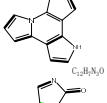
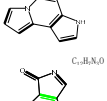
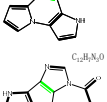
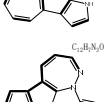








































Five kinds of energies calculated for aaptourinamine

	Stretch	Bond	Stretch-Bond	Torsion	Total Energy	
<div><div>G-64</div><div></div></div>	0.6193	29.4203	-0.188	-10.49	24.8857	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)8-2-1-3-9-11(8)15(12)6-14-9/h1-6,13H
<div><div>G-61</div><div></div></div>	0.8158	29.443	-0.1702	-11.61	27.6437	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-14-15(12)11(7)9/h1-6,13H
<div><div>H-41</div><div></div></div>	0.5838	24.2838	-0.2751	-6.96	28.6774	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)14-12(10)15(7)9/h1-6,13H
<div><div>G-77</div><div></div></div>	0.8842	36.8875	-0.1325	-11.61	29.8313	InChI=1S/C12H7N3O/c16-12-14-6-7-2-1-3-8-9-4-5-13-11(9)15(12)10(7)9/h1-6,13H
<div><div>G-72</div><div></div></div>	0.8379	35.9095	-0.1491	-10.49	30.7624	InChI=1S/C12H7N3O/c16-10-6-14-9-3-1-2-7-8-4-5-13-12(8)15(10)11(7)9/h1-6,13H
<div><div>F-36</div><div></div></div>	0.5524	24.9718	-0.2552	-3.18	30.9923	InChI=1S/C12H7N3O/c16-10-6-11-14-12-7(4-5-13-12)8-2-1-3-9(10)15(8)11/h1-6H, 0H, 13, 14
<div><div>H-89</div><div></div></div>	0.6614	27.2712	-0.2188	-7.96	33.3615	InChI=1S/C12H7N3O/c16-11-10-8(4-5-13-10)9-3-1-2-7-6-14-12(11)15(7)9/h1-6,13H
<div><div>H11-99</div><div></div></div>	0.6236	28.8637	-0.2704	-7.1	33.9255	InChI=1S/C12H7N3O/c16-12-10-6-8-7(4-5-13-8)9-2-1-3-11(14-12)15(9)10/h1-6,13H
<div><div>A-205</div><div></div></div>	0.6377	28.5779	-0.1138	-7.7000	34.6231	InChI=1S/C12H7N3O/c16-12-9-7(3-4-13-9)8-2-1-5-15-6-14-10(12)11(8)15/h1-6,13H
<div><div>H11-144</div><div></div></div>	0.552	28.2809	-0.1965	-4.18	35.5961	InChI=1S/C12H7N3O/c16-12-9-6-14-10-3-1-2-8(15)(9)10(7)-4-5-13-11(7)12/h1-6,13H
<div><div>A-2</div><div></div></div>	0.5225	35.5435	-0.4186	-5.11	36.5923	InChI=1S/C12H7N3O/c16-9-6-14-12-10(9)11-7(3-4-13-11)8-2-1-5-15(8)12/h1-6,13H
<div><div>G-13</div><div></div></div>	0.8976	35.7206	-0.0883	-8.83	36.7221	InChI=1S/C12H7N3O/c16-10-6-14-15-11-7(2-1-3-9(10)11)8-4-5-13-12(8)14-10/h1-6,13H
<div><div>B-15</div><div></div></div>	0.6383	37.0653	-0.4954	-6.8300	36.7441	InChI=1S/C12H7N3O/c16-10-6-8-11-7(3-4-13-11)9-2-1-5-15(9)12(8)14-10/h1-6,13H
<div><div>A-43</div><div></div></div>	0.7851	29.5535	-0.1306	-5.04	36.8764	InChI=1S/C12H7N3O/c16-12-9-6-14-15-5-1-2-8(11)(9)15)7-3-4-13-10(7)12/h1-6,13H
<div><div>H-58</div><div></div></div>	1.0299	33.8094	-0.2722	-8.89	37.8158	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)12(14-10)15(7)9/h1-6,13H
<div><div>A-7</div><div></div></div>	0.569	35.9588	-0.3973	-6.77	38.4748	InChI=1S/C12H7N3O/c16-9-6-14-11-10-7(3-4-13-10)8-2-1-5-15(8)12(9)11/h1-6,13H
<div><div>G-32</div><div></div></div>	1.0393	37.8963	-0.1479	-8.83	38.7282	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-8-4-5-13-11(8)15(6-14-12)10(7)9/h1-6,13H
<div><div>O-249</div><div></div></div>	0.5836	37.7969	-0.4667	-6.83	38.925	InChI=1S/C12H7N3O/c16-10-6-7-8-2-1-5-15(8)9-3-4-13-12(9)11(7)14-10/h1-6,13H

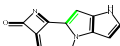
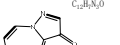
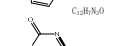
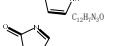
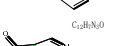
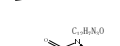
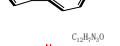
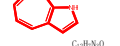
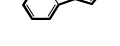
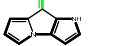
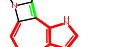
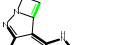

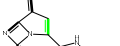
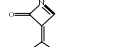
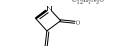
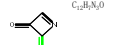
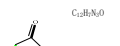
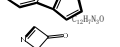
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B-36		0.5700	37.8115	-0.4635	-6.8300	39.4375	InChI=1S/C12H7N3O/c16-10-6-9-12(14-10)11-7(3-4-13-11)8-2-1-5-15(8)9/h1-6,13H
n-112		0.5505	36.5458	-0.3962	-4.18	40.0021	InChI=1S/C12H7N3O/c16-9-6-14-12-10(9)7-2-1-5-15(7)8-3-4-13-11(8)12/h1-6,13H
o-246		0.6213	37.8819	-0.4702	-4.9	40.4893	InChI=1S/C12H7N3O/c16-10-6-7-11-9(3-4-13-11)15-5-1-2-8(15)12(7)14-10/h1-6,13H
n-116		0.5705	36.6427	-0.3974	-3.18	40.6556	InChI=1S/C12H7N3O/c16-9-6-14-12-7-2-1-5-15(7)8-3-4-13-11(8)10(9)12/h1-6,13H
A-77		0.7588	39.8004	-0.4695	-6.83	42.5764	InChI=1S/C12H7N3O/c16-12-11-8(6-14-12)10-7(3-4-13-10)9-2-1-5-15(9)11/h1-6,13H
n-188		0.6841	40.6443	-0.4488	-5.17	43.2659	InChI=1S/C12H7N3O/c16-12-10-7(6-14-12)8-2-1-5-15(8)9-3-4-13-11(9)10/h1-6,13H
A-79		0.6046	40.439	-0.4409	-5.17	43.4986	InChI=1S/C12H7N3O/c16-12-10-9(6-14-12)15-5-1-2-8(15)7-3-4-13-11(7)10/h1-6,13H
n-187		0.711	40.6044	-0.455	-4.24	44.1716	InChI=1S/C12H7N3O/c16-12-10-7(6-14-12)11-9(3-4-13-11)15-5-1-2-8(10)15/h1-6,13H
G1-79		0.981	54.2429	-0.311	-10.49	44.8958	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-10(7)11-12(8)15(9)6-14-11/h1-6,13H
C-43		0.6313	54.2300	-0.2471	-5.7000	45.9080	InChI=1S/C12H7N3O/c16-10-6-9-11-7(2-1-4-13-9)8-3-5-14-12(8)15(10)11/h1-6,14H
C-39		0.8105	54.9447	-0.2788	-10.5500	46.8038	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-5-13-11)8-2-1-4-14-15(10)12(8)9/h1-6,13H
n-123		0.8613	35.2223	-0.0886	-2.12	47.2803	InChI=1S/C12H7N3O/c16-9-6-14-11-10-8(3-4-13-10)15-5-1-2-7(9)12(11)15/h1-6,13H
n-198		0.917	38.6938	-0.099	-5.17	47.865	InChI=1S/C12H7N3O/c16-12-9-10-8(3-4-13-10)15-5-1-2-7(6-14-12)11(9)15/h1-6,13H
n-210		1.0813	37.8015	-0.1408	-4.11	48.1425	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-10(9)8(6-14-12)11(7)15/h1-6,13H
n-113		0.8463	37.3669	-0.0777	-2.12	48.6871	InChI=1S/C12H7N3O/c16-9-6-14-7-2-1-5-15-8-3-4-13-11(8)10(9)12(7)15/h1-6,13H
G1-55		1.3235	55.7794	-0.287	-10.55	49.9772	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)9-6-14-15(10)12(8)9/h1-6,13H
A2-61		0.8459	51.0599	-0.301	-5.9	51.7907	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-5-13-11)8-2-1-4-14-12(10)15(8)9/h1-6,13H
D-16		0.7350	52.8473	-0.2477	-3.1800	54.2489	InChI=1S/C12H7N3O/c16-9-6-10-13-4-1-2-8-7-3-5-14-11(7)12(9)15(8)10/h1-6,14H

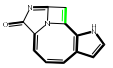
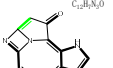
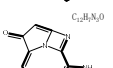
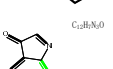
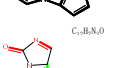
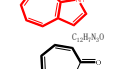
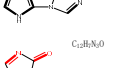
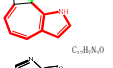
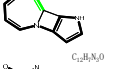
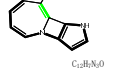
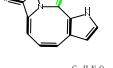
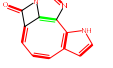
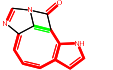
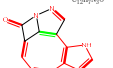
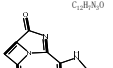
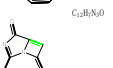
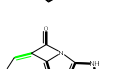
G1-38		0.9427	56.1479	-0.2363	-5.04	54.8006	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15-11(7)9(10)6-14-15/h1-6,13H
	$C_{12}H_7N_3O$						
H1-75		0.7912	54.3054	-0.2516	-4.18	55.8908	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)12-14-6-9(10)15(8)12/h1-6,13H
	$C_{12}H_7N_3O$						
I-85		0.9012	52.3096	-0.1927	-3.91	57.1763	InChI=1S/C12H7N3O/c16-9-6-7-10-8(2-4-14-10)15-5-1-3-13-11(9)12(7)15/h1-6,14H
	$C_{12}H_7N_3O$						
H1-51		1.0726	56.0431	-0.2987	-6.9	57.5894	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)9-6-14-12(10)15(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
H-148		1.2972	83.1531	-0.6288	-13.54	60.1273	InChI=1S/C12H7N3O/c16-12-14-10-6-7-2-1-3-8(7)9-4-5-13-11(9)15(10)12/h1-6,13H
	$C_{12}H_7N_3O$						
I-86		0.9725	55.0755	-0.1842	-1.19	60.6569	InChI=1S/C12H7N3O/c16-9-6-7-12-10(9)11-8(2-4-14-11)15(12)5-1-3-13-7/h1-6,14H
	$C_{12}H_7N_3O$						
H-149		1.2305	83.0582	-0.6034	-13.54	63.052	InChI=1S/C12H7N3O/c16-12-14-11-10-9(4-5-13-10)8-3-1-2-7(8)6-15(11)12/h1-6,13H
	$C_{12}H_7N_3O$						
H11-68		0.8853	81.6821	-0.661	-8.56	63.1592	InChI=1S/C12H7N3O/c16-11-6-10-14-9-3-1-2-7(9)8-4-5-13-12(8)15(10)11/h1-6,13H
	$C_{12}H_7N_3O$						
F-44		0.8885	81.6812	-0.6786	-8.56	64.7771	InChI=1S/C12H7N3O/c16-11-6-10-14-12-8(4-5-13-12)7-2-1-3-9(7)15(10)11/h1-6H, (H,13,14)
	$C_{12}H_7N_3O$						
F-39		0.854	82.0203	-0.6834	-12.54	66.0692	InChI=1S/C12H7N3O/c16-11-6-10-8-3-1-2-7(8)9-4-5-13-12(9)14-15(10)11/h1-6H, (H,13,14)
	$C_{12}H_7N_3O$						
G1-108		1.2199	75.9162	-0.6734	-7.83	67.6958	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)8-6-14-12(8)15(9)10/h1-6,13H
	$C_{12}H_7N_3O$						
G1-80		1.1488	75.9844	-0.6595	-6.77	68.3645	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)12-9(6-14-12)15(8)10/h1-6,13H
	$C_{12}H_7N_3O$						
H11-60		0.787	82.1482	-0.6714	-10.55	68.7169	InChI=1S/C12H7N3O/c16-11-6-10-12-8(4-5-13-12)7-2-1-3-9(7)14-15(10)11/h1-6,13H
	$C_{12}H_7N_3O$						
C-42		1.3450	78.3761	-0.4861	-5.7600	69.0697	InChI=1S/C12H7N3O/c16-10-6-9-11-7(2-1-4-13-11)8-3-5-14-12(8)15(9)10/h1-6,14H
	$C_{12}H_7N_3O$						
C-44		1.1679	78.3801	-0.4984	-6.7600	71.5441	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-5-13-11)8-2-1-4-14-12(8)15(9)10/h1-6,13H
	$C_{12}H_7N_3O$						
H-52		0.8016	87.3188	-0.5391	-7.82	72.1239	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)14-12(9)15(7)10/h1-6,13H
	$C_{12}H_7N_3O$						
B-138		1.2784	92.3785	-0.4982	-12.5400	72.1450	InChI=1S/C12H7N3O/c16-12-14-11-9-6-10-8(3-4-13-10)7(9)2-1-5-15(11)12/h1-6,13H
	$C_{12}H_7N_3O$						
B-40		0.7982	87.0260	-0.5086	-5.7600	72.4208	InChI=1S/C12H7N3O/c16-10-6-9-11-7(2-1-5-15(9)10)8-3-4-13-12(8)14-11/h1-6,13H
	$C_{12}H_7N_3O$						
H11-2		1.2809	92.7054	-0.5258	-12.48	72.6091	InChI=1S/C12H7N3O/c16-12-14-11-3-1-2-8-7-4-5-13-9(7)6-10(8)15(11)12/h1-6,13H
	$C_{12}H_7N_3O$						

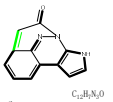
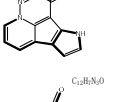
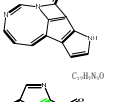
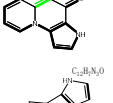
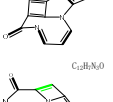
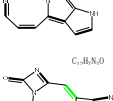
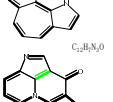
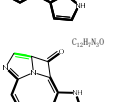
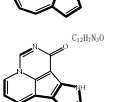
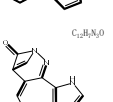
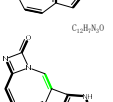
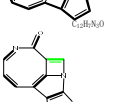
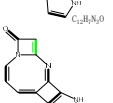
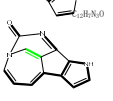

C-66		1.7689	79.1033	-0.3733	-5.7000	74.4022	InChI=1S/C12H7N3O/c16-12-10-7(3-5-14-10)8-2-1-4-13-9-6-15(12)11(8)9/h1-6,14H
	$C_{12}H_7N_3O$						
A-159		1.5223	82.2859	-0.2297	-7.69	75.4238	InChI=1S/C12H7N3O/c16-12-10-11-8(2-1-5-15(11)12)7-3-4-13-9(7)6-14-10/h1-6,13H
	$C_{12}H_7N_3O$						
G1-97		1.0219	78.9743	-0.5496	-6.04	77.8141	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-11(8)15-6-14-12(15)10(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
B-13		1.0570	79.4923	-0.7905	-6.8300	78.5829	InChI=1S/C12H7N3O/c16-10-6-8-11-7(3-4-13-11)9-2-1-5-15(9)14-12(8)10/h1-6,13H
	$C_{12}H_7N_3O$						
G1-60		1.1444	77.2593	-0.6814	-7.1	79.5073	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15-9(6-14-15)11(7)10/h1-6,13H
	$C_{12}H_7N_3O$						
B-30		0.9009	77.6844	-0.7592	-4.9700	79.6273	InChI=1S/C12H7N3O/c16-10-6-9-11(10)14-12-7(3-4-13-12)8-2-1-5-15(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
G-19		2.0473	89.6073	-0.2082	-7.83	79.7694	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-8-4-5-13-11(8)14-6-15(12)10(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
G-18		1.7607	86.3927	-0.2874	-9.82	80.1332	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8-7-4-5-13-10(7)6-14-15(12)11(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
B-190		1.5813	82.5811	-0.8318	-7.8300	80.1895	InChI=1S/C12H7N3O/c16-12-11-8(6-14-11)10-7(3-4-13-10)9-2-1-5-15(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
o-81		1.244	78.5981	-0.8352	-3.91	80.5002	InChI=1S/C12H7N3O/c16-9-6-7-11-8(3-4-13-11)15-5-1-2-10(15)14-12(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
H-103		1.7507	72.8837	-0.4563	-7.96	80.6798	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)9-3-1-2-7-6-10(14-12)15(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
H1-53		0.912	79.7585	-0.3846	-7.83	81.0946	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-8(7)6-11-14-12(10)15(9)11/h1-6,13H
	$C_{12}H_7N_3O$						
C-17		1.4916	88.4519	-0.3243	-9.8200	81.8663	InChI=1S/C12H7N3O/c16-12-9-6-10-7(3-5-13-10)8-2-1-4-14-15(12)11(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
H11-156		1.5683	79.0011	-0.3076	-5.84	82.1499	InChI=1S/C12H7N3O/c16-9-6-11-14-10-3-1-2-8(15(10)11)7-4-5-13-12(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
B-128		1.1807	82.3227	-0.8142	-7.1000	82.1757	InChI=1S/C12H7N3O/c16-12-8-6-9-7(3-4-13-9)10-2-1-5-15(10)11(8)14-12/h1-6,13H
	$C_{12}H_7N_3O$						
A-50		2.0704	89.0358	-0.1434	-4.97	82.4838	InChI=1S/C12H7N3O/c16-12-9-6-14-11-8(3-4-13-11)7-2-1-5-15(12)10(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
H1-139		1.1673	75.4039	-0.4689	-2.2499	83.0307	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-12(7)14-11-6-9(10)15(8)11/h1-6,13H
	$C_{12}H_7N_3O$						
F-34		0.9843	85.2549	-0.6054	-5.17	83.3222	InChI=1S/C12H7N3O/c16-11-6-10-7(11)2-1-3-9-8-4-5-13-12(8)14-15(9)10/h1-6H, (H,13,14)
	$C_{12}H_7N_3O$						
B-177		1.5548	85.6303	-0.8151	-5.1100	83.8586	InChI=1S/C12H7N3O/c16-12-8-6-14-11(8)10-7(3-4-13-10)9-2-1-5-15(9)12/h1-6,13H
	$C_{12}H_7N_3O$						

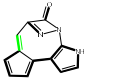
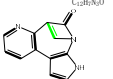
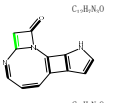
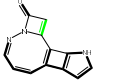
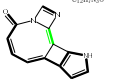
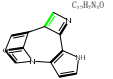
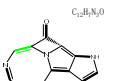
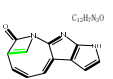
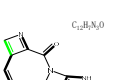
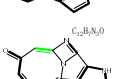
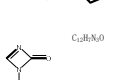
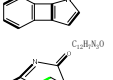
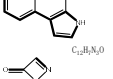
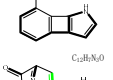
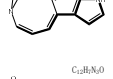
H-96		1.445	89.9564	-0.6485	-8.89	84.2638	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-14-11(7)15(9)12/h1-6,13H
A2-65		1.1108	75.2129	-0.3873	-2.25	84.631	InChI=1S/C12H7N3O/c16-12-9-6-10-13-4-1-2-8(15(9)10)7-3-5-14-11(7)12/h1-6,14H
I-85		1.6193	72.7872	-0.2913	-3.05	84.9833	InChI=1S/C12H7N3O/c16-12-7-6-8-11(7)15(5-1-3-13-8)9-2-4-14-10(9)12/h1-6,14H
D-15		1.6918	79.0777	-0.6035	-5.1700	85.0092	InChI=1S/C12H7N3O/c16-10-6-9-11(10)12-7(3-5-13-12)8-2-1-4-14-15(8)9/h1-6,13H
o-152		0.9309	86.2884	-0.655	-3.18	85.3147	InChI=1S/C12H7N3O/c16-10-6-8-7(10)2-1-5-15-9-3-4-13-11(9)14-12(8)15/h1-6,13H
G-37		0.9748	90.3349	-0.5259	-7.7	85.7224	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)8-2-1-3-9-14-6-15(9)11(8)12/h1-6,13H
F-32		1.3256	77.2465	-0.376	-5.3	86.0534	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(15(7)10)8-4-5-13-11(8)14-12/h1-6H, 10, 13, 14, 16
H11-82		1.3344	91.8828	-0.6199	-7.83	86.6297	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)9-3-1-2-8-10(6-14-8)15(9)12/h1-6,13H
B-175		0.9905	82.8896	-0.7618	-3.2500	86.9107	InChI=1S/C12H7N3O/c16-11-8-6-14-12(8)15-5-1-2-9(15)7-3-4-13-10(7)11/h1-6,13H
B-194		0.9614	81.7212	-0.7108	-5.9700	87.1129	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)8-2-1-5-15(8)9-6-14-11(9)12/h1-6,13H
G-82		2.284	96.201	-0.297	-12.61	87.436	InChI=1S/C12H7N3O/c16-12-14-6-7-2-1-3-9-8-4-5-13-10(8)11(9)15(7)12/h1-6,13H
x4-8		3.0846	101.9716	-0.3211	-8.56	87.5633	InChI=1S/C12H7N3O/c16-9-6-14-12-10-8(15(9)12)3-1-2-7-4-5-13-11(7)10/h1-6,13H
A-193		0.8324	90.9855	-0.5203	-6.04	87.7987	InChI=1S/C12H7N3O/c16-11-9-7(8-3-4-13-10(8)11)2-1-5-15-6-14-12(9)15/h1-6,13H
G-36		1.2165	88.634	-0.6581	-9.82	88.9444	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-14-15(7)11(9)12/h1-6,13H
n-130		1.3745	83.0542	-0.7384	-5.97	88.9725	InChI=1S/C12H7N3O/c16-12-10-7(6-14-10)8-2-1-5-15(8)9-3-4-13-11(9)12/h1-6,13H
A-100		1.0557	89.4209	-0.7002	-7.1	89.1989	InChI=1S/C12H7N3O/c16-12-10-7(8-3-4-13-11(8)12)2-1-5-15-9(10)6-14-15/h1-6,13H
o-212		1.686	85.8072	-0.8108	-5.17	89.4196	InChI=1S/C12H7N3O/c16-12-7-6-8-9(3-4-13-8)15-5-1-2-10(15)11(7)14-12/h1-6,13H
I-62		1.9738	79.8974	-0.6684	-2.25	89.4926	InChI=1S/C12H7N3O/c16-9-6-7-10(9)12-14-3-1-5-15(12)8-2-4-13-11(7)8/h1-6,13H
B-212		1.6979	86.0119	-0.8287	-6.0400	89.4981	InChI=1S/C12H7N3O/c16-12-8-6-15-5-1-2-9(15)7-3-4-13-10(7)11(8)14-12/h1-6,13H

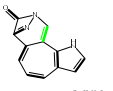
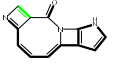
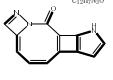
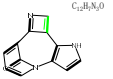
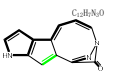
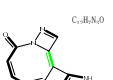
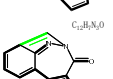
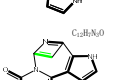
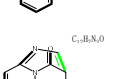
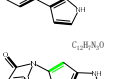
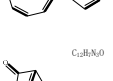
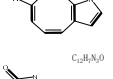
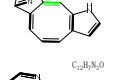
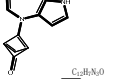
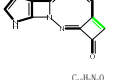
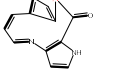
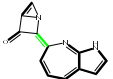
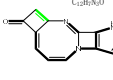
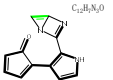
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A-93		2.4599	97.9078	-0.3783	-12.48	89.9282	InChI=1S/C12H7N3O/c16-12-14-6-9-10-7(2-1-5-15(9)12)8-3-4-13-11(8)10/h1-6,13H
G-74		2.3269	97.8878	-0.3522	-10.49	90.5347	InChI=1S/C12H7N3O/c16-10-6-14-9-3-1-2-8-7-4-5-13-11(7)12(8)15(9)10/h1-6,13H
C-13		1.6486	83.4726	-0.2891	-5.0400	91.6469	InChI=1S/C12H7N3O/c16-12-9-6-15-11(9)8(2-1-4-14-15)7-3-5-13-10(7)12/h1-6,13H
o-12		1.7845	83.452	-0.748	-3.25	92.16	InChI=1S/C12H7N3O/c16-12-9-2-1-5-15(9)8-3-4-13-10(8)7-6-14-11(7)12/h1-6,13H
A-29		2.3045	98.5626	-0.3666	-9.49	92.7921	InChI=1S/C12H7N3O/c16-9-6-14-12-10-7(2-1-5-15(9)12)8-3-4-13-11(8)10/h1-6,13H
q11-33		3.0117	105.9451	-0.2067	-9.56	93.2161	InChI=1S/C12H7N3O/c16-10-6-9-14-12-8(15(9)10)3-1-2-7-4-5-13-11(7)12/h1-6,13H
n-168		1.679	80.5456	-0.2721	-2.25	93.639	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-8(9)6-14-10(12)11(7)15/h1-6,13H
n11-45		3.0985	106.4455	-0.25	-9.56	93.6818	InChI=1S/C12H7N3O/c16-10-6-9-14-8-3-1-2-7-4-5-13-11(7)12(8)15(9)10/h1-6,13H
n-129		1.2359	89.5579	-0.636	-4.18	94.2099	InChI=1S/C12H7N3O/c16-12-10-9(3-4-13-10)15-5-1-2-8-7(6-14-8)11(12)15/h1-6,13H
o-177		1.5068	86.1471	-0.7589	-1.32	94.5221	InChI=1S/C12H7N3O/c16-12-7-6-14-10(7)8-2-1-5-15(8)9-3-4-13-11(9)12/h1-6,13H
x4-58		3.9161	108.2528	-0.251	-6.9	94.6147	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9(8)11-14-6-15(11)12/h1-6,13H
I-37		1.466	82.2125	-0.3364	-2.25	94.8563	InChI=1S/C12H7N3O/c16-12-7-6-8-9(2-4-13-8)15-5-1-3-14-10(12)11(7)15/h1-6,13H
n-136		1.3111	89.4414	-0.6109	-5.24	94.9039	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)15-5-1-2-7-6-14-9(7)11(12)15/h1-6,13H
q-65		3.8442	110.3677	-0.2714	-11.55	95.068	InChI=1S/C12H7N3O/c16-12-14-10-6-8-9(15(10)12)3-1-2-7-4-5-13-11(7)8/h1-6,13H
F-11		1.5166	84.39	-0.3455	-1.52	95.0843	InChI=1S/C12H7N3O/c16-11-9-3-1-2-8-7-4-5-13-12(7)14-6-10(11)15(8)9/h1-6H, (H, 13, 14)
o-120		1.818	86.4643	-0.7624	-0.53	95.9977	InChI=1S/C12H7N3O/c16-12-7-6-14-10(7)11-8(3-4-13-11)15-5-1-2-9(12)15/h1-6,13H
G-14		2.2582	95.4504	-0.2845	-8.83	96.8994	InChI=1S/C12H7N3O/c16-10-6-14-15-9(10)3-1-2-8-7-4-5-13-11(7)12(8)15/h1-6,13H
q-66		3.9336	112.4572	-0.2893	-11.61	97.2231	InChI=1S/C12H7N3O/c16-12-14-11-8-3-1-2-7-4-5-13-10(7)9(8)6-15(11)12/h1-6,13H

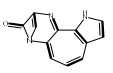
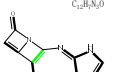
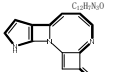
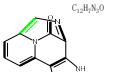
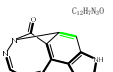
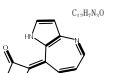
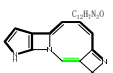
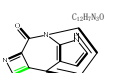
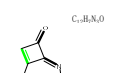
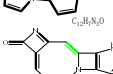

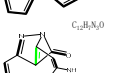
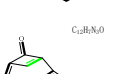
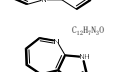

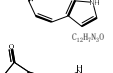
o-165		1.5203	94.507	-0.6811	-5.17	97.6925	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-8(9)6-10(15)11(7)14-12/h1-6,13H
A-5	 C ₂₂ H ₉ N ₃ O	2.3393	96.6582	-0.371	-8.83	98.2585	InChI=1S/C12H7N3O/c16-9-6-14-15-5-1-2-7-8-3-4-13-11(8)10(7)12(9)15/h1-6,13H
A-91	 C ₂₂ H ₉ N ₃ O	1.7078	52.2594	-0.3866	32.0397	99.635	InChI=1S/C12H7N3O/c16-12-14-6-9-10-7(3-4-13-10)8-2-1-5-15(12)11(8)9/h1-6,13H
G-33	 C ₂₂ H ₉ N ₃ O	2.3699	99.4261	-0.3702	-8.83	100.6877	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8-7-4-5-13-10(7)11(8)15(9)6-14-12/h1-6,13H
n-169	 C ₂₂ H ₉ N ₃ O	2.2114	87.2917	-0.1542	0.47	100.7267	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-12(9)14-6-8(11)10(7)15/h1-6,13H
A-214	 C ₂₂ H ₉ N ₃ O	2.3372	100.4604	-0.4130	-8.8300	102.1544	InChI=1S/C12H7N3O/c16-12-11-9-7(8-3-4-13-10(8)9)2-1-5-15(11)6-14-12/h1-6,13H
x4-52	 C ₂₂ H ₉ N ₃ O	3.959	109.8063	-0.2959	-9.89	102.3922	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)10(8)9-6-14-15(9)12/h1-6,13H
A-31	 C ₂₂ H ₉ N ₃ O	1.4793	50.2142	-0.3625	36.679	102.7852	InChI=1S/C12H7N3O/c16-9-6-14-11-10-7(3-4-13-10)8-2-1-5-15(9)12(8)11/h1-6,13H
n-192	 C ₂₂ H ₉ N ₃ O	0.8701	107.2225	-1.0434	-6.17	102.8584	InChI=1S/C12H7N3O/c16-12-7(6-14-12)10-8-2-1-5-15(8)9-3-4-13-11(9)10/h1-6,13H/b10-7+
x4-2	 C ₂₂ H ₉ N ₃ O	2.3628	103.7329	-0.4647	-8.96	103.0488	InChI=1S/C12H7N3O/c16-9-6-14-15-8-3-1-2-7-4-5-13-11(7)10(8)12(9)15/h1-6,13H
n11-43	 C ₂₂ H ₉ N ₃ O	1.3674	73.165	-1.7878	31.5974	104.3785	InChI=1S/C12H7N3O/c16-10-6-9-11-8(14-15(9)10)3-1-2-7-4-5-13-12(7)11/h1-6,13H
q11-37	 C ₂₂ H ₉ N ₃ O	1.3653	73.6564	-1.7615	30.1092	104.7756	InChI=1S/C12H7N3O/c16-10-6-9-8-3-1-2-7-4-5-13-11(7)12(8)14-15(9)10/h1-6,13H
q-6	 C ₂₂ H ₉ N ₃ O	2.3066	108.5089	-0.3431	-7.83	104.9584	InChI=1S/C12H7N3O/c16-9-6-8-11-7(4-5-13-11)2-1-3-10-14-12(9)15(8)10/h1-6,13H/b2-1-,10-3-
A-137	 C ₂₂ H ₉ N ₃ O	1.1253	108.9979	-1.0393	-6.17	105.2014	InChI=1S/C12H7N3O/c16-12-8(6-14-12)11-10-7(3-4-13-10)9-2-1-5-15(9)11/h1-6,13H/b11-8-
A-53	 C ₂₂ H ₉ N ₃ O	1.0628	108.1536	-1.0467	-5.24	105.2761	InChI=1S/C12H7N3O/c16-12-8(6-14-12)11-10-7(3-4-13-10)9-2-1-5-15(9)11/h1-6,13H/b11-8+
n-110	 C ₂₂ H ₉ N ₃ O	0.8206	105.7112	-1.0454	-3.18	105.3514	InChI=1S/C12H7N3O/c16-9-6-14-12(9)10-7-2-1-5-15(7)8-3-4-13-11(8)10/h1-6,13H/b12-10-
H-56	 C ₂₂ H ₉ N ₃ O	2.9978	106.9247	-0.1965	-7.89	105.8668	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-12(8)15(9)11(7)14-10/h1-6,13H
A-11	 C ₂₂ H ₉ N ₃ O	1.1011	107.603	-1.0384	-3.18	108.3786	InChI=1S/C12H7N3O/c16-9-6-14-11(9)12-10-7(3-4-13-10)8-2-1-5-15(8)12/h1-6,13H/b12-11-
H11-108	 C ₂₂ H ₉ N ₃ O	3.0223	107.6649	-0.2252	-6.83	108.4432	InChI=1S/C12H7N3O/c16-11-6-10-8(14-11)2-1-3-9-7-4-5-13-12(7)15(9)10/h1-6,13H







q-60		2.9096	106.833	-0.5107	-6.17	109.9364	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)9-6-10(14-12)15(8)9/h1-6,13H/b2-1-,8-3-
s11-60		2.7662	111.0263	-0.3239	-5.11	110.0418	InChI=1S/C12H7N3O/c16-8-6-10-14-9-3-1-2-7-4-5-13-11(7)12(8)15(9)10/h1-6,13H/b3-1-,7-2-,12-11+
n-111		2.5506	103.7403	-0.2097	-3.12	110.2534	InChI=1S/C12H7N3O/c16-9-6-14-7-2-1-5-15-8-3-4-13-11(8)12(15)10(7)9/h1-6,13H
q11-39		2.689	111.2961	-0.3554	-5.11	110.33	InChI=1S/C12H7N3O/c16-9-6-10-14-12-11-7(4-5-13-11)2-1-3-8(9)15(10)12/h1-6,13H/b2-1-,8-3-
n-124		2.5201	103.2878	-0.1805	-2.12	111.0444	InChI=1S/C12H7N3O/c16-9-6-14-10-7(9)2-1-5-15-8-3-4-13-11(8)12(10)15/h1-6,13H
x4-64		1.5564	67.7639	-1.6827	47.1595	111.0755	InChI=1S/C12H7N3O/c16-12-14-6-9-10-8(15(9)12)3-1-2-7-4-5-13-11(7)10/h1-6,13H
G1-40		6.5832	107.3583	-1.6272	-7.7	112.324	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-12(8)15-6-14-10(9)11(7)15/h1-6,13H
x4-48		2.869	113.6808	-0.4064	-8.96	112.5396	InChI=1S/C12H7N3O/c16-12-11-9-8(15(11)6-14-12)3-1-2-7-4-5-13-10(7)9/h1-6,13H
n-195		2.6158	106.6636	-0.2669	-4.24	112.7755	InChI=1S/C12H7N3O/c16-12-9-7(6-14-12)2-1-5-15-8-3-4-13-10(8)11(9)15/h1-6,13H
n-209		2.6741	106.4948	-0.2824	-4.11	112.8499	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-10(9)11(15)8(7)6-14-12/h1-6,13H
q-13		2.2015	110.804	-0.4099	-6.17	112.8842	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)9-6-14-12(11)15(8)9/h1-6,13H/b2-1-,8-3-
C-69		2.7279	128.6412	-0.4780	-10.5500	114.1289	InChI=1S/C12H7N3O/c16-12-14-4-1-2-8-7-3-5-13-10(7)9-6-15(12)11(8)9/h1-6,13H/b2-1-,14-4+
x4-60		4.6873	124.2552	0.1194	-8.83	114.4048	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)10-11(8)15(12)6-14-10/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,10-9-
x4-22		4.6468	125.1605	0.0804	-8.83	114.9034	InChI=1S/C12H7N3O/c16-12-9-10-7(4-5-13-10)2-1-3-8-11(9)15(12)6-14-8/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,10-9-
x4-50		4.1308	125.0374	-0.114	-8.89	118.4166	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9-6-14-15(12)11(8)9/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,10-9+
q11-5		4.0247	117.4642	-0.2412	-7.23	121.1339	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)11(14-12)15(8)9/h1-6,13H/b2-1-,8-3-
s11-29		3.9762	118.0425	-0.2667	-6.17	121.948	InChI=1S/C12H7N3O/c16-12-9-6-8-11-7(4-5-13-11)2-1-3-10(14-12)15(8)9/h1-6,13H/b3-1-,7-2-,11-8+
C-21		3.0042	133.2379	-0.2830	-4.9700	122.1485	InChI=1S/C12H7N3O/c16-12-9-6-13-4-1-2-7-8-3-5-14-11(8)15(12)10(7)9/h1-6,14H/b2-1-,4-1-,7-2-,9-6+,13-4-,13-6-
H1-140		2.5244	119.6951	-0.7109	-6.9	122.8513	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-12(7)9-6-10(14-11)15(8)9/h1-6,13H/b3-1-,8-2-,14-10-

H-47	 <chem>C12H9N3O</chem>	1.6481	28.7932	-0.4814	84.484	124.1106	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8-9-4-5-13-12(9)15(10)14-11(7)8/h1-6,13H
F-18	 <chem>C12H9N3O</chem>	2.0887	77.9619	-1.1284	44.1027	124.3702	InChI=1S/C12H7N3O/c16-12-10-6-15(12)14-11-9(4-5-13-11)7-2-1-3-8(7)10/h1-6H, 8H, 13, 14)/b9-7-
x4-20	 <chem>C12H9N3O</chem>	1.1336	84.4457	-1.3435	40.4106	124.7909	InChI=1S/C12H7N3O/c16-12-9-10-7(4-5-13-10)2-1-3-8-6-14-15(12)11(8)9/h1-6,13H/b2-1-,3-1-,7-27,8-3-,10-9-
A-1	 <chem>C12H9N3O</chem>	0.9952	54.7149	-0.038	56.4489	126.1308	InChI=1S/C12H7N3O/c16-9-6-14-15-5-1-2-8-7-3-4-13-11(7)10(9)12(8)15/h1-6,13H
A1-4	 <chem>C12H9N3O</chem>	3.2129	138.9044	-0.5068	-7.83	127.0571	InChI=1S/C12H7N3O/c16-12-9-10-7(3-5-14-10)8-2-1-4-13-6-15(12)11(8)9/h1-6,14H/b4-1-,8-2-,13-6-
n-134	 <chem>C12H9N3O</chem>	0.8786	46.1517	-0.1079	63.1328	127.2811	InChI=1S/C12H7N3O/c16-12-9-8(3-4-13-9)15-5-1-2-7-6-14-10(12)11(7)15/h1-6,13H
I-102	 <chem>C12H9N3O</chem>	2.7308	121.5186	-0.3719	-5.04	127.7407	InChI=1S/C12H7N3O/c16-12-8-6-7-10-9(2-4-13-10)15(11(7)8)5-1-3-14-12/h1-6,13H/b5-1-,14-3+
D-14	 <chem>C12H9N3O</chem>	1.6916	122.2259	-0.5548	-4.2400	128.0222	InChI=1S/C12H7N3O/c16-12-10-6-9-11-7(3-5-13-11)8(15(9)10)2-1-4-14-12/h1-6,13H/b2-1-,14-4-
B-105	 <chem>C12H9N3O</chem>	2.8686	148.5867	-0.5111	-12.4799	129.7706	InChI=1S/C12H7N3O/c16-12-14-10-6-9-7(2-1-5-15(10)12)8-3-4-13-11(8)9/h1-6,13H/b5-1-,7-2-,9-6+
q11-25	 <chem>C12H9N3O</chem>	3.6296	124.0211	-0.2448	-3.45	129.9949	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)12-14-6-9(11)15(8)12/h1-6,13H/b2-1-,8-3-
s11-8	 <chem>C12H9N3O</chem>	4.068	68.8545	-3.0109	46.9092	130.2112	InChI=1S/C12H7N3O/c16-12-8-6-15(12)14-9-3-1-2-7-4-5-13-11(7)10(8)9/h1-6,13H
n-133	 <chem>C12H9N3O</chem>	0.8942	47.9496	-0.1088	66.8213	130.2552	InChI=1S/C12H7N3O/c16-12-7-6-14-8-2-1-5-15(11(7)8)9-3-4-13-10(9)12/h1-6,13H
s11-14	 <chem>C12H9N3O</chem>	3.5949	124.9767	-0.2794	-3.45	130.4249	InChI=1S/C12H7N3O/c16-12-8-6-14-9-3-1-2-7-4-5-13-10(7)11(12)15(8)9/h1-6,13H/b3-1-,7-2-,11-10+
A-202	 <chem>C12H9N3O</chem>	1.0737	56.3958	-0.1513	58.2053	130.6125	InChI=1S/C12H7N3O/c16-12-9-10-7(3-4-13-10)8-2-1-5-15(6-14-12)11(8)9/h1-6,13H
q11-20	 <chem>C12H9N3O</chem>	4.1591	69.0939	-3.0512	45.9075	130.6856	InChI=1S/C12H7N3O/c16-12-9-6-15(12)14-11-8(9)3-1-2-7-4-5-13-10(7)11/h1-6,13H
H11-3	 <chem>C12H9N3O</chem>	2.9677	149.4584	-0.5274	-12.48	130.7805	InChI=1S/C12H7N3O/c16-12-14-10-3-1-2-7-8-4-5-13-11(8)9(7)6-15(10)12/h1-6,13H/b3-1-,7-2-,9-6+
C-32	 <chem>C12H9N3O</chem>	1.9183	128.6555	-0.4576	-5.0400	130.9211	InChI=1S/C12H7N3O/c16-12-9-6-15-10(9)7(2-1-4-14-12)8-3-5-13-11(8)15/h1-6,13H/b2-1-,14-4+
B-57	 <chem>C12H9N3O</chem>	2.6619	147.1573	-0.5574	-8.5800	132.5643	InChI=1S/C12H7N3O/c16-10-6-9-14-12-7(2-1-5-15(9)10)8-3-4-13-11(8)12/h1-6,13H/b5-1-,7-2-,14-12+
B-241	 <chem>C12H9N3O</chem>	2.9513	44.9555	-0.5605	77.5437	134.7103	InChI=1S/C12H7N3O/c16-12-14-11-9-6-15(12)5-1-2-7(9)8-3-4-13-10(8)11/h1-6,13H

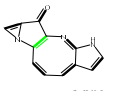
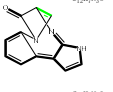
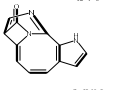
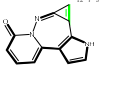
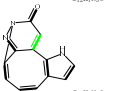
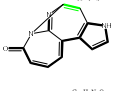
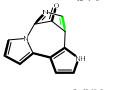
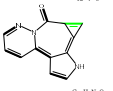
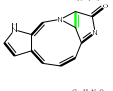
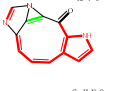
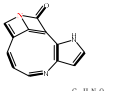
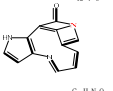
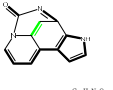
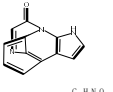
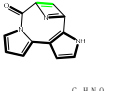
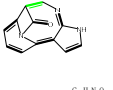
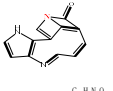
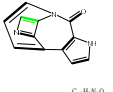
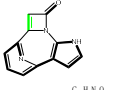
H-51		2.6408	148.4282	-0.5944	-11.6099	135.6414	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8-9-4-5-13-11(9)12(8)14-15(7)10/h1-6,13H/b2-1-,8-3-,14-12+
C-23		3.2976	61.9535	-1.8659	65.6327	135.9833	InChI=1S/C12H7N3O/c16-12-9-6-15(12)11-8(2-1-4-14-11)7-3-5-13-10(7)9/h1-6,13H
G-54		2.6609	154.4301	-0.7693	-8.83	136.2258	InChI=1S/C12H7N3O/c16-12-10-7(8-4-5-13-11(8)10)2-1-3-9-14-6-15(9)12/h1-6,13H/b2-1-,9-3-
H-105		2.9182	76.9794	-1.4983	58.6159	137.5541	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-8(7)9-4-5-13-11(9)15(12)14-10/h1-6,13H/b7-6-
C-20		3.1491	65.7909	-1.7024	66.4517	137.7385	InChI=1S/C12H7N3O/c16-12-9-6-15(12)11-8(3-5-14-11)7-2-1-4-13-10(7)9/h1-6,14H
C-45		2.6844	152.0928	-0.7452	-8.5600	137.7756	InChI=1S/C12H7N3O/c16-10-6-9-13-4-1-2-8-7-3-5-14-11(7)12(8)15(9)10/h1-6,14H/b2-1-,13-4-
C-40		2.5410	151.4197	-0.7800	-11.4800	137.9523	InChI=1S/C12H7N3O/c16-10-6-9-11-7(2-1-4-14-15(9)10)8-3-5-13-12(8)11/h1-6,13H/b2-1-,14-4-
G1-104		2.7991	156.4763	-0.9461	-9.49	138.6197	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-11(8)10(7)12-14-6-15(9)12/h1-6,13H/b3-1-,7-2-,12-10+
o-159		1.0971	77.5375	-0.871	61.5742	138.9759	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)9-3-4-13-11(9)10-8(7)6-14-10/h1-6,13H
D-6		2.2250	132.6663	-0.4987	-1.5200	140.1740	InChI=1S/C12H7N3O/c16-12-9-6-13-4-1-2-8-7-3-5-14-10(7)11(12)15(8)9/h1-6,14H/b2-1-,9-6-,13-4-
H-24		1.7686	84.6723	-1.022	58.9871	140.4791	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-10(8)14-11(9)15(12)6-7/h1-6,13H/b2-1-,9-3-
H-118		2.3503	156.7711	-0.8374	-8.89	140.8419	InChI=1S/C12H7N3O/c16-12-10-7(6-14-10)2-1-3-9-8-4-5-13-11(8)15(9)12/h1-6,13H/b2-1-,9-3-
H1-77		4.7748	139.4743	-1.8664	-4.84	140.9399	InChI=1S/C12H7N3O/c16-7-2-1-3-9-8-4-5-13-11(8)12-14-10(6-7)15(9)12/h1-6,13H/b2-1-,9-3-,10-6-
G-78		4.4797	157.8209	-1.964	-13.2753	141.703	InChI=1S/C12H7N3O/c16-12-14-6-15(12)9-3-1-2-7-8-4-5-13-11(8)10(7)9/h1-6,13H
H11-11		1.994	30.9462	-0.998	99.6897	142.0054	InChI=1S/C12H7N3O/c16-12-14-10-3-1-2-7-8-4-5-13-11(8)15(12)6-9(7)10/h1-6,13H
G-69		4.379	155.7441	-2.0578	-13.2796	142.86	InChI=1S/C12H7N3O/c16-10-6-14-15(10)9-3-1-2-7-8-4-5-13-12(8)11(7)9/h1-6,13H
q-17		4.2168	68.1477	-3.2131	61.2493	142.9036	InChI=1S/C12H7N3O/c16-12-9-6-8-10(15(12)14-9)3-1-2-7-4-5-13-11(7)8/h1-6,13H
B-216		2.4789	82.2492	-1.1737	63.5064	143.2974	InChI=1S/C12H7N3O/c16-12-9-6-15(12)5-1-2-7-8-3-4-13-11(8)14-10(7)9/h1-6,13H/b5-1-,7-2-
A2-62		2.5644	86.1721	-1.5585	43.4267	144.0817	InChI=1S/C12H7N3O/c16-11-10-6-8-7(3-5-13-8)9-2-1-4-14-12(11)15(9)10/h1-6,13H

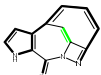

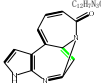
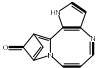
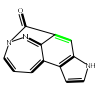


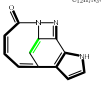
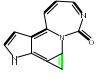
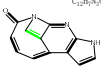
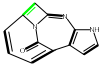
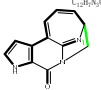
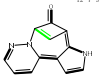
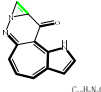
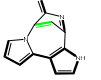
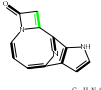
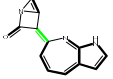
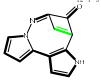
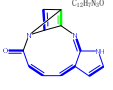
q-19		4.5819	69.6001	-3.3022	60.8835	144.5361	InChI=1S/C12H7N3O/c16-12-11-8-3-1-2-7-4-5-13-10(7)9(8)6-15(12)14-11/h1-6,13H
H11-56		2.3778	159.1064	-0.8929	-5.11	144.5552	InChI=1S/C12H7N3O/c16-12-8-6-14-9(8)2-1-3-10-7-4-5-13-11(7)15(10)12/h1-6,13H/b2-1-,10-3-
G-50		2.6133	154.234	-0.761	-10.9499	144.8616	InChI=1S/C12H7N3O/c16-12-10-8(9-4-5-13-11(9)10)3-1-2-7-6-14-15(7)12/h1-6,13H/b3-1-,7-2-
o-156		1.1137	78.1529	-0.8374	67.818	145.7529	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)9-3-4-13-11(9)8-6-14-10(7)8/h1-6,13H
B-137		3.2711	84.5124	-1.4540	58.3158	146.0074	InChI=1S/C12H7N3O/c16-12-11-9-6-10-8(3-4-13-10)7(9)2-1-5-15(12)14-11/h1-6,13H/b5-1-,7-2-
G1-66		2.8169	156.3919	-0.9602	-12.48	146.442	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)11(7)9-6-14-15(9)10/h1-6,13H/b3-1-,7-2-,11-9+
H-94		2.3892	32.7235	-0.399	96.9511	147.7955	InChI=1S/C12H7N3O/c16-12-11-9(4-5-13-11)8-3-1-2-7-6-15(12)14-10(7)8/h1-6,13H
H1-66		3.2496	48.1462	-1.9478	93.1193	148.1237	InChI=1S/C12H7N3O/c16-11-3-1-2-9-7-4-5-13-12(7)8-6-10(14-8)15(9)11/h1-6,13H
H11-46		2.8633	29.846	29.846	107.7825	148.1649	InChI=1S/C12H7N3O/c16-12-8-6-14-10-3-1-2-9(15(10)12)7-4-5-13-11(7)8/h1-6,13H
H11-14		2.7415	87.1542	-1.4825	59.5647	149.0216	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8-7-4-5-13-10(7)6-11(8)15(12)14-9/h1-6,13H/b3-1-,8-2-
p-7		4.5254	91.5109	-4.6569	54.6639	150.7167	InChI=1S/C12H7N3O/c16-12-11-8-6-9-7(4-5-13-9)2-1-3-10(8)15(12)14-11/h1-6,13H/b2-1-,3-1-,7-2-,8-6+,9-6+,10-3+
p-9		4.5194	91.6308	-4.6656	54.6701	150.8581	InChI=1S/C12H7N3O/c16-12-11-8-3-1-2-7-4-5-13-9(7)6-10(8)15(12)14-11/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,9-6+,10-6+
I-20		7.3872	59.0496	-7.9195	71.0039	152.7793	InChI=1S/C12H7N3O/c16-11-7-6-8(11)10(7)15-5-1-3-13-12-9(15)2-4-14-12/h1-6,14H
H-37		3.4887	155.3092	-0.5153	-7.89	152.992	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-12(8)15(9)14-11(7)10/h1-6,13H/b2-1-,9-3-,14-11+
X22-18		7.0901	68.7746	-7.7869	71.3871	153.5187	InChI=1S/C12H7N3O/c16-12-11-8(3-5-14-11)13-4-1-2-7-9-6-10(7)15(9)12/h1-6,14H/b2-1-,13-4+
r-10		17.3588	123.7754	-14.6496	16.8223	155.1197	InChI=1S/C12H7N3O/c16-11-9-6-15(9)10(11)8-3-1-2-7-4-5-13-12(7)14-8/h1-6H, (H,13,14)/b10-8-
o-155		3.106	151.3302	-0.5394	-1.19	156.2356	InChI=1S/C12H7N3O/c16-10-6-8-7(10)2-1-5-15-9-3-4-13-11(9)12(15)14-8/h1-6,13H/b5-1-,7-2+,14-12-
H1-67		16.7809	126.3095	-14.2019	19.1284	156.8769	InChI=1S/C12H7N3O/c16-9-3-1-2-7(9)8-4-5-13-11(8)12-14-10-6-15(10)12/h1-6,13H
G-43		3.3271	90.6008	-1.2005	54.0222	157.0728	InChI=1S/C12H7N3O/c16-12-11-8-2-1-3-10(11)15(12)14-6-9-7(8)4-5-13-9/h1-6,13H/b14-6+




















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	$C_{12}H_7N_3O$						
r-53		2.7071	167.6187	-1.7583	-7.82	157.3238	InChI=1S/C12H7N3O/c16-10-6-9-8-3-1-2-7-4-5-13-11(7)14-12(8)15(9)10/h1-6H,13,14
	$C_{12}H_7N_3O$						
A2-71		3.2725	158.2689	-0.6628	-4.97	158.8646	InChI=1S/C12H7N3O/c16-10-6-9-11(10)13-4-1-2-8-7-3-5-14-12(7)15(8)9/h1-6,14H/b4-1-,8-2-,13-11+
	$C_{12}H_7N_3O$						
H-132		2.798	31.1583	-0.5604	115.6226	159.4333	InChI=1S/C12H7N3O/c16-12-11-10-8(4-5-13-10)9-3-1-2-7(6-14-11)15(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
C-50		3.1302	94.0206	-1.2338	52.9116	160.0377	InChI=1S/C12H7N3O/c16-12-11-8-2-1-4-14-15(12)10(11)6-9-7(8)3-5-13-9/h1-6,13H/b2-1-,14-4-
	$C_{12}H_7N_3O$						
X22-46		18.0557	125.7998	-14.8688	19.4838	161.0879	InChI=1S/C12H7N3O/c16-12-9-6-15(9)11(12)7-2-1-4-13-8-3-5-14-10(7)8/h1-6,14H/b11-7+
	$C_{12}H_7N_3O$						
H11-105		3.6496	160.6467	-0.615	-6.04	161.1676	InChI=1S/C12H7N3O/c16-12-8-6-15-10(3-1-2-9(8)14-12)7-4-5-13-11(7)15/h1-6,13H/b2-1-,8-6-,10-3-
	$C_{12}H_7N_3O$						
B-192		1.5016	80.1299	-1.0333	81.1686	161.6153	InChI=1S/C12H7N3O/c16-12-10-9(6-14-10)7-2-1-5-15(12)11-8(7)3-4-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
o-78		7.8248	148.7515	-1.804	-4.97	162.0732	InChI=1S/C12H7N3O/c16-10-6-7-8-2-1-5-15(8)9-3-4-13-12(9)14-11(7)10/h1-6,13H
	$C_{12}H_7N_3O$						
o-166		3.2452	158.1813	-0.6059	-5.11	162.2884	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)10(15)6-8(7)14-12/h1-6,13H/b5-1-,7-2-,10-6-
	$C_{12}H_7N_3O$						
G1-112		13.9898	127.837	-10.4114	18.1837	162.3633	InChI=1S/C12H7N3O/c16-9-3-1-2-7(9)8-4-5-13-10(8)11-12-14-6-15(11)12/h1-6,13H
	$C_{12}H_7N_3O$						
s12-29		4.3499	87.0169	-4.0771	66.4326	163.1137	InChI=1S/C12H7N3O/c16-12-11-8-3-1-2-7-4-5-13-9(7)6-10(11)15(12)14-8/h1-6,13H/b3-1-,7-2-,9-6+
	$C_{12}H_7N_3O$						
A-30		5.4966	50.2811	-1.2698	93.0716	163.2547	InChI=1S/C12H7N3O/c16-9-6-14-11-7-2-1-5-15(9)12(11)10-8(7)3-4-13-10/h1-6,13H
	$C_{12}H_7N_3O$						
o-119		7.531	89.0651	-3.535	164.2332	164.2332	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)10(14-15)8(12)6-7/h1-6,13H/b5-1-,7-2+
	$C_{12}H_7N_3O$						
C-9		18.7375	127.6179	-14.9205	19.2514	164.7115	InChI=1S/C12H7N3O/c16-11-9-6-15(9)10(11)7-2-1-4-13-12-8(7)3-5-14-12/h1-6,14H/b10-7-
	$C_{12}H_7N_3O$						
G1-109		17.6603	128.9041	-11.5244	18.1827	165.9109	InChI=1S/C12H7N3O/c16-10-3-1-2-7(10)8-4-5-13-11(8)15-9-6-14-12(9)15/h1-6,13H
	$C_{12}H_7N_3O$						
p-29		4.0771	106.9416	-4.2777	58.1877	165.9211	InChI=1S/C12H7N3O/c16-12-14-11-8-6-9-7(4-5-13-9)2-1-3-10(8)15(11)12/h1-6,13H/b2-1-,3-1-,7-2-,8-6-,9-6+,13-3+
	$C_{12}H_7N_3O$						
i-64		2.9907	157.3911	-0.7352	1.67	165.968	InChI=1S/C12H7N3O/c16-9-6-7-10(9)12-11-8(2-4-14-11)15(12)5-1-3-13-7/h1-6,14H/b5-1-,12-10+,13-3+
	$C_{12}H_7N_3O$						
i-7		2.9894	157.392	-0.7353	1.67	165.968	InChI=1S/C12H7N3O/c16-9-6-7-10(9)12-11-8(2-4-14-11)15(12)5-1-3-13-7/h1-6,14H/b5-1-,12-10+,13-3-
	$C_{12}H_7N_3O$						

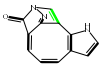





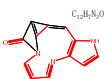



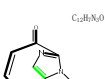


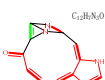


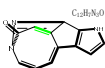


p-30	 <chem>C12H9N2O</chem>	4.075	106.9531	-4.2805	58.1904	166.072	InChI=1S/C12H7N3O/c16-12-14-11-8-3-1-2-7-4-5-13-9(7)6-10(8)15(11)12/h1-6,13H/b2-1-,3-1-,7-22,8-3-,9-6-,10-6+
p1-41	 <chem>C12H9N2O</chem>	4.5469	176.7374	-1.9815	-7.83	166.2458	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-8-6-14-12(8)15(9)11/h1-6,13H/b3-1-,7-2-,11-10+
G1-98	 <chem>C12H9N2O</chem>	3.4195	165.0788	-0.6594	-3.25	166.8311	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)15(9)12-8(10)6-14-12/h1-6,13H/b3-1-,9-2-
I-18	 <chem>C12H9N2O</chem>	4.1692	108.2632	-4.408	59.6754	167.5354	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-4-13-8-3-5-14-11(8)12(7)15(9)10/h1-6,14H/b2-1-,4-1-,7-2-,12-11-,13-4-,13-8+
G1-62	 <chem>C12H9N2O</chem>	3.5077	164.5886	-0.6669	-5.97	167.7829	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-12(7)15(8)9-6-14-11(9)10/h1-6,13H/b3-1-,8-2-
H11-7	 <chem>C12H9N2O</chem>	3.0631	37.9922	-0.2656	114.6803	168.173	InChI=1S/C12H7N3O/c16-12-14-9-3-1-2-7-6-10(9)15(12)11-8(7)4-5-13-11/h1-6,13H
q11-27	 <chem>C12H9N2O</chem>	12.137	127.5572	-11.2718	17.3642	168.4159	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(8)14-15-6-9(12)15/h1-6,13H
B-16	 <chem>C12H9N2O</chem>	3.2126	50.0954	-1.0409	106.4528	168.4822	InChI=1S/C12H7N3O/c16-10-6-9-11-8(3-4-13-11)7-2-1-5-15(10)14-12(7)9/h1-6,13H
H-152	 <chem>C12H9N2O</chem>	2.5804	84.0007	-1.5158	76.6733	168.9105	InChI=1S/C12H7N3O/c16-12-14-10-8-3-1-2-7(6-8)9-4-5-13-11(9)15(10)12/h1-6,13H
G-79	 <chem>C12H9N2O</chem>	3.8974	33.0044	-1.4275	117.0167	169.0122	InChI=1S/C12H7N3O/c16-12-14-6-9-7-2-1-3-10(9)15(12)11-8(7)4-5-13-11/h1-6,13H
G1-106	 <chem>C12H9N2O</chem>	14.3817	126.8967	-10.5145	16.9573	169.0291	InChI=1S/C12H7N3O/c16-9-3-1-2-8(7-4-5-13-10(7)9)11-12-14-6-15(11)12/h1-6,13H
o-252	 <chem>C12H9N2O</chem>	4.6276	65.719	-1.9825	88.4398	169.2713	InChI=1S/C12H7N3O/c16-12-14-10-7-2-1-5-15(12)9-3-4-13-11(9)8(10)6-7/h1-6,13H/b5-1-,7-2-
F-72	 <chem>C12H9N2O</chem>	3.1261	53.3931	-2.1278	109.0562	169.8379	InChI=1S/C12H7N3O/c16-12-14-11-9(4-5-13-11)8-3-1-2-7-6-10(8)15(7)12/h1-6H, (H,13,14,16)
H11-1	 <chem>C12H9N2O</chem>	3.3604	106.0349	-0.6828	63.3373	170.2006	InChI=1S/C12H7N3O/c16-12-14-10-3-1-2-7-6-9(15(10)12)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
x6-37	 <chem>C12H9N2O</chem>	7.5678	63.9245	-7.3201	87.0127	170.6488	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-9(7)6-8-11-14-12(8)15(10)11/h1-6,13H/b3-1-,7-2-,9-6+
G-20	 <chem>C12H9N2O</chem>	3.3819	31.5376	-1.0286	122.7399	170.708	InChI=1S/C12H7N3O/c16-12-12-9-3-1-2-7-8-4-5-13-11(8)15(12)6-14-10(7)9/h1-6,13H
q1-48	 <chem>C12H9N2O</chem>	4.7885	58.1365	-4.4497	107.7514	171.0032	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-9-6-14-11(8)15(9)12/h1-6,13H/b2-1-,8-3-
q1-49	 <chem>C12H9N2O</chem>	4.7889	58.1364	-4.4501	107.7516	171.0032	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-9-6-15(9)11(8)14-12/h1-6,13H/b2-1-,8-3-,14-11+
F-51	 <chem>C12H9N2O</chem>	4.5821	67.5758	-1.5187	93.8878	171.0266	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-7-4-5-13-11(7)14-6-10(8)15(9)12/h1-6H, (H,13,14)




















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k-42		12.1389	131.6509	-12.0904	33.2123	171.6974	InChI=1S/C12H7N3O/c16-12-8-6-7(8)11-10-9(2-4-14-10)13-3-1-5-15(11)12/h1-6,14H/b5-1-,13-3+
B-43		2.4270	26.1226	-0.6467	134.6101	172.0471	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-4-13-11)8-2-1-5-15(10)12(8)14-9/h1-6,13H
r-16		6.1125	176.8878	-2.1651	-9.8995	172.1875	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-11(7)14-15(12)10(8)9/h1-6H, (H,13,14)/b3-1-,7-2-
A2-12		4.6544	67.2507	-1.6348	94.9893	172.7055	InChI=1S/C12H7N3O/c16-12-8-6-9-7(3-5-13-9)10-2-1-4-14-11(8)15(10)12/h1-6,13H
G-44		3.3196	93.4663	-1.0526	72.9197	173.1638	InChI=1S/C12H7N3O/c16-12-10-7-2-1-3-9(10)15(12)6-14-11-8(7)4-5-13-11/h1-6,13H/b4-6+
B-42		1.9532	32.2233	-1.1398	125.9839	173.3647	InChI=1S/C12H7N3O/c16-10-6-8-11-7(3-4-13-11)9-2-1-5-15(9)12(10)14-8/h1-6,13H
F-68		3.8858	90.6198	-0.8942	70.9244	173.4242	InChI=1S/C12H7N3O/c16-12-14-11-8(4-5-13-11)7-2-1-3-10-9(7)6-15(10)12/h1-6H, (H,13,14,16)/b8-7-
I-89		15.1994	123.8905	-14.1899	31.8556	173.8152	InChI=1S/C12H7N3O/c16-11-8-6-7(8)10(11)15-5-1-3-13-12-9(15)2-4-14-12/h1-6,14H
o-89		1.6097	81.7025	-1.1105	88.8545	173.8596	InChI=1S/C12H7N3O/c16-12-11-8(6-14-11)7-2-1-5-15(12)9-3-4-13-10(7)9/h1-6,13H
H1-9		3.8199	93.7507	-0.8348	63.9008	174.5586	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-9(7)6-10-12(8)14-15(10)11/h1-6,13H/b3-1-,8-2-
s11-5		5.5537	71.9083	-2.7465	88.19	174.6283	InChI=1S/C12H7N3O/c16-12-8-6-14-9-3-1-2-7-4-5-13-10(7)11(8)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,9-3-,11-10+
r-54		4.3989	108.2	-4.4905	66.513	175.1858	InChI=1S/C12H7N3O/c16-10-6-9-11-8(15(9)10)3-1-2-7-4-5-13-12(7)14-11/h1-6H, (H,13,14)
H-162		3.9607	29.7555	-1.1196	129.6123	175.4641	InChI=1S/C12H7N3O/c16-12-14-9-6-7-2-1-3-10(15(7)12)8-4-5-13-11(8)9/h1-6,13H
s12-32		4.5328	110.6982	-4.4613	57.2459	176.0986	InChI=1S/C12H7N3O/c16-12-8-6-10-7(4-5-13-10)2-1-3-9-11(8)15(12)14-9/h1-6,13H/b3-1-,7-2-,10-6+
H11-51		4.7254	125.1139	-1.5559	39.5355	176.3135	InChI=1S/C12H7N3O/c16-12-10-6-15(12)11-8(4-5-13-11)7-2-1-3-9(7)14-10/h1-6,13H/b4-9-
p1-36		6.1545	75.2028	-6.9142	70.9122	176.6051	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-8-6-15(11)12(8)14-9/h1-6,13H/b3-1-,7-2-,11-10-,14-12+
q11-4		25.5681	141.1312	-17.3474	10.1934	176.7601	InChI=1S/C12H7N3O/c16-12-9-6-15(9)8-3-1-2-7-4-5-13-10(7)11(8)14-12/h1-6,13H
p-10		6.1297	87.3151	-3.7965	82.3765	176.7952	InChI=1S/C12H7N3O/c16-12-11-9-3-1-2-7-4-5-13-8(7)6-10(14-11)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-6+,9-3-,10-6-

F-9		19, 2943	146, 6623	-14, 997	13, 7703	177, 83	InChI=1S/C12H7N3O/c16-11-9-6-15(9)8-3-1-2-7-4-5-13-12(7)14-10(8)11/h1-6H, (H, 13, 14)
F-30		4, 8708	125, 1208	-1, 5796	39, 6364	177, 8631	InChI=1S/C12H7N3O/c16-12-9-6-15(12)10-3-1-2-7(10)8-4-5-13-11(8)14-9/h1-6H, (H, 13, 14)/b8-7-
q11-18		5, 7529	74, 0277	-2, 6645	89, 6845	178, 7669	InChI=1S/C12H7N3O/c16-12-8-6-14-11-10-7(4-5-13-10)2-1-3-9(8)15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 9-3-, 11-10+
H1-84		19, 8453	127, 6083	-15, 565	32, 3122	178, 7784	InChI=1S/C12H7N3O/c16-11-3-1-2-10-7-4-5-13-12(7)8-6-9(8)14-15(10)11/h1-6, 13H
q-42		5, 1943	72, 2889	-3, 0381	88, 3295	178, 9836	InChI=1S/C12H7N3O/c16-10-6-8-11-7(4-5-13-11)2-1-3-9-12(8)14-15(9)10/h1-6, 13H/b2-1-, 9-3+
H1-27		3, 625	54, 8508	-1, 9648	117, 2584	179, 0005	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-9(7)6-10-14-12(8)15(10)11/h1-6, 13H
B-180		2, 3329	31, 1598	-1, 4478	130, 8328	179, 1354	InChI=1S/C12H7N3O/c16-11-8-6-14-12(11)15-5-1-2-9(15)7-3-4-13-10(7)8/h1-6, 13H
D-8		24, 7489	122, 6888	-16, 4964	38, 7076	179, 1979	InChI=1S/C12H7N3O/c16-12-9-6-8(9)11-7(3-5-13-11)10-2-1-4-14-15(10)12/h1-6, 13H
s12-48		10, 3475	135, 2974	-6, 1342	16, 8237	179, 6105	InChI=1S/C12H7N3O/c16-12-11-10-8(14-12)3-1-2-7-4-5-13-9(7)6-15(10)11/h1-6, 13H/b3-1-, 7-2-, 9-6+
x9-43		9, 7586	139, 6265	-7, 2259	16, 0495	179, 882	InChI=1S/C12H7N3O/c16-12-9-7(4-5-13-9)2-1-3-8-10-11(12)15(10)6-14-8/h1-6, 13H/b2-1-, 8-3+
X23-8		4, 4837	184, 9719	-1, 8971	-4, 04	179, 9794	InChI=1S/C12H7N3O/c16-12-9-10-8(3-5-14-10)13-4-1-2-7-6-15(12)11(7)9/h1-6, 14H/b2-1-, 13-4-
X23-17		4, 4829	184, 9713	-1, 8969	-4, 04	179, 9795	InChI=1S/C12H7N3O/c16-12-9-10-8(3-5-14-10)13-4-1-2-7-6-15(12)11(7)9/h1-6, 14H/b2-1-, 13-4+
B-119		2, 0791	24, 3021	-0, 8850	143, 6051	180, 0002	InChI=1S/C12H7N3O/c16-12-14-9-6-10-7(2-1-5-15(10)12)8-3-4-13-11(8)9/h1-6, 13H
G-71		3, 5874	32, 3843	-1, 3496	130, 1585	180, 2907	InChI=1S/C12H7N3O/c16-10-6-14-11-7-2-1-3-9(11)15(10)12-8(7)4-5-13-12/h1-6, 13H
B-77		6, 5449	76, 0963	-2, 2443	85, 0898	180, 3398	InChI=1S/C12H7N3O/c16-12-9-6-8(14-9)11-7(3-4-13-11)10-2-1-5-15(10)12/h1-6, 13H
F-21		5, 0303	76, 9726	-1, 3805	95, 4579	180, 3607	InChI=1S/C12H7N3O/c16-12-8-6-14-11-7(4-5-13-11)9-2-1-3-10(8)15(9)12/h1-6H, (H, 13, 14)
X22-33		4, 4933	184, 9202	-1, 8946	-2, 98	180, 5989	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-9-3-5-14-10(9)8-6-15(12)11(7)8/h1-6, 14H/b2-1-, 13-4+
B-198		2, 1032	86, 7524	-1, 0825	87, 1370	180, 6371	InChI=1S/C12H7N3O/c16-12-11-8(3-4-13-11)7-2-1-5-15(12)9-6-14-10(7)9/h1-6, 13H
H11-69		2, 4242	89, 6617	-0, 84	82, 6258	180, 6661	InChI=1S/C12H7N3O/c16-11-6-10-9-3-1-2-8(14-9)7-4-5-13-12(7)15(10)11/h1-6, 13H

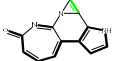
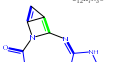
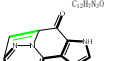
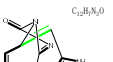
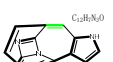
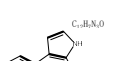
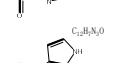
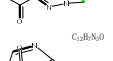
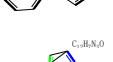
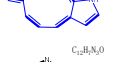
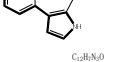
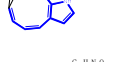
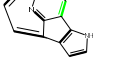
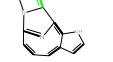
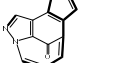
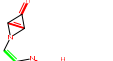
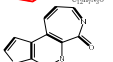
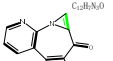
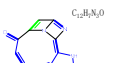
H1-73		3.2291	82.5713	-0.6564	81.7596	180.8385	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-9-10(6-7)15(12)14-9/h1-6,13H
	$C_{12}H_7N_3O$						
k1-23		12.6307	124.8361	-10.6346	32.2657	181.0101	InChI=1S/C12H7N3O/c16-12-9-7-6-15(11(7)9)5-1-3-13-8-2-4-14-10(8)12/h1-6,14H/b5-1-,13-3+
	$C_{12}H_7N_3O$						
H1-135		3.1397	54.6767	-1.8121	117.6126	181.9984	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)14-10-6-9(7)15(10)11/h1-6,13H
	$C_{12}H_7N_3O$						
k-14		4.6813	59.9744	-5.7698	111.0014	182.4278	InChI=1S/C12H7N3O/c16-12-7-6-9(12)15-5-1-3-13-8-2-4-14-10(8)11(7)15/h1-6,14H/b5-1-,13-3+
	$C_{12}H_7N_3O$						
B-129		2.7518	47.0601	-0.3761	117.2884	182.5027	InChI=1S/C12H7N3O/c16-12-9-6-10-7(3-4-13-10)8-2-1-5-15(12)14-11(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
o-217		2.4967	32.8873	-1.4343	131.4104	182.6763	InChI=1S/C12H7N3O/c16-12-7-6-8(14-12)9-2-1-5-15(9)10-3-4-13-11(7)10/h1-6,13H
	$C_{12}H_7N_3O$						
o-222		2.4949	32.8575	-1.4083	131.8529	182.7319	InChI=1S/C12H7N3O/c16-12-7-6-8(14-12)11-10(3-4-13-11)15-5-1-2-9(7)15/h1-6,13H
	$C_{12}H_7N_3O$						
H1-57		4.2946	103.1244	-0.6537	61.08	183.0038	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9-12(14-15(9)10)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
	$C_{12}H_7N_3O$						
D-24		16.2347	140.6010	-13.0611	28.5334	183.1472	InChI=1S/C12H7N3O/c16-12-14-4-1-2-9-7-3-5-13-11(7)8-6-10(8)15(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
H1-102		4.5341	76.2478	-2.3341	92.3412	183.1818	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)14-12-9(7)6-15(10)12/h1-6,13H/b3-1-,7-2-
	$C_{12}H_7N_3O$						
H-76		4.9167	69.1839	-1.8255	106.5246	183.285	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(15(7)12)14-11-8(9)4-5-13-11/h1-6H, (H,13,14)
	$C_{12}H_7N_3O$						
H-101		5.8232	39.8649	-0.801	117.0571	183.3269	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-15(12)11(9)14-7/h1-6,13H
	$C_{12}H_7N_3O$						
D-4		3.5715	49.9432	-2.3423	110.6633	183.3468	InChI=1S/C12H7N3O/c16-12-8-6-10(12)15-9(2-1-4-14-15)7-3-5-13-11(7)8/h1-6,13H
	$C_{12}H_7N_3O$						
s11-17		9.6254	141.8565	-7.1825	15.1173	183.8615	InChI=1S/C12H7N3O/c16-12-9-6-15(9)14-8-3-1-2-7-4-5-13-11(7)10(8)12/h1-6,13H
	$C_{12}H_7N_3O$						
B-87		2.4120	32.0922	-1.4678	133.3005	184.0518	InChI=1S/C12H7N3O/c16-12-10-6-8(14-12)11-7(3-4-13-11)9-2-1-5-15(9)10/h1-6,13H
	$C_{12}H_7N_3O$						
B-39		1.9130	94.1783	-0.5022	88.0528	184.2918	InChI=1S/C12H7N3O/c16-10-6-9-12-11-7(3-4-13-11)8(14-12)2-1-5-15(9)10/h1-6,13H/b5-1-,8-2-
	$C_{12}H_7N_3O$						
r-46		21.4879	155.8057	-15.9717	16.6769	184.3004	InChI=1S/C12H7N3O/c16-12-10(9-6-15(9)12)8-3-1-2-7-4-5-13-11(7)14-8/h1-6H, (H,13,14)/b10-8+
	$C_{12}H_7N_3O$						
B-64		2.7833	68.1035	-1.4902	101.9827	185.4752	InChI=1S/C12H7N3O/c16-12-8-6-9(12)14-15-5-1-2-10(15)7-3-4-13-11(7)8/h1-6,13H/b14-9+
	$C_{12}H_7N_3O$						
r1-28		8.1016	65.9566	-7.9122	98.8439	185.7817	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)14-11-8-6-9(11)15(8)10/h1-6H, (H,13,14)/b3-1-,7-2-
	$C_{12}H_7N_3O$						

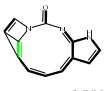
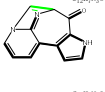
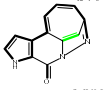
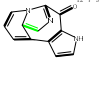
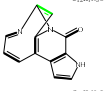
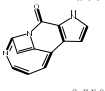
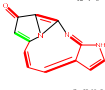
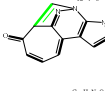
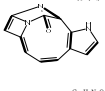
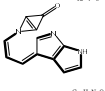
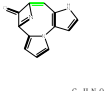
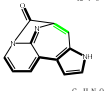
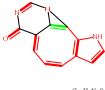
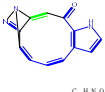
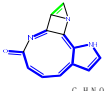
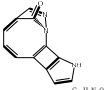
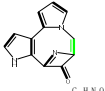
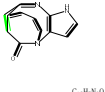
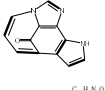
p1-23		7.0286	88.2227	-6.2578	92.9829	185.8994	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11-8(6-14-11)15(9)12/h1-6,13H/b3-1-,7-2-,12-10+
r-51		18.071	152.1334	-14.4942	13.1802	185.9392	InChI=1S/C12H7N3O/c16-12-10-8(15-6-9(10)15)3-1-2-7-4-5-13-11(7)14-12/h1-6H,(H,13,14,16)
H11-81		2.3408	78.2946	-1.2903	100.4996	186.2417	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)9-3-1-2-7-6-10(14-7)15(9)12/h1-6,13H/b2-1-,9-3-
H1-55		18.4	149.9367	-14.4214	23.1417	186.7559	InChI=1S/C12H7N3O/c16-10-3-1-2-7(10)8-4-5-13-11(8)12-9-6-15(9)14-12/h1-6,13H
H11-8		4.6756	52.9127	-1.0674	108.569	186.8569	InChI=1S/C12H7N3O/c16-12-14-7-2-1-3-8-9-4-5-13-11(9)15(12)(10)8(6-7)h1-6,13H
p-28		4.7141	82.2546	-3.9506	100.0256	186.9254	InChI=1S/C12H7N3O/c16-12-14-11-9-3-1-2-7-4-5-13-8(7)6-10(11)15(9)12/h1-6,13H/b2-1-,9-3-,10-6-
q1-9		7.1364	88.7328	-6.1786	91.9165	187.7356	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-11-9(6-14-11)15(8)12/h1-6,13H/b2-1-,8-3-
G1-87		5.2311	66.2549	-0.8107	104.058	187.8009	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-10(8)12-11(7)14-6-15(9)12/h1-6,13H/b3-1-,7-2-
H11-123		6.3211	64.9993	0.3543	90.322	187.8322	InChI=1S/C12H7N3O/c16-11-6-10-12-7(4-5-13-12)9-3-1-2-8(11)14-15(9)10/h1-6,13H
G-42		2.5515	90.9628	-0.8953	79.2273	187.9293	InChI=1S/C12H7N3O/c16-12-10-7-2-1-3-8(10)9-4-5-13-11(9)15(12)14-6-7/h1-6,13H
q1-54		5.2484	53.8557	-4.6202	126.9986	187.9864	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-6-9-14-11(8)15(9)12/h1-6,13H/b2-1-,8-3-
C-51		21.5486	157.2139	-15.6416	16.7246	188.1383	InChI=1S/C12H7N3O/c16-12-10(9-6-15(9)12)7-2-1-4-13-11-8(7)3-5-14-11/h1-6,14H/b10-7+
X22-3		4.0731	148.6576	-3.8749	39.8264	188.16	InChI=1S/C12H7N3O/c16-10-6-9-11-8(15(9)10)2-1-4-13-7-3-5-14-12(7)11/h1-6,14H/b2-1-,4-1-,8-2-,12-11-,13-4-,13-7-
s11-37		29.1859	149.729	-18.1174	13.5391	188.2658	InChI=1S/C12H7N3O/c16-12-10-8(14-9-6-15(9)12)3-1-2-7-4-5-13-11(7)10/h1-6,13H
X22-2		4.0174	148.627	-3.8165	38.7633	188.3089	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-4-13-8-3-5-14-11(8)12(7)15(9)10/h1-6,14H/b2-1-,4-1-,7-2-,12-11-,13-4-,13-8-
o-75		2.1657	32.9716	-1.0209	139.214	188.867	InChI=1S/C12H7N3O/c16-10-6-7-11-9(3-4-13-11)15-5-1-2-8(15)12(10)14-7/h1-6,13H
r-4		5.0505	53.4778	-5.0751	117.6826	188.9603	InChI=1S/C12H7N3O/c16-11-9-6-15-10(11)8(9)3-1-2-7-4-5-13-12(7)14-15/h1-6H,(H,13,14)/b3-1-,7-2-
x4-40		5.3879	76.3699	-2.4702	94.9236	189.3458	InChI=1S/C12H7N3O/c16-12-10-11-9-7(4-5-13-9)2-1-3-8(6-14-10)15(11)12/h1-6,13H/b2-1-,3-1-,7-29,8-3-,11-9+
X22-21		21.7735	157.2358	-16.0054	19.3404	189.4612	InChI=1S/C12H7N3O/c16-12-10(9-6-15(9)12)7-2-1-4-13-8-3-5-14-11(7)8/h1-6,14H/b10-7-

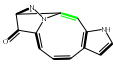
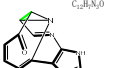
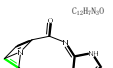
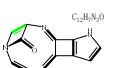
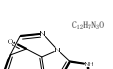

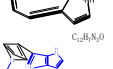
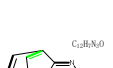
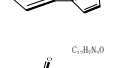
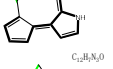
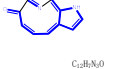
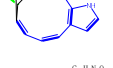
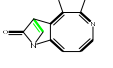
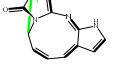
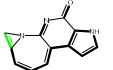
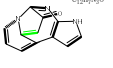
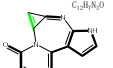
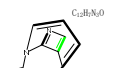
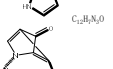
q-49		3.167	56.3556	-2.3104	117.5566	189.7924	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9-6-15(12)14-11(8)9/h1-6,13H/t2-1-,8-3+
	$C_{12}H_7N_3O$						
o-82		2.1749	32.8485	-0.9936	139.812	189.7929	InChI=1S/C12H7N3O/c16-10-6-7-8-2-1-5-15(8)9-3-4-13-11(9)12(10)14-7/h1-6,13H
	$C_{12}H_7N_3O$						
A-78		3.4893	34.8422	-2.1022	124.3005	190.0713	InChI=1S/C12H7N3O/c16-12-10-9(6-14-12)7-2-1-5-15(10)11-8(7)3-4-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
q1-18		6.364	90.4827	-5.7725	94.3089	190.1406	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-8-6-14-11(8)15(9)12/h1-6,13H/t2-1-,9-3+
	$C_{12}H_7N_3O$						
o-86		5.7944	37.6499	-1.6408	130.1714	190.6841	InChI=1S/C12H7N3O/c16-12-11-7-2-1-5-15(12)9-3-4-13-10(8)7(6)14-11/h1-6,13H
	$C_{12}H_7N_3O$						
A2-20		3.2034	70.8554	-1.1244	115.3354	190.8621	InChI=1S/C12H7N3O/c16-12-8-2-1-4-13-10-6-9(15)(10)12(11-7(8)3-5-14-11/h1-6,14H/t2-1-,4-1-,8-2-,13-4-,13-10-
	$C_{12}H_7N_3O$						
x2-17		19.3346	126.3221	-11.3978	47.475	191.0323	InChI=1S/C12H7N3O/c16-12-10-7-6-9-8(2-4-14-9)13-3-1-5-15(12)11(7)10/h1-6,14H/t5-1-,7-6-,13-3+
	$C_{12}H_7N_3O$						
I-13		11.9386	156.9465	-10.5928	11.4469	191.3651	InChI=1S/C12H7N3O/c16-12-7-6-9-13-3-1-5-15(9)8-2-4-14-11(8)10(7)12/h1-5,10,14H
	$C_{12}H_7N_3O$						
o-51		3.109	69.592	-1.3498	105.2136	191.5327	InChI=1S/C12H7N3O/c16-11-7-6-8(11)14-12-10(3-4-13-12)15-5-1-2-9(7)15/h1-6,13H/t14-8+
	$C_{12}H_7N_3O$						
o-180		3.4364	70.5752	-1.2293	102.2899	191.7114	InChI=1S/C12H7N3O/c16-12-8-6-7(14-8)9-2-1-5-15(9)10-3-4-13-11(10)12/h1-6,13H
	$C_{12}H_7N_3O$						
H1-46		4.7226	59.1239	-0.9962	113.0796	191.7272	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)15-9(7)6-14-12(10)15/h1-6,13H/t3-1-,7-2-
	$C_{12}H_7N_3O$						
E-36		8.3379	135.9304	0.1856	19.6237	191.7293	InChI=1S/C12H7N3O/c16-11-6-10-8(11)2-1-3-9-7-4-5-13-12(7)15(10)14-9/h1-6,13H/t3-1-,8-2+
	$C_{12}H_7N_3O$						
A2-41		3.6878	77.7517	-0.9857	103.5818	191.8679	InChI=1S/C12H7N3O/c16-12-11-10-6-8-7(3-5-13-8)9(15)(10)12(2-1-4-14-11/h1-6,13H/t2-1-,4-1-,9-2-,14-4-,14-11-
	$C_{12}H_7N_3O$						
x6-40		15.7612	123.1308	-10.7783	37.906	191.9173	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-10-14-12-11(9)15(10)12/h1-6,13H/t3-1-,7-2-,8-6+
	$C_{12}H_7N_3O$						
H11-67		4.3531	29.3777	-1.1756	145.7394	192.017	InChI=1S/C12H7N3O/c16-11-6-8-12-7(4-5-13-12)9-2-1-3-10(14-8)15(9)11/h1-6,13H
	$C_{12}H_7N_3O$						
I-19		4.471	49.9794	-2.7877	117.9557	192.5579	InChI=1S/C12H7N3O/c16-11-7-6-8(11)12-14-3-1-5-15(12)9-2-4-13-10(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
B-21		6.3858	52.7413	-1.4743	97.3776	192.6615	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(10)14-12(9)11-8(7)3-4-13-11/h1-6,13H/t5-1-,7-2-
	$C_{12}H_7N_3O$						
B-66		2.3806	31.5196	-1.4024	143.2325	192.6658	InChI=1S/C12H7N3O/c16-12-8-6-10(14-12)15-5-1-2-9(15)7-3-4-13-11(7)8/h1-6,13H
	$C_{12}H_7N_3O$						
x7-16		15.9834	152.0666	-10.9336	16.8512	193.1598	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10(9)12-8-6-14-15(8)12/h1-6,13H
	$C_{12}H_7N_3O$						

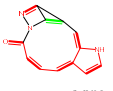
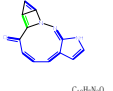
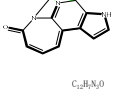
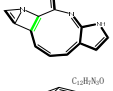
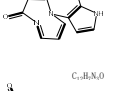
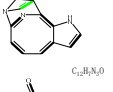
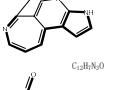
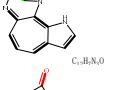
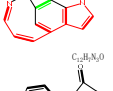
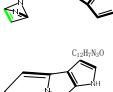
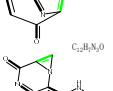
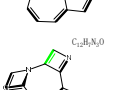
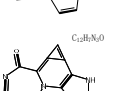
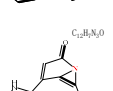
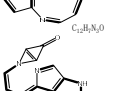
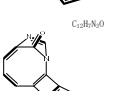
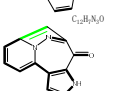
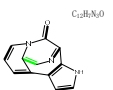

H-106		7.9994	150.2604	-1.8262	17.9143	193.2735	InChI=1S/C12H7N3O/c16-12-11-10-9(4-5-13-10)8-3-1-2-7(8)6-15(12)14-11/h1-6,13H/b7-6+
	$C_{12}H_7N_3O$						
B-117		5.1653	34.0296	-0.9789	133.5773	193.2756	InChI=1S/C12H7N3O/c16-12-9-6-10-7(2-1-5-15(10)12)8-3-4-13-11(8)14-9/h1-6,13H
	$C_{12}H_7N_3O$						
q-22		5.6087	79.3971	-2.3508	96.5773	193.5204	InChI=1S/C12H7N3O/c16-12-11-8-3-1-2-7-4-5-13-10(7)9(6-14-11)15(8)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,10-9+
	$C_{12}H_7N_3O$						
A2-56		4.5262	55.1997	-1.2475	117.7667	194.1001	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-4-13-12(10)15(9)11-8(7)3-5-14-11/h1-6,14H/b4-1-,7-2-,13-12+
	$C_{12}H_7N_3O$						
r-15		4.1907	85.3634	-4.4024	106.0149	194.1454	InChI=1S/C12H7N3O/c16-12-9-6-15(12)11-8(9)3-1-2-7-4-5-13-10(7)14-11/h1-6H, (H,13,14)
	$C_{12}H_7N_3O$						
r1-7		13.2254	117.6991	-10.7014	61.2287	194.1483	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-10-8-6-15(9)11(8)10/h1-6H, (H,13,14)/b3-1-,7-2-
	$C_{12}H_7N_3O$						
q11-65		3.5248	52.533	-2.7291	119.3861	194.2395	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-9(8)6-15(12)14-11/h1-6,13H/b2-1-,8-3+
	$C_{12}H_7N_3O$						
o-36		2.4785	31.8613	-1.2981	144.4271	194.3986	InChI=1S/C12H7N3O/c16-12-7-6-14-11(12)8-2-1-5-15(8)9-3-4-13-10(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
o-126		2.3875	74.6673	-1.7146	108.4398	194.4732	InChI=1S/C12H7N3O/c16-10-7-2-1-5-15-9-3-4-13-11(9)14-12(15)8(10)6-7/h1-6,13H/b5-1-,7-2+
	$C_{12}H_7N_3O$						
s11-39		3.5121	53.2085	-2.7216	119.4333	194.6104	InChI=1S/C12H7N3O/c16-12-10-8-6-15(12)14-9(8)3-1-2-7-4-5-13-11(7)10/h1-6,13H/b3-1-,7-2-,11-10-
	$C_{12}H_7N_3O$						
G1-68		15.3827	151.5405	-10.9756	18.1523	195.3412	InChI=1S/C12H7N3O/c16-10-3-1-2-8(7-4-5-13-11(7)10)12-9-6-14-15(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
x9-25		15.9444	153.012	-10.9392	16.551	196.0665	InChI=1S/C12H7N3O/c16-12-8(11-9-6-14-15(9)11)3-1-2-7-4-5-13-10(7)12/h1-6,13H
	$C_{12}H_7N_3O$						
H-23		4.6117	137.4506	-1.8718	55.6449	196.1947	InChI=1S/C12H7N3O/c16-12-7-2-1-3-8-9-4-5-13-10(9)11(8)14-15(12)6-7/h1-6,13H/b2-1-,8-3-,14-11+
	$C_{12}H_7N_3O$						
B-52		2.0557	32.9466	-0.9800	147.5796	196.2259	InChI=1S/C12H7N3O/c16-9-6-10-14-12(9)11-7(3-4-13-11)8-2-1-5-15(8)10/h1-6,13H
	$C_{12}H_7N_3O$						
G-63		4.759	39.4986	-1.1245	131.5732	196.3838	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-9-10(7)14-6-15(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
B-115		5.3757	32.2214	-0.8095	132.4213	196.4807	InChI=1S/C12H7N3O/c16-12-9-6-10-7(2-1-5-15(10)14-9)8-3-4-13-11(8)12/h1-6,13H
	$C_{12}H_7N_3O$						
s12-30		7.4878	87.0626	-5.6032	102.1504	196.6345	InChI=1S/C12H7N3O/c16-12-10-11-8(14-10)3-1-2-7-4-5-13-9(7)6-15(11)12/h1-6,13H/b3-1-,7-2-,9-6+
	$C_{12}H_7N_3O$						
H1-125		4.1118	96.1394	-0.2098	90.2526	196.9734	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)8-6-15(10)12(8)14-9/h1-6,13H/b3-1-,9-2-
	$C_{12}H_7N_3O$						
o-202		5.3947	40.399	-1.4307	137.4653	197.1262	InChI=1S/C12H7N3O/c16-12-8-6-14-10-7(8)2-1-5-15(12)9-3-4-13-11(9)10/h1-6,13H
	$C_{12}H_7N_3O$						

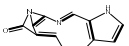


















G-76		3. 8322	87. 1896	-2. 5874	105. 2713	197. 5654	InChI=1S/C12H7N3O/c16-12-14-6-15(12)11-8-2-1-3-9(11)10-7(8)4-5-13-10/h1-6, 13H
A-80		3. 5692	35. 8233	-2. 1671	132. 2546	197. 5835	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(9(10)6-14-12)11-8(7)3-4-13-11/h1-6, 13H
r-32		22. 0594	167. 2708	-14. 9091	16. 3014	197. 6605	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)14-10(8)9-6-15(9)12/h1-6H, (H, 13, 14)
B-75		2. 6207	67. 9332	-1. 1617	113. 2062	197. 6812	InChI=1S/C12H7N3O/c16-12-8-6-10(14-8)15-5-1-2-9(15)7-3-4-13-11(7)12/h1-6, 13H
X-20		3. 6396	39. 3416	0. 3498	138. 6864	198. 0779	InChI=1S/C13H11N3O/c1-16-8-9-3-2-5-14-11(7-12(16)17)13-10(9)4-6-15-13/h2-8, 15H, H3/h3-2-, 9-8-, 11-7-, 14-5-
B-251		19. 5566	152. 7600	-11. 6943	13. 4288	198. 3912	InChI=1S/C12H7N3O/c16-12-11-8(3-4-13-11)7-2-1-5-15-6-9(15)10(7)14-12/h1-6, 13H
x2-4		20. 5461	140. 7699	-11. 5038	28. 2621	198. 5072	InChI=1S/C12H7N3O/c16-12-7-6-9-8(2-4-14-9)13-3-1-5-15-10(7)11(12)15/h1-6, 14H/h5-1-, 7-6-, 13-3+
X23-6		6. 7308	87. 8405	-5. 1731	110. 7353	198. 6276	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-4-13-9-3-5-14-11(9)15(12)10(7)8/h1-6, 14H/h2-1-, 13-4-
q-67		5. 5478	117. 6032	-0. 6777	71. 8415	198. 7185	InChI=1S/C12H7N3O/c16-12-14-11-8-3-1-2-7-4-5-13-10(7)9(6-8)15(11)12/h1-6, 13H/h2-1-, 3-1-, 7-2-, 8-3-, 10-9-
G-68		3. 6332	85. 1245	-2. 6736	105. 2229	198. 9734	InChI=1S/C12H7N3O/c16-10-6-14-15(10)12-8-2-1-3-9(12)11-7(8)4-5-13-11/h1-6, 13H
H11-87		5. 2578	71. 6006	-1. 8279	122. 284	199. 4523	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-14-11(15(10)12)6-9-7(8)4-5-13-9/h1-6, 13H
r-2		5. 3419	51. 5049	-4. 9031	131. 0908	199. 4916	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-12(7)14-15-9(8)6-10(11)15/h1-6H, (H, 13, 14)/h3-1-, 7-2-
F-6		6. 0618	85. 816	-2. 0488	91. 8315	199. 955	InChI=1S/C12H7N3O/c16-11-7-2-1-3-9-8-4-5-13-12(8)14-15(9)10(11)6-7/h1-6H, (H, 13, 14)/h3-1-, 7-2-
o-144		8. 3812	62. 9362	0. 3676	103. 6842	200. 059	InChI=1S/C12H7N3O/c16-10-6-8-11-7(10)2-1-5-15(14-11)9-3-4-13-12(8)9/h1-6, 13H
G1-42		12. 7837	153. 9825	-6. 5026	20. 2053	200. 0878	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-12(8)14-6-15-10(7)11(9)15/h1-6, 13H
B-62		24. 8968	131. 2636	-16. 4417	40. 6715	200. 2822	InChI=1S/C12H7N3O/c16-12-8-6-9(8)14-11-7(3-4-13-11)10-2-1-5-15(10)12/h1-6, 13H/h14-9-
s12-42		13. 8088	157. 3361	-8. 7276	16. 0777	200. 4169	InChI=1S/C12H7N3O/c16-12-14-8-3-1-2-7-4-5-13-9(7)6-10-11(8)15(10)12/h1-6, 13H/h3-1-, 7-2-, 9-6+
A-165		11. 1724	155. 4483	-6. 3101	16. 6695	200. 6597	InChI=1S/C12H7N3O/c16-12-11-10-8(2-1-5-15(10)11)7-3-4-13-9(7)6-14-12/h1-6, 13H/h14-6-
G-45		2. 975	85. 2699	-0. 8383	102. 7676	201. 1512	InChI=1S/C12H7N3O/c16-12-10-7-2-1-3-9(10)14-6-15(12)11-8(7)4-5-13-11/h1-6, 13H


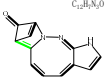
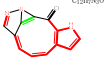
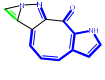
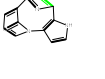
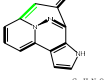
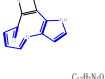
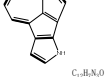
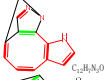
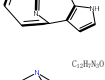
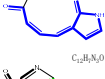
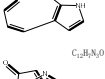
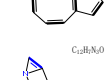
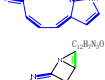
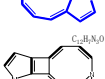
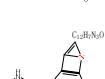
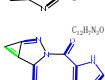
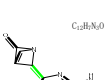

H1-28	 <chem>C12H9N3O</chem>	26.0732	157.6419	-17.051	14.5391	201.2877	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)9-6-15(9)12(8)14-10/h1-6,13H
r1-31	 <chem>C12H9N3O</chem>	13.9961	135.3994	-13.918	53.0801	201.6113	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)14-12-8-6-9(8)15(10)12/h1-6H, (H,13,14)/b3-1-,7-2-
H11-141	 <chem>C12H9N3O</chem>	4.9332	42.611	-0.7141	126.1791	201.8289	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(15(10)14-7)8-4-5-13-11(8)12/h1-6,13H
H-159	 <chem>C12H9N3O</chem>	2.8113	88.3997	-1.4149	106.5172	202.3606	InChI=1S/C12H7N3O/c16-12-14-11-9-3-1-2-7(15(11)12)6-10-8(9)4-5-13-10/h1-6,13H
H-153	 <chem>C12H9N3O</chem>	2.7674	88.9402	-1.415	106.2531	202.5799	InChI=1S/C12H7N3O/c16-12-14-11-7-2-1-3-10(15(11)12)8-4-5-13-9(8)6-7/h1-6,13H
H1-2	 <chem>C12H9N3O</chem>	32.5001	151.524	-18.9256	18.3715	202.7886	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-12(8)15-6-10(15)14-11(7)9/h1-6,13H
H1-1	 <chem>C12H9N3O</chem>	10.1248	157.0471	-6.7654	15.6791	203.0717	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)9-6-15(9)14-12(7)10/h1-6,13H
A-200	 <chem>C12H9N3O</chem>	4.3229	48.8463	-0.9987	122.7673	203.5869	InChI=1S/C12H7N3O/c16-12-9-7-2-1-5-15(12)6-14-11(9)10-8(7)3-4-13-10/h1-6,13H
p1-11	 <chem>C12H9N3O</chem>	5.2979	47.8191	-4.6813	145.9246	203.7847	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)12-8-6-9(14-12)15(8)10/h1-6,13H/b3-1-,7-2-,12-11-
H11-145	 <chem>C12H9N3O</chem>	5.8911	35.3454	-0.7056	136.0079	204.0675	InChI=1S/C12H7N3O/c16-12-8-6-15-9(2-1-3-10(15)14-8)7-4-5-13-11(7)12/h1-6,13H
q1-33	 <chem>C12H9N3O</chem>	5.254	56.2389	-4.8825	126.2473	204.1585	InChI=1S/C12H7N3O/c16-12-10-6-8-9(15(10)14-8)3-1-2-7-4-5-13-11(7)12/h1-6,13H/b2-1-,9-3-
B-236	 <chem>C12H9N3O</chem>	5.9406	51.4285	-1.3711	114.7518	204.3059	InChI=1S/C12H7N3O/c16-12-14-11-7-2-1-5-15(12)6-9(11)10-8(7)3-4-13-10/h1-6,13H/b5-1-,7-2-
s11-42	 <chem>C12H9N3O</chem>	9.918	158.9866	0.5146	15.8662	204.4707	InChI=1S/C12H7N3O/c16-10-6-8-12-11-7(4-5-13-11)2-1-3-9(14-12)15(8)10/h1-6,13H/b2-1-,3-1-,7-2-,9-3+,12-11+
A-60	 <chem>C12H9N3O</chem>	5.1618	45.5747	-0.2571	131.3653	204.7129	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-11(12)9(6-14-15)10-7(8)3-4-13-10/h1-6,13H
x5-10	 <chem>C12H9N3O</chem>	51.1042	154.7884	-28.9274	11.0764	204.7688	InChI=1S/C12H7N3O/c16-11-9-10(11)15(9)6-8-3-1-2-7-4-5-13-12(7)14-8/h1-6H, (H,13,14)/b8-6-
C-62	 <chem>C12H9N3O</chem>	27.5081	154.8625	-17.4980	14.8557	204.7839	InChI=1S/C12H7N3O/c16-12-11-8(2-1-4-14-12)7-3-5-13-10(7)9-6-15(9)11/h1-6,13H
C-15	 <chem>C12H9N3O</chem>	22.9529	152.5482	-12.4385	20.3836	204.8985	InChI=1S/C12H7N3O/c16-11-9-6-15(9)12-8(2-1-4-14-12)7-3-5-13-10(7)11/h1-6,13H
p1-13	 <chem>C12H9N3O</chem>	4.2278	164.4442	-1.435	19.8872	205.0896	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)12-14-10-6-8(9)15(10)12/h1-6,13H/b3-1-,7-2-,12-11+
G-62	 <chem>C12H9N3O</chem>	5.1842	43.9755	-1.2443	129.1464	205.0977	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-10-9(7)6-14-15(10)12/h1-6,13H

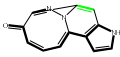
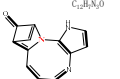
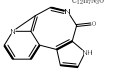
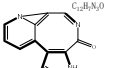
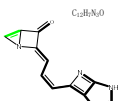
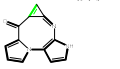
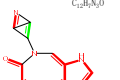
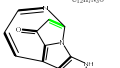
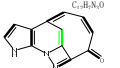
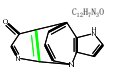
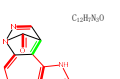
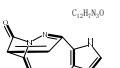
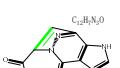
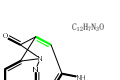
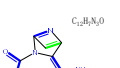
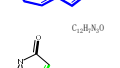
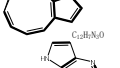
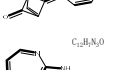
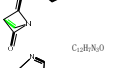
r-58		17.095	150.7892	-11.6145	35.5085	205.1282	InChI=1S/C12H7N3O/c16-12-14-11-7(4-5-13-11)2-1-3-8-9-6-15(12)10(8)9/h1-6H, (H, 13, 14, 16)/b3-1-, 7-2-
B-226		5.1240	34.9950	-0.3474	142.0440	205.1912	InChI=1S/C12H7N3O/c16-11-9-6-15-5-1-2-8(12(15)14-9)7-3-4-13-10(7)11/h1-6, 13H
H11-74		4.2806	38.0105	-1.9891	138.6704	205.1943	InChI=1S/C12H7N3O/c16-12-11-9(4-5-13-11)8-3-1-2-7-6-10(8)15(12)14-7/h1-6, 13H
B-203		6.9680	37.0691	-1.8861	131.5896	205.3937	InChI=1S/C12H7N3O/c16-11-10-8(3-4-13-10)7-2-1-5-15-9(7)6-14-12(11)15/h1-6, 13H
C-67		5.0187	62.2587	-3.0194	131.6022	205.5432	InChI=1S/C12H7N3O/c16-12-11-8(3-5-14-11)7-2-1-4-13-10-6-9(7)15(10)12/h1-6, 14H/b2-1-, 4-1-, 7-2-, 13-4-, 13-10+
A2-18		5.0013	62.1845	-3.0195	131.7378	205.5477	InChI=1S/C12H7N3O/c16-12-11-8(3-5-14-11)7-2-1-4-13-10-6-9(7)15(10)12/h1-6, 14H/b2-1-, 4-1-, 7-2-, 13-4-, 13-10+
x5-27		12.4707	131.9353	-9.5242	46.568	205.8154	InChI=1S/C12H7N3O/c16-9-6-8-3-1-2-7-4-5-13-11(7)14-12-10(9)15(8)12/h1-6H, (H, 13, 14)/b3-1-, 7-2-
H1-6		2.9475	32.0025	-1.5479	151.0325	206.0314	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15-6-9(10)11(7)14-15/h1-6, 13H
q11-50		2.7391	78.1386	-1.0227	122.7792	206.4645	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8-6-9(14-11)15(8)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3-, 11-10+
A-168		50.6349	164.1033	-28.9094	10.0558	206.5689	InChI=1S/C12H7N3O/c16-11-9-10(11)15(9)5-1-2-7-6-14-12-8(7)3-4-13-12/h1-6, 13H/b5-1-, 7-2+
o-37		2.9999	70.9155	-1.7767	116.6809	206.7321	InChI=1S/C12H7N3O/c16-12-8-6-7-9(3-4-13-7)15-5-1-2-10(15)11(12)14-8/h1-6, 13H/b8-6-
B-133		4.1872	39.2540	-0.8166	146.7820	207.0045	InChI=1S/C12H7N3O/c16-12-10-6-9-7(3-4-13-9)8-2-1-5-15(12)11(8)14-10/h1-6, 13H
x4-62		12.7983	151.7478	-6.7907	19.3227	207.057	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)11-10(8)15(11)6-14-12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 11-9-
q1-8		7.6014	57.5418	-8.1189	116.5029	207.2088	InChI=1S/C12H7N3O/c16-10-6-9-12-8(15(9)14-12)3-1-2-7-4-5-13-11(7)10/h1-6, 13H/b2-1-, 8-3+, 9-6+
p1-20		17.4418	138.4803	-14.5626	41.6261	207.2405	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11(14-9)8-6-15(8)12/h1-6, 13H/b3-1-, 7-2-, 12-10-, 14-11-
G-23		7.2049	135.7461	0.0109	48.1927	207.3029	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-10(8)11(9)15(12)14-6-7/h1-6, 13H/b3-1-, 7-2-
B-223		2.9610	70.5162	-1.7344	116.8846	207.4899	InChI=1S/C12H7N3O/c16-12-8-6-15-5-1-2-9(15)7-3-4-13-10(7)11(12)14-8/h1-6, 13H/b8-6-
o-204		4.3926	65.6973	-1.3025	129.7869	207.5686	InChI=1S/C12H7N3O/c16-12-8-6-9-7(8)2-1-5-15(12)10-3-4-13-11(10)14-9/h1-6, 13H/b14-9-
A-197		5.021	47.1283	-0.1921	134.4048	208.1973	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-14-10(11(12)15)9-7(8)3-4-13-9/h1-6, 13H


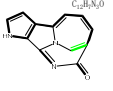
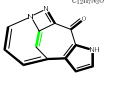
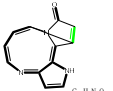
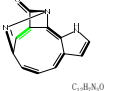
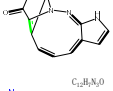

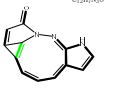
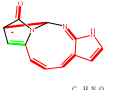
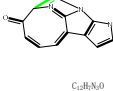
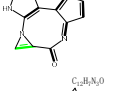
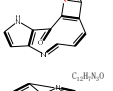
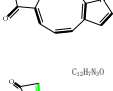
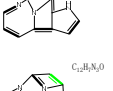
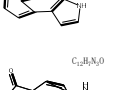
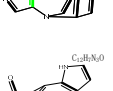
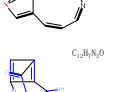


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	$C_{12}H_7N_3O$						
G1-65		25.5558	157.1772	-13.2852	22.1485	208.4285	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-12(7)14-6-9-11(10)15(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
r-26		14.6717	155.5602	-10.2728	20.9095	208.4836	InChI=1S/C12H7N3O/c16-12-9-6-9-8(15)9(10)3-1-2-7-4-5-13-11(7)14-12/h1-6H,13,14,16
	$C_{12}H_7N_3O$						
B-228		5.7565	134.8823	-2.0770	70.7178	208.5443	InChI=1S/C12H7N3O/c16-12-9-6-15(12)5-1-2-7-8-3-4-13-10(8)11(7)14-9/h1-6,13H/b5-1-,7-2-,14-11+
	$C_{12}H_7N_3O$						
G-3		4.8578	46.7798	-0.1851	137.1473	208.5629	InChI=1S/C12H7N3O/c16-11-7-2-1-3-8-9-4-5-13-12(9)15(10)11(8)11-14-6-7/h1-6,13H
	$C_{12}H_7N_3O$						
s12-24		10.3107	141.2797	-6.6163	42.8587	208.8339	InChI=1S/C12H7N3O/c16-12-11-10-8(14-12)3-1-2-7-4-5-13-9(7)6-15(10)11/h1-6,13H/b3-1-,7-2-,9-6-
	$C_{12}H_7N_3O$						
k1-15		8.4273	71.8097	-7.7112	105.1349	208.9446	InChI=1S/C12H7N3O/c16-12-10-8-6-9(10)15(8)5-1-3-13-7-2-4-14-11(7)12/h1-6,14H/b5-1-,13-3+
	$C_{12}H_7N_3O$						
H-49		5.7122	35.2984	-2.2899	147.3529	208.9858	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)14-12(7)15(9)10/h1-6,13H
	$C_{12}H_7N_3O$						
F-71		19.8158	165.3877	-13.9605	16.0914	209.0142	InChI=1S/C12H7N3O/c16-12-14-11-9(4-5-13-11)7-2-1-3-8(7)10-6-15(10)12/h1-6H,13,14,16)/b9-7-
	$C_{12}H_7N_3O$						
p1-26		17.2208	144.0024	-11.5533	37.0872	209.3657	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-14-11(9)8-6-15(8)12/h1-6,13H/b3-1-,7-2-,12-10-
	$C_{12}H_7N_3O$						
q1-21		7.4753	57.8675	-8.14	117.4465	209.531	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-8-6-15(9)11(8)14-12/h1-6,13H/b2-1-,9-3+,14-11+
	$C_{12}H_7N_3O$						
i-9		7.1186	90.4082	-3.9051	96.4049	209.5406	InChI=1S/C12H7N3O/c16-12-7-6-15(12)9-2-1-4-13-8-3-5-14-11(8)10(7)9/h1-6,14H/b2-1-,4-1-,9-2+,11-10+,13-4+,13-8+
	$C_{12}H_7N_3O$						
r-49		5.9773	87.5197	-4.645	112.9676	209.6268	InChI=1S/C12H7N3O/c16-12-8-6-10-14-11-7(4-5-13-11)2-1-3-9(8)15(10)12/h1-6H,13,14
	$C_{12}H_7N_3O$						
H-104		22.6259	155.2592	-12.3555	16.4426	209.6434	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-15(7)11(9)14-12/h1-6,13H
	$C_{12}H_7N_3O$						
B-50		6.6254	35.7588	-1.9484	138.6494	209.8548	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(9)12(10)14-11-8(7)3-4-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
H1-85		17.1281	134.0246	-12.5559	44.0856	209.8655	InChI=1S/C12H7N3O/c16-11-3-1-2-9-7-4-5-13-12(7)14-8-6-10(8)15(9)11/h1-6,13H
	$C_{12}H_7N_3O$						
B-193		5.0650	110.0433	-2.0341	92.7341	210.7179	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)7-2-1-5-15(12)11-9(7)6-14-11/h1-6,13H
	$C_{12}H_7N_3O$						
k-18		4.5711	59.3064	-4.9526	136.6344	211.0917	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-8-2-4-14-10(8)9(7)11(12)15/h1-6,14H/b5-1-,13-3-
	$C_{12}H_7N_3O$						
B-191		2.4485	143.5660	-1.2992	50.2164	211.2176	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)11-9(6-14-11)10-7(8)3-4-13-10/h1-6,13H
	$C_{12}H_7N_3O$						

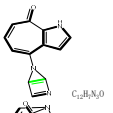
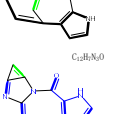
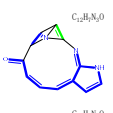
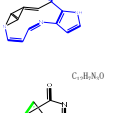
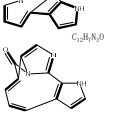
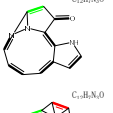
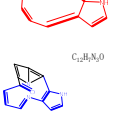
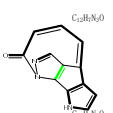
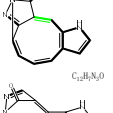
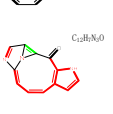
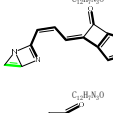
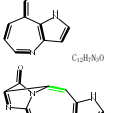

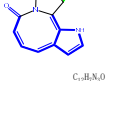


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r1-30		13, 6228	130, 0755	-13, 6869	59, 2201	211, 6549	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)14-15-9-6-8(9)11(10)15/h1-6H, (H, 13, 14)/b3-1-, 7-2-
H1-26		3, 0129	30, 4782	-1, 7338	163, 8402	212, 1507	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)9-6-15(10)12(8)14-9/h1-6, 13H
r-50		18, 2604	138, 7853	-13, 8047	50, 6023	212, 3206	InChI=1S/C12H7N3O/c16-12-10-8(9-6-15(9)10)3-1-2-7-4-5-13-11(7)14-12/h1-6H, (H, 13, 14, 16)
I-60		11, 1663	149, 5885	26, 2881	33, 7741	212, 3763	InChI=1S/C12H7N3O/c16-12-10-7-6-8-9(2-4-13-8)15(11(7)10)5-1-3-14-12/h1-6, 13H/b5-1-, 14-3+
s11-7		7, 2525	79, 8439	-3, 4351	102, 8563	212, 4776	InChI=1S/C12H7N3O/c16-12-8-6-15(12)9-3-1-2-7-4-5-13-10(7)11(8)14-9/h1-6, 13H/b2-1-, 3-1-, 7-2-, 9-3+, 11-10+
A2-25		2, 6093	41, 1356	-1, 8464	152, 18	212, 5822	InChI=1S/C12H7N3O/c16-12-10-9-6-15(12)11-8(3-5-14-11)7(9)2-1-3-13-10/h1-6, 14H
s11-12		5, 0499	72, 3172	-3, 9054	120, 8153	212, 5874	InChI=1S/C12H7N3O/c16-12-9-6-15(12)11-8(14-9)3-1-2-7-4-5-13-10(7)11/h1-6, 13H
X-37		5, 2930	143, 5597	-1, 2149	48, 0688	212, 8026	InChI=1S/C12H7N3O/c16-12-10-9-6-7(2-1-4-14-15(9)12)8-3-5-13-11(8)10/h1-6, 13H/b2-1-, 14-4-
B-123		7, 5545	136, 6673	-7, 2378	63, 1012	212, 9245	InChI=1S/C12H7N3O/c16-12-8(7-3-4-13-11(7)12)2-1-5-15-9-6-10(15)14-9/h1-6, 13H/b5-1-, 8-2-
G1-83		4, 8075	61, 8324	-1, 2756	127, 5212	212, 9374	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-10(7)12-11(9)14-6-15(8)12/h1-6, 13H/b2-1-, 8-2-
s11-28		17, 2082	168, 4311	-10, 0486	11, 566	213, 0093	InChI=1S/C12H7N3O/c16-12-9-6-15(9)11-8(14-12)3-1-2-7-4-5-13-10(7)11/h1-6, 13H
B-199		2, 3608	143, 1694	-1, 2461	51, 5418	213, 1124	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)9-6-14-11(9)10-7(8)3-4-13-10/h1-6, 13H
I-108		15, 8954	147, 6461	-12, 3373	36, 1603	213, 1998	InChI=1S/C12H7N3O/c16-12-11-8-6-7(8)10-9(2-4-13-10)15(11)5-1-3-14-12/h1-6, 13H
X22-5		13, 5548	167, 4098	-8, 5998	24, 3772	213, 4219	InChI=1S/C12H7N3O/c16-10-6-7-11-8(3-5-14-11)13-4-1-2-9-12(7)15(9)10/h1-6, 14H/b2-1-, 13-4-
A-153		50, 9257	167, 9063	-28, 83	11, 9843	213, 4331	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)5-1-2-8-7-3-4-13-9(7)6-14-8/h1-6, 13H/b5-1-, 8-2-
G-30		7, 3067	142, 7552	0, 102	48, 7656	214, 0817	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8-7-4-5-13-10(7)11(8)15(12)6-14-9/h1-6, 13H/b2-1-, 9-3+
H-86		3, 6126	36, 5293	-0, 2964	149, 7942	214, 2306	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(15(7)14-9)8-4-5-13-11(8)12/h1-6, 13H
B-204		3, 3999	28, 8555	-1, 6264	167, 8730	214, 2956	InChI=1S/C12H7N3O/c16-12-11-10-8(3-4-13-10)7-2-1-5-15(12)9(7)6-14-11/h1-6, 13H

p11-21		15.864	175.8799	-10.8751	17.7359	214.5693	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-14-11-10(8)15(11)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,9-6+,14-6+,14-11-
H-3		19.2266	275.0135	-21.4631	41.071	214.8764	InChI=1S/C12H7N3O/c16-12-11-9(12)5-1-3-13-10-7-6-8(7)10/h1-6,14H/b5-1-,13-3-
G-9		5.3458	51.7549	0.0592	139.3191	215.0071	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-8-4-5-13-12(8)15(6-14-9)10(7)11/h1-6,13H
X-16		5.2752	108.8523	-2.4107	86.7488	215.3045	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-4-14-15(12)11(9)10-8(7)3-5-13-10/h1-6,13H/b2-1-,14-4-
H1-20		4.3423	56.264	-0.8856	142.0287	215.4433	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)15-9(10)6-14-12(7)15/h1-6,13H/b3-1-,7-2-
B-184		2.1380	36.7230	-1.2350	160.1929	215.7348	InChI=1S/C12H7N3O/c16-12-9-6-14-11(12)10-7(3-4-13-10)8-2-1-5-15(8)9/h1-6,13H
B-237		4.9748	33.6539	-0.8207	147.7988	215.8487	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)7-2-1-5-15-6-9(7)11(12)14-15/h1-6,13H
x4-45		4.311	81.5439	-3.1881	117.5249	215.8899	InChI=1S/C12H7N3O/c16-12-9-8-3-1-2-7-4-5-13-10(7)11(9)15(12)6-14-8/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,11-10-
X-6		53.4083	161.0656	-28.2317	12.0036	215.9809	InChI=1S/C12H7N3O/c16-11-9-10(11)15(9)12-8(3-5-14-12)7-2-1-4-13-6-7/h1-6,14H
H1-56		4.6419	119.2208	-0.9384	74.9623	216.0661	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12-9(7)6-15(10)14-12/h1-6,13H/b3-1-,7-2-
I-106		19.9866	107.8697	-25.0051	86.6182	216.3031	InChI=1S/C12H7N3O/c16-12-10-9(2-4-13-10)15(5-1-3-14-12)11-7-6-8(7)11/h1-6,13H/b5-1-,14-3+
H-90		5.2782	37.1637	-0.9237	144.2541	216.3191	InChI=1S/C12H7N3O/c16-11-10-8(4-5-13-10)9-3-1-2-7-6-15(9)12(11)14-7/h1-6,13H
B-215		5.9125	87.0923	-2.5727	112.9176	216.4565	InChI=1S/C12H7N3O/c16-12-8-6-15(12)5-1-2-9-7-3-4-13-10(7)11(8)14-9/h1-6,13H/b5-1-,9-2-
n-189		3.8995	35.705	-2.3341	145.6413	216.4998	InChI=1S/C12H7N3O/c16-12-11-8(6-14-12)7-2-1-5-15(11)9-3-4-13-10(7)9/h1-6,13H
I-81		22.6642	155.3525	-13.7035	32.7432	216.7913	InChI=1S/C12H7N3O/c16-11-7-6-8(7)12-14-3-1-5-15(12)9-2-4-13-10(9)11/h1-6,13H
r1-35		18.2206	148.6619	-14.6596	41.2837	216.86	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)14-12-10(9)8-6-15(8)12/h1-6H, (8,13,14)/b3-1-,7-2-
x6-42		18.022	129.0963	-10.3151	46.0087	216.9411	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-11-14-12(10)15(9)11/h1-6,13H/b3-1-,7-2-,8-6+
x7-22		19.494	127.594	-11.0706	54.7524	216.9785	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-14-6-8-11(9)15(8)12/h1-6,13H/b3-1-,7-2-,12-10+
p1-3		13.2792	130.404	-11.8999	72.5279	217.1502	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)12-14-8-6-9(8)15(10)12/h1-6,13H/b3-1-,7-2-,12-11+

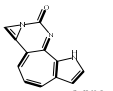
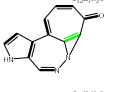
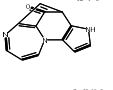
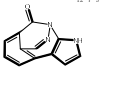
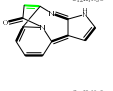
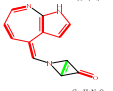
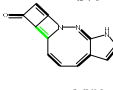
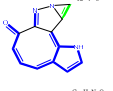
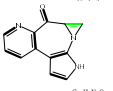
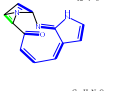
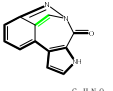
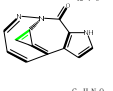
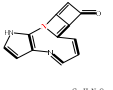
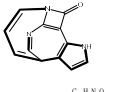
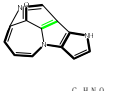
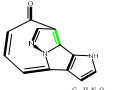
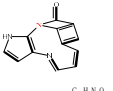
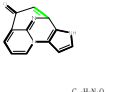
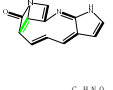
q1-34		5.414	52.1131	-5.9233	150.3894	217.2416	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)2-1-3-9-8-6-10(14-8)15(9)12/h1-6,13H/b2-1-,9-3-
r-7		4.8695	56.2857	-6.0286	148.5868	217.2528	InChI=1S/C12H7N3O/c16-11-8-6-10(11)15-9(8)3-1-2-7-4-5-13-12(7)14-15/h1-6H, (H,13,14)/b3-1-,7-2-
x9-18		7.8384	129.4834	-6.8365	62.6153	217.3212	InChI=1S/C12H7N3O/c16-12-9-7(4-5-13-9)2-1-3-8-6-14-15-10(8)11(12)15/h1-6,13H/b2-1-,8-3-
q1-43		16.0301	126.4601	-12.589	60.3424	217.3597	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-9-6-15(9)14-11(8)12/h1-6,13H/b2-1-,8-3-
o-158		3.8951	65.3956	-2.1932	143.8704	217.4127	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)10-3-4-13-11(10)9-6-8(7)14-9/h1-6,13H
H-40		2.947	25.0821	-0.6278	162.7278	217.5138	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)12(10)14-15(7)9/h1-6,13H
H-10		18.6535	144.7436	-14.2666	35.8553	217.5173	InChI=1S/C12H7N3O/c16-9-2-1-4-13-7-3-5-14-11(7)10-8-6-15(8)12(9)10/h1-6,14H/b2-1-,13-4+
A-65		4.4854	82.4943	-0.3995	99.4697	217.6143	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(12)14-6-9(10)11-8(7)3-4-13-11/h1-6,13H
x4-53		4.4424	61.1269	-2.736	130.9901	217.6354	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-9(8)6-14-15(11)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,11-10-
H-98		7.242	72.2202	-2.6825	126.3838	217.8616	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)9-3-1-2-7-6-10(14-9)15(7)12/h1-6,13H/b2-1-,3-1-,7-2-,9-3-
r1-25		14.2187	139.1267	-9.0182	46.7141	218.3283	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)14-12-10-8(9)6-15(10)12/h1-6H, (H,13,14)/b3-1-,7-2-
q-57		11.895	121.8665	-1.3248	75.8599	218.4648	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9-6-14-11(8)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,10-9+
q11-36		4.6024	64.9014	-2.6906	127.0552	218.4982	InChI=1S/C12H7N3O/c16-10-6-8-9-3-1-2-7-4-5-13-11(7)12(8)14-15(9)10/h1-6,13H/b2-1-,9-3+
r1-33		17.6288	148.2085	-14.2203	39.9018	218.7731	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-10-8-6-15(8)11(9)10/h1-6H, (H,13,14)/b3-1-,7-2-
p1-50		16.8053	130.3852	-14.9644	69.4028	218.8639	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10-8-6-15(8)12(10)14-9/h1-6,13H/b3-1-,7-2-,11-10+,14-12+
A-201		4.5481	102.8645	-0.4156	101.6327	218.9168	InChI=1S/C12H7N3O/c16-12-11-9-7(8-3-4-13-10(8)9)2-1-5-15(12)6-14-11/h1-6,13H/b5-1-,7-2-,11-9-
X22-58		18.8506	149.248	-14.0842	32.5856	218.9386	InChI=1S/C12H7N3O/c16-12-10-8(15-6-9(10)15)2-1-4-13-7-3-5-14-11(7)12/h1-6,14H/b2-1-,13-4+
q1-1		13.307	175.3259	-12.9425	27.4648	218.9829	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)2-1-3-10-8-6-9(8)14-15(10)12/h1-6,13H/b2-1-,10-3-
r-20		30.3949	152.4808	-16.8526	36.3121	219.1508	InChI=1S/C12H7N3O/c16-12-8-6-15(12)10(8)9-3-1-2-7-4-5-13-11(7)14-9/h1-6H, (H,13,14)/b10-9-




















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X22-52		4.543	51.7791	-5.6918	159.745	219.5177	InChI=1S/C12H7N3O/c16-11-7-6-10(11)15-9(7)2-1-4-13-8-3-5-14-12(8)15/h1-6,14H/b2-1-,13-4-
A-86		13.3463	162.4563	-6.7739	20.1917	219.6635	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)8-2-1-5-15-9(6-14-12)11(8)15/h1-6,13H/b4-6-
A-143		13.3485	162.4604	-6.7754	20.1829	219.6635	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)8-2-1-5-15-9(6-14-12)11(8)15/h1-6,13H/b4-6-
F-9		18.8514	193.4215	-14.6965	15.6642	219.6932	InChI=1S/C12H7N3O/c16-11-9(15-6-10(11)15)3-1-2-8-7-4-5-13-12(7)14-8/h1-6H, (H, 13, 14)/b2-1-,9-3-
o-123		15.6464	145.7608	-12.0142	38.0359	219.9552	InChI=1S/C12H7N3O/c16-11-7-6-8(7)14-12-10(3-4-13-12)15-5-1-2-9(11)15/h1-6,13H/b4-8-
x6-6		29.0043	129.3372	-23.0957	72.4015	219.9775	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-15(9)12-10-11(12)14-10/h1-6,13H/b3-1-,7-2-,8-6+
C-37		4.6772	55.4682	-1.0003	144.9773	220.0923	InChI=1S/C12H7N3O/c16-9-6-10-13-4-1-2-7-8-3-5-14-12(8)15(10)11(7)9/h1-6,14H/b2-1-,13-4-
H1-33		3.6828	88.5684	-0.6983	108.5312	220.1362	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9-11(10)14-15(9)12-8(7)4-5-13-12/h1-6,13H/b3-1-,7-2+
n-119		3.8495	33.1956	-2.3513	155.4802	220.2087	InChI=1S/C12H7N3O/c16-9-6-14-12-10(9)7-2-1-5-15(12)8-3-4-13-11(7)8/h1-6,13H
x4-35		3.8875	54.7172	-3.6095	146.2687	220.2441	InChI=1S/C12H7N3O/c16-12-8-6-14-15(12)9-3-1-2-7-4-5-13-11(7)10(8)9/h1-6,13H
q11-19		5.1089	66.8269	-3.2904	129.3441	220.6268	InChI=1S/C12H7N3O/c16-12-8-6-9-11-7(4-5-13-11)2-1-3-10(8)15(12)14-9/h1-6,13H/b2-1-,10-3-
H1-65		3.2289	31.6704	-1.6311	163.644	220.7408	InChI=1S/C12H7N3O/c16-11-3-1-2-9-7-4-5-13-12(7)8-6-10(11)15(9)14-8/h1-6,13H
E-21		3.6303	77.7746	-1.8124	129.7378	220.7776	InChI=1S/C12H7N3O/c16-12-8-6-10-7(4-5-13-10)9-2-1-3-11(8)15(12)14-9/h1-6,13H/b8-6+
p1-12		5.0759	48.5427	-5.8702	161.2696	220.9824	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)12-8-6-9(14-8)12/h1-6,13H/b3-1-,7-2-,12-11+
q-43		2.5072	69.2206	-2.0999	148.8891	221.0597	InChI=1S/C12H7N3O/c16-10-6-8-11-7(4-5-13-11)2-1-3-9-14-12(8)15(9)10/h1-6,13H/b2-1-,9-3-
X22-6		30.3767	152.0426	-16.5553	36.4732	221.0696	InChI=1S/C12H7N3O/c16-12-8-6-15(12)11(8)7-2-1-4-13-9-3-5-14-10(7)9/h1-6,14H/b11-7-
C-19		31.0585	153.2240	-16.9772	34.5824	221.1188	InChI=1S/C12H7N3O/c16-12-9-6-15(12)10(9)7-2-1-4-13-11-8(7)3-5-14-11/h1-6,14H/b10-7-
n-117		3.84	33.0644	-2.3236	153.659	221.1803	InChI=1S/C12H7N3O/c16-9-6-14-11-7-2-1-5-15(12)9(11)8-3-4-13-10(7)8/h1-6,13H




















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


















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


















q11-46	 <chem>C12H9N3O</chem>	17.5136	184.3489	-9.4517	11.9214	227.7688	InChI=1S/C12H7N3O/c16-12-14-11-8(9-6-15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6,13H
G1-41	 <chem>C12H9N3O</chem>	5.4911	168.0252	-3.1772	28.2141	227.8499	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-9(7)6-14-15(8)12(10)15/h1-6,13H
I-94	 <chem>C12H9N3O</chem>	3.8015	29.2239	-2.0357	168.6921	227.883	InChI=1S/C12H7N3O/c16-12-7-6-8-11(12)15(5-1-3-13-8)9-2-4-14-10(7)9/h1-6,14H
G-17	 <chem>C12H9N3O</chem>	5.5686	96.0939	-1.442	94.7596	228.0403	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-8-4-5-13-11(8)15(12)14-6-10(7)9/h1-6,13H
F-42	 <chem>C12H9N3O</chem>	5.5017	37.1308	-1.8323	163.7139	228.0867	InChI=1S/C12H7N3O/c16-11-6-8-10-3-1-2-9(15(10)11)7-4-5-13-12(7)14-8/h1-6H, (H,13,14)
X-7	 <chem>C12H9N3O</chem>	53.8869	172.2992	-28.1117	10.3475	228.1907	InChI=1S/C12H7N3O/c16-11-9-10(11)15(9)6-7-2-1-4-13-12-8(7)3-5-14-12/h1-6,14H/b7-6-
r-37	 <chem>C12H9N3O</chem>	6.0171	85.9405	-5.7194	128.7364	228.2057	InChI=1S/C12H7N3O/c16-10-6-9-11(10)8-3-1-2-7-4-5-13-12(7)14-15(8)9/h1-6H, (H,13,14)/b3-1-,7-2-
p1-43	 <chem>C12H9N3O</chem>	16.6821	125.3602	-12.2721	73.126	228.2855	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10-8-6-15(8)14-12(9)10/h1-6,13H/b3-1-,7-2-,11-10+
C-10	 <chem>C12H9N3O</chem>	22.8992	169.1708	-12.2867	23.9828	228.3335	InChI=1S/C12H7N3O/c16-11-9-6-15(9)12-8(3-5-14-12)7-2-1-4-13-10(7)11/h1-6,14H
r1-42	 <chem>C12H9N3O</chem>	13.3497	155.283	-10.2791	52.3339	228.3955	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-10-6-8-11(9)15(8)10/h1-6H, (H,13,14)/b3-1-,7-2-
H11-75	 <chem>C12H9N3O</chem>	4.9464	97.4025	-2.0096	99.4759	228.4168	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-10-9(7)6-15(12)14-10/h1-6,13H
C-63	 <chem>C12H9N3O</chem>	26.5390	127.2790	-16.4157	65.3674	228.4815	InChI=1S/C12H7N3O/c16-12-11-8(3-5-13-11)7-2-1-4-14-15(12)10-6-9(7)10/h1-6,13H/b2-1-,14-4-
X22-41	 <chem>C12H9N3O</chem>	6.0202	85.1302	-5.7045	132.7059	228.5261	InChI=1S/C12H7N3O/c16-10-6-9-11(10)8-2-1-4-13-7-3-5-14-12(7)15(8)9/h1-6,14H/b2-1-,13-4+
A-172	 <chem>C12H9N3O</chem>	5.695	97.3315	-2.2893	113.6657	228.9442	InChI=1S/C12H7N3O/c16-12-9-10-8(3-4-13-10)7-2-1-5-15(12)11(9)14-6-7/h1-6,13H/b5-1-,7-2+
n-150	 <chem>C12H9N3O</chem>	7.8432	70.0965	0.5004	122.2938	229.1199	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-9-3-4-13-10(9)7(6-14-8)11(12)15/h1-6,13H
G1-82	 <chem>C12H9N3O</chem>	4.5136	57.4885	-1.2218	148.9697	229.1829	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)12-8(10)6-14-15(9)12/h1-6,13H/b3-1-,9-2-
X23-15	 <chem>C12H9N3O</chem>	5.4255	78.0872	-4.0815	140.1474	229.3894	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-4-13-9-3-5-14-11(9)15(12)10(7)8/h1-6,14H/b2-1-,13-4+
o-148	 <chem>C12H9N3O</chem>	4.1498	32.9299	-0.6266	164.9834	229.4777	InChI=1S/C12H7N3O/c16-10-6-8-11-9(3-4-13-11)15-5-1-2-7(10)12(15)14-8/h1-6,13H
r-33	 <chem>C12H9N3O</chem>	5.2931	112.437	-4.7317	112.26	229.5214	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)14-9-6-15(12)10(8)9/h1-6H, (H,13,14)/b3-1-,7-2-

B-187		6.3594	34.7582	-1.9179	160.8514	229.5353	InChI=1S/C12H7N3O/c16-11-9-6-14-12-8(2-1-5-15(9)12)7-3-4-13-10(7)11/h1-6,13H
	$C_{12}H_7N_3O$						
X22-40		4.8741	52.6574	-5.327	168.3175	229.5603	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-4-13-8-3-5-14-12(8)15(9)11(7)10/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
B-58		14.4718	171.9581	-11.8850	33.5445	230.0207	InChI=1S/C12H7N3O/c16-12-8-6-9(8)14-15-5-1-2-10(15)7-3-4-13-11(7)12/h1-6,13H/b14-9-
	$C_{12}H_7N_3O$						
o-176		9.3388	94.2249	0.3614	102.6403	230.0974	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(14-10(7)8)9-3-4-13-11(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
B-55		10.0110	82.6531	-1.5205	115.5414	230.1907	InChI=1S/C12H7N3O/c16-9-6-10-14-12-8(2-1-5-15(10)12)7-3-4-13-11(7)9/h1-6,13H/b10-6+
	$C_{12}H_7N_3O$						
x12-47		19.3885	133.1544	-10.7308	59.3525	230.2168	InChI=1S/C12H7N3O/c16-12-11-9-6-8-7(4-5-13-8)2-1-3-10(14-12)15(9)11/h1-6,13H/b3-1-,7-2-,8-6+
	$C_{12}H_7N_3O$						
o-127		5.4239	43.3885	-0.496	155.9307	230.6668	InChI=1S/C12H7N3O/c16-11-7-6-9-10(3-4-13-9)15-5-1-2-8(11)14-12(7)15/h1-6,13H
	$C_{12}H_7N_3O$						
H11-36		6.2618	35.3051	-2.1832	162.7873	231.0737	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(15(12)14-7)8-4-5-13-11(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
G-40		6.1572	41.4521	-1.7434	156.7944	231.1564	InChI=1S/C12H7N3O/c16-9-6-14-10-3-1-2-7-8-4-5-13-12(8)15(10)11(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
x7-30		20.3482	132.4381	-11.3554	66.4233	231.2409	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)8-6-14-12-11(9)15(8)12/h1-6,13H/b3-1-,7-2-,10-8+
	$C_{12}H_7N_3O$						
o-118		4.7946	40.6438	-0.5251	162.3902	231.2451	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-10-3-4-13-8(10)6-9(11)14-12(7)15/h1-6,13H
	$C_{12}H_7N_3O$						
x8-19		12.6105	162.9416	-9.5	44.6892	231.2846	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)14-12-10-8(9)6-15(10)12/h1-6H, (H,13,14)/b3-1-,7-2-
	$C_{12}H_7N_3O$						
G-15		5.8282	39.0806	-1.8029	160.7818	231.3071	InChI=1S/C12H7N3O/c16-10-6-14-12-7-2-1-3-9(10)15(12)11-8(7)4-5-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
H-95		5.3762	66.5584	-3.0319	147.1722	231.4534	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-15(12)11(7)14-9/h1-6,13H
	$C_{12}H_7N_3O$						
B-167		4.0089	83.5312	-2.3711	131.8013	232.0434	InChI=1S/C12H7N3O/c16-12-10-9-6-7(2-1-5-15(9)12)8-3-4-13-11(8)14-10/h1-6,13H
	$C_{12}H_7N_3O$						
F-16		25.4538	145.7628	-16.7352	58.2731	232.1061	InChI=1S/C12H7N3O/c16-12-9-6-7(9)2-1-3-10-8-4-5-13-11(8)14-15(10)12/h1-6H, (H,13,14)/b3-1-,7-2-
	$C_{12}H_7N_3O$						
H1-13		11.2978	201.4482	-4.407	0.2928	232.1665	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15-6-9(15)11(7)14-10/h1-6,13H
	$C_{12}H_7N_3O$						
H1-128		26.8766	129.5682	-11.9062	72.6757	232.1763	InChI=1S/C12H7N3O/c16-9-3-1-2-7(9)8-4-5-13-12(8)15-10-6-11(15)14-10/h1-6,13H
	$C_{12}H_7N_3O$						
H-97		3.7037	34.0406	-1.1905	171.5263	232.2515	InChI=1S/C12H7N3O/c16-12-11-9(4-5-13-11)8-3-1-2-7-6-10(8)14-15(7)12/h1-6,13H
	$C_{12}H_7N_3O$						











o-129		5.4166	111.5226	-2.3068	90.8058	232.5158	InChI=1S/C12H7N3O/c16-12-8-6-7(14-8)11-9(3-4-13-11)15-5-1-2-10(12)15/h1-6,13H
E-45		2.6309	87.4731	-1.4917	137.3528	232.5638	InChI=1S/C12H7N3O/c16-11-6-10-14-8-2-1-3-9(15(10)11)12-7(8)4-5-13-12/h1-6,13H
r1-27		9.5498	70.995	-7.6582	122.0955	232.633	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)14-15-8-6-9(15)11(8)10/h1-6H, 8H, 13, 14)/b3-1-, 7-2-
X23-44		18.3949	167.5106	-9.0148	39.9135	232.7164	InChI=1S/C12H7N3O/c16-12-10-8(3-5-14-10)13-4-1-2-7-6-9-11(12)15(7)9/h1-6,14H/b2-1-, 13-4-
q1-32		5.2401	48.3767	-5.4399	165.6213	232.7223	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)2-1-3-8-9-6-10(8)15(12)14-9/h1-6,13H/b2-1-, 8-3+
C-61		11.5383	201.0088	-4.4427	0.1180	232.7302	InChI=1S/C12H7N3O/c16-12-10-7(2-1-4-14-12)8-3-5-13-11(8)15-6-9(10)15/h1-6,13H
x2-18		19.4285	147.9367	-13.5681	66.9484	232.9439	InChI=1S/C12H7N3O/c16-12-10-7-6-9-8(2-4-14-9)13-3-1-5-15(12)11(7)10/h1-6,14H/b5-1-, 7-6-, 13-3+
q1-42		30.1319	124.7522	-11.8872	59.0494	232.9637	InChI=1S/C12H7N3O/c16-12-8(15-9-6-10(15)14-9)3-1-2-7-4-5-13-11(7)12/h1-6,13H
X22-4		7.6323	183.696	-8.0542	34.7744	233.1502	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-4-13-9-3-5-14-12(9)15(10)11(7)8/h1-6,14H/b2-1-, 13-4-
F-69		15.9111	199.066	-7.0721	10.0136	233.1561	InChI=1S/C12H7N3O/c16-12-14-11-8(4-5-13-11)9-3-1-2-7-6-10(7)15(9)12/h1-6H, 8H, 13, 14, 16)
x7-17		18.2895	149.2043	-15.4691	52.1892	233.6744	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11-8(6-14-9)15(11)12/h1-6,13H/b3-1-, 7-2-, 12-10-, 14-6+
B-208		11.8450	110.0315	0.2354	74.3510	233.6863	InChI=1S/C12H7N3O/c16-12-9-6-15-5-1-2-7(10(9)14-15)8-3-4-13-11(8)12/h1-6,13H
o-70		15.2078	168.682	-12.9434	38.1839	233.7024	InChI=1S/C12H7N3O/c16-11-10-9(3-4-13-10)15-5-1-2-7-6-8(7)14-12(11)15/h1-6,13H/b5-1-, 7-2-, 14-12-
A-160		13.6497	152.8499	-6.4192	46.7986	233.7059	InChI=1S/C12H7N3O/c16-12-11-10-8(2-1-5-15(10)11)7-3-4-13-9(7)6-14-12/h1-6,13H/b14-6-
H1-5		18.882	147.977	-15.0609	62.804	233.7534	InChI=1S/C12H7N3O/c16-10-3-1-2-7(8-4-5-13-12(8)10)11-9-6-15(9)14-11/h1-6,13H
G1-90		18.0752	140.2962	-11.6047	72.2171	233.76	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)12(15(9)10)8-6-14-8/h1-6,13H/b12-8+
r-38		12.6606	184.8085	-9.2839	26.6117	233.8792	InChI=1S/C12H7N3O/c16-9-6-10-14-12-7(4-5-13-12)2-1-3-8-11(9)15(8)10/h1-6H, 8H, 13, 14)/b3-1-, 7-2-
C-49		10.1922	146.7333	0.6096	51.2103	234.0225	InChI=1S/C12H7N3O/c16-12-10-7-2-1-4-14-15(12)6-9(10)11-8(7)3-5-13-11/h1-6,13H/b2-1-, 14-4-
B-92		20.6992	144.3666	-15.1999	69.6780	234.0546	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)14-10-6-9(10)11-7(8)3-4-13-11/h1-6,13H/b14-10-

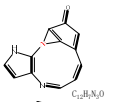
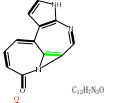
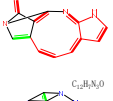
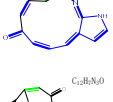
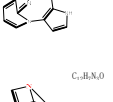
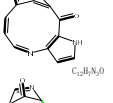
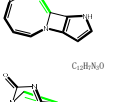
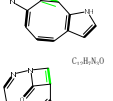
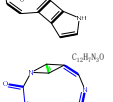
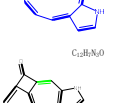
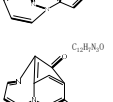
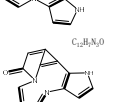
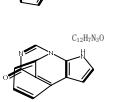
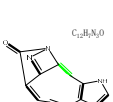
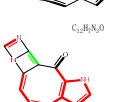
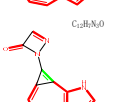

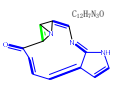

q-34		5.5639	66.0165	-3.0827	146.0699	234.0986	InChI=1S/C12H7N3O/c16-12-8-6-9-10(12)14-9)3-1-2-7-4-5-13-11(7)8/h1-6,13H/b2-1-,10-3-
	<chem>C12H7N3O</chem>						
H-55		6.5222	49.7558	-1.7669	155.2879	234.2652	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)12(14-7)15(9)10/h1-6,13H/b2-1-,9-3-
	<chem>C12H7N3O</chem>						
k-30		6.0001	85.0581	-5.6872	135.7164	234.3206	InChI=1S/C12H7N3O/c16-9-6-8-10(9)12-11-7(2-4-14-11)13-3-1-5-15(8)12/h1-6,14H/b5-1-,13-3+
	<chem>C12H7N3O</chem>						
B-169		3.8988	92.6715	-0.6888	118.0569	234.4115	InChI=1S/C12H7N3O/c16-12-14-11-9-6-7(2-1-5-15(9)12)8-3-4-13-10(8)11/h1-6,13H
	<chem>C12H7N3O</chem>						
A-54		4.4632	89.1429	-3.0975	124.7452	234.567	InChI=1S/C12H7N3O/c16-12-9(6-14-12)10-7-2-1-5-15(10)11-8(7)3-4-13-11/h1-6,13H/b10-9+
	<chem>C12H7N3O</chem>						
A-138		4.4627	89.1406	-3.0973	124.7462	234.567	InChI=1S/C12H7N3O/c16-12-9(6-14-12)10-7-2-1-5-15(10)11-8(7)3-4-13-11/h1-6,13H/b10-9-
	<chem>C12H7N3O</chem>						
B-118		5.4979	72.4402	-1.2768	131.5807	234.7420	InChI=1S/C12H7N3O/c16-12-11-8(3-4-13-11)7-2-1-5-15-9(7)6-10(15)14-12/h1-6,13H/b14-10-
	<chem>C12H7N3O</chem>						
x4-10		5.237	57.8784	-4.2308	156.6333	234.863	InChI=1S/C12H7N3O/c16-9-6-14-11-8-3-1-2-7-4-5-13-10(7)12(11)15(8)9/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,12-10+
	<chem>C12H7N3O</chem>						
x9-22		5.7086	97.0237	-4.8935	118.8518	234.906	InChI=1S/C12H7N3O/c16-12-10-8(15-9(10)6-14-15)3-1-2-7-4-5-13-11(7)12/h1-6,13H/b2-1-,8-3+
	<chem>C12H7N3O</chem>						
H11-55		6.3126	180.2328	-0.0963	43.0576	234.9871	InChI=1S/C12H7N3O/c16-12-9-6-7(14-9)2-1-3-10-8-4-5-13-11(8)15(10)12/h1-6,13H/b2-1-,10-3-
	<chem>C12H7N3O</chem>						
G1-107		19.4549	186.8631	-6.3525	20.8858	234.9956	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-9(7)6-14-12-11(8)15(10)12/h1-6,13H
	<chem>C12H7N3O</chem>						
A-3		6.8185	45.5305	-1.6038	150.2606	235.0039	InChI=1S/C12H7N3O/c16-9-6-14-15-5-1-2-7-8-3-4-13-11(8)12(15)10(7)9/h1-6,13H
	<chem>C12H7N3O</chem>						
n-183		4.473	84.6969	-0.4592	117.5213	235.1446	InChI=1S/C12H7N3O/c16-12-9-7-2-1-5-15(12)8-3-4-13-10(8)11(9)14-6-7/h1-6,13H
	<chem>C12H7N3O</chem>						
x7-37		42.4627	144.8357	-27.9588	46.3108	235.1549	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)9-11-12(9)15(11)6-14-8/h1-6,13H/b3-1-,7-2-,10-9-,14-6-
	<chem>C12H7N3O</chem>						
H-67		6.4168	44.4882	-1.9093	157.6008	235.1678	InChI=1S/C12H7N3O/c16-10-8-3-1-2-7-6-14-12(10)15(7)11-9(8)4-5-13-11/h1-6,13H/b2-1-,8-3-
	<chem>C12H7N3O</chem>						
p1-59		19.5343	141.4102	-13.0237	60.1465	235.2569	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-8-6-15(8)12(9)14-11/h1-6,13H/b3-1-,7-2-,11-10+
	<chem>C12H7N3O</chem>						
A-114		3.4111	121.5172	-1.6734	98.4001	235.2985	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(12)9(10)6-14-11-8(7)3-4-13-11/h1-6,13H
	<chem>C12H7N3O</chem>						
H-157		5.3406	34.793	-1.6585	172.1692	235.308	InChI=1S/C12H7N3O/c16-12-14-10-7-2-1-3-9(15(12)6-7)8-4-5-13-11(8)10/h1-6,13H
	<chem>C12H7N3O</chem>						
H-35		16.4049	190.4723	-20.7734	46.8782	235.3859	InChI=1S/C12H7N3O/c16-12(10-7-6-8(7)10)15-5-1-3-13-11-9(15)2-4-14-11/h1-6,14H
	<chem>C12H7N3O</chem>						

B-32		4.0310	53.8065	-2.0160	153.6411	235.7093	InChI=1S/C12H7N3O/c16-10-6-9-11-7(2-1-5-15(9)14-11)8-3-4-13-12(8)10/h1-6,13H
q11-56		14.7876	131.044	-11.0555	70.2386	235.9875	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(12)14-15-6-9(8)15/h1-6,13H/b2-1-,8-3-
C-64		35.3079	175.0093	-15.8221	18.2245	236.1323	InChI=1S/C12H7N3O/c16-12-11-8(3-5-14-11)7-2-1-4-13-10(7)9-6-15(9)12/h1-6,14H
A2-2		4.846	103.887	-2.8188	107.8602	236.2458	InChI=1S/C12H7N3O/c16-12-10-8(3-5-13-10)7-2-1-4-14-11-9(7)6-15(11)12/h1-6,13H
F-38		7.1382	52.8548	-2.3348	151.3416	236.2717	InChI=1S/C12H7N3O/c16-11-6-9-7-2-1-3-10(9)15(11)14-12-8(7)4-5-13-12/h1-6H,(H,13,14)
r-40		5.212	53.1064	-5.5346	168.0242	236.3113	InChI=1S/C12H7N3O/c16-12-9-6-10-8(9)3-1-2-7-4-5-13-11(7)14-15(10)12/h1-6H,(H,13,14)/b3-1-,7-2-
r-42		21.662	156.4119	-15.0252	62.5204	236.5194	InChI=1S/C12H7N3O/c16-12-10-8(9-6-15(9)12)3-1-2-7-4-5-13-11(7)14-10/h1-6H,(H,13,14)
l-74		16.8217	129.1038	-11.7042	74.4554	236.6476	InChI=1S/C12H7N3O/c16-9-6-7-10-12(7)15(5-1-3-13-10)8-2-4-14-11(8)9/h1-6,14H
A-206		5.6489	34.7901	-1.9616	163.9372	236.6877	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)7-2-1-5-15-6-14-9(7)11(12)15/h1-6,13H
s12-45		11.9854	148.9434	-6.8837	49.096	236.7013	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-10-11(12)15(10)14-8/h1-6,13H/b3-1-,7-2-,9-6-
l-36		13.3774	213.0623	-1.6772	0.74	236.7718	InChI=1S/C12H7N3O/c16-12-7-6-13-3-1-5-15-8-2-4-14-10(8)9(12)11(7)15/h1-6,14H/b5-1-,7-6-,13-3-
B-162		3.6082	155.1536	-1.3118	75.5759	236.8136	InChI=1S/C12H7N3O/c16-12-14-11-9-6-7(2-1-5-15(11)12)8-3-4-13-10(8)9/h1-6,13H/b5-1-,7-2+
H-102		8.3104	69.148	-2.949	127.886	236.8199	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-15(9)11(7)14-12/h1-6,13H
x9-23		5.5449	58.9511	-4.6161	151.7238	236.8921	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-8-6-14-15(9)11(8)12/h1-6,13H/b2-1-,9-3+
n-145		15.8594	200.659	-11.8811	29.0824	236.9182	InChI=1S/C12H7N3O/c16-12-11-9(3-4-13-11)15(12)5-1-2-7-8-6-14-10(7)8/h1-6,13H/b5-1-,7-2-
A-157		3.3946	120.0503	-1.7466	100.9181	236.9842	InChI=1S/C12H7N3O/c16-12-10-8-2-1-5-15(12)11(10)14-6-9-7(8)3-4-13-9/h1-6,13H
n-176		4.5784	86.4905	-0.4668	117.6719	236.9969	InChI=1S/C12H7N3O/c16-12-10-7-6-14-8(10)2-1-5-15(12)9-3-4-13-11(7)9/h1-6,13H
p-3		5.3453	93.8672	-4.345	128.9922	237.0443	InChI=1S/C12H7N3O/c16-11-9-6-8-7(4-5-13-8)2-1-3-10-14-12(11)15(9)10/h1-6,13H/b2-1-,9-6-,10-3-
x4-47		13.4872	192.5869	-6.6971	10.1273	237.5042	InChI=1S/C12H7N3O/c16-12-11-10-9-7(4-5-13-9)2-1-3-8(6-14-12)15(10)11/h1-6,13H/b2-1-,8-3-

C-55		33, 9860	174, 3142	-15, 0482	17, 3311	237, 5734	InChI=1S/C12H7N3O/c16-12-11-7(2-1-4-13-11)8-3-5-14-10(8)9-6-15(9)12/h1-6, 14H
O-149		4, 6514	95, 6722	-1, 7943	117, 1836	237, 8869	InChI=1S/C12H7N3O/c16-10-6-8-7(10)2-1-5-15-9-3-4-13-12(9)11(8)14-15/h1-6, 13H/b5-1-, 7-2+
K1-16		22, 535	148, 0259	-12, 0882	42, 6975	237, 9141	InChI=1S/C12H7N3O/c16-12-7-6-9-11(7)15(9)5-1-3-13-8-2-4-14-10(8)12/h1-6, 14H/b5-1-, 13-3+
O-253		5, 9063	60, 5419	-3, 1271	153, 8771	238, 3723	InChI=1S/C12H7N3O/c16-12-14-9-6-8-7(9)2-1-5-15(12)10-3-4-13-11(8)10/h1-6, 13H/b5-1-, 7-2-, 14-9-
B-130		4, 1157	87, 4054	-2, 0463	138, 5348	238, 4131	InChI=1S/C12H7N3O/c16-12-8-6-10-7(3-4-13-10)9-2-1-5-15(12)11(8)14-9/h1-6, 13H
P1-14		28, 9104	126, 1455	-11, 5132	66, 7335	238, 435	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-11(7)12(8)15-9-6-10(15)14-9/h1-6, 13H
H1-134		5, 0438	70, 585	-2, 743	149, 1579	238, 5059	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)15(11)10-6-9(7)14-10/h1-6, 13H/b3-1-, 7-2-
O-20		5, 6163	39, 0538	-1, 1884	166, 3329	238, 577	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-12(9)14-8(11)6-10(7)15/h1-6, 13H
P11-14		18, 0268	118, 6225	-12, 7712	99, 8425	238, 7343	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-9(7)6-14-15(12)11(8)10/h1-6, 13H/b2-1-, 8-3-, 14-6-
X4-4		13, 6235	194, 1125	-6, 8663	13, 0311	238, 7979	InChI=1S/C12H7N3O/c16-8-6-14-9-3-1-2-7-4-5-13-10(7)12-11(8)15(9)12/h1-6, 13H/b2-1-, 9-3-
H-73		6, 2084	73, 3471	-2, 3343	153, 5252	238, 8004	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-15(12)11(7)14-10-8(9)4-5-13-10/h1-6, 13H/b2-1-, 9-3-
X4-38		7, 7595	143, 7756	-3, 2322	67, 2917	238, 9582	InChI=1S/C12H7N3O/c16-12-9-8-3-1-2-7-4-5-13-10(7)11(9)15(12)14-6-8/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3-, 11-10-
X9-48		12, 3702	126, 511	-8, 4338	82, 1383	239, 1765	InChI=1S/C12H7N3O/c16-12-9-7(4-5-13-9)2-1-3-8-10-11(8)15(12)6-14-10/h1-6, 13H/b2-1-, 8-3-
X7-32		17, 7841	147, 9991	-15, 4866	56, 7966	239, 1875	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-9(7)10-11-12(14-6-8)15(10)11/h1-6, 13H/b3-1-, 7-2-, 10-9-, 14-6+
O-167		5, 7022	43, 7935	-0, 1122	164, 9248	239, 3381	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-8(7)10(14-12)11-9(15)3-4-13-11/h1-6, 13H
X23-46		22, 3422	135, 698	-11, 2101	63, 0155	239, 3771	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-13-8-3-5-14-10(8)12-11(9)15(7)12/h1-6, 14H/b1-6, 13-4-
X6-5		22, 89	150, 1825	-12, 3508	59, 3132	239, 4146	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-15-12-10(9)11(12)14-15/h1-6, 13H/b3-1-, 7-2-, 8-6+
O-243		2, 4676	61, 6351	-1, 8065	171, 6128	239, 4483	InChI=1S/C12H7N3O/c16-10-6-7-8-2-1-5-15(10)9-3-4-13-12(9)11(7)14-8/h1-6, 13H/b5-1-, 8-2+
O-54		6, 4289	122, 9127	-2, 2845	85, 882	239, 5157	InChI=1S/C12H7N3O/c16-12-7-6-8(12)14-10-2-1-5-15(10)9-3-4-13-11(7)9/h1-6, 13H/b14-8+

x6-26		13.4144	161.1687	-9.0753	41.6756	239.5438	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-12-11(10)14-15(9)12/h1-6,13H/b3-1-,7-2-,8-6+
x7-31		19.522	139.2145	-18.4576	58.5042	239.7469	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)9-11-12(9)15(11)14-6-8/h1-6,13H/b3-1-,7-2-,10-9-,14-6-
o-172		6.407	43.7696	-2.0468	155.4234	239.7625	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-10-3-4-13-9(10)6-8(7)11(15)14-12/h1-6,13H
x9-41		5.3661	58.3066	-4.9588	160.8194	239.8689	InChI=1S/C12H7N3O/c16-12-9-7(4-5-13-9)2-1-3-8-10-11(12)15(8)6-14-10/h1-6,13H/b2-1-,8-3+
q-59		10.526	109.9774	-1.7253	94.982	240.0184	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-10(7)8-6-15(9)11(8)14-12/h1-6,13H/b2-1-,9-3-
t1-4		19.8556	191.9848	-21.8644	45.7405	240.0277	InChI=1S/C12H7N3O/c16-12-14-3-1-5-15(12)9-2-4-13-11(9)10-7-6-8(7)10/h1-6,13H
B-81		6.2613	119.3281	-2.2587	87.2091	240.0513	InChI=1S/C12H7N3O/c16-11-8-6-10(11)15-5-1-2-9(15)7-3-4-13-12(7)14-8/h1-6,13H/b4-8+
q-4		6.3747	55.9861	-3.4749	151.8547	240.1564	InChI=1S/C12H7N3O/c16-10-6-9-11-7(4-5-13-11)2-1-3-8-12(10)14-15(8)9/h1-6,13H/b2-1-,9-3-
G-38		4.9734	27.2877	-1.9936	175.6906	240.1849	InChI=1S/C12H7N3O/c16-10-6-14-15-9-3-1-2-7(11)9(10)8-4-5-13-12(8)15/h1-6,13H
H11-22		5.4495	50.9886	-1.0178	164.796	240.3637	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-7-4-5-13-11(7)10(6-14-8)15(9)12/h1-6,13H
q-64		4.2659	50.798	-2.6957	169.6562	240.4826	InChI=1S/C12H7N3O/c16-12-14-8-6-10-11-7(4-5-13-11)2-1-3-9(8)15(10)12/h1-6,13H/b2-1-,9-3-
o-199		3.5552	90.3155	-2.1622	139.1277	240.6488	InChI=1S/C12H7N3O/c16-12-8-6-14-10(8)7-2-1-5-15(12)9-3-4-13-11(7)9/h1-6,13H
r-8		19.0369	144.5411	-13.5798	66.397	240.8203	InChI=1S/C12H7N3O/c16-11-9-6-14-12-7(4-5-13-12)2-1-3-8-10(11)15(8)9/h1-6H, (H,13,14)/b3-1-,7-2-,9-6-
F-31		6.4483	78.6891	-1.5998	132.0745	240.9216	InChI=1S/C12H7N3O/c16-12-8-6-15-9(2-1-3-10(8)15)7-4-5-13-11(7)14-12/h1-6H, (H,13,14,16)/b9-7-
q-53		3.9676	56.3652	-2.3623	163.5474	240.9891	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)10-6-9(8)14-15(10)12/h1-6,13H/b2-1-,8-3+
r1-5		23.063	146.3055	-12.5068	66.4165	241.1032	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-15-6-8-10(9)11(8)15/h1-6H, (H,13,14)/b3-1-,7-2-
x7-21		5.0425	57.3162	-4.8088	160.4361	241.4273	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-8-6-14-15(12)11(8)9/h1-6,13H/b3-1-,7-2-,12-10-
H-50		3.935	103.5715	-0.8197	113.2415	241.7669	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-12(8)15(10)11(7)14-9/h1-6,13H
A-139		19.5803	203.4857	-11.7371	16.8385	241.7915	InChI=1S/C12H7N3O/c16-11-8(7-3-4-13-10(7)11)2-1-5-15-9-6-14-12(9)15/h1-6,13H/b5-1-,8-2-














k-45		4.2593	177.6282	-1.4932	64.1788	241.8893	InChI=1S/C12H7N3O/c16-12-10-7-6-9(10)15(12)5-1-3-13-8-2-4-14-11(7)8/h1-6,14H/b5-1-,13-3+
	$C_{12}H_7N_3O$						
H11-13		4.1047	101.1007	-2.1306	127.2043	241.9395	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(15)(12)14-9)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
	$C_{12}H_7N_3O$						
G-11		3.1031	84.7821	-1.6985	133.0256	241.9454	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(10-6-14-15(9)10)8-4-5-13-11(8)12/h1-6,13H
	$C_{12}H_7N_3O$						
p11-19		18.266	151.9113	-14.6336	59.9277	242.1453	InChI=1S/C12H7N3O/c16-12-11-10-9(15(10)11)3-1-2-7-4-5-13-8(7)6-14-12/h1-6,13H/b2-1-,9-3-,14-6-
	$C_{12}H_7N_3O$						
x5-40		4.4562	117.3397	-3.7726	118.3995	242.1633	InChI=1S/C12H7N3O/c16-12-9-10-8(6-15(10)12)3-1-2-7-4-5-13-11(7)14-9/h1-6H, 6H, 13, 14)/b3-1-,7-2-
	$C_{12}H_7N_3O$						
q11-57		4.2369	96.3689	-2.4449	128.9925	242.1651	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)9-6-10(8)15(12)14-9/h1-6,13H/b2-1-,8-3+
	$C_{12}H_7N_3O$						
o-229		13.8239	74.8653	-2.6136	118.8357	242.3582	InChI=1S/C12H7N3O/c16-10-6-7-8-2-1-5-15(12(7)14-8)9-3-4-13-11(9)10/h1-6,13H
	$C_{12}H_7N_3O$						
x9-30		13.269	134.2138	-8.222	78.6737	242.4382	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-9-6-14-15(12)11(8)9/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
q11-84		6.8166	151.1206	-2.2285	68.4219	242.5161	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-9(6-8)15(12)14-11/h1-6,13H/b2-1-,8-3+
	$C_{12}H_7N_3O$						
x7-33		18.0067	146.8751	-14.6132	64.2142	242.5671	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-9(7)10-11-12(14-6-8)15(10)11/h1-6,13H/b3-1-,7-2-,10-9-,14-6-
	$C_{12}H_7N_3O$						
p1-51		7.3995	60.1603	-5.842	152.6547	242.7183	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10-8-6-15(9)12(10)14-8/h1-6,13H/b3-1-,7-2-,11-10+
	$C_{12}H_7N_3O$						
B-231		15.8109	190.0125	-9.2424	18.4947	243.0287	InChI=1S/C12H7N3O/c16-12-9-6-15(9)5-1-2-7-8-3-4-13-10(8)11(7)14-12/h1-6,13H/b5-1-,7-2-,11-11+
	$C_{12}H_7N_3O$						
A1-36		7.6389	192.5339	-5.7235	25.9137	243.1508	InChI=1S/C12H7N3O/c16-12-9-7(3-5-14-9)8-2-1-4-13-6-15-10(8)11(12)15/h1-6,14H/b4-1-,8-2-,13-6-
	$C_{12}H_7N_3O$						
i-25		24.1093	149.7976	-16.3959	74.1693	243.3247	InChI=1S/C12H7N3O/c16-12-10-7(9-6-15(9)12)2-1-4-13-8-3-5-14-11(8)10/h1-6,14H/b2-1-,4-1-,7-2-,11-10-,13-4-,13-8-
	$C_{12}H_7N_3O$						
x4-44		4.0233	60.6437	-3.6465	164.3112	243.4323	InChI=1S/C12H7N3O/c16-12-11-9-8(15(12)6-14-11)3-1-2-7-4-5-13-10(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
H1-59		5.6797	59.7057	-3.5645	153.2934	243.6019	InChI=1S/C12H7N3O/c16-7-2-1-3-9-8-4-5-13-11(8)12-10(6-7)15(9)14-12/h1-6,13H/b2-1-,9-3-,10-6-
	$C_{12}H_7N_3O$						
B-132		5.7484	120.8495	-2.7801	91.6077	243.7016	InChI=1S/C12H7N3O/c16-11-9-6-8-7(3-4-13-8)10-2-1-5-15(10)12(11)14-9/h1-6,13H/b9-6-
	$C_{12}H_7N_3O$						
C-33		8.8174	121.8181	-1.7139	91.4490	244.1836	InChI=1S/C12H7N3O/c16-12-10-6-9-7(2-1-4-14-12)8-3-5-13-11(8)15(9)10/h1-6,13H/b2-1-,14-4+
	$C_{12}H_7N_3O$						
X23-39		12.6662	140.5264	-6.5939	74.6008	244.2204	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-13-8-3-5-14-12(8)15-10(7)11(9)15/h1-6,14H/b2-1-,13-4+
	$C_{12}H_7N_3O$						


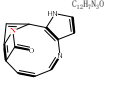
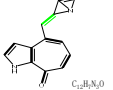
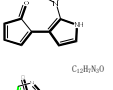
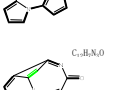
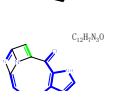
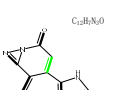
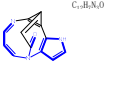
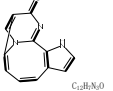
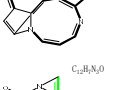
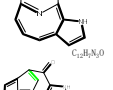
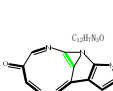
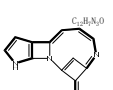
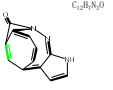
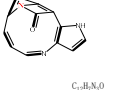
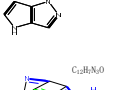
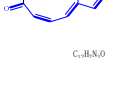


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G1-70		22.7006	191.9953	-7.1368	22.3382	244.2428	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)14-6-9-11(7)15(9)10/h1-6,13H
x5-16		9.6604	151.1014	-4.5219	81.3766	244.3857	InChI=1S/C12H7N3O/c16-12-9-8-3-1-2-7-4-5-13-10(7)14-11(9)15(12)6-8/h1-6H, (H,13,14)/b3-1+,7-2-
r1-3		23.4002	150.5176	-19.8241	49.1417	244.6427	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-12(7)14-15-10-9(6-8)11(10)15/h1-6H, (H,13,14)/b3-1-,7-2-,9-6-
o-228		10.6027	83.5608	-1.282	117.718	244.6467	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(12(7)14-8)9-3-4-13-11(9)10/h1-6,13H/b8-6-
X23-43		9.931	199.4421	-8.3852	24.6845	244.8222	InChI=1S/C12H7N3O/c16-12-9-8(3-5-14-9)13-4-1-2-7-6-15-10(7)11(12)15/h1-6,14H/b2-1-,13-4-
n-164		5.4442	110.0688	-0.3498	112.1621	244.9565	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-9(8)11(15)10(12)14-6-7/h1-6,13H/b5-1-,7-2-,11-10+
q-62		3.4502	57.4982	-2.569	166.9192	245.0278	InChI=1S/C12H7N3O/c16-12-14-11-8-6-15(12)9(11)3-1-2-7-4-5-13-10(7)8/h1-6,13H/b2-1-,9-3+
C-18		4.7642	139.0906	-1.4021	98.2811	245.1282	InChI=1S/C12H7N3O/c16-12-9-6-15(12)14-4-1-2-7-8-3-5-13-11(8)10(7)9/h1-6,13H/b2-1-,14-4-
r1-8		42.296	163.4048	-27.7993	40.791	245.2317	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-6-8-10-11(8)15(9)10/h1-6H, (H,13,14)/b3-1-,7-2-,8-6-
o-109		8.0714	111.6225	0.0953	105.6517	245.7193	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-10-3-4-13-9(10)6-8(12)11(7)14-15/h1-6,13H
I-38		3.9166	30.2351	-2.1878	185.3701	246.0198	InChI=1S/C12H7N3O/c16-12-7-6-9-11(12)13-3-1-5-15(9)8-2-4-14-10(7)8/h1-6,14H
k-34		13.524	131.016	-8.036	80.8169	246.2373	InChI=1S/C12H7N3O/c16-9-6-7-10-11-8(2-4-14-11)13-3-1-5-15(9)12(7)10/h1-6,14H/b5-1-,13-3+
G-57		5.6497	27.6794	-2.3909	179.2026	246.4004	InChI=1S/C12H7N3O/c16-12-10-7-2-1-3-9(10)15(6-14-12)11-8(7)4-5-13-11/h1-6,13H
p-22		7.1483	83.2387	-5.2395	146.5137	246.5805	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-10-11(8)14-15(10)12/h1-6,13H/b2-1+,8-3-,10-6-
x9-45		5.332	98.9018	-4.6174	133.3593	246.7828	InChI=1S/C12H7N3O/c16-11-9-8(15-6-14-12(9)15)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,8-3+
x4-7		13.3077	200.0333	-10.0222	29.9886	246.7987	InChI=1S/C12H7N3O/c16-9-6-14-15(9)12-8-3-1-2-7-4-5-13-11(7)10(8)12/h1-6,13H
x4-27		9.5534	177.9296	-4.7002	41.2341	247.0075	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)10-11(12)15(10)14-6-8/h1-6,13H/b2-1-,8-3-
r1-36		17.9625	166.7592	-15.3786	49.6958	247.1399	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-6-8-10-11(9)15(8)10/h1-6H, (H,13,14)/b3-1-,7-2-,8-6-













r1-2		16.8995	196.3954	-20.94	46.0335	247.1777	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)14-15(10)11-8-6-9(8)11/h1-6H, (H, 13, 14)/b3-1-, 7-2-
x4-67		13.1097	202.0803	-9.8911	30.0306	247.2342	InChI=1S/C12H7N3O/c16-12-14-6-15(12)11-8-3-1-2-7-4-5-13-10(7)9(8)11/h1-6, 13H
C-7		5.1063	54.8837	-2.8419	160.9390	247.3043	InChI=1S/C12H7N3O/c16-12-10-6-9-7(3-5-13-9)8-2-1-4-14-15(11(8)12/h1-6, 13H
A-71		7.2056	100.2634	-2.4286	125.8972	247.5054	InChI=1S/C12H7N3O/c16-12-10-9-6-14-8(2-1-5-15(9)12)7-3-4-13-11(7)10/h1-6, 13H/b5-1-, 8-2-
C-12		9.7206	141.5892	0.6069	64.8715	247.5450	InChI=1S/C12H7N3O/c16-11-9-6-15-10(11)7(2-1-4-13-9)8-3-5-14-12(8)15/h1-6, 14H/b2-1-, 13-4-
G1-89		14.5711	147.5792	-6.6587	64.6324	247.7116	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-10(7)12-11(8)15(12)6-14-9/h1-6, 13H/b3-1-, 8-2-, 14-6-
r-56		14.1727	174.0853	-8.2223	47.5102	247.8864	InChI=1S/C12H7N3O/c16-10-6-8-11-9(15(10)11)3-1-2-7-4-5-13-12(7)14-8/h1-6H, (H, 13, 14)/b3-1-, 7-2-
A2-47		3.4687	27.7277	-1.898	191.2126	247.8985	InChI=1S/C12H7N3O/c16-11-8-6-15-9(2-1-4-14-12(11)15)7-3-5-13-10(7)8/h1-6, 13H
E-49		6.8805	76.3303	-2.9643	149.0215	248.0216	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)8-2-1-3-10-9(14-8)6-15(10)12/h1-6, 13H
p-23		18.3878	192.7632	-4.4081	34.9412	248.331	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)6-9(8)11-14-15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 9-6+, 10-6+
x4-26		5.4209	39.1241	-3.3105	173.9208	248.3489	InChI=1S/C12H7N3O/c16-12-8-6-14-15-9(12)3-1-2-7-4-5-13-10(7)11(8)15/h1-6, 13H/b2-1-, 9-3-
X22-19		21.8182	145.537	-12.1232	86.8778	248.4024	InChI=1S/C12H7N3O/c16-12-10-8(3-5-14-10)13-4-1-2-7-6-9-11(7)15(9)12/h1-6, 14H/b2-1-, 13-4+
p-18		18.3809	192.9279	-4.414	34.9543	248.5777	InChI=1S/C12H7N3O/c16-12-9-6-10-7(4-5-13-10)2-1-3-8(9)11-14-15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 9-6+, 10-6+
x5-29		13.1789	155.2125	-7.5702	71.0744	248.6186	InChI=1S/C12H7N3O/c16-9-6-8-3-1-2-7-4-5-13-11(7)14-12-10(8)15(9)12/h1-6H, (H, 13, 14)/b3-1-, 7-2-
H1-76		4.9197	107.4836	-0.0935	111.886	248.9923	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)12-14-8(10)6-15(9)12/h1-6, 13H/b3-1-, 9-2-
X23-40		24.7121	139.5452	-12.0807	67.0138	249.073	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-13-8-3-5-14-10(8)12-11(9)15(7)12/h1-6, 14H/b2-1-, 13-4+
p11-2		42.8472	204.8605	-19.4144	12.5587	249.3673	InChI=1S/C12H7N3O/c16-12-10-9-3-1-2-7-4-5-13-8(7)6-14-15(9)11(10)12/h1-6, 13H/b2-1-, 9-3-, 14-6-
F-50		23.0936	225.5882	-16.0852	15.5754	249.486	InChI=1S/C12H7N3O/c16-12-8(10-6-15(10)12)2-1-3-9-7-4-5-13-11(7)14-9/h1-6H, (H, 13, 14)/b3-1-, 8-2+
p11-4		12.1768	162.1413	-8.5657	60.3536	249.4895	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-14-15-10(8)11(12)15/h1-6, 13H/b2-1-, 8-3+, 14-6-




















H11-101		4.0329	26.8049	-1.2942	189.3571	249.5407	InChI=1S/C12H7N3O/c16-12-8-6-15-9(2-1-3-10(15)14-12)7-4-5-13-11(7)8/h1-6,13H
x7-29		23.8673	165.0777	-8.2491	48.499	249.5926	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)8-6-14-12-11(8)15(9)12/h1-6,13H/h3-1-,7-2-,10-8+
r-18		22.2436	165.0788	-12.336	53.6117	249.7376	InChI=1S/C12H7N3O/c16-12-8-6-14-11-7(4-5-13-11)2-1-3-9-10(8)15(9)12/h1-6H,(H,13,14)
C-58		5.3603	41.4412	-2.1247	178.0747	250.1303	InChI=1S/C12H7N3O/c16-12-9-6-10-13-4-1-2-7(9)8-3-5-14-11(8)15(10)12/h1-6,14H/h2-1-,4-1-,7-2-,13-4-,13-10+
o-235		5.21	51.484	-2.9099	166.0265	250.1985	InChI=1S/C12H7N3O/c16-12-11-8(3-4-13-11)15-5-1-2-7-6-9(15)10(7)14-12/h1-6,13H
x7-13		15.8869	187.2353	-2.6093	37.7076	250.2268	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)12-10(9)8-6-14-15(8)12/h1-6,13H/h3-1-,7-2-,12-11-
i-17		21.8277	194.4602	-2.7117	41.8852	250.3106	InChI=1S/C12H7N3O/c16-10-6-9-11-8(15(9)10)2-1-4-13-7-3-5-14-12(7)11/h1-6,14H/h2-1-,4-1-,8-2-,12-11-,13-4-,13-7+
q11-34		5.9552	60.2068	-2.4695	165.1718	250.4044	InChI=1S/C12H7N3O/c16-10-6-8-9-3-1-2-7-4-5-13-11(7)12(14-8)15(9)10/h1-6,13H/h2-1-,9-3-
B-104		5.6802	142.2327	-1.7178	96.5892	250.4420	InChI=1S/C12H7N3O/c16-12-10-6-9-7(2-1-5-15(12)14-10)8-3-4-13-11(8)9/h1-6,13H/h5-1-,7-2-,9-6-
H1-24		9.9967	132.6683	-1.2407	92.4927	250.4728	InChI=1S/C12H7N3O/c16-7-2-1-3-8-9-4-5-13-11(9)15-10(6-7)14-12(8)15/h1-6,13H/h2-1-,8-3-,10-6+
q11-51		5.9818	64.9528	-3.7205	157.5638	250.6523	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-9-8(14-11)6-15(9)12/h1-6,13H/h2-1-,9-3-
x7-45		5.5433	57.8411	-4.9641	171.6764	250.75	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-9(7)12-10-11(8)15(12)6-14-10/h1-6,13H/h3-1-,7-2-,12-9-
q-3		4.8193	82.8594	-1.8844	145.8899	250.8262	InChI=1S/C12H7N3O/c16-11-8-6-15-9(14-12(11)15)3-1-2-7-4-5-13-10(7)8/h1-6,13H/h2-1-,9-3-
r-1		7.0467	87.4517	-5.6003	147.4985	251.1746	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-12(7)14-15-6-9(11)10(8)15/h1-6H,(H,13,14)/h3-1-,7-2-
E-69		3.3161	66.7527	-1.8883	171.0041	251.2007	InChI=1S/C12H7N3O/c16-12-14-9-3-1-2-7-6-10(15(7)12)11-8(9)4-5-13-11/h1-6,13H/h3-1-,7-2-
q-63		3.8657	76.8125	-2.6842	167.1431	251.3735	InChI=1S/C12H7N3O/c16-12-14-11-9-6-8(15(11)12)3-1-2-7-4-5-13-10(7)9/h1-6,13H/h2-1-,3-1-,7-2-,8-3+,10-9-
i-97		4.4035	56.9392	-2.0406	164.5005	251.3736	InChI=1S/C12H7N3O/c16-12-7-6-8-9(2-4-13-8)15-5-1-3-14-10(7)11(12)15/h1-6,13H
n-181		7.2394	117.6548	-1.1854	113.5702	251.6484	InChI=1S/C12H7N3O/c16-12-7-6-14-8-2-1-5-15(12)9-3-4-13-11(9)10(7)8/h1-6,13H/h5-1-,8-2+
o-174		3.7657	31.5544	-0.7364	186.2093	251.7181	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)8(14-12)6-10(7)15/h1-6,13H

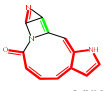
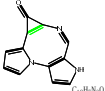
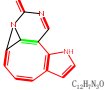
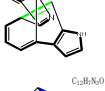

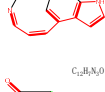
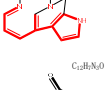
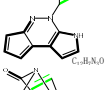
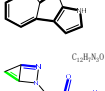
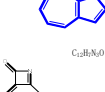
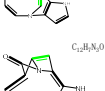
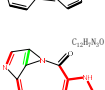
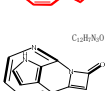
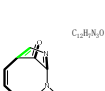
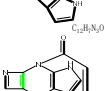
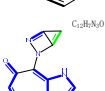
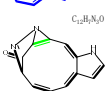
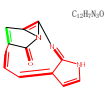

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n-194		7.0032	185.1097	-6.1428	52.9697	252.1672	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(12)9-3-4-13-8(9)6-14-11(7)10/h1-6,13H/b14-6-
x22-56		8.5409	70.4234	-5.9156	153.3137	252.1868	InChI=1S/C12H7N3O/c16-11-7-2-1-4-13-8-3-5-14-12(8)15-9(7)6-10(11)15/h1-6,14H/b2-1-,13-4-
A1-14		23.8825	187.8476	-7.7691	28.1988	252.2367	InChI=1S/C12H7N3O/c16-9-6-13-4-1-2-8-7-3-5-14-10(7)12-11(8)15(9)12/h1-6,14H/b4-1-,8-2-,13-6-
q1-15		19.1588	138.1681	-13.1283	83.3674	252.2892	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-14-11(12)8-6-15(8)9/h1-6,13H/b2-1-,9-3+
i-26		5.7249	73.7027	-5.0045	171.5353	252.3243	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-9-3-5-14-10(9)11-8(7)6-15(11)12/h1-6,14H/b4-1-,7-2-,11-10-,13-9+
n-193		6.8514	44.5674	-1.9978	165.742	252.4068	InChI=1S/C12H7N3O/c16-12-11-9-7(6-14-12)2-1-5-15(11)8-3-4-13-10(8)9/h1-6,13H
x4-21		9.9261	101.8665	-2.1327	132.8988	252.4378	InChI=1S/C12H7N3O/c16-12-9-10-7(4-5-13-10)2-1-3-8-6-14-11(9)15(8)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,10-9-
x23-38		14.2054	177.3543	-11.6833	45.1948	252.7335	InChI=1S/C12H7N3O/c16-12-10-8(3-5-14-10)13-4-1-2-7-6-9-11(12)15(7)9/h1-6,14H/b2-1-,13-4+
x6-25		26.4263	162.6429	-13.7198	64.5062	252.8078	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-11-12(14-9)15(10)11/h1-6,13H/b3-1-,7-2-,8-6-
B-17		4.2555	111.9752	-0.6511	112.7018	253.0623	InChI=1S/C12H7N3O/c16-10-6-8-11-7(3-4-13-11)9-2-1-5-15(10)12(8)14-9/h1-6,13H
p1-4		6.925	49.039	-6.2115	177.8933	253.1348	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)11-8-6-9(11)15(10)14-8/h1-6,13H/b3-1-,7-2-,12-11+
k-35		5.2902	53.5092	-4.9584	182.6693	253.157	InChI=1S/C12H7N3O/c16-12-9-6-8-10(12)11-7(2-4-14-11)13-3-1-5-15(8)9/h1-6,14H/b5-1-,13-3-
C-31		4.5094	152.1671	-1.1217	91.7676	253.4230	InChI=1S/C12H7N3O/c16-12-9-6-15(12)11-8(2-1-4-13-9)7-3-5-14-10(7)11/h1-6,14H/b2-1-,13-4-
x22-26		5.8647	44.0112	-5.9157	193.9551	253.4457	InChI=1S/C12H7N3O/c16-12-8-6-10-7(8)2-1-4-13-9-3-5-14-11(9)15(10)12/h1-6,14H/b2-1-,13-4-
x3-1		48.7512	192.1299	-28.4528	17.1455	253.4581	InChI=1S/C12H7N3O/c16-11-9-7(10(9)11)6-15-5-1-3-13-12-8(15)2-4-14-12/h1-6,14H
H1-10		4.6118	153.7749	-2.0879	92.8563	253.4924	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15(10)9-6-14-11(7)9/h1-6,13H/b3-1-,7-2-
o-48		6.0904	119.4549	-2.3993	100.366	253.5482	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(7)9-3-4-13-10(9)11(12)14-8/h1-6,13H/b8-6-
H1-114		8.0294	68.666	-2.9376	150.7624	253.7246	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)14-12-8(10)6-15(9)12/h1-6,13H/b3-1-,9-2-

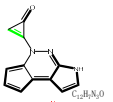
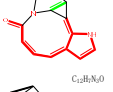
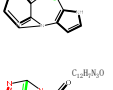
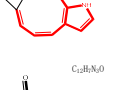
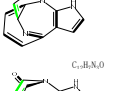
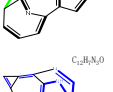

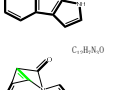
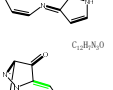
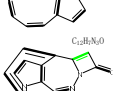
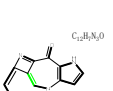
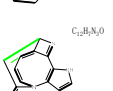
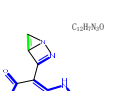
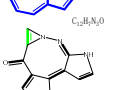
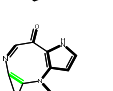
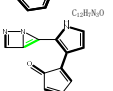
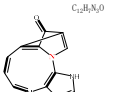
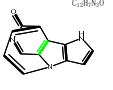
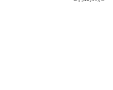
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B-240		4.6792	46.2645	-3.0613	175.6048	254.0438	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)7-2-1-5-15-6-9(7)11(15)14-12/h1-6,13H
x6-9		11.5288	167.7379	-9.8669	60.3518	254.0903	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-11-12(10)15(11)14-9/h1-6,13H/b3-1-,7-2-,9-6-
H1-92		20.5394	223.2765	-16.7461	19.5878	254.0922	InChI=1S/C12H7N3O/c16-10-3-1-2-7(10)8-4-5-13-11(8)14-12-9-6-15(9)12/h1-6,13H/b14-12+
s12-27		29.0318	172.0983	-14.2302	54.3891	254.2569	InChI=1S/C12H7N3O/c16-10-6-9-7(4-5-13-9)2-1-3-8-11-12(14-8)15(10)11/h1-6,13H/b3-1-,7-2-,9-6+
E-68		4.947	72.2397	-2.0556	164.0325	254.6338	InChI=1S/C12H7N3O/c16-12-14-9-2-1-3-10-8(6-15(10)12)11-7(9)4-5-13-11/h1-6,13H/b2-1-,10-3-,14-9-
H-21		6.9076	118.9248	-0.9475	107.5276	254.8234	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-11(8)14(10(6-7)15(9)12/h1-6H,(11,13,14)
H-156		5.9188	100.8961	-2.1218	108.01	254.8435	InChI=1S/C12H7N3O/c16-12-14-10-7-2-1-3-8(10)9-4-5-13-11(9)15(12)6-7/h1-6,13H
X22-25		13.0892	146.603	-8.229	88.2361	254.9007	InChI=1S/C12H7N3O/c16-12-10-7-6-15(12)9(10)2-1-4-13-8-3-5-14-11(7)8/h1-6,14H/b2-1-,13-4+
i-29		24.6233	161.0985	-14.1982	57.5133	254.9335	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-11(8)10(7)9-6-15(9)12/h1-6,14H/b2-1-,4-1-,7-2-,11-10-,13-4-,13-8-
H-43		6.5888	190.3462	-5.8819	52.3769	255.1843	InChI=1S/C12H7N3O/c16-12-10-7-6-8-9(2-4-13-8)15(12)5-1-3-14-11(7)10/h1-6,13H/b5-1-,14-3-
H-154		16.2898	200.6342	-10.7414	33.6743	255.4128	InChI=1S/C12H7N3O/c16-12-14-9-6-7(9)2-1-3-10-8-4-5-13-11(8)15(10)12/h1-6,13H/b2-1-,10-3-,14-9-
x6-23		17.8619	161.4558	-15.1498	57.4501	255.4637	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-14-12-11-10(9)15(11)12/h1-6,13H/b3-1-,7-2-,8-6-,14-12-
o-238		12.9095	185.9725	-7.7885	33.5751	255.5117	InChI=1S/C12H7N3O/c16-12-10-9(3-4-13-10)15-5-1-2-7-6-8(7)11(15)14-12/h1-6,13H
i-92		9.9306	139.8422	0.4315	71.8231	256.0786	InChI=1S/C12H7N3O/c16-12-8-6-7-10-9(2-4-14-10)15(11(7)12)5-1-3-13-8/h1-6,14H/b2-1-,13-3-
o-161		20.458	147.6474	-14.1842	76.9119	256.3173	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)10-3-4-13-11(10)14-9-6-8(7)9/h1-6,13H/b14-9-
X23-35		30.1852	215.028	-12.0192	17.1317	256.5074	InChI=1S/C12H7N3O/c16-11-8-6-7-2-1-4-13-9-3-5-14-12(9)15(7)10(8)11/h1-6,14H/b2-1-,13-4+
q-51		4.5349	127.3422	-1.1165	116.5954	256.5454	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-10(7)8-6-15(12)11(8)14-9/h1-6,14H/b2-1-,9-3-
n-179		7.5424	188.5377	-6.3193	52.1952	257.1546	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(12)9-3-4-13-11(9)14-6-8(7)10/h1-6,13H/b14-6-

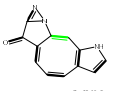
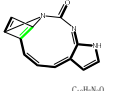
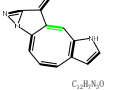
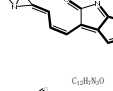
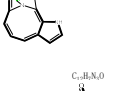
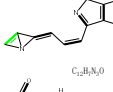
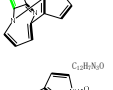
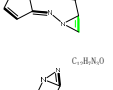
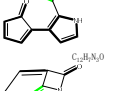
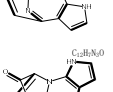
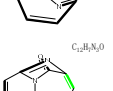
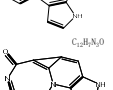
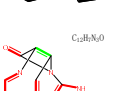
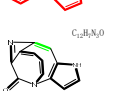
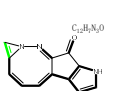
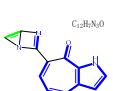
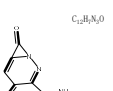
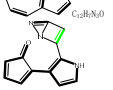

k-44		8.3404	75.7174	-6.0544	153.939	257.2	InChI=1S/C12H7N3O/c16-12-7-6-9-10(7)11-8(2-4-14-11)13-3-1-5-15(9)12/h1-6,14H/b5-1-,13-3+
X22-36		5.7993	125.0833	-4.5824	117.772	257.2844	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-11(8)10-6-9(7)15(10)12/h1-6,14H/b2-1-,4-1-,7-2-,11-10+,13-4-,13-8-
H1-104		25.5643	130.7463	-18.955	86.2928	257.2864	InChI=1S/C12H7N3O/c16-10-3-1-2-7(6-9-12-14-15(9)12)8-4-5-13-11(8)10/h1-6,13H/b2-1-,4-1-,7-2-,11-10+,13-4-,13-8-
H1-91		20.656	140.3052	-10.9525	101.7782	257.3211	InChI=1S/C12H7N3O/c16-10-3-1-2-7(10)8-4-5-13-11(8)15-6-9-12(15)14-9/h1-6,13H
o-46		5.0864	97.5237	-1.1765	133.7896	257.4603	InChI=1S/C12H7N3O/c16-12-7-6-14-11(12)10-9(3-4-13-10)15-5-1-2-8(7)15/h1-6,13H
o-236		12.759	83.607	-0.969	117.6476	257.5933	InChI=1S/C12H7N3O/c16-12-11-9(3-4-13-11)15-5-1-2-7-8(14-12)6-10(7)15/h1-6,13H/b14-8+
q1-41		5.6011	92.2448	-4.349	150.0649	257.6397	InChI=1S/C12H7N3O/c16-12-8-6-10-14-9(15(8)10)3-1-2-7-4-5-13-11(7)12/h1-6,13H/b2-1-,9-3-
q-44		17.6711	199.3149	-2.1887	34.9525	257.8894	InChI=1S/C12H7N3O/c16-10-6-9-8(12-14-15(10)12)3-1-2-7-4-5-13-11(7)9/h1-6,13H
H1-33		27.4289	142.9561	-11.8093	61.8563	257.954	InChI=1S/C12H7N3O/c16-9-6-7-10-11(7)13-3-1-5-15(9)8-2-4-14-12(8)10/h1-6,14H/b5-1-,13-3-
q11-6		6.7384	50.826	-4.5119	171.2138	258.241	InChI=1S/C12H7N3O/c16-12-8-6-15-9(8)3-1-2-7-4-5-13-10(7)11(15)14-12/h1-6,13H/b2-1-,9-3-
k-29		5.2626	55.3263	-4.8876	188.4584	258.3039	InChI=1S/C12H7N3O/c16-9-6-8-10-11-7(2-4-14-11)13-3-1-5-15(8)12(9)10/h1-6,14H/b5-1-,13-3-
n11-49		27.0632	161.0275	-15.9562	64.5644	258.3346	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(14-8)9-6-15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,11-10+
o-182		6.9611	43.412	-1.7331	173.4356	258.5233	InChI=1S/C12H7N3O/c16-11-8-6-14-12-7(8)2-1-5-15(12)9-3-4-13-10(9)11/h1-6,13H
G1-105		12.5475	144.813	-7.4628	82.0408	258.6533	InChI=1S/C12H7N3O/c16-7-2-1-3-8-9-4-5-13-11(9)15-10(8)12(15)14-6-7/h1-6,13H/b2-1-,8-3-,14-6-
A2-72		6.6669	146.1773	-1.6266	92.9011	258.6606	InChI=1S/C12H7N3O/c16-11-8-6-10(11)15-9(2-1-4-13-8)7-3-5-14-12(7)15/h1-6,14H/b4-1-,9-2-,13-8+
F-17		6.9231	101.0194	-2.8697	134.1431	258.8913	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(9)15(12)14-11-8(7)4-5-13-11/h1-6H,13,14/b8-7+
X23-19		5.3187	152.751	-2.6261	93.7299	259.0993	InChI=1S/C12H7N3O/c16-12-10-9-6-7(15(9)12)2-1-4-13-8-3-5-14-11(8)10/h1-6,14H/b2-1-,4-1-,7-2-,11-10+,13-4-,13-8-
n-34		48.4137	209.511	-28.6597	14.1045	259.3571	InChI=1S/C12H7N3O/c16-12-10-7(11(10)12)2-1-5-15-9-3-4-13-8(9)6-14-15/h1-6,13H/b5-1-
p1-15		10.0152	159.036	-3.4143	75.0497	259.4243	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9-12(8)14-15(9)10/h1-6,13H/b3-1-,7-2-,11-8-







































o-191		$C_{22}H_{15}N_2O$	38, 1671	212, 3142	-17, 1727	16, 2177	259, 513	InChI=1S/C12H7N3O/c16-10-6-7(10)14-12-8-2-1-5-15(8)9-3-4-13-11(9)12/h1-6, 13H/b14-12+
H11-79		$C_{22}H_{15}N_2O$	34, 8458	195, 5731	-19, 0718	29, 2528	259, 6126	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-9(7)14-10-6-15(10)12/h1-6, 13H/b14-9-
H-158		$C_{22}H_{15}N_2O$	8, 1429	144, 3713	-4, 3734	90, 116	259, 8753	InChI=1S/C12H7N3O/c16-12-14-11-10-9(4-5-13-10)7-2-1-3-8(6-7)15(11)12/h1-6, 13H
q1-10		$C_{22}H_{15}N_2O$	13, 2267	201, 5409	-10, 7817	38, 7069	259, 9083	InChI=1S/C12H7N3O/c16-12-8(11-9-6-15(9)14-11)3-1-2-7-4-5-13-10(7)12/h1-6, 13H
n-197		$C_{22}H_{15}N_2O$	4, 5189	88, 5521	-3, 167	148, 4849	259, 931	InChI=1S/C12H7N3O/c16-12-8(6-14-12)11-7-2-1-5-15(11)9-3-4-13-10(7)9/h1-6, 13H/b11-8-
l-24		$C_{22}H_{15}N_2O$	6, 1072	144, 9669	-1, 4745	93, 8383	260, 203	InChI=1S/C12H7N3O/c16-12-7-6-8(12)13-3-1-5-15-9-2-4-14-10(9)11(7)15/h1-6, 14H/b5-1-, 11-7-, 13-3-
q11-47		$C_{22}H_{15}N_2O$	24, 1679	185, 7488	-17, 2976	54, 5068	260, 257	InChI=1S/C12H7N3O/c16-12-14-11-10-7(4-5-13-10)2-1-3-8-6-9(8)15(11)12/h1-6, 13H/b2-1-, 8-3-
H1-79		$C_{22}H_{15}N_2O$	13, 901	230, 7199	-13, 1747	26, 1209	260, 404	InChI=1S/C12H7N3O/c16-11-3-1-2-7(11)8-4-5-13-12(8)15-10-6-9(10)14-15/h1-6, 13H
A-25		$C_{22}H_{15}N_2O$	5, 902	196, 5552	-3, 4926	39, 3143	260, 5356	InChI=1S/C12H7N3O/c16-9-6-14-12-11-8(2-1-5-15(11)12)7-3-4-13-10(7)9/h1-6, 13H/b14-6-
G1-92		$C_{22}H_{15}N_2O$	12, 9713	200, 6004	-7, 4304	28, 9174	260, 6451	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)12-9(6-14-10)15(8)12/h1-6, 13H/b3-1-, 8-2-, 14-6-
p-26		$C_{22}H_{15}N_2O$	8, 8996	180, 233	-1, 4115	62, 443	260, 8044	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-10-14-11(8)15(10)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3-, 9-6-, 10-6+
q11-8		$C_{22}H_{15}N_2O$	7, 3917	84, 0495	-2, 5999	151, 7288	260, 8485	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)11(12)14-15(8)9/h1-6, 13H/b2-1-, 8-3-
X22-1		$C_{22}H_{15}N_2O$	19, 9243	196, 3831	-11, 4111	56, 1196	260, 9643	InChI=1S/C12H7N3O/c16-10-6-9-12(15(9)10)7-2-1-4-13-8-3-5-14-11(7)8/h1-6, 14H/b12-7-
l-85		$C_{22}H_{15}N_2O$	10, 2578	131, 5551	-1, 3562	93, 7602	261, 0058	InChI=1S/C12H7N3O/c16-12-7-6-13-3-1-5-15-8-2-4-14-10(8)9(7)11(12)15/h1-6, 14H/b5-1-, 7-6-, 13-3-
A1-5		$C_{22}H_{15}N_2O$	8, 253	134, 7216	-0, 6129	99, 4584	261, 0967	InChI=1S/C12H7N3O/c16-12-9-7-2-1-4-13-6-15(12)11(9)10-8(7)3-5-14-10/h1-6, 14H/b4-1-, 7-2-, 13-6-
H-124		$C_{22}H_{15}N_2O$	6, 4236	108, 1481	-0, 8204	119, 6288	261, 2754	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(15(7)12)8-4-5-13-11(8)14-9/h1-6H, (H, 13, 14)
D-7		$C_{22}H_{15}N_2O$	4, 6561	109, 5842	-0, 2227	125, 2347	261, 3295	InChI=1S/C12H7N3O/c16-12-8-6-15-9(2-1-4-13-8)7-3-5-14-10(7)11(12)15/h1-6, 14H/b2-1-, 13-4+
H1-47		$C_{22}H_{15}N_2O$	4, 7989	32, 0724	-2, 0761	195, 4624	261, 7746	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)15-6-9(7)14-12(10)15/h1-6, 13H/b3-1-, 7-2-
H1-41		$C_{22}H_{15}N_2O$	10, 7754	131, 1185	0, 5318	90, 9029	262, 0923	InChI=1S/C12H7N3O/c16-11-3-1-2-9-7-4-5-13-12(7)10-6-8(11)14-15(9)10/h1-6, 13H/b3-1-, 9-2-














H-37		4.6245	156.2567	-1.1982	81.6515	262.1231	InChI=1S/C12H7N3O/c16-12-10-7-6-8(10)13-3-1-5-15(12)9-2-4-14-11(7)9/h1-6,14H/b5-1-,13-3-
	$C_{12}H_7N_3O$						
p1-18		6.6031	57.268	-4.9208	176.3891	262.3674	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11-8(9)6-15(12)14-11/h1-6,13H/b3-1-,7-2-,12-10-
	$C_{12}H_7N_3O$						
E-10		5.2814	92.9363	-1.317	139.6695	262.4445	InChI=1S/C12H7N3O/c16-12-10-3-1-2-8-7-4-5-13-9(7)6-11(12)15(10)14-8/h1-6,13H
	$C_{12}H_7N_3O$						
D-17		6.8018	135.1242	-1.3988	108.6573	262.5971	InChI=1S/C12H7N3O/c16-10-6-9-12-11-7(3-5-14-11)8(15(9)10)2-1-4-13-12/h1-6,14H/b2-1-,4-1-,8-2-,13-4-,13-12+
	$C_{12}H_7N_3O$						
H1-89		30.1418	164.2134	-20.1493	71.7347	262.687	InChI=1S/C12H7N3O/c16-11-3-1-2-8(11)7-4-5-13-9(7)6-10-12-14-15(10)12/h1-6,13H/b10-6-
	$C_{12}H_7N_3O$						
B-51		6.2016	30.9990	-2.3326	189.5883	262.7778	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(9)12(14-10)11-8(7)3-4-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
o-56		20.4834	198.8954	-14.0958	40.5978	262.8579	InChI=1S/C12H7N3O/c16-10-8-6-7(8)2-1-5-15-9-3-4-13-11(9)14-12(10)15/h1-6,13H/b5-1-,7-2-
	$C_{12}H_7N_3O$						
H11-85		6.4286	35.297	-2.758	195.489	263.0725	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(15(12)14-7)11-8(9)4-5-13-11/h1-6,13H/b2-1-,9-3-
	$C_{12}H_7N_3O$						
X22-59		20.3671	143.2058	-19.6823	95.5263	263.0896	InChI=1S/C12H7N3O/c16-12-7(11-9-6-15(9)11)2-1-4-13-8-3-5-14-10(8)12/h1-6,14H/b2-1-,11-7-,13-4-
	$C_{12}H_7N_3O$						
H-49		25.4235	132.0458	-16.6204	110.4888	263.0973	InChI=1S/C12H7N3O/c16-12-8-6-7(8)10-11-9(2-4-14-11)15(12)5-1-3-13-10/h1-6,14H/b5-1-,13-3+
	$C_{12}H_7N_3O$						
p1-46		24.8224	130.8342	-11.4915	111.1514	263.143	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9-14-12(8)15(9)10/h1-6,13H/b3-1-,7-2-,11-8+
	$C_{12}H_7N_3O$						
s11-62		18.3945	149.4417	-12.2035	74.974	263.1573	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(12)15-6-9(15)14-8/h1-6,13H/b3-1-,7-2-,11-10-
	$C_{12}H_7N_3O$						
j-5		17.1725	209.2014	-10.0568	27.5804	263.1925	InChI=1S/C12H7N3O/c16-12-9-2-1-4-13-7-3-5-14-8(7)6-10-11(12)15(9)10/h1-6,14H/b4-1-,8-6-,9-2-,13-7+
	$C_{12}H_7N_3O$						
x7-14		15.3351	182.0236	-7.5145	61.3871	263.2702	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10-8-6-14-15(9)12(8)10/h1-6,13H/b3-1-,7-2-,11-10+
	$C_{12}H_7N_3O$						
p1-39		20.5694	225.0862	-16.4734	16.0036	263.3057	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11(9)14-12-8-6-15(8)12/h1-6,13H/b14-12+
	$C_{12}H_7N_3O$						
H11-61		5.5278	108.7324	-1.5361	110.77	263.3921	InChI=1S/C12H7N3O/c16-11-6-9-7-2-1-3-10(9)14-15(11)12-8(7)4-5-13-12/h1-6,13H
	$C_{12}H_7N_3O$						
X22-23		14.2153	171.8228	-7.4163	71.9234	263.5907	InChI=1S/C12H7N3O/c16-12-10-7-2-1-4-13-9-3-5-14-11(9)15(12)6-8(7)10/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
q-58		5.923	157.99	-2.4029	89.5247	263.7001	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9-6-15(12)11(8)14-9/h1-6,13H/b2-1-,8-3+
	$C_{12}H_7N_3O$						
i-6		7.2029	175.8223	-3.197	54.6172	263.9338	InChI=1S/C12H7N3O/c16-12-8-2-1-4-13-7-3-5-14-11(7)9-6-10(12)15(8)9/h1-6,14H/b4-1-,8-2-,11-9+,13-7+
	$C_{12}H_7N_3O$						












x6-31		21.6554	148.8334	-10.9746	95.9225	264.1004	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-11-12(14-11)15(9)10/h1-6,13H/h3-1-,7-2-,8-6+
n-51		34.102	207.3871	-17.9195	21.67	264.3604	InChI=1S/C12H7N3O/c16-12-10-9-2-1-5-15(9)8-3-4-13-7(8)6-14-11(10)12/h1-6,13H/h14-6-
x4-63		12.0486	156.3884	-7.6906	84.8926	264.4537	InChI=1S/C12H7N3O/c16-12-14-6-8-10-7(4-5-13-10)2-1-3-9-11(8)15(9)12/h1-6,13H/h2-1-,3-1-,7-2-,9-3+,10-8+
H-114		5.0618	78.2275	-2.1214	159.683	264.6516	InChI=1S/C12H7N3O/c16-12-11-7-2-1-3-10(15)(12)14-11)8-4-5-13-9(8)6-7/h1-6,13H/h2-1-,3-1-,7-2-,9-6+,10-3-,10-8-
p1-5		8.0875	63.9747	-5.5327	160.1358	264.8685	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)12-8-6-9(10)15(12)14-8/h1-6,13H/h3-1-,7-2-,12-11+
X-26		7.2363	194.8996	-3.5280	37.1332	265.0089	InChI=1S/C12H7N3O/c16-12-11-10-9-8(3-5-13-9)7(6-15(10)11)2-1-4-14-12/h1-6,13H/h2-1-,14-4-
X-44		7.2359	194.8999	-3.5295	37.1377	265.0089	InChI=1S/C12H7N3O/c16-12-11-10-9-8(3-5-13-9)7(6-15(10)11)2-1-4-14-12/h1-6,13H/h2-1-,14-4+
H11-132		38.591	207.9669	-17.5451	21.3116	265.0898	InChI=1S/C12H7N3O/c16-11-6-10(11)15-12-8(4-5-13-12)7-2-1-3-9(7)14-15/h1-6,13H
H-121		5.1059	77.9291	-2.1462	160.2427	265.1049	InChI=1S/C12H7N3O/c16-12-11-9-3-1-2-7(15)(12)14-11)6-10-8(9)4-5-13-10/h1-6,13H/h2-1-,3-1-,7-2-,7-6-,9-3-,9-8-,10-6+
q1-2		14.1784	226.9194	-13.1928	21.0411	265.1164	InChI=1S/C12H7N3O/c16-12-9(15-10-6-8(10)14-15)3-1-2-7-4-5-13-11(7)12/h1-6,13H
o-164		5.1972	100.7554	-2.1069	132.8425	265.1308	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-8(10(7)14-12)11-9(15)3-4-13-11/h1-6,13H/h5-1-,7-2+
i-30		7.9178	164.4559	-2.6681	83.6337	265.1378	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-11(8)10-6-9(7)15(10)12/h1-6,14H/h2-1-,4-1-,7-2-,11-10+,13-4-,13-8+
x9-31		16.1107	174.6704	-7.08	67.0555	265.2259	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-11-9(6-14-8)15(11)12/h1-6,13H/h2-1-,8-3+
A2-15		6.5305	132.3135	-1.8611	114.3836	265.3256	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-4-14-12(15(9)10)11-8(7)3-5-13-11/h1-6,13H/h2-1-,4-1-,7-2-,14-4-,14-12+
H-15		7.4784	115.4107	-1.2753	124.0781	265.4118	InChI=1S/C12H7N3O/c16-10-7-2-1-3-9-8-4-5-13-11(8)15(9)12(10)14-6-7/h1-6,13H/h2-1-,9-3-
G1-103		6.8029	173.9611	-2.8735	82.1857	265.6056	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)15(10)12-9(7)6-14-12/h1-6,13H/h3-1-,7-2+
p1-2		14.3271	226.7848	-13.1853	22.8881	265.733	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)12(10)15-9-6-8(9)14-15/h1-6,13H
s12-23		11.386	135.1393	-7.4922	95.171	265.8802	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-10-11(12)15(10)14-8/h1-6,13H/h3-1-,7-2-,9-6+
x5-33		13.4776	190.8223	-6.1163	46.8948	266.0537	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)14-11-9(6-8)15(11)12/h1-6H, (H,13,14)




















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x7-42		15, 8541	180, 0457	-7, 8204	62, 7807	266, 1268	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)9-11-12(9)15(8)6-14-11/h1-6, 13H/h3-1-, 7-2-, 10-9-
o-91		3, 5601	70, 1685	-2, 1492	181, 7983	266, 3691	InChI=1S/C12H7N3O/c16-12-11-7-6-9-10(3-4-13-9)15(12)5-1-2-8(7)14-11/h1-6, 13H/h5-1-, 8-2-
x9-21		15, 6755	176, 8735	-6, 5579	66, 5831	266, 4055	InChI=1S/C12H7N3O/c16-12-9-7(4-5-13-9)2-1-3-8-6-14-11-10(8)15(11)12/h1-6, 13H/h2-1-, 8-3-
E-41		7, 4241	50, 4435	-1, 4671	181, 8499	266, 4793	InChI=1S/C12H7N3O/c16-11-6-9-10-3-1-2-8(14-9)7-4-5-13-12(7)15(10)11/h1-6, 13H
H-117		4, 7838	41, 1789	-1, 8213	197, 2288	266, 4958	InChI=1S/C12H7N3O/c16-12-10-7-2-1-3-9(14-10)8-4-5-13-11(8)15(12)6-7/h1-6, 13H
H-27		19, 4829	137, 0406	-14, 566	104, 8203	266, 6294	InChI=1S/C12H7N3O/c16-12-8-6-7(8)10-11-9(2-4-14-11)15(12)5-1-3-13-10/h1-6, 14H/h5-1-, 13-3-
E-23		7, 7035	102, 5525	-1, 8888	132, 5002	266, 7656	InChI=1S/C12H7N3O/c16-12-8-6-14-9-2-1-3-10(8)15(12)11-7(9)4-5-13-11/h1-6, 13H/h2-1-, 3-1-, 8-6-, 9-2-, 10-3-, 14-6-, 14-9-
j-18		17, 826	194, 6525	-9, 7922	45, 7128	266, 8761	InChI=1S/C12H7N3O/c16-12-10-7-2-1-4-13-8-3-5-14-9(8)6-15(12)11(7)10/h1-6, 14H/h4-1-, 7-2-, 9-6-, 13-8+
p-1		6, 4531	51, 092	-5, 6309	187, 882	266, 9787	InChI=1S/C12H7N3O/c16-12-10-6-8-7(4-5-13-8)2-1-3-9-11(12)14-15(9)10/h1-6, 13H/h2-1-, 9-3-, 10-6-
H11-59		4, 9501	82, 2704	-2, 9986	163, 4752	267, 0869	InChI=1S/C12H7N3O/c16-11-6-10-7-2-1-3-9(14-15(10)11)12-8(7)4-5-13-12/h1-6, 13H
o-85		7, 0036	96, 354	-0, 2394	137, 4813	267, 1519	InChI=1S/C12H7N3O/c16-12-10-7-6-15(5-1-2-8(7)14-10)9-3-4-13-11(9)12/h1-6, 13H
o-242		6, 8631	75, 2938	-2, 8969	169, 9071	267, 1796	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(10)9-3-4-13-12(9)11(7)14-8/h1-6, 13H/h5-1-, 7-2-, 8-6+
p1-19		14, 4831	221, 9069	-11, 2218	21, 439	267, 2292	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10(9)12-8-6-15(8)14-12/h1-6, 13H
F-8		10, 3947	163, 1443	-8, 58	83, 6789	267, 284	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7(8)9-4-5-13-12(9)14-15-6-10(11)15/h1-6H, (H, 13, 14)/b9-7-
n-107		5, 5884	177, 2905	-4, 7305	63, 0496	267, 5498	InChI=1S/C12H7N3O/c16-9-6-14-10-7-2-1-5-15(12(7)10)8-3-4-13-11(8)9/h1-6, 13H/h4-6-
G1-91		11, 8586	210, 3654	-6, 7359	40, 2902	267, 5749	InChI=1S/C12H7N3O/c16-10-3-1-2-7(10)8-4-5-13-11(8)12-9-6-14-15(9)12/h1-6, 13H
X22-48		13, 8852	124, 7053	-6, 8774	116, 1307	267, 8009	InChI=1S/C12H7N3O/c16-11-8-6-15-10(11)7(8)2-1-4-13-9-3-5-14-12(9)15/h1-6, 14H/h2-1-, 13-4-
n-208		7, 2749	46, 2621	-1, 9566	180, 8363	267, 9216	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-11(8)10(7)9(15)6-14-12/h1-6, 13H




















p-5		18.3766	166.4133	-4.1907	70.7777	267.9266	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-9(7)6-10(8)15-12(11)14-15/h1-6,13H/t2-1-,3-1-,7-2-,8-3-,9-6+,10-6+
r-59		32.0088	125.3754	-14.2495	111.3093	267.9708	InChI=1S/C12H7N3O/c16-12-14-11-7(4-5-13-11)2-1-3-8-9-6-10(8)15(9)12/h1-6H,(H,13,14,16)/b3-1-,7-2-
p-2		18.3715	166.554	-4.2002	70.8092	268.0247	InChI=1S/C12H7N3O/c16-11-8-6-9-7(4-5-13-9)2-1-3-10(8)15-12(11)14-15/h1-6,13H/t2-1-,3-1-,7-2-,8-6+,9-6+,10-3+
F-67		20.9385	234.1669	-16.9853	19.2653	268.0811	InChI=1S/C12H7N3O/c16-12-8(7-4-5-13-11(7)14-12)2-1-3-9-10-6-15(9)10/h1-6H,(H,13,14,16)/b2-1-,9-3-
s11-21		5.1918	36.7051	-3.9748	196.3846	268.2974	InChI=1S/C12H7N3O/c16-12-8-6-15-9(14-8)3-1-2-7-4-5-13-10(7)11(12)15/h1-6,13H/b3-1-,7-2-,11-10+
E-48		21.1506	237.2349	-16.7622	15.7369	268.3125	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)8(14-12)2-1-3-9-10-6-15(9)10/h1-6,13H/b2-1-,9-3-
B-31		3.0771	84.2254	-1.7887	160.4054	268.3231	InChI=1S/C12H7N3O/c16-10-6-9-11(10)14-8-2-1-5-15(9)12-7(8)3-4-13-12/h1-6,13H
H11-140		13.7916	193.1917	-11.4221	45.3476	268.3574	InChI=1S/C12H7N3O/c16-12-10-6-15(10)14-9-3-1-2-7(9)8-4-5-13-11(8)12/h1-6,13H/b14-9+
H1-88		23.7434	147.8239	-9.4002	100.1206	268.3744	InChI=1S/C12H7N3O/c16-10-3-1-2-7(10)8-4-5-13-11(8)9-6-15-12(9)14-15/h1-6,13H
E-63		5.1	88.8566	-2.7873	157.876	268.6071	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-7-4-5-13-11(7)15(12)10(8)6-14-9/h1-6,13H/t2-1-,3-1-,8-2-,9-3-
E-37		5.7431	44.5414	-1.5221	193.104	268.6402	InChI=1S/C12H7N3O/c16-10-6-11-14-8-2-1-3-9(10)15(11)12-7(8)4-5-13-12/h1-6,13H/b2-1-,9-3-
H11-45		5.4958	118.9425	-0.635	121.2882	268.8245	InChI=1S/C12H7N3O/c16-12-9-6-8-7(4-5-13-8)10-2-1-3-11(14-9)15(10)12/h1-6,13H
I-100		12.751	155.6641	-8.5346	81.9144	268.8941	InChI=1S/C12H7N3O/c16-12-10-7-6-8-9(2-4-13-8)15(11(7)10)5-1-3-14-12/h1-6,13H/b5-1-,14-3-
X-25		8.4729	139.0849	-2.1481	110.2644	269.1313	InChI=1S/C12H7N3O/c16-12-10-9-6-7(2-1-4-13-10)8-3-5-14-11(8)15(9)12/h1-6,14H/t2-1-,4-1-,7-2-,13-4+,13-10-
o-87		8.8396	135.8842	-3.1814	102.6043	269.1346	InChI=1S/C12H7N3O/c16-12-11-7-2-1-5-15(12)10-3-4-13-9(10)6-8(7)14-11/h1-6,13H/b8-6+
H-87		13.3643	195.2826	-8.9015	43.2838	269.3	InChI=1S/C12H7N3O/c16-12-10-9(4-5-13-10)8-3-1-2-7-6-15(7)14-11(8)12/h1-6,13H/t2-1-,8-3-,14-11+
q1-56		15.5807	230.9341	-12.1394	16.9766	269.3425	InChI=1S/C12H7N3O/c16-11-8(12-14-9-6-15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6,13H
q11-16		13.7263	218.4223	-4.9944	30.089	269.3626	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)11(8)14-15(9)12/h1-6,13H
H1-127		23.7944	144.494	-9.8049	104.8398	269.4558	InChI=1S/C12H7N3O/c16-10-3-1-2-7(10)8-4-5-13-12(8)9-6-11-14-15(9)11/h1-6,13H

		23.9013	141.2334	-9.583	97.9737	269.5304	InChI=1S/C12H7N3O/c16-12-8(9-6-10-14-15(9)10)3-1-2-7-4-5-13-11(7)12/h1-6,13H
q1-38	<chem>C12H7N3O</chem>						
		16.2511	211.6004	-10.1616	50.9467	269.7676	InChI=1S/C12H7N3O/c16-12-10-6-9(15(10)12)8-3-1-2-7-4-5-13-11(7)14-8/h1-6H, 1H,13,14)/b9-8-
r-23	<chem>C12H7N3O</chem>						
		6.3657	92.5972	-1.4865	143.5781	269.9233	InChI=1S/C12H7N3O/c16-12-7-6-8-10(7)11-9(2-4-14-11)15(12)5-1-3-13-8/h1-6,14H/b5-1-,13-3-
h1-32	<chem>C12H7N3O</chem>						
		10.4798	123.2725	-1.52	106.0255	269.9784	InChI=1S/C12H7N3O/c16-12-7-6-9-10(7)11-8(2-4-13-11)15(9)5-1-3-14-12/h1-6,13H/b5-1-,13-3-
l-103	<chem>C12H7N3O</chem>						
		18.3526	163.195	-7.9358	67.5321	270.0092	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-13-8-3-5-14-10(8)12-11(7)15(9)12/h1-6,14H/b2-1-,13-4+
x23-26	<chem>C12H7N3O</chem>						
		15.3136	176.3069	-10.2613	69.2743	270.2289	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-5-14-11)13-4-1-2-8-12(10)15(8)9/h1-6,14H/b2-1-,13-4-
x22-42	<chem>C12H7N3O</chem>						
		23.9818	142.1045	-9.3106	99.5616	270.2334	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10(9)8-6-15-12(8)14-15/h1-6,13H
p1-35	<chem>C12H7N3O</chem>						
		16.074	230.9498	-12.1172	18.1087	270.2944	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-11(7)10(8)12-14-9-6-15(9)12/h1-6,13H
p1-54	<chem>C12H7N3O</chem>						
		15.9428	194.0952	-9.6289	39.08	270.3136	InChI=1S/C12H7N3O/c16-12-8-6-7(8)2-1-5-15-9-3-4-13-10(9)11(15)14-12/h1-6,13H/b5-1-,7-2-,14-11-
o-223	<chem>C12H7N3O</chem>						
		42.5397	222.7128	-19.5289	10.2338	270.3293	InChI=1S/C12H7N3O/c16-10-6-9(10)15-12-8(14-15)3-1-2-7-4-5-13-11(7)12/h1-6,13H
s11-23	<chem>C12H7N3O</chem>						
		41.3849	223.0005	-19.4366	9.1582	270.3331	InChI=1S/C12H7N3O/c16-10-6-9(10)15-8-3-1-2-7-4-5-13-11(7)12(8)14-15/h1-6,13H
q11-1	<chem>C12H7N3O</chem>						
		14.0218	189.1175	-7.0613	63.1346	270.3507	InChI=1S/C12H7N3O/c16-12-10-7-6-15(12)5-1-3-13-8-2-4-14-11(8)9(7)10/h1-6,14H/b3-1-,13-3+
k-25	<chem>C12H7N3O</chem>						
		6.8208	167.1528	-2.8989	92.9133	270.4957	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15(10)9-6-14-11(7)9/h1-6,13H/b3-1-,7-2+
G1-67	<chem>C12H7N3O</chem>						
		4.1291	82.8702	-2.2261	167.5477	270.5926	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-7-4-5-13-10(7)6-11(8)15(12)14-9/h1-6,13H/b3-1-,8-2+
E-62	<chem>C12H7N3O</chem>						
		12.2136	226.2923	-6.2463	28.6998	270.6062	InChI=1S/C12H7N3O/c16-12-11-8-6-10-7(4-5-13-10)2-1-3-9(8)14-15(11)12/h1-6,13H/b3-1-,7-2-,10-6+
s12-36	<chem>C12H7N3O</chem>						
		16.2637	211.7792	-9.9640	49.3043	270.6401	InChI=1S/C12H7N3O/c16-12-10-6-9(15(10)12)7-2-1-4-13-11-8(7)3-5-14-11/h1-6,14H/b9-7-
C-25	<chem>C12H7N3O</chem>						
		17.5367	223.2863	-14.3443	23.8666	270.6582	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-11(14-12)9-6-15(8)9/h1-6,13H/b2-1-,8-3+,14-11+
q1-12	<chem>C12H7N3O</chem>						
		7.6194	45.6854	-1.7747	184.6738	270.6881	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-14-10(12)11(15)9-7(8)3-4-13-9/h1-6,13H/b5-1?,8-2-
A-208	<chem>C12H7N3O</chem>						
		23.5662	141.5112	-9.2103	99.4094	270.6925	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)11(9)8-6-10-14-15(8)10/h1-6,13H
p1-9	<chem>C12H7N3O</chem>						

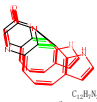
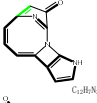
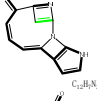
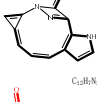

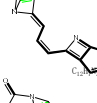
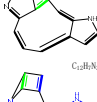
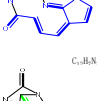
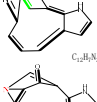
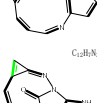
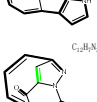
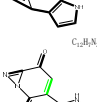
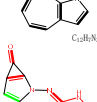
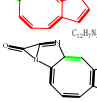
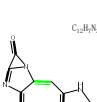
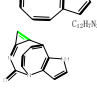
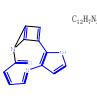
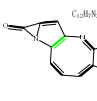

x2-13		39,3498	168,5154	-17,2945	58,8043	270,6955	InChI=1S/C12H7N3O/c16-12-7-6-9-8(2-4-14-9)13-3-1-5-15-10(7)11(12)15/h1-6,14H/b5-1-,7-6-,13-3+
i-3		4,8713	96,4335	-4,2493	160,1313	270,9458	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-4-13-8-3-5-14-10(8)11(12)15(7)9/h1-6,14H/b4-1-,7-2-,11-10-,13-8+
G1-88		8,0354	169,9014	-4,4073	75,8332	271,0592	InChI=1S/C12H7N3O/c16-7-2-1-3-9-8-4-5-13-10(8)12-11(9)15(12)14-6-7/h1-6,13H/b2-1-,9-3-,14-6-
H1-6		11,2898	198,8486	-8,1654	44,0154	271,099	InChI=1S/C12H7N3O/c16-9-2-1-4-13-8-3-5-14-10(8)7-6-15-11(7)12(9)15/h1-6,14H/b2-1-,13-4+
I-79		14,1355	135,5532	-8,2835	97,688	271,1617	InChI=1S/C12H7N3O/c16-9-6-7-10-11-8(2-4-14-11)15(12(7)10)5-1-3-13-9/h1-6,14H/b5-1-,7-6-,13-3-
H11-42		9,8659	155,4035	-2,2372	68,4777	271,4306	InChI=1S/C12H7N3O/c16-12-8-6-15(12)10-3-1-2-9(14-10)7-4-5-13-11(7)8/h1-6,13H
x5-36		4,2497	126,3441	-3,3479	134,3575	271,4568	InChI=1S/C12H7N3O/c16-12-10-9-6-8(15(9)12)3-1-2-7-4-5-13-11(7)14-10/h1-6H, (H,13,14)
H-151		5,1668	83,207	-3,0573	169,3248	271,7613	InChI=1S/C12H7N3O/c16-12-14-11-9-3-1-2-7(6-15(11)12)10-8(9)4-5-13-10/h1-6,13H
H11-84		5,277	69,3427	-2,6884	178,0846	271,7748	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-11(15(12)14-9)6-10-7(8)4-5-13-10/h1-6,13H/b3-1-,8-2-
C-35		9,1177	126,0855	-2,0546	115,1748	271,9517	InChI=1S/C12H7N3O/c16-10-6-9-11(10)7-2-1-4-14-15(9)12-8(7)3-5-13-12/h1-6,13H/b2-1-,14-4-
q1-7		5,9748	145,3667	-2,5233	106,2465	271,9987	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)2-1-3-8-6-9-10(8)14-15(9)12/h1-6,13H/b2-1-,8-3-
H11-21		6,5446	124,1839	-0,6853	117,8515	272,0377	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-7-4-5-13-9(7)6-11(14-8)15(10)12/h1-6,13H
o-221		3,5493	89,1536	-2,2485	156,1442	272,0458	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(11(8)14-12)9-3-4-13-10(7)9/h1-6,13H
x5-44		8,4426	137,4746	-4,848	119,036	272,0946	InChI=1S/C12H7N3O/c16-12-9-8-3-1-2-7-4-5-13-10(7)14-11(9)15(12)6-8/h1-6H, (H,13,14)/b3-1-,7-2-
p1-29		30,4155	162,9516	-19,9368	71,048	272,1779	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8(10)6-9-12-14-15(9)12/h1-6,13H/b9-6-
H11-32		15,7146	197,7946	-5,4254	39,1802	272,2209	InChI=1S/C12H7N3O/c16-12-9-6-15(12)14-10-3-1-2-7(10)8-4-5-13-11(8)9/h1-6,13H/b14-10-
A-45		8,8134	51,1013	-1,6087	181,0185	272,306	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-11(9(12)6-14-15)10-7(8)3-4-13-10/h1-6,13H/b5-1?,8-2-
q1-26		30,2024	162,9467	-19,9862	69,851	272,3173	InChI=1S/C12H7N3O/c16-11-8(6-9-12-14-15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b9-6+
A1-28		6,6847	164,3812	-4,5534	88,6674	272,9472	InChI=1S/C12H7N3O/c16-12-8-6-13-4-1-2-9-7-3-5-14-10(7)11(8)15(9)12/h1-6,14H/b2-1-,4-1-,8-6-,9-2-,13-4-,13-6-

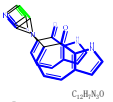
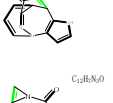
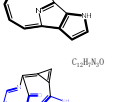
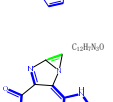
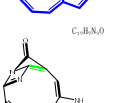
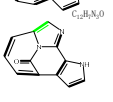
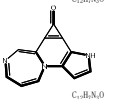
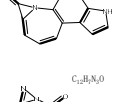
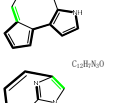
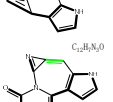
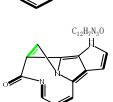
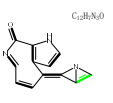
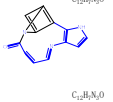
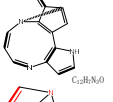
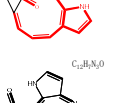
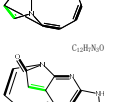



o-173		6.8653	48.2711	-1.7671	185.6399	272.9663	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-10(9)8(6-7)11(15)14-12/h1-6,13H/b5-1-,7-2-
	$C_{12}H_7N_3O$						
B-12		38.8658	210.4918	-17.5920	26.6353	273.0177	InChI=1S/C12H7N3O/c16-10-6-9(10)15-5-1-2-8-7-3-4-13-11(7)14-12(8)15/h1-6,13H
	$C_{12}H_7N_3O$						
o-6		6.569	97.3444	-0.4426	146.2064	273.058	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-6-8(7)10(11)14-12-9(15)3-4-13-12/h1-6,13H
	$C_{12}H_7N_3O$						
B-230		12.6115	180.9988	-9.5379	62.0081	273.1227	InChI=1S/C12H7N3O/c16-11-9-6-15(9)5-1-2-7-8-3-4-13-12(8)14-10(7)11/h1-6,13H/b5-1-,7-2-
	$C_{12}H_7N_3O$						
q1-31		17.1212	217.3519	-15.2517	30.3928	273.338	InChI=1S/C12H7N3O/c16-11-8(14-12-9-6-15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b14-12-
	$C_{12}H_7N_3O$						
n-8		14.9452	183.1758	-7.3706	52.1885	273.3404	InChI=1S/C12H7N3O/c16-9-6-14-12-8(3-4-13-12)15-5-1-2-7-10(9)11(7)15/h1-6,13H/b14-6+
	$C_{12}H_7N_3O$						
F-59		40.1116	198.9502	-21.1729	23.627	273.491	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(9)8-4-5-13-11(8)14-10-6-15(10)12/h1-6H,13,14/b8-7-
	$C_{12}H_7N_3O$						
q11-59		20.2107	184.408	-10.8242	55.7734	273.5907	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(8)14-9-6-15(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
H-54		6.8255	125.5488	-0.6988	114.7904	274.1684	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8-9-4-5-13-11(9)15(10)12(8)14-7/h1-6,13H
	$C_{12}H_7N_3O$						
x4-6		16.2471	209.2332	-5.3887	28.3282	274.3784	InChI=1S/C12H7N3O/c16-9-6-14-12-11-10-7(4-5-13-10)2-1-3-8(9)15(11)12/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
X-39		11.1132	151.2987	-2.9123	96.6153	274.3875	InChI=1S/C12H7N3O/c16-12-10-9-6-7(2-1-4-13-10)8-3-5-14-11(8)15(9)12/h1-6,14H/b2-1-,4-1-,7-2-,13-4-,13-10+
	$C_{12}H_7N_3O$						
H1-39		7.4904	177.622	-5.6039	75.3332	274.7072	InChI=1S/C12H7N3O/c16-12-10-7-6-13-3-1-5-15(12)8-2-4-14-11(8)9(7)10/h1-6,14H/b5-1-,7-6-,13-3-
	$C_{12}H_7N_3O$						
H-150		7.3724	139.3043	-2.3279	120.6349	274.7694	InChI=1S/C12H7N3O/c16-12-14-10-6-7-2-1-3-9(15(10)12)8-4-5-13-11(7)8/h1-6,13H
	$C_{12}H_7N_3O$						
H1-7		6.6098	59.3041	-3.9741	180.9843	274.8727	InChI=1S/C12H7N3O/c16-7-2-1-3-8-9-4-5-13-12(9)15-10(6-7)11(8)14-15/h1-6,13H/b2-1-,4-1-,7-2-,13-4-,10-6+
	$C_{12}H_7N_3O$						
H1-63		25.04	191.7285	-15.6019	47.2029	274.8918	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)12(14-8)9-6-15(9)10/h1-6,13H/b3-1-,8-2-
	$C_{12}H_7N_3O$						
H1-78		12.7327	222.6855	-4.8014	14.209	275.0531	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)12(14-8)15-6-9(10)15/h1-6,13H/b3-1-,8-2-
	$C_{12}H_7N_3O$						
H1-5		15.7571	196.9395	-9.5163	46.4494	275.1376	InChI=1S/C12H7N3O/c16-10-2-1-4-13-7-3-5-14-11(7)8-6-9-12(10)15(8)9/h1-6,14H/b2-1-,13-4+
	$C_{12}H_7N_3O$						
q11-26		7.2065	141.3603	-0.1822	106.5311	275.2076	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-11(7)8-6-10(12)15(9)14-8/h1-6,13H/b2-1-,9-3-
	$C_{12}H_7N_3O$						
A2-43		18.2608	168.3353	-13.2196	69.5441	275.2699	InChI=1S/C12H7N3O/c16-12-11-7(3-5-14-11)9-2-1-4-13-8-6-10(8)15(9)12/h1-6,14H/b4-1-,9-2-,13-8-
	$C_{12}H_7N_3O$						

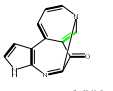
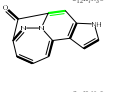
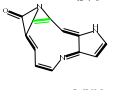
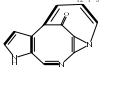
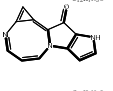
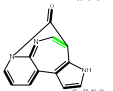
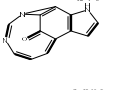
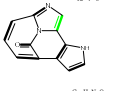
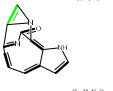
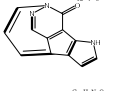
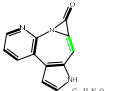
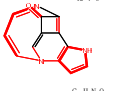
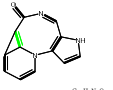
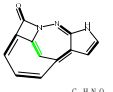
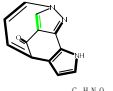
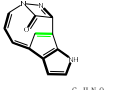
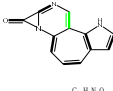
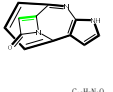

H11-120		7.9895	113.8385	-1.3477	132.1924	275.2775	InChI=1S/C12H7N3O/c16-11-8-2-1-3-9-7-4-5-13-12(7)15(9)10(11)6-14-8/h1-6,13H/b2-1-,9-3-
B-232		7.6716	48.8210	-1.5878	190.3081	275.3252	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-9(11(12)14-15)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-
H11-76		10.0745	126.3189	-2.8752	129.7801	275.4223	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-9-14-10(6-7)15(9)12/h1-6,13H/b2-1-,3-1-,7-2+,9-3+
X22-55		26.2292	243.8188	0.3743	1.53	275.5194	InChI=1S/C12H7N3O/c16-11-7-2-1-4-13-9-3-5-14-12(9)15-6-8(11)10(7)15/h1-6,14H/b2-1-,13-4-
B-195		2.9391	87.3509	-1.7340	164.1195	275.5687	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(9-6-14-10(9)11)12-8(7)3-4-13-12/h1-6,13H
x4-61		16.8119	208.357	-5.7384	26.788	275.6575	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-9(6-14-12)15(8)11/h1-6,13H/b2-1-,8-3-
X22-34		16.3042	172.5104	-13.7678	90.2156	275.6871	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-9-3-5-14-11(9)15(12)10-6-8(7)10/h1-6,14H/b2-1-,13-4-
B-239		6.0569	115.5031	-0.2536	130.0077	275.7503	InChI=1S/C12H7N3O/c16-12-10-9-6-15(12)5-1-2-7(9)8-3-4-13-11(8)14-10/h1-6,13H
X23-30		51.6988	163.949	-29.8209	70.0776	275.802	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)7-2-1-4-13-8-3-5-14-9(8)6-7/h1-6,14H/b2-1-,4-1+,7-2+,7-6-,9-6-,13-4+,13-8-
I-86		4.4177	54.2127	-1.5254	189.8087	275.8522	InChI=1S/C12H7N3O/c16-12-7-6-9-10(7)13-3-1-5-15(9)8-2-4-14-11(8)12/h1-6,14H
o-232		26.2116	197.3671	-11.8989	54.3868	276.0241	InChI=1S/C12H7N3O/c16-12-11-10(3-4-13-11)15(12)5-1-2-7-8-6-9(7)14-8/h1-6,13H/b5-1-
x7-18		17.0302	177.5692	-6.6691	72.4619	276.0585	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-12-8(6-14-11)15(9)12/h1-6,13H/b3-1-,7-2-,11-10-
q1-61		5.0171	86.072	-4.0934	169.4279	276.1309	InChI=1S/C12H7N3O/c16-11-10-7(4-5-13-10)2-1-3-8-6-9-14-12(11)15(8)9/h1-6,13H/b2-1-,8-3-
q11-61		4.6015	58.1414	-3.3169	190.4479	276.3832	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-14-9(8)6-15(11)12/h1-6,13H/b2-1-,8-3+
r-45		21.7479	185.3757	-10.6078	64.7796	276.3953	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-11(7)14-6-9(10)15(8)12/h1-6H,13,14
H1-44		11.8119	168.5367	-5.6766	77.8494	276.8031	InChI=1S/C12H7N3O/c16-9-6-7-10-11(7)13-3-1-5-15(9)8-2-4-14-12(8)10/h1-6,14H/b5-1-,13-3+
B-176		3.0637	88.1284	-1.8602	167.7954	277.0013	InChI=1S/C12H7N3O/c16-10-7-2-1-5-15(12-9(10)6-14-12)11-8(7)3-4-13-11/h1-6,13H
q11-14		16.1289	212.0865	-5.4804	44.5816	277.1225	InChI=1S/C12H7N3O/c16-12-9-6-14-11-8(15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6,13H
s11-1		16.139	211.9739	-5.4697	44.5989	277.1847	InChI=1S/C12H7N3O/c16-12-9-6-14-8-3-1-2-7-4-5-13-10(7)11(8)15(9)12/h1-6,13H

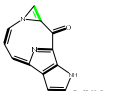
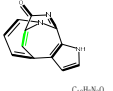
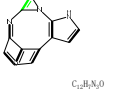
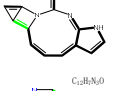
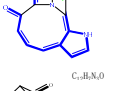
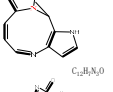
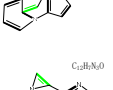
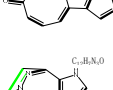
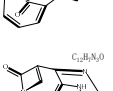
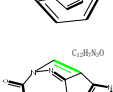
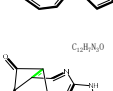
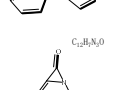
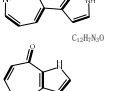
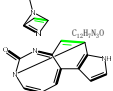
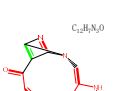
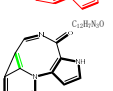
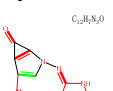
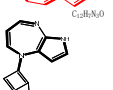
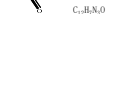
s11-32		7.4786	194.4991	-1.6047	61.4967	277.3735	InChI=1S/C12H7N3O/c16-12-10-9-6-8(14-15(9)12)3-1-2-7-4-5-13-11(7)10/h1-6,13H/b3-1-,7-2-,11-10-
x7-48		13.2181	239.0131	-8.41	15.2593	277.3751	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)9(8)11-12-14-6-15(11)12/h1-6,13H
r-19		17.6553	143.2303	-9.3937	111.7988	277.4144	InChI=1S/C12H7N3O/c16-12-8-6-15(12)9-3-1-2-7-4-5-13-11(7)14-10(8)9/h1-6H,(H,13,14)
p1-37		7.2071	89.4664	-5.3907	166.3174	277.7072	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-8-6-15(9)12(8)14-11/h1-6,13H/b3-1-,7-2-,11-10+
H-109		5.7459	78.967	-2.7912	175.8216	277.8076	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(15(12)14-9)8-4-5-13-11(7)8/h1-6,13H/b7-6-
C-48		12.0928	184.3321	-8.8533	56.4076	278.0940	InChI=1S/C12H7N3O/c16-12-10-7(3-5-14-10)8-2-1-4-13-9-6-15(9)11(8)12/h1-6,14H/b2-1-,13-4-
q-16		4.0725	54.2207	-3.0311	198.4354	278.133	InChI=1S/C12H7N3O/c16-12-11-8-6-15(12)9(14-11)3-1-2-7-4-5-13-10(7)8/h1-6,13H/b2-1-,9-3-
k-38		5.9834	82.1597	-5.3412	179.2775	278.1828	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-8-2-4-14-10(8)9(12)11(7)15/h1-6,14H/b5-1-,13-3+
q11-11		4.0203	117.3499	-3.1354	139.5078	278.3459	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)11(14-9)15(8)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,11-10+
E-24		6.9557	73.431	-3.75	169.2907	278.3973	InChI=1S/C12H7N3O/c16-12-9-6-15(12)14-10-3-1-2-7(9)11-8(10)4-5-13-11/h1-6,13H/b14-10-
E-4		7.475	74.7653	-2.0193	169.1013	278.5342	InChI=1S/C12H7N3O/c16-12-8-6-15-10(8)3-1-2-9(14-15)7-4-5-13-11(7)12/h1-6,13H
o-171		14.0977	195.5782	-8.99	45.8534	278.6145	InChI=1S/C12H7N3O/c16-12-10-2-1-5-15(10)9-3-4-13-11(9)7-6-8(7)14-12/h1-6,13H/b14-8-
s11-55		21.8922	206.0038	-16.5636	46.0932	278.8171	InChI=1S/C12H7N3O/c16-12-14-10-3-1-2-7-4-5-13-11(7)8-6-9(8)15(10)12/h1-6,13H/b3-1-,7-2-,11-8+
p1-25		8.1162	61.4223	-5.4189	173.079	278.8189	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-8-6-15(12)14-11(8)9/h1-6,13H/b3-1-,7-2-,12-10-
F-33		21.934	223.0169	-15.085	21.5659	278.9946	InChI=1S/C12H7N3O/c16-12-10-6-15(10)9-3-1-2-7(9)8-4-5-13-11(8)14-12/h1-6H,(H,13,14,16)/b8-7-
q-61		18.463	188.2292	-11.0039	55.2189	279.568	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9-6-15(9)11(8)14-12/h1-6,13H/b2-1-,8-3-
G1-69		10.2691	189.9755	-7.383	65.1971	279.5942	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15-9(6-14-10)11(7)15/h1-6,13H/b3-1-,7-2-,14-6-
s11-61		24.3443	166.8828	-16.6638	65.5752	279.6296	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)10(12)9-6-15(9)14-8/h1-6,13H/b3-1-,7-2-,11-10+
s11-31		5.307	115.589	-2.8561	149.8005	279.6963	InChI=1S/C12H7N3O/c16-12-10-8-6-14-9(15(8)12)3-1-2-7-4-5-13-11(7)10/h1-6,13H/b2-1-,3-1-,7-2-,9-3-,11-10-

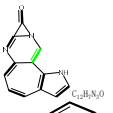
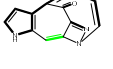
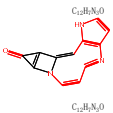
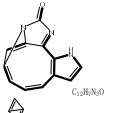
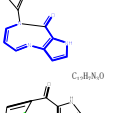
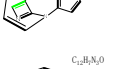
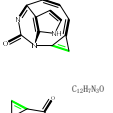
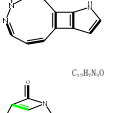
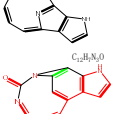
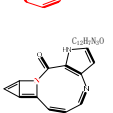
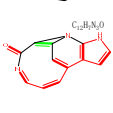
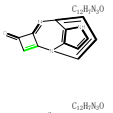
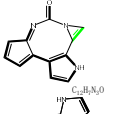
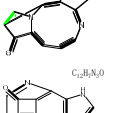
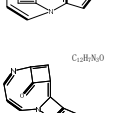
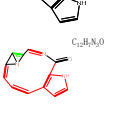
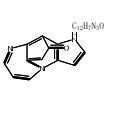


s12-6		6.347	104.381	-5.1005	161.8141	279.8449	InChI=1S/C12H7N3O/c16-12-8-6-9-7(4-5-13-9)2-1-3-10-14-11(8)15(10)12/h1-6,13H/b2-1-,3-1-,7-2-,8-6-,9-6-,10-3+
H1-42		8.1298	128.0553	-3.6113	107.0311	279.8549	InChI=1S/C12H7N3O/c16-12-8-6-7-10(8)13-3-1-5-15(12)9-2-4-14-11(7)9/h1-6,14H/b5-1-,13-3-
I-11		6.5998	138.0683	-5.6709	128.6945	280.115	InChI=1S/C12H7N3O/c16-12-8-6-15(12)11-7(8)2-1-4-13-9-3-5-14-10(9)11/h1-6,14H/b2-1-,4-1-,7-2-,11-10-,13-4-,13-9+
F-35		7.3647	41.5509	-3.1719	201.8181	280.1486	InChI=1S/C12H7N3O/c16-11-6-10-7-2-1-3-9(11)15(10)14-12-8(7)4-5-13-12/h1-6H, (H,13,14)
I-82		18.975	137.0755	-12.4504	99.354	280.4558	InChI=1S/C12H7N3O/c16-12-10-7-6-9(7)15(5-1-3-13-10)8-2-4-14-11(8)12/h1-6,14H/b5-1-,13-3-
H11-41		5.112	76.1242	-2.0431	181.4048	280.7742	InChI=1S/C12H7N3O/c16-12-9-6-15(12)10-3-1-2-7(9)8-4-5-13-11(8)14-10/h1-6H, (H,13,14)
H11-158		8.247	76.1061	-2.777	171.8843	280.7794	InChI=1S/C12H7N3O/c16-11-6-10-9-3-1-2-7(11)8-4-5-13-12(8)15(10)14-9/h1-6,13H/b3-1-,7-2-
H-110		5.564	69.4222	-3.0255	185.0469	280.8484	InChI=1S/C12H7N3O/c16-12-11-8-3-1-2-7(6-15(12)14-11)10-9(8)4-5-13-10/h1-6,13H/b7-6-
A2-7		5.2075	103.292	-1.869	152.6436	281.1129	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-4-13-12(9)15(10)11-8(7)3-5-14-11/h1-6,14H
A2-4		4.2734	92.4946	-1.9569	164.8948	281.1491	InChI=1S/C12H7N3O/c16-12-9-6-15(12)11-10-8(3-5-13-10)7(9)2-1-4-14-11/h1-6,13H/b2-1-,4-1-,7-2-,14-4-,14-11+
A-154		25.7166	218.7105	-10.2464	33.8365	281.1715	InChI=1S/C12H7N3O/c16-12-10-11(12)15-5-1-2-9(15)7-3-4-13-8(7)6-14-10/h1-6,13H/b14-6-
B-178		5.5621	134.3960	-2.8733	125.8273	281.3962	InChI=1S/C12H7N3O/c16-12-9-6-14-10(9)7-2-1-5-15(12)11-8(7)3-4-13-11/h1-6,13H
B-45		7.0862	33.6130	-2.1727	205.4868	281.4349	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-4-13-11)8-2-1-5-15(9)12(10)14-8/h1-6,13H
H11-31		6.3162	68.2397	-4.0796	183.1139	281.4543	InChI=1S/C12H7N3O/c16-12-9-6-15(12)14-10-3-1-2-7(9)8-4-5-13-11(8)10/h1-6,13H/b14-10-
H11-64		5.2526	125.1335	-1.9385	140.5917	281.8557	InChI=1S/C12H7N3O/c16-11-6-9-7-2-1-3-10(15(9)11)14-12-8(7)4-5-13-12/h1-6H, (H,13,14)
D-10		7.4589	118.7892	-2.2445	146.3350	281.9242	InChI=1S/C12H7N3O/c16-12-8-6-13-4-1-2-9-7-3-5-14-10(7)11(8)15(9)12/h1-6,14H/b2-1-,4-1-,8-6-,9-2-,13-4-,13-6-
D-9		6.6261	78.6423	-2.7199	173.8510	282.0449	InChI=1S/C12H7N3O/c16-12-8-6-15(12)9-2-1-4-13-11(8)10-7(9)3-5-14-10/h1-6,14H/b2-1-,4-1-,9-2-,13-4-,13-11-
q1-20		7.1574	124.9421	-4.7741	139.6512	282.2053	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-8-6-15(12)11(8)14-9/h1-6,13H/b2-1-,9-3+
p1-42		18.5858	148.1898	-12.281	110.2526	282.3388	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11(9)15-8-6-14-12(8)15/h1-6,13H

x4-9		19.8651	173.9418	-9.0431	72.3495	282.4306	InChI=1S/C12H7N3O/c16-9-6-14-8-3-1-2-7-4-5-13-10(7)12-11(8)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,12-10-
H-43		9.7589	183.1233	-0.4698	62.8536	282.4359	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)15(9)12(10)14-7/h1-6,13H/b2-1-,9-3-
H1-42		6.1155	147.9819	-3.1386	121.5911	282.4394	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-12(7)15(9)11-6-8(10)14-11/h1-6,13H/b3-1-,9-2-
q11-54		24.1465	219.166	-17.3339	33.4006	282.5366	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8-6-9(8)15(12)14-11/h1-6,13H/b2-1-,8-3-
x4-66		20.1145	175.6835	-9.2798	69.8529	282.7059	InChI=1S/C12H7N3O/c16-12-14-6-8-3-1-2-7-4-5-13-9(7)11-10(8)15(11)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,11-9-
F-19		31.7268	222.4865	-16.9974	32.8786	282.7382	InChI=1S/C12H7N3O/c16-12-8-6-15(12)10(8)3-1-2-9-7-4-5-13-11(7)14-9/h1-6H, (H,13,14)/b2-1-,10-3-
s12-41		18.8176	175.5205	-12.533	71.5772	282.8291	InChI=1S/C12H7N3O/c16-12-14-8-3-1-2-7-4-5-13-9(7)6-10-11(8)15(10)12/h1-6,13H/b3-1-,7-2-,9-6-
r1-37		31.155	161.9261	-15.8418	91.2495	283.181	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)14-8-6-9-11(8)15(9)10/h1-6H, (H,13,14)/b3-1-,7-2-
s11-56		20.2113	138.2119	-5.6082	86.9825	283.3825	InChI=1S/C12H7N3O/c16-12-14-8-3-1-2-7-4-5-13-11(7)10-6-9(8)15(10)12/h1-6,13H/b3-1-,7-2-,11-10-
X22-50		11.9073	182.9028	-5.2772	75.4771	283.4417	InChI=1S/C12H7N3O/c16-12-7-6-15-9(11)(12)15)2-1-4-13-8-3-5-14-10(7)8/h1-6,14H/b2-1-,13-4-
H-71		26.1328	156.0144	-16.6645	101.6278	283.4926	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(7)14-15(12)11-8(9)4-5-13-11/h1-6,13H/b2-1-,9-3-,14-10-
H11-149		6.2858	34.7141	-2.3357	215.1499	283.607	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-6-10(11)15(14-7)12-9(8)4-5-13-12/h1-6,13H/b2-1-,8-3-
q-5		19.9815	175.3068	-1.8891	71.9789	283.6541	InChI=1S/C12H7N3O/c16-10-6-8-9(15-12(10)14-15)3-1-2-7-4-5-13-11(7)8/h1-6,13H
x5-7		36.2137	241.0198	-17.5869	16.5188	283.6602	InChI=1S/C12H7N3O/c16-11-9-6-8-3-1-2-7-4-5-13-12(7)14-15(8)10(9)11/h1-6H, (H,13,14)/b3-1-,7-2-
p-12		11.3561	226.5495	-5.5322	46.7539	283.6822	InChI=1S/C12H7N3O/c16-12-11-14-9-6-8-7(4-5-13-8)2-1-3-10(9)15(11)12/h1-6,13H/b2-1-,3-1-,7-2-,8-6+,9-6+,10-3+
p-11		11.3579	226.5228	-5.5296	46.7439	283.6852	InChI=1S/C12H7N3O/c16-12-11-14-8-3-1-2-7-4-5-13-9(7)6-10(8)15(11)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,9-6+,10-6+
o-255		32.1644	161.3824	-15.8338	96.5502	283.9396	InChI=1S/C12H7N3O/c16-12-14-9-6-8(9)7-2-1-5-15(12)10-3-4-13-11(7)10/h1-6,13H/b14-9-
H-3		32.1635	161.3787	-15.833	96.5467	283.9396	InChI=1S/C12H7N3O/c16-10-2-1-4-13-8-3-5-14-11(8)7-6-9-12(7)15(9)10/h1-6,14H/b2-1-,13-4+
r-22		13.8999	223.3773	-6.2927	50.4139	283.9833	InChI=1S/C12H7N3O/c16-12-10-6-8-9(15(10)12)3-1-2-7-4-5-13-11(7)14-8/h1-6H, (H,13,14)




















q1-30		18,6139	148,5902	-12,3521	109,1813	284,0614	InChI=1S/C12H7N3O/c16-11-8(15-9-6-14-12(9)15)3-1-2-7-4-5-13-10(7)11/h1-6,13H
o-71		5,7086	33,498	-1,789	212,1177	284,1755	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(14-12(7)10)9-3-4-13-11(8)9/h1-6,13H
H-127		29,3564	193,3415	-11,9977	49,7231	284,4018	InChI=1S/C12H7N3O/c16-12-11-10-8(4-5-13-10)9(14-11)3-1-2-7-6-15(7)12/h1-6,13H/b2-1-,9-3-
H-50		26,3107	171,2122	-12,454	82,3967	284,5098	InChI=1S/C12H7N3O/c16-12-11-8-6-7(8)10-9(2-4-14-10)15(12)5-1-3-13-11/h1-6,14H
p1-44		17,0289	173,0059	-11,6986	83,094	284,6302	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)12-11(8)14-9-6-15(9)12/h1-6,13H/b3-1-,7-2-,12-10-
s12-35		10,6871	182,9374	-3,5507	86,6145	284,8534	InChI=1S/C12H7N3O/c16-12-8-6-9-7(4-5-13-9)2-1-3-10-14-11(8)15(10)12/h1-6,13H/b2-1-,3-1-,7-2-,8-6-,9-6-,10-3+
H-77		4,5077	121,8012	-1,0678	133,9233	284,8888	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-14-11(15(7)12)10-8(9)4-5-13-10/h1-6,13H
I-32		24,9057	232,3668	-8,9476	19,8525	284,8904	InChI=1S/C12H7N3O/c16-12-9-8-6-13-3-1-5-15(8)7-2-4-14-11(7)10(9)12/h1-6,14H
G-29		24,1763	197,8558	-10,9561	60,9463	285,5162	InChI=1S/C12H7N3O/c16-12-10-3-1-2-8-7-4-5-13-9(7)6-14-11(8)15(10)12/h1-6,13H
H-91		24,6936	204,8164	-6,1077	40,7249	285,7901	InChI=1S/C12H7N3O/c16-12-11-9(4-5-13-11)8-3-1-2-7(8)6-10-14-15(10)12/h1-6,13H/b7-6-
H-68		7,5599	36,4479	-2,742	211,7965	285,8006	InChI=1S/C12H7N3O/c16-10-8-3-1-2-7-6-15(12(10)14-7)11-9(8)4-5-13-11/h1-6,13H/b2-1-,8-3-
H1-119		19,4506	160,2801	-7,126	90,6457	285,8536	InChI=1S/C12H7N3O/c16-11-3-1-2-10-7-4-5-13-8(7)6-9-12(14-9)15(10)11/h1-6,13H
D-13		7,7136	148,1636	-1,6579	104,7636	286,0760	InChI=1S/C12H7N3O/c16-12-8-6-15-9(2-1-4-14-12)7-3-5-13-10(7)11(8)15/h1-6,14H/b2-1-,14-4+
C-68		21,1280	242,3229	-16,6603	16,0694	286,1138	InChI=1S/C12H7N3O/c16-12-10-7(3-5-13-10)8(2-1-4-14-12)11-9-6-15(9)11/h1-6,13H/b2-1-,11-8-,14-4+
H-7		33,7945	117,9504	-13,625	118,2906	286,2965	InChI=1S/C12H7N3O/c16-10-2-1-4-13-7-3-5-14-12(7)11-8-6-9(11)15(8)10/h1-6,14H/b2-1-,13-4+
k-17		6,0656	51,6611	-4,8573	212,9572	286,6337	InChI=1S/C12H7N3O/c16-12-9-6-7-10-8(2-4-14-10)13-3-1-5-15(9)11(7)12/h1-6,14H/b5-1-,13-3-
x4-30		11,2802	211,0477	-5,3628	46,4336	286,6464	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)10-11(12)15(10)6-14-8/h1-6,13H/b2-1-,8-3+
I-2		6,0242	48,2635	-5,1651	209,3984	286,6912	InChI=1S/C12H7N3O/c16-12-7-6-15-9(7)2-1-4-13-8-3-5-14-10(8)11(12)15/h1-6,14H/b4-1-,9-2-,11-10-,13-8-
B-22		5,4204	104,2680	-1,4774	157,9607	286,9300	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(10)12(9)14-11-8(7)3-4-13-11/h1-6,13H

















B-221		6.5173	31.6942	-1.7927	212.9590	286.9998	InChI=1S/C12H7N3O/c16-10-9-6-15-5-1-2-7(9)8-3-4-13-11(8)14-12(10)15/h1-6,13H
	$C_{12}H_7N_3O$						
H11-115		7.6332	128.7719	-1.1949	120.0252	287.0608	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-7-4-5-13-9(7)6-11(12)15(10)14-8/h1-6,13H
	$C_{12}H_7N_3O$						
J-22		19.7783	191.6137	-13.2327	68.5785	287.1839	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-9(8)6-10-11(7)15(10)12/h1-6,14H/b2-1-,4-1-,7-2-,9-6-,10-6-,13-4-,13-8+
	$C_{12}H_7N_3O$						
A-161		13.2003	176.6799	-5.2391	62.1327	287.295	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-10(11)12(15)14-6-9-7(8)3-4-13-9/h1-6,13H/b14-6-
	$C_{12}H_7N_3O$						
I-105		16.8959	178.7622	-12.945	73.9829	287.5264	InChI=1S/C12H7N3O/c16-12-10-9(2-4-14-10)15-5-1-3-13-8-6-7(8)11(12)15/h1-6,14H/b5-1-,11-7-,13-3-
	$C_{12}H_7N_3O$						
B-161		4.6252	104.7459	-1.6566	157.4616	287.6029	InChI=1S/C12H7N3O/c16-12-9-6-14-11-8(2-1-5-15(11)12)7-3-4-13-10(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
A1-37		8.0578	183.4658	-5.5308	68.5642	287.8516	InChI=1S/C12H7N3O/c16-12-8-2-1-4-13-6-15-10(11(12)15)9-7(8)3-5-14-9/h1-6,14H/b4-1-,8-2-,13-6-
	$C_{12}H_7N_3O$						
H11-88		4.6197	123.2683	-1.0363	135.6416	287.979	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-14-6-9(15(10)12)11-7(8)4-5-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
s11-64		18.5167	147.6865	-12.5738	96.2652	288.0306	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8(14-12)9-6-15(9)11/h1-6,13H/b3-1-,7-2-,11-10-
	$C_{12}H_7N_3O$						
A-110		13.6224	171.2839	-3.7172	76.226	288.1044	InChI=1S/C12H7N3O/c16-12-10-9-6-14-15(12)5-1-2-7(9)8-3-4-13-11(8)10/h1-6,13H/b5-1-,7-2-
	$C_{12}H_7N_3O$						
C-27		22.5306	196.0763	-9.7045	67.1223	288.3716	InChI=1S/C12H7N3O/c16-12-10-6-9-7(3-5-13-9)8-2-1-4-14-11(8)15(10)12/h1-6,13H
	$C_{12}H_7N_3O$						
x3-15		7.8575	102.2105	-2.1166	146.8784	288.5054	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-11(12)9(7)10-8(15)2-4-14-10/h1-6,14H/b5-1-,13-3-
	$C_{12}H_7N_3O$						
n-196		8.5974	198.7193	-6.8282	68.6978	288.5113	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(11(7)10)9-3-4-13-8(9)6-14-12/h1-6,13H/b14-6-
	$C_{12}H_7N_3O$						
F-49		10.1085	136.7281	-4.3294	119.4384	288.7137	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(9)15(12)14-11-8(7)4-5-13-11/h1-6H,13,14
	$C_{12}H_7N_3O$						
B-210		9.5604	52.6997	-1.7961	194.9800	288.7293	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-9(12)11(14-15)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-
	$C_{12}H_7N_3O$						
B-161		7.0404	158.9899	-1.9899	103.8464	288.9494	InChI=1S/C12H7N3O/c16-12-11-9-6-7(2-1-5-15(12)14-11)8-3-4-13-10(8)9/h1-6,13H/b5-1-,7-2+
	$C_{12}H_7N_3O$						
q-25		12.3965	226.0416	-4.1159	47.6053	288.9612	InChI=1S/C12H7N3O/c16-12-11-14-6-8-9(15(11)12)3-1-2-7-4-5-13-10(7)8/h1-6,13H
	$C_{12}H_7N_3O$						
H11-71		5.9359	135.2562	-1.5825	138.6355	288.9812	InChI=1S/C12H7N3O/c16-11-6-10-8-2-1-3-9(15(10)11)7-4-5-13-12(7)14-8/h1-6H,13,14
	$C_{12}H_7N_3O$						
G-47		7.0575	39.1919	-2.9015	209.7581	289.1149	InChI=1S/C12H7N3O/c16-12-9-6-14-15(12)10-3-1-2-7(9)8-4-5-13-11(8)10/h1-6,13H
	$C_{12}H_7N_3O$						

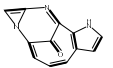
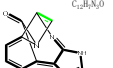
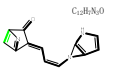
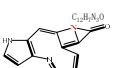
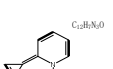
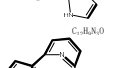
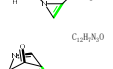
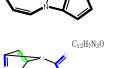
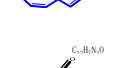
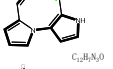
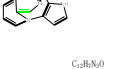
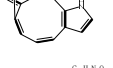
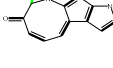
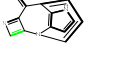
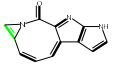

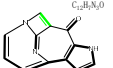
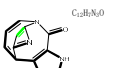
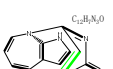
B-229		17.6381	171.6536	-12.6392	86.4873	289.1327	InChI=1S/C12H7N3O/c16-12-9-6-15(9)5-1-2-8-7-3-4-13-10(7)11(12)14-8/h1-6,13H/b5-1-,8-2-
B-160		7.7494	35.2983	-2.4813	207.1461	289.1777	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-5-15(9)11(14-12)10-8(7)3-4-13-10/h1-6,13H
H11-128		21.8027	140.4274	-11.416	107.0879	289.2247	InChI=1S/C12H7N3O/c16-11-7-2-1-3-9(11)14-10-6-15(10)12-8(7)4-5-13-12/h1-6,13H/b14-9-
r-61		15.0662	261.0521	-13.0769	20.8317	289.2957	InChI=1S/C12H7N3O/c16-12-14-11-7(4-5-13-11)2-1-3-9-8-6-10(8)15(9)12/h1-6H,10,13,14,16/h3-1-,7-2-
p1-58		6.0689	98.6288	-3.448	159.6167	289.4837	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)8-6-10-14-12(9)15(8)10/h1-6,13H/b3-1-,7-2-,11-8+
X23-18		12.588	150.9674	-6.6538	122.0965	289.6586	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-4-13-9-3-5-14-10(9)11(8)15(7)12/h1-6,14H/b2-1-,4-1-,7-2-,11-10-,13-4-,13-9-
o-247		5.3963	29.0694	-2.2083	218.5866	289.7053	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(9)8-3-4-13-12(8)11(7)14-10/h1-6,13H
H1-12		13.6232	233.6199	-3.5258	33.2125	289.7779	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)14-11(7)9-6-15(9)10/h1-6,13H/b3-1-,7-2-
H-75		7.3619	99.6933	-1.7569	149.2065	289.913	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(14-15(7)12)11-8(9)4-5-13-11/h1-6,13H
A2-28		7.0864	79.7175	-2.6946	178.7574	290.0521	InChI=1S/C12H7N3O/c16-12-8-6-15(12)9-2-1-4-13-11(8)10-7(9)3-5-14-10/h1-6,14H/b2-1-,4-1-,9-2-,13-4-,13-11-
H1-8		5.3078	110.2044	-1.5256	154.5449	290.3109	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)9-6-15(10)14-12(7)9/h1-6,13H/b3-1-,7-2-
n-154		8.1594	107.1358	-2.5207	139.1281	290.5949	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-12(9)14-6-8(7)10(11)15/h1-6,13H
A1-27		14.3706	228.9544	-4.5298	46.8009	290.6989	InChI=1S/C12H7N3O/c16-12-10-9-6-13-4-1-2-7(9)8-3-5-14-11(8)15(10)12/h1-6,14H
H1-137		28.0223	129.3267	-12.569	116.8018	290.7083	InChI=1S/C12H7N3O/c16-9-3-1-2-8(7-4-5-13-12(7)9)15-10-6-11(15)14-10/h1-6,13H
B-112		6.1615	85.8902	-2.8633	173.4481	290.7209	InChI=1S/C12H7N3O/c16-12-14-9-6-10-11-8(3-4-13-11)7(9)2-1-5-15(10)12/h1-6,13H/b5-1-,7-2-
x6-38		32.714	141.7503	-11.8596	89.7757	290.8523	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-15-11-10(9)12(15)14-11/h1-6,13H/b3-1-,7-2-,8-6+
n-148		10.9952	191.2585	-7.7524	66.347	290.8549	InChI=1S/C12H7N3O/c16-12-10-9(3-4-13-10)15-5-1-2-7-8(6-14-12)11(7)15/h1-6,13H/b14-6-
x5-8		32.9039	213.5949	-11.9245	41.9265	290.8942	InChI=1S/C12H7N3O/c16-11-9-8-3-1-2-7-4-5-13-12(7)14-15(6-8)10(9)11/h1-6H,10,13,14/h3-1-,7-2-
I-29		25.5735	153.7118	-13.6396	104.3575	290.9358	InChI=1S/C12H7N3O/c16-11-7-6-9(10(7)11)15-5-1-3-13-12-8(15)2-4-14-12/h1-6,14H














q-24		10.4092	230.6242	-3.5182	46.8936	290.9757	InChI=1S/C12H7N3O/c16-12-11-14-9-3-1-2-7-4-5-13-10(7)8(9)6-15(11)12/h1-6,13H
B-141		9.2282	78.8221	-2.9975	171.0734	291.0696	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-10(11)(12)14-15)6-9-7(8)3-4-13-9/h1-6,13H/b5-1-,8-2-
x2-14		44.4644	189.6656	-18.4986	61.9548	291.2005	InChI=1S/C12H7N3O/c16-12-10-9-6-8-7(2-4-14-8)13-3-1-5-15(9)11(10)12/h1-6,14H/b5-1-,9-6-,13-3+
q11-43		4.5044	158.3045	-3.3019	117.2972	291.3085	InChI=1S/C12H7N3O/c16-12-14-11-9-6-8(15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,8-3-
k1-17		17.9319	229.4727	-21.3013	50.107	291.3448	InChI=1S/C12H7N3O/c16-12-10-9(2-4-14-10)13-3-1-5-15(12)11-7-6-8(7)11/h1-6,14H/b5-1-,13-3+
o-141		3.5206	88.0862	-1.9453	174.5027	291.3469	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(12-8(7)6-14-12)9-3-4-13-10(9)11/h1-6,13H
E-71		20.6928	187.4377	-12.484	74.5703	291.4551	InChI=1S/C12H7N3O/c16-12-14-9-3-1-2-7-6-10(7)15(12)11-8(9)4-5-13-11/h1-6,13H/b3-1-,7-2-
C-8		12.3938	217.1513	-7.1334	47.6213	291.5055	InChI=1S/C12H7N3O/c16-12-9-6-15(9)14-4-1-2-7-8-3-5-13-11(8)10(7)12/h1-6,13H/b2-1-,14-4-
H-25		9.9046	139.9782	-6.6209	126.5344	291.6181	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-10(8)11(14-9)15(12)6-7/h1-6,13H/b2-1-,9-3-
X-50		12.2879	210.9911	-4.7381	48.8809	291.6769	InChI=1S/C12H7N3O/c16-12-14-4-1-2-7-6-9-11(15(9)12)10-8(7)3-5-13-10/h1-6,13H/b2-1-,14-4-
X22-20		13.7344	258.0083	-12.7329	24.775	291.9741	InChI=1S/C12H7N3O/c16-12-11-8(3-5-14-11)13-4-1-2-9-7-6-10(7)15(9)12/h1-6,14H/b2-1-,13-4-
X-45		6.3093	205.6155	-3.6019	61.8586	292.2587	InChI=1S/C12H7N3O/c16-12-10-9-6-7(2-1-4-14-12)8-3-5-13-11(8)15(9)10/h1-6,13H/b2-1-,14-4-
o-80		3.4822	86.4737	-2.0468	177.6747	292.6788	InChI=1S/C12H7N3O/c16-10-6-9-12(10)14-7-2-1-5-15(9)8-3-4-13-11(7)8/h1-6,13H
H11-6		7.683	268.4263	-4.4179	8.4085	292.7019	InChI=1S/C12H7N3O/c16-12-14-9-3-1-2-7(9)8-4-5-13-11(8)10-6-15(10)12/h1-6,13H/b14-9-
I-5		8.7978	65.3071	-5.46	186.1112	292.7397	InChI=1S/C12H7N3O/c16-12-7-6-15-9(12)2-1-4-13-8-3-5-14-10(8)11(7)15/h1-6,14H/b4-1-,9-2-,11-10-,13-8-
I-69		3.2079	84.4988	-1.3605	180.5918	292.7656	InChI=1S/C12H7N3O/c16-9-6-8-10(9)12-11-7(2-4-14-11)15(8)5-1-3-13-12/h1-6,14H/b5-1-,13-3-
I-21		8.6576	135.6167	-3.0317	122.9783	292.8707	InChI=1S/C12H7N3O/c16-12-7-6-8(12)13-3-1-5-15-9-2-4-14-10(9)11(7)15/h1-6,14H/b5-1-,11-7-,13-3-
x9-28		21.1302	210.026	-17.2398	39.0098	292.9666	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-11-9(6-14-12)15(8)11/h1-6,13H/b2-1-,8-3-,14-6-
I-71		5.6294	40.2371	-2.3325	217.4854	293.0702	InChI=1S/C12H7N3O/c16-9-6-8-12-10(9)11-7(2-4-14-11)15(8)5-1-3-13-12/h1-6,14H




















H1-32		5, 1603	103, 2288	-2, 081	154, 662	293, 0743	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15-6-9(7)11(10)14-15/h1-6, 13H
	$C_{12}H_7N_3O$						
B-260		8, 5683	248, 1879	-4, 7627	9, 9399	293, 0793	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)7-2-1-5-15-6-9(15)14-11(7)12/h1-6, 13H/h5-1-, 7-2-, 14-11+
	$C_{12}H_7N_3O$						
s12-21		31, 2077	201, 4535	-12, 3343	61, 8444	293, 1498	InChI=1S/C12H7N3O/c16-12-10-11(12)15-6-8-7(4-5-13-8)2-1-3-9(15)14-10/h1-6, 13H/h3-1-, 7-2-, 8-6+
	$C_{12}H_7N_3O$						
H-74		4, 5634	182, 402	-1, 5605	91, 6426	293, 5195	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-14-10(7)15(12)11-8(9)4-5-13-11/h1-6, 13H/h2-1-, 9-3-
	$C_{12}H_7N_3O$						
B-145		5, 7368	101, 1529	-1, 7681	166, 8863	293, 6345	InChI=1S/C12H7N3O/c16-12-14-11-8-2-1-5-15(12)10(11)6-9-7(8)3-4-13-9/h1-6, 13H
	$C_{12}H_7N_3O$						
H11-159		7, 9901	79, 6953	-2, 4983	187, 9395	293, 6772	InChI=1S/C12H7N3O/c16-9-6-11-14-10-3-1-2-7(9)8-4-5-13-12(8)15(10)11/h1-6, 13H/h3-1-, 7-2-
	$C_{12}H_7N_3O$						
B-93		11, 8470	251, 6173	-6, 7214	21, 8394	293, 7612	InChI=1S/C12H7N3O/c16-12-14-9-6-8(9)11-7(3-4-13-11)10-2-1-5-15(10)12/h1-6, 13H/h14-9-
	$C_{12}H_7N_3O$						
X23-34		32, 0489	216, 5674	-11, 9538	47, 1326	293, 7919	InChI=1S/C12H7N3O/c16-11-9-7-2-1-4-13-8-3-5-14-12(8)15(6-7)10(9)11/h1-6, 14H/h2-1-, 13-4+
	$C_{12}H_7N_3O$						
s11-30		6, 4487	54, 9346	-3, 9252	200, 778	293, 8397	InChI=1S/C12H7N3O/c16-12-8-6-15-9(14-12)3-1-2-7-4-5-13-10(7)11(8)15/h1-6, 13H/h3-1-, 7-2-, 11-10+
	$C_{12}H_7N_3O$						
o-121		10, 0241	58, 1264	-1, 8532	187, 3662	294, 0756	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-2-8(12)14-10(7)11-9(15)3-4-13-11/h1-6, 13H/h5-1-, 8-2+
	$C_{12}H_7N_3O$						
x9-40		11, 7677	234, 6095	-7, 7937	34, 9084	294, 0771	InChI=1S/C12H7N3O/c16-11-8(10-12-14-6-15(10)12)3-1-2-7-4-5-13-9(7)11/h1-6, 13H
	$C_{12}H_7N_3O$						
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	$C_{12}H_7N_3O$						
X-5		44, 5570	257, 0095	-25, 6236	4, 6138	294, 1319	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)14-4-1-2-7-6-9-8(7)3-5-13-9/h1-6, 13H/h2-1-, 14-4-
	$C_{12}H_7N_3O$						
s11-44		8, 3999	158, 6513	-2, 1565	119, 9889	294, 2659	InChI=1S/C12H7N3O/c16-10-6-9-8-3-1-2-7-4-5-13-11(7)12(14-8)15(9)10/h1-6, 13H/h2-1-, 3-1-, 7-2-, 8-3-, 12-11-
	$C_{12}H_7N_3O$						
H11-10		8, 1236	108, 6759	-1, 3066	148, 7546	294, 3151	InChI=1S/C12H7N3O/c16-12-14-7-2-1-3-9-8-4-5-13-11(8)10(6-7)15(9)12/h1-6, 13H/h2-1-, 9-3-
	$C_{12}H_7N_3O$						
A-4		8, 3685	102, 7647	-2, 0791	161, 61	294, 4907	InChI=1S/C12H7N3O/c16-9-6-14-12-10(9)7-2-1-5-15(12)11-8(7)3-4-13-11/h1-6, 13H
	$C_{12}H_7N_3O$						
H11-137		44, 0623	184, 3229	-25, 3071	79, 0991	294, 5293	InChI=1S/C12H7N3O/c16-10-6-8(10)14-11-3-1-2-9-7-4-5-13-12(7)15(9)11/h1-6, 13H/h14-11+
	$C_{12}H_7N_3O$						
o-185		6, 644	92, 8431	-2, 3819	160, 0428	294, 5434	InChI=1S/C12H7N3O/c16-11-8-6-7-2-1-5-15(12(8)14-7)9-3-4-13-10(9)11/h1-6, 13H
	$C_{12}H_7N_3O$						
o-117		5, 372	37, 4698	-1, 98	221, 4925	294, 6236	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-10(9)8(11)6-14-12(7)15/h1-6, 13H
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













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B-188		9, 3533	41, 4057	-1, 9806	210, 8432	294, 9903	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-9(11)6-14-12(15)10-7(8)3-4-13-10/h1-6, 13H
H1-130		20, 2525	207, 9265	-14, 8336	78, 2157	294, 994	InChI=1S/C12H7N3O/c16-11(15-9-6-10(15)14-9)3-1-2-7-8-4-5-13-12(7)8/h1-6, 13H/b3-1-, 7-2-
q11-49		21, 6102	144, 0373	-14, 364	106, 7932	295, 1502	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(14-12)15-6-9(8)15/h1-6, 13H/b2-1-, 8-3-
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G-73		8, 8233	109, 9891	-2, 3756	157, 3214	295, 4664	InChI=1S/C12H7N3O/c16-10-6-14-12-8-2-1-3-9(15(10)12)11-7(8)4-5-13-11/h1-6, 13H
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B-153		6, 8672	111, 3130	-2, 0928	147, 8142	295, 5493	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-5-15(12)14-11(9)10-8(7)3-4-13-10/h1-6, 13H/b5-1-, 7-2+
o-73		14, 7205	145, 1396	-11, 8205	125, 4861	295, 7119	InChI=1S/C12H7N3O/c16-10-6-8-7(11(10)14-8)2-1-5-15-9-3-4-13-12(9)15/h1-6, 13H/b5-1-, 7-2+
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A2-13		20, 824	220, 0057	-8, 6841	58, 4345	296, 2445	InChI=1S/C12H7N3O/c16-12-11-14-4-1-2-8-7-3-5-13-9(7)6-10(8)15(11)12/h1-6, 13H/b4-1-, 8-2-, 14-11-
o-52		14, 4828	144, 5772	-12, 0062	125, 3053	296, 3553	InChI=1S/C12H7N3O/c16-11-7-6-9(11)14-8(7)2-1-5-15-10-3-4-13-12(10)15/h1-6, 13H/b5-1-, 8-2+
X22-14		15, 6579	225, 0955	-14, 8935	53, 1926	296, 3706	InChI=1S/C12H7N3O/c16-12-8-6-7(8)10-2-1-4-13-9-3-5-14-11(9)15(10)12/h1-6, 14H/b2-1-, 13-4+
A2-48		7, 0453	103, 9001	-2, 187	147, 9216	296, 5383	InChI=1S/C12H7N3O/c16-11-8-6-15-9(2-1-4-14-12(8)15)7-3-5-13-10(7)11/h1-6, 13H


















H-113		12.0377	127.6125	-4.5764	131.5908	296.6551	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7(6-8)9-4-5-13-11(9)15(12)14-10/h1-6,13H
I-21		17.2459	136.032	-6.9574	135.4018	296.6672	InChI=1S/C12H7N3O/c16-12-10-7-6-15(12)9(7)2-1-4-13-8-3-5-14-11(8)10/h1-6,14H/b4-1-,9-2-,11-10-,13-8+
H11-110		24.8109	142.9468	-15.4294	109.1981	296.8875	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)9-3-1-2-8(14-12)10-6-15(9)10/h1-6,13H
H1-99		18.486	175.116	-1.9853	89.0687	297.0752	InChI=1S/C12H7N3O/c16-7-2-1-3-8-9-4-5-13-11(9)15-12(14-15)10(8)6-7/h1-6,13H
H11-54		6.6152	75.7646	-3.6273	193.0825	297.1153	InChI=1S/C12H7N3O/c16-12-8-6-15(12)10-3-1-2-9(8)14-11-7(10)4-5-13-11/h1-6H, (H, 13, 14)
H1-64		6.1788	108.2245	-2.7994	153.7978	297.1289	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)9-6-10(7)15(11)14-9/h1-6,13H
C-34		21.6078	203.4406	-10.1791	48.4315	297.1846	InChI=1S/C12H7N3O/c16-12-9-6-15(9)11-8(2-1-4-14-12)7-3-5-13-10(7)11/h1-6,13H/b2-1-,14-4+
A-105		5.5083	162.3974	-1.7363	108.8302	297.2877	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-9(6-14-15)10(12)11-7(8)3-4-13-11/h1-6,13H/b5-1-,8-2-,10-9-
B-95		19.5405	191.1884	-14.4006	81.6326	297.2948	InChI=1S/C12H7N3O/c16-12-14-10-6-9(10)7-2-1-5-15(12)11-8(7)3-4-13-11/h1-6,13H/b14-10-
o-114		9.6353	39.2994	-1.9162	214.1047	297.428	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-10-3-4-13-11(10)8(12)6-9(7)14-15/h1-6,13H
F-53		6.7207	125.6429	-1.9378	135.9501	297.434	InChI=1S/C12H7N3O/c16-12-7-2-1-3-8-9-4-5-13-11(9)14-15(12)10(8)6-7/h1-6H, (H, 13, 14)
H-138		6.2768	44.9232	-1.9508	221.8401	297.4528	InChI=1S/C12H7N3O/c16-12-11-10-8(4-5-13-10)9-3-1-2-7(14-11)6-15(9)12/h1-6,13H
A1-45		10.1659	229.8211	-4.8325	47.6967	297.5411	InChI=1S/C12H7N3O/c16-11-7-2-1-4-13-6-9-10(11)15(9)12-8(7)3-5-14-12/h1-6,14H/b4-1-,7-2-,13-6-
H11-121		9.0685	155.9967	-2.2475	111.702	297.5727	InChI=1S/C12H7N3O/c16-11-8-2-1-3-10-7-4-5-13-12(7)15(10)6-9(11)14-8/h1-6,13H/b2-1-,9-6-,10-3-
B-258		6.9446	99.3367	-1.8167	161.2175	297.5977	InChI=1S/C12H7N3O/c16-12-11-10-8(3-4-13-10)7-2-1-5-15(12)6-9(7)14-11/h1-6,13H
n-212		14.4712	204.7823	-5.8267	60.1729	297.607	InChI=1S/C12H7N3O/c16-12-14-6-8-7-2-1-5-15(12)9-3-4-13-11(9)10(7)8/h1-6,13H/b5-1-,7-2+,14-6-
B-94		17.4231	186.9124	-11.2809	81.3505	297.7857	InChI=1S/C12H7N3O/c16-12-11-8(3-4-13-11)7-2-1-5-15(12)14-10-6-9(7)10/h1-6,13H/b5-1-,7-2+,14-10-
o-28		6.0495	58.9995	-3.1459	200.0194	297.9848	InChI=1S/C12H7N3O/c16-12-8-6-9-10(3-4-13-9)15-5-1-2-7(8)11(12)14-15/h1-6,13H/b8-6+
F-48		9.6974	99.1846	-3.2244	160.3447	297.9965	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-8-4-5-13-11(8)14-15(12)6-10(7)9/h1-6H, (H, 13, 14)




















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F-65		6, 4299	73, 3604	-3, 8282	207, 4953	298, 0671	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-9(6-15(10)12)14-11-7(8)4-5-13-11/h1-6H, 13H/b5-1-, 7-2+
o-116		14, 6332	144, 5564	-11, 9185	127, 9342	298, 4505	InChI=1S/C12H7N3O/c16-11-7(8-6-9(11)14-8)2-1-5-15-10-3-4-13-12(10)15/h1-6, 13H/b5-1-, 7-2+
X22-28		16, 5132	233, 4715	-9, 9173	51, 8886	298, 5332	InChI=1S/C12H7N3O/c16-12-11-7-2-1-4-13-8-3-5-14-9(8)6-10(7)15(11)12/h1-6, 14H/b2-1-, 10-6+, 13-4+
A-85		2, 4687	293, 7689	-2, 0948	5, 3058	298, 8915	InChI=1S/C12H9N3O/c16-12(9-4-3-6-13-9)15-7-2-1-5-11(15)10-8-14-10/h1-8, 13H/b11-10-
H11-118		11, 7533	210, 0306	-3, 943	57, 4536	298, 9313	InChI=1S/C12H7N3O/c16-12-11-9-3-1-2-8(14-9)7-4-5-13-12(7)15-6-10(11)15/h1-6, 13H
n-163		5, 9784	162, 5785	-0, 4543	107, 9834	298, 9669	InChI=1S/C12H7N3O/c16-12-7-6-14-8(12)2-1-5-15-9-3-4-13-10(9)11(7)15/h1-6, 13H/b5-1-, 8-2+, 11-7-
q1-39		13, 4721	101, 0377	-6, 867	175, 6205	299, 0417	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)2-1-3-8-9-6-10(14-8)15(9)12/h1-6, 13H/b2-1-, 8-3+
n-52		32, 3312	225, 7906	-11, 1171	25, 967	299, 3202	InChI=1S/C12H7N3O/c16-12-9-10-8(3-4-13-10)15-5-1-2-7(15)6-14-11(9)12/h1-6, 13H/b14-6-
o-16		5, 3588	39, 2434	-1, 7954	221, 4673	299, 4435	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-10(8)11(12)14-6-9(7)15/h1-6, 13H
q11-60		6, 0429	116, 2057	-3, 3222	166, 5322	299, 5979	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-14-9(6-8)15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3-, 11-10+
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x6-32		27, 7306	241, 9086	-15, 1481	23, 528	299, 9921	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-11-12(14-10)15(9)11/h1-6, 13H/b3-1-, 7-2-, 8-6+, 14-12-
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B-142		20, 5455	216, 7082	-7, 8283	46, 5778	300, 2691	InChI=1S/C12H7N3O/c16-12-11(14-12)10-6-8-7(3-4-13-8)9-2-1-5-15(9)10/h1-6, 13H


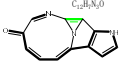

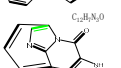


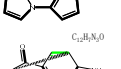
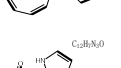
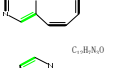
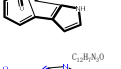

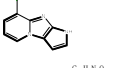
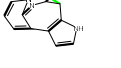

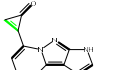




r-44		9.1747	111.8845	-4.6926	152.6189	300.3489	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-11(7)14-15(12)9(10)6-8/h1-6H, (H, 13, 14)/b3-1-, 7-2-
	$C_{12}H_7N_3O$						
r-39		15.2313	161.1512	-8.4927	115.6467	300.4079	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-11(7)14-15(12)6-9(8)10/h1-6H, (H, 13, 14)/b3-1-, 7-2-
	$C_{12}H_7N_3O$						
H1-38		20.842	169.4887	-11.5396	85.1789	300.9023	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-12(7)14-11(10)9-6-15(8)9/h1-6, 13H/b3-1-, 8-2-
	$C_{12}H_7N_3O$						
B-143		7.9237	116.0139	-4.2187	153.4215	301.0019	InChI=1S/C12H7N3O/c16-12-11-10-6-9-7(3-4-13-9)8(14-11)2-1-5-15(10)12/h1-6, 13H/b5-1-, 8-2?
	$C_{12}H_7N_3O$						
A-112		2.5761	304.6855	-2.3943	-4.24	301.0355	InChI=1S/C12H7N3O/c16-12-10(8-6-14-8)11-7(3-4-13-11)9-2-1-5-15(9)12/h1-6, 13H/b14-8+
	$C_{12}H_7N_3O$						
o-125		3.4669	90.7347	-2.1484	184.6101	301.1951	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(12-8(11)6-14-12)9-3-4-13-10(7)9/h1-6, 13H
	$C_{12}H_7N_3O$						
x4-3		6.4604	41.5972	-5.2892	223.7605	301.4445	InChI=1S/C12H7N3O/c16-9-6-14-15-8-3-1-2-7-4-5-13-11(7)12(15)10(8)9/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 12-11+
	$C_{12}H_7N_3O$						
H11-148		13.8732	128.2455	-11.2374	135.8671	301.4773	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(14-15-6-10(12)15)11-7(8)4-5-13-11/h1-6, 13H/b14-9+
	$C_{12}H_7N_3O$						
C-2		40.2315	253.1360	-17.3688	11.6605	301.5344	InChI=1S/C12H7N3O/c16-10-6-9(10)15-12-8(2-1-4-14-15)7-3-5-13-11(7)12/h1-6, 13H
	$C_{12}H_7N_3O$						
r-34		8.8097	161.6291	-2.6475	124.8409	301.6949	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)14-10-6-9(8)15(10)12/h1-6H, (H, 13, 14)
	$C_{12}H_7N_3O$						
X22-47		19.6785	189.6369	-14.7218	89.7401	301.9421	InChI=1S/C12H7N3O/c16-12-9-6-15(9)8-2-1-4-13-7-3-5-14-11(7)10(8)12/h1-6, 14H/b2-1-, 4-1-, 8-2+, 11-10-, 13-4-, 13-7-
	$C_{12}H_7N_3O$						
s11-35		6.8559	133.6553	-4.6747	135.9639	302.0117	InChI=1S/C12H7N3O/c16-12-8-6-10-9(14-15(10)12)3-1-2-7-4-5-13-11(7)8/h1-6, 13H/b3-1-, 7-2-, 11-8-
	$C_{12}H_7N_3O$						
H1-58		4.9507	43.5491	-1.7905	221.3928	302.2293	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)12-8(10)6-15(9)14-12/h1-6, 13H/b3-1-, 9-2-
	$C_{12}H_7N_3O$						
s12-17		40.5849	173.1501	-25.5486	87.8927	302.2481	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)14-8-3-1-2-7-4-5-13-9(7)6-8/h1-6, 13H/b14-8+
	$C_{12}H_7N_3O$						
x9-3		20.3066	195.0032	-16.5436	60.362	302.4612	InChI=1S/C12H7N3O/c16-9-6-14-12-11-8(15(11)12)3-1-2-7-4-5-13-10(7)9/h1-6, 13H/b2-1-, 8-3-, 14-6-
	$C_{12}H_7N_3O$						
H1-40		7.4167	152.8202	-1.2914	121.3212	302.5034	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)15-10(7)6-9(11)14-15/h1-6, 13H/b3-1-, 7-2-
	$C_{12}H_7N_3O$						
n-127		11.1374	219.357	-3.7543	51.0967	302.5613	InChI=1S/C12H7N3O/c16-9-6-14-11-7-2-1-5-15(9)8-3-4-13-12(8)10(7)11/h1-6, 13H/b5-1-, 7-2-, 14-6-
	$C_{12}H_7N_3O$						
B-83		7.5012	37.0390	-2.2485	218.6705	302.5676	InChI=1S/C12H7N3O/c16-12-10-6-9-7(2-1-5-15(10)14-9)8-3-4-13-11(8)12/h1-6, 13H
	$C_{12}H_7N_3O$						
X22-54		19.2882	188.397	-14.5791	91.3053	302.646	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-10(8)11(7)15-6-9(12)15/h1-6, 14H/b2-1-, 4-1-, 7-2+, 11-10-, 13-4-, 13-8-
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
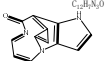




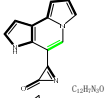





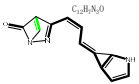




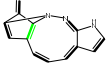

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H11-96	 $C_{12}H_7N_3O$	7.3353	41.4689	-3.0228	221.087	302.8328	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-9(6-15(12)14-10)11-7(8)4-5-13-11/h1-6,13h/b3-1-,8-2-
s11-63	 $C_{12}H_7N_3O$	20.0209	138.1235	-13.7646	115.304	302.8552	InChI=1S/C12H7N3O/c16-12-10-8-6-15(8)9(14-12)3-1-2-7-4-5-13-11(7)10/h1-6,13h/b3-1-,7-2-,11-10+
I-80	 $C_{12}H_7N_3O$	15.5783	194.0006	-7.7059	78.5793	302.9181	InChI=1S/C12H7N3O/c16-9-6-7-10-11-8(2-4-14-11)15(12(7)10)5-1-3-13-9/h1-6,14h/b5-1-,7-6-,13-3-
s12-46	 $C_{12}H_7N_3O$	10.1718	178.9314	-6.6244	86.38	303.2843	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-9(7)6-15-10(11)12(15)14-8/h1-6,13h/b3-1-,7-2-,9-6-
G-22	 $C_{12}H_7N_3O$	5.4373	135.5597	-2.0593	151.1189	303.5955	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8(11-14-6-15(11)12)7-4-5-13-10(7)9/h1-6,13h
A2-11	 $C_{12}H_7N_3O$	4.6757	95.9807	-2.2352	182.6854	303.6264	InChI=1S/C12H7N3O/c16-12-8-6-10-13-4-1-2-9(15(10)12)7-3-5-14-11(7)8/h1-6,14h
H11-43	 $C_{12}H_7N_3O$	7.4931	43.2313	-2.9238	222.7176	303.6958	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(14-9)15(12)11-8(7)4-5-13-11/h1-6,13h/b2-1-,3-1-,7-2-,10-3-
X22-39	 $C_{12}H_7N_3O$	30.021	249.9632	-15.4549	20.7086	303.7422	InChI=1S/C12H7N3O/c16-10-6-9-12-8(15(9)12)2-1-4-13-7-3-5-14-11(7)10/h1-6,14h/b2-1-,9-6-,13-4-
s12-44	 $C_{12}H_7N_3O$	10.5576	220.9262	-7.8409	55.6651	304.045	InChI=1S/C12H7N3O/c16-9-6-8-7(4-5-13-8)2-1-3-10-14-12-11(9)15(10)12/h1-6,13h/b3-1-,7-2-,8-6+
H11-78	 $C_{12}H_7N_3O$	7.3305	44.4049	-3.2601	218.1927	304.2572	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-10-14-9(7)6-15(10)12/h1-6,13h
H11-93	 $C_{12}H_7N_3O$	4.9465	185.128	-1.6694	98.7347	304.3009	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-10(6-14-9)15(12)11-7(8)4-5-13-11/h1-6,13h/b3-1-,8-2-
B-10	 $C_{12}H_7N_3O$	41.4955	254.0969	-17.8805	11.8608	304.4054	InChI=1S/C12H7N3O/c16-10-6-9(10)15-5-1-2-7-8-3-4-13-11(8)12(7)14-15/h1-6,13h
k-8	 $C_{12}H_7N_3O$	26.418	158.8026	-7.2203	80.5648	304.5097	InChI=1S/C12H7N3O/c16-12-7-6-9-11(12)15(9)5-1-3-13-8-2-4-14(7)8/h1-6,14h/b5-1-,13-3-
I-84	 $C_{12}H_7N_3O$	9.7814	72.3471	-3.7419	186.2711	304.7295	InChI=1S/C12H7N3O/c16-12-10-7-6-9(10)15(5-1-3-13-7)8-2-4-14-11(8)12/h1-6,14h/b5-1-,13-3-
o-162	 $C_{12}H_7N_3O$	16.7362	207.4445	-10.2922	69.3679	304.862	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)10-3-4-13-11(10)7-6-9(7)14-8/h1-6,13h/b14-9-
n-190	 $C_{12}H_7N_3O$	19.5651	220.5445	-14.3328	49.744	304.9913	InChI=1S/C12H7N3O/c16-12-10-7(8(10)6-14-12)2-1-5-15-9-3-4-13-11(9)15/h1-6,13h/b5-1-,7-2-
n-101	 $C_{12}H_7N_3O$	19.5658	220.5332	-14.3324	49.7448	304.9966	InChI=1S/C12H7N3O/c16-12-10-7(8(10)6-14-12)2-1-5-15-9-3-4-13-11(9)15/h1-6,13h/b5-1-,7-2+
B-99	 $C_{12}H_7N_3O$	13.4720	250.1730	-7.7562	27.7937	305.1494	InChI=1S/C12H7N3O/c16-12-11-7(3-4-13-11)9-2-1-5-15(9)10-6-8(10)14-12/h1-6,13h/b14-8-










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	$C_{12}H_7N_3O$						
n-7		18, 9768	222, 2016	-14, 1298	49, 7678	305, 3636	InChI=1S/C12H7N3O/c16-9-6-14-11-7(10(9)11)2-1-5-15-8-3-4-13-12(8)15/h1-6, 13H/b5-1-, 7-2-
	$C_{12}H_7N_3O$						
A1-50		26, 9993	219, 4469	-13, 2157	37, 4615	305, 5073	InChI=1S/C12H7N3O/c16-12-10-7(3-5-14-10)8-2-1-4-13-6-9-11(12)15(8)9/h1-6, 14H/b4-1-, 8-2-, 13-6-
	$C_{12}H_7N_3O$						
H1-39		19, 6153	188, 8091	-10, 0866	79, 9601	305, 5401	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-12(7)15-6-9(15)11(10)14-8/h1-6, 13H
	$C_{12}H_7N_3O$						
G1-61		1, 8677	311, 2616	-2, 0541	-8, 83	305, 589	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-11(8)12(10(7)9)15-6-14-15/h1-6, 13H
	$C_{12}H_7N_3O$						
H11-98		8, 3586	133, 4658	-0, 7802	134, 8468	305, 8243	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(14-12)15(9)11-8(7)4-5-13-11/h1-6, 13H/b3-1-, 7-2+
	$C_{12}H_7N_3O$						
H11-124		10, 2981	201, 26	-0, 3261	66, 6895	306, 2006	InChI=1S/C12H7N3O/c16-10-6-11-14-8(10)2-1-3-9-7-4-5-13-12(7)15(9)11/h1-6, 13H/b2-1-, 9-3-
	$C_{12}H_7N_3O$						
G-35		1, 9851	310, 9121	-1, 9498	-9, 89	306, 3266	InChI=1S/C12H7N3O/c16-12-10-7(8-4-5-13-11(8)12)2-1-3-9(10)15-6-14-15/h1-6, 13H
	$C_{12}H_7N_3O$						
x6-34		23, 7337	156, 1097	-9, 1143	107, 2446	306, 5943	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-9(7)6-8-11(10)15-12(8)14-15/h1-6, 13H/b3-1-, 7-2-, 9-6+
	$C_{12}H_7N_3O$						
r-57		31, 2949	250, 4438	-15, 5206	19, 774	306, 6803	InChI=1S/C12H7N3O/c16-10-6-9-11-8(15(9)11)3-1-2-7-4-5-13-12(7)14-10/h1-6H, 13, 14, 16
	$C_{12}H_7N_3O$						
A1-51		34, 5919	248, 2518	-17, 3154	23, 0055	306, 7655	InChI=1S/C12H7N3O/c16-11-8-6-13-4-1-2-9-7-3-5-14-12(7)15(9)10(8)11/h1-6, 14H/b4-1-, 9-2-, 13-6+
	$C_{12}H_7N_3O$						
o-10		6, 7797	110, 1949	-1, 4068	152, 7016	306, 8749	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-8-3-4-13-12(8)14-10(11)9(15)6-7/h1-6, 13H
	$C_{12}H_7N_3O$						
C-16		18, 9666	197, 6738	-14, 4028	79, 0292	307, 0189	InChI=1S/C12H7N3O/c16-12-10-6-9(10)7-2-1-4-14-15(12)11-8(7)3-5-13-11/h1-6, 13H/b2-1-, 14-4-
	$C_{12}H_7N_3O$						
k-19		30, 4342	225, 9135	-12, 0752	55, 6604	307, 0989	InChI=1S/C12H7N3O/c16-12-7-6-9-10-8(2-4-14-10)13-3-1-5-15(9)11(7)12/h1-6, 14H/b5-1-, 13-3+
	$C_{12}H_7N_3O$						
C-6		8, 0074	64, 1834	-4, 5520	202, 2741	307, 2047	InChI=1S/C12H7N3O/c16-11-9-6-10(11)15-12-8(3-5-13-12)7(9)2-1-4-14-15/h1-6, 13H/b2-1-, 14-4-
	$C_{12}H_7N_3O$						
A2-42		12, 4027	163, 8404	-2, 0406	114, 4077	307, 2167	InChI=1S/C12H7N3O/c16-10-6-9-12-11-7(3-5-14-11)8(15(9)10)2-1-4-13-12/h1-6, 14H/b2-1-, 4-1-, 8-2+, 13-4-, 13-12-
	$C_{12}H_7N_3O$						
A-37		29, 2812	227, 6797	-10, 7759	35, 6279	307, 2906	InChI=1S/C12H7N3O/c16-12-8-6-14-15-5-1-2-9(15)7-3-4-13-11(7)10(8)12/h1-6, 13H/b4-6-
	$C_{12}H_7N_3O$						
n-177		5, 8192	180, 2048	-2, 1477	103, 3098	307, 5775	InChI=1S/C12H7N3O/c16-12-10-7-6-14-8(7)2-1-5-15(12)9-3-4-13-11(9)10/h1-6, 13H/b5-1-, 8-2-, 10-7-
	$C_{12}H_7N_3O$						
H1-3		10, 6413	232, 0947	-6, 4387	49, 5121	307, 7018	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12(7)14-15-6-9(10)15/h1-6, 13H/b3-1-, 7-2-, 14-12+
	$C_{12}H_7N_3O$						

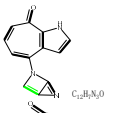
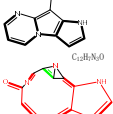
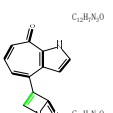
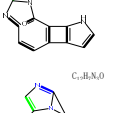
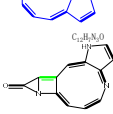
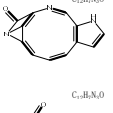
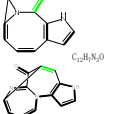
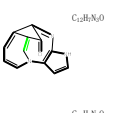
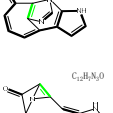
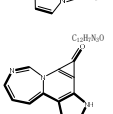
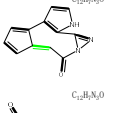
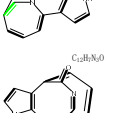
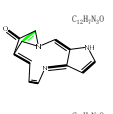
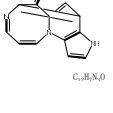


A-107		24.0724	209.0615	-8.7431	54.245	307.7393	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9(10(11)15)6-14-12-8(7)3-4-13-12/h1-6,13H/b14-6-
x6-39		20.5695	236.8543	-10.214	44.2202	307.8399	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-10-14-12-11(9)15(10)12/h1-6,13H/b3-1-,7-2-,8-6-
x4-33		10.4858	138.1653	-4.4392	134.0543	307.8787	InChI=1S/C12H7N3O/c16-12-10-8-6-14-15(12)9(10)3-1-2-7-4-5-13-11(7)8/h1-6,13H/b2-1-,3-1-,7-2-,9-3+,11-8+
H-108		18.1378	217.4184	-7.3148	61.0241	307.9327	InChI=1S/C12H7N3O/c16-12-11-14-6-7-2-1-3-8(7)9-4-5-13-10(9)15(11)12/h1-6,13H/b7-6-,14-11-
n-36		26.6206	224.327	-10.1106	50.3647	308.1897	InChI=1S/C12H7N3O/c16-12-10-9-2-1-5-15(9)8-3-4-13-7(8)6-14-11(10)12/h1-6,13H/b14-6+
p11-13		13.4443	227.119	-8.2575	53.2706	308.2052	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-4-5-13-8(7)6-14-12-10(11)15(9)12/h1-6,13H/b2-1-,9-3-,14-6-
o-67		6.9898	112.3869	-1.3514	148.2508	308.2365	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)15-5-1-2-7-6-9(15)11(12)14-7/h1-6,13H
B-18		6.5229	144.6333	-2.0717	127.7113	308.2606	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(14-11(9)10)12-8(7)3-4-13-12/h1-6,13H
B-63		16.1107	153.8981	-13.4576	130.0974	308.3420	InChI=1S/C12H7N3O/c16-12-8-6-10(8)14-9-2-1-5-15(12)11-7(9)3-4-13-11/h1-6,13H/b14-10-
q-54		18.2331	201.0827	-3.348	81.7647	308.3466	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)9(8)6-10-14-15(10)12/h1-6,13H
r-55		10.6421	262.9812	-6.3266	35.5792	308.3575	InChI=1S/C12H7N3O/c16-10-6-9-11(15(9)10)8-3-1-2-7-4-5-13-12(7)14-8/h1-6H,13,14)/b11-8-
H-72		7.0436	43.349	-2.2995	228.6278	308.4244	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-15(12)14-10(7)11-8(9)4-5-13-11/h1-6,13H/b2-1-,9-3-
H-48		5.5311	99.8454	-2.2335	176.073	308.4907	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-12(8)11(7)14-15(9)10/h1-6,13H/b2-1-,9-3-
G1-84		5.3865	187.0784	-3.431	94.5286	308.6075	InChI=1S/C12H7N3O/c16-9-3-1-2-7-6-14-15-11(9)12(15)10-8(7)4-5-13-10/h1-6,13H/b3-1-,7-2+
x4-57		18.4226	242.8169	-4.4932	36.7144	308.7869	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)10-11(14-6-8)15(10)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,10-9+
B-4		10.3668	303.4465	-3.2479	-3.9087	308.7922	InChI=1S/C12H7N3O/c16-10-6-8(10)12-14-11-7(3-4-13-11)9-2-1-5-15(9)12/h1-6,13H
s12-39		14.7554	190.8557	-6.4966	81.1357	308.8113	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-10-11(14-8)15(10)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,9-6-,10-6-
E-17		5.5457	79.9682	-1.908	193.8849	308.8335	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(14-12)8-4-5-13-11(8)15(7)10/h1-6,13H/b3-1-,7-2-
o-215		14.7878	143.457	-12.4736	138.6018	308.8979	InChI=1S/C12H7N3O/c16-12-8-6-9(14-12)7(8)2-1-5-15-10-3-4-13-11(10)15/h1-6,13H/b5-1-,7-2+

n-132	 <chem>C12H9N3O</chem>	2.4709	304.0531	-2.2557	-3.31	308.928	InChI=1S/C12H7N3O/c16-12-10(7-6-14-7)8-2-1-5-15(8)9-3-4-13-11(9)12/h1-6,13H/b10-7+
E-42	 <chem>C12H9N3O</chem>	8.2856	144.3312	-2.6235	117.6	308.9398	InChI=1S/C12H7N3O/c16-11-6-10-8-2-1-3-9(14-15(10)11)7-4-5-13-12(7)8/h1-6,13H
H1-69	 <chem>C12H9N3O</chem>	17.7727	173.9	-2.2712	100.868	308.9584	InChI=1S/C12H7N3O/c16-7-2-1-3-8-9-4-5-13-11(9)12-14-15(12)10(8)6-7/h1-6,13H
p-27	 <chem>C12H9N3O</chem>	10.671	137.7607	-7.1259	139.2835	309.412	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-8(7)6-10-11(14-12)15(9)10/h1-6,13H/b2-1-,9-3-,10-6-
H1-61	 <chem>C12H9N3O</chem>	18.4604	160.361	-4.5148	117.174	309.6399	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)12-8(14-12)6-15(9)10/h1-6,13H
H11-77	 <chem>C12H9N3O</chem>	5.384	111.0578	-1.6609	167.7345	309.7541	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-10-14-6-9(7)15(10)12/h1-6,13H
q-20	 <chem>C12H9N3O</chem>	7.7586	151.8445	-2.8499	105.595	309.8593	InChI=1S/C12H7N3O/c16-12-11-8-3-1-2-7-4-5-13-10(7)9(6-8)15(12)14-11/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,10-9-
o-188	 <chem>C12H9N3O</chem>	10.3032	302.596	-3.2276	-3.9779	309.8834	InChI=1S/C12H7N3O/c16-10-6-7(10)11-8-2-1-5-15(8)9-3-4-13-12(9)14-11/h1-6,13H
F-61	 <chem>C12H9N3O</chem>	20.0377	139.1646	-13.1334	120.613	310.295	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(10-6-15(9)10)8-4-5-13-11(8)14-12/h1-6H,13,14,16
I-63	 <chem>C12H9N3O</chem>	12.0989	265.2713	-9.7472	26.4171	310.3671	InChI=1S/C12H7N3O/c16-9-6-7-10(9)11(7)15-5-1-3-13-12-8(15)2-4-14-12/h1-6,14H
A-59	 <chem>C12H9N3O</chem>	2.7376	304.7561	-2.2573	-4.31	310.4219	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)9-2-1-5-15(9)11(12)8-6-14-8/h1-6,13H/b11-8+
A-103	 <chem>C12H9N3O</chem>	2.737	304.7563	-2.2566	-4.31	310.4219	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)9-2-1-5-15(9)11(12)8-6-14-8/h1-6,13H/b11-8-
B-1	 <chem>C12H9N3O</chem>	10.3706	304.5912	-3.2159	-4.8400	310.4467	InChI=1S/C12H7N3O/c16-10-6-8(10)12-11-7(3-4-13-11)9-2-1-5-15(9)14-12/h1-6,13H
x6-35	 <chem>C12H9N3O</chem>	23.0123	151.9938	-10.935	118.592	310.4601	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-15-11(9)10-12(15)14-10/h1-6,13H/b3-1-,7-2-,8-6+
C-5	 <chem>C12H9N3O</chem>	4.7265	104.6521	-2.1768	172.1481	310.7083	InChI=1S/C12H7N3O/c16-12-9-6-15-11(12)8(2-1-4-14-15)7-3-5-13-10(7)9/h1-6,13H
H1-103	 <chem>C12H9N3O</chem>	6.8398	88.0435	-4.8906	189.5491	310.8708	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)15-6-9(7)12(14-10/h1-6,13H/b3-1-,7-2-,14-12+
A2-70	 <chem>C12H9N3O</chem>	16.7605	141.4378	-11.7505	119.1067	311.096	InChI=1S/C12H7N3O/c16-12-9-6-15(9)8-2-1-4-13-11(12)10-7(8)3-5-14-10/h1-6,14H/b2-1-,4-1-,8-2-,13-4-,13-11+
I-33	 <chem>C12H9N3O</chem>	31.0903	251.7363	-15.2745	22.6369	311.3173	InChI=1S/C12H7N3O/c16-12-7-6-9-11-8(2-4-14-11)15(9)5-1-3-13-10(7)12/h1-6,14H/b5-1-,9-6-,13-3-
n-186	 <chem>C12H9N3O</chem>	5.2656	180.5498	-1.8871	106.1715	311.3351	InChI=1S/C12H7N3O/c16-12-9-10-7(6-14-10)2-1-5-15(12)8-3-4-13-11(8)9/h1-6,13H/b5-1-,7-2-,10-9+

o-196		$C_{12}H_8N_2O$	10.292	303.4448	-3.2463	-1.9195	311.3793	InChI=1S/C12H7N3O/c16-9-6-7(9)11-12-8(3-4-13-12)15-5-1-2-10(15)14-11/h1-6,13H
G1-113		$C_{12}H_8N_2O$	15.5678	192.9938	-7.8869	86.8553	311.4334	InChI=1S/C12H7N3O/c16-7-2-1-3-9-8-4-5-13-10(8)11-12(14-6-7)15(9)11/h1-6,13H/b2-1-,9-3-,14-6-
C-3		$C_{12}H_8N_2O$	10.7671	308.7869	-3.1372	-4.7643	311.4427	InChI=1S/C12H7N3O/c16-10-6-9(10)15-11-7(2-1-4-13-11)8-3-5-14-12(8)15/h1-6,14H
H-99		$C_{12}H_8N_2O$	5.557	100.0915	-2.0407	182.0111	311.4489	InChI=1S/C12H7N3O/c16-12-10-8(4-5-13-10)9-3-1-2-7-6-14-11(9)15(7)12/h1-6,13H
n-64		$C_{12}H_8N_2O$	2.4733	304.3156	-2.2843	0.34	311.4764	InChI=1S/C12H7N3O/c16-12-9-2-1-5-15(9)8-3-4-13-11(8)10(12)7-6-14-7/h1-6,13H/b10-7-
n-158		$C_{12}H_8N_2O$	2.4747	304.314	-2.2851	0.34	311.4764	InChI=1S/C12H7N3O/c16-12-9-2-1-5-15(9)8-3-4-13-11(8)10(12)7-6-14-7/h1-6,13H/b10-7+
C-54		$C_{12}H_8N_2O$	9.1065	44.1380	-3.0624	224.2046	311.6774	InChI=1S/C12H7N3O/c16-12-9-6-10-11-8(3-5-13-11)7(9)2-1-4-14-15(10)12/h1-6,13H/b2-1-,14-4-
H-129		$C_{12}H_8N_2O$	5.3118	98.435	-2.2713	184.8172	311.7376	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7(6-14-10)15(12)11-9(8)4-5-13-11/h1-6,13H/b2-1-,3-1-,7-2-,8-3-
H1-68		$C_{12}H_8N_2O$	27.2378	156.5714	-6.4043	101.8232	311.7959	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12-14-15(12)6-9(7)10/h1-6,13H
r1-17		$C_{12}H_8N_2O$	29.3397	248.9029	-15.3466	29.2529	311.8398	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-11(7)14-12-10-9(6-8)15(10)12/h1-6H, (H,13,14)/b3-1-,7-2-,9-6-
o-193		$C_{12}H_8N_2O$	10.416	306.8439	-3.1975	-3.8472	311.8672	InChI=1S/C12H7N3O/c16-10-6-8(10)7-2-1-5-15-9-3-4-13-11(9)14-12(7)15/h1-6,13H
B-219		$C_{12}H_8N_2O$	4.9835	33.8328	-2.1425	239.7607	311.8971	InChI=1S/C12H7N3O/c16-12-9-6-15-5-1-2-8(11(15)14-12)7-3-4-13-10(7)9/h1-6,13H
k-43		$C_{12}H_8N_2O$	13.4211	178.1531	-7.9712	106.6194	311.9131	InChI=1S/C12H7N3O/c16-12-10-7-6-15(12)5-1-3-13-8-2-4-14-11(8)9(7)10/h1-6,14H/b5-1-,13-3+
F-1		$C_{12}H_8N_2O$	10.6378	306.5472	-3.1774	-4.8266	311.9631	InChI=1S/C12H7N3O/c16-11-6-8(11)10-3-1-2-9-7-4-5-13-12(7)14-15(9)10/h1-6H, (H,13,14)
H11-53		$C_{12}H_8N_2O$	6.8963	74.9445	-3.8231	208.2216	312.0012	InChI=1S/C12H7N3O/c16-12-9-6-15(12)10-3-1-2-8(14-9)11-7(10)4-5-13-11/h1-6,13H/b14-8-
o-35		$C_{12}H_8N_2O$	14.8701	148.4509	-12.0268	136.4392	312.2119	InChI=1S/C12H7N3O/c16-11-8-6-7(10(11)14-8)2-1-5-15-9-3-4-13-12(9)15/h1-6,13H/b5-1-,7-2+
o-104		$C_{12}H_8N_2O$	2.8789	309.1423	-2.3387	-5.3	312.489	InChI=1S/C12H7N3O/c16-12-11(14-12)8-6-7-2-1-5-15(7)9-3-4-13-10(8)9/h1-6,13H
o-102		$C_{12}H_8N_2O$	2.9152	309.1682	-2.3145	-6.23	312.5084	InChI=1S/C12H7N3O/c16-12-11(14-12)7-6-8-10(3-4-13-8)15-5-1-2-9(7)15/h1-6,13H
B-8		$C_{12}H_8N_2O$	42.9601	256.4993	-17.9518	13.2809	312.5399	InChI=1S/C12H7N3O/c16-10-6-8(10)14-12-11-7(3-4-13-11)9-2-1-5-15(9)12/h1-6,13H/b14-12-











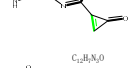








B-49		4.6223	41.2763	-1.5848	234.1641	312.5505	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(9)14-12(10)11-8(7)3-4-13-11/h1-6,13H
I-59		19.3807	144.5724	-13.8023	127.6449	312.8513	InChI=1S/C12H7N3O/c16-12-10-7-6-9(7)15(5-1-3-14-12)8-2-4-13-11(8)10/h1-6,13H/b5-1-,14-3+
I-101		19.359	144.5778	-13.7938	127.6361	312.8514	InChI=1S/C12H7N3O/c16-12-10-7-6-9(7)15(5-1-3-14-12)8-2-4-13-11(8)10/h1-6,13H/b5-1-,14-3-
H-65		2.5449	242.9961	-1.2733	49.2237	312.8624	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-15(7)14-11(12)10-8(9)4-5-13-10/h1-6,13H/b2-1-,9-3-,14-11-
o-34		5.9523	34.7442	-2.3034	234.0187	312.9849	InChI=1S/C12H7N3O/c16-11-9-6-7-2-1-5-15(9)8-3-4-13-12(8)14-10(7)11/h1-6,13H
H11-18		23.2814	232.1553	-5.7974	42.6815	313.0631	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8(14-9)7-4-5-13-11(7)10-6-15(10)12/h1-6,13H
B-233		2.9313	309.8885	-2.3299	-5.1700	313.1706	InChI=1S/C12H7N3O/c16-12-11(14-12)8-6-15-5-1-2-9(15)7-3-4-13-10(7)8/h1-6,13H
I-40		19.1833	274.6317	-21.4888	40.8831	313.2456	InChI=1S/C12H7N3O/c16-12-11-9(2-4-14-11)15(12)5-1-3-13-10-7-6-8(7)10/h1-6,14H/b5-1-,13-3+
p1-60		6.9333	46.1842	-5.8893	238.397	313.2881	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-8-6-15(11)12(9)14-8/h1-6,13H/b3-1-,7-2-,11-10+
A-8		21.772	237.3524	-9.6321	39.4809	313.3255	InChI=1S/C12H7N3O/c16-9-6-14-12-8(3-4-13-12)7-2-1-5-15-10(7)11(9)15/h1-6,13H/b14-6-
o-218		8.1538	70.3117	-2.0678	195.134	313.509	InChI=1S/C12H7N3O/c16-12-8-6-9-10(3-4-13-9)15-5-1-2-7(8)11(15)14-12/h1-6,13H
o-17		7.2768	35.9741	-1.6428	234.7928	313.5715	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-8(7)14-11(12)10-9(15)3-4-13-10/h1-6,13H
H11-30		19.3321	227.2583	-12.0315	71.803	313.6043	InChI=1S/C12H7N3O/c16-12-9-6-15(12)14-10(9)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
o12-2		25.8203	285.5071	-16.9956	10.0278	313.75	InChI=1S/C12H7N3O/c16-12-10-11(15(10)12)14-8-3-1-2-7-4-5-13-9(7)6-8/h1-6,13H/b14-8-
o-205		6.9058	117.4832	-2.7311	166.9211	313.8136	InChI=1S/C12H7N3O/c16-12-9-6-8(14-9)7-2-1-5-15(12)10-3-4-13-11(7)10/h1-6,13H
D-23		17.0747	173.8824	-10.2052	102.8610	313.8785	InChI=1S/C12H7N3O/c16-12-10-9-6-15(9)8(2-1-4-14-12)7-3-5-13-11(7)10/h1-6,13H/b2-1-,14-4-
q11-44		9.1851	119.441	-5.7176	159.3183	313.9117	InChI=1S/C12H7N3O/c16-12-14-11-8-6-15(12)9(8)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,9-3+
r-6		6.4136	112.7865	-4.2017	172.3164	314.1385	InChI=1S/C12H7N3O/c16-11-9-6-8-3-1-2-7-4-5-13-12(7)14-15(9)10(8)11/h1-6H,(8,13,14)/b3-1-,7-2-
C-47		4.0441	246.7152	-2.1891	50.2445	314.3742	InChI=1S/C12H7N3O/c16-12-10-7(8-3-5-13-11(8)12)2-1-4-14-15-6-9(10)15/h1-6,13H/b2-1-,14-4-

n-109		6.8879	94.5107	-1.7716	177.9344	314.4407	InChI=1S/C12H7N3O/c16-9-6-14-7-2-1-5-15-8-3-4-13-11(8)10(7)12(9)15/h1-6,13H
	$C_{12}H_7N_3O$						
X22-17		12.9427	258.9273	-8.3136	36.5793	314.558	InChI=1S/C12H7N3O/c16-12-10-9(3-5-14-10)13-4-1-2-7-8-6-15(12)11(7)8/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
H11-9		7.2846	120.2866	-1.2434	156.5472	314.8573	InChI=1S/C12H7N3O/c16-12-14-8-2-1-3-10-7-4-5-13-9(7)6-11(8)15(10)12/h1-6,13H
	$C_{12}H_7N_3O$						
H-125		7.8197	48.1039	-2.5023	226.1072	315.0028	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(14-10)8-4-5-13-11(8)15(7)12/h1-6,13H/b2-1-,3-1-,7-2+,9-3-
	$C_{12}H_7N_3O$						
H1-131		24.395	143.2772	-10.1126	141.074	315.0464	InChI=1S/C12H7N3O/c16-10-3-1-2-7(8-4-5-13-12(8)10)9-6-11-14-15(9)11/h1-6,13H
	$C_{12}H_7N_3O$						
k-46		27.787	240.7844	-1.1068	46.1786	315.1659	InChI=1S/C12H7N3O/c16-12-8-6-7-10-9(2-4-14-10)13-3-1-5-15(12)11(7)8/h1-6,14H/b5-1-,13-3+
	$C_{12}H_7N_3O$						
C-73		9.7606	178.4313	-4.4364	99.6347	315.2187	InChI=1S/C12H7N3O/c16-12-14-4-1-2-7-8-3-5-13-11(8)10-6-9(7)15(10)12/h1-6,13H/b2-1-,14-4+
	$C_{12}H_7N_3O$						
s12-43		10.4399	245.8797	-7.155	43.6944	315.58	InChI=1S/C12H7N3O/c16-10-6-9-7(4-5-13-9)2-1-3-8-11-12(10)15(11)14-8/h1-6,13H/b3-1-,7-2-,9-6+
	$C_{12}H_7N_3O$						
X-9		26.7636	219.1431	-12.4290	62.8759	315.6816	InChI=1S/C12H7N3O/c16-11-9-10(11)15-6-7(2-1-4-13-9)8-3-5-14-12(8)15/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
H1-82		15.7637	214.8021	-17.2171	79.2096	315.7159	InChI=1S/C12H7N3O/c16-11-3-1-2-9(7-4-5-13-12(7)11)15-10-6-8(10)14-15/h1-6,13H
	$C_{12}H_7N_3O$						
j-21		11.6271	215.2692	-9.5678	82.5521	315.8051	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-9(8)6-10-11(7)15(10)12/h1-6,14H/b2-1-,4-1-,7-2+,9-6+,10-6+,13-4-,13-8-
	$C_{12}H_7N_3O$						
s11-16		15.5125	173.749	-10.9072	110.6101	315.847	InChI=1S/C12H7N3O/c16-12-8-6-15(8)9-3-1-2-7-4-5-13-10(7)11(12)14-9/h1-6,13H/b2-1-,3-1-,7-2-,9-3+,11-10+
	$C_{12}H_7N_3O$						
A2-34		24.5537	237.0201	-13.3672	59.2125	316.1424	InChI=1S/C12H7N3O/c16-12-8-6-9(8)13-4-1-2-10-7-3-5-14-11(7)15(10)12/h1-6,14H/b4-1-,10-2-,13-9-
	$C_{12}H_7N_3O$						
H-83		14.6426	209.0033	-9.6537	70.3497	316.2562	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)10-3-1-2-7-6-9(7)14-15(10)12/h1-6,13H/b2-1-,10-3-,14-9-
	$C_{12}H_7N_3O$						
F-28		12.9435	269.8555	-4.3151	32.165	316.3337	InChI=1S/C12H7N3O/c16-12-10-6-14-11-8(4-5-13-11)7-2-1-3-9(7)15(10)12/h1-6H,(H,13,14)/b8-7-,10-6-
	$C_{12}H_7N_3O$						
H-83		16.3631	177.7765	-11.4741	103.5919	316.3829	InChI=1S/C12H7N3O/c16-11-10-9(4-5-13-10)8-3-1-2-7(8)6-15-12(11)14-15/h1-6,13H/b7-6+
	$C_{12}H_7N_3O$						
x4-31		9.4491	98.3008	-5.0371	174.7189	316.59	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)11-10(12)14-6-15(8)11/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
x6-30		24.8518	158.4784	-9.4787	115.8438	316.7002	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-11(10)12-14-15(9)12/h1-6,13H/b3-1-,7-2-,8-6+
	$C_{12}H_7N_3O$						
H11-114		9.7836	115.6472	-2.2443	162.4648	317.2073	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-6-10(11)15(14-9)12-8(7)4-5-13-12/h1-6,13H/b3-1-,7-2+
	$C_{12}H_7N_3O$						




















H1-111	 C ₂₂ H ₂₀ N ₂ O	21.8696	141.2111	-11.7677	147.5788	317.2772	InChI=1S/C12H7N3O/c16-10-3-1-2-9(7)-4-5-13-11(7)1015-6-8-12(15)14-8/h1-6,13H
I-67	 C ₂₂ H ₂₀ N ₂ O	10.6191	309.7027	-3.3023	-1.9184	317.3861	InChI=1S/C12H7N3O/c16-9-6-7(9)10-11-8(2-4-13-11)15-5-1-3-14-12(10)15/h1-6,13H
x7-7	 C ₂₂ H ₂₀ N ₂ O	29.981	247.4215	-15.76	41.6674	317.4129	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11-8(6-14-9)15(11)12/h1-6,13H/b3-1-,7-2-,12-10-,14-6+
H1-98	 C ₂₂ H ₂₀ N ₂ O	24.69	144.6163	-10.2797	142.0617	317.4648	InChI=1S/C12H7N3O/c16-10-3-1-2-7(8-4-5-13-11(8)10)9-6-15-12(9)14-15/h1-6,13H
C-60	 C ₂₂ H ₂₀ N ₂ O	27.3000	235.8692	-12.5884	40.8583	317.7645	InChI=1S/C12H7N3O/c16-12-10-7(8-3-5-14-11(8)10)2-1-4-13-9-6-15(9)12/h1-6,14H/b2-1-,13-4+
p1-56	 C ₂₂ H ₂₀ N ₂ O	10.5399	138.1545	-7.0148	149.9369	317.8991	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-12-14-6-8(9)15(11)12/h1-6,13H/b3-1-,7-2-,11-10+
j-15	 C ₂₂ H ₂₀ N ₂ O	17.3743	224.8466	-9.7016	67.7158	317.9955	InChI=1S/C12H7N3O/c16-12-11-7-6-9-8(3-5-14-9)13-4-1-2-10(7)15(11)12/h1-6,14H/b4-1-,9-6+,10-2-,13-8-
p11-16	 C ₂₂ H ₂₀ N ₂ O	15.5012	174.0018	-10.518	121.137	318.0092	InChI=1S/C12H7N3O/c16-12-10-11-9(15(11)12)3-1-2-7-4-5-13-8(7)6-14-10/h1-6,13H/b2-1-,3-1-,7-2-,8-6+,9-3+,14-6-,14-10+
q-47	 C ₂₂ H ₂₀ N ₂ O	10.4253	143.2734	-6.3676	139.8607	318.13	InChI=1S/C12H7N3O/c16-10-6-9-11-7(4-5-13-11)2-1-3-8-12(14-10)15(8)9/h1-6,13H/b2-1-,8-3-
o-57	 C ₂₂ H ₂₀ N ₂ O	5.0965	33.3123	-1.7411	245.7002	318.2781	InChI=1S/C12H7N3O/c16-11-7-6-9-10(3-4-13-9)15-5-1-2-8(7)14-12(11)15/h1-6,13H
o-30	 C ₂₂ H ₂₀ N ₂ O	6.403	72.8361	-2.0772	204.76	318.3322	InChI=1S/C12H7N3O/c16-11-8-6-15-5-1-2-7(8)10(11)14-12-9(15)3-4-13-12/h1-6,13H/b14-10-
G1-35	 C ₂₂ H ₂₀ N ₂ O	15.2986	95.351	-4.1313	175.2603	318.5861	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-12(8)15-6-14-10(7)11(9)15/h1-6,13H
j-13	 C ₂₂ H ₂₀ N ₂ O	16.9481	229.8972	-11.6096	61.8524	318.7452	InChI=1S/C12H7N3O/c16-12-9-2-1-4-13-7-3-5-14-8(7)6-10-11(12)15(9)10/h1-6,14H/b4-1-,8-6-,9-2-,13-7+
A1-39	 C ₂₂ H ₂₀ N ₂ O	24.7572	244.1837	-8.8446	47.1399	318.8529	InChI=1S/C12H7N3O/c16-12-9-10-7(3-5-14-10)8-2-1-4-13-6-15(8)11(9)12/h1-6,14H
H-44	 C ₂₂ H ₂₀ N ₂ O	20.8228	204.1442	-6.3144	79.5227	319.1696	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8(7)9-4-5-13-11(9)12-14-15(10)12/h1-6,13H/b7-6+
H-12	 C ₂₂ H ₂₀ N ₂ O	5.7848	34.6729	-1.4201	238.8613	319.1793	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-10(8)11(12)14-15(9)6-7/h1-6,13H
B-111	 C ₂₂ H ₂₀ N ₂ O	9.4622	61.1771	-4.2654	212.0121	319.2151	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-9(6-10(15)14-12)11-7(8)3-4-13-11/h1-6,13H/b5-1-,8-2-,14-10+
j-14	 C ₂₂ H ₂₀ N ₂ O	22.411	199.5597	-13.7771	90.4627	319.3004	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-9(8)6-15-10(7)11(12)15/h1-6,14H/b4-1-,7-2-,9-6+,13-8+
I-87	 C ₂₂ H ₂₀ N ₂ O	6.7931	38.4503	-2.4454	234.2248	319.3318	InChI=1S/C12H7N3O/c16-12-9-6-7-10-8(2-4-14-10)15(9)5-1-3-13-11(7)12/h1-6,14H/b5-1-,13-3-




















o-98		3.1688	315.5445	-2.2232	-6.23	319.4161	InChI=1S/C12H7N3O/c16-12-11(14-12)7-2-1-5-15-9-3-4-13-8(9)6-10(7)15/h1-6,13H
r1-32		18.4483	242.8025	-13.6118	47.2087	319.5661	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-11(7)14-12-10-9(6-8)15(10)12/h1-6H, 11, 13, 14)/b3-1-, 7-2-, 9-6-
E-46		14.6171	146.549	-10.8119	135.8597	319.7265	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(14-15-6-10(8)15)7-4-5-13-11(7)12/h1-6,13H/b3-1-, 8-2-, 9-6-
X-48		20.4304	225.4575	-8.0750	55.8505	319.7574	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-14-12-11(15(9)12)10-8(7)3-5-13-10/h1-6,13H/b2-1-, 14-4-
A-41		27.4174	235.6397	-10.6258	55.6913	319.7926	InChI=1S/C12H7N3O/c16-11-8-6-14-12-7(3-4-13-12)9-2-1-5-15(9)10(8)11/h1-6,13H/b14-6-
H11-92		6.8026	143.8225	-2.8103	151.6169	319.9262	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(14-7)15(12)11-8(9)4-5-13-11/h1-6,13H/b2-1-, 9-3-
H11-15		11.5506	263.256	-0.8694	21.2869	320.1346	InChI=1S/C12H7N3O/c16-12-10-3-1-2-7-8-4-5-13-11(8)9(7)6-15(12)14-10/h1-6,13H/b3-1-, 7-2-, 9-6-
X-30		5.7308	191.2725	-3.7435	100.8806	320.1388	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-14-15-11(9)12(15)10-8(7)3-5-13-10/h1-6,13H/b2-1-, 14-4-
A-9		10.1036	123.629	-2.5861	159.0908	320.1731	InChI=1S/C12H7N3O/c16-9-6-14-10-7-2-1-5-15(11(9)10)12-8(7)3-4-13-12/h1-6,13H
r-11		9.7513	260.2814	-4.9889	29.6158	320.2472	InChI=1S/C12H7N3O/c16-11-8-6-15-9(10(11)15)3-1-2-7-4-5-13-12(7)14-8/h1-6H, 11, 13, 14)/b3-1-, 7-2-
H-123		19.257	228.1598	-12.0637	81.2697	321.2139	InChI=1S/C12H7N3O/c16-12-10-6-7(15(12)14-10)2-1-3-8-9-4-5-13-11(8)9/h1-6,13H/b2-1-, 8-3-
H1-132		24.8723	153.6644	-7.3158	127.5475	321.2518	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15-11(14-15)6-9(7)10/h1-6,13H
F-60		19.4982	145.9334	-12.2227	125.9493	321.5251	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(15-6-10(8)15)7-4-5-13-11(7)14-12/h1-6H, 11, 13, 14, 16)
x6-29		23.9086	211.226	-14.5201	91.6976	321.615	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-8(7)6-9-11-12(14-9)15(10)11/h1-6,13H/b3-1-, 7-2-, 8-6-
E-28		7.3988	96.5711	-3.8492	188.6252	322.108	InChI=1S/C12H7N3O/c16-12-9-6-15(12)10-3-1-2-8(14-9)7-4-5-13-11(7)10/h1-6,13H/b14-8-
r-41		16.1938	221.0346	-9.957	88.9855	322.146	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-11(7)14-6-9(8)15(10)12/h1-6H, 11, 13, 14)/b3-1-, 7-2-, 9-6-
o-94		21.8996	201.629	-12.7759	88.5456	322.1473	InChI=1S/C12H7N3O/c16-12-11-10-9(3-4-13-10)15(12)5-1-2-7-6-8(7)14-11/h1-6,13H/b5-1-, 7-2-, 14-11-
H-27		5.9223	122.0041	-2.1837	164.9335	322.1898	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-10(8)11(14-6-7)15(9)12/h1-6,13H
H1-117		3.4496	314.6995	-2.1369	-4.97	322.2114	InChI=1S/C12H7N3O/c16-7-2-1-3-9-8-4-5-13-11(8)14-12-10(6-7)15(9)12/h1-6,13H/b2-1-, 9-3-, 10-6-

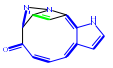
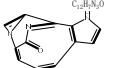
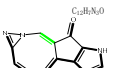
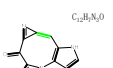
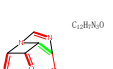

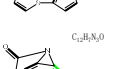
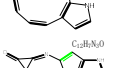
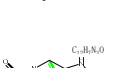
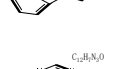
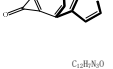
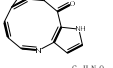
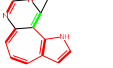
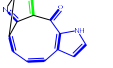
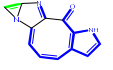
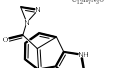

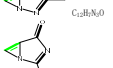
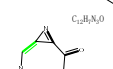
x8-42		11, 6931	232, 5301	-8, 1839	59, 9533	322, 2381	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)14-12-9-6-8(10)15(9)12/h1-6H, (H, 13, 14)/b3-1+, 7-2-
o-60		10, 2032	83, 4459	-1, 4717	186, 9894	322, 3706	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(9)(7)6-14-10)8-3-4-13-11(8)12/h1-6, 13H
H1-4		23, 0032	229, 2796	-10, 8701	60, 4065	322, 6853	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12(7)14-9-6-15(9)10/h1-6, 13H/b3-1-, 7-2-, 14-12+
q-23		9, 0954	146, 3492	-3, 7305	128, 4647	322, 8845	InChI=1S/C12H7N3O/c16-12-11-9-3-1-2-7-4-5-13-10(7)8(14-11)6-15(9)12/h1-6, 13H/b2-1-, 9-3-
G-21		7, 2744	110, 2844	-5, 6755	184, 311	322, 8981	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(10-6-14-15(10)12)8-4-5-13-11(8)9/h1-6, 13H
X-49		18, 3921	206, 7738	-7, 2790	74, 8771	322, 9435	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-14-12-11(15(9)12)10-8(7)3-5-13-10/h1-6, 13H/b2-1-, 14-4+
X22-51		5, 2454	103, 8589	-4, 5579	198, 9348	323, 0094	InChI=1S/C12H7N3O/c16-11-9-6-7-2-1-4-13-8-3-5-14-12(8)15(9)10(7)11/h1-6, 14H/b2-1-, 13-4-
j-2		43, 849	183, 4522	-19, 6747	105, 5004	323, 0448	InChI=1S/C12H7N3O/c16-12-10-9-2-1-4-13-7-3-5-14-8(7)6-15(9)11(10)12/h1-6, 14H/b4-1-, 8-6+, 9-2-, 13-7+
G-7		7, 1878	111, 0751	-2, 2408	179, 4143	323, 1684	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-8-4-5-13-12(8)14-6-15(9)10(7)11/h1-6, 13H
j-16		34, 9177	176, 2139	-11, 6661	102, 2709	323, 1887	InChI=1S/C12H7N3O/c16-12-11-9-2-1-4-13-7-3-5-14-8(7)6-10(11)15(9)12/h1-6, 14H/b2-1-, 4-1-, 8-6+, 9-2-, 10-6+, 13-4-, 13-7-
H1-70		5, 8149	109, 6856	-1, 8814	179, 8445	323, 3168	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12-14-6-9(7)15(10)12/h1-6, 13H
x8-33		30, 6646	246, 8901	-15, 9943	44, 9422	323, 5791	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-6-8-10-11(9)15(8)10/h1-6H, (H, 13, 14)/b3-1-, 7-2-, 8-6-
r1-21		17, 042	248, 406	-12, 8016	49, 6107	323, 7516	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-6-8-10-11(9)15(8)10/h1-6H, (H, 13, 14)/b3-1-, 7-2-, 8-6+
H-115		19, 4701	229, 9522	-12, 1241	80, 9088	323, 8598	InChI=1S/C12H7N3O/c16-12-10-7(6-15(12)14-10)2-1-3-8-9-4-5-13-11(8)9/h1-6, 13H/b2-1-, 8-3-
G-5		6, 7184	33, 5261	-1, 9776	238, 8266	323, 9794	InChI=1S/C12H7N3O/c16-11-9-6-14-15-10(11)3-1-2-7(9)8-4-5-13-12(8)15/h1-6, 13H
x3-19		17, 7343	221, 0329	-9, 3046	51, 7688	324, 1335	InChI=1S/C12H7N3O/c16-12-9-7-6-15(5-1-3-13-10(7)9)8-2-4-14-11(8)12/h1-6, 14H/b5-1-, 13-3-
q1-13		13, 6833	101, 3802	-7, 5023	186, 2112	324, 2038	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-8-6-15(9)14-11(8)12/h1-6, 13H/b2-1-, 9-3+
B-261		11, 5541	185, 1853	-8, 6438	103, 4119	324, 2391	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-9(15)14-11(12)10-7(8)3-4-13-10/h1-6, 13H/b5-1-, 8-2-, 14-11-
C-52		11, 9271	120, 1919	-5, 3248	175, 5246	324, 2574	InChI=1S/C12H7N3O/c16-12-10-7-2-1-4-13-6-9(10)15(12)11-8(7)3-5-14-11/h1-6, 14H/b2-1-, 4-1-, 7-2-, 9-6-, 13-4?, 13-6?

A-151		28.1914	208.0815	-10.9522	72.0548	324.5239	InChI=1S/C12H7N3O/c16-12-10-8-2-1-5-15(11)(10)12)14-6-9-7(8)3-4-13-9/h1-6,13H/b14-6-
	$C_{12}H_7N_3O$						
H-45		16.5552	228.1068	-6.7528	59.958	324.9105	InChI=1S/C12H7N3O/c16-12-10-7-6-8(7)13-3-1-5-15(12)9-2-4-14-11(9)10/h1-6,14H/b5-1-,10-7-,13-3+
	$C_{12}H_7N_3O$						
H-13		7.5134	121.769	-1.6206	163.9985	324.9178	InChI=1S/C12H7N3O/c16-10-7-2-1-3-9-8-4-5-13-11(8)14-12(10)15(9)6-7/h1-6,13H
	$C_{12}H_7N_3O$						
o-227		24.5225	166.3196	-9.1128	115.0129	324.9256	InChI=1S/C12H7N3O/c16-10-6-9-11-7(14-11)2-1-5-15(9)8-3-4-13-12(8)10/h1-6,13H
	$C_{12}H_7N_3O$						
x4-14		28.8571	239.6461	-16.4459	55.8546	325.044	InChI=1S/C12H7N3O/c16-12-9-10-7(4-5-13-10)2-1-3-8-14-6-15(8)11(9)12/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
A2-39		20.6112	203.2816	-7.6498	90.225	325.1266	InChI=1S/C12H7N3O/c16-12-10-6-9-7(2-1-4-13-9)8-3-5-14-11(8)15(10)12/h1-6,14H
	$C_{12}H_7N_3O$						
F-46		12.1969	171.3321	-8.4357	118.9971	325.1852	InChI=1S/C12H7N3O/c16-11-7-2-1-3-9(11)10-6-15(10)14-12-8(7)4-5-13-12/h1-6H, (H,13,14)/b8-7-
	$C_{12}H_7N_3O$						
j-12		16.1788	251.3693	-12.7943	48.9753	325.3577	InChI=1S/C12H7N3O/c16-10-6-8-7(3-5-14-8)13-4-1-2-9-11-12(10)15(9)11/h1-6,14H/b4-1-,8-6+,9-2-,13-7-
	$C_{12}H_7N_3O$						
A-171		8.1382	184.821	-5.6108	105.8705	325.3578	InChI=1S/C12H7N3O/c16-11-9-8(3-4-13-9)7-2-1-5-15-10(11)12(15)14-6-7/h1-6,13H/b5-1-,7-2-,14-6-
	$C_{12}H_7N_3O$						
r-21		14.6329	215.965	-6.6379	95.3195	325.4156	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)14-11(8)15(9)12/h1-6H, (H,13,14)
	$C_{12}H_7N_3O$						
H11-134		42.2807	270.6401	-17.5813	16.0664	325.4455	InChI=1S/C12H7N3O/c16-11-6-8(11)9-2-1-3-10-7-4-5-13-12(7)15(10)14-9/h1-6,13H
	$C_{12}H_7N_3O$						
H11-125		16.4648	144.5879	-11.662	131.6228	325.4553	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(10-6-15(10)14-9)8-4-5-13-11(8)12/h1-6,13H/b3-1-,7-2-,14-9-
	$C_{12}H_7N_3O$						
X23-14		35.1847	178.0543	-11.384	118.2383	325.4594	InChI=1S/C12H7N3O/c16-12-10-7-2-1-4-13-8-3-5-14-11(8)15(12)9(10)6-7/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
o-207		8.1708	111.2585	-1.3792	170.7013	325.5857	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(12)9-3-4-13-11(9)10(8)14-7/h1-6,13H/b5-1-,7-2-
	$C_{12}H_7N_3O$						
o-15		11.3896	146.0053	-3.1998	138.6949	325.6652	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-8(9)6-10(15)11(12)14-7/h1-6,13H/b5-1-,7-2-
	$C_{12}H_7N_3O$						
G-8		6.1099	34.1798	-1.9431	242.3326	325.7278	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-8-4-5-13-12(8)15(9)6-14-10(7)11/h1-6,13H
	$C_{12}H_7N_3O$						
o-61		5.3564	65.0881	-1.9593	219.5756	325.8005	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(6-8(7)14-10)9-3-4-13-11(9)12/h1-6,13H
	$C_{12}H_7N_3O$						
H11-112		19.3263	170.7741	-11.382	105.2929	325.8254	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(14-12)10-6-15(10)11-7(8)4-5-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
x2-2		44.6647	170.9174	-19.846	112.1233	325.8786	InChI=1S/C12H7N3O/c16-12-10-9-6-8-7(2-4-14-8)13-3-1-5-15(9)11(10)12/h1-6,14H/b5-1-,9-6-,13-3+
	$C_{12}H_7N_3O$						

E-12		9, 2618	74, 2055	-3, 5044	206, 8067	325, 9341	InChI=1S/C12H7N3O/c16-11-9-3-1-2-8-7-4-5-13-12(7)15(9)10(11)6-14-8/h1-6, 13H/b2-1-, 9-3-
q-14		8, 1924	141, 9647	-2, 7498	150, 3899	325, 9495	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-4-5-13-10(7)8-6-15(9)12(11)14-8/h1-6, 13H/b2-1-, 9-3-
H-163		23, 503	237, 7916	-10, 716	50, 8736	326, 2605	InChI=1S/C12H7N3O/c16-12-14-11-8(9-4-5-13-10(9)11)3-1-2-7-6-15(7)12/h1-6, 13H/b2-1-, 8-3-, 14-11+
X22-15		11, 2117	275, 7946	-7, 5539	31, 8228	326, 283	InChI=1S/C12H7N3O/c16-12-7-6-9-8(3-5-14-9)13-4-1-2-10-11(7)15(10)12/h1-6, 14H/b2-1-, 4-1-, 7-6+, 9-6+, 10-2+, 13-4-, 13-8-
E-9		5, 6676	32, 6603	-1, 488	253, 2698	326, 3254	InChI=1S/C12H7N3O/c16-11-9-6-15-10(11)3-1-2-8(14-9)7-4-5-13-12(7)15/h1-6, 13H/b2-1-, 10-3-
x4-37		13, 419	231, 0312	-5, 0512	73, 1905	326, 4661	InChI=1S/C12H7N3O/c16-12-11-9-8(6-14-15(11)12)3-1-2-7-4-5-13-10(7)9/h1-6, 13H
H11-34		6, 402	104, 3469	-2, 3727	176, 2397	326, 5063	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-8(10)9-4-5-13-11(9)15(12)14-7/h1-6, 13H
G1-85		20, 3665	192, 0836	-8, 7673	69, 7877	326, 5209	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-10(7)12-11(9)15(12)6-14-8/h1-6, 13H/b3-1-, 8-2-
H-42		8, 1063	125, 9041	-1, 8084	164, 0574	326, 5657	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9-8-4-5-13-11(8)15(7)12(10)14-9/h1-6, 13H/b2-1-, 9-3-
H11-26		30, 7559	226, 4123	-3, 1898	60, 7433	326, 821	InChI=1S/C12H7N3O/c16-12-9-6-10-8(4-5-13-10)7(9)2-1-3-11-14-15(11)12/h1-6, 13H/b3-1-, 7-2-
n-172		9, 5084	83, 932	-3, 139	205, 0707	326, 9305	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-14-10(7)9(12)11-8(15)3-4-13-11/h1-6, 13H/b5-1-, 7-2+
B-217		5, 9470	36, 5117	-1, 7935	246, 7211	326, 9660	InChI=1S/C12H7N3O/c16-12-9-6-15-5-1-2-7(11(12)14-15)8-3-4-13-10(8)9/h1-6, 13H
H11-40		19, 0493	227, 477	-11, 769	89, 5236	327, 1579	InChI=1S/C12H7N3O/c16-12-9-6-15(12)10(14-9)3-1-2-7-8-4-5-13-11(7)8/h1-6, 13H/b3-1-, 7-2-
H1-45		12, 4953	221, 744	-6, 8788	71, 3658	327, 1913	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-9(7)6-10(8)15-12(11)14-15/h1-6, 13H/b3-1-, 8-2-
G1-102		17, 2769	258, 4896	-7, 9662	25, 5658	327, 271	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-8(7)6-14-12-11(10)15(9)12/h1-6, 13H
x5-46		21, 2722	254, 0267	-11, 7759	37, 9909	327, 3277	InChI=1S/C12H7N3O/c16-12-10-9-8(6-15(9)10)3-1-2-7-4-5-13-11(7)14-12/h1-6H, 0L, 13, 14, 16) /b3-1-, 7-2-
o-72		9, 6465	85, 3861	-1, 3028	190, 7921	327, 566	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(9)8-3-4-13-12(8)14-11(7)10/h1-6, 13H
B-249		12, 1788	185, 5793	-8, 0506	105, 6709	327, 5795	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-6-9(15)10(11)14-12-8(7)3-4-13-12/h1-6, 13H/b5-1-, 7-2-
x4-12		28, 843	239, 7963	-16, 5141	54, 2626	327, 6644	InChI=1S/C12H7N3O/c16-12-9-10-7(4-5-13-10)2-1-3-8-6-14-15(8)11(9)12/h1-6, 13H/b2-1-, 8-3-




















C-70		15, 4224	229, 9853	-8, 2708	69, 6491	327, 7104	InChI=1S/C12H7N3O/c16-12-14-4-1-2-7-8-3-5-13-11(8)15(12)10-6-9(7)10/h1-6, 13H/b2-1-, 14-4+
H1-74		10, 2011	161, 177	-4, 0584	137, 0456	327, 9363	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9-14-12(15(9)10)-11-8(7)4-5-13-11/h1-6, 13H/b3-1-, 7-2+
J-6		19, 2812	186, 7255	-11, 9631	105, 5102	328, 1127	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-9(8)6-15-10(7)11(12)15/h1-6, 14H/b4-1-, 7-2+, 9-6+, 13-8-
H11-160		14, 8974	277, 8875	-10, 9147	37, 22	328, 2241	InChI=1S/C12H7N3O/c16-12-8(7-4-5-13-11(7)12)2-1-3-9-10-6-15(10)14-9/h1-6, 13H/b3-1-, 8-2-
x5-37		27, 1838	291, 4628	-17, 2036	15, 7491	328, 4594	InChI=1S/C12H7N3O/c16-12-10-9(15(10)12)6-8-3-1-2-7-4-5-13-11(7)14-8/h1-6H, (H, 13, 14)/b8-6+
H1-14		5, 1122	102, 3543	-1, 7656	192, 1384	328, 6005	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)15-10(11)6-9(7)14-15/h1-6, 13H/b3-1-, 7-2-
q1-24		15, 515	162, 4007	-5, 1711	140, 3574	328, 7814	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-6-9-11(14-9)15(8)12/h1-6, 13H/b2-1-, 8-3-
r-43		14, 0148	219, 797	-6, 4437	96, 359	328, 7999	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-11(7)14-9(8)6-15(10)12/h1-6H, (H, 13, 14)/b3-1-, 7-2-
o-19		5, 3063	38, 6774	-1, 5446	251, 8438	328, 8518	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-10-3-4-13-11(10)8(7)6-9(12)14-15/h1-6, 13H/b5-1-, 7-2+
o-85		6, 0951	27, 3608	-2, 4223	256, 3581	329, 0251	InChI=1S/C12H7N3O/c16-10-6-7-8-2-1-5-15(12(10)14-8)9-3-4-13-11(7)9/h1-6, 13H
G-27		24, 4014	201, 9059	-10, 4277	95, 783	329, 2019	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-8-4-5-13-11(8)14-6-10(7)15(9)12/h1-6H, (H, 13, 14)
q1-47		25, 8758	160, 9622	-9, 2859	126, 9452	329, 2413	InChI=1S/C12H7N3O/c16-10-6-9-8(12-14-15(9)12)3-1-2-7-4-5-13-11(7)10/h1-6, 13H/b2-1-, 8-3+, 9-6+
x6-19		25, 1396	130, 4511	-18, 0599	162, 6484	329, 2563	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-9(7)6-8(10)11-12-14-15(11)12/h1-6, 13H/b3-1-, 7-2-, 9-6+, 11-8+
x6-28		25, 1398	130, 4462	-18, 0624	162, 6538	329, 2563	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-9(7)6-8(10)11-12-14-15(11)12/h1-6, 13H/b3-1-, 7-2-, 9-6+, 11-8-
D-12		6, 3423	186, 5784	-1, 2905	115, 3382	329, 3851	InChI=1S/C12H7N3O/c16-12-8-6-10-11-7(3-5-14-11)9(15(10)12)2-1-4-13-8/h1-6, 14H/b2-1-, 4-1-, 9-2-, 13-4-, 13-8-
B-149		7, 9676	47, 8663	-3, 0484	244, 2945	329, 4064	InChI=1S/C12H7N3O/c16-12-11-8-2-1-5-15(12(10(14-11)6-9-7(8)3-4-13-9/h1-6, 13H
A2-52		22, 2939	297, 6044	-16, 8012	18, 3984	329, 4496	InChI=1S/C12H7N3O/c16-11-8(7-3-5-13-10(7)11)2-1-4-14-12-9-6-15(9)12/h1-6, 13H/b4-1-, 8-2-, 14-12+
n-39		32, 1661	235, 7711	-14, 0655	58, 758	329, 5284	InChI=1S/C12H7N3O/c16-11-7-6-14-12-9(3-4-13-12)15-5-1-2-8(15)10(7)11/h1-6, 13H/b14-6+
B-245		22, 7354	214, 2626	-11, 1336	96, 2573	329, 8089	InChI=1S/C12H7N3O/c16-11-8(7-3-4-13-10(7)11)2-1-5-15-6-9-12(15)14-9/h1-6, 13H/b5-1-, 8-2-

G-80		20.8215	184.3881	-10.7917	116.717	329.9656	InChI=1S/C12H7N3O/c16-12-14-6-9-7(4-5-13-9)8-2-1-3-10-11(8)15(10)12/h1-6,13H/b14-6+
X-38		27.2207	299.0374	-17.4719	15.2944	330.1413	InChI=1S/C12H7N3O/c16-12-10-9(15(10)12)6-7-2-1-4-13-11(8)7(3-5-14-11)/h1-6,14H
q1-25		3.8077	320.7917	-3.8746	-6.9	330.3065	InChI=1S/C12H7N3O/c16-11-9(15-6-8-12(15)14-8)3-1-2-7-4-5-13-10(7)11/h1-6,13H
B-222		6.9967	25.6906	-2.5947	252.3510	330.3711	InChI=1S/C12H7N3O/c16-12-9-6-15-5-1-2-7(9)8-3-4-13-10(8)11(15)14-12/h1-6,13H
H1-86		29.2675	232.3062	-14.6918	54.3331	330.5339	InChI=1S/C12H7N3O/c16-11-3-1-2-9-7-4-5-13-12(7)15(9)10-6-8(10)14-11/h1-6,13H/b3-1-,9-2-,14-8-
H11-58		19.5947	247.5686	-12.2697	67.4285	330.604	InChI=1S/C12H7N3O/c16-11-6-10-9(14-5-10(11)3-1-2-7-8-4-5-13-12(7)8)/h1-6,13H/b3-1-,7-2-
H1-52		6.097	110.2737	-2.5903	185.4815	330.8791	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)8-6-15(9)12(10)14-8/h1-6,13H
B-234		9.1254	116.6030	-1.7667	178.0672	331.1962	InChI=1S/C12H7N3O/c16-12-11-8-6-15(12)5-1-2-9(14-11)7-3-4-13-10(7)8/h1-6,13H/b5-1-,9-2-
xS-42		14.0647	223.2202	-6.5934	94.1026	331.2831	InChI=1S/C12H7N3O/c16-12-10-9-8(6-15(10)12)3-1-2-7-4-5-13-11(7)14-9/h1-6H,(H,13,14)/b3-1-,7-2-
F-70		10.4757	201.8327	-7.0701	100.2318	331.2863	InChI=1S/C12H7N3O/c16-12-14-11-8(4-5-13-11)7-2-1-3-9-10(6-7)15(9)12/h1-6H,(H,13,14,16)/b8-7-
p1-40		4.254	321.4149	-3.7151	-5.8399	331.3219	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11(9)15-6-8-12(15)14-8/h1-6,13H
A2-6		22.6442	255.5083	-15.3912	59.6908	331.3838	InChI=1S/C12H7N3O/c16-12-9-6-15(12)11(9)14-4-1-2-7-8-3-5-13-10(7)8/h1-6,13H/b4-1-,7-2-,14-11+
r-31		19.0139	203.7369	-10.9016	116.8254	331.6135	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)14-6-9-10(8)15(9)12/h1-6H,(H,13,14)
B-109		3.0749	333.9557	-2.4695	-6.1700	331.6171	InChI=1S/C12H7N3O/c16-12-8(14-12)6-10-11-7(3-4-13-11)9-2-1-5-15(9)10/h1-6,13H/b10-6+
F-13		8.1316	84.0056	-2.6531	209.865	331.625	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10-9(11)6-15(10)14-12-8(7)4-5-13-12/h1-6H,(H,13,14)/b8-7+
o-79		16.1713	176.2141	-12.2469	126.979	331.6479	InChI=1S/C12H7N3O/c16-10-6-7-8(14-11(7)10)2-1-5-15-9-3-4-13-12(9)15/h1-6,13H/b5-1-,8-2+
o-145		9.7408	80.0743	-1.7626	202.6726	331.6808	InChI=1S/C12H7N3O/c16-10-6-9-11-7(10)2-1-5-15(9)8-3-4-13-12(8)14-11/h1-6,13H
C-53		6.4407	125.8465	-3.0804	172.2254	331.7248	InChI=1S/C12H7N3O/c16-12-10-7-2-1-4-13-9(10)6-15(12)11-8(7)3-5-14-11/h1-6,14H
k1-18		16.8175	158.1135	-11.22	147.9749	331.7926	InChI=1S/C12H7N3O/c16-12-7-6-9-11(7)15(9)5-1-3-13-8-2-4-14-10(8)12/h1-6,14H/b5-1-,13-3-

p11-24		10.9482	147.4734	-3.4674	143.1155	331.9131	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9-12(10)14-15(8)9/h1-6,13H/b3-1-,7-2-,11-8-
q11-48		10.0202	190.8876	-5.1363	97.5052	332.0808	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(14-12)9-6-15(8)9/h1-6,13H/b2-1-,8-3+
H11-139		16.8839	190.0491	-3.7657	95.6086	332.1529	InChI=1S/C12H7N3O/c16-12-9-6-15-10(14-15)3-1-2-7(9)8-4-5-13-11(8)12/h1-6,13H/b3-1-,7-2-,9-6+
o-13		16.927	190.8585	-8.8846	93.8056	332.4291	InChI=1S/C12H7N3O/c16-12-10-2-1-5-15(10)9-3-4-13-7(9)6-8-11(12)14-8/h1-6,13H/b8-6+
x4-32		9.878	187.6349	-1.1636	107.9719	332.4739	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)10-11(12)15(8)6-14-10/h1-6,13H/b2-1-,8-3+
o-107		2.901	334.5617	-2.4463	-6.17	332.6181	InChI=1S/C12H7N3O/c16-12-8(14-12)6-7-9-2-1-5-15(9)10-3-4-13-11(7)10/h1-6,13H/b7-6+
p-24		15.463	217.275	-6.2119	96.1616	332.8611	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-10-11(14-8)15(10)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,9-6-,10-6+
o-3		18.2406	222.3613	-9.4373	84.4834	332.9272	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-8(9)6-10(15)14-11(7)12/h1-6,13H/b5-1-,7-2-,14-11+
H1-25		5.0164	102.2729	-2.2529	204.1877	332.9873	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)9-6-14-12(8)15(9)10/h1-6,13H
A-188		30.1092	206.1159	-11.8249	78.2583	333.0942	InChI=1S/C12H7N3O/c16-11-9-7-2-1-5-15(10)9)11)6-14-12-8(7)3-4-13-12/h1-6,13H/b14-6-
X22-44		10.4703	243.6752	-7.9162	56.9717	333.2431	InChI=1S/C12H7N3O/c16-12-7-6-15-9(11)7)15)2-1-4-13-8-3-5-14-10(8)12/h1-6,14H/b14-6-,13-4-
x4-43		16.8683	220.0994	-5.7104	88.6999	333.322	InChI=1S/C12H7N3O/c16-12-11-9-8(14-6-15(11)12)3-1-2-7-4-5-13-10(7)9/h1-6,13H
q1-5		11.6463	109.3915	-7.3654	192.9686	333.4662	InChI=1S/C12H7N3O/c16-12-8-6-15-9(11)8)14-15)3-1-2-7-4-5-13-10(7)12/h1-6,13H/b2-1-,9-3+
q1-44		18.001	227.8925	-12.7477	77.8378	333.5158	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-11(12)14-9-6-15(8)9/h1-6,13H/b2-1-,8-3+
G-41		25.3092	164.5878	-11.5449	135.9675	333.6094	InChI=1S/C12H7N3O/c16-12(15-6-14-15)10-7-2-1-3-9(10)11-8(7)4-5-13-11/h1-6,13H
H11-113		28.17	264.4491	-19.4634	41.5302	333.6596	InChI=1S/C12H7N3O/c16-12-9(14-15-6-10(12)15)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
H11-97		31.7296	272.4363	15.0725	36.2329	333.6722	InChI=1S/C12H7N3O/c16-12-9-6-15(9)10(14-12)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
B-242		13.5278	196.6577	-6.6820	87.6995	333.8300	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)9-2-1-5-15(9)6-8-11(12)14-8/h1-6,13H/b8-6+
B-79		19.5665	194.5424	-13.1393	117.7632	334.0500	InChI=1S/C12H7N3O/c16-12-9-6-10(14-9)15(12)5-1-2-7-8-3-4-13-11(7)8/h1-6,13H/b5-1-,7-2-

F-25		18.0432	281.6491	-10.3816	47.6965	334.1887	InChI=1S/C12H7N3O/c16-12-10-6-7(15(10)12)2-1-3-9-8-4-5-13-11(8)14-9/h1-6H, (H, 13, 14)/b3-1-, 7-2-
A2-38		13.7883	240.6196	-9.4275	64.3984	334.5143	InChI=1S/C12H7N3O/c16-12-8-2-1-4-13-9-6-10(9)15(12)11-7(8)3-5-14-11/h1-6, 14H/b4-1-, 8-2-, 13-9-
n-12		6.4967	154.4565	-3.5067	148.8136	334.6785	InChI=1S/C12H7N3O/c16-9-6-14-11(9)12-7-2-1-5-15(12)8-3-4-13-10(7)8/h1-6, 13H/b12-11-
X23-4		7.2476	339.466	-5.0468	-5.7	335.0525	InChI=1S/C12H7N3O/c16-12-11-9-7(6-15(11)12)2-1-4-13-8-3-5-14-10(8)9/h1-6, 14H/b2-1-, 13-4-
X23-21		7.2457	339.4678	-5.0468	-5.7	335.0525	InChI=1S/C12H7N3O/c16-12-11-9-7(6-15(11)12)2-1-4-13-8-3-5-14-10(8)9/h1-6, 14H/b2-1-, 13-4+
r1-29		18.8639	223.1337	-11.7074	97.9347	335.4465	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)14-8-6-9-11(8)15(9)10/h1-6H, (H, 13, 14)/b3-1-, 7-2-
o-5		16.4295	178.6009	-12.2921	127.8096	335.4469	InChI=1S/C12H7N3O/c16-11-7(8-6-14-10(8)11)2-1-5-15-9-3-4-13-12(9)15/h1-6, 13H/b5-1-, 7-2+
p11-20		22.7589	217.8445	-13.3048	82.3133	335.4713	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)6-14-11-10(8)15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3-, 9-6+, 14-6-, 14-11+
H11-122		11.1866	99.7375	-2.7149	175.0327	335.5051	InChI=1S/C12H7N3O/c16-11-6-10-7-2-1-3-9(11)14-15(10)12-8(7)4-5-13-12/h1-6, 13H/b3-1-, 7-2-
q-10		19.4414	180.8494	-2.156	113.7445	335.5104	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)9(8)6-15-12(11)14-15/h1-6, 13H
B-98		15.8167	305.5684	-13.2833	22.6707	335.5370	InChI=1S/C12H7N3O/c16-12-8(7-3-4-13-11(7)12)2-1-5-15-10-6-9(10)14-15/h1-6, 13H/b5-1-, 8-2-
A1-42		17.6926	215.6149	-10.2434	77.8047	335.6108	InChI=1S/C12H7N3O/c16-9-6-13-4-1-2-7-8-3-5-14-12(8)15-10(7)11(9)15/h1-6, 14H/b4-1-, 7-2-, 13-6-
H-66		18.1452	185.7179	-10.4126	102.6894	335.6184	InChI=1S/C12H7N3O/c16-10-8-3-1-2-7-6-15(7)12(10)14-11-9(8)4-5-13-11/h1-6, 13H/b2-1-, 8-3-
A2-50		22.0931	202.3427	-12.5906	81.7261	335.7968	InChI=1S/C12H7N3O/c16-11-8-2-1-4-14-12(11)15-6-9(15)10-7(8)3-5-13-10/h1-6, 13H
B-257		8.4961	42.0850	-3.8879	239.5820	335.8619	InChI=1S/C12H7N3O/c16-11-10-8(3-4-13-10)7-2-1-5-15-6-9(7)14-12(11)15/h1-6, 13H
H-57		7.3856	122.383	-2.2018	173.7937	335.9411	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8-9-4-5-13-11(9)15(7)12(8)14-10/h1-6, 13H
s11-40		4.2513	102.4648	-2.7962	210.8065	336.2329	InChI=1S/C12H7N3O/c16-12-10-8-6-15(12)9(14-8)3-1-2-7-4-5-13-11(7)10/h1-6, 13H/b3-1-, 7-2-, 11-10-
o-233		15.8038	311.7954	-13.5174	27.6972	336.309	InChI=1S/C12H7N3O/c16-12-11-10(3-4-13-11)15(12)5-1-2-8-7-6-9(7)14-8/h1-6, 13H/b5-1-, 8-2+
o-248		6.0276	90.7349	-1.4137	196.8781	336.4234	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(12(7)14-10)9-3-4-13-11(8)9/h1-6, 13H

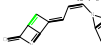
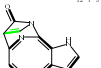
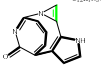

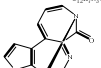
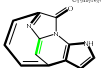
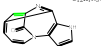
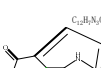
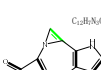
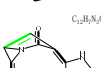
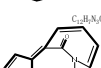
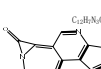
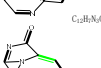
p1-16		$C_{22}H_{18}N_2O$	27.9003	118.2154	-12.4422	165.3428	336.4681	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)12-11-9(6-8)15(12)14-11/h1-6,13H/h3-1-,7-2-,9-6-,12-10+
o-254		$C_{22}H_{18}N_2O$	2.0165	299.8684	-1.751	35.6676	336.5124	InChI=1S/C12H7N3O/c16-12-14-10-8-6-7(8)2-1-5-15(12)9-3-4-13-11(9)10/h1-6,13H/h5-1-,7-2-
q11-45		$C_{22}H_{18}N_2O$	12.7815	209.7689	-5.8231	103.0075	336.5238	InChI=1S/C12H7N3O/c16-12-14-8-6-10-9(15)(10)12(3)-1-2-7-4-5-13-11(7)8/h1-6,13H/h2-1-,9-3+
s11-53		$C_{22}H_{18}N_2O$	11.1238	209.9077	-5.1073	105.4582	336.7171	InChI=1S/C12H7N3O/c16-12-14-8-3-1-2-7-4-5-13-10(7)11-9(6-8)15(11)12/h1-6,13H/h3-1-,7-2-,11-10-
s12-16		$C_{22}H_{18}N_2O$	54.8706	211.7163	-32.8787	71.295	336.8211	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)9-3-1-2-7-4-5-13-8(7)6-14-9/h1-6,13H/h2-1-,3-1-,7-2-,8-6+,9-3+,14-6-,14-9+
i-28		$C_{22}H_{18}N_2O$	14.7854	208.7932	-6.4856	114.8468	336.9067	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-10(8)11-9(6-7)15(11)12/h1-6,14H/h2-1-,4-1-,7-2-,11-10+,13-4-,13-8+
H-60		$C_{22}H_{18}N_2O$	26.0085	218.0912	-9.7625	96.1033	337.3351	InChI=1S/C12H7N3O/c16-12-9(8-4-5-13-11(8)12)3-1-2-7-6-10-14-15(7)10/h1-6,13H/h2-1-,9-3-
G-6		$C_{22}H_{18}N_2O$	10.0939	128.7254	-3.46	160.0812	337.4775	InChI=1S/C12H7N3O/c16-12-10-3-1-2-8-7-4-5-13-9(7)6-14-15(10)11(8)12/h1-6,13H
H11-106		$C_{22}H_{18}N_2O$	10.1817	126.4028	-2.7997	167.3055	337.918	InChI=1S/C12H7N3O/c16-11-6-9-7-2-1-3-10(14-11)15(9)12-8(7)4-5-13-12/h1-6,13H
x9-1		$C_{22}H_{18}N_2O$	35.3336	235.4143	-22.3718	71.0153	338.154	InChI=1S/C12H7N3O/c16-9-6-14-15-11-8(12(11)15)3-1-2-7-4-5-13-10(7)9h1-6,13H/h2-1-,8-3-,14-6-
o-18		$C_{22}H_{18}N_2O$	7.7278	35.6726	-2.2317	249.6561	338.2417	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-10(8)11(12)14-9(15)6-7/h1-6,13H
o-179		$C_{22}H_{18}N_2O$	7.858	70.9104	-2.4469	224.9587	338.3936	InChI=1S/C12H7N3O/c16-12-8-6-9-7(8)2-1-5-15(14-9)10-3-4-13-11(10)12/h1-6,13H
i-99		$C_{22}H_{18}N_2O$	25.8483	245.7115	-13.318	48.2028	338.3965	InChI=1S/C12H7N3O/c16-12-8-6-7(8)11-10-9(2-4-13-10)15(11)5-1-3-14-12/h1-6,13H/h5-1-,11-7-,14-3+
E-16		$C_{22}H_{18}N_2O$	8.1091	72.7688	-3.2688	224.3353	338.4704	InChI=1S/C12H7N3O/c16-12-8-6-15-10(8)3-1-2-9(14-12)7-4-5-13-11(7)15/h1-6,13H/h2-1-,10-3-,14-9+
B-68		$C_{22}H_{18}N_2O$	11.8574	109.6420	-2.7712	186.5797	338.5070	InChI=1S/C12H7N3O/c16-12-8-6-10-14-9(2-1-5-15(10)12)7-3-4-13-11(7)8/h1-6,13H
C-36		$C_{22}H_{18}N_2O$	14.4312	92.3847	-3.8004	196.1578	338.5475	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-5-13-11)8-2-1-4-14-15(9)12(8)10/h1-6,13H
H-84		$C_{22}H_{18}N_2O$	7.3195	44.3855	-3.0549	243.7567	338.6053	InChI=1S/C12H7N3O/c16-12-10-7-2-1-3-9(15(6-7)14-10)8-4-5-13-11(8)12/h1-6,13H
B-102		$C_{22}H_{18}N_2O$	13.1263	221.6240	-10.6649	88.0241	338.7482	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)10-6-9(10)14-11-7(8)3-4-13-11/h1-6,13H/h14-9-
G-12		$C_{22}H_{18}N_2O$	6.7823	126.9748	-1.5787	176.1931	338.8253	InChI=1S/C12H7N3O/c16-11-9-3-1-2-8(12-14-6-15(9)12)7-4-5-13-10(7)11/h1-6,13H




















A1-19		17,5665	253,4454	-9,8606	32,0108	338,8317	InChI=1S/C12H7N3O/c16-12-10-7(3-5-14-10)8-2-1-4-13-6-9-11(8)15(9)12/h1-6,14H/b2-1-,4-1-,8-2-,9-6+,13-4-,13-6-
H11-109		10,3379	203,4154	-4,026	85,4265	338,8862	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)7-2-1-3-10(14-12)15-6-9(7)15/h1-6,13H/b14-10-
G-52		5,7939	108,1391	-2,1437	193,9557	338,9486	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7(6-14-10)15(12)11-9(8)4-5-13-11/h1-6,13H/b2-1-,3-1-,7-2+,8-3-
s11-4		22,0201	269,3135	-7,729	32,9072	338,9592	InChI=1S/C12H7N3O/c16-12-10-6-8-9(14-15(10)12)3-1-2-7-4-5-13-11(7)8/h1-6,13H
H11-104		10,0448	191,2616	-2,4097	106,2139	338,9683	InChI=1S/C12H7N3O/c16-12-10-6-7(14-12)2-1-3-9-8-4-5-13-11(8)15(9)10/h1-6,13H/b2-1-,9-3-
i-12		16,1725	220,287	-5,893	87,2593	339,0965	InChI=1S/C12H7N3O/c16-12-10-6-7-9(15(10)12)2-1-4-13-8-3-5-14-11(7)8/h1-6,14H/b2-1-,4-1-,9-2+,11-7+,13-4-,13-8-
A1-49		55,5152	218,7234	-29,0852	52,3091	339,4702	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)9-2-1-4-13-6-8-7(9)3-5-14-8/h1-6,14H/b2-1-,4-1-,8-6-,9-2-,9-7+,13-4-,13-6+
o-9		9,4343	111,4506	-2,7987	181,5331	339,6004	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-10(9)8(6-7)11(12)14-15/h1-6,13H/b5-1-,7-2-
x9-42		30,3636	233,7751	-23,8712	59,1604	339,6402	InChI=1S/C12H7N3O/c16-12-9-8(11(9)15-6-14-15)3-1-2-7-4-5-13-10(7)12/h1-6,13H/b2-1-,8-3+
i-51		13,4506	120,4575	-4,6611	166,5437	339,7146	InChI=1S/C12H7N3O/c16-12-10-7-6-9(10)15(5-1-3-14-12)8-2-4-13-11(7)8/h1-6,13H/b5-1-,14-3-
X-34		27,8730	299,1631	-16,0762	16,9733	339,9600	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)9-8(3-5-14-9)7-2-1-4-13-6-7/h1-6,14H
p-14		20,2351	162,081	-3,9076	134,5841	339,9657	InChI=1S/C12H7N3O/c16-11-8-6-9-7(4-5-13-9)2-1-3-10(11)15-12(8)14-15/h1-6,13H/b2-1-,8-6+,10-3+
o-230		25,6556	238,1183	-14,0606	91,9452	339,9695	InChI=1S/C12H7N3O/c16-12-11-9(3-4-13-11)15(12)5-1-2-7-8-6-14-10(7)8/h1-6,13H/b5-1-,7-2+
o-77		6,7134	145,262	-2,141	153,9927	340,149	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(14-12(8)10)9-3-4-13-11(7)9/h1-6,13H
H1-122		21,1659	219,0202	-17,1838	99,1204	340,1576	InChI=1S/C12H7N3O/c16-10-3-1-2-8(7-4-5-13-11(7)10)14-12-9-6-15(9)12/h1-6,13H/b14-12+
H-160		18,8293	246,3922	-11,7981	85,2565	340,4883	InChI=1S/C12H7N3O/c16-12-14-10-6-7(15(10)12)2-1-3-8-9-4-5-13-11(8)9/h1-6,13H/b2-1-,8-3-
o-213		6,89	28,3364	-2,491	257,0335	340,6312	InChI=1S/C12H7N3O/c16-12-8-6-15-5-1-2-7(8)10(14-12)11-9(15)3-4-13-11/h1-6,13H
o-214		6,8892	28,3366	-2,4911	257,0333	340,6312	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-5-15(9)8-3-4-13-11(8)10(7)14-12/h1-6,13H
p11-22		47,5233	255,5096	-26,997	51,4866	340,6455	InChI=1S/C12H7N3O/c16-12-14-6-9-7(4-5-13-9)2-1-3-8-10-11(8)15(10)12/h1-6,13H/b2-1-,8-3-,14-6-

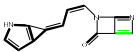
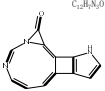

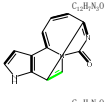

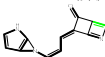
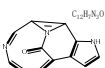
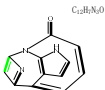
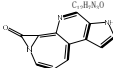


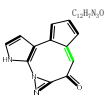





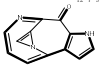
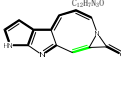
q1-4		15.001	163.3035	-9.7754	142.7326	340.8909	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-9-6-15(12)14-11(8)9/h1-6,13H/b2-1-,8-3-
H1-43		32.1367	270.6311	-22.0138	42.194	340.9394	InChI=1S/C12H7N3O/c16-9(12-14-10-6-15(10)12)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
A-12		7.8283	163.8026	-3.318	145.9023	341.0126	InChI=1S/C12H7N3O/c16-9-6-14-10(9)11-7-2-1-5-15(11)12-8(7)3-4-13-12/h1-6,13H/b11-10-
H1-107		15.4403	166.0341	-3.1273	149.5285	341.2372	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9-12(14-9)15(10)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
o-239		23.6941	212.579	-10.3956	83.8807	341.2591	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(10)9-3-4-13-12(9)14-11(7)8/h1-6,13H/b5-1-,7-2+,8-6-,14-11-
n-46		29.4146	212.8899	-11.5776	74.2928	341.2777	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(11(10)12)9-3-4-13-8(9)6-14-7/h1-6,14H/b14-6-
C-41		4.4506	351.5815	-4.3287	-5.7000	341.4528	InChI=1S/C12H7N3O/c16-10-6-9-11(15(9)10)7-2-1-4-13-12-8(7)3-5-14-12/h1-6,14H/b11-7-
H11-47		16.6399	257.5302	-6.462	65.7434	341.4878	InChI=1S/C12H7N3O/c16-12-10-6-14-9-3-1-2-7(9)8-4-5-13-11(8)15(10)12/h1-6,13H/b10-6-,14-9-
H11-154		26.4572	163.5921	-4.3551	128.0526	341.5085	InChI=1S/C12H7N3O/c16-10-6-9-7(8-4-5-13-12(8)10)2-1-3-11-14-15(9)11/h1-6,13H
B-227		5.3579	34.9085	-1.6482	272.4896	341.5742	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-6-9(11)14-12(15)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-
H-155		18.8088	247.4619	-11.7108	84.8688	341.6548	InChI=1S/C12H7N3O/c16-12-14-11-7(6-15(11)12)2-1-3-8-9-4-5-13-10(8)9/h1-6,13H/b2-1-,8-3-
q-15		11.6599	174.3275	-4.9924	95.8393	341.8057	InChI=1S/C12H7N3O/c16-12-11-9-6-8(15(12)14-11)3-1-2-7-4-5-13-10(7)9/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,10-9-
p-6		6.8366	153.3183	-5.0923	162.1241	342.1793	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-4-5-13-8(7)6-10-14-12(11)15(9)10/h1-6,13H/b2-1-,9-3-,10-6-
A-81		25.284	273.2003	-14.4318	39.9912	342.2298	InChI=1S/C12H7N3O/c16-12-11-9(6-14-12)15(11)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
A-126		25.3688	273.0574	-14.4581	40.0425	342.3124	InChI=1S/C12H7N3O/c16-12-11-9(6-14-12)15(11)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
A1-47		15.5637	210.0589	-7.7078	98.726	342.3528	InChI=1S/C12H7N3O/c16-9-6-13-4-1-2-8-7-3-5-14-10(7)12-11(9)15(8)12/h1-6,14H/b4-1-,8-2+,13-6-
G1-101		26.5141	272.8521	-17.2613	46.5652	342.5345	InChI=1S/C12H7N3O/c16-9(11-12-14-6-15(11)12)3-1-2-7-8-4-5-13-10(7)8/h1-6,13H/b3-1-,7-2-
q-29		3.0595	347.1067	-2.7817	-11.68	342.5562	InChI=1S/C12H7N3O/c16-12-11(14-12)15-6-8-9(15)3-1-2-7-4-5-13-10(7)8/h1-6,13H
B-19		24.7065	166.7659	-6.6243	113.1278	342.6312	InChI=1S/C12H7N3O/c16-10-6-9-7(8-3-4-13-11(8)10)2-1-5-15-12(9)14-15/h1-6,13H




















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q1-22		20.386	163.2682	-4.2615	133.6545	342.8138	InChI=1S/C12H7N3O/c16-11-9-6-8(15-12(9)14-15)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,8-3+
A2-10		14.9032	103.8318	-3.3891	199.3327	342.865	InChI=1S/C12H7N3O/c16-10-6-8-11-7(3-5-13-11)9-2-1-4-14-12(8)15(9)10/h1-6,13H
H1-87		23.2985	178.7529	-11.9692	132.0101	342.9071	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-12(7)15(11)10-6-9(10)14-8/h1-6,13H/b3-1-,8-2+
n-118		25.2097	272.0734	-14.3146	39.8165	342.9219	InChI=1S/C12H7N3O/c16-9-6-14-11-7(10(9)11)2-1-5-15-8-3-4-13-12(8)15/h1-6,13H/b5-1-,7-2+
A-10		24.9594	274.4688	-14.3194	40.0533	342.9464	InChI=1S/C12H7N3O/c16-9-6-14-12-11(9)15(12)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
n-50		29.8255	211.6253	-11.8679	77.7922	343.038	InChI=1S/C12H7N3O/c16-11-9-7-2-1-5-15(10(9)11)8-3-4-13-12(8)14-6-7/h1-6,13H/b14-6-
B-213		7.0012	158.2152	-2.2356	147.8170	343.1748	InChI=1S/C12H7N3O/c16-12-9-6-15-5-1-2-7(10(9)14-12)8-3-4-13-11(8)15/h1-6,13H
o-25		6.4069	27.2816	-2.2409	269.506	343.3921	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-10(9)8(7)6-14-12(11)15/h1-6,13H
A-196		6.6402	152.9018	-2.7797	163.7295	343.43	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-6-14-12(15)9(11)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-,12-9-
H11-117		8.2266	33.6961	-0.9124	254.2511	343.4601	InChI=1S/C12H7N3O/c16-12-8-6-15-10(3-1-2-9(12)14-15)7-4-5-13-11(7)8/h1-6,13H
p-20		11.4904	200.1261	-5.614	123.1249	343.687	InChI=1S/C12H7N3O/c16-12-9-6-8-7(4-5-13-8)2-1-3-10-11(14-9)15(10)12/h1-6,13H/b2-1-,3-1-,7-2-,8-6+,9-6+,10-3-
I-34		27.8883	240.394	-11.2846	67.7402	343.6948	InChI=1S/C12H7N3O/c16-12-10-9-6-7-8(2-4-13-7)15(9)5-1-3-14-11(10)12/h1-6,13H/b5-1-,14-3+
E-22		2.4454	322.4384	-1.3686	11.1954	343.7677	InChI=1S/C12H7N3O/c16-12-9-6-7(9)2-1-3-10-8-4-5-13-11(8)15(12)14-10/h1-6,13H/b3-1-,7-2-
B-225		19.5656	196.7825	-13.0672	124.1779	343.9435	InChI=1S/C12H7N3O/c16-11-9-6-15(12(11)14-9)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
X22-16		23.3267	247.3793	-8.642	67.9826	343.9956	InChI=1S/C12H7N3O/c16-12-7-6-10-9(15(10)12)2-1-4-13-8-3-5-14-11(7)8/h1-6,14H/b2-1-,4-1-,9-2+,11-7-,13-4-,13-8-
k-40		28.9282	209.2907	-16.1624	105.9713	344.1004	InChI=1S/C12H7N3O/c16-12-10-7-6-9(7)15(12)5-1-3-13-8-2-4-14-11(8)10/h1-6,14H/b5-1-,13-3+
H-19		10.5753	105.831	-4.2094	185.789	344.1949	InChI=1S/C12H7N3O/c16-12-7-2-1-3-8-9-4-5-13-11(9)15(12)14-10(8)6-7/h1-6,13H
H-48		15.6444	233.7757	-9.5521	76.382	344.296	InChI=1S/C12H7N3O/c16-12-10-7-6-8(7)13-3-1-5-15(12)9-2-4-14-11(9)10/h1-6,14H/b5-1-,10-7-,13-3-


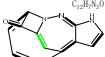
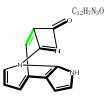
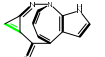






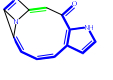
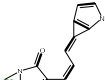




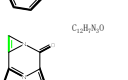


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I-90		30, 9747	214, 5762	-12, 3833	75, 3276	344, 538	InChI=1S/C12H7N3O/c16-12-10-8-6-7-9(2-4-14-7)15(11(10)12)5-1-3-13-8/h1-6, 14H/b5-1-, 13-3-
B-80		19, 6052	194, 1136	-13, 2924	133, 7561	344, 7994	InChI=1S/C12H7N3O/c16-12-9-6-10(12)15(14-9)5-1-2-7-8-3-4-13-11(7)8/h1-6, 13H/b5-1-, 7-2-
A2-27		7, 8706	59, 8038	-2, 6803	244, 8379	345, 1971	InChI=1S/C12H7N3O/c16-12-11-8-6-15(12)9(2-1-4-13-11)7-3-5-14-10(7)8/h1-6, 14H/b4-1-, 9-2-, 13-11+
X22-45		13, 0133	255, 3054	-8, 5552	50, 7956	345, 2312	InChI=1S/C12H7N3O/c16-12-10-6-9-8(15(9)10)2-1-4-13-7-3-5-14-11(7)12/h1-6, 14H/b2-1-, 13-4-
H1-120		11, 8082	116, 4633	-4, 5121	178, 3122	345, 4397	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)8-6-15(9)12(8)14-10/h1-6, 13H/b3-1-, 9-2-, 14-12-
o-150		19, 2749	196, 1112	-4, 7853	106, 7636	345, 7449	InChI=1S/C12H7N3O/c16-10-6-7-11(14-7)12-9(3-4-13-12)15-5-1-2-8(10)15/h1-6, 13H/b7-6+
o-58		6, 7927	78, 2316	-3, 4083	224, 6331	345, 8865	InChI=1S/C12H7N3O/c16-11-8-6-7-2-1-5-15(12(11)14-8)9-3-4-13-10(7)9/h1-6, 13H/b8-6-
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X22-7		8, 6989	196, 5303	-5, 2672	118, 8898	345, 966	InChI=1S/C12H7N3O/c16-12-8-6-15(12)11-7(8)2-1-4-13-9-3-5-14-10(9)11/h1-6, 14H/b2-1-, 4-1-, 7-2-, 11-10-, 13-4-, 13-9-
B-148		10, 4175	85, 0375	-3, 0521	215, 5314	346, 0132	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-10(14-12(11)15)6-9-7(8)3-4-13-9/h1-6, 13H/b10-6-
k-28		5, 4225	325, 9488	-1, 4559	0, 87	346, 0175	InChI=1S/C12H7N3O/c16-9-6-8-12-10(9)11-7(2-4-14-11)13-3-1-5-15(8)12/h1-6, 14H/b5-1-, 13-3+
H11-63		19, 1861	247, 2316	-12, 1016	91, 9471	346, 2341	InChI=1S/C12H7N3O/c16-11-6-10-14-9(15(10)11)3-1-2-7-8-4-5-13-12(7)8/h1-6, 13H/b3-1-, 7-2-
o-208		16, 8387	214, 3139	-10, 0793	101, 8748	346, 6231	InChI=1S/C12H7N3O/c16-12-7-6-9(7)14-8-2-1-5-15(12)10-3-4-13-11(8)10/h1-6, 13H/b14-9-
n-114		12, 9075	155, 019	-4, 5817	141, 6958	346, 8738	InChI=1S/C12H7N3O/c16-9-6-14-11(9)12-7-2-1-5-15(12)8-3-4-13-10(7)8/h1-6, 13H/b12-11+
G-70		13, 9741	208, 9391	-5, 7467	124, 9914	347, 2313	InChI=1S/C12H7N3O/c16-10-6-14-12-8(4-5-13-12)7-2-1-3-9-11(7)15(9)10/h1-6, 13H/b14-6+
x4-46		11, 0851	146, 8777	-4, 591	156, 5231	347, 3151	InChI=1S/C12H7N3O/c16-12-9-8-3-1-2-7-4-5-13-10(7)11(9)14-6-15(8)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3-, 11-10-
B-54		19, 4473	192, 9077	-12, 6764	138, 0841	347, 5067	InChI=1S/C12H7N3O/c16-9-6-10-14-12(9)15(10)5-1-2-7-8-3-4-13-11(7)8/h1-6, 13H/b5-1-, 7-2-
X-27		32, 8016	246, 0185	-12, 7483	37, 7256	347, 5645	InChI=1S/C12H7N3O/c16-12-10-9-6-7(2-1-4-14-12)8-3-5-13-11(8)15(9)10/h1-6, 13H/b2-1-, 14-4+














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H1-141 <chem>C12H7N3O</chem>						
	15, 8426	170, 8558	-12, 1393	146, 6974	347, 7367	InChI=1S/C12H7N3O/c16-12-8-6-7(10(8)14-12)2-1-5-15-9-3-4-13-11(9)15/h1-6, 13H/b5-1-, 7-2+
o-211 <chem>C12H7N3O</chem>						
	9, 0394	151, 7148	-4, 2375	150, 8343	347, 8085	InChI=1S/C12H7N3O/c16-12-8-6-15(12)11-10-7(4-5-13-10)2-1-3-9(8)14-11/h1-6, 13H/b2-1-, 3-1-, 7-2-, 9-3-, 11-10-
s11-10 <chem>C12H7N3O</chem>						
	12, 8241	205, 0944	-5, 1018	94, 6472	347, 988	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10(14-12)15-6-9(15)11-7(8)4-5-13-11/h1-6, 13H
H11-111 <chem>C12H7N3O</chem>						
	46, 3916	257, 1949	-26, 7209	60, 8682	348, 1159	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-14-10-11-12(10)15(9)11/h1-6, 13H/b3-1-, 7-2-, 8-6+, 14-10-
x6-7 <chem>C12H7N3O</chem>						
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B-202 <chem>C12H7N3O</chem>						
	12, 9559	129, 7493	-9, 3496	190, 5005	348, 4503	InChI=1S/C12H7N3O/c16-10-6-9-12-11-7(3-5-14-11)8(15(9)12)2-1-4-13-10/h1-6, 14H/b2-1-, 9-6-, 13-4+
D-19 <chem>C12H7N3O</chem>						
	10, 435	114, 626	-4, 0662	189, 6572	348, 667	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(14-9)15(12)11-8(7)4-5-13-11/h1-6, 13H/b2-1-, 3-1-, 7-2+, 9-3-
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B-86 <chem>C12H7N3O</chem>						
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o-203 <chem>C12H7N3O</chem>						
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n-125 <chem>C12H7N3O</chem>						
	14, 5623	171, 3439	-4, 6292	132, 4518	349, 5789	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-4-14-15(12)11(9)10-8(7)3-5-13-10/h1-6, 13H/b2-1-, 14-4+
X-33 <chem>C12H7N3O</chem>						
	7, 1555	231, 1202	-3, 8667	79, 642	349, 6081	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)9-6-15(9)12(10)14-8/h1-6, 13H
H1-54 <chem>C12H7N3O</chem>						
	13, 1158	198, 9243	-6, 5594	127, 9609	349, 9043	InChI=1S/C12H7N3O/c16-12-7-6-10-9(15(10)12)2-1-4-13-8-3-5-14-11(7)8/h1-6, 14H/b2-1-, 4-1-, 9-2-, 11-7+, 13-4-, 13-8-
i-23 <chem>C12H7N3O</chem>						
	22, 864	218, 0959	-8, 2691	105, 2427	350, 0516	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-10(15(9)12)6-14-11-7(8)4-5-13-11/h1-6H, (H, 13, 14)
F-64 <chem>C12H7N3O</chem>						
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A-69 <chem>C12H7N3O</chem>						
	31, 7238	322, 6931	-16, 6811	5, 9921	350, 127	InChI=1S/C12H7N3O/c16-12-11-9(15(11)12)6-7-2-1-4-13-8-3-5-14-10(7)8/h1-6, 14H/b7-6-
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X22-8		8, 3567	195, 4239	-5, 1717	127, 0533	350, 3507	InChI=1S/C12H7N3O/c16-12-7-6-15(12)9-2-1-4-13-8-3-5-14-11(8)10(7)9/h1-6, 14H/b2-1-, 4-1+, 9-2+, 11-10+, 13-4+, 13-8-
x3-5		30, 6802	211, 7078	-16, 4982	92, 7628	350, 6896	InChI=1S/C12H7N3O/c16-12-9-7-6-15(5-1-3-13-11(9)12)8-2-4-14-10(7)8/h1-6, 14H/b2-1-, 4-1+, 9-2+, 11-10+, 13-4+, 13-3+
q-50		12, 8393	207, 8316	-3, 8111	114, 6303	350, 9989	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9(6-8)11-14-15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 10-9-
B-140		18, 9131	195, 0910	-9, 4755	130, 2210	351, 2580	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)11-10(14-11)6-9-7(8)3-4-13-9/h1-6, 13H/b10-6+
B-186		19, 9836	197, 8071	-12, 9876	132, 7640	351, 2701	InChI=1S/C12H7N3O/c16-11-9-6-14-12(11)15(9)5-1-2-7-8-3-4-13-10(7)8/h1-6, 13H/b5-1-, 7-2-
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F-12		9, 9313	93, 9073	-3, 821	211, 1584	351, 7119	InChI=1S/C12H7N3O/c16-11-8-6-15-9(2-1-3-10(11)15)7-4-5-13-12(7)14-8/h1-6H, (H, 13, 14)
X-21		32, 0847	326, 1695	-16, 6754	3, 1212	351, 7200	InChI=1S/C12H7N3O/c16-12-10-9(15(10)12)6-7-2-1-4-13-11-8(7)3-5-14-11/h1-6, 14H/b7-6-
C-71		3, 2809	301, 8370	-2, 1021	33, 6623	351, 8446	InChI=1S/C12H7N3O/c16-12-14-4-1-2-8-7-3-5-13-9(7)6-10-11(8)15(10)12/h1-6, 13H/b2-1-, 14-4+
x6-8		36, 2323	245, 9439	-24, 022	67, 4751	352, 0725	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-15-11-10(14-9)12(11)15/h1-6, 13H/b3-1-, 7-2-, 8-6-, 14-10-
o-47		8, 0347	32, 6852	-2, 5691	271, 1097	352, 0924	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-2-8(7)14-11(12)10-9(15)3-4-13-10/h1-6, 13H
C-72		25, 4956	293, 7610	-6, 7510	19, 6725	352, 1818	InChI=1S/C12H7N3O/c16-12-14-4-1-2-7-8-3-5-13-11(8)10(7)9-6-15(9)12/h1-6, 13H/b2-1-, 14-4+
H11-57		24, 7558	242, 1763	-6, 3139	75, 4533	352, 2242	InChI=1S/C12H7N3O/c16-11-6-9-7(8-4-5-13-12(8)9)2-1-3-10-14-15(10)11/h1-6, 13H/b3-1-, 7-2-, 9-6+
p1-49		18, 3122	157, 8525	-4, 4159	162, 9778	352, 2746	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10-8(9)6-15-12(10)14-15/h1-6, 13H/b3-1-, 7-2-, 11-10-
n-175		9, 249	43, 0967	-3, 3568	261, 357	352, 4087	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-8-3-4-13-10(8)9(11)12(15)14-6-7/h1-6, 13H/b5-1-, 7-2+
A2-29		26, 3864	177, 0612	-17, 3042	5, 0238352, 47	352, 4726	InChI=1S/C12H7N3O/c16-12-11-10-8(3-5-14-10)7(2-1-4-13-11)9-6-15(9)12/h1-6, 14H/b2-1-, 4-1-, 7-2+, 13-4-, 13-11+
i-83		7, 1166	211, 6778	-5, 6091	112, 3748	352, 5915	InChI=1S/C12H7N3O/c16-12-9-7-6-13-3-1-5-15(11(7)9)8-2-4-14-10(8)12/h1-6, 14H/b5-1-, 7-6-, 13-3-
B-44		8, 4456	32, 7371	-3, 2322	265, 2683	352, 6131	InChI=1S/C12H7N3O/c16-10-6-9-11-8(3-4-13-11)7-2-1-5-15(9)14-12(7)10/h1-6, 13H

B-179		$C_{22}H_{23}N_2O$	22.1370	224.1673	-13.2651	116.7235	352.7252	InChI=1S/C12H7N3O/c16-12-9-6-14-11(9)15(12)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
A1-6		$C_{22}H_{23}N_2O$	21.8975	284.5503	-8.227	42.8425	352.8862	InChI=1S/C12H7N3O/c16-12-11-9-7(8-3-5-14-10(8)9)2-1-4-13-6-15(11)12/h1-6,14H/b4-1-,7-2-,11-9-,13-6-
H-29		$C_{22}H_{23}N_2O$	10.9934	90.9764	-3.1155	206.659	352.8959	InChI=1S/C12H7N3O/c16-12-7-2-1-3-8-9-4-5-13-10(9)15(6-7)11(8)14-12/h1-6,13H/b2-1-,8-3-
H11-12		$C_{22}H_{23}N_2O$	9.2379	95.0732	-3.8468	218.0315	353.2159	InChI=1S/C12H7N3O/c16-12-14-9-2-1-3-10-7-4-5-13-11(7)8(9)6-15(10)12/h1-6,13H/b2-1-,10-3-
F-62		$C_{22}H_{23}N_2O$	15.0158	242.1577	-8.0848	78.1088	353.3531	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(7)15(12)14-11-8(9)4-5-13-11/h1-6H, (H,13,14)/b3-1-,7-2-
o-110		$C_{22}H_{23}N_2O$	17.0761	177.0623	-12.6082	146.7406	353.422	InChI=1S/C12H7N3O/c16-11-7(10-8(11)6-14-10)2-1-5-15-9-3-4-13-12(9)15/h1-6,13H/b5-1-,7-2-
A1-21		$C_{22}H_{23}N_2O$	11.6947	228.2749	-3.2068	96.4631	353.427	InChI=1S/C12H7N3O/c16-12-8-2-1-4-13-6-9-11(15(9)12)10-7(8)3-5-14-10/h1-6,14H/b2-1-,4-1-,8-2-,9-6-,13-4-,13-6-
H1-16		$C_{22}H_{23}N_2O$	11.0594	177.9608	-4.1784	140.3135	353.4631	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)15(11)10-6-9(7)14-10/h1-6,13H/b3-1-,7-2+
A-158		$C_{22}H_{23}N_2O$	15.3142	283.8904	-6.0637	35.6041	353.5351	InChI=1S/C12H7N3O/c16-12-11-10-8(2-1-5-15(11)12)7-3-4-13-9(7)6-14-10/h1-6,13H
x9-46		$C_{22}H_{23}N_2O$	38.0515	229.067	-23.8994	80.7424	353.7788	InChI=1S/C12H7N3O/c16-12-9-7(4-5-13-9)2-1-3-8-10-11(8)15(10)6-14-12/h1-6,13H/b2-1-,8-3-,14-6-
H11-90		$C_{22}H_{23}N_2O$	24.3526	163.9546	-16.628	153.2787	354.178	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(14-10-6-15(10)12)11-7(8)4-5-13-11/h1-6,13H/b14-9+
H-35		$C_{22}H_{23}N_2O$	15.9689	227.0712	-3.4489	94.6273	354.3727	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8(7)9-4-5-13-11(9)15-12(10)14-15/h1-6,13H/b7-6-
q-46		$C_{22}H_{23}N_2O$	9.9801	227.5151	-3.9076	110.2736	354.6103	InChI=1S/C12H7N3O/c16-10-6-8-11-7(4-5-13-11)2-1-3-9-12(14-8)15(9)10/h1-6,13H/b2-1-,9-3+
A-170		$C_{22}H_{23}N_2O$	27.9465	232.8078	-10.1632	86.4161	355.1117	InChI=1S/C12H7N3O/c16-11-9-10(11)15-5-1-2-7(6-14-9)8-3-4-13-12(8)15/h1-6,13H/b14-6-
q1-19		$C_{22}H_{23}N_2O$	19.7557	209.9681	-13.8179	116.8716	355.342	InChI=1S/C12H7N3O/c16-11-8(9-6-15-12(9)14-15)3-1-2-7-4-5-13-10(7)11/h1-6,13H
q1-23		$C_{22}H_{23}N_2O$	7.2804	157.7975	-2.4385	168.4003	355.417	InChI=1S/C12H7N3O/c16-11-8-6-15-9(14-12(8)15)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,9-3-
s11-51		$C_{22}H_{23}N_2O$	13.2577	205.9148	-3.0692	125.4356	355.7266	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)9-6-10(14-8)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,11-9+
A2-69		$C_{22}H_{23}N_2O$	24.0255	227.9868	-12.5083	74.7545	355.8438	InChI=1S/C12H7N3O/c16-12-10-7(3-5-14-10)8-2-1-4-13-11(12)9-6-15(8)9/h1-6,14H/b4-1-,8-2-,13-11+
B-91		$C_{22}H_{23}N_2O$	8.5383	282.3750	-7.4345	68.4081	355.9379	InChI=1S/C12H7N3O/c16-12-10-6-9-7(2-1-5-15(10)12)8-3-4-13-11(8)14-9/h1-6,13H/b5-1-,7-2-,10-6-

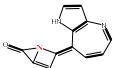
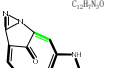
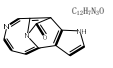
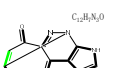
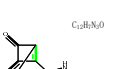
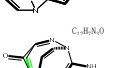
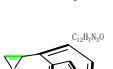
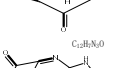

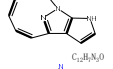
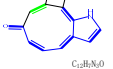
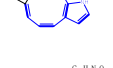
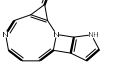
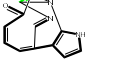
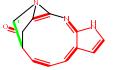
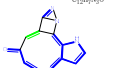
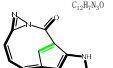
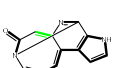
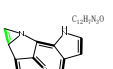
G1-99		10.9977	174.2464	-1.8165	151.5534	356.0999	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-11(7)10(9)12-14-6-15(8)12/h1-6,13H/b3-1-,8-2-
o-251		26.0913	203.7383	-9.3129	93.8813	356.12	InChI=1S/C12H7N3O/c16-12-14-11-7-2-1-5-15(12)10-3-4-13-9(10)6-8(7)11/h1-6,13H/b5-1-,7-2-,8-6-,14-11-
B-46	 C ₁₂ H ₇ N ₃ O	17.6995	89.6610	-3.6359	210.5486	356.2227	InChI=1S/C12H7N3O/c16-10-6-9-11-7(3-4-13-11)8-2-1-5-15(9)12(8)14-10/h1-6,13H
E-67	 C ₁₂ H ₇ N ₃ O	25.1885	166.5068	-16.8885	148.1195	356.429	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(14-10-6-15(10)12)7-4-5-13-11(7)8/h1-6,13H/b14-9+
q1-57	 C ₁₂ H ₇ N ₃ O	8.4494	180.4311	-5.574	143.4827	356.4295	InChI=1S/C12H7N3O/c16-11-10-7(4-5-13-10)2-1-3-9-8-6-15(9)12(11)14-8/h1-6,13H/b2-1-,9-3-
E-27	 C ₁₂ H ₇ N ₃ O	5.9458	96.7895	-2.2615	223.6454	356.468	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(14-10)8-4-5-13-11(8)15(7)12/h1-6,13H/b2-1-,3-1-,7-2-,9-3-
o-170	 C ₁₂ H ₇ N ₃ O	18.6294	173.4723	-13.674	139.3953	356.5295	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(10-6-8(10)14-12)9-3-4-13-11(7)9/h1-6,13H/b14-8-
G1-63	 C ₁₂ H ₇ N ₃ O	29.1437	289.4842	-18.4399	40.5821	357.019	InChI=1S/C12H7N3O/c16-10(12-9-6-14-15(9)12)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
B-235	 C ₁₂ H ₇ N ₃ O	8.6235	70.3362	-3.1036	241.9506	357.1469	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-9(11(15)14-12)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-
C-46	 C ₁₂ H ₇ N ₃ O	18.9583	193.5453	-6.9511	134.2526	357.1578	InChI=1S/C12H7N3O/c16-10-6-9-11-7(2-1-4-13-10)8-3-5-14-12(8)15(9)11/h1-6,14H/b2-1-,9-6-,13-4-
o-113	 C ₁₂ H ₇ N ₃ O	5.1407	38.9076	-1.4712	278.4769	357.1695	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-8(12)14-10(7)11-9(15)3-4-13-11/h1-6,13H/b5-1-,7-2+
C-14	 C ₁₂ H ₇ N ₃ O	12.8227	146.6011	-2.9815	165.6015	357.1712	InChI=1S/C12H7N3O/c16-12-10-6-9-7(2-1-4-14-15(9)10)8-3-5-13-11(8)12/h1-6,13H
D-3	 C ₁₂ H ₇ N ₃ O	17.7607	201.6942	-8.8305	124.2492	357.3225	InChI=1S/C12H7N3O/c16-12-8-6-15-9(2-1-4-14-15)7-3-5-13-11(7)10(8)12/h1-6,13H
p11-18	 C ₁₂ H ₇ N ₃ O	35.7288	217.797	-18.888	91.1	357.3365	InChI=1S/C12H7N3O/c16-12-10-9-3-1-2-7-4-5-13-8(7)6-14-11(10)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-6-,9-3-,14-6-,14-11+
G-16	 C ₁₂ H ₇ N ₃ O	30.3066	317.8375	-11.7133	13.8911	357.337	InChI=1S/C12H7N3O/c16-12(15-6-14-15)9-3-1-2-7-8-4-5-13-11(8)10(7)9/h1-6,13H
X-3	 C ₁₂ H ₇ N ₃ O	23.7712	254.4892	-7.4976	66.1850	357.3994	InChI=1S/C12H7N3O/c16-12-9-10-8(3-5-13-10)7-2-1-4-14-15(6-7)11(9)12/h1-6,13H
H1-81	 C ₁₂ H ₇ N ₃ O	18.066	235.2784	-14.2733	87.0236	357.4388	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)15(11)14-10-6-9(7)10/h1-6,13H/b3-1-,7-2+
B-253	 C ₁₂ H ₇ N ₃ O	20.6503	286.7302	-7.6626	31.9001	357.4569	InChI=1S/C12H7N3O/c16-12-11(14-12)15-5-1-2-7-8-3-4-13-10(8)9(7)6-15/h1-6,13H
H-116	 C ₁₂ H ₇ N ₃ O	7.098	82.984	-2.6601	233.2515	357.6086	InChI=1S/C12H7N3O/c16-12-10-7-2-1-3-9(15(12)6-7)8-4-5-13-11(8)14-10/h1-6,13H




















q1-40		19,3674	129,8165	-11,7222	190,3512	357,6256	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)2-1-3-8-9-6-10(14-12)15(8)9/h1-6,13H/b2-1-,8-3-,14-10-
F-7		11,7877	145,3081	-3,3714	169,1319	357,6466	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7-6-10(11)15(9)14-12-8(7)4-5-13-12/h1-6H,(H,13,14)/b2-1-,9-3+
B-152		6,6045	138,8015	-3,0580	178,6818	357,6659	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-5-15(11(9)14-12)10-8(7)3-4-13-10/h1-6,13H
B-59		18,5091	148,5981	-14,3403	166,2510	357,7080	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(14-10-6-9(10)11)12-8(7)3-4-13-12/h1-6,13H/b14-10-
x3-12		27,8299	243,9356	-10,6665	75,718	357,7978	InChI=1S/C12H7N3O/c16-12-9-7-6-15(5-1-3-13-11(9)12)8-2-4-14-10(7)8/h1-6,14H/b5-1-,13-3-
x4-15		6,3976	182,3631	-2,4661	138,787	358,0612	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)10(12)9-6-14-15(8)9/h1-6,13H/b2-1-,8-3+
G-81		7,428	171,7295	-2,4283	153,372	358,076	InChI=1S/C12H7N3O/c16-12-14-6-10-7-2-1-3-9(15(10)12)11-8(7)4-5-13-11/h1-6,13H
E-72		19,5873	214,2455	-12,3519	107,7775	358,4599	InChI=1S/C12H7N3O/c16-12-14-9-3-1-2-8(10-6-15(10)12)11-7(9)4-5-13-11/h1-6,13H/b14-9+
H-16		26,2718	253,645	-0,7124	65,0697	358,4805	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7(6-8)9-4-5-13-10(9)11-14-15(11)12/h1-6,13H
q1-55		17,8728	131,0019	-11,355	197,2071	358,9308	InChI=1S/C12H7N3O/c16-9-6-10-14-12-8(15(10)12)3-1-2-7-4-5-13-11(7)9/h1-6,13H/b2-1-,8-3-,10-6-
H11-16		36,2382	296,197	-22,6558	40,0081	359,0486	InChI=1S/C12H7N3O/c16-12-9(14-10-6-15(10)12)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
H-82		13,7007	213,0682	-5,7623	101,7744	359,1671	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-15(7)11(14-12)10-8(9)4-5-13-10/h1-6,13H/b2-1-,9-3+
C-22		7,1790	129,7094	-3,3371	185,8726	359,3948	InChI=1S/C12H7N3O/c16-12-9-6-10-7(2-1-4-14-15(10)12)8-3-5-13-11(8)9/h1-6,13H
G1-114		16,7974	216,327	-6,4338	107,2498	359,5419	InChI=1S/C12H7N3O/c16-9-3-1-2-7-6-14-12-11(15(9)12)10-8(7)4-5-13-10/h1-6,13H/b3-1-,7-2+
H11-65		13,0264	194,3278	-4,4929	125,5378	359,6479	InChI=1S/C12H7N3O/c16-11-6-9-12-7(4-5-13-12)8-2-1-3-10(14-8)15(9)11/h1-6,13H
s11-34		19,1708	201,7029	-9,1767	119,7062	359,8846	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8(14-11)9-6-15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,11-10+
B-196		22,3495	224,8795	-13,4467	121,4834	359,9655	InChI=1S/C12H7N3O/c16-12-11-9(6-14-11)15(12)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
q-38		7,9099	203,0362	-5,1618	135,7849	360,1542	InChI=1S/C12H7N3O/c16-12-8-6-14-11-9(15(11)12)3-1-2-7-4-5-13-10(7)8/h1-6,13H/b2-1-,3-1-,7-29,9-3-,10-8+
o-160		18,3373	192,6342	-4,6111	130,7229	360,1678	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)9-3-4-13-11(9)10-8(6-7)14-10/h1-6,13H/b8-6+




















o-200		37.3962	93.5428	-3.6922	142.5601	360.2204	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(12)9-3-4-13-11(9)14-10(7)8/h1-6,13H/b5-1-,7-2+
X-41	 C ₁₂ H ₇ N ₃ O	12.4474	145.9632	-4.1576	177.3891	360.3239	InChI=1S/C12H7N3O/c16-12-9-10-8(3-5-13-10)7-2-1-4-14-11(9)15(12)6-7/h1-6,13H/b2-1-,14-4-
A2-35	 C ₁₂ H ₇ N ₃ O	10.4039	216.2386	-0.6621	98.691	360.75	InChI=1S/C12H7N3O/c16-12-9-6-10-7(2-1-4-13-9)8-3-5-14-11(8)15(10)12/h1-6,14H/b2-1-,4-1-,7-2-,13-4-,13-9+
H11-48	 C ₁₂ H ₇ N ₃ O	6.0277	334.9954	-1.0624	-2.2999	360.8441	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(14-7)8-4-5-13-11(8)15(10)12/h1-6,13H/b10-6-
x4-1	 C ₁₂ H ₇ N ₃ O	9.3239	228.0712	-4.9477	107.2163	361.3278	InChI=1S/C12H7N3O/c16-9-6-14-15-8-3-1-2-7-4-5-13-11(7)10(9)12(8)15/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,11-10+
F-14	 C ₁₂ H ₇ N ₃ O	13.9031	150.8384	-3.7384	166.2317	361.4487	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-6-10(11)15(7)14-12-9(8)4-5-13-12/h1-6H,13,14/b3-1-,7-2+
j-20	 C ₁₂ H ₇ N ₃ O	52.0822	248.7604	-28.1838	78.4327	361.4616	InChI=1S/C12H7N3O/c16-10-6-9-8(3-5-14-9)13-4-1-2-7-11-12(7)15(10)11/h1-6,14H/b4-1-,7-2-,9-6-,13-8+
I-14	 C ₁₂ H ₇ N ₃ O	16.2538	159.1262	-7.5876	160.0194	361.5319	InChI=1S/C12H7N3O/c16-10-6-9-8-2-1-4-13-7-3-5-14-11(7)12(10)15(8)9/h1-6,14H/b4-1-,8-2-,12-11+,13-7+
o-76	 C ₁₂ H ₇ N ₃ O	16.3222	223.0386	-5.4969	90.0877	361.5466	InChI=1S/C12H7N3O/c16-10-6-9-12-8(3-4-13-12)15(9)5-1-2-7-11(10)14-7/h1-6,13H/b5-1-,7-2+,9-6-
x4-17	 C ₁₂ H ₇ N ₃ O	5.7543	181.7657	-2.2622	147.1579	361.5525	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)9(11)12-14-6-15(8)12/h1-6,13H/b2-1-,8-3+
B-89	 C ₁₂ H ₇ N ₃ O	19.8214	193.0310	-13.0852	149.5271	361.6426	InChI=1S/C12H7N3O/c16-12-9-6-10(14-12)15(9)5-1-2-7-8-3-4-13-11(7)8/h1-6,13H/b5-1-,7-2-
H11-35	 C ₁₂ H ₇ N ₃ O	8.4306	118.5863	-3.6794	200.3334	362.1659	InChI=1S/C12H7N3O/c16-12-8-6-10-7(4-5-13-10)11-3-1-2-9(8)14-15(11)12/h1-6,13H
n-95	 C ₁₂ H ₇ N ₃ O	7.908	171.4089	-3.2122	154.4457	362.2157	InChI=1S/C12H7N3O/c16-12-8(6-14-12)11-7-2-1-5-15(11)9-3-4-13-10(7)9/h1-6,13H/b11-8+
q11-52	 C ₁₂ H ₇ N ₃ O	7.9409	197.7129	-5.0617	140.5474	362.5136	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8-9(6-14-11)15(8)12/h1-6,13H/b2-1-,3-1-,7-2?,8-3-,11-10-
q-12	 C ₁₂ H ₇ N ₃ O	21.827	257.3791	-12.4492	52.9452	362.5401	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)9-6-15(9)12(11)14-8/h1-6,13H/b2-1-,8-3-
p1-45	 C ₁₂ H ₇ N ₃ O	20.6389	168.0479	-3.6582	149.8415	362.6076	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9(10)15-12(8)14-15/h1-6,13H/b3-1-,7-2-,11-8-
o-241	 C ₁₂ H ₇ N ₃ O	25.6755	187.3657	-4.841	140.9863	363.208	InChI=1S/C12H7N3O/c16-10-6-7-11-8(14-11)2-1-5-15(10)9-3-4-13-12(7)9/h1-6,13H/b5-1-,8-2+
B-82	 C ₁₂ H ₇ N ₃ O	9.4375	65.5313	-5.1913	248.0615	364.3133	InChI=1S/C12H7N3O/c16-11-9-6-10(11)15-5-1-2-8(14-9)7-3-4-13-12(7)15/h1-6,13H/b14-9+
I-35	 C ₁₂ H ₇ N ₃ O	11.7233	214.5309	1.3352	93.9193	364.3158	InChI=1S/C12H7N3O/c16-12-7-6-9-10(12)11-8(2-4-14-11)15(9)5-1-3-13-7/h1-6,14H/b5-1-,13-3-




















q-36		15.4264	217.9696	-7.0823	118.0978	364.7496	InChI=1S/C12H7N3O/c16-12-9-6-8(11-14-15(11)12)3-1-2-7-4-5-13-10(7)9/h1-6,13H/b2-1-,3-1-,7-2?,8-3+,10-9-
H11-44		9.568	108.0083	-3.784	209.3507	364.9065	InChI=1S/C12H7N3O/c16-12-9-6-14-10-3-1-2-7(9)8-4-5-13-11(8)15(10)12/h1-6,13H/b2-1-,3-1-,7-2-,10-3-
q11-41		16.049	216.3937	-5.6033	106.6339	365.0018	InChI=1S/C12H7N3O/c16-10-6-9-8(10)3-1-2-7-4-5-13-11(7)12-14-15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,10-3-
q11-23		7.6519	115.3346	-2.871	203.023	365.0165	InChI=1S/C12H7N3O/c16-11-8-6-15-9(11)3-1-2-7-4-5-13-10(7)12(15)14-8/h1-6,13H/b2-1-,9-3-
B-34		12.0145	78.8127	-3.8106	234.7978	365.2996	InChI=1S/C12H7N3O/c16-10-6-9-12-11-8(3-4-13-11)7(10)2-1-5-15(9)14-12/h1-6,13H/b5-1-,7-2-
G-75		16.3341	217.3653	-6.8775	122.052	365.3625	InChI=1S/C10H6N2/c1-2-6-7-4-5-11-10(7)12-8(3-1)9(6)12/h1-5,11H
X22-29		19.6855	241.6703	-10.4099	103.9702	365.901	InChI=1S/C12H7N3O/c16-12-11-7-2-1-4-13-8-3-5-14-10(8)9(6-7)15(11)12/h1-6,14H/b2-1-,13-4-
H1-31		33.0881	294.2946	-22.2101	45.0104	366.1205	InChI=1S/C12H7N3O/c16-10(12-9-6-15(9)14-12)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
s12-20		31.8228	256.098	-14.339	66.1397	366.1429	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-9(7)6-15(14-8)11(10)12/h1-6,13H/b3-1-,7-2-,9-6-
G-67		9.6824	200.1228	-4.4344	140.1312	366.4059	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)8-2-1-3-9-11(8)15(9)6-14-12/h1-6,13H/b14-6-
x4-42		35.1516	276.8718	-18.756	57.1519	366.4869	InChI=1S/C12H7N3O/c16-12(15-6-14-15)10-8-3-1-2-7-4-5-13-11(7)9(8)10/h1-6,13H
A-166		27.4867	238.6362	-9.4751	89.6954	366.692	InChI=1S/C12H7N3O/c16-12-9-10-8(3-4-13-10)7-2-1-5-15(11)9(12)14-6-7/h1-6,13H
H1-106		37.9115	238.0814	-3.5103	80.7127	366.8203	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9(12-14-15(10)12)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
G1-32		3.6964	368.8892	-1.9363	-10.49	366.9746	InChI=1S/C12H7N3O/c16-9-3-1-2-7-8-4-5-13-11(8)10(7)12(9)15-6-14-15/h1-6,13H
G1-111		39.1638	301.6379	-20.1433	38.0727	367.0445	InChI=1S/C12H7N3O/c16-10(15-9-6-14-12(9)15)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
o-184		21.9403	241.2134	-13.9223	77.8546	367.0457	InChI=1S/C12H7N3O/c16-12-7-6-8(7)14-10-2-1-5-15(10)9-3-4-13-11(9)12/h1-6,13H/b14-8-
i-96		8.7106	78.2311	-3.2675	234.5267	367.0629	InChI=1S/C12H7N3O/c16-12-7-6-9(12)15-5-1-3-13-10(7)11-8(15)2-4-14-11/h1-6,14H/b5-1-,13-3-
G-25		8.3426	343.5923	-5.2559	14.4754	367.2447	InChI=1S/C12H7N3O/c16-12-10-3-1-2-7-8-4-5-13-11(8)9(7)6-14-15(10)12/h1-6,13H/b2-1-,10-3-,14-6-
H-119		8.9371	166.9977	-5.4604	161.7183	367.5905	InChI=1S/C12H7N3O/c16-12-11-10-9(4-5-13-10)7-2-1-3-8(6-7)15(12)14-11/h1-6,13H




















o-90		24.7623	261.9209	-13.7079	51.5598	368.1457	InChI=1S/C12H7N3O/c16-12-10-8-6-7(8)2-1-5-15(12)9-3-4-13-11(9)14-10/h1-6,13H/b5-1-,7-2-
n-155		9.6764	42.55	-3.2076	276.531	368.3403	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-11(8)10(12)9(15)6-14-7/h1-6,13H/b5-1-,7-2-
D-1		11.8480	359.8022	-3.5368	-4.8238	368.3830	InChI=1S/C12H7N3O/c16-10-6-8(10)12-11-7(3-5-13-11)9-2-1-4-14-15(9)12/h1-6,13H
E-57		6.7918	306.9802	-3.6346	44.7111	368.5699	InChI=1S/C12H7N3O/c16-12-10-3-1-2-8-7-4-5-13-11(7)9(14-8)6-15(10)12/h1-6,13H/b2-1-,9-6-,10-3-
I-88		33.2745	233.3379	-12.0615	90.5583	368.5794	InChI=1S/C12H7N3O/c16-12-9-7-6-13-3-1-5-15(11)9(12)8-2-4-14-10(7)8/h1-6,14H/b5-1-,7-6-,13-3-
o-53		6.8147	76.7257	-2.7153	242.2632	368.6395	InChI=1S/C12H7N3O/c16-12-8-6-10(12)15-5-1-2-7(14-8)11-9(15)3-4-13-11/h1-6,13H/b14-8+
H11-127		14.1733	239.5553	-8.3514	82.1033	368.7102	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(12)14-15-6-10(15)11-7(8)4-5-13-11/h1-6,13H/b4-9-
q-52		2.4677	378.3159	-2.2351	-7.1	368.9684	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-10(7)8-6-14-11(8)15(9)12/h1-6,13H/b2-1-,9-3-
B-53		6.6415	98.0687	-2.7796	231.2525	369.3214	InChI=1S/C12H7N3O/c16-9-6-10-14-11(9)7-2-1-5-15(10)12-8(7)3-4-13-12/h1-6,13H
o-26		29.9898	82.4332	-0.903	182.6085	369.5068	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-10-3-4-13-9(10)6-8(7)14-12(11)15/h1-6,13H
H-133		2.3951	305.9491	-1.4391	48.3945	369.5692	InChI=1S/C12H7N3O/c16-12-11-14-8-3-1-2-7(6-8)9-4-5-13-10(9)15(11)12/h1-6,13H/b4-11-
H-22		10.7236	110.7754	-5.053	214.8156	369.728	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-11(8)15(12)10(6-7)14-9/h1-6,13H/b2-1-,3-1-,7-2-,9-3-
o-49		6.0466	34.8679	-2.2957	285.5235	370.1044	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-5-15(9)8-3-4-13-10(8)11(12)14-7/h1-6,13H
B-11		41.2144	197.1890	-17.7926	125.0926	370.1200	InChI=1S/C12H7N3O/c16-10-6-9(10)15-5-1-2-8-7-3-4-13-11(7)12(15)14-8/h1-6,13H
E-54		13.4086	207.011	-4.9089	117.0614	370.3933	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8(14-12)7-4-5-13-11(7)10-6-15(9)10/h1-6,13H
X22-24		18.059	222.3667	-10.5004	131.4791	370.4035	InChI=1S/C12H7N3O/c16-12-11-7-2-1-4-13-9-3-5-14-10(9)8(7)6-15(11)12/h1-6,14H/b2-1-,13-4+
s11-48		13.7836	214.2104	-5.8742	134.0995	370.6094	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-9(6-14-8)15(11)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,11-10+
n-53		28.0244	235.953	-10.2332	95.4831	370.8986	InChI=1S/C12H7N3O/c16-12-10-11(12)15-5-1-2-7(6-14-10)9-8(15)3-4-13-9/h1-6,13H/b14-6-
H11-136		40.3957	182.6014	-18.6435	141.8413	370.9652	InChI=1S/C12H7N3O/c16-10-6-9(10)15-8-2-1-3-11(15)14-12-7(8)4-5-13-12/h1-6H,13(14)




















X22-9		14.7307	300.1629	-9.418	61.0408	370.9844	InChI=1S/C12H7N3O/c16-12-10-6-9(15(10)12)7-2-1-4-13-8-3-5-14-11(7)8/h1-6,14H/b9-7-
p-15		21.1393	165.9135	-3.5988	160.4256	371.0786	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-9(7)6-10(11)15-12(8)14-15/h1-6,13H/b2-1-,8-3+,10-6+
A1-29		28.7316	203.1437	-6.0521	107.4882	371.1511	InChI=1S/C12H7N3O/c16-12-10-9-6-13-4-1-2-8(15(9)12)7-3-5-14-11(7)10/h1-6,14H/b2-1-,4-1-,8-2-,9-6-,13-4-,13-6-
H-39		9.2966	97.8013	-2.0925	213.9225	371.3012	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8-9-4-5-13-12(9)15(7)14-11(8)10/h1-6,13H/b2-1-,8-3-
n-161		14.4154	123.8091	-3.327	191.502	371.5831	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)10(7)8(12)6-14-15/h1-6,13H/b5-1-,7-2+
B-69		11.4242	125.3384	-3.9610	190.8051	371.6340	InChI=1S/C12H7N3O/c16-11-9-6-10(11)14-15-5-1-2-7(9)8-3-4-13-12(8)15/h1-6,13H/b14-10+
H1-29		17.5339	185.5619	-12.4778	128.6816	371.6371	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12(10)14-15-6-9(7)15/h1-6,13H/b3-1-,7-2+
H1-48		32.5244	236.9127	-18.4822	78.5267	371.6996	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)14-12(10)15-6-9(7)15/h1-6,13H/b3-1-,7-2-
E-8		4.1293	349.9685	-0.7266	-2.38	371.8685	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10-8-4-5-13-12(8)15(14-10)6-9(7)11/h1-6,13H/b3-1-,7-2+,9-6+
p1-47		24.5875	147.461	-10.1	193.7638	371.9059	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-11(7)10-9(6-8)15-12(10)14-15/h1-6,13H/b3-1-,7-2-,9-6+,11-10-
q1-17		24.0602	145.3116	-9.9427	196.7868	371.9232	InChI=1S/C12H7N3O/c16-10-6-8-9(15-12(8)14-15)3-1-2-7-4-5-13-11(7)10/h1-6,13H/b2-1-,8-6+,9-3+
A1-40		32.0292	260.58	-14.8056	70.0872	372.1395	InChI=1S/C12H7N3O/c16-11-8-6-13-4-1-2-9-7-3-5-14-12(7)15(9)10(8)11/h1-6,14H/b4-1-,9-2-,13-6-
G1-100		16.6557	272.0284	-5.5065	41.4828	372.2318	InChI=1S/C12H7N3O/c16-9-3-1-2-7-6-14-12(9)15(12)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
xS-31		12.8003	277.0201	-6.1549	54.5863	372.63	InChI=1S/C12H7N3O/c16-10-8-3-1-2-7-4-5-13-11(7)14-12-9(10)15(12)6-8/h1-6H,(H,13,14)/b3-1-,7-2-
p1-33		16.0141	214.9551	-8.2407	128.1811	372.7541	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)11-9(6-8)12-14-15(11)12/h1-6,13H/b3-1-,7-2-,9-6+,11-10-
H11-25		4.1354	331.8086	-1.6928	28.7373	372.7771	InChI=1S/C12H7N3O/c16-12-9-6-7(8-4-5-13-11(8)9)2-1-3-10-14-15(10)12/h1-6,13H/b3-1-,7-2+
B-48		7.9979	105.6074	-2.4001	227.4461	372.8104	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(10)12(14-9)11-8(7)3-4-13-11/h1-6,13H/b5-1-,7-2-
i-20		15.5268	202.5069	-9.3695	116.0623	372.8175	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-10(8)11(12)15-6-9(7)15/h1-6,14H/b4-1-,7-2-,11-10-,13-8-
o-128		3.9621	347.8911	-0.6529	-1.45	372.8191	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-10-3-4-13-11(10)9(14-15)6-8(7)12/h1-6,13H/b5-1-,7-2+,8-6+


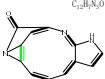
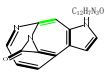
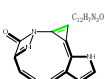
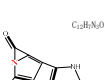
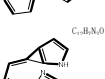
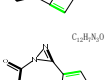
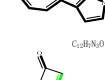
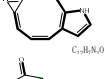
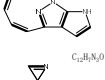
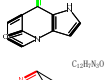
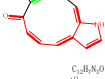
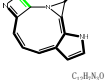
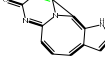
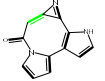
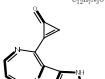
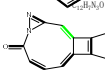
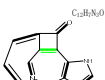
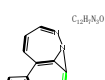
H-11		7.7682	101.0018	-1.8472	217.5197	373.1574	InChI=1S/C12H7N3O/c16-11-7-2-1-3-8-9-4-5-13-12(9)15(6-7)14-10(8)11/h1-6,13H
	$C_{12}H_7N_3O$						
H-92		18.759	215.631	-12.3191	123.0106	373.4137	InChI=1S/C12H7N3O/c16-12-10-9(4-5-13-10)7-2-1-3-8(6-7)11-14-15(11)12/h1-6,13H
	$C_{12}H_7N_3O$						
o-151		10.2508	108.5215	-2.5487	205.4285	373.4321	InChI=1S/C12H7N3O/c16-10-6-9-12-11-8(3-4-13-11)15(9)5-1-2-7(10)14-12/h1-6,13H/b5-1-,7-2+
	$C_{12}H_7N_3O$						
X-43		26.8871	351.7298	-16.9523	7.7793	373.5181	InChI=1S/C12H7N3O/c16-12-10-11(15(10)12)14-4-1-2-7-6-9-8(7)3-5-13-9/h1-6,13H/b2-1-,14-4+
	$C_{12}H_7N_3O$						
o-168		10.7184	203.1599	-1.2724	108.7099	373.5567	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-10(8)11(14-12)9(15)6-7/h1-6,13H
	$C_{12}H_7N_3O$						
A-89		3.2826	303.0629	-2.9036	67.9105	373.5658	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)11(9-6-14-9)10-7(8)3-4-13-10/h1-6,13H/b11-9-
	$C_{12}H_7N_3O$						
A-144		3.2847	303.062	-2.9043	67.9121	373.5658	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)11(9-6-14-9)10-7(8)3-4-13-10/h1-6,13H/b11-9+
	$C_{12}H_7N_3O$						
p1-32		12.7142	181.5779	-8.2325	176.9694	373.7968	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)9-6-8-12(14-8)15(9)10/h1-6,13H/b3-1-,7-2-,11-9+
	$C_{12}H_7N_3O$						
p1-17		15.7571	184.3735	-8.4936	163.1543	373.8377	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)10-8-6(15)14-12(8)10/h1-6,13H/b3-1-,7-2-,11-10+
	$C_{12}H_7N_3O$						
i-22		12.3699	144.2187	-8.6058	192.0903	374.0981	InChI=1S/C12H7N3O/c16-12-10-9-6-7(15(9)12)2-1-4-13-8-3-5-14-11(8)10/h1-6,14H/b2-1-,4-1-,7-2-,11-10+,13-4-,13-8+
	$C_{12}H_7N_3O$						
H1-105		21.1779	167.9882	-2.7615	159.696	374.2126	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9(10)12-14-15(12)11-8(7)4-5-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
X22-43		8.7583	216.9879	-7.5247	149.3884	374.2401	InChI=1S/C12H7N3O/c16-10-6-9-11-7(10)2-1-4-13-8-3-5-14-12(8)15(9)11/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
X22-49		9.8106	248.2682	-6.8284	116.1364	374.3756	InChI=1S/C12H7N3O/c16-11-7-6-15-9(10(7)11)2-1-4-13-8-3-5-14-12(8)15/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
X23-28		24.2086	246.3291	-9.9084	96.0881	374.6283	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-10(8)11-9(6-7)15(11)12/h1-6,14H/b2-1-,4-1-,7-2-,11-10-,13-4-,13-8-
	$C_{12}H_7N_3O$						
H11-33		7.4581	147.2728	-3.3255	185.5401	374.6385	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(9)14-15(12)11-8(7)4-5-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
E-70		15.0309	229.3004	-5.0131	117.0212	374.6747	InChI=1S/C12H7N3O/c16-12-14-8-2-1-3-10-11(15(10)12)6-9-7(8)4-5-13-9/h1-6,13H/b2-1-,10-3-,11-6-,14-8-
	$C_{12}H_7N_3O$						
o-210		6.9856	158.9022	-2.3393	173.9435	375.2987	InChI=1S/C12H7N3O/c16-12-8-6-15-5-1-2-7(10(8)14-12)11-9(15)3-4-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
o-157		11.0529	252.6149	-4.6084	92.0685	375.7524	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)10-3-4-13-8(10)6-9-11(7)14-9/h1-6,13H/b9-6+
	$C_{12}H_7N_3O$						
X22-53		19.4596	232.8245	-11.2555	102.4595	375.7914	InChI=1S/C12H7N3O/c16-12-10-6-8-7(3-5-14-8)13-4-1-2-9-11(12)15(9)10/h1-6,14H/b2-1-,10-6+,13-4+
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


















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q11-13		32.3262	104.4232	-1.9383	169.2389	375.894	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)11(9)14-15(8)12/h1-6,13H/b2-1-,8-3-
B-20		10.9926	196.8951	-3.1754	128.9184	375.9011	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(12(9)14-10)11-8(7)3-4-13-11/h1-6,13H
G-4		34.3503	306.7886	-0.6493	25.9443	375.9638	InChI=1S/C12H7N3O/c16-12-9(15-6-14-15)3-1-2-7-8-4-5-13-11(8)10(7)12/h1-6,13H
C-24		9.9285	333.9921	-6.2759	26.6744	376.0325	InChI=1S/C12H7N3O/c16-12-10-6-9-7(2-1-4-14-15(10)12)8-3-5-13-11(8)9/h1-6,13H/b2-1-,10-6-,14-4-
n-202		3.3104	304.3819	-2.8024	69.9947	376.0421	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)9-3-4-13-11(9)10(7)8-6-14-8/h1-6,13H/b10-8+
o-42		4.2829	336.5798	-1.4156	27.9592	376.3951	InChI=1S/C12H7N3O/c16-11-8-6-7-2-1-5-15(7)9-3-4-13-12(9)14-10(8)11/h1-6,13H/b8-6-,14-10+
G1-54		9.0853	101.5378	-4.2033	234.7189	376.4993	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-11(7)8-6-14-15(9)12(8)10/h1-6,13H
X-51		40.7009	178.1793	-13.6208	127.4517	376.6416	InChI=1S/C12H7N3O/c16-12-14-4-1-2-7-6-9-11(15(9)12)10-8(7)3-5-13-10/h1-6,13H/b2-1-,14-4+
o-111		6.8323	71.5989	-3.1054	264.3496	377.0699	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-6-8(11)10(7)14-12-9(15)3-4-13-12/h1-6,13H/b5-1-,7-2-
H11-142		29.2906	87.3477	-0.6664	194.6325	377.1724	InChI=1S/C12H7N3O/c16-12-8-6-15-10(3-1-2-9(8)14-15)7-4-5-13-11(7)12/h1-6,13H
I-78		30.8332	146.5095	-1.9266	131.4504	377.2	InChI=1S/C12H7N3O/c16-9-6-7-10-8(2-4-14-10)15-5-1-3-13-11(7)12(9)15/h1-6,14H
x4-25		10.3645	210.9421	-2.1629	126.8696	377.3435	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-10(7)8-6-14-15(9)11(8)12/h1-6,13H/b2-1-,9-3+
H-26		13.0317	161.4802	-4.5056	174.7297	377.4772	InChI=1S/C12H7N3O/c16-12-7-2-1-3-8-9-4-5-13-10(9)15(12)11(8)14-6-7/h1-6,13H/b2-1-,3-1-,7-2-,8-3-
A-162		27.2801	243.3722	-9.1879	95.3855	377.5027	InChI=1S/C12H7N3O/c16-12-9-10-7(3-4-13-10)8-2-1-5-15(6-14-8)11(9)12/h1-6,13H
H1-17		24.1073	230.853	-18.0462	97.4676	377.6856	InChI=1S/C12H7N3O/c16-9-3-1-2-8(7-4-5-13-11(7)9)12-14-10-6-15(10)12/h1-6,13H
X-32		9.5610	307.7570	-5.8589	52.9577	377.9733	InChI=1S/C12H7N3O/c16-12-11-9-6-7(2-1-4-14-15(11)12)8-3-5-13-10(8)9/h1-6,13H/b2-1-,11-9+,14-4-
x9-44		6.0257	327.4753	-2.1886	26.0059	378.4639	InChI=1S/C12H7N3O/c16-12-9-7(4-5-13-9)2-1-3-8-11-10(12)14-6-15(8)11/h1-6,13H/b2-1-,8-3+
k-27		9.0743	181.696	-6.6891	174.533	378.6925	InChI=1S/C12H7N3O/c16-9-6-8-12-10(9)11-7(2-4-14-11)13-3-1-5-15(8)12/h1-6,14H/b5-1-,13-3+




















G-51		23, 8946	217, 9301	-7, 3242	126, 2462	378, 8251	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7(15(10)12)6-14-11-9(8)4-5-13-11/h1-6, 13H/h14-6+
	$C_{12}H_7N_3O$						
x7-15		18, 2071	186, 3008	-7, 3792	158, 2424	379, 2397	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11-8(9)6-14-15(11)12/h1-6, 13H/h3-1-, 7-2-, 12-10-
	$C_{12}H_7N_3O$						
q1-58		38, 9115	233, 0783	-26, 5945	92, 9067	379, 2409	InChI=1S/C12H7N3O/c16-11-10-7(4-5-13-10)2-1-3-8-6-9(8)15-12(11)14-15/h1-6, 13H/h2-1-, 8-3-
	$C_{12}H_7N_3O$						
B-47		9, 3124	108, 5350	-2, 9316	219, 3928	379, 2905	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(12(10)14-9)11-8(7)3-4-13-11/h1-6, 13H
	$C_{12}H_7N_3O$						
G1-8		10, 2334	146, 4419	-2, 3512	195, 8886	379, 3802	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-12(7)11(10)9-6-14-15(8)9/h1-6, 13H/h3-1-, 8-2-
	$C_{12}H_7N_3O$						
G1-61		10, 2352	146, 3976	-2, 3533	195, 9353	379, 3802	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-12(7)11(10)9-6-14-15(8)9/h1-6, 13H/h3-1-, 8-2-
	$C_{12}H_7N_3O$						
o-186		4, 7682	79, 6515	-1, 9862	261, 9724	379, 6236	InChI=1S/C12H7N3O/c16-12-7-6-10-14-8(7)2-1-5-15(10)9-3-4-13-11(9)12/h1-6, 13H
	$C_{12}H_7N_3O$						
q1-51		19, 8475	151, 5249	-4, 6765	179, 909	379, 6393	InChI=1S/C12H7N3O/c16-11-9-6-8(12-14-15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6, 13H/h2-1-, 8-3+
	$C_{12}H_7N_3O$						
n-41		41, 5621	301, 4429	-18, 6991	37, 8313	379, 8706	InChI=1S/C12H7N3O/c16-11-9-7(6-14-10(9)11)2-1-5-15-8-3-4-13-12(8)15/h1-6, 13H/h5-1-, 7-2+
	$C_{12}H_7N_3O$						
s11-13		6, 4836	132, 8394	-3, 74	224, 8715	379, 8864	InChI=1S/C12H7N3O/c16-12-8-6-9-11-7(4-5-13-11)2-1-3-10(14-8)15(9)12/h1-6, 13H/h2-1-, 3-1-, 7-2-, 10-3-, 11-9+
	$C_{12}H_7N_3O$						
o-154		10, 7415	186, 4911	-1, 3167	139, 0622	379, 9356	InChI=1S/C12H7N3O/c16-10-6-7-11-9(3-4-13-11)15-5-1-2-8(10)14-12(7)15/h1-6, 13H
	$C_{12}H_7N_3O$						
q-32		20, 5237	171, 7874	-2, 2849	159, 7858	380, 0552	InChI=1S/C12H7N3O/c16-12-8-6-10-14-15(10)9(12)3-1-2-7-4-5-13-11(7)8/h1-6, 13H/h2-1-, 9-3+
	$C_{12}H_7N_3O$						
k-20		31, 7332	203, 2749	-12, 9333	136, 3011	380, 2208	InChI=1S/C12H7N3O/c16-12-9-7-6-15(11(9)12)5-1-3-13-8-2-4-14-10(7)8/h1-6, 14H/h5-1-, 13-3+
	$C_{12}H_7N_3O$						
G-58		7, 7547	178, 3329	-2, 0206	160, 4325	380, 378	InChI=1S/C12H7N3O/c16-12-11-8-2-1-3-9(15(11)6-14-12)10-7(8)4-5-13-10/h1-6, 13H
	$C_{12}H_7N_3O$						
x4-18		13, 8077	127, 1981	-5, 3276	208, 9544	380, 4401	InChI=1S/C12H7N3O/c16-12-10-8-6-14-15(12)9(8)3-1-2-7-4-5-13-11(7)10/h1-6, 13H/h2-1-, 3-1-, 7-2-, 9-3+, 11-10-
	$C_{12}H_7N_3O$						
q-11		21, 8723	191, 5779	-6, 127	140, 6933	380, 5765	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)9(6-8)15-12(11)14-15/h1-6, 13H/h2-1-, 3-1-, 7-2-, 8-3+, 10-9-
	$C_{12}H_7N_3O$						
B-146		5, 8114	306, 8303	-4, 1638	63, 8805	380, 6165	InChI=1S/C12H7N3O/c16-12-11-14-10-6-9-8(3-4-13-9)7(10)2-1-5-15(11)12/h1-6, 13H/h5-1-, 7-2-, 14-11-
	$C_{12}H_7N_3O$						
n-54		41, 5804	302, 1261	-18, 7673	37, 9675	380, 7042	InChI=1S/C12H7N3O/c16-11-9-7(6-14-10(9)11)2-1-5-15-8-3-4-13-12(8)15/h1-6, 13H/h5-1-, 7-2-
	$C_{12}H_7N_3O$						
E-5		17, 7844	190, 6341	-2, 4951	138, 0758	380, 8977	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(14-15(7)10)8-4-5-13-11(8)12/h1-6, 13H
	$C_{12}H_7N_3O$						

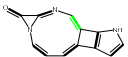
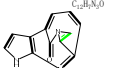
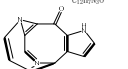
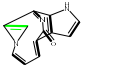
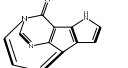
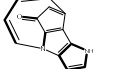
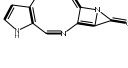
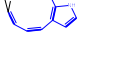
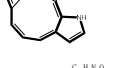
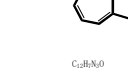
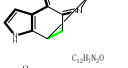
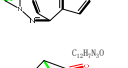
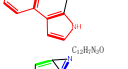
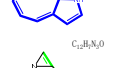
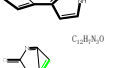
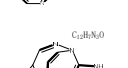
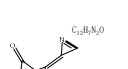
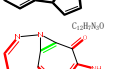

xS-45		19.1363	241.4263	-8.2395	67.4453	380.9713	InChI=1S/C12H7N3O/c16-12-10-9-6-8(15(9)10)3-1-2-7-4-5-13-11(7)14-12/h1-6H, (H, 13, 14, 16)
B-134		8.7183	95.3234	-3.4991	232.5639	381.0257	InChI=1S/C12H7N3O/c16-12-10-6-9-7(3-4-13-9)8-2-1-5-15(10)14-11(8)12/h1-6, 13H
o-44		3.8275	328.5753	-1.7103	40.1384	381.0944	InChI=1S/C12H7N3O/c16-12-7-6-8-9(3-4-13-8)15-5-1-2-10(15)14-11(7)12/h1-6, 13H/b7-6-, 14-11+
o-14		12.6666	148.1222	-4.8182	184.2659	381.4021	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-7(11(12)14-8)10-9(15)3-4-13-10/h1-6, 13H/b5-1-, 8-2-
F-56		6.8464	324.1257	-4.3256	48.4684	381.404	InChI=1S/C12H7N3O/c16-12-10-3-1-2-7-8-4-5-13-11(8)14-9(7)6-15(10)12/h1-6H, (H, 13, 14)/b2-1-, 9-6+, 10-3-
G1-64		12.9837	280.9963	-5.6158	44.8392	381.473	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-12(7)15-9(6-14-8)11(10)15/h1-6, 13H/b3-1-, 8-2-
E-56		5.746	109.6698	-2.6643	231.0018	381.6102	InChI=1S/C12H7N3O/c16-12-7-2-1-3-10-8-4-5-13-11(8)9(7)6-15(12)14-10/h1-6, 13H/b3-1-, 7-2+
A1-35		65.4155	299.7358	-36.5455	36.1949	381.6798	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)6-13-4-1-2-7-8-3-5-14-9(7)8/h1-6, 14H/b4-1-, 7-2-, 13-6+
A2-55		12.6811	376.8157	-2.9406	-3.9061	381.7175	InChI=1S/C12H7N3O/c16-10-6-8(10)12-13-4-1-2-9-7-3-5-14-11(7)15(9)12/h1-6, 14H
s12-7		33.5121	302.0714	-11.4204	33.4162	381.8104	InChI=1S/C12H7N3O/c16-12-8-6-10-7(4-5-13-10)2-1-3-9-11(8)15(12)14-9/h1-6, 13H/b3-1-, 7-2-, 10-6-
n-38		41.6362	299.5563	-19.1408	40.9285	382.0145	InChI=1S/C12H7N3O/c16-11-7-6-14-8(10(7)11)2-1-5-15-9-3-4-13-12(9)15/h1-6, 13H/b5-1-, 8-2-
n-27		41.6417	299.5758	-19.1411	40.9232	382.0531	InChI=1S/C12H7N3O/c16-11-7-6-14-8(10(7)11)2-1-5-15-9-3-4-13-12(9)15/h1-6, 13H/b5-1-, 8-2+
o-122		18.906	149.5705	-14.5719	186.3231	382.4127	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(14-9-6-8(9)12)10-3-4-13-11(7)10/h1-6, 13H/b14-9-
B-67		8.2463	154.0109	-3.3952	183.2734	382.6586	InChI=1S/C12H7N3O/c16-12-9-6-10-7(2-1-5-15(12)14-10)8-3-4-13-11(8)9/h1-6, 13H
G1-57		5.1452	378.8144	-1.9874	-4.31	382.6774	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-12(7)15(9)11(10)8-6-14-8/h1-6, 13H/b11-8+
p11-8		24.0195	362.1523	-14.0581	2.3418	382.7947	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)8-3-1-2-7-4-5-13-9(7)6-14-8/h1-6, 13H/b2-1-, 3-1-, 7-27, 8-3-, 9-6+, 14-6+, 14-8-
q-26		19.1611	222.3701	-5.7734	125.1465	383.0988	InChI=1S/C12H7N3O/c16-12-11-14-8-3-1-2-7-4-5-13-10(7)9(6-8)15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 10-9-
A-40		28.9064	219.9518	-12.6774	112.3738	383.1125	InChI=1S/C12H7N3O/c16-11-8-6-14-9-2-1-5-15(10(8)11)12-7(9)3-4-13-12/h1-6, 13H/b14-6-
A-97		28.9037	219.9567	-12.6751	112.3776	383.1125	InChI=1S/C12H7N3O/c16-12-9-6-14-15(11(9)12)5-1-2-7-8-3-4-13-10(7)8/h1-6, 13H/b5-1-, 7-2-




















s11-22		45.6984	221.2654	-20.2391	109.0682	383.5982	InChI=1S/C12H7N3O/c16-9-6-8(9)15-10-3-1-2-7-4-5-13-11(7)12(15)14-10/h1-6,13H/b2-1-,3-1-,7-2-,10-3+,12-11-
H-7		31.4162	237.5892	-0.4189	91.6489	383.7032	InChI=1S/C12H7N3O/c16-10-8-3-1-2-7(6-8)9-4-5-13-11(9)15-12(10)14-15/h1-6,13H
F-45		16.0704	208.1672	-7.8066	142.9849	383.8432	InChI=1S/C12H7N3O/c16-11-6-10-9-3-1-2-8(15(9)10)7-4-5-13-12(7)14-11/h1-6H, (H,13,14,16)
H1-108		22.9479	228.36	-12.6454	106.985	383.9893	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9-12(15(9)10)14-11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
r-47		36.2934	122.4188	-5.9502	154.0971	384.012	InChI=1S/C12H7N3O/c16-12-10-8-6-15(12)9(10)3-1-2-7-4-5-13-11(7)14-8/h1-6H, (H,13,14)/b3-1-,7-2-
p1-8		27.4471	251.7443	0.1078	91.3611	384.0151	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-11(7)12-8(9)6-10-14-15(10)12/h1-6,13H/b3-1-,7-2-,12-11-
x9-27		6.7249	331.3418	-2.1824	27.9438	384.0773	InChI=1S/C12H7N3O/c16-12-8-6-14-15-9(11(8)15)3-1-2-7-4-5-13-10(7)12/h1-6,13H/b2-1-,9-3+
E-35		17.1464	230.9232	0.4309	98.0555	384.2176	InChI=1S/C12H7N3O/c16-11-6-10-12-7(4-5-13-12)8-2-1-3-9(11)15(10)14-8/h1-6,13H
o-231		5.2354	396.1676	-4.3733	-6.1106	384.4764	InChI=1S/C12H7N3O/c16-12-11-9(3-4-13-11)15(12)5-1-2-7-6-8-10(7)14-8/h1-6,13H/b5-1-,7-2+
H-139		2.8751	321.2462	-2.2854	54.0038	384.5051	InChI=1S/C12H7N3O/c16-12-11(14-12)15-6-7-2-1-3-8(7)9-4-5-13-10(9)15/h1-6,13H
p1-28		21.5905	170.6936	-3.6864	167.9083	384.519	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)9-6-8(10)12-14-15(9)12/h1-6,13H/b3-1-,7-2-,11-9-
X-31		24.0536	224.7255	-6.7368	86.1720	384.5838	InChI=1S/C12H7N3O/c16-9-6-7-2-1-4-13-12-10(9)15(12)11-8(7)3-5-14-11/h1-6,14H/b2-1-,13-4+
x4-11		22.193	267.0774	-10.6831	77.1749	384.6324	InChI=1S/C12H7N3O/c16-9-6-14-11-10-7(4-5-13-10)2-1-3-8-12(11)15(8)9/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,11-10-
H11-116		6.9576	98.683	-0.3222	235.294	384.8603	InChI=1S/C12H7N3O/c16-11-9-6-15-12-8(4-5-13-12)7(9)2-1-3-10(11)14-15/h1-6,13H
B-162		12.1079	101.9582	-3.6023	220.0471	385.0658	InChI=1S/C12H7N3O/c16-10-9-6-14-12(10)15-5-1-2-7(9)8-3-4-13-11(8)15/h1-6,13H
B-197		12.1058	101.9626	-3.6014	220.0521	385.0658	InChI=1S/C12H7N3O/c16-11-8(7-3-4-13-10(7)11)2-1-5-15-9-6-14-12(9)15/h1-6,13H/b5-1-,8-2-
F-22		32.3923	90.7082	-1.2189	175.0698	385.2188	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-8(10)9-4-5-13-11(9)14-15(7)12/h1-6H, (H,13,14)
G-39		8.0588	180.4439	-1.9583	163.7656	385.4359	InChI=1S/C12H7N3O/c16-10-6-14-15-9-3-1-2-8(12(10)15)7-4-5-13-11(7)9/h1-6,13H
H1-44		34.7146	317.9273	-0.913	24.4868	385.5878	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)9(7)6-15-12(10)14-15/h1-6,13H/b3-1-,7-2-,9-6-











H11-151		10.3889	246.9327	-5.0409	93.0635	385.6224	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10(15-6-9(11)15)14-12-8(7)4-5-13-12/h1-6H, (H, 13, 14)
r-24		28.6283	260.1755	-15.9036	60.9602	385.7178	InChI=1S/C12H7N3O/c16-12-8-6-10-9(15(10)12)3-1-2-7-4-5-13-11(7)14-8/h1-6H, (H, 13, 14)
C-59		22.0180	224.8696	-8.4195	115.8410	385.7520	InChI=1S/C12H7N3O/c16-12-11-8-2-1-4-14-10(15(11)12)6-9-7(8)3-5-13-9/h1-6, 13H/b2-1-, 14-4-
s11-50		20.5703	231.4414	-15.2791	110.2615	386.1579	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-11(7)8-6-10(8)15(12)14-9/h1-6, 13H/b3-1-, 7-2-, 11-8+
X23-22		20.1554	243.1066	-12.0305	121.0635	386.1651	InChI=1S/C12H7N3O/c16-12-11-8-6-7(15(11)12)2-1-4-13-9-3-5-14-10(8)9/h1-6, 14H/b2-1-, 13-4+
B-29		21.3203	221.5702	-13.4457	138.1159	386.1938	InChI=1S/C12H7N3O/c16-10-6-9-12(10)14-15(9)5-1-2-7-8-3-4-13-11(7)8/h1-6, 13H/b5-1-, 7-2-
H1-100		10.8615	316.3868	-3.3016	44.764	386.4151	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-10(8)6-9(7)12-14-15(11)12/h1-6, 13H/b3-1-, 7-2-
q-45		29.8538	302.6913	-1.3228	50.5487	386.4229	InChI=1S/C12H7N3O/c16-10-6-9-11-7(4-5-13-11)2-1-3-8-12(14-8)15(9)10/h1-6, 13H/b2-1-, 8-3+
E-11		16.3085	190.5955	-5.7162	151.568	386.6361	InChI=1S/C12H7N3O/c16-11-7-2-1-3-9-8-4-5-13-12(8)15(14-9)10(11)6-7/h1-6, 13H/b3-1-, 7-2-
n-201		30.8459	249.3627	-1.7002	106.769	386.8984	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(12)9-3-4-13-11(9)10(7)8-6-14-8/h1-6, 13H/b10-8-
x6-33		14.8256	210.6749	-11.1197	152.5941	386.9951	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-8(7)6-15-11-10(9)14-12(11)15/h1-6, 13H/b3-1-, 7-2-, 8-6+
s11-33		2.2266	363.2665	-2.1468	13.8607	387.0896	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8-9(6-14-8)15(11)12/h1-6, 13H/b3-1-, 7-2-, 11-10+
s11-66		16.0458	204.1664	-5.5498	147.7744	387.1428	InChI=1S/C12H7N3O/c16-10-6-8-12-11-7(4-5-13-11)2-1-3-9(14-10)15(8)12/h1-6, 13H/b3-1-, 7-2-, 12-11+
B-26		13.3250	239.7498	-7.9708	108.4249	387.3239	InChI=1S/C12H7N3O/c16-10-6-8-12(14-8)11-7(3-4-13-11)9-2-1-5-15(9)10/h1-6, 13H/b8-6+
l-70		12.3622	374.8131	-2.963	-0.989	387.3557	InChI=1S/C12H7N3O/c16-9-6-7(9)10-12-11-8(2-4-14-11)15(12)5-1-3-13-10/h1-6, 14H
H1-133		28.4088	323.5817	-0.7958	25.3718	387.7236	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)9(7)6-10-14-15(10)11/h1-6, 13H/b3-1-, 7-2-, 9-6+
n-152		10.381	147.2249	-2.8163	178.2509	387.7757	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)10(12)8(7)6-14-15/h1-6, 13H/b5-1-, 7-2+
C-38		13.6934	182.8836	-7.9419	157.0088	388.0407	InChI=1S/C12H7N3O/c16-10-6-9-12-8(2-1-4-14-15(9)12)7-3-5-13-11(7)10/h1-6, 13H
q1-16		50.3245	260.6623	-31.441	85.7042	388.6626	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-6-9(8)11-14-15(11)12/h1-6, 13H/b2-1-, 8-3-

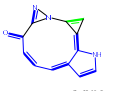
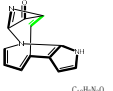
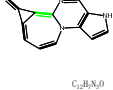
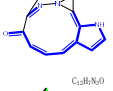
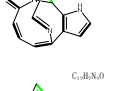
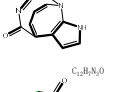
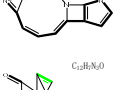
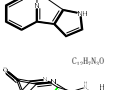
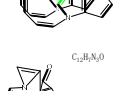
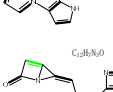
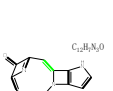
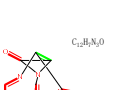
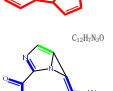
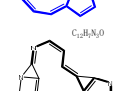
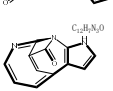
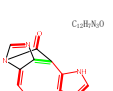
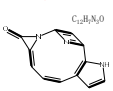
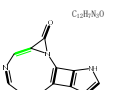

q-33		20.5913	171.5996	-2.3227	170.0114	388.7535	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)9(11)6-15-12(8)14-15/h1-6,13H/b2-1-,8-3+
	$C_{12}H_7N_3O$						
I-31		30.0355	241.9833	-11.511	104.7319	389.0207	InChI=1S/C12H7N3O/c16-12-10-9-6-7-8(2-4-13-7)15(9)5-1-3-14-11(10)12/h1-6,13H/b5-1-,14-3-
	$C_{12}H_7N_3O$						
r-48		16.6312	210.4221	-7.3584	150.5829	389.0624	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-11(7)14-9(6-8)15(10)12/h1-6H,(H,13,14)/b3-1-,7-2-
	$C_{12}H_7N_3O$						
B-163		9.4638	90.8963	-2.6880	233.3984	389.4499	InChI=1S/C12H7N3O/c16-12-9-6-14-11-10-8(3-4-13-10)7(9)2-1-5-15(11)12/h1-6,13H
	$C_{12}H_7N_3O$						
o-45		29.1464	189.7053	-15.527	135.5273	389.4922	InChI=1S/C12H7N3O/c16-12-8-6-7(8)2-1-5-15-9-3-4-13-10(9)11(12)14-15/h1-6,13H/b5-1-,7-2+
	$C_{12}H_7N_3O$						
x3-11		29.5878	230.4044	-10.2537	111.7192	389.6294	InChI=1S/C12H7N3O/c16-12-9-7-6-15(5-1-3-13-7)8-2-4-14-11(8)10(9)12/h1-6,14H
	$C_{12}H_7N_3O$						
X23-13		26.8622	295.6441	-17.6454	71.3918	389.7792	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)7-2-1-4-13-8-3-5-14-9(8)6-7/h1-6,14H/b2-1-,4-1+,7-2+,9-6-,13-4+,13-8-
	$C_{12}H_7N_3O$						
H1-72		9.1275	260.4201	-3.8942	92.8823	389.9076	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12(14-10)15-6-9(7)15/h1-6,13H/b3-1-,7-2-,14-12-
	$C_{12}H_7N_3O$						
B-220		7.0604	49.9000	-2.5844	293.1526	390.2323	InChI=1S/C12H7N3O/c16-12-9-6-15-5-1-2-7(9)8-3-4-13-10(8)11(12)14-15/h1-6,13H
	$C_{12}H_7N_3O$						
H11-70		11.0727	195.7445	-3.2136	163.4121	390.3056	InChI=1S/C12H7N3O/c16-11-6-10-14-8-2-1-3-9(15(10)11)7-4-5-13-12(7)8/h1-6,13H
	$C_{12}H_7N_3O$						
r-60		26.9576	235.5927	-15.6562	143.7479	390.4587	InChI=1S/C12H7N3O/c16-12-14-11-7(4-5-13-11)2-1-3-8-6-9-10(8)15(9)12/h1-6H,(H,13,14,16)/b3-1-,7-2-
	$C_{12}H_7N_3O$						
A2-88		24.6288	199.683	-8.8464	138.9161	390.4691	InChI=1S/C12H7N3O/c16-10-6-9-12-13-4-1-2-7(10)8-3-5-14-11(8)15(9)12/h1-6,14H/b4-1-,7-2-,13-12+
	$C_{12}H_7N_3O$						
o-190		43.2162	212.8658	-17.9671	122.5941	390.506	InChI=1S/C12H7N3O/c16-10-6-8(10)7-2-1-5-15-9-3-4-13-12(9)11(7)14-15/h1-6,13H
	$C_{12}H_7N_3O$						
B-155		4.3637	333.3225	-1.5723	33.7911	390.5621	InChI=1S/C12H7N3O/c16-11-9-6-7(8-3-4-13-10(8)9)2-1-5-15-12(11)14-15/h1-6,13H/b5-1-,7-2+
	$C_{12}H_7N_3O$						
o-136		8.9617	119.1315	-1.7455	217.4528	390.6212	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(9-6-14-10(7)9)8-3-4-13-11(8)12/h1-6,13H
	$C_{12}H_7N_3O$						
A2-45		9.761	90.2414	-3.6611	249.2791	391.02	InChI=1S/C12H7N3O/c16-10-9-6-15-11-8(3-5-14-11)7(9)2-1-4-13-12(10)15/h1-6,14H/b4-1-,7-2-,13-12-
	$C_{12}H_7N_3O$						
q11-62		2.3064	366.0954	-2.0956	13.5149	391.058	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-9(6-14-11)15(8)12/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
q1-50		17.4953	178.1749	-7.34	172.7485	391.3076	InChI=1S/C12H7N3O/c16-11-8-6-15-9(12(15)14-8)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,9-3-
	$C_{12}H_7N_3O$						
H11-126		18.3915	182.4848	-13.3984	151.815	391.8406	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(15-6-10(15)14-8)7-4-5-13-11(7)12/h1-6,13H/b2-1-,9-3+,14-8-
	$C_{12}H_7N_3O$						
















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A-178		16, 6905	221, 7856	-6, 6724	134, 3578	392, 18	InChI=1S/C12H7N3O/c16-12-11-10-9-8(3-4-13-9)7(6-14-10)2-1-5-15(11)12/h1-6, 13H/t5-1-, 7-2-, 11-10-
A-75		3, 8797	307, 3977	-2, 9374	80, 4911	392, 3123	InChI=1S/C12H7N3O/c16-12-10(9-6-14-9)7-2-1-5-15(12)11-8(7)3-4-13-11/h1-6, 13H/t10-9+
A2-33		16, 0641	201, 1743	-8, 1536	158, 8676	392, 5144	InChI=1S/C12H7N3O/c16-12-8-2-1-4-13-11(9-6-15(9)12)10-7(8)3-5-14-10/h1-6, 14H/t2-1-, 4-1-, 8-2-, 13-4-, 13-11-
o-201		11, 0175	270, 0908	-5, 4091	98, 6238	393, 2011	InChI=1S/C12H7N3O/c16-12-7-6-9-10(3-4-13-9)15(12)5-1-2-8-11(7)14-8/h1-6, 13H/t5-1-, 8-2+
G-60		27, 0622	135, 2239	-12, 9603	202, 5701	393, 3255	InChI=1S/C12H7N3O/c16-10-6-14-15-9-3-1-2-8(12(9)15)7-4-5-13-11(7)10/h1-6, 13H/t14-6-
E-64		6, 1087	276, 6665	-4, 7719	98, 5734	393, 3497	InChI=1S/C12H7N3O/c16-12-10-3-1-2-8-7-4-5-13-9(7)6-11(14-8)15(10)12/h1-6, 13H/t2-1-, 10-3-
B-70		15, 9929	218, 6936	-4, 0322	129, 8326	393, 4414	InChI=1S/C12H7N3O/c16-12-9-6-10-14-15(10)5-1-2-7(9)8-3-4-13-11(8)12/h1-6, 13H/t5-1-, 7-2-, 9-6+
o-206		3, 9124	331, 1109	-1, 4793	44, 3327	393, 5433	InChI=1S/C12H7N3O/c16-12-7-6-9-8(14-9)2-1-5-15(12)10-3-4-13-11(7)10/h1-6, 13H/t5-1-, 7-6-, 8-2+
o-134		7, 2819	71, 3418	-3, 2078	277, 0413	393, 6694	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(10-6-8(12)14-10)9-3-4-13-11(7)9/h1-6, 13H
A2-54		30, 4286	200, 372	-16, 4849	142, 8395	393, 6884	InChI=1S/C12H7N3O/c16-11-8-2-1-4-14-12(15-6-9(11)15)10-7(8)3-5-13-10/h1-6, 13H/t2-1-, 4-1-, 8-2-, 14-4-, 14-12+
A2-57		9, 6726	200, 2529	-2, 8935	153, 8267	394, 0419	InChI=1S/C12H7N3O/c16-10-9-6-7-2-1-4-13-12(10)15(9)11-8(7)3-5-14-11/h1-6, 14H/t4-1-, 7-2-, 13-12+
B-224		11, 1261	117, 2096	-4, 2309	220, 9679	394, 0717	InChI=1S/C12H7N3O/c16-11-9-6-15-5-1-2-7(10(11)14-9)8-3-4-13-12(8)15/h1-6, 13H/t9-6+
o-133		4, 1566	321, 3279	-2, 7564	59, 2623	394, 2847	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-12(9)14-10(15)6-8(7)11/h1-6, 13H/t5-1-, 7-2-, 8-6+
B-65		2, 8312	316, 1776	-1, 4743	61, 6931	394, 5034	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-10(14-15)6-9(12)11-7(8)3-4-13-11/h1-6, 13H/t5-1-, 8-2-, 9-6-
H11-66		12, 5431	113, 2213	-5, 7391	227, 4253	394, 8312	InChI=1S/C12H7N3O/c16-11-6-9-7-2-1-3-10(14-9)15(11)12-8(7)4-5-13-12/h1-6, 13H
q11-32		23, 6086	137, 2225	-11, 0093	201, 3456	395, 061	InChI=1S/C12H7N3O/c16-10-6-9-8-3-1-2-7-4-5-13-11(7)12(10)14-15(8)9/h1-6, 13H/t2-1-, 8-3-
H1-73		16, 7969	209, 8785	-6, 013	136, 7235	395, 0625	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9(10)15-12(14-15)11-8(7)4-5-13-11/h1-6, 13H
B-147		3, 1789	327, 7203	-2, 1795	55, 2962	395, 1918	InChI=1S/C12H7N3O/c16-12-11(14-12)15-5-1-2-8-7-3-4-13-9(7)6-10(8)15/h1-6, 13H

B-200		8.7272	338.1042	-5.1547	45.1324	395.5303	InChI=1S/C12H7N3O/c16-12-11-14-6-9-7(2-1-5-15(11)12)8-3-4-13-10(8)9/h1-6,13H/b5-1-,7-2-,9-6+,14-11-
H11-91		16.9959	254.9599	-4.8991	101.1766	395.5609	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(10-6-15(10)12)14-11-7(8)4-5-13-11/h1-6H, (H,13,14)
A-102		5.6286	258.8255	-2.9818	100.1163	395.5672	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)8-2-1-5-15-9(6-14-8)11(12)15/h1-6,13H/b5-1-,8-2-,14-6-
B-252		39.2827	231.5208	-21.4907	110.9525	395.6011	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-6-9(15)11(14-12)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-
A-199		11.7548	156.7419	-4.7505	191.6494	395.9290	InChI=1S/C12H7N3O/c16-12-9-10-8(3-4-13-10)7-2-1-5-15(12)6-14-11(7)9/h1-6,13H/b5-1-,7-2-
I-77		17.696	160.2131	-4.4082	183.6305	396.0395	InChI=1S/C12H7N3O/c16-9-6-7-10-11-8(2-4-14-11)15(12(9)10)5-1-3-13-7/h1-6,14H/b5-1-,13-3-
p11-17		17.774	288.1218	-10.1447	71.3682	396.4794	InChI=1S/C12H7N3O/c16-12-11-10-9(15(11)12)3-1-2-7-4-5-13-8(7)6-14-10/h1-6,13H/b2-1-,9-3+,14-6-
q1-14		22.5516	185.2736	-7.6494	163.2958	396.6427	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-6-9-11(12)14-15(8)9/h1-6,13H/b2-1-,8-3-
s11-58		32.6573	296.473	-0.7614	48.4964	396.6741	InChI=1S/C12H7N3O/c16-9-6-8-11(9)12-7(4-5-13-12)2-1-3-10-14-15(8)10/h1-6,13H/b3-1-,7-2-,12-11-
s12-34		26.1805	285.8108	-17.4528	90.2972	396.7302	InChI=1S/C12H7N3O/c16-12-10-11(15(10)12)14-8-3-1-2-7-4-5-13-9(7)6-8/h1-6,13H/b14-8+
H1-15		27.2143	146.5195	-0.7758	155.923	396.9648	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)10-6-9(7)14-15(10)11/h1-6,13H/b3-1-,7-2-
E-13		5.5988	240.6331	-3.0768	126.0427	396.9994	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9(14-15-6-10(12)15)7-4-5-13-11(7)8/h1-6,13H/b14-9+
X-24		35.1853	107.5470	-4.9518	167.0259	397.3322	InChI=1S/C12H7N3O/c16-12-10-11-9-8(3-5-14-9)7(6-15(11)12)2-1-4-13-10/h1-6,14H/b2-1-,13-4+
p1-22		10.2506	223.494	-3.7893	156.0392	397.3872	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11-8(14-11)6-15(9)12/h1-6,13H/b3-1-,7-2-,12-10+
H11-143		21.4571	280.5736	-8.6731	62.0497	397.5504	InChI=1S/C12H7N3O/c16-12-9-6-15(9)10-3-1-2-8(14-10)7-4-5-13-11(7)12/h1-6,13H
o-175		8.7028	91.2252	-2.8035	251.6476	397.862	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)8(7)6-10(15)14-12/h1-6,13H/b5-1-,7-2+
A-38		43.1149	213.7075	-19.9262	125.5195	398.287	InChI=1S/C12H7N3O/c16-11-9-6-14-15-5-1-2-7(10(9)11)8-3-4-13-12(8)15/h1-6,13H/b14-6-
A-140		31.4001	247.7778	-1.9229	117.2207	398.667	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)8-2-1-5-15(12)11(8)9-6-14-9/h1-6,13H/b11-9-
X-28		16.8013	264.5596	-6.1221	68.0765	398.7473	InChI=1S/C12H7N3O/c16-12-10-8(3-5-13-10)7-2-1-4-14-15-9(6-7)11(12)15/h1-6,13H/b2-1-,14-4-

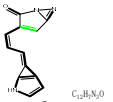
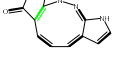
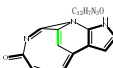
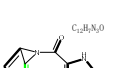
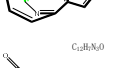
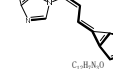
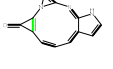
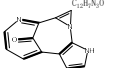
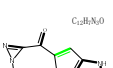
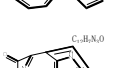

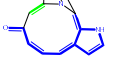
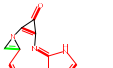
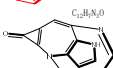
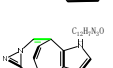
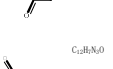
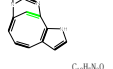
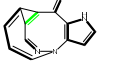
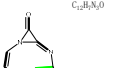
o-226		16.9773	255.9126	-6.8639	103.0625	398.8468	InChI=1S/C12H7N3O/c16-10-6-7-11(14-7)8-2-1-5-15(8)9-3-4-13-12(9)10/h1-6,13H/b7-6+
o-55		9.7556	94.0681	-3.3881	248.7674	398.9458	InChI=1S/C12H7N3O/c16-11-8-6-14-12(11)15-5-1-2-7(8)10-9(15)3-4-13-10/h1-6,13H
A2-14		6.362	316.5023	-4.4833	69.0862	399.0445	InChI=1S/C12H7N3O/c16-12-11-14-4-1-2-7-6-9(15(11)12)10-8(7)3-5-13-10/h1-6,13H/b4-1-,7-2-,14-11-
n-157		10.4864	227.1501	-4.5453	140.1875	399.4082	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-8-3-4-13-12(8)14-6-9(15)10(7)11/h1-6,13H
B-173		10.6494	166.9557	-3.2741	182.3572	399.6050	InChI=1S/C12H7N3O/c16-12-11-10-8(3-4-13-10)7-2-1-5-15(12)9(6-7)14-11/h1-6,13H
B-2		40.7988	199.3532	-18.4767	145.0187	399.6152	InChI=1S/C12H7N3O/c16-10-6-9(10)11-7-2-1-5-15(14-11)12-8(7)3-4-13-12/h1-6,13H
A2-1		4.7056	375.359	-1.2214	8.3403	399.7589	InChI=1S/C12H7N3O/c16-12-11-14-4-1-2-7-8-3-5-13-10(8)9(7)6-15(11)12/h1-6,13H/b4-1-,7-2-,9-6-,14-11-
x3-20		22.6505	193.1365	-10.1245	120.0192	400.0334	InChI=1S/C12H7N3O/c16-12-10-7-6-15(5-1-3-14-12)8-2-4-13-11(8)9(7)10/h1-6,13H/b5-1-,14-3-
o-240		13.869	213.3357	-5.2186	155.2466	400.0802	InChI=1S/C12H7N3O/c16-10-6-8-11(14-8)7-2-1-5-15(10)9-3-4-13-12(7)9/h1-6,13H/b8-6+
A-90		5.8297	259.6163	-3.1021	101.7362	400.2021	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-9(6-14-12)11(15)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-,14-6-
A-147		5.8288	259.6198	-3.1013	101.7392	400.2021	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-9(6-14-12)11(15)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-,14-6-
q-37		21.0764	264.5947	-12.3504	104.5835	400.2749	InChI=1S/C12H7N3O/c16-12-8-6-15(12)11-9(14-11)3-1-2-7-4-5-13-10(7)8/h1-6,13H/b2-1-,9-3+
B-214		20.9788	223.1406	-13.3699	150.8684	400.3782	InChI=1S/C12H7N3O/c16-12-9-6-15(11(9)14-12)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
B-73		8.5003	110.7119	-4.2030	240.9151	400.7151	InChI=1S/C12H7N3O/c16-12-9-6-10-14-11-8(3-4-13-11)7(9)2-1-5-15(10)12/h1-6,13H
o-143		13.1384	78.941	-4.0751	254.6704	401.012	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(10-6-8(7)14-10)9-3-4-13-11(9)12/h1-6,13H/b5-1-,7-2-
q11-31		15.7286	222.1347	-6.5177	146.3709	401.1255	InChI=1S/C12H7N3O/c16-10-6-9-8-3-1-2-7-4-5-13-11(7)12(14-10)15(8)9/h1-6,13H/b2-1-,8-3-
p1-34		14.7745	192.8863	-9.7113	179.2925	401.141	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)12-14-11-9(6-8)15(11)12/h1-6,13H/b3-1-,7-2-,9-6-,12-10+
q11-9		10.6633	99.1836	-6.2713	247.1434	401.2129	InChI=1S/C12H7N3O/c16-12-8-6-15-9(8)3-1-2-7-4-5-13-10(7)11(12)14-15/h1-6,13H/b2-1-,9-3-
A-186		32.7492	215.2297	-12.1799	137.6089	401.7052	InChI=1S/C12H7N3O/c16-11-9-7-2-1-5-15(6-14-10(9)11)12-8(7)3-4-13-12/h1-6,13H/b14-6-

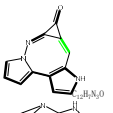
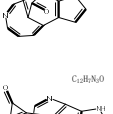
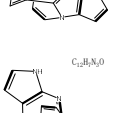
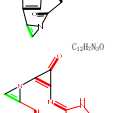
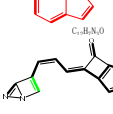
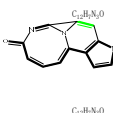
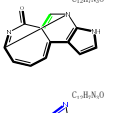
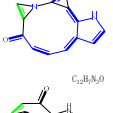
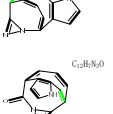
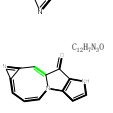
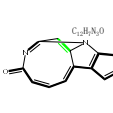
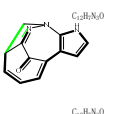
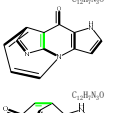
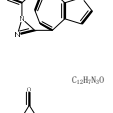
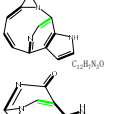
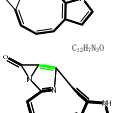
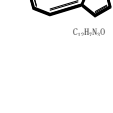


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X22-31		15, 8218	187, 3031	-9, 6674	181, 7438	401, 7984	InChI=1S/C12H7N3O/c16-12-7-6-10-11-8(3-5-14-11)13-4-1-2-9(7)15(10)12/h1-6, 14H/b2-1-, 4-1-, 9-2-, 11-10+, 13-4-, 13-8-
s11-11		30, 6095	88, 8487	-2, 4147	212, 229	401, 9704	InChI=1S/C12H7N3O/c16-12-8-6-10-11-7(4-5-13-11)2-1-3-9(8)14-15(10)12/h1-6, 13H/b3-1-, 7-2-, 11-10+
H-69		24, 304	236, 4696	-8, 4314	122, 4646	402, 1769	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(6-10-14-15(10)12)11-8(9)4-5-13-11/h1-6, 13H/b7-6+
H-14		9, 689	163, 971	-2, 3686	186, 9409	402, 3238	InChI=1S/C12H7N3O/c16-10-7-2-1-3-9-8-4-5-13-11(8)15(6-7)12(10)14-9/h1-6, 13H/b2-1-, 7-3-
p1-38		9, 0938	87, 4765	-4, 5203	274, 5111	402, 3338	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-14-11-8(9)6-15(11)12/h1-6, 13H/b3-1-, 7-2-, 12-10+
j-11		29, 1422	296, 5739	-16, 9884	70, 4396	402, 6073	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)7-2-1-4-13-8-3-5-14-9(8)6-7/h1-6, 14H/b2-1-, 4-1-, 7-2-, 7-6+, 9-6+, 13-4+, 13-8+
H-144		4, 2011	335, 5062	-3, 6905	56, 6177	402, 9528	InChI=1S/C12H7N3O/c16-12-9(14-12)6-7-2-1-3-10-8-4-5-13-11(8)15(7)10/h1-6, 13H/b7-6+
B-72		9, 5468	92, 1662	-3, 2993	248, 6108	403, 0349	InChI=1S/C12H7N3O/c16-12-9-6-10-11-8(3-4-13-11)7(9)2-1-5-15(12)14-10/h1-6, 13H
H11-146		26, 5225	181, 7576	-2, 6243	175, 1671	403, 4782	InChI=1S/C12H7N3O/c16-12-8-2-1-3-11-14-15(11)10(12)6-9-7(8)4-5-13-9/h1-6, 13H/b3-1-, 8-2-
n-180		3, 943	308, 6081	-3, 0076	90, 1258	404, 1097	InChI=1S/C12H7N3O/c16-12-10(8-6-14-8)7-2-1-5-15(12)9-3-4-13-11(7)9/h1-6, 13H/b10-8+
H1-124		14, 404	217, 317	-4, 5402	157, 8046	404, 278	InChI=1S/C12H7N3O/c16-7-2-1-3-9-8-4-5-13-11(8)15-10(6-7)12(15)14-9/h1-6, 13H/b2-1-, 9-3-, 10-6-
r-30		28, 0444	257, 366	-16, 1202	103, 6407	404, 6738	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)14-15(12)10-6-9(8)10/h1-6H, (H, 13, 14)/b3-1-, 7-2-
X-47		26, 8267	301, 7881	-10, 1582	38, 2390	404, 7158	InChI=1S/C12H7N3O/c16-12-10-8(3-5-13-10)7-2-1-4-14-11-9(6-7)15(11)12/h1-6, 13H/b2-1-, 4-1-, 7-2-, 14-4-, 14-11+
E-18		17, 1108	188, 7346	-11, 7536	171, 9912	405, 0279	InChI=1S/C12H7N3O/c16-12-10-6-15(10)9-3-1-2-8(14-12)7-4-5-13-11(7)9/h1-6, 13H/b14-8+
r1-26		14, 4322	206, 558	-10, 0021	172, 1751	405, 0906	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-12(7)14-15-9-6-8(10)11(9)15/h1-6H, (H, 13, 14)/b3-1-, 7-2-
B-90		8, 6524	383, 4929	-1, 3744	-1, 2400	405, 1161	InChI=1S/C12H7N3O/c16-12-10-6-9-11-7(3-4-13-11)8(14-9)2-1-5-15(10)12/h1-6, 13H/b5-1-, 8-2-, 10-6-
H1-62		37, 4178	242, 0817	-19, 5418	101, 3663	405, 1623	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)12(14-10)9-6-15(8)9/h1-6, 13H/b3-1-, 8-2-, 14-12+
s11-27		13, 0446	125, 5835	-4, 4157	209, 2359	405, 399	InChI=1S/C12H7N3O/c16-12-8-6-15-11(8)10-7(4-5-13-10)2-1-3-9(12)14-15/h1-6, 13H/b3-1-, 7-2-, 11-10+

p1-57		45.0512	265.1361	-24.3066	74.1772	405.5603	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9(8)15-12(10)14-15/h1-6,13H/b3-1-,7-2-,11-8+
B-156		11.1099	134.2884	-4.3342	217.2857	405.5885	InChI=1S/C12H7N3O/c16-10-9-6-7-2-1-5-15(12(10)14-9)11-8(7)3-4-13-11/h1-6,13H/b9-6-
n-173		10.528	233.6527	-4.4348	142.5101	405.6015	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-8(9)6-14-12(15)10(7)11/h1-6,13H
p1-7		18.6708	182.993	-8.3884	187.611	406.065	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)12-9-6-8(10)14-15(9)12/h1-6,13H/b3-1-,7-2-,12-11+
G1-93		25.0414	260.1715	-10.2187	86.8008	406.0666	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)12-9(6-14-8)15(10)12/h1-6,13H/b3-1-,8-2-
B-101		14.5919	224.5256	-10.4700	126.4957	406.2290	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(10-6-9(10)14-12)11-7(8)3-4-13-11/h1-6,13H/b4-9-
H11-72		19.1255	297.9108	-7.2137	95.8822	406.347	InChI=1S/C12H7N3O/c16-11-6-9-8(14-9)2-1-3-10-7-4-5-13-12(7)15(10)11/h1-6,13H/b2-1-,9-6-,10-3-
E-47		17.9316	205.7924	-11.9457	142.5112	406.6189	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8(14-10-6-15(9)10)7-4-5-13-11(7)12/h1-6,13H/b2-1-,9-3-,14-87
o-2		3.91	332.5461	-0.8276	40.7799	406.7397	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-8(14-10(7)12)11-9(15)3-4-13-11/h1-6,13H/b5-1-,7-2-,14-10+
k-37		75.7039	298.6089	-44.7342	46.0788	406.7574	InChI=1S/C12H7N3O/c16-12-9-8-6-15(8)5-1-3-13-7-2-4-14-11(7)10(9)12/h1-6,14H/b5-1-,13-3+
F-40		6.0562	422.5676	-4.548	-7.09	407.7498	InChI=1S/C12H7N3O/c16-11-6-10-9(15(10)11)3-1-2-8-7-4-5-13-12(7)14-8/h1-6H, (H,13,14)/b2-1-,9-3-
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X-36		22.4627	218.3116	-6.8948	154.3305	408.0401	InChI=1S/C12H7N3O/c16-12-11-10-9-8(3-5-14-9)7(6-15(11)12)2-1-4-13-10/h1-6,14H/b2-1-,13-4+
p1-61		11.7442	205.621	-5.6811	181.2857	408.2126	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-8-6-14-12(9)15(8)11/h1-6,13H/b3-1-,7-2-,11-10+
A2-17		28.1088	300.1096	-18.1858	90.5473	408.3433	InChI=1S/C12H7N3O/c16-10-6-9-12(15(9)10)14-4-1-2-7-8-3-5-13-11(7)8/h1-6,13H/b4-1-,7-2-,14-12+
A2-9		38.5085	148.005	-2.2015	132.8147	408.6141	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-4-13-11(9)15(12)10-8(7)3-5-14-10/h1-6,14H/b2-1-,4-1-,7-2-,13-4-,13-11+
x4-23		14.3688	131.3423	-5.2323	235.0337	408.8757	InChI=1S/C12H7N3O/c16-12-9-10-7(4-5-13-10)2-1-3-8-11(9)14-6-15(8)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,10-9-
q11-58		10.8047	321.1137	-8.1516	71.1154	409.0259	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-11(7)8-6-10(14-8)15(9)12/h1-6,13H/b2-1-,9-3-
C-29		4.6772	409.1886	-1.3878	-6.9000	409.0847	InChI=1S/C12H7N3O/c16-12-9-6-13-4-1-2-8-7-3-5-14-10(7)11(8)15(9)12/h1-6,14H/b2-1-,9-6-,13-4-




















H11-29		15, 509	360, 778	-6, 23	13, 3573	409, 2413	InChI=1S/C12H7N3O/c16-12-11-6-10-8(4-5-13-10)7-2-1-3-9(7)14-15(11)12/h1-6, 13H/b1-6+, 14-9+
H1-96		35, 5576	285, 8959	-18, 4848	107, 8659	409, 6079	InChI=1S/C12H7N3O/c16-10(15-6-9-12(15)14-9)3-1-2-7-8-4-5-13-11(7)8/h1-6, 13H/b3-1-, 7-2-
X22-10		14, 3582	268, 9758	-6, 302	121, 8439	409, 9068	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-4-13-8-3-5-14-10(8)11(7)15(9)12/h1-6, 14H/b2-1-, 4-1+, 7-2-, 11-10-, 13-4+, 13-8-
B-168		22, 2631	202, 4280	-10, 5421	145, 2049	409, 9229	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)7-2-1-5-15-9(6-7)11(15)14-12/h1-6, 13H/b1-6, 13H/b4-11+
B-127		18, 5362	245, 7404	-0, 7296	120, 2535	409, 9749	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-12(14-15)9(11)6-10-7(8)3-4-13-10/h1-6, 13H/b5-1-, 8-2-
B-27		10, 3319	290, 0698	-3, 9610	102, 4724	410, 0598	InChI=1S/C12H7N3O/c16-10-6-9-11(14-9)7-2-1-5-15(10)12-8(7)3-4-13-12/h1-6, 13H/b9-6+
n-47		29, 9418	236, 7207	-11, 1637	128, 1542	410, 266	InChI=1S/C12H7N3O/c16-12-7-6-14-8-2-1-5-15(11(7)12)9-3-4-13-10(8)9/h1-6, 13H/b14-6-
X22-11		15, 0521	267, 8199	-6, 6042	125, 823	410, 6209	InChI=1S/C12H7N3O/c16-12-10-6-7-9(15(10)12)2-1-4-13-8-3-5-14-11(7)8/h1-6, 14H/b2-1-, 4-1+, 9-2+, 11-7+, 13-4+, 13-8-
F-24		14, 402	289, 6439	-6, 0627	83, 2499	411, 245	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-8(7)9-4-5-13-11(9)14-15(10)12/h1-6H, 6H, 13, 14)/b9-8-, 10-6-
B-189		9, 8923	343, 2398	-5, 6494	54, 1731	411, 4031	InChI=1S/C12H7N3O/c16-12-9-6-14-11-7(2-1-5-15(9)12)8-3-4-13-10(8)11/h1-6, 13H/b5-1-, 7-2-, 9-6-, 14-11+
q1-28		25, 7905	237, 6206	-13, 3513	142, 7206	411, 4976	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-6-9-11(14-12)15(8)9/h1-6, 13H/b2-1-, 8-3-, 14-11-
A1-46		15, 0399	317, 2185	-6, 9849	53, 8231	411, 5688	InChI=1S/C12H7N3O/c16-9-6-13-4-1-2-8-7-3-5-14-10(7)12-11(9)15(8)12/h1-6, 14H/b4-1-, 8-2-, 13-6-
H1-83		5, 4295	378, 3863	-1, 4205	15, 99	411, 7236	InChI=1S/C12H7N3O/c16-11-3-1-2-10-7-4-5-13-12(7)15(10)14-9-6-8(9)11/h1-6, 13H/b3-1-, 10-2-, 14-9+
A2-49		34, 0664	259, 5813	-18, 142	72, 4809	411, 9961	InChI=1S/C12H7N3O/c16-11-10-8(3-5-13-10)7-2-1-4-14-12(11)15-6-9(7)15/h1-6, 13H/b4-1-, 7-2-, 14-12-
s11-36		23, 1218	261, 8095	-7, 5335	119, 7223	412, 2107	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8-6-9(14-8)15(11)12/h1-6, 13H/b3-1-, 7-2-, 11-10+
G-26		9, 0995	343, 0371	-5, 665	55, 9812	412, 3139	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-8-4-5-13-10(8)11(7)14-6-15(9)12/h1-6, 13H/b2-1-, 9-3-, 14-6-
s11-65		21, 6676	206, 8672	-8, 0977	161, 038	412, 5423	InChI=1S/C12H7N3O/c16-10-6-9-12-11-7(4-5-13-11)2-1-3-8(10)14-15(9)12/h1-6, 13H/b3-1-, 7-2-, 12-11+
q1-11		56, 3338	297, 5131	-35, 4473	66, 0221	412, 5729	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-11(14-8)9-6-15(9)12/h1-6, 13H/b2-1-, 8-3+
X23-48		21, 9523	201, 5274	-11, 6095	152, 3051	412, 8202	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-9(8)10-11(12)15(10)6-7/h1-6, 14H/b2-1-, 13-4-

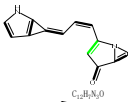
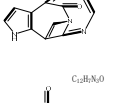
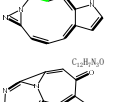
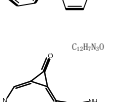
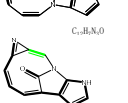
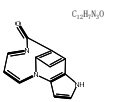
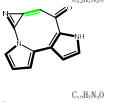
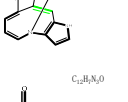
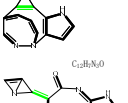
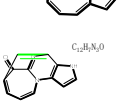
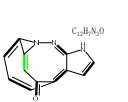
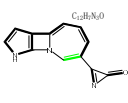
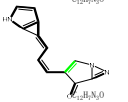
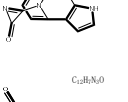
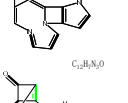
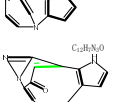



o-38		5.2712	339.6806	-1.204	39.009	413.3015	InChI=1S/C12H7N3O/c16-12-7-6-15(9-3-4-13-10(7)9)5-1-2-8-11(12)14-8/h1-6,13H/b5-1-,8-2+
H11-103		11.6128	261.8223	-6.5209	96.4561	413.3017	InChI=1S/C12H7N3O/c16-12-10-6-15(10)9-3-1-2-8(14-12)11-7(9)4-5-13-11/h1-6,13H/b14-8+
E-34		9.7071	238.6297	-3.8805	147.2322	415.108	InChI=1S/C12H7N3O/c16-11-6-10-9-3-1-2-8(14-15(9)10)7-4-5-13-12(7)11/h1-6,13H/b10-6-
o-132		44.9042	274.6467	-13.125	81.7624	415.1714	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-10(9)12(15)14-8(11)6-7/h1-6,13H/b5-1-,7-2+,14-12+
G-56		10.8898	265.8503	-7.3089	122.2273	415.3505	InChI=1S/C12H7N3O/c16-12-11-8-2-1-3-10(15(11)12)14-6-9-7(8)4-5-13-9/h1-6,13H/b14-6-
q-2		34.9799	161.3317	-6.651	183.5588	415.8205	InChI=1S/C12H7N3O/c16-11-9-6-8(15-12(11)14-15)3-1-2-7-4-5-13-10(7)9/h1-6,13H/b2-1-,3-1-,7-2-,8-3+,10-9-
I-26		39.4171	282.4875	-16.0584	77.2491	415.8239	InChI=1S/C12H7N3O/c16-12-7-6-9-13-3-1-5-15(9)8-2-4-14-11(8)10(7)12/h1-6,14H
A2-44		26.6274	205.4175	-12.4222	174.5697	416.1063	InChI=1S/C12H7N3O/c16-12-10-6-8-11-7(3-5-14-11)9(15(10)12)2-1-4-13-8/h1-6,14H/b2-1-,4-1-,9-2+,13-4-,13-8-
r-27		47.3423	293.3871	-28.3765	69.6384	416.2701	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-12(7)14-15-6-9(15)10(8)11/h1-6H,14H/b2-1-,4-1-,9-2+,13-4-,13-8-
H-107		11.3733	351.1073	-5.9723	40.0656	416.6119	InChI=1S/C12H7N3O/c16-12-11-14-10-9(4-5-13-10)8-3-1-2-7(8)6-15(11)12/h1-6,13H/b7-6+,14-11+
B-41		3.5876	367.6267	-1.8386	37.5476	416.8128	InChI=1S/C12H7N3O/c16-10-6-9-7(8-3-4-13-11(8)9)2-1-5-15-12(10)14-15/h1-6,13H/b5-1-,7-2+,9-6+
B-121		10.1904	119.9854	-3.9390	245.2591	416.8571	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(10-6-9(11)14-10)12-8(7)3-4-13-12/h1-6,13H
D-21		37.6310	101.7245	-0.8324	204.4411	417.4198	InChI=1S/C12H7N3O/c16-12-10-8-6-15(12)9(2-1-4-13-8)7-3-5-14-11(7)10/h1-6,14H/b2-1-,13-4+
q1-53		43.142	272.9663	-29.0933	95.8204	417.4465	InChI=1S/C12H7N3O/c16-11-9-6-15(9)12-8(14-12)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,8-3+
n-108		13.797	225.0084	-5.7352	143.9402	417.8372	InChI=1S/C12H7N3O/c16-9-6-14-15-5-1-2-7-10(9)11(7)12-8(15)3-4-13-12/h1-6,13H/b5-1-,7-2-,14-6-
k-16		14.2652	238.3662	-10.899	163.0535	417.8653	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-8-2-4-14-10(8)11(15)9(7)12/h1-6,14H/b5-1-,13-3+
H-28		10.6616	270.0842	-2.5097	107.9448	418.0164	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-11(8)15(9)10(6-7)14-12/h1-6,13H/b2-1-,9-3-
H1-116		6.8317	376.3778	-1.6488	18.8174	418.2076	InChI=1S/C12H7N3O/c16-7-2-1-3-10-8-4-5-13-11(8)15(10)12-9(6-7)14-12/h1-6,13H/b2-1-,9-6+,10-3-
p1-31		13.186	256.0042	-6.3984	135.211	418.2742	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9-12(14-8)15(9)10/h1-6,13H/b3-1-,7-2-,11-8+

	33.1114	329.6061	-12.0708	62.797	418.4548	InChI=1S/C12H7N3O/c16-12-7(6-10-14-15(10)12)2-1-3-8-9-4-5-13-11(8)9/h1-6,13H/b2-1-,8-3-
	8.1998	274.4753	-3.9283	118.0544	418.8747	InChI=1S/C12H7N3O/c16-10-6-9-11-8(10)3-1-2-7-4-5-13-12(7)14-15(9)11/h1-6H,(H,13,14)/b3-1-,7-2-
	13.707	256.0018	-4.1224	114.2555	419.1308	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9-12(14-10)15(9)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2-,14-12+
	12.9063	253.3421	-5.2919	139.6867	419.1834	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)8-2-1-3-9-10(6-14-8)15(9)12/h1-6,13H/b2-1-,3-1-,8-2-,9-3-,10-6-,14-6-,14-8-
	46.4349	346.2874	-19.6216	38.4811	419.4754	InChI=1S/C12H7N3O/c16-12-10-11(12)15(6-14-10)5-1-2-7-8-3-4-13-9(7)8/h1-6,13H/b5-1-,7-2-
	39.6345	299.5055	-22.6694	69.1183	419.5641	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-12(7)14-9-6-15(9)10(8)11/h1-6H,(H,13,14)/b3-1-,7-2-
	12.8826	287.9336	-4.6364	71.4206	419.8102	InChI=1S/C12H7N3O/c16-11-7-2-1-4-13-10(11)9-6-15(9)12-8(7)3-5-14-12/h1-6,14H
	9.4541	288.9039	-4.9602	106.8930	420.6262	InChI=1S/C12H7N3O/c16-11-9-6-10-8(3-4-13-10)7(9)2-1-5-15-12(11)14-15/h1-6,13H/b5-1-,7-2-
	10.9704	113.7608	-3.1505	247.3011	421.4933	InChI=1S/C12H7N3O/c16-9-6-10-14-12(9)7-2-1-5-15(10)8-3-4-13-11(7)8/h1-6,13H
	14.6902	191.0045	-9.9452	210.7976	421.4943	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-10(7)11-12-14-9(6-8)15(11)12/h1-6,13H/b3-1-,7-2-,9-6-,11-10+
	42.5105	330.1977	-19.7335	38.7267	421.7303	InChI=1S/C12H7N3O/c16-11-9-10(11)15-6-8(15)3-1-2-7-4-5-13-12(7)14-9/h1-6H,(H,13,14)/b3-1-,7-2-
	28.5182	244.978	-10.9357	138.0366	421.8263	InChI=1S/C12H7N3O/c16-12-7-6-8-10-9(2-4-14-10)15(11(7)12)5-1-3-13-8/h1-6,14H/b5-1-,13-3-
	28.2133	156.5812	-6.5905	207.4458	422.0654	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7(6-15-12(11)14-15)10-8(9)4-5-13-10/h1-6,13H/b7-6+
	9.8748	334.6597	-4.9325	65.7759	422.1236	InChI=1S/C12H7N3O/c16-12-11-14-9-6-8(15(11)12)3-1-2-7-4-5-13-10(7)9/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,10-9-
	14.8398	208.2431	-6.2049	159.3172	422.4126	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(14-6-8(7)10)9-3-4-13-11(9)12/h1-6,13H/b5-1-,7-2-,14-6-
	7.0239	368.7743	-1.7311	34.8647	422.4965	InChI=1S/C12H7N3O/c16-12-11-14-9-6-7(2-1-5-15(11)12)8-3-4-13-10(8)9/h1-6,13H/b5-1-,7-2-,14-11-
	47.4611	272.479	-23.0086	95.8691	422.608	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9(8)12-14-15(10)12/h1-6,13H/b3-1-,7-2-,11-8+
	11.1202	113.3175	-3.2751	245.6974	422.8723	InChI=1S/C12H7N3O/c16-12-10-6-8(14-12)7-2-1-5-15(10)9-3-4-13-11(7)9/h1-6,13H
	6.2419	364.8261	-0.7995	27.2967	422.9695	InChI=1S/C12H7N3O/c16-10-3-1-2-7-6-9(15-12(10)14-15)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+

B-126		17.1357	353.5146	-5.4672	24.8415	423.0857	InChI=1S/C12H7N3O/c16-12-8-6-9-7(3-4-13-9)10-2-1-5-15(10)14-11(8)12/h1-6,13H/b8-6+,14-11+
A1-26		14.2232	227.3943	-5.835	147.4151	423.1151	InChI=1S/C12H7N3O/c16-12-10-7-2-1-4-13-6-9(10)15(12)11-8(7)3-5-14-11/h1-6,14H/b2-1-,4-1-,7-2-,9-6+,13-4-,13-6-
I-72		41.0449	200.2737	-18.5419	173.8625	423.2859	InChI=1S/C12H7N3O/c16-9-6-7(9)12-11-10-8(2-4-14-10)15(12)5-1-3-13-11/h1-6,14H
H11-17		20.0378	223.1456	-12.7431	145.1855	423.4554	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(10-6-15(10)12)8-4-5-13-11(8)14-9/h1-6H,11(13,14)
xS-12		41.6476	327.6544	-19.36	43.1568	423.6578	InChI=1S/C12H7N3O/c16-11-9-10(11)15-6-8(15)3-1-2-7-4-5-13-12(7)14-9/h1-6H,11(13,14)/b3-1-,7-2-
H-59		17.6614	301.1117	-10.083	107.3286	423.7168	InChI=1S/C12H7N3O/c16-11-9(8-4-5-13-10(8)11)3-1-2-7-6-15-12(7)14-15/h1-6,13H/b2-1-,9-3-
H1-121		24.7106	186.2007	-15.7712	189.3037	423.8207	InChI=1S/C12H7N3O/c16-11-3-1-2-9-7-4-5-13-8(7)6-10-12(14-11)15(9)10/h1-6,13H/b3-1-,9-2-,14-12-
H11-100		11.3107	89.7304	-3.9303	268.9902	424.0463	InChI=1S/C12H7N3O/c16-12-9-6-15-10(14-12)3-1-2-7(9)8-4-5-13-11(8)15/h1-6,13H/b3-1-,7-2-
p1-52		46.3614	261.1107	-26.5075	112.242	424.0732	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-12(14-11)15-6-8(9)15/h1-6,13H/b3-1-,7-2-,11-10-
H-33		42.4539	167.6417	-5.5452	179.3323	424.5622	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9(15-12(7)14-15)8-4-5-13-11(8)10/h1-6,13H/b7-6+
H-70		24.6988	242.0923	-8.7705	140.7063	425.0937	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7(11-14-15(11)12)6-10-8(9)4-5-13-10/h1-6,13H/b2-1-,3-1-,7-2-,7-6-,9-3+,9-8+,10-6-
o-181		17.895	296.2275	-0.7618	95.5488	425.3649	InChI=1S/C12H7N3O/c16-12-10-6-8-7(14-8)2-1-5-15(10)9-3-4-13-11(9)12/h1-6,13H/b5-1-,7-2-,10-6-
H1-136		13.386	237.6454	-3.4279	130.4353	425.7003	InChI=1S/C12H7N3O/c16-11-3-1-2-7-8-4-5-13-12(8)15-9(7)6-10(15)14-11/h1-6,13H/b3-1-,7-2-,14-10-
H-62		18.7494	113.1154	0.4264	223.0127	425.7237	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-6-15(14-10(7)11)12-9(8)4-5-13-12/h1-6,13H
n-138		11.3296	154.2074	-3.516	211.4942	425.7329	InChI=1S/C12H7N3O/c16-11-9-7-2-1-5-15(12(9)14-6-7)8-3-4-13-10(8)11/h1-6,13H
H-45		24.7334	210.4218	-5.4986	175.0062	425.7541	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9(12-14-15(10)12)8-4-5-13-11(7)8/h1-6,13H/b7-6+
E-59		6.048	288.3555	-4.033	117.2931	426.4338	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8-7-4-5-13-11(7)10(6-14-8)15(9)12/h1-6,13H/b2-1-,9-3-
q-39		9.7493	157.7733	-4.9035	220.9339	426.5751	InChI=1S/C12H7N3O/c16-12-8-6-15-9(11(15)14-12)3-1-2-7-4-5-13-10(7)8/h1-6,13H/b2-1-,9-3-
s12-37		19.6614	261.1851	-7.5654	122.4141	426.9298	InChI=1S/C12H7N3O/c16-12-11-9-6-8-7(4-5-13-8)2-1-3-10(14-9)15(11)12/h1-6,13H/b3-1-,7-2-,8-6-

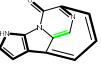
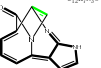
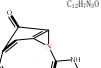
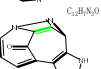
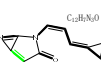
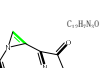

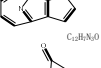
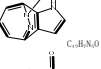
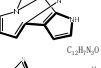
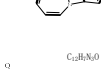
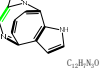
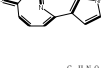

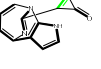
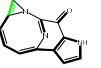
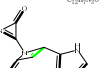
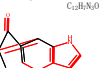
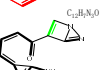
x5-11		58,9177	267,1308	-33,5843	88,5578	427,1074	InChI=1S/C12H7N3O/c16-11-9-10(11)15(9)8-3-1-2-7-4-5-13-12(7)14-6-8/h1-6H, (H, 13, 14)
n-37		43,1635	216,9249	-19,7439	148,2142	427,1236	InChI=1S/C12H7N3O/c16-12-8-6-14-15-5-1-2-7(10(8)12)11-9(15)3-4-13-11/h1-6, 13H/b14-6-
o-93		8,655	171,2507	-2,4238	200,6392	427,4907	InChI=1S/C12H7N3O/c16-12-11-8-6-7(14-11)2-1-5-15(12)9-3-4-13-10(8)9/h1-6, 13H/b5-1-, 7-2-
o-39		16,8175	284,8075	-1,4015	107,8789	427,9361	InChI=1S/C12H7N3O/c16-12-10-6-8-9(3-4-13-8)15(10)5-1-2-7-11(12)14-7/h1-6, 13H/b5-1-, 7-2+
H1-115		23,7915	208,9441	-8,9835	169,2083	428,5144	InChI=1S/C12H7N3O/c16-7-2-1-3-10-8-4-5-13-11(8)9(6-7)12-14-15(10)12/h1-6, 13H/b2-1-, 9-6+, 10-3-
n-55		35,6201	233,9994	-15,4841	139,215	428,8988	InChI=1S/C12H7N3O/c16-12-9-7-2-1-5-15(6-14-11(9)12)8-3-4-13-10(7)8/h1-6, 13H/b14-6-
E-39		18,7952	181,6983	-4,7446	176,4615	429,4183	InChI=1S/C12H7N3O/c16-11-6-8-10-3-1-2-9(14-15(10)11)7-4-5-13-12(7)8/h1-6, 13H
B-144		17,5118	239,9575	-6,1261	139,6164	429,5412	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-10(11(15)14-12)6-9-7(8)3-4-13-9/h1-6, 13H/b5-1-, 8-2-, 10-6+, 14-11+
o-244		24,0463	285,6107	-13,8808	109,8294	429,6235	InChI=1S/C12H7N3O/c16-10-6-8-7(11(8)14-10)2-1-5-15-9-3-4-13-12(9)15/h1-6, 13H/b1-7-, 7-2+
q-41		28,2041	170,6939	-5,7242	204,1974	430,1464	InChI=1S/C12H7N3O/c16-10-6-9-11-7(4-5-13-11)2-1-3-8(10)12-14-15(9)12/h1-6, 13H/b2-1-, 8-3+
B-14		26,2597	177,0629	-3,7344	202,3775	430,1767	InChI=1S/C12H7N3O/c16-10-6-9-11-8(3-4-13-11)7(10)2-1-5-15-12(9)14-15/h1-6, 13H/b5-1-, 7-2-
x4-24		10,8816	276,6831	-7,1206	119,1811	430,4757	InChI=1S/C12H7N3O/c16-12-9-10-7(4-5-13-10)2-1-3-8-11(9)15(8)6-14-12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 10-9-
H-34		41,4222	173,5108	-4,9031	182,7742	430,4758	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9(12-14-15(7)12)8-4-5-13-11(8)10/h1-6, 13H/b7-6-
X-40		28,7128	271,8828	-9,1544	107,7547	430,5360	InChI=1S/C12H7N3O/c16-12-10-9-6-7(2-1-4-13-9)8-3-5-14-11(8)15(10)12/h1-6, 14H
x7-36		28,041	266,7163	-22,1944	118,642	430,5736	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-11(7)10-9(8)12(10)15-6-14-15/h1-6, 13H/b3-1-, 7-2-, 11-10-
o-147		6,3847	94,4552	-2,0196	287,7538	430,7088	InChI=1S/C12H7N3O/c16-9-6-10-14-11-7(9)2-1-5-15(10)8-3-4-13-12(8)11/h1-6, 13H/b5-1-, 7-2-
n-194		13,6155	225,8832	-5,8859	157,0082	430,9128	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(6-14-12)8-3-4-13-11(8)9(7)10/h1-6, 13H/b5-1-, 7-2-, 14-6-
C-1		12,3328	307,7674	-3,9600	103,8312	431,3015	InChI=1S/C12H7N3O/c16-10-6-9(10)11-7-2-1-4-14-15(11)12-8(7)3-5-13-12/h1-6, 13H
A2-66		5,7022	385,9717	-1,1302	20,7343	431,3694	InChI=1S/C12H7N3O/c16-11-8-6-15-9(2-1-4-13-10(8)11)7-3-5-14-12(7)15/h1-6, 14H/b4-1-, 8-6+, 9-2-, 13-10+

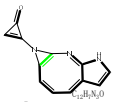
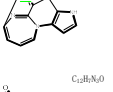
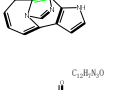
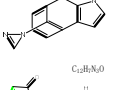
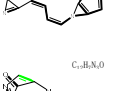
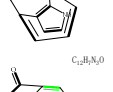
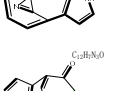
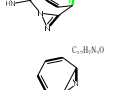
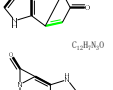
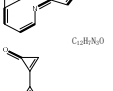
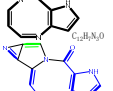
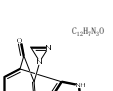
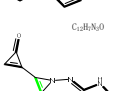
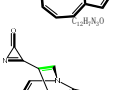
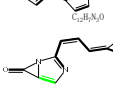
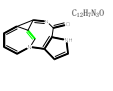
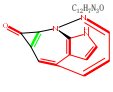
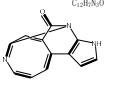
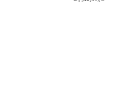
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	<chem>C12H7N3O</chem>						
s11-3		11.3015	329.8128	-6.2257	79.8201	432.211	InChI=1S/C12H7N3O/c16-12-9-6-8-11-7(4-5-13-11)2-1-3-10(14-8)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,10-3+,11-8+
	<chem>C12H7N3O</chem>						
q-1		14.1359	128.427	-4.5503	239.5969	432.8718	InChI=1S/C12H7N3O/c16-12-8-6-15-9(11)(12)14-15(3-1-2-7-4-5-13-10(7)8)/h1-6,13H/b2-1-,9-3-
	<chem>C12H7N3O</chem>						
H1-97		35.261	367.5303	-24.3244	39.895	433.0871	InChI=1S/C12H7N3O/c16-10(14-12-9-6-15(9)12)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-,14-12-
	<chem>C12H7N3O</chem>						
A-180		13.396	259.5742	-7.0592	124.9311	433.4148	InChI=1S/C12H7N3O/c16-12-11-10-9-8(3-4-13-9)7(6-14-12)2-1-5-15(10)11/h1-6,13H/b5-1-,7-2+,14-6-
	<chem>C12H7N3O</chem>						
o-112		10.6532	89.2497	-3.7913	276.59	433.4179	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-11(8)10(7)14-6-9(12)15/h1-6,13H
	<chem>C12H7N3O</chem>						
o-225		10.5882	106.1123	-4.3093	268.2282	433.5861	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(14-11(7)8)9-3-4-13-12(9)10/h1-6,13H/b8-6-
	<chem>C12H7N3O</chem>						
o-224		10.5873	106.1127	-4.3087	268.2355	433.5862	InChI=1S/C12H7N3O/c16-12-8-6-10(14-12)15-5-1-2-7(8)11-9(15)3-4-13-11/h1-6,13H
	<chem>C12H7N3O</chem>						
q1-29		27.4315	217.1627	-14.669	185.868	434.0516	InChI=1S/C12H7N3O/c16-9-6-8-12-14-10(15(8)12)3-1-2-7-4-5-13-11(7)9/h1-6,13H/b2-1-,8-6-,10-3-
	<chem>C12H7N3O</chem>						
q1-36		21.3166	217.4147	-4.6911	165.5887	434.2783	InChI=1S/C12H7N3O/c16-12-8-6-10-14-15(10)9(8)3-1-2-7-4-5-13-11(7)12/h1-6,13H/b2-1-,9-3+
	<chem>C12H7N3O</chem>						
X23-27		37.6366	265.2255	-16.4262	112.4022	434.3538	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-10(8)11-9(6-7)15(11)12/h1-6,14H/b2-1-,4-1-,7-2-,11-10+,13-4-,13-8-
	<chem>C12H7N3O</chem>						
o-50		12.5262	142.8663	-4.0064	233.1761	435.358	InChI=1S/C12H7N3O/c16-12-8-6-9(12)14-15-5-1-2-7(8)11-10(15)3-4-13-11/h1-6,13H/b14-9+
	<chem>C12H7N3O</chem>						
o-63		25.8307	247.5647	-14.7347	127.9842	435.3591	InChI=1S/C12H7N3O/c16-12-10-8-6-7(8)2-1-5-15(14-10)9-3-4-13-11(9)12/h1-6,13H/b5-1-,7-2-
	<chem>C12H7N3O</chem>						
j-3		58.8966	272.8244	-31.9211	86.3458	435.6512	InChI=1S/C12H7N3O/c16-12-10-11(12)15(10)7-2-1-4-13-8-3-5-14-9(8)6-7/h1-6,14H/b2-1-,4-1-,7-2+,7-6+,9-6+,13-4-,13-8+
	<chem>C12H7N3O</chem>						
x7-19		54.8848	268.6388	-28.8255	112.5158	435.9409	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11(15(9)12)8-6-14-8/h1-6,13H/b3-1-,7-2-,11-8+,12-10+
	<chem>C12H7N3O</chem>						
B-254		19.3978	119.4070	0.2696	223.1006	436.2248	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-6-9(14-12(11)15)10-7(8)3-4-13-10/h1-6,13H
	<chem>C12H7N3O</chem>						
H-80		15.3772	210.2573	-4.4337	163.2048	436.311	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-15(10(7)14-12)11-8(9)4-5-13-11/h1-6,13H/b2-1-,9-3-
	<chem>C12H7N3O</chem>						
H11-80		24.1841	286.613	-13.3339	87.6126	436.3662	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)8-2-1-3-9(14-8)10-6-15(10)12/h1-6,13H
	<chem>C12H7N3O</chem>						
B-164		4.1753	326.4802	-3.5774	96.0822	436.8150	InChI=1S/C12H7N3O/c16-12-10-8(3-4-13-10)7-2-1-5-15(12)11-9(6-7)14-11/h1-6,13H/b5-1-,7-2+,9-6-
	<chem>C12H7N3O</chem>						

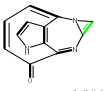
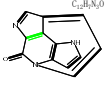
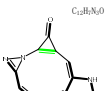
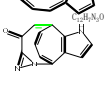
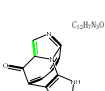
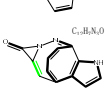
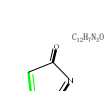
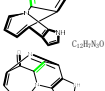
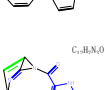
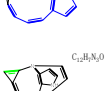
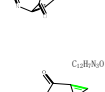
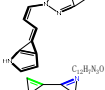
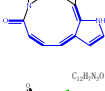
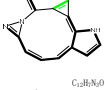
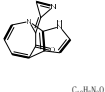
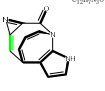
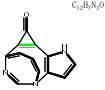
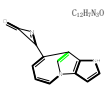
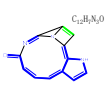
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A2-3		40, 1941	204, 6816	-1, 9358	116, 1892	437, 4215	InChI=1S/C12H7N3O/c16-12-8-2-1-4-14-11-9(6-15(11)12)10-7(8)3-5-13-10/h1-6, 13H/b4-1-, 8-2-, 14-11-
s11-18		33, 0605	213, 4451	-5, 5896	168, 068	437, 6464	InChI=1S/C12H7N3O/c16-12-8-6-9(12)15-10(14-15)3-1-2-7-4-5-13-11(7)8/h1-6, 13H/b3-1-, 7-2-, 11-8-
A2-63		26, 6227	272, 1981	-11, 0367	113, 3979	437, 7401	InChI=1S/C12H7N3O/c16-10-6-9-12-14-4-1-2-8(15(9)12)7-3-5-13-11(7)10/h1-6, 13H
I-16		5, 3445	390, 1145	-1, 2643	20, 0589	437, 7894	InChI=1S/C12H7N3O/c16-12-7-6-13-3-1-5-15-8-2-4-14-10(8)11(15)9(7)12/h1-6, 14H/b5-1-, 7-6+, 11-9+, 13-3-
H11-34		6, 1053	371, 0272	-1, 0262	50, 7809	438, 0128	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-10(14-9)6-15(12)11-7(8)4-5-13-11/h1-6, 13H/b3-1-, 8-2-, 10-6+
I-98		29, 6416	240, 3748	-2, 2587	93, 0731	438, 3743	InChI=1S/C12H7N3O/c16-12-10-7-6-9(10)15(5-1-3-14-12)8-2-4-13-11(7)8/h1-6, 13H/b5-1-, 14-3+
B-24		13, 5272	289, 0356	-2, 3639	110, 6306	438, 5470	InChI=1S/C12H7N3O/c16-10-6-8-12(14-8)15-5-1-2-9(15)7-3-4-13-11(7)10/h1-6, 13H/b8-6+
o-4		11, 2385	191, 6347	-4, 238	189, 6789	438, 6667	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-10-3-4-13-9(10)6-8(7)11(12)14-15/h1-6, 13H/b5-1-, 7-2+
n-40		29, 388	228, 7723	-10, 501	152, 1026	438, 9068	InChI=1S/C12H7N3O/c16-12-9-7-2-1-5-15(14-6-7)8-3-4-13-11(8)10(9)12/h1-6, 13H
r-35		31, 0665	281, 8318	-23, 8393	88, 9774	438, 9889	InChI=1S/C12H7N3O/c16-12-8(10-9-6-15(9)10)3-1-2-7-4-5-13-11(7)14-12/h1-6H, (H, 13, 14, 16)/b3-1-, 7-2-, 10-8+
o-27		9, 2155	119, 5684	-1, 9931	257, 9555	439, 9163	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-10(9)8(6-7)14-12(11)15/h1-6, 13H
F-37		17, 2243	237, 6246	-6, 8365	154, 3888	440, 0133	InChI=1S/C12H7N3O/c16-11-6-10-9-3-1-2-7(11)8-4-5-13-12(8)14-15(9)10/h1-6H, (H, 13, 14)/b2-1-, 8-7-, 9-3+, 10-6-
H-141		6, 0338	390, 3097	-2, 5098	37, 7923	440, 3037	InChI=1S/C12H7N3O/c16-12-10(14-12)7-2-1-3-9-8-4-5-13-11(8)15(9)6-7/h1-6, 13H
H-10		33, 1265	305, 2755	-11, 626	97, 7105	440, 3121	InChI=1S/C12H7N3O/c16-11-7(6-15-12(11)14-15)2-1-3-8-9-4-5-13-10(8)9/h1-6, 13H/b2-1-, 8-3-
H-143		22, 0742	186, 8198	-12, 9146	212, 547	440, 5718	InChI=1S/C12H7N3O/c16-12-11(14-12)15-7-2-1-3-10(15)8-4-5-13-9(8)6-7/h1-6, 13H
I-30		5, 4594	420, 9913	-1, 3202	2, 4	440, 6082	InChI=1S/C12H7N3O/c16-12-7-6-13-3-1-5-15-8-2-4-14-10(8)11(15)9(7)12/h1-6, 14H/b5-1-, 7-6+, 11-9+, 13-3+
n-162		11, 0617	142, 8319	-2, 4058	242, 0201	440, 8303	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-14-11(12)9(7)10-8(15)3-4-13-10/h1-6, 13H/b5-1-, 7-2+
q-40		25, 3855	168, 3784	-6, 4861	220, 3222	440, 8509	InChI=1S/C12H7N3O/c16-10-6-8-11-7(4-5-13-11)2-1-3-9(10)15-12(8)14-15/h1-6, 13H/b2-1-, 9-3+

H1-71		27.7442	166.2168	-0.691	183.6354	440.907	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-11(8)12-14-9(7)6-15(10)12/h1-6,13h/b3-1-,7-2-
H11-38		18.3831	261.2861	-5.7578	143.3085	440.9325	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(15(9)12)14-11-8(7)4-5-13-11/h1-6h,(H,13,14)/b9-6-
s11-25		20.4563	280.446	-7.4178	94.2085	441.7953	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)12(14-8)15-6-9(11)15/h1-6,13h/b2-1-,3-1-,7-2-,8-3-,12-10-
H11-83		13.1215	308.3287	-3.0582	94.3841	441.9333	InChI=1S/C12H7N3O/c16-12-11-7(4-5-13-11)10-3-1-2-8-9(14-8)6-15(10)12/h1-6,13h/b2-1-,9-6+,10-3-
G-49		19.3638	243.3415	-8.5373	164.2615	442.3374	InChI=1S/C12H7N3O/c16-12-11-8-2-1-3-9(14-6-15(11)12)10-7(8)4-5-13-10/h1-6,13h/b1-8+,9-6-
n-131		13.6246	164.3127	-3.5853	224.3902	442.3669	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(9(10)6-14-7)8-3-4-13-11(8)12/h1-6,13h
H1-37		32.0051	339.0933	-0.5383	49.937	442.7323	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-12(7)15(9)6-8-11(10)14-8/h1-6,13h/b3-1-,8-6+,9-2-
B-255		9.9845	121.8987	-3.1551	268.2289	444.2806	InChI=1S/C12H7N3O/c16-12-11-7-2-1-5-15(12)6-9(14-11)10-8(7)3-4-13-10/h1-6,13h
H1-80		28.9638	387.1369	-20.9407	44.7785	444.9692	InChI=1S/C12H7N3O/c16-11(15-10-6-9(10)14-15)3-1-2-7-8-4-5-13-12(7)8/h1-6,13h/b3-1-,7-2-
H1-11		17.29	239.3982	-4.2537	168.1118	445.0442	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15(10)6-9-11(7)14-9/h1-6,13h/b3-1-,7-2+
E-50		16.0984	303.4664	-10.9586	79.9601	445.2336	InChI=1S/C12H7N3O/c16-12-11-8(4-5-13-11)9-3-1-2-7-6-10(7)15(12)14-9/h1-6,13h/b3-1-,7-2-
H11-89		20.1185	125.5402	0.3321	232.4967	445.44	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-14-9(6-15(10)12)11-7(8)4-5-13-11/h1-6,13h
x5-30		13.678	317.1055	-7.8027	67.6148	445.5954	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-12(7)14-15-9(6-8)10(11)15/h1-6h,(H,13,14)/b3-1-,7-2-
H11-147		4.2429	344.843	-1.6071	84.913	445.9834	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-14-15(10)6-9(12)11-7(8)4-5-13-11/h1-6,13h/b3-1-,8-2-,9-6-
A2-81		30.7967	381.8482	-20.3529	41.3775	445.9847	InChI=1S/C12H7N3O/c16-11-9-6-15(9)12(11)14-4-1-2-7-8-3-5-13-10(7)8/h1-6,13h/b4-1-,7-2-,14-12-
o-198		13.2282	384.8515	-3.4294	46.4006	446.5643	InChI=1S/C12H7N3O/c16-10-6-7(10)8-2-1-5-15-9-3-4-13-11(9)12(15)14-8/h1-6,13h
H11-50		20.3525	262.5275	-6.2512	139.5763	446.7743	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(15(10)12)8-4-5-13-11(8)14-7/h1-6h,(H,13,14)/b10-6-
o-32		11.441	144.8331	-3.6187	239.6874	447.6102	InChI=1S/C12H7N3O/c16-12-8-6-15-5-1-2-7(11(12)14-8)10-9(15)3-4-13-10/h1-6,13h/b8-6-
A2-31		30.9743	388.4952	-20.1535	41.3593	447.996	InChI=1S/C12H7N3O/c16-12-11(9-6-15(9)12)13-4-1-2-7-8-3-5-14-10(7)8/h1-6,14h/b4-1-,7-2-,13-11+

o-131		5.2523	401.8744	-1.3802	17.24	448.1023	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-10(9)12(15)14-6-8(7)11/h1-6,13H/b5-1-,7-2-,8-6-,14-12-
H11-150		21.2587	120.6305	0.1132	231.3328	448.1873	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10-9(11)6-15(14-10)12-8(7)4-5-13-12/h1-6,13H
s11-52		23.3324	226.3885	-2.0801	123.1009	448.3755	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11-9(14-8)6-15(11)12/h1-6,13H/b3-1-,7-2-,11-10+
q11-29		23.852	179.2223	-13.0797	215.8213	448.5412	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)12-14-15(12)9(1)6-8/h1-6,13H/b2-1-,8-3?
n-142		27.9944	168.3973	-11.9776	237.6052	448.6427	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(11)7(8-6-14-8)9-3-4-13-10(9)12/h1-6,13H/b11-8+
H11-95		18.4133	423.5314	-14.2717	12.7394	448.7571	InChI=1S/C12H7N3O/c16-12-9(14-12)3-1-2-7-8-4-5-13-11(8)15-6-10(7)15/h1-6,13H/b3-1-,7-2-
H1-94		44.6497	310.494	-27.7063	96.2767	448.9616	InChI=1S/C12H7N3O/c16-7(6-10-12-14-15(10)12)2-1-3-8-9-4-5-13-11(8)9/h1-6,13H/b2-1-,8-3-,10-6-
B-244		29.8333	307.8213	-12.4353	112.7730	449.4524	InChI=1S/C12H7N3O/c16-12-11-9(14-11)6-15(12)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
H-122		7.9072	294.471	-5.2645	129.4008	450.218	InChI=1S/C12H7N3O/c16-12-11-14-9-3-1-2-7(15(11)12)6-10-8(9)4-5-13-10/h1-6,13H/b2-1-,3-1-,7-2-,7-6-,9-3-,9-8-,10-6+,14-11+
B-110		8.4499	119.8740	-3.9032	278.1428	450.4195	InChI=1S/C12H7N3O/c16-12-9-6-10-11-7(3-4-13-11)8(14-9)2-1-5-15(10)12/h1-6,13H/b5-1-,8-2-
i-15		21.9471	242.6314	-8.4386	155.6394	450.7177	InChI=1S/C12H7N3O/c16-10-6-9-12-11-7(3-5-14-11)13-4-1-2-8(10)15(9)12/h1-6,14H/b4-1-,8-2-,12-11-,13-7+
H1-129		37.9257	291.8006	-17.0545	122.6116	450.8782	InChI=1S/C12H7N3O/c16-10(9-6-11-14-15(9)11)3-1-2-7-8-4-5-13-12(7)8/h1-6,13H/b3-1-,7-2-
X23-36		35.5755	361.6302	-16.7489	48.5656	452.1322	InChI=1S/C12H7N3O/c16-12-9-10-8(3-5-14-10)13-4-1-2-7-6-15(7)11(9)12/h1-6,14H/b2-1-,13-4+
n-137		14.0185	253.4141	-6.434	142.7367	452.7306	InChI=1S/C12H7N3O/c16-12-9-7-2-1-5-15(6-14-10(7)9)8-3-4-13-11(8)12/h1-6,13H/b5-1-,7-2-,14-6-
o-1		4.3324	386.2022	-1.4882	54.5744	453.659	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-8-3-4-13-11(8)9(15)6-14-10(7)12/h1-6,13H/b5-1-,7-2+,9-6-,14-10+
i-27		26.1576	396.5689	-18.8152	31.8228	453.808	InChI=1S/C12H7N3O/c16-12-9-2-1-4-13-8-3-5-14-11(8)7-6-10(7)15(9)12/h1-6,14H/b4-1-,9-2-,11-7-,13-8+
X22-38		49.2765	343.3314	-24.8616	51.2894	454.0522	InChI=1S/C12H7N3O/c16-10-6-7(10)11-9-2-1-4-13-8-3-5-14-12(8)15(9)11/h1-6,14H/b2-1-,13-4-
s12-33		21.5032	174.6845	-9.1315	212.826	454.0639	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7-4-5-13-9(7)6-15(12)11(10)14-8/h1-6,13H/b3-1-,7-2-,9-6-
q-7		14.7354	131.0188	-3.3814	240.7674	454.7878	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-10(7)8-6-15(9)14-11(8)12/h1-6,13H/b2-1-,9-3-




















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F-52		30, 4118	116, 3083	-1, 5718	228, 2096	455, 9466	InChI=1S/C12H7N3O/c16-12-7-2-1-3-10-8-4-5-13-11(8)14-9(7)6-15(10)12/h1-6H, (H, 13, 14)
X23-47		16, 2578	311, 213	-10, 2721	109, 6841	456, 3918	InChI=1S/C12H7N3O/c16-11-7-2-1-4-13-8-3-5-14-12(8)15-9(6-7)10(11)15/h1-6, 14H/b2-1-, 13-4-
B-85		20, 6389	129, 7882	0, 3234	227, 3057	456, 5246	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-10(12)6-9(14-15)11-7(8)3-4-13-11/h1-6, 13H
B-28		30, 1443	313, 3940	-12, 3300	115, 9743	456, 9533	InChI=1S/C12H7N3O/c16-10-6-9-12(14-9)15(10)5-1-2-7-8-3-4-13-11(7)8/h1-6, 13H/b5-1-, 7-2-
B-248		11, 7109	302, 0143	-5, 5247	96, 9935	457, 0196	InChI=1S/C12H7N3O/c16-12-10-7(3-4-13-10)8-2-1-5-15-6-9(15)11(12)14-8/h1-6, 13H/b5-1-, 8-2-
E-1		12, 8008	304, 3642	-4, 5826	123, 9164	457, 1528	InChI=1S/C12H7N3O/c16-11-6-8(11)10-3-1-2-9-7-4-5-13-12(7)15(10)14-9/h1-6, 13H
E-2		12, 8031	304, 3628	-4, 5825	123, 9200	457, 1533	InChI=1S/C12H7N3O/c16-11-6-10(11)15-9-3-1-2-8(14-15)7-4-5-13-12(7)9/h1-6, 13H
B-135		17, 5216	232, 6777	-6, 0462	151, 3991	457, 1800	InChI=1S/C12H7N3O/c16-11-10-6-9-7(3-4-13-9)8-2-1-5-15(12)11)14-8/h1-6, 13H/b10-6+
o-99		8, 9979	374, 1875	-2, 3464	66, 9474	457, 508	InChI=1S/C12H7N3O/c16-12-10(14-12)7-2-1-5-15-8-3-4-13-11(8)9(15)6-7/h1-6, 13H
E-33		10, 0664	291, 0211	-6, 3202	134, 5538	457, 6312	InChI=1S/C12H7N3O/c16-12-10-6-14-8-2-1-3-9(15)10(12)11-7(8)4-5-13-11/h1-6, 13H/b10-6-, 14-8+
H1-142		40, 9193	222, 495	-9, 5011	150, 6661	457, 6818	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-12(7)9-6-10(14-8)15(9)11/h1-6, 13H/b3-1-, 8-2-
H11-119		18, 6861	243, 6485	-9, 0381	153, 2403	458, 0606	InChI=1S/C12H7N3O/c16-11-8-2-1-3-9(15-6-10(11)15)7-4-5-13-12(7)14-8/h1-6H, (H, 13, 14)
B-5		45, 4174	203, 8970	-19, 2428	193, 2612	458, 2123	InChI=1S/C12H7N3O/c16-10-6-8(10)12-14-9-2-1-5-15(12)11-7(9)3-4-13-11/h1-6, 13H
H-88		36, 7731	260, 6384	-19, 5216	129, 1949	458, 2484	InChI=1S/C12H7N3O/c16-11-10-8(4-5-13-10)9-3-1-2-7-6-15(7)12(11)14-9/h1-6, 13H/b2-1-, 9-3-
q-30		7, 3484	339, 3393	-4, 091	94, 3142	458, 2538	InChI=1S/C12H7N3O/c16-12-11(14-12)15-8-3-1-2-7-4-5-13-10(7)9(15)6-8/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 10-9-
x3-10		35, 7824	124, 9855	-4, 4295	190, 5335	458, 5641	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-11(12)9(7)10-8(15)2-4-14-10/h1-6, 14H/b5-1-, 13-3+
H1-93		38, 7888	297, 1687	-17, 1392	125, 8827	458, 8206	InChI=1S/C12H7N3O/c16-10(9-6-15-12(9)14-15)3-1-2-7-8-4-5-13-11(7)8/h1-6, 13H/b3-1-, 7-2-
o-139		13, 2107	255, 7504	-6, 1328	154, 8829	459, 8502	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(14-9-6-8(7)9)10-3-4-13-11(10)12/h1-6, 13H/b5-1-, 7-2-, 14-9-

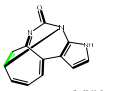
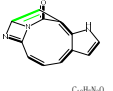
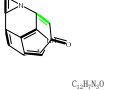
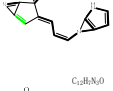
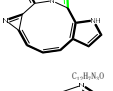
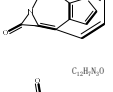
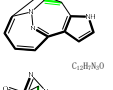
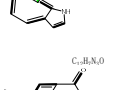
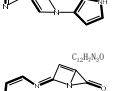
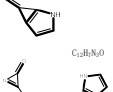
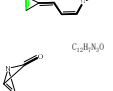
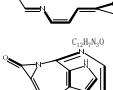
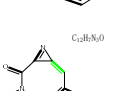
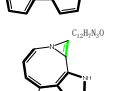
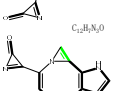
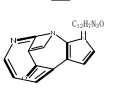
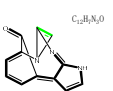
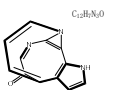

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o-59		9,8089	106,7539	-4,07	296,5981	460,6573	InChI=1S/C12H7N3O/c16-11-8-6-7-2-1-5-15(12(11)14-7)9-3-4-13-10(8)9/h1-6, 13H
G1-78		9,3374	158,6259	-3,8307	254,9371	460,81	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-10(7)11-12(9)15(8)6-14-11/h1-6, 13H
G-10		34,2046	236,4184	-1,7806	171,963	461,0401	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8(11(9)15-6-14-15)7-4-5-13-10(7)12/h1-6, 13H
o-146		23,3257	285,1249	-15,2076	147,2464	461,6591	InChI=1S/C12H7N3O/c16-10-6-8-11(14-8)7(10)2-1-5-15-9-3-4-13-12(9)15/h1-6, 13H/b5-1-, 7-2-
B-185		11,4243	162,0162	-3,6609	233,7016	462,4641	InChI=1S/C12H7N3O/c16-11-9-6-14-10(11)7-2-1-5-15(9)12-8(7)3-4-13-12/h1-6, 13H
H1-19		27,3842	246,8254	-5,8965	137,6607	462,5736	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-9(7)6-10(11)15-12(8)14-15/h1-6, 13H/b3-1-, 8-2-
H-31		24,1309	171,9646	-3,773	231,0461	462,6938	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8(10)9-4-5-13-12(9)15-11(7)14-15/h1-6, 13H
H11-62		31,3014	175,841	-7,5325	198,9007	462,9271	InChI=1S/C12H7N3O/c16-11-6-8-9-2-1-3-10(15(11)14-9)7-4-5-13-12(7)8/h1-6, 13H
i-24		21,0285	366,8348	-16,418	63,3099	463,1092	InChI=1S/C12H7N3O/c16-12-11-10-8(3-5-14-10)13-4-1-2-7-6-9(7)15(11)12/h1-6, 14H/b4-1-, 7-2-, 11-10-, 13-8+
k-32		58,7003	327,7866	-30,6852	72,9821	464,4104	InChI=1S/C12H7N3O/c16-9-6-7(9)11-12-10-8(2-4-14-10)13-3-1-5-15(11)12/h1-6, 14H/b5-1-, 13-3-
q1-6		13,1394	253,5441	-8,0067	187,0666	464,5178	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-11-8(14-11)6-15(9)12/h1-6, 13H/b2-1-, 9-3-
G-2		4,2059	305,752	-3,4806	135,3752	464,5826	InChI=1S/C12H7N3O/c16-12-9-3-1-2-8(11(12)15-6-14-15)7-4-5-13-10(7)9/h1-6, 13H
r-12		50,36	331,8359	-24,3013	74,823	464,7951	InChI=1S/C12H7N3O/c16-10-6-8(10)11-9-3-1-2-7-4-5-13-12(7)14-15(9)11/h1-6H, (H, 13, 14)/b3-1-, 7-2-
B-238		5,6111	308,6107	-3,8788	128,2634	465,0462	InChI=1S/C12H7N3O/c16-12-10(14-12)9-6-15-5-1-2-7(9)8-3-4-13-11(8)15/h1-6, 13H
H11-37		33,8031	362,4331	-19,9895	84,2452	465,297	InChI=1S/C12H7N3O/c16-12-9-6-14-10(15(9)12)3-1-2-7-8-4-5-13-11(7)8/h1-6, 13H/b3-1-, 7-2-
o-234		13,8556	241,4753	-5,761	171,6303	466,3149	InChI=1S/C12H7N3O/c16-12-11-9(3-4-13-11)15-5-1-2-7-8(6-15)10(7)14-12/h1-6, 13H/b4-10-
X-4		34,7281	276,2723	-12,8916	128,3278	466,5022	InChI=1S/C12H7N3O/c16-11-9-6-7-2-1-4-14-15(10(9)11)12-8(7)3-5-13-12/h1-6, 13H/b2-1-, 14-4-
A2-8		29,6333	185,3333	0,0617	177,2056	466,628	InChI=1S/C12H7N3O/c16-12-9-6-10-13-4-1-2-7(9)8-3-5-14-11(8)15(10)12/h1-6, 14H/b2-1-, 4-1-, 7-2-, 13-4-, 13-10-

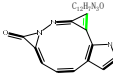
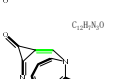

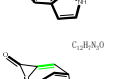
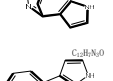
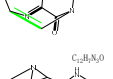
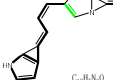
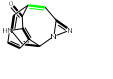
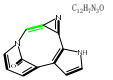
H1-30		14.5001	281.2593	-6.6309	128.4592	467.514	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-11(7)12(9)14-10-6-15(8)10/h1-6,13H/b3-1-,8-2+
n-182		70.4081	106.0874	-2.6801	164.1376	467.78	InChI=1S/C12H7N3O/c16-12-11-9-7(6-14-11)2-1-5-15(12)8-3-4-13-10(8)9/h1-6,13H/b5-1-,7-2-
s12-18		65.2568	321.9806	-23.7271	73.2959	468.0456	InChI=1S/C12H7N3O/c16-12-8-6-9-7(4-5-13-9)2-1-3-10-14-15(10)11(8)12/h1-6,13H/b3-1-,7-2-,9-6+
H-36		20.1355	201.1598	-5.9547	204.0948	468.0947	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-9(15-12(10)14-15)8-4-5-13-11(7)8/h1-6,13H/b7-6+
H11-152		15.997	208.7885	-3.9339	199.7616	469.2695	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10-14-6-9(11)15(10)12-8(7)4-5-13-12/h1-6,13H/b3-1-,7-2-
H11-28		16.9922	285.1541	-8.841	140.0194	469.7302	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(14-15(10)12)11-8(7)4-5-13-11/h1-6,13H/b10-6-,7-9?
B-37		7.7809	244.2875	-2.9872	170.6874	470.3701	InChI=1S/C12H7N3O/c16-10-6-9-11(14-10)7-2-1-5-15(9)12-8(7)3-4-13-12/h1-6,13H
o-130		10.3113	115.9426	-2.6044	291.9782	470.4342	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)8(14-7)6-10(12)15/h1-6,13H
q1-27		34.9416	226.7454	-11.6374	187.3512	471.2955	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-8-6-9-11(14-8)15(9)12/h1-6,13H/b2-1-,8-3-
o-140		15.12	263.9429	-11.2623	148.57	471.4065	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(10-6-8(10)14-7)9-3-4-13-11(9)12/h1-6,13H/b5-1-,7-2-,14-8-
B-61		40.5091	366.9093	-24.6072	58.9434	471.4340	InChI=1S/C12H7N3O/c16-12-9-6-10(9)14-15(12)5-1-2-7-8-3-4-13-11(7)8/h1-6,13H/b5-1-,7-2-
p1-21		49.5003	337.5004	-27.4487	78.5804	471.5873	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)12-11(14-12)8-6-15(8)9/h1-6,13H/b3-1-,7-2-,12-10-
s11-9		49.0535	361.086	-16.5826	68.6329	471.6874	InChI=1S/C12H7N3O/c16-12-9-6-8(9)11-7(4-5-13-11)2-1-3-10-14-15(10)12/h1-6,13H/b3-1-,7-2-,12-8+
A-64		23.6511	209.1926	-10.162	210.4172	473.2291	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(10(11)9-6-14-9)12-8(7)3-4-13-12/h1-6,13H/b10-9+
B-163		4.9405	371.1543	-3.7825	91.1762	473.5028	InChI=1S/C12H7N3O/c16-12-10-9(14-10)6-7-2-1-5-15(12)11-8(7)3-4-13-11/h1-6,13H/b9-6+
n-43		26.5761	288.6748	-8.8186	140.1245	474.8718	InChI=1S/C12H7N3O/c16-12-9-7-2-1-5-15(6-14-7)8-3-4-13-11(8)10(9)12/h1-6,13H
o-97		7.4287	326.9653	-2.9058	118.3599	475.0624	InChI=1S/C12H7N3O/c16-12-11(14-12)7-2-1-5-15-6-8(7)10-9(15)3-4-13-10/h1-6,13H
p1-30		18.4584	280.8982	-11.3441	164.1557	475.4006	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)8-6-9-12(14-10)15(8)9/h1-6,13H/b3-1-,7-2-,11-8+,14-12-
G-46		10.9404	298.5454	-7.0494	147.9523	475.5558	InChI=1S/C12H7N3O/c16-12-11-9-3-1-2-7(6-14-15(11)12)10-8(9)4-5-13-10/h1-6,13H/b1-9+,14-6-

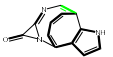
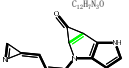
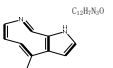
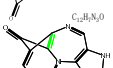
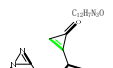


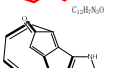
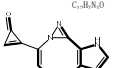
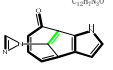
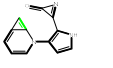
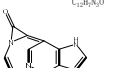
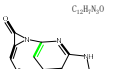
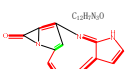

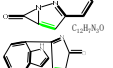
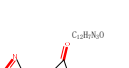
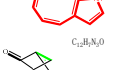
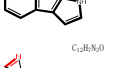
E-38		13.639	239.1646	-6.0659	198.0443	478.8388	InChI=1S/C12H7N3O/c16-11-6-10-9-3-1-2-8(14-11)7-4-5-13-12(7)15(9)10/h1-6,13H/b2-1-,9-3-,10-6+,14-8-
	$C_{12}H_7N_3O$						
H1-126		19.6108	251.7064	-11.3912	165.5354	476.2105	InChI=1S/C12H7N3O/c16-11-3-1-2-8-7-4-5-13-9(7)6-10-12(14-8)15(10)11/h1-6,13H/b3-1-,8-2-
	$C_{12}H_7N_3O$						
I-91		14.6465	169.7737	-4.5927	245.7693	476.2608	InChI=1S/C12H7N3O/c16-12-9-6-7-10(12)11-8(2-4-14-11)15(9)5-1-3-13-7/h1-6,14H/b5-1-,13-3-
	$C_{12}H_7N_3O$						
p1-53		19.3993	209.3147	-11.038	234.1386	476.3942	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-10(7)11-12-14-8(9)6-15(11)12/h1-6,13H/b3-1-,7-2-,11-10+
	$C_{12}H_7N_3O$						
H-147		25.0168	439.3958	-17.3921	14.729	476.3971	InChI=1S/C12H7N3O/c16-12-11(14-12)10-8(4-5-13-10)9-3-1-2-7-6-15(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
s12-31		27.1816	363.1546	-16.5929	78.3867	476.74	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)8-3-1-2-7-4-5-13-9(7)6-14-8/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,9-6+,14-6-,14-8+
	$C_{12}H_7N_3O$						
o-96		70.2255	129.1134	-0.3704	173.36	477.0705	InChI=1S/C12H7N3O/c16-12-9-6-7-8(14-9)2-1-5-15(12)10-3-4-13-11(7)10/h1-6,13H/b5-1-,8-2+
	$C_{12}H_7N_3O$						
H-6		23.0429	189.5113	-6.0834	231.6986	477.2086	InChI=1S/C12H7N3O/c16-11-7-2-1-3-9(12-14-15(12)6-7)8-4-5-13-10(8)11/h1-6,13H/b2-1-,7-6-,9-3-
	$C_{12}H_7N_3O$						
H-3		22.9858	232.2597	-3.4305	188.7217	477.3862	InChI=1S/C12H7N3O/c16-11-7-2-1-3-8(11)9-4-5-13-12(9)15-10(6-7)14-15/h1-6,13H/b7-6-
	$C_{12}H_7N_3O$						
B-33		11.4094	237.6571	-6.0927	188.2746	477.4251	InChI=1S/C12H7N3O/c16-10-6-9-12-14-8(2-1-5-15(9)12)7-3-4-13-11(7)10/h1-6,13H/b9-6-
	$C_{12}H_7N_3O$						
B-88		14.1308	178.1172	-5.6147	226.8957	477.4608	InChI=1S/C12H7N3O/c16-12-10-6-9(14-12)7-2-1-5-15(10)11-8(7)3-4-13-11/h1-6,13H
	$C_{12}H_7N_3O$						
H11-133		44.6084	264.607	-19.612	151.7783	477.5938	InChI=1S/C12H7N3O/c16-11-6-10(11)15-9-3-1-2-8(14-15)12-7(9)4-5-13-12/h1-6,13H
	$C_{12}H_7N_3O$						
B-206		20.4377	296.6558	-9.7353	127.1744	478.1293	InChI=1S/C12H7N3O/c16-11-8-6-15-5-1-2-9(15)7-3-4-13-12(7)14-10(8)11/h1-6,13H/b8-6+,14-10+
	$C_{12}H_7N_3O$						
x5-34		32.1173	416.6908	-22.01	30.7674	478.2888	InChI=1S/C12H7N3O/c16-12-10-9-6-8(9)3-1-2-7-4-5-13-11(7)14-15(10)12/h1-6H,13,14/b3-1-,7-2-,10-9-
	$C_{12}H_7N_3O$						
x7-46		16.0951	263.5092	-11.2466	187.3522	478.7525	InChI=1S/C12H7N3O/c16-8-3-1-2-7-4-5-13-9(7)11-12-10(8)14-6-15(11)12/h1-6,13H/b3-1-,7-2-,11-9-
	$C_{12}H_7N_3O$						
H11-23		26.5115	197.4967	-9.2987	196.9212	479.0314	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-8-4-5-13-11(8)15(12)6-10(7)14-9/h1-6,13H
	$C_{12}H_7N_3O$						
A1-30		32.3166	264.6705	-12.9051	156.5332	479.9345	InChI=1S/C12H7N3O/c16-12-11-8-6-13-4-1-2-9(15(11)12)7-3-5-14-10(7)8/h1-6,14H/b4-1-,9-2-,13-6-
	$C_{12}H_7N_3O$						
B-38		26.3658	323.4106	-14.1996	131.4817	480.8151	InChI=1S/C12H7N3O/c16-10-6-9-12(14-10)15(9)5-1-2-7-8-3-4-13-11(7)8/h1-6,13H/b5-1-,7-2-
	$C_{12}H_7N_3O$						
H1-138		36.5188	170.9108	-4.1722	245.6742	481.7835	InChI=1S/C12H7N3O/c16-10-3-1-2-9-7-4-5-13-12(7)8(10)6-11-14-15(9)11/h1-6,13H/b3-1-,9-2+
	$C_{12}H_7N_3O$						

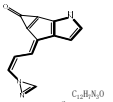
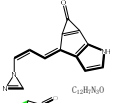
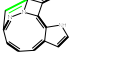
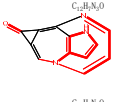
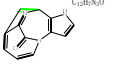
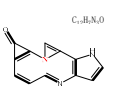
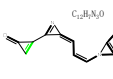
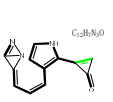
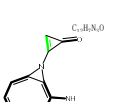
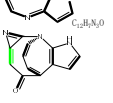
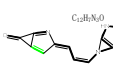
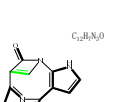
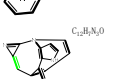
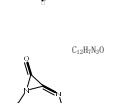
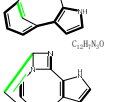
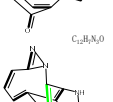
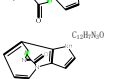
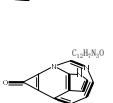
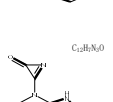
H11-39		14,995	335,5305	-8,837	105,4118	482,2364	InChI=1S/C12H7N3O/c16-12-10-6-9-7(4-5-13-9)8-2-1-3-11(14-8)15(10)12/h1-6,13H/b10-6-
s11-2		6,4251	360,3669	-3,9391	95,202	482,5814	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)11(14-8)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,11-10-
A-108		5,3993	305,6151	-3,8571	149,2747	482,8402	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(10(11)9-6-14-9)12-8(7)3-4-13-12/h1-6,13H/b10-9-
o-124		38,2443	359,5606	-23,7052	77,9954	483,0718	InChI=1S/C12H7N3O/c16-11-7-6-9(7)14-8(11)2-1-5-15-10-3-4-13-12(10)15/h1-6,13H/b5-1-,8-2-
o-197		43,6927	202,0178	-19,8559	215,3135	483,3586	InChI=1S/C12H7N3O/c16-10-6-7(10)12-14-8-2-1-5-15(12)9-3-4-13-11(8)9/h1-6,13H
x4-41		27,4234	262,5196	-8,2632	148,5392	484,3867	InChI=1S/C12H7N3O/c16-12-11-10-9-7(4-5-13-9)2-1-3-8(6-14-10)15(11)12/h1-6,13H/b2-1-,8-3+
o-183		11,2003	177,7562	-2,6419	240,0897	484,6597	InChI=1S/C12H7N3O/c16-11-8-6-7-2-1-5-15(12(7)14-8)9-3-4-13-10(9)11/h1-6,13H
X23-20		32,7579	404,5339	-22,1232	57,4884	484,9333	InChI=1S/C12H7N3O/c16-12-10-8-6-7(8)2-1-4-13-9-3-5-14-11(9)15(10)12/h1-6,14H/b2-1-,10-8-,13-4-
X22-60		50,9748	312,0827	-23,2406	103,4997	484,9758	InChI=1S/C12H7N3O/c16-11-7-2-1-4-13-8-3-5-14-12(8)15-6-9(15)10(7)11/h1-6,14H/b2-1-,13-4-
o-40		6,8449	315,8798	-2,7449	137,7514	485,0558	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(14-11(8)12)9-3-4-13-10(7)9/h1-6,13H/b8-6-,14-11+
H11-49		9,7741	296,0713	-4,2852	161,6086	485,8526	InChI=1S/C12H7N3O/c16-12-10-6-14-8-2-1-3-9(15(10)12)7-4-5-13-11(7)8/h1-6,13H/b10-6-,14-8?
x4-34		18,8643	265,9221	-6,7289	179,5035	486,3198	InChI=1S/C12H7N3O/c16-12-11-8-6-14-9(15(11)12)3-1-2-7-4-5-13-10(7)8/h1-6,13H/b2-1-,9-3+
H-8		15,5544	262,4972	-6,0425	169,8835	486,3522	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10(15-12(11)14-15)8-4-5-13-9(8)6-7/h1-6,13H/b2-1-,3-1-,7-2-,9-6+,10-3+,10-8+
o-108		25,2097	413,0662	-15,6831	35,0456	486,6476	InChI=1S/C12H7N3O/c16-12-11(14-12)15-5-1-2-7-6-8(7)10-9(15)3-4-13-10/h1-6,13H/b5-1-,7-2-
H-111		13,7764	286,5892	-7,3514	163,5519	487,8977	InChI=1S/C12H7N3O/c16-12-11-14-9-3-1-2-7(6-15(11)12)10-8(9)4-5-13-10/h1-6,13H/b7-6?,14-11-
o-250		7,7451	243,8332	-2,8344	191,2963	488,064	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(12(8)14-10)9-3-4-13-11(7)9/h1-6,13H
H-85		7,0181	408,587	-1,5677	31,0612	488,6959	InChI=1S/C12H7N3O/c16-11-10-9(4-5-13-10)7-2-1-3-8(6-7)15-12(11)14-15/h1-6,13H
p1-10		19,971	276,2716	-11,9098	174,1788	489,6852	InChI=1S/C12H7N3O/c16-10-3-1-2-7-4-5-13-11(7)12-8-6-9(14-10)15(8)12/h1-6,13H/b3-1-,7-2-,12-11+,14-9-
B-35		29,4666	261,6122	-12,4034	153,3560	490,6897	InChI=1S/C12H7N3O/c16-10-6-9-12-14-11-8(3-4-13-11)7(10)2-1-5-15(9)12/h1-6,13H/b5-1-,7-2-,9-6+,14-12+

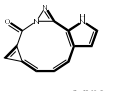
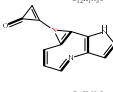
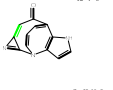
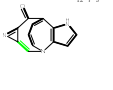
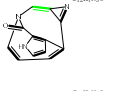
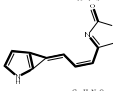
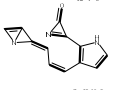
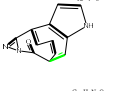
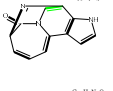
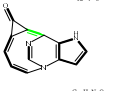
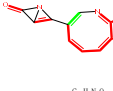
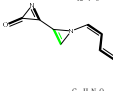
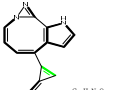
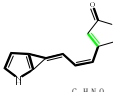
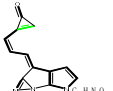
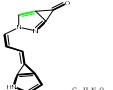
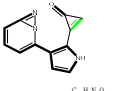
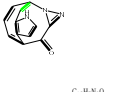
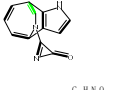
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B-211		20, 9676	208, 0068	-4, 3459	198, 6477	491, 8809	InChI=1S/C12H7N3O/c16-10-7-2-1-5-15-6-9(10)12(15)14-11-8(7)3-4-13-11/h1-6, 13H/b5-1-, 7-2-
I-13		20, 6709	321, 7143	-9, 5137	125, 8399	492, 3697	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-4-13-8-3-5-14-10(8)11(7)15(9)12/h1-6, 14H/b2-1-, 4-1-, 7-2-, 11-10-, 13-4-, 13-8-
H-20		29, 6734	169, 5819	-1, 364	186, 8487	492, 8094	InChI=1S/C12H7N3O/c16-12-7-2-1-3-10-8-4-5-13-11(8)9(6-7)14-15(10)12/h1-6, 13H
B-150		3, 8110	316, 3044	-2, 4339	160, 6584	492, 9003	InChI=1S/C12H7N3O/c16-11-9-6-7-2-1-5-15(14-10(9)11)12-8(7)3-4-13-12/h1-6, 13H/b9-6+, 14-10+
E-61		32, 8075	190, 4475	-4, 7519	171, 8887	493, 1829	InChI=1S/C12H7N3O/c16-12-8-2-1-3-9-7-4-5-13-11(7)15(12)6-10(8)14-9/h1-6, 13H
k-41		33, 5864	401, 2117	-22, 4158	64, 0164	493, 3655	InChI=1S/C12H7N3O/c16-12-11-8-6-7(8)10-9(2-4-14-10)13-3-1-5-15(11)12/h1-6, 14H/b5-1-, 11-8-, 13-3+
n-149		2, 7566	323, 3734	-2, 1323	152, 3304	493, 6298	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-11(9)8(6-14-15)10(7)12/h1-6, 13H/b5-1-, 7-2-, 10-8-
H11-S		15, 0025	331, 0532	-8, 8023	103, 4357	493, 6742	InChI=1S/C12H7N3O/c16-12-14-9-3-1-2-7(10-6-15(10)12)8-4-5-13-11(8)9/h1-6, 13H/b14-9+
B-103		44, 3322	409, 5198	-24, 5352	46, 3141	493, 8548	InChI=1S/C12H7N3O/c16-12-14-9-6-10(9)15(12)5-1-2-7-8-3-4-13-11(7)8/h1-6, 13H/b5-1-, 7-2-
r-17		41, 5179	384, 9292	-21, 7348	55, 8266	493, 9054	InChI=1S/C12H7N3O/c16-12-9-6-8(9)10-3-1-2-7-4-5-13-11(7)14-15(10)12/h1-6H, (H, 13, 14)/b3-1-, 7-2-
F-4		6, 103	337, 8632	-4, 9206	140, 2904	494, 3954	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10-8-4-5-13-12(8)14-15(10)6-9(7)11/h1-6H, (H, 13, 14)/b3-1-, 7-2+, 9-6+
G1-58		8, 9592	381, 9419	-4, 0671	93, 0752	494, 5243	InChI=1S/C12H7N3O/c16-10-3-1-2-7-8-4-5-13-12(8)15(10)11(7)9-6-14-9/h1-6, 13H/b11-9+
H11-96		13, 8205	457, 5465	-9, 0367	14, 7483	495, 6627	InChI=1S/C12H7N3O/c16-12-8(14-12)2-1-3-9-7-4-5-13-11(7)10-6-15(9)10/h1-6, 13H/b2-1-, 9-3-
r1-19		30, 2093	346, 7206	-20, 16	84, 0866	495, 7694	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-10(9)11-8-6-15(8)11/h1-6H, (H, 13, 14)/b3-1-, 7-2-, 11-10+
r1-34		30, 2095	346, 7198	-20, 1599	84, 0802	495, 7694	InChI=1S/C12H7N3O/c16-9-3-1-2-7-4-5-13-12(7)14-10(9)11-8-6-15(8)11/h1-6H, (H, 13, 14)/b3-1-, 7-2-, 11-10-
H-64		15, 3087	176, 3736	-4, 2285	258, 9622	497, 6912	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-6-10(11)14-15(7)12-9(8)4-5-13-12/h1-6, 13H/b2-1-, 8-3-
r-5		13, 101	294, 0564	-10, 3844	183, 9353	497, 7215	InChI=1S/C12H7N3O/c16-11-8-6-15-9(10(8)11)3-1-2-7-4-5-13-12(7)14-15/h1-6H, (H, 13, 14)/b3-1-, 7-2-
H-128		32, 7791	365, 9397	-19, 5399	110, 5883	498, 8001	InChI=1S/C12H7N3O/c16-12-11-14-6-7(15(11)12)2-1-3-8-9-4-5-13-10(8)9/h1-6, 13H/b2-1-, 8-3-

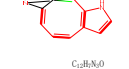

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s11-38		44.5491	170.8566	-8.8544	209.7928	500.351	InChI=1S/C12H7N3O/c16-12-8-6-10-14-9(15(10)12)3-1-2-7-4-5-13-11(7)8/h1-6,13H/b2-1-,3-1-,7-2-,9-3-,11-8+
H1-23		11.6836	291.1883	-4.1	168.9386	500.6245	InChI=1S/C12H7N3O/c16-7-2-1-3-9-8-4-5-13-11(8)10(6-7)15-12(9)14-15/h1-6,13H/b2-1-,9-3-,10-6+
o-11		30.069	327.9502	-12.1056	124.1393	500.7148	InChI=1S/C12H7N3O/c16-11-7(6-8-10(11)14-8)2-1-5-15-9-3-4-13-12(9)15/h1-6,13H/b5-1-,7-2+
q-21		52.026	385.49	-15.1559	56.5832	500.7518	InChI=1S/C12H7N3O/c16-12-11-8(14-11)3-1-2-7-4-5-13-10(7)9-6-15(9)12/h1-6,13H/b2-1-,8-3+
C-57		18.3781	282.3149	-6.4475	172.8341	502.1458	InChI=1S/C12H7N3O/c16-12-11-8-2-1-4-13-9(6-15(11)12)10-7(8)3-5-14-10/h1-6,14H/b2-1-,13-4-
E-7		27.2909	194.6153	-3.7697	188.6216	502.7499	InChI=1S/C12H7N3O/c16-12-8-6-15-10(12)3-1-2-9(14-15)7-4-5-13-11(7)8/h1-6,13H
s12-19		62.4404	341.5027	-20.1788	98.5112	502.7801	InChI=1S/C12H7N3O/c16-12-8-6-9-7(4-5-13-9)2-1-3-10-14-15(10)11(8)12/h1-6,13H/b3-1-,7-2-,9-6-
n-141		4.4875	301.913	-3.3071	176.2196	503.378	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(11(7)8-6-14-8)9-3-4-13-10(9)12/h1-6,13H/b11-8-
A2-22		20.1301	476.7627	-12.9076	19.0512	503.5611	InChI=1S/C12H7N3O/c16-12-9-6-10(15(9)12)13-4-1-2-7-8-3-5-14-11(7)8/h1-6,14H/b4-1-,7-2-,13-10+
o-101		64.4286	385.3272	-42.6067	60.359	503.7176	InChI=1S/C12H7N3O/c16-12-10(14-12)8-6-7(8)2-1-5-15-9-3-4-13-11(9)15/h1-6,13H/b5-1-,7-2+
A1-22		41.1515	436.9778	-24.6839	39.6379	503.8292	InChI=1S/C12H7N3O/c16-12-11-9(15(11)12)6-13-4-1-2-7-8-3-5-14-10(7)8/h1-6,14H/b4-1-,7-2-,13-6+
A2-23		23.1784	269.3333	-11.935	188.8555	504.3166	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-4-14-11(15(9)12)10-8(7)3-5-13-10/h1-6,13H/b2-1-,4-1-,7-2-,14-4-,14-11+
B-139		22.1829	377.2852	-2.7719	77.4439	504.5369	InChI=1S/C12H7N3O/c16-12-11-9(14-11)6-8-7(3-4-13-8)10-2-1-5-15(10)12/h1-6,13H/b9-6+
B-256		11.6134	449.5147	-9.6907	24.7796	506.5129	InChI=1S/C12H7N3O/c16-12-11(14-12)7-2-1-5-15-6-9(15)10-8(7)3-4-13-10/h1-6,13H/b5-1-,7-2+
q-28		11.9572	450.3436	-9.8034	23.2338	506.9304	InChI=1S/C12H7N3O/c16-12-11(14-12)8-3-1-2-7-4-5-13-10(7)9-6-15(8)9/h1-6,13H/b2-1-,8-3-
A2-46		41.078	189.4408	-1.688	175.4447	507.3965	InChI=1S/C12H7N3O/c16-10-7-2-1-4-13-12-9(10)6-15(12)11-8(7)3-5-14-11/h1-6,14H/b4-1-,7-2-,13-12+
F-47		30.4995	346.4942	-7.6898	63.4116	507.5261	InChI=1S/C12H7N3O/c16-11-7-2-1-3-9(11)15-6-10(15)14-12-8(7)4-5-13-12/h1-6H,13(14)/b8-7-
A-26		17.2088	313.7283	-9.8066	129.7395	508.5933	InChI=1S/C12H7N3O/c16-9-6-14-12-11-10-8(3-4-13-10)7(9)2-1-5-15(11)12/h1-6,13H/b5-1-,7-2-,14-6-




















B-171	 <chem>C12H9N3O</chem>	7.6313	370.6679	-3.3594	107.5132	508.6998	InChI=1S/C12H7N3O/c16-12-11(14-12)15-5-1-2-7-6-9(15)10-8(7)3-4-13-10/h1-6,13H
o-187	 <chem>C12H9N3O</chem>	44.7844	274.2274	-19.4033	168.2264	509.6677	InChI=1S/C12H7N3O/c16-10-6-8(10)11-7-2-1-5-15(14-11)9-3-4-13-12(7)9/h1-6,13H
B-157	 <chem>C12H9N3O</chem>	64.6153	131.3070	-2.9553	207.3351	510.2658	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-5-15(12)11(14-9)10-8(7)3-4-13-10/h1-6,13H/b5-1-,7-2+
q-48	 <chem>C12H9N3O</chem>	28.9304	422.7677	-18.5593	59.0598	510.6603	InChI=1S/C12H7N3O/c16-12-10-3-1-2-7-4-5-13-11(7)8-6-9(8)14-15(10)12/h1-6,13H/b2-1-,10-3-,14-9-
C-56	 <chem>C12H9N3O</chem>	24.1269	291.8084	-9.1694	156.8045	511.7807	InChI=1S/C12H7N3O/c16-12-11-8-2-1-4-13-6-9(15(11)12)10-7(8)3-5-14-10/h1-6,14H/b2-1-,9-6-,13-4-
H-32	 <chem>C12H9N3O</chem>	17.3203	250.6551	-1.6068	221.3161	511.793	InChI=1S/C12H7N3O/c16-10-6-7-2-1-3-8(10)9-4-5-13-11(9)12-14-15(7)12/h1-6,13H
B-207	 <chem>C12H9N3O</chem>	3.3676	314.4998	-2.0115	172.9804	513.2982	InChI=1S/C12H7N3O/c16-11-8-6-15-5-1-2-9(14-10(8)11)7-3-4-13-12(7)15/h1-6,13H/b8-6+,14-10+
o-66	 <chem>C12H9N3O</chem>	26.9378	322.9294	-7.3883	117.0577	514.0534	InChI=1S/C12H7N3O/c16-12-10-8(14-10)6-7-2-1-5-15(7)9-3-4-13-11(9)12/h1-6,13H/b8-6+
B-243	 <chem>C12H9N3O</chem>	5.3702	309.6318	-2.5067	172.2856	514.3673	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(6-9-10(11)14-9)12-8(7)3-4-13-12/h1-6,13H/b9-6+
E-30	 <chem>C12H9N3O</chem>	14.3732	348.9453	-7.2207	108.6946	514.3833	InChI=1S/C12H7N3O/c16-12-10-6-7-2-1-3-9(14-15(10)12)8-4-5-13-11(7)8/h1-6,13H/b10-6-,14-9+
H-137	 <chem>C12H9N3O</chem>	23.3864	228.3339	-7.2017	183.9421	514.6981	InChI=1S/C12H7N3O/c16-12-10-8-3-1-2-7(14-10)6-15(12)11-9(8)4-5-13-11/h1-6,13H
A-6	 <chem>C12H9N3O</chem>	17.5678	320.6604	-7.3681	132.9228	517.1849	InChI=1S/C12H7N3O/c16-9-6-15-8-2-1-5-14-11(9)12(14,15)10-7(8)3-4-13-10/h1-6,13H
A-15	 <chem>C12H9N3O</chem>	17.5698	320.6424	-7.3694	132.9357	517.1849	InChI=1S/C12H7N3O/c16-9-6-14-8-2-1-5-15-11(9)12(15)10-7(8)3-4-13-10/h1-6,13H/b5-1-,8-2-,14-6-
H-136	 <chem>C12H9N3O</chem>	32.2381	410.5806	-18.6836	85.3755	517.428	InChI=1S/C12H7N3O/c16-12-11-14-7(6-15(11)12)2-1-3-8-9-4-5-13-10(8)9/h1-6,13H/b2-1-,8-3-
o-169	 <chem>C12H9N3O</chem>	44.0592	390.8025	-26.8	72.7839	517.4701	InChI=1S/C12H7N3O/c16-12-7(8-6-9(8)14-12)2-1-5-15-10-3-4-13-11(10)15/h1-6,13H/b5-1-,7-2+
H-5	 <chem>C12H9N3O</chem>	19.8938	224.9747	-10.5674	239.9182	518.1268	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9(15-10(6-7)14-15)8-4-5-13-11(8)12/h1-6,13H/b2-1-,7-6-,9-3+
C-4	 <chem>C12H9N3O</chem>	21.1163	289.4894	-9.0025	174.9886	518.8057	InChI=1S/C12H7N3O/c16-11-9-6-15-12-8(3-5-13-12)7(10(9)11)2-1-4-14-15/h1-6,13H/b2-1-,14-4-
B-247	 <chem>C12H9N3O</chem>	7.1070	401.5440	-5.4404	86.0725	519.4280	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15(12)6-9-11(14-9)10-7(8)3-4-13-10/h1-6,13H/b9-6+
x4-16	 <chem>C12H9N3O</chem>	34.7057	279.4893	-2.4058	195.3734	519.4702	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9(12)11(8)15-6-14-15/h1-6,13H/b2-1-,3-1-,7-2-,8-3-,10-9+


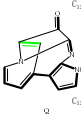

















H-112		10.7647	336.0059	-5.4077	140.1532	519.9452	InChI=1S/C12H7N3O/c16-12-11-14-6-7-2-1-3-9(15(11)12)8-4-5-13-10(7)8/h1-6,13H/b7-9?,14-11-
n-48		33.9968	481.4187	-14.0268	14.1138	519.964	InChI=1S/C12H7N3O/c16-12-9-10-8(3-4-13-10)15(11(9)12)5-1-2-7-6-14-7/h1-6,13H/b5-1-,7-2-
A1-23		31.5605	402.3908	-18.4958	66.3832	520.0129	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)8-2-1-4-13-6-9-7(8)3-5-14-9/h1-6,14H/b2-1+,4-1-,8-2-,8-7+,9-6-,13-4-,13-6+
n-170		60.464	209.6654	-15.6087	176.7022	520.2091	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-9-3-4-13-8(9)6-14-10(7)11(12)15/h1-6,13H
B-6		56.7353	335.7516	-19.2223	121.9497	520.2093	InChI=1S/C12H7N3O/c16-10-6-9(10)11-7(3-4-13-11)8-2-1-5-15-12(8)14-15/h1-6,13H
H-2		59.78	337.2705	-22.8093	115.4289	520.6033	InChI=1S/C12H7N3O/c16-10-6-7(10)2-1-3-9-8-4-5-13-11(8)12-14-15(9)12/h1-6,13H/b2-1-,9-3-
x4-28		42.0517	430.0337	-3.6306	26.2637	520.7946	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9(8)11(12)15-6-14-15/h1-6,13H
I-68		24.167	227.172	-7.7117	204.3085	520.902	InChI=1S/C12H7N3O/c16-9-6-8-10-11-7(2-4-14-11)15(8)5-1-3-13-12(9)10/h1-6,14H/b5-1-,13-3-
q11-3		40.534	470.4479	-19.0189	14.1099	521.1795	InChI=1S/C12H7N3O/c16-10-6-8(10)9-3-1-2-7-4-5-13-11(7)12-14-15(9)12/h1-6,13H/b2-1-,9-3-
G1-39		7.6569	380.1387	-3.6516	114.9553	522.74	InChI=1S/C12H7N3O/c16-9-3-1-2-8-7-4-5-13-11(7)10(9)12(8)15-6-14-15/h1-6,13H
o-105		12.382	474.8578	-7.5714	25.4591	522.8668	InChI=1S/C12H7N3O/c16-12-11(14-12)10-8(3-4-13-10)15-5-1-2-7-6-9(7)15/h1-6,13H
A-116		7.5023	357.8306	-4.3312	145.4798	523.2895	InChI=1S/C12H7N3O/c16-12-11-8-6-14-9(2-1-5-15(11)12)7-3-4-13-10(7)8/h1-6,13H/b5-1-,9-2-,11-8+
F-58		14.4809	368.1225	-8.5212	123.0395	524.4219	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(15(9)12)14-11-8(7)4-5-13-11/h1-6H,(H,13,14)/b2-1-,9-3-
x5-38		20.5419	358.1564	-9.9801	131.5015	525.2484	InChI=1S/C12H7N3O/c16-12-10-9-6-8(15(10)12)3-1-2-7-4-5-13-11(7)14-9/h1-6H,(H,13,14)/b3-1-,7-2-
H11-27		34.3787	417.4561	-20.222	82.4347	526.6918	InChI=1S/C12H7N3O/c16-12-10-6-7(14-15(10)12)2-1-3-8-9-4-5-13-11(8)9/h1-6,13H/b2-1-,8-3-
o-245		23.8471	243.6354	-9.2964	199.7692	526.8428	InChI=1S/C12H7N3O/c16-10-6-9-12(14-10)7-2-1-5-15(9)8-3-4-13-11(7)8/h1-6,13H
x4-13		56.7995	407.2539	-13.8339	53.8484	528.177	InChI=1S/C12H7N3O/c16-12-9-8(15-6-14-15)3-1-2-7-4-5-13-11(7)10(9)12/h1-6,13H/b2-1-,3-1-,7-2?,8-3+,9-8-,11-10-
E-19		22.5443	252.6839	-2.945	158.5938	528.2917	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-3-10(14-15(7)12)8-4-5-13-11(8)9/h1-6,13H
x9-32		49.3841	442.7775	-20.0128	33.2467	529.217	InChI=1S/C12H7N3O/c16-12-10-7(4-5-13-10)2-1-3-9-11(15(9)12)8-6-14-8/h1-6,13H/b2-1-,9-3-,11-8-

A-161		64.5008	422.1344	-12.8372	50.0416	529.5293	InChI=1S/C12H7N3O/c16-12-9-7(2-1-5-15-6-14-15)8-3-4-13-11(8)10(9)12/h1-6,13H/b5-1-,7-2-
A-164		64.4956	422.1389	-12.8387	50.0417	529.5293	InChI=1S/C12H7N3O/c16-12-9-7(2-1-5-15-6-14-15)8-3-4-13-11(8)10(9)12/h1-6,13H/b5-1-,7-2-
s11-15		27.8887	218.0288	-3.4304	186.8062	530.7711	InChI=1S/C12H7N3O/c16-12-9-6-8-3-1-2-7-4-5-13-10(7)11(12)15(9)14-8/h1-6,13H/b3-1-,7-2-,11-10+
x3-18		17.1198	237.5195	-6.6959	252.472	530.8629	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-11(9(7)12)10-8(15)2-4-14-10/h1-6,14H/b5-1-,13-3-
o-88		74.5028	174.0144	-0.8599	173.7279	531.1528	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(12)9-3-4-13-11(9)8(6-7)14-10/h1-6,13H
X22-61		15.0096	504.5486	-5.7686	6.5529	531.4198	InChI=1S/C12H7N3O/c16-12-7-2-1-4-13-8-3-5-14-10(8)9-6-15(9)11(7)12/h1-6,14H/b2-1-,13-4+
o-169		85.2448	407.7816	-50.4001	59.1498	531.5637	InChI=1S/C12H7N3O/c16-10-6-7(10)11-8(14-11)2-1-5-15-9-3-4-13-12(9)15/h1-6,13H/b5-1-,8-2+
q-31		39.5672	431.4769	-23.3095	69.0953	532.4619	InChI=1S/C12H7N3O/c16-10-6-8(10)11-7(4-5-13-11)2-1-3-9-12-14-15(9)12/h1-6,13H/b2-1-,9-3-
i-1		55.7208	336.1653	-27.4489	115.9848	533.5404	InChI=1S/C12H7N3O/c16-10-6-9(10)15-8-2-1-4-13-7-3-5-14-11(7)12(8)15/h1-6,14H/b2-1-,4-1-,8-2+,12-11-,13-4-,13-7-
B-25		14.0538	283.2203	-1.0748	210.5397	533.8624	InChI=1S/C12H7N3O/c16-10-6-9-12(14-9)15-5-1-2-7(10)8-3-4-13-11(8)15/h1-6,13H/b9-6+
o-43		29.1812	362.5097	-21.6032	134.2685	534.3421	InChI=1S/C12H7N3O/c16-11-8-6-7(14-10(8)11)2-1-5-15-9-3-4-13-12(9)15/h1-6,13H/b5-1-,7-2+
H11-52		35.4676	314.0187	-9.3026	121.1356	535.6238	InChI=1S/C12H7N3O/c16-12-8-6-15(12)11-7(4-5-13-11)9-2-1-3-10(8)14-9/h1-6,13H
o-142		13.9255	266.7158	-5.9232	212.1313	536.8329	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15(12-8(6-7)14-12)9-3-4-13-10(9)11/h1-6,13H/b5-1-,7-2-,8-6+
H-120		19.0317	379.7294	-10.7438	106.8113	537.0635	InChI=1S/C12H7N3O/c16-12-11-14-10-9(4-5-13-10)7-2-1-3-8(6-7)15(11)12/h1-6,13H/b14-11-
B-56		68.3263	106.8393	-6.4000	241.3061	537.4364	InChI=1S/C12H7N3O/c16-9-6-10-14-12-11-8(3-4-13-11)7(9)2-1-5-15(10)12/h1-6,13H/b5-1-,7-2+,10-6-
H11-157		6.2378	358.4387	-3.436	152.0061	537.6199	InChI=1S/C12H7N3O/c16-10-6-9-12-8(4-5-13-12)7(10)2-1-3-11-14-15(9)11/h1-6,13H/b3-1-,7-2+
o-92		6.1719	420.607	-4.4464	95.1141	537.8444	InChI=1S/C12H7N3O/c16-12-11-8(14-11)6-7-2-1-5-15(12)9-3-4-13-10(7)9/h1-6,13H/b8-6-
A1-38		33.4126	330.8115	-13.968	152.4089	538.5182	InChI=1S/C12H7N3O/c16-11-9-7-2-1-4-13-6-15(10(9)11)12-8(7)3-5-14-12/h1-6,14H/b4-1-,7-2-,13-6-
H-142		11.7763	376.0464	-4.6876	121.8824	539.0595	InChI=1S/C12H7N3O/c16-12-11(14-12)15-8-3-1-2-7(6-8)9-4-5-13-10(9)15/h1-6,13H




















q11-22		25.5728	443.8257	-8.0346	57.4771	539.152	InChI=1S/C12H7N3O/c16-12-9-6-8(9)3-1-2-7-4-5-13-10(7)11-14-15(11)12/h1-6,13H/b2-1-,8-3-
X22-37		49.0223	385.9611	-22.7423	84.8135	539.7301	InChI=1S/C12H7N3O/c16-10-6-9(10)15-8-2-1-4-13-7-3-5-14-11(7)12(8)15/h1-6,14H/b2-1-,4-1-,8-2-,12-11-,13-4-,13-7+
o-153		11.8654	286.9106	-4.4862	202.8484	539.9066	InChI=1S/C12H7N3O/c16-10-6-8-12(14-8)15-5-1-2-7(10)11-9(15)3-4-13-11/h1-6,13H/b8-6+
o-8		5.9099	313.5441	-2.8623	192.6171	540.2982	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(6-8-11(12)14-8)9-3-4-13-10(7)9/h1-6,13H/b8-6+
B-246		20.4189	277.7493	-7.3434	212.1976	543.0819	InChI=1S/C12H7N3O/c16-12-11-8(3-4-13-11)7-2-1-5-15(12)6-9-10(7)14-9/h1-6,13H/b5-1-,7-2+,9-6+
H11-4		42.272	449.3267	-27.8614	49.5383	544.3496	InChI=1S/C12H7N3O/c16-12-14-9(10-6-15(10)12)3-1-2-7-8-4-5-13-11(7)8/h1-6,13H/b3-1-,7-2-
q11-42		21.6786	461.2642	-18.89	67.5798	544.5193	InChI=1S/C12H7N3O/c16-12-11(14-12)10-7(4-5-13-10)2-1-3-8-9-6-15(8)9/h1-6,13H/b2-1-,8-3-
H-17		27.5576	284.4669	-9.3889	181.4634	545.1328	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9(11-14-15(11)12)8-4-5-13-10(8)6-7/h1-6,13H/b2-1-,3-1+,7-2-,7-6+,9-3+,9-8+,10-6+
H11-24		35.4996	184.506	0.2029	215.4248	546.5195	InChI=1S/C12H7N3O/c16-12-8-2-1-3-10-7-4-5-13-11(7)9(14-8)6-15(10)12/h1-6,13H
n-167		21.7644	312.0941	-8.1315	183.8997	546.5702	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15-6-14-11(9(7)12)10-8(15)3-4-13-10/h1-6,13H/b5-1-,7-2+,11-9+
x5-41		36.1623	408.9338	-22.5447	82.6439	546.6424	InChI=1S/C12H7N3O/c16-12-10-9(15(10)12)8-3-1-2-7-4-5-13-11(7)14-6-8/h1-6H,11,13,14
B-250		55.8257	427.8550	-32.4853	58.7815	546.7424	InChI=1S/C12H7N3O/c16-12-11(14-12)9-6-15(9)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
B-7		53.1996	384.3254	-24.9124	100.6858	547.7187	InChI=1S/C12H7N3O/c16-10-6-9(10)7-2-1-5-15-12(14-15)11-8(7)3-4-13-11/h1-6,13H/b5-1-,7-2+
H-46		29.6639	423.367	-18.102	100.504	547.8796	InChI=1S/C12H7N3O/c16-10-6-7(12-14-15(10)12)2-1-3-8-9-4-5-13-11(8)9/h1-6,13H/b2-1-,8-3-
H-1		28.2799	432.948	-7.1062	89.735	548.8865	InChI=1S/C12H7N3O/c16-10-6-7(10)2-1-3-8-9-4-5-13-11(9)15-12(8)14-15/h1-6,13H/b2-1-,8-3-
B-205		28.3325	416.2083	-14.2854	101.2601	549.5034	InChI=1S/C12H7N3O/c16-12-9-6-15(14-11(9)12)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-
H11-131		63.209	328.2761	-21.4668	153.2239	550.2088	InChI=1S/C12H7N3O/c16-10-6-8(10)12-7(4-5-13-12)9-2-1-3-11-14-15(9)11/h1-6,13H
H-63		7.6693	312.2742	-3.6849	200.6819	551.8636	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7(15-12(11)14-15)6-10-8(9)4-5-13-10/h1-6,13H/b2-1-,3-1-,7-2+,7-6-,9-3+,9-8+,10-6-
H-140		8.8495	381.2359	-4.4102	132.551	552.0011	InChI=1S/C12H7N3O/c16-12-11(14-12)15-6-7-2-1-3-9(15)8-4-5-13-10(7)8/h1-6,13H

J-19		33, 8998	405, 9618	-20, 0515	90, 9701	553, 6468	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)7-2-1-4-13-8-3-5-14-9(8)6-7/h1-6,14H/b2-1-,4-1-,7-2-,7-6+,9-6+,13-4-,13-8-
	$C_{12}H_7N_3O$						
B-9		47, 0158	313, 7818	-20, 3052	177, 3003	553, 7674	InChI=1S/C12H7N3O/c16-10-6-9(10)14-12-7-2-1-5-15(12)11-8(7)3-4-13-11/h1-6,13H/b4-12-
	$C_{12}H_7N_3O$						
H-145		61, 9606	436, 9493	-39, 0581	62, 4658	554, 1098	InChI=1S/C12H7N3O/c16-12-11(14-12)15-6-7(15)2-1-3-8-9-4-5-13-10(8)9/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
H1-18		23, 0563	255, 0699	-3, 52	234, 5017	554, 4645	InChI=1S/C12H7N3O/c16-10-3-1-2-8-7-4-5-13-11(7)9(10)6-15-12(8)14-15/h1-6,13H/b3-1-,8-2+
	$C_{12}H_7N_3O$						
H11-129		92, 9968	423, 2239	-41, 5388	67, 8374	556, 566	InChI=1S/C12H7N3O/c16-10-6-9(10)15-11(14-15)3-1-2-7-8-4-5-13-12(7)8/h1-6,13H/b3-1-,7-2-
	$C_{12}H_7N_3O$						
o-41		7, 6221	327, 8079	-2, 2259	197, 8619	562, 4258	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-2-8(10)7(12)11-9(15)3-4-13-11/h1-6,13H/b7-6+,14-10+
	$C_{12}H_7N_3O$						
q1-59		35, 2977	250, 999	-7, 1099	184, 1047	562, 4889	InChI=1S/C12H7N3O/c16-11-10-7(4-5-13-10)2-1-3-8-9-6-14-12(11)15(8)9/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
q1-60		35, 2955	251, 0004	-7, 1093	184, 1049	562, 4889	InChI=1S/C12H7N3O/c16-11-10-7(4-5-13-10)2-1-3-8-9-6-15(9)12(11)14-8/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
q-9		5, 3794	510, 7308	-4, 4858	39, 0562	565, 5103	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)9-6-15(9)14-11(8)12/h1-6,13H/b2-1-,8-3-,14-11+
	$C_{12}H_7N_3O$						
x4-65		118, 5101	117, 6217	0, 7239	121, 6109	567, 3897	InChI=1S/C12H7N3O/c16-12-14-6-8-9-3-1-2-7-4-5-13-10(7)11(8)15(9)12/h1-6,13H/b2-1-,3-1-,7-2-,9-3-,11-10+
	$C_{12}H_7N_3O$						
H11-153		14, 8429	212, 3338	-5, 0959	286, 9912	567, 9757	InChI=1S/C12H7N3O/c16-11-7-2-1-3-10-14-9(11)6-15(10)12-8(7)4-5-13-12/h1-6,13H/b3-1-,7-2-
	$C_{12}H_7N_3O$						
H11-138		31, 0733	314, 8555	-2, 351	180, 7329	569, 5849	InChI=1S/C12H7N3O/c16-12-9-6-7(8-4-5-13-11(8)12)2-1-3-10-14-15(9)10/h1-6,13H/b3-1-,7-2+
	$C_{12}H_7N_3O$						
B-100		25, 3840	366, 0297	-12, 3389	120, 5242	570, 2147	InChI=1S/C12H7N3O/c16-12-11-7(3-4-13-11)8-2-1-5-15(12)10-6-9(10)14-8/h1-6,13H/b5-1-,8-2-,14-9-
	$C_{12}H_7N_3O$						
H-79		27, 2404	204, 4452	-0, 9662	255, 4377	574, 6805	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-15(12)11(14-7)10-8(9)4-5-13-10/h1-6,13H/b2-1-,9-3-
	$C_{12}H_7N_3O$						
o-195		57, 2798	363, 0401	-24, 4922	148, 6	575, 2101	InChI=1S/C12H7N3O/c16-10-6-7(10)11-9(3-4-13-11)15-5-1-2-8-12(14-8)/h1-6,13H
	$C_{12}H_7N_3O$						
H-146		37, 6185	391, 4367	-18, 3924	119, 1527	576, 3995	InChI=1S/C12H7N3O/c16-12-10(14-12)8-3-1-2-7-6-15(7)11-9(8)4-5-13-11/h1-6,13H/b2-1-,8-3+
	$C_{12}H_7N_3O$						
o-84		35, 6083	234, 1044	-7, 3865	229, 8095	578, 4437	InChI=1S/C12H7N3O/c16-10-6-8-7-2-1-5-15(12(10)14-8)9-3-4-13-11(7)9/h1-6,13H
	$C_{12}H_7N_3O$						
q1-52		52, 0835	230, 2145	-9, 4445	203, 4246	578, 555	InChI=1S/C12H7N3O/c16-11-9-6-14-12-8(15(9)12)3-1-2-7-4-5-13-10(7)11/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
B-166		8, 3668	361, 1655	-5, 0258	180, 9595	579, 4220	InChI=1S/C12H7N3O/c16-12-10(14-12)9-6-7-2-1-5-15(9)11-8(7)3-4-13-11/h1-6,13H
	$C_{12}H_7N_3O$						

o-103		9.2134	389.6344	-4.4371	151.8766	580.9726	InChI=1S/C12H7N3O/c16-12-11(14-12)9-6-7-2-1-5-15(9)8-3-4-13-10(7)8/h1-6,13H
	$C_{12}H_7N_3O$						
o-100		9.2659	389.4437	-4.4386	152.8028	581.6421	InChI=1S/C12H7N3O/c16-12-11(14-12)8-6-15-5-1-2-7(8)10-9(15)3-4-13-10/h1-6,13H
	$C_{12}H_7N_3O$						
H11-135		56.9281	338.4564	-21.3536	151.2871	581.8178	InChI=1S/C12H7N3O/c16-10-6-9(10)15-11-3-1-2-8(14-11)7-4-5-13-12(7)15/h1-6,13H
	$C_{12}H_7N_3O$						
G-28		7.2136	559.1289	-6.823	19.4606	582.526	InChI=1S/C12H7N3O/c16-12-10-3-1-2-7(9-6-14-9)8-4-5-13-11(8)15(10)12/h1-6,13H/b2-1-,9-7-,10-3-
	$C_{12}H_7N_3O$						
o-33		29.128	205.1976	-1.6662	258.6443	582.7638	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(14-10(7)12)9-3-4-13-11(8)9/h1-6,13H
	$C_{12}H_7N_3O$						
o-194		47.5457	318.1315	-20.0676	201.4043	584.923	InChI=1S/C12H7N3O/c16-10-6-8(10)14-12-7-2-1-5-15(12)9-3-4-13-11(7)9/h1-6,13H/b14-12+
	$C_{12}H_7N_3O$						
G-1		4.8466	585.3746	-4.055	-8.8242	584.9703	InChI=1S/C12H7N3O/c16-11-9-3-1-2-7(10(9)11)8-4-5-13-12(8)15-6-14-15/h1-6,13H
	$C_{12}H_7N_3O$						
X-29		46.7691	357.4902	-13.7856	109.0789	586.5769	InChI=1S/C12H7N3O/c16-11-9-8(3-5-13-9)7-2-1-4-14-12-10(11)15(12)6-7/h1-6,13H/b2-1-,14-4-
	$C_{12}H_7N_3O$						
H-134		8.2966	351.9734	-4.8319	197.0684	589.1494	InChI=1S/C12H7N3O/c16-12-11-14-7-2-1-3-10(15(11)12)8-4-5-13-9(8)6-7/h1-6,13H/b2-1-,3-1-,7-2-,7-6-,9-6-,10-3-,10-8-,14-11+
	$C_{12}H_7N_3O$						
q11-30		23.6355	453.4107	-5.9429	102.6509	589.34	InChI=1S/C12H7N3O/c16-11-8-3-1-2-7-4-5-13-10(7)12-14-15(12)6-9(8)11/h1-6,13H/b2-1-,8-3+,9-6+
	$C_{12}H_7N_3O$						
s11-24		25.8052	474.9788	-9.4184	72.1017	592.0316	InChI=1S/C12H7N3O/c16-9-6-8(9)12-11-7(4-5-13-11)2-1-3-10-14-15(10)12/h1-6,13H/b3-1-,7-2-,12-11+
	$C_{12}H_7N_3O$						
B-158		112.3698	138.3066	-6.2273	214.5581	593.3360	InChI=1S/C12H7N3O/c16-12-9-6-7-2-1-5-15(9)14-11(12)10-8(7)3-4-13-10/h1-6,13H
	$C_{12}H_7N_3O$						
q11-24		119.0408	164.2401	-16.2932	174.6628	594.1339	InChI=1S/C12H7N3O/c16-12-8-6-15-9(12)3-1-2-7-4-5-13-10(7)11(8)14-15/h1-6,13H/b2-1-,9-3-
	$C_{12}H_7N_3O$						
X23-5		17.3383	395.5576	-8.105	151.0733	594.5359	InChI=1S/C12H7N3O/c16-12-11-8-6-7(15(11)12)2-1-4-13-9-3-5-14-10(8)9/h1-6,14H/b2-1-,13-4-
	$C_{12}H_7N_3O$						
A-48		110.8024	191.1679	-11.5963	141.2124	595.2185	InChI=1S/C12H7N3O/c16-12-8-6-14-9-2-1-5-15(12)11(8)10-7(9)3-4-13-10/h1-6,13H/b5-1-,9-2?
	$C_{12}H_7N_3O$						
x4-39		28.4676	567.4099	-18.9209	11.6416	596.5025	InChI=1S/C12H7N3O/c16-12-11-10(15(11)12)9-7(4-5-13-9)2-1-3-8-6-14-8/h1-6,13H/b2-1-,8-3-
	$C_{12}H_7N_3O$						
E-58		56.366	304.5087	-1.6749	151.5082	596.8912	InChI=1S/C12H7N3O/c16-12-7-2-1-3-9-8-4-5-13-11(8)10(6-7)15(12)14-9/h1-6,13H/b3-1-,7-2-
	$C_{12}H_7N_3O$						
F-5		116.5159	182.4432	-7.0139	169.0299	597.4067	InChI=1S/C12H7N3O/c16-11-9-6-15-10(11)3-1-2-7(9)8-4-5-13-12(8)14-15/h1-6H,13,14
	$C_{12}H_7N_3O$						
s11-26		41.1956	221.3895	-3.2479	221.1417	597.7032	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-11(7)9-6-10(12)15(9)14-8/h1-6,13H/b3-1-,7-2-,11-9+
	$C_{12}H_7N_3O$						

s11-19		32, 5894	520, 617	-1, 6299	32, 073	599, 5328	InChI=1S/C12H7N3O/c16-12-8-6-15-9(14-15)3-1-2-7-4-5-13-11(7)10(8)12/h1-6, 13H/b3-1-, 7-2-, 8-6+, 11-10-
B-159		106, 2673	168, 7315	-6, 9524	173, 8143	599, 8938	InChI=1S/C12H7N3O/c16-10-9-6-7-2-1-5-15(9)12(10)14-11-8(7)3-4-13-11/h1-6, 13H/b14-12-
A-174		110, 4153	188, 1457	-10, 6784	140, 6899	600, 1554	InChI=1S/C12H7N3O/c16-12-10-11-9-8(3-4-13-9)7(6-14-10)2-1-5-15(11)12/h1-6, 13H/b5-1-, 7-2+
s12-1		59, 2945	444, 2272	-34, 8579	86, 1374	600, 5944	InChI=1S/C12H7N3O/c16-12-11-10-8(14-10)3-1-2-7-4-5-13-9(7)6-15(11)12/h1-6, 13H/b3-1-, 7-2-, 9-6-, 11-10+
p-25		31, 3362	535, 9802	-2, 3182	31, 4898	603, 5707	InChI=1S/C12H7N3O/c16-12-10-3-1-2-7-4-5-13-8(7)6-9-11(14-9)15(10)12/h1-6, 13H/b2-1-, 9-6+, 10-3-
B-3		80, 2990	484, 5911	-39, 7794	56, 9957	604, 8136	InChI=1S/C12H7N3O/c16-10-6-9(10)12-14-15(12)5-1-2-7-8-3-4-13-11(7)8/h1-6, 13H/b5-1-, 7-2-
s11-41		32, 8314	494, 664	-5, 1573	77, 7814	605, 1568	InChI=1S/C12H7N3O/c16-12-11-10-7(4-5-13-10)2-1-3-8-9(14-8)6-15(11)12/h1-6, 13H/b3-1-, 7-2-, 9-6-, 11-10+
s12-38		63, 5595	452, 6179	-37, 5274	77, 6939	605, 233	InChI=1S/C12H7N3O/c16-12-11-10-8(14-10)3-1-2-7-4-5-13-9(7)6-15(11)12/h1-6, 13H/b3-1-, 7-2-, 9-6-, 11-10-
x3-16		81, 1163	131, 415	-6, 0587	252, 8722	606, 6167	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-10(7)9(12)11-8(15)2-4-14-11/h1-6, 14H/b5-1-, 13-3+
o-137		10, 4623	280, 5907	-5, 6046	266, 679	607, 4944	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(10-6-8(7)14-10)9-3-4-13-11(9)12/h1-6, 13H/b5-1-, 7-2-, 8-6+
o-138		10, 4623	280, 5907	-5, 6046	266, 679	607, 4944	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(10-6-8(7)14-10)9-3-4-13-11(9)12/h1-6, 13H/b5-1-, 7-2+
H-81		83, 8146	132, 7448	-2, 0764	218, 0375	607, 5426	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-6-10(14-12)15(7)11-8(9)4-5-13-11/h1-6, 13H/b2-1-, 9-3-
x4-49		100, 7238	78, 9635	-1, 278	208, 6361	609, 2112	InChI=1S/C12H7N3O/c16-12-9-8-3-1-2-7-4-5-13-10(7)11(9)15(8)6-14-12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 11-10+
o-83		83, 1147	155, 1226	-2, 4533	209, 5822	610, 4506	InChI=1S/C12H7N3O/c16-10-6-9-7-2-1-5-15(9)8-3-4-13-11(8)12(10)14-7/h1-6, 13H
q11-57		19, 3409	484, 0376	-7, 1388	100, 4018	611, 173	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-10(7)11-8(14-11)6-15(9)12/h1-6, 13H/b2-1-, 8-6+, 9-3-
o-115		121, 1788	137, 1193	-12, 1887	211, 5004	613, 1668	InChI=1S/C12H7N3O/c16-11-7-2-1-5-15-9-3-4-13-12(9)14-8(7)6-10(11)15/h1-6, 13H
p-19		36, 3524	542, 6912	-1, 6868	30, 967	614, 5603	InChI=1S/C12H7N3O/c16-12-10-6-9-7(4-5-13-9)2-1-3-8-11(14-8)15(10)12/h1-6, 13H/b2-1-, 8-3+, 10-6-
n-160		37, 4044	527, 7858	-21, 214	47, 597	616, 1988	InChI=1S/C12H7N3O/c16-11-7(10(11)8-6-14-8)2-1-5-15-9-3-4-13-12(9)15/h1-6, 13H/b5-1-, 7-2-, 10-8+
A2-64		18, 8474	458, 7429	-4, 8857	120, 3507	617, 7947	InChI=1S/C12H7N3O/c16-10-6-9(10)15-8-2-1-4-14-12(15)11-7(8)3-5-13-11/h1-6, 13H

n-159		9.8923	373.3664	-4.988	200.8884	618.5545	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(11)(12)8-6-14-8)9-3-4-13-10(7)9/h1-6,13H/b11-8-
G-53		21.7228	540.4176	-14.1698	72.5792	622.4466	InChI=1S/C12H7N3O/c16-12-10-8(3-1-2-7-6-14-7)9-4-5-13-11(9)15(10)12/h1-6,13H/b3-1-,7-2-
x4-55		35.9644	497.5163	-6.2288	88.2876	625.1611	InChI=1S/C12H7N3O/c16-12-9-3-1-2-7-4-5-13-10(7)11(15(9)12)8-6-14-8/h1-6,13H/b2-1-,9-3-,11-8-
I-28		20.499	413.0557	-10.8252	154.8829	626.8357	InChI=1S/C12H7N3O/c16-11-7-6-8-9(2-4-13-8)15-5-1-3-14-12(15)7(11)/h1-6,13H
A2-60		181.5459	141.6323	-18.4344	149.7095	629.3483	InChI=1S/C12H7N3O/c16-11-7-2-1-4-13-10-6-9(11)15(10)12-8(7)3-5-14-12/h1-6,14H/b4-1-,7-2-,13-10-
o-135		51.3558	51.3558	-1.9351	263.1238	629.4345	InChI=1S/C12H7N3O/c16-12-7-6-10-14-8(12)2-1-5-15(10)9-3-4-13-11(7)9/h1-6,13H
H1-112		51.3419	285.6661	-5.2579	152.7529	631.9066	InChI=1S/C12H7N3O/c16-11-3-1-2-10-7-4-5-13-9(7)6-8(11)12-14-15(10)12/h1-6,13H/b3-1-,10-2-
o-178		7.9808	385.6085	-4.3072	200.308	632.9609	InChI=1S/C12H7N3O/c16-12-7-6-15(9-3-4-13-11(9)12)5-1-2-8-10(7)14-8/h1-6,13H/b5-1-,8-2+
H1-50		161.1305	188.3019	-16.5316	137.0661	634.7372	InChI=1S/C12H7N3O/c16-9-3-1-2-7-6-10-14-12(9)15(10)11-8(7)4-5-13-11/h1-6,13H/b3-1-,7-2+
B-116		11.4350	446.7503	-5.1116	152.5187	636.2027	InChI=1S/C12H7N3O/c16-12-9(14-12)6-10-7-2-1-5-15(10)11-8(7)3-4-13-11/h1-6,13H/b10-6+
H-4		50.8879	330.9189	-14.6343	209.4347	638.2767	InChI=1S/C12H7N3O/c16-11-7-2-1-3-9(11)8-4-5-13-10(8)12-14-15(12)6-7/h1-6,13H/b7-6-
A-76		46.8207	549.5131	-24.4362	53.3533	638.8785	InChI=1S/C12H7N3O/c16-12-11(9-6-14-9)15(12)5-1-2-7-8-3-4-13-10(7)8/h1-6,13H/b5-1-,7-2-,11-9+
x4-29		33.8434	521.6337	-2.2975	79.9158	641.2281	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-10(7)11(9(8)12)15-6-14-15/h1-6,13H/b2-1-,3-1-,7-29,8-3+,11-9-,11-10-
H11-130		30.7082	530.2823	-3.6247	81.121	646.3184	InChI=1S/C12H7N3O/c16-10-6-9(10)7-2-1-3-11-14-15(11)12-8(7)4-5-13-12/h1-6,13H/b3-1-,7-2+
o-69		88.2494	183.3953	-5.1615	258.8157	655.8837	InChI=1S/C12H7N3O/c16-12-8-6-10-7(14-8)2-1-5-15(10)9-3-4-13-11(9)12/h1-6,13H
o-192		45.3109	477.3198	-20.603	124.4462	658.8215	InChI=1S/C12H7N3O/c16-10-6-9(10)15-5-1-2-7-11(14-7)12-8(15)3-4-13-12/h1-6,13H/b5-1-,7-2+
o-106		12.5848	449.9503	-5.1905	169.0786	661.2269	InChI=1S/C12H7N3O/c16-12-8(14-12)6-10-7-2-1-5-15(10)9-3-4-13-11(7)9/h1-6,13H/b10-6+
B-172		113.7871	209.4162	-11.0960	187.9011	665.9597	InChI=1S/C12H7N3O/c16-11-10-8(3-4-13-10)7-2-1-5-15-9(6-7)14-12(11)15/h1-6,13H
o-209		156.8627	172.7787	-10.4908	195.8172	680.1633	InChI=1S/C12H7N3O/c16-12-7-6-9-11-10(3-4-13-11)15(12)5-1-2-8(7)14-9/h1-6,13H

x3-9		81, 1163	131, 415	-6, 0587	285, 4218	689, 2473	InChI=1S/C12H7N3O/c16-12-7-6-15-5-1-3-13-10(7)9(12)11-8(15)2-4-14-11/h1-6, 14H/b5-1-, 13-3-
x4-59		147, 6248	257, 6234	-13, 1834	138, 7773	691, 3369	InChI=1S/C12H7N3O/c16-12-8-3-1-2-7-4-5-13-9(7)11-10(8)14-6-15(11)12/h1-6, 13H/b2-1-, 3-1-, 7-2-, 8-3+, 11-9-
o-62		175, 5508	214, 8686	-13, 4074	185, 8839	692, 3203	InChI=1S/C12H7N3O/c16-12-10-7-2-1-5-15(9(6-7)14-10)8-3-4-13-11(8)12/h1-6, 13H
s11-20		171, 9744	198, 0843	-10, 8864	174, 1847	693, 4302	InChI=1S/C12H7N3O/c16-12-8-6-15-11(12)10-7(4-5-13-10)2-1-3-9(8)14-15/h1-6, 13H/b3-1-, 7-2-, 11-10+
B-108		71, 7100	257, 8296	-7, 7718	236, 8467	694, 7424	InChI=1S/C12H7N3O/c16-12-8-2-1-5-15-10(6-9(12)14-15)11-7(8)3-4-13-11/h1-6, 13H/b5-1-, 8-2-
n-74		11, 7073	429, 6718	-5, 3127	208, 2608	695, 1251	InChI=1S/C12H7N3O/c16-12-7-2-1-5-15(11(12)8-6-14-8)9-3-4-13-10(7)9/h1-6, 13H/b11-8+
p-13		12, 9049	684, 8786	-5, 6729	-10, 75	709, 4234	InChI=1S/C12H7N3O/c16-12-11(14-12)15-9-3-1-2-7-4-5-13-8(7)6-10(9)15/h1-6, 13H/b2-1-, 3-1-, 7-27, 8-6+, 9-3+, 10-6+
A-118		58, 4707	619, 5777	-27, 1136	52, 0104	711, 5618	InChI=1S/C12H7N3O/c16-12-11(9-6-14-9)15(12)5-1-2-7-8-3-4-13-10(7)8/h1-6, 13H/b5-1-, 7-2-, 11-9-
o-219		87, 7034	197, 5438	-5, 045	265, 9833	722, 5407	InChI=1S/C12H7N3O/c16-12-8-6-7-2-1-5-15(11(7)14-12)9-3-4-13-10(8)9/h1-6, 13H
B-218		76, 0661	314, 2668	-3, 1857	248, 8399	765, 7155	InChI=1S/C12H7N3O/c16-11-8-6-15-5-1-2-9(14-12(11)15)7-3-4-13-10(7)8/h1-6, 13H
s11-47		195, 679	281, 7681	-15, 7946	152, 2319	776, 5139	InChI=1S/C12H7N3O/c16-10-6-8-12-11-7(4-5-13-11)2-1-3-9(14-8)15(10)12/h1-6, 13H/b3-1-, 7-2-, 12-11+
B-201		170, 3337	121, 7425	-5, 7893	263, 9435	804, 0994	InChI=1S/C12H7N3O/c16-11-8-2-1-5-15-9(6-14-12(11)15)10-7(8)3-4-13-10/h1-6, 13H
o-31		155, 0843	274, 2628	-17, 4045	306, 8765	863, 3481	InChI=1S/C12H7N3O/c16-12-9-6-14-11(12)7-2-1-5-15(9)8-3-4-13-10(7)8/h1-6, 13H
C-11		162, 7668	259, 6384	-33, 8478	369, 1963	960, 8567	InChI=1S/C12H7N3O/c16-11-9-6-13-4-1-2-7-8-3-5-14-12(8)15(9)10(7)11/h1-6, 14H/b2-1-, 9-6-, 13-4?
B-259		194, 8672	704, 8841	-10, 6092	76, 6735	972, 0031	InChI=1S/C12H7N3O/c16-12-11(14-12)10-8(3-4-13-10)7-2-1-5-15-6-9(7)15/h1-6, 13H
A-92		296, 6812	157, 9234	-17, 0657	157, 6324	1007, 5428	InChI=1S/C12H7N3O/c16-12-14-6-9-7-2-1-5-15(12)11(9)10-8(7)3-4-13-10/h1-6, 13H
s11-46		484, 2379	525, 8648	-12, 8248	230, 6381	1058, 2742	InChI=1S/C12H7N3O/c16-10-6-8-9-3-1-2-7-4-5-13-11(7)12(8)15(10)14-9/h1-6, 13H/b3-1-, 7-2-, 12-11-
A2-21		732, 8354	338, 8582	-21, 9599	304, 307	1356, 0904	InChI=1S/C12H7N3O/c16-12-8-2-1-4-14-11-10(15(11)12)6-9-7(8)3-5-13-9/h1-6, 13H/b2-1-, 4-1-, 8-2-, 14-4-, 14-11-
o-237		238, 8518	840, 113	-21, 3841	119, 8159	1440, 7624	InChI=1S/C12H7N3O/c16-12-11-10(3-4-13-11)15-5-1-2-9(15)7-6-8(7)14-12/h1-6, 13H/b14-8-