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Supplementary

New Crystal Forms for Biologically Active Compounds. Part 2: Anastrozole as N-substituted 1,2,4-Triazole in Halogen Bonding and Lp-π Interactions with 1,4-Diiodotetrafluorobenzene

Mariya A. Kryukova, Alexander V. Sapegin, Alexander S. Novikov, Mikhail Krasavin and Daniil M. Ivanov *

Saint Petersburg State University, Institute of Chemistry, Universitetskaya Nab. 7/9, Saint Petersburg 199034, Russian Federation; mary_kryukova@mail.ru (M.A.K.); sapegin_yar@mail.ru (A.V.S.); ja2-88@mail.ru (A.S.N.); krasavintm@gmail.com (M.K.)

* Correspondence: st024644@student.spbu.ru

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Table S1. Parameters of the C–I···N XBs including 1,2,4-triazole moiety in CCDC structures.

Structure	Doi	*d*(I···N), Å	∠(C–I···N), °	Motif
CUJGEV	10.1016/j.tetlet.2015.07.006	3.162(4)	175.04(17)	***d***
FALNEN	10.1039/c1ce05577a	3.372(4)	157.18(17)	***b***
FARCIN	10.1002/slct.201600644	3.210(8)	173.6(2)	***c***
FARCIN01	10.1039/c7nj02034a	3.210(8)	173.6(2)	***c***
LEFROF	10.1107/S160053681203139X	3.085(5)	173.91(12)	***e***
MIXWUN	10.1016/j.cclet.2013.05.010	2.839(4)	175.89(15)	***d***
		2.844(4)	165.74(17)	
		2.918(5)	174.51(17)	
NEWGON	10.1016/j.jfluchem.2013.01.025	3.378(3)	172.15(11)	***d***
		3.365(3)	159.60(11)	
NEWGUT	10.1016/j.jfluchem.2013.01.025	3.224(4)	167.1(5)	***d***
		3.224(4)	159.4(7)	
OYOHER	10.1021/acs.jmedchem.6b00849	3.1321(19)	177.57(8)	***c***
		3.122(2)	176.08(7)	
SUKNUJ	10.1016/j.bmc.2015.08.031	3.020(4)	166.52(12)	***a***
SUKPAR	10.1016/j.bmc.2015.08.031	3.062(4)	173.74(14)	***e***
UMOTOG	10.1016/j.ica.2010.12.038	3.294(4)	158.38(14)	***b***

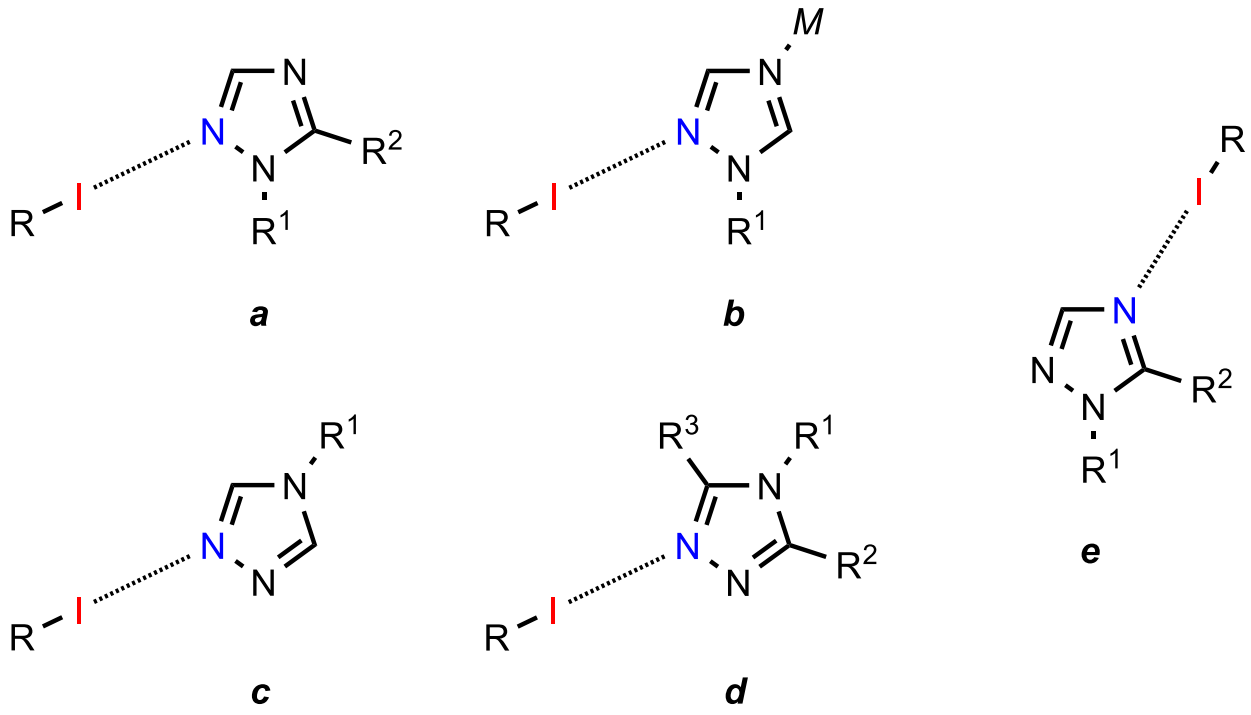

Figure S1. Structural motifs around the C–I···N XBs including 1,2,4-triazole moiety in CCDC structures.

Table S2. Parameters of the lp(I)···C interactions including 1,2,4-triazole moiety in CCDC structures.

Structure	Doi	*d*(C···I), Å	∠(C···I–R), °	Motif
ARONAY	10.1039/C6RA10627G	3.582(5)	98.38(10) 123.07(10) 154.75(9)	***d***
AXATEA	10.1002/marc.201600001	3.476(5)	–	***a***
EBAHAR	10.1021/ic049961v	3.669(8)	–	***a***
EMIYUV	10.1039/c0ce00431f	3.647(3)	123.33(7)	***d***
CISHOC	10.1002/zaac.200700306	3.640(2)	–	***a***
CISHUI	10.1002/zaac.200700306	3.594(5)	–	***a***
DEKGIM	10.11862/CJIC.2017.165	3.644(4)	94.22(6) 97.11(5)	***d***
GUXGAJ	10.1021/ef500264z	3.591(2)	–	***a***
ICEGUV	10.1002/zaac.201600270	3.6632(6)	–	***a***
ICEHUW	10.1002/zaac.201600270	3.604(3)	–	***a***
		3.670(3)	–	***a***
ICEJOS	10.1002/zaac.201600270	3.4363(2)	–	***a***
		3.581(2)	–	***a***
IDIFEH	10.1055/s-2006-926281	3.530(4)	80.09(13)	***c***
IKIKOE	10.1016/j.poly.2016.02.034	3.482(4)	–	***a***
LUGCEX	10.1107/S2056989015009019	3.546(4)	–	***a***
LUGCIB	10.1107/S2056989015009019	3.532(3)	–	***a***
LUGCUN	10.1107/S2056989015009019	3.504(3)	–	***a***
MUPKOY	10.1021/cg901438x	3.613(12)	106.10(19)	***d***
NEJFOA	10.1021/acs.jmedchem.7b00272	3.569(8)	–	***a***
		3.492(8)	–	***a***
NEJFUG	10.1021/acs.jmedchem.7b00272	3.638(8)	–	***b***
NEZBAY	–	3.641(3)	–	***a***
PUFWOE	10.1002/chem.201405395	3.646(5)	134.91(7) 134.30(7)	***e***

RAGZOR	10.1016/j.tetlet.2016.12.016	3.513(4)	–	***a***
RUWQIL	–	3.664(4)	–	***a***
TUMGEP	10.1016/j.molstruc.2015.04.045	3.600(5)	96.52(8)	***f***
UNETEN	10.1021/cg101264h	3.65(2)	–	***b***
UNETUD	10.1021/cg101264h	3.518(2)	–	***a***
XIWFOB	10.1021/acs.organomet.8b00856	3.4392(14)	–	***a***
		3.5564(14)	–	***a***
XIWGOC	10.1021/acs.organomet.8b00856	3.606(3)	–	***b***

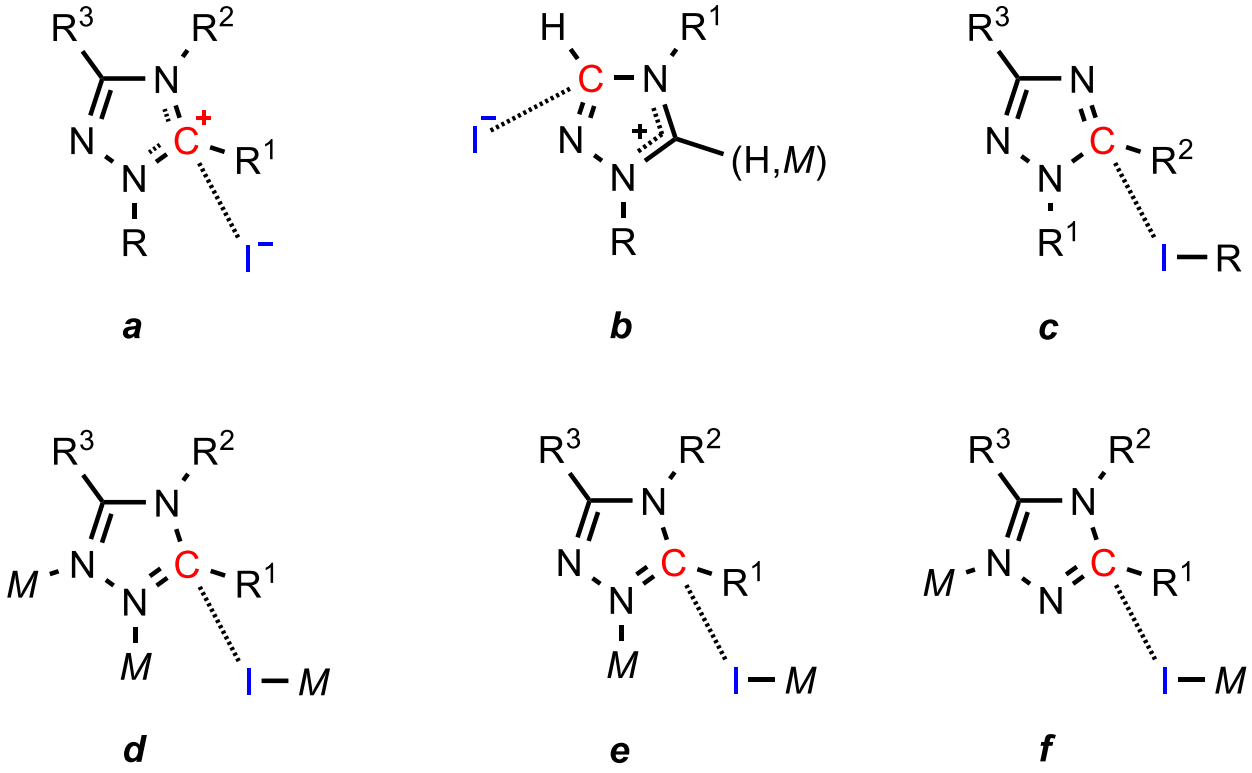

Figure 2S. Structural motifs around the lp(I)···C interactions including 1,2,4-triazole moiety in CCDC structures.

Table 3S. Crystal data and structure refinement for **ASZ**·1.5(**1,4-FIB**).

Identification Code	**ASZ·1.5(1,4-FIB)**
CCDC number	1960975
Empirical formula	$C_{26}H_{19}F_6I_3N_5$
Formula weight	896.16
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	5.5263(2)
b/Å	15.1686(6)
c/Å	18.1482(9)
α/°	76.254(4)
β/°	85.962(4)
γ/°	89.956(3)
Volume/Å^3	1473.86(11)
Z	2
ρ_{calc}g/cm^3	2.019
μ/mm^{-1}	3.244

F(000)	846.0
Crystal size/mm^3	0.21 × 0.18 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.464 to 52
Index ranges	–6 ≤ h ≤ 6, –18 ≤ k ≤ 18, –22 ≤ l ≤ 22
Reflections collected	5678
Independent reflections	5678 [R_{int} = 0.0337, R_{sigma} = 0.0547]
Data/restraints/parameters	5678/0/342
Goodness-of-fit on F^2	1.102
Final R indexes [I≥2σ (I)]	R_1 = 0.0482, wR_2 = 0.0973
Final R indexes [all data]	R_1 = 0.0586, wR_2 = 0.1025
Largest diff. peak/hole / e·Å^{-3}	2.05/–1.10

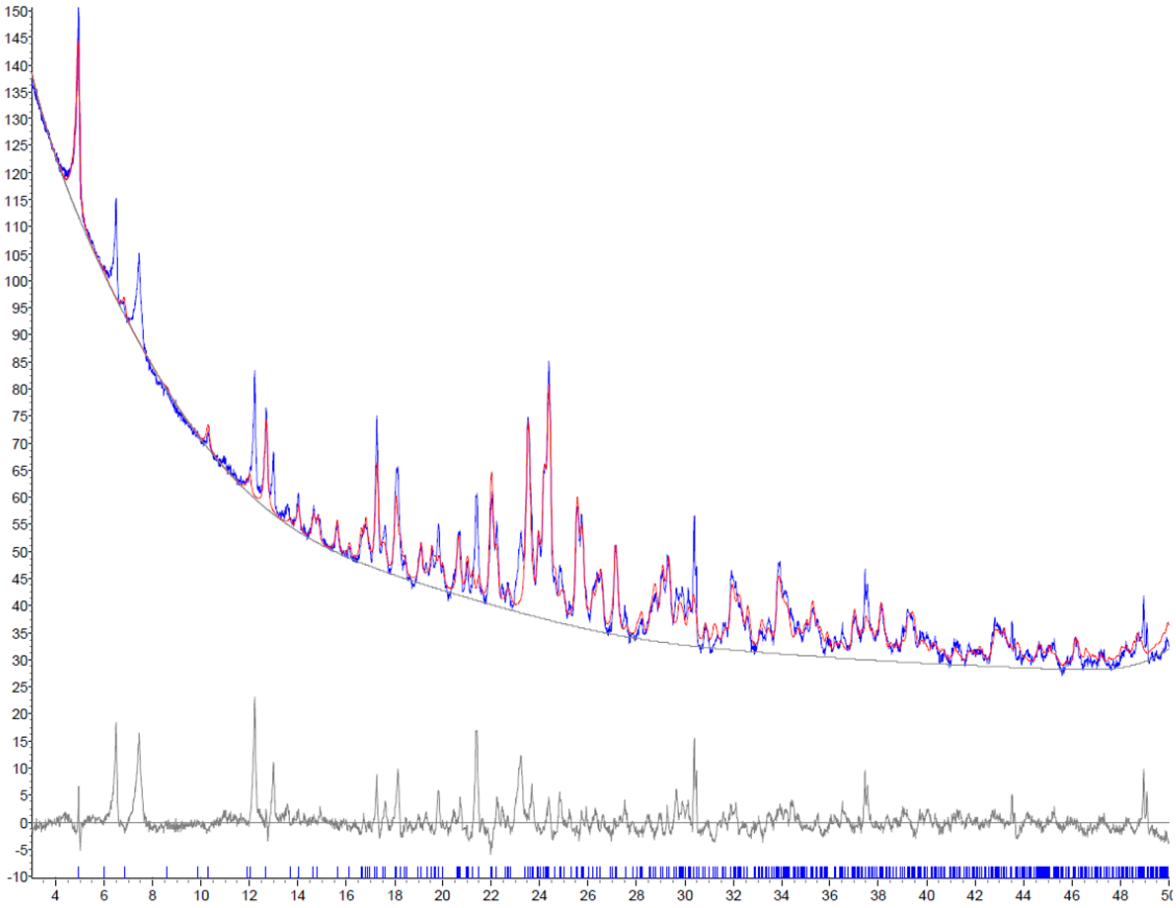

Figure 3S. Powder X-ray diffraction data (blue line) of mixture, obtained by mechanical grinding of 2**ASZ** + 3(**1,4-FIB)** mixture with MeOH additions. Modeled data (red line) in accordance with **ASZ**·1.5(**1,4-FIB**) single-crystal XRD experiment. Difference between them (gray line).

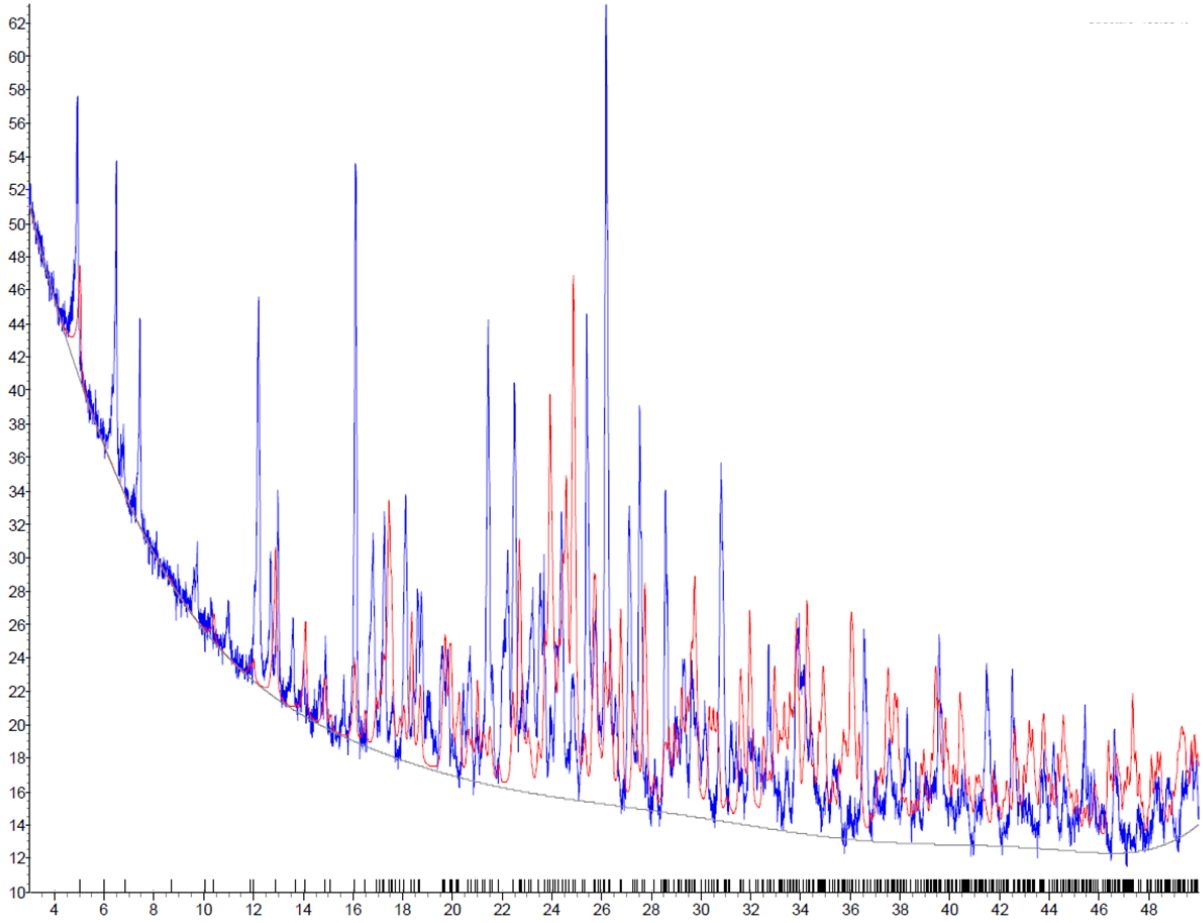

Figure 4S. Powder X-ray diffraction data (blue line) of mixture, obtained by grinding of crystalline material grown from 2**ASZ** + 3(**1,4-FIB)** solution in methanol. Modeled data (red line) in accordance with ASZ·1.5(1,4-FIB) single-crystal XRD experiment.

Table 4S. Cartesian atomic coordinates of model supramolecular cluster.

Atom	X	Y	Z
I	2.840734	11.890266	13.942739
I	7.973362	15.815034	16.579376
F	4.677981	11.601274	16.486893
F	6.319779	16.037805	13.831970
F	4.351388	14.539371	12.812199
F	6.472732	13.233896	17.633257
C	4.869960	14.198959	13.984936
C	6.011050	13.533816	16.437662
C	6.437855	14.669949	15.757229
C	5.886221	14.965157	14.517679
C	5.040803	12.732362	15.853931
C	4.436894	13.046380	14.647788
I	3.362059	6.517623	15.847074
F	3.184596	5.674784	18.948410
F	1.007568	4.586539	14.893939
C	1.146225	4.470848	16.228433
C	2.152993	5.171233	16.882494
C	2.267375	4.999594	18.248636
I	-0.806137	2.105097	19.317462
F	-0.628674	2.947937	16.216126

F	1.548354	4.036182	20.270597
C	1.409697	4.151873	18.936103
C	0.402929	3.451488	18.282042
C	0.288547	3.623126	16.915900
N	6.191075	10.062730	13.453952
N	4.495948	8.769016	12.984505
N	4.547036	1.360210	9.963871
N	4.883061	8.408136	14.234604
C	3.752223	6.963083	11.465397
C	5.276733	9.749460	12.553739
H	5.192145	10.162239	11.725615
C	4.412159	7.196500	10.252221
H	4.624622	8.066630	10.002552
C	5.448840	6.413126	8.072019
C	4.050172	2.157674	10.617932
C	3.387683	3.177448	11.454848
C	3.354014	8.144698	12.325170
H	2.909165	8.804811	11.769570
H	2.722319	7.848698	12.998571
C	3.447352	5.666988	11.839899
H	3.003696	5.512106	12.643409
C	5.157989	5.369366	7.013567
H	4.210586	5.222517	6.959062
H	5.596392	4.546497	7.245653
H	5.482819	5.674911	6.162585
C	4.971087	7.739923	7.581474
C	4.751035	6.141183	9.418821
N	4.611986	8.749539	7.214005
C	1.853165	3.011069	11.252652
H	1.640474	3.115191	10.322550
H	1.387875	3.676532	11.764296
H	1.584754	2.136549	11.546275
C	5.891458	9.218047	14.475481
H	6.360309	9.211817	15.278991
C	4.448325	4.837249	9.823213
H	4.686787	4.122640	9.278163
C	3.758235	2.905140	12.917692
H	3.466908	2.023098	13.162086
H	3.329487	3.552113	13.483841
H	4.709950	2.967844	13.024944
C	3.796583	4.591058	11.027599
C	6.989148	6.535708	8.293556
H	7.336180	5.694542	8.599487
H	7.165975	7.212254	8.949374
H	7.413399	6.774049	7.465431
I	10.779437	11.901050	21.221798
I	5.646809	7.976282	18.585161
F	8.942190	12.190042	18.677643
F	7.300392	7.753511	21.332566
F	9.268783	9.251945	22.352337
F	7.147439	10.557420	17.531280
C	8.750211	9.592357	21.179600
C	7.609121	10.257500	18.726874
C	7.182316	9.121368	19.407308
C	7.733950	8.826159	20.646857
C	8.579368	11.058954	19.310605
C	9.183277	10.744936	20.516749
I	8.367034	11.890266	13.942739
I	13.499662	15.815034	16.579376

F	10.204281	11.601274	16.486893
F	11.846079	16.037805	13.831970
F	9.877688	14.539371	12.812199
F	11.999032	13.233896	17.633257
C	10.396260	14.198959	13.984936
C	11.537350	13.533816	16.437662
C	11.964155	14.669949	15.757229
C	11.412521	14.965157	14.517679
C	10.567103	12.732362	15.853931
C	9.963194	13.046380	14.647788
N	0.624835	9.417226	4.128317
N	2.319962	10.710939	4.597763
N	2.268874	18.119746	7.618397
N	1.932849	11.071820	3.347664
C	3.063687	12.516873	6.116871
C	1.539177	9.730496	5.028529
H	1.623764	9.317716	5.856653
C	2.403750	12.283456	7.330048
H	2.191288	11.413326	7.579716
C	1.367070	13.066830	9.510249
C	2.765738	17.322282	6.964336
C	3.428227	16.302508	6.127420
C	3.461895	11.335258	5.257098
H	3.906745	10.675145	5.812698
H	4.093591	11.631258	4.583697
C	3.368558	13.812968	5.742369
H	3.812213	13.967850	4.938859
C	1.657921	14.110590	10.568701
H	2.605324	14.257439	10.623206
H	1.219518	14.933459	10.336615
H	1.333091	13.805045	11.419683
C	1.844823	11.740033	10.000794
C	2.064875	13.338773	8.163447
N	2.203924	10.730417	10.368263
C	4.962745	16.468887	6.329617
H	5.175436	16.364765	7.259718
H	5.428035	15.803424	5.817973
H	5.231156	17.343407	6.035993
C	0.924451	10.261909	3.106787
H	0.455601	10.268139	2.303277
C	2.367585	14.642707	7.759055
H	2.129122	15.357316	8.304105
C	3.057675	16.574816	4.664576
H	3.349002	17.456858	4.420182
H	3.486423	15.927842	4.098427
H	2.105959	16.512112	4.557324
C	3.019327	14.888897	6.554670
C	-0.173238	12.944248	9.288712
H	-0.520270	13.785414	8.982781
H	-0.350065	12.267702	8.632894
H	-0.597489	12.705907	10.116837
N	6.139486	-5.751369	4.128317
N	7.834613	-4.457656	4.597763
N	7.783525	2.951150	7.618397
N	7.447500	-4.096776	3.347664
C	8.578339	-2.651722	6.116871
C	7.053828	-5.438099	5.028529
H	7.138416	-5.850879	5.856653
C	7.918402	-2.885139	7.330048

H	7.705940	-3.755270	7.579716
C	6.881721	-2.101766	9.510249
C	8.280389	2.153687	6.964336
C	8.942878	1.133912	6.127420
C	8.976547	-3.833338	5.257098
H	9.421397	-4.493450	5.812698
H	9.608243	-3.537338	4.583697
C	8.883209	-1.355628	5.742369
H	9.326865	-1.200746	4.938859
C	7.172572	-1.058005	10.568701
H	8.119976	-0.911157	10.623206
H	6.734169	-0.235137	10.336615
H	6.847742	-1.363551	11.419683
C	7.359474	-3.428563	10.000794
C	7.579527	-1.829823	8.163447
N	7.718575	-4.438178	10.368263
C	10.477397	1.300291	6.329617
H	10.690087	1.196170	7.259718
H	10.942687	0.634828	5.817973
H	10.745807	2.174812	6.035993
C	6.439103	-4.906687	3.106787
H	5.970252	-4.900457	2.303277
C	7.882236	-0.525889	7.759055
H	7.643774	0.188721	8.304105
C	8.572326	1.406221	4.664576
H	8.863654	2.288262	4.420182
H	9.001074	0.759247	4.098427
H	7.620611	1.343517	4.557324
C	8.533978	-0.279698	6.554670
C	5.341413	-2.224348	9.288712
H	4.994381	-1.383182	8.982781
H	5.164586	-2.900893	8.632894
H	4.917162	-2.462689	10.116837
I	4.720163	2.105097	19.317462
F	4.897626	2.947937	16.216126
F	7.074654	4.036182	20.270597
C	6.935997	4.151873	18.936103
C	5.929229	3.451488	18.282042
C	5.814847	3.623126	16.915900
I	8.888359	6.517623	15.847074
F	8.710896	5.674784	18.948410
F	6.533868	4.586539	14.893939
C	6.672525	4.470848	16.228433
C	7.679293	5.171233	16.882494
C	7.793675	4.999594	18.248636