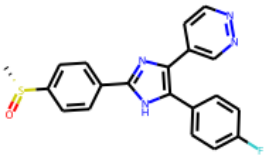
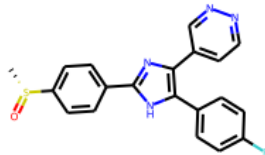
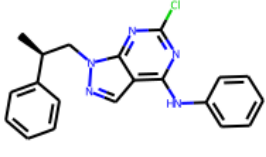
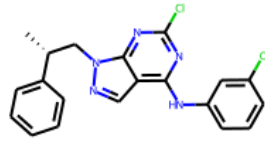
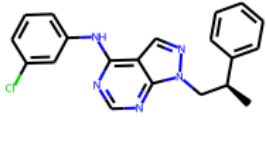
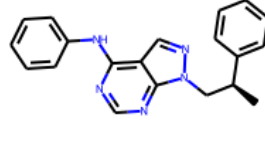
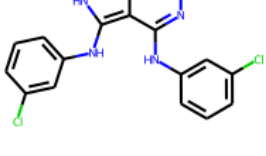
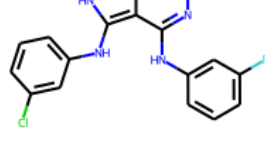
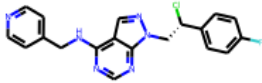
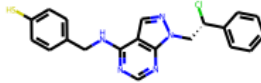
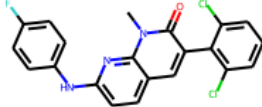
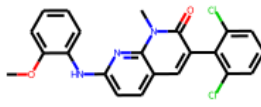
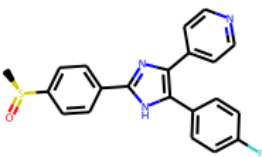
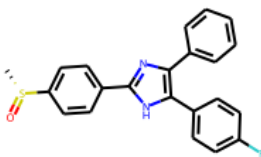
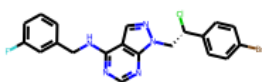
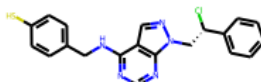
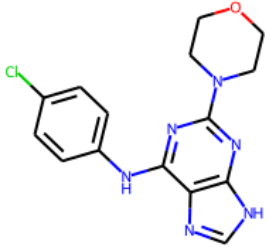
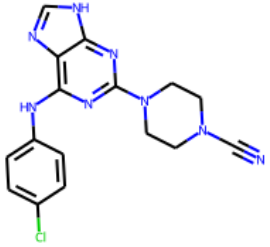
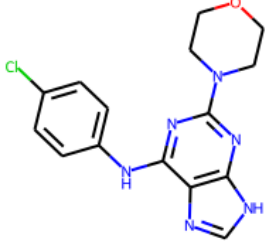
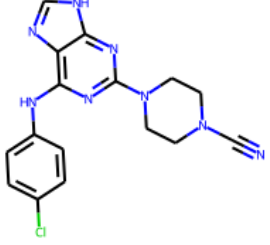
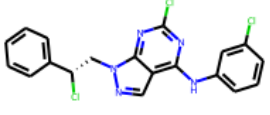
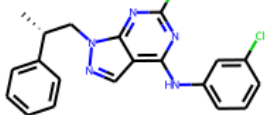
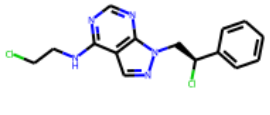
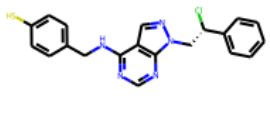
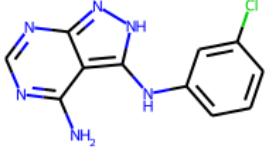
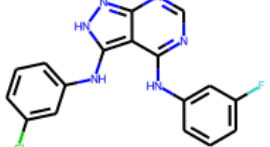
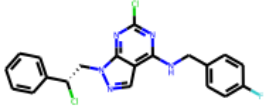
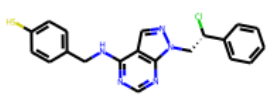
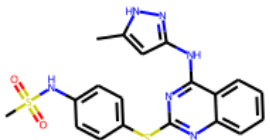
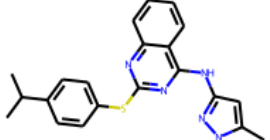
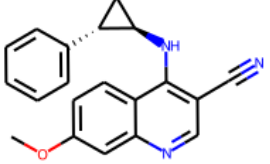
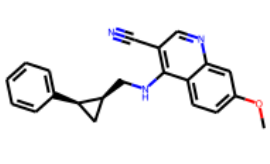
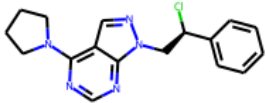
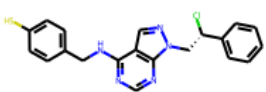
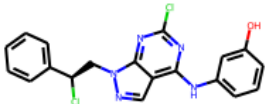
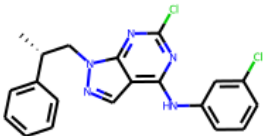
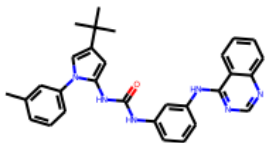
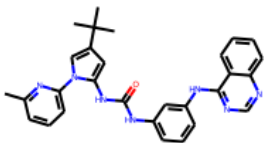
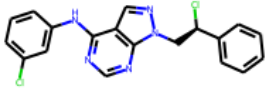
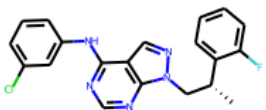


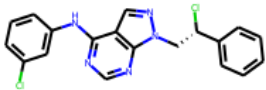
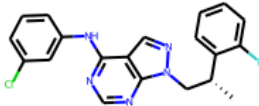
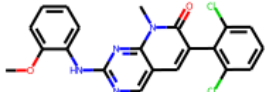
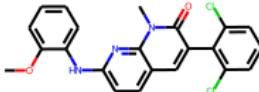
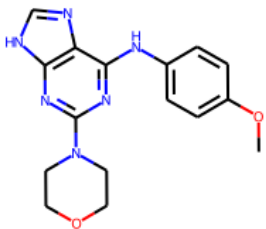
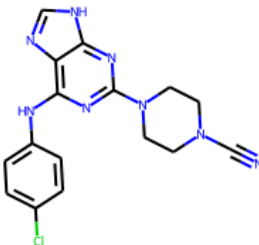
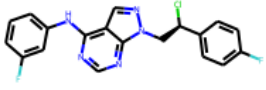
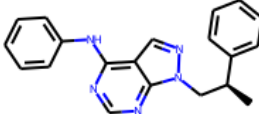
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0		[1.0]		<chem>C[S@@](=O)c1ccc(-c2nc(-c3ccnnc3)c(-c3ccc(F)cc3)[nH]2)cc1</chem>	0.709527	2.560076	2.763322	4	0.805595
1		[0.9631067961165048]		<chem>Clc1nc(Nc2cccc(Cl)c2)c2cnn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.812670	2.803140	2.415127	4	0.800810
2		[0.9525316455696202]		<chem>C[C@@H](Cn1ncc2c(Nc3ccccc3)ncnc21)c1ccccc1</chem>	0.582066	3.453236	4.511770	4	0.858060
3		[0.9335142469470827]		<chem>Fc1cccc(Nc2ncnc3n[nH]c(Nc4cccc(Cl)c4)c23)c1</chem>	0.648843	2.528773	3.556390	4	0.786036

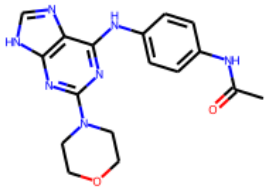
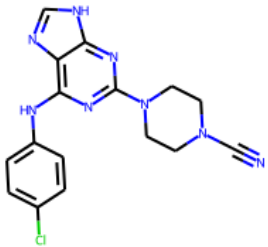
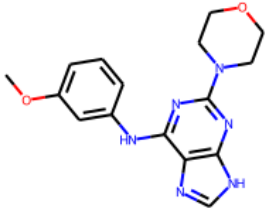
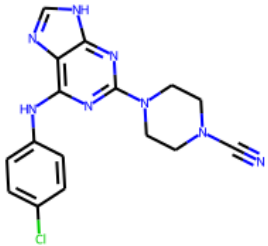
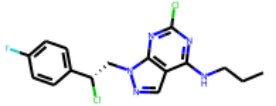
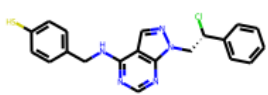
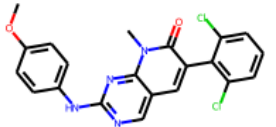
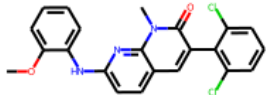
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4		[0.9122098890010091]		<chem>Sc1ccc(CNc2ncnc3c2enn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643
5		[0.9105760963026656]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
6		[0.9077901430842608]		<chem>C[S@@](=O)c1ccc(-c2nc(-c3ccccc3)c(-c3ccc(F)cc3)[nH]2)cc1</chem>	0.693247	2.498708	3.629723	4	0.800488
7		[0.9036742800397219]		<chem>Sc1ccc(CNc2ncnc3c2enn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643

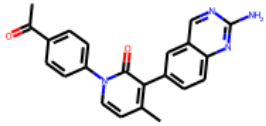
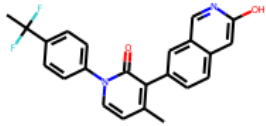
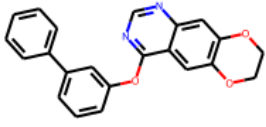
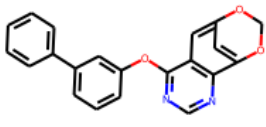
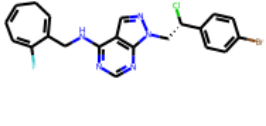
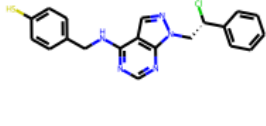
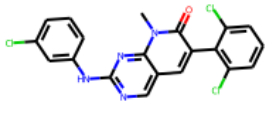
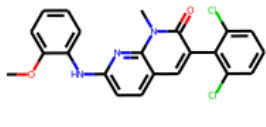
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8		[0.8751418842224744]		<chem>N#CN1CCN(c2nc(Nc3ccc(Cl)cc3)c3nc[nH]c3n2)CC1</chem>	0.582066	3.453236	4.511770	4	0.832190
9		[0.8751418842224744]		<chem>N#CN1CCN(c2nc(Nc3ccc(Cl)cc3)c3nc[nH]c3n2)CC1</chem>	0.582066	3.453236	4.511770	4	0.832190
10		[0.8729729729729729]		<chem>Clc1nc(Nc2cccc(Cl)c2)c2cnn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.812670	2.803140	2.415127	4	0.800810
11		[0.8715313463514902]		<chem>Sc1ccc(CNc2ncnc3c2cnn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643

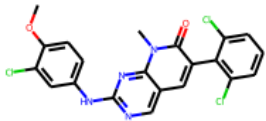
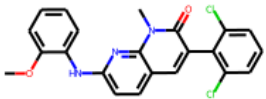
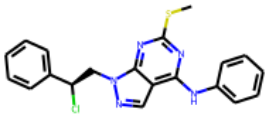
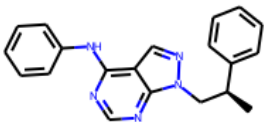
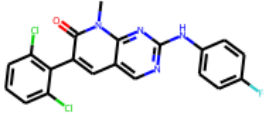
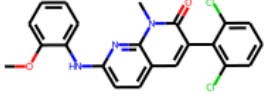
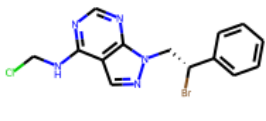
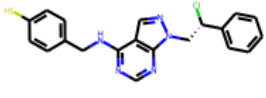
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12		[0.864314789687924]		<chem>Fc1cccc(Nc2ncnc3n[nH]c(Nc4cccc(Cl)c4)c23)c1</chem>	0.648843	2.528773	3.556390	4	0.786036
13		[0.8641975308641975]		<chem>Sc1ccc(CNc2ncnc3c2cnn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643
14		[0.8505747126436781]		<chem>C[C@@H](C)c1ccc(Sc2nc(Nc3cc(C)[nH]n3)c3ccccc3n2)cc1</chem>	0.789802	3.119093	1.773532	4	0.800611
15		[0.8269230769230769]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

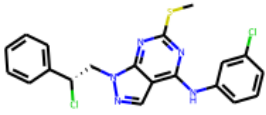
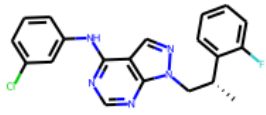
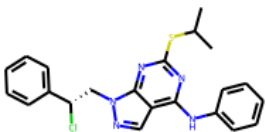
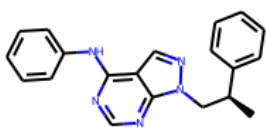
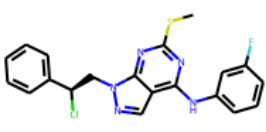
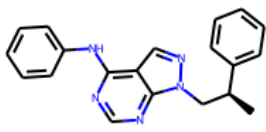
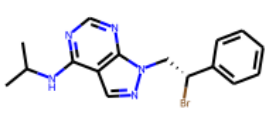
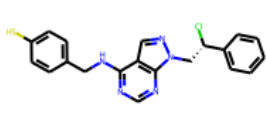
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16		[0.8228460793804453]		<chem>Sc1ccc(CNc2ncnc3c2cnn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643
17		[0.8197725284339458]		<chem>Clc1nc(Nc2cccc(Cl)c2)c2cnn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.812670	2.803140	2.415127	4	0.800810
18		[0.812254516889238]		<chem>CC(C)(C)c1cc(NC(=O)Nc2cccc(Nc3ncnc4ccccc34)c2)n(-c2cccc(C)n2)c1</chem>	0.511693	2.495788	5.669147	5	0.771803
19		[0.8091743119266055]		<chem>Clc1cccc(Nc2ncnc3c2cnn3C[C@@H](C)c2ccccc2F)c1</chem>	0.812670	2.803140	2.415127	4	0.793690

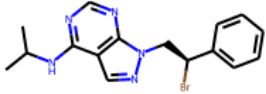
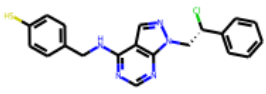
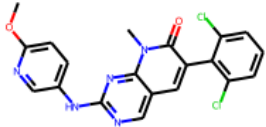
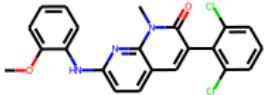
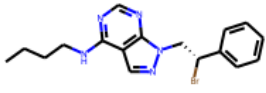
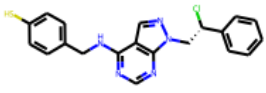
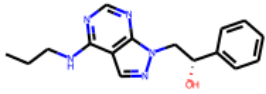
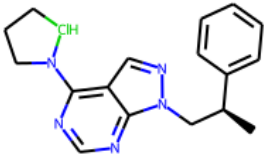
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20		[0.8091743119266055]		<chem>Clc1cccc(Nc2ncnc3c2cnn3C[C@@H](C)c2ccccc2F)c1</chem>	0.812670	2.803140	2.415127	4	0.793690
21		[0.8064257028112449]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
22		[0.8047464940668824]		<chem>N#CN1CCN(c2nc(Nc3ccc(Cl)cc3)c3nc[nH]c3n2)CC1</chem>	0.582066	3.453236	4.511770	4	0.832190
23		[0.8011527377521613]		<chem>C[C@@H](Cn1ncc2c(Nc3ccccc3)ncnc21)c1ccccc1</chem>	0.582066	3.453236	4.511770	4	0.858060

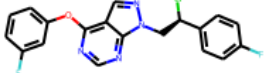
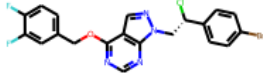
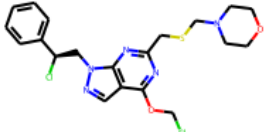
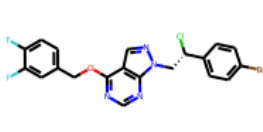
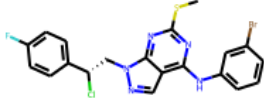
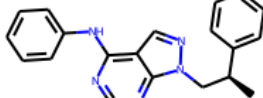
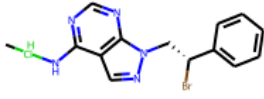
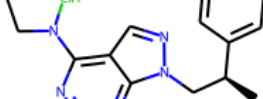
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24		[0.7972251867662753]		<chem>N#CN1CCN(c2nc(Nc3ccc(Cl)cc3)c3nc[nH]c3n2)CC1</chem>	0.582066	3.453236	4.511770	4	0.832190
25		[0.7824267782426778]		<chem>N#CN1CCN(c2nc(Nc3ccc(Cl)cc3)c3nc[nH]c3n2)CC1</chem>	0.582066	3.453236	4.511770	4	0.832190
26		[0.779707495429616]		<chem>Sc1ccc(CNc2ncnc3c2enn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643
27		[0.7676282051282052]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857

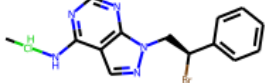
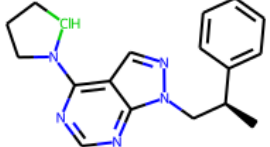
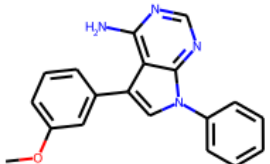
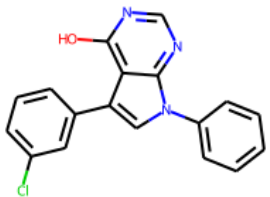
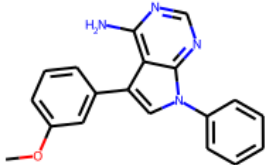
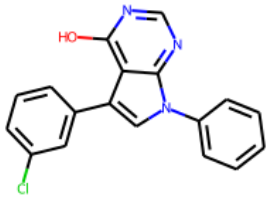
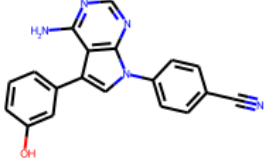
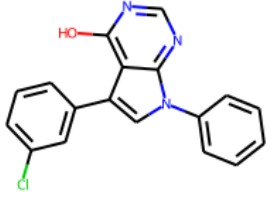
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28		[0.7672493100275989]		<chem>Cc1ccn(-c2ccc(C(C)(F)F)cc2)c(=O)c1-c1ccc2cc(O)ncc2c1</chem>	0.773249	2.760402	2.523284	4	0.781500
29		[0.764642082429501]		<chem>c1ccc(-c2ccc(Oc3ncnc4c3cc(cc34)OCO3)c2)cc1</chem>	0.582066	3.453236	4.511770	5	0.847750
30		[0.7606382978723404]		<chem>Sc1ccc(CNc2ncnc3c2enn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643
31		[0.7529880478087649]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857

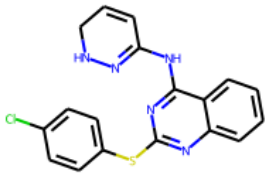
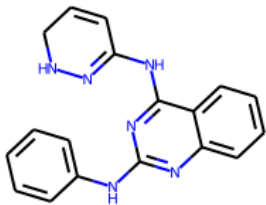
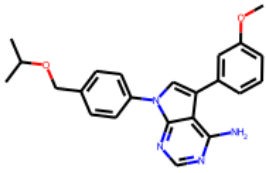
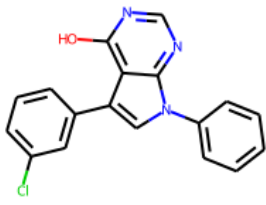
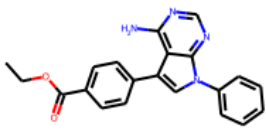
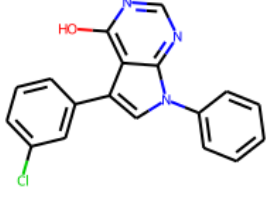
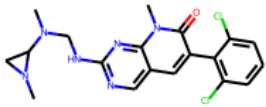
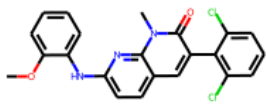
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32		[0.750388802488336]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
33		[0.7491007194244604]		<chem>C[C@@H](Cn1ncc2c(Nc3ccccc3)nnc21)c1ccccc1</chem>	0.582066	3.453236	4.511770	4	0.858060
34		[0.7468253968253968]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
35		[0.7463414634146341]		<chem>Sc1ccc(CNc2nnc3c2cnn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643

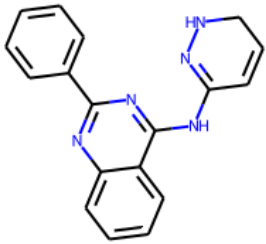
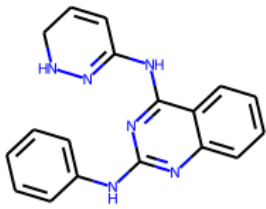
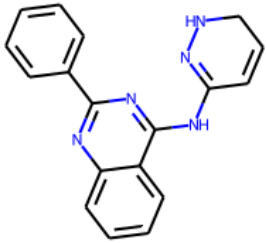
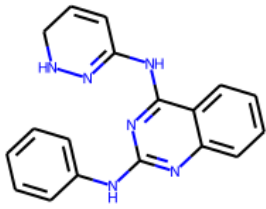
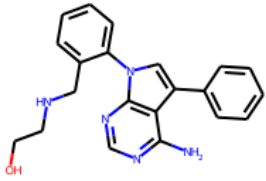
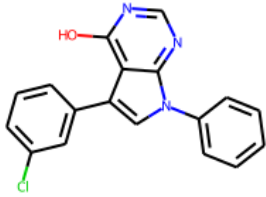
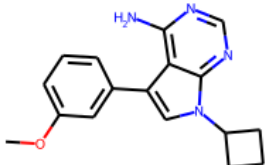
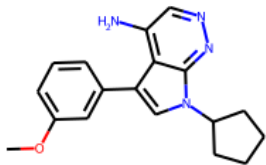
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36		[0.742714404662781]		<chem>Clc1cccc(Nc2ncnc3c2cnn3C[C@@H](C)c2ccccc2F)c1</chem>	0.812670	2.803140	2.415127	4	0.793690
37		[0.7383259911894273]		<chem>C[C@@H](Cn1ncc2c(Nc3ccccc3)nnc21)c1ccccc1</chem>	0.582066	3.453236	4.511770	4	0.858060
38		[0.7318777292576419]		<chem>C[C@@H](Cn1ncc2c(Nc3ccccc3)nnc21)c1ccccc1</chem>	0.582066	3.453236	4.511770	4	0.858060
39		[0.7289272030651341]		<chem>Sc1ccc(CNc2ncnc3c2cnn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643

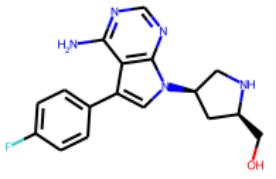
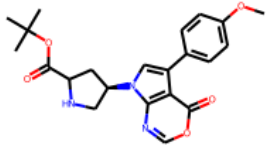
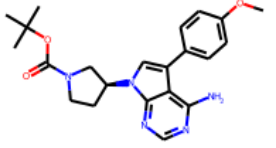
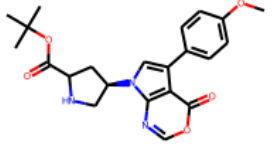
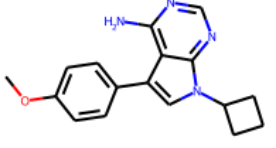
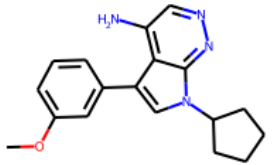
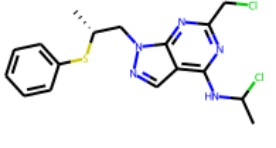
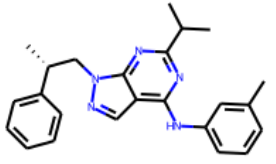
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40		[0.7289272030651341]		<chem>Sc1ccc(CNc2ncnc3c2enn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643
41		[0.7248475609756098]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
42		[0.7243346007604563]		<chem>Sc1ccc(CNc2ncnc3c2enn3C[C@H](Cl)c2ccccc2)cc1</chem>	0.773249	2.760402	2.523284	4	0.788643
43		[0.7217235188509874]		<chem>C[C@@H](Cn1ncc2c(N3CCCC13)ncnc21)c1ccccc1</chem>	0.618172	2.645624	3.611880	4	0.778794

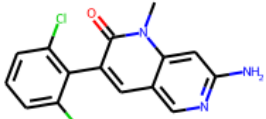
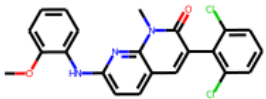
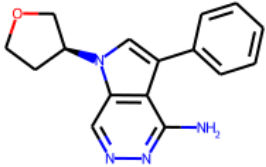
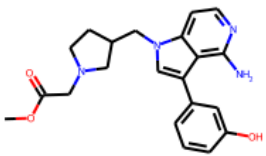
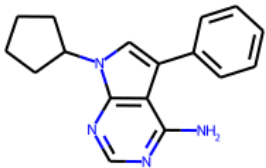
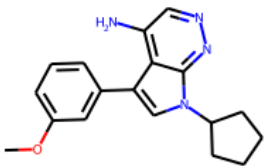
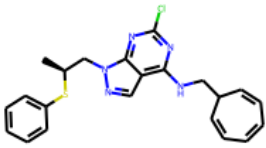
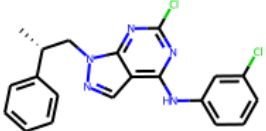
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44		[0.7177280550774526]		<chem>Fc1ccc(COc2ncnc3c2enn3C[C@H](Cl)c2ccc(Br)cc2)cc1F</chem>	0.709527	2.560076	2.763322	4	0.846183
45		[0.7112387202625102]		<chem>Fc1ccc(COc2ncnc3c2enn3C[C@H](Cl)c2ccc(Br)cc2)cc1F</chem>	0.709527	2.560076	2.763322	4	0.846183
46		[0.7097872340425532]		<chem>C[C@@H](Cn1ncc2c(Nc3ccccc3)nnc21)c1ccccc1</chem>	0.582066	3.453236	4.511770	4	0.858060
47		[0.7088607594936709]		<chem>C[C@@H](Cn1ncc2c(N3CCCCI3)nnc21)c1ccccc1</chem>	0.618172	2.645624	3.611880	4	0.778794

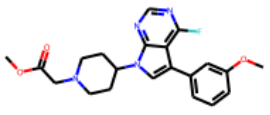
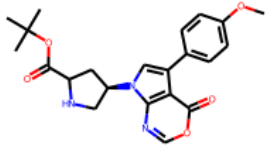
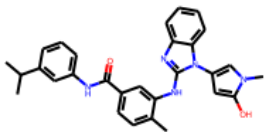
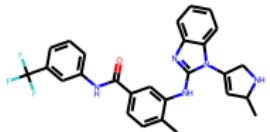
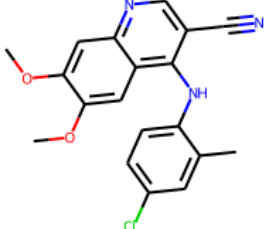
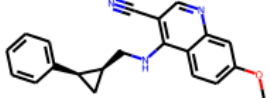
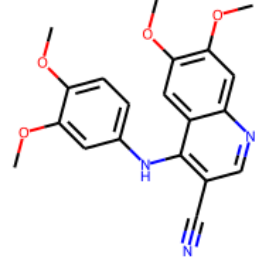
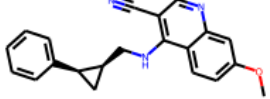
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48		[0.7088607594936709]		<chem>C[C@@H](Cn1ncc2c(N3CCCC13)nnc21)c1ccccc1</chem>	0.618172	2.645624	3.611880	4	0.778794
49		[0.7066436583261432]		<chem>Clc1cccc(-c2cn(-c3ccccc3)c3nnc(O)c23)c1</chem>	0.789759	3.120557	2.191082	4	0.824512
50		[0.7066436583261432]		<chem>Clc1cccc(-c2cn(-c3ccccc3)c3nnc(O)c23)c1</chem>	0.789759	3.120557	2.191082	4	0.824512
51		[0.7035775127768313]		<chem>Clc1cccc(-c2cn(-c3ccccc3)c3nnc(O)c23)c1</chem>	0.789759	3.120557	2.191082	4	0.824512

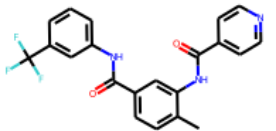
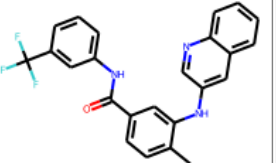
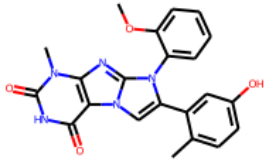
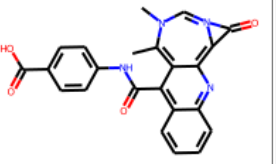
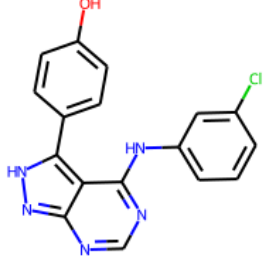
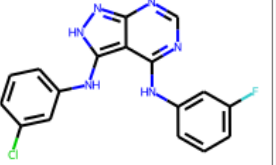
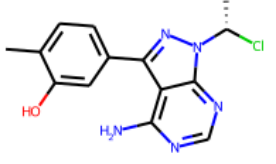
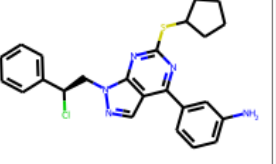
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52		[0.687]		<chem>C1ccc(Nc2nc(Nc3ccccc3)nc3ccccc23)n[nH]1</chem>	0.618172	2.645624	3.611880	4	0.818496
53		[0.6836065573770492]		<chem>Clc1cccc(-c2cn(-c3ccccc3)c3ncnc(O)c23)c1</chem>	0.789759	3.120557	2.191082	4	0.824512
54		[0.6825795644891123]		<chem>Clc1cccc(-c2cn(-c3ccccc3)c3ncnc(O)c23)c1</chem>	0.789759	3.120557	2.191082	4	0.824512
55		[0.6795162509448224]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857

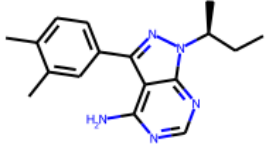
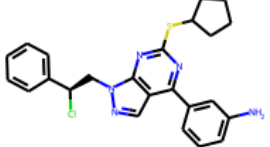
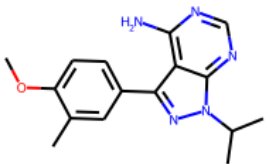
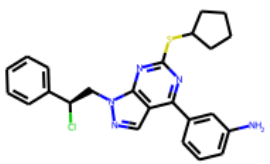
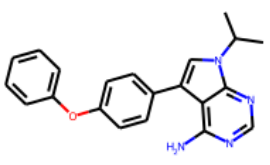
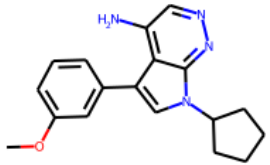
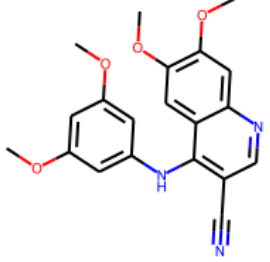
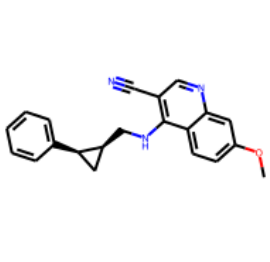
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56		[0.6730575176589304]		<chem>C1ccc(Nc2nc(Nc3ccccc3)nc3ccccc23)n[nH]1</chem>	0.618172	2.645624	3.611880	4	0.818496
57		[0.6730575176589304]		<chem>C1ccc(Nc2nc(Nc3ccccc3)nc3ccccc23)n[nH]1</chem>	0.618172	2.645624	3.611880	4	0.818496
58		[0.6618819776714514]		<chem>Clc1cccc(-c2cn(-c3ccccc3)c3nnc(O)c23)c1</chem>	0.789759	3.120557	2.191082	4	0.824512
59		[0.6614420062695925]		<chem>COc1cccc(-c2cn(C3CCCC3)c3nnc(N)c23)c1</chem>	0.618172	2.645624	3.611880	4	0.828369

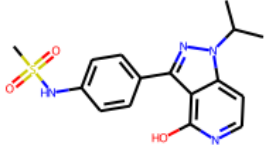
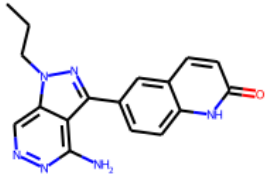
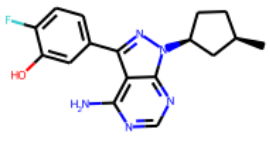
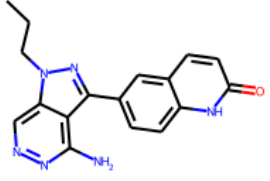
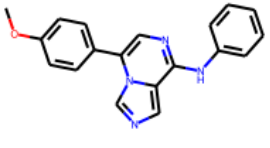
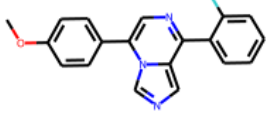
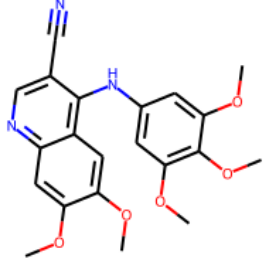
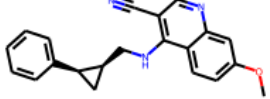
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60		[0.6448345712356516]		<chem>COc1ccc(-c2cn([C@H]3CNC(C(=O)OC(C)(C)C)C3)c3ncoc(=O)c23)cc1</chem>	0.709527	2.560076	2.763322	4	0.791833
61		[0.634527687296417]		<chem>COc1ccc(-c2cn([C@H]3CNC(C(=O)OC(C)(C)C)C3)c3ncoc(=O)c23)cc1</chem>	0.709527	2.560076	2.763322	4	0.791833
62		[0.6310452418096724]		<chem>COc1cccc(-c2cn(C3CCCC3)c3ncc(N)c23)c1</chem>	0.618172	2.645624	3.611880	4	0.828369
63		[0.6270523846755277]		<chem>CC(C)c1nc(Nc2cccc(C)c2)c2cnn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.582066	3.453236	4.511770	4	0.771524

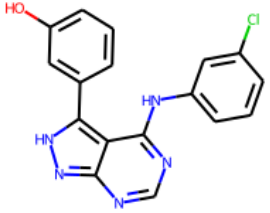
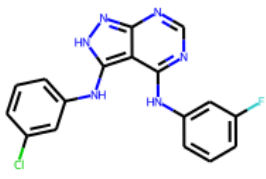
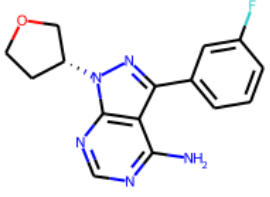
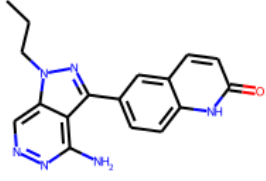
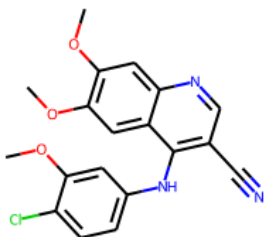
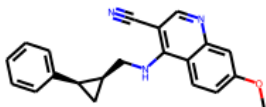
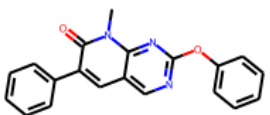
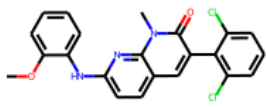
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64		[0.6256938937351308]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
65		[0.6236559139784946]		<chem>COC(=O)CN1CC(Cn2cc(-c3cccc(O)c3)c3c(N)nccc32)CC1</chem>	0.582066	3.453236	4.511770	4	0.822500
66		[0.6208791208791209]		<chem>COc1cccc(-c2cn(C3CCCC3)c3nccc(N)c23)c1</chem>	0.618172	2.645624	3.611880	4	0.828369
67		[0.6201427438540841]		<chem>Clc1nc(Nc2cccc(Cl)c2)c2cnn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.812670	2.803140	2.415127	4	0.800810

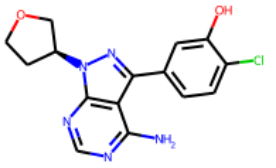
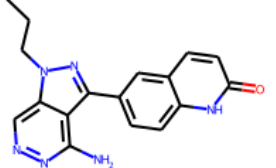

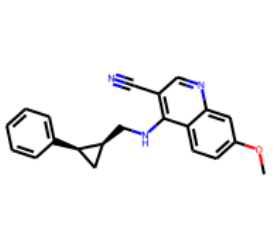
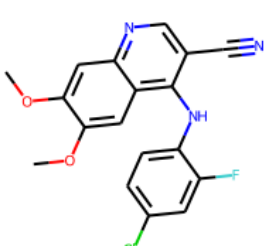
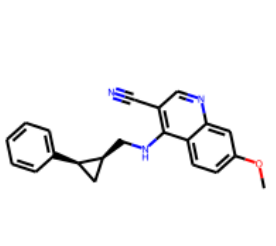
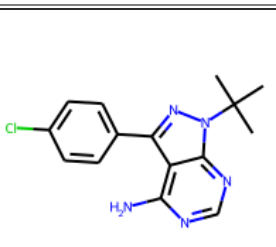
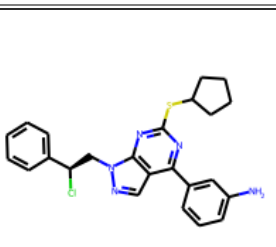
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68		[0.59734219269103]		<chem>COc1ccc(-c2cn([C@H]3CNC(C(=O)OC(C)(C)C)C3)c3ncoc(=O)c23)cc1</chem>	0.709527	2.560076	2.763322	4	0.791833
69		[0.5907894736842105]		<chem>Cc1ccc(C(=O)Nc2cccc(C(F)(F)F)c2)cc1Nc1nc2cccc2n1-c1CNC(C)c1</chem>	0.837081	4.329537	2.430174	5	0.773214
70		[0.582089552238806]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
71		[0.5786993402450519]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

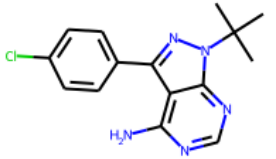
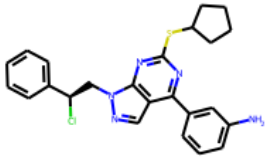
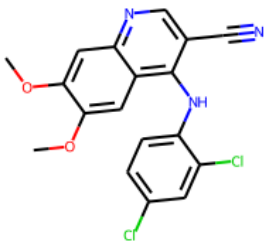
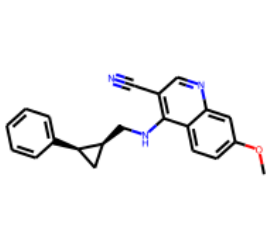
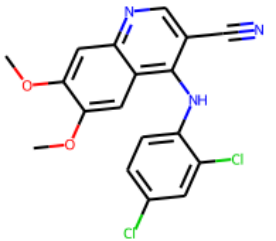
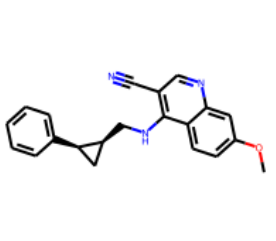
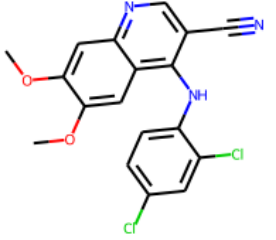
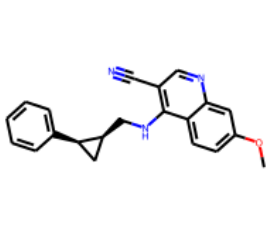
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72		[0.5786314525810324]		<chem>Cc1ccc(C(=O)Nc2cccc(C(F)(F)F)c2)cc1Nc1cc2ccccc2nc1</chem>	0.801881	4.739956	1.893492	4	0.736596
73		[0.5759625390218522]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
74		[0.5752636625119847]		<chem>Fc1cccc(Nc2ncnc3n[nH]c(Nc4cccc(Cl)c4)c23)c1</chem>	0.648843	2.528773	3.556390	4	0.786036
75		[0.5751724137931035]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611

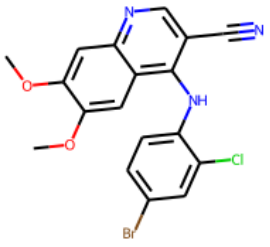
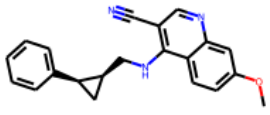
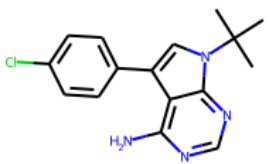
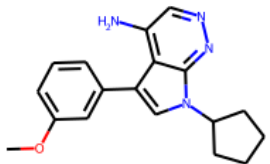
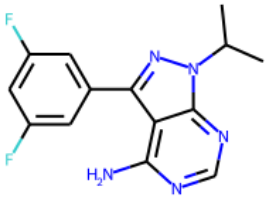
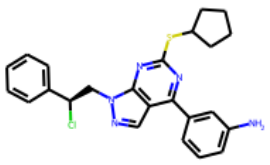
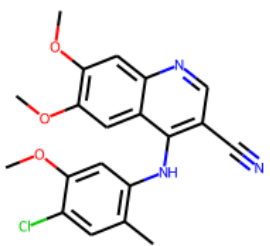
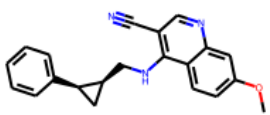
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76		[0.5750174459176552]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
77		[0.5745276417074877]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
78		[0.5737451737451738]		<chem>COc1cccc(-c2cn(C3CCCC3)c3nccc(N)c23)c1</chem>	0.618172	2.645624	3.611880	4	0.828369
79		[0.5727611940298507]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

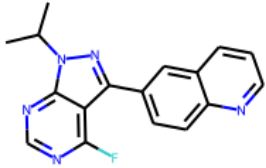
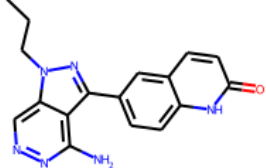
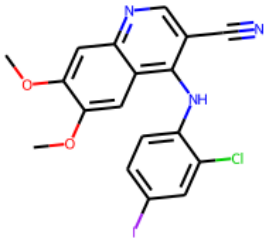
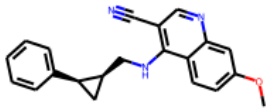
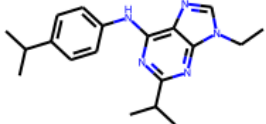
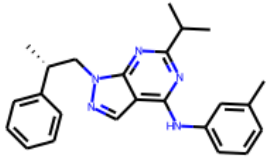
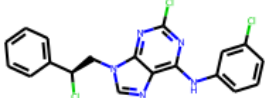
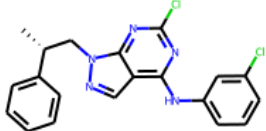
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80		[0.5720620842572062]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891
81		[0.5718270571827058]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891
82		[0.5711592836946278]		<chem>COc1ccc(-c2enc(-c3ccccc3F)c3cnen23)cc1</chem>	0.836239	3.357318	2.011011	4	0.800881
83		[0.5710332103321033]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

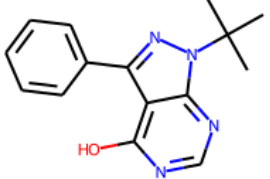
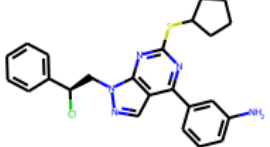
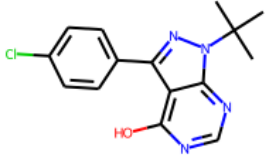
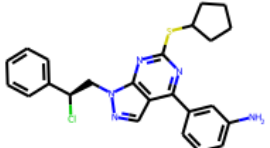
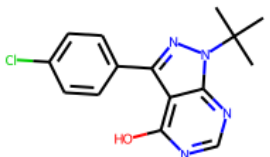
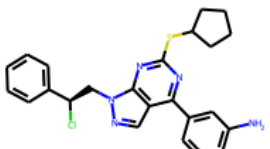
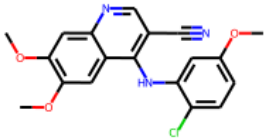
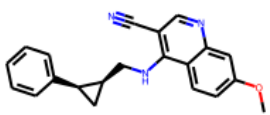
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84		[0.568738229755179]		<chem>Fc1cccc(Nc2ncnc3n[nH]c(Nc4cccc(Cl)c4)c23)c1</chem>	0.648843	2.528773	3.556390	4	0.786036
85		[0.5677731673582296]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891
86		[0.5652173913043478]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)enc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
87		[0.5645896656534954]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857

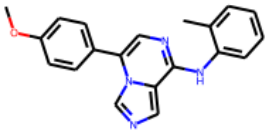
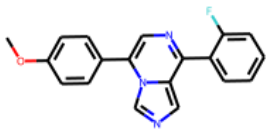
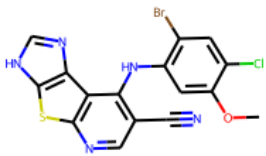
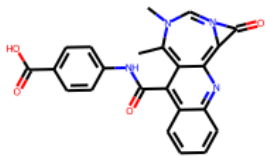
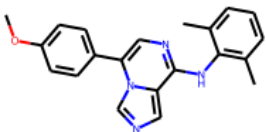
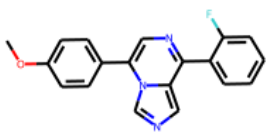
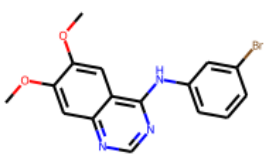
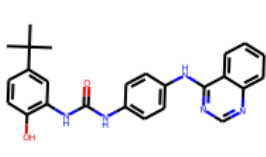
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88		[0.563858695652174]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891
89		[0.5630550621669627]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
90		[0.5626666666666666]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
91		[0.5624548736462094]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611

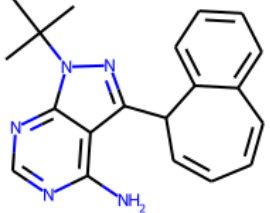
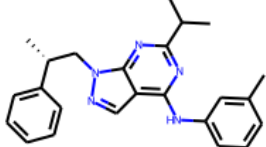
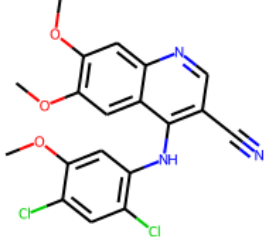
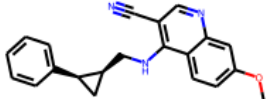
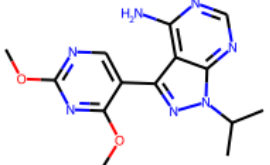
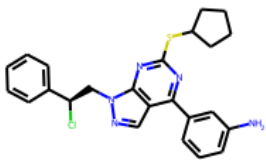
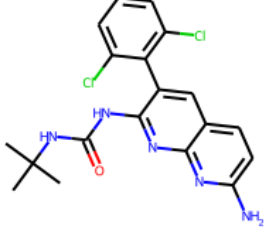
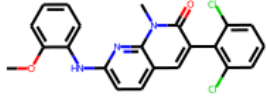
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92		[0.5624548736462094]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2nn3C[C@@H](Cl)c2cccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
93		[0.5609756097560976]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
94		[0.5609756097560976]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
95		[0.5609756097560976]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

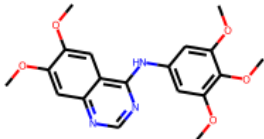
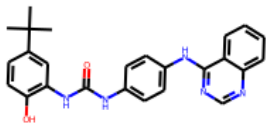
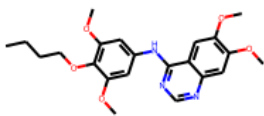
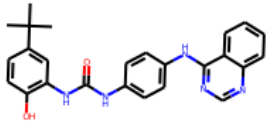
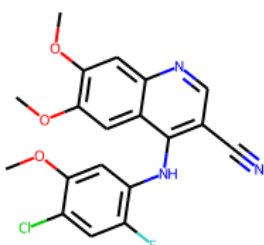
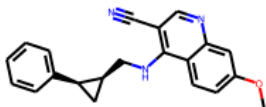
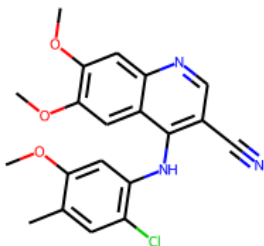
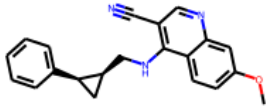
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96		[0.560888888888889]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
97		[0.5604311008468053]		<chem>COc1cccc(-c2cn(C3CCCC3)c3ncc(N)c23)c1</chem>	0.618172	2.645624	3.611880	4	0.828369
98		[0.5578571428571428]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
99		[0.5572052401746724]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

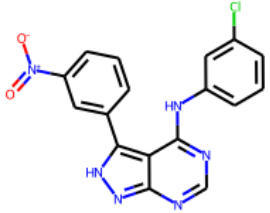
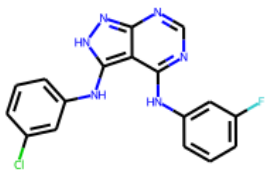
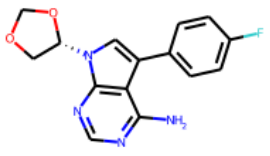
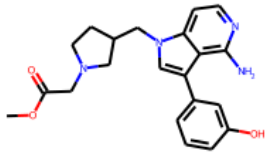
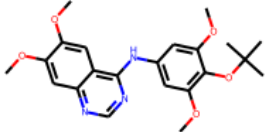
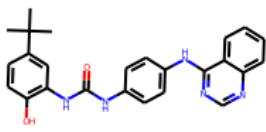
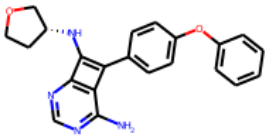
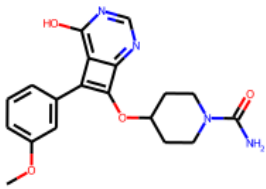
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100		[0.5553956834532374]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891
101		[0.5546666666666666]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
102		[0.5541158536585366]		<chem>CC(C)c1nc(Nc2cccc(C)c2)c2cnn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.582066	3.453236	4.511770	4	0.771524
103		[0.5540641312453393]		<chem>Clc1nc(Nc2cccc(Cl)c2)c2cnn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.812670	2.803140	2.415127	4	0.800810

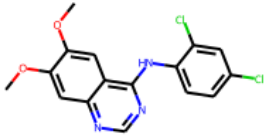
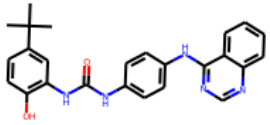
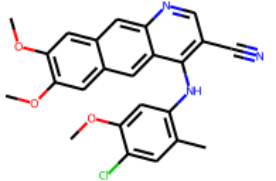
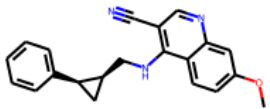
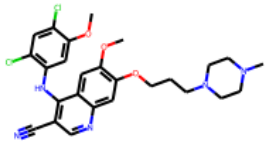
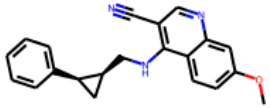
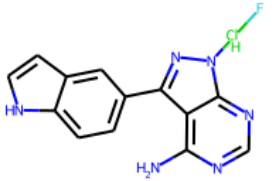
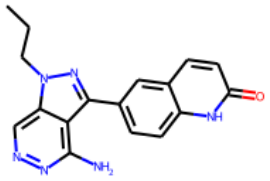
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104		[0.55394641564084]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
105		[0.5538132573057734]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
106		[0.5538132573057734]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
107		[0.5517241379310345]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

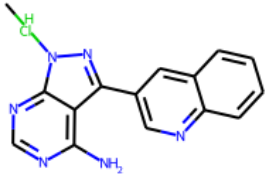
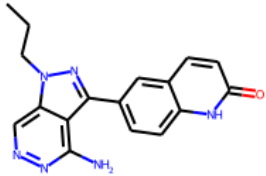
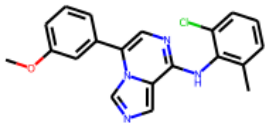
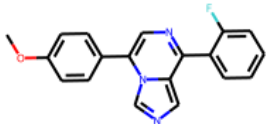
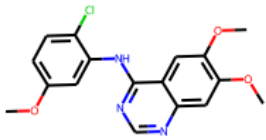
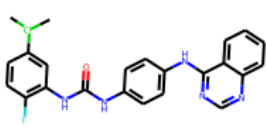
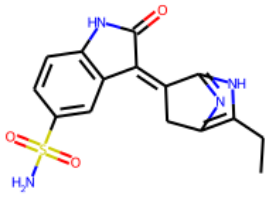
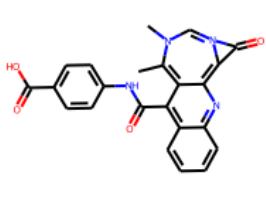
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108		[0.5497335701598579]		<chem>COc1ccc(-c2enc(-c3ccccc3F)c3cnen23)cc1</chem>	0.836239	3.357318	2.011011	4	0.800881
109		[0.5487012987012987]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
110		[0.5485008818342152]		<chem>COc1ccc(-c2enc(-c3ccccc3F)c3cnen23)cc1</chem>	0.836239	3.357318	2.011011	4	0.800881
111		[0.5482587064676617]		<chem>CC(C)(C)c1cc(NC(=O)Nc2ccc(Nc3ncnc4ccccc34)cc2)c(O)cc1</chem>	0.718099	4.269790	-0.023583	4	0.763474

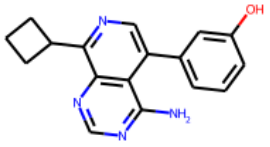
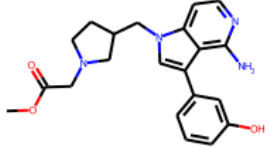
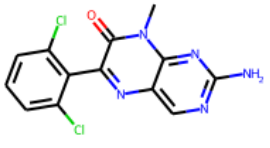
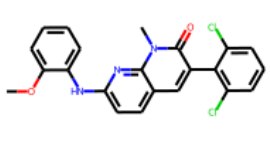
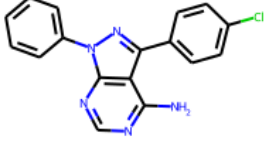
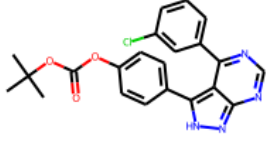
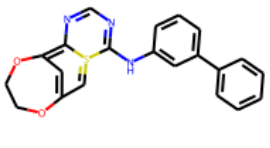
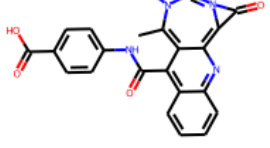
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112		[0.5470588235294118]		<chem>CC(C)c1nc(Nc2cccc(C)c2)c2enn(C[C@@H](C)c3ccccc3)c2n1</chem>	0.582066	3.453236	4.511770	4	0.771524
113		[0.5459227467811159]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)enc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
114		[0.5431773236651285]		<chem>Nc1cccc(-c2nc(SC3CCCC3)nc3c2cnn3C[C@@H](Cl)c2ccccc2)c1</chem>	0.693247	2.498708	3.629723	5	0.805611
115		[0.5430711610486891]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857

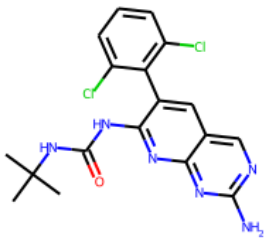
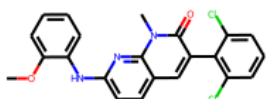
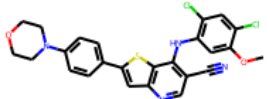
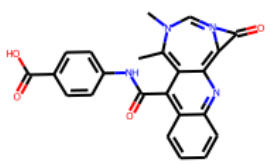
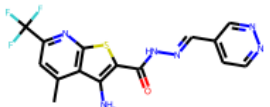
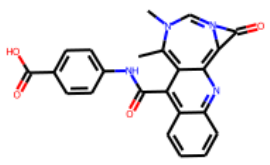
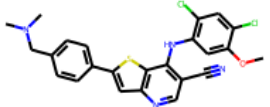
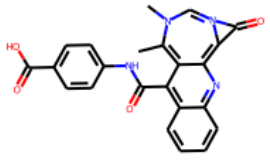
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116		[0.5412221144519883]		<chem>CC(C)(C)c1cc(NC(=O)Nc2ccc(Nc3ncnc4ccccc34)cc2)c(O)cc1</chem>	0.718099	4.269790	-0.023583	4	0.763474
117		[0.5409219190968956]		<chem>CC(C)(C)c1cc(NC(=O)Nc2ccc(Nc3ncnc4ccccc34)cc2)c(O)cc1</chem>	0.718099	4.269790	-0.023583	4	0.763474
118		[0.540133779264214]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
119		[0.5398981324278438]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

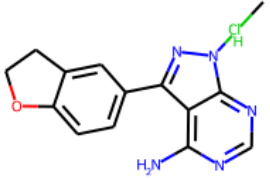

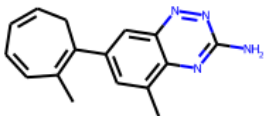
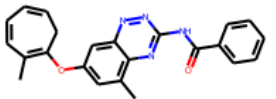
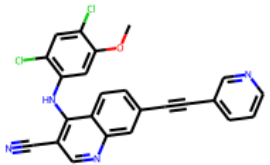
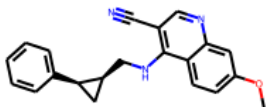
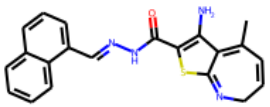
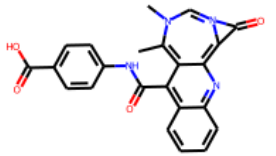
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120		[0.5394853593611357]		<chem>Fc1cccc(Nc2ncnc3n[nH]c(Nc4cccc(Cl)c4)c23)c1</chem>	0.648843	2.528773	3.556390	4	0.786036
121		[0.5391737891737892]		<chem>COC(=O)CN1CC(Cn2cc(-c3cccc(O)c3)c3c(N)nccc32)CC1</chem>	0.582066	3.453236	4.511770	4	0.822500
122		[0.5380997177798683]		<chem>CC(C)(C)c1cc(NC(=O)Nc2ccc(Nc3ncnc4cccc34)cc2)c(O)cc1</chem>	0.718099	4.269790	-0.023583	4	0.763474
123		[0.5364751452550033]		<chem>COc1cccc(-c2c(O[C@H]3CCN(C(N)=O)CC3)c3ncnc(O)c32)c1</chem>	0.528532	2.861050	5.353921	4	0.767083

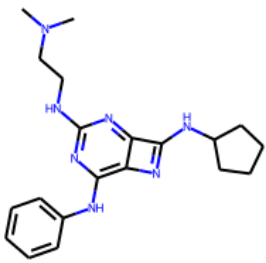
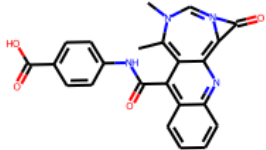
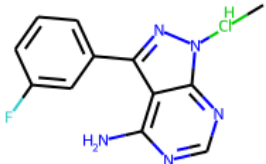
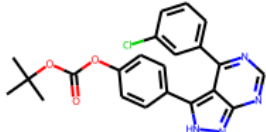
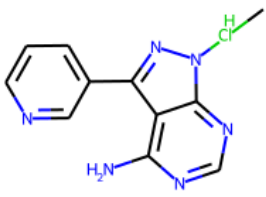
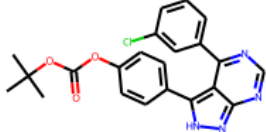
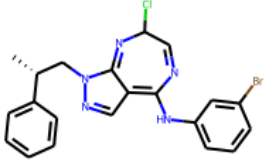
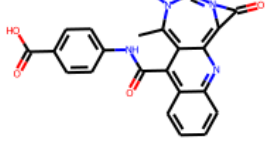
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124		[0.5336538461538461]		<chem>CC(C)(C)c1cc(NC(=O)Nc2ccc(Nc3ncnc4ccccc34)cc2)c(O)cc1</chem>	0.718099	4.269790	-0.023583	4	0.763474
125		[0.529567519858782]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)enc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
126		[0.5278900565885206]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)enc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
127		[0.5267341040462428]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891

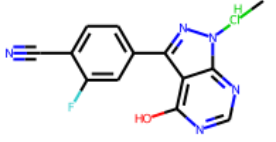
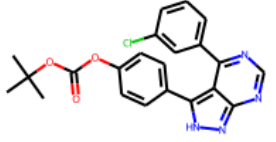
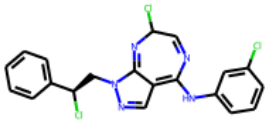
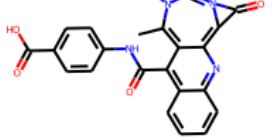
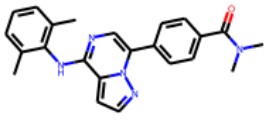
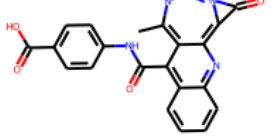
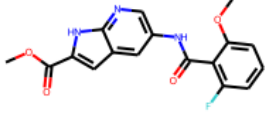
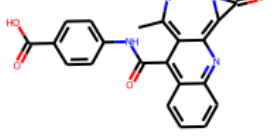
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128		[0.5263157894736842]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891
129		[0.5255354200988468]		<chem>COc1ccc(-c2cnc(-c3ccccc3F)c3cncn23)cc1</chem>	0.836239	3.357318	2.011011	4	0.800881
130		[0.5247895229186156]		<chem>Cl(C)(C)c1cc(NC(=O)Nc2ccc(Nc3ncnc4ccccc34)cc2)c(F)cc1</chem>	0.802754	4.453978	1.994952	4	0.757125
131		[0.5245641838351822]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

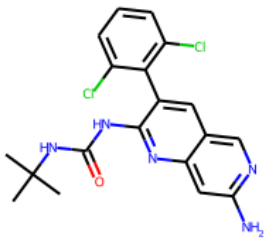
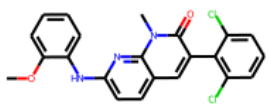
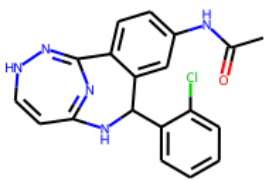
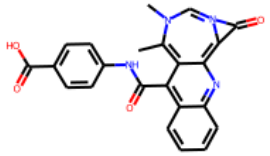
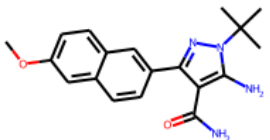
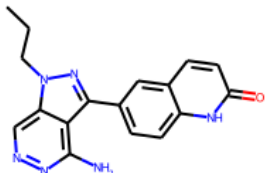
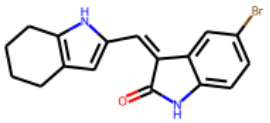
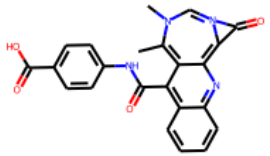
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132		[0.5220913107511046]		<chem>COC(=O)CN1CC(Cn2cc(-c3ccccc(O)c3)c3c(N)nccc32)CC1</chem>	0.582066	3.453236	4.511770	4	0.822500
133		[0.5215243472124206]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
134		[0.5202808112324493]		<chem>CC(C)(C)OC(=O)Oc1ccc(-c2[nH]nc3ncnc(-c4cccc(Cl)c4)c23)cc1</chem>	0.821471	2.730201	2.924359	4	0.823833
135		[0.5196078431372549]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

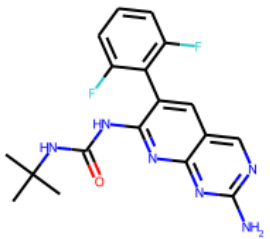
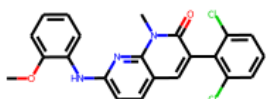
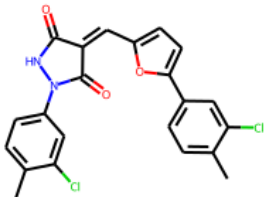
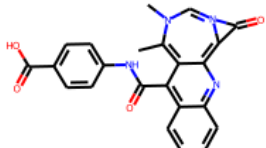
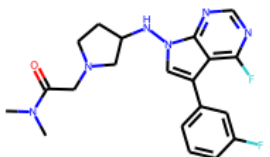
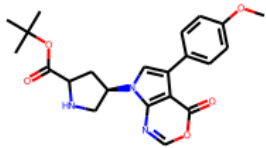

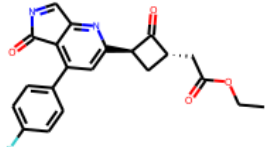
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136		[0.5194805194805194]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
137		[0.5179240235420011]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
138		[0.5161821173889194]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
139		[0.5140237324703344]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

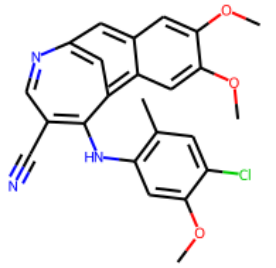
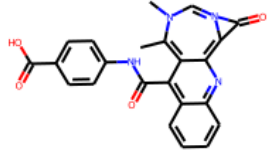
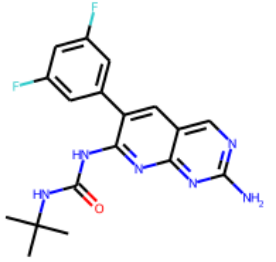
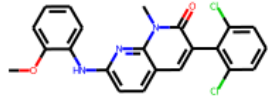
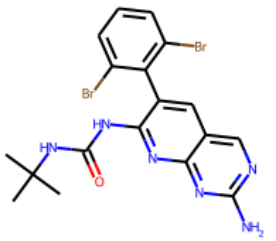
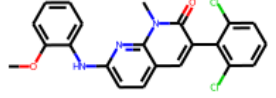
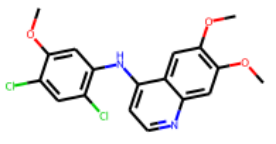
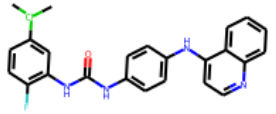
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140		[0.5136157337367625]		<chem>CC(C)(C)OC(=O)Oc1ccc(-c2[nH]nc3ncnc(-c4cccc(Cl)c4)c23)cc1</chem>	0.821471	2.730201	2.924359	4	0.823833
141		[0.5082508250825083]		<chem>C1ccccc(C)c1Oc1cc(C)c2nc(NC(=O)c3ccccc3)nnc2c1</chem>	0.693247	2.498708	3.629723	4	0.794857
142		[0.4991624790619765]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969
143		[0.4991587212563096]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

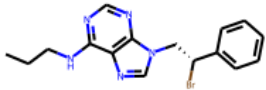
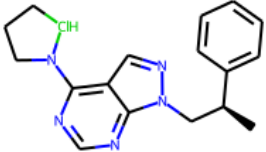
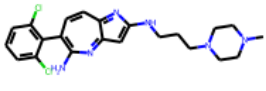
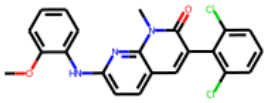
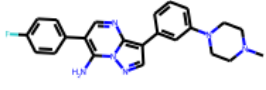
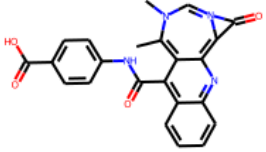
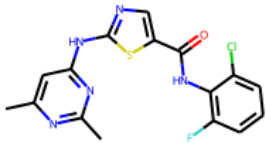
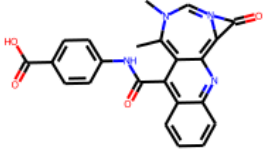
	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
144		[0.49305169538632576]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
145		[0.49029126213592233]		<chem>CC(C)(C)OC(=O)Oc1ccc(-c2[nH]nc3ncnc(-c4cccc(Cl)c4)c23)cc1</chem>	0.821471	2.730201	2.924359	4	0.823833
146		[0.4859887910328263]		<chem>CC(C)(C)OC(=O)Oc1ccc(-c2[nH]nc3ncnc(-c4cccc(Cl)c4)c23)cc1</chem>	0.821471	2.730201	2.924359	4	0.823833
147		[0.48321408915795266]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

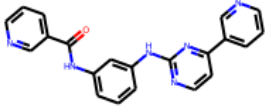
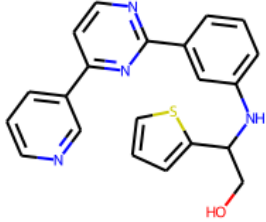
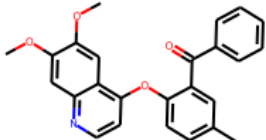
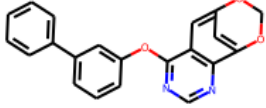
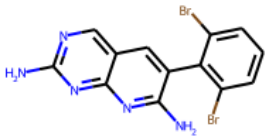
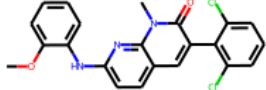
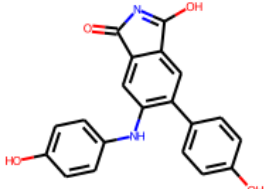
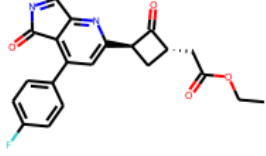
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148		[0.4821981424148607]		<chem>CC(C)(C)OC(=O)Oc1ccc(-c2[nH]nc3ncnc(-c4cccc(Cl)c4)c23)cc1</chem>	0.821471	2.730201	2.924359	4	0.823833
149		[0.4817880794701987]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
150		[0.4811946902654867]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
151		[0.480113636363635]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

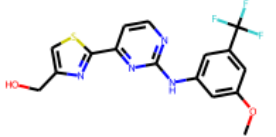
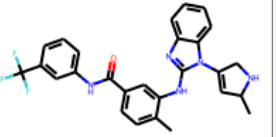
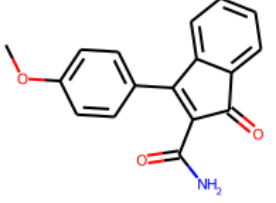
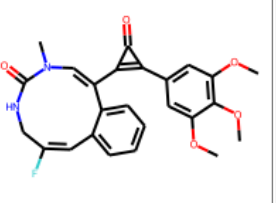
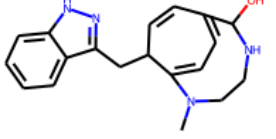
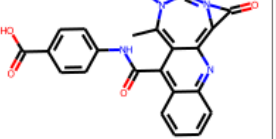
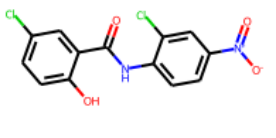
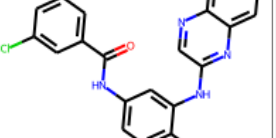
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152		[0.47988505747126436]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
153		[0.4714285714285714]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
154		[0.47091800981079185]		<chem>C(CC)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)nncc21</chem>	0.518739	2.583386	5.711228	4	0.891891
155		[0.4668141592920354]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

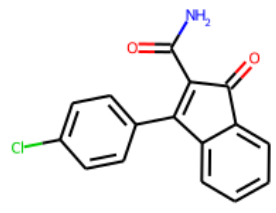
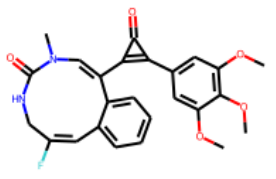
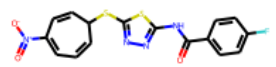
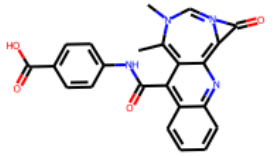
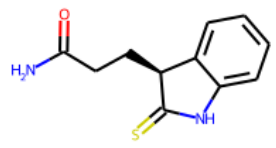
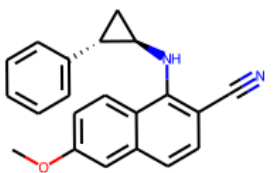
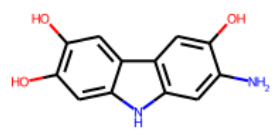
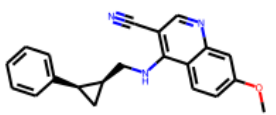
	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
156		[0.4626038781163435]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
157		[0.46102819237147596]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
158		[0.46092307692307694]		<chem>COc1ccc(-c2cn([C@H]3CNC(C(=O)OC(C)(C)C)C3)c3ncoc(=O)c23)cc1</chem>	0.709527	2.560076	2.763322	4	0.791833
159		[0.45710627400768244]		<chem>CCOC(=O)C[C@@H]1C[C@@H](c2cc(-c3ccc(F)cc3)c3c(=O)ncc3n2)C1=O</chem>	0.814616	2.897929	3.830811	4	0.733397

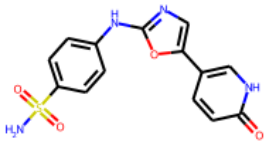
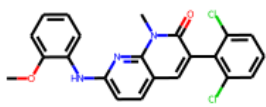
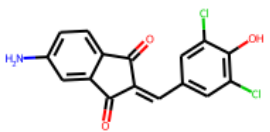
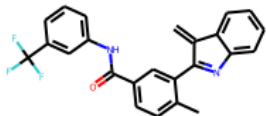
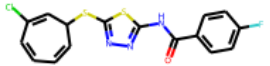
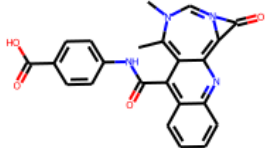
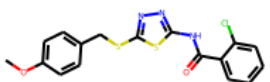
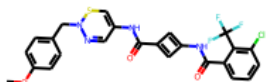
	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
160		[0.45419211549139366]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
161		[0.45396600566572237]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
162		[0.4515905947441217]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
163		[0.4500998003992016]		<chem>Cl(C)(C)c1cc(NC(=O)Nc2ccc(Nc3ccnc4ccccc34)cc2)c(F)cc1</chem>	0.522453	2.355392	5.398832	4	0.845766

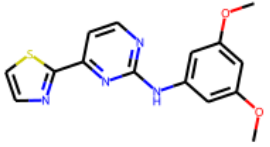
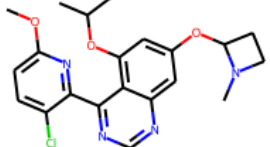
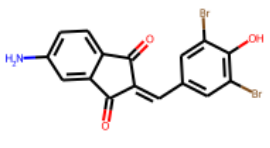
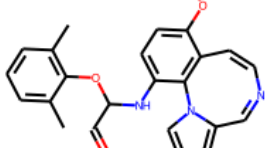
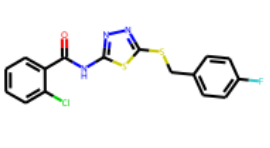
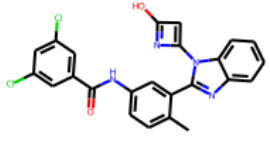
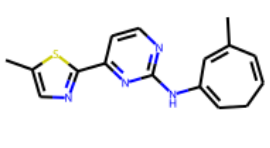
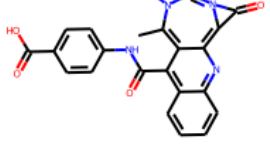
	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
164		[0.4477498093058734]		<chem>C[C@@H](Cn1ncc2c(N3CCCC13)nnc21)c1ccccc1</chem>	0.618172	2.645624	3.611880	4	0.778794
165		[0.44202389318341534]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
166		[0.43993231810490696]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
167		[0.43495475113122173]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

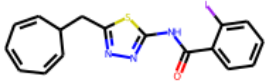
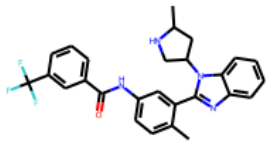
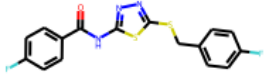
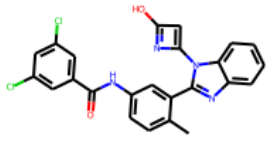
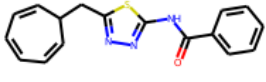
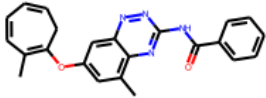
	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
168		[0.43478260869565216]		<chem>OCC(Nc1cccc(/c2nccc(-c3ccnc3)n2)c1)c1cccs1</chem>	0.582066	3.453236	4.511770	4	0.869905
169		[0.4338807260155575]		<chem>c1ccc(-c2cccc(Oc3ncnc4c3cc(cc34)OCO3)c2)cc1</chem>	0.582066	3.453236	4.511770	5	0.847750
170		[0.4214939024390244]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
171		[0.4146825396825397]		<chem>CCOC(=O)C[C@@H]1C[C@@H](c2cc(-c3ccc(F)cc3)c3c(=O)ncc3n2)C1=O</chem>	0.814616	2.897929	3.830811	4	0.733397

	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
172		[0.4095052083333333]		<chem>Cc1ccc(C(=O)Nc2cccc(C(F)(F)F)c2)cc1Nc1nc2ccccc2n1-c1CNC(C)c1</chem>	0.837081	4.329537	2.430174	5	0.773214
173		[0.40523338048090524]		<chem>COc1cc(C2=C(c3cn(C(=O)NCc(F)cc4ccccc43)C)C2=O)cc(OC)c1OC</chem>	0.618172	2.645624	3.611880	4	0.774782
174		[0.4028011204481793]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
175		[0.39980059820538383]		<chem>Cc1ccc(NC(=O)c2cc(Cl)cc(Cl)c2)cc1Nc1nc2ccccc2nc1</chem>	0.520232	2.229788	3.986566	4	0.818238

	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
176		[0.39151943462897526]		<chem>COc1cc(C2=C(c3cn(C(=O)NCc(F)cc4ccccc43)C)C2=O)cc(OC)c1OC</chem>	0.618172	2.645624	3.611880	4	0.774782
177		[0.3749271137026239]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
178		[0.369281045751634]		<chem>COc1ccc2c(N[C@@H]3C[C@H]3c3ccccc3)c(C#N)ccc2c1</chem>	0.693247	2.498708	3.629723	4	0.772905
179		[0.3687031082529475]		<chem>COc1ccc2c(NC[C@H]3C[C@H]3c3ccccc3)c(C#N)cnc2c1</chem>	0.709527	2.560076	2.763322	4	0.790969

	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
180		[0.36623748211731044]		<chem>COc1ccccc1Nc1ccc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1</chem>	0.773249	2.760402	2.523284	4	0.821857
181		[0.3437738731856379]		<chem>Cc1ccc(C(=O)Nc2cccc(C(F)(F)F)c2)cc1-c1nc2ccccc2c1=C</chem>	0.814616	2.897929	3.830811	4	0.746365
182		[0.3431603773584906]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357
183		[0.3431516936671576]		<chem>COc1ccc(Cn2ncc(NC(=O)c3cc(NC(=O)c4cccc(Cl)c4C(F)(F)F)c3)cs2)cc1</chem>	0.814616	2.897929	3.830811	4	0.744310

	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
184		[0.34279475982532753]		<chem>COc1ccc(Cl)c(-c2ncnc3cc(OC(N4C)CC4)cc(OC(C)C)c23)n1</chem>	0.710142	2.759610	3.436126	4	0.773833
185		[0.3385345997286296]		<chem>COc1ccc(NC(C=O)Oc2c(C)cccc2C)c2c1ccncc1ccn12</chem>	0.563628	3.441104	4.745130	4	0.822733
186		[0.33811475409836067]		<chem>Cc1ccc(NC(=O)c2cc(Cl)cc(Cl)c2)cc1-c1nc2ccccc2n1-c1cc(O)n1</chem>	0.821471	2.730201	2.924359	5	0.800890
187		[0.3367756741250717]		<chem>Cn1c(C)c2c(C(=O)Nc3ccc(C(=O)O)cc3)c3ccccc3nc2c2C(=O)n2=C1</chem>	0.563628	3.441104	4.745130	5	0.732357

	src known mol	similarity	mol	smiles	qed	logP	SAS	rings	kinase inhibition likelihood
188		[0.32419465387251545]		<chem>Cc1ccc(NC(=O)c2cccc(C(F)(F)F)c2)cc1-c1nc2ccccc2n1-c1CNC(C)C1</chem>	0.814616	2.897929	3.830811	5	0.804286
189		[0.3068340306834031]		<chem>Cc1ccc(NC(=O)c2cc(Cl)cc(Cl)c2)cc1-c1nc2ccccc2n1-c1cc(O)n1</chem>	0.821471	2.730201	2.924359	5	0.800890
190		[0.3055555555555556]		<chem>C1ccccc(C)c1Oc1cc(C)c2nc(NC(=O)c3ccccc3)nnc2c1</chem>	0.693247	2.498708	3.629723	4	0.794857