

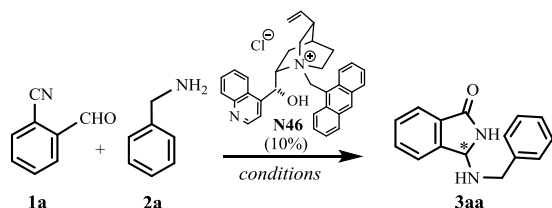
Asymmetric tandem hemiaminal-heterocyclization-Aza-Mannich

reaction of 2-formylbenzonitriles and amines using chiral phase transfer catalysis: an experimental and theoretical study

Amedeo Capobianco, Antonia Di Mola, Valentina Intintoli, Antonio Massa, Vito Capaccio, Lukas Roiser, Mario Waser and Laura Palombi

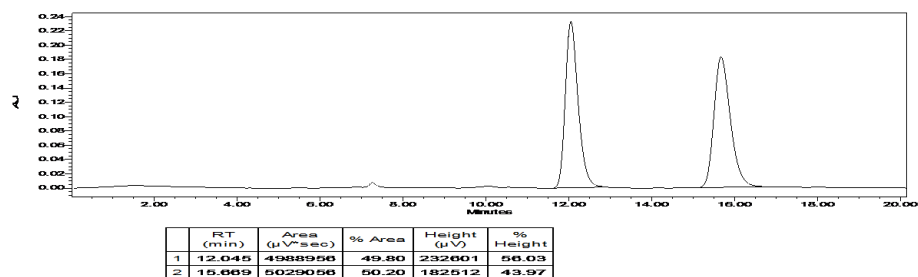
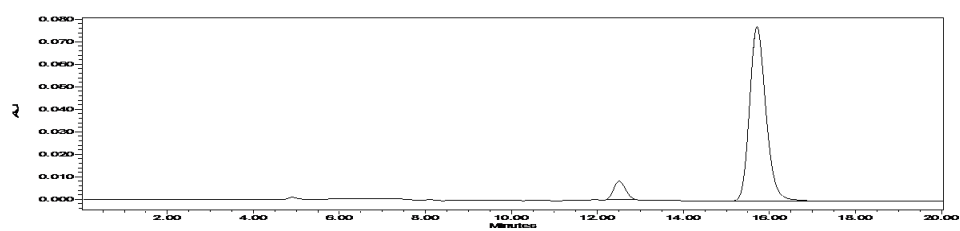
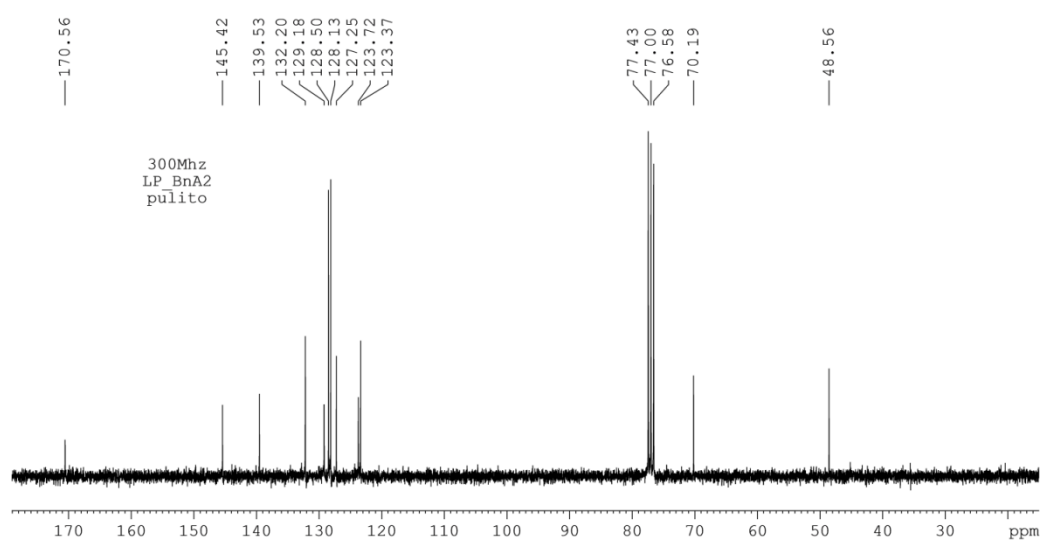
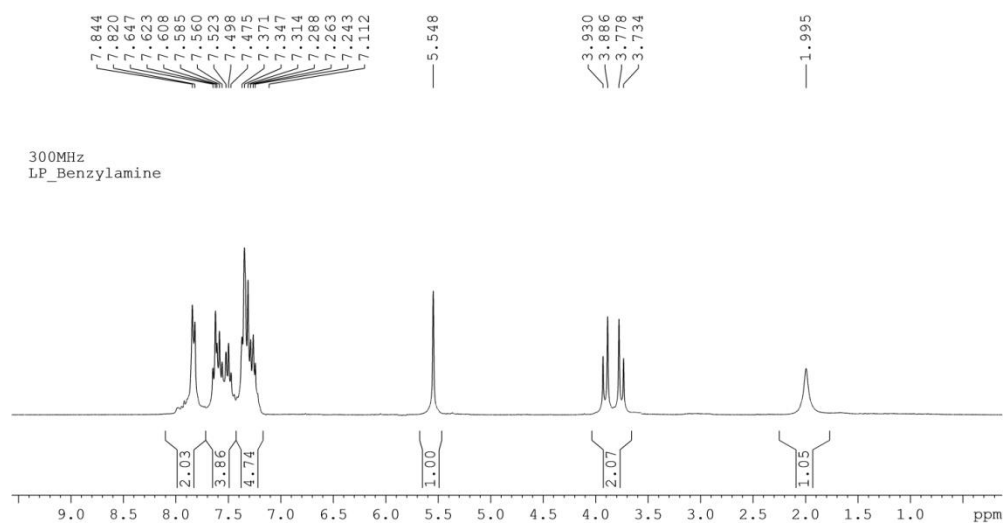
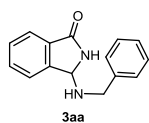
General remarks. All reactions were performed using commercially available compounds without further purification and technical grade solvents. All the reactions were monitored by thin layer chromatography (TLC) using *Merck Silica Gel 60 F254* plates and were visualized by fluorescence quenching at 254 nm. Column chromatographic purification of products was carried out using silica gel 60 (70–230 mesh, Merck). The NMR spectra were recorded on Bruker DRX 500, 400, 300, 250 spectrometers (500 MHz, 400 MHz, 300 MHz, 250 MHz, 1H; 100 MHz, 75 MHz, 62,5 MHz 13C). Spectra were referenced to residual CHCl₃ (7.26 ppm, 1H; 77.00 ppm, 13C), CD₃OD (or (CH₃)₂SO (2.5 ppm, 1H; 39.52 ppm, 13C) when indicated. Yields are given for isolated products showing one spot on a TLC plate and no impurities detectable in the NMR spectrum. Mass spectral analyses were carried out using an electrospray spectrometer, Waters 4 micro quadrupole. Elemental analyses were performed with FLASH EA 1112 series-Thermo Scientific for CHNS-O apparatus. HPLC analyses were performed with a Waters 1525 HPLC, by calibrating the chiral methods with the corresponding racemic mixtures, using diacel chiralpak AD and $\lambda = 254$ nm. Optical rotations were measured on a Perkin-Elmer Polarimeter with a sodium lamp at $\lambda = 589$ nm

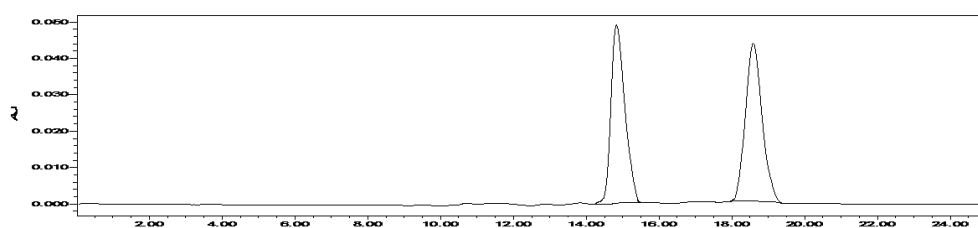
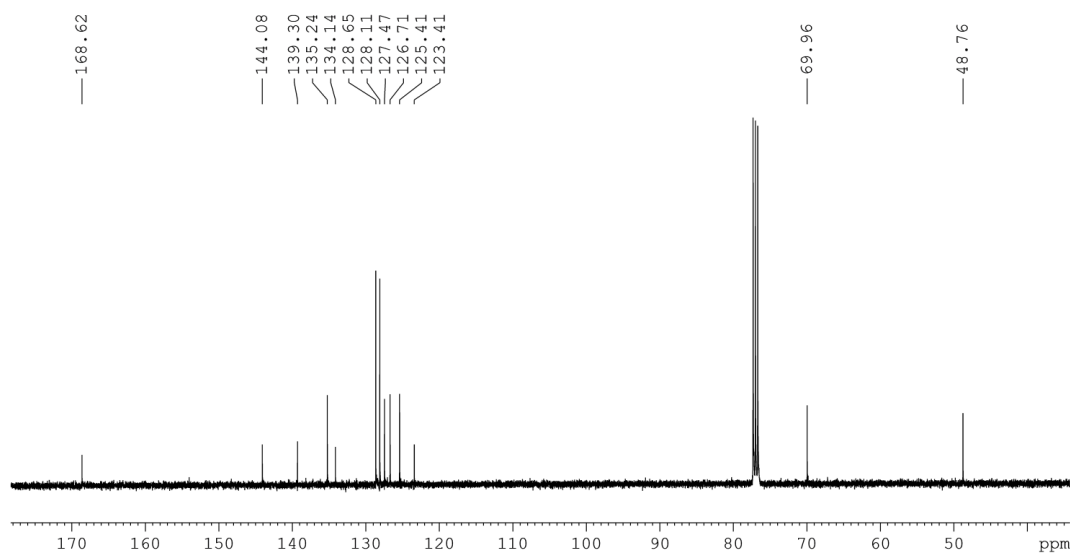
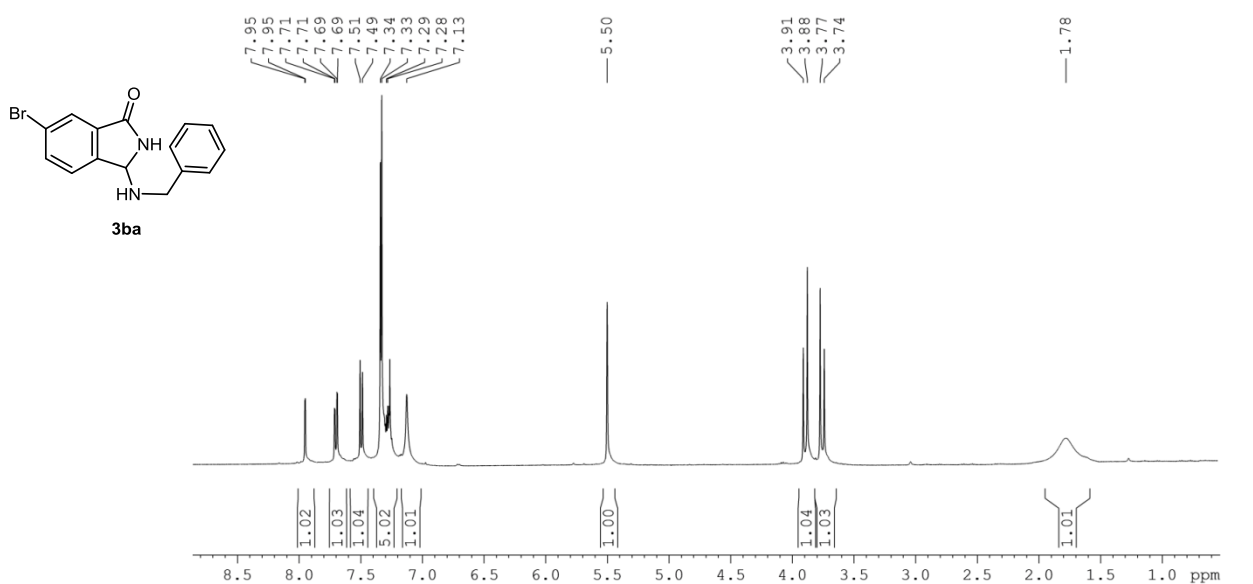
Chart 1	p 2
NMR spectra and HPLC traces of compounds 3	pp 3-14
NMR spectra of catalyst QDOH-1 and QDOH-2	p 15
Additional computational data.....	pp 16-21
Cartesian coordinates	pp 22-153

Chart 1. Tandem reaction of **1a** with **2a** with **N46** under different condition

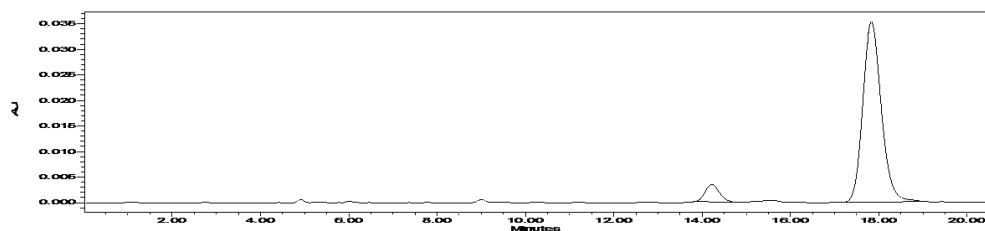
Entry	Base (1 eq.)	[C] mM	T (°C)	Time (h)	Yield ^a (%)	e.e. ^b (%)
1	K ₂ CO ₃	50	25	1	70	30
2	K ₂ CO ₃	33	25	8	71	30
3	K ₂ CO ₃	50	-10	3	86	32
4	K₂CO₃	50	-20	8	86	56 (98)^c
5	K ₂ CO ₃	50	-40	24	84	32
6	K ₂ CO ₃	100	-20	8	88	44
7 ^d	K ₂ CO ₃	50	-20	1	96	40
6	Cs ₂ CO ₃	50	-20	4	96	30
7	LiOH	50	-20	21	80	48
8	KOH	50	-20	1/2	50	24
9 ^e	KOH	50	-20	1/2	59	33
10 ^{f,g}	-	50	20	1	75	17
11 ^{f,g}	-	50	-20	72	-	-
12 ^{g,h}	-	20	20	1	90	15
13 ^{g,i}	-	50	20	1	66	20

^a Yields refer to isolated products. ^b E.e. determined on HPLC equipped with chiral column. ^c In parenthesis e.e. after reverse crystallization. ^d K₂CO₃ has been added as aqueous solution 0.9 M. ^e Catalyst loading 20% mol. ^f Base-free reaction under biphasic conditions (Toluene/H₂O). ^g Toluene/H₂O ratio 1/30. ^h Toluene/H₂O ratio 1/2. ⁱ Toluene/H₂O ratio 1/20.

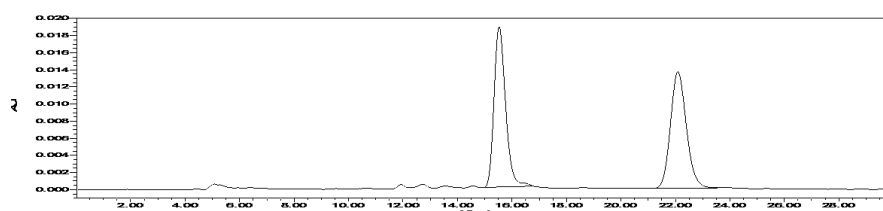
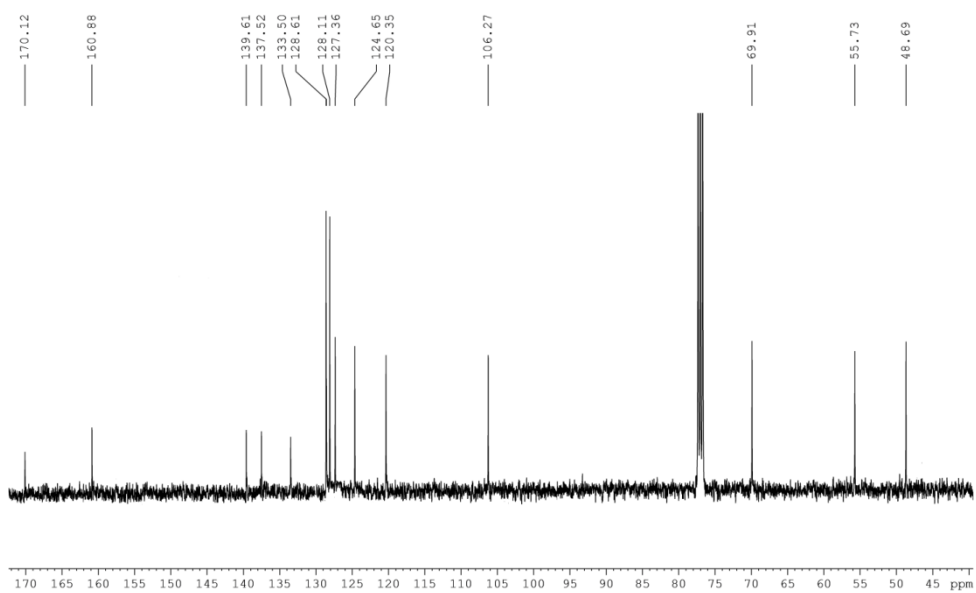
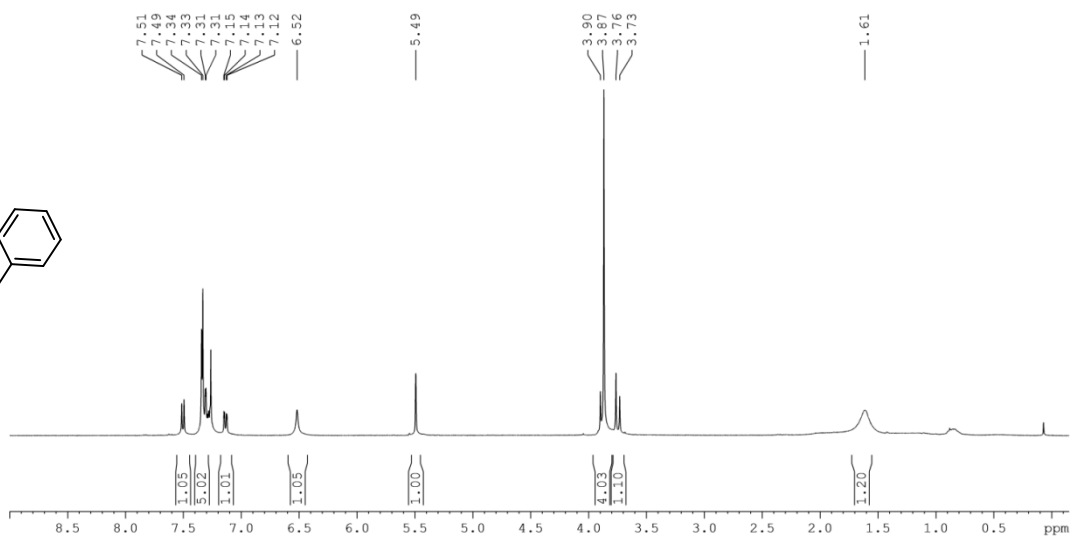
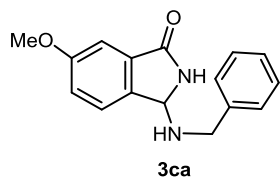




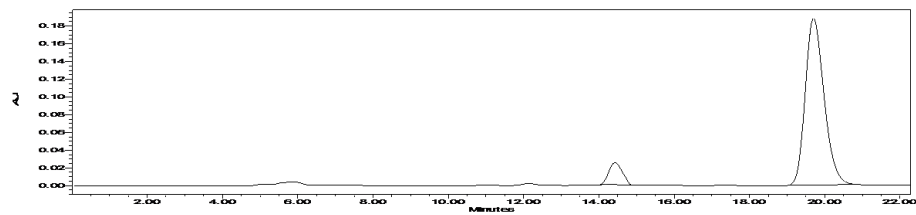
	RT (min)	Area (μV·sec)	% Area	Height (μV)	% Height
1	14.831	1193472	49.99	46959	53.83
2	18.588	1194048	50.01	40278	46.17



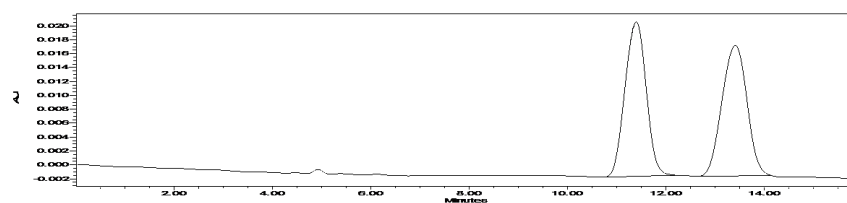
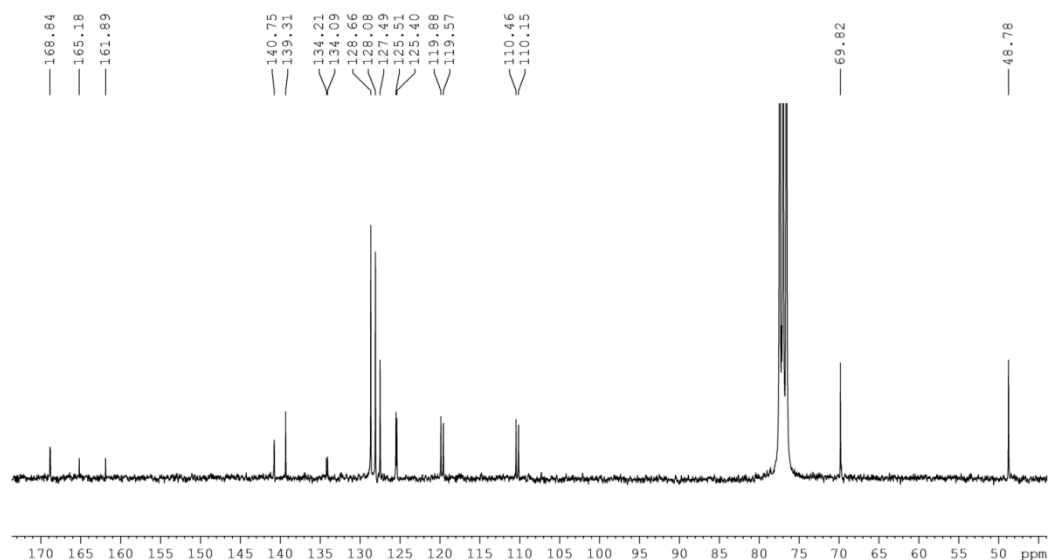
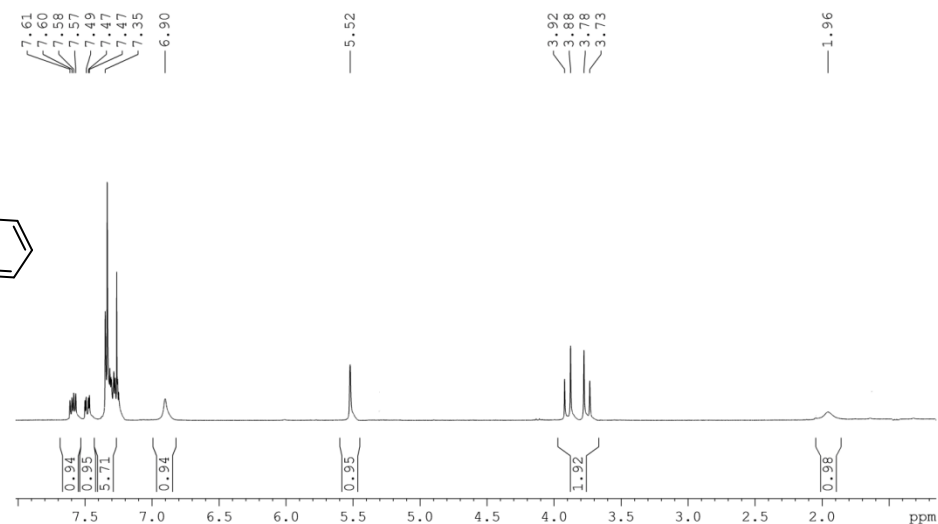
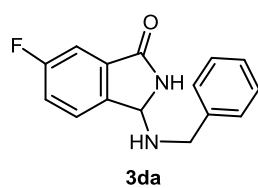
	RT (min)	Area (μV·sec)	% Area	Height (μV)	% Height
1	14.219	76024	6.91	3432	8.84
2	17.831	1024710	93.09	35383	91.16



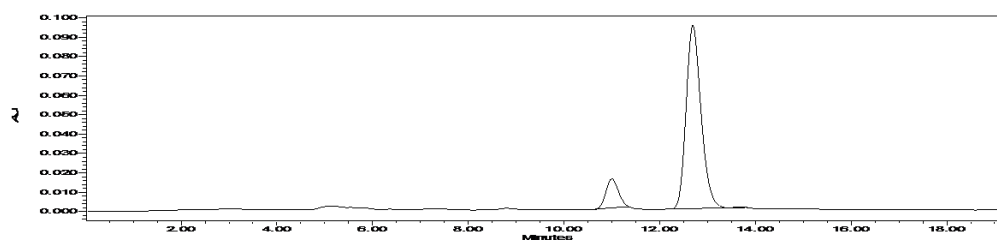
	RT (min)	Area (μV·sec)	% Area	Height (μV)	% Height
1	15.528	552120	50.03	18755	57.92
2	22.087	551391	49.97	13625	42.08



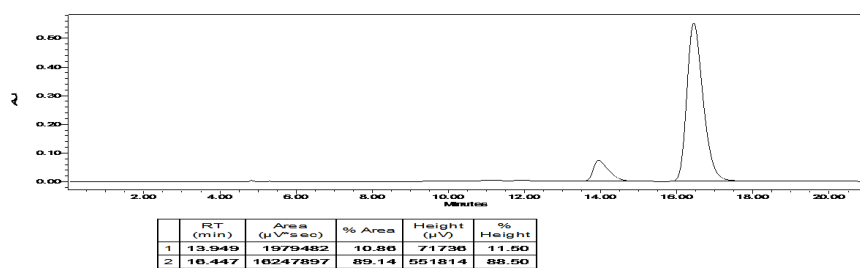
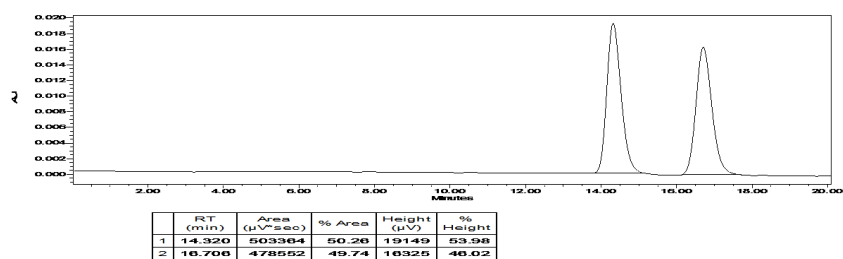
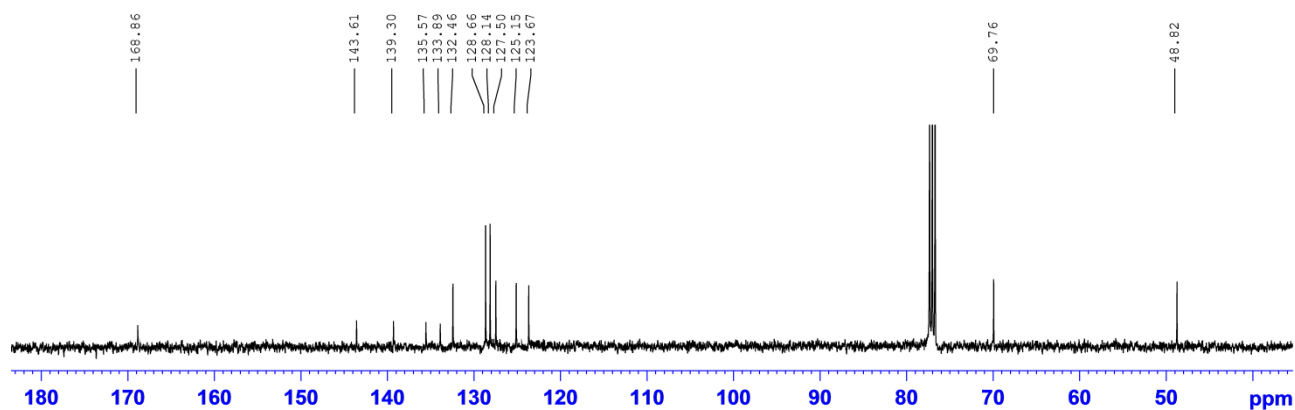
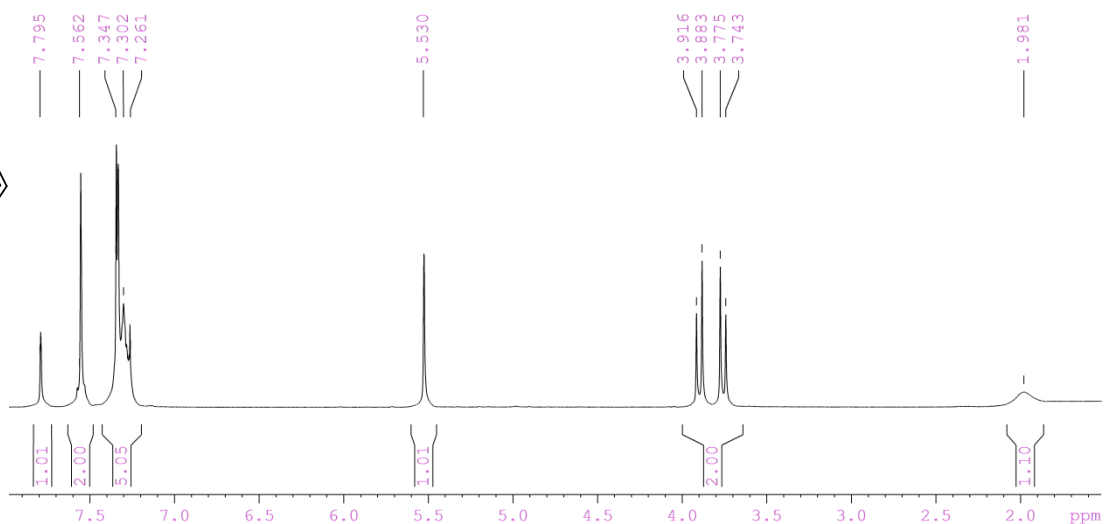
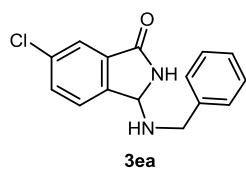
	RT (min)	Area (μV·sec)	% Area	Height (μV)	% Height
1	14.426	475324	6.78	21543	10.26
2	19.702	6534718	93.22	188035	89.72

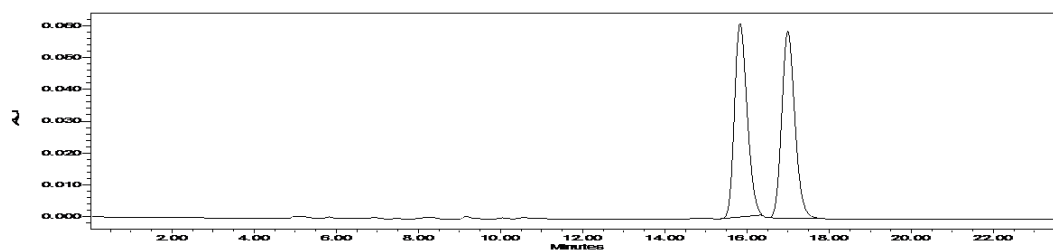
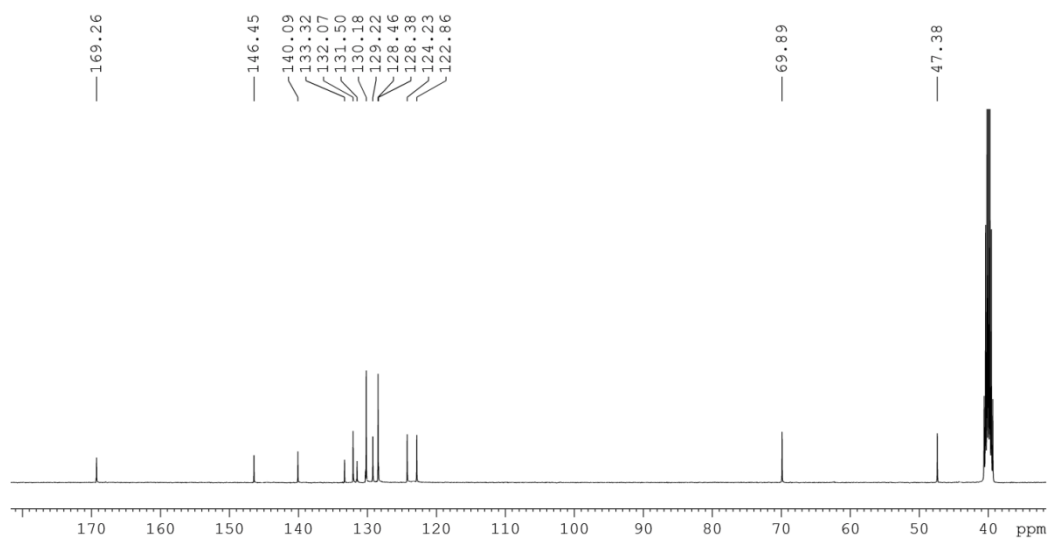
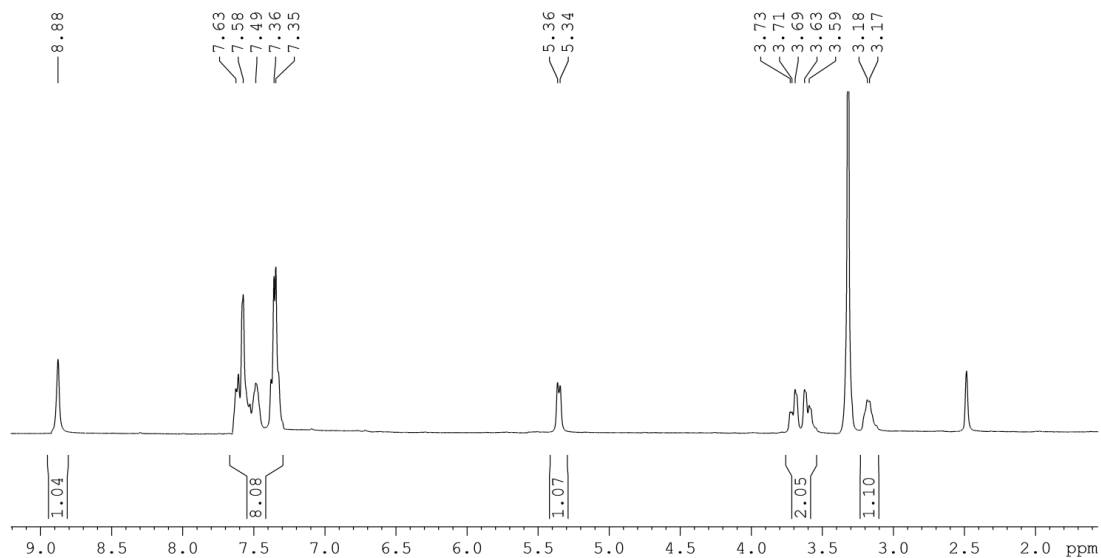
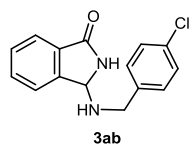


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1	11.395	666662	50.17	22218	54.20
2	13.406	662232	49.83	18777	45.80

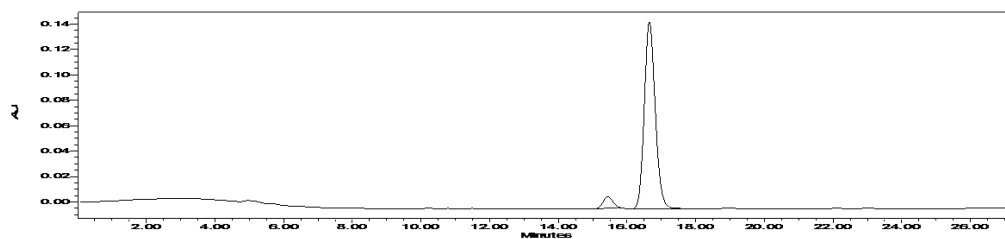


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1	10.999	270901	11.65	15000	13.70
2	12.692	2054709	88.35	94519	86.30

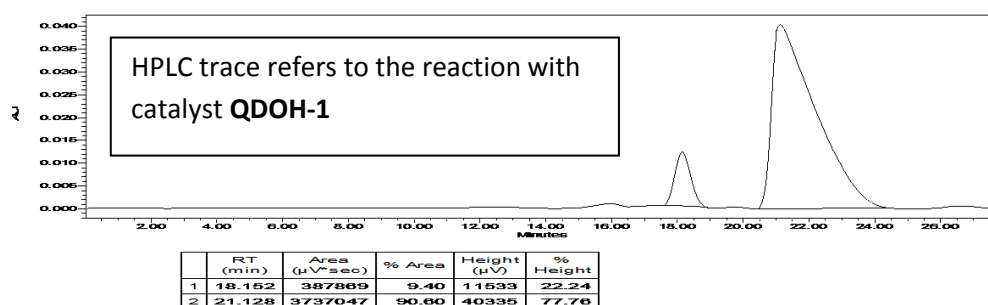
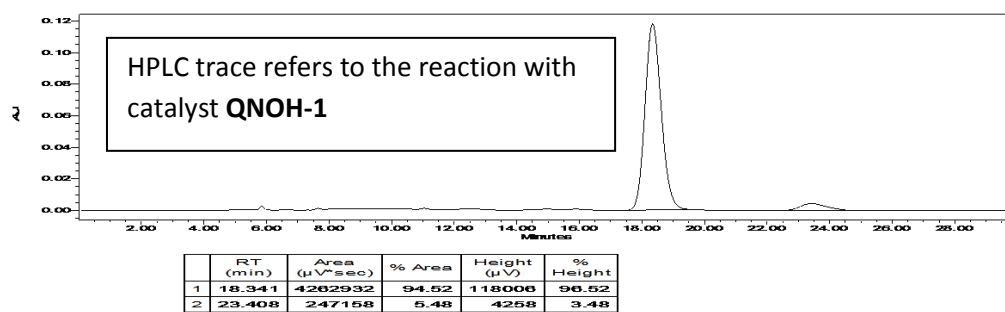
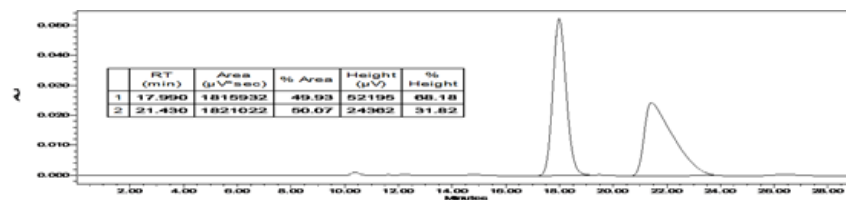
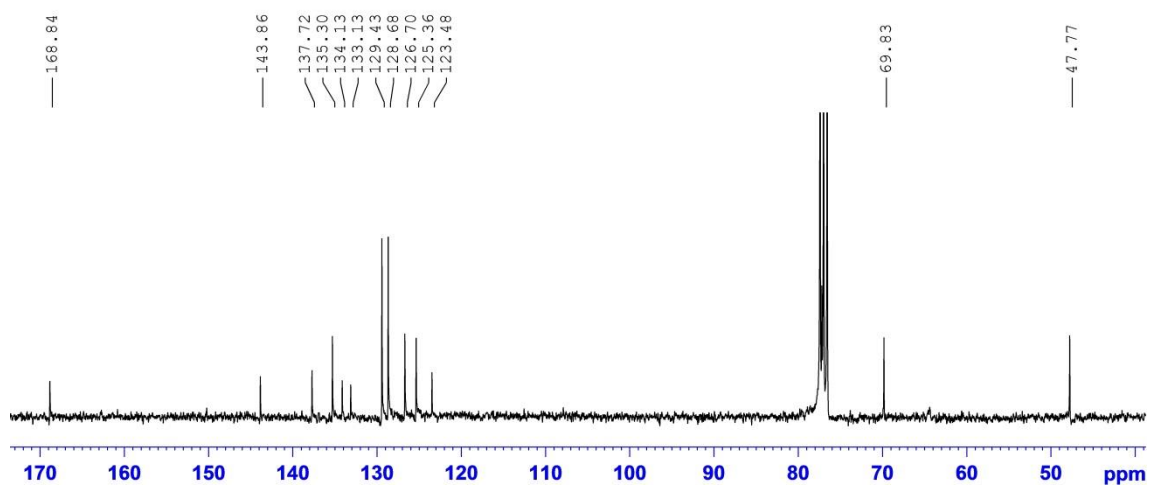
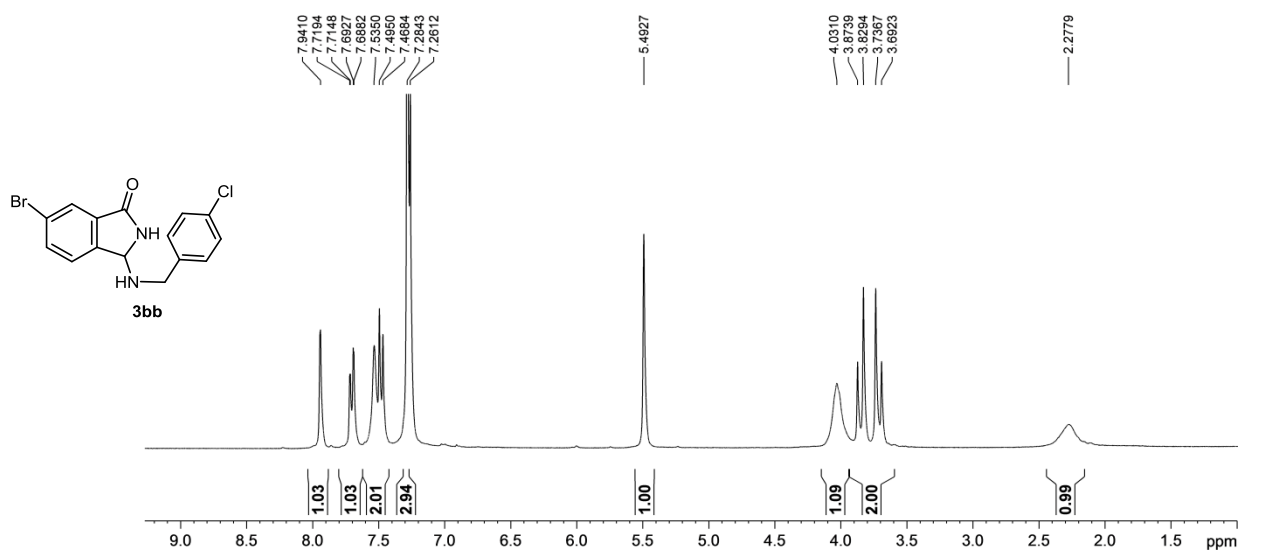


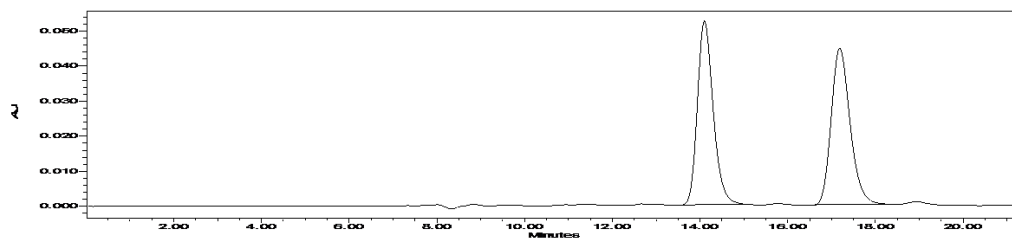
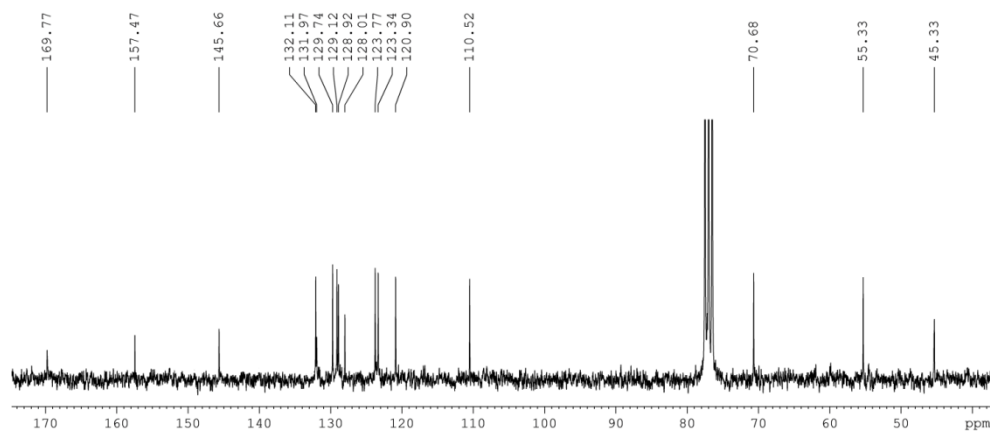
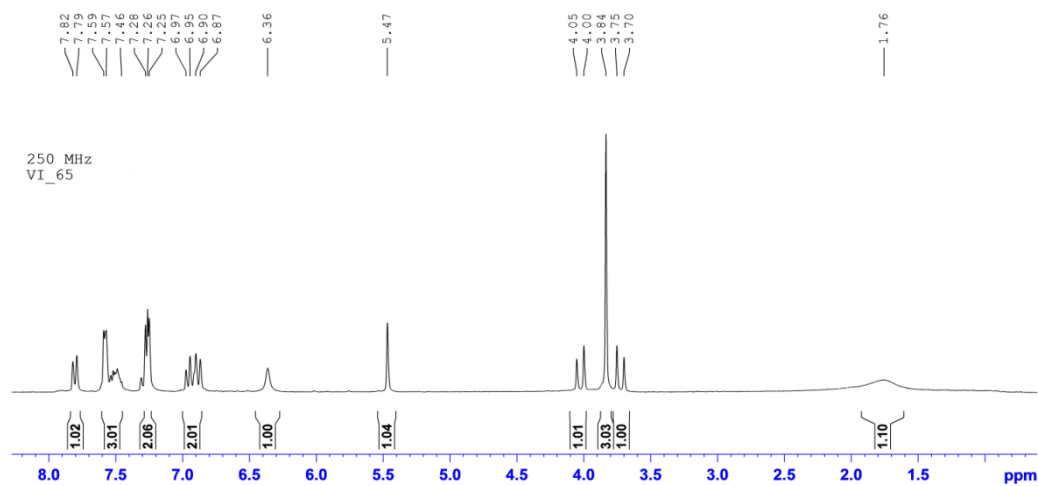
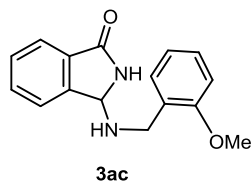


	RT (min)	Area (μV·sec)	% Area	Height (μV)	% Height
1	15.831	1297716	49.78	60803	50.85
2	16.993	1309398	50.22	58767	49.15

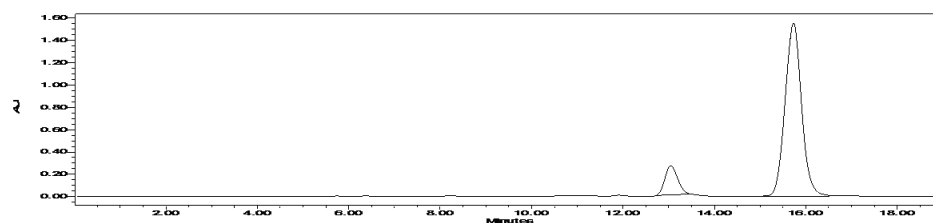


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1	15.440	174114	5.07	9074	5.81
2	16.649	3259248	94.93	147192	94.19

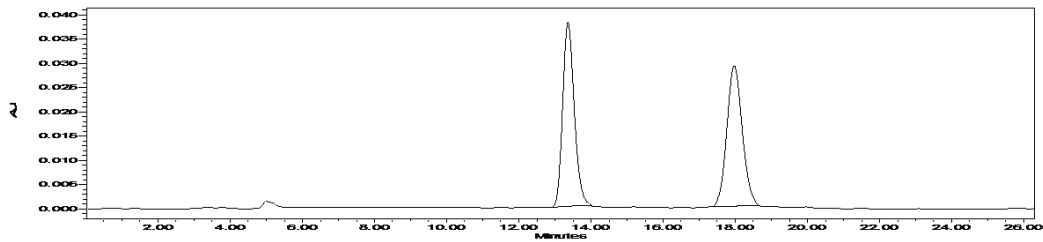
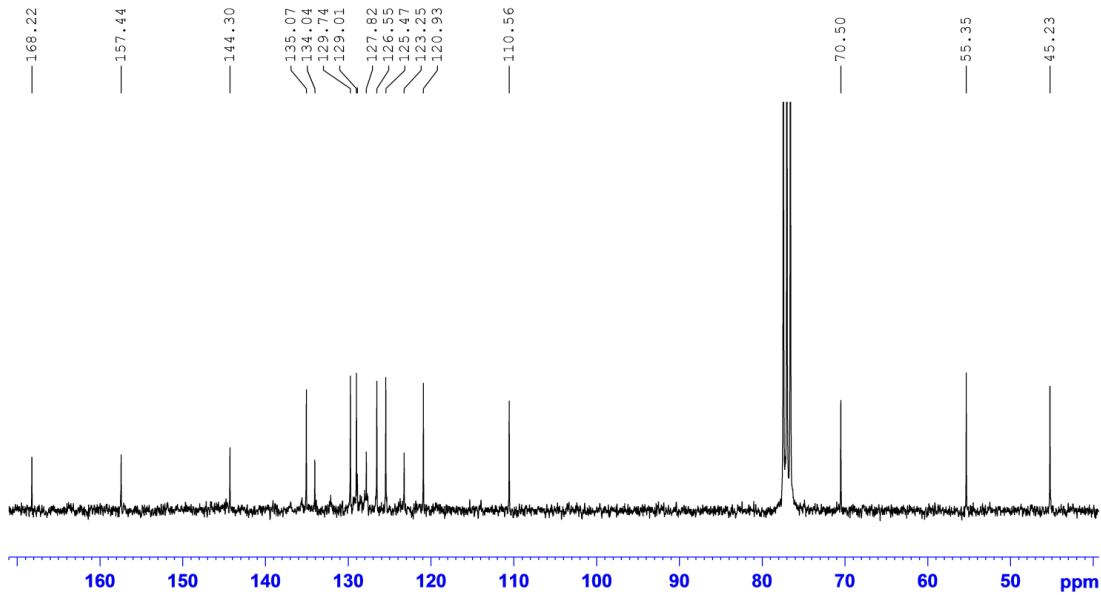
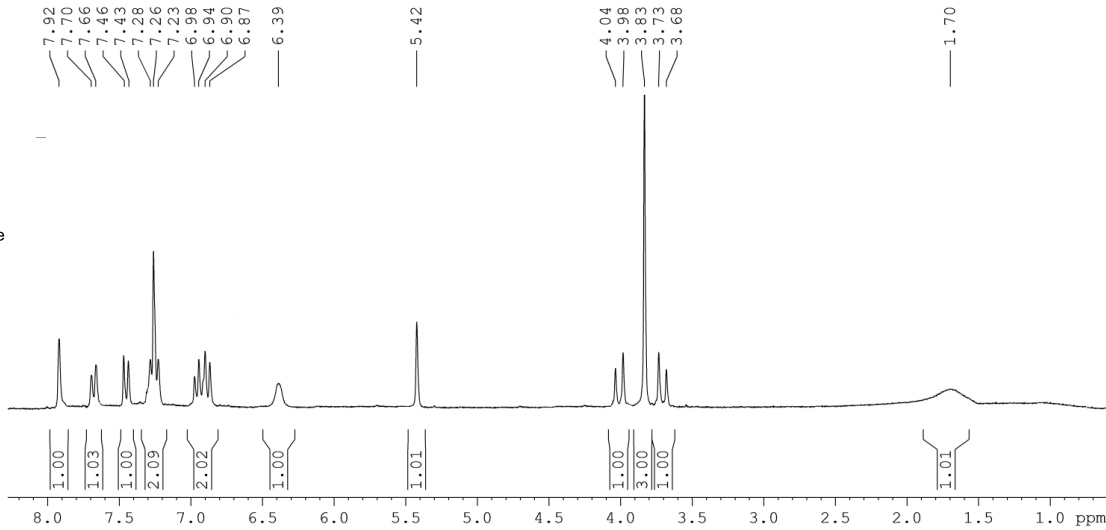
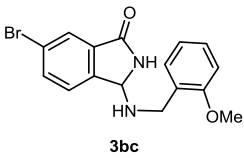




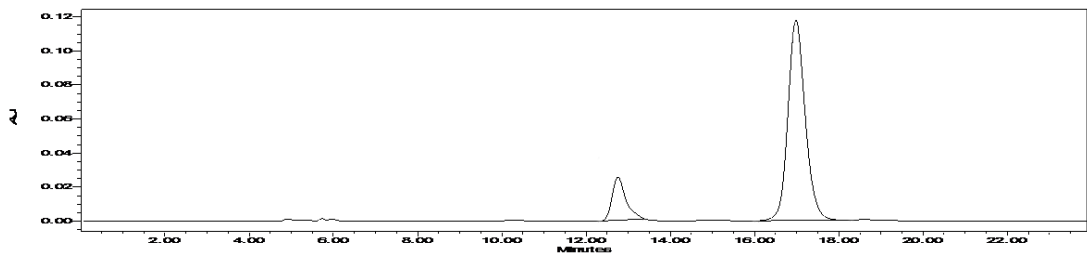
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1	14.100	1309098	49.72	52425	54.09
2	17.185	1323803	50.28	44502	45.91



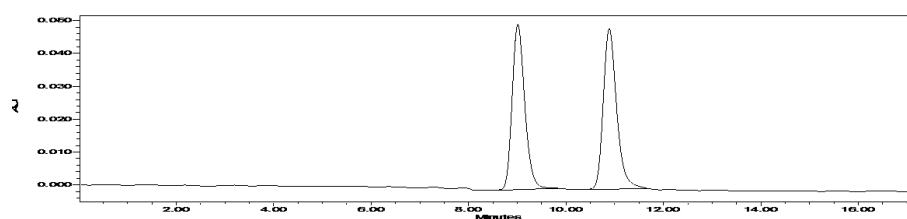
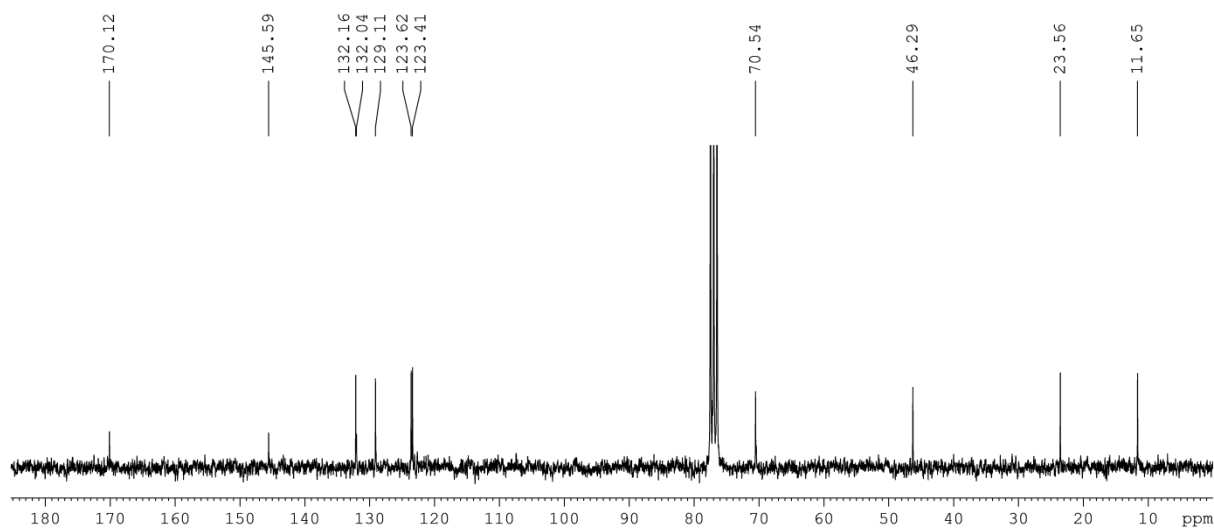
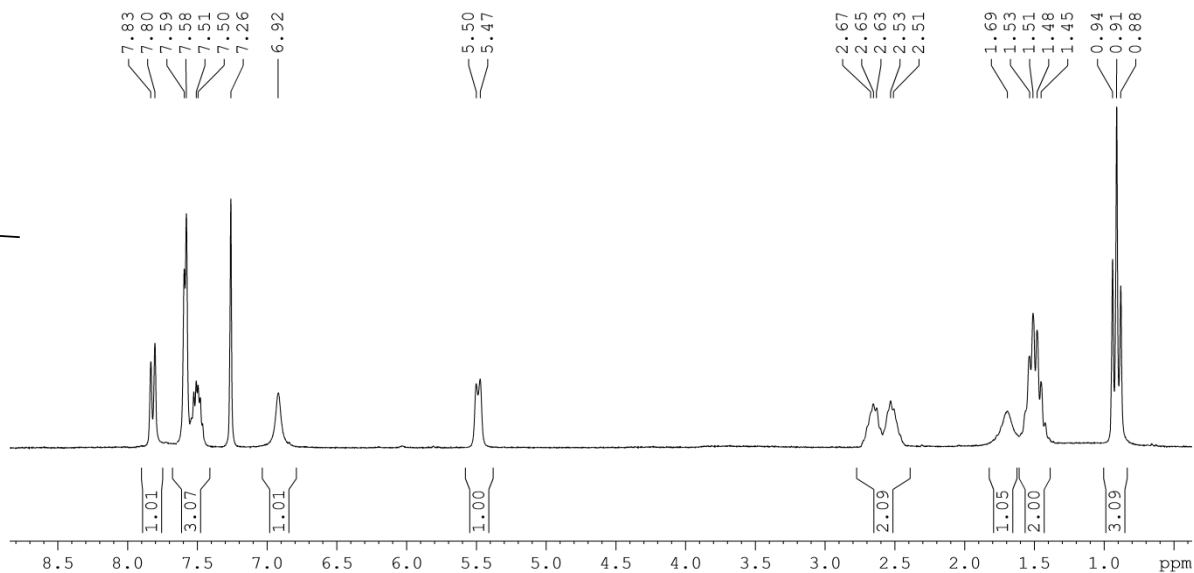
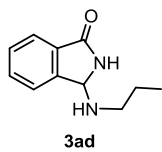
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	13.046	5037708	11.48	260309	14.36
2	15.730	38860388	88.52	1552887	85.64



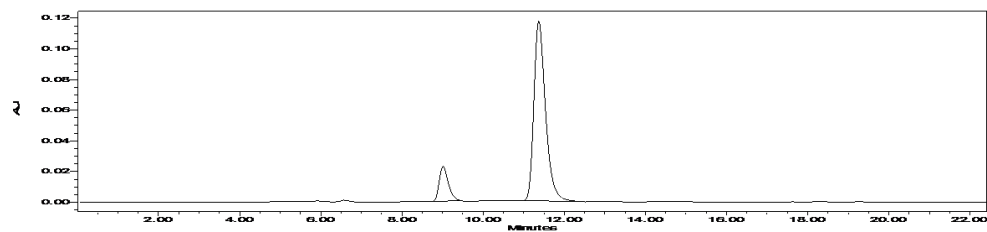
	RT (min)	Area (μV ² sec)	% Area	Height (μV)	% Height
1	13.363	841811	50.40	37903	57.14
2	17.969	828400	49.60	28435	42.86



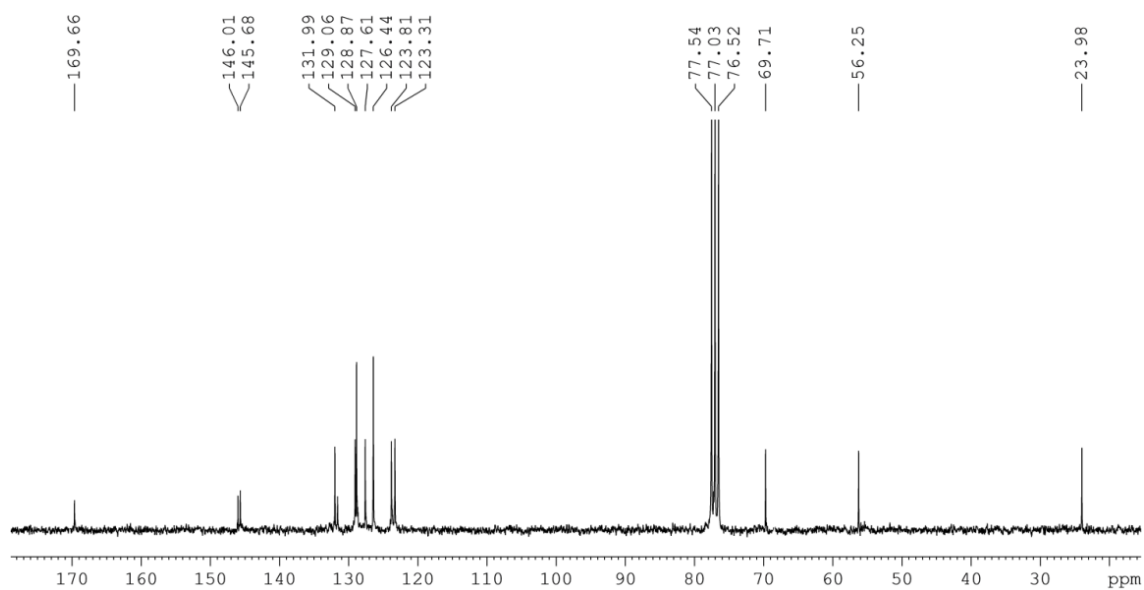
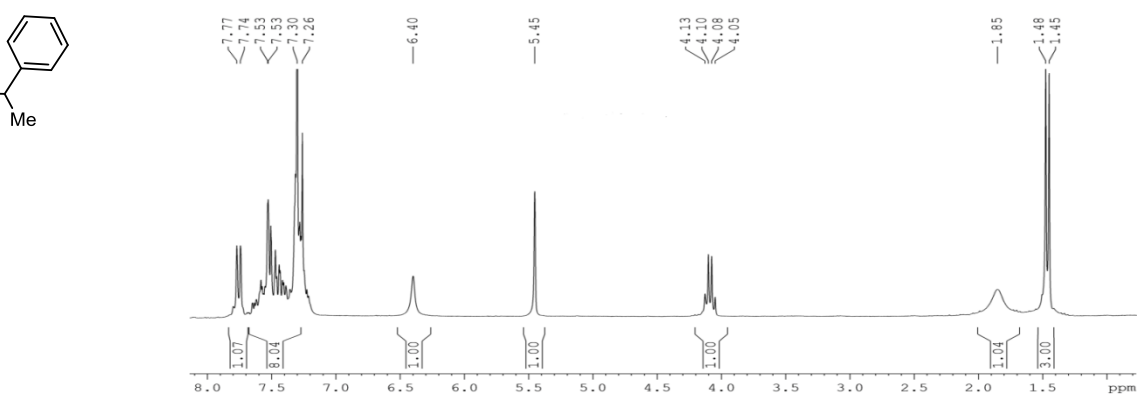
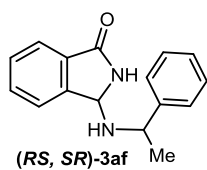
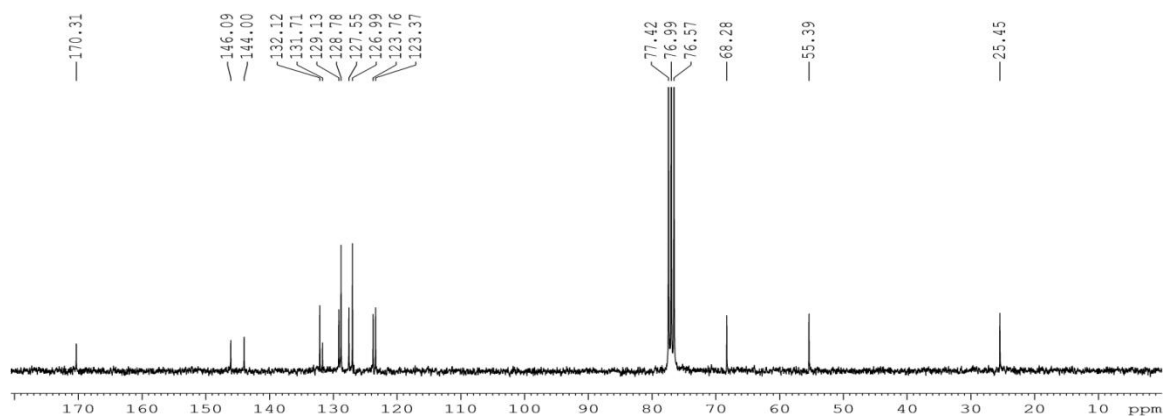
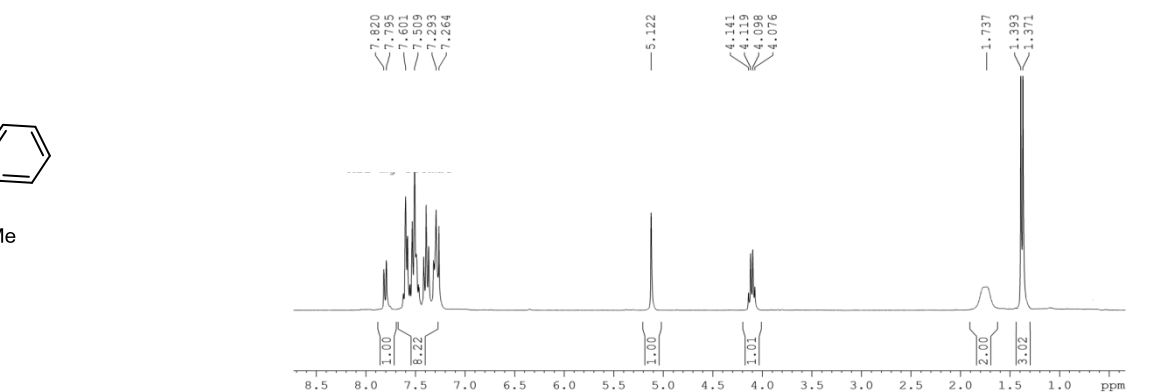
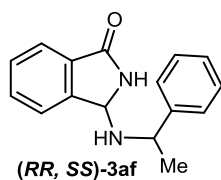
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1	12.755	573802	14.59	25250	17.64
2	16.982	3358812	85.41	117899	82.36



	RT (min)	Area (μV·sec)	% Area	Height (μV)	% Height
1	9.011	907783	49.27	50253	50.89
2	10.887	934630	50.73	48892	49.31



	RT (min)	Area (μV·sec)	% Area	Height (μV)	% Height
1	9.016	352458	13.15	22767	16.27
2	11.374	2327492	86.85	117194	83.73



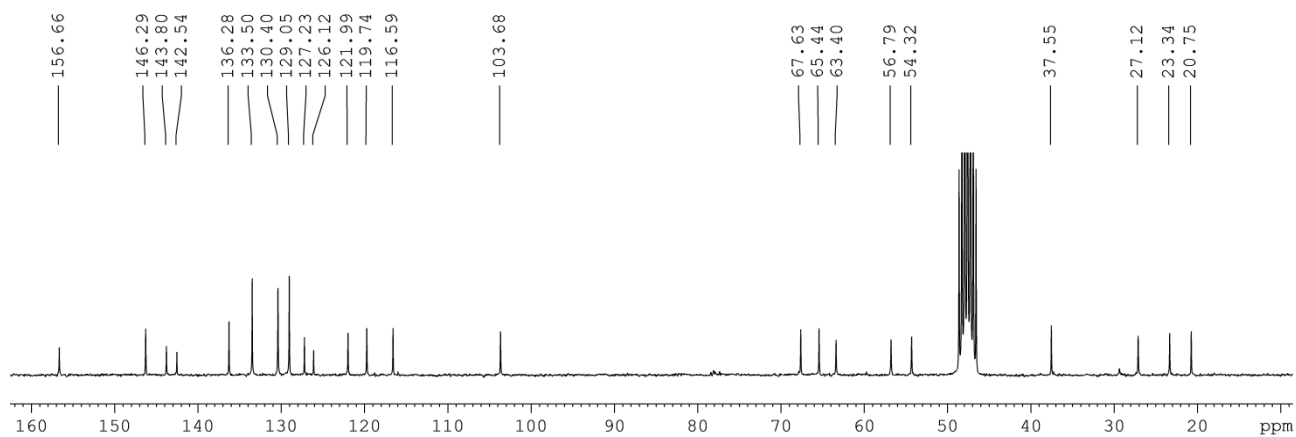
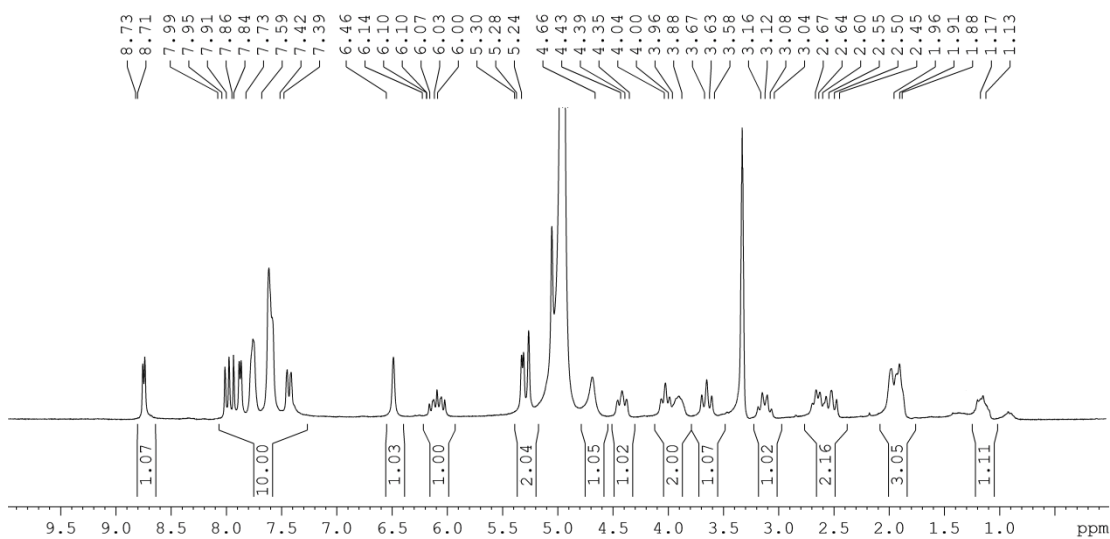
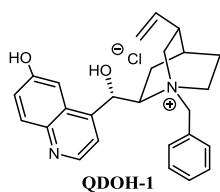
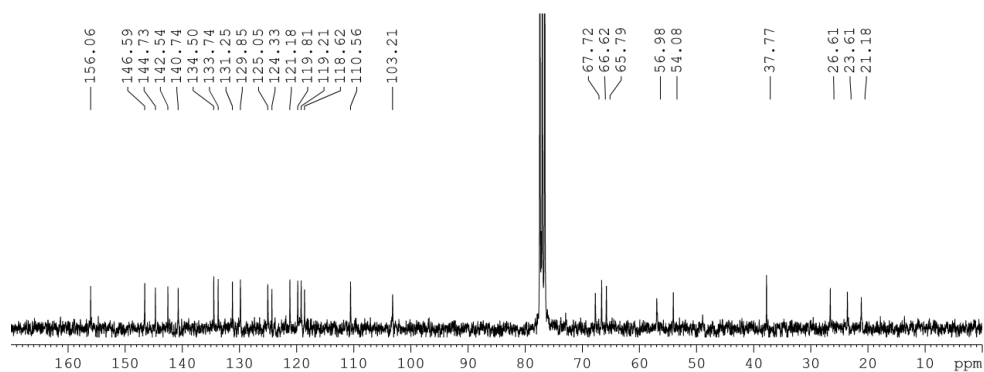
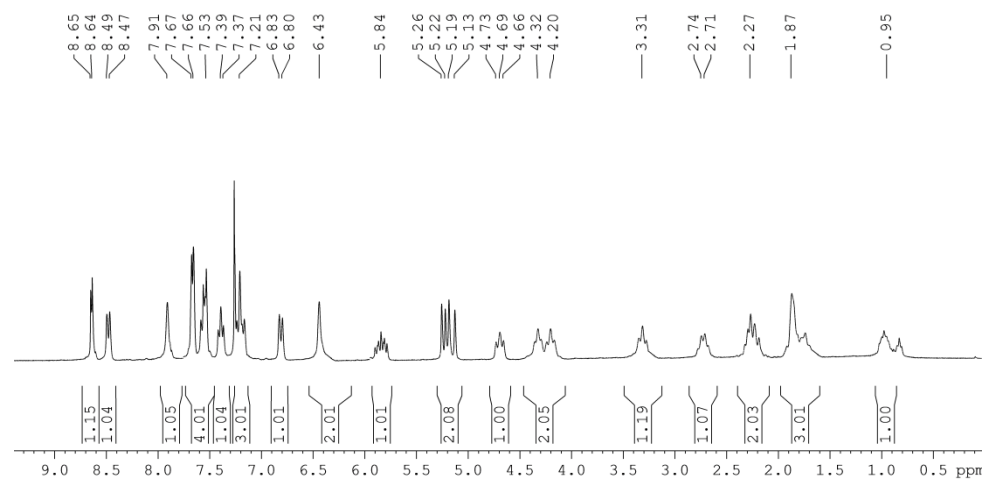
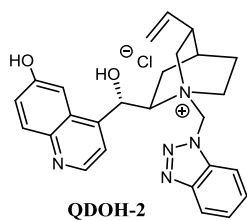
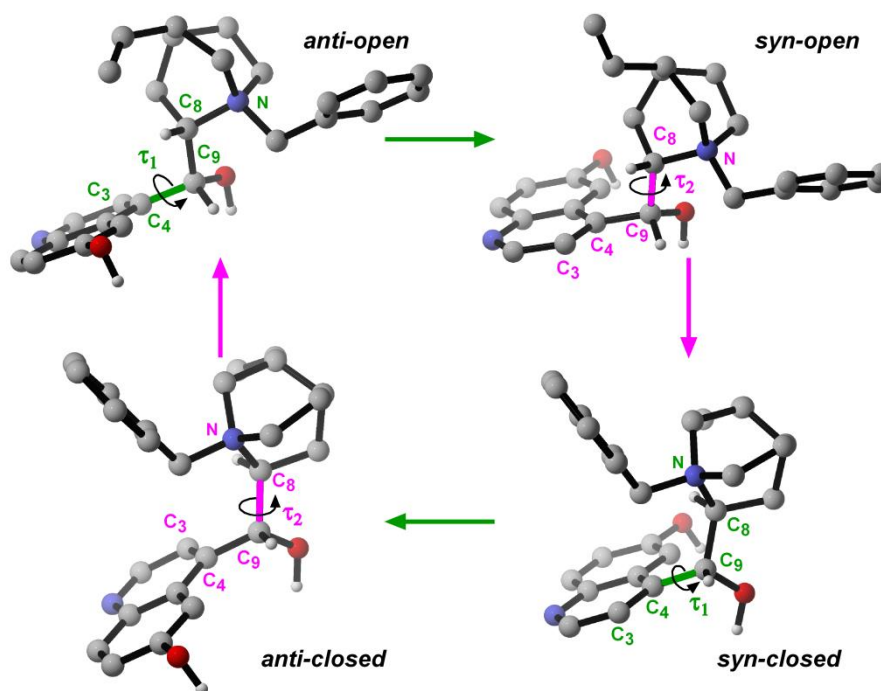
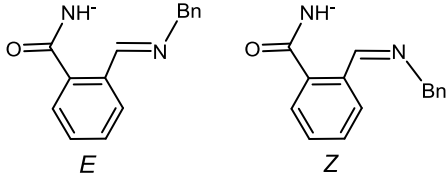


Figure S1. The most relevant conformations of QNHOH-1 ammonium cation and definition of dihedral angles.**Table S1.** Relative energies (kcal/mol, referred to the most stable conformer 1-AO) of the conformers of QNOH-1 ammonium cation. A(S)O(C) denotes Anti(Syn) Open(Closed) conformations, see Figure S1.

#	Conformation	Rel. energy
1	AO	0.0
2	AO	0.2
3	AO	0.3
4	AO	0.5
5	AO	0.6
6	AO	0.6
7	SO	0.8
8	AO	1.0
9	AO	1.0
10	AO	1.5
11	AO	2.0
12	AO	3.1
13	SO	3.1
14	AO	3.2
15	SO	3.2
16	SO	3.2
17	SO	3.2
18	AO	3.3
19	AO	3.4
20	AO	3.4
21	SO	3.5
22	AO	3.5
23	AO	3.5
24	SO	3.6
25	AO	3.8
26	AO	3.9
27	SO	4.4
28	SO	4.5
29	AO	4.6
30	SO	4.7
31	SC	4.9
32	AO	4.9
33	AO	5.0
34	AO	5.1
35	AO	5.2
36	SO	5.2
37	SO	5.3
38	AO	5.3
39	SO	5.4
40	SC	5.5
41	AO	5.6

42	SO	5.6
43	AO	5.6
44	SO	5.7
45	AO	5.7
46	AC	5.8
47	SC	5.8
48	AO	5.8
49	SO	5.9
50	SO	6.1
51	SC	6.5
52	SC	6.7
53	SC	6.8
54	SC	6.9
55	SC	7.1
56	SC	7.2
57	AC	7.3
58	SC	7.3
59	SC	7.5
60	SC	7.9
61	AC	8.0
62	AC	8.2

Table S2. Relative energies (kcal/mol, referred to the most stable 1-*E*) of the conformers of the **A** intermediate, *E* and *Z* configurations.

 <i>E</i> <i>Z</i>		
#	Configuration	Rel. energy
1	<i>E</i>	0.0
2	<i>E</i>	0.1
3	<i>E</i>	0.4
4	<i>E</i>	0.6
5	<i>E</i>	1.7
6	<i>E</i>	2.0
7	<i>E</i>	2.2
8	<i>E</i>	2.4
9	<i>Z</i>	3.7
10	<i>Z</i>	3.9
11	<i>Z</i>	4.0
12	<i>Z</i>	4.3
13	<i>Z</i>	4.4
14	<i>Z</i>	6.1
15	<i>Z</i>	6.2
16	<i>Z</i>	6.3
17	<i>Z</i>	6.3
18	<i>Z</i>	6.4
19	<i>Z</i>	6.9
20	<i>Z</i>	7.8

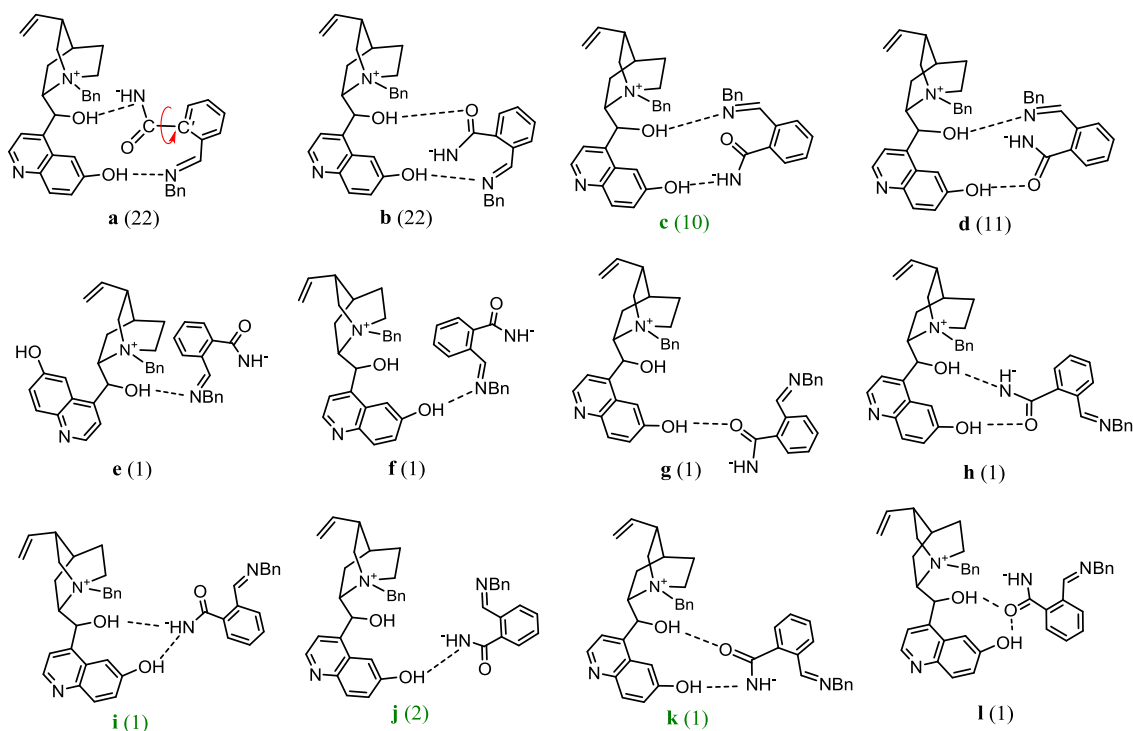


Figure S2. Schematic representation of the hydrogen bond patterns of QNOH-1:A binary complexes. The number of unique complexes detected for each pattern is reported in parentheses; arrangements allowing for proton transfer have been highlighted in green, see also Figure S3.

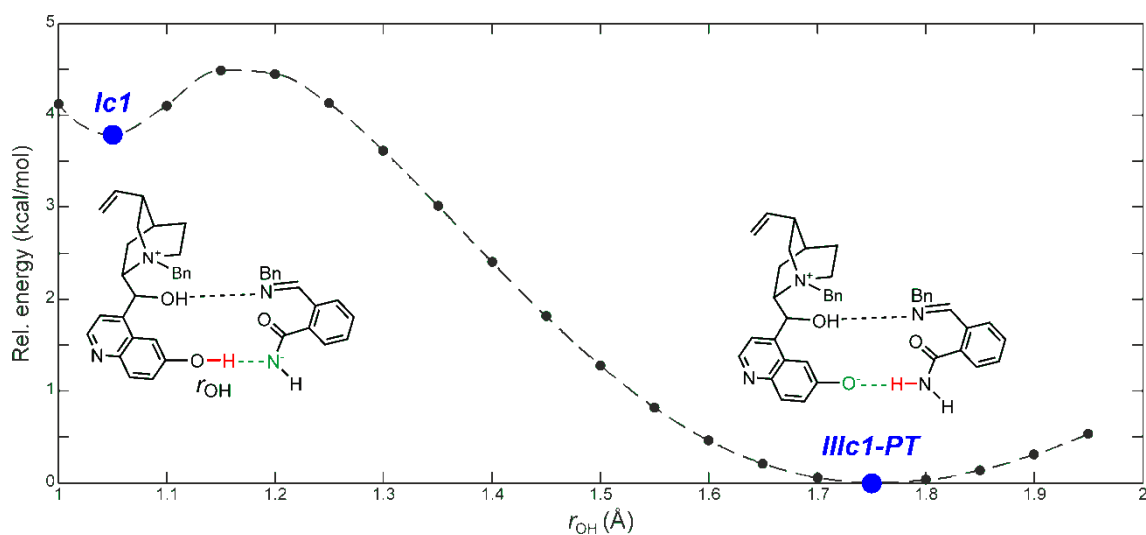


Figure S3. Potential energy profile of the most stable QNOH-1:A binary complex of pattern **c** along the r_{OH} coordinate. Energy refers to **IIIC1-PT**. The range $1.00 \leq r_{\text{OH}} \leq 1.95$ Å with steps of 0.05 Å was explored, fixing in each computation the value of r_{OH} while optimizing all other internal coordinates of the molecule. Please note that **Ic1** and **IIIC1-PT** have been indicated as **Ic** and **IIc-PT**, respectively in the main article (see Figure 3 of the main article).

Table S3. Relative energies (kcal/mol, referred to non-interacting ammonium cation QNOH-1 and A intermediate in their most stable conformations) of pre-reactive binary complexes (I,RC) and their corresponding transition states (II,TS) for the ring closure process. Complexes have been numbered according to increasing energy; *E* / *Z* indicate the configuration of the A intermediate; a, b, ... denote the pattern of hydrogen bonds, see Figure S2; *R* / *S* indicate the enantiomer of the final product.

	I (RC)	II (TS)
b1E-R†	-38.7	-30.0
b2E-R†	-38.6	-27.8
h1E-R	-37.0	-13.0
d1E-R	-36.9	-27.4
b3E-R	-36.8	-25.4
b4E-R	-36.8	-25.2
d2E-S†	-36.4	-28.3
b5Z-S	-34.6	-21.0
d3E-S	-34.2	-27.7
b6E-R	-34.2	-22.9
d4E-S	-33.7	-26.5
b7E-R	-33.6	-23.5
b8E-R	-33.5	-23.8
d5E-S	-33.5	-25.6
b9E-R	-33.0	-22.7
b10Z-S	-32.6	-23.9
b11E-S	-32.0	-21.0
b13Z-R	-29.7	-19.4
e1E-R	-29.6	-22.9
d6Z-S	-29.0	-15.0
b15E-S	-28.9	-19.4
d7Z-R	-28.3	-16.7
a16Z-S	-28.3	-16.8
i1E-S	-28.3	-10.2
d8Z-S	-27.6	-10.6
d9Z-R	-27.6	-14.1
b16Z-S	-27.4	-15.2
g1Z-S	-27.1	-14.2
d10Z-S	-26.3	-12.2
a19Z-S	-25.7	-18.8
d11Z-R	-25.7	-12.9
a20Z-S	-24.7	-17.7
b18Z-R	-23.3	-10.0
b19Z-R	-21.8	-12.6
b20Z-S	-21.1	-11.9
f1Z-R	-19.7	-15.7
b21Z-R	-17.0	-8.7
b22Z-S	-16.1	-6.6

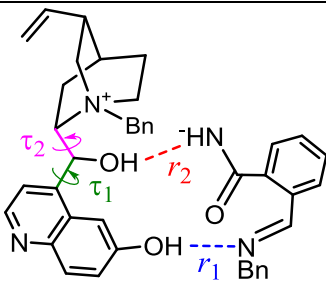
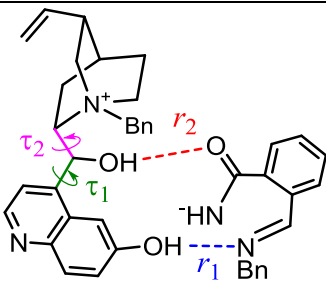
† RC/TS for **b1E-R**, **b2E-R** and **d2E-S** have been denoted as **Ib1/Iib1-R**, **Ib2/Iib2-R** and **Id/IId-S**, respectively, in Figure 3 of the main article.

Table S4. Relative energies (kcal/mol, referred to non-interacting ammonium cation QNOH-1 and A intermediate in their most stable conformations) of starting binary complexes (I,BC) giving rise to pre-reaction arrangements upon torsion about the C-C' bond (See Figure S2). BC have been numbered according to increasing energy; *E* / *Z* indicate the configuration assumed by the A intermediate; a-l denote the pattern of hydrogen bonds, see Figure S2. Energies of the proton transferred complexes (III-PT, PC) have been reported for **c**, **i**, **j** and **k** patterns (see Figure 3 in the main article).

	I (BC)	III-PT (PC)
a1E†	-40.7	
a2E†	-40.6	
c1E†	-39.5	-42.5
k1E	-38.7	-36.7
a3E	-38.5	
a4E	-38.5	
c2E	-36.9	-39.6
c3E	-36.5	-39.3
j1Z	-36.5	-38.1
c4E	-36.2	-38.6
c5E	-35.1	-38.5
a5E	-34.4	
a6E	-34.3	
a7E	-34.0	
c6Z	-33.8	-35.8
a8E	-33.7	
a9Z	-33.6	
a10Z	-33.2	
a11E	-32.5	
a12Z	-31.3	
a13Z	-30.8	
c7Z	-30.8	-31.6
j2Z	-30.8	-35.9
c8Z	-30.8	-33.3
l1E	-30.5	
b12Z	-29.7	
a14Z	-29.3	
c9Z	-29.2	-31.4
b14Z	-29.2	
c10Z	-29.1	-33.6
a15E	-28.4	
i1E	-28.3	-30.9
b17Z	-27.3	
a17Z	-26.8	
a18Z	-25.8	
a21Z	-21.8	
a22Z	-17.8	

† BC/PC for **a1E-R**, **a2E-R** and **c1E** have been denoted as **Ia1**, **Ia2** and **Ic/IIIc-PT**, respectively, in Figure 3 of the main article.

Table S5. Geometrical parameters of the two most stable conformers of patterns **a** and **b**. **Ia1(Ib1)** is more stable (by ca 0.1 kcal/mol) than **Ia2(Ib2)**, see Figure 3 of the main article and Tables S3, S4.

				
	$\tau_1/\text{degrees}$	$\tau_2/\text{degrees}$	$r_1/\text{\AA}$	$r_2/\text{\AA}$
Ia1	99.1	165.5	1.85	1.59
Ia2	101.9	163.9	1.83	1.63
Ib1	100.4	171.2	1.81	1.61
Ib2	101.5	166.6	1.82	1.65

Cartesian coordinates (Å) of the conformers of ammonium cation QNOH-1

AO, SO, AC, SC denote Anti(Syn) Open(Closed) conformations.

01 AO; Energy (including ZPVE) = -1267.304620 Hartree

H	-2.788115	-2.735617	1.951721
C	-1.907424	-2.734847	1.302945
C	0.411700	-1.912928	1.013140
C	0.040742	-0.716816	0.123959
C	-0.705032	-2.136365	2.036407
C	-2.170301	-1.908053	0.035215
H	0.550300	-2.810487	0.400036
H	0.404088	0.203064	0.589077
H	-3.231936	-1.704588	-0.103619
H	-1.704975	-3.769741	1.016428
H	1.363957	-1.689825	1.500913
H	-0.368022	-2.801176	2.835530
H	-1.767023	-2.369609	-0.864770
N	-1.487694	-0.558116	0.151433
C	-1.130184	-0.774565	2.628309
H	-1.881751	-0.973952	3.401821
C	-1.828599	0.022791	1.509432
H	-2.915009	-0.026216	1.597997
H	-1.536169	1.074436	1.493120
C	0.035257	-0.091291	3.304516
H	0.485070	-0.699629	4.089729
C	0.556931	1.108618	3.062237
H	1.406289	1.464635	3.635823
H	0.177067	1.793116	2.307585
C	0.660620	-0.783939	-1.279428
O	0.110847	-1.897527	-1.946005
C	-1.949454	0.365242	-0.963636
H	-1.724302	-0.166997	-1.890091
H	-1.315527	1.254145	-0.896214
H	0.456863	-1.919158	-2.852483
H	0.431565	0.136846	-1.830851
H	2.274131	-2.947146	-1.619646
C	2.822699	-2.058885	-1.325553
C	2.169667	-0.871382	-1.123232
N	4.962107	-1.108341	-0.764569
C	2.933151	0.271885	-0.731872
C	4.225889	-2.125807	-1.138280
C	4.334135	0.084706	-0.559144
C	2.376878	1.556126	-0.510718
H	4.740218	-3.070509	-1.301413
H	6.194037	1.021954	-0.025721
C	3.176812	2.603093	-0.112108
H	1.321872	1.759398	-0.662748
C	4.570247	2.416309	0.072649
H	5.184520	3.256086	0.386194
C	5.129342	1.187838	-0.153035
O	2.590444	3.807710	0.092150
H	3.258617	4.461415	0.348656
C	-3.406575	0.746400	-0.916084
C	-6.104598	1.483538	-0.900511
C	-3.827187	1.877249	-0.209433
C	-4.347872	0.005058	-1.637212
C	-5.691550	0.368184	-1.625508
C	-5.170408	2.240545	-0.196313
H	-3.101628	2.486341	0.323603
H	-4.026877	-0.854759	-2.220612
H	-6.412179	-0.214673	-2.189695
H	-5.484225	3.120174	0.356053
H	-7.151384	1.769997	-0.894084

02 AO

H	-2.779677	-3.140271	1.042969
C	-1.880743	-2.923612	0.458757
C	0.416075	-2.011515	0.504924
C	0.050163	-0.635353	-0.071805
C	-0.731001	-2.516708	1.383217
C	-2.147168	-1.781133	-0.535386
H	0.594882	-2.719619	-0.311645
H	0.382572	0.157224	0.605993
H	-3.210301	-1.554630	-0.614861
H	-1.620835	-3.826754	-0.098823
H	1.349527	-1.917600	1.065238
H	-0.404122	-3.362694	1.991885
H	-1.742640	-1.975935	-1.526873
N	-1.480684	-0.504409	-0.054193
C	-1.236530	-1.385072	2.300155
H	-2.034595	-1.793785	2.929137
C	-1.870726	-0.297640	1.395871
H	-2.960755	-0.331806	1.427375
H	-1.546688	0.708613	1.675343
C	-0.167146	-0.837973	3.209138
H	0.665600	-0.307263	2.745092
C	-0.186072	-0.982459	4.530620
H	0.608702	-0.590356	5.156815
H	-0.999524	-1.501333	5.032130
C	0.706750	-0.351302	-1.433829
O	0.148209	-1.239917	-2.374525
C	-1.924026	0.675639	-0.904447
H	-1.664518	0.405222	-1.929937
H	-1.309436	1.521436	-0.584541
H	0.510895	-1.032718	-3.250772
H	0.504656	0.686067	-1.728537
H	2.256360	-2.410692	-2.283748
C	2.829457	-1.640267	-1.779575
C	2.211411	-0.517900	-1.292673
N	4.993884	-0.923286	-1.009073
C	3.008663	0.472306	-0.639234
C	4.228255	-1.796385	-1.615837
C	4.402875	0.204842	-0.522300
C	2.494146	1.684660	-0.117950
H	4.713363	-2.689535	-2.003956
H	6.290887	0.931062	0.205157
C	3.327563	2.585188	0.507037
H	1.446086	1.948338	-0.209785
C	4.713882	2.315994	0.634338
H	5.356302	3.040994	1.127152
C	5.232274	1.155577	0.127136
O	2.781186	3.728727	0.986288
H	3.466980	4.275767	1.398277
C	-3.386005	1.023330	-0.802070
C	-6.091614	1.713038	-0.661487
C	-3.831155	1.948789	0.146547
C	-4.305117	0.470007	-1.699088
C	-5.653140	0.808351	-1.625695
C	-5.178787	2.287659	0.220939
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H	-3.961449	-0.220586	-2.465705

H	-6.357505	0.373521	-2.327119
H	-5.514522	3.006435	0.961224
H	-7.141985	1.980466	-0.606002

03 AO

H	-4.917535	-1.396689	0.458747
C	-3.963855	-1.704675	0.019704
C	-1.540276	-2.030788	0.436454
C	-1.100791	-0.690860	-0.181096
C	-2.902174	-1.862666	1.111155
C	-3.475161	-0.662281	-0.997272
H	-1.597863	-2.797691	-0.343210
H	-0.516679	-0.126635	0.549126
H	-4.262106	0.040368	-1.276517
H	-4.125749	-2.653652	-0.496980
H	-0.775500	-2.338040	1.154074
H	-3.126638	-2.724295	1.744573
H	-3.060076	-1.112861	-1.896773
N	-2.351503	0.172855	-0.392937
C	-2.889675	-0.572584	1.954618
H	-3.854723	-0.505640	2.471295
C	-2.804549	0.617405	0.982273
H	-3.772883	1.102168	0.839420
H	-2.093260	1.357946	1.331401
C	-1.811920	-0.617267	3.013094
H	-1.928361	-1.449004	3.708228
C	-0.774907	0.200582	3.179702
H	-0.070078	0.038502	3.988315
H	-0.570642	1.061039	2.544762
C	-0.221500	-0.881172	-1.421813
O	-0.976032	-1.567344	-2.395204
C	-2.156957	1.373543	-1.309524
H	-3.113426	1.902172	-1.273206
H	-2.042776	0.950451	-2.310759
H	-0.451278	-1.626463	-3.209172
H	0.086722	0.095044	-1.804612
H	0.445667	-3.478515	-1.899405
C	1.200690	-2.950846	-1.326472
C	1.032563	-1.629841	-0.999685
N	3.326818	-3.070094	-0.204237
C	2.052705	-0.975765	-0.243318
C	2.370719	-3.628973	-0.906550
C	3.181697	-1.757154	0.130205
C	2.000912	0.389407	0.144090
H	2.502737	-4.676994	-1.167241
H	5.069850	-1.764345	1.161380
C	3.024113	0.944795	0.877471
H	1.164222	1.021357	-0.139448
C	4.148040	0.165714	1.256988
H	4.935004	0.640434	1.833418
C	4.219722	-1.148177	0.887926
O	3.028361	2.239113	1.274656
H	2.225318	2.682455	0.951179
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C	1.094542	4.141479	-0.610128
C	0.000683	2.474501	-1.966352
C	-0.999272	3.166539	0.107980
C	0.060672	4.046275	0.321628
C	1.049616	3.366792	-1.768342
H	-0.029958	1.890334	-2.882784
H	-1.829254	3.182114	0.806056
H	0.059261	4.679952	1.202467
H	1.827353	3.459087	-2.518776
H	1.911035	4.839035	-0.449782

04 AO

H	-2.804281	-3.060066	1.258475
C	-1.920350	-2.896165	0.634771
C	0.377812	-2.006165	0.541904
C	0.005795	-0.628801	-0.019067
C	-0.727595	-2.469503	1.496551
C	-2.189498	-1.800272	-0.410499
H	0.486806	-2.726320	-0.276852
H	0.352714	0.150047	0.669612
H	-3.253393	-1.582639	-0.502252
H	-1.702088	-3.832809	0.116247
H	1.346418	-1.918184	1.036663
H	-0.386631	-3.304694	2.112721
H	-1.781195	-2.036368	-1.391825
N	-1.527008	-0.502876	0.021121
C	-1.190546	-1.299132	2.383754
H	-1.959489	-1.678947	3.068491
C	-1.896116	-0.267741	1.469788
H	-2.983072	-0.343728	1.522815
H	-1.608607	0.758409	1.713584
C	-0.108428	-0.664075	3.227510
H	-0.319747	0.350122	3.567935
C	1.019586	-1.250149	3.620300
H	1.723107	-0.729746	4.261918
H	1.280509	-2.266544	3.337293
C	0.633228	-0.339961	-1.392759
O	0.052170	-1.226853	-2.322827
C	-1.997176	0.653231	-0.847509
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H	-1.384116	1.511015	-0.558153
H	0.396371	-1.018816	-3.206219
H	0.423138	0.697712	-1.680947
H	2.157257	-2.405587	-2.272048
C	2.744765	-1.631552	-1.790331
C	2.140736	-0.506654	-1.291578
N	4.931979	-0.905382	-1.095888
C	2.956826	0.488329	-0.669601
C	4.148447	-1.784251	-1.670682
C	4.354729	0.224783	-0.597448
C	2.456509	1.702097	-0.138640
H	4.622365	-2.679169	-2.068462
H	6.264085	0.960625	0.061573
C	3.307697	2.608618	0.452435
H	1.404239	1.958918	-0.191664
C	4.698389	2.344318	0.534213
H	5.355074	3.073913	1.000900
C	5.202860	1.181972	0.017537
O	2.774493	3.753517	0.944045
H	3.472213	4.302810	1.332280
C	-3.460013	0.990143	-0.721702
C	-6.169658	1.653288	-0.530686
C	-3.893154	1.932873	0.215432
C	-4.394147	0.407231	-1.583643
C	-5.743877	0.732248	-1.485005
C	-5.242366	2.258485	0.315233
H	-3.170997	2.424363	0.862972
H	-4.061387	-0.295740	-2.343773
H	-6.459588	0.274145	-2.159687
H	-5.568310	2.990569	1.046861

H	-7.221522	1.909692	-0.455017
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05 AO

H	-2.747236	-2.550001	2.194563
C	-1.871010	-2.590577	1.540960
C	0.428104	-1.756931	1.156424
C	0.030292	-0.650442	0.169602
C	-0.676284	-1.903940	2.206443
C	-2.159698	-1.888603	0.203889
H	0.575581	-2.704003	0.625778
H	0.375012	0.310745	0.558093
H	-3.226228	-1.716883	0.060135
H	-1.648815	-3.642755	1.347854
H	1.381088	-1.476160	1.612155
H	-0.321569	-2.485007	3.061056
H	-1.758392	-2.424896	-0.654461
N	-1.501139	-0.520799	0.189921
C	-1.124196	-0.500593	2.672932
H	-1.864680	-0.641669	3.469374
C	-1.848727	0.173055	1.491185
H	-2.932654	0.105876	1.592294
H	-1.585036	1.225129	1.371043
C	0.032258	0.266650	3.270477
H	0.505332	-0.257488	4.101122
C	0.521107	1.451965	2.914408
H	1.367022	1.880636	3.441140
H	0.113078	2.054989	2.106462
C	0.645603	-0.821575	-1.228026
O	0.064904	-1.963137	-1.816558
C	-1.983009	0.295053	-0.998331
H	-1.747415	-0.308412	-1.877064
H	-1.366632	1.198659	-1.003200
H	0.395952	-2.048979	-2.725008
H	0.431518	0.066252	-1.836971
H	2.184383	-3.042490	-1.457771
C	2.765266	-2.159422	-1.215553
C	2.153938	-0.939618	-1.075227
N	4.936763	-1.254958	-0.714299
C	2.958186	0.195643	-0.751502
C	4.164462	-2.265835	-1.031425
C	4.352114	-0.032870	-0.571800
C	2.452423	1.514948	-0.600349
H	4.646065	-3.234386	-1.146073
H	6.249799	0.858415	-0.092732
C	3.296585	2.547571	-0.260891
H	1.401595	1.735253	-0.770385
C	4.683578	2.318091	-0.067178
H	5.312914	3.160900	0.197780
C	5.192345	1.060873	-0.225933
O	2.883358	3.826586	-0.094800
H	1.928018	3.889475	-0.246359
C	-3.446113	0.653460	-0.974134
C	-6.157832	1.338318	-0.986432
C	-3.878579	1.842544	-0.378903
C	-4.382774	-0.173560	-1.602137
C	-5.733288	0.163661	-1.603304
C	-5.228454	2.180696	-0.379378
H	-3.156859	2.515510	0.077096
H	-4.052165	-1.080231	-2.102955
H	-6.450573	-0.486391	-2.093167
H	-5.552309	3.105556	0.086294
H	-7.210037	1.603683	-0.989475

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H	-4.681057	-1.628766	-0.995287
C	-3.591339	-1.553085	-0.962693
C	-1.556602	-1.699216	0.419859
C	-0.957322	-0.465608	-0.295863
C	-3.081712	-1.610208	0.477404
C	-3.157332	-0.221463	-1.584917
H	-1.282946	-2.602273	-0.131788
H	-0.392308	0.141596	0.415099
H	-3.978098	0.498302	-1.637895
H	-3.172583	-2.382368	-1.538583
H	-1.116671	-1.785667	1.416666
H	-3.485409	-2.485327	0.992389
H	-2.728418	-0.351948	-2.574031
N	-2.101388	0.462697	-0.720407
C	-3.536245	-0.328798	1.202016
H	-4.611284	-0.206726	1.027173
C	-2.790775	0.869479	0.569417
H	-3.467717	1.691811	0.327906
H	-2.010983	1.237570	1.237204
C	-3.301999	-0.367371	2.687050
H	-2.264519	-0.451350	3.014217
C	-4.275321	-0.307823	3.590646
H	-4.065621	-0.352732	4.654366
H	-5.317933	-0.215354	3.295830
C	0.005157	-0.832899	-1.433399
O	-0.747885	-1.495343	-2.423453
C	-1.645526	1.680785	-1.507243
H	-2.535100	2.311981	-1.584945
H	-1.416737	1.308251	-2.508114
H	-0.172793	-1.675756	-3.183940
H	0.450709	0.083396	-1.839316
H	0.421911	-3.486981	-1.803666
C	1.174919	-3.035239	-1.167108
C	1.129447	-1.695480	-0.874797
N	3.143176	-3.381412	0.170694
C	2.142190	-1.149335	-0.027386
C	2.206586	-3.837837	-0.625045
C	3.121132	-2.053757	0.475343
C	2.221426	0.220575	0.337030
H	2.237960	-4.898847	-0.863155
H	4.864539	-2.272484	1.715039
C	3.214866	0.659760	1.182930
H	1.513302	0.944724	-0.055463
C	4.183010	-0.242674	1.694799
H	4.948137	0.144009	2.359598
C	4.134730	-1.561440	1.342190
O	3.334737	1.948494	1.578153
H	2.618902	2.478565	1.188087
C	-0.466589	2.476341	-0.994911
C	1.730884	4.062888	-0.265371
C	0.638790	2.609621	-1.845560
C	-0.470273	3.177112	0.216011
C	0.629351	3.951369	0.584909
C	1.730496	3.394080	-1.488012
H	0.640554	2.102813	-2.807601
H	-1.337753	3.162271	0.866690
H	0.611821	4.490816	1.526393
H	2.574484	3.484651	-2.163316
H	2.576592	4.682942	0.017041

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H	-2.772537	-3.172659	0.948841
C	-1.874467	-2.932448	0.372720
C	0.418900	-2.015846	0.447985
C	0.049957	-0.622576	-0.084519
C	-0.726585	-2.551421	1.310333
C	-2.145787	-1.758775	-0.583184
H	0.597988	-2.697020	-0.391057
H	0.381763	0.148391	0.618433
H	-3.209689	-1.532547	-0.651992
H	-1.610078	-3.815492	-0.214098
H	1.352878	-1.938133	1.009779
H	-0.397181	-3.415461	1.891604
H	-1.743600	-1.920041	-1.581434
N	-1.481561	-0.496083	-0.062185
C	-1.235134	-1.451380	2.263062
H	-2.032626	-1.881562	2.878214
C	-1.871804	-0.337184	1.393333
H	-2.961785	-0.374547	1.423777
H	-1.549616	0.660324	1.703951
C	-0.167355	-0.930199	3.188785
H	0.669985	-0.393983	2.739534
C	-0.192069	-1.102943	4.506743
H	0.602227	-0.727927	5.143910
H	-1.009453	-1.628811	4.994340
C	0.706230	-0.294309	-1.437159
O	0.143929	-1.150089	-2.405559
C	-1.929134	0.710048	-0.872717
H	-1.662097	0.478471	-1.905594
H	-1.323199	1.548338	-0.518173
H	0.516848	-0.925718	-3.273271
H	0.505997	0.752629	-1.698527
H	2.236540	-2.341984	-2.338700
C	2.817788	-1.590055	-1.816348
C	2.210604	-0.472336	-1.302049
N	4.985995	-0.915124	-1.024004
C	3.017021	0.492636	-0.625852
C	4.212660	-1.765482	-1.654929
C	4.407011	0.206185	-0.511985
C	2.516216	1.703133	-0.077501
H	4.689639	-2.653584	-2.063953
H	6.302838	0.887783	0.240800
C	3.362597	2.577701	0.565365
H	1.467170	1.966667	-0.175924
C	4.745097	2.284744	0.695074
H	5.376858	2.999957	1.211015
C	5.248242	1.131168	0.164760
O	2.957085	3.751892	1.104184
H	2.009026	3.881137	0.948209
C	-3.393934	1.044352	-0.767039
C	-6.104278	1.713298	-0.621587
C	-3.851131	1.932407	0.210999
C	-4.303387	0.517676	-1.689636
C	-5.653825	0.845555	-1.613798
C	-5.201144	2.261175	0.287607
H	-3.146627	2.377916	0.909395
H	-3.950577	-0.144202	-2.477145
H	-6.350989	0.431090	-2.334435
H	-5.546059	2.951447	1.050415
H	-7.156523	1.972790	-0.564364

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H	-2.798366	-3.102565	1.167528
C	-1.914245	-2.911923	0.552019
C	0.380685	-2.012458	0.492906
C	0.006181	-0.620686	-0.029929
C	-0.725862	-2.507211	1.430308
C	-2.188621	-1.783377	-0.456372
H	0.493473	-2.708635	-0.345809
H	0.351836	0.139540	0.679990
H	-3.253211	-1.564749	-0.537297
H	-1.688164	-3.829117	0.002941
H	1.347883	-1.936098	0.992247
H	-0.383989	-3.359941	2.021516
H	-1.783592	-1.986549	-1.446069
N	-1.527126	-0.498765	0.013171
C	-1.195302	-1.366640	2.351725
H	-1.967402	-1.769093	3.019782
C	-1.897308	-0.306597	1.467602
H	-2.984489	-0.381265	1.516970
H	-1.607309	0.711321	1.741849
C	-0.119783	-0.757130	3.221905
H	-0.341065	0.240393	3.602925
C	1.012157	-1.348785	3.594571
H	1.709356	-0.848743	4.258908
H	1.282854	-2.350721	3.272400
C	0.634976	-0.293461	-1.394757
O	0.053211	-1.153716	-2.348836
C	-1.999311	0.680636	-0.822079
H	-1.752233	0.421377	-1.853305
H	-1.390882	1.531566	-0.504589
H	0.407401	-0.931011	-3.224715
H	0.425886	0.751809	-1.655751
H	2.145844	-2.348681	-2.311466
C	2.738862	-1.588616	-1.814606
C	2.142310	-0.467167	-1.295816
N	4.927327	-0.893602	-1.098208
C	2.964255	0.508943	-0.655323
C	4.138857	-1.755780	-1.693466
C	4.358718	0.231322	-0.582509
C	2.473894	1.722854	-0.105674
H	4.607441	-2.646837	-2.105784
H	6.273999	0.933989	0.098432
C	3.335218	2.610421	0.497995
H	1.419463	1.975540	-0.168021
C	4.723250	2.327939	0.584831
H	5.367368	3.054042	1.069371
C	5.215981	1.170191	0.053903
O	2.940082	3.788639	1.036436
H	1.986254	3.909355	0.911796
C	-3.463845	1.008384	-0.692587
C	-6.176641	1.656336	-0.497739
C	-3.905847	1.919007	0.271718
C	-4.390622	0.449656	-1.578288
C	-5.741979	0.767108	-1.477887
C	-5.256722	2.237197	0.373126
H	-3.189336	2.390941	0.939921
H	-4.050654	-0.228944	-2.357162
H	-6.452148	0.327920	-2.170690
H	-5.589743	2.944392	1.125707
H	-7.229773	1.906967	-0.420638

09 AO

H	-3.905741	-3.130546	0.681297
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C	-2.911122	-3.068748	0.230093
C	-0.561160	-2.368610	0.567410
C	-0.694371	-1.017352	-0.157275
C	-1.870165	-2.695031	1.285894
C	-2.887510	-2.009748	-0.882014
H	-0.322571	-3.156594	-0.155370
H	-0.383965	-0.211871	0.512665
H	-3.893412	-1.706375	-1.175828
H	-2.682050	-4.044646	-0.205134
H	0.272595	-2.294591	1.270141
H	-1.726924	-3.514258	1.994909
H	-2.338947	-2.333061	-1.763733
N	-2.187332	-0.746803	-0.392958
C	-2.365668	-1.436043	2.024940
H	-3.272684	-1.712328	2.575953
C	-2.772222	-0.398764	0.961803
H	-3.856198	-0.363030	0.825337
H	-2.421200	0.597438	1.217119
C	-1.348945	-0.965477	3.039059
H	-1.113096	-1.723390	3.786602
C	-0.728555	0.209684	3.116444
H	-0.010235	0.399648	3.907073
H	-0.895883	1.032835	2.424769
C	0.187447	-0.933910	-1.409209
O	-0.295765	-1.865143	-2.351145
C	-2.481708	0.349696	-1.415031
H	-3.569492	0.339348	-1.517622
H	-2.054138	-0.010348	-2.353514
H	0.218441	-1.772854	-3.168906
H	0.134269	0.078119	-1.819242
H	1.681245	-3.160463	-1.857508
C	2.225930	-2.394723	-1.315992
C	1.629778	-1.200022	-1.006577
N	4.292490	-1.772979	-0.249420
C	2.388307	-0.223026	-0.289094
C	3.564720	-2.633426	-0.917435
C	3.721764	-0.575799	0.068103
C	1.893001	1.053390	0.072653
C	4.033063	-3.583486	-1.166220
H	5.520925	0.069071	1.052200
C	2.684815	1.936165	0.772326
H	0.895344	1.381590	-0.199939
C	4.008757	1.583978	1.138673
H	4.618365	2.293735	1.691759
C	4.509153	0.358969	0.788730
O	2.156376	3.142956	1.091738
H	2.811103	3.675587	1.568072
C	-2.018358	1.750341	-1.085618
C	-1.229843	4.389755	-0.541007
C	-0.951117	2.335480	-1.774774
C	-2.734016	2.540506	-0.175075
C	-2.334695	3.841905	0.107628
C	-0.551499	3.641303	-1.497730
H	-0.439627	1.787177	-2.561047
H	-3.627028	2.146486	0.301554
H	-2.897743	4.432453	0.822783
H	0.285279	4.072259	-2.037557
H	-0.916975	5.405103	-0.320262

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H	-4.800792	-1.384121	-0.891474
C	-3.709019	-1.335304	-0.884189
C	-1.643854	-1.600584	0.437737
C	-1.026557	-0.369626	-0.266904
C	-3.164739	-1.466785	0.538402
C	-3.260509	0.010743	-1.460524
C	-1.408863	-2.499285	-0.138128
H	-0.407800	0.190753	0.437161
H	-4.058668	0.757121	-1.441555
H	-3.324208	-2.148133	-1.504876
H	-1.185654	-1.710629	1.423439
H	-3.587341	-2.354465	1.015044
H	-2.878964	-0.082421	-2.472946
N	-2.148130	0.617553	-0.609542
C	-3.553867	-0.205278	1.318879
H	-4.623599	-0.022862	1.149792
C	-2.773609	0.992870	0.720893
H	-3.416955	1.856939	0.540942
H	-1.955111	1.288483	1.378700
C	-3.333311	-0.254935	2.810726
H	-3.475715	0.696677	3.323460
C	-3.009100	-1.328436	3.525221
H	-2.887798	-1.262754	4.601488
H	-2.859564	-2.307934	3.079569
C	-0.127436	-0.732331	-1.457222
O	-0.944854	-1.318908	-2.443724
C	-1.671353	1.851137	-1.359501
H	-2.539311	2.515837	-1.385460
H	-1.484393	1.514357	-2.381478
H	-0.403836	-1.496276	-3.229750
H	0.344379	0.179459	-1.843926
H	0.152861	-3.383572	-1.952984
C	0.952829	-2.991871	-1.334125
C	0.978596	-1.665641	-0.982886
N	2.965579	-3.477152	-0.110502
C	2.051155	-1.199984	-0.161836
C	1.973429	-3.859371	-0.877088
C	3.014078	-2.164736	0.251435
C	2.205363	0.146737	0.259927
H	1.948415	-4.909132	-1.161460
H	4.808234	-2.510008	1.385083
C	3.256803	0.506151	1.072808
H	1.508762	0.916751	-0.059488
C	4.212474	-0.455512	1.491298
H	5.027464	-0.130673	2.129431
C	4.090748	-1.753695	1.083891
O	3.446618	1.769119	1.520012
H	2.732246	2.342054	1.192879
C	-0.448721	2.579225	-0.848503
C	1.828043	4.046249	-0.111022
C	0.639551	2.705656	-1.721615
C	-0.393961	3.227131	0.390397
C	0.744636	3.940363	0.762801
C	1.770361	3.431366	-1.360488
H	0.596484	2.241950	-2.704127
H	-1.245258	3.217951	1.062128
H	0.772819	4.437874	1.726874
H	2.599833	3.518952	-2.053929
H	2.703916	4.621379	0.174522

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H	-4.324685	-2.329944	-0.939159
C	-3.267569	-2.058142	-0.881737
C	-1.290728	-1.780542	0.565128

C	-0.853008	-0.556813	-0.274877
C	-2.813405	-1.924733	0.572665
C	-3.056472	-0.712517	-1.580900
H	-0.860427	-2.687818	0.134240
H	-0.371699	0.184937	0.367759
H	-3.980397	-0.132466	-1.642132
H	-2.684067	-2.832479	-1.386264
H	-0.887453	-1.685720	1.576709
H	-3.099594	-2.807456	1.149401
H	-2.635029	-0.821296	-2.575643
N	-2.109498	0.169162	-0.772364
C	-3.480782	-0.671692	1.171405
H	-4.550714	-0.712139	0.935804
C	-2.865809	0.567294	0.482110
H	-3.631777	1.285169	0.181132
H	-2.149748	1.069604	1.134923
C	-3.330807	-0.566401	2.663511
H	-2.310684	-0.511268	3.045395
C	-4.355504	-0.539523	3.510000
H	-4.204269	-0.474258	4.582606
H	-5.383169	-0.584080	3.157465
C	0.151272	-0.895234	-1.387972
O	-0.529667	-1.666838	-2.350695
C	-1.809003	1.382571	-1.639700
H	-2.789574	1.818366	-1.852828
H	-1.412920	0.980291	-2.574811
H	0.072378	-1.842604	-3.091245
H	0.514827	0.038856	-1.834395
H	0.773194	-3.523585	-1.609882
C	1.499979	-2.975453	-1.020196
C	1.348963	-1.630159	-0.799161
N	3.529135	-3.085758	0.267110
C	2.335357	-0.956335	-0.012659
C	2.609258	-3.660860	-0.466775
C	3.405323	-1.747697	0.497566
C	2.308877	0.430505	0.273193
H	2.719809	-4.728198	-0.664658
H	5.210334	-1.747436	1.663527
C	3.300259	1.003698	1.038765
C	1.529291	1.079680	-0.110375
C	4.361137	0.216856	1.553896
H	5.133727	0.688026	2.155847
C	4.407034	-1.123989	1.285173
O	3.228328	2.335647	1.279830
H	3.987741	2.615601	1.813293
C	-0.865441	2.416904	-1.076452
C	0.906598	4.384188	-0.152966
C	0.357526	2.637321	-1.719514
C	-1.215238	3.241971	-0.000297
C	-0.327972	4.206181	0.467634
C	1.240126	3.612126	-1.261441
H	0.620803	2.051757	-2.597124
H	-2.192051	3.157791	0.464470
H	-0.609471	4.827702	1.311215
H	2.189437	3.759245	-1.765646
H	1.599619	5.132280	0.217478

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H	-2.973603	-3.398255	-1.646130
C	-2.187263	-2.824936	-1.149229
C	-1.455199	-1.766377	0.988367
C	-0.915813	-0.586166	0.147073
C	-2.621595	-2.453392	0.270665
C	-1.917127	-1.537705	-1.945935
H	-0.654353	-2.492429	1.149677
H	-0.958041	0.349884	0.708088
H	-2.705624	-1.319807	-2.670286
H	-1.281415	-3.432373	-1.120140
H	-1.767665	-1.410981	1.974192
H	-2.924599	-3.345600	0.823705
H	-0.959048	-1.569801	-2.465393
N	-1.881143	-0.342232	-1.015959
C	-3.808244	-1.478580	0.159927
H	-4.528717	-1.904000	-0.547734
C	-3.262880	-0.156678	-0.418216
H	-3.903565	0.229172	-1.213437
H	-3.164914	0.616651	0.347544
C	-4.519035	-1.233614	1.462364
H	-3.937401	-0.764091	2.256711
C	-5.789449	-1.557434	1.683283
H	-6.261689	-1.377597	2.643613
H	-6.401068	-2.017014	0.910582
C	0.534965	-0.791680	-0.330374
O	0.743634	-2.087937	-0.866090
C	-1.534304	0.894371	-1.838157
H	-2.306194	0.940820	-2.609898
H	-0.587309	0.690679	-2.338204
H	1.153644	-2.650936	-0.191380
H	0.734591	-0.108547	-1.162097
H	0.219121	-0.299808	2.427603
C	1.238967	-0.247348	2.061914
C	1.556443	-0.464257	0.744823
N	3.530014	0.170862	2.673355
C	2.933861	-0.378416	0.358223
C	2.264780	0.062411	2.991667
C	3.875328	-0.041095	1.371453
C	3.386352	-0.590519	-0.965820
H	2.002839	0.230075	4.033964
H	5.944006	0.349605	1.809013
C	4.722667	-0.455405	-1.269871
H	2.703853	-0.891683	-1.752306
C	5.662600	-0.108646	-0.265723
H	6.712365	-0.006796	-0.527860
C	5.244161	0.088651	1.022084
O	5.106087	-0.669260	-2.552022
H	6.064889	-0.553934	-2.635556
C	-1.483417	2.178842	-1.052584
C	-1.404764	4.586284	0.370889
C	-0.298008	2.603162	-0.442270
C	-2.620695	2.987215	-0.962844
C	-2.583553	4.183291	-0.252213
C	-0.260597	3.797758	0.271029
H	0.610811	2.011635	-0.531490
H	-3.537944	2.687198	-1.463718
H	-3.472672	4.802364	-0.193751
H	0.664896	4.115113	0.740189
H	-1.374142	5.519198	0.924472

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H	2.021190	0.844662	-3.162195
C	1.170713	0.453944	-2.596062
C	-0.597177	0.967605	-0.947839
C	0.127300	0.347984	0.256596
C	0.429276	1.593928	-1.894729

C	1.646160	-0.555142	-1.536966
H	-1.159126	0.197099	-1.483984
H	0.222993	1.086480	1.059075
H	2.685376	-0.844644	-1.692458
H	0.507890	-0.054971	-3.300290
H	-1.318324	1.702149	-0.579797
H	-0.066254	2.240581	-2.622294
H	1.024632	-1.448308	-1.493172
N	1.582933	0.071711	-0.155108
C	1.463599	2.412103	-1.097783
H	2.162242	2.856229	-1.814650
C	2.268974	1.421171	-0.218892
H	3.265898	1.239262	-0.622271
H	2.370593	1.775634	0.810751
C	0.848684	3.531305	-0.299526
H	0.201375	3.257904	0.534797
C	1.048198	4.817720	-0.569754
H	0.576586	5.601271	0.014383
H	1.689901	5.130953	-1.389967
C	-0.601720	-0.854503	0.880789
O	-0.553357	-1.928224	-0.030540
C	2.262553	-0.825789	0.868405
H	1.746417	-1.785373	0.796763
H	2.055506	-0.373541	1.842448
H	-0.984769	-2.700412	0.369682
H	-0.078049	-1.133351	1.803479
H	-1.196770	0.337800	3.155330
C	-2.079532	0.226468	2.530373
C	-1.995897	-0.402268	1.311318
N	-4.434715	0.624080	2.318468
C	-3.194472	-0.547530	0.539758
C	-3.316271	0.730392	2.992865
C	-4.388125	-0.007300	1.112580
C	-3.280655	-1.183378	-0.726813
H	-3.366465	1.230925	3.957429
H	-6.498313	0.304718	0.859290
C	-4.484393	-1.269218	-1.387390
H	-2.407243	-1.615566	-1.195316
C	-5.666895	-0.730354	-0.821331
C	-6.607390	-0.810453	-1.360392
C	-5.611005	-0.116972	0.398986
O	-4.498306	-1.888029	-2.595034
H	-5.397001	-1.885405	-2.957373
C	3.745807	-1.004629	0.675913
C	6.499768	-1.384277	0.374364
C	4.651398	-0.144392	1.304048
C	4.234422	-2.073163	-0.081801
C	5.605045	-2.259257	-0.237508
C	6.021863	-0.329848	1.149826
H	4.284635	0.668358	1.926095
H	3.538339	-2.770828	-0.541278
H	5.971718	-3.092461	-0.828040
H	6.715769	0.344066	1.641524
H	7.568721	-1.530886	0.256936

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H	-2.957745	-3.426362	-1.602726
C	-2.173897	-2.842134	-1.114707
C	-1.443901	-1.753018	1.008568
C	-0.911274	-0.581958	0.150774
C	-2.607606	-2.455785	0.301397
C	-1.913315	-1.563150	-1.927974
H	-0.639411	-2.472749	1.179901
H	-0.956435	0.361269	0.699114
H	-2.705138	-1.358303	-2.652596
H	-1.264421	-3.443879	-1.080261
H	-1.757486	-1.386007	1.989781
H	-2.904574	-3.342787	0.865847
H	-0.956785	-1.596332	-2.450235
N	-1.880501	-0.356612	-1.012604
C	-3.799724	-1.488827	0.180628
H	-4.518771	-1.925879	-0.521480
C	-3.261683	-0.170829	-0.412978
H	-3.906202	0.203543	-1.210593
H	-3.164935	0.610846	0.344395
C	-4.510446	-1.233102	1.481077
H	-3.930250	-0.752924	2.270086
C	-5.779162	-1.560493	1.706428
H	-6.251483	-1.373032	2.665256
H	-6.389235	-2.030867	0.939024
C	0.539899	-0.787075	-0.326211
O	0.754807	-2.088463	-0.847549
C	-1.542031	0.872705	-1.849179
H	-2.317009	0.907693	-2.618361
H	-0.595872	0.667529	-2.350353
H	1.153707	-2.645896	-0.161490
H	0.735024	-0.113761	-1.167141
H	0.217973	-0.240270	2.419656
C	1.238862	-0.194756	2.056121
C	1.560915	-0.440726	0.744021
N	3.526871	0.240117	2.661765
C	2.938213	-0.364289	0.360572
C	2.260267	0.137021	2.980311
C	3.875955	-0.002421	1.367660
C	3.398109	-0.610079	-0.958924
H	1.996242	0.328348	4.017916
H	5.943208	0.400929	1.805392
C	4.736252	-0.486238	-1.255814
H	2.704286	-0.932137	-1.729362
C	5.673026	-0.112155	-0.256931
H	6.717600	-0.025478	-0.536806
C	5.248996	0.119265	1.020576
O	5.250388	-0.711561	-2.488117
H	4.544616	-0.972694	-3.099546
C	-1.493467	2.165403	-1.076998
C	-1.419355	4.585958	0.324427
C	-0.307117	2.601143	-0.476636
C	-2.634263	2.969016	-0.988662
C	-2.599337	4.171483	-0.288814
C	-0.271786	3.802242	0.225639
H	0.604084	2.013102	-0.564423
H	-3.552753	2.659804	-1.481566
H	-3.491263	4.786559	-0.231040
H	0.654583	4.128300	0.687012
H	-1.390488	5.523891	0.869562

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H	2.049892	-0.798397	-3.252233
C	1.191460	-0.876647	-2.578613
C	-0.590043	0.365199	-1.388853
C	0.139169	0.423285	-0.038142
C	0.438582	0.453966	-2.519805
C	1.649658	-1.247149	-1.158323
H	-1.155158	-0.567290	-1.479319

H	0.236642	1.466825	0.277675
H	2.684631	-1.588398	-1.142443
H	0.541014	-1.667579	-2.959888
H	-1.303547	1.192874	-1.425261
H	-0.056116	0.660236	-3.472213
H	1.013292	-1.994833	-0.687926
N	1.593551	-0.023532	-0.263034
C	1.455877	1.569713	-2.202731
H	2.141038	1.638480	-3.056697
C	2.285829	1.112666	-0.987742
H	3.261828	0.729249	-1.288405
H	2.445621	1.907139	-0.257481
C	0.768125	2.908077	-2.075422
H	0.177366	3.166738	-2.954555
C	0.801380	3.770891	-1.063362
H	0.252444	4.705063	-1.118529
H	1.369202	3.609440	-0.150718
C	-0.582692	-0.307940	1.105336
O	-0.540932	-1.693525	0.849110
C	2.276104	-0.306376	1.067499
H	1.773952	-1.190893	1.465595
C	2.050370	0.553235	1.704688
H	-0.956894	-2.162561	1.590291
H	-0.051387	-0.091644	2.040471
H	-1.157209	1.849440	2.501670
C	-2.047403	1.445539	2.026093
C	-1.974200	0.299218	1.272280
N	-4.408893	1.682412	1.688969
C	-3.181948	-0.209561	0.692936
C	-3.281796	2.110201	2.201825
C	-4.373216	0.538289	0.950293
C	-3.279532	-1.387187	-0.094620
H	-3.321950	3.020922	2.795268
H	-6.492295	0.671918	0.629835
C	-4.493199	-1.792720	-0.600353
H	-2.407619	-1.990566	-0.307170
C	-5.674453	-1.052560	-0.342953
H	-6.623864	-1.394904	-0.745998
C	-5.606595	0.083941	0.413533
O	-4.518840	-2.925722	-1.347145
H	-5.421887	-3.101306	-1.651591
C	3.764371	-0.527422	0.986040
C	6.527870	-0.947453	0.892977
C	4.648970	0.546106	1.128341
C	4.279817	-1.817916	0.828445
C	5.655079	-2.026582	0.775598
C	6.023864	0.338713	1.076214
H	4.262737	1.549022	1.292670
H	3.602067	-2.665531	0.761135
H	6.043875	-3.032081	0.652897
H	6.700815	1.179464	1.186893
H	7.600240	-1.109984	0.855133

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H	2.026787	0.835270	-3.167432
C	1.175655	0.444437	-2.602442
C	-0.597415	0.959454	-0.959690
C	0.125203	0.342800	0.247358
C	0.430557	1.584749	-1.905549
C	1.650202	-0.561687	-1.540067
H	-1.157881	0.187172	-1.495062
H	0.218398	1.082916	1.048567
H	2.690299	-0.849837	-1.692326
H	0.515414	-0.066762	-3.307465
H	-1.320036	1.694032	-0.594754
H	-0.063837	2.229181	-2.635839
H	1.030436	-1.456167	-1.495785
N	1.582143	0.067791	-0.159938
C	1.461503	2.406160	-1.107573
H	2.161302	2.849604	-1.823697
C	2.266089	1.418486	-0.224262
H	3.264660	1.237608	-0.624016
H	2.363649	1.775063	0.805031
C	0.842571	3.526356	-0.313763
H	0.194788	3.254132	0.520588
C	1.039091	4.812328	-0.588208
H	0.564484	5.596631	-0.007543
H	1.681147	5.124408	-1.408580
C	-0.605322	-0.858458	0.871644
O	-0.562245	-1.932469	-0.040597
C	2.260093	-0.826919	0.867146
H	1.747529	-1.783440	0.793504
H	2.046878	-0.375201	1.840111
H	-0.972844	-2.709726	0.371621
H	-0.081045	-1.140253	1.792785
H	-1.185054	0.346365	3.140879
C	-2.071666	0.235870	2.521277
C	-1.997128	-0.401084	1.304508
N	-4.424103	0.643698	2.314737
C	-3.198411	-0.545620	0.540327
C	-3.302118	0.748403	2.985514
C	-4.386056	0.004919	1.114158
C	-3.295853	-1.191988	-0.724188
H	-3.346742	1.255195	3.947014
H	-6.496317	0.329801	0.869688
C	-4.504907	-1.275864	-1.373524
H	-2.415651	-1.628025	-1.180808
C	-5.682127	-0.723828	-0.806531
H	-6.614202	-0.812678	-1.354575
C	-5.615563	-0.101992	0.406095
O	-4.658312	-1.881033	-2.576988
H	-3.808114	-2.241183	-2.872828
C	3.744840	-1.000571	0.681837
C	6.501555	-1.370567	0.394634
C	4.644099	-0.136715	1.314124
C	4.241094	-2.067691	-0.072863
C	5.613144	-2.249056	-0.221350
C	6.015951	-0.317379	1.167008
H	4.271292	0.674928	1.934029
H	3.549832	-2.768151	-0.535367
H	5.985992	-3.081310	-0.809357
H	6.704918	0.359158	1.662030
H	7.571618	-1.513494	0.282940

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H	2.049627	-0.805155	-3.247403
C	1.191280	-0.885340	-2.573924
C	-0.594840	0.352881	-1.386915
C	0.134724	0.417386	-0.036587
C	0.432909	0.442339	-2.518573
C	1.650454	-1.250550	-1.152527
H	-1.156929	-0.581759	-1.474722
H	0.228643	1.462411	0.275211
H	2.686337	-1.588938	-1.135815

H	0.544659	-1.680031	-2.954021
H	-1.311521	1.177675	-1.425308
H	-0.062870	0.644202	-3.471345
H	1.016480	-1.998735	-0.679589
N	1.590548	-0.024832	-0.260773
C	1.445758	1.562958	-2.204692
H	2.130136	1.632608	-3.059195
C	2.278269	1.112005	-0.989216
H	3.255404	0.731243	-1.289486
H	2.435634	1.908876	-0.261112
C	0.752610	2.898811	-2.079686
H	0.159429	3.153033	-2.958469
C	0.784314	3.764174	-1.069760
H	0.231650	4.696060	-1.126103
H	1.354494	3.607184	-0.157795
C	-0.585098	-0.311089	1.109925
O	-0.543068	-1.698400	0.859165
C	2.275374	-0.301437	1.070024
H	1.776750	-1.186488	1.471389
H	2.047540	0.559373	1.704834
H	-0.936994	-2.164195	1.614325
H	-0.053092	-0.091456	2.043702
H	-1.158098	1.850226	2.499127
C	-2.048575	1.446862	2.023676
C	-1.976950	0.295897	1.274678
N	-4.406594	1.688764	1.673496
C	-3.183156	-0.211734	0.695441
C	-3.280132	2.115324	2.191494
C	-4.372049	0.542202	0.941200
C	-3.283898	-1.397541	-0.085401
H	-3.320979	3.028517	2.780992
H	-6.489088	0.688007	0.605346
C	-4.497215	-1.796146	-0.594606
H	-2.403374	-1.998930	-0.276090
C	-5.676776	-1.046436	-0.352413
H	-6.612743	-1.401423	-0.770705
O	-5.606992	0.091588	0.397273
-4.653545	-2.913611	-1.346822	
H	-3.798208	-3.356966	-1.456664
C	3.764245	-0.517858	0.987147
C	6.528976	-0.928383	0.888448
C	4.645361	0.559260	1.123810
C	4.283916	-1.807061	0.832789
C	5.659758	-2.011030	0.777108
C	6.020831	0.356568	1.068824
H	4.255998	1.561320	1.285842
H	3.609116	-2.657382	0.770305
H	6.051818	-3.015545	0.656759
H	6.695019	1.200128	1.174831
H	7.601807	-1.087204	0.848135

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H	-4.398073	-2.263516	-0.870968
C	-3.340682	-1.989120	-0.833795
C	-1.322707	-1.757608	0.567600
C	-0.909998	-0.513678	-0.254943
C	-2.844967	-1.905725	0.611543
C	-3.154070	-0.620649	-1.492569
H	-0.898436	-2.653188	0.107705
H	-0.400278	0.207325	0.389805
H	-4.079383	-0.039943	-1.502260
H	-2.769023	-2.743500	-1.380107
H	-0.902189	-1.673383	1.572536
H	-3.116839	-2.815920	1.151219
-2.764793	-0.693751	-2.503714	
N	-2.180518	0.231537	-0.684528
C	-3.487505	-0.678908	1.270067
H	-4.562890	-0.699766	1.047300
C	-2.894871	0.588272	0.604327
H	-3.669220	1.315141	0.348928
H	-2.156974	1.067220	1.250216
C	-3.338192	-0.575291	2.767629
H	-3.687712	0.364832	3.195088
C	-2.846795	-1.507554	3.578618
H	-2.793719	-1.340145	4.649353
H	-2.485787	-2.467314	3.219616
C	0.050839	-0.821370	-1.415380
O	-0.668188	-1.553607	-2.381214
C	-1.906040	1.474377	-1.518496
H	-2.894242	1.904816	-1.705010
H	-1.519238	1.105069	-2.470801
-0.088328	-1.714650	-3.142668	
H	0.405033	0.125738	-1.841462
H	0.627392	-3.449851	-1.732382
C	1.387161	-2.926602	-1.161974
C	1.263431	-1.585989	-0.898902
N	3.470828	-3.095315	0.028758
C	2.293710	-0.945632	-0.141802
C	2.510948	-3.639653	-0.677145
C	3.375980	-1.762194	0.298079
C	2.299017	0.433789	0.176957
H	2.598755	-4.703196	-0.888939
H	5.233284	-1.810808	1.378757
C	3.334017	0.977593	0.904588
H	1.509312	1.099943	-0.151831
C	4.406654	0.165555	1.352317
H	5.212298	0.613393	1.928305
C	4.421470	-1.169379	1.052222
O	3.292658	2.305130	1.175688
H	4.088422	2.566499	1.663623
-0.968153	2.502400	-0.934991	
C	0.791189	4.463657	0.025229
C	0.254370	2.740900	-1.571749
C	-1.324045	3.306112	0.155661
C	-0.443535	4.268034	0.640582
C	1.131435	3.711629	-1.094756
H	0.522221	2.173962	-2.460214
H	-2.300038	3.206050	0.619762
H	-0.729807	4.873878	1.493928
H	2.081672	3.871143	-1.593342
H	1.478679	5.210396	0.408624

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H	2.782928	-3.716664	1.153734
C	2.207058	-2.839781	1.464174
C	-0.003934	-1.734916	1.428151
C	0.308065	-0.801600	0.249040
C	0.714930	-3.067318	1.218486
C	2.658523	-1.593907	0.682710
H	0.318619	-1.273619	2.368125
H	-0.423764	-0.971390	-0.543626
H	3.595969	-1.775178	0.154770
H	2.397615	-2.676664	2.527562
H	-1.088088	-1.866168	1.473824

H	0.323343	-3.829150	1.896790
H	2.754982	-0.710148	1.309931
N	1.635443	-1.249454	-0.383186
C	0.526814	-3.516660	-0.246448
C	0.997045	-4.502092	-0.351006
C	1.320147	-2.539424	-1.131157
H	2.286586	-2.958842	-1.418037
H	0.789071	-2.257068	-2.041384
C	-0.937187	-3.680994	-0.581259
H	-1.444179	-4.391867	0.071875
C	-1.648212	-3.081591	-1.533075
H	-2.704364	-3.300208	-1.651114
H	-1.234249	-2.365104	-2.238694
C	0.230424	0.678380	0.632882
O	1.235826	0.937552	1.583847
C	2.203791	-0.291801	-1.425108
H	1.366179	-0.059810	-2.089987
H	2.912755	-0.902289	-1.991858
H	1.437572	1.886569	1.573425
H	0.381046	1.290954	-0.260133
H	-0.533664	1.170819	3.188739
C	-1.371636	1.172879	2.500778
C	-1.166626	0.961781	1.162824
N	-3.753925	1.384648	2.218001
C	-2.295590	0.982265	0.286245
C	-2.688030	1.385838	2.980705
C	-3.573047	1.186115	0.880911
C	-2.209422	0.812436	-1.117838
H	-2.847207	1.552700	4.044041
H	-5.688272	1.338957	0.525464
C	-3.346837	0.814924	-1.893196
H	-1.256482	0.692237	-1.623200
C	-4.621967	0.999414	-1.301075
H	-5.508708	0.998540	-1.929216
C	-4.724523	1.186316	0.050984
O	-3.203351	0.638256	-3.229676
H	-4.070324	0.666716	-3.661915
C	2.681922	0.983687	-0.972563
C	4.136468	3.400789	-0.290686
C	4.124006	0.985357	-0.328700
C	2.313228	2.211894	-1.325806
C	2.927976	3.412591	-0.982162
C	4.737588	2.184036	0.022255
H	4.636080	0.055435	-0.107369
H	1.385519	2.235562	-1.892890
H	2.465500	4.352886	-1.263874
H	5.695819	2.164089	0.531152
H	4.618663	4.333707	-0.017416

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H	-2.924336	-3.637588	-1.467034
C	-2.156794	-3.014403	-1.001467
C	-1.486499	-1.791975	1.076592
C	-0.955103	-0.668014	0.159358
C	-2.616510	-2.559019	0.384358
C	-1.903417	-1.777442	-1.879164
H	-0.671710	-2.478376	1.320396
H	-1.021228	0.303829	0.652459
H	-2.683575	-1.626833	-2.629185
H	-1.238442	-3.597830	-0.921413
H	-1.852352	-1.365767	2.015635
H	-2.905975	-3.421622	0.990291
H	-0.935886	-1.821237	-2.380661
N	-1.909872	-0.524195	-1.028926
C	-3.817491	-1.611083	0.207099
H	-4.520564	-2.101199	-0.479178
C	-3.301044	-0.326512	-0.458258
H	-3.940616	-0.011733	-1.284826
H	-3.210649	0.501824	0.244864
C	-4.549681	-1.382373	1.505127
H	-4.928133	-2.302541	1.949878
C	-4.778621	-0.233389	2.135543
H	-5.325776	-0.223233	3.072454
H	-4.458853	0.735437	1.763048
C	0.504526	-0.876770	-0.287361
O	0.758107	-2.206300	-0.709036
C	-1.580734	0.667341	-1.923489
H	-2.360885	0.664711	-2.688221
H	-0.637124	0.441844	-2.420698
H	1.141933	-2.707359	0.027344
H	0.691165	-0.264407	-1.175049
H	0.147890	-0.202864	2.424492
C	1.167471	-0.130878	2.060597
C	1.504222	-0.426681	0.763753
N	3.432693	0.434536	2.649625
C	2.879008	-0.306409	0.377706
C	2.171466	0.290799	2.969942
C	3.796598	0.146436	1.367499
C	3.349977	-0.591166	-0.926088
H	1.894818	0.519468	3.996697
H	5.842108	0.663464	1.782840
C	4.680358	-0.414529	-1.234976
H	2.687447	-0.979414	-1.691126
C	5.596358	0.045776	-0.254360
H	6.642227	0.177540	-0.518480
C	5.160267	0.314259	1.014599
O	5.081034	-0.697643	-2.498345
H	6.033046	-0.539828	-2.588602
C	-1.529087	1.993605	-1.210408
C	-1.446667	4.468818	0.091948
C	-0.329868	2.471321	-0.670307
C	-2.679426	2.782903	-1.113511
C	-2.640445	4.012073	-0.462088
C	-0.290184	3.699888	-0.017689
H	0.587532	1.894625	-0.767872
H	-3.609153	2.440529	-1.561389
H	-3.539886	4.615409	-0.397050
H	0.646314	4.058752	0.396324
H	-1.414310	5.428105	0.598488

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H	2.107838	0.666660	-3.221436
C	1.247627	0.283140	-2.664741
C	-0.573370	0.825686	-1.093902
C	0.162519	0.391137	0.178454
C	0.434898	1.439479	-2.071133
C	1.709809	-0.633267	-1.518838
H	-1.053976	-0.036242	-1.566382
H	0.226718	1.237060	0.872707
H	2.749900	-0.936335	-1.636876
H	0.635548	-0.299582	-3.357336
H	-1.360248	1.525408	-0.806017
H	-0.076223	1.989379	-2.864617
H	1.086472	-1.518682	-1.403047

N	1.629026	0.114260	-0.199650
C	1.416344	2.357752	-1.322290
H	2.103970	2.788406	-2.061143
C	2.279763	1.465444	-0.397755
H	3.267842	1.269427	-0.816441
H	2.405406	1.907513	0.593908
C	0.782464	3.507376	-0.573580
H	1.400838	3.946395	0.209934
C	-0.407725	4.044929	-0.827791
H	-0.763129	4.900773	-0.263235
H	-1.064216	3.671806	-1.609320
C	-0.523841	-0.752335	0.943601
O	-0.454462	-1.917756	0.153066
C	2.331534	-0.660028	0.904601
H	1.847104	-1.638738	0.924173
H	2.103624	-0.123159	1.829919
H	-0.852122	-2.653856	0.645129
H	0.018707	-0.914225	1.882990
H	-1.133277	0.611024	3.117443
C	-2.016755	0.424372	2.512127
C	-1.925582	-0.301523	1.349066
N	-4.382174	0.747656	2.288913
C	-3.126659	-0.543712	0.605996
C	-3.262335	0.935007	2.942374
C	-4.328664	0.017280	1.140044
C	-3.205905	-1.292373	-0.597438
H	-3.316831	1.513296	3.862117
H	-6.446343	0.260606	0.877020
C	-4.411009	-1.459678	-1.239993
H	-2.326006	-1.750409	-1.027711
C	-5.601344	-0.896667	-0.715076
H	-6.542673	-1.041536	-1.238959
C	-5.552406	-0.179623	0.447961
O	-4.419454	-2.181567	-2.389072
H	-5.322335	-2.237272	-2.736291
C	3.820933	-0.807845	0.734027
C	6.587400	-1.128983	0.481746
C	4.695857	0.138276	1.277316
C	4.347468	-1.930911	0.089906
C	5.724201	-2.088516	-0.042541
C	6.072238	-0.018179	1.146702
H	4.301170	0.995558	1.817268
H	3.676106	-2.693025	-0.299566
H	6.121372	-2.965006	-0.543913
H	6.742215	0.721726	1.572112
H	7.661152	-1.253227	0.383707

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H	2.839682	-3.608156	1.166986
C	2.229879	-2.746900	1.455613
C	-0.012623	-1.713440	1.358498
C	0.305512	-0.755254	0.198869
C	0.753038	-3.022775	1.168406
C	2.668279	-1.494933	0.676878
H	0.274778	-1.248899	2.308257
H	-0.399342	-0.913183	-0.623188
H	3.615654	-1.659006	0.161071
H	2.385554	-2.571469	2.522747
H	-1.093397	-1.873556	1.387121
H	0.365682	-3.795971	1.835357
H	2.740512	-0.609250	1.303570
N	1.656187	-1.168178	-0.405717
C	0.633719	-3.491281	-0.294657
H	1.165493	-4.444218	-0.387192
C	1.383987	-2.458792	-1.169175
H	2.361992	-2.832715	-1.478546
H	0.618114	-2.183428	-2.062255
C	-0.789445	-3.712627	-0.734689
H	-1.442629	-2.840579	-0.790361
C	-1.281176	-4.909399	-1.040767
H	-2.316340	-5.038933	-1.339410
H	-0.662637	-5.802907	-1.002288
C	0.192180	0.717420	0.612089
O	1.185213	0.974601	1.576256
C	2.224924	-0.191013	-1.430353
H	1.398384	0.023612	-2.114010
H	2.962250	-0.781522	-1.981474
H	1.357855	1.929200	1.598770
H	0.338981	1.351981	-0.266033
H	-0.592367	1.091642	3.178816
C	-1.426359	1.118028	2.486520
C	-1.212599	0.965986	1.141621
N	-3.806963	1.337895	2.200463
C	-2.336742	1.024077	0.260476
C	-2.745593	1.305579	2.968617
C	-3.617791	1.202046	0.856893
C	-2.243009	0.924154	-1.149775
H	-2.910725	1.423614	4.037563
H	-5.730522	1.376632	0.497656
C	-3.375346	0.978148	-1.931210
H	-1.287998	0.825440	-1.654958
C	-4.653875	1.132980	-1.337807
H	-5.536965	1.167205	-1.970355
C	-4.764310	1.246874	0.021448
O	-3.224223	0.880849	-3.274698
H	-4.087493	0.944778	-3.710571
C	2.862125	1.096776	-0.955144
C	4.045107	3.535327	-0.225969
C	4.093042	1.121194	-0.290468
C	2.270021	2.314249	-1.306212
C	2.849005	3.525578	-0.938541
C	4.671095	2.330223	0.084001
H	4.623375	0.200980	-0.070867
H	1.353406	2.321097	-1.891365
H	2.368677	4.457523	-1.218052
H	5.620559	2.328410	0.609389
H	4.498713	4.476697	0.066974

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H	-2.894282	-3.669990	-1.419430
C	-2.131502	-3.033396	-0.964194
C	-1.467493	-1.777688	1.096569
C	-0.949592	-0.661084	0.162800
C	-2.591336	-2.565547	0.417525
C	-1.893452	-1.804875	-1.858168
H	-0.645055	-2.451637	1.349399
H	-1.023370	0.316187	0.643747
H	-2.677363	-1.671024	-2.607330
H	-1.207223	-3.606825	-0.879847
H	-1.836278	-1.342001	2.030120
H	-2.870119	-3.423462	1.035003
H	-0.927050	-1.845287	-2.362188
N	-1.909469	-0.541508	-1.023111
C	-3.802536	-1.632255	0.231910

H	-4.502069	-2.138173	-0.446527
C	-3.300799	-0.350714	-0.450077
H	-3.946379	-0.051323	-1.277847
H	-3.215477	0.486096	0.243528
C	-4.534104	-1.394809	1.528725
H	-4.902991	-2.313008	1.985450
C	-4.772415	-0.240382	2.145580
H	-5.317554	-0.223978	3.083579
H	-4.462651	0.726894	1.760750
C	0.510883	-0.861823	-0.285222
O	0.775648	-2.193162	-0.695232
C	-1.595220	0.643327	-1.932089
H	-2.379792	0.626347	-2.691974
H	-0.652590	0.419893	-2.432131
H	1.155554	-2.686446	0.048532
H	0.689856	-0.257042	-1.179932
H	0.146923	-0.137282	2.412096
C	1.167560	-0.072054	2.050360
C	1.509264	-0.393712	0.759718
N	3.430825	0.500691	2.634376
C	2.884542	-0.284324	0.377655
C	2.167481	0.365502	2.953879
C	3.798928	0.185931	1.361268
C	3.363339	-0.599474	-0.920047
H	1.888331	0.614633	3.975110
H	5.844516	0.706393	1.777790
C	4.696602	-0.436973	-1.220358
H	2.688938	-1.003129	-1.668911
C	5.609849	0.043560	-0.245427
H	6.651459	0.156988	-0.526709
C	5.167752	0.342334	1.011942
O	5.227266	-0.720432	-2.433653
H	4.534731	-1.044087	-3.030069
C	-1.549100	1.976994	-1.232614
C	-1.475467	4.463970	0.047715
C	-0.349013	2.469677	-0.708082
C	-2.705332	2.757099	-1.131183
C	-2.670539	3.982167	-0.490814
C	-0.313493	3.704040	-0.066424
H	0.572247	1.899858	-0.808899
H	-3.636551	2.402812	-1.566378
H	-3.574524	4.588256	-0.422029
H	0.623735	4.074067	0.335870
H	-1.446610	5.427793	0.545773

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H	2.116699	0.655910	-3.223902
C	1.255302	0.270704	-2.670264
C	-0.573616	0.810560	-1.107553
C	0.159651	0.382991	0.168676
C	0.435735	1.425551	-2.082931
C	1.715365	-0.641424	-1.520091
H	-1.048690	-0.055147	-1.579070
H	0.218976	1.232057	0.859407
H	2.756342	-0.943236	-1.633739
H	0.648703	-0.315751	-3.364591
H	-1.364696	1.507606	-0.824865
H	-0.074514	1.971537	-2.879648
H	1.093234	-1.527639	-1.403375
N	1.628245	0.109689	-0.203654
C	1.410780	2.349463	-1.332577
H	2.098929	2.781692	-2.069974
C	2.274898	1.462668	-0.403572
H	3.264836	1.269147	-0.819023
H	2.396070	1.907754	0.587289
C	0.769268	3.497586	-0.587956
H	1.382305	3.939430	0.198148
C	-0.421596	4.030704	-0.848273
H	-0.782728	4.885642	-0.285991
H	-1.073199	3.655020	-1.632672
C	-0.527031	-0.758711	0.935763
O	-0.463010	-1.925605	0.145767
C	2.329910	-0.659311	0.904833
H	1.849876	-1.640245	0.924290
H	2.096082	-0.122007	1.828397
H	-0.843297	-2.663435	0.648930
H	0.016882	-0.922210	1.873793
H	-1.121040	0.614896	3.105020
C	-2.008288	0.430707	2.504422
C	-1.926277	-0.302493	1.343815
N	-4.370768	0.767783	2.284629
C	-3.130105	-0.541735	0.607704
C	-3.247509	0.951242	2.935415
C	-4.325894	0.030932	1.141283
C	-3.220524	-1.300649	-0.592668
H	-3.296432	1.534831	3.852027
H	-6.443615	0.289417	0.885208
C	-4.430414	-1.462661	-1.225729
H	-2.334427	-1.764740	-1.008411
C	-5.615529	-0.885828	-0.701230
H	-6.548406	-1.040574	-1.233026
C	-5.556103	-0.161434	0.453754
O	-4.577864	-2.173494	-2.371010
H	-3.720621	-2.534349	-2.644766
C	3.820623	-0.800586	0.740280
C	6.589467	-1.108948	0.498872
C	4.688944	0.151742	1.283362
C	4.354960	-1.923287	0.101008
C	5.732916	-2.074576	-0.024997
C	6.066496	0.001630	1.158127
H	4.288229	1.008987	1.818880
H	3.688820	-2.690289	-0.286847
H	6.136294	-2.950880	-0.521685
H	6.731306	0.746272	1.583373
H	7.664154	-1.228233	0.405118

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H	-2.940854	-3.365003	-1.824664
C	-2.175132	-2.789615	-1.298688
C	-1.501377	-1.783223	0.889002
C	-0.962312	-0.576704	0.085222
C	-2.638414	-2.474971	0.126508
C	-1.927817	-1.471659	-2.049632
H	-0.691113	-2.496122	1.061937
H	-1.018798	0.342643	0.671778
H	-2.718668	-1.244657	-2.768532
H	-1.255396	-3.375512	-1.276427
H	-1.857078	-1.446394	1.866288
H	-2.922171	-3.399827	0.633927
H	-0.967520	-1.466426	-2.566218
N	-1.919687	-0.308724	-1.078321
C	-3.836261	-1.524474	0.026570
H	-4.522329	-1.924244	-0.732025
C	-3.307197	-0.165723	-0.486687

H	-3.945100	0.249916	-1.269272
H	-3.222761	0.569545	0.316985
C	-4.633721	-1.313372	1.289531
H	-5.388671	-0.529322	1.224995
C	-4.506894	-1.992539	2.425771
H	-5.142340	-1.773279	3.277516
H	-3.779550	-2.789121	2.555832
C	0.494541	-0.753589	-0.383648
O	0.723551	-2.033514	-0.949023
C	-1.582750	0.961548	-1.852375
H	-2.349750	1.029152	-2.627669
H	-0.630388	0.786189	-2.352671
H	1.130053	-2.609300	-0.283010
H	0.694504	-0.047624	-1.196425
H	0.146521	-0.305522	2.380061
C	1.170144	-0.246251	2.025913
C	1.502586	-0.441593	0.709122
N	3.454414	0.161528	2.670357
C	2.884399	-0.348301	0.339759
C	2.185475	0.048670	2.972072
C	3.814556	-0.029190	1.369268
C	3.352362	-0.538516	-0.982232
H	1.911465	0.199428	4.013888
H	5.878492	0.350420	1.837637
C	4.692609	-0.402720	-1.267854
H	2.678821	-0.824872	-1.781702
C	5.621389	-0.074299	-0.247400
H	6.674500	0.029580	-0.495345
C	5.187756	0.103604	1.038219
O	5.090550	-0.598309	-2.548541
H	6.051034	-0.488477	-2.618151
C	-1.546686	2.215542	-1.018105
C	-1.488654	4.568832	0.493945
C	-0.357903	2.642236	-0.416115
C	-2.699185	2.993316	-0.872436
C	-2.672128	4.162597	-0.118117
C	-0.330453	3.810163	0.340768
H	0.560645	2.073845	-0.547119
H	-3.621651	2.691422	-1.362301
H	-3.573220	4.758482	-0.016535
H	0.598019	4.130232	0.802127
H	-1.466211	5.481183	1.081074

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H	-2.924316	-3.389738	-1.795691
C	-2.160859	-2.805235	-1.276613
C	-1.486142	-1.778499	0.901389
C	-0.956465	-0.575446	0.086389
C	-2.621350	-2.483026	0.147811
C	-1.924944	-1.491421	-2.038341
H	-0.671511	-2.485329	1.078972
H	-1.016821	0.348356	0.665340
H	-2.720402	-1.274563	-2.755312
H	-1.237232	-3.384940	-1.253147
H	-1.841215	-1.435952	1.876941
H	-2.897574	-3.405775	0.663076
H	-0.967238	-1.484160	-2.559655
N	-1.919355	-0.321609	-1.075733
C	-3.825128	-1.540304	0.045228
H	-4.511889	-1.949482	-0.707713
C	-3.305650	-0.182323	-0.479829
H	-3.948797	0.223885	-1.263122
H	-3.222519	0.559157	0.318236
C	-4.618694	-1.324414	1.309903
H	-5.377792	-0.544617	1.242957
C	-4.483949	-1.995113	2.450258
H	-5.117026	-1.773085	3.303040
H	-3.752228	-2.787248	2.582970
C	0.500602	-0.747116	-0.384524
O	0.736950	-2.028739	-0.943624
C	-1.592751	0.945366	-1.859523
H	-2.362417	1.002719	-2.632943
H	-0.640614	0.772459	-2.361217
H	1.130931	-2.603524	-0.269094
H	0.694748	-0.045412	-1.202542
H	0.146831	-0.266767	2.371206
C	1.171294	-0.209762	2.019481
C	1.508354	-0.422336	0.705254
N	3.451958	0.211558	2.662028
C	2.889819	-0.333438	0.339358
C	2.181756	0.100380	2.963117
C	3.815876	0.001827	1.366437
C	3.365552	-0.544563	-0.980645
H	1.905506	0.265872	4.002036
H	5.878069	0.390049	1.839738
C	4.707515	-0.415924	-1.257609
H	2.680874	-0.844829	-1.767930
C	5.632688	-0.069920	-0.238172
H	6.680868	0.021284	-0.502692
C	5.193278	0.130154	1.039334
O	5.236553	-0.610486	-2.488871
H	4.538249	-0.857575	-3.114448
C	-1.561973	2.205255	-1.033907
C	-1.513519	4.568449	0.462976
C	-0.374116	2.642759	-0.437871
H	-2.718680	2.977183	-0.889985
C	-2.696292	4.151318	-0.143104
C	-0.351291	3.815624	0.311400
H	0.547384	2.078767	-0.567143
H	-3.640894	2.666804	-1.375083
H	-3.600627	4.742436	-0.042589
H	0.576590	4.143980	0.768064
H	-1.494761	5.484534	1.044368

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H	0.748934	4.017966	-1.538984
C	0.449371	3.003917	-1.262427
C	-0.161073	1.473064	0.590451
C	0.546620	0.333739	-0.183180
C	0.467589	2.828277	0.257551
C	1.431362	2.003769	-1.885133
H	-1.217539	1.496602	0.315154
H	0.969756	-0.394834	0.513782
H	2.388255	2.466288	-2.140161
H	-0.556209	2.823715	-1.649479
H	-0.115624	1.267425	1.663151
H	-0.093370	3.629165	0.745041
H	1.023682	1.516267	-2.767203
N	1.780965	0.914943	-0.881948
C	1.935731	2.860147	0.721206
H	2.421878	3.723654	0.252513
C	2.609897	1.568875	0.210014
H	3.594621	1.773601	-0.215303
H	2.718322	0.827897	1.005063

C	2.099557	2.981534	2.210607
H	1.660364	2.187260	2.815134
C	2.736602	3.985685	2.804756
H	2.823504	4.042677	3.884952
H	3.192484	4.788115	2.229117
C	-0.388203	-0.460255	-1.109650
O	-0.906774	0.405795	-2.091717
C	2.611676	-0.129130	-1.615848
H	3.469547	0.426141	-2.004625
H	2.010984	-0.449506	-2.469044
H	-1.451340	-0.113386	-2.704789
H	0.195334	-1.250130	-1.594610
H	0.001987	-2.716722	0.196774
C	-1.007639	-2.344731	0.355255
C	-1.427805	-1.181918	-0.248670
N	-3.118335	-2.717066	1.425057
C	-2.771533	-0.747054	-0.013451
C	-1.880376	-3.077102	1.186452
C	-3.567204	-1.574320	0.839678
C	-3.366099	0.428915	-0.554884
H	-1.532102	-3.993628	1.657699
H	-5.484480	-1.852562	1.769082
C	-4.667676	0.755927	-0.255815
H	-2.791927	1.078496	-1.204529
C	-5.455921	-0.066925	0.589329
H	-6.478957	0.228748	0.796563
C	-4.911686	-1.200665	1.117978
O	-5.282287	1.864588	-0.736198
H	-4.671474	2.358633	-1.304200
C	3.061493	-1.313912	-0.797143
C	3.913776	-3.551896	0.661002
C	2.462414	-2.562813	-0.991154
C	4.131928	-1.214743	0.099522
C	4.547611	-2.322792	0.831313
C	2.879815	-3.674385	-0.263143
H	1.685747	-2.684243	-1.741849
H	4.661707	-0.274054	0.215416
H	5.375856	-2.227446	1.525604
H	2.403782	-4.635541	-0.428095
H	4.238996	-4.416052	1.231092

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H	0.741443	4.016395	-1.543941
C	0.444612	3.001927	-1.265960
C	-0.161908	1.472153	0.588269
C	0.549169	0.333215	-0.182754
C	0.464171	2.828237	0.254176
C	1.429113	2.003634	-1.887614
H	-1.217716	1.493861	0.310581
H	0.974704	-0.392747	0.515514
H	2.385045	2.468072	-2.142921
H	-0.560873	2.818677	-1.651790
H	-0.117549	1.268010	1.661332
H	-0.098739	3.628297	0.740723
H	1.022657	1.514112	-2.769087
N	1.781627	0.916533	-0.883147
C	1.932310	2.863825	0.717604
H	2.416429	3.728131	0.248263
C	2.609586	1.573764	0.207326
H	3.593518	1.780524	-0.218897
H	2.720492	0.834014	1.003179
C	2.095999	2.986486	2.206898
H	1.659113	2.191162	2.811756
C	2.730057	3.992717	2.800740
H	2.816701	4.050432	3.880931
C	3.183315	4.796310	2.225399
C	-0.383268	-0.464988	-1.108086
O	-0.899633	0.397938	-2.092972
C	2.613900	-0.126639	-1.616196
H	3.470310	0.429833	-2.006469
H	2.013130	-0.449437	-2.468430
H	-1.463736	-0.116543	-2.692165
H	0.201766	-1.256321	-1.589097
H	0.005039	-2.719083	0.204311
C	-1.004708	-2.346169	0.360213
C	-1.422986	-1.185355	-0.246196
N	-3.117576	-2.719658	1.427900
C	-2.768756	-0.749594	-0.013861
C	-1.879767	-3.078215	1.192130
C	-3.566072	-1.576816	0.839040
C	-3.359864	0.422928	-0.557391
H	-1.530958	-3.993647	1.665237
H	5.485132	-1.852253	1.763014
C	-4.663145	0.753033	-0.265123
H	-2.799556	1.082472	-1.205927
C	-5.451997	-0.068487	0.578869
H	-6.479588	0.210482	0.795966
C	-4.908592	-1.203284	1.112376
O	-5.164692	1.888929	-0.812109
H	-6.085287	2.010723	-0.534955
C	3.067079	-1.309349	-0.796196
C	3.925755	-3.543389	0.664486
C	2.470786	-2.559963	-0.987915
C	4.137951	-1.206513	0.099532
C	4.556809	-2.312553	0.832580
C	2.891387	-3.669531	-0.258715
H	1.693862	-2.684218	-1.737822
H	4.665622	-0.264431	0.213693
H	5.385331	-2.214284	1.526143
H	2.417512	-4.632034	-0.422059
H	4.253457	-4.406016	1.235486

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H	-2.429357	1.206845	3.099881
C	-1.606693	1.130726	2.384386
C	-0.356630	2.283164	0.562577
C	-0.264510	0.921109	-0.165280
C	-1.602582	2.342933	1.450351
C	-1.779334	-0.148215	1.549119
H	0.535241	2.426962	1.178953
H	-0.254486	1.052847	-1.251483
H	-2.788378	-0.557768	1.623300
H	-0.669590	1.080702	2.941552
H	-0.375080	3.095473	-0.169416
H	-1.603169	3.270913	2.027091
H	-1.059010	-0.919439	1.824154
N	-1.575461	0.154176	0.078654
C	-2.864901	2.269746	0.572725
H	-3.722570	2.081408	1.228494
C	-2.696917	1.066440	-0.379012
H	-3.603822	0.464746	-0.417388
H	-2.439552	1.376742	-1.396463
C	-3.140628	3.527259	-0.204347
H	-2.375724	3.842002	-0.915270

C	-4.245747	4.253054	-0.064389
H	-4.404090	5.163028	-0.634072
H	-5.031411	3.961232	0.628349
C	0.990015	0.114826	0.219077
O	1.108074	-0.008861	1.627428
C	-1.597619	-1.129850	-0.742706
H	-0.795257	-1.756220	-0.355028
H	-1.349285	-0.832530	-1.765122
H	1.773816	0.616933	1.951812
H	0.894817	-0.906765	-0.163031
H	1.457958	2.454260	-1.299466
C	2.329705	1.836568	-1.116147
C	2.264065	0.669252	-0.398859
N	4.694826	1.613134	-1.510093
C	3.473442	-0.081873	-0.223013
C	3.571025	2.269157	-1.649936
C	4.659601	0.443515	-0.809983
C	3.534891	-1.310942	0.476611
H	3.609491	3.199436	-2.212346
H	6.764078	0.140609	-1.129465
C	4.728585	-1.988894	0.583296
C	2.658391	-1.727644	0.958585
C	5.912640	-1.467825	0.002070
H	6.844786	-2.018367	0.099907
C	5.872823	-0.279458	-0.675249
O	4.731973	-3.162388	1.261556
H	5.625703	-3.536825	1.271357
C	-2.891885	-1.900791	-0.703173
C	-5.246060	-3.409693	-0.676887
C	-3.857522	-1.722744	-1.698714
C	-3.107823	-2.858547	0.292450
C	-4.282211	-3.604859	0.310134
C	-5.031212	-2.470752	-1.683696
H	-3.687985	-1.000668	-2.493599
H	-2.348596	-3.030916	1.051178
H	-4.437993	-4.346184	1.086816
H	-5.773102	-2.325313	-2.461885
H	-6.158852	-3.996514	-0.667643

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H	-3.942150	-2.224133	-1.946531
C	-2.955858	-1.965366	-1.553136
C	-1.497028	-1.885620	0.457057
C	-0.737101	-0.813278	-0.359602
C	-2.953019	-1.956631	-0.017852
C	-2.586957	-0.557381	-2.038048
H	-1.011965	-2.850948	0.321683
H	-0.161786	-0.176378	0.316285
H	-3.467405	0.070987	-2.193451
H	-2.237851	-2.703057	-1.924339
H	-1.442300	-1.637455	1.520996
H	-3.441108	-2.850112	0.377355
H	-2.013151	-0.551047	-2.964286
N	-1.781132	0.138820	-0.958011
C	-3.690432	-0.688380	0.453149
H	-4.614648	-0.583613	-0.127442
C	-2.759944	0.500964	0.146727
H	-3.318678	1.375189	-0.191101
H	-2.159618	0.791024	1.012500
C	-4.057674	-0.700587	1.910702
H	-3.236763	-0.795594	2.622000
C	-5.306973	-0.605633	2.355435
H	-5.535605	-0.630023	3.415932
H	-6.145804	-0.502795	1.671214
C	0.223921	-1.375903	-1.465418
O	0.279082	-2.782593	-1.339232
C	-1.157167	1.404739	-1.535585
H	-1.945024	1.856048	-2.143944
H	-0.357958	1.077197	-2.203816
H	0.917825	-3.111660	-1.991205
H	-0.178071	-1.122575	-2.454035
H	1.529694	0.040742	-3.375811
C	2.096439	-0.044204	-2.451567
C	1.605769	-0.755371	-1.385845
N	4.080557	0.604546	-1.259101
C	2.409866	-0.855477	-0.206784
C	3.346002	0.618326	-2.343502
C	3.632715	-0.125449	-0.196551
C	2.037322	-1.603855	0.934899
H	3.722971	1.190969	-3.187962
H	5.357239	0.422638	0.966301
C	2.839386	-1.602068	2.054902
H	1.142632	-2.216343	0.934130
C	4.047178	-0.858031	2.078007
H	4.663822	-0.868058	2.972845
C	4.432313	-0.144284	0.975732
O	2.439006	-2.333118	3.122057
H	3.096358	-2.273610	3.831777
C	-0.651020	2.390256	-0.511946
C	0.265778	4.244442	1.375143
C	0.652762	2.311023	-0.013633
C	-1.479162	3.431468	-0.078529
C	-1.025849	4.350435	0.862450
C	1.106709	3.227842	0.930254
H	1.328172	1.543293	-0.376143
H	-2.480283	3.535086	-0.489537
H	-1.678613	5.153475	1.188505
H	2.121046	3.149297	1.308214
H	0.620462	4.961707	2.108304

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H	3.286043	3.112083	-0.715900
C	2.398719	2.813595	-1.281980
C	-0.065976	2.607297	-1.246619
C	-0.091346	1.121794	-0.840755
C	1.125729	3.294829	-0.580119
C	2.335793	1.283179	-1.413264
H	-0.000900	2.704119	-2.333895
H	-0.654580	1.004091	0.085588
H	3.294617	0.813859	-1.193507
H	2.478245	3.251994	-2.279539
H	-1.013941	3.056500	-0.941719
H	1.031578	4.381144	-0.652131
H	2.007240	0.958930	-2.403143
N	1.334347	0.728327	-0.424739
C	1.190927	2.865621	0.900132
H	2.007415	3.424307	1.373260
C	1.582588	1.378594	0.924730
H	2.644569	1.243839	1.133138
H	1.017688	0.803877	1.660540
C	-0.086685	3.230912	1.619929
H	-0.307440	4.297826	1.575528
C	-0.944987	2.436457	2.255199
H	-1.841448	2.843724	2.710645

H	-0.811218	1.362200	2.359552
C	-0.743468	0.228065	-1.931575
O	-1.698132	1.065488	-2.559904
C	1.475359	-0.780407	-0.297680
H	1.367126	-1.177118	-1.308088
H	0.619224	-1.106980	0.297823
H	-2.218450	0.517560	-3.166835
H	0.019936	-0.078247	-2.664083
H	-0.289452	-2.362726	-2.616187
C	-1.054753	-2.257652	-1.851459
C	-1.421045	-1.019280	-1.388723
N	-2.561551	-3.398046	-0.367779
C	-2.464751	-0.942781	-0.409077
C	-1.656265	-3.422323	-1.314489
C	-2.971976	-2.179551	0.086367
C	-3.007402	0.270344	0.085779
H	-1.352104	-4.399991	-1.681669
H	-4.329668	-3.113121	1.467539
C	-3.965590	0.251507	1.074228
H	-2.714583	1.228702	-0.328211
C	-4.444844	-0.977871	1.595254
H	-5.203028	-0.970595	2.374039
C	-3.964346	-2.159567	1.101259
O	-4.436343	1.440799	1.522357
H	-5.133086	1.295748	2.180486
C	2.769418	-1.257398	0.308695
C	5.148378	-2.224425	1.416862
C	2.878032	-1.456376	1.688543
C	3.854717	-1.578185	-0.512470
C	5.041329	-2.053242	0.038838
C	4.063386	-1.931248	2.240945
H	2.028391	-1.252084	2.335017
H	3.765182	-1.472136	-1.590896
H	5.876272	-2.299886	-0.608650
H	4.135493	-2.081673	3.313078
H	6.071469	-2.599535	1.846920

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H	-3.218353	-3.428900	-1.241903
C	-2.246844	-2.953493	-1.083139
C	-0.571034	-2.225373	0.610719
C	-0.318948	-0.975880	-0.271810
C	-1.995324	-2.753788	0.413306
C	-2.242571	-1.580890	-1.774914
H	0.137542	-3.006952	0.330958
H	0.000281	-0.127966	0.341455
H	-3.252269	-1.233950	-2.008134
H	-1.473971	-3.589895	-1.514669
H	-0.383060	-1.980180	1.659026
H	-2.117878	-3.697605	0.950291
H	-1.640589	-1.572920	-2.682740
N	-1.667767	-0.521600	-0.849483
C	-3.016254	-1.722515	0.922649
H	-4.005508	-2.010086	0.547869
C	-2.627975	-0.360470	0.318552
H	-3.497110	0.179947	-0.060011
H	-2.124044	0.281947	1.044559
C	-3.093700	-1.631225	2.421641
H	-2.188407	-1.313465	2.940328
C	-4.185995	-1.918751	3.122885
H	-4.198097	-1.855821	4.206156
H	-5.107101	-2.229699	2.635694
C	0.793512	-1.225202	-1.320537
O	0.490742	-2.409615	-2.019449
C	-1.578468	0.798020	-1.621828
H	-2.350331	0.728593	-2.390257
H	-0.617140	0.803154	-2.134502
H	1.167707	-2.544449	-2.701456
H	0.855144	-0.387302	-2.024614
H	2.188493	-3.465619	-0.644096
C	2.667956	-2.554740	-0.301993
C	2.122172	-1.328720	-0.583173
N	4.499480	-1.589364	0.928043
C	2.814072	-0.162083	-0.136701
C	3.865967	-2.632841	0.451736
C	3.988720	-0.358105	0.642486
C	2.394462	1.156818	-0.427614
H	4.292497	-3.609070	0.672265
H	5.562379	0.605772	1.745039
C	3.074240	2.238583	0.085773
H	1.553556	1.353535	-1.082810
C	4.225295	2.046190	0.891386
H	4.752138	2.910352	1.286483
C	4.672629	0.778129	1.148324
O	2.605074	3.475428	-0.207476
H	3.174079	4.151963	0.190840
C	-1.800382	2.057670	-0.818962
C	-2.303500	4.438426	0.569724
C	-0.844643	2.583732	0.056199
C	-3.006842	2.742435	-0.991660
C	-3.258903	3.926050	-0.304194
C	-1.097268	3.764881	0.748041
H	0.108936	2.088474	0.206423
H	-3.752674	2.349470	-1.678094
H	-4.199330	4.445957	-0.454398
H	-0.341941	4.161551	1.418631
H	-2.495712	5.362258	1.105761

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H	-3.584917	-3.053778	-1.346140
C	-2.566698	-2.709450	-1.147331
C	-0.875697	-2.210872	0.621075
C	-0.438252	-1.007063	-0.249841
C	-2.345635	-2.562801	0.359767
C	-2.364484	-1.338270	-1.813901
H	-0.250453	-3.071211	0.375804
H	-0.016914	-0.218825	0.377990
H	-3.312319	-0.866584	-2.083336
H	-1.867419	-3.433012	-1.564930
H	-0.711850	-1.978874	1.676366
H	-2.601746	-3.490834	0.876558
H	-1.728424	-1.392530	-2.697913
N	-1.700443	-0.370781	-0.847271
C	-3.255510	-1.421127	0.846096
H	-4.251089	-1.573379	0.413966
C	-2.666043	-0.108997	0.297342
H	-3.437102	0.561808	-0.086444
H	-2.098559	0.429290	1.059947
C	-3.401765	-1.346848	2.340543
H	-2.489954	-1.175271	2.913605
C	-4.562207	-1.481430	2.975192
H	-4.625866	-1.435371	4.057523
H	-5.490322	-1.645114	2.432749
C	0.649269	-1.395902	-1.282626

O	0.257481	-2.583362	-1.929227
C	-1.427709	0.938222	-1.582571
H	-2.215617	1.012713	-2.334394
H	-0.488673	0.810906	-2.121715
H	0.927503	-2.800948	-2.596539
H	0.777064	-0.601249	-2.026965
H	1.864749	-3.700050	-0.473119
C	2.412758	-2.810993	-0.180273
C	1.963563	-1.563674	-0.533050
N	4.308391	-1.915360	1.004542
C	2.735440	-0.429595	-0.141289
C	3.599784	-2.935029	0.582596
C	3.888966	-0.667655	0.654988
C	2.400871	0.904086	-0.486630
H	3.953045	-3.925554	0.860722
H	5.520323	0.237912	1.725216
C	3.136389	1.959132	0.003468
H	1.568016	1.112590	-1.150878
C	4.275506	1.725601	0.817288
H	4.836956	2.581724	1.176117
C	4.645249	0.444553	1.117854
O	2.833775	3.255065	-0.246599
H	2.017640	3.315274	-0.769402
C	-1.435125	2.205438	-0.754825
C	-1.491819	4.660064	0.606685
C	-0.474115	2.504594	0.219635
C	-2.428433	3.150438	-1.025308
C	-2.456875	4.370158	-0.352694
C	-0.502779	3.721564	0.894558
H	0.305733	1.795531	0.475758
H	-3.183912	2.934579	-1.776523
H	-3.234355	5.091639	-0.581635
H	0.254628	3.932685	1.642771
H	-1.509737	5.610416	1.130075

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H	-0.549603	-4.198002	-1.304387
C	-0.294403	-3.155896	-1.095781
C	0.238091	-1.481718	0.662675
C	-0.527910	-0.430103	-0.176457
C	-0.320051	-2.882340	0.408672
C	-1.317759	-2.241263	-1.778621
H	1.296094	-1.463238	0.394396
H	-0.994366	0.312560	0.476577
H	-2.249303	-2.762614	-2.011705
H	0.703308	-2.959171	-1.494864
H	0.161202	-1.226260	1.723267
H	0.281259	-3.623687	0.941636
H	-0.927220	-1.783483	-2.683966
N	-1.726246	-1.118384	-0.840125
C	-1.781117	-2.940702	0.894957
H	-2.221118	-3.864827	0.497126
C	-2.527123	-1.741484	0.288615
H	-3.492508	-2.032933	-0.129746
H	-2.685937	-0.944278	1.014185
C	-1.865659	-3.019111	2.398181
H	-1.349920	-3.886169	2.810562
C	-2.473555	-2.185853	3.238624
H	-2.446803	-2.371189	4.307343
H	-3.027611	-1.305775	2.924741
C	0.364598	0.361022	-1.146211
O	0.927123	-0.527859	-2.081520
C	-2.608728	-0.164770	-1.634761
H	-3.425962	-0.790040	-2.005213
H	-2.016629	0.149361	-2.496164
H	1.463112	-0.018377	-2.710216
H	-0.258214	1.093953	-1.671396
H	-0.136270	2.663675	0.038185
C	0.889411	2.348862	0.217050
C	1.364620	1.178005	-0.324263
N	2.978641	2.878562	1.265862
C	2.728565	0.819264	-0.067276
C	1.725949	3.165174	1.009938
C	3.482961	1.728478	0.739377
C	3.375818	-0.351931	-0.546012
H	1.332933	4.086990	1.433028
H	5.385056	2.146407	1.645004
C	4.692484	-0.602907	-0.235919
H	2.849268	-1.071597	-1.158027
C	5.440236	0.301091	0.559713
H	6.480362	0.084751	0.789201
C	4.841790	1.435628	1.031300
O	5.247563	-1.743128	-0.718668
H	6.168258	-1.813071	-0.424637
C	-3.141382	1.028746	-0.880962
C	-4.155762	3.279418	0.447920
C	-2.613714	2.300275	-1.125929
C	-4.220655	0.908240	0.002737
C	-4.716952	2.023405	0.670188
C	-3.111697	3.418826	-0.462191
H	-1.830296	2.431108	-1.867924
H	-4.694547	-0.056656	0.156569
H	-5.551767	1.912176	1.354226
H	-2.689609	4.397575	-0.666269
H	-4.545763	4.149296	0.966418

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H	3.805367	0.798577	2.650269
C	2.987140	0.342361	2.087195
C	2.383134	-1.509566	0.486543
C	1.449798	-0.468873	-0.180257
C	3.530802	-0.803676	1.226662
C	2.350745	1.410512	1.172305
H	1.795196	-2.101069	1.189869
H	1.278427	-0.703434	-1.234064
H	2.964880	2.310128	1.078555
H	2.243846	-0.028481	2.791402
H	2.782840	-2.192489	-0.268835
H	4.072124	-1.521328	1.847720
H	1.354237	1.697959	1.511785
N	2.201972	0.866804	-0.228962
C	4.479702	-0.172340	0.193807
H	5.123813	0.547455	0.711596
C	3.586478	0.579664	-0.804008
H	4.018562	1.538893	-1.093664
H	3.408556	-0.006454	-1.710462
C	5.361439	-1.155525	-0.524369
H	4.860941	-1.944534	-1.086475
C	6.689957	-1.107718	-0.500830
H	7.293471	-1.844029	-1.021607
H	7.219932	-0.329540	0.042910
C	0.073745	-0.386959	0.513523
O	0.236618	-0.599594	1.908565
C	1.613269	1.907010	-1.186594

H	1.817654	1.517674	-2.187030
H	2.234900	2.791923	-1.029148
H	-0.643952	-0.627120	2.315188
H	-0.343920	0.605180	0.355722
H	0.446815	-2.770907	-0.934525
C	-0.552326	-2.525428	-0.737682
C	-0.915277	-1.387421	-0.063447
N	-2.835805	-3.235918	-1.023851
C	-2.310328	-1.155011	0.162510
C	-1.550806	-3.421541	-1.196770
C	-3.226770	-2.114507	-0.354101
C	-2.812583	-0.023606	0.850115
H	-1.251694	-4.321395	-1.729955
H	-5.298715	-2.644720	-0.578701
C	-4.169211	0.157856	0.996140
H	-2.158255	0.745356	1.249666
C	-5.084530	-0.794485	0.479976
H	-6.152077	-0.635734	0.607822
C	-4.618271	-1.902125	-0.175495
O	-4.591046	1.275936	1.635919
H	-5.558709	1.281819	1.691377
C	0.157813	2.257738	-1.062809
C	-2.558004	2.879356	-0.855939
C	-0.278147	3.205874	-0.132506
C	-0.772324	1.650241	-1.912766
C	-2.125490	1.955887	-1.806181
C	-1.633687	3.508099	-0.024030
H	0.440982	3.713552	0.505713
H	-0.436423	0.927303	-2.653070
H	-2.842194	1.468350	-2.459299
H	-1.966871	4.239194	0.705318
H	-3.615064	3.106028	-0.760203

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H	3.740851	0.921063	2.781260
C	2.940797	0.444499	2.208965
C	2.408158	-1.466218	0.638122
C	1.496753	-0.448636	-0.089786
C	3.513624	-0.729209	1.407739
C	2.334349	1.478298	1.237677
H	1.795670	-2.055188	1.321754
H	1.364059	-0.713512	-1.142556
H	2.946103	2.379147	1.143326
H	2.176425	0.097323	2.902042
H	2.864693	-2.147369	-0.087298
H	4.029703	-1.424177	2.075462
H	1.322503	1.766974	1.526349
N	2.247720	0.888935	-0.149697
C	4.498263	-0.144794	0.380804
H	5.130716	0.583540	0.905452
C	3.654024	0.592182	-0.662608
H	4.094623	1.548193	-0.949910
H	3.499650	-0.006060	-1.563357
C	5.414151	-1.190576	-0.200987
H	5.967871	-1.745230	0.556288
C	5.620778	-1.481061	-1.482775
H	6.320915	-2.260844	-1.764081
H	5.130896	-0.964208	-2.302864
C	0.097210	-0.351935	0.554131
O	0.212116	-0.528384	1.959354
C	1.690676	1.888958	-1.167134
H	1.911965	1.450681	-2.143241
H	2.317550	2.775162	-1.042368
H	-0.682462	-0.562699	2.333703
H	-0.318145	0.634451	0.358435
H	0.568596	-2.761915	-0.829740
C	-0.477353	-2.523683	-0.662812
C	-0.867911	-1.372695	-0.027180
N	-2.745341	-3.273405	-0.970414
C	-2.270215	-1.150793	0.162140
C	-1.455192	-3.445021	-1.116567
C	-3.163641	-2.138983	-0.340412
C	-2.800754	-0.005444	0.804444
H	-1.134118	-4.355259	-1.618572
H	-5.223344	-2.710099	-0.577553
C	-4.162247	0.157213	0.926693
H	-2.164594	0.786868	1.187490
C	-5.054195	-0.826419	0.428885
H	-6.125779	-0.683029	0.539460
C	-4.560842	-1.944529	-0.187657
O	-4.612247	1.286170	1.526687
H	-5.580850	1.279530	1.562650
C	0.236359	2.256538	-1.088164
C	-2.477548	2.906141	-0.955363
C	-0.207408	3.249803	-0.210495
C	-0.684244	1.617958	-1.925720
C	-2.036465	1.937703	-1.856054
C	-1.562290	3.565775	-0.137857
H	0.505277	3.783416	0.413646
H	-0.342327	0.857697	-2.624609
H	-2.746042	1.426164	-2.498476
H	-1.901025	4.332234	0.551467
H	-3.534024	3.145715	-0.889879

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H	0.571657	4.114149	-1.455101
C	0.330666	3.078126	-1.203569
C	-0.212829	1.473468	0.609225
C	0.576640	0.397541	-0.176222
C	0.335987	2.872605	0.313507
C	1.378570	2.152193	-1.831949
H	-1.265835	1.435472	0.321892
H	1.036416	-0.314829	0.514063
H	2.308045	2.676706	-2.066851
H	-0.657129	2.846439	-1.608553
H	-0.155687	1.251353	1.677488
H	-0.288760	3.630260	0.792295
H	1.011649	1.656137	-2.726985
N	1.780678	1.068912	-0.843958
C	1.784626	2.981597	0.801365
C	2.231372	3.874117	0.342699
C	2.551936	1.746170	0.272331
H	3.528294	2.018634	-0.134222
H	2.691976	0.996387	1.053668
C	1.980605	3.094830	2.292921
H	3.019023	3.041752	2.621239
C	1.025905	3.263064	3.203064
H	1.271419	3.347737	4.256581
H	-0.027334	3.328626	2.944126
C	-0.290035	-0.440852	-1.128931
O	-0.841374	0.400494	-2.114552
C	2.684315	0.092084	-1.585711
H	3.505849	0.708593	-1.960272
H	2.111544	-0.255050	-2.447712

H	-1.336118	-0.146979	-2.745131
H	0.349868	-1.189023	-1.609361
H	0.217674	-2.673888	0.177942
C	-0.816904	-2.368020	0.317069
C	-1.298341	-1.232153	-0.292425
N	-2.922376	-2.878876	1.339767
C	-2.671467	-0.884567	-0.084635
C	-1.658579	-3.157573	1.128215
C	-3.431240	-1.765492	0.746914
C	-3.327802	0.253294	-0.635908
H	-1.262423	-4.051209	1.605504
H	-5.347926	-2.171990	1.629204
C	-4.655848	0.490934	-0.370965
H	-2.782001	0.942980	-1.268319
C	-5.408717	-0.384879	0.452650
H	-6.453892	-0.158146	0.634717
C	-4.803739	-1.481805	0.993140
O	-5.329783	1.557358	-0.867401
H	-4.738185	2.088612	-1.422256
C	3.206971	-1.070187	-0.778451
C	4.202482	-3.263298	0.656787
C	2.690556	-2.353029	-0.986119
C	4.267212	-0.910831	0.121593
C	4.753798	-1.996977	0.841958
C	3.178940	-3.442740	-0.269642
H	1.923565	-2.516258	-1.738584
H	4.733604	0.061557	0.248065
H	5.572814	-1.855121	1.539254
H	2.765271	-4.430573	-0.444999
H	4.584145	-4.110545	1.217295

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H	-3.080902	-3.682692	-1.148393
C	-2.130861	-3.163294	-0.997129
C	-0.519363	-2.296204	0.714120
C	-0.315968	-1.071647	-0.213409
C	-1.903265	-2.913377	0.494180
C	-2.180076	-1.809720	-1.724677
H	0.251188	-3.038674	0.500380
H	-0.038287	-0.189393	0.370363
H	-3.199802	-1.521211	-1.989561
H	-1.330260	-3.778596	-1.406892
H	-0.407550	-1.989097	1.757973
H	-1.981489	-3.851053	1.051122
H	-1.557444	-1.792576	-2.618596
N	-1.681768	-0.701505	-0.814144
C	-2.973622	-1.920602	0.976631
H	-3.942162	-2.274384	0.597887
C	-2.662149	-0.560898	0.338525
H	-3.552910	-0.075703	-0.064025
H	-2.189922	0.126843	1.040156
C	-3.073111	-1.876571	2.480652
H	-3.219638	-2.857799	2.932021
C	-3.023294	-0.811368	3.276255
H	-3.119041	-0.924024	4.351254
H	-2.904889	0.205498	2.912962
C	0.809223	-1.307506	-1.251812
O	0.591007	-2.550175	-1.877262
C	-1.652454	0.605653	-1.611214
H	-2.423664	0.489772	-2.375047
H	-0.693012	0.641175	-2.126647
H	1.271487	-2.672600	-2.558148
H	0.808588	-0.512164	-2.006243
H	2.346093	-3.398106	-0.422789
C	2.771554	-2.435826	-0.158424
C	2.145218	-1.271752	-0.522500
N	4.561955	-1.264022	0.947464
C	2.766048	-0.033129	-0.178977
C	3.984838	-2.379482	0.572745
C	3.968488	-0.093094	0.580244
C	2.251252	1.229963	-0.552163
H	4.475309	-3.306576	0.861705
H	5.503097	1.053012	1.558269
C	2.867963	2.389137	-0.138123
H	1.378304	1.322956	-1.188183
C	4.052172	2.333767	0.640483
H	4.531007	3.257817	0.953660
C	4.589195	1.120268	0.977294
O	2.305199	3.566455	-0.502027
H	2.827599	4.306782	-0.157491
C	-1.924504	1.869473	-0.829852
C	-2.524987	4.244888	0.530029
C	-0.996758	2.438188	0.049081
C	-3.151506	2.511268	-1.023261
C	-3.451425	3.692309	-0.350532
C	-1.298023	3.615438	0.727336
H	-0.027252	1.979977	0.212886
H	-3.875474	2.086448	-1.713984
H	-4.407236	4.178425	-0.516160
H	-0.564842	4.043686	1.403025
H	-2.755365	5.165407	1.056554

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H	0.563867	4.109833	-1.463723
C	0.325494	3.073604	-1.210470
C	-0.214386	1.471010	0.604996
C	0.578422	0.395380	-0.177442
C	0.330958	2.871037	0.306954
C	1.376645	2.149617	-1.836266
H	-1.266679	1.430491	0.315939
H	1.039831	-0.314555	0.514349
H	2.305081	2.676213	-2.070806
H	-0.661573	2.838553	-1.615156
H	-0.157725	1.251185	1.673788
H	-0.296539	3.627674	0.783694
H	1.012037	1.651021	-2.730795
N	1.781016	1.068897	-0.845934
C	1.778994	2.984946	0.795357
H	2.223721	3.877621	0.335013
C	2.549830	1.750409	0.269289
C	3.525696	2.024578	-0.137359
H	2.691443	1.002628	1.052270
C	1.974035	3.101882	2.286731
H	3.012381	3.051684	2.615806
C	1.018431	3.270285	3.195910
H	1.263034	3.358063	4.249399
H	-0.034704	3.333074	2.935895
C	-0.285335	-0.446419	-1.130083
O	-0.834563	0.393263	-2.117294
C	2.687327	0.092893	-1.585174
H	3.507019	0.710601	-1.961746
H	2.115441	-0.258388	-2.446101
H	-1.347345	-0.150414	-2.736612
H	0.356519	-1.195037	-1.607579

H	0.217715	-2.682924	0.175649
C	-0.816430	-2.374919	0.313422
C	-1.294203	-1.238072	-0.294445
N	-2.924333	-2.887076	1.333362
C	-2.668670	-0.888138	-0.087347
C	-1.661469	-3.165777	1.122798
C	-3.431100	-1.770361	0.741610
C	-3.318945	0.250288	-0.635537
H	-1.266171	-4.060735	1.598442
H	-5.349781	-2.173273	1.618720
C	-4.647109	0.494663	-0.372445
H	-2.786070	0.948940	-1.266056
C	-5.402277	-0.381818	0.446702
H	-6.450567	-0.170143	0.640642
C	-4.800591	-1.484311	0.985719
O	-5.206053	1.601216	-0.924017
H	-6.137556	1.665080	-0.664728
C	3.213518	-1.065442	-0.774448
C	4.214800	-3.251013	0.668484
C	2.700205	-2.350297	-0.977282
C	4.273601	-0.900339	0.124751
C	4.763044	-1.982684	0.848914
C	3.191447	-3.436226	-0.257025
H	1.933379	-2.518010	-1.728908
H	4.737518	0.073688	0.247783
H	5.581898	-1.836269	1.545478
H	2.780126	-4.425674	-0.428789
H	4.598734	-4.095282	1.231938

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H	-3.897093	0.775688	-2.210111
C	-3.130666	-0.003224	-2.261529
C	-2.295347	-2.111540	-1.272752
C	-1.212898	-1.451221	-0.395379
C	-3.510391	-1.189939	-1.374009
C	-1.775402	0.547167	-1.788655
H	-1.895889	-2.317513	-2.270853
H	-1.348012	-1.750122	0.648193
H	-1.769075	1.636063	-1.749138
H	-3.043766	-0.315418	-3.304953
H	-2.550737	-3.073002	-0.823973
H	-4.364265	-1.727217	-1.794490
H	-0.944556	0.219362	-2.417275
N	-1.481044	0.060160	-0.384332
C	-3.861059	-0.657848	0.029015
H	-4.768870	-0.049224	-0.064729
C	-2.723221	0.283381	0.459592
H	-2.994111	1.330788	0.321238
H	-2.427553	0.146598	1.500926
C	-4.177291	-1.792647	0.974044
H	-4.973845	-2.441511	0.608677
C	-3.620812	-2.078216	2.148206
H	-3.956205	-2.935532	2.722315
H	-2.828032	-1.487995	2.600713
C	0.206426	-1.876745	-0.846472
O	0.047301	-3.256241	-1.132993
C	-0.309634	0.827076	0.212346
H	0.521960	0.693558	-0.481867
H	-0.068021	0.315868	1.147530
H	0.924106	-3.622987	-1.325528
H	0.468687	-1.335074	-1.764147
H	0.267258	-2.999629	1.588669
C	1.145423	-2.388295	1.400640
C	1.293673	-1.718770	0.209378
N	3.255279	-1.610176	2.244884
C	2.498282	-0.979829	-0.006441
C	2.149134	-2.299282	2.392088
C	3.442046	-0.960390	1.063734
C	2.801760	-0.269774	-1.196218
H	2.017283	-2.821456	3.337112
H	5.350064	-0.234417	1.735431
C	3.982902	0.427337	-1.313293
H	2.134051	-0.265264	-2.050717
C	4.920104	0.449366	-0.248293
H	5.847441	1.004280	-0.362431
C	4.650491	-0.230731	0.906246
O	4.217011	1.084955	-2.474025
H	5.081220	1.522589	-2.440037
C	-0.551884	2.295802	0.444703
C	-0.923468	5.030239	0.897675
C	-1.056987	2.748497	1.667719
C	-0.203580	3.229878	-0.535761
C	-0.394644	4.590807	-0.313602
C	-1.248255	4.108364	1.890848
H	-1.289162	2.036730	2.455996
H	0.235065	2.892706	-1.472256
H	-0.120410	5.306030	-1.082144
H	-1.640540	4.448542	2.843565
H	-1.069350	6.091182	1.073594

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H	-2.430860	1.092612	3.246225
C	-1.606572	1.031078	2.531203
C	-0.313201	2.254383	0.781072
C	-0.290869	0.949639	-0.048325
C	-1.548610	2.299974	1.679627
C	-1.818316	-0.183769	1.614566
H	0.589886	2.311744	1.393869
H	-0.296082	1.163726	-1.121653
H	-2.835806	-0.573486	1.674393
H	-0.676002	0.910820	3.089014
H	-0.315043	3.120988	0.114447
H	-1.508744	3.185454	2.319470
H	-1.113084	-0.986798	1.827641
N	-1.624467	0.212492	0.165113
C	-2.805586	2.352332	0.786918
H	-3.673505	2.187605	1.436595
C	-2.726912	1.183279	-0.210195
H	-3.655720	0.614700	-0.220174
H	-2.509863	1.499339	-1.231997
C	-2.971011	3.709791	0.149921
H	-3.301179	4.476261	0.849983
C	-2.724590	4.065286	-1.108417
H	-2.856977	5.094787	-1.424532
H	-2.389191	3.373497	-1.876364
C	0.937840	0.072035	0.255546
O	1.069085	-0.153981	1.650444
C	-1.701368	-1.010066	-0.742988
H	-0.918059	-1.689947	-0.410122
H	-1.453614	-0.650537	-1.745805
H	1.757778	0.427301	2.008381
H	0.800542	-0.916106	-0.194340
H	1.469963	2.491017	-1.106585
C	2.321430	1.831951	-0.979823

C	2.223378	0.622095	-0.340918
N	4.672883	1.554244	-1.419690
C	3.407465	-0.180441	-0.232076
C	3.571194	2.256245	-1.500597
C	4.604772	0.342519	-0.798077
C	3.434722	-1.453924	0.385825
H	3.636856	3.220661	-1.999540
H	6.694437	-0.008804	-1.163165
C	4.606489	-2.175317	0.435799
H	2.550048	-1.872359	0.851029
C	5.801262	-1.657377	-0.125739
H	6.715131	-2.243533	-0.075104
C	5.794278	-0.427613	-0.725659
O	4.578058	-3.388482	1.040238
H	5.459952	-3.789855	1.019885
C	-3.021506	-1.736350	-0.736090
C	-5.432519	-3.151097	-0.757034
C	-3.996164	-1.456740	-1.698607
C	-3.256306	-2.749061	0.199095
C	-4.459297	-3.448180	0.194257
C	-5.198174	-2.158724	-1.706938
H	-3.811527	-0.691601	-2.448997
H	-2.489954	-2.999594	0.928665
H	-4.630346	-4.230509	0.926279
H	-5.947482	-1.936175	-2.459540
H	-6.368478	-3.700344	-0.765460

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H	-2.422632	1.251111	3.112832
C	-1.611225	1.147011	2.388083
C	-0.327597	2.265186	0.565567
C	-0.291291	0.902037	-0.166198
C	-1.563512	2.366945	1.465005
C	-1.845362	-0.115889	1.545002
H	0.576254	2.377830	1.170897
H	-0.278442	1.038164	-1.251555
H	-2.872257	-0.478427	1.618461
H	-0.671929	1.053261	2.935422
H	-0.336096	3.076710	-0.167020
H	-1.517648	3.280090	2.062921
H	-1.160573	-0.921358	1.811643
N	-1.631459	0.189722	0.076531
C	-2.825993	2.352148	0.597437
H	-3.686278	2.168665	1.254788
C	-2.714118	1.151007	-0.370204
H	-3.644087	0.585360	-0.415208
H	-2.443086	1.464155	-1.382926
C	-3.115461	3.609623	-0.184521
C	-3.924919	3.519699	-0.909497
C	-2.497545	4.779750	-0.051866
H	-2.790734	5.634932	-0.651841
H	-1.688702	4.939155	0.656107
C	0.933535	0.046379	0.207850
O	1.053100	-0.100766	1.613899
C	-1.710413	-1.083125	-0.758585
H	-0.924425	-1.740713	-0.389611
H	-1.467049	-0.781847	-1.780992
H	1.714428	0.525536	1.947071
H	0.801531	-0.966941	-0.185006
H	1.462658	2.372258	-1.305381
C	2.318957	1.733353	-1.123297
C	2.224574	0.565717	-0.407142
N	4.677013	1.453659	-1.512257
C	3.414262	-0.213621	-0.231488
C	3.568966	2.137140	-1.653848
C	4.612940	0.285134	-0.815017
C	3.448811	-1.448334	0.467599
H	3.631075	3.067348	-2.214236
H	6.712009	-0.061043	-1.131420
C	4.628899	-2.148245	0.574682
H	2.552815	-1.832774	0.944662
C	5.826122	-1.652435	-0.004152
H	6.734131	-2.235824	0.106786
C	5.812427	-0.465050	-0.679020
O	4.736283	-3.330291	1.227323
H	3.875863	-3.583180	1.595875
C	-3.029447	-1.809971	-0.709144
C	-5.432207	-3.239361	-0.664448
C	-3.996030	-1.599329	-1.697297
C	-3.269086	-2.761309	0.287415
C	-4.467577	-3.467381	0.314745
C	-5.193806	-2.308178	-1.673117
H	-3.807291	-0.884493	-2.494691
H	-2.509737	-2.959952	1.039668
H	-4.641617	-4.203616	1.092425
H	-5.936111	-2.139195	-2.446175
H	-6.364029	-3.795352	-0.647943

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H	-2.434424	1.254905	3.108344
C	-1.620501	1.152605	2.386138
C	-0.337549	2.270992	0.563527
C	-0.295439	0.907194	-0.166407
C	-1.575875	2.370264	1.459876
C	-1.846133	-0.113840	1.545973
H	0.564353	2.385481	1.171374
H	-0.282185	1.041572	-1.252087
H	-2.870855	-0.482475	1.619463
H	-0.682081	1.064766	2.935930
H	-0.346448	3.081754	-0.169909
H	-1.534859	3.285131	2.055541
H	-1.156559	-0.914415	1.815257
N	-1.632781	0.189238	0.076842
C	-2.836544	2.348383	0.589766
H	-3.697613	2.164629	1.246029
C	-2.719188	1.144148	-0.373383
H	-3.646688	0.574380	-0.416462
H	-2.449231	1.454785	-1.387171
C	-3.128486	3.602200	-0.197163
H	-3.935075	3.506663	-0.924641
C	-2.515869	4.775277	-0.066019
H	-2.810469	5.627527	-0.669478
H	-1.710037	4.939893	0.644178
C	0.931418	0.056552	0.211204
O	1.048005	-0.083331	1.618019
C	-1.705094	-1.086637	-0.754408
H	-0.917293	-1.740057	-0.381956
H	-1.461111	-0.787723	-1.777375
H	1.727315	0.525417	1.946958
H	0.803533	-0.958099	-0.179530
H	1.464761	2.387231	-1.296310
C	2.319518	1.745991	-1.114727
C	2.221698	0.577184	-0.403289
N	4.679375	1.465631	-1.501364

C	3.410720	-0.206330	-0.229013
C	3.572860	2.149936	-1.642148
C	4.611987	0.293128	-0.808337
C	3.439270	-1.441361	0.462578
C	3.636531	3.082296	-2.198887
H	6.709730	-0.058466	-1.120741
C	4.615842	-2.148681	0.569975
H	2.550870	-1.840453	0.937855
C	5.814691	-1.652770	-0.002910
H	6.732879	-2.226089	0.095181
C	5.806615	-0.459689	-0.673007
O	4.588214	-3.326243	1.240948
H	5.473013	-3.721410	1.253420
C	-3.021324	-1.818620	-0.704676
C	-5.418209	-3.257901	-0.659050
C	-3.988542	-1.613135	-1.693324
C	-3.257275	-2.769800	0.292905
C	-4.452872	-3.480829	0.320623
C	-5.183413	-2.326825	-1.668671
H	-3.802626	-0.898405	-2.491467
H	-2.497245	-2.964529	1.045467
H	-4.623998	-4.216997	1.099011
H	-5.926232	-2.161659	-2.442064
H	-6.347707	-3.817767	-0.642211

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H	-4.017687	-1.954698	-2.117308
C	-3.027159	-1.736433	-1.711008
C	-1.543830	-1.862185	0.281950
C	-0.790397	-0.718228	-0.438758
C	-3.005699	-1.884514	-0.182839
C	-2.661479	-0.288470	-2.057599
H	-1.059336	-2.810522	0.054829
H	-0.203641	-0.153431	0.289623
H	-3.541297	0.354933	-2.133796
H	-2.313379	-2.432941	-2.160647
H	-1.488263	-1.704331	1.362702
H	-3.490404	-2.818219	0.109635
H	-2.098875	-0.189154	-2.985729
N	-1.838885	0.292184	-0.923782
C	-3.725587	-0.674877	0.424860
H	-4.652424	-0.497149	-0.137645
C	-2.797981	0.544478	0.224038
H	-3.356983	1.449571	-0.020366
H	-2.183631	0.743278	1.105306
C	-4.095691	-0.778443	1.883163
H	-4.510664	0.133785	2.312339
C	-3.965536	-1.853284	2.655271
H	-4.269828	-1.829579	3.696557
H	-3.560506	-2.792619	2.289436
C	0.152412	-1.168302	-1.608900
O	0.193445	-2.580923	-1.633196
C	-1.217919	1.606893	-1.382249
H	-2.008950	2.111547	-1.942848
H	-0.421190	1.344398	-2.080942
H	0.826537	-2.845263	-2.318979
H	-0.255840	-0.809030	-2.561618
H	1.454682	0.456353	-3.355609
C	2.031622	0.251613	-2.457350
C	1.542105	-0.573106	-1.476139
N	4.050635	0.708506	-1.234966
C	2.359852	-0.825916	-0.329508
C	3.297235	0.871233	-2.293719
C	3.602203	-0.132177	-0.258371
C	1.988489	-1.691973	0.726011
H	3.673427	1.533586	-3.070037
H	5.366133	0.226869	0.917424
C	2.812282	-1.842966	1.819568
H	1.077652	-2.277515	0.677413
C	4.042854	-1.142225	1.901578
H	4.678436	-1.279008	2.772518
C	4.425207	-0.312126	0.883247
O	2.413470	-2.685208	2.802247
H	3.078245	-2.710967	3.507111
C	-0.712568	2.496536	-0.275136
C	0.195369	4.198593	1.753185
C	0.584531	2.367320	0.231012
C	-1.538673	3.507479	0.226912
C	-1.090174	4.351684	1.237407
H	1.033200	3.209169	1.245182
H	1.259444	1.622421	-0.179374
H	-2.535101	3.646945	-0.185083
H	-1.741647	5.132942	1.614905
H	2.042129	3.095134	1.628368
H	0.547365	4.858239	2.539807

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H	3.850680	-2.329238	1.399937
C	2.859150	-1.878418	1.309673
C	0.500863	-2.207965	0.640401
C	0.497726	-0.800675	-0.002980
C	1.898220	-2.825477	0.588009
C	2.970368	-0.559752	0.528328
H	0.190399	-2.124638	1.684604
H	-0.123594	-0.800826	-0.903415
H	3.919347	-0.475450	-0.008390
H	2.484651	-1.672492	2.315061
H	-0.228872	-2.835639	0.124261
H	1.897495	-3.797682	1.087099
H	2.836644	0.302606	1.173882
N	1.903433	-0.492618	-0.545345
C	2.359247	-2.971443	-0.864045
H	3.430228	-3.214366	-0.855736
C	2.202895	-1.594942	-1.551857
H	3.116173	-1.303930	-2.071683
H	1.377558	-1.584512	-2.268850
C	1.663412	-4.035545	-1.677380
H	1.887311	-4.012232	-2.744100
C	0.849560	-4.979419	-1.213453
H	0.414612	-5.714118	-1.883132
H	0.588586	-5.067200	-0.162344
C	-0.067300	0.267481	0.945842
O	0.737867	0.278080	2.102557
C	1.979275	0.817734	-1.334167
H	1.104473	0.809513	-1.990612
H	2.864030	0.704941	-1.965457
H	0.480069	1.036287	2.650456
H	-0.038089	1.245534	0.458558
H	-1.118988	-0.777728	3.226277
C	-1.872532	-0.590183	2.469053
C	-1.521126	-0.058985	1.255212
N	-4.205795	-0.691686	1.883385
C	-2.553489	0.192848	0.299673
C	-3.231330	-0.891410	2.736475

C	-3.883731	-0.150858	0.673989
C	-2.325696	0.770626	-0.972617
H	-3.502709	-1.317200	3.700276
H	-5.943503	-0.186916	0.058540
C	-3.371260	0.988561	-1.841074
H	-1.333004	1.065658	-1.293579
C	-4.695258	0.637240	-1.474467
H	-5.508715	0.816026	-2.172429
C	-4.938250	0.084375	-0.246473
O	-3.091012	1.545676	-3.044035
H	-3.905451	1.652496	-3.558616
C	2.080276	2.131626	-0.592367
C	2.298788	4.661302	0.597230
C	3.272197	2.528007	0.024624
C	1.023307	3.045064	-0.655225
C	1.125824	4.298646	-0.059280
C	3.374606	3.776985	0.629483
H	4.135893	1.869939	0.021795
H	0.112839	2.785344	-1.190681
H	0.292988	4.991498	-0.117719
H	4.303071	4.064556	1.111812
H	2.383101	5.637327	1.064098

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H	3.758300	0.812221	2.284542
C	3.016954	0.008102	2.278028
C	2.289135	-2.089769	1.192415
C	1.190363	-1.439521	0.325379
C	3.466396	-1.128089	1.356627
C	1.660846	0.535687	1.782171
H	1.880485	-2.344298	2.175216
H	1.328192	-1.700628	-0.729145
H	1.625531	1.624697	1.769071
H	2.905399	-0.350637	3.304115
H	2.586549	-3.029334	0.724137
H	4.328404	-1.650093	1.778143
H	0.825347	0.170416	2.382702
N	1.409838	0.077467	0.359958
C	3.844362	-0.518019	-0.004875
H	4.704901	0.142831	0.145359
C	2.656218	0.362699	-0.457910
H	2.866098	1.424779	-0.325414
H	2.391839	0.189554	-1.504395
C	4.223599	-1.552376	-1.031019
H	3.438375	-2.227701	-1.372806
H	5.452172	-1.684791	-1.521252
H	5.692636	-2.453186	-2.248888
H	6.261450	-1.028815	-1.209237
C	-0.216606	-1.925206	0.760774
O	-0.010601	-3.307317	0.999936
C	0.222931	0.818663	-0.240058
H	-0.615510	0.639123	0.435025
H	0.017006	0.323253	-1.192392
H	-0.874100	-3.710487	1.179268
H	-0.493703	-1.422528	1.696418
H	-0.266203	-3.000363	-1.693774
C	-1.156120	-2.411467	-1.491072
C	-1.313015	-1.768992	-0.286212
N	-3.285862	-1.662904	-2.310904
C	-2.533501	-1.063017	-0.049490
C	-2.165814	-2.324743	-2.476552
C	-3.481794	-1.041983	-1.115746
C	-2.849162	-0.386472	1.156478
H	-2.026843	-2.824893	-3.432340
H	-5.407707	-0.344429	-1.765786
C	-4.044868	0.281886	1.292082
H	-2.180242	-0.385756	2.009958
C	-4.985937	0.306657	0.230644
H	-5.924823	0.838241	0.359964
C	-4.705428	-0.342661	-0.938892
O	-4.289788	0.907745	2.467911
H	-5.163859	1.326253	2.446234
C	0.415514	2.300223	-0.430742
C	0.687851	5.057849	-0.805114
C	0.918858	2.804354	-1.634118
C	0.019972	3.193282	0.569679
C	0.161482	4.565923	0.386924
C	1.060308	4.176191	-1.818055
H	1.189426	2.123119	-2.436902
H	-0.416403	2.813448	1.490619
H	-0.149898	5.248955	1.170357
H	1.451633	4.556423	-2.755884
H	0.794714	6.128021	-0.950895

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H	3.307243	2.875112	-1.195053
C	2.371246	2.532275	-1.645157
C	-0.084296	2.408070	-1.400325
C	-0.109927	0.955960	-0.882671
C	1.171480	3.117530	-0.894708
C	2.285758	0.997308	-1.595658
H	-0.098347	2.414973	-2.492855
H	-0.634249	0.901073	0.075092
H	3.248260	0.541032	-1.365073
H	2.366802	2.855112	-2.688947
H	-0.998355	2.909663	-1.073232
H	1.095542	4.193692	-1.065554
H	1.911934	0.566232	-2.526896
N	1.327964	0.569572	-0.506124
C	1.365334	2.842874	0.607123
H	2.251871	3.392411	0.941193
C	1.669513	1.334812	0.759423
H	2.728676	1.151435	0.944576
H	1.091491	0.878452	1.567535
C	0.197862	3.291387	1.446761
H	-0.741181	2.745991	1.338476
C	0.257045	4.315954	2.291958
H	-0.607327	4.625693	2.870170
H	1.175395	4.881093	2.433231
C	-0.807435	-0.012913	-1.883713
O	-1.728640	0.786974	-2.601580
C	1.438391	-0.925142	-0.239166
H	1.274395	-1.413732	-1.200295
H	0.602775	-1.167536	0.422557
H	-2.273961	0.195297	-3.142989
H	-0.058127	-0.422134	-2.578892
H	-0.410596	-2.681313	-2.251803
C	-1.186592	-2.466868	-1.521717
C	-1.526191	-1.173619	-1.215440
N	-2.760217	-3.385452	0.044839
C	-2.588099	-0.956367	-0.278800
C	-1.833153	-3.544136	-0.867232
C	-3.145748	-2.111796	0.341701
C	-3.106506	0.320558	0.052241

H	-1.550037	-4.565875	-1.109997
H	-4.569877	-2.839306	1.779164
C	-4.101539	0.443455	0.995831
H	-2.771941	1.212097	-0.465679
C	-4.630868	-0.701882	1.644143
H	-5.412979	-0.581460	2.388957
C	-4.166825	-1.945741	1.314152
O	-4.560315	1.687846	1.274010
H	-5.282120	1.639177	1.919032
C	2.746188	-1.379923	0.353987
C	5.145086	-2.300395	1.456542
C	2.900757	-1.465283	1.741184
C	3.794788	-1.789741	-0.475266
C	4.991675	-2.241833	0.073427
C	4.096203	-1.917521	2.290428
H	2.077738	-1.188754	2.395166
H	3.670320	-1.771708	-1.555577
H	5.798474	-2.558063	-0.579451
H	4.204505	-1.980157	3.368233
H	6.076189	-2.658034	1.884269

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H	3.820588	0.977838	2.626804
C	3.015620	0.496217	2.065778
C	2.475158	-1.373974	0.454598
C	1.503980	-0.361618	-0.199920
C	3.594867	-0.631519	1.203156
C	2.340047	1.544776	1.157132
H	1.909055	-1.999388	1.146413
H	1.335262	-0.596248	-1.254267
H	2.921508	2.466103	1.066093
H	2.288187	0.100585	2.772475
H	2.911559	-2.019889	-0.312753
H	4.150558	-1.326398	1.836904
H	1.334336	1.794761	1.498803
N	2.209875	0.999943	-0.244998
C	4.517200	0.026349	0.174227
H	5.133681	0.774022	0.690513
C	3.602526	0.767166	-0.819545
H	4.000941	1.746347	-1.091948
H	3.448795	0.187664	-1.734199
C	5.451128	-0.885548	-0.581759
H	5.994205	-0.408441	-1.397865
C	5.665145	-2.173408	-0.328887
H	6.370652	-2.747676	-0.920371
H	5.157989	-2.704179	0.472235
C	0.128944	-0.330885	0.499951
O	0.303925	-0.548155	1.892913
C	1.581241	2.017741	-1.201881
H	1.793686	1.632785	-2.202335
H	2.171279	2.924743	-1.050435
H	-0.574174	-0.609892	2.301337
H	-0.322730	0.647660	0.350405
H	0.623447	-2.685156	-0.967047
C	-0.423145	-2.482317	-0.761459
C	-0.825796	-1.363026	-0.078586
N	-2.678207	-3.285527	-1.026930
C	-2.226952	-1.187890	0.160622
C	-1.388708	-3.416488	-1.215390
C	-3.107958	-2.183906	-0.348221
C	-2.768930	-0.080116	0.856989
H	-1.058681	-4.301280	-1.755558
H	-5.157769	-2.803327	-0.546456
C	-4.130098	0.041184	1.022544
H	-2.143349	0.715788	1.249862
C	-5.009722	-0.949192	0.516492
H	-6.081151	-0.838465	0.660670
C	-4.504814	-2.032913	-0.150023
O	-4.592402	1.137345	1.672369
H	-5.558861	1.101437	1.737255
C	0.115242	2.317004	-1.070289
C	-2.618699	2.844429	-0.845421
C	-0.347212	3.248135	-0.135546
C	-0.798303	1.679228	-1.915717
C	-2.160650	1.937746	-1.800035
C	-1.711509	3.503390	-0.018032
H	0.358567	3.779296	0.498320
H	-0.441591	0.969978	-2.659442
H	-2.864151	1.426583	-2.449409
H	-2.065048	4.221900	0.714150
H	-3.682267	3.035051	-0.743584

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H	-4.446579	-2.273417	-0.644133
C	-3.379599	-2.043613	-0.697065
C	-1.255535	-1.813877	0.544788
C	-0.898333	-0.547804	-0.268781
C	-2.770673	-1.955045	0.703371
C	-3.187925	-0.699589	-1.410274
H	-0.868359	-2.707390	0.041749
H	-0.392616	0.172889	0.377333
H	-4.110735	-0.115796	-1.426580
H	-2.904089	-2.851901	-1.261030
H	-0.754600	-1.761228	1.514201
H	-3.006881	-2.861007	1.266333
H	-2.817202	-0.805849	-2.426129
N	-2.195765	0.174146	-0.652563
C	-3.360949	-0.723248	1.399772
H	-4.451915	-0.764375	1.282689
C	-2.858526	0.542636	0.659263
H	-3.675720	1.227089	0.420955
H	-2.110292	1.073078	1.249600
C	-3.070952	-0.595871	2.875168
H	-3.372834	0.354392	3.316317
C	-2.517899	-1.519857	3.655234
H	-2.366518	-1.333948	4.713446
H	-2.200290	-2.490403	3.284397
O	0.032864	-0.824778	-1.469013
C	-0.634323	-1.509926	-2.503111
C	-1.970728	1.409891	-1.516732
H	-2.970281	1.828992	-1.663032
H	-1.624090	1.030845	-2.480764
H	-0.891107	-2.392668	-2.191817
H	0.335503	0.128079	-1.910533
H	0.867662	-3.375891	-2.033481
C	1.528601	-2.841869	-1.359641
C	1.291609	-1.541432	-0.994744
N	3.558490	-2.971812	-0.075819
C	2.255787	-0.889816	-0.160554
C	2.674305	-3.517703	-0.871743
C	3.367698	-1.668252	0.274645
C	2.180457	0.471335	0.224081
H	2.843642	-4.552803	-1.160638
H	5.177976	-1.682392	1.431687

C	3.155929	1.027631	1.021710
H	1.383978	1.121450	-0.120936
C	4.246761	0.246481	1.479256
H	5.001592	0.700398	2.115984
C	4.345763	-1.066469	1.107645
O	3.038635	2.337568	1.348741
H	3.802130	2.615696	1.877249
C	-1.018345	2.454367	-0.988131
C	0.756618	4.444714	-0.120834
C	0.172573	2.701725	-1.679719
C	-1.337697	3.266212	0.107936
C	-0.448617	4.241315	0.547742
C	1.056795	3.687797	-1.248988
H	0.408616	2.132214	-2.575482
H	-2.294177	3.163886	0.610272
H	-0.706757	4.852572	1.406126
H	1.979860	3.857825	-1.793164
H	1.450617	5.202921	0.226663

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H	3.172107	3.158945	-0.669388
C	2.301635	2.830824	-1.245535
C	-0.135591	2.492254	-1.241510
C	-0.106437	1.020956	-0.800725
C	1.000933	3.246841	-0.546984
C	2.305714	1.300334	-1.398051
H	-0.020726	2.564402	-2.327010
H	-0.650139	0.907813	0.141536
H	3.287240	0.874550	-1.193378
H	2.369308	3.284294	-2.237218
H	-1.120317	2.894891	-1.002770
H	0.856564	4.326987	-0.623364
H	1.982706	0.972266	-2.398470
N	1.342675	0.688326	-0.404524
C	1.101649	2.814721	0.925784
H	1.898510	3.401198	1.400629
C	1.580615	1.344923	0.939858
H	2.650680	1.258622	1.131682
H	1.044260	0.747516	1.681681
C	-0.155935	3.004692	1.743765
H	-0.210084	2.405976	2.653479
C	-1.145778	3.852279	1.475053
H	-1.997739	3.941892	2.141141
H	-1.143425	4.494578	0.598496
C	-0.734127	0.081011	-1.867833
O	-1.692269	0.876014	-2.542392
C	1.558112	-0.812918	-0.285061
H	1.458473	-1.212342	-1.295611
H	0.726693	-1.181743	0.321115
H	-2.185847	0.296416	-3.143124
H	0.044573	-0.236401	-2.578499
H	-0.199955	-2.531544	-2.421358
C	-0.988974	-2.408038	-1.683995
C	-1.394817	-1.158579	-1.288698
N	-2.526384	-3.513549	-0.204597
C	-2.471186	-1.061279	-0.347638
C	-1.585992	-3.560165	-1.115601
C	-2.975983	-2.285272	0.180546
C	-3.051277	0.161483	0.074482
H	-1.250722	-4.546439	-1.428649
H	-4.374378	-3.184989	1.543596
C	-4.053638	0.166128	1.017868
C	-2.752530	1.106968	-0.363774
C	-4.534569	-1.048824	1.570274
H	-5.327315	-1.022003	2.313392
C	-4.010600	-2.241075	1.151601
O	-4.566674	1.363985	1.390953
H	-5.294132	1.232407	2.017762
C	2.882098	-1.224671	0.305034
C	5.322004	-2.060482	1.386967
C	3.006312	-1.451652	1.679030
C	3.985195	-1.449956	-0.524377
C	5.201520	-1.859624	0.013932
C	4.221644	-1.861661	2.218403
H	2.146174	-1.320963	2.330598
H	3.888668	-1.317142	-1.599313
H	6.049573	-2.032317	-0.640557
H	4.305651	-2.035264	3.286168
H	6.268460	-2.385500	1.807043

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H	3.839830	1.149984	2.017231
C	3.158213	0.299780	2.112801
C	2.464568	-1.870974	1.170218
C	1.319411	-1.318764	0.302141
C	3.610713	-0.857872	1.215431
C	1.733548	0.705926	1.703607
H	2.100161	-2.062471	2.184895
H	1.472952	-1.600774	-0.745876
H	1.604087	1.787795	1.689382
H	3.151573	-0.004190	3.162038
H	2.766514	-2.831063	0.753406
H	4.518258	-1.315913	1.615728
H	0.971146	0.272640	2.354996
N	1.441496	0.211203	0.300829
C	3.867640	-0.284955	-0.187687
H	4.706187	0.419704	-0.118268
C	2.629391	0.556080	-0.573314
H	2.799821	1.624939	-0.439227
H	2.318468	0.379341	-1.606124
C	4.219404	-1.302627	-1.248103
H	4.056675	-0.977854	-2.276225
C	4.752586	-2.501977	-1.031263
H	5.016209	-3.151878	-1.859171
H	4.960865	-2.877189	-0.032747
C	-0.045745	-1.878502	0.775128
O	0.247449	-3.239667	1.041748
C	0.189250	0.871745	-0.255562
H	-0.608401	0.646950	0.453831
H	-0.022825	0.357677	-1.196418
H	-0.587836	-3.689612	1.241397
H	-0.332228	-1.371273	1.705731
H	-0.080583	-2.999227	-1.658472
C	-1.001644	-2.464328	-1.445864
C	-1.171809	-1.811313	-0.248490
N	-3.190345	-1.860827	-2.229332
C	-2.427641	-1.176143	0.004184
C	-2.036300	-2.457697	-2.408812
C	-3.397749	-1.230622	-1.041003
C	-2.756325	-0.497034	1.205277
H	-1.888337	-2.966110	-3.358908
H	-5.374919	-0.657209	-1.659354
C	-3.984831	0.105272	1.355275
H	-2.068495	-0.439917	2.042018

C	-4.948103	0.055212	0.314622
H	-5.913055	0.534900	0.454351
C	-4.655788	-0.599348	-0.849135
O	-4.239759	0.739392	2.524667
H	-5.134622	1.111693	2.513515
C	0.280966	2.361390	-0.461197
C	0.360367	5.129279	-0.852951
C	0.721958	2.891099	-1.678058
C	-0.150202	3.232240	0.544075
C	-0.104991	4.610232	0.352875
C	0.767711	4.268360	-1.870360
H	1.018900	2.226099	-2.485070
H	-0.539957	2.828885	1.475822
H	-0.443049	5.275460	1.140533
H	1.112912	4.668182	-2.818129
H	0.392590	6.203246	-1.005702

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H	1.198627	1.374339	-2.854453
C	0.432756	1.153906	-2.105418
C	-0.682497	1.916588	-0.039941
C	0.096698	0.989127	0.910517
C	0.209914	2.366248	-1.197188
C	0.859145	-0.045887	-1.241664
H	-1.545181	1.393005	-0.458688
H	0.576792	1.568376	1.705751
H	1.707408	-0.575327	-1.675015
H	-0.487812	0.900460	-2.637174
H	-1.061946	2.765266	0.536049
H	-0.266188	3.180692	-1.747431
H	0.049387	-0.758537	-1.076890
N	1.237928	0.428826	0.127223
C	1.574798	2.826318	-0.659999
H	2.179840	3.162522	-1.508681
C	2.267948	1.583047	-0.058039
H	3.057263	1.207863	-0.710602
H	2.700238	1.789031	0.924651
C	1.469823	3.967579	0.316567
H	0.984605	3.766327	1.272511
C	1.923922	5.191411	0.064249
H	1.817431	5.996056	0.784422
H	2.418169	5.429508	-0.874685
C	-0.842139	0.024857	1.682613
O	-0.090870	-0.549559	2.730286
C	1.998476	-0.683774	0.897507
H	1.280916	-1.497466	0.949515
H	2.144257	-0.294724	1.906154
H	-0.705882	-0.976143	3.347497
H	-1.569890	0.732471	2.105910
H	-0.241570	-2.607258	1.358641
C	-1.142284	-2.318951	0.828719
C	-1.620956	-1.031481	0.901251
N	-2.964708	-3.069490	-0.546143
C	-2.899972	-0.764914	0.309290
C	-1.837607	-3.298739	0.081857
C	-3.512049	-1.829009	-0.419766
C	-3.608911	0.455638	0.445962
H	-1.426351	-4.302989	0.006889
H	-5.208846	-2.435117	-1.591036
C	-4.841524	0.623899	-0.142444
H	-3.217287	1.284140	1.024675
C	-5.428314	-0.418517	-0.904463
H	-6.399221	-0.264930	-1.367939
C	-4.774985	-1.612538	-1.032294
O	-5.467958	1.812385	0.032476
H	-6.330697	1.801551	-0.408838
C	3.292902	-1.164233	0.295798
C	5.698347	-2.134344	-0.752348
C	4.512308	-0.598775	0.681062
C	3.294863	-2.241550	-0.595716
C	4.490725	-2.720881	-1.123141
C	5.708691	-1.076736	0.155019
H	4.528591	0.211688	1.405767
H	2.355484	-2.719140	-0.866336
H	4.478758	-3.558784	-1.812406
H	6.648744	-0.630201	0.462429
H	6.631983	-2.510374	-1.158291

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H	1.210104	1.186309	-3.019423
C	0.442194	1.005188	-2.261969
C	-0.726268	1.908047	-0.282011
C	0.087900	1.112929	0.755186
C	0.157897	2.284356	-1.470542
C	0.898930	-0.092458	-1.285578
H	-1.565389	1.313642	-0.650793
H	0.534593	1.798964	1.481221
H	1.763426	-0.637838	-1.663109
H	-0.459686	0.668094	-2.778818
H	-1.136754	2.793523	0.212330
H	-0.345566	3.022929	-2.099402
H	0.108389	-0.807129	-1.052545
N	1.314989	0.529315	0.030029
C	1.492295	2.850362	-0.952860
H	2.082971	3.154263	-1.825502
C	2.242425	1.693812	-0.272592
H	3.022272	1.290695	-0.920236
H	2.703098	1.980422	0.674219
C	1.268752	4.084546	-0.112728
H	0.736352	4.872463	-0.646066
C	1.630935	4.308984	1.147415
H	1.401555	5.254962	1.626528
H	2.172259	3.589181	1.755829
C	-0.811261	0.186003	1.613813
O	-0.038718	-0.281378	2.699203
C	2.060618	-0.471424	0.904342
H	1.358029	-1.277076	1.090577
H	2.238254	0.043674	1.850356
H	-0.639860	-0.663240	3.357965
H	-1.557007	0.902481	1.985888
H	-0.128300	-2.449371	1.463761
C	-1.049674	-2.226134	0.937814
C	-1.566403	-0.951375	0.927212
N	-2.882025	-3.131751	-0.326726
C	-2.864562	-0.766662	0.345040
C	-1.733092	-3.279645	0.285761
C	-3.462005	-1.900704	-0.283725
C	-3.602983	0.443289	0.396126
H	-1.294302	-4.275090	0.277758
H	-5.165803	-2.643283	-1.362281
C	-4.850780	0.532231	-0.176877
H	-3.220540	1.328357	0.890945
C	-5.426065	-0.583588	-0.836676
H	-6.409911	-0.492665	-1.289076

C	-4.743532	-1.767065	-0.881742
O	-5.502468	1.716655	-0.086197
H	-6.369542	1.654547	-0.514831
C	3.335767	-1.013977	0.314345
C	5.703077	-2.100420	-0.706224
C	4.562350	-0.385618	0.549949
C	3.312700	-2.209151	-0.412174
C	4.489073	-2.747548	-0.925846
C	5.739351	-0.921813	0.036286
H	4.600717	0.519926	1.149668
H	2.367872	-2.726702	-0.566889
H	4.458098	-3.674907	-1.488250
H	6.685444	-0.425100	0.224978
H	6.622127	-2.520186	-1.102452

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H	1.191471	1.364181	-2.856301
C	0.426999	1.144897	-2.105547
C	-0.687216	1.913374	-0.041640
C	0.093610	0.989676	0.911167
C	0.203295	2.360138	-1.201462
C	0.856697	-0.051174	-1.238285
H	-1.549868	1.387416	-0.457674
H	0.573369	1.571709	1.704574
H	1.706129	-0.579723	-1.670399
H	-0.493738	0.888007	-2.635355
H	-1.065715	2.763870	0.532313
H	-0.274374	3.171934	-1.754284
H	0.048888	-0.765383	-1.071063
N	1.295074	0.428856	0.129011
C	1.567692	2.824241	-0.666649
C	2.171653	3.158445	-1.516843
C	2.263056	1.584228	-0.060652
H	3.052602	1.208071	-0.712332
H	2.695461	1.794290	0.921148
C	1.461320	3.968770	0.305969
H	0.978432	3.769522	1.263555
C	1.911776	5.192870	0.048444
H	1.804813	5.999859	0.765921
H	2.403866	5.428691	-0.892191
C	-0.845312	0.027170	1.685752
O	-0.093717	-0.545364	2.733890
C	1.998585	-0.679762	0.902719
H	1.282387	-1.494248	0.959106
H	2.145402	-0.286338	1.909536
H	-0.707499	-0.977549	3.348470
H	-1.571904	0.736209	2.109072
H	-0.239477	-2.601637	1.364765
C	-1.139527	-2.316956	0.832122
C	-1.623777	-1.029813	0.904856
N	-2.953153	-3.067517	-0.551493
C	-2.900553	-0.766986	0.310286
C	-1.827768	-3.296174	0.082021
C	-3.504516	-1.830504	-0.425009
C	-3.618169	0.453043	0.446818
H	-1.414491	-4.299524	0.007032
H	-5.190546	-2.440788	-1.611609
C	-4.847088	0.614230	-0.149471
H	-3.218253	1.271767	1.036657
C	-5.424272	-0.428491	-0.920436
H	-6.391638	-0.257429	-1.380486
C	-4.766223	-1.616905	-1.047421
O	-5.582332	1.746204	-0.047677
H	-5.116621	2.398350	0.498174
C	3.292651	-1.160600	0.300636
C	5.697235	-2.131010	-0.749009
C	4.511964	-0.591671	0.681004
C	3.294322	-2.241534	-0.586509
C	4.489757	-2.721045	-1.114702
C	5.707926	-1.069825	0.154175
H	4.528580	0.221712	1.402410
H	2.355101	-2.721704	-0.853048
H	4.477618	-3.561737	-1.800535
H	6.647947	-0.620508	0.457595
H	6.630563	-2.507091	-1.155605

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H	1.244000	1.459422	-2.860252
C	0.448525	1.223333	-2.147648
C	-0.749113	1.937470	-0.121936
C	0.082143	1.115595	0.873992
C	0.143924	2.436835	-1.260525
C	0.864060	0.046316	-1.248187
H	-1.540900	1.323443	-0.557683
H	0.533547	1.781191	1.617993
H	1.707783	-0.504049	-1.663368
H	-0.435865	0.934803	-2.720928
H	-1.224517	2.753502	0.427246
H	-0.363957	3.212349	-1.838240
H	0.046889	-0.653301	-1.061770
N	1.300140	0.567521	0.106202
C	1.475211	2.958012	-0.700784
H	2.078173	3.324967	-1.541388
C	2.231477	1.742177	-0.122249
H	3.005920	1.380798	-0.800107
H	2.691610	1.967291	0.843480
C	1.356668	4.086199	0.298133
H	2.217406	4.217834	0.954441
C	0.340637	4.939655	0.394207
H	0.360977	5.749839	1.115823
H	-0.537374	4.879969	-0.243732
C	-0.790822	0.148609	1.715848
O	-0.003464	-0.286490	2.804349
C	2.041252	-0.497878	0.903063
H	1.333539	-1.311172	1.025023
H	2.224985	-0.055136	1.883596
H	-0.589466	-0.696154	3.460068
H	-1.573592	0.827383	2.084521
H	-0.040556	-2.466479	1.677306
C	-0.927700	-2.280410	1.083011
C	-1.479167	-1.022164	1.013685
N	-2.623504	-3.259212	-0.309064
C	-2.742528	-0.890699	0.345346
C	-1.525434	-3.363625	0.396998
C	-3.247224	-2.048457	-0.321272
C	-3.536619	0.284752	0.347755
H	-1.056175	-4.344203	0.438969
H	-4.829821	-2.857802	-1.526746
C	-4.741755	0.322673	-0.315825
H	-3.233624	1.178586	0.880255
C	-5.214803	-0.811455	-1.023345
H	-6.164060	-0.759335	-1.549719
C	-4.482411	-1.965773	-1.016232
O	-5.453240	1.474721	-0.266258

H	-6.287208	1.371480	-0.748988
C	3.308772	-1.006733	0.267727
C	5.656524	-2.032844	-0.855183
C	4.541514	-0.400694	0.528285
C	3.270310	-2.151551	-0.535418
C	4.436747	-2.659544	-1.099995
C	5.708752	-0.906994	-0.035660
H	4.592444	0.463976	1.184801
H	2.321142	-2.654893	-0.708535
H	4.394278	-3.548167	-1.721123
H	6.659799	-0.427727	0.172338
H	6.568145	-2.429268	-1.290711

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H	-0.601170	2.135385	-2.577940
C	-0.514149	1.487984	-1.701656
C	-0.149323	1.381264	0.750123
C	0.529351	0.007611	0.507392
C	-0.028777	2.278872	-0.483761
C	0.510382	0.385982	-1.999725
H	-1.207674	1.237831	0.968551
H	1.290529	-0.176398	1.269917
H	1.214620	0.688239	-2.778597
H	-1.501027	1.057042	-1.507563
H	0.294237	1.858093	1.627977
H	-0.626282	3.183153	-0.346304
H	0.055723	-0.555123	-2.300841
N	1.364000	0.121802	-0.777351
C	1.447539	2.645637	-0.714489
H	1.551140	3.040675	-1.731987
C	2.256300	1.340443	-0.595423
H	3.036420	1.277860	-1.355938
H	2.727122	1.235994	0.384828
C	1.975408	3.677780	0.242952
H	1.961309	3.415296	1.301426
C	2.445729	4.862339	-0.135323
H	2.809204	5.585883	0.587101
H	2.481730	5.149728	-1.183364
C	-0.463658	-1.177134	0.673953
O	0.273189	-2.380303	0.587089
C	2.247343	-1.096265	-1.061232
H	2.596456	-0.944582	-2.085831
H	1.591028	-1.963098	-1.031287
H	-0.295975	-3.110419	0.878640
H	-0.786948	-1.030154	1.713555
H	-0.777341	-2.492714	-1.668486
C	-1.676247	-1.960027	-1.373123
C	-1.711927	-1.245673	-0.199317
N	-3.951181	-1.424974	-1.926473
C	-2.966349	-0.677090	0.198983
C	-2.812912	-2.008516	-2.212806
C	-4.046916	-0.785090	-0.728417
C	-3.210023	-0.057112	1.451168
H	-2.758340	-2.547447	-3.156094
H	-6.103470	-0.308088	-1.125139
C	-4.449815	0.460175	1.750538
H	-2.445661	0.011784	2.216939
C	-5.510149	0.391181	0.810901
H	-6.479346	0.813295	1.063118
C	-5.306703	-0.221286	-0.393967
O	-4.618577	1.030909	2.967061
H	-5.531887	1.339855	3.065805
C	3.431635	-1.247522	-0.138219
C	5.680092	-1.510440	1.511089
C	3.322071	-1.861694	1.114549
C	4.684992	-0.792740	-0.562985
C	5.802622	-0.919752	0.255148
C	4.440925	-1.984441	1.935042
H	2.363358	-2.254835	1.436870
H	4.790215	-0.344259	-1.548002
H	6.767137	-0.562254	-0.090374
H	4.343585	-2.460580	2.905559
H	6.550016	-1.609727	2.152645

57 AC

H	-0.557283	-1.478751	-2.597884
C	-0.329245	-1.575551	-1.533316
C	-0.751774	-2.863707	0.550175
C	-0.566535	-1.526936	1.311548
C	-1.243683	-2.614815	-0.877984
C	-0.557941	-0.217145	-0.851847
H	0.196311	-3.400731	0.508270
H	-1.158460	-1.530277	2.231303
H	-1.230671	0.420342	-1.428207
H	0.717923	-1.879732	-1.444388
H	-1.449568	-3.500857	1.099795
H	-1.235337	-3.548618	-1.444804
H	0.364004	0.335834	-0.677962
N	-1.235781	-0.418491	0.484020
C	-2.666717	-2.030698	-0.835978
H	-2.895517	-1.608011	-1.821261
C	-2.651888	-0.894680	0.204527
H	-3.212684	-0.029430	-0.147085
H	-3.063877	-1.211277	1.167636
C	-3.729959	-3.038346	-0.499282
H	-3.637998	-3.540564	0.464248
C	-4.747824	-3.335997	-1.300986
H	-5.488833	-4.078987	-1.024074
H	-4.873561	-2.848265	-2.264597
C	0.889163	-1.344879	1.836070
O	0.898999	-0.271268	2.752365
C	-1.312120	0.876158	1.289574
H	-0.298467	1.088488	1.613166
H	-1.901515	0.626675	2.176123
H	1.735981	-0.296568	3.242805
H	0.996240	-2.286800	2.395340
H	2.263399	-3.467435	0.993643
C	2.599360	-2.555273	0.509592
C	2.049948	-1.338032	0.842899
N	4.085185	-1.611188	-1.119604
C	2.631108	-0.168653	0.247644
C	3.605822	-2.648525	-0.479457
C	3.623183	-0.382098	-0.757881
C	2.293354	1.169446	0.582664
H	4.005969	-3.624059	-0.746456
H	4.927201	0.537866	-2.195988
C	2.859737	2.228510	-0.089924
H	1.621033	1.385224	1.401344
C	3.810172	2.013415	-1.119617
H	4.244920	2.863589	-1.638207
C	4.184811	0.736469	-1.430283
O	2.475586	3.478497	0.268998
H	2.962277	4.138312	-0.248432
C	-1.894426	2.053518	0.553487

C	-2.935147	4.296846	-0.751925
C	-3.258146	2.351557	0.635887
C	-1.051575	2.909128	-0.163722
C	-1.570649	4.021567	-0.818726
C	-3.777971	3.464727	-0.018627
H	-3.914668	1.719484	1.229449
H	0.018836	2.715792	-0.194957
H	-0.907537	4.678852	-1.371918
H	-4.837756	3.686403	0.053077
H	-3.339227	5.167397	-1.258848

58 SC

H	1.149610	1.227603	-3.008457
C	0.384787	1.064564	-2.243705
C	-0.723790	1.984501	-0.237908
C	0.086226	1.163326	0.781222
C	0.151576	2.345412	-1.438064
C	0.817516	-0.054842	-1.281093
H	-1.583130	1.414294	-0.597509
H	0.566898	1.835623	1.498333
H	1.655491	-0.628450	-1.676204
H	-0.532871	0.760309	-2.753157
H	-1.102614	2.876700	0.269608
H	-0.339718	3.103993	-2.052515
H	0.005665	-0.742895	-1.038540
N	1.279127	0.545333	0.030056
C	1.510812	2.866467	-0.939015
H	2.094943	3.161164	-1.819253
C	2.237651	1.680965	-0.284584
H	2.988916	1.257298	-0.952292
H	2.728270	1.944158	0.653779
C	1.340628	4.098875	-0.083615
H	0.807308	4.901155	-0.594224
C	1.752950	4.308772	1.163597
H	1.561384	5.257105	1.654552
H	2.302088	3.575361	1.748325
C	-0.814863	0.260515	1.664093
O	-0.035485	-0.162433	2.763005
C	2.006935	-0.484603	0.884599
H	1.282998	-1.272023	1.066163
H	2.210815	0.014588	1.833754
H	-0.629470	-0.537401	3.432216
H	-1.567076	0.982775	2.013200
H	-0.142832	-2.376210	1.691011
C	-1.036623	-2.181113	1.109825
C	-1.553501	-0.908533	1.012932
N	-2.790117	-3.145562	-0.217307
C	-2.824691	-0.758530	0.367630
C	-1.680354	-3.264117	0.470373
C	-3.376635	-1.918662	-0.254336
C	-3.587339	0.442158	0.351216
H	-1.241664	-4.257539	0.532947
H	-5.005004	-2.716598	-1.407840
C	-4.803135	0.492303	-0.290013
H	-3.233824	1.332785	0.861193
C	-5.321804	-0.647391	-0.958000
H	-6.280136	-0.560684	-1.458921
C	-4.624053	-1.819481	-0.931329
O	-5.580578	1.599820	-0.329487
H	-5.161935	2.320467	0.166136
C	3.257057	-1.058979	0.271518
C	5.575711	-2.203301	-0.795894
C	4.505171	-0.469785	0.495697
C	3.187748	-2.244928	-0.467179
C	4.339927	-2.811879	-1.004242
C	5.658057	-1.034995	-0.041012
H	4.578786	0.428253	1.103645
H	2.226064	-2.733274	-0.612263
H	4.273592	-3.732107	-1.575341
H	6.621210	-0.568563	0.138409
H	6.475907	-2.645689	-1.210414

59 SC

H	-0.734763	1.721051	-2.878771
C	-0.607841	1.224374	-1.913433
C	-0.140525	1.532089	0.514239
C	0.528345	0.134579	0.466211
C	-0.091628	2.205966	-0.858396
C	0.421896	0.100074	-2.067426
H	-1.180780	1.435408	0.824984
H	1.314212	0.067921	1.223467
H	1.095497	0.278741	-2.908807
H	-1.581102	0.821975	-1.617375
H	0.365769	2.155453	1.257147
H	-0.698392	3.114778	-0.848974
H	-0.029041	-0.881004	-2.197327
N	1.318940	0.045314	-0.848803
C	1.375165	2.540458	-1.186443
H	1.433435	2.762028	-2.260794
C	2.202787	1.282091	-0.893300
H	2.959529	1.102176	-1.658428
H	2.699983	1.324382	0.076327
C	1.853283	3.768632	-0.455093
H	1.255411	4.654844	-0.666822
C	2.886994	3.882138	0.374877
H	3.119129	4.838034	0.832908
H	3.550757	3.060359	0.627466
C	-0.452290	-1.008277	0.849916
O	0.300283	-2.199394	0.964879
C	2.209072	-1.195267	-0.962887
H	2.522974	-1.207446	-2.009871
H	1.564558	-2.050615	-0.771167
H	-0.261022	-2.880669	1.368717
H	-0.767131	-0.684391	1.851766
H	-0.762792	-2.733952	-1.199932
C	-1.668745	-2.169505	-1.001949
C	-1.707950	-1.247685	0.016633
N	-3.951218	-1.773163	-1.633322
C	-2.966488	-0.625427	0.306765
C	-2.808315	-2.383888	-1.809449
C	-4.048366	-0.916038	-0.579841
C	-3.213656	0.217286	1.420046
H	-2.751752	-3.098790	-2.632536
H	-6.109138	-0.534615	-1.054105
C	-4.456274	0.775055	1.618360
H	-2.451396	0.427315	2.161378
C	-5.516832	0.523224	0.711194
H	-6.488420	0.978901	0.881707
C	-5.311192	-0.306461	-0.355479
O	-4.628848	1.562662	2.706651
H	-5.540985	1.888737	2.739103
C	3.422352	-1.190566	-0.064562
C	5.717179	-1.199962	1.541792
C	3.355858	-1.629226	1.262303

C	4.656425	-0.780168	-0.581803
C	5.796595	-0.780407	0.215626
C	4.497782	-1.627877	2.060477
H	2.411450	-1.984252	1.661152
H	4.731059	-0.468415	-1.620910
H	6.745933	-0.459547	-0.200881
H	4.433947	-1.971649	3.087950
H	6.605744	-1.203236	2.164992

60 SC

H	-0.364359	-1.369611	-2.742521
C	-0.194741	-1.507322	-1.671689
C	-0.713902	-2.906117	0.328364
C	-0.594025	-1.600576	1.153420
C	-1.113235	-2.597524	-1.116029
C	-0.508754	-0.189665	-0.948096
H	0.236180	-3.441175	0.338461
H	-1.229751	-1.654743	2.041701
H	-1.174074	0.447937	-1.533353
H	0.854104	-1.784670	-1.535025
H	-1.459339	-3.561035	0.789531
H	-1.045914	-3.503853	-1.723279
H	0.381468	0.387212	-0.701739
N	-1.250120	-0.473110	0.338369
C	-2.555463	-2.057650	-1.117775
H	-2.731842	-1.590248	-2.096109
C	-2.636221	-0.975119	-0.032290
H	-3.206442	-0.108971	-0.366244
H	-3.070849	-1.347546	0.898256
C	-3.571789	-3.159405	-0.963017
H	-3.474071	-3.942588	-1.714437
C	-4.540304	-3.262275	-0.056820
H	-5.211758	-4.114476	-0.065266
H	-4.724563	-2.518324	0.712648
C	0.827915	-1.406482	1.758735
O	0.762575	-0.374019	2.719520
C	-1.405258	0.780029	1.196023
H	-0.416315	1.001730	1.583458
H	-2.032709	0.475411	2.038152
H	1.569959	-0.406488	3.256929
H	0.932484	-2.368792	2.282396
H	2.289305	-3.455630	0.888349
C	2.629250	-2.514732	0.466328
C	2.036332	-1.326412	0.828001
N	4.171475	-1.463467	-1.040167
C	2.616820	-0.117779	0.315616
C	3.685037	-2.539804	-0.473933
C	3.663104	-0.262802	-0.646009
C	2.227343	1.195397	0.689893
H	4.119873	-3.492928	-0.766436
H	5.014706	0.750866	-1.972130
C	2.800214	2.297149	0.095686
H	1.505954	1.357057	1.478440
C	3.809214	2.150624	-0.889504
H	4.248927	3.032642	-1.346719
C	4.230746	0.897825	-1.236962
O	2.363275	3.519808	0.487221
H	2.854540	4.215197	0.023206
C	-1.981839	1.975337	0.485022
C	-3.020881	4.249108	-0.768728
C	-3.355287	2.236059	0.515725
C	-1.129874	2.883563	-0.152334
C	-1.647778	4.011096	-0.781888
C	-3.873953	3.364392	-0.113135
H	-4.021433	1.562391	1.049947
H	-0.054073	2.720540	-0.139770
H	-0.976820	4.709985	-1.270871
H	-4.941362	3.556738	-0.081429
H	-3.424137	5.131618	-1.255117

61 AC

H	-0.712503	1.687691	-2.869758
C	-0.574216	1.195355	-1.903799
C	-0.131292	1.507210	0.523328
C	0.574102	0.127173	0.477104
C	-0.087574	2.192158	-0.846741
C	0.482413	0.096356	-2.056294
H	-1.173044	1.380748	0.819088
H	1.357498	0.081764	1.238512
H	1.156005	0.293478	-2.893471
H	-1.537174	0.768440	-1.608684
H	0.348383	2.133934	1.279660
H	-0.726697	3.077525	-0.846315
H	0.054923	-0.894303	-2.191902
N	1.373949	0.057801	-0.832745
C	1.361113	2.559100	-1.180820
H	1.427709	2.762103	-2.258319
C	2.224740	1.316350	-0.873415
H	2.991752	1.155195	-1.633008
H	2.715432	1.391906	0.099588
C	1.933447	3.754044	-0.460391
H	2.999387	3.915575	-0.622988
C	1.265401	4.598103	0.320490
H	1.768039	5.437849	0.788979
H	0.202396	4.496387	0.521524
C	-0.378144	-1.041369	0.855471
O	0.405519	-2.211575	0.976913
C	2.291912	-1.162408	-0.945378
H	2.608103	-1.166862	-1.991714
H	1.666461	-2.032328	-0.755644
H	-0.139887	-2.907662	1.377028
H	-0.708221	-0.725594	1.854896
H	-0.629337	-2.773175	-1.198900
C	-1.550575	-2.231697	-1.007142
C	-1.620959	-1.313603	0.013032
N	-3.835925	-1.886667	-1.658700
C	-2.896869	-0.723833	0.294394
C	-2.677625	-2.476895	-1.825305
C	-3.963184	-1.035517	-0.603490
C	-3.174006	0.106425	1.410120
H	-2.597282	-3.182557	-2.649189
H	-6.026955	-0.696315	-1.097860
C	-4.431329	0.633225	1.599626
H	-2.423697	0.329819	2.159815
C	-5.476062	0.364255	0.679283
H	-6.458268	0.799580	0.841673
C	-5.241469	-0.454844	-0.389600
O	-4.634142	1.409071	2.691143
H	-5.556870	1.704495	2.720860
C	3.502946	-1.131104	-0.045059
C	5.796115	-1.092592	1.562801
C	3.443056	-1.565139	1.283694
C	4.729773	-0.701003	-0.563305
C	5.869301	-0.678001	0.234794

C	4.583940	-1.539438	2.082706
H	2.505083	-1.936142	1.683149
H	4.798960	-0.393206	-1.604029
H	6.813326	-0.342682	-0.182374
H	4.525447	-1.879400	3.111773
H	6.684116	-1.078046	2.186663

62 AC

H	-0.514499	-1.401723	-2.674758
C	-0.321859	-1.516298	-1.605077
C	-0.825424	-2.838286	0.444707
C	-0.648742	-1.514057	1.229712
C	-1.261296	-2.562680	-0.997880
C	-0.567376	-0.167920	-0.911125
H	0.113259	-3.393266	0.437390
H	-1.266858	-1.525959	2.131871
H	-1.221655	0.479409	-1.498012
H	0.719951	-1.827710	-1.487045
H	-1.566156	-3.461157	0.952736
H	-1.223696	-3.482038	-1.586258
H	0.349827	0.380518	-0.700545
N	-1.286576	-0.388420	0.399835
C	-2.675279	-1.974754	-0.991525
H	-2.861142	-1.513802	-1.971014
C	-2.693790	-0.854347	0.071230
H	-3.242357	0.020179	-0.277291
H	-3.131277	-1.193249	1.014849
C	-3.802105	-2.940406	-0.722823
H	-4.780014	-2.475045	-0.597819
C	-3.703063	-4.263951	-0.638927
H	-4.579401	-4.875761	-0.451367
H	-2.760132	-4.790913	-0.756880
C	0.790878	-1.348607	1.800242
O	0.775570	-0.294133	2.738766
C	-1.382261	0.892412	1.224820
H	-0.377512	1.095034	1.580442
H	-1.996741	0.629932	2.090249
H	1.594419	-0.336411	3.257791
H	0.878714	-2.301946	2.343055
H	2.176443	-3.458357	0.945457
C	2.533638	-2.536441	0.496471
C	1.981243	-1.324380	0.843153
N	4.077659	-1.561147	-1.058694
C	2.586235	-0.143960	0.294915
C	3.571103	-2.611169	-0.461590
C	3.610531	-0.338520	-0.681674
C	2.241934	1.187406	0.649125
H	3.973847	-3.582202	-0.740822
H	4.967826	0.609029	-2.050970
C	2.835521	2.259552	0.022126
H	1.542611	1.387166	1.448798
C	3.821451	2.064147	-0.977791
H	4.278136	2.923858	-1.460379
C	4.200661	0.792944	-1.306354
O	2.443216	3.502384	0.396817
H	2.945496	4.172237	-0.092087
C	-1.941595	2.084060	0.494258
C	-2.945552	4.352503	-0.796098
C	-3.305759	2.386127	0.551685
C	-1.080002	2.947970	-0.189850
C	-1.580821	4.073104	-0.837349
C	-3.807312	3.511815	-0.095453
H	-3.977096	1.747019	1.120759
H	-0.009835	2.751028	-0.200522
H	-0.903303	4.737614	-1.363822
H	-4.867551	3.736673	-0.043138
H	-3.334927	5.233226	-1.296893

Cartesian coordinates (Å) of the conformers of A intermediate

01 E; Enegy (including ZPVE) = -763.906282 Hartree

C	4.039478	-1.018548	0.262591
C	4.980545	-0.297337	-0.470955
C	4.617119	0.901273	-1.078570
C	3.310852	1.372965	-0.945799
C	2.370435	0.654388	-0.211905
C	2.732743	-0.550414	0.400478
C	1.716238	-1.316933	1.226975
N	0.461605	-1.459185	0.501712
C	-0.472941	-0.672152	0.859759
C	-2.307014	-1.921529	-0.240540
C	-3.564846	-2.005436	-0.824515
C	-4.332486	-0.849486	-0.967382
C	-3.829649	0.373970	-0.537535
C	-2.558829	0.479138	0.035934
C	-1.797630	-0.691655	0.193911
C	-2.000087	1.850192	0.408082
O	-0.735285	1.956454	0.456248
N	-2.911288	2.768732	0.624908
H	4.323401	-1.957814	0.731888
H	5.993363	-0.676568	-0.571889
H	5.345619	1.464468	-1.654508
H	3.021927	2.307198	-1.419128
H	1.350624	1.027483	-0.113096
H	2.113159	-2.313857	1.449088
H	1.569716	-0.796166	2.187862
H	-0.345372	0.043545	1.676993
H	-1.699653	-2.811372	-0.101393
H	-3.947873	-2.965089	-1.159248
H	-5.319884	-0.903967	-1.417809
H	-4.407052	1.285882	-0.645929
H	-2.391485	3.627178	0.837667

02 E

C	4.068265	-1.006962	0.304481
C	5.023064	-0.316438	-0.440932
C	4.678762	0.871284	-1.080106
C	3.377899	1.363282	-0.967050
C	2.423707	0.675844	-0.221216
C	2.767187	-0.518438	0.422472
C	1.733717	-1.251297	1.257169
N	0.491929	-1.418166	0.514737
C	-0.458980	-0.641257	0.851559
C	-2.256072	-1.934505	-0.254056
C	-3.516948	-2.056019	-0.825830
C	-4.324897	-0.926028	-0.950891
C	-3.855969	0.309498	-0.517651
C	-2.579939	0.455079	0.033500
C	-1.779658	-0.691883	0.182537

C	-2.130595	1.869878	0.391802
O	-3.044964	2.706132	0.634098
N	-0.826732	2.055947	0.357531
H	4.336693	-1.937882	0.799784
H	6.031458	-0.710961	-0.526565
H	5.418119	1.410306	-1.665285
H	3.104652	2.288854	-1.466107
H	1.406960	1.064515	-0.136425
H	2.123055	-2.240557	1.523389
H	1.570489	-0.695914	2.195797
H	-0.351423	0.092789	1.655193
H	-1.620272	-2.805608	-0.123366
H	-3.872854	-3.026434	-1.159460
H	-5.317422	-1.011506	-1.384873
H	-4.465385	1.203637	-0.599493
H	-0.677981	3.043009	0.595017

03 E

C	-2.806867	0.576422	0.644489
C	-3.942574	1.174021	1.187240
C	-5.211573	0.728155	0.824501
C	-5.337528	-0.318248	-0.087514
C	-4.200531	-0.910490	-0.630951
C	-2.924250	-0.473251	-0.268533
C	-1.694936	-1.160407	-0.831549
N	-0.571376	-0.248525	-0.945511
C	0.472712	-0.542460	-0.277216
C	1.456512	1.711057	-0.563503
C	2.507230	2.616373	-0.509234
C	3.774139	2.172714	-0.127308
C	3.971613	0.833148	0.188002
C	2.929169	-0.097239	0.119392
C	1.652381	0.356726	-0.258617
C	3.217767	-1.571869	0.399076
O	2.493080	-2.416439	-0.207428
N	4.207225	-1.776082	1.238359
H	-1.818293	0.930034	0.923629
H	-3.835026	1.990218	1.895702
H	-6.096729	1.194274	1.246682
H	-6.322212	-0.669204	-0.382109
H	-4.303279	-1.721071	-1.348902
H	-1.450582	-2.034814	-0.204691
H	-1.936050	-1.541221	-1.831780
H	0.543104	-1.454277	0.320624
H	0.456619	2.035713	-0.835338
H	2.339613	3.661721	-0.752056
H	4.604448	2.871779	-0.075274
H	4.947182	0.468617	0.491856
H	4.296033	-2.795927	1.311481

04 E

C	-2.821131	0.573745	0.636087
C	-3.957994	1.199898	1.142435
C	-5.226329	0.754049	0.776736
C	-5.350091	-0.320724	-0.101696
C	-4.211493	-0.941933	-0.608547
C	-2.936204	-0.505255	-0.242573
C	-1.704487	-1.221953	-0.761860
N	-0.582260	-0.315338	-0.924046
C	0.456587	-0.563510	-0.229292
C	1.407776	1.690380	-0.567227
C	2.442202	2.615811	-0.537227
C	3.720675	2.200245	-0.163901
C	3.944133	0.867706	0.162276
C	2.921927	-0.085002	0.109813
C	1.629564	0.342767	-0.249204
C	3.312388	-1.531072	0.419882
O	4.327022	-1.688170	1.156886
N	2.562851	-2.440869	-0.165539
H	-1.832834	0.927489	0.916451
H	-3.852692	2.038815	1.824271
H	-6.112569	1.242622	1.170330
H	-6.334041	-0.671632	-0.398797
H	-4.311930	-1.775284	-1.300285
H	-1.461394	-2.058377	-0.084475
H	-1.941738	-1.660239	-1.739145
H	0.528793	-1.437355	0.423073
H	0.397912	1.994257	-0.826495
H	2.251263	3.655481	-0.787261
H	4.537547	2.915740	-0.122845
H	4.926017	0.521381	0.467243
H	2.960225	-3.345002	0.115726

05 E

C	4.033387	-0.983730	0.323408
C	4.969682	-0.296797	-0.448012
C	4.596684	0.862299	-1.122817
C	3.285550	1.327810	-1.020627
C	2.349211	0.643291	-0.249882
C	2.722101	-0.520554	0.431963
C	1.714797	-1.245996	1.305993
N	0.460873	-1.450299	0.593699
C	-0.469883	-0.629111	0.875086
C	-2.281949	-1.919423	-0.233277
C	-3.521237	-2.007290	-0.857819
C	-4.278959	-0.852200	-1.044193
C	-3.792161	0.375108	-0.602398
C	-2.546874	0.482795	0.022609
C	-1.786759	-0.685461	0.200257
C	-1.989252	1.855412	0.418187
O	-0.752020	2.017006	0.203795
N	-2.801703	2.756294	0.921537
H	4.324516	-1.891261	0.847358
H	5.986396	-0.671205	-0.524903
H	5.321687	1.399708	-1.727068
H	2.989364	2.230933	-1.546729
H	1.325557	1.012898	-0.179798
H	2.123075	-2.221397	1.592468
H	1.561147	-0.665621	2.230716
H	-0.336809	0.160098	1.622472
H	-1.678727	-2.807708	-0.068228
H	-3.894833	-2.969277	-1.195827
H	-5.244817	-0.907358	-1.538633
H	-4.373448	1.279071	-0.764688
H	-3.727173	2.336179	1.024985

06 E

C	-2.831579	0.676776	0.576466
C	-3.969235	1.192643	1.195755
C	-5.223894	0.657172	0.917709
C	-5.335545	-0.397917	0.012652
C	-4.198913	-0.907325	-0.607623
C	-2.935156	-0.378786	-0.329856

C	-1.708256	-0.983083	-0.986221
N	-0.577729	-0.075442	-0.971979
C	0.490395	-0.496064	-0.420388
C	1.585874	1.725837	-0.601533
C	2.681552	2.570392	-0.483846
C	3.903221	2.052532	-0.052006
C	4.008927	0.701893	0.262912
C	2.919314	-0.167108	0.139030
C	1.694482	0.360019	-0.309385
C	3.106445	-1.661893	0.435328
O	2.604078	-2.449781	-0.415107
N	3.773079	-2.010975	1.513341
H	-1.853738	1.098448	0.788992
H	-3.872886	2.015810	1.897812
H	-6.109979	1.059765	1.399157
H	-6.310172	-0.820445	-0.213863
H	-4.290664	-1.726022	-1.318165
H	-1.472018	-1.942904	-0.496568
H	-1.952748	-1.211499	-2.031533
H	0.574458	-1.505107	-0.005717
H	0.620580	2.107168	-0.921162
H	2.585966	3.625377	-0.723130
H	4.770395	2.701090	0.036779
H	4.959245	0.295040	0.598767
H	4.025693	-1.164076	2.025987

07 E

C	3.951124	-1.090527	0.262129
C	4.902009	-0.529339	-0.590261
C	4.668855	0.714284	-1.169976
C	3.482680	1.395460	-0.893031
C	2.535919	0.833183	-0.042805
C	2.764391	-0.416054	0.543728
C	1.716391	-1.012410	1.462924
N	0.501013	-1.316119	0.714707
C	-0.466235	-0.504353	0.875621
C	-2.184039	-1.943915	-0.206235
C	-3.421761	-2.129149	-0.808019
C	-4.262417	-1.031657	-1.006006
C	-3.853613	0.236522	-0.608608
C	-2.594772	0.446843	-0.038828
C	-1.763766	-0.665121	0.181449
C	-2.179358	1.883703	0.302251
O	-3.051080	2.576532	0.888758
N	-0.977459	2.293098	-0.060530
H	4.132418	-2.063343	0.712601
H	5.822082	-1.065943	-0.802209
H	5.406159	1.152799	-1.835722
H	3.296497	2.366959	-1.341212
H	1.610613	1.367499	0.170666
H	2.100242	-1.941879	1.896556
H	1.516613	-0.310462	2.287775
H	-0.385297	0.363586	1.542405
H	-1.526694	-2.786346	-0.011225
H	-3.738622	-3.123540	-1.108147
H	-5.237540	-1.170058	-1.464893
H	-4.503197	1.096409	-0.744205
H	-0.521962	1.538389	-0.577692

08 E

C	-2.803022	0.616533	0.614295
C	-3.930474	1.183653	1.205752
C	-5.201465	0.707841	0.893345
C	-5.339065	-0.338592	-0.017446
C	-4.211535	-0.899605	-0.610363
C	-2.932660	-0.431797	-0.297894
C	-1.714955	-1.089656	-0.918759
N	-0.587085	-0.179912	-0.991168
C	0.472840	-0.526700	-0.376498
C	1.525621	1.703295	-0.648798
C	2.598496	2.576208	-0.548580
C	3.828969	2.102640	-0.085288
C	3.967524	0.765648	0.264594
C	2.909832	-0.139875	0.127375
C	1.667742	0.346684	-0.319726
C	3.193307	-1.605860	0.489339
O	3.874686	-1.771427	1.535785
N	2.754189	-2.561805	-0.304359
H	-1.813089	0.993388	0.854833
H	-3.814004	1.999773	1.912828
H	-6.079729	1.150783	1.353143
H	-6.326138	-0.713377	-0.272030
H	-4.323412	-1.710198	-1.326988
H	-1.468431	-2.004030	-0.353206
H	-1.971000	-1.402072	-1.938775
H	0.547997	-1.485524	0.152066
H	0.549631	2.053810	-0.971234
H	2.476990	3.622529	-0.812958
H	4.672183	2.781371	0.009431
H	4.908009	0.385952	0.651660
H	2.286837	-2.131473	-1.104455

09 Z

C	2.043546	0.677274	0.016797
C	3.057347	1.494833	-0.477784
C	4.267591	0.946545	-0.901796
C	4.461834	-0.430513	-0.826998
C	3.449417	-1.249818	-0.330235
C	2.234757	-0.706281	0.090513
C	1.111352	-1.602083	0.575486
N	0.484941	-1.040630	1.767603
C	-0.683929	-0.539066	1.687309
C	-2.086431	-1.891300	0.156158
C	-3.024646	-2.051351	-0.856546
C	-3.543353	-0.924031	-1.493008
C	-3.122625	0.342164	-1.104262
C	-2.179628	0.519216	-0.086029
C	-1.649464	-0.616680	0.544725
C	-1.737243	1.918963	0.324962
O	-0.799734	1.981833	1.180010
N	-2.388162	2.897211	-0.255661
H	1.101608	1.110175	0.356919
H	2.901247	2.568750	-0.531664
H	5.054851	1.589402	-1.284753
H	5.402481	-0.867587	-1.150105
H	3.604992	-2.324687	-0.268094
H	0.406812	-1.753674	-0.253604
H	1.524617	-2.583673	0.836031
H	-1.069726	-0.067071	2.592185
H	-1.682058	-2.763935	0.664367
H	-3.348991	-3.046716	-1.145510
H	-4.276222	-1.035051	-2.287271
H	-3.513790	1.234852	-1.579973
H	-1.976549	3.761240	0.112052

10 Z

C	2.152247	0.720347	-0.035488
C	3.191437	1.516887	-0.510452
C	4.414211	0.948409	-0.867750
C	4.594782	-0.426959	-0.745921
C	3.556277	-1.225713	-0.269054
C	2.330284	-0.662081	0.085101
C	1.178876	-1.527836	0.557836
N	0.551000	-0.926296	1.729031
C	-0.630063	-0.457081	1.643075
C	-1.991321	-1.922676	0.186676
C	-2.980900	-2.165752	-0.760286
C	-3.629108	-1.089129	-1.362162
C	-3.278501	0.209439	-1.008935
C	-2.279451	0.471668	-0.067860
C	-1.624807	-0.616010	0.537233
C	-1.961350	1.935786	0.232004
O	-2.755823	2.794836	-0.240872
N	-0.873661	2.120299	0.949317
H	1.197506	1.166054	0.252818
H	3.046163	2.589927	-0.601922
H	5.221982	1.574772	-1.235107
H	5.545034	-0.879208	-1.015592
H	3.701518	-2.299194	-0.168978
H	0.484239	-1.673617	-0.280615
H	1.563428	-2.515212	0.840307
H	-1.007286	0.067511	2.522460
H	-1.496159	-2.756528	0.679333
H	-3.247159	-3.186626	-1.018203
H	-4.406632	-1.262617	-2.100918
H	-3.772255	1.067855	-1.452060
H	-0.780852	3.134374	1.072912

11 Z

C	-3.291743	-1.285228	-0.252926
C	-4.542609	-0.808592	-0.631855
C	-4.941494	0.479102	-0.272401
C	-4.078508	1.285124	0.464942
C	-2.824039	0.805257	0.840440
C	-2.419455	-0.484059	0.490537
C	-1.065973	-1.015901	0.916400
N	-0.402467	-1.705275	-0.185882
C	0.679501	-1.236686	-0.669250
C	0.536359	1.232142	-0.555475
C	1.077278	2.502397	-0.394800
C	2.427462	2.634645	-0.071533
C	3.215118	1.499628	0.083200
C	2.685123	0.214779	-0.072526
C	1.323195	0.083996	-0.388410
C	3.560999	-1.019646	0.121490
O	2.957925	-2.133671	0.132362
N	4.843838	-0.770605	0.248984
H	-2.973201	-2.283385	-0.538838
H	-5.208749	-1.441648	-1.210961
H	-5.916822	0.851702	-0.570767
H	-4.376923	2.291389	0.744233
H	-2.146784	1.441099	1.406798
H	-0.473006	-0.203046	1.354392
H	-1.218680	-1.764531	1.705483
H	1.152115	-1.826258	-1.454455
H	-0.511839	1.118126	-0.823806
H	0.451737	3.380743	-0.525677
H	2.863578	3.621305	0.058270
H	4.267704	1.578374	0.332125
H	5.290580	-1.685082	0.375602

12 Z

C	3.249055	-1.245795	-0.375492
C	4.486019	-0.758212	-0.786755
C	4.935833	0.483568	-0.338673
C	4.137106	1.234380	0.520107
C	2.897238	0.744527	0.928289
C	2.442929	-0.501512	0.491020
C	1.107441	-1.044601	0.960424
N	0.412432	-1.746786	-0.112499
C	-0.669092	-1.272819	-0.591456
C	-0.493328	1.193351	-0.476269
C	-1.021399	2.474138	-0.351356
C	-2.382206	2.629476	-0.095596
C	-3.191752	1.505523	0.027459
C	-2.676782	0.211552	-0.083343
C	-1.300981	0.056463	-0.334370
C	-3.654184	-0.950044	0.093158
O	-4.883914	-0.659504	0.071341
N	-3.080566	-2.119929	0.265877
H	2.889746	-2.206250	-0.731889
H	5.100984	-1.347836	-1.460544
H	5.899597	0.864836	-0.662491
H	4.474720	2.206083	0.868476
H	2.269353	1.339611	1.588015
H	1.293104	-1.786438	1.749047
H	0.521615	-0.234775	1.413697
H	-1.170039	-1.879105	-1.345721
H	0.562872	1.063989	-0.702252
H	-0.376044	3.340870	-0.461321
H	-2.810293	3.623398	0.001857
H	-4.257136	1.595376	0.211035
H	-3.845620	-2.796692	0.364840

13 Z

C	-3.250606	-1.247600	-0.372026
C	-4.487284	-0.759159	-0.783074
C	-4.934170	0.484894	-0.338280
C	-4.132831	1.237044	0.516882
C	-2.893285	0.746218	0.924948
C	-2.442040	-0.502140	0.491176
C	-1.107086	-1.046517	0.960500
N	-0.412220	-1.748234	-0.112957
C	0.668844	-1.273484	-0.592198
C	0.491870	1.192482	-0.475910
C	1.019116	2.473540	-0.350274
C	2.379827	2.629576	-0.094515
C	3.190045	1.506028	0.027855
C	2.675925	0.211756	-0.083616
C	1.300182	0.055981	-0.334679
C	3.654145	-0.949218	0.092439
O	4.883710	-0.657729	0.071202
N	3.081709	-2.119807	0.264407
H	-2.893329	-2.209580	-0.726267
H	-5.104307	-1.349822	-1.454053
H	-5.897737	0.866843	-0.661860
H	-4.468215	2.210438	0.862627

H	-2.263208	1.342354	1.581621
H	-0.520749	-0.237498	1.414521
H	-1.293362	-1.788940	1.748395
H	1.169812	-1.87188	-1.346927
H	-0.564258	1.062654	-0.701856
H	0.373178	3.339905	-0.459654
H	2.807344	3.623672	0.003510
H	4.255341	1.596676	0.211515
H	3.847465	-2.795809	0.363292

14 Z

C	2.095702	0.718086	-0.185935
C	3.117972	1.497589	-0.721405
C	4.386539	0.955887	-0.932681
C	4.630171	-0.374938	-0.603877
C	3.608576	-1.156947	-0.065990
C	2.338406	-0.620029	0.143497
C	1.206483	-1.470582	0.685458
N	0.543339	-0.765772	1.777891
C	-0.645236	-0.334187	1.630892
C	-1.919782	-1.929553	0.197480
C	-2.852628	-2.226804	-0.791363
C	-3.500819	-1.187327	-1.454716
C	-3.228628	0.131937	-1.103605
C	-2.300400	0.446892	-0.107705
C	-1.615536	-0.603331	0.525717
C	-2.000239	1.902257	0.264992
O	-0.799447	2.138039	0.588809
N	-2.969129	2.787650	0.235721
H	1.105333	1.143601	-0.013746
H	2.923881	2.536381	-0.973933
H	5.180526	1.569613	-1.348306
H	5.615518	-0.805029	-0.759311
H	3.801685	-2.195193	0.194754
H	0.534089	-1.722982	-0.144737
H	1.613857	-2.409556	1.077694
H	-1.037899	0.275543	2.448631
H	-1.420233	-2.734540	0.731565
H	-3.070274	-3.260868	-1.041089
H	-4.218933	-1.402978	-2.240712
H	-3.733573	0.943224	-1.621379
H	-3.841366	2.311623	0.000256

15 Z

C	3.237587	-1.245872	-0.419183
C	4.465494	-0.763807	-0.863463
C	4.932204	0.476469	-0.429049
C	4.160066	1.232660	0.448934
C	2.929038	0.749277	0.889828
C	2.458765	-0.495250	0.466174
C	1.137361	-1.030004	0.981626
N	0.400046	-1.738021	-0.059360
C	-0.678407	-1.247096	-0.527578
C	-0.516289	1.236488	-0.368027
C	-1.080617	2.499667	-0.234560
C	-2.454369	2.618512	-0.023591
C	-3.245271	1.476849	0.041285
C	-2.691233	0.197874	-0.059874
C	-1.305817	0.082110	-0.267967
C	-3.644189	-1.002032	0.040542
O	-4.780649	-0.819355	-0.471948
N	-3.241020	-2.099887	0.646357
H	2.867576	-2.207214	-0.762335
H	5.060457	-1.357322	-1.551494
H	5.889332	0.852260	-0.777690
H	4.511436	2.202661	0.787966
H	2.322086	1.346949	1.566567
H	1.345317	-1.769701	1.766146
H	0.568243	-0.215924	1.448078
H	-1.214894	-1.871761	-1.247210
H	0.546571	1.135947	-0.575998
H	-0.455449	3.384547	-0.308074
H	-2.906777	3.601307	0.075985
H	-4.321207	1.548358	0.166785
H	-2.306609	-1.944974	1.027290

16 Z

C	-1.978298	0.483770	0.324801
C	-3.014232	1.315686	-0.097321
C	-4.102536	0.795785	-0.794694
C	-4.153969	-0.570025	-1.067532
C	-3.118976	-1.401974	-0.647819
C	-2.021557	-0.884484	0.044625
N	-0.868301	-1.794892	0.423529
C	-0.271884	-1.402422	1.694194
C	0.851122	-0.801416	1.690305
C	2.482140	-1.659093	0.033301
C	3.389559	-1.511236	-1.011356
C	3.577969	-0.253481	-1.579721
C	2.846672	0.832786	-1.109027
C	1.925604	0.701610	-0.065058
C	1.760758	-0.563984	0.521529
C	1.132061	1.899353	0.468888
O	0.818921	1.817631	1.693635
N	0.816328	2.888268	-0.332263
H	-1.142291	0.899347	0.884514
H	-2.963637	2.378968	0.119450
H	-4.907164	1.448567	-1.120434
H	-5.001417	-0.989126	-1.602713
H	-3.161910	-2.467936	-0.861192
H	-1.246817	-2.818105	0.530180
H	-0.144947	-1.800777	-0.404470
H	1.237668	-0.481201	2.657782
H	2.331310	-2.636210	0.486763
H	3.948685	-2.369501	-1.371970
H	4.295430	-0.118640	-2.383929
H	3.003208	1.814439	-1.548510
H	1.141318	2.667769	-1.274758

17 Z

C	3.207122	-1.244809	-0.414931
C	4.436474	-0.767385	-0.860944
C	4.910165	0.469563	-0.424854
C	4.143145	1.227161	0.456618
C	2.911271	0.747943	0.899344
C	2.433584	-0.493675	0.474580
C	1.110593	-1.022025	0.992622
N	0.375481	-1.750100	-0.035367
C	-0.707296	-1.272764	-0.506289
C	-0.506077	1.211270	-0.422590
C	-1.041476	2.488751	-0.285949
C	-2.401213	2.636005	-0.022795
C	-3.212232	1.508517	0.075714

C	-2.692397	0.219476	-0.066324
C	-1.312202	0.075171	-0.287455
C	-3.585423	-1.020186	0.069306
O	-3.022233	-2.023668	0.589982
N	-4.831285	-0.964691	-0.346239
H	2.830840	-2.202956	-0.760047
H	5.026985	-1.361907	-1.552056
H	5.868143	0.841923	-0.774963
H	4.499361	2.195126	0.796643
H	2.308079	1.347124	1.578173
H	1.317678	-1.745003	1.793172
H	0.540883	-0.200025	1.444257
H	-1.241927	-1.907208	-1.216079
H	0.551362	1.088384	-0.645754
H	-0.400684	3.360082	-0.383107
H	-2.829996	3.626065	0.103643
H	-4.272496	1.624733	0.284685
H	-4.993978	-0.051531	-0.773495

18 Z

C	-1.375026	-0.435629	1.313034
C	-1.984412	0.668479	1.906938
C	-3.105501	1.247206	1.318639
C	-3.620406	0.713534	0.137368
C	-3.013036	-0.391303	-0.451018
C	-1.883646	-0.975765	0.130216
C	-1.182074	-2.123864	-0.562695
N	-0.567399	-1.649755	-1.815112
C	0.508984	-0.970605	-1.757140
C	1.942068	-1.754692	0.124525
C	2.774715	-1.536729	1.216078
C	3.063503	-0.228875	1.606831
C	2.535379	0.837706	0.889230
C	1.671586	0.638602	-0.191804
C	1.367862	-0.680113	-0.568524
C	1.139578	1.882211	-0.920319
O	1.970419	2.826543	-1.020126
N	-0.096441	1.891984	-1.369322
H	-0.486813	-0.875119	1.761758
H	-1.575994	1.081096	2.824610
H	-3.576175	2.112109	1.776067
H	-4.494427	1.161402	-0.326013
H	-3.407407	-0.801958	-1.377306
H	-0.461546	-2.574614	0.125897
H	-1.908422	-2.896067	-0.835627
H	0.866118	-0.558445	-2.705621
H	1.747031	-2.770161	-0.212239
H	3.208214	-2.379390	1.746460
H	3.716793	-0.044969	2.455375
H	2.787019	1.861664	1.146340
H	-0.568308	1.035527	-1.075805

19 Z

C	-3.277721	-1.300031	-0.172609
C	-4.535561	-0.821969	-0.525654
C	-4.910770	0.479656	-0.191527
C	-4.017189	1.298268	0.493470
C	-2.755791	0.817156	0.842950
C	-2.375425	-0.486177	0.519087
C	-1.013513	-1.018224	0.916264
N	-0.386752	-1.721542	-0.199695
C	0.659291	-1.240443	-0.745635
C	0.536972	1.231606	-0.676563
C	1.086708	2.500458	-0.524273
C	2.425835	2.624276	-0.160840
C	3.188975	1.482060	0.060989
C	2.653342	0.197850	-0.083608
C	1.308346	0.080359	-0.475523
C	3.517071	-1.047802	0.158605
O	3.258180	-2.034416	-0.586073
N	4.443093	-1.014692	1.090312
H	-2.977765	-2.309218	-0.439571
H	-5.225847	-1.464902	-1.064171
H	-5.891974	0.853066	-0.468867
H	-4.297240	2.315201	0.752383
H	-2.054404	1.462556	1.367441
H	-0.403647	-0.202050	1.323607
H	-1.145396	-1.758117	1.716601
H	1.115710	-1.830134	-1.537447
H	-0.505798	1.122847	-0.967659
H	0.477256	3.382549	-0.697128
H	2.874788	3.607338	-0.050958
H	4.234446	1.580778	0.341567
H	4.396627	-0.113199	1.567678

20 Z

C	-2.720977	-0.673218	-0.870764
C	-3.922529	-0.239802	-1.433198
C	-4.897003	0.353067	-0.636849
C	-4.665011	0.511042	0.730276
C	-3.468386	0.076165	1.288920
C	-2.481901	-0.519079	0.494826
C	-1.181390	-0.957031	1.143633
N	-0.350235	-1.765514	0.267059
C	0.715199	-1.296179	-0.255926
C	0.464945	1.209341	-0.279378
C	0.999575	2.490324	-0.215903
C	2.373325	2.653157	-0.035757
C	3.196267	1.535809	0.049512
C	2.683261	0.240739	-0.069044
C	1.289736	0.077103	-0.189935
C	3.684664	-0.322805	-0.019070
O	4.349983	-1.004791	1.045861
N	3.804396	-1.699398	-1.075874
H	-1.963667	-1.139010	-1.493953
H	-4.093635	-0.368260	-2.497897
H	-5.831347	0.690541	-1.074732
H	-5.419235	0.972216	1.360934
H	-3.291629	0.198626	2.355304
H	-0.661832	-0.073879	1.540490
H	-1.433683	-1.589687	2.003811
H	1.320256	-2.013785	-0.813009
H	-0.604696	1.081704	-0.424536
H	0.348789	3.354935	-0.302081
H	2.799664	3.650062	0.031913
H	4.266100	1.652445	0.198543
H	3.167283	-1.354982	-1.798033

Cartesian coordinates (Å) of IIIb1-R, IIIb2-R and IIId-S products

IIIb1-R

H	2.914262	4.362058	-1.268285
C	1.870289	4.060953	-1.399192
C	-0.259382	3.528546	-0.252380
C	-0.081476	2.005380	-0.304011
C	1.108393	4.194215	-0.076162
C	1.782657	2.601770	-1.877353
H	-0.725024	3.875682	-1.182050
H	-0.147764	1.572127	0.695548
H	2.743402	2.224302	-2.230983
H	1.430953	4.711135	-2.160038
H	-0.940666	3.772380	0.566466
H	0.995236	5.244699	0.202302
H	1.027135	2.457614	-2.648262
N	1.369557	1.709721	-0.725506
C	1.917915	3.454280	1.008778
H	2.870010	3.980911	1.136611
C	2.239991	2.040429	0.464026
H	3.272575	1.970409	0.117786
H	2.069249	1.259813	1.211387
C	1.231779	3.413606	2.349254
C	-1.149533	1.301065	-1.152608
O	-1.085600	1.746464	-2.489259
C	1.505344	0.249064	-1.108768
H	0.881500	0.131622	-1.997431
H	1.074829	-0.337697	-0.285491
C	3.255474	-0.421542	-2.767208
C	4.511422	-0.922857	-3.099959
C	2.900966	-0.220903	-1.428549
H	6.399641	-1.633336	-2.350079
C	3.817715	-0.550806	-0.424092
C	5.071946	-1.053360	-0.757132
C	5.422128	-1.236736	-2.093800
C	-3.433251	-1.318287	-2.095170
C	-3.014243	-3.199254	-0.011403
C	-4.468020	-1.664165	-1.228525
C	-2.201953	-1.924561	-1.890629
C	-1.985030	-2.836672	-0.863650
C	-4.258345	-2.594637	-0.205647
H	-5.442435	-1.198111	-1.336595
H	-5.076822	-2.836754	0.464980
H	-2.846883	-3.873325	0.822270
C	-0.913396	-1.685043	-2.587190
O	-0.677057	-0.854575	-3.471142
H	-1.156255	0.950005	-3.053897
N	-0.016404	-2.526834	-2.019218
H	0.968833	-2.478861	-2.250638
H	-3.570698	-0.586655	-2.886357
C	-0.515187	-3.194426	-0.802434
H	-0.343414	-4.277179	-0.900381
N	0.095855	-2.635640	0.384815
C	1.349979	-3.267599	0.760453
H	1.969161	-3.368267	-0.142643
H	1.211314	-4.291351	1.149654
C	2.136671	-2.445298	1.758864
C	3.710392	-0.875893	3.472410
C	1.586564	-1.334303	2.402145
C	3.469869	-2.783724	2.013890
C	4.253436	-2.007491	2.861418
C	2.374094	-0.552658	3.251991
H	0.535589	-1.094635	2.259937
H	3.904420	-3.649924	1.518924
H	5.290891	-2.276604	3.037516
H	1.936890	0.315293	3.739304
H	4.322161	-0.260888	4.125234
H	-0.964008	0.224984	-1.109285
H	-3.181502	2.975233	-1.912878
C	-3.416621	2.403431	-1.020666
C	-2.502803	1.517892	-0.507037
N	-5.042264	1.846520	0.667588
C	-2.851658	0.740033	0.641291
C	-4.675858	2.541147	-0.391423
C	-4.160470	0.948919	1.177809
C	-2.009337	-0.234067	1.200389
H	-5.401675	3.248188	-0.789233
H	-5.551505	0.309859	2.694559
C	-2.424639	-1.106951	2.229840
H	-1.037546	-0.440970	0.765095
C	-3.743541	-0.835451	2.781642
H	-4.072435	-1.469673	3.601879
C	-4.559725	0.138675	2.282204
H	3.550975	-0.431472	0.622766
H	5.768791	-1.313194	0.034087
H	4.772766	-1.076158	-4.142031
H	2.532970	-0.197492	-3.549605
O	-1.721081	-2.089853	2.642072
H	-0.568191	-2.584804	1.175040
C	1.693526	4.038430	3.428864
H	0.307889	2.838426	2.425531
H	1.168275	3.994988	4.377571
H	2.613327	4.618059	3.398903

IIIb2-R

H	1.910755	4.582721	-2.027381
C	1.107436	3.992849	-1.577824
C	-0.334474	3.661427	0.411488
C	-0.203581	2.137617	0.193894
C	0.907805	4.386168	-0.111385
C	1.472440	2.501902	-1.654370
H	-1.211028	4.021581	-0.133567
H	-0.245424	1.596937	1.144947
H	2.533800	2.349381	-1.858014
H	0.187040	4.173854	-2.136331
H	-0.501930	3.873154	1.470646
H	0.776862	5.467633	-0.020767
H	0.888249	1.960879	-2.398771
N	1.215747	1.834643	-0.323124
C	2.153941	3.947786	0.681350
H	3.039900	4.317807	0.151958
C	2.185305	2.404109	0.685811
H	3.174388	2.021985	0.429396
H	1.893809	1.988433	1.655386
C	2.190865	4.482725	2.086263
H	1.390623	4.156775	2.751994
C	3.125284	5.312888	2.539595
H	3.106744	5.686654	3.558274
H	3.942179	5.648325	1.904985
C	-1.330815	1.577052	-0.694610
O	-1.447701	2.305492	-1.898044
C	1.412980	0.329754	-0.411198

H	0.626980	-0.049551	-1.057519
H	1.245658	-0.063797	0.595857
C	-3.358701	-0.730227	-2.195501
C	-2.988916	-3.124546	-0.716204
C	-4.400769	-1.275147	-1.448690
C	-2.144609	-1.403285	-2.180015
C	-1.952571	-2.571356	-1.449126
C	-4.215009	-2.456108	-0.722977
H	-5.361904	-0.771611	-1.414351
H	-5.038390	-2.851012	-0.135969
H	-2.840680	-4.009397	-0.105851
C	-0.848941	-1.021861	-2.796832
O	-0.567186	0.038483	-3.368046
H	-1.326075	1.660897	-2.623432
N	0.003063	-2.047855	-2.549441
H	0.995762	-1.949646	-2.729666
H	-3.479046	0.198407	-2.747129
C	-0.496249	-2.976376	-1.517355
H	-0.361317	-4.008523	-1.875494
N	0.160796	-2.727331	-0.251082
C	1.419434	-3.439973	-0.099598
H	2.056961	-3.203246	-0.965622
H	1.287554	-4.537002	-0.110990
C	2.181112	-3.036640	1.144527
C	3.711677	-2.244881	3.359358
C	1.612754	-2.250585	2.148727
C	3.511586	-3.446550	1.277497
C	4.274377	-3.055416	2.372045
C	2.380274	-1.854239	3.246963
H	0.562033	-1.974700	2.092403
H	3.960880	-4.057872	0.497079
H	5.309420	-3.375072	2.451970
H	1.927448	-1.241718	4.021629
H	4.304616	-1.932827	4.213821
H	-1.124233	0.531645	-0.921506
H	-3.428289	3.328174	-0.811347
C	-3.578044	2.539327	-0.080619
C	-2.617870	1.575563	0.104238
N	-5.056117	1.506940	1.512420
C	-2.865609	0.506116	1.022480
C	-4.780468	2.473037	0.659396
C	-4.132615	0.527231	1.686831
C	-1.979482	-0.565303	1.231169
H	-5.539074	3.242195	0.526202
H	-5.411424	-0.535129	3.056032
C	-2.323837	-1.698521	2.002268
H	-1.032272	-0.620009	0.702246
C	-3.600818	-1.621986	2.694603
H	-3.866854	-2.467805	3.324532
C	-4.451508	-0.565718	2.545821
O	-1.596843	-2.745546	2.086622
H	-0.479969	-2.878775	0.545508
C	2.745235	-0.116707	-0.950944
C	5.174543	-1.052464	-1.972743
C	2.928504	-0.252459	-2.334103
C	3.782533	-0.472990	-0.087159
C	4.994417	-0.934697	-0.597463
C	4.138016	-0.714357	-2.843153
H	2.114982	0.006747	-3.011287
H	3.631534	-0.423523	0.990111
H	5.788808	-1.219637	0.085290
H	4.269662	-0.815852	-3.915645
H	6.116882	-1.418628	-2.367865

IIId-S

H	2.901788	3.459758	-2.331895
C	2.030002	2.801185	-2.403255
C	-0.350154	2.499462	-1.821557
C	-0.111366	1.618163	-0.589085
C	0.767058	3.537353	-1.951182
C	2.207747	1.554233	-1.523537
H	-0.365758	1.859388	-2.711757
H	-0.592011	2.054571	0.294194
H	3.244481	1.421812	-1.213985
H	1.936180	2.487002	-3.446472
H	-1.334695	2.967319	-1.734222
H	0.494418	4.320417	-2.663697
H	1.818815	0.642538	-1.980709
N	1.388847	1.699577	-0.254057
C	1.063436	4.173534	-0.577686
H	1.846512	4.927159	-0.717166
C	1.641872	3.063072	0.335334
H	2.723454	3.158697	0.450652
H	1.187247	3.073442	1.330171
C	-0.133636	4.862607	0.022213
H	-0.974749	4.235790	0.321267
C	-0.216231	6.179882	0.185927
H	-1.101437	6.646764	0.605835
H	0.602175	6.837770	-0.097727
O	-0.607752	0.142507	-0.776630
O	0.157288	-0.566424	-1.627717
C	1.754455	0.602488	0.727556
H	1.639127	-0.317502	0.148025
H	0.987331	0.633385	1.507646
C	-3.943376	-2.161968	0.806542
C	-2.251437	-3.602330	-0.951363
C	-4.427009	-2.655668	-0.401950
C	-2.606491	-2.389023	1.108003
C	-1.779146	-3.115428	0.258959
C	-3.586742	-3.358518	-1.273556
H	-5.460058	-2.473983	-0.682210
H	-3.982317	-3.716696	-2.219260
H	-1.595367	-4.142451	-1.626504
C	-1.797776	-1.907386	2.262740
O	-2.164320	-1.236860	3.228513
H	0.448671	-2.048059	-0.615187
N	-0.531721	-2.347319	2.036058
H	0.168940	-2.283185	2.763013
H	-4.575427	-1.585068	1.475766
C	-0.393995	-3.233823	0.850496
H	-0.221860	-4.252895	1.228294
N	0.638055	-2.923853	-0.086170
C	1.966406	-3.001149	0.491457
H	2.088631	-3.997310	0.940249
H	2.115227	-2.281664	1.322391
C	3.085112	-2.765662	-0.499043
C	5.256716	-2.159725	-2.168282
C	4.391989	-3.086381	-0.115853
C	2.871671	-2.160203	-1.739289
C	3.957098	-1.856282	-2.564869
C	5.471314	-2.787384	-0.940167
H	4.563075	-3.558358	0.849507
H	1.865546	-1.889704	-2.046692
H	3.781086	-1.374762	-3.522820
H	6.479727	-3.039106	-0.624721

H	6.097155	-1.917277	-2.811613
H	-0.633138	-0.297651	0.248170
H	-1.662820	-0.417972	-3.151617
C	-2.432781	-0.045870	-2.483996
C	-2.081002	0.264231	-1.196078
N	-4.750419	0.523781	-2.131518
C	-3.118651	0.680249	-0.307631
C	-3.773213	0.110075	-2.906671
C	-4.438994	0.781675	-0.827990
C	-2.913508	0.874991	1.081024
H	-4.038330	-0.116955	-3.938814
H	-6.496886	1.210942	-0.365883
C	-3.979193	1.071660	1.927139
H	-1.928154	0.740850	1.515239
C	-5.285550	1.247893	1.403279
H	-6.100366	1.438517	2.094676
C	-5.501200	1.115338	0.056537
O	-3.829795	1.057316	3.279769
H	-3.137028	0.392297	3.473422
C	3.125887	0.724333	1.342494
C	5.651250	0.896806	2.543951
C	3.283236	1.353621	2.582430
C	4.247654	0.165020	0.721003
C	5.502612	0.252235	1.318499
C	4.537588	1.445707	3.177788
H	2.414270	1.766136	3.090109
H	4.141621	-0.354505	-0.227745
H	6.359582	-0.196042	0.824838
H	4.643868	1.936321	4.140095
H	6.629365	0.963587	3.010195

Cartesian coordinates (Å) of amide coordinated to betaine

IIIClE-PT (denoted as IIIC-PT in the main article)

H	3.805569	2.644078	-1.389698
C	2.856356	2.189941	-1.691202
C	0.398859	2.474681	-1.826655
C	0.096818	1.511178	-0.667516
C	1.716353	3.203926	-1.561358
C	2.543834	0.962521	-0.818623
H	0.474421	1.905564	-2.758591
H	-0.557381	1.984224	0.071999
H	3.389677	0.680266	-0.190391
H	2.958476	1.864875	-2.730411
H	-0.435443	3.172875	-1.929529
H	1.849907	4.024741	-2.270446
H	2.225213	0.104007	-1.409746
N	1.397927	1.270236	0.120629
C	1.725362	3.760846	-0.124614
H	2.669571	4.296423	0.023092
C	1.712065	2.557230	0.848792
H	2.683184	2.412574	1.323840
H	0.959347	2.672404	1.633467
C	0.598332	4.723598	0.140983
H	-0.409394	4.309089	0.195562
C	0.773404	6.031861	0.301922
H	-0.062951	6.700772	0.477196
H	1.764139	6.479107	0.262751
C	-0.606492	0.233252	-1.156895
O	0.139235	-0.352041	-2.196184
C	1.209453	0.122593	1.104013
H	1.239375	-0.794620	0.508413
H	0.205084	0.241528	1.519740
C	-3.376633	-2.159456	1.459879
C	-2.403442	-3.038878	-0.986951
C	-4.252450	-2.356100	0.395614
C	-2.009515	-2.388626	1.311361
C	-1.521317	-2.881133	0.084969
C	-3.761779	-2.769334	-0.837763
H	-5.310298	-2.150952	0.525010
H	-4.433308	-2.892219	-1.681795
H	-2.013175	-3.395648	-1.935218
C	-1.036084	-2.005147	2.392039
O	0.104413	-2.478600	2.420027
H	0.171739	-1.323781	-2.023560
N	-1.462112	-1.091245	3.286989
H	-0.784015	-0.838037	3.995295
H	-3.756663	-1.764295	2.396879
C	-0.112116	-3.301202	-0.130662
N	0.322370	-3.986048	0.600679
N	0.526747	-2.949041	-1.175697
C	1.833355	-3.571279	-1.401128
H	1.684897	-4.34459	-2.165633
H	2.203953	-4.067766	-0.494471
C	2.844355	-2.568181	-1.905969
C	4.685850	-0.675758	-2.846117
C	4.008524	-2.295016	-1.187895
C	2.620863	-1.899067	-3.113817
C	3.531714	-0.956543	-3.580021
C	4.926777	-1.351931	-1.652906
H	4.202663	-2.830693	-0.261395
H	1.721698	-2.114349	-3.686095
H	3.343652	-0.441056	-4.517118
H	5.827512	-1.147098	-1.081721
H	5.396307	0.060435	-3.209827
H	-0.706709	-0.474170	-0.326635
H	-1.620108	0.444482	-3.671115
C	-2.359770	0.667164	-2.909181
C	-2.015615	0.608752	-1.582438
N	-4.646128	1.219147	-2.395972
C	-3.015832	0.868282	-0.592853
C	-3.688505	0.989876	-3.270071
C	-4.331341	1.147344	-1.075811
C	-2.784422	0.799296	0.792921
H	-3.961542	1.046161	-4.322532
H	-6.361475	1.563328	-0.492197
C	-3.816518	0.879168	1.748251
H	-1.800301	0.546019	1.171436
C	-5.129048	1.210880	1.224294
H	-5.933766	1.324407	1.946713
C	-5.367416	1.336816	-0.114258
O	-3.643781	0.633120	2.995404
H	-2.304698	-0.482673	3.179894
C	2.206286	0.075185	2.231685
C	4.005685	-0.025224	4.371481
C	1.881125	0.658966	3.459988
C	3.431853	-0.580326	2.094361
C	4.330481	-0.624909	3.157142
C	2.775895	0.612606	4.524288
H	0.916835	1.146906	3.585050

H	3.675696	-1.072595	1.156857
H	5.279716	-1.137656	3.038672
H	2.510378	1.068087	5.472876
H	4.704064	-0.064966	5.201407

IIIC2E-PT

H	3.783328	3.790903	-1.412582
C	2.845355	3.307365	-1.702898
C	0.441191	3.061415	-1.208552
C	0.566876	1.743779	-0.422414
C	1.667461	3.937570	-0.958664
C	2.886996	1.806409	-1.375046
H	0.350153	2.849026	-2.279823
H	0.114455	1.866007	0.565755
H	3.900737	1.471951	-1.150778
H	2.726224	3.433328	-2.782108
H	-0.482063	3.553706	-0.893074
H	1.491374	4.959398	-1.305356
H	2.470964	1.178885	-2.161289
N	2.058196	1.513487	-0.130924
C	1.996528	3.937578	0.547093
H	2.845228	4.616223	0.699260
C	2.466449	2.521825	0.923442
H	3.556011	2.458414	0.991316
H	2.053181	2.192400	1.873635
C	0.840154	4.476194	1.357246
H	0.563253	5.494055	1.080662
C	0.144161	3.873886	2.318617
H	-0.674290	4.388749	2.810720
H	0.339556	2.861258	2.665668
C	-0.157185	0.570702	-1.113310
O	0.571195	0.142745	-2.240680
C	2.386564	0.088032	0.323434
H	3.454228	-0.031843	0.133551
H	1.857599	-0.577894	-0.357196
C	-3.788052	-2.067491	0.280080
C	-2.311509	-2.124490	-2.068544
C	-4.370036	-1.653695	-0.914926
C	-2.476678	-2.540859	0.310582
C	-1.727487	-2.578911	-0.881314
C	-3.627007	-1.674030	-2.091196
H	-5.393595	-1.293193	-0.919781
H	-4.063469	-1.324831	-3.021798
H	-1.722064	-2.146564	-2.980643
C	-1.886730	-3.012904	1.613235
O	-1.144735	-3.995537	1.661843
H	0.496789	-0.843223	-2.269693
N	-2.248614	-2.314466	2.706721
H	-1.877385	-2.662245	3.581995
H	-4.353282	-2.014894	1.205953
C	-0.362269	-3.152095	-0.961745
H	-0.183531	-4.072558	-0.401135
N	0.538942	-2.642088	-1.708291
C	1.760587	-3.432983	-1.880104
H	1.783160	-3.740996	-2.932250
H	1.726401	-4.344673	-1.269044
C	3.023159	-2.661635	-1.570998
C	5.419224	-1.310622	-1.035184
C	3.728344	-2.909853	-0.391720
C	3.516364	-1.711623	-2.470104
C	4.708818	-1.042044	-2.206320
C	4.922730	-2.241210	-0.123722
H	3.346621	-3.642216	0.315094
H	2.971230	-1.509323	-3.389476
H	5.090791	-0.317783	-2.920001
H	5.466132	-2.452935	0.792122
H	6.355879	-0.798463	-0.836777
H	-0.247856	-0.261439	-0.402461
H	-1.137966	1.167998	-3.551466
C	-1.886319	1.291863	-2.775810
C	-1.565141	1.023399	-1.468192
N	-4.162398	1.827590	-2.218353
C	-2.577466	1.141810	-0.465717
C	-3.197575	1.697519	-3.105396
C	-3.872667	1.546113	-0.921930
C	-2.393419	0.808261	0.890215
H	-3.450136	1.916533	-4.141678
H	-5.901700	1.943536	-0.323781
C	-3.461720	0.732111	1.807366
H	-1.427562	0.478505	1.255129
C	-4.740483	1.224807	1.327228
H	-5.562826	1.234280	2.038746
C	-4.930049	1.609889	0.032681
O	-3.351563	0.224725	2.979109
H	-2.697795	-1.374094	2.717645
C	2.108591	-0.193693	1.775224
C	1.640203	-0.527871	4.516287
C	0.844109	-0.562505	2.237808
C	3.150767	-0.053693	2.699357
C	2.922173	-0.224743	4.060483
C	0.604059	-0.702267	3.603045
H	0.035322	-0.756255	1.539195
H	4.146917	0.202668	2.345219
H	3.739938	-0.111341	4.764879
H	-0.398645	-0.937669	3.942200
H	1.452210	-0.638409	5.579499

IIIC3E-PT

H	0.435665	4.081564	-3.083643
C	0.373392	2.992749	-2.998231
C	-1.138409	1.028005	-2.958310
C	-1.041626	0.821452	-1.436918
C	-1.054803	2.519642	-3.285218
C	0.780051	2.539734	-1.584835
H	-0.316254	0.496842	-3.448549
H	-2.038180	0.767564	-0.986663
H	1.233167	3.347902	-1.009342
H	1.068460	2.561912	-3.723216
H	-2.073688	0.588491	-3.312870
H	-1.316039	2.699136	-4.330863
H	1.444465	1.676446	-1.603935
N	-0.441402	2.094661	-0.811915
C	-2.012924	3.310122	-2.373139
H	-1.948455	4.367586	-2.651228
C	-1.494702	3.174742	-0.920650
H	-1.027167	4.096291	-0.571508
H	-2.294233	2.907471	-0.224707
C	-3.449137	2.879254	-2.512638
H	-3.712332	1.889999	-2.135845
C	-4.390284	3.633835	-3.071757
H	-5.413294	3.285911	-3.170856
H	-4.167324	4.628367	-3.451116
C	-0.307447	-0.484404	-1.083614
O	0.956843	-0.513603	-1.702656

C	-0.088268	1.844763	0.646763
H	0.764596	1.162462	0.642518
H	-0.950168	1.326543	1.078981
C	-1.071576	-2.746523	2.856017
C	1.176003	-3.268065	1.306920
C	-0.898961	-4.003702	2.284018
C	-0.124490	-1.740714	2.662893
C	1.030778	-2.015769	1.908342
C	0.216862	-4.260236	1.493679
H	-1.651906	-4.770581	2.434551
H	0.344715	-5.229910	1.023405
H	2.058150	-3.460252	0.703794
C	-0.353233	-0.340918	3.161943
O	0.590463	0.448473	3.276821
H	1.589972	-0.830881	-1.009832
N	-1.626645	0.002799	3.434603
H	-1.755528	0.955475	3.753293
H	-1.978169	-2.532700	3.413433
C	2.137196	-1.040304	1.716258
H	2.644176	-0.657520	2.605066
N	2.521516	-0.728860	0.543350
C	3.691495	0.136707	0.404893
H	4.094033	0.433090	1.382662
H	3.369442	1.046355	-0.119325
C	4.745837	-0.563720	-0.422022
C	6.650905	-1.917518	-1.958486
C	4.536884	-0.766083	-1.789275
C	5.912027	-1.048139	0.168574
C	6.864319	-1.719970	-0.596877
C	5.483098	-1.440575	-2.554222
H	3.625727	-0.393712	-2.253783
H	6.076625	-0.897991	1.232543
H	7.770954	-2.089588	-0.127945
H	5.312396	-1.592428	-3.615512
H	7.391103	-2.441238	-2.555295
H	-0.185501	-0.559899	0.003410
H	-0.059551	-2.132674	-3.238316
C	-0.929770	-2.368423	-2.634701
C	-1.198955	-1.639948	-1.503585
N	-2.823486	-3.810796	-2.275485
C	-2.327093	-1.995079	-0.698432
C	-1.780163	-3.441421	-2.988804
C	-3.093980	-3.117599	-1.138669
C	-2.669330	-1.343366	0.501245
H	-1.575839	-4.014380	-3.891463
H	-4.769180	-4.387109	-0.670753
C	-3.685550	-1.805417	1.361444
H	-2.075143	-0.509852	0.860173
C	-4.467487	-2.922297	0.862509
H	-5.282894	-3.271840	1.491040
C	-4.184828	-3.539309	-0.322005
O	-3.902978	-1.316301	2.527422
H	-2.473882	-0.525782	3.121868
C	0.229797	3.076612	1.452625
C	0.826244	5.321106	3.013711
C	-0.780329	3.738941	2.156981
C	1.545315	3.533650	1.563152
C	1.842780	4.653990	2.334361
C	-0.485603	4.858217	2.929392
H	-1.802618	3.371074	2.109683
H	2.346943	2.999005	1.059492
H	2.869123	4.997248	2.413005
H	-1.278435	5.362682	3.471919
H	1.057375	6.191619	3.619153

IIIC4E-PT

H	2.893491	0.687553	-4.541065
C	1.926983	0.589836	-4.037320
C	0.209284	1.733084	-2.671239
C	0.671275	1.153035	-1.327050
C	1.426146	1.957707	-3.571444
C	2.044820	-0.333742	-2.813562
H	-0.491309	1.041836	-3.152334
H	0.883106	1.966846	-0.626449
H	2.981902	-0.890008	-2.819213
H	1.224866	0.148607	-4.749046
H	-0.322194	2.666819	-2.473456
H	1.164121	2.584716	-4.427660
H	1.207144	-1.023865	-2.718457
N	2.044336	0.491135	-1.542114
C	2.551765	2.629631	-2.754283
H	3.385221	2.817688	-3.442417
C	3.045196	1.612477	-1.707122
H	3.982153	1.143501	-2.012007
H	3.194288	2.056315	-0.720998
C	2.104514	3.969876	-2.221347
H	1.796644	4.657591	-3.009692
C	2.036290	4.386678	-0.959895
H	1.684147	5.386496	-0.728888
H	2.319813	3.777726	-0.105274
C	-0.369317	0.253180	-0.655441
O	-0.603156	-0.882815	-1.452489
C	2.398530	-0.375407	-0.348154
H	1.698417	-1.216306	-0.374210
H	2.182459	0.237745	0.532037
C	2.190133	-2.091262	2.635938
C	0.360364	-3.303730	0.936124
C	2.604011	-3.121474	1.796079
C	0.857704	-1.671986	2.653889
C	-0.076262	-2.300583	1.808054
C	1.689173	-3.719496	0.932782
H	3.642040	-3.439714	1.802398
H	2.006944	-4.514069	0.264653
H	-0.365041	-3.772572	0.277462
C	0.427127	-0.517218	3.527902
O	-0.681239	-0.495898	4.051201
H	-1.214193	-1.436215	-0.906550
N	1.332868	0.478711	3.685004
H	2.147776	0.478808	3.085856
H	2.908828	-1.618349	3.299843
C	-1.521774	-1.952863	1.807238
H	-2.008433	-1.836530	2.776934
N	-2.153695	-1.816746	0.711642
C	-3.573600	-1.485301	0.806319
H	-3.663547	-0.399918	0.943515
H	-4.019531	-1.957282	1.693409
C	-4.338809	-1.884949	-0.433558
C	-5.830260	-2.612414	-2.692559
C	-3.913024	-2.928422	-1.256031
C	-5.518915	-1.208913	-0.754419
C	-6.262626	-1.569729	-1.873602
C	-4.654110	-3.289334	-2.381140
H	-2.995406	-3.458105	-1.014715
H	-5.846913	-0.383958	-0.125913
H	-7.175417	-1.031927	-2.111701

H	-4.310892	-4.102556	-3.013895
H	-6.406085	-2.892650	-3.569232
H	0.008101	-0.057704	0.327731
H	-2.668623	0.329204	-2.108862
C	-2.700071	0.985860	-1.244666
C	-1.621046	1.071763	-0.398826
N	-4.008921	2.471866	0.118445
C	-1.703530	1.905466	0.761714
C	-3.872779	1.716516	-0.952549
C	-2.954727	2.568924	0.969437
C	-0.659127	2.070331	1.692916
H	-4.729561	1.649475	-1.620762
H	-4.052699	3.867804	2.289132
C	-0.800956	2.827437	2.879334
H	0.300084	1.587310	1.534340
C	-2.086078	3.489252	3.046639
H	-2.210461	4.089751	3.944546
C	-3.098545	3.367866	2.142412
O	0.111641	2.949177	3.765780
H	0.933967	1.422879	3.894170
C	3.824043	-0.860252	-0.305929
C	6.445169	-1.818790	-0.112332
C	4.189227	-2.056640	-0.931688
C	4.779287	-0.163833	0.438961
C	6.085133	-0.638251	0.533279
C	5.494737	-2.529875	-0.842950
H	3.439937	-2.636861	-1.465128
H	4.498554	0.746711	0.963561
H	6.817017	-0.090147	1.117652
H	5.765557	-3.460047	-1.331956
H	7.461494	-2.191790	-0.035608

IIIC5E-PT

H	-4.431672	0.512152	-2.584228
C	-3.415476	0.249296	-2.276745
C	-1.672815	-1.516891	-2.239073
C	-1.228090	-1.000150	-0.846093
C	-3.156164	-1.243681	-2.495494
C	-3.242799	0.563651	-0.786916
H	-1.090024	-1.004600	-3.005839
H	-0.824844	-1.814577	-0.234481
H	-4.203034	0.627682	-0.267094
H	-2.707708	0.841576	-2.859245
H	-1.446024	-2.583046	-2.326160
H	-3.415683	-1.533910	-3.517041
H	-2.677087	1.476905	-0.612572
N	-2.504195	-0.569011	-0.090488
C	-4.018435	-2.028209	-1.492854
H	-5.039668	-1.630594	-1.533663
C	-3.432930	-1.766578	-0.090487
H	-4.222693	-1.552631	0.631952
H	-2.850562	-2.615956	0.273912
C	-4.078553	-3.504190	-1.771855
H	-3.132940	-4.046019	-1.728235
C	-5.198389	-4.158498	-2.064680
H	-5.195667	-5.223214	-2.274760
H	-6.158321	-3.649111	-2.107770
C	-0.129621	0.083955	-0.953859
O	-0.663757	1.184445	-1.637935
C	-2.261915	-0.113551	1.341033
H	-3.229640	0.275100	1.671222
H	-1.575006	0.731997	1.271137
C	4.312112	0.481213	0.696055
C	3.421901	2.115089	-1.367583
C	4.957589	0.457834	-0.534985
C	3.216363	1.319499	0.908677
C	2.792688	2.175877	-0.121015
C	4.494513	1.256048	-1.578016
H	5.798140	-0.210776	-0.688538
H	4.968719	1.209598	-2.553363
C	3.068137	2.761769	-2.165022
C	2.417474	1.263587	2.178080
O	1.573425	2.130611	2.429642
H	-0.062362	1.959338	-1.462157
N	2.662176	0.232882	3.017506
H	2.062512	0.221141	3.834557
H	4.642231	-0.185623	1.486927
C	1.758459	3.225951	0.065871
H	1.948323	3.980069	0.835933
N	0.751037	3.315033	-0.705630
C	-0.141517	4.455642	-0.524347
H	-0.322361	4.901099	-1.507624
H	0.330777	5.220642	0.109451
C	-1.460366	4.041171	0.093644
C	-3.892020	3.405887	1.329208
C	-1.473237	3.434375	1.353478
C	-2.670754	4.306981	-0.547773
C	-3.882971	3.989812	0.064861
C	-2.684235	3.129191	1.970873
H	-0.531125	3.202080	1.849683
H	-2.665156	4.773442	-1.529746
H	-4.817799	4.204288	-0.444248
H	-2.685052	2.671627	2.956772
H	-4.834074	3.168257	1.814386
H	0.193989	0.383411	0.058323
H	0.599313	0.525621	-3.503265
C	1.277385	-0.164738	-3.012613
C	1.078405	-0.500795	-1.692981
N	3.240678	-1.540289	-3.198797
C	2.030061	-1.363940	-1.064033
C	2.366693	-0.707628	-3.726101
C	3.092704	-1.855692	-1.888208
C	2.020108	-1.675475	0.307506
H	2.508790	-0.444781	-4.773203
H	4.860593	-3.083056	-1.925916
C	3.087341	-2.338104	0.945237
H	1.247677	-1.265626	0.940667
C	4.080905	-2.921153	0.063213
H	4.870635	-3.506491	0.528251
C	4.080549	-2.686395	-1.280478
O	3.237632	-2.384992	2.221236
H	2.999006	-0.701570	2.703032
C	-1.742318	-1.158731	2.292152
C	-0.678850	-3.097510	4.009657
C	-0.395167	-1.135469	2.647755
C	-2.574942	-2.122669	2.875566
C	-2.045567	-3.083358	3.730247
C	0.149722	-2.116481	3.474104
H	0.232783	-0.327731	2.281566
H	-3.641924	-2.123978	2.673316
H	-2.701416	-3.825981	4.173332
H	1.221999	-2.133637	3.647714
H	-0.265114	-3.866756	4.654161

IIc6Z-PT

H	2.795229	-1.654019	-4.064247
C	2.374073	-0.957674	-3.333894
C	2.772085	1.173762	-2.065860
C	2.086598	0.470022	-0.868548
C	3.393805	0.141496	-3.017730
C	2.046020	-1.723256	-2.037915
H	2.023843	1.752788	-2.605888
H	2.435407	0.887318	0.078913
H	2.512838	-2.710970	-2.009590
H	1.464110	-0.521796	-3.742535
H	3.533671	1.870494	-1.705284
H	3.722016	0.631475	-3.938232
H	0.972230	-1.836129	-1.872241
N	2.592446	-0.980400	-0.838451
C	4.587351	-0.539630	-2.327737
H	4.846364	-1.439337	-2.898195
C	4.104874	-0.953154	-0.926627
H	4.459502	-1.948905	-0.653416
H	4.441014	-0.252422	-0.158492
C	5.816592	0.319728	-2.230990
H	5.712982	1.261837	-1.691385
C	6.991081	-0.007759	-2.761760
H	7.853847	0.645798	-2.681921
H	7.129084	-0.943969	-3.297600
C	0.538052	0.597536	-0.922087
O	0.116323	0.554218	-2.265991
C	2.194874	-1.731078	0.430993
H	2.347980	-2.785775	0.186659
H	1.123949	-1.584810	0.579430
C	-3.968592	-3.967796	0.922627
C	-4.190859	-3.575515	-1.816803
C	-4.915175	-4.683994	0.194786
C	-3.132172	-3.046447	0.291403
C	-3.250103	-2.839605	-1.092582
C	-5.026830	-4.487159	-1.178401
H	-5.553306	-5.402946	0.698232
H	-5.758310	-5.045225	-1.753787
H	-4.274992	-3.419751	-2.889122
C	-2.049204	-2.348412	1.075942
O	-0.918757	-2.226867	0.591051
H	-0.829983	0.262692	-2.240650
N	-2.403961	-1.905368	2.288169
H	-3.378736	-1.940419	2.552909
H	-3.856918	-4.146331	1.988328
C	-2.414943	-1.862885	-1.849098
H	-1.875513	-2.277016	-2.706038
N	-2.293625	-0.612331	-1.659873
C	-2.968599	0.064844	-0.562893
H	-2.292490	0.063375	0.303567
H	-3.882871	-0.466100	-0.259107
C	-3.283708	1.502976	-0.908406
C	-3.872353	4.178929	-1.482266
C	-3.522190	1.906195	-2.222303
C	-3.346444	2.449395	0.116956
C	-3.634363	3.780523	-0.167231
C	-3.816540	3.238550	-2.508206
H	-3.465181	1.174319	-3.023471
H	-3.138579	2.142563	1.140776
H	-3.651646	4.509383	0.637881
H	-3.998206	3.542171	-3.535197
H	-4.092027	5.218618	-1.706061
H	0.074832	-0.234536	-0.376114
H	0.401477	3.069744	-2.032144
C	0.167936	3.080935	-0.972602
C	0.138154	1.908458	-0.254257
N	-0.462230	4.402621	0.934142
C	-0.275343	1.956311	1.114891
C	-0.134717	4.304627	-0.336986
C	-0.551926	3.254119	1.651751
C	-0.474135	0.816159	1.921832
H	-0.096066	5.231046	-0.907590
H	-1.193573	4.333339	3.399330
C	-0.944254	0.885569	3.251807
H	-0.293110	-0.180504	1.530261
C	-1.184074	2.223208	3.766464
H	-1.538789	2.300211	4.791439
C	-0.993729	3.339701	3.005322
O	-1.163955	-0.148703	3.972528
H	-1.772656	-1.332387	2.899595
C	3.001859	-1.375316	1.656353
C	4.510875	-0.776275	3.940912
N	2.695910	-0.255808	2.435538
C	4.059569	-2.202753	2.049773
C	4.811435	-1.906165	3.182453
C	3.449658	0.043819	3.567757
H	1.846253	0.371715	2.182386
H	4.291072	-3.093437	1.470271
H	5.627042	-2.559735	3.474912
H	3.193418	0.913590	4.164218
H	5.094202	-0.543864	4.826309

IIc7Z-PT

H	-3.450720	-3.415598	-2.891292
C	-2.881846	-2.971548	-2.069882
C	-2.704123	-2.715864	0.403825
C	-2.252896	-1.256843	0.143742
C	-3.591380	-3.226449	-0.737283
C	-2.772692	-1.453886	-2.293143
H	-1.820538	-3.350153	0.459061
H	-2.520081	-0.614741	0.986296
H	-1.767111	-1.145515	-2.584271
H	-1.884496	-3.411428	-2.053355
H	-3.223717	-2.782469	1.363219
H	-3.786674	-4.293986	-0.606702
H	-3.486750	-1.091127	-3.036412
N	-3.104118	-0.709327	-1.016084
C	-4.918328	-2.448514	-0.758111
H	-5.415955	-2.644414	-1.715466
C	-4.559819	-0.953518	-0.672932
H	-5.155589	-0.352641	-1.362887
H	-4.705681	-0.553847	0.333870
C	-5.864385	-2.826592	0.347167
H	-5.509299	-2.669804	1.366480
C	-7.077471	-3.331853	0.144593
H	-7.724019	-3.604041	0.972605
H	-7.465520	-3.491658	-0.858606
C	-0.728660	-1.127878	-0.087243
O	-0.287478	-2.180780	-0.915989
C	-2.913495	0.779331	-1.275686
H	-3.375211	0.948003	-2.251987
H	-1.844278	0.956705	-1.405666
C	2.568080	3.745316	-1.587356
C	4.077394	1.419425	-1.522038

C	3.954783	3.824325	-1.498750
C	1.925123	2.509841	-1.667439
C	2.685435	1.325507	-1.610677
C	4.711421	2.657744	-1.476182
C	4.439593	4.794095	-1.451045
H	5.794103	2.706284	-1.417991
H	4.671525	0.510241	-1.503063
C	0.428145	2.487865	-1.836329
O	-0.127653	1.672199	-2.580389
H	0.692190	-2.058741	-0.981580
N	-0.227765	3.444377	-1.145565
H	-1.239584	3.407741	-1.212831
H	1.971053	4.650665	-1.610794
C	2.033432	-0.013608	-1.648315
H	1.256256	-0.138231	-2.402346
N	2.259420	-1.025836	-0.903179
C	3.198660	-0.976545	0.208115
H	2.703770	-1.464794	1.054625
H	3.419974	0.053827	0.519665
C	4.484696	-1.729888	-0.070055
C	6.899562	-3.094387	-0.481007
C	5.347218	-1.989584	1.000537
C	4.841914	-2.167529	-1.345220
C	6.044202	-2.846091	-1.549380
C	6.546290	-2.662984	0.798440
H	5.067761	-1.660317	1.999225
H	4.174300	-1.982539	-2.182126
H	6.308510	-3.181124	-2.547978
H	7.205601	-2.856056	1.639434
H	7.835316	-3.621245	-0.640249
H	-0.518580	-0.172644	-0.582161
H	-0.033700	-3.275465	1.419861
C	0.281374	-2.339065	1.866723
C	0.016036	-1.138640	1.245332
N	1.521355	-1.291501	3.636948
C	0.554039	0.059040	1.820175
C	1.022692	-2.369661	3.066364
C	1.308203	-0.099062	3.028429
C	0.444413	1.338960	1.240185
H	1.215090	-3.321612	3.557330
H	2.473802	0.921858	4.520751
C	1.036427	2.498644	1.795124
H	-0.123957	1.463443	0.328712
C	1.785478	2.287825	3.024260
H	2.252510	3.163868	3.467284
C	1.906755	1.061823	3.603916
O	0.950013	3.671112	1.293607
H	0.180036	3.705026	-0.211887
C	-3.546954	1.700859	-0.262261
C	-4.747892	3.479425	1.541454
C	-2.946148	1.976796	0.970899
C	-4.748292	2.342108	-0.585002
C	-5.346802	3.224298	0.309562
C	-3.546376	2.856455	1.868093
H	-1.994047	1.526951	1.236467
H	-5.213648	2.159555	-1.550894
H	-6.275865	3.716688	0.040919
H	-3.062880	3.061057	2.817878
H	-5.210078	4.170351	2.239372

IIIC8Z-PT

H	3.582057	-2.161849	-3.068290
C	3.039603	-1.315971	-2.636386
C	3.222949	0.871404	-1.484477
C	1.952552	0.497075	-0.681882
C	4.001190	-0.377961	-1.903399
C	2.008563	-1.840412	-1.630125
H	2.924143	1.413536	-2.384129
H	1.953670	0.973278	0.304904
H	2.235606	-2.857060	-1.297330
H	2.530561	-0.778434	-3.437950
H	3.848226	1.549301	-0.896800
H	4.835842	-0.098527	-2.551867
H	0.989395	-1.823963	-2.012324
N	2.023360	-1.005684	-0.363469
C	4.528004	-1.115936	-0.660302
H	4.855637	-2.115681	-0.970046
C	3.349185	-1.256759	0.323478
H	3.301037	-2.258576	0.754348
H	3.411530	-0.539602	1.145562
C	5.689046	-0.429376	0.003245
H	5.507106	0.576511	0.383517
C	6.892264	-0.977429	0.144157
H	7.707961	-0.443892	0.621429
H	7.102539	-1.982214	-0.214949
C	0.651518	0.946090	-1.398592
O	0.558501	0.393949	-2.691183
C	0.877801	-1.503465	0.523081
H	0.786523	-2.563676	0.276564
H	-0.036551	-1.005605	0.197761
C	-5.387984	0.227159	0.888204
C	-5.062306	-0.411433	-1.801087
C	-6.497437	-0.100693	0.112814
C	-4.111660	0.232412	0.327349
C	-3.942168	-0.108958	-1.025329
C	-6.334630	-0.412471	-1.233816
H	-7.485897	-0.111730	0.560349
H	-7.196745	-0.656263	-1.845980
H	-4.936859	-0.631549	-2.857584
C	-2.890601	0.551877	1.148597
O	-1.837864	-0.059552	0.932123
H	-0.276407	-0.133621	-2.719212
N	-3.016473	1.498066	2.087241
H	-3.849095	2.070964	2.096101
H	-5.512244	0.457625	1.942523
C	-2.584609	-0.016937	-1.641872
H	-2.129871	0.977483	-1.579920
N	-1.897232	-0.910631	-2.231665
C	-2.383342	-2.290760	-2.325574
H	-2.181169	-2.635341	-3.343775
H	-3.461774	-2.359248	-2.151755
C	-1.670953	-3.187599	-1.333939
C	-0.427679	-4.886195	0.515224
C	-2.020336	-3.138979	0.020221
C	-0.687264	-4.085859	-1.748397
C	-0.065163	-4.932489	-0.829183
C	-1.403847	-3.982263	0.939506
H	-2.769447	-2.426289	0.354672
H	-0.412427	-4.132019	-2.799779
H	0.692202	-5.633306	-1.167752
H	-1.682333	-3.934920	1.987914
H	0.045899	-5.551457	1.231377
H	-0.202736	0.627764	-0.793001
H	1.234190	2.569753	-3.516279
C	1.031986	3.127641	-2.607627

C	0.662131	2.468636	-1.459656
N	0.972127	5.278623	-1.522993
C	0.345334	3.244988	-0.302352
C	1.165687	4.535712	-2.593383
C	0.563734	4.654248	-0.387931
C	-0.163325	2.684467	0.880637
H	1.467081	5.054678	-3.501735
H	0.503191	6.502085	0.717515
C	-0.421421	3.439835	2.041299
H	-0.431455	1.635947	0.900885
C	-0.129077	4.859986	1.939118
H	-0.317195	5.466629	2.822039
C	0.323241	5.431801	0.783865
O	-0.903351	2.931378	3.116606
H	-2.166497	1.888149	2.559184
C	1.084561	-1.369285	2.012105
C	1.437650	-1.241000	4.791556
C	1.480496	-2.500098	2.736141
C	0.845359	-0.178729	2.704119
C	1.025745	-0.114666	4.083515
C	1.660276	-2.438793	4.114911
H	1.636302	-3.441189	2.212274
H	0.497814	0.707170	2.188089
H	0.821161	0.820822	4.594497
H	1.965786	-3.326459	4.659999
H	1.572051	-1.190945	5.867786

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H	1.779695	-4.512902	-0.408951
C	1.764534	-3.466900	-0.727504
C	2.977811	-1.697247	-2.028993
C	2.417717	-0.725693	-0.963341
C	3.070738	-3.117842	-1.450627
C	1.627915	-2.566791	0.515455
H	2.310859	-1.693480	-2.890522
H	3.045911	0.163920	-0.893705
H	1.907903	-3.086701	1.435496
H	0.916811	-3.311291	-1.394278
H	3.961198	-1.356183	-2.364590
H	3.271241	-3.838744	-2.247337
H	0.625923	-2.151935	0.651302
N	2.585299	-1.398648	0.406527
C	4.195312	-3.161769	-0.399558
H	4.070513	-4.070558	0.201560
C	4.000147	-1.929329	0.499611
H	4.189490	-2.160067	1.549785
H	4.656175	-1.104904	0.209182
C	5.581522	-3.173477	-0.979926
C	5.860800	-2.315878	-1.592873
C	6.458060	-4.154401	-0.785911
H	7.446672	-4.129244	-1.233018
H	6.214746	-5.019306	-0.173300
C	0.948726	-0.281683	-1.242232
O	0.331437	-1.224067	-2.091014
C	2.341981	-0.443322	1.570548
H	2.273705	-1.089952	2.449627
H	1.359525	0.003915	1.419174
C	-4.140681	-0.975556	2.925519
C	-4.427501	-2.561458	0.657820
C	-5.267575	-1.778184	2.777572
C	-3.153359	-0.956284	1.939418
C	-3.300712	-1.750293	0.795124
C	-5.411175	-2.571345	1.641365
H	-6.028571	-1.789414	3.551386
H	-6.290638	-3.195617	1.519056
H	-4.547138	-3.159852	-0.241144
C	-1.925233	-0.097730	2.073031
O	-0.820349	-0.543273	1.736221
H	-0.640318	-1.033919	-2.009214
N	-2.125300	1.140566	2.545516
H	-3.078057	1.450898	2.681734
H	-4.015825	-0.373004	3.821270
C	-2.317127	-1.694075	-0.327331
H	-1.682157	-2.574770	-0.470305
N	-2.160226	-0.750018	-1.163971
C	-2.953515	0.486282	-1.074345
H	-2.646696	1.108205	-1.921014
H	-2.671765	1.037619	-0.168500
C	-4.448899	0.251539	-1.111785
C	-7.199265	-0.271308	-1.149575
C	-5.010256	-0.513692	-2.137596
C	-5.280087	0.763200	-0.116316
C	-6.648728	0.503393	-0.131821
C	-6.376586	-0.775872	-2.156364
H	-4.366404	-0.918394	-2.914862
H	-4.847732	1.353482	0.688348
H	-7.282421	0.898635	0.656511
H	-6.801209	-1.375412	-2.956204
H	-8.264635	-0.480368	-1.160627
H	0.393822	-0.242854	-0.299012
H	1.611001	0.397480	-3.773004
C	1.352710	1.264205	-3.171259
C	0.945996	1.107120	-1.865965
N	1.156933	3.656120	-3.062101
C	0.558791	2.266525	-1.120157
C	1.437243	2.556308	-3.731464
C	0.727663	3.526702	-1.781097
C	0.066335	2.234468	0.202069
H	1.764130	2.678472	-4.762662
H	0.566053	5.661578	-1.557219
C	-0.232536	3.400806	0.937645
H	-0.097368	1.289051	0.705455
C	-0.019909	4.658816	0.240994
H	-0.244548	5.569531	0.790883
C	0.426457	4.712317	-1.046104
O	-0.663386	3.387799	2.143535
H	-1.403679	1.905279	2.472849
C	3.421419	0.592143	1.767448
C	5.423769	2.508256	2.177218
C	3.410691	1.793970	1.052520
C	4.431348	0.376141	2.711501
C	5.428888	1.325140	2.913663
C	4.410648	2.742661	1.251196
H	2.603293	2.003461	0.357147
H	4.431434	-0.536867	3.302065
H	6.204052	1.144395	3.651427
H	4.386336	3.670601	0.688798
H	6.199633	3.250832	2.334878

IIIC10Z-PT

H	-5.113723	2.170432	-1.669460
C	-4.419724	1.359874	-1.911635
C	-3.552284	-0.854225	-1.246998
C	-2.293309	-0.328129	-0.545788

C	-4.699482	0.137235	-1.035716
C	-2.966152	1.805683	-1.681760
H	-3.357033	-0.980219	-2.318421
H	-2.268074	-0.680527	0.489034
H	-2.289716	1.476411	-2.469527
H	-4.552757	1.112888	-2.967943
H	-3.785118	-1.841971	-0.841069
H	-5.659191	-0.316547	-1.293588
H	-2.896690	2.885695	-1.560563
N	-2.428747	1.194603	-0.402962
C	-4.730823	0.607458	0.434380
H	-5.582238	1.286778	0.550412
C	-3.442127	1.430435	0.693726
H	-3.641277	2.503429	0.706690
H	-2.962800	1.155211	1.637037
C	-4.909468	-0.525147	1.411972
H	-4.088956	-1.236392	1.516426
C	-6.013208	-0.699706	2.132637
H	-6.118626	-1.535353	2.816745
H	-6.851170	-0.010052	2.061463
C	-0.976156	-0.792346	-1.185822
O	-0.821898	-0.205975	-2.458968
C	-1.084345	1.804455	-0.044294
H	-0.460365	1.663275	-0.929707
H	-0.667830	1.194018	0.763139
C	4.837610	-1.281384	1.326599
C	4.746960	-1.360224	-1.451760
C	6.008139	-1.483534	0.599621
C	3.618397	-1.105278	0.672069
C	3.578718	-1.111248	-0.729918
C	5.959644	-1.542314	-0.791014
H	6.952929	-1.605326	1.119127
H	6.863471	-1.726409	-1.362609
H	4.705331	-1.412396	-2.536103
C	2.342681	-0.879035	1.443363
O	1.495047	-0.085120	1.031638
H	0.150641	-0.067859	-2.587364
N	2.220228	-1.593848	2.578896
H	2.862299	-2.361396	2.721135
H	4.874035	-1.237424	2.411339
C	2.289609	-0.894931	-1.446854
H	1.532914	-1.673082	-1.304128
N	1.976283	0.075164	-2.208287
C	2.933886	1.183188	-2.414337
H	2.537534	1.785878	-3.235499
H	3.907222	0.797229	-2.731158
C	3.103995	2.048755	-1.181646
C	3.350612	3.612796	1.132420
C	2.112166	2.967954	-0.832859
C	4.237690	1.945512	-0.372167
C	4.359666	2.720358	0.779132
C	2.226560	3.742906	0.318561
H	1.249683	3.088543	-1.484558
H	5.029552	1.249743	-0.638421
H	5.245100	2.623390	1.400331
H	1.445306	4.453477	0.575069
H	3.444062	4.214154	2.031502
H	-0.151247	-0.487010	-0.531015
H	-1.291925	-2.415158	-3.340442
C	-1.212786	-2.975133	-2.414461
C	-1.010895	-2.311874	-1.228898
N	-1.262143	-5.119129	-1.323325
C	-0.884541	-3.069043	-0.019529
C	-1.327910	-4.383913	-2.414321
C	-1.040316	-4.486732	-0.142012
C	-0.610298	-2.499823	1.239117
H	-1.491801	-4.911243	-3.352359
H	-1.080623	-6.345642	0.943831
C	-0.452542	-3.272952	2.411529
H	-0.426547	-1.433876	1.333848
C	-0.675516	-4.701885	2.255597
H	-0.586948	-5.312922	3.150847
C	-0.944738	-5.271688	1.045517
O	-0.107425	-2.774020	3.536098
H	1.286871	-1.740834	3.007207
C	-1.137644	3.254643	0.361185
C	-1.100801	5.941871	1.149772
C	-1.170765	3.597169	1.715776
C	-1.069588	4.275417	-0.594029
C	-1.056010	5.611419	-0.203776
C	-1.155596	4.932804	2.109148
H	-1.187612	2.813252	2.468578
H	-1.001191	4.026282	-1.650434
H	-0.996905	6.391937	-0.955223
H	-1.176068	5.183732	3.164596
H	-1.082496	6.982940	1.455745

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H	-2.439539	0.581851	-3.565683
C	-1.670253	0.055712	-2.994036
C	-0.638206	-2.165819	-2.505932
C	-0.543472	-1.735134	-1.024866
C	-1.808326	-1.456995	-3.195147
C	-1.837695	0.381177	-1.500462
H	0.296160	-1.899407	-3.005017
H	-0.630086	-2.593351	-0.351244
H	-2.810518	0.825030	-1.276780
H	-0.690456	0.396214	-3.332600
H	-0.755459	-3.251178	-2.573230
H	-1.816355	-1.701386	-4.260383
H	-1.048338	1.039320	-1.131346
N	-1.780530	-0.889445	-0.677282
C	-3.135315	-1.898600	-2.548867
H	-3.921923	-1.220230	-2.900280
C	-2.987457	-1.732993	-1.020397
H	-3.859133	-1.242316	-0.589506
H	-2.844045	-2.691532	-0.511650
C	-3.543343	-3.303764	-2.894186
H	-2.880756	-4.102226	-2.557999
C	-4.643503	-3.609832	-3.575305
H	-4.893727	-4.637860	-3.817087
H	-5.331728	-2.840575	-3.917490
C	0.765614	-1.022071	-0.690146
O	0.982625	-0.027933	-1.683456
C	-1.767951	-0.551917	0.808968
H	-0.969745	0.177472	0.955142
H	-1.503613	-1.478121	1.329600
C	-0.039549	4.200113	-2.270221
C	-0.740422	4.008260	0.390080
C	-1.185167	4.840279	-1.817570
C	0.790480	3.473358	-1.407151
C	0.425766	3.364483	-0.050762
C	-1.539668	4.743971	-0.474348
H	-1.798051	5.408929	-2.509669
H	-2.431087	5.238667	-0.100733

H	-1.003577	3.917483	1.439175
C	1.952276	2.804871	-2.114767
O	1.834256	2.521001	-3.306125
H	1.918363	0.236061	-1.663618
N	3.108725	2.568018	-1.464690
H	3.819491	2.103855	-2.017411
H	0.234979	4.240619	-3.317999
C	1.152952	2.572155	0.977386
H	2.247952	2.605211	1.031308
N	0.482271	1.902630	1.829194
C	1.239591	1.220167	2.881069
H	1.193083	1.861515	3.770670
H	2.297887	1.096250	2.610582
C	0.593557	-0.110318	3.198522
C	-0.682712	-2.553595	3.707572
C	1.202209	-1.313940	2.840126
C	-0.659592	-0.141347	3.817965
C	-1.293033	-1.353505	4.076961
C	0.564303	-2.531263	3.085484
H	2.177723	-1.293254	2.359763
H	-1.145484	0.794608	4.084432
H	-2.266650	-1.362134	4.558561
H	1.048338	-3.459276	2.794848
H	-1.176438	-3.500073	3.906893
H	0.669425	-0.540159	0.291819
H	1.099166	-3.818485	-1.224016
C	1.982461	-3.292504	-0.873127
C	1.958803	-1.953209	-0.570735
N	4.328968	-3.479366	-0.339029
C	3.169599	-1.338901	-0.114769
C	3.193527	-4.015319	-0.736814
C	4.332458	-2.158243	-0.027759
C	3.238758	0.013840	0.252568
H	3.209612	-5.076147	-0.978335
H	6.425254	-2.171446	0.485642
C	4.425715	0.651032	0.669503
H	2.348706	0.625685	0.222133
C	5.594028	-0.215815	0.744614
H	6.525809	0.235124	1.077638
C	5.541635	-1.541613	0.418411
O	4.475114	1.895954	0.952065
H	3.344408	2.662458	-0.474848
C	-3.046539	0.027478	1.350876
C	-5.363826	1.141203	2.448928
C	-3.247589	1.409770	1.323157
C	-4.004768	-0.790529	1.957295
C	-5.160192	-0.237251	2.500769
C	-4.405297	1.964680	1.862586
H	-2.480534	2.051196	0.895195
H	-3.837020	-1.864120	2.013095
H	-5.897746	-0.880463	2.970079
H	-4.551554	3.040026	1.834991
H	-6.263938	1.572700	2.875305

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H	-1.268896	-5.017693	-0.910984
C	-0.692914	-4.186294	-1.329212
C	1.480216	-2.999993	-1.324295
C	1.020384	-1.849381	-0.417505
C	0.774900	-4.293371	-0.909627
C	-1.251745	-2.840292	-0.839851
H	1.238983	-2.762727	-2.366592
H	1.682924	-1.751444	0.449226
H	-1.317397	-2.096358	-1.632709
H	-0.782939	-4.234949	-2.417630
H	2.567058	-3.088704	-1.252663
H	1.249727	-5.159485	-1.377097
H	-2.226220	-2.952355	-0.363105
N	-0.329582	-2.243511	0.204077
C	0.817389	-4.449867	0.623842
H	0.328288	-5.396808	0.877467
C	-0.029543	-3.305788	1.236496
H	-0.993085	-3.664664	1.601334
H	0.489507	-2.808860	2.060758
C	2.219340	-4.491687	1.172148
H	2.801695	-3.570507	1.127686
C	2.771633	-5.586000	1.687362
H	3.791670	-5.587489	2.057603
H	2.219617	-6.520863	1.754774
C	1.017889	-0.485224	-1.123719
O	0.114895	-0.510909	-2.206563
C	-0.972683	-1.028975	0.853346
H	-1.247361	-0.363525	0.029360
H	-0.190457	-0.542464	1.441438
C	-0.119918	5.227125	1.699424
C	-1.144788	4.991755	-0.876553
C	-0.761132	6.311581	1.104085
C	0.008626	4.020788	1.013935
C	-0.521337	3.894017	-0.281379
C	-1.267620	6.195539	-0.187013
H	-0.863450	7.244473	1.648893
H	-1.756200	7.040540	-0.660919
H	-1.516806	4.909847	-1.893706
C	0.659110	2.820903	1.652181
O	0.172075	1.699519	1.475408
H	-0.339264	0.367332	-2.223305
N	1.747892	3.060297	2.396675
H	2.172597	3.976363	2.346296
H	0.262934	5.311734	2.712437
C	-0.302931	2.636155	-1.048066
H	0.731698	2.281154	-1.058206
N	-1.142950	1.945921	-1.711302
C	-2.554643	2.318406	-1.737387
H	-2.722543	2.904152	-2.651754
H	-2.827743	2.959684	-0.891161
C	-3.472727	1.114471	-1.773680
C	-5.293840	-1.017010	-1.935725
C	-3.166990	-0.025813	-2.523062
C	-4.698211	1.170679	-1.105499
C	-5.608446	0.119175	-1.192585
C	-4.068259	-1.086786	-2.597436
H	-2.228160	-0.082686	-3.065306
H	-4.945098	2.049074	-0.514678
H	-6.558632	0.184861	-0.670784
H	-3.814846	-1.965805	-3.183229
H	-5.997445	-1.841269	-1.999615
H	0.714605	0.276320	-0.396398
H	2.099087	-0.647316	-3.609478
C	2.828965	-0.352260	-2.862480
C	2.443574	-0.186033	-1.554562
N	5.113018	0.217468	-2.367317
C	3.413114	0.239602	-0.591337
C	4.177882	-0.137963	-3.224094
C	4.749280	0.412497	-1.073257
C	3.113735	0.504385	0.760118

H	4.487075	-0.275359	-4.258919
H	6.760326	0.939322	-0.514643
C	4.080762	0.970069	1.677769
H	2.096091	0.419533	1.129607
C	5.435445	1.083987	1.162571
H	6.200281	1.416340	1.860659
C	5.745949	0.825064	-0.140311
O	3.804054	1.299168	2.883760
H	2.377084	2.281484	2.696020
C	-2.180964	-1.328058	1.699911
C	-4.451818	-1.800437	3.262439
C	-2.056280	-1.577395	3.069892
C	-3.454622	-1.291052	1.127451
C	-4.585664	-1.530728	1.902326
C	-3.186045	-1.818294	3.846310
H	-1.073223	-1.569825	3.534333
H	-3.559762	-1.059542	0.070438
H	-5.568454	-1.495189	1.441573
H	-3.078314	-2.009716	4.909166
H	-5.332225	-1.985062	3.870219

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H	-5.495892	1.115589	-2.340928
C	-4.620151	0.462087	-2.400945
C	-3.463355	-1.498738	-1.431245
C	-2.456245	-0.689895	-0.600402
C	-4.799207	-0.753231	-1.487620
C	-3.350382	1.216587	-1.974444
H	-3.072778	-1.636486	-2.445949
H	-2.501607	-0.981988	0.454579
H	-2.499435	1.009422	-2.621381
H	-4.513821	0.144899	-3.441603
H	-3.568735	-2.490840	-0.985664
H	-5.591215	-1.407045	-1.860856
H	-3.517190	2.292571	-1.916076
N	-2.925619	0.775644	-0.589941
C	-5.177485	-0.236489	-0.084481
H	-6.149167	0.263435	-0.162435
C	-4.132460	0.834680	0.317626
H	-4.535260	1.845333	0.232135
H	-3.770212	0.690140	1.339104
C	-5.306025	-1.337578	0.935201
H	-4.393833	-1.856637	1.232498
C	-6.466062	-1.706330	1.470556
H	-6.528641	-2.515405	2.191079
H	-7.395796	-1.208635	1.204252
C	-0.997586	-0.888485	-1.045095
O	-0.822005	-0.401360	-2.355827
C	-1.810969	1.661169	-0.063446
H	-1.015610	1.598534	-0.808991
H	-1.450077	1.191979	0.854015
C	4.085492	1.827346	2.160184
C	4.145823	2.602940	-0.504345
C	5.209176	2.470223	1.652566
C	2.989600	1.549113	1.339523
C	3.021967	1.941488	-0.005617
C	5.240946	2.855767	0.314748
H	6.052440	2.679721	2.302768
H	6.114894	3.355581	-0.090700
H	4.171643	2.891425	-1.551669
C	1.767934	0.857480	1.882621
O	0.651168	1.137644	1.433990
H	0.082407	0.001077	-2.352852
N	1.978986	-0.046434	2.849820
H	2.924862	-0.316822	3.078629
H	4.049487	1.559662	3.212413
C	1.924804	1.638456	-0.976189
H	1.342858	2.498110	-1.322146
N	1.644135	0.514197	-1.500528
C	2.367599	-0.699903	-1.077014
H	1.963316	-1.521512	-1.678975
H	2.114615	-0.930202	-0.032021
C	3.868161	-0.619315	-1.258974
C	6.637124	-0.379470	-1.594979
C	4.401649	-0.249663	-2.496409
C	4.734752	-0.884593	-0.199226
C	6.112692	-0.762838	-0.363168
C	5.777606	-0.127827	-2.663975
H	3.730788	-0.039107	-3.326076
H	4.323522	-1.167132	0.767252
H	6.775256	-0.960693	0.474236
H	6.180528	0.166257	-3.628686
H	7.710580	-0.278653	-1.723571
H	-0.343425	-0.337467	-0.358078
H	-0.873903	-2.789799	-2.991027
C	-0.678454	-3.194582	-2.002990
C	-0.668114	-2.363484	-0.909007
N	-0.182679	-5.128748	-0.661548
C	-0.358419	-2.907688	0.376738
C	-0.429286	-4.574548	-1.830894
C	-0.137674	-4.320228	0.428974
C	-0.242390	-2.131833	1.547738
H	-0.443887	-5.236784	-2.694742
H	0.313357	-5.977302	1.728397
C	0.118032	-2.689009	2.793738
H	-0.374446	-1.053225	1.517295
C	0.280818	-4.133634	2.818118
H	0.529446	-4.583451	3.776518
C	0.163630	-4.900838	1.696446
O	0.314712	-1.986328	3.845521
H	1.213646	-0.644265	3.238441
C	-2.191832	3.097024	0.182869
C	-2.814101	5.781890	0.670004
C	-2.665672	3.498918	1.435345
C	-2.006742	4.060821	-0.813545
C	-2.321168	5.395929	-0.574419
C	-2.981191	4.832758	1.676618
H	-2.775135	2.765607	2.230156
H	-1.601350	3.764886	-1.778744
H	-2.172273	6.134444	-1.355463
H	-3.346539	5.132620	2.653523
H	-3.055182	6.823027	0.860148

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H	3.265890	1.471888	-2.647650
C	2.280227	1.603180	-2.190892
C	0.769735	3.140225	-0.951219
C	0.246178	1.911202	-0.168501
C	2.214801	2.918329	-1.411602
C	2.031523	0.447620	-1.215709
H	0.128159	3.299042	-1.821959
H	-0.058444	2.193160	0.842579
H	2.963652	-0.031200	-0.907352
H	1.523852	1.601152	-2.977569

H	0.714078	4.031017	-0.319352
H	2.537501	3.745832	-2.048375
H	1.362817	-0.320026	-1.606356
N	1.422747	0.965224	0.074881
C	3.134409	2.786145	-0.190700
H	4.083697	2.346548	-0.530122
C	2.482800	1.776646	0.782937
H	3.214900	1.067364	1.176610
H	1.988058	2.278559	1.617862
C	3.462039	4.060929	0.544836
H	4.006932	3.920584	1.479240
C	3.162109	5.297263	0.157053
H	3.454471	6.154449	0.754823
H	2.623327	5.508491	-0.762410
C	-0.955633	1.222383	-0.834229
O	-0.760578	1.058748	-2.228930
C	1.050691	-0.253135	0.907773
H	1.989925	-0.794565	1.057291
H	0.428050	-0.874597	0.264038
C	-2.569481	-2.945044	0.377623
C	-0.220040	-3.644554	1.706551
C	-2.600756	-3.267634	1.732869
C	-1.354780	-2.950856	-0.312990
C	-0.168659	-3.324939	0.347828
C	-1.425424	-3.602851	2.400110
H	-3.545359	-3.248032	2.267222
H	-1.448076	-3.845939	3.457855
H	0.699191	-3.938939	2.202923
C	-1.281883	-2.428382	-1.717954
O	-0.284296	-1.771149	-2.072246
H	-0.626193	0.106655	-2.403609
N	-2.312309	-2.674688	-2.543360
H	-2.233537	-2.183346	-3.429073
H	-3.489547	-2.676946	-0.139644
C	1.121243	-3.460607	-0.375345
H	1.067729	-3.727120	-1.437328
N	2.232359	-3.311848	0.222143
C	3.438535	-3.540014	-0.565626
H	3.211137	-3.884650	-1.584949
H	4.009330	-4.332114	-0.065236
C	4.274833	-2.280239	-0.627588
C	5.769822	0.089920	-0.737984
C	4.627887	-1.609534	0.548486
C	4.682910	-1.755943	-1.854541
C	5.428787	-0.577658	-1.912179
C	5.369949	-0.431545	0.494699
H	4.311474	-2.014705	1.506470
H	4.407671	-2.267644	-2.773095
H	5.739761	-0.181686	-2.874248
H	5.645697	0.077041	1.414563
H	6.354421	1.004151	-0.778851
H	-1.081349	0.231909	-0.385251
H	-1.424014	3.849900	0.100526
C	-2.316444	3.262088	-0.085525
C	-2.254301	1.971588	-0.556474
N	-4.720818	3.241233	0.038390
C	-3.490148	1.270337	-0.750775
C	-3.569611	3.859936	0.185540
C	-4.693360	1.960874	-0.412125
C	-3.555364	-0.056711	-1.208162
H	-3.603834	4.885844	0.547168
H	-6.836081	1.793197	-0.289084
C	-4.761595	-0.779313	-1.313694
H	-2.643090	-0.531840	-1.530652
C	-5.962488	-0.041874	-0.963467
H	-6.907455	-0.572578	-1.050771
C	-5.926262	1.256244	-0.545234
O	-4.837934	-2.011639	-1.673532
H	-3.292230	-2.679762	-2.175112
C	0.364201	0.040769	2.215442
C	-0.915943	0.520740	4.659926
C	1.106506	0.374909	3.353678
C	-1.024999	-0.081497	2.325991
C	-1.661573	0.159071	3.540552
C	0.470830	0.622110	4.566537
H	2.191097	0.423482	3.297539
H	-1.620500	-0.397067	1.471443
H	-2.739669	0.054556	3.610025
H	1.059402	0.881209	5.440669
H	-1.411871	0.708535	5.607003

Cartesian coordinates (Å) of the TS for the ring-closure process

IIa16Z-S			
H	-4.73875	0.29825	-3.07762
C	-3.95769	-0.20453	-2.50020
C	-3.45386	-1.99561	-0.84764
C	-2.40238	-1.04003	-0.23195
C	-4.57924	-1.19902	-1.51695
C	-3.15615	0.84327	-1.71532
H	-2.95735	-2.62758	-1.58782
H	-2.29128	-1.22999	0.83811
H	-2.17125	1.03781	-2.13196
H	-3.29707	-0.72782	-3.19296
H	-3.86763	-2.64165	-0.06802
H	-5.25580	-1.87518	-2.04614
H	-3.66731	1.80536	-1.64000
N	-2.95426	0.38389	-0.28324
C	-5.34397	-0.39318	-0.46003
H	-5.94814	0.35991	-0.98480
C	-4.30021	0.35748	0.39989
H	-4.58603	1.39742	0.57566
H	-4.15026	-0.12546	1.36885
C	-6.27292	-1.17145	0.43755
H	-6.69882	-0.59741	1.26161
C	-6.61452	-2.44978	0.30556
H	-7.30533	-2.91514	1.00098
H	-6.23305	-3.07916	-0.49363
C	-1.00888	-1.16958	-0.85853
O	-1.14146	-1.17401	-2.27389
C	-2.04993	1.39140	0.42006
H	-2.50904	2.36492	0.23267
H	-1.09888	1.38406	-0.11516
C	0.15675	5.09546	-0.37876
C	2.84111	4.32302	-0.15091
C	1.05451	5.88861	0.33037
C	0.60745	3.91566	-0.95888
C	1.94072	3.52873	-0.85911
C	2.39131	5.50016	0.44490
H	0.71911	6.81124	0.79485
H	3.08821	6.12329	0.99757

H	3.88322	4.02296	-0.07387
C	-0.25644	2.96900	-1.73817
O	-1.42678	3.26113	-2.05167
H	-0.29939	-1.48282	-2.64783
N	0.43198	1.84819	-1.95940
H	0.00765	1.23028	-2.65265
H	-0.88746	5.37195	-0.49319
C	2.36831	2.28031	-1.58198
H	2.59845	2.42883	-2.63852
N	3.03275	1.30952	-1.00868
C	2.72953	1.02220	0.38468
H	1.67269	0.70913	0.46898
H	2.83004	1.91938	1.01354
C	3.61413	-0.07448	0.93396
C	5.25805	-2.10862	1.94727
C	4.98212	-0.08697	0.65425
C	3.08220	-1.09637	1.72090
C	3.89426	-2.10742	2.22839
C	5.79867	-1.09592	1.15696
H	5.39499	0.68800	0.01421
H	2.01159	-1.11559	1.91743
H	3.45728	-2.90443	2.82335
H	6.85970	-1.09647	0.92417
H	5.89469	-2.90015	2.33137
H	-0.39437	-0.30599	-0.57066
H	-1.88215	-3.39775	0.66947
C	-0.85148	-3.43765	0.33317
C	-0.27830	-2.41771	-0.38810
N	1.15000	-4.77138	0.25863
C	1.09345	-2.54833	-0.77327
C	-0.09350	-4.59312	0.63678
C	1.75100	-3.76754	-0.43449
C	1.81588	-1.52984	-1.44195
H	-0.55525	-5.39987	1.20299
H	3.58429	-4.88195	-0.56439
C	3.16244	-1.69390	-1.74659
H	1.36721	-0.56021	-1.65061
C	3.78926	-2.94678	-1.46365
H	4.83729	-3.05208	-1.72549
C	3.10775	-3.94168	-0.82461
O	3.89924	-0.71845	-2.25384
H	3.54485	0.20890	-1.80639
C	-1.86602	1.13808	1.89327
C	-1.48591	0.73104	4.63822
C	-0.86480	0.27593	2.35366
C	-2.66050	1.80750	2.82809
C	-2.47570	1.60370	4.19244
C	-0.67754	0.06940	3.71687
H	-0.21748	-0.23428	1.64316
H	-3.41856	2.50732	2.48420
H	-3.09696	2.13485	4.90642
H	0.10776	-0.59818	4.05721
H	-1.33637	0.57590	5.70199

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H	1.77651	-3.56367	-2.73259
C	1.75992	-2.51763	-2.41377
C	3.04581	-0.40526	-2.21893
C	2.34375	-0.15278	-0.86157
C	3.15682	-1.90479	-2.50670
C	1.27840	-2.43617	-0.95851
H	2.45838	0.07303	-3.00714
H	2.99919	0.39641	-0.18180
H	0.26338	-2.06177	-0.86447
H	1.07118	-1.96595	-3.05616
H	4.03882	0.05446	-2.21962
H	3.58451	-2.06329	-3.50019
H	1.33231	-3.39651	-0.43961
N	2.16574	-1.50164	-0.15786
C	4.04407	-2.58283	-1.44502
H	3.90823	-3.66725	-1.53631
C	3.53644	-2.13089	-0.05955
H	3.45236	-2.97105	0.63382
H	4.19249	-1.38209	0.39140
C	5.50936	-2.28266	-1.59352
H	5.80487	-1.23737	-1.49291
C	6.43578	-3.20473	-1.83576
H	7.48279	-2.94339	-1.94945
H	6.17745	-4.25655	-1.93274
C	1.02941	0.64257	-1.00877
O	0.22849	0.11958	-2.04121
C	1.57560	-1.37449	1.24063
H	1.46945	-2.40190	1.59756
H	0.56054	-0.99377	1.13141
C	-3.74738	-3.87620	-0.54713
C	-5.37266	-1.78095	-1.45946
C	-5.02618	-4.14257	-1.02626
C	-3.28703	-2.56367	-0.54359
C	-4.08827	-1.51566	-0.98833
C	-5.83458	-3.09618	-1.47774
H	-5.40284	-5.16077	-1.04093
H	-6.83690	-3.30774	-1.83841
H	-6.00691	-0.96510	-1.79525
C	-1.97831	-2.11641	0.02701
O	-1.28582	-2.84689	0.74402
H	-0.57606	-0.28159	-1.61462
N	-1.74720	-0.82705	-0.32923
H	-1.29403	-0.32796	0.44070
H	-3.10277	-4.66368	-0.16774
C	-3.52115	-0.11638	-0.96089
H	-3.13105	0.22190	-1.92420
N	-3.99224	0.85021	-0.21205
C	-4.46903	0.52299	1.12566
H	-5.05978	-0.40369	1.14454
H	-5.11940	1.34036	1.45804
C	-3.27939	0.39075	2.06149
C	-0.87901	0.10365	3.48163
C	-2.39418	1.46883	2.18511
C	-2.96215	-0.81666	2.67844
C	-1.76511	-0.96498	3.38007
C	-1.20171	1.32743	2.88673
H	-2.63612	2.40810	1.69264
H	-3.62831	-1.66925	2.56181
H	-1.51786	-1.92501	3.82318
H	-0.51942	2.16975	2.96995
H	0.05775	-0.00901	4.02112
H	0.47769	0.58903	-0.06065
H	3.42697	2.01444	-1.56385
C	2.54577	2.64225	-1.50156
C	1.29767	2.12628	-1.24383
N	1.73943	4.90044	-1.63487
C	0.19608	3.04183	-1.16861
C	2.71768	4.03188	-1.69827
C	0.49334	4.42403	-1.36681
C	-1.13738	2.65432	-0.88293

H	3.71107	4.42297	-1.91147
H	-0.30591	6.41704	-1.42782
C	-2.15047	3.60071	-0.79058
H	-1.39427	1.60872	-0.75314
C	-1.83449	4.98023	-0.98881
H	-2.64746	5.69539	-0.91105
C	-0.56011	5.37345	-1.27098
O	-3.41778	3.31738	-0.52059
H	-3.61141	2.26829	-0.43065
C	2.40178	-0.55245	2.19587
C	3.89639	0.92990	4.04426
C	2.27518	0.84073	2.25906
C	3.27250	-1.19074	3.08304
C	4.01915	-0.45614	4.00030
C	3.02103	1.57706	3.17446
H	1.57769	1.35991	1.60569
H	3.35621	-2.27490	3.06730
H	4.68803	-0.96767	4.68499
H	2.90977	2.65593	3.21242
H	4.47361	1.50494	4.76134

I Ia20Z-S

H	-2.64239	-1.39495	3.32248
C	-2.35759	-0.56700	2.66737
C	-3.00707	1.65094	1.75164
C	-2.34326	1.22995	0.41859
C	-3.51280	0.42494	2.51725
C	-1.99394	-1.12068	1.28281
H	-2.26599	2.18271	2.35344
H	-2.84946	1.69482	-0.43288
H	-0.92091	-1.14847	1.10244
H	-1.49147	-0.06098	3.09780
H	-3.84096	2.32950	1.55080
H	-3.87896	0.72296	3.50315
H	-2.38634	-2.12701	1.11932
N	-2.61715	-0.26707	0.19728
C	-4.62501	-0.25953	1.71473
H	-4.77914	-1.26204	2.13765
C	-4.11608	-0.44064	0.26447
H	-4.34410	-1.43416	-0.12115
H	-4.54328	0.30413	-0.41475
C	-5.96550	0.43140	1.69807
H	-6.69467	-0.00253	1.01265
C	-6.32316	1.48002	2.43327
H	-7.32136	1.89866	2.35786
H	-5.64873	1.95723	3.13889
C	-0.85030	1.61610	0.34592
O	-0.18607	1.30314	1.54499
C	-2.09629	-0.69309	-1.17059
H	-1.00732	-0.68018	-1.10111
H	-2.41608	0.08775	-1.86744
C	2.81409	-3.36713	2.75965
C	4.81722	-1.41949	2.48307
C	4.02497	-3.50796	3.43097
C	2.61272	-2.24236	1.96709
C	3.60054	-1.27423	1.82048
C	5.02188	-2.53861	3.28794
H	4.20362	-4.37598	4.05827
H	5.97000	-2.66317	3.80263
H	5.59550	-0.67161	2.35988
C	1.41691	-1.99139	1.10748
O	0.58628	-2.87358	0.86219
H	0.46198	0.56759	1.36353
N	1.45410	-0.71723	0.64387
H	1.06846	-0.66300	-0.30283
H	2.02991	-4.11481	2.83330
C	3.29428	-0.07441	0.95703
H	2.99300	0.80725	1.52922
N	3.95685	0.21569	-0.14096
C	4.31518	-0.86896	-1.04116
H	4.67674	-1.75825	-0.50489
H	5.12821	-0.51774	-1.68743
C	3.10314	-1.23775	-1.88126
C	0.66821	-1.77279	-3.16461
C	2.55851	-2.51948	-1.85956
C	2.43016	-0.22585	-2.57779
C	1.22049	-0.48919	-3.21301
C	1.34460	-2.78759	-2.49230
H	3.05938	-3.30451	-1.29709
H	2.84728	0.77929	-2.58202
H	0.70515	0.30761	-3.74292
H	0.91501	-3.78401	-2.43826
H	-0.28405	-1.98045	-3.64648
H	-0.38372	1.08053	-0.49287
H	-2.70946	3.73593	0.41429
C	-1.70824	4.01593	0.10831
C	-0.68563	3.10047	0.02724
N	-0.32390	5.83919	-0.61870
C	0.60095	3.57115	-0.39396
C	-1.47927	5.37377	-0.21310
C	0.70642	4.95677	-0.72018
C	1.73797	2.73827	-0.53452
H	-2.29720	6.08761	-0.13206
H	2.00105	6.51415	-1.43664
C	2.94642	3.24876	-0.99567
H	1.68911	1.68708	-0.26977
C	3.02904	4.63586	-1.33334
H	3.98441	5.00546	-1.69259
C	1.95038	5.45747	-1.19277
O	4.04631	2.52868	-1.15146
H	3.96600	1.54173	-0.70060
C	-2.54405	-2.05066	-1.64347
C	-3.30232	-4.55657	-2.61271
C	-3.62228	-2.16951	-2.52530
C	-1.83154	-3.19289	-1.26340
C	-2.21863	-4.44133	-1.74468
C	-4.00322	-3.41846	-3.00681
H	-4.16059	-1.27908	-2.84359
H	-0.96347	-3.09807	-0.61030
H	-1.66077	-5.32444	-1.44889
H	-4.83830	-3.50116	-3.69507
H	-3.59518	-5.53089	-2.99154

I Ib1E-R (denoted as I Ib1-R in the main article)

H	3.058397	4.333447	-1.191060
C	2.003873	4.068331	-1.314879
C	-0.121797	3.560992	-0.148655
C	0.009408	2.034284	-0.255319
C	1.266252	4.185217	0.023472
C	1.865132	2.626749	-1.832310
H	-0.589446	3.949724	-1.060706
H	-0.061696	1.564218	0.733311
H	2.808561	2.231988	-2.212102
H	1.573931	4.753201	-2.050058

H	-0.783494	3.801361	0.686925
H	1.183875	5.230182	0.331726
H	1.092329	2.525582	-2.593107
N	1.446057	1.715615	-0.698094
C	2.072431	3.395256	1.073886
H	3.041246	3.890907	1.199522
C	2.342409	1.988758	0.485845
H	3.367068	1.893316	0.122123
H	2.159319	1.193258	1.213311
C	1.408367	3.335206	2.424389
C	-1.088564	1.393402	-1.128294
O	-1.038446	1.865519	-2.450216
C	1.536442	0.262632	-1.120063
H	0.923456	0.186418	-2.020376
H	1.075125	-0.322549	-0.314481
C	3.354097	-0.334900	-2.741630
C	4.605619	-0.866244	-3.043210
C	2.922151	-0.248281	-1.413681
H	6.402828	-1.747873	-2.252058
C	3.747387	-0.730987	-0.393375
C	4.996848	-1.263442	-0.694976
C	5.429885	-1.326576	-2.018614
C	-3.265129	-1.262995	-2.380843
C	-3.186218	-3.203338	-0.351807
C	-4.433129	-1.626011	-1.711295
C	-2.071706	-1.877844	-2.026614
C	-2.020345	-2.834530	-1.011936
C	-4.391297	-2.594373	-0.707225
H	-5.375502	-1.148984	-1.962974
H	-5.303117	-2.865511	-0.183390
H	-3.149077	-3.922057	0.461768
C	-0.727482	-1.550165	-2.601439
O	-0.556356	-0.616003	-3.436649
H	-0.996064	1.052560	-3.011877
N	0.168206	-2.332544	-2.042939
H	1.140881	-2.200551	-2.314848
H	-3.266677	-0.501162	-3.156434
C	-0.650603	-3.324204	-0.620333
H	-0.328734	-4.276736	-1.057693
N	-0.258588	-3.001504	0.598627
C	0.966410	-3.619998	1.064486
H	1.559753	-4.019503	0.226724
H	0.742928	-4.481332	1.716601
C	1.852375	-2.672468	1.855076
C	3.539779	-0.987051	3.350200
C	1.377237	-1.463225	2.370101
C	3.181855	-3.028159	2.109818
C	4.020313	-2.197331	2.847349
C	2.214361	-0.629049	3.115596
H	0.343002	-1.180776	2.199500
H	3.565608	-3.966290	1.714127
H	5.050838	-2.490409	3.026857
H	1.826849	0.306370	3.513281
H	4.190000	-0.335866	3.926300
H	-0.946342	0.311571	-1.126496
H	-2.978764	3.286665	-1.722239
C	-3.246856	2.674439	-0.867441
C	-2.422550	1.658891	-0.456925
N	-4.859430	2.201758	0.863078
C	-2.836558	0.840603	0.635938
C	-4.455293	2.910380	-0.167064
C	-4.073716	1.161342	1.261198
C	-2.104882	-0.286685	1.073855
H	-5.102961	3.726916	-0.481426
H	-5.460509	0.607064	2.812167
C	-2.595687	-1.108737	2.070814
H	-1.187899	-0.592971	0.581337
C	-3.810717	-0.758865	2.727491
H	-4.165483	-1.406027	3.523782
C	-4.521915	0.342507	2.334367
H	3.407769	-0.705858	0.638850
H	5.624209	-1.641013	0.106923
H	4.930091	-0.930803	-4.076785
H	2.693246	-0.003859	-5.540270
O	-1.984539	-2.241544	2.432238
H	-1.289313	-2.508957	1.703338
C	1.919956	3.889521	3.519994
H	0.458370	2.803279	2.494856
H	1.411033	3.831168	4.476776
H	2.866546	4.424511	3.494931

Iib2E-R (denoted as Iib2-R in the main article)

H	2.067401	4.495833	-2.059325
C	1.260112	3.932808	-1.583221
C	-0.125430	3.648323	0.450992
C	-0.075795	2.123323	0.207989
C	1.128782	4.323130	-0.108539
C	1.568704	2.430814	-1.678047
H	-1.000038	4.059204	-0.059002
H	-0.117713	1.574141	1.154609
H	2.621797	2.245242	-1.897104
H	0.326880	4.148777	-2.106808
H	-0.244614	3.852223	1.518393
H	1.047194	5.408295	-0.005167
H	0.954687	1.910243	-2.414411
N	1.313384	1.760897	-0.345777
C	2.379174	3.821814	0.637682
H	3.262872	4.141124	0.072632
C	2.326955	2.278840	0.648864
H	3.290623	1.843433	0.382258
H	2.026511	1.883058	1.624481
C	2.500013	4.357627	2.037129
H	1.699784	4.093341	2.729575
C	3.507007	5.118207	2.455823
H	3.549473	5.495479	3.472508
H	4.324805	5.391448	1.793291
C	-1.252510	1.629817	-0.662505
O	-1.381587	2.371236	-1.847593
C	1.444519	0.249639	-0.462574
H	0.679351	-0.077378	-1.163284
H	1.214877	-0.155101	0.528027
C	-3.289182	-0.540568	-2.412431
C	-3.235752	-2.938569	-0.952768
C	-4.446416	-1.010727	-1.792333
C	-2.118037	-1.278871	-2.299031
C	-2.079018	-2.463952	-1.558606
C	-4.418852	-2.206277	-1.074483
H	-5.368727	-0.441718	-1.860093
H	-5.322027	-2.562528	-0.587950
H	-3.208316	-3.842796	-0.351575
C	-0.785803	-0.889200	-2.870492
O	-0.556065	0.270431	-3.326589
H	-1.218776	1.717596	-2.572628
N	0.044592	-1.897497	-2.734100
H	1.013446	-1.718533	-2.988264

H	-3.284864	0.397097	-2.962524
C	-0.717831	-3.080575	-1.374953
H	-0.487955	-3.969096	-1.976006
N	-0.159855	-2.915862	-0.192728
C	1.132376	-3.559916	-0.061601
H	1.775770	-3.279059	-0.915660
H	1.051893	-4.660781	-0.099234
C	1.885142	-3.167291	1.193427
C	3.434189	-2.390849	3.411273
C	1.391390	-2.248460	2.121108
C	3.160575	-3.704189	1.404548
C	3.930695	-3.322351	2.497033
C	2.161053	-1.862186	3.221313
H	0.401067	-1.827093	1.985838
H	3.560213	-4.417656	0.686447
H	4.920364	-3.748029	2.635841
H	1.758549	-1.145070	3.931321
H	4.032486	-2.089283	4.265625
H	-1.095447	0.581719	-0.913213
H	-3.214443	3.544131	-0.610458
C	-3.385757	2.741434	0.099168
C	-2.512006	1.687990	0.181630
N	-4.835401	1.812594	1.787704
C	-2.821303	0.615090	1.071250
C	-4.529338	2.763178	0.935076
C	-4.008046	0.730273	1.847969
C	-2.051215	-0.568530	1.148479
H	-5.210330	3.610953	0.884244
H	-5.271328	-0.239346	3.295888
C	-2.474813	-1.635527	1.916288
H	-1.174430	-0.720224	0.527517
C	-3.633786	-1.502172	2.730628
H	-3.928151	-2.346591	3.346200
C	-4.370549	-0.349033	2.699504
O	-1.848484	-2.821874	1.905794
H	-1.189407	-2.846915	1.125534
C	2.784732	-0.245347	-0.940462
C	5.218361	-1.285815	-1.846396
C	3.062071	-0.310264	-2.312285
C	3.732106	-0.720481	-0.030291
C	4.944530	-1.237703	-0.482389
C	4.274468	-0.822224	-2.762964
H	2.317274	0.038291	-3.025947
H	3.511476	-0.713862	1.035637
H	5.665025	-1.616529	0.235763
H	4.478556	-0.867950	-3.827860
H	6.161144	-1.692724	-2.198495

I Ib10Z-S

H	-3.07976	-4.16172	1.69453
C	-3.07950	-3.10418	1.41593
C	-4.05077	-1.36840	-0.06358
C	-2.65246	-0.71606	-0.13227
C	-3.93032	-2.87802	0.16248
C	-1.63734	-2.65517	1.13146
H	-4.60009	-0.93406	0.77390
H	-2.49663	-0.21749	-1.09492
H	-1.21533	-2.03654	1.92590
H	-3.48333	-2.52227	2.24672
H	-4.61298	-1.14501	-0.97427
H	-4.92330	-3.31750	0.28878
H	-0.97008	-3.50048	0.94699
N	-1.59526	-1.83489	-0.14063
C	-3.21686	-3.54151	-1.03070
H	-2.94416	-4.56282	-0.73833
C	-1.92431	-2.74224	-1.30142
C	-1.06847	-3.40225	-1.44858
H	-2.01774	-2.09546	-2.18016
C	-4.05940	-3.62094	-2.27304
H	-4.41516	-2.67384	-2.68070
C	-4.38168	-4.75871	-2.88030
H	-5.00145	-4.77166	-3.77083
H	-4.03659	-5.71918	-2.50508
C	-2.42840	0.33496	0.97622
O	-2.78706	-0.16671	2.23679
C	-0.22370	-1.22211	-0.34093
H	-0.05860	-0.57095	0.51713
H	-0.30071	-0.60854	-1.24385
C	2.73191	-0.68452	3.32737
C	4.20844	1.13239	1.77838
C	4.11624	-0.81289	3.22601
C	2.10298	0.35446	2.65362
C	2.82942	1.27171	1.89384
C	4.84688	0.08865	2.45080
H	4.62849	-1.61570	3.74804
H	5.92344	-0.02411	2.36366
H	4.77641	1.81959	1.15734
C	0.62574	0.61201	2.62624
O	-0.20587	-0.25309	3.02892
H	-1.95016	-0.13900	2.76612
N	0.43102	1.78725	2.07468
H	-0.51809	2.13893	1.97808
H	2.13512	-1.37464	3.91807
C	2.04498	2.35099	1.17913
H	2.06495	3.33371	1.64996
N	1.96092	2.36916	-0.13838
C	2.07990	1.09967	-0.84059
H	1.31027	1.08802	-1.63118
H	1.88350	0.24327	-0.18341
C	3.43018	0.88289	-1.49080
C	5.91272	0.46315	-2.71428
C	4.14967	-0.28697	-1.24815
C	3.96714	1.84701	-2.34724
C	5.20136	1.63873	-2.95592
C	5.38483	-0.49950	-1.85773
H	3.74420	-1.02567	-0.55804
H	3.40882	2.76296	-2.52711
H	5.61046	2.39322	-3.62163
H	5.93559	-1.41437	-1.65666
H	6.87635	0.30288	-3.18890
H	-1.37560	0.61110	0.98864
H	-4.93306	1.03786	1.75493
C	-4.50103	1.74971	1.05931
C	-3.21690	1.57863	0.60376
N	-4.78146	3.79488	-0.17285
C	-2.64082	2.59136	-0.22579
C	-5.24834	2.87181	0.63598
C	-3.49064	3.67944	-0.58647
C	-1.28455	2.60253	-0.64795
H	-6.27284	2.99716	0.98189
H	-3.62820	5.52802	-1.67452
C	-0.75982	3.67927	-1.35092
H	-0.60054	1.80956	-0.36203
C	-1.64253	4.72715	-1.76123
H	-1.21789	5.54019	-2.34198

C	-2.95707	4.72173	-1.39498
O	0.52455	3.79798	-1.66177
H	1.15004	3.25495	-0.96578
C	0.92312	-2.19341	-0.43444
C	3.16277	-3.85556	-0.56396
C	1.40998	-2.62277	-1.67155
C	1.58058	-2.58184	0.73680
C	2.69622	-3.41105	0.67260
C	2.52216	-3.45812	-1.73575
H	0.93203	-2.28393	-2.58823
H	1.22807	-2.20204	1.69376
H	3.21087	-3.69171	1.58628
H	2.89999	-3.78046	-2.70054
H	4.03788	-4.49591	-0.61498

IIb11E-S

H	2.02873	-4.16648	0.05783
C	1.79300	-3.15670	-0.29121
C	2.44739	-1.30928	-1.82910
C	2.06584	-0.31995	-0.70090
C	2.88217	-2.65547	-1.24176
C	1.70376	-2.21049	0.91594
H	1.57697	-1.45490	-2.47320
H	2.68162	0.57844	-0.74128
H	2.15664	-2.62730	1.81941
H	0.82817	-3.18116	-0.80204
H	3.24650	-0.88748	-2.44636
H	3.05501	-3.37700	-2.04465
H	0.68216	-1.93200	1.16207
N	2.47147	-0.93400	0.63727
C	4.17193	-2.47353	-0.41917
C	4.32529	-3.38288	0.17461
C	3.93925	-1.28512	0.53604
H	4.28186	-1.50889	1.54925
H	4.45064	-0.38214	0.19326
C	5.40151	-2.24800	-1.25375
H	5.40827	-1.35433	-1.87905
C	6.45008	-3.06502	-1.26872
H	7.31246	-2.87071	-1.89807
H	6.48033	-3.96084	-0.65307
C	0.58369	0.10626	-0.78506
O	-0.23168	-1.01623	-1.04351
C	2.27406	0.03395	1.79824
H	2.61477	-0.50941	2.68311
H	1.20178	0.16785	1.91580
C	2.31599	2.45240	1.08988
C	2.96160	3.67811	0.95512
C	2.98336	1.35477	1.64529
C	4.77820	4.78218	1.28778
C	4.29560	1.52083	2.09988
C	4.94094	2.74685	1.96986
C	4.27650	3.82510	1.38972
C	-3.46966	2.05228	2.06529
C	-0.92608	1.73756	3.24026
C	-2.80531	3.13678	2.63946
C	-2.84734	0.80853	2.07493
C	-1.58027	0.66852	2.63966
C	-1.54749	2.98409	3.22968
H	-3.27559	4.11556	2.63066
H	-1.05424	3.84195	3.67654
H	0.05070	1.59129	3.69516
C	-3.43114	-0.46534	1.53427
H	-0.87243	-1.12512	-0.30218
H	-4.44170	2.17318	1.59847
C	-1.05696	-0.72125	2.48567
H	0.26479	0.56244	0.16416
H	2.44529	1.21150	-2.59587
C	1.44206	1.61464	-2.66754
C	0.40970	1.17208	-1.87156
N	0.06927	3.21071	-3.82309
C	-0.87963	1.76761	-2.06867
C	1.22614	2.62818	-3.62894
C	-0.97618	2.79376	-3.05972
C	-2.03343	1.40356	-1.33712
H	2.05723	2.96042	-4.24858
H	-2.27380	4.20667	-4.02647
C	-3.25999	2.01089	-1.58740
H	-1.99342	0.61547	-0.59449
C	-3.33449	3.05003	-2.56613
H	-4.30257	3.51402	-2.72868
C	-2.23134	3.42550	-3.27359
H	4.81286	0.68891	2.57192
H	5.95807	2.86172	2.33039
H	2.43206	4.51763	0.51668
H	1.28017	2.36057	0.77079
O	-4.38164	1.67988	-0.97150
H	-4.23896	0.77782	-0.37695
N	-4.12593	-0.40402	0.41202
H	-3.79301	-1.15455	2.31435
C	-4.83235	-1.61755	0.04530
H	-5.44981	-1.39568	-0.83287
H	-5.51221	-1.94930	0.84880
C	-3.86535	-2.74479	-0.26566
C	-1.89450	-4.69633	-0.69059
C	-2.91005	-2.58231	-1.27409
C	-3.82390	-3.89721	0.51904
C	-2.84477	-4.86994	0.31229
C	-1.93443	-3.55055	-1.48793
H	-2.90849	-1.66784	-1.86406
H	-4.55517	-4.02611	1.31394
H	-2.82330	-5.75808	0.93728
H	-1.19335	-3.40017	-2.26793
H	-1.12829	-5.44922	-0.85322
O	-0.13098	-1.18628	3.16318
N	-1.75825	-1.31655	1.48965
H	-1.71510	-2.33862	1.51708

IIb13Z-R

H	-5.33446	-0.58752	-2.17444
C	-4.37379	-0.98644	-1.83645
C	-3.23086	-2.75832	-0.52861
C	-2.20540	-1.69219	-0.08544
C	-4.58740	-2.11107	-0.81908
C	-3.56105	0.13958	-1.17912
H	-2.86287	-3.23586	-1.43977
H	-1.80811	-1.91246	0.91177
H	-2.74192	0.49787	-1.80445
H	-3.82801	-1.36946	-2.70011
H	-3.31882	-3.53567	0.23528
H	-5.28320	-2.85717	-1.21190
H	-4.18759	0.98747	-0.89356
N	-2.94650	-0.35445	0.11415
C	-5.16555	-1.49044	0.46711
H	-6.00802	-0.84788	0.18397

C	-4.06201	-0.61339	1.09707
H	-4.45113	0.35724	1.40797
H	-3.59944	-1.09727	1.96354
C	-5.66624	-2.50441	1.45771
C	-4.92994	-3.20676	1.85054
C	-6.93040	-2.58287	1.86142
H	-7.25713	-3.33840	2.56847
H	-7.68574	-1.89251	1.49349
C	-1.00704	-1.58868	-1.04800
O	-1.42292	-1.46881	-2.38500
C	-1.99050	0.67734	0.68739
H	-1.17778	0.76139	-0.03329
H	-1.60883	0.24306	1.61716
C	0.20465	3.93489	-2.08287
C	1.83971	4.27996	0.16521
C	0.54498	5.21576	-1.65061
C	0.69263	2.82817	-1.40021
C	1.49849	3.00037	-0.26890
C	1.36365	5.38754	-0.53504
H	0.17986	6.08491	-2.18958
H	1.62580	6.38685	-0.20248
H	2.44814	4.40927	1.05656
C	0.45348	1.40566	-1.82432
O	-0.59904	1.11363	-2.47781
H	-1.07689	-0.58733	-2.67807
N	1.41763	0.63970	-1.37377
H	1.28835	-0.34704	-1.60490
H	-0.42368	3.77802	-2.95524
C	1.82953	1.79469	0.52870
H	0.99601	1.27111	0.99283
N	2.97181	1.49753	1.05078
C	4.25701	1.95108	0.53345
H	4.71467	2.64441	1.24730
H	4.07750	2.49626	-0.40014
C	5.16995	0.76585	0.30214
C	6.85820	-1.41470	-0.14293
C	6.53367	0.86502	0.57559
C	4.65339	-0.43214	-0.19638
C	5.49466	-1.52045	-0.40926
C	7.37775	-0.21860	0.34665
H	6.93639	1.79267	0.97554
H	3.58896	-0.51180	-0.40833
H	5.07834	-2.45316	-0.77775
H	8.43826	-0.13223	0.56353
H	7.51371	-2.26399	-0.31068
H	-0.42528	-0.71105	-0.77727
H	-0.88559	-3.91562	-2.46214
C	-0.17721	-3.89041	-1.64006
C	-0.09488	-2.78188	-0.83275
N	1.63611	-4.98153	-0.49784
C	0.91098	-2.73752	0.18355
C	0.69979	-4.97580	-1.42204
C	1.76449	-3.87881	0.28339
C	1.14205	-1.62596	1.02557
H	0.62633	-5.86323	-2.04824
H	3.46581	-4.72043	1.29354
C	2.23113	-1.55365	1.90719
H	0.50253	-0.75157	0.96780
C	3.05912	-2.73708	1.99793
H	3.89610	-2.69683	2.68964
C	2.82891	-3.84209	1.23200
O	2.51662	-0.49726	2.59823
H	2.91548	0.64688	1.75153
C	-2.56899	2.04956	0.91011
C	-3.50295	4.65032	1.30478
C	-3.09080	2.42905	2.14936
C	-2.50018	2.98726	-0.12494
C	-2.96602	4.28295	0.07242
C	-3.56301	3.72424	2.34389
H	-3.11134	1.71554	2.97018
H	-2.06059	2.69442	-1.07703
H	-2.89387	5.00804	-0.73232
H	-3.96391	4.01362	3.31002
H	-3.86270	5.66259	1.46062

I Ib15E-S

H	-3.70549	-0.34786	-3.42299
C	-2.77161	-0.69549	-2.96860
C	-1.72642	-2.45843	-1.56063
C	-1.69754	-1.59477	-0.28363
C	-2.95029	-2.10842	-2.40503
C	-2.33276	0.24819	-1.83734
H	-0.61172	-2.27678	-2.12875
H	-2.18038	-2.10783	0.55131
H	-2.85366	1.20561	-1.85625
H	-2.00365	-0.69067	-3.74652
H	-1.74302	-3.51334	-1.27860
H	-3.07588	-2.83386	-3.21383
H	-1.26196	0.44596	-1.84438
N	-2.63501	-0.39418	-0.50095
C	-4.19226	-2.11543	-1.49253
H	-5.07152	-1.92442	-2.12095
C	-4.05051	-0.92852	-0.52718
H	-4.67905	-0.09026	-0.82991
H	-4.31375	-1.18407	0.50063
C	-4.38539	-3.46932	-0.85338
H	-4.52463	-4.26904	-1.58161
C	-4.38977	-3.78802	0.43853
H	-4.53488	-4.81582	0.75416
H	-4.26469	-3.06080	1.23681
C	-0.24687	-1.24433	0.13162
O	0.51830	-0.95277	-1.01612
C	-2.49704	0.60984	0.63908
H	-1.57700	1.15980	0.44344
H	-2.38270	0.00753	1.54566
C	-0.15532	3.18871	1.80608
C	2.61025	2.94136	2.27880
C	0.36688	3.42786	3.07563
C	0.71493	2.81010	0.79051
C	2.08965	2.71816	1.00865
C	1.73748	3.29116	3.30947
H	-0.29220	3.71268	3.89011
H	2.13042	3.46415	4.30686
H	3.67558	2.83105	2.45571
C	0.33790	2.43200	-0.60633
O	-0.76998	2.68317	-1.10978
H	0.95024	-0.06812	-0.94051
N	1.37612	1.77646	-1.15510
H	1.34081	1.71705	-2.17536
H	-1.22002	3.28315	1.60300
C	2.90934	2.39398	-0.20386
H	3.02563	3.22940	-0.91040
N	3.92080	1.56523	-0.06592
C	4.78997	1.42694	-1.22151
H	5.64639	0.81078	-0.92356

H	5.18642	2.40363	-1.54541
C	4.06311	0.78394	-2.38812
C	2.52643	-0.34104	-4.44605
C	3.44715	-0.45990	-2.21699
C	3.89933	1.45446	-3.59953
C	3.13709	0.89690	-4.62716
C	2.68588	-1.01932	-3.23679
H	3.53551	-0.96935	-1.25917
H	4.36058	2.43034	-3.73556
H	3.01611	1.43322	-5.56410
H	2.19940	-1.97650	-3.07702
H	1.92801	-0.77569	-5.24162
H	-0.24360	-0.37976	0.80939
H	-1.24079	-3.83212	0.71650
C	-0.25675	-3.61305	1.11697
C	0.37288	-2.40536	0.91677
N	1.53838	-4.49938	2.44331
C	1.66830	-2.22567	1.50720
C	0.36555	-4.63073	1.87544
C	2.18531	-3.31540	2.27415
C	2.43105	-1.03706	1.40073
H	-0.14533	-5.58222	2.01281
H	3.80804	-4.01401	3.49421
C	3.67204	-0.92213	2.02120
H	2.07525	-0.19297	0.81873
C	4.16343	-2.01759	2.79768
H	5.13144	-1.89617	3.27383
C	3.44586	-3.16987	2.91542
O	4.43944	0.15025	1.93766
H	4.15322	0.77194	1.08421
C	-3.64900	1.57348	0.78743
C	-5.76736	3.37358	1.09877
C	-4.69769	1.29012	1.66947
C	-3.65272	2.78532	0.08806
C	-4.71348	3.67588	0.24119
C	-5.75425	2.18174	1.82136
H	-4.68208	0.37219	2.25304
H	-2.79998	3.03860	-0.53732
H	-4.70599	4.61510	-0.30277
H	-6.56080	1.95153	2.51021
H	-6.58919	4.07252	1.21920

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H	1.76837	-3.78158	-2.14127
C	1.88619	-2.72100	-1.90189
C	3.37117	-0.73394	-2.03843
C	2.88682	-0.33025	-0.62440
C	3.30632	-2.25213	-2.22420
C	1.61988	-2.50438	-0.40579
H	2.72567	-0.25044	-2.77628
H	3.67043	0.19443	-0.07364
H	0.66338	-2.02774	-0.21001
H	1.16470	-2.14741	-2.48674
H	4.39124	-0.37454	-2.20369
H	3.57494	-2.51498	-3.25072
H	1.66237	-3.43179	0.17158
N	2.68502	-1.60947	0.19708
C	4.26994	-2.94365	-1.24074
H	4.03222	-4.01418	-1.23155
C	3.99691	-2.35972	0.16199
H	3.93406	-3.14521	0.91837
H	4.77078	-1.65054	0.46728
C	5.72134	-2.79107	-1.60106
H	6.11115	-1.77263	-1.62690
C	6.52833	-3.80935	-1.88203
H	7.56829	-3.65308	-2.14949
H	6.17472	-4.83733	-1.85758
C	1.63990	0.57368	-0.66307
O	0.67726	0.06995	-1.55899
C	2.29546	-1.34014	1.64713
H	2.24550	-2.32899	2.11043
H	1.27328	-0.95931	1.63126
C	-3.17907	-3.48726	-0.01623
C	-4.44813	-1.40491	-1.40864
C	-4.31616	-3.74377	-0.77587
C	-2.68538	-2.18790	0.03453
C	-3.31896	-1.14392	-0.63556
C	-4.94156	-2.70584	-1.47302
H	-4.72132	-4.74979	-0.82895
H	-5.83359	-2.91197	-2.05698
H	-4.95975	-0.59375	-1.91867
C	-1.49111	-1.74761	0.82100
O	-0.92175	-2.45103	1.66066
H	-0.09579	-0.20916	-1.00092
N	-1.16891	-0.48638	0.43616
H	-0.73354	0.04607	1.19201
H	-2.67085	-4.27130	0.53769
C	-2.73784	0.24443	-0.47468
H	-2.19622	0.60416	-1.35453
N	-3.30620	1.20244	0.22444
C	-4.09826	0.81100	1.38320
H	-4.18404	1.69592	2.02623
H	-3.57977	0.03983	1.97607
C	-5.48913	0.31513	1.03497
C	-8.02849	-0.61114	0.29457
C	-6.29089	1.05981	0.16548
C	-5.97852	-0.88965	1.53735
C	-7.23997	-1.35368	1.16908
C	-7.55105	0.60169	-0.20375
H	-5.90257	1.99123	-0.23901
H	-5.35029	-1.48784	2.19399
H	-7.60041	-2.30298	1.55493
H	-8.16249	1.18828	-0.88368
H	-9.00911	-0.97340	0.00022
H	1.19992	0.60223	0.34077
H	4.06562	1.70365	-1.54162
C	3.25382	2.41047	-1.41129
C	2.00122	2.01651	-1.00300
N	2.63339	4.72770	-1.54849
C	0.99475	3.02864	-0.86096
C	3.52179	3.77320	-1.67855
C	1.38494	4.37204	-1.14297
C	-0.33318	2.76855	-0.44282
H	4.51700	4.06783	-2.00660
H	0.74874	6.42318	-1.20437
C	-1.26414	3.79352	-0.31590
H	-0.65402	1.75437	-0.24559
C	-0.84964	5.13569	-0.58824
H	-1.59209	5.91923	-0.47371
C	0.42461	5.40990	-0.98799
O	-2.52613	3.61910	0.03725
H	-2.81465	2.58366	0.11510
C	3.24628	-0.43983	2.39356
C	5.01759	1.20852	3.80562
C	4.33448	-0.98692	3.08148

C	3.04256	0.94359	2.44566
C	3.92569	1.76286	3.14256
C	5.21798	-0.16946	3.77943
H	4.48459	-2.06392	3.08401
H	2.18482	1.39463	1.95354
H	3.75303	2.83364	3.17135
H	6.05550	-0.61081	4.31002
H	5.70325	1.84774	4.35272

IIb18Z-R

H	-4.31807	-0.66749	2.99844
C	-3.34584	-0.86790	2.53702
C	-1.10946	0.04225	2.01470
C	-1.41852	0.41939	0.55155
C	-2.34786	0.23735	2.89023
C	-3.47904	-0.93997	1.00679
H	-0.78050	-0.99890	2.07818
H	-1.21172	1.48021	0.36366
H	-2.89899	-1.75676	0.57387
H	-2.99443	-1.83339	2.90972
H	-0.28497	0.65688	2.38616
H	-2.07746	0.19529	3.94792
H	-4.51911	-1.03789	0.69515
N	-2.95233	0.33023	0.37842
C	-2.99576	1.59574	2.57224
H	-3.85520	1.72826	3.23936
C	-3.53581	1.51150	1.12634
H	-4.61867	1.37800	1.10828
H	-3.28636	2.40344	0.54566
C	-2.06309	2.76016	2.78108
H	-1.20497	2.84501	2.11209
C	-2.23028	3.66960	3.73606
H	-1.52885	4.48653	3.86905
H	-3.07397	3.62636	4.42116
C	-0.49432	-0.30575	-0.47151
O	-0.72300	0.14014	-1.78693
C	-3.36443	0.41978	-1.08578
H	-2.96318	-0.47051	-1.56433
H	-2.82377	1.27604	-1.49009
C	3.07301	3.99732	-1.74414
C	5.22575	3.25369	-0.10080
C	4.33378	4.55736	-1.94406
C	2.90488	3.07962	-0.71670
C	3.96892	2.69468	0.10242
C	5.40025	4.18940	-1.12253
H	4.48842	5.28244	-2.73719
H	6.37974	4.62993	-1.28370
H	6.06484	2.95074	0.51996
C	1.61262	2.42396	-0.32857
O	0.56652	2.48397	-1.02342
H	-0.26800	1.01196	-1.82072
N	1.82876	1.81609	0.82177
H	1.07607	1.27998	1.23371
H	2.22219	4.26680	-2.36314
C	3.66148	1.62638	1.13712
H	3.58778	1.99310	2.16265
N	4.16174	0.39951	1.03564
C	4.70410	-0.06784	-0.23925
H	5.62552	-0.61872	-0.00814
H	4.99334	0.77057	-0.88528
C	3.81060	-0.99741	-1.03938
C	2.16515	-2.74629	-2.49470
C	4.00242	-2.37834	-0.97832
C	2.78015	-0.50218	-1.84478
C	1.96755	-1.36840	-2.57236
C	3.18292	-3.25095	-1.69097
H	4.78828	-2.77320	-0.33735
H	2.62142	0.57333	-1.91607
H	1.16136	-0.96835	-3.17924
H	3.33457	-4.32389	-1.61136
H	1.51752	-3.42199	-3.04674
H	0.49002	0.05824	-0.17053
H	-1.91892	-2.20658	-1.87467
C	-1.22300	-2.62817	-1.15492
C	-0.41998	-1.81746	-0.38952
N	-0.27626	-4.64060	-0.23508
C	0.57380	-2.43818	0.43715
C	-1.11813	-4.03426	-1.03958
C	0.57678	-3.86434	0.48709
C	1.57566	-1.72918	1.14328
H	-1.76676	-4.67083	-1.63919
H	1.51409	-5.60018	1.33993
C	2.58097	-2.38403	1.83437
H	1.67084	-0.65432	1.06333
C	2.51721	-3.80626	1.95079
H	3.29019	-4.30346	2.52908
C	1.54918	-4.51578	1.29674
O	3.61901	-1.75289	2.37293
H	3.79351	-0.80521	1.91015
C	-4.84786	0.53949	-1.32465
C	-7.58510	0.76128	-1.86876
C	-5.45365	1.79618	-1.42069
C	-5.62496	-0.60289	-1.53920
C	-6.98751	-0.49464	-1.80331
C	-6.81507	1.90756	-1.68393
H	-4.85312	2.69500	-1.30227
H	-5.15595	-1.58427	-1.51515
H	-7.57737	-1.39019	-1.97013
H	-7.27163	2.88927	-1.75792
H	-8.64631	0.84780	-2.07940

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H	4.61599	-0.79998	-3.18964
C	3.88092	-0.20562	-2.63965
C	3.42625	1.91783	-1.45299
C	2.56239	1.12410	-0.44547
C	4.53649	1.03806	-2.03272
C	3.27974	-1.05540	-1.51025
H	2.79482	2.24695	-2.27861
H	2.60627	1.57848	0.54996
H	3.89642	-1.92525	-1.27335
H	3.08899	0.09549	-3.32838
H	3.83329	2.81317	-0.97557
H	5.08844	1.59201	-2.79682
H	2.26220	-1.39142	-1.71298
N	3.22679	-0.24794	-0.23002
C	5.49995	0.58850	-0.92002
H	6.13723	-0.20922	-1.32092
C	4.64124	0.01368	0.22664
H	5.04225	-0.93291	0.58952
H	4.56704	0.70814	1.07018
C	6.39232	1.68780	-0.41459
H	5.89704	2.53769	0.05668
C	7.71765	1.67348	-0.51626

H	8.32517	2.49535	-0.15177
H	8.24190	0.83781	-0.97383
C	1.06716	1.06429	-0.85656
O	0.92755	0.65662	-2.19509
C	2.46294	-1.01003	0.83507
H	1.47559	-1.14786	0.40245
H	2.41696	-0.34685	1.70560
C	-2.61551	-2.73952	-2.10649
C	-4.54619	-2.59831	-0.07521
C	-3.92615	-3.14291	-2.35494
C	-2.28687	-2.26860	-0.84226
C	-3.24642	-2.16760	0.16720
C	-4.88061	-3.08486	-1.33865
H	-4.20479	-3.51268	-3.33724
H	-5.90018	-3.40203	-1.53666
H	-5.30350	-2.51374	0.69874
C	-0.91086	-1.87963	-0.39194
O	0.05941	-1.74941	-1.20086
H	0.45063	-0.20169	-2.14921
N	-0.94160	-1.73948	0.91328
H	-0.11158	-1.42285	1.40334
H	-1.84517	-2.79870	-2.87010
C	-2.80365	-1.52505	1.46546
H	-2.71569	-2.19683	2.31978
N	-3.08932	-0.27400	1.76644
C	-3.34828	0.64162	0.65419
H	-2.55390	0.58295	-0.10960
H	-3.29755	1.65938	1.06078
C	-4.69817	0.47260	-0.01572
C	-7.19936	0.11686	-1.23005
C	-4.81229	0.42460	-1.40426
C	-5.85429	0.35751	0.76061
C	-7.09614	0.17845	0.15981
C	-6.05372	0.24543	-2.01073
H	-3.91321	0.48766	-2.01369
H	-5.76273	0.38084	1.84356
H	-7.98695	0.08500	0.77495
H	-6.12341	0.19112	-3.09359
H	-8.16781	-0.02918	-1.69953
H	0.53837	0.35811	-0.21769
H	0.98151	3.22945	-2.53354
C	0.59530	3.44322	-1.54286
C	0.48637	2.44672	-0.60388
N	-0.29038	5.10869	-0.04874
C	-0.15396	2.75531	0.63779
C	0.19885	4.76069	-1.21554
C	-0.49905	4.12095	0.86452
C	-0.53881	1.78434	1.59716
H	0.31572	5.55268	-1.95307
H	-1.35790	5.52149	2.24971
C	-1.29728	2.12998	2.70243
H	-0.38611	0.72599	1.41812
C	-1.52706	3.51115	2.97834
H	-2.07768	3.76319	3.87916
C	-1.13869	4.47096	2.08607
O	-1.87011	1.21626	3.49383
H	-2.34247	0.49077	2.87846
C	3.00998	-2.36621	1.19152
C	3.90861	-4.91996	1.87210
C	2.51013	-3.48889	0.52336
C	3.93787	-2.53515	2.22305
C	4.39080	-3.80752	2.55856
C	2.96476	-4.76074	0.85949
H	1.75086	-3.35200	-0.24526
H	4.29395	-1.66899	2.77663
H	5.11030	-3.93120	3.36149
H	2.57097	-5.62869	0.34040
H	4.25736	-5.91299	2.13786

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H	5.16209	1.67742	2.12670
C	4.44505	0.85184	2.17657
C	3.70730	-1.27931	1.15245
C	2.47383	-0.68349	0.45026
C	4.84192	-0.25463	1.19511
C	3.02845	1.34322	1.83190
H	3.43386	-1.54987	2.17695
H	2.46447	-0.93412	-0.61787
H	2.27329	0.95228	2.51206
H	4.44995	0.47004	3.20070
H	4.00514	-2.19416	0.63551
H	5.77506	-0.73081	1.50685
H	2.96381	2.43170	1.79826
N	2.63376	0.85114	0.45516
C	5.02943	0.38055	-0.19496
H	5.86220	1.09040	-0.13540
C	3.74501	1.18435	-0.51025
H	3.91143	2.25941	-0.42381
H	3.36635	0.96960	-1.51380
C	5.35362	-0.62833	-1.26417
H	4.56865	-1.33614	-1.53381
C	6.53209	-0.70267	-1.87475
H	6.73313	-1.45535	-2.62999
H	7.33857	-0.01234	-1.63844
C	1.14838	-1.20041	1.05857
O	1.10941	-0.93974	2.44174
C	1.33642	1.50937	0.02667
H	0.61217	1.25448	0.80600
H	1.06119	1.02903	-0.92104
C	-3.74913	0.32079	3.20286
C	-5.29062	-0.93181	1.22144
C	-5.08104	-0.01149	3.45440
C	-3.20670	0.03973	1.95798
C	-3.96771	-0.59135	0.96397
C	-5.84742	-0.62689	2.46605
H	-5.52444	0.21207	4.42014
H	-6.88389	-0.88098	2.66752
H	-5.87629	-1.44016	0.45988
C	-1.83089	0.44059	1.50713
O	-0.93919	0.87096	2.30535
H	0.32038	-0.36156	2.59050
N	-1.77395	0.25859	0.21449
H	-0.96261	0.59686	-0.28991
H	-3.13188	0.80770	3.95237
C	-3.22821	-1.02551	-0.27695
H	-2.59294	-1.89030	-0.06982
N	-3.59854	-0.93606	-1.52614
C	-4.35959	0.24569	-1.91667
H	-5.20721	0.43302	-1.24262
H	-4.76860	0.06802	-2.91769
C	-3.45404	1.46343	-1.92201
C	-1.60648	3.56257	-1.72201
C	-3.69426	2.54165	-1.07399
C	-2.28319	1.45252	-2.68817
C	-1.36464	2.49313	-2.58729

C	-2.77796	3.58713	-0.97203
H	-4.58964	2.54290	-0.45635
H	-2.07439	0.59564	-3.32637
H	-0.45453	2.47480	-3.18304
H	-2.96907	4.41148	-0.29063
H	-0.88265	4.36822	-1.63179
H	0.30556	-0.71188	0.57486
H	2.04082	-3.29032	2.53679
C	1.60739	-3.60884	1.59456
C	1.05153	-2.68633	0.74272
N	1.08364	-5.44660	0.13407
C	0.39848	-3.15806	-0.44062
C	1.60629	-4.97780	1.24278
C	0.46207	-4.56163	-0.69302
C	-0.35717	-2.34108	-1.32334
H	2.06762	-5.70348	1.91036
H	-0.09815	-6.14761	-2.02866
C	-1.08753	-2.88738	-2.36543
H	-0.46910	-1.27771	-1.14687
C	-0.93935	-4.27637	-2.65550
H	-1.48251	-4.67477	-3.50686
C	-0.18640	-5.08094	-1.84727
O	-1.94026	-2.17109	-3.11065
H	-2.60510	-1.61955	-2.49376
C	1.36553	3.00904	-0.11071
C	1.24377	5.79309	-0.32466
C	1.86970	3.65245	-1.24554
C	0.76593	3.76884	0.89773
C	0.70873	5.15644	0.79265
C	1.81858	5.03926	-1.34755
H	2.28534	3.07023	-2.06451
H	0.31114	3.25594	1.74326
H	0.23481	5.73690	1.57774
H	2.21207	5.52996	-2.23208
H	1.19693	6.87431	-0.40935

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H	5.04911	1.21546	2.36292
C	4.04192	1.35532	1.95778
C	1.72658	0.49687	1.90548
C	1.85833	-0.24694	0.56358
C	3.04606	0.44088	2.67483
C	4.01626	1.03352	0.45363
H	1.44759	1.54170	1.73919
H	1.58175	-1.30244	0.66970
H	3.43758	1.75866	-0.12057
H	3.76981	2.40405	2.10227
H	0.92346	0.04482	2.49318
H	2.90019	0.75926	3.70983
H	5.02134	0.97068	0.03661
N	3.36234	-0.30964	0.22228
C	3.59903	-0.99536	2.64649
H	4.51978	-1.01624	3.24023
C	3.97709	-1.30814	1.18112
H	5.05577	-1.25930	1.02078
H	3.62449	-2.29533	0.87060
C	2.64559	-2.00593	3.23130
H	1.75097	-2.24815	2.65446
C	2.83987	-2.59558	4.40677
H	2.12544	-3.30473	4.81138
H	3.72229	-2.38571	5.00725
C	0.84393	0.26478	-0.50161
O	0.86015	-0.51024	-1.67458
C	3.58820	-0.79670	-1.20235
H	3.11827	-0.06291	-1.85113
H	3.01073	-1.71866	-1.28958
C	-2.94898	-3.63795	-0.78656
C	-5.05404	-2.36149	0.56057
C	-4.26558	-4.04052	-1.00177
C	-2.70190	-2.60231	0.10465
C	-3.74223	-1.94773	0.76579
C	-5.30939	-3.41090	-0.32204
H	-4.48123	-4.84959	-1.69332
H	-6.33385	-3.72802	-0.49318
H	-5.87340	-1.84999	1.05731
C	-1.34490	-2.10573	0.50313
O	-0.28556	-2.45466	-0.08629
H	0.41072	-1.34569	-1.41320
N	-1.50518	-1.29355	1.52913
H	-0.67252	-0.84884	1.90335
H	-2.11400	-4.12076	-1.28586
C	-3.36502	-0.77289	1.64678
C	-3.44519	-0.95029	2.71961
N	-3.58721	0.47504	1.27391
C	-3.61344	0.74367	-0.16287
H	-2.77739	0.24905	-0.68624
H	-3.45074	1.82185	-0.28758
C	-4.91378	0.38501	-0.85591
C	-7.33138	-0.28316	-2.10908
C	-4.91823	-0.28886	-2.07625
C	-6.13542	0.73298	-0.27393
C	-7.33600	0.40059	-0.89309
C	-6.11796	-0.62404	-2.70057
H	-3.97138	-0.58293	-2.52450
H	-6.13193	1.24579	0.68455
H	-8.27884	0.67283	-0.42667
H	-6.10406	-1.16411	-3.64309
H	-8.26815	-0.54808	-2.59068
H	-0.09583	0.06854	0.02103
C	2.23000	1.62018	-2.47416
C	1.64502	2.26727	-1.82733
C	0.86506	1.74761	-0.82046
N	0.98097	4.52883	-1.34561
C	0.01167	2.64703	-0.10224
C	1.67896	3.66382	-2.04452
C	0.13479	4.03758	-0.40102
C	-0.96602	2.23232	0.83627
H	2.31996	4.06912	-2.82549
H	-0.56394	6.01464	0.07052
C	-1.83502	3.13710	1.42395
H	-1.12733	1.18500	1.06319
C	-1.64723	4.53223	1.17679
C	-2.31240	5.22920	1.67689
C	-0.69425	4.96090	0.29684
O	-2.85228	2.76321	2.19361
H	-3.14036	1.76227	1.96324
C	5.03103	-1.00284	-1.58466
C	7.67790	-1.39140	-2.40904
C	5.74456	0.03201	-2.19781
C	5.65196	-2.24428	-1.41544
C	6.96956	-2.43630	-1.81957
C	7.06218	-0.15701	-2.60273
H	5.25850	0.99015	-2.37041
H	5.09706	-3.07063	-0.97742
H	7.43851	-3.40558	-1.68460

H	7.60202	0.65440	-3.07993
H	8.70358	-1.54343	-2.72984

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H	-3.62433	0.02330	-3.09997
C	-2.80526	0.39809	-2.47797
C	-0.64363	-0.12999	-1.40738
C	-1.21441	-0.32779	0.01246
C	-1.64558	-0.60038	-2.46133
C	-3.28774	0.62325	-1.03389
H	-0.41629	0.92613	-1.58246
H	-0.92029	-1.30420	0.42066
H	-4.37431	0.58064	-0.95932
H	-2.47985	1.35335	-2.89798
H	0.30010	-0.67393	-1.51990
H	-1.15935	-0.65468	-3.43936
H	-2.94131	1.57078	-0.61909
N	-2.74678	-0.45921	-0.12599
C	-2.21004	-1.97921	-2.08168
H	-2.91578	-2.28443	-2.86277
C	-3.01551	-1.80002	-0.77224
H	-4.09112	-1.84095	-0.95343
H	-2.75945	-2.56098	-0.02995
C	-1.16428	-3.05521	-1.96184
H	-0.36562	-2.90336	-1.23368
C	-1.17898	-4.16856	-2.68894
H	-0.41399	-4.93018	-2.57604
H	-1.95688	-4.35644	-3.42555
C	-0.63828	0.68134	1.05339
O	-1.01001	0.34380	2.36804
C	-3.42916	-0.42931	1.23521
H	-3.19974	0.54096	1.66469
H	-2.91236	-1.17874	1.83710
C	3.47892	-2.15175	3.73449
C	5.46523	-0.64922	2.43030
C	4.78428	-2.12793	4.22971
C	3.18746	-1.43937	2.58188
C	4.16853	-0.67742	1.93502
C	5.77012	-1.39010	3.57596
H	5.03617	-2.69063	5.12353
H	6.78328	-1.38051	3.96689
H	6.22246	-0.04655	1.93607
C	1.87682	-1.43748	1.84754
O	0.78420	-1.80353	2.35534
H	-0.43952	-0.42590	2.60114
N	2.12381	-0.98467	0.63209
H	1.32353	-0.92421	0.01263
H	2.69626	-2.72772	4.21981
C	3.66682	0.22654	0.83538
C	3.10812	1.06323	1.27171
N	4.23333	0.53055	-0.30442
C	4.76300	-0.57098	-1.08997
H	5.10647	-1.40152	-0.45696
H	5.62434	-0.21822	-1.67058
C	3.68553	-1.07453	-2.04089
C	1.63004	-1.94144	-3.74863
C	3.05244	-0.17779	-2.90782
C	3.27233	-2.40707	-2.03864
C	2.25168	-2.83955	-2.88280
C	2.03668	-0.60760	-3.75967
H	3.34767	0.86870	-2.90287
H	3.73685	-3.10526	-1.34680
H	1.93394	-3.87842	-2.85952
H	1.56077	0.10279	-4.43096
H	0.83061	-2.28062	-4.40185
H	0.43298	0.50430	0.94927
H	-2.58781	2.36046	2.01683
C	-1.89253	2.85310	1.34451
C	-0.83730	2.16389	0.79192
N	-1.22382	4.93359	0.34723
C	0.13944	2.90933	0.05115
C	-2.05637	4.23025	1.07902
C	-0.12405	4.30047	-0.13964
C	1.36186	2.37168	-0.43625
H	0.59628	6.13774	-0.99065
C	2.32137	3.17794	-1.03132
H	1.59990	1.31966	-0.32744
C	2.01249	4.55463	-1.26775
H	2.76185	5.15951	-1.76878
C	0.83175	5.08853	-0.84181
O	3.52165	2.74885	-1.39859
H	3.78552	1.80068	-0.95931
C	-4.91797	-0.66021	1.20958
C	-7.68903	-1.04740	1.27239
C	-5.79017	0.43000	1.12993
C	-5.45135	-1.94493	1.35055
C	-6.82925	-2.13875	1.37594
C	-7.16836	0.23912	1.15433
H	-5.38416	1.43733	1.06072
H	-4.78412	-2.79725	1.45488
H	-7.23132	-3.14046	1.48799
H	-7.83342	1.09447	1.09403
H	-8.76349	-1.19860	1.29776
H	-2.91036	4.76017	1.49740

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H	-4.82676	-3.51569	0.12399
C	-4.59353	-2.49096	0.43045
C	-4.14415	-0.17992	-0.33916
C	-2.62055	-0.26767	-0.16999
C	-4.69351	-1.54275	-0.76792
C	-3.17177	-2.40866	1.01154
H	-4.59469	0.11826	0.61429
H	-2.10816	0.00663	-1.09864
H	-2.75170	-3.39475	1.21555
H	-5.31114	-2.20507	1.20401
H	-4.37358	0.59923	-1.07021
H	-5.72891	-1.45358	-1.10629
H	-3.12333	-1.79314	1.90956
N	-2.24314	-1.74816	0.01571
C	-3.83070	-2.12596	-1.90541
H	-4.26924	-3.08499	-2.20374
C	-2.42238	-2.41357	-1.32496
H	-2.25745	-3.48100	-1.16594
H	-1.62894	-2.03516	-1.97577
C	-3.78362	-1.24316	-3.12436
H	-3.27740	-0.28196	-3.02668
C	-4.32866	-1.57481	-4.29066
H	-4.28990	-0.90996	-5.14723
H	-4.83500	-2.52750	-4.42814
C	-2.09319	0.66683	0.93359
O	-2.70939	0.40022	2.16528
C	-0.80589	-1.85526	0.50164
H	-0.82551	-1.46757	1.52218

H	-0.20260	-1.18860	-0.12564
C	-0.25018	-4.01198	1.66461
C	0.33387	-5.27574	1.69161
C	-0.22135	-3.24209	0.49683
C	1.42266	-6.75887	0.57591
C	0.43781	-3.74157	-0.63064
C	1.02033	-5.00472	-0.60564
C	0.96205	-5.77620	0.55386
C	0.19825	2.52240	2.73414
C	2.34057	2.83090	0.94839
C	0.53377	3.78706	2.25314
C	0.93893	1.42444	2.31552
C	1.99440	1.56814	1.41403
C	1.60531	3.93908	1.37300
H	-0.04685	4.65449	2.55277
H	1.85348	4.92547	0.99248
H	3.14131	2.94288	0.22239
C	0.64941	-0.00133	2.67877
O	-0.39783	-0.33721	3.30882
H	-1.95894	0.23503	2.79487
N	1.57998	-0.77259	2.16739
H	1.45581	-1.77488	2.30010
H	-0.64138	2.37650	3.40916
C	2.62749	0.30577	0.90030
H	3.56861	0.00049	1.37209
N	2.40626	0.01213	-0.36518
C	3.21619	-1.08752	-0.87572
H	2.86379	-1.31586	-1.89062
H	3.05715	-2.00171	-0.27992
C	4.70348	-0.78390	-0.93703
C	7.44294	-0.20632	-1.10498
C	5.65378	-1.71916	-0.52890
C	5.14135	0.45276	-1.42423
C	6.49966	0.73816	-1.51032
C	7.01678	-1.43606	-0.61285
H	5.32232	-2.67817	-0.13672
H	4.40373	1.19111	-1.73191
H	6.82643	1.70100	-1.89243
H	7.74349	-2.17349	-0.28411
H	8.50330	0.01934	-1.16766
H	-1.01658	0.52300	1.03082
H	-3.99335	2.50912	1.67041
C	-3.30276	2.88640	0.92307
C	-2.28526	2.09454	0.46070
N	-2.60884	4.74877	-0.44703
C	-1.36094	2.64431	-0.47750
C	-3.42510	4.20975	0.42879
C	-1.56990	3.98773	-0.89353
C	-0.23315	1.93886	-0.95032
H	-4.23976	4.83876	0.78399
H	-0.81932	5.59150	-2.11431
C	0.70193	2.55017	-1.76152
H	-0.00348	0.93687	-0.60680
C	0.46760	3.87833	-2.21716
H	1.40273	4.33051	-2.87584
C	-0.63710	4.56955	-1.79592
H	0.51319	-3.12913	-1.52632
H	1.53158	-5.38066	-1.48614
H	0.31055	-5.86186	2.60460
H	-0.70740	-3.60058	2.56250
O	1.84369	1.94198	-2.10561
H	2.00649	1.15795	-1.45628

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H	-4.59583	-2.73427	1.91280
C	-4.13866	-1.82742	1.50715
C	-4.20727	-0.12333	-0.29782
C	-2.66381	-0.10886	-0.24954
C	-4.74128	-1.49025	0.13969
C	-2.62467	-2.05057	1.34973
H	-4.58470	0.64231	0.38441
H	-2.24245	0.13514	-1.22965
H	-2.36677	-3.11163	1.36127
H	-4.31434	-1.00438	2.20137
H	-4.55359	0.13313	-1.30274
H	-5.83272	-1.46703	0.19670
H	-2.03180	-1.52985	2.10586
N	-2.16438	-1.54291	-0.00008
C	-4.29618	-2.57555	-0.85904
H	-4.48515	-3.55462	-0.40229
C	-2.77630	-2.41201	-1.07312
H	-2.26093	-3.37272	-1.04597
H	-2.54781	-1.92487	-2.02652
C	-5.02464	-2.52701	-2.17304
H	-4.91657	-1.61168	-2.75612
C	-5.77506	-3.51875	-2.64268
H	-6.29512	-3.43812	-3.59154
H	-5.89762	-4.44751	-2.09069
C	-2.12239	0.92721	0.75964
O	-2.78260	0.85426	1.99453
C	-0.64736	-1.58345	-0.11779
H	-0.24288	-0.95606	0.67537
H	-0.40790	-1.12266	-1.08021
C	0.12963	2.73407	2.49538
C	2.38624	2.88554	0.83306
C	0.51772	3.95638	1.94780
C	0.87662	1.59911	2.20601
C	1.99184	1.66562	1.36792
C	1.64344	4.03029	1.12748
H	-0.06561	4.85010	2.14766
H	1.93056	4.98286	0.69251
H	3.23279	2.93441	0.15362
C	0.55277	0.20257	2.65353
O	-0.56158	-0.10239	3.17300
H	-2.07146	0.62304	2.64485
N	1.55397	-0.58437	2.33231
H	1.42491	-1.57611	2.51435
H	-0.75788	2.65126	3.11774
C	2.62876	0.35715	0.99049
H	3.56332	0.09473	1.49928
N	2.40849	-0.05891	-0.24110
C	3.17054	-1.24214	-0.62090
H	2.83874	-1.54186	-1.62418
H	2.93186	-2.09009	0.04348
C	4.67625	-1.03981	-0.64746
C	7.45486	-0.66776	-0.75832
C	5.54505	-2.01300	-0.15394
C	5.21645	0.13061	-1.19152
C	6.59410	0.31427	-1.24898
C	6.92667	-1.83239	-0.20939
H	5.13371	-2.92082	0.28193
H	4.54362	0.89912	-1.56544
H	6.99949	1.22697	-1.67602
H	7.58859	-2.59838	0.18412
H	8.53001	-0.52172	-0.79961

H	-1.05993	0.75111	0.91628
H	-3.98871	2.89812	1.18322
C	-3.25302	3.16290	0.43071
C	-2.23892	2.29651	0.11945
N	-2.43847	4.83131	-1.11202
C	-1.24885	2.71254	-0.82060
C	-3.31220	4.42023	-0.22300
C	-1.39859	3.99971	-1.40541
C	-0.11428	1.93378	-1.13633
H	-4.12546	5.10493	0.01145
H	-0.53600	5.43051	-2.75902
C	0.87921	2.42263	-1.96096
H	0.07360	0.98186	-0.65601
C	0.70750	3.69152	-2.58322
H	1.48990	4.04775	-3.24599
C	-0.40039	4.45021	-2.31271
O	2.01898	1.75117	-2.16935
H	2.11055	1.02124	-1.45155
C	-0.02366	-2.95047	-0.02239
C	1.29362	-5.41301	0.14847
C	0.40854	-3.60482	-1.17854
C	0.21796	-3.54007	1.22367
C	0.86874	-4.76708	1.30847
C	1.06380	-4.83073	-1.09537
H	0.24824	-3.14057	-2.14895
H	-0.09783	-3.02796	2.13002
H	1.05438	-5.21255	2.28042
H	1.40233	-5.32428	-2.00051
H	1.81017	-6.36514	0.21563

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H	-1.98442	4.06337	-2.80797
C	-2.14387	3.07717	-2.36307
C	-3.45977	1.74237	-0.74425
C	-2.17058	0.95964	-0.41103
C	-3.12400	3.16753	-1.18915
C	-0.80377	2.52776	-1.85316
H	-3.97909	1.23724	-1.56075
H	-2.16995	0.62699	0.63318
H	-0.39028	1.74419	-2.48917
H	-2.54305	2.40748	-3.12711
H	-4.13137	1.74111	0.11842
H	-4.03605	3.68990	-1.49011
H	-0.05473	3.31310	-1.73145
N	-0.97987	1.93279	-0.47186
C	-2.44096	3.93777	-0.04395
H	-2.01792	4.86006	-0.46031
C	-1.28793	3.05817	0.48719
H	-0.37049	3.63406	0.61234
H	-1.53518	2.58738	1.44454
C	-3.37710	4.31479	1.07038
H	-3.85996	3.49163	1.59888
C	-3.63934	5.56793	1.42824
H	-4.33252	5.79666	2.23117
H	-3.16876	6.41080	0.92774
C	-1.98208	-0.29150	-1.29016
O	-2.08453	0.01973	-2.65621
C	0.28664	1.21423	-0.04061
H	0.42315	0.40258	-0.75361
H	0.08095	0.79968	0.95261
C	3.56984	-0.74985	-3.10219
C	4.47211	-2.48968	-1.09208
C	4.93576	-0.96645	-2.92279
C	2.67246	-1.41277	-2.27696
C	3.10989	-2.28168	-1.27401
C	5.38108	-1.83473	-1.92615
H	5.65521	-0.46475	-3.56290
H	6.44602	-2.00051	-1.79319
H	4.82310	-3.15023	-0.30334
C	1.17610	-1.33267	-2.35878
O	0.57692	-0.45083	-3.03894
H	-1.20910	-0.23780	-3.03911
N	0.69266	-2.28003	-1.58732
H	-0.31070	-2.42478	-1.53725
H	3.19450	-0.08808	-3.87830
C	2.03693	-2.85997	-0.37174
H	1.81199	-3.91870	-0.50157
N	1.90493	-2.40884	0.87096
C	2.51468	-1.11676	1.14687
H	2.28354	-0.38863	0.35003
H	3.61258	-1.19223	1.12997
C	2.12550	-0.47347	2.45918
C	1.43583	0.96266	4.78064
C	0.84862	-0.58629	3.01660
C	3.05489	0.35284	3.09978
C	2.71937	1.06559	4.24680
C	0.50553	0.12972	4.16376
H	0.11924	-1.25065	2.56638
H	4.05328	0.44882	2.67879
H	3.46060	1.69991	4.72484
H	-0.49044	0.02142	4.58376
H	1.16876	1.51378	5.67730
H	-0.99336	-0.69710	-1.09125
H	-4.44110	-0.77888	-2.33202
C	-4.21136	-1.42879	-1.49421
C	-2.99178	-1.34511	-0.86784
N	-4.92356	-3.25887	-0.10719
C	-2.68158	-2.29397	0.15646
C	-5.15235	-2.39207	-1.06636
C	-3.69904	-3.23772	0.48358
C	-1.41595	-2.39186	0.79366
H	-6.12798	-2.44142	-1.54659
H	-4.20892	-4.93729	1.69633
C	-1.12902	-3.43485	1.66415
H	-0.61160	-1.70584	0.54975
C	-2.17526	-4.34260	2.01806
H	-1.93826	-5.12883	2.72800
C	-3.41321	-4.23978	1.45339
O	0.06764	-3.64542	2.20053
H	0.83347	-3.09924	1.70545
C	1.53237	2.05783	-0.02869
C	3.92361	3.49465	-0.00656
C	2.33573	2.10471	-1.17375
C	1.95098	2.70579	1.13534
C	3.14090	3.42932	1.14355
C	3.52538	2.82463	-1.16301
H	2.03263	1.54565	-2.05906
H	1.36543	2.61069	2.04855
H	3.46486	3.92182	2.05520
H	4.14988	2.84639	-2.05050
H	4.85526	4.05183	0.00356

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H	-4.56126	1.87852	-2.73361
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C	-4.09406	1.25143	-1.96873
C	-3.97128	0.74349	0.47778
C	-2.46208	0.49452	0.24827
C	-4.52208	1.71592	-0.57381
C	-2.56311	1.36844	-2.08688
H	-4.49593	-0.20974	0.39567
H	-1.89996	0.67696	1.16578
H	-2.11205	0.47496	-2.53006
H	-4.39520	0.21648	-2.12812
H	-4.13962	1.13100	1.48652
H	-5.61180	1.76755	-0.50353
H	-2.26323	2.24348	-2.67040
N	-1.94646	1.57465	-0.71639
C	-3.91514	3.11331	-0.35189
H	-4.10604	3.71399	-1.24951
C	-2.39664	2.92094	-0.18754
H	-1.82671	3.68351	-0.72355
H	-2.09349	2.95387	0.86194
C	-4.48237	3.85013	0.82898
H	-4.35785	3.37796	1.80426
C	-5.11287	5.03719	0.74109
C	-5.51996	5.51130	1.61720
H	-5.24710	5.51812	-0.21470
C	-2.17578	-0.95710	-0.23053
O	-3.18839	-1.42531	-1.07925
C	-0.42484	1.59011	-0.85550
H	-0.24084	2.12964	-1.78909
H	-0.08318	0.56698	-1.02124
C	-0.55177	-3.86090	-1.64090
C	2.16912	-3.48551	-1.03384
C	0.12813	-4.78909	-0.85427
C	0.14176	-2.75296	-2.11040
C	1.48815	-2.55194	-1.80496
C	1.47969	-4.60241	-0.55942
H	-0.39470	-5.65581	-0.46162
H	1.99807	-5.32748	0.06095
C	3.20821	-3.31743	-0.76697
C	-0.44739	-1.62759	-2.89942
O	-1.66032	-1.58719	-3.24310
H	-2.74879	-1.66253	-1.93649
N	0.48728	-0.71830	-3.09072
H	0.24919	0.07886	-3.67531
H	-1.60749	-3.97572	-1.87207
C	2.08533	-1.25026	-2.26955
H	2.62378	-1.29372	-3.22850
N	2.53857	-0.43885	-1.32542
H	-1.22236	-0.97246	-0.76174
H	-4.09688	-2.40157	1.05092
C	-3.12685	-2.47815	1.53104
C	-2.03432	-1.84668	0.99304
N	-1.83063	-3.43260	3.32426
C	-0.76112	-2.04617	1.60823
C	-2.97409	-3.25498	2.70468
C	-0.72381	-2.85340	2.78179
C	0.44707	-1.52742	1.08986
C	-3.84491	-3.74158	3.14080
H	0.53820	-3.69357	4.30491
C	1.66282	-1.80127	1.68731
H	0.47681	-0.95207	0.17320
C	1.69007	-2.57708	2.88203
H	2.65418	-2.76811	3.34286
C	0.53265	-3.08348	3.40703
O	2.82529	-1.38380	1.18270
H	2.69564	-0.97892	0.24733
C	0.32412	2.28151	0.25929
C	1.76157	3.65745	2.23786
C	0.44874	1.74929	1.54833
C	0.94837	3.50062	-0.02431
C	1.66841	4.18201	0.95205
C	1.15315	2.43986	2.53140
H	0.03680	0.77581	1.79150
H	0.88179	3.91494	-1.02797
H	2.16047	5.11714	0.70531
H	1.24347	2.00821	3.52319
H	2.32090	4.18607	3.00345
C	3.21092	0.73397	-1.85193
C	4.22994	1.33007	-0.90671
H	3.70845	0.51283	-2.81357
H	2.46323	1.51950	-2.08380
C	5.48956	1.71613	-1.36802
C	6.41844	2.30185	-0.50992
C	6.09681	2.50521	0.82942
C	4.84254	2.12032	1.29964
C	3.91679	1.54059	0.43794
H	5.74786	1.55104	-2.41170
H	7.39509	2.59205	-0.88664
H	6.82001	2.95485	1.50351
H	4.58125	2.27059	2.34375
H	2.94475	1.23256	0.81111

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H	4.71793	-1.90731	-2.86932
C	4.20268	-1.19245	-2.22099
C	4.16746	-0.12197	0.03113
C	2.62455	-0.18393	-0.05236
C	4.80076	-1.23346	-0.81231
C	2.71345	-1.56718	-2.14250
H	4.49577	0.84724	-0.35077
H	2.17508	-0.24174	0.94423
H	2.53595	-2.59759	-2.46398
H	4.30910	-0.19375	-2.64363
H	4.49292	-0.18815	1.07299
H	5.88526	-1.10133	-0.85261
H	2.06478	-0.90129	-2.71831
N	2.23604	-1.52403	-0.70125
C	4.46359	-2.60541	-0.20266
H	4.70921	-3.37697	-0.94280
C	2.94554	-2.62398	0.05938
H	2.49037	-3.56872	-0.24479
H	2.71177	-2.46760	1.11556
C	5.21964	-2.91263	1.05974
H	5.04252	-2.24778	1.90612
C	6.07256	-3.92414	1.18787
H	6.60886	-4.10127	2.11438
H	6.26579	-4.61142	0.36762
C	2.04438	1.06545	-0.76609
O	2.72977	1.36566	-1.95077
C	0.72671	-1.78606	-0.68568
H	0.54235	-2.40226	-1.56960
H	0.21406	-0.83905	-0.85127
C	-0.31881	3.20111	-2.12349
C	-2.60894	2.76199	-0.55744
C	-0.83830	4.22669	-1.33475
C	-0.95758	1.96752	-2.12437
C	-2.08789	1.73841	-1.33923

C	-1.97946	4.00758	-0.56210
H	-0.34530	5.19374	-1.30795
H	-2.36860	4.80737	0.06065
H	-3.46763	2.57479	0.08178
C	-0.48800	0.74342	-2.85181
O	0.62528	0.69333	-3.44906
H	2.04723	1.29703	-2.66720
N	-1.37504	-0.21235	-2.68291
H	-1.14361	-1.11651	-3.08738
H	0.58367	3.34157	-2.71318
C	-2.60039	0.32509	-1.29562
H	-3.47763	0.10190	-1.91473
N	-2.43257	-0.30843	-0.14726
C	-3.10404	-1.59883	-0.06017
H	-2.82418	-2.05289	0.90046
H	-2.73773	-2.28789	-0.84060
C	-4.61761	-1.51540	-0.14670
C	-7.41548	-1.34588	-0.25736
C	-5.34853	-2.35206	-0.98914
C	-5.30589	-0.58140	0.63564
C	-6.69288	-0.49904	0.58434
C	-6.73999	-2.27180	-1.04544
H	-4.82193	-3.07314	-1.61059
H	-4.73660	0.08418	1.28128
H	-7.21462	0.22866	1.19931
H	-7.29408	-2.92804	-1.71055
H	-8.49841	-1.27804	-0.30079
H	0.99535	0.88610	-0.99925
H	3.86783	3.10992	-0.57825
C	3.10315	3.14967	0.19076
C	2.09407	2.22279	0.21446
N	2.23128	4.30318	2.12469
C	1.07058	2.36197	1.19633
C	3.12672	4.17169	1.17357
C	1.19540	3.41727	2.13975
C	-0.06260	1.52580	1.23619
H	3.93523	4.90094	1.16341
H	0.29452	4.36285	3.84886
C	-1.06277	1.70954	2.17117
C	-0.23339	0.76813	0.48235
C	-0.91305	2.73466	3.14905
H	-1.69898	2.85913	3.88748
C	0.18009	3.56121	3.12562
O	-2.17087	0.96169	2.16928
H	-2.22432	0.44423	1.27393
C	0.17704	-2.49629	0.52659
C	-0.97713	-3.87013	2.67874
C	-0.18497	-3.84084	0.40406
C	-0.05276	-1.84421	1.74193
C	-0.62092	-2.52960	2.81162
C	-0.76004	-4.52634	1.47020
H	-0.03016	-4.35244	-0.54365
H	0.18277	-0.79136	1.85840
H	-0.80643	-2.00389	3.74275
H	-1.04437	-5.56718	1.35299
H	-1.43358	-4.39724	3.51062

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H	3.67175	3.65261	2.42205
C	3.42840	2.81931	1.75627
C	3.28019	2.09653	-0.64970
C	2.01667	1.30880	-0.23050
C	3.51638	3.27785	0.29805
C	1.99228	2.34629	2.04630
H	4.13659	1.42079	-0.61890
H	1.32844	1.17082	-1.07169
H	1.42945	3.08544	2.62333
H	4.12800	2.00548	1.93880
H	3.17658	2.46163	-1.67594
H	4.49465	3.72570	0.09987
H	1.95496	1.38557	2.56887
N	1.21985	2.19055	0.75040
C	2.40318	4.31209	0.06670
H	2.43711	5.02409	0.90346
C	1.06878	3.55741	0.11488
H	0.31689	4.09635	0.69235
H	0.66043	3.37129	-0.87936
C	2.60609	5.10797	-1.19736
H	3.59091	5.57068	-1.26416
C	1.73960	5.31289	-2.18575
H	2.01414	5.92064	-3.04151
H	0.73072	4.81038	-2.19200
C	2.38931	-0.09266	0.32417
O	3.47921	-0.03863	1.20259
C	-0.17979	1.64212	1.07893
H	-0.40604	2.05714	2.06507
H	-0.10172	0.56001	1.20149
C	1.97350	-3.32543	1.66293
C	-0.64359	-4.04933	0.93783
C	1.75274	-4.42122	0.82946
C	0.87929	-2.60554	2.12404
C	-0.42349	-2.95047	1.75857
C	0.45182	-4.78121	0.47552
H	2.59406	-4.98866	0.44372
H	0.28998	-5.62800	-0.18464
H	-1.65184	-4.29922	0.62114
C	0.94775	-1.35975	2.95391
O	2.03743	-0.81993	3.29276
H	3.15387	-0.43218	2.05320
N	-0.27900	-0.94177	3.18095
H	-0.37878	-0.10179	3.74557
H	2.97773	-3.01281	1.93715
C	-1.50915	-2.00677	2.19901
H	-2.05602	-2.28952	3.10995
N	-2.15445	-1.36039	1.24098
C	-3.20360	-0.50362	1.75317
H	-2.77183	0.44656	2.12174
H	-3.68477	-0.96414	2.63773
C	-4.28228	-0.15737	0.75094
C	-6.34369	0.50244	-1.03775
C	-4.64776	-1.03952	-0.26821
C	-4.97551	1.04853	0.87138
C	-6.00206	1.37735	-0.00924
C	-5.66308	-0.70716	-1.16204
H	-4.13037	-1.98799	-0.36473
H	-4.69501	1.74557	1.65850
H	-6.52466	2.32410	0.09843
H	-5.92654	-1.39996	-1.95604
H	-7.13704	0.75852	-1.73389
H	1.52457	-0.50242	0.84732
H	4.81342	-0.78363	-0.76648
C	3.97089	-1.22070	-1.29189
C	2.68994	-1.00625	-0.85277
N	3.22965	-2.63151	-3.10653
C	1.62791	-1.67317	-1.52746

C	4.18612	-2.03989	-2.42925
C	1.95266	-2.46890	-2.65997
C	0.29170	-1.60515	-1.08941
H	5.20243	-2.19712	-2.78619
H	1.15934	-3.73456	-4.20716
C	-0.71389	-2.28589	-1.74272
H	0.02285	-1.08628	-0.17846
C	-0.39855	-3.04862	-2.90260
H	-1.20415	-3.57214	-3.40776
C	0.89691	-3.13776	-3.33919
O	-1.97810	-2.26084	-1.30704
H	-2.02206	-1.83781	-0.37429
C	-1.28503	2.01727	0.12061
C	-3.37930	2.73882	-1.59792
C	-2.07179	3.14648	0.38528
C	-1.58719	1.23832	-0.99775
C	-2.63056	1.59519	-1.84989
C	-3.10073	3.51442	-0.47303
H	-1.88005	3.73884	1.27801
H	-1.02110	0.33892	-1.20714
H	-2.86476	0.96023	-2.69803
H	-3.70040	4.39200	-0.25188
H	-4.19902	3.00948	-2.25578

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H	4.54735	-2.08073	-3.03645
C	4.09039	-1.35441	-2.35780
C	4.18375	-0.34870	-0.06490
C	2.63875	-0.32112	-0.11169
C	4.72758	-1.45718	-0.97099
C	2.58810	-1.65539	-2.23647
C	4.55909	0.61968	-0.40246
H	2.21152	-0.37696	0.89474
H	2.34777	-2.66734	-2.57577
H	4.23442	-0.35395	-2.76404
H	4.52794	-0.50491	0.96191
H	5.81610	-1.37610	-1.04645
H	1.95624	-0.94296	-2.77511
N	2.16268	-1.62493	-0.77942
C	4.33981	-2.82009	-0.36957
H	4.51889	-3.58166	-1.14179
C	2.83673	-2.77473	-0.06163
H	2.32281	-3.68842	-0.36765
H	2.63467	-2.61479	0.99838
C	5.19612	-3.18464	0.81632
C	6.26428	-3.16479	0.59894
C	4.80555	-3.52563	2.04141
H	5.53818	-3.76924	2.80384
H	3.76465	-3.59257	2.34427
C	2.10973	0.97306	-0.78470
O	2.79584	1.27407	-1.96892
C	0.64354	-1.81183	-0.72080
H	0.40111	-2.39940	-1.60984
H	0.17353	-0.83813	-0.85433
C	-0.16807	3.24415	-2.08069
C	-2.45992	2.86675	-0.50073
C	-0.63623	4.27305	-1.26494
C	-0.85765	2.03836	-2.09971
C	-1.98790	1.83838	-1.30719
C	-1.77890	4.08508	-0.48630
H	-0.10302	5.21788	-1.22280
H	-2.12904	4.88761	0.15605
H	-3.32002	2.70268	0.14291
C	-0.44641	0.81326	-2.85907
O	0.65431	0.73586	-3.47622
H	2.10527	1.25351	-2.68060
N	-1.36607	-0.11223	-2.69542
H	-1.17802	-1.01437	-3.12602
H	0.73291	3.35842	-2.67826
C	-2.55683	0.44616	-1.28678
H	-3.44770	0.27149	-1.90220
N	-2.40692	-0.21590	-0.15188
C	-3.13547	-1.47595	-0.08050
H	-2.87206	-1.95677	0.87200
H	-2.80360	-2.16909	-0.87286
C	-4.64428	-1.32326	-0.15868
C	-7.43224	-1.02668	-0.25734
C	-5.41653	-2.12679	-0.99683
C	-5.28589	-0.35851	0.62592
C	-6.66802	-0.21292	0.58037
C	-6.80308	-1.98343	-1.04692
H	-4.92639	-2.87128	-1.62050
H	-4.68405	0.28098	1.26821
H	-7.15298	0.53859	1.19682
H	-7.38941	-2.61455	-1.70861
H	-8.51109	-0.90926	-0.29632
H	1.05102	0.84715	-1.01050
H	4.02977	2.92404	-0.56153
C	3.27340	2.98096	0.21469
C	2.22204	2.10192	0.22492
N	2.47026	4.12966	2.18157
C	1.21409	2.26636	1.21915
C	3.35265	3.97709	1.22120
C	1.39336	3.29404	2.18418
C	0.04430	1.48209	1.25090
H	4.19567	4.66605	1.22226
H	0.54675	4.24457	3.91828
C	-0.94119	1.69283	2.19564
H	-0.16431	0.74723	0.48468
C	-0.73940	2.68997	3.19256
H	-1.51488	2.83504	3.93811
C	0.39124	3.46444	3.17935
O	-2.08315	0.99781	2.18620
H	-2.16332	0.50062	1.28184
C	0.09192	-2.51859	0.49266
C	-1.08645	-3.87541	2.64312
C	-0.07882	-1.88054	1.72503
C	-0.33985	-3.84081	0.35326
C	-0.92648	-4.51801	1.41833
C	-0.65976	-2.55751	2.79343
H	0.21321	-0.84380	1.85687
H	-0.23243	-4.33982	-0.60752
H	-1.26625	-5.54043	1.28750
H	-0.79935	-2.04201	3.73816
H	-1.55291	-4.39503	3.47413

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H	-4.98578	-1.18685	-3.75907
C	-4.18070	-1.56980	-3.12341
C	-3.46990	-2.10321	-0.82329
C	-2.65862	-0.81731	-0.58888
C	-4.68944	-1.80700	-1.70061
C	-3.01500	-0.57231	-3.06023
H	-2.83900	-2.84156	-1.32752

H	-3.02616	-0.32351	0.31298
H	-3.09519	0.19226	-3.83457
H	-3.82444	-2.50470	-3.56377
H	-3.75664	-2.51644	0.14641
H	-5.39443	-2.64150	-1.67253
H	-2.03972	-1.05503	-3.11094
N	-3.02175	0.16651	-1.72606
C	-5.39733	-0.52037	-1.23270
H	-6.27153	-0.36434	-1.87502
C	-4.42504	0.66229	-1.46944
H	-4.70162	1.25043	-2.34927
H	-4.38033	1.33271	-0.60938
C	-5.88164	-0.59559	0.19087
H	-5.12522	-0.65741	0.97423
C	-7.16697	-0.60052	0.52984
H	-7.48202	-0.66955	1.56581
H	-7.95122	-0.53514	-0.22091
C	-1.13641	-1.05770	-0.44831
O	-0.65514	-1.66628	-1.60371
C	-2.07431	1.33712	-1.86896
H	-2.33115	1.79022	-2.82897
H	-1.07274	0.90547	-1.97684
C	4.60974	2.34887	0.34500
C	4.50924	0.88342	-2.04534
C	5.78502	2.02605	-0.33070
C	3.39459	1.93939	-0.18745
C	3.33741	1.19107	-1.36157
C	5.73178	1.30768	-1.52636
H	6.74531	2.33856	0.06896
H	6.65091	1.05615	-2.04724
H	4.47446	0.28028	-2.94826
C	2.04471	2.25540	0.38294
O	1.90948	2.76292	1.52442
H	0.31310	-1.23493	-1.74977
N	1.12756	1.92137	-0.50525
H	0.17436	2.09329	-0.19442
H	4.61765	2.91877	1.26942
C	1.98230	0.66373	-1.77632
C	1.54961	1.11361	-2.67137
N	1.64288	-0.59201	-1.56245
C	2.23574	-1.25565	-0.39987
H	1.61323	-2.13747	-0.19556
H	2.17049	-0.61771	0.49637
C	3.66818	-1.71504	-0.58574
C	6.32062	-2.52910	-0.98272
C	4.02854	-2.42843	-1.73214
C	4.64758	-1.42601	0.36281
C	5.96700	-1.82885	0.16753
C	5.34450	-2.83153	-1.93212
H	3.26841	-2.63864	-2.48073
H	4.38050	-0.84720	1.24409
H	6.72198	-1.58174	0.90865
H	5.61249	-3.38114	-2.83028
H	7.34982	-2.83834	-1.14040
H	-0.64626	-0.08535	-0.30345
H	-1.23463	-3.75408	-0.12535
C	-1.06759	-3.23524	0.81251
C	-0.90624	-1.87039	0.82645
N	-0.86484	-3.40597	3.20402
C	-0.56884	-1.24946	2.07026
C	-1.03050	-3.96034	2.02536
C	-0.62055	-2.06744	3.23753
C	-0.16091	0.10358	2.20267
H	-1.17725	-5.03891	2.01005
H	-0.45344	-2.10292	5.38033
C	0.11012	0.65090	3.44002
H	0.02229	0.71502	1.32799
C	-0.04743	-0.14451	4.61078
H	0.15578	0.31599	5.57234
C	-0.38317	-1.46499	4.50490
O	0.51641	1.91891	3.60668
H	0.90129	2.27868	2.75526
C	-2.11191	2.42814	-0.82064
C	-1.80658	4.58592	0.95294
C	-2.09741	2.22083	0.56401
C	-2.00296	3.73884	-1.29598
C	-1.84907	4.80880	-0.41998
C	-1.93811	3.28951	1.44243
H	-2.16109	1.22831	0.98999
H	-2.00904	3.92251	-2.36721
H	-1.74913	5.81447	-0.81503
H	-1.88467	3.09525	2.50911
H	-1.66447	5.41470	1.63844

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H	-5.57028	-0.14268	-1.79244
C	-4.59294	-0.60759	-1.95630
C	-2.95262	-2.25950	-1.14007
C	-2.04518	-1.24927	-0.42314
C	-4.41305	-1.81399	-1.03240
C	-3.46071	0.39593	-1.68006
H	-2.66500	-2.32238	-2.19528
H	-1.91728	-1.53348	0.62867
H	-2.65520	0.34737	-2.41235
H	-4.54488	-0.91739	-3.00342
H	-2.79106	-3.24734	-0.70189
H	-5.08792	-2.62590	-1.31388
H	-3.84247	1.41299	-1.60475
N	-2.80452	0.08772	-0.34771
C	-4.72860	-1.35795	0.40657
H	-5.78542	-1.07109	0.44501
C	-3.89144	-0.08379	0.68708
H	-4.50145	0.82059	0.64606
H	-3.40070	-0.12281	1.66365
C	-4.50992	-2.43839	1.43240
H	-3.48917	-2.79282	1.57897
C	-5.49173	-2.97918	2.14714
H	-5.30215	-3.76681	2.86877
H	-6.52272	-2.65256	2.03272
C	-0.63119	-1.12192	-1.02680
O	-0.66584	-0.51006	-2.27895
C	-1.85816	1.20749	0.05268
H	-1.15183	1.31470	-0.77586
H	-1.31782	0.83047	0.92619
C	5.35711	0.31249	0.99385
C	4.69721	0.36695	-1.73791
C	6.36221	0.34802	0.02769
C	4.03286	0.33110	0.58136
C	3.69495	0.35820	-0.77377
C	6.03221	0.37565	-1.32832
H	7.40557	0.34977	0.32814
H	6.82189	0.39276	-2.07358
H	4.44032	0.35489	-2.79369
C	2.83336	0.35079	1.47785
O	2.88577	0.07261	2.70140

H	0.20421	0.08861	-2.31841
N	1.79124	0.67770	0.73609
H	0.90167	0.69987	1.23043
H	5.58423	0.28147	2.05532
C	2.22294	0.22228	-1.07470
H	1.92333	-0.82260	-0.95165
N	1.54070	0.85146	-2.01445
C	1.96076	2.21106	-2.34870
H	1.33612	2.55098	-3.18272
H	3.00247	2.23995	-2.69856
C	1.81716	3.17280	-1.18540
C	1.48435	4.78178	1.08825
C	0.55311	3.63260	-0.81263
C	2.91853	3.55432	-0.41842
C	2.75454	4.35161	0.71200
C	0.37826	4.42685	0.31706
H	-0.30219	3.36686	-1.43025
H	3.90994	3.20420	-0.69716
H	3.62027	4.63012	1.30562
H	-0.61556	4.77331	0.59177
H	1.35719	5.39811	1.97323
H	-0.03896	-0.51468	-0.33579
H	-0.49140	-2.81681	-3.11384
C	-0.08759	-3.26274	-2.21110
C	-0.02443	-2.52210	-1.05736
N	0.88903	-5.19695	-1.16140
C	0.59769	-3.10613	0.08940
C	0.37643	-4.59886	-2.21132
C	1.02487	-4.46118	-0.02347
C	0.86312	-2.40165	1.29257
H	0.30482	-5.19093	-3.12198
H	1.94848	-6.11503	0.99128
C	1.56536	-2.99215	2.32279
H	0.58787	-1.35973	1.39537
C	1.91914	-4.36756	2.23320
H	2.43953	-4.81464	3.07392
C	1.65321	-5.07581	1.09472
O	1.93329	-2.32862	3.43533
H	2.13206	-1.37855	3.21499
C	-2.52748	2.51348	0.39709
C	-3.65470	4.98251	1.08935
C	-2.76051	2.83831	1.73613
C	-2.85117	3.44992	-0.59139
C	-3.41606	4.67454	-0.24879
C	-3.32263	4.06399	2.08223
H	-2.47977	2.13567	2.51705
H	-2.63413	3.23533	-1.63472
H	-3.65356	5.39384	-1.02564
H	-3.48940	4.30450	3.12703
H	-4.08607	5.94151	1.35757

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H	2.56619	1.08044	-4.47175
C	1.62004	0.87923	-3.95860
C	-0.15816	1.81596	-2.51865
C	0.39904	1.26128	-1.19993
C	1.00234	2.18173	-3.44563
C	1.83694	-0.06245	-2.76317
H	-0.79967	1.06367	-2.99167
H	0.56134	2.08364	-0.49610
H	2.80893	-0.55311	-2.81044
H	0.95116	0.39504	-4.67486
H	-0.77839	2.68509	-2.28581
H	0.65748	2.80187	-4.27778
H	1.04678	-0.80514	-2.65420
N	1.81726	0.73154	-1.47297
C	2.08218	2.93838	-2.64087
H	2.87044	3.22973	-3.34730
C	2.70714	1.94025	-1.64680
H	3.66779	1.56529	-2.00420
H	2.86221	2.36909	-0.65481
C	1.52628	4.21131	-2.04770
H	1.11419	4.88576	-2.79915
C	1.47781	4.58714	-0.77273
H	1.03834	5.53909	-0.49440
H	1.86039	3.98820	0.04994
C	-0.52826	0.24627	-0.51958
O	-0.62770	-0.92455	-1.27086
C	2.29360	-0.12685	-0.31281
H	1.65563	-1.01530	-0.32384
H	2.08232	0.44432	0.59846
C	2.67945	-1.69105	2.59109
C	1.13992	-3.62248	1.25878
C	3.29660	-2.79101	1.99727
C	1.29679	-1.57863	2.52765
C	0.52067	-2.54408	1.88359
C	2.53036	-3.74241	1.32276
H	4.37837	-2.88912	2.02667
H	3.02025	-4.58341	0.84016
H	0.54025	-4.36019	0.73303
C	0.49731	-0.41833	3.04503
O	1.07013	0.63657	3.43822
H	-1.00885	-1.58881	-0.56676
N	-0.77713	-0.70943	2.91973
H	-1.44719	0.01642	3.15982
H	3.25205	-0.91279	3.08813
C	-0.96942	-2.34900	1.91221
H	-1.47971	-2.83877	2.75249
N	-1.60671	-2.24957	0.76581
C	-3.04851	-2.18315	0.88678
H	-3.35943	-1.18260	1.23748
H	-3.41174	-2.89571	1.65009
C	-3.75947	-2.45624	-0.42096
C	-5.10716	-2.92523	-2.83820
C	-3.15667	-3.19766	-1.43691
C	-5.04816	-1.95667	-0.62933
C	-5.72003	-2.18810	-1.82534
C	-3.82477	-3.42943	-2.63860
H	-2.15286	-3.58114	-1.27917
H	-5.51963	-1.36249	0.15124
H	-6.71851	-1.78555	-1.97084
H	-3.33953	-4.00382	-3.42284
H	-5.62512	-3.10224	-3.77613
H	-0.13135	0.00979	0.47749
H	-2.86038	-0.06282	-1.90294
C	-2.94327	0.67005	-1.10600
C	-1.86906	0.93150	-0.29601
N	-4.37429	2.17980	0.12202
C	-2.04499	1.83980	0.78913
C	-4.17276	1.33149	-0.85976
C	-3.32895	2.42357	0.96392
C	-1.03183	2.10015	1.73863
H	-5.02288	1.12616	-1.50894
H	-4.52393	3.71410	2.20276
C	-1.30166	2.81180	2.88709

H	-0.05035	1.65099	1.64976
C	-2.56779	3.44192	3.03907
H	-2.74755	4.03064	3.93314
C	-3.54315	3.26181	2.09308
O	-0.40507	2.89542	3.88967
H	0.21042	2.11498	3.80160
C	3.75152	-0.50416	-0.37339
C	6.44143	-1.27634	-0.36573
C	4.15593	-1.67394	-1.02344
C	4.70604	0.25962	0.30259
C	6.04499	-0.12183	0.30533
C	5.49416	-2.05455	-1.02803
H	3.41080	-2.31108	-1.49405
H	4.39654	1.14398	0.85490
H	6.77524	0.47604	0.84117
H	5.79401	-2.96716	-1.53340
H	7.48444	-1.57705	-0.36021

IId2E-S (denoted as IId-S in the main article)

H	3.713850	2.570104	-1.826335
C	2.770813	2.052084	-2.026635
C	0.301595	2.240192	-2.070224
C	0.080285	1.464839	-0.762319
C	1.602773	3.041183	-1.984287
C	2.528520	0.945966	-0.987487
H	0.363821	1.527087	-2.899285
H	-0.538864	2.041544	-0.065503
H	3.412726	0.759831	-0.376262
H	2.847507	1.593215	-3.016321
H	-0.561302	2.886403	-2.250348
H	1.670697	3.755231	-2.808767
H	2.192274	0.013566	-1.440319
N	1.429168	1.364938	-0.031975
C	1.666637	3.799259	-0.642632
H	2.596564	4.378057	-0.626912
C	1.751132	2.745119	0.489287
H	2.754665	2.686044	0.913764
H	1.047593	2.952495	1.300596
C	0.521784	4.759144	-0.454234
H	-0.471052	4.330596	-0.310949
C	0.663032	6.081216	-0.466357
H	-0.186292	6.745777	-0.344899
H	1.637729	6.544763	-0.600460
C	-0.616393	0.106289	-1.003617
O	0.108290	-0.682928	-1.894391
C	1.311957	0.367895	1.107788
H	1.279104	-0.620593	0.637701
H	0.339330	0.555538	1.572423
C	-3.685549	-2.090257	1.324423
C	-2.287640	-3.371727	-0.745201
C	-4.367907	-2.561688	0.205228
C	-2.307743	-2.253788	1.392320
C	-1.611424	-2.924007	0.385716
C	-3.667290	-3.180465	-0.832268
H	-5.442699	-2.427604	0.128256
H	-4.202098	-3.520323	-1.714233
H	-1.741155	-3.862311	-1.545398
C	-1.410107	-1.674518	2.445211
O	-1.816726	-0.868657	3.325633
H	0.350112	-1.531652	-1.362560
N	-0.182751	-2.103988	2.234572
H	0.528678	-1.773172	2.883941
H	-4.204771	-1.571391	2.125615
C	-0.139777	-3.133272	0.603106
H	0.104426	-4.054264	1.149109
N	0.704077	-2.710175	-0.316506
C	2.071078	-3.163005	-0.115491
H	2.119946	-4.265960	-0.091876
H	2.454402	-2.830080	0.866428
C	3.008826	-2.640765	-1.183627
C	4.747117	-1.578044	-3.120336
C	4.343141	-2.360100	-0.873716
C	2.569261	-2.420790	-2.492046
C	3.428334	-1.887416	-3.451004
C	5.206870	-1.828816	-1.829420
H	4.710316	-2.558521	0.131707
H	1.540793	-2.650272	-2.753014
H	3.064648	-1.711034	-4.459156
H	6.236418	-1.607148	-1.564239
H	5.413739	-1.154597	-3.865372
H	-0.721816	-0.423461	-0.047928
H	-1.587378	-0.057359	-3.538229
C	-2.335186	0.288326	-2.832701
C	-2.019994	0.406498	-1.503581
N	-4.616931	0.980919	-2.467942
C	-3.047255	0.803555	-0.596476
C	-3.645818	0.601593	-3.266817
C	-4.337803	1.060733	-1.135777
C	-2.862665	0.858645	0.805061
H	-3.888419	0.527428	-4.325611
H	-6.371431	1.594314	-0.674943
C	-3.931075	1.058371	1.649956
H	-1.903189	0.622881	1.251260
C	-5.208076	1.373380	1.112494
H	-6.025625	1.562078	1.801267
C	-5.397593	1.383579	-0.243690
O	-3.823185	0.905271	2.987197
H	-3.060295	0.286650	3.165257
C	2.386234	0.453581	2.159976
C	4.325865	0.575888	4.173957
C	2.137790	1.157120	3.342880
C	3.607525	-0.209644	2.008945
C	4.575591	-0.143343	3.007261
C	3.102689	1.221630	4.343590
H	1.176116	1.644337	3.485975
H	3.797286	-0.787366	1.108561
H	5.520382	-0.661529	2.876668
H	2.895463	1.768498	5.257668
H	5.078487	0.624433	4.954624

IId3E-S

H	-4.22954	1.39386	2.84781
C	-3.26475	0.88177	2.76839
C	-0.80939	1.14568	2.74505
C	-0.64216	0.97688	1.22316
C	-2.12220	1.85299	3.07065
C	-3.07123	0.30598	1.35579
H	-0.80525	0.15781	3.21792
H	-0.07018	1.81378	0.80724
H	-3.99220	0.35118	0.77174
H	-3.26571	0.06069	3.49061
H	0.05370	1.69814	3.12497
H	-2.14385	2.15909	4.12073
H	-2.69769	-0.71576	1.35675

N	-2.04164	1.12632	0.58708
C	-2.27606	3.08518	2.15885
H	-3.20598	3.59506	2.44194
C	-2.44380	2.57844	0.71651
C	-3.48724	2.62615	0.39112
H	-1.84932	3.15050	0.00819
C	-1.14394	4.06180	2.37408
H	-1.09365	4.43996	3.39579
C	-0.22877	4.47977	1.50351
H	0.54162	5.17957	1.80978
H	-0.18948	4.16069	0.46452
C	0.08503	-0.34768	0.88093
O	-0.73763	-1.43482	1.16760
C	-2.11094	0.69222	-0.88056
H	-3.17193	0.51246	-1.06847
H	-1.59420	-0.27019	-0.94466
C	3.79638	-1.59102	-1.18263
C	2.00185	-3.50071	-0.19093
C	4.17948	-2.43681	-0.14447
C	2.51402	-1.69338	-1.70616
C	1.62549	-2.66594	-1.23989
C	3.27818	-3.37634	0.35899
H	5.16956	-2.34602	0.29242
H	3.57072	-4.01260	1.18899
H	1.29752	-4.23090	0.19770
C	1.92212	-0.73872	-2.70266
O	2.51276	0.32099	-3.05572
H	-0.76188	-1.99368	0.29775
N	0.72402	-1.15565	-3.04784
H	0.24108	-0.54853	-3.70784
H	4.46454	-0.82524	-1.56706
C	0.27980	-2.75249	-1.89696
H	0.22773	-3.36882	-2.80161
N	-0.78880	-2.60170	-1.16017
C	-2.05234	-2.78199	-1.85225
H	-2.08425	-3.75426	-2.37329
H	-2.16764	-2.01413	-2.63706
C	-3.22501	-2.67915	-0.90024
C	-5.39062	-2.47609	0.87749
C	-4.39712	-2.01755	-1.27431
C	-3.15551	-3.24664	0.37505
C	-4.22702	-3.14370	1.25855
C	-5.47520	-1.91695	-0.39589
H	-4.46485	-1.57439	-2.26618
H	-2.24348	-3.75422	0.67748
H	-4.15306	-3.58646	2.24759
H	-6.37927	-1.40055	-0.70612
H	-6.22659	-2.39785	1.56609
H	0.34836	-0.35439	-0.18815
H	0.60361	-1.81309	3.07910
C	1.45772	-1.20869	2.79454
C	1.38565	-0.41213	1.67874
N	3.74740	-0.60000	3.23440
C	2.55712	0.29936	1.28909
C	2.65400	-1.25663	3.54628
C	3.71851	0.15139	2.09939
C	2.65262	1.03720	0.08628
H	2.69642	-1.87303	4.44310
H	5.79191	0.67151	2.33193
C	3.86613	1.51033	-0.35847
H	1.80182	1.12890	-0.57531
C	5.00730	1.42960	0.48430
H	5.94147	1.84909	0.12447
C	4.92672	0.77787	1.68479
O	4.02773	1.99581	-1.60862
H	3.44819	1.44674	-2.20661
C	-1.59092	1.70061	-1.87102
C	-0.64364	3.58628	-3.71260
C	-0.24308	1.73858	-2.22208
C	-2.47136	2.60333	-2.47919
C	-2.00037	3.54431	-3.38897
C	0.23553	2.67407	-3.13625
H	0.43578	0.99672	-1.82637
H	-3.53216	2.56790	-2.23889
H	-2.69318	4.24019	-3.85163
H	1.28804	2.65154	-3.39941
H	-0.27854	4.31790	-4.42659

IId4E-S

H	4.18516	-0.05469	-2.60324
C	3.15127	0.07904	-2.27051
C	1.12919	1.48643	-2.34863
C	0.79439	1.02959	-0.90546
C	2.63642	1.48277	-2.60069
C	3.08441	-0.11386	-0.75664
H	0.65912	0.80151	-3.05700
H	0.27089	1.82853	-0.36905
H	4.04352	0.09434	-0.27293
H	2.52844	-0.67692	-2.75691
H	0.69343	2.47333	-2.53051
H	2.84202	1.74065	-3.64314
H	2.74910	-1.10643	-0.47693
N	2.12407	0.89341	-0.13870
C	3.33532	2.48837	-1.66673
H	4.41332	2.28565	-1.69057
C	2.80926	2.23866	-0.23600
H	3.62404	2.23606	0.49083
H	2.08111	2.99245	0.07276
C	3.12190	3.92288	-2.06155
H	2.08975	4.27532	-2.06662
C	4.10175	4.75599	-2.39771
H	3.90069	5.78197	-2.68838
H	5.14197	4.43880	-2.39631
C	-0.09439	-0.24127	-0.83650
O	0.63799	-1.37262	-1.18636
C	1.94575	0.49198	1.32194
H	2.95198	0.21641	1.65352
H	1.33321	-0.41708	1.31769
C	-4.15137	-1.25769	0.60818
C	-2.43891	-3.23377	-0.39996
C	-4.47810	-1.93514	-0.56438
C	-2.96294	-1.56163	1.26017
C	-2.12191	-2.56838	0.78075
C	-3.61612	-2.90785	-1.07369
H	-5.39065	-1.68682	-1.09821
H	-3.86170	-3.41243	-2.00350
H	-1.76402	-3.99039	-0.79040
C	-2.40606	-0.80494	2.43118
O	-2.93120	0.25614	2.86824
H	0.50623	-2.02865	-0.40181
N	-1.29563	-1.38586	2.83470
H	-0.84896	-0.93742	3.63280
H	-4.78609	-0.46836	1.00169
C	-0.88909	-2.88535	1.57324
H	-1.02513	-3.60348	2.39065

N	0.27515	-2.80320	0.98274
C	1.40135	-3.26455	1.77664
H	1.23147	-4.29059	2.14575
H	1.52365	-2.63489	2.67464
C	2.68291	-3.21661	0.97478
C	5.02452	-3.03766	-0.56305
C	3.86101	-2.70907	1.52654
C	2.69634	-3.64922	-0.35541
C	3.85527	-3.55653	-1.12068
C	5.02698	-2.62194	0.76636
H	3.86169	-2.37116	2.56093
H	1.77784	-4.03065	-0.79351
H	3.84648	-3.88600	-2.15556
H	5.93470	-2.22365	1.21071
H	5.92876	-2.96589	-1.16020
H	-0.46679	-0.34590	0.19517
H	-0.53356	-1.39141	-3.22126
C	-1.34446	-0.72332	-2.95209
C	-1.30554	-0.06244	-1.74897
N	-3.48150	0.21766	-3.54431
C	-2.42447	0.74560	-1.39558
C	-2.44642	-0.54238	-3.81819
C	-3.49261	0.83871	-2.33318
C	-2.57397	1.35212	-0.12633
H	-2.46074	-1.05443	-4.77937
H	-5.44320	1.65870	-2.71687
C	-3.76331	1.93892	0.24091
H	-1.80709	1.24735	0.62941
C	-4.79550	2.10659	-0.72142
H	-5.70568	2.61252	-0.41498
C	-4.65455	1.57776	-1.97533
O	-4.01335	2.30497	1.51803
H	-3.60009	1.60695	2.09683
C	1.36783	1.55986	2.21458
C	0.26046	3.51397	3.88880
C	-0.00071	1.58086	2.48018
C	2.18825	2.50755	2.83789
C	1.63677	3.48286	3.66211
C	-0.55939	2.55251	3.30626
C	-0.63327	0.79748	2.08323
H	3.26545	2.47773	2.69239
H	2.28418	4.21279	4.13794
H	-1.62805	2.52583	3.49282
H	-0.16476	4.27438	4.53638

IId5E-S

H	-0.66299	4.51922	-2.84471
C	-0.75962	3.42881	-2.85800
C	-2.22405	1.50173	-2.34397
C	-1.52871	1.13612	-1.02575
C	-2.19929	3.01956	-2.53568
C	0.18160	2.78766	-1.82379
H	-1.69917	1.01240	-3.17208
H	-2.25334	1.09517	-0.20524
H	0.91043	3.50272	-1.44147
H	-0.47917	3.08309	-3.85639
H	-3.24465	1.11143	-2.32375
H	-2.87715	3.32076	-3.33841
H	0.68512	1.90055	-2.20809
N	-0.61354	2.30814	-0.62901
C	-2.61032	3.72420	-1.22632
H	-2.61135	4.80439	-1.41117
C	-1.51252	3.43045	-0.17231
H	-0.86678	4.29496	-0.00493
H	-1.93717	3.12846	0.78970
C	-3.98687	3.33711	-0.75414
C	-4.12540	2.31469	-0.40038
C	-5.02466	4.16786	-0.75840
H	-6.00736	3.85100	-0.42511
H	-4.92627	5.19648	-1.09793
C	-0.81134	-0.22889	-1.09317
O	0.16723	-0.23111	-2.08624
C	0.31555	1.86732	0.48930
H	1.00653	1.14352	0.04590
H	-0.31293	1.33247	1.20814
C	-0.65988	-3.43474	1.97840
C	1.03123	-3.54753	-0.25481
C	-0.76391	-4.48858	1.07366
C	0.27950	-2.43639	1.75169
C	1.14976	-2.50811	0.66339
C	0.06532	-4.53233	-0.04836
H	-1.50946	-5.26279	1.22708
H	-0.04113	-5.34004	-0.76621
H	1.68615	-3.57963	-1.12074
C	0.39334	-1.15986	2.53486
O	-0.44671	-0.82168	3.41175
H	1.03063	-0.52618	-1.59780
N	1.43299	-0.47943	2.09592
H	1.61013	0.40070	2.57836
H	-1.32359	-3.35927	2.83545
C	2.18973	-1.43679	0.53539
H	3.11821	-1.62687	1.08592
N	2.24540	-0.74233	-0.57932
C	3.43190	0.09288	-0.70744
H	3.53066	0.77093	0.15835
H	3.29380	0.73439	-1.59047
C	4.72981	-0.68032	-0.86289
C	7.12916	-2.09233	-1.20100
C	4.78151	-1.80784	-1.68817
C	5.89123	-0.27663	-0.20471
C	7.08589	-0.97530	-0.37211
C	5.97128	-2.50778	-1.85811
H	3.87320	-2.13481	-2.18728
H	5.85899	0.59039	0.45137
H	7.97968	-0.65182	0.15337
H	5.99591	-3.38256	-2.50138
H	8.05716	-2.64127	-1.32936
H	-0.34957	-0.43552	-0.11840
H	-1.38050	-1.62879	-3.35112
C	-2.05016	-1.87840	-2.53508
C	-1.88429	-1.28247	-1.31210
N	-3.91096	-3.20279	-1.75848
C	-2.74320	-1.67445	-0.24331
C	-3.08626	-2.82791	-2.70887
C	-3.73640	-2.65285	-0.52388
C	-2.59676	-1.19968	1.08112
H	-3.22853	-3.29017	-3.68439
H	-5.33165	-3.83654	0.30145
C	-3.33590	-1.73831	2.11055
H	-1.80778	-0.50339	1.34127
C	-4.37127	-2.66883	1.82268
H	-4.96298	-3.05000	2.64904
C	-4.56651	-3.10405	0.53952
O	-3.07479	-1.45959	3.40258
H	-2.12089	-1.17488	3.47159

C	1.05398	2.97974	1.18658
C	2.43740	4.99700	2.54964
C	0.54374	3.51441	2.37383
C	2.28320	3.44641	0.70796
C	2.96746	4.45471	1.38122
C	1.22810	4.51988	3.05017
H	-0.38637	3.12540	2.78132
H	2.71720	3.00549	-0.18623
H	3.92030	4.80703	0.99953
H	0.82257	4.92119	3.97318
H	2.97378	5.77872	3.07799

IId6Z-S

H	2.71207	0.53553	-4.36279
C	2.33873	0.73967	-3.35519
C	2.79045	1.92696	-1.19692
C	2.15305	0.69560	-0.51085
C	3.37775	1.53771	-2.56117
C	2.07598	-0.59511	-2.63365
H	2.01113	2.67331	-1.34878
H	2.53812	0.57623	0.50396
H	2.55113	-1.44494	-3.13110
H	1.40809	1.30168	-3.42114
H	3.56243	2.35915	-0.55383
H	3.67102	2.43424	-3.11350
H	1.00763	-0.79907	-2.53111
N	2.66442	-0.55690	-1.23977
C	4.59749	0.62271	-2.35925
H	4.83453	0.14936	-3.32011
C	4.17208	-0.46054	-1.35291
C	4.53652	-1.44935	-1.64075
H	4.53879	-0.24455	-0.34645
C	5.82879	1.33566	-1.87501
H	5.75361	1.83448	-0.90809
C	6.96954	1.38994	-2.55527
H	7.83182	1.92980	-2.17769
H	7.07941	0.89887	-3.51927
C	0.59290	0.77548	-0.46896
O	0.12818	1.52012	-1.54532
C	2.31752	-1.84501	-0.50284
H	2.49137	-2.64532	-1.22713
H	1.25058	-1.80843	-0.28376
C	-4.81695	-3.15656	-1.00205
C	-4.92951	-0.96899	-2.76150
C	-6.02994	-2.77828	-1.57540
C	-3.67369	-2.44098	-1.32765
C	-3.71837	-1.35133	-2.19652
C	-6.08253	-1.69348	-2.45196
C	-6.93737	-3.32543	-1.33887
H	-7.03258	-1.40156	-2.88987
H	-4.97716	-0.10606	-3.42048
C	-2.28864	-2.72213	-0.83224
O	-2.02953	-3.52201	0.09700
H	-0.86562	1.20317	-1.72966
N	-1.45500	-1.98172	-1.54515
H	-0.47812	-2.05231	-1.27458
H	-4.74491	-3.99412	-0.31445
C	-2.42282	-0.58657	-2.38151
H	-1.95067	-0.69435	-3.35949
N	-2.26355	0.60291	-1.81703
C	-3.00347	0.83234	-0.58605
H	-2.69737	0.12477	0.20487
H	-4.08110	0.65556	-0.73132
C	-2.83165	2.23972	-0.05776
C	-2.58784	4.83967	0.96862
C	-2.49431	3.30323	-0.89547
C	-3.04499	2.49454	1.29984
C	-2.92830	3.78248	1.81179
C	-2.37149	4.59441	-0.38514
H	-2.31706	3.10466	-1.94798
H	-3.28924	1.66598	1.96316
H	-3.07717	3.95557	2.87385
H	-2.10487	5.41281	-1.04860
H	-2.48721	5.84529	1.36695
H	0.18244	-0.23807	-0.52497
H	0.76909	3.34352	0.36217
C	0.42617	2.68073	1.14996
C	0.20006	1.35149	0.88856
N	-0.23914	2.46861	3.45111
C	-0.36855	0.54728	1.92520
C	0.19301	3.19260	2.44477
C	-0.54010	1.16620	3.19900
C	-0.79799	-0.79939	1.75529
H	0.38718	4.24446	2.64788
H	-1.18935	0.88882	5.22906
C	-1.37250	-1.50099	2.79585
H	-0.75395	-1.28514	0.78633
C	-1.48603	-0.89364	4.07905
H	-1.92565	-1.47725	4.88162
C	-1.08351	0.39763	4.26693
O	-1.84933	-2.74907	2.67753
H	-1.87051	-3.03326	1.72669
C	3.10063	-2.09095	0.76145
C	4.54060	-2.58907	3.10689
C	2.67291	-1.55802	1.98073
C	4.24096	-2.90037	0.73506
C	4.96038	-3.14488	1.89996
C	3.39337	-1.80124	3.14671
H	1.75953	-0.97113	2.02813
H	4.56143	-3.35407	-0.20003
H	5.84199	-3.77677	1.86735
H	3.04493	-1.38541	4.08648
H	5.09830	-2.78439	4.01734

IId7Z-R

H	4.35474	2.79684	-1.31963
C	3.32688	2.57774	-1.62608
C	0.94846	3.21126	-1.39862
C	0.58169	2.09719	-0.40684
C	2.38219	3.68379	-1.14850
C	2.85775	1.23639	-1.03855
H	0.86646	2.82182	-2.41910
H	0.12155	2.51724	0.49642
H	2.30237	0.63005	-1.75279
H	3.31425	2.51084	-2.71724
H	0.22605	4.02491	-1.29915
H	2.57851	4.61970	-1.67770
H	3.68672	0.66011	-0.62712
N	1.89762	1.48202	0.10934
C	2.61748	3.88768	0.36071
H	3.64278	4.24983	0.49695
C	2.51953	2.49801	1.03835
H	3.50318	2.10833	1.30680
H	1.90376	2.52526	1.94193

C	1.68740	4.90147	0.97244
H	0.62756	4.64773	1.01376
C	2.09132	6.07632	1.44548
H	1.39121	6.79112	1.86520
H	3.13979	6.36483	1.42684
C	-0.40140	1.05891	-0.98502
O	0.16793	0.37495	-2.05915
C	1.62085	0.18334	0.85262
H	1.26416	-0.53058	0.10068
H	0.80299	0.42135	1.53925
C	-4.12368	-3.85641	1.28781
C	-2.90239	-4.00267	-1.24271
C	-4.52453	-4.82323	0.36690
C	-3.10058	-2.98823	0.93653
C	-2.49682	-3.04472	-0.32030
C	-3.91374	-4.89672	-0.88638
H	-5.31542	-5.52212	0.62200
H	-4.23794	-5.65110	-1.59729
H	-2.44812	-4.03890	-2.22944
C	-2.50991	-1.91835	1.79855
O	-3.06063	-1.48225	2.83445
H	0.01554	-0.64021	-1.85385
N	-1.36587	-1.54382	1.23905
H	-0.92789	-0.75172	1.70315
H	-4.58287	-3.77374	2.26835
C	-1.52860	-1.92608	-0.62158
H	-2.08171	-1.01426	-0.87772
N	-0.37602	-2.03798	-1.25734
C	0.38422	-3.23083	-0.93909
H	-0.04777	-4.13227	-1.40547
H	0.35415	-3.41445	0.14909
C	1.83607	-3.14162	-1.35764
C	4.55599	-3.03758	-2.07274
C	2.28707	-2.22916	-2.31474
C	2.76681	-4.01170	-0.77814
C	4.11128	-3.96759	-1.13233
C	3.63781	-2.17351	-2.66443
H	1.57808	-1.56171	-2.79382
H	2.42834	-4.72463	-0.02953
H	4.81534	-4.65246	-0.66808
H	3.97088	-1.45483	-3.40870
H	5.60585	-2.99457	-2.34691
H	-0.64332	0.35317	-0.18607
H	-1.11156	2.02509	-3.40283
C	-1.85940	2.24218	-2.64750
C	-1.68845	1.78382	-1.36452
N	-3.97461	3.26751	-2.12659
C	-2.74079	2.00480	-0.42304
C	-3.01521	2.98717	-2.97757
C	-3.86069	2.76756	-0.86555
C	-2.75690	1.46775	0.89004
H	-3.13573	3.36927	-3.98974
H	-5.76337	3.60113	-0.31381
C	-3.84844	1.63239	1.71664
H	-1.93616	0.86094	1.24710
C	-4.93189	2.45143	1.29261
H	-5.76321	2.58913	1.97642
C	-4.93175	3.00081	0.04119
O	-3.94639	1.06214	2.93178
H	-3.45943	0.19550	2.95101
C	2.79192	-0.37033	1.62110
C	4.92383	-1.45090	3.07210
C	2.94936	-0.07076	2.97794
C	3.69837	-1.23710	1.00462
C	4.76220	-1.77038	1.72649
C	4.01219	-0.60384	3.69975
H	2.22693	0.57069	3.47781
H	3.56189	-1.51010	-0.03833
H	5.45268	-2.44813	1.23378
H	4.12116	-0.36850	4.75355
H	5.74950	-1.87325	3.63642

IId8z-S

H	-3.14446	-3.76000	-2.28006
C	-2.70335	-3.16273	-1.47699
C	-2.95385	-2.39314	0.88765
C	-2.39000	-1.03350	0.40891
C	-3.64129	-3.13266	-0.26762
C	-2.48623	-1.72254	-1.97692
H	-2.12192	-3.00285	1.23999
H	-2.75444	-0.21970	1.03976
H	-1.42547	-1.50825	-2.11735
H	-1.74288	-3.59287	-1.19457
H	-3.64892	-2.24335	1.71859
H	-3.89938	-4.14958	0.03932
H	-3.02182	-1.51135	-2.90652
N	-3.01157	-0.72891	-0.96386
C	-4.91071	-2.37518	-0.69277
H	-5.23298	-2.76656	-1.66547
C	-4.51283	-0.89690	-0.84988
H	-4.95423	-0.44952	-1.74346
H	-4.81851	-0.30073	0.01327
C	-6.05837	-2.51170	0.26819
H	-5.89734	-2.12853	1.27653
C	-7.22464	-3.06785	-0.04446
H	-8.02278	-3.16279	0.68439
H	-7.41939	-3.45362	-1.04237
C	-0.83155	-1.00971	0.38634
O	-0.33981	-2.28253	0.09483
C	-2.72567	0.69122	-1.44522
H	-2.99775	0.69159	-2.50425
H	-1.64920	0.85374	-1.37762
C	3.70789	2.35949	-2.26233
C	4.61107	-0.29996	-2.16262
C	5.07423	2.08257	-2.23205
C	2.81408	1.29831	-2.24915
C	3.24817	-0.02829	-2.19011
C	5.51854	0.76140	-2.19160
H	5.79397	2.89545	-2.24254
H	6.58383	0.55193	-2.16739
H	4.96729	-1.32370	-2.09507
C	1.32590	1.41286	-2.34050
O	0.69784	2.50139	-2.28840
H	0.57671	-2.17412	-0.40424
N	0.83653	0.19402	-2.45858
H	-0.16550	0.11583	-2.60375
H	3.33267	3.37820	-2.30075
C	2.16099	-1.08117	-2.06718
H	1.97211	-1.66813	-2.96781
N	1.98632	-1.73882	-0.92282
C	2.55746	-1.13962	0.28034
H	1.93146	-1.45139	1.12774
H	2.53008	-0.03900	0.27393
C	3.97539	-1.58729	0.58867
C	6.58611	-2.41285	1.20272

C	4.85404	-0.73306	1.25691
C	4.41805	-2.86364	0.23575
C	5.71389	-3.27413	0.53923
C	6.15064	-1.13914	1.56215
C	4.52080	0.26852	1.52167
H	3.73788	-3.51858	-0.30130
H	6.04615	-4.26869	0.25412
H	6.82485	-0.45692	2.07246
H	7.59844	-2.73039	1.43510
H	-0.48709	-0.31122	-0.38207
H	-0.79145	-2.28575	2.78983
C	-0.42930	-1.26523	2.85729
C	-0.35079	-0.47460	1.73608
N	0.51025	0.43489	4.27744
C	0.21891	0.83090	1.87279
C	0.00364	-0.76382	4.10590
C	0.63762	1.22485	3.17703
C	0.43392	1.72268	0.78849
H	-0.07298	-1.39160	4.99196
H	1.54849	2.77804	4.35084
C	1.05846	2.93999	0.97409
H	0.13942	1.46024	-0.21887
C	1.45474	3.33395	2.28385
H	1.93224	4.30123	2.40310
C	1.24474	2.50169	3.34611
O	1.32034	3.79776	-0.02365
H	1.08579	3.38713	-0.90120
C	-3.47566	1.77642	-0.71466
C	-4.85238	3.83217	0.59290
C	-2.98830	2.30446	0.48417
C	-4.64772	2.30663	-1.26290
C	-5.33482	3.32651	-0.61262
C	-3.67683	3.32274	1.13746
H	-2.05237	1.94239	0.90017
H	-5.01832	1.93186	-2.21416
H	-6.24019	3.73250	-1.05202
H	-3.28150	3.72634	2.06380
H	-5.38404	4.63206	1.09829

IId9Z-R

H	4.08439	-1.08750	-3.11580
C	3.35891	-0.42758	-2.63126
C	2.98843	1.70445	-1.44720
C	1.88835	1.00942	-0.60988
C	4.06327	0.70930	-1.88766
C	2.54161	-1.23184	-1.61765
H	2.53926	2.13349	-2.34284
H	1.84082	1.45584	0.38760
H	3.05739	-2.14329	-1.30057
H	2.69034	-0.01713	-3.39107
H	3.41962	2.53331	-0.87862
H	4.78806	1.20682	-2.53779
H	1.54937	-1.50080	-1.97533
N	2.35315	-0.43509	-0.33684
C	4.78597	0.11841	-0.66198
H	5.36073	-0.75509	-0.99347
C	3.70297	-0.34343	0.33657
H	3.92110	-1.33153	0.75002
H	3.58906	0.35288	1.17144
C	5.73732	1.07787	-0.00342
H	5.30251	1.99187	0.40303
C	7.04648	0.87132	0.09998
H	7.70212	1.59618	0.57131
H	7.50951	-0.03295	-0.28800
C	0.46602	1.07965	-1.23048
O	0.42847	0.48130	-2.45902
C	1.40291	-1.24259	0.53413
H	1.74305	-2.27665	0.42812
H	0.42094	-1.19328	0.05470
C	-5.63156	-1.03210	0.21497
C	-4.37984	-1.57688	-2.24662
C	-6.38499	-1.44125	-0.88408
C	-4.25541	-0.92529	0.07223
C	-3.62660	-1.18447	-1.14582
C	-5.76117	-1.71515	-2.10318
H	-7.46201	-1.54644	-0.79518
H	-6.35977	-2.02776	-2.95363
H	-3.89606	-1.75953	-3.20250
C	-3.27636	-0.53014	1.13072
O	-3.60089	0.01009	2.20951
H	-0.17088	-0.35470	-2.39163
N	-2.06020	-0.82698	0.67990
H	-1.29812	-0.54727	1.29617
H	-6.09274	-0.80714	1.17200
C	-2.15643	-0.83465	-1.18180
H	-2.06051	0.25377	-1.27797
N	-1.20524	-1.47876	-1.84800
C	-1.30618	-2.92779	-1.95533
H	-1.04802	-3.22697	-2.98000
H	-2.33336	-3.27404	-1.76951
C	-0.37769	-3.65676	-0.99962
C	1.38309	-4.91872	0.79303
C	-0.69400	-3.75744	0.36106
C	0.82471	-4.20792	-1.44597
C	1.70401	-4.83348	-0.56001
C	0.17861	-4.37833	1.25039
H	-1.62174	-3.31897	0.71942
H	1.07521	-4.14825	-2.50362
H	2.63120	-5.26322	-0.92954
H	-0.08016	-4.44217	2.30361
H	2.05917	-5.41151	1.48627
H	-0.19842	0.55314	-0.53880
H	0.82238	2.85503	-3.24652
C	0.35562	3.31056	-2.37989
C	0.01799	2.53913	-1.29305
N	-0.45483	5.33389	-1.36109
C	-0.73641	3.16421	-0.25000
C	0.09817	4.70027	-2.36897
C	-0.89147	4.57975	-0.31617
C	-1.37518	2.46105	0.80487
H	0.39380	5.30585	-3.22371
H	-1.64382	6.32512	0.68689
C	-2.07234	3.12371	1.79390
H	-1.40423	1.38043	0.79829
C	-2.12512	4.54639	1.77974
H	-2.66186	5.04574	2.57976
C	-1.56627	5.24407	0.74673
O	-2.71802	2.50478	2.79637
H	-2.88659	1.54540	2.59808
C	1.39259	-0.87920	1.99690
C	1.33880	-0.34543	4.75019
C	1.97674	-1.76575	2.90769
C	0.77959	0.27753	2.48861
C	0.74821	0.54253	3.85516
C	1.95429	-1.50064	4.27361

H	2.43002	-2.68343	2.53917
H	0.31037	0.98556	1.81350
H	0.24778	1.43735	4.21198
H	2.40714	-2.20238	4.96686
H	1.31049	-0.14317	5.81610

I1e1E-R

H	3.45304	2.92192	-2.07502
C	2.66722	2.16228	-2.13862
C	0.22375	1.75772	-2.32011
C	0.03662	1.33899	-0.84879
C	1.31893	2.82051	-2.44138
C	2.55431	1.38380	-0.82130
H	0.50738	0.87452	-2.90205
H	-0.77180	1.91204	-0.38173
H	3.37848	1.57535	-0.12913
H	2.94143	1.46610	-2.93587
H	-0.73165	2.11751	-2.71055
H	1.31691	3.25918	-3.44282
H	2.46761	0.31114	-0.98674
N	1.28446	1.78095	-0.07594
C	1.09732	3.92906	-1.39693
H	1.89652	4.66958	-1.51336
C	1.23864	3.28559	0.00521
H	2.15535	3.59230	0.51628
H	0.38205	3.54255	0.62613
C	-0.22120	4.63729	-1.55727
H	-1.12173	4.05785	-1.34685
C	-0.33780	5.90479	-1.94080
H	-1.30780	6.37648	-2.05936
H	0.53697	6.51494	-2.15391
C	-0.29790	-0.16585	-0.73137
O	0.71209	-0.93086	-1.30658
C	1.41752	1.15679	1.29993
H	2.32750	1.58601	1.73432
H	1.63175	0.10166	1.10924
C	5.35399	-0.44788	-0.36674
C	3.72482	-2.55514	-1.22960
C	5.49579	-0.95800	-1.65561
C	4.40722	-1.00365	0.48543
C	3.60567	-2.06277	0.06845
C	4.67482	-2.00218	-2.08764
H	6.23361	-0.53659	-2.33226
H	4.77251	-2.38360	-3.09971
H	3.06959	-3.35375	-1.56686
C	4.04439	-0.44188	1.83387
O	4.45249	0.68802	2.18127
H	0.96200	-1.64038	-0.59890
N	3.20057	-1.27096	2.42621
H	2.83201	-0.93107	3.31376
H	5.94608	0.39188	-0.01336
C	2.58826	-2.60794	1.02878
H	2.91483	-3.43808	1.66434
N	1.33413	-2.52921	0.66536
C	0.37296	-3.33515	1.40337
H	0.16989	-2.91394	2.40165
H	0.77285	-4.34717	1.57882
C	-0.92373	-3.42629	0.63051
C	-3.29196	-3.58189	-0.86462
C	-2.09151	-2.81405	1.08197
C	-0.95063	-4.10499	-0.59250
C	-2.12449	-4.18891	-1.33148
C	-3.27186	-2.88978	0.34065
H	-2.08048	-2.26213	2.01990
H	-0.03575	-4.56358	-0.96118
H	-2.13173	-4.72089	-2.27873
H	-4.16825	-2.38947	0.69873
H	-4.20576	-3.63170	-1.44909
H	-0.41963	-0.43666	0.32623
H	-0.79380	-1.42673	-3.05295
C	-1.70515	-1.03816	-2.61232
C	-1.64553	-0.38881	-1.40747
N	-4.10022	-0.81369	-2.75248
C	-2.86804	0.05589	-0.81899
C	-2.95619	-1.21922	-3.24926
C	-4.06856	-0.19283	-1.53957
C	-2.94755	0.67710	0.45504
H	-2.99784	-1.72682	-4.21195
H	-6.20931	-0.00192	-1.53827
C	-4.16618	1.03558	0.98292
H	-2.05106	0.84896	1.04483
C	-5.36476	0.79804	0.26229
H	-6.30576	1.09692	0.71244
C	-5.30912	0.20003	-0.96653
O	-4.29915	1.62623	2.19716
H	-3.42154	1.71503	2.60615
C	0.25982	1.25061	2.26835
C	-1.77897	1.20129	4.20704
C	-0.23090	2.44049	2.81779
C	-0.25055	0.03806	2.75156
C	-1.25730	0.00747	3.70987
C	-1.25845	2.41627	3.76087
H	0.20475	3.39859	2.55665
H	0.16875	-0.88722	2.36438
H	-1.63027	-0.94507	4.07392
H	-1.62983	3.35037	4.17080
H	-2.56635	1.18555	4.95518

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H	2.89033	-0.06095	3.33912
C	2.42489	-0.57396	2.49256
C	2.55597	-2.53148	0.95618
C	2.03233	-1.61297	-0.17458
C	3.31496	-1.71561	2.00141
C	2.22690	0.42399	1.34635
H	1.70558	-3.03553	1.42029
H	2.44541	-1.91194	-1.14263
H	1.20520	0.79474	1.26593
H	1.45548	-0.96366	2.81170
H	3.22220	-3.29345	0.53973
H	3.60702	-2.36285	2.83382
H	2.88108	1.29442	1.44104
N	2.62676	-0.21038	0.02503
C	4.56902	-1.11617	1.33658
H	4.97437	-0.36330	2.02673
C	4.12809	-0.40054	0.04628
H	4.57930	0.58677	-0.03972
H	4.36876	-0.97018	-0.85508
C	5.64619	-2.15052	1.13103
H	5.90597	-2.68970	2.04227
C	6.29813	-2.45341	0.01173
H	7.06328	-3.22283	0.01160
H	6.12610	-1.95543	-0.93799
C	0.50401	-1.64546	-0.31429

O	-0.03157	-1.42231	0.97991
C	2.21706	0.69757	-1.13424
H	1.15773	0.92921	-0.97964
H	2.32620	0.08915	-2.03762
C	-1.37483	4.91522	0.01773
C	-3.63891	3.99401	-1.35011
C	-2.28986	5.82340	-0.50946
C	-1.58798	3.55395	-0.16259
C	-2.71403	3.08779	-0.83486
C	-3.41856	5.36180	-1.18884
H	-2.13410	6.89075	-0.38350
H	-4.13722	6.07224	-1.58648
H	-4.52724	3.63393	-1.86237
C	-0.72431	2.46865	0.40864
O	0.09188	2.71702	1.32623
H	-0.98140	-1.64125	1.00615
N	-1.02268	1.30781	-0.16273
H	-0.73305	0.52280	0.42449
H	-0.50106	5.23991	0.57564
C	-2.90505	1.60078	-0.99220
H	-2.62965	1.20656	-1.97256
N	-3.82171	0.91327	-0.37120
C	-4.17858	1.27661	0.99279
H	-5.23795	1.03884	1.14511
H	-4.04493	2.34924	1.18534
C	-3.33359	0.46711	1.96223
C	-1.69274	-1.09214	3.61939
C	-3.48421	-0.92338	2.00696
C	-2.35112	1.06339	2.75066
C	-1.52952	0.29002	3.57040
C	-2.67482	-1.69985	2.83454
H	-4.23708	-1.39405	1.37768
H	-2.19221	2.13768	2.69529
H	-0.75517	0.77200	4.16031
H	-2.80890	-2.77780	2.86397
H	-1.05541	-1.69707	4.25818
H	0.17558	-0.84441	-0.99250
H	1.90646	-4.00043	-1.00159
C	0.83683	-4.03655	-1.17032
C	0.01754	-2.96399	-0.90665
N	-0.98718	-5.42680	-1.88172
C	-1.38178	-3.10282	-1.18347
C	0.29176	-5.24427	-1.66210
C	-1.82064	-4.37839	-1.65115
C	-2.32787	-2.05740	-1.02012
H	0.95181	-6.08606	-1.86275
H	-3.51273	-5.55631	-2.25552
C	-3.67806	-2.27302	-1.28247
H	-2.01719	-1.05867	-0.71921
C	-4.10230	-3.56707	-1.72048
H	-5.16171	-3.70360	-1.91322
C	-3.20550	-4.57574	-1.90571
O	-4.61848	-1.35491	-1.15399
H	-4.23391	-0.39242	-0.83077
C	3.01892	1.96762	-1.26165
C	4.48225	4.32967	-1.56693
C	2.67490	3.10614	-0.52559
C	4.08672	2.02933	-2.16316
C	4.81805	3.20268	-2.31505
C	3.41201	4.27851	-0.67759
H	1.82653	3.07763	0.15837
H	4.34287	1.15223	-2.75371
H	5.64273	3.23964	-3.01981
H	3.13822	5.15864	-0.10417
H	5.04802	5.24865	-1.68577

Ilg1Z-S

H	-5.44889	0.97831	-2.40842
C	-4.54107	0.36669	-2.42300
C	-3.36705	-1.57249	-1.43881
C	-2.45555	-0.75918	-0.50623
C	-4.73110	-0.89025	-1.57098
C	-3.34193	1.15820	-1.87470
H	-2.89993	-1.64372	-2.42672
H	-2.56119	-1.10096	0.53121
H	-2.43241	1.00423	-2.45345
H	-4.34109	0.09661	-3.46323
H	-3.45442	-2.58910	-1.04803
H	-5.45706	-1.56665	-2.02908
H	-3.56161	2.22287	-1.79227
N	-3.00505	0.68237	-0.47352
C	-5.24344	-0.44775	-0.18700
H	-6.22786	0.01377	-0.32334
C	-4.28115	0.64892	0.33369
H	-4.72122	1.64495	0.25478
H	-3.99578	0.47699	1.37557
C	-5.40154	-1.59071	0.78018
H	-4.49469	-2.10632	1.09852
C	-6.57754	-2.00027	1.24539
H	-6.65770	-2.83772	1.93057
H	-7.50389	-1.51044	0.95402
C	-0.95540	-0.83994	-0.87267
O	-0.70554	-0.18949	-2.08055
C	-1.99553	1.60662	0.18347
H	-1.09361	1.55226	-0.42954
H	-1.79703	1.15495	1.15841
C	4.42075	1.40675	2.32298
C	4.01889	2.59031	-0.19193
C	5.47534	2.03702	1.66593
C	3.17416	1.37938	1.71170
C	2.97016	1.94682	0.45676
C	5.27053	2.63234	0.41903
H	6.45961	2.06961	2.12373
H	6.09880	3.11720	-0.08916
H	3.87273	3.01647	-1.18041
C	1.92710	0.78319	2.28559
O	1.92521	0.08139	3.32203
H	0.14784	0.39380	-1.85643
N	0.91095	1.14712	1.51619
H	0.01991	0.75268	1.80234
H	4.54687	0.94486	3.29770
C	1.60689	1.74457	-0.17250
H	0.99751	2.64940	-0.24389
N	1.43246	0.88063	-1.16438
C	2.25013	-0.33455	-1.11564
H	1.77154	-1.05890	-1.78923
H	2.22195	-0.78919	-0.11013
C	3.69458	-0.17169	-1.54602
C	6.36121	0.18584	-2.33560
C	3.99980	0.46526	-2.75184
C	4.73930	-0.64214	-0.75194
C	6.06516	-0.46265	-1.13981
C	5.32189	0.64574	-3.14445
H	3.18711	0.84324	-3.36770
H	4.51135	-1.12153	0.19747

H	6.86718	-0.81797	-0.49892
H	5.54467	1.14836	-4.08171
H	7.39420	0.33264	-2.63748
H	-0.37866	-0.34924	-0.07982
H	-0.84547	-2.54842	-2.97226
C	-0.59789	-3.03826	-2.03600
C	-0.54844	-2.30764	-0.87458
N	0.00320	-5.08033	-0.91188
C	-0.11465	-2.96209	0.31873
C	-0.31643	-4.42346	-2.00300
C	0.12613	-4.36413	0.23924
C	0.13486	-2.29033	1.54314
H	-0.37415	-5.00474	-2.92166
H	0.69976	-6.12394	1.33234
C	0.61693	-2.96951	2.64256
H	0.02439	-1.21604	1.61742
C	0.78016	-4.38261	2.57971
H	1.13398	-4.89455	3.46895
C	0.54426	-5.05265	1.41217
O	0.94320	-2.36239	3.79480
H	1.14823	-1.40189	3.63113
C	-2.43620	3.03704	0.34649
C	-3.17077	5.71659	0.66134
C	-3.12603	3.45226	1.48899
C	-2.09320	3.98407	-0.62307
C	-2.46348	5.31677	-0.47015
C	-3.49675	4.78438	1.64367
H	-3.35884	2.73366	2.27123
H	-1.52244	3.67502	-1.49617
H	-2.18892	6.04343	-1.22799
H	-4.02895	5.09565	2.53670
H	-3.45429	6.75695	0.78505

IIh1E-R

H	-2.64731	-2.31002	-2.45982
C	-1.67224	-2.21546	-1.97324
C	-0.02523	-3.27312	-0.43489
C	0.25035	-1.86351	0.14240
C	-1.45578	-3.35994	-0.98038
C	-1.62461	-0.88262	-1.21376
H	0.68683	-3.46748	-1.24155
H	0.53872	-1.92068	1.19548
H	-2.61378	-0.44361	-1.06351
H	-0.89189	-2.23542	-2.73585
H	0.12414	-4.02811	0.34241
H	-1.61032	-4.32045	-1.47925
H	-0.98900	-0.14515	-1.70051
N	-1.06621	-1.09140	0.18036
C	-2.46411	-3.18142	0.16240
H	-3.44642	-2.98446	-0.29098
C	-2.06013	-1.91646	0.95477
H	-2.91607	-1.26347	1.14857
H	-1.58499	-2.16338	1.90798
C	-2.62294	-4.34599	1.10683
H	-3.23497	-4.13949	1.98598
C	-2.10724	-5.56267	0.95800
H	-2.29045	-6.33989	1.69270
H	-1.49239	-5.83646	0.10509
C	1.36178	-1.11181	-0.61482
O	1.18787	-1.20544	-2.01301
C	-0.92913	0.27530	0.83087
H	-1.87832	0.81987	0.68179
H	-0.18452	0.80248	0.24591
C	1.83436	3.03485	0.10604
C	-0.37887	4.02950	1.54489
C	2.01020	3.61381	1.36214
C	0.54664	2.97980	-0.41493
C	-0.55165	3.48224	0.28059
C	0.90986	4.09599	2.07670
H	3.00364	3.67422	1.79594
H	1.06055	4.51666	3.06664
H	-1.24361	4.36749	2.10750
C	0.08523	2.24944	-1.63325
O	0.82203	1.52800	-2.35158
H	1.02641	-0.29654	-2.34765
N	-1.22445	2.42470	-1.71200
H	-1.76578	1.96302	-2.43430
H	2.67722	2.63135	-0.44900
C	-1.87905	3.27325	-0.42328
H	-2.19621	4.18233	-0.97457
N	-2.82122	2.67427	0.34344
C	-4.15632	2.74288	-0.19930
H	-4.28926	3.57455	-0.92044
H	-4.87999	2.91159	0.61443
C	-4.55208	1.44619	-0.88841
C	-5.13488	-1.03528	-2.09045
C	-4.97786	0.35569	-0.12072
C	-4.42893	1.26947	-2.26905
C	-4.70937	0.04096	-2.86813
C	-5.27229	-0.87206	-0.71093
H	-5.08741	0.48519	0.95493
H	-4.12261	2.11477	-2.88407
H	-4.61074	-0.07275	-3.94418
H	-5.62521	-1.69875	-0.09860
H	-5.37007	-1.98833	-2.55593
H	1.34219	-0.05310	-0.32757
H	2.21623	-3.35119	0.91268
C	3.00963	-2.72167	0.52414
C	2.75169	-1.60968	-0.23702
N	5.39734	-2.39696	0.42896
C	3.87180	-0.84439	-0.69276
C	4.35032	-3.07735	0.82287
C	5.17208	-1.27946	-0.31920
C	3.73482	0.33400	-1.46407
H	4.54230	-3.96723	1.41968
H	7.27893	-0.86847	-0.42868
C	4.84480	1.05495	-1.83256
H	2.75876	0.69058	-1.77649
C	6.14601	0.62935	-1.46430
H	6.99698	1.22483	-1.77805
C	6.29812	-0.51391	-0.72828
O	4.75415	2.20301	-2.55286
H	3.82258	2.35863	-2.78007
C	-0.52822	0.27424	2.27915
C	0.18722	0.40958	4.98074
C	-1.50864	0.40535	3.26682
C	0.81794	0.24453	2.65914
C	1.17418	0.30607	4.00308
C	-1.15492	0.46654	4.61138
H	-2.55043	0.49531	2.96846
H	1.59815	0.19672	1.90121
H	2.22222	0.28503	4.28475
H	-1.92460	0.57550	5.36891
H	0.46513	0.46243	6.02893

IIIE-S

H	2.49362	-2.95125	-1.17470
C	1.67852	-2.24583	-1.36265
C	0.49801	-0.87409	-3.09048
C	0.36883	0.23026	-2.01468
C	1.72517	-1.75066	-2.81267
C	1.82104	-1.04095	-0.41943
H	-0.40410	-1.48895	-3.06974
H	0.35112	1.22639	-2.46708
H	2.81109	-0.98605	0.04046
H	0.73157	-2.74987	-1.16278
H	0.57358	-0.42367	-4.08529
H	1.74521	-2.59453	-3.50752
H	1.06460	-1.01385	0.36573
N	1.66027	0.25223	-1.19195
C	3.00222	-0.90519	-2.97961
H	3.83932	-1.46564	-2.54618
C	2.80300	0.39152	-2.16587
H	3.69404	0.63710	-1.58905
H	2.55955	1.24643	-2.80631
C	3.34544	-0.58750	-4.40791
H	2.60577	-0.01739	-4.97193
C	4.47450	-0.96028	-5.00268
H	4.67643	-0.72105	-6.04177
H	5.23728	-1.52280	-4.46970
C	-0.90171	0.06731	-1.16178
O	-1.08076	-1.29734	-0.86970
C	1.63389	1.43096	-0.22639
H	0.84684	1.20636	0.49640
H	1.35449	2.30545	-0.82175
C	0.43410	-4.78605	1.19348
C	1.62334	-2.55953	2.42386
C	1.80475	-4.76947	1.43538
C	-0.32216	-3.67655	1.55466
C	0.25404	-2.56739	2.16560
C	2.39410	-3.65997	2.05056
H	2.41859	-5.62035	1.15513
H	3.46219	-3.66054	2.24944
H	2.07884	-1.70302	2.91329
C	-1.80227	-3.53300	1.37456
O	-2.54308	-4.46461	1.06963
H	-1.44330	-1.43628	0.04018
N	-2.11600	-2.23749	1.62240
H	-3.11787	-2.10046	1.75663
H	-0.05740	-5.63550	0.72817
C	-0.67689	-1.43645	2.52564
H	-1.12725	-1.55877	3.52488
N	-0.34325	-0.21402	2.12622
C	-1.04565	0.83711	2.85198
H	-0.90593	0.74024	3.94338
H	-2.14119	0.80944	2.68909
C	-0.55323	2.19266	2.39944
C	0.52570	4.57400	1.37563
C	-1.20870	2.89362	1.38285
C	0.63414	2.71730	2.91401
C	1.17514	3.89579	2.40576
C	-0.67439	4.07477	0.87106
H	-2.14418	2.50549	0.98504
H	1.15175	2.17961	3.70516
H	2.11119	4.27714	2.80447
H	-1.19708	4.60564	0.08052
H	0.94676	5.49212	0.97669
H	-0.79546	0.63462	-0.22959
H	-1.27869	0.93600	-3.84443
C	-2.16005	0.97957	-3.21337
C	-2.13020	0.60977	-1.89175
N	-4.51128	1.50872	-3.16188
C	-3.35600	0.69850	-1.16013
C	-3.37179	1.42301	-3.80065
C	-4.51587	1.14916	-1.84652
C	-3.45552	0.36089	0.21158
H	-3.37739	1.71124	-4.85044
H	-6.61612	1.57753	-1.68826
C	-4.66033	0.45780	0.86560
H	-2.58103	0.02218	0.75742
C	-5.82327	0.89683	0.18394
H	-6.75534	0.95520	0.73621
C	-5.74530	1.23520	-1.13884
O	-4.81398	0.14084	2.17907
H	-3.95201	-0.09729	2.55594
C	2.91928	1.67127	0.51800
C	5.23356	2.18827	1.99506
C	3.13230	1.02918	1.74156
C	3.86080	2.59237	0.05491
C	5.01643	2.84900	0.78793
C	4.28863	1.28108	2.47324
H	2.35264	0.37158	2.12430
H	3.68162	3.12133	-0.87891
H	5.74112	3.56903	0.42131
H	4.44575	0.78326	3.42527
H	6.13217	2.39093	2.56950

Cartesian coordinates (Å) of the starting binary complexes

IaIE (denoted as IaI in the main article)

H	-1.758731	4.436487	2.238839
C	-0.970641	3.846757	1.762911
C	0.416372	3.527621	-0.266927
C	0.282811	2.001526	-0.073023
C	-0.810641	4.248540	0.293184
C	-1.330579	2.355465	1.844646
H	1.301787	3.872331	0.272727
H	0.267697	1.484337	-1.038752
H	-2.385414	2.192434	2.077728
H	-0.031960	4.021066	2.292681
H	0.564570	3.757677	-1.325283
H	-0.681724	5.330597	0.205796
H	-0.719177	1.810219	2.562907
N	-1.113832	1.696522	0.502098
C	-2.073883	3.815097	-0.472082
H	-2.946553	4.193357	0.073249
C	-2.120422	2.270841	-0.466691
H	-3.100981	1.911025	-0.158116
H	-1.884886	1.842782	-1.446898
C	-2.135789	4.344702	-1.878095
H	-1.359752	3.999831	-2.562780
C	-3.064240	5.192355	-2.310986
H	-3.064394	5.562545	-3.331136
H	-3.856899	5.547192	-1.656481

C	1.453177	1.429600	0.765275
O	1.636577	2.140370	1.950150
C	-1.294888	0.191088	0.616351
H	-0.549152	-0.137239	1.340821
H	-1.051312	-0.211444	-0.371393
C	3.116885	-1.168557	2.642984
C	2.589936	-3.053826	0.678721
C	4.161533	-1.698001	1.890854
C	1.797750	-1.582942	2.441718
C	1.529931	-2.510687	1.414613
C	3.900369	-2.661072	0.918405
H	5.179905	-1.367288	2.071881
H	4.710338	-3.091070	0.337455
H	2.373093	-3.778459	-0.100639
C	0.708058	-1.025967	3.346268
O	-0.172514	-1.818114	3.758897
H	1.428878	1.464893	2.695519
N	0.818304	0.268306	3.615062
H	0.078646	0.511643	4.278583
H	3.308168	-0.421261	3.406348
C	0.142756	-2.843679	1.021434
C	-0.610201	-2.861145	1.816416
N	-0.162589	-3.063534	-0.201146
C	-1.533783	-3.463290	-0.485214
H	-2.170024	-3.359974	0.408145
H	-1.513619	-4.531080	-0.740038
C	-2.176439	-2.707237	-1.631488
C	-3.532619	-1.288571	-3.642042
C	-1.526511	-1.710783	-2.359116
C	-3.508501	-3.002907	-1.942838
C	-4.182806	-2.302666	-2.935998
C	-2.202400	-1.000821	-3.354449
H	-0.486073	-1.476009	-2.160600
H	-4.026896	-3.776839	-1.380920
H	-5.218610	-2.542291	-3.157029
H	-1.679684	-0.224551	-3.905699
H	-4.057937	-0.736966	-4.415348
H	1.258979	0.378047	0.996676
H	3.537140	3.172956	0.823365
C	3.644097	2.431487	0.038973
C	2.693410	1.455434	-0.114570
N	4.985980	1.571371	-1.769719
C	2.902674	0.458510	-1.115918
C	4.769432	2.452253	-0.820303
C	4.074916	0.567274	-1.914376
C	2.036197	-0.646338	-1.308589
H	5.514034	3.237893	-0.705563
H	5.222204	-0.321910	-3.503437
C	2.342864	-1.632166	-2.223238
H	1.165350	-0.779411	-0.674812
C	3.491646	-1.500606	-3.048203
H	3.693467	-2.281993	-3.773954
C	4.328140	-0.428958	-2.897013
O	1.611807	-2.756638	-2.372611
H	0.981400	-2.863474	-1.608463
C	-2.651372	-0.284737	1.066733
C	-5.110708	-1.302679	1.919327
C	-2.841483	-0.634930	2.408190
C	-3.692678	-0.476357	0.151764
C	-4.918587	-0.978868	0.577564
C	-4.070098	-1.136638	2.831130
H	-2.012404	-0.563542	3.110122
H	-3.537857	-0.260801	-0.904017
H	-5.713324	-1.133352	-0.145644
H	-4.208451	-1.412157	3.871801
H	-6.064966	-1.700252	2.251081

Ib1E-R (denoted as Ib1 in the main article)

H	1.766765	4.487787	-2.099793
C	0.987334	3.867063	-1.649527
C	-0.436890	3.475383	0.334113
C	-0.275486	1.955782	0.110016
C	0.796009	4.225259	-0.172662
C	1.389252	2.390014	-1.759613
H	-1.310327	3.823539	-0.223040
H	-0.270861	1.421188	1.066571
H	2.460065	2.270214	-1.938990
H	0.052953	4.032337	-2.190341
H	-0.622101	3.677422	1.392365
H	0.653145	5.302652	-0.054891
H	0.842154	1.843901	-2.528350
N	1.134444	1.684868	-0.442810
C	2.048949	3.781897	0.606750
H	2.928571	4.177762	0.085604
C	2.106807	2.238114	0.571666
H	3.098931	1.885468	0.290150
H	1.840019	1.789158	1.534271
C	2.081072	4.283351	2.024026
H	1.288230	3.928609	2.684072
C	3.002471	5.118647	2.494384
H	2.981120	5.468709	3.521415
H	3.811216	5.482675	1.865064
C	-1.417161	1.370314	-0.753933
O	-1.556890	2.054435	-1.965499
C	1.334646	0.187557	-0.601015
H	0.611904	-0.122696	-1.354910
H	1.080071	-0.253549	0.367659
C	-2.926084	-1.029278	-2.830217
C	-2.652523	-2.897670	-0.797862
C	-4.047966	-1.466996	-2.133538
C	-1.656049	-1.539095	-2.547560
C	-1.515501	-2.452681	-1.484681
C	-3.914298	-2.420872	-1.125003
H	-5.027213	-1.066770	-2.378787
H	-4.785669	-2.771283	-0.580663
H	-2.531458	-3.611990	0.011457
C	-0.490764	-1.027312	-3.374508
O	-0.382026	0.254172	-3.470935
H	-1.240971	1.404927	-2.661177
N	0.265227	-1.937512	-3.908230
H	0.978709	-1.452161	-4.462487
H	-3.023658	-0.281741	-3.612111
C	-0.176195	-2.865405	-1.014348
H	0.611637	-2.925524	-1.772897
N	0.059913	-3.105537	0.219675
C	1.398904	-3.567453	0.559252
H	2.060905	-3.540140	-0.319662
H	1.313174	-4.619197	0.862484
C	2.055561	-2.791991	1.684582
C	3.428476	-1.354075	3.669842
C	1.418797	-1.771560	2.390750
C	3.382927	-3.100336	2.003554
C	4.065192	-2.391065	2.985187
C	2.103122	-1.052356	3.373376
H	0.382201	-1.526508	2.185198

H	3.891003	-3.893115	1.458892
H	5.097169	-2.640859	3.212721
H	1.590730	-0.258217	3.908655
H	3.960393	-0.794893	4.433094
H	-1.220548	0.313889	-0.954362
H	-3.491940	3.133534	-0.917823
C	-3.629920	2.399947	-0.130815
C	-2.690100	1.422410	0.072909
N	-5.050335	1.560791	1.627678
C	-2.944231	0.437141	1.075413
C	-4.789263	2.433204	0.682022
C	-4.151492	0.553751	1.818191
C	-2.094897	-0.672502	1.309401
H	-5.524503	3.221213	0.530079
H	-5.376730	-0.325960	3.352655
C	-2.455318	-1.661318	2.200264
H	-1.194730	-0.809954	0.719176
C	-3.638892	-1.521375	2.973256
H	-3.882866	-2.304457	3.684187
C	-4.456616	-0.440551	2.788147
O	-1.745488	-2.797806	2.364440
H	-1.103950	-2.909964	1.610033
C	2.709203	-0.241252	-1.038473
C	5.204897	-1.161903	-1.886379
C	2.977817	-0.390981	-2.403095
C	3.694858	-0.564578	-0.101753
C	4.939530	-1.023309	-0.525701
C	4.224004	-0.844491	-2.825066
H	2.196792	-0.155560	-3.123284
H	3.485581	-0.473757	0.962554
H	5.694602	-1.281875	0.210549
H	4.425576	-0.961267	-3.885172
H	6.173324	-1.524808	-2.216521

Ia5E

H	5.040877	2.664541	1.816299
C	4.474530	1.891135	1.289987
C	3.837189	0.972169	-0.939096
C	2.452646	0.659098	-0.326474
C	4.489591	2.152828	-0.216985
C	3.019249	1.913328	1.777334
H	4.472114	0.088656	-0.838397
H	1.674393	0.677979	-1.096747
H	2.764114	2.851088	2.277882
H	4.915653	0.917126	1.503724
H	3.734082	1.192486	-2.005688
H	5.516111	2.285171	-0.570699
H	2.778607	1.079790	2.436063
N	2.064949	1.824723	0.601186
C	3.668730	3.425487	-0.491337
H	4.006397	4.190893	0.220995
C	2.195748	3.101649	-0.203920
H	1.702290	3.892169	0.364389
H	1.623486	2.930461	-1.116630
C	3.914533	3.971384	-1.874962
H	4.968439	4.156948	-2.082928
C	3.023033	4.250903	-2.822406
H	3.346303	4.647101	-3.779569
H	1.952013	4.118544	-2.699112
C	2.420329	-0.735520	0.354615
O	3.476168	-0.927290	1.245871
C	0.640113	1.696071	1.150505
H	0.673081	2.112138	2.159098
H	0.429536	0.634826	1.275348
C	0.905419	-3.271509	2.166378
C	-1.669688	-3.165052	1.148077
C	0.426640	-4.318953	1.385687
C	0.111210	-2.156677	2.452338
C	-1.192188	-2.105190	1.926280
C	-0.869410	-4.269051	0.877665
H	1.066239	-5.169145	1.168516
H	-1.251325	-5.078574	0.263068
H	-2.673047	-3.104419	0.735084
C	0.666790	-1.001892	3.273786
O	-0.149186	-0.141799	3.688474
H	3.026136	-1.076101	2.151417
N	1.983520	-1.010433	3.449956
H	2.200440	-0.216747	4.058103
H	1.917294	-3.291134	2.558205
C	-2.095979	-0.937117	2.100028
H	-2.363751	-0.631231	3.112308
N	-2.574402	-0.347523	1.074631
C	-3.499836	0.755894	1.300275
H	-2.966692	1.692461	1.099160
H	-3.820721	0.786982	2.352641
C	-4.710840	0.690427	0.394571
C	-7.005592	0.632141	-1.215845
C	-5.178131	-0.515649	-0.128225
C	-5.405183	1.867623	0.100940
C	-6.546424	1.841416	-0.694468
C	-6.317443	-0.544200	-0.931848
H	-4.642513	-1.436517	0.084487
H	-5.040681	2.812189	0.498792
H	-7.073997	2.764879	-0.914074
H	-6.666691	-1.489816	-1.335702
H	-7.892297	0.609433	-1.841883
H	1.478227	-0.845105	0.895555
H	4.475808	-2.297635	-0.522458
C	3.559247	-2.467636	-1.077233
C	2.417756	-1.785473	-0.744066
N	2.455239	-3.675371	-2.850333
C	1.219812	-2.086830	-1.456980
C	3.526225	-3.402399	-2.141402
C	1.299732	-3.034762	-2.512916
C	-0.031541	-1.512309	-1.137190
H	4.436655	-3.934845	-2.410852
H	0.199062	-4.059357	-4.051707
C	-1.169438	-1.847196	-1.839570
H	-0.133452	-0.852718	-0.283052
C	-1.081429	-2.762051	-2.924107
H	-1.988975	-3.004466	-3.467790
C	0.118130	-3.340218	-3.242497
O	-2.384930	-1.353627	-1.536113
H	-2.372748	-0.915383	-0.638348
C	-0.447943	2.381809	0.360595
C	-2.585369	3.646752	-0.940539
C	-0.994366	3.563364	0.870018
C	-0.983875	1.843482	-0.814990
C	-2.047082	2.469801	-1.458936
C	-2.055658	4.195234	0.224879
H	-0.596826	3.983168	1.790769
H	-0.591555	0.921444	-1.232049
H	-2.465413	2.025124	-2.356285
H	-2.471602	5.108214	0.638743
H	-3.422049	4.126855	-1.438414

Ib8E-R

H	5.160867	2.154135	1.996349
C	4.552782	1.455498	1.414643
C	3.930138	0.704032	-0.888032
C	2.498557	0.491039	-0.342313
C	4.661053	1.777985	-0.076929
C	3.083622	1.589141	1.844576
H	4.475696	-0.239109	-0.816212
H	1.756358	0.612087	-1.138182
H	2.896341	2.529756	2.369967
H	4.902153	0.441031	1.605870
H	3.891392	0.992602	-1.942588
H	5.710514	1.824009	-0.381748
H	2.739648	0.759092	2.468001
N	2.183979	1.648052	0.621495
C	3.980867	3.136429	-0.319822
H	4.354480	3.830457	0.445852
C	2.473110	2.940306	-0.115157
H	2.026089	3.748190	0.467207
H	1.934812	2.863867	-1.060932
C	4.340791	3.724150	-1.660629
H	5.416042	3.802373	-1.822868
C	3.522120	4.154739	-2.617187
H	3.921824	4.565193	-3.538774
H	2.439222	4.135913	-2.534949
C	2.319369	-0.923308	0.275827
O	3.362797	-1.265665	1.139499
C	0.731329	1.649623	1.097781
H	0.755266	2.091297	2.095868
H	0.429626	0.611937	1.237745
C	0.693318	-3.281140	2.250196
C	-1.850958	-2.963109	1.211671
C	0.126933	-4.299010	1.488924
C	0.000878	-2.097757	2.520820
C	-1.291062	-1.937958	1.981889
C	-1.154585	-4.141582	0.968353
H	0.688439	-5.207847	1.294563
H	-1.604178	-4.921972	0.362171
H	-2.836604	-2.815431	0.778289
C	0.726863	-1.016796	3.306379
O	2.008741	-1.111798	3.362029
H	2.936919	-1.332297	2.046499
N	-0.015681	-0.086693	3.833159
H	0.617835	0.558417	4.317435
H	1.701545	-3.376261	2.640036
C	-2.091413	-0.692226	2.120224
H	-2.280287	-0.303778	3.121405
N	-2.555789	-0.120669	1.078086
C	-3.397955	1.056135	1.257991
H	-2.839809	1.933370	0.911376
H	-3.627917	1.213251	2.322718
C	-4.677067	0.947891	0.456104
C	-7.079371	0.791306	-0.978278
C	-5.328037	-0.277131	0.296363
C	-5.240510	2.092027	-0.112321
C	-6.436592	2.017726	-0.821292
C	-6.520810	-0.355941	-0.418604
H	-4.895182	-1.174354	0.731106
H	-4.734170	3.047683	0.002550
H	-6.862538	2.916352	-1.257520
H	-7.013627	-1.315986	-0.539271
H	-8.008548	0.729711	-1.536473
H	1.376527	-0.960432	0.825956
H	4.241562	-2.569420	-0.734410
C	3.301130	-2.651598	-1.268409
C	2.212846	-1.920464	-0.866607
N	2.082388	-3.692978	-3.070321
C	0.979292	-2.115642	-1.556045
C	3.185204	-3.524072	-2.378049
C	0.976324	-3.005887	-2.665511
C	-0.228375	-1.489879	-1.171009
H	4.055099	-4.093751	-2.699848
H	-0.220051	-3.874530	-4.229238
C	-1.400692	-1.716121	-1.861798
H	-0.272212	-0.868858	-0.283936
C	-1.392896	-2.572111	-2.996960
H	-2.326398	-2.728168	-3.528303
C	-0.238331	-3.200514	-3.378488
O	-2.576370	-1.167961	-1.505233
H	-2.505878	-0.748197	-0.600348
C	-0.256870	2.408187	0.244421
C	-2.207127	3.831318	-1.183318
C	-0.719481	3.644933	0.705523
C	-0.785867	1.892985	-0.944211
C	-1.755427	2.598467	-1.651359
C	-1.686617	4.355063	-0.002077
H	-0.330944	4.048040	1.637524
H	-0.460645	0.930276	-1.324487
H	-2.166871	2.174346	-2.561654
H	-2.037791	5.310257	0.374719
H	-2.969141	4.375759	-1.732444

Ia7E

H	-5.142424	-2.037028	2.218621
C	-4.544907	-1.338682	1.625924
C	-4.044715	-0.508883	-0.679383
C	-2.572547	-0.381082	-0.224866
C	-4.766227	-1.587185	0.133010
C	-3.058705	-1.551844	1.943773
H	-4.540259	0.453209	-0.531050
H	-1.890678	-0.496435	-1.073628
H	-2.872811	-2.514946	2.426347
H	-4.831725	-0.318916	1.883214
H	-4.088671	-0.752071	-1.745094
H	-5.834564	-1.578079	-0.101222
H	-2.636274	-0.758437	2.560629
N	-2.242812	-1.592132	0.666337
C	-4.161381	-2.959520	-0.217312
H	-4.517104	-3.675417	0.536277
C	-2.635202	-2.838593	-0.100407
H	-2.192080	-3.688719	0.421565
H	-2.150784	-2.747660	-1.072959
C	-4.635688	-3.458935	-1.558338
H	-5.721421	-3.525548	-1.631028
C	-3.907865	-3.818337	-2.612629
H	-4.391144	-4.162989	-3.521137
H	-2.821964	-3.803738	-2.628830
C	-2.291931	0.997557	0.435335
O	-3.258175	1.348334	1.377018
C	-0.762425	-1.659172	1.053060
H	-0.737644	-2.090340	2.055522
H	-0.408561	-0.634768	1.163713
C	-0.348902	3.276842	2.227852

C	2.087945	2.757249	1.017392
C	0.240578	4.241928	1.418013
C	0.262678	2.038184	2.448583
C	1.496787	1.777513	1.824308
C	1.468691	3.984360	0.813060
H	-0.258244	5.193186	1.258630
H	1.936466	4.729280	0.176637
H	3.033370	2.532642	0.530881
C	-0.434532	0.986094	3.301427
O	0.237892	-0.006270	3.674372
H	-2.756976	1.424348	2.265085
N	-1.719043	1.224278	3.546615
H	-2.040137	0.479600	4.170409
H	-1.309570	3.460966	2.697175
C	2.200404	0.471411	1.914682
H	2.396397	0.049026	2.900331
N	2.586785	-0.109970	0.846445
C	3.381962	-1.330822	0.979321
H	2.858331	-2.130451	0.445430
H	3.482459	-1.625886	2.032707
C	4.742223	-1.113255	0.356166
C	7.233110	-0.628916	-0.822850
C	5.857525	-0.841768	1.148781
C	4.883001	-1.134829	-1.033528
C	6.120791	-0.891898	-1.621662
C	7.099912	-0.604292	0.563432
H	5.751796	-0.817904	2.230844
H	4.011135	-1.336031	-1.652525
H	6.219737	-0.910893	-2.702810
H	7.962544	-0.398097	1.189894
H	8.200281	-0.444382	-1.280443
H	-1.313226	0.971808	0.920783
H	-4.160984	2.812566	-0.363986
C	-3.264395	2.845478	-0.973530
C	-2.205497	2.024745	-0.682859
N	-2.121702	3.847349	-2.847404
C	-1.021785	2.146263	-1.469781
C	-3.173348	3.739801	-2.068634
C	-1.041346	3.068445	-2.553661
C	0.160961	1.420926	-1.204518
H	-4.021461	4.380000	-2.304807
H	0.083513	3.888356	-4.194596
C	1.286071	1.579328	-1.985744
H	0.228677	0.770394	-0.340549
C	1.250731	2.465208	-3.096861
H	2.146051	2.565192	-3.702422
C	0.120594	3.190259	-3.364033
O	2.441939	0.935084	-1.738841
H	2.429123	0.528766	-0.824318
C	0.129940	-2.462346	0.138247
C	1.879253	-3.994456	-1.430392
C	0.557920	-1.995882	-1.109744
C	0.590414	-3.704109	0.586762
C	1.460344	-4.466708	-0.189186
C	1.422618	-2.759437	-1.889672
C	0.229208	-1.031503	-1.484131
H	0.273475	-4.071505	1.559741
H	1.813644	-5.424039	0.179821
H	1.747538	-2.380431	-2.853823
H	2.560792	-4.582832	-2.036450

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H	5.131900	-1.941274	-2.242671
C	4.531986	-1.257538	-1.635442
C	4.045863	-0.470434	0.691827
C	2.567761	-0.355789	0.253595
C	4.775423	-1.522308	-0.148648
C	3.044070	-1.485012	-1.941962
H	4.526792	0.500983	0.559062
H	1.895418	-0.490102	1.107116
H	2.869522	-2.447941	-2.429826
H	4.806048	-0.232292	-1.884171
H	4.103373	-0.735041	1.751766
H	5.846266	-1.497740	0.072921
H	2.608681	-0.691477	-2.556247
N	2.247796	-1.559017	-0.650210
C	4.198977	-2.910107	0.187918
H	4.554939	-3.607925	-0.582218
C	2.670341	-2.809926	0.093561
H	2.232313	-3.659186	-0.434432
H	2.197554	-2.739343	1.073717
C	4.700342	-3.423461	1.513667
H	5.787674	-3.481750	1.566782
C	3.993949	-3.801670	2.575966
H	4.495887	-4.153237	3.471625
H	2.908450	-3.796037	2.611290
C	2.265377	1.026858	-0.388793
O	3.237967	1.407501	-1.316410
C	0.765121	-1.652673	-1.009932
H	0.733389	-2.108355	-2.001291
H	0.396839	-0.635615	-1.138569
C	0.371194	3.195829	-2.314692
C	-2.085321	2.718869	-1.134684
C	-0.229588	4.188456	-1.547063
C	-0.242393	1.956838	-2.521141
C	-1.487385	1.715547	-1.905955
C	-1.468441	3.952197	-0.957610
H	0.271226	5.141288	-1.404522
H	-1.944427	4.715097	-0.349271
H	-3.035562	2.508168	-0.651167
C	0.525021	0.918005	-3.325248
O	1.788278	1.120562	-3.463743
H	2.762716	1.423526	-2.201442
N	-0.162201	-0.086501	-3.786280
H	0.496882	-0.683044	-4.297888
H	1.347593	3.355526	-2.760323
C	-2.190626	0.406666	-1.957054
H	-2.363015	-0.054155	-2.929915
N	-2.586955	-0.136367	-0.872446
C	-3.367664	-1.370231	-0.967402
H	-2.838911	-2.143481	-0.399960
H	-3.455862	-1.704511	-2.010063
C	-4.734698	-1.145409	-0.361917
C	-7.236707	-0.641064	0.784173
C	-5.838784	-0.871813	-1.169653
C	-4.892489	-1.159356	1.023853
C	-6.133594	-0.906333	1.597779
C	-7.086643	-0.624344	-0.600701
H	-5.719632	-0.854126	-2.250483
H	-4.029076	-1.361847	1.656167
H	-6.248148	-0.919192	2.677706
H	-7.940547	-0.416811	-1.238574
H	-8.208303	-0.448770	1.229068
H	1.293451	0.993583	-0.886413
H	4.126222	2.825146	0.466228

C	3.217620	2.854221	1.057729
C	2.159915	2.042832	0.736961
N	2.043992	3.841948	2.919094
C	0.960634	2.166357	1.499525
C	3.110569	3.736571	2.160654
C	0.964719	3.074340	2.594341
C	-0.221895	1.450978	1.201655
H	3.957931	4.368275	2.420770
H	-0.187779	3.884711	4.220877
C	-1.361263	1.609285	1.962151
H	-0.278281	0.808152	0.330894
C	-1.342529	2.483340	3.083271
H	-2.249254	2.583043	3.671602
C	-0.212927	3.196486	3.381711
O	-2.515021	0.973880	1.687671
H	-2.477447	0.553759	0.780173
C	-0.108448	-2.449568	-0.071249
C	-1.843053	-3.969473	1.525917
C	-0.541782	-1.963723	1.167351
C	-0.555367	-3.705187	-0.494938
C	-1.417643	-4.461858	0.294799
C	-1.399390	-2.721205	1.961256
H	-0.225354	-0.987886	1.521928
H	-0.235215	-4.087912	-1.460945
H	-1.760755	-5.429642	-0.056085
H	-1.729516	-2.327099	2.917576
H	-2.519613	-4.552632	2.142512

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H	3.199086	1.532631	-2.668115
C	2.223714	1.649061	-2.185544
C	0.732361	3.156810	-0.887891
C	0.236567	1.913208	-0.110738
C	2.168209	2.951874	-1.384464
C	2.007029	0.476540	-1.223215
H	0.070655	3.320626	-1.742716
H	-0.044725	2.176497	0.912512
H	2.951620	0.006755	-0.939895
H	1.447486	1.652990	-2.952626
H	0.684103	4.039655	-0.244182
H	2.471056	3.791999	-2.014512
H	1.336052	-0.292136	-1.608528
N	1.422809	0.969859	0.089041
C	3.116168	2.805868	-0.187002
H	4.059785	2.378022	-0.555749
C	2.493617	1.776464	0.784827
H	3.239691	1.066034	1.149506
H	2.016191	2.262577	1.639060
C	3.453531	4.070286	0.561804
H	4.022854	3.917694	1.479677
C	3.135732	5.310995	0.203291
H	3.437245	6.160054	0.808134
H	2.572638	5.534014	-0.698684
C	-0.972050	1.224844	-0.762987
O	-0.799486	1.055132	-2.152085
C	1.075316	-0.268638	0.904182
H	2.022564	-0.803618	1.025454
H	0.445582	-0.879856	0.255844
C	-2.524287	-3.024549	0.448709
C	-0.126392	-3.728599	1.667851
C	-2.509150	-3.400944	1.790084
C	-1.340521	-2.975436	-0.290710
C	-0.131051	-3.349461	0.322407
C	-1.306113	-3.742933	2.404471
H	-3.435909	-3.421361	2.355530
H	-1.289030	-4.031562	3.450902
H	0.816274	-4.023548	2.118632
C	-1.345227	-2.401989	-1.688979
O	-0.386442	-1.596924	-1.955038
H	-0.677209	0.084003	-2.301627
N	-2.347662	-2.719169	-2.469002
H	-2.209786	-2.216275	-3.351384
H	-3.459772	-2.753948	-0.031601
C	1.129709	-3.420488	-0.456274
H	1.030307	-3.585695	-1.535570
N	2.267128	-3.329885	0.104448
C	3.435653	-3.495319	-0.751612
H	3.162843	-3.762826	-1.783110
H	4.028171	-4.322702	-0.340671
C	4.274251	-2.235414	-0.759905
C	5.771038	0.137036	-0.773645
C	4.637046	-1.619035	0.442498
C	4.675563	-1.656407	-1.964412
C	5.422023	-0.477370	-1.974218
C	5.379525	-0.439935	0.436636
H	4.325396	-2.066182	1.383068
H	4.391714	-2.124514	-2.903446
H	5.725800	-0.038363	-2.919879
H	5.661765	0.026144	1.376905
H	6.355446	1.052301	-0.777663
H	-1.092190	0.236675	-0.306719
H	-1.453393	3.816922	0.291016
C	-2.340349	3.239733	0.054810
C	-2.269558	1.975088	-0.474003
N	-4.752093	3.229449	0.117493
C	-3.505728	1.298806	-0.728814
C	-3.603562	3.827599	0.320829
C	-4.715008	1.966024	-0.394267
C	-3.559554	-0.011815	-1.252610
H	-3.641564	4.835688	0.729613
H	-6.859621	1.805865	-0.328400
C	-4.764382	-0.668710	-1.408895
H	-2.648798	-0.498259	-1.563003
C	-5.974279	0.000564	-1.070453
H	-6.911012	-0.530079	-1.209441
C	-5.945577	1.280601	-0.587673
O	-4.865497	-1.931136	-1.861408
H	-3.946162	-2.309408	-2.061398
C	0.409546	-0.007983	2.230014
C	-0.849604	0.396820	4.700350
C	1.154015	0.361536	3.356258
C	-0.967980	-0.205996	2.367749
C	-1.594862	-0.003560	3.594380
C	0.527934	0.572159	4.581168
H	2.233565	0.465272	3.282797
H	-1.556671	-0.558305	1.523249
H	-2.663672	-0.170144	3.684312
H	1.118277	0.858650	5.445574
H	-1.336387	0.555362	5.657486

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H	3.078079	1.111882	-2.844159
C	2.118886	1.284843	-2.346515
C	0.669036	2.958040	-1.196467

C	0.231300	1.827932	-0.233488
C	2.077675	2.690468	-1.740648
H	1.956235	0.257775	-1.219031
H	-0.041370	3.006394	-2.025936
H	-0.011473	2.224550	0.755448
H	2.913907	-0.174992	-0.922714
H	1.316258	1.170628	-3.076543
H	0.648982	3.918754	-0.673970
H	2.331558	3.430760	-2.503683
H	1.266598	-0.554892	-1.464239
N	1.442942	0.938893	0.037926
C	3.090022	2.733891	-0.589841
H	4.025424	2.277625	-0.945063
C	2.543828	1.839058	0.547233
H	3.320081	1.184820	0.952081
H	2.115438	2.429041	1.361227
C	3.429882	4.098656	-0.046285
H	4.040511	4.090563	0.857284
C	3.071220	5.268870	-0.567226
H	3.380920	6.201516	-0.106768
H	2.466551	5.348630	-1.466592
C	-0.988790	1.046976	-0.753770
O	-0.840916	0.713543	-2.112903
C	1.157179	-0.150879	1.058473
H	2.101923	-0.690064	1.178481
H	0.461538	-0.838182	0.578707
C	-2.547792	-2.779889	0.808599
C	-0.108998	-3.259648	2.043318
C	-2.477557	-2.855452	2.195383
C	-1.398827	-2.908338	0.020890
C	-0.167968	-3.174776	0.645482
C	-1.249931	-3.088587	2.816118
H	-3.378194	-2.738488	2.790764
H	-1.186840	-3.150659	3.898246
H	0.849305	-3.473647	2.506640
C	-1.554303	-2.750145	-1.476660
O	-2.584934	-3.266582	-2.001517
H	-0.706800	-0.273253	-2.140789
N	-0.621891	-2.045905	-2.093601
H	-0.865387	-2.078412	-3.090513
H	-3.501340	-2.623937	0.312676
C	1.067514	-3.430838	-0.134707
H	0.936802	-3.809854	-1.153316
N	2.217920	-3.240090	0.373765
C	3.371001	-3.588246	-0.447588
H	3.079987	-4.020847	-1.416123
H	3.945119	-4.347971	0.097891
C	4.235829	-2.366742	-0.668899
C	5.741543	-0.033725	-1.062438
C	4.698493	-1.627970	0.425843
C	4.543691	-1.930977	-1.957711
C	5.294865	-0.771866	-2.156051
C	5.444501	-0.467850	0.231837
H	4.459188	-1.964290	1.431696
H	4.182790	-2.494832	-2.814038
H	5.525659	-0.444335	-3.165370
H	5.803201	0.094756	1.089515
H	6.326965	0.868253	-1.214703
H	-1.099128	0.116782	-0.177923
H	-1.452138	3.697381	0.127224
C	-2.343663	3.120701	-0.092142
C	-2.284644	1.825108	-0.542663
N	-4.752835	3.161584	-0.093511
C	-3.526832	1.155691	-0.794152
C	-3.598896	3.748552	0.106508
C	-4.729077	1.870402	-0.531699
C	-3.605702	-0.183043	-1.245685
H	-3.625395	4.779459	0.454466
H	-6.877773	1.775942	-0.517134
C	-4.827045	-0.808510	-1.394737
H	-2.703100	-0.716249	-1.509479
C	-6.027134	-0.092287	-1.131808
H	-6.973429	-0.606167	-1.268061
C	-5.973738	1.210803	-0.721448
O	-4.954795	-2.092702	-1.774609
H	-4.055915	-2.514038	-1.892340
C	0.612135	0.332183	2.376773
C	-0.421839	1.174465	4.839350
C	1.466621	0.771208	3.393561
C	-0.764562	0.291627	2.620974
C	-1.279585	0.712384	3.843767
C	0.953266	1.196852	4.615379
H	2.542321	0.765823	3.236500
H	-1.441765	-0.103736	1.866738
H	-2.349777	0.669859	4.019314
H	1.628127	1.535481	5.394900
H	-0.822219	1.504194	5.792871

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H	-4.418271	-3.230414	1.316571
C	-4.021610	-2.256410	1.017549
C	-4.031845	-0.479776	-0.721192
C	-2.521029	-0.298042	-0.460699
C	-4.457389	-1.917126	-0.411066
C	-2.486094	-2.290898	1.085200
H	-4.581756	0.201949	-0.067875
H	-2.002294	0.014846	-1.372288
H	-2.091966	-3.309240	1.122069
H	-4.396484	-1.496789	1.705623
H	-4.268359	-0.213803	-1.754865
H	-5.541183	-2.017235	-0.513125
H	-2.086462	-1.723028	1.926763
N	-1.902810	-1.678469	-0.167466
C	-3.754677	-2.892317	-1.373286
H	-3.909664	-3.910496	-0.997472
C	-2.243820	-2.573979	-1.335768
H	-1.652660	-3.483149	-1.227106
H	-1.911699	-2.045524	-2.235075
C	-4.276184	-2.828279	-2.782000
H	-4.151480	-1.878689	-3.303977
C	-4.870811	-3.843870	-3.400655
H	-5.248115	-3.748825	-4.413774
H	-5.003544	-4.806618	-2.912868
C	-2.255068	0.763203	0.639081
O	-3.078573	0.584539	1.747902
C	-0.395342	-1.535013	-0.048122
H	-0.228161	-0.856499	0.788947
H	-0.071225	-1.048679	-0.974076
C	-0.226861	2.499836	3.002399
C	1.901925	2.684466	1.235106
C	0.130618	3.736668	2.473536
C	0.482237	1.340398	2.676039
C	1.542468	1.434859	1.753191
C	1.211610	3.833462	1.599866
H	-0.430704	4.624552	2.748591

H	1.502965	4.794847	1.188149
H	2.721010	2.740946	0.523748
C	0.086673	0.023160	3.325683
O	1.004745	-0.755932	3.680357
H	-2.435819	0.369740	2.520124
N	-1.219801	-0.160354	3.459853
H	-1.357967	-1.043147	3.957905
H	-1.067963	2.412970	3.682706
C	2.216246	0.228082	1.219729
H	2.381244	-0.606946	1.906907
N	2.546136	0.166908	-0.012758
C	3.253825	-1.027970	-0.473862
H	2.722520	-1.406566	-1.355644
H	3.248292	-1.819480	0.289201
C	4.671810	-0.660162	-0.852582
C	7.284002	0.080430	-1.525780
C	5.750073	-1.107723	-0.090586
C	4.909946	0.168237	-1.953074
C	6.208785	0.537767	-2.287820
C	7.052999	-0.742881	-0.427282
H	5.568372	-1.745684	0.770857
H	4.071230	0.527542	-2.545649
H	6.384448	1.181632	-3.144370
H	7.885760	-1.099824	0.171118
H	8.297898	0.366533	-1.788247
H	-1.209643	0.715657	0.957201
H	-4.339733	2.499957	0.882819
C	-3.572114	2.867176	0.210309
C	-2.439370	2.127629	-0.004905
N	-2.823530	4.643356	-1.241116
C	-1.423565	2.672772	-0.848639
C	-3.719699	4.118938	-0.437919
C	-1.671191	3.940635	-1.442382
C	-0.179656	2.036436	-1.076196
H	-4.626847	4.698707	-0.275412
H	-0.876413	5.478367	-2.721569
C	0.799870	2.642056	-1.833127
H	0.059334	1.096907	-0.592131
C	0.536829	3.889147	-2.459887
H	1.318726	4.337580	-3.064586
C	-0.666057	4.514897	-2.267696
O	2.031134	2.111085	-1.988700
H	2.184741	1.405436	-1.300733
C	0.386212	-2.799482	0.194115
C	1.999898	-5.032602	0.663135
C	0.846276	-3.577459	-0.874497
C	0.759643	-3.134918	1.499627
C	1.561085	-4.251393	1.729769
C	1.644679	-4.692649	-0.641419
H	0.600297	-3.296071	-1.896256
H	0.468833	-2.498104	2.334895
H	1.853395	-4.500606	2.744886
H	1.999100	-5.286639	-1.477625
H	2.629853	-5.897566	0.846236

Ib4E-R

H	-4.592036	-3.024945	1.214232
C	-4.121448	-2.078666	0.933647
C	-4.003580	-0.265995	-0.756478
C	-2.486715	-0.183724	-0.479277
C	-4.517898	-1.684208	-0.491765
C	-2.595085	-2.233417	1.005359
H	-4.520953	0.428822	-0.090076
H	-1.945220	0.116792	-1.381777
H	-2.288101	-3.281458	0.975330
H	-4.444390	-1.305771	1.633928
H	-4.211644	0.045589	-1.783769
H	-5.603917	-1.716912	-0.611801
H	-2.150489	-1.762119	1.884097
N	-1.957291	-1.602949	-0.216355
C	-3.857629	-2.677789	-1.467141
H	-4.063923	-3.693256	-1.108775
C	-2.332301	-2.435975	-1.419478
H	-1.783322	-3.375316	-1.345924
H	-1.974555	-1.890624	-2.298517
C	-4.368785	-2.566848	-2.876513
H	-4.223460	-1.606335	-3.372279
C	-4.977665	-3.555302	-3.524556
H	-5.346146	-3.429011	-4.537501
H	-5.131065	-4.526889	-3.061026
C	-2.150747	0.839255	0.633991
O	-2.947805	0.666043	1.768035
C	-0.448267	-1.546410	-0.066115
H	-0.265658	-0.915784	0.803927
H	-0.076652	-1.043901	-0.965516
C	-0.191044	2.266956	3.177014
C	1.881973	2.585381	1.359303
C	0.131549	3.535707	2.706532
C	0.537266	1.142986	2.777097
C	1.560999	1.303765	1.824889
C	1.184557	3.699147	1.806466
H	-0.438953	4.397627	3.039422
H	1.442173	4.686167	1.435187
H	2.672494	2.693250	0.621751
C	0.128565	-0.205847	3.336489
O	-1.118595	-0.510924	3.223644
H	-2.319015	0.315194	2.465753
N	1.076079	-0.909024	3.878983
H	0.642946	-1.767047	4.238555
H	-1.018219	2.132038	3.868114
C	-2.219182	0.126968	1.216235
H	2.353447	-0.754662	1.852521
N	2.565125	0.131371	-0.013225
C	3.235492	-1.058446	-0.537976
H	2.689660	-1.375689	-1.435142
H	3.210090	-1.886138	0.185071
C	4.662020	-0.712696	-0.904207
C	7.289561	0.001582	-1.542584
C	5.722779	-1.143907	-0.108429
C	4.925206	0.086619	-2.019900
C	6.232222	0.443002	-2.337852
C	7.033304	-0.792028	-0.427509
H	5.520377	-1.757980	0.765699
H	4.099597	0.434667	-2.637042
H	6.428148	1.063355	-3.207192
H	7.852550	-1.136178	0.196416
H	8.309779	0.276779	-1.791929
H	-1.099658	0.749673	0.918898
H	-4.193369	2.626829	0.944368
C	-3.420685	2.986020	0.273170
C	-2.310201	2.221894	0.028962
N	-2.635639	4.775483	-1.142021
C	-1.286894	2.759052	-0.810210
C	-3.540342	4.255550	-0.345511
C	-1.502892	4.049074	-1.367237

C	-0.061095	2.096285	-1.060001
H	-4.430782	4.854582	-0.162541
H	-0.668769	5.602947	-2.601411
C	0.937956	2.704468	-1.788258
C	0.153320	1.133697	-0.609978
C	0.707312	3.975730	-2.378709
H	1.503066	4.424873	-2.964487
C	-0.482549	4.622222	-2.174868
O	2.159961	2.152029	-1.944387
H	2.286258	1.426688	-1.272126
C	0.247557	-2.864412	0.140072
C	1.684374	-5.218191	0.576569
C	0.765430	-3.584536	-0.940729
C	0.466822	-3.323587	1.442109
C	1.179887	-4.499352	1.658699
C	1.478655	-4.759863	-0.723531
H	0.626934	-3.214200	-1.954349
H	0.092393	-2.740771	2.281060
H	1.351033	-4.847124	2.672464
H	1.882240	-5.310423	-1.567182
H	2.246312	-6.131180	0.746938

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H	3.472771	2.769650	-2.341099
C	2.610595	2.096369	-2.333706
C	0.140286	1.926882	-2.250754
C	0.091719	1.367271	-0.814094
C	1.310900	2.898405	-2.408180
C	2.602675	1.245948	-1.055602
H	0.266474	1.096233	-2.952635
H	-0.615004	1.938074	-0.202765
H	3.501354	1.381517	-0.450151
H	2.697014	1.435026	-3.200270
H	-0.815918	2.405536	-2.476824
H	1.239312	3.428344	-3.361422
H	2.471629	0.185437	-1.264441
N	1.442332	1.642447	-0.150308
C	1.314212	3.917741	-1.254301
H	2.170512	4.586450	-1.394088
C	1.522901	3.135493	0.066990
H	2.501067	3.326663	0.514730
H	0.746905	3.392783	0.785406
C	0.064441	4.756149	-1.213995
H	-0.862434	4.246056	-0.946009
C	0.037062	6.055693	-1.493126
H	-0.887596	6.623292	-1.470867
H	0.942828	6.597100	-1.756019
C	-0.352479	-0.110468	-0.807640
O	0.539378	-0.873330	-1.570039
C	1.663431	0.885980	1.147908
H	2.626901	1.237216	1.534131
H	1.805202	-0.154490	0.848971
C	5.260049	-0.713639	-0.330817
C	3.465825	-2.455568	-1.520755
C	5.364461	-0.987677	-1.691064
C	4.268640	-1.298997	0.458481
C	3.378136	-2.203169	-0.145973
C	4.450820	-1.850332	-2.295105
H	6.144339	-0.517425	-2.283192
H	4.507428	-2.056493	-3.359554
H	2.752915	-3.138543	-1.974834
C	4.100689	-0.798138	1.889795
O	4.743160	0.247482	2.192204
H	0.722013	-1.707890	-1.046800
N	3.229809	-1.472693	2.605489
H	3.165047	-1.004032	3.514866
H	5.921057	-0.001608	0.152738
C	2.310182	-2.912611	0.605016
H	2.600605	-3.520515	1.462264
N	1.104279	-2.856519	0.191226
C	0.098387	-3.654768	0.903998
H	0.064878	-3.361362	1.961584
H	0.389375	-4.712457	0.874662
C	-1.260444	-3.479009	0.270770
C	-3.764480	-3.164065	-0.945857
C	-2.278810	-2.780376	0.916968
C	-1.503746	-4.008022	-1.001160
C	-2.745661	-3.853074	-1.606292
C	-3.528105	-2.625957	0.314341
H	-2.097467	-2.348881	1.899143
H	-0.708860	-4.544396	-1.514732
H	-2.921688	-4.267387	-2.594846
H	-4.307709	-2.066036	0.824641
H	-4.732015	-3.032736	-1.420995
H	-0.388993	-0.491328	0.221321
H	-1.169188	-1.074118	-3.188831
C	-1.995789	-0.667227	-2.617269
C	-1.770372	-0.159543	-1.364789
N	-4.358148	-0.211701	-2.511190
C	-2.889368	0.325057	-0.620338
C	-3.306505	-0.665942	-3.150108
C	-4.164184	0.267354	-1.249296
C	-2.800509	0.807443	0.712117
H	-3.475709	-1.060985	-4.150536
H	-6.270031	0.645996	-1.028220
C	-3.931116	1.215221	1.382640
H	-1.846392	0.832400	1.232459
C	-5.202964	1.163703	0.755918
H	-6.070776	1.491354	1.318889
C	-5.308769	0.702573	-0.527260
O	-3.909200	1.681893	2.654979
H	-2.995612	1.666186	2.989470
C	0.599009	0.936706	2.222629
C	-1.272174	0.797585	4.319680
C	0.201047	2.093625	2.900509
C	0.084806	-0.295227	2.653838
C	-0.840606	-0.368961	3.688408
C	-0.743471	2.026533	3.926249
H	0.646709	3.056492	2.679398
H	0.456926	-1.202339	2.184045
H	-1.214378	-1.334844	4.014253
H	-1.040247	2.936506	4.438619
H	-1.992187	0.746684	5.131228

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H	2.975688	-0.878207	3.260209
C	2.399036	-1.216123	2.394653
C	2.120411	-3.020826	0.694368
C	1.694592	-1.917171	-0.307126
C	3.052486	-2.445537	1.762159
C	2.361600	-0.092976	1.352131
H	1.225802	-3.437535	1.161721
H	1.983960	-2.185490	-1.326804
H	1.438477	0.486864	1.368415

H	1.384797	-1.454068	2.721033
H	2.637083	-3.826291	0.162777
H	3.257292	-3.205803	2.521161
H	3.191945	0.605056	1.480532
N	2.555786	-0.669182	-0.039006
C	4.364021	-2.008128	1.080379
H	4.913974	-1.383442	1.797460
C	3.993152	-1.141639	-0.134951
H	4.620626	-0.253641	-0.200852
H	4.060571	-1.686931	-1.078895
C	5.247623	-3.184313	0.753998
H	5.510923	-3.778653	1.628942
C	5.725723	-3.557414	-0.430430
H	6.357256	-4.435921	-0.514537
H	5.533813	-3.019358	-1.353927
C	0.178937	-1.667671	-0.329928
O	-0.250419	-1.569183	1.019248
C	2.283512	0.386533	-1.106803
H	1.257515	0.732397	-0.943152
H	2.347924	-0.143030	-2.061854
C	-0.249929	4.865782	-0.143207
C	-2.668134	4.735697	-1.486719
C	-0.719987	5.982863	-0.825270
C	-0.966498	3.667950	-0.130736
C	-2.205501	3.613295	-0.789293
C	-1.935219	5.917883	-1.504142
H	-0.139897	6.900846	-0.831633
H	-2.311238	6.781573	-2.043762
H	-3.620170	4.681601	-2.009519
C	-0.379151	2.481412	0.608068
O	0.315212	2.741900	1.637210
H	-1.194700	-1.330027	1.054059
N	-0.658894	1.305839	0.091319
H	-0.321382	0.618344	0.768516
H	0.689678	4.896896	0.399906
C	-3.093773	2.416311	-0.825906
H	-3.391791	2.105225	-1.833556
N	-3.626297	1.754435	0.118066
C	-3.353169	2.020773	1.523556
C	-4.302359	2.351004	1.966317
H	-2.621549	2.820231	1.676174
C	-2.898731	0.760148	2.234898
C	-2.087029	-1.549734	3.605586
C	-3.614585	-0.432937	2.101219
C	-1.771483	0.784508	3.059800
C	-1.371228	-0.361791	3.743863
C	-3.207377	-1.583880	2.775949
H	-4.493681	-0.465666	1.462448
H	-1.176997	1.692502	3.120622
H	-0.487563	-0.329875	4.375002
H	-3.767821	-2.506093	2.653746
H	-1.769503	-2.445501	4.130807
H	-0.039059	-0.731228	-0.856996
H	1.076936	-4.155409	-1.291875
C	0.021621	-3.963787	-1.442448
C	-0.569003	-2.785542	-1.053519
N	-2.035782	-4.890158	-2.264729
C	-1.971816	-2.622195	-1.310080
C	-0.748100	-4.984322	-2.046764
C	-2.649057	-3.727345	-1.906916
C	-2.704058	-1.437537	-1.011842
H	-0.263046	-5.912196	-2.343873
H	-4.530758	-4.486603	-2.614770
C	-4.064460	-1.380184	-1.269357
H	-2.207593	-0.548211	-0.618098
C	-4.732366	-2.496406	-1.847014
H	-5.797814	-2.406815	-2.033589
C	-4.042626	-3.629662	-2.161695
O	-4.843738	-0.318039	-1.015649
H	-4.355507	0.419210	-0.521396
C	3.223096	1.565618	-1.087456
C	4.917700	3.791217	-1.119781
C	2.986114	2.643211	-0.226450
C	4.301275	1.623604	-1.976679
C	5.146990	2.729388	-1.992271
C	3.837796	3.745527	-0.240729
H	2.136752	2.626872	0.457397
H	4.476167	0.801218	-2.666843
H	5.979393	2.763148	-2.687980
H	3.649067	4.575732	0.433324
H	5.574230	4.655709	-1.131363

Ia13Z

H	5.263562	0.031734	2.043919
C	4.330495	-0.479808	1.792114
C	3.304292	-2.463275	0.701242
C	2.169845	-1.531314	0.223072
C	4.606611	-1.675714	0.876323
C	3.394394	0.502308	1.068250
H	3.018802	-2.896197	1.662916
H	1.755384	-1.877430	-0.729564
H	2.566399	0.842883	1.694025
H	3.856006	-0.822049	2.713585
H	3.436538	-3.286405	-0.006191
H	5.378513	-2.318765	1.307595
H	3.929332	1.370853	0.677837
N	2.783338	-0.168816	-0.142055
C	5.083182	-1.132538	-0.484043
H	5.867772	-0.389748	-0.297265
C	3.880300	-0.429138	-1.146943
H	4.166406	0.534201	-1.571510
H	3.431773	-1.040375	-1.936562
C	5.647814	-2.187531	-1.394366
H	4.968770	-2.985796	-1.696547
C	6.903217	-2.192596	-1.832567
H	7.276656	-2.980031	-2.479371
H	7.602557	-1.406801	-1.556665
C	1.004494	-1.436637	1.235947
O	1.463452	-1.237646	2.548615
C	1.710514	0.699031	-0.771812
H	0.900992	0.755325	-0.043850
H	1.360581	0.140471	-1.646182
C	-1.016683	4.015348	2.488034
C	-2.261849	4.406471	0.034840
C	-1.578498	5.253816	2.184455
C	-1.071487	2.962725	1.576067
C	-1.709397	3.161021	0.337337
C	-2.201968	5.450600	0.955531
H	-1.536817	6.059619	2.910774
H	-2.642077	6.412617	0.712571
H	-2.735339	4.557637	-0.931932
C	-0.521597	1.580858	1.878934
O	-1.107529	0.645544	1.263975
H	1.128766	-0.327769	2.798924
N	0.517835	1.391259	2.666355

H	0.869732	2.271300	3.041284
H	-0.554527	3.857694	3.459018
C	-1.700396	2.098534	-0.717673
H	-0.708763	1.846142	-1.105174
N	-2.679323	1.521893	-1.288067
C	-4.043458	1.726942	-0.798874
H	-4.612285	2.243817	-1.580051
H	-4.061785	2.354275	0.101276
C	-4.679679	0.383296	-0.512587
C	-5.789823	-2.132315	-0.001047
C	-5.854227	-0.011604	-1.151243
C	-4.061649	-0.488255	0.389732
C	-4.613839	-1.741832	0.638863
C	-6.411488	-1.263621	-0.894788
H	-6.332120	0.660694	-1.860043
H	-3.130388	-0.186481	0.868212
H	-4.116306	-2.422078	1.325132
H	-7.325281	-1.562011	-1.400445
H	-6.216231	-3.112758	0.190340
H	0.327346	-0.621307	0.984481
H	1.097021	-3.705166	2.746953
C	0.403345	-3.785229	1.916503
C	0.194255	-2.711281	1.089207
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C	-0.782149	-2.832435	0.048674
C	-0.290371	-4.995470	1.679358
C	-1.396540	-4.106601	-0.116625
C	-1.169741	-1.761455	-0.802273
H	-0.112253	-5.849818	2.330580
H	-2.783195	-5.264191	-1.285798
C	-2.120048	-1.951154	-1.784310
H	-0.799347	-0.755954	-0.628155
C	-2.681458	-3.241673	-1.987262
H	-3.421579	-3.359627	-2.772436
C	-2.336435	-4.281572	-1.169097
O	-2.568521	-0.963297	-2.586416
H	-2.470703	-0.071286	-2.153284
C	2.130805	2.094859	-1.152673
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C	2.576578	2.391081	-2.443956
C	1.984724	3.132121	-0.224947
C	2.301818	4.440650	-0.575576
C	2.898850	3.699871	-2.793700
H	2.657259	1.597916	-3.183703
H	1.607124	2.905903	0.769829
H	2.176050	5.237221	0.150856
H	3.242843	3.919842	-3.799203
H	3.007517	5.746014	-2.135153

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C	4.304501	-2.388497	0.686949
C	3.560970	-0.041632	1.092668
H	2.520426	-3.304786	1.442856
H	1.489565	-1.907168	-0.890750
H	2.841974	0.429269	1.763188
H	3.739059	-1.572843	2.606405
H	2.817909	-3.682407	-0.251194
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N	2.803512	-0.470854	-0.149055
C	4.861039	-1.834245	-0.638641
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C	3.820484	-0.842783	-1.203575
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C	5.178015	-2.899859	-1.650429
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C	6.393208	-3.118215	-2.143948
H	6.578770	-3.907053	-2.865854
H	7.245852	-2.514926	-1.841393
C	0.786519	-1.499992	1.096715
O	1.259193	-1.348280	2.407563
C	1.922095	0.659804	-0.644840
H	1.201779	0.828501	0.153937
H	1.417114	0.271081	-1.535570
C	-0.116696	3.992619	2.234477
C	-1.475336	4.445706	-0.148963
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H	-1.154559	-0.172500	2.352290
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C	-4.781652	1.088018	-0.562435
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H	-6.349756	1.683112	-1.910504
H	-3.390103	0.251222	0.850281
H	-4.863376	-1.669840	1.424314
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H	0.663668	-3.702418	2.666899
C	-0.066168	-3.730434	1.865122
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C	-2.545311	-1.724212	-1.773298
H	-0.934466	-0.713471	-0.827100
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C	-3.042192	-3.970451	-1.020669
O	-2.896688	-0.719344	-2.596613
H	-2.657446	0.161987	-2.183086
C	2.614680	1.967090	-0.926259
C	3.768172	4.460769	-1.421733
C	3.108576	2.273817	-2.197117
C	2.680425	2.926570	0.090331
C	3.257850	4.168114	-0.158272
C	3.690881	3.514594	-2.442120
H	3.022664	1.546788	-3.001608
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H	3.299270	4.910496	0.632803
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H	2.948798	1.177396	-4.419339
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C	2.070686	-0.040968	-2.840686
H	-0.475046	1.306368	-3.088833
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H	3.011832	-0.587954	-2.886410
H	1.300097	0.631207	-4.738720
H	-0.363517	2.854927	-2.241831
H	1.163895	3.014846	-4.156460
H	1.236288	-0.741700	-2.834731
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C	2.516138	2.913401	-2.457350
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C	2.022447	4.172639	-1.785548
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O	-0.590777	-0.790874	-1.567484
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C	2.268708	-2.219956	2.470872
C	0.428312	-3.286281	0.692674
C	2.672261	-3.188385	1.556597
C	0.940930	-1.787773	2.535074
C	0.004962	-2.343770	1.639557
C	1.750540	-3.717201	0.654133
H	3.708141	-3.514780	1.535387
H	2.059156	-4.466101	-0.069145
H	-0.305180	-3.698087	0.005059
C	0.535782	-0.714399	3.540587
O	-0.541551	-0.864139	4.149095
H	-1.172747	-1.412811	-1.065102
N	1.340772	0.334326	3.691091
H	2.145212	0.297798	3.068477
H	2.993091	-1.795179	3.160889
C	-1.433831	-1.978285	1.663758
H	-1.882843	-1.812084	2.645300
N	-2.095401	-1.877842	0.578844
C	-3.517421	-1.558798	0.693774
H	-3.626923	-0.487860	0.910012
H	-3.961998	-2.098894	1.541316
C	-4.272148	-1.882753	-0.575518
C	-5.727964	-2.484194	-2.895518
C	-3.820435	-2.861391	-1.461762
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C	-6.187653	-1.507143	-2.012991
C	-4.543130	-3.159892	-2.616197
H	-2.896172	-3.389525	-1.244911
H	-5.817273	-0.438702	-0.181789
H	-7.108830	-0.972188	-2.224029
H	-4.178194	-3.922576	-3.297819
H	-6.289900	-2.715435	-3.795186
H	-0.012488	-0.121533	0.281142
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C	-2.704976	1.044166	-1.258647
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C	6.461957	-1.740142	-0.286115
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C	4.776211	-0.162523	0.413308
C	6.087762	-0.627275	0.463769
C	5.519401	-2.394168	-1.077449
H	3.463833	-2.471536	-1.702434
H	4.485231	0.693093	1.018484
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C	1.911333	0.804804	-4.007865
C	0.157388	1.838610	-2.602432
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C	1.383165	2.134896	-3.467455
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H	-0.529070	1.172826	-3.137383
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H	1.232466	0.402135	-4.763636
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H	1.125005	2.810739	-4.287062
H	1.172361	-0.888032	-2.804366
N	1.991507	0.548238	-1.523142
C	2.484226	2.768910	-2.589984

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H	1.684851	4.793140	-2.712632
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H	2.228653	3.733646	0.127338
C	-0.435661	0.230739	-0.694917
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C	2.349853	-0.389319	-0.378198
H	1.682181	-1.251116	-0.482097
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C	2.288740	-2.222482	2.340393
C	0.325061	-3.364528	0.751234
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H	3.643296	-3.614022	1.418307
H	1.881893	-4.635163	-0.016694
H	-0.454721	-3.796992	0.130313
C	0.708262	-0.599212	3.387425
O	1.536550	0.385264	3.249410
H	-1.269646	-1.443024	-1.037630
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C	-1.446393	-1.940376	1.729117
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C	-3.554405	-1.486255	0.821431
H	-3.630932	-0.407084	1.008661
H	-3.984578	-1.990555	1.697997
C	-4.353984	-1.830726	-0.414827
C	-5.882512	-2.479825	-2.674537
C	-3.972827	-2.681330	-1.250925
C	-5.509859	-1.108260	-0.722849
C	-6.270957	-1.429776	-1.843502
C	-4.731624	-3.204290	-2.374677
H	-3.074132	-3.445876	-1.018987
H	-5.808202	-0.280753	-0.082617
H	-7.164231	-0.856236	-2.072303
H	-4.422367	-4.024561	-3.015736
H	-6.472522	-2.729815	-3.550920
H	-0.054644	-0.164740	0.252580
H	-2.769561	0.477946	-2.115137
C	-2.759264	1.073015	-1.207261
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H	4.372769	0.686324	1.065749
H	6.730322	-0.047935	1.175806
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H	7.486633	-2.007058	-0.149640

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H	-3.626490	1.568004	-1.815231
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H	-0.100615	1.069683	-2.887879
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H	-3.562513	2.349421	-0.236945
H	-3.125065	3.950420	-2.145572
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H	0.550512	3.376092	-0.163650
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C	-2.192196	4.784234	0.275194
H	-2.812976	4.183641	0.941312
C	-2.139124	6.102979	0.436822
H	-2.708620	6.604256	1.212861
H	-1.522066	6.727848	-0.204473
C	-2.041477	-0.319761	-1.352612
O	-2.193863	-0.196577	-2.738045
C	0.599338	0.790437	-0.392770
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H	0.342320	0.595106	0.652929
C	2.911558	-2.536354	-3.057670
C	3.761331	-2.808756	-0.435021
C	4.263313	-2.726872	-2.785213
C	1.963489	-2.487407	-2.034173
C	2.398487	-2.622314	-0.697461
C	4.691181	-2.864448	-1.467583
H	4.978575	-2.776576	-3.600524
H	5.740966	-3.023229	-1.243392
H	4.093454	-2.943189	0.589752
C	0.493251	-2.242584	-2.361916
O	-0.359021	-2.878485	-1.696947
H	-1.383570	-0.666997	-3.124582
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H	1.013405	-0.929615	-3.706600
H	2.579021	-2.438953	-4.087773
C	1.422133	-2.628004	0.427557
H	0.518269	-3.206612	0.247104
N	1.499545	-2.036612	1.559537
C	2.623503	-1.193318	1.932682

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H	3.354951	-1.814221	2.466756
C	2.222984	-0.045336	2.837194
C	1.620332	2.230338	4.368172
C	0.897754	0.302193	3.098679
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C	2.949419	1.872961	4.134027
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H	4.280136	0.481332	3.179549
H	3.755834	2.477268	4.538665
H	-0.439319	1.694646	4.046411
H	1.385747	3.113295	4.954337
H	-1.190025	-0.968165	-1.140122
H	-4.583660	-0.527025	-2.297130
C	-4.474669	-0.961598	-1.309330
C	-3.245125	-0.980400	-0.702138
N	-5.535633	-2.080787	0.541400
C	-3.125981	-1.626623	0.566814
C	-5.591539	-1.520475	-0.644640
C	-4.314704	-2.152808	1.144164
C	-1.889922	-1.797644	1.244926
H	-6.569209	-1.487208	-1.122570
H	-5.150984	-3.188840	2.834670
C	-1.832894	-2.475430	2.446095
H	-0.965576	-1.455724	0.791800
C	-3.031015	-2.961193	3.041105
H	-2.955130	-3.474394	3.994505
C	-4.230801	-2.804853	2.405445
O	-0.688667	-2.722587	3.112997
H	0.109296	-2.432829	2.585488
C	2.010811	1.304674	-0.509915
C	4.699538	2.056612	-0.680307
C	2.799856	0.881292	-1.584334
C	2.585988	2.100653	0.486018
C	3.923088	2.478346	0.397052
C	4.137228	1.254469	-1.672015
H	2.362445	0.234046	-2.339807
H	2.000735	2.399448	1.353677
H	4.361049	3.085205	1.183550
H	4.739975	0.908463	-2.505747
H	5.744768	2.343497	-0.740768

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H	-0.848920	3.879282	-3.333254
C	-1.250160	3.021859	-2.786184
C	-2.797064	2.261185	-1.008967
C	-1.757879	1.186517	-0.621171
C	-2.103156	3.488098	-1.602083
C	-0.088030	2.165412	-2.262338
H	-3.472231	1.844129	-1.759913
H	-1.789287	0.985744	0.455762
H	0.065181	1.244408	-2.825307
H	-1.862796	2.426834	-3.466399
H	-3.400817	2.526794	-0.137286
H	-2.848708	4.216590	-1.931670
H	0.853309	2.719422	-2.236534
N	-0.348727	1.770419	-0.823464
C	-1.175098	4.133531	-0.556461
H	-0.542890	4.864865	-1.073784
C	-0.271146	3.021257	0.020166
H	0.773177	3.332131	0.036271
H	-0.562073	2.729048	1.034756
C	-1.910180	4.847185	0.544137
H	-2.550421	4.234790	1.180481
C	-1.818383	6.154621	0.768450
H	-2.374981	6.635775	1.566272
H	-1.181686	6.790206	0.157606
C	-1.999156	-0.151450	-1.358825
O	-2.106758	0.026176	-2.744003
C	0.685504	0.762516	-0.357735
H	0.562689	-0.102679	-1.007943
H	0.407486	0.505289	0.668742
C	2.852385	-2.243601	-3.140328
C	3.625094	-2.852128	-0.549540
C	4.194522	-2.465885	-2.853894
C	1.873268	-2.347567	-2.149979
C	2.268727	-2.629594	-0.827867
C	4.583034	-2.781534	-1.552968
H	4.936947	-2.394836	-3.643186
H	5.626239	-2.969129	-1.320053
H	3.927469	-3.108249	0.461022
C	0.438535	-2.065414	-2.555030
O	0.274343	-0.956910	-3.194074
H	-1.266900	-0.379509	-3.117187
N	-0.448974	-2.949511	-2.212014
H	-1.359499	-2.635675	-2.567635
H	2.541844	-1.977358	-4.146192
C	1.252061	-2.701283	0.254381
H	0.324098	-3.204805	-0.021222
N	1.310857	-2.223523	1.440736
C	2.461918	-1.479188	1.927988
H	3.033820	-1.027561	1.103781
H	3.137116	-2.180783	2.435399
C	2.086967	-0.381165	2.902477
C	1.551590	1.817671	4.565154
C	0.774943	0.035773	3.125639
C	3.126384	0.299336	3.546791
C	2.865634	1.389211	4.368668
C	0.509419	1.133132	3.948121
H	-0.053533	-0.488609	2.658723
H	4.153283	-0.018573	3.378943
H	3.686444	1.908298	4.854281
H	-0.518373	1.446602	4.106525
H	1.343448	2.671851	5.201851
H	-1.183623	-0.845858	-1.143890
H	-4.523533	-0.149827	-2.380241
C	-4.463968	-0.653734	-1.421546
C	-3.257089	-0.775489	-0.780396
N	-5.634188	-1.851253	0.310847
C	-3.210234	-1.513033	0.441501
C	-5.626886	-1.202557	-0.830843
C	-4.439193	-2.025486	0.941942
C	-2.007553	-1.789168	1.141575
H	-6.585929	-1.088214	-1.332681
H	-5.373158	-3.150426	2.521355
C	-2.016714	-2.562602	2.285343
H	-1.055345	-1.439168	0.758561
C	-3.253290	-3.039249	2.804593
H	-3.231798	-3.630880	3.714113
C	-4.424050	-2.776753	2.150007
O	-0.903899	-2.908758	2.957699
H	-0.085877	-2.632836	2.452734
C	2.121352	1.208452	-0.429139
C	4.846247	1.806193	-0.524597

C	2.878181	0.865815	-1.554677
C	2.737635	1.851628	0.648727
C	4.096548	2.150956	0.598965
C	4.236687	1.164224	-1.602005
C	2.392271	0.345371	-2.377620
H	2.162933	2.091459	1.541479
H	4.570367	2.638459	1.445408
H	4.819663	0.883342	-2.473508
H	5.907889	2.031140	-0.556570

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H	-3.248806	-3.181311	-3.050253
C	-2.765628	-2.773100	-2.158453
C	-2.833918	-2.647675	0.339723
C	-2.367121	-1.178701	0.180629
C	-3.589346	-3.114630	-0.912589
C	-2.673242	-1.242108	-2.290100
H	-1.957961	-3.281883	0.470333
H	-2.695783	-0.578878	1.031727
H	-1.657838	-0.885510	-2.478743
H	-1.765065	-3.195718	-2.074172
H	-3.461098	-2.746200	1.229973
H	-3.771781	-4.191017	-0.858337
N	-3.331726	-0.853264	-3.070736
N	-3.133654	-0.580089	-1.007958
C	-4.924484	-2.358272	-1.022271
H	-5.315298	-2.496040	-2.037429
C	-4.606042	-0.869141	-0.802873
H	-5.158088	-0.231835	-1.496438
H	-4.840781	-0.546855	0.214947
C	-5.973803	-2.822126	-0.051308
H	-5.730728	-2.734712	1.008407
C	-7.150362	-3.322725	-0.416452
H	-7.876766	-3.660517	0.315747
H	-7.426327	-3.414634	-1.464275
C	-0.827992	-1.034601	0.037947
O	-0.321976	-2.174242	-0.621373
C	-2.956489	0.925923	-1.161804
H	-3.438973	1.156652	-2.115767
H	-1.888319	1.115928	-1.303108
C	2.894071	3.306402	-2.319618
C	4.195038	0.885711	-1.956739
C	4.282740	3.251025	-2.385507
C	2.132963	2.156860	-2.094995
C	2.797145	0.931486	-1.902321
C	4.937244	2.034925	-2.206813
H	4.852240	4.155716	-2.575606
H	6.020105	1.979056	-2.258388
H	4.699925	-0.066298	-1.813877
C	0.620664	2.262621	-2.035498
O	-0.066004	1.262611	-2.386207
H	0.664054	-2.053310	-0.642000
N	0.176424	3.411050	-1.555857
H	-0.846123	3.376884	-1.539933
H	2.371629	4.248852	-2.444257
C	2.052224	-0.333969	-1.657284
H	1.274990	-0.580035	-2.378735
N	2.218912	-1.164734	-0.701413
C	3.156939	-0.911023	0.381600
H	2.645444	-1.191742	1.311123
H	3.414516	0.153706	0.466281
C	4.422930	-1.739727	0.280389
C	6.791347	-3.238751	0.196894
C	5.402032	-1.580569	1.266879
C	4.643372	-2.656324	-0.747310
C	5.822635	-3.401815	-0.788257
C	6.577235	-2.322029	1.226937
H	5.236660	-0.866264	2.070598
H	3.889099	-2.787801	-1.517357
H	5.980219	-4.112884	-1.593793
H	7.328555	-2.184923	1.998805
H	7.708228	-3.819104	0.164396
H	-0.600835	-0.146976	-0.562300
H	-0.491290	-2.935218	1.935061
C	-0.081445	-1.977806	2.237007
C	-0.166944	-0.883264	1.407984
N	1.171721	-0.784398	3.906451
C	0.469892	0.327577	1.830331
C	0.581666	-1.878107	3.480417
C	1.133672	0.306198	3.093302
C	0.525695	1.508162	1.045709
H	0.627986	-2.747320	4.133692
H	2.328579	1.430809	4.483614
C	1.217470	2.629915	1.475753
H	0.015958	1.549010	0.093568
C	1.876401	2.592193	2.741826
H	2.414416	3.480348	3.058437
C	1.828941	1.472080	3.520552
O	1.313271	3.767005	0.786009
H	0.861452	3.688227	-0.143896
C	-3.581392	1.752501	-0.066451
C	-4.757562	3.346246	1.917088
C	-2.920646	1.985886	1.143623
C	-4.830716	2.346799	-0.276303
C	-5.417352	3.136191	0.708069
C	-3.506785	2.772649	2.131530
H	-1.933638	1.567372	1.316670
H	-5.343356	2.201248	-1.224194
H	-6.385716	3.591999	0.528236
H	-2.978070	2.945187	3.063455
H	-5.212120	3.964130	2.685082

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H	-3.198845	-3.159395	-3.046811
C	-2.711300	-2.770543	-2.148882
C	-2.765061	-2.714008	0.357262
C	-2.291894	-1.247271	0.217821
C	-3.521055	-3.152990	-0.905468
C	-2.634004	-1.234829	-2.244637
H	-1.891176	-3.351613	0.490419
H	-2.592243	-0.666029	1.091738
H	-1.622498	-0.871665	-2.448010
H	-1.706024	-3.185093	-2.085708
H	-3.398957	-2.818764	1.241890
H	-3.697709	-4.231234	-0.880814
H	-3.308542	-0.830644	-3.003552
N	-3.078090	-0.611945	-0.936407
C	-4.860493	-2.399399	-0.986053
H	-5.256575	-2.509406	-2.002462
C	-4.548070	-0.915540	-0.724551
H	-5.111520	-0.260452	-1.391749
H	-4.772785	-0.627348	0.305434
C	-5.903275	-2.893517	-0.022634
H	-5.653797	-2.838504	1.037748

C	-7.081774	-3.383567	-0.395555
H	-7.803137	-3.743826	0.330833
H	-7.364576	-3.443533	-1.443828
C	-0.755708	-1.111532	0.031597
O	-0.252756	-2.270467	-0.589138
C	-2.907643	0.901857	-1.021739
H	-3.335294	1.173755	-1.990772
H	-1.838779	1.114037	-1.069419
C	2.637226	3.343865	-2.241110
C	4.134837	1.082074	-1.682928
C	4.021062	3.440095	-2.139955
C	1.981455	2.118555	-2.103671
C	2.742798	0.975628	-1.793377
C	4.775873	2.301998	-1.867802
H	4.508222	4.401351	-2.272169
H	5.856937	2.362489	-1.791558
H	4.719887	0.192322	-1.466016
C	0.472444	2.134273	-2.281245
O	-0.146309	3.107713	-1.716175
H	0.732182	-2.142719	-0.625408
N	-0.050526	1.188190	-3.013556
H	-1.048066	1.411499	-3.100150
H	2.038445	4.228152	-2.436232
C	2.075988	-0.335617	-1.590653
H	1.293744	-0.570933	-2.313655
N	2.272650	-1.198998	-0.668245
C	3.198277	-0.966641	0.429824
H	2.692279	-1.309671	1.341245
H	3.416421	0.101860	0.567956
C	4.493248	-1.745339	0.299976
C	6.922879	-3.136513	0.156409
C	5.393113	-1.718968	1.370624
C	4.821623	-2.477983	-0.840357
C	6.031637	-3.170262	-0.910815
C	6.599355	-2.406130	1.300971
H	5.139631	-1.152501	2.264186
H	4.127964	-2.509302	-1.675517
H	6.274433	-3.737047	-1.804684
H	7.288124	-2.373937	2.139816
H	7.864100	-3.674667	0.100353
H	-0.546668	-0.249565	-0.612048
H	-0.296123	-2.921745	2.001273
C	0.080940	-1.934809	2.249227
C	-0.071527	-0.885124	1.375266
N	1.323945	-0.602179	3.823823
C	0.507687	0.372754	1.726437
C	0.773185	-1.741113	3.467344
C	1.207231	0.448477	2.966321
C	0.464046	1.515421	0.893747
H	0.879411	-2.573432	4.160363
H	2.372607	1.708882	4.262882
C	1.088312	2.695590	1.251873
H	-0.082006	1.506493	-0.037870
C	1.790967	2.761951	2.490780
H	2.279191	3.695017	2.754000
C	1.840846	1.673722	3.317105
O	1.062259	3.791624	0.487931
H	0.592878	3.584739	-0.393062
C	-3.585768	1.681190	0.076779
C	-4.858363	3.174006	2.075544
C	-2.970940	1.875906	1.317474
C	-4.834830	2.265338	-0.158076
C	-5.469637	3.005021	0.834812
C	-3.606645	2.612320	2.313382
H	-1.980917	1.470791	1.506305
H	-5.309358	2.152460	-1.129934
H	-6.437340	3.454675	0.637196
H	-3.115765	2.756015	3.270418
H	-5.351436	3.751972	2.850723

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H	-2.718039	-0.933895	3.588509
C	-2.266047	-0.197195	2.918466
C	-2.440283	2.082446	1.953671
C	-1.901412	1.515663	0.619366
C	-3.193969	1.005072	2.735186
C	-2.006570	-0.842933	1.551150
H	-1.595689	2.442002	2.547256
H	-2.339997	2.045301	-0.232039
H	-0.958189	-1.075077	1.372250
H	-1.319936	0.133179	3.353307
H	-3.107693	2.925548	1.755861
H	-3.498502	1.392534	3.711005
H	-2.593707	-1.752233	1.401161
N	-2.443101	0.090123	0.438200
C	-4.416475	0.547573	1.931938
H	-4.789644	-0.381131	2.385547
C	-3.947362	0.202837	0.495797
H	-4.356998	-0.749894	0.164117
H	-4.232561	0.973100	-0.227576
C	-5.576635	1.509754	1.873813
H	-6.368068	1.226013	1.178923
C	-5.720536	2.623449	2.586726
H	-6.607959	3.239591	2.482721
H	-4.975472	2.964183	3.300335
C	-0.368735	1.614233	0.490140
O	0.283466	1.196302	1.664572
H	-1.972077	-0.473888	-0.906211
C	-0.934474	-0.792580	-0.749745
H	-1.995290	0.363302	-1.610391
C	2.305959	-3.588386	2.830818
C	4.712490	-2.298900	2.402505
C	3.407575	-3.907931	3.617488
C	2.385011	-2.636663	1.810068
C	3.611344	-1.985944	1.596225
C	4.622340	-3.263247	3.399565
H	3.312286	-4.646722	4.407196
H	5.488691	-3.498105	4.009450
H	5.653080	-1.778917	2.238008
C	1.139907	-2.292121	1.007364
O	1.015711	-1.065905	0.657443
H	0.684312	0.307757	1.457704
N	0.274483	-3.219023	0.712980
H	0.613091	-4.122210	1.045559
H	1.350965	-4.068487	3.024734
C	3.849128	-0.919139	0.585594
H	4.335474	-0.025150	0.993546
N	3.659246	-0.899288	-0.669701
C	3.058911	-2.003431	-1.399835
H	2.753339	-2.832701	-0.753376
H	3.841326	-2.385344	-2.069985
C	1.882630	-1.552099	-2.243408
C	-0.264167	-0.815671	-3.892941
C	0.839382	-2.446181	-2.492948
C	1.842687	-0.285974	-2.832105

C	0.767591	0.086010	-3.637763
C	-0.217730	-2.088232	-3.326805
H	0.844259	-3.418422	-2.008114
H	2.653440	0.415933	-2.663600
H	0.745309	1.080077	-4.075547
H	-1.020236	-2.796508	-3.512997
H	-1.099433	-0.530299	-4.526400
H	-0.047796	0.987389	-0.351258
H	-1.776505	4.059104	0.602025
C	-0.746518	4.138907	0.277443
C	0.067910	3.039452	0.158521
N	0.962072	5.670225	-0.444358
C	1.408965	3.256490	-0.301836
C	-0.255547	5.431187	-0.026276
C	1.790618	4.597686	-0.596029
C	2.340492	2.206616	-0.514679
H	-0.915279	6.289807	0.086552
H	3.363934	5.881358	-1.303380
C	3.590847	2.483760	-1.036777
H	2.073971	1.179668	-0.277976
C	3.970563	3.825646	-1.315292
C	4.965656	3.995998	-1.712538
C	3.096917	4.850576	-1.092690
O	4.513010	1.545583	-1.324261
H	4.152097	0.616671	-1.174290
C	-2.795161	-1.620433	-1.430778
C	-4.255620	-3.755065	-2.483873
C	-3.806509	-1.389319	-2.367618
C	-2.502331	-2.929255	-1.035987
C	-3.239004	-3.989969	-1.559357
C	-4.536050	-2.452215	-2.892974
H	-4.016894	-0.372716	-2.694275
H	-1.661069	-3.104434	-0.361025
H	-3.006503	-5.006883	-1.257199
H	-5.316061	-2.265535	-3.624482
H	-4.820825	-4.585966	-2.895410

Ia20Z-S

H	-2.795160	-0.592082	3.373540
C	-2.325809	0.085574	2.655118
C	-2.352021	2.354644	1.647832
C	-1.909037	1.708138	0.312251
C	-3.150596	1.363801	2.498612
C	-2.231545	-0.613299	1.293101
H	-1.458177	2.666803	2.193659
H	-2.309276	2.260416	-0.543317
H	-1.225205	-0.977714	1.082948
H	-1.322734	0.333995	3.007298
H	-2.959915	3.241249	1.448331
H	-3.359220	1.796764	3.480143
H	-2.935941	-1.443035	1.204621
N	-2.616565	0.348780	0.185513
C	-4.454960	1.001170	1.779896
H	-4.868842	0.103683	2.259742
C	-4.097723	0.628637	0.320748
H	-4.624798	-0.268122	-0.006187
H	-4.323618	1.442819	-0.374681
C	-5.538637	2.050168	1.782616
H	-6.400962	1.815473	1.157617
C	-5.535440	3.187782	2.471682
H	-6.374702	3.873620	2.417762
H	-4.710433	3.479887	3.115563
C	-0.369455	1.660650	0.163322
O	0.248573	1.148464	1.310484
C	-2.340684	-0.249403	-1.187432
H	-1.261896	-0.378626	-1.263354
H	-2.644001	0.518062	-1.905722
C	1.786011	-3.486670	3.020856
C	4.125655	-2.007303	3.060501
C	2.678603	-3.637639	4.075999
C	2.037229	-2.589386	1.980873
C	3.238966	-1.863649	1.985149
C	3.854864	-2.890000	4.098931
H	2.457354	-4.331645	4.881232
H	4.557665	-2.993807	4.919486
H	5.044747	-1.426598	3.070284
C	1.004078	-2.467793	0.880864
O	0.427745	-3.523330	0.523669
H	0.591269	0.216686	1.069529
N	0.833727	-1.249265	0.386456
H	0.261473	-1.362863	-0.454261
H	0.867481	-4.063835	2.981742
C	3.682419	-0.911091	0.929477
H	4.032515	0.050271	1.324011
N	3.809275	-1.045224	-0.328299
C	3.422812	-2.243605	-1.057099
H	3.114903	-3.063315	-0.397594
H	4.316961	-2.575889	-1.600450
C	2.310412	-1.945045	-2.047941
C	0.132052	-1.376500	-3.722327
C	1.352295	-2.922382	-2.321573
C	2.196273	-0.695768	-2.663322
C	1.107843	-0.408257	-3.484273
C	0.269496	-2.641350	-3.152609
H	1.415649	-3.885438	-1.825185
H	2.946953	0.067338	-2.484422
H	1.022057	0.576730	-3.934598
H	-0.482628	-3.404085	-3.332163
H	-0.724425	-1.149329	-4.350948
H	-0.104223	1.042579	-0.708640
H	-1.639192	4.185776	0.106923
C	-0.581708	4.200090	-0.124948
C	0.180613	3.056297	-0.143547
N	1.260440	5.625252	-0.718322
C	1.568001	3.194195	-0.485709
C	-0.000588	5.458085	-0.409742
C	2.041724	4.509111	-0.768537
C	2.465510	2.097686	-0.592258
H	-0.623109	6.350326	-0.377060
H	3.732971	5.703275	-1.347075
C	3.776468	2.307135	-0.983643
H	2.127534	1.090083	-0.364876
C	4.242328	3.623716	-1.254436
H	5.280102	3.744144	-1.548995
C	3.399647	4.690544	-1.143192
O	4.688943	1.331464	-1.142191
H	4.319622	0.418373	-0.919650
C	-3.029935	-1.558124	-1.474381
C	-4.278445	-3.981005	-2.095796
C	-4.233415	-1.573228	-2.186598
C	-2.440433	-2.769498	-1.095123
C	-3.069866	-3.973527	-1.401910
C	-4.858654	-2.778457	-2.493307
H	-4.677658	-0.635662	-2.513984
H	-1.481687	-2.794421	-0.574183

H	-2.604843	-4.908105	-1.103624
H	-5.790720	-2.777337	-3.049151
H	-4.762200	-4.922687	-2.336198

Ta12Z

H	-3.545955	-4.095396	1.014119
C	-3.454438	-3.013230	0.886857
C	-4.185348	-1.029844	-0.417323
C	-2.746086	-0.485756	-0.279331
C	-4.185793	-2.560214	-0.380115
C	-1.967594	-2.640883	0.770585
H	-4.781106	-0.655432	0.418456
H	-2.474304	0.124897	-1.146595
H	-1.580237	-2.154287	1.667589
H	-3.885136	-2.516840	1.758255
H	-4.639502	-0.657867	-1.339603
H	-5.212707	-2.935207	-0.383528
H	-1.342587	-3.503927	0.530597
N	-1.768264	-1.669897	-0.372278
C	-3.425204	-3.118932	-1.596677
H	-3.244361	-4.186341	-1.423582
C	-2.066615	-2.390192	-1.666863
H	-1.250113	-3.091072	-1.843276
H	-2.049867	-1.627163	-2.451690
C	-4.170475	-2.974745	-2.894385
H	-4.406937	-1.957518	-3.209155
C	-4.546579	-4.000713	-3.651905
H	-5.094336	-3.852687	-4.577094
H	-4.319589	-5.026515	-3.371277
C	-2.564449	0.380514	0.989805
O	-3.108780	-0.234491	2.124688
C	-0.345813	-1.144831	-0.402166
H	-0.216176	-0.557289	0.507657
H	-0.297449	-0.473103	-1.266214
C	2.247922	-0.844632	3.893360
C	3.877990	0.236955	1.928566
C	3.606502	-1.147602	3.877824
C	1.682489	0.002040	2.937847
C	2.515690	0.557522	1.945897
C	4.424608	-0.609922	2.887584
H	4.024455	-1.800633	4.637808
H	5.484746	-0.841090	2.864316
H	4.516522	0.670809	1.162950
C	0.184582	0.281128	2.917989
O	-0.169374	1.413483	2.503212
-H	-2.314672	-0.405013	2.723104
N	-0.668922	-0.675452	3.245111
-H	-0.194388	-1.522173	3.553781
H	1.613888	-1.263208	4.670549
C	1.988387	1.513234	0.927134
H	1.437331	2.367067	1.312491
N	2.113602	1.446697	-0.343099
C	2.807239	0.344060	-0.996511
H	2.197518	0.054883	-1.862400
H	2.896952	-0.539829	-0.353084
C	4.182866	0.747804	-1.490103
C	6.730415	1.411110	-2.446193
C	5.156415	-0.240455	-1.660252
C	4.497692	2.072813	-1.797859
C	5.765910	2.401230	-2.272899
C	6.421953	0.086967	-2.138800
H	4.916725	-1.272154	-1.409245
H	3.749715	2.848148	-1.660550
H	6.000594	3.435521	-2.506021
H	7.170124	-0.689947	-2.263924
H	7.718731	1.670134	-2.813331
H	-1.511899	0.592151	1.177941
H	-5.013879	1.304179	1.749850
C	-4.477255	2.012991	1.128049
C	-3.208539	1.723294	0.696265
N	-4.486455	4.155931	0.026016
C	-2.506688	2.711192	-0.063112
C	-5.074855	3.243432	0.764215
C	-3.208072	3.907714	-0.379363
C	-1.158450	2.564376	-0.483759
H	-6.087935	3.464489	1.096158
H	-3.097222	5.808456	-1.382874
C	-0.526267	3.566541	-1.191479
H	-0.584009	1.692332	-0.192169
C	-1.245402	4.743778	-1.541888
H	-0.726275	5.510603	-2.108123
C	-2.542900	4.906594	-1.142532
O	0.762847	3.508354	-1.577593
H	1.224829	2.710446	-1.187341
C	0.741227	-2.186033	-0.464310
C	2.952904	-3.894418	-0.524466
C	1.273127	-2.608284	-1.686040
C	1.324638	-2.630135	0.725804
C	2.426863	-3.479437	0.697879
C	2.372136	-3.462408	-1.716439
H	0.849850	-2.239760	-2.618029
H	0.927917	-2.278346	1.674673
H	2.881642	-3.801002	1.629561
H	2.784217	-3.777860	-2.669572
H	3.819236	-4.547930	-0.549231

Ib10

H	-3.546745	-4.156166	0.761806
C	-3.436903	-3.070919	0.687171
C	-4.101381	-1.018264	-0.531875
C	-2.660214	-0.496306	-0.340030
C	-4.113312	-2.547440	-0.583082
C	-1.942311	-2.715953	0.644959
H	-4.709368	-0.690936	0.314731
H	-2.360808	0.134405	-1.183449
H	-1.565414	-2.298497	1.579599
H	-3.897351	-2.611455	1.564219
H	-4.536402	-0.586985	-1.437229
H	-5.142223	-2.911280	-0.646564
N	-1.325440	-3.573963	0.368838
N	-1.690037	-1.686032	-0.436529
C	-3.312300	-3.045681	-1.800737
H	-3.159105	-4.125385	-1.686775
C	-1.936323	-2.344401	-1.774143
H	-1.125833	-3.055694	-1.935671
H	-1.861680	-1.552994	-2.526729
C	-4.004381	-2.806837	-3.113957
H	-4.202852	-1.767044	-3.377352
C	-4.377602	-3.777491	-3.942495
H	-4.887662	-3.563025	-4.876101
H	-4.186104	-4.823108	-3.713222
C	-2.511617	0.341212	0.953861
O	-3.057463	-0.308891	2.067088
C	-0.264232	-1.175145	-0.369430

H	-0.166399	-0.698032	0.605559
H	-0.182985	-0.419553	-1.158618
C	2.049904	-1.234045	3.747299
C	3.732780	-0.049117	1.888554
C	3.381214	-1.626962	3.671260
C	1.543900	-0.228855	2.919700
C	2.392796	0.357033	1.963559
C	4.229000	-1.028622	2.739888
H	3.758620	-2.397747	4.336631
H	5.271444	-1.324068	2.675410
H	4.393152	0.421639	1.164999
C	0.069660	0.104417	3.040943
O	-0.708848	-0.923722	3.025642
H	-2.261076	-0.572843	2.621082
N	-0.240387	1.362578	3.133555
H	-1.260575	1.431353	3.225398
H	1.373324	-1.711317	4.449723
C	1.874545	1.403811	1.042355
H	1.248375	2.166375	1.506188
N	2.042316	1.495709	-0.222597
C	2.784297	0.498845	-0.985788
C	2.194648	0.303370	-1.892254
H	2.880114	-0.453120	-0.451171
C	4.156603	0.987632	-1.402783
C	6.697305	1.810128	-2.244295
C	5.184932	0.056499	-1.567763
C	4.412611	2.337117	-1.655582
C	5.677577	2.744346	-2.073765
C	6.448139	0.462899	-1.990172
H	4.989581	-0.993658	-1.358286
H	3.622919	3.071031	-1.522047
H	5.867025	3.796151	-2.265668
H	7.238274	-0.271521	-2.113271
H	7.682141	2.131444	-2.568794
H	-1.457386	0.555177	1.143501
H	-4.982949	1.185903	1.732027
C	-4.453713	1.930547	1.147100
C	-3.180393	1.680718	0.703911
N	-4.482758	4.131972	0.166839
C	-2.490720	2.714565	-0.000875
C	-5.065056	3.171953	0.847552
C	-3.200885	3.922140	-0.246781
C	-1.141863	2.605610	-0.424818
H	-6.081582	3.362215	1.187286
H	-3.100403	5.882635	-1.129972
C	-0.509770	3.658401	-1.055025
H	-0.566434	1.710676	-0.218184
C	-1.235686	4.849717	-1.335515
H	-0.719077	5.655875	-1.846518
C	-2.539147	4.972921	-0.940865
O	0.783052	3.625322	-1.425439
H	1.235152	2.819372	-1.035910
C	0.821483	-2.210665	-0.498975
C	3.032559	-3.909032	-0.655910
C	1.394304	-2.508149	-1.739062
C	1.360295	-2.773603	0.661748
C	2.463551	-3.619129	0.582954
C	2.494087	-3.357480	-1.818406
H	1.000143	-2.048237	-2.642911
H	0.925778	-2.519441	1.626449
H	2.885458	-4.036569	1.491779
H	2.939775	-3.575006	-2.783777
H	3.899454	-4.559703	-0.716068

Ia18Z

H	-3.250135	0.356423	-3.165254
C	-2.529465	0.719369	-2.425645
C	-0.464246	0.215627	-1.172309
C	-1.157781	-0.308962	0.092999
C	-1.278862	-0.166218	-2.408956
C	-3.153646	0.715898	-1.020275
H	-0.372662	1.306264	-1.137932
H	-0.819375	-1.328949	0.296597
H	-4.240373	0.645562	-1.060458
H	-2.267894	1.746184	-2.693898
H	0.546260	-0.203540	-1.186890
H	-0.688402	-0.023684	-3.316582
H	-2.877820	1.595123	-0.434440
N	-2.656598	-0.480416	-0.241774
C	-1.732116	-1.632818	-2.297206
H	-2.270499	-1.904304	-3.212446
C	-2.749759	-1.700841	-1.132362
H	-3.777316	-1.736186	-1.499105
H	-2.577085	-2.569547	-0.492391
C	-0.589583	-2.601010	-2.119893
H	0.091047	-2.426565	-1.282668
C	-0.385250	-3.637282	-2.930101
H	0.444664	-4.321051	-2.777994
H	-1.038332	-3.836911	-3.777170
C	-0.739137	0.445519	1.383955
O	-1.227857	-0.180935	2.537180
C	-3.493191	-0.710358	1.004887
H	-3.397804	0.195790	1.596387
H	-2.991669	-1.508705	1.552025
C	3.461941	-3.424842	2.661623
C	5.100050	-1.665922	2.011118
C	4.785123	-3.774946	2.922203
C	3.147326	-2.205477	2.060938
C	4.185700	-1.319347	1.736873
C	5.812674	-2.895145	2.593647
H	5.012486	-4.733579	3.378237
H	6.846307	-3.158954	2.793520
H	6.306475	-0.966373	1.771078
C	1.713674	-1.854373	1.703200
O	1.520341	-1.515147	0.502511
H	-0.555515	-0.936245	2.678691
N	0.789828	-1.912913	2.641905
H	1.208389	-2.166176	3.535046
H	2.655660	-4.109616	2.910944
C	3.911675	0.045672	1.188843
H	3.713419	0.831694	1.925674
N	3.934362	0.409313	-0.027043
C	4.129303	-0.595036	-1.070541
H	3.836611	-1.586852	-0.714754
H	5.199812	-0.614410	-1.315293
C	3.334936	-0.235283	-2.304849
C	1.903315	0.396977	-4.629867
C	3.457501	1.027636	-2.892531
C	2.479640	-1.171351	-2.886070
C	1.774213	-0.862172	-4.048671
C	2.741753	1.344869	-4.043322
H	4.113529	1.769250	-2.445215
H	2.355617	-2.144133	-2.417347
H	1.109960	-1.603258	-4.483767
H	2.843759	2.330499	-4.487353

H	1.350262	0.641759	-5.531898
H	0.344649	0.285235	1.335113
H	-2.819764	1.822911	2.512529
C	-2.093131	2.470898	2.034684
C	-0.971260	1.945829	1.436877
N	-1.436020	4.742823	1.594146
C	0.019934	2.866918	0.962834
C	-2.291702	3.869773	2.072276
C	-0.277372	4.257787	1.067041
C	1.289632	2.471574	0.458940
H	0.434865	6.255391	0.706991
C	2.226947	3.415188	0.092224
H	1.549285	1.421537	0.364062
C	1.909319	4.800819	0.161298
H	2.663267	5.515793	-0.152381
C	0.691813	5.203625	0.630541
O	3.464605	3.101014	-0.332613
H	3.610029	2.111036	-0.285661
C	-4.945155	-1.027074	0.750563
C	-7.660553	-1.602286	0.377780
C	-5.894851	-0.000249	0.738376
C	-5.377392	-2.349021	0.604479
C	-6.725883	-2.635382	0.412508
C	-7.244393	-0.283651	0.546882
H	-5.574843	1.028199	0.891768
H	-4.656269	-3.160955	0.652027
H	-7.047269	-3.665754	0.300043
H	-7.969592	0.523531	0.539472
H	-8.712541	-1.825901	0.232141
H	-3.199356	4.268782	2.521337

Ib22Z-S

H	-3.278983	0.466629	-3.164434
C	-2.483247	0.649443	-2.436197
C	-0.418766	-0.195719	-1.382030
C	-1.036767	-0.252028	0.028404
C	-1.467774	-0.496759	-2.449844
C	-3.085909	0.788327	-1.023272
H	-0.020567	0.803335	-1.579500
H	-0.816125	-1.206345	0.518855
H	-4.172409	0.690558	-1.033654
H	-1.989553	1.585295	-2.712641
H	0.434818	-0.882296	-1.427551
H	-0.987514	-0.573325	-3.429421
H	-2.824246	1.734817	-0.550605
N	-2.573152	-0.304135	-0.117469
C	-2.215483	-1.801710	-2.136006
H	-3.001664	-1.931842	-2.888819
C	-2.898693	-1.635553	-0.756823
C	-3.985277	-1.680746	-0.843975
H	-2.574793	-2.402030	-0.046899
C	-1.339861	-3.023004	-2.169958
H	-0.464872	-3.021944	-1.518053
C	-1.582218	-4.078493	-2.941373
H	-0.930678	-4.946623	-2.939047
H	-2.443180	-4.110384	-3.605139
C	-0.401751	0.786173	1.004062
O	-0.795759	0.591907	2.333743
C	-3.237005	-0.250074	1.252927
H	-2.953672	0.703586	1.687838
H	-2.742186	-1.026197	1.841878
C	2.848086	-2.104023	3.900041
C	4.980858	-0.608324	2.971922
C	4.012293	-2.024554	4.655660
C	2.741753	-1.477738	2.655960
C	3.820413	-0.703989	2.195389
C	5.092137	-1.283922	4.182564
H	4.076705	-2.535372	5.611881
H	6.008349	-1.212755	4.760671
H	5.800489	0.016327	2.624995
C	1.485966	-1.754726	1.853632
O	0.367178	-1.767603	2.479859
H	-0.369689	-0.273490	2.599525
N	1.720468	-2.028636	0.600555
H	0.835784	-2.323681	0.174484
H	1.989700	-2.666785	4.253592
C	3.746919	0.242256	1.034223
H	3.529041	1.274735	1.337348
N	3.962824	0.088371	-0.207130
C	4.233961	-1.221755	-0.783652
H	4.115771	-2.021112	-0.047744
H	5.273654	-1.200857	-1.137658
C	3.308020	-1.471061	-1.959389
C	1.571569	-1.976533	-4.108208
C	2.990090	-0.461272	-2.869625
C	2.755783	-2.741050	-2.146575
C	1.901371	-2.995032	-3.213975
C	2.122251	-0.710234	-3.933757
H	3.409908	0.532903	-2.751462
H	2.971630	-3.519756	-1.421076
H	1.474102	-3.985708	-3.340309
H	1.881336	0.091231	-4.626750
H	0.890718	-2.173072	-4.931868
H	0.658050	0.512446	0.897771
H	-2.277462	2.584368	1.856417
C	-1.558353	3.018950	1.169693
C	-0.531749	2.261590	0.653685
N	-0.794896	5.036810	0.104308
C	0.468830	2.943589	-0.109345
C	-1.663500	4.390714	0.846194
C	0.282580	4.337912	-0.343941
C	1.663202	2.328757	-0.564444
H	1.114264	6.113257	-1.223966
C	2.660393	3.071208	-1.160025
H	1.832359	1.268565	-0.424242
C	2.452059	4.451514	-1.433610
H	3.243908	5.000715	-1.932665
C	1.290838	5.057479	-1.044942
O	3.853922	2.547767	-1.498795
H	3.935251	1.631417	-1.103866
C	-4.733968	-0.419040	1.247009
C	-7.517691	-0.700314	1.337451
C	-5.565221	0.701674	1.155386
C	-5.315049	-1.679867	1.414109
C	-6.698903	-1.821364	1.453386
C	-6.949413	0.563306	1.193553
H	-5.123538	1.691969	1.065813
H	-4.678907	-2.554887	1.525887
H	-7.137051	-2.805418	1.585245
H	-7.582314	1.442158	1.124139
H	-8.596936	-0.809998	1.373429
H	-2.501958	4.968345	1.231717

Ia2E (denoted as Ia2 in the main article)

H	2.384024	3.969431	-2.553556
C	1.371361	3.580907	-2.409324
C	-0.547377	3.407656	-0.846243
C	-0.315618	1.914471	-0.549828
C	0.786100	4.109965	-1.094600
C	1.384867	2.041083	-2.384963
H	-1.172707	3.492875	-1.739917
H	-0.307175	1.719185	0.529559
H	2.352569	1.627977	-2.675418
H	0.763347	3.917796	-3.252818
H	-1.089994	3.859513	-0.012394
H	0.643330	5.192205	-1.149181
H	0.600476	1.606015	-3.003111
N	1.118025	1.553874	-0.978888
C	1.767929	3.776304	0.043279
H	2.704439	4.312143	-0.146108
C	2.065191	2.261674	-0.036623
H	3.069084	2.073978	-0.419581
H	1.966188	1.768605	0.935934
C	1.265315	4.181649	1.403361
C	-1.432508	1.049764	-1.133578
O	-1.606608	1.350342	-2.542277
C	1.328421	0.052296	-0.883632
H	0.669562	-0.380589	-1.637606
H	0.982754	-0.224535	0.118304
C	3.027065	-1.055990	-2.344603
C	4.295130	-1.581406	-2.581118
C	2.732947	-0.441170	-1.122817
H	6.262239	-1.924693	-1.775845
C	3.717155	-0.391705	-0.128541
C	4.982454	-0.919594	-0.366257
C	5.275835	-1.508867	-1.594795
C	-2.956614	-2.117739	-2.384574
C	-2.441354	-3.258044	0.090938
C	-4.012798	-2.478414	-1.552580
C	-1.629997	-2.342337	-2.008062
C	-1.371683	-2.889980	-0.735009
C	-3.755073	-3.065999	-0.315452
H	-5.036185	-2.306721	-1.872390
H	-4.573163	-3.360620	0.334244
H	-2.231044	-3.687855	1.065911
C	-0.518559	-1.996163	-2.989069
O	0.424617	-2.810105	-3.122382
H	-1.349175	0.487639	-3.053618
N	-0.677273	-0.835453	-3.612017
H	0.094599	-0.720909	-4.273048
H	-3.144992	-1.659069	-3.349826
C	0.006664	-3.002286	-0.210899
H	0.800833	-3.182660	-0.942741
N	0.259119	-2.863903	1.035787
C	1.635284	-3.077120	1.459982
H	2.294329	-3.246467	0.593950
H	1.652493	-3.997267	2.058300
C	2.210826	-1.947999	2.291545
C	3.452164	0.141154	3.701311
C	1.497626	-0.797954	2.628750
C	3.546173	-2.052348	2.697259
C	4.163632	-1.020549	3.394130
C	2.116491	0.243693	3.325471
H	0.451843	-0.700933	2.355806
H	4.112573	-2.944005	2.437778
H	5.203697	-1.116453	3.691076
H	1.546206	1.134960	3.573398
H	3.934578	0.952462	4.237111
H	-1.190412	-0.011967	-1.079156
H	-3.525223	2.672785	-1.794248
C	-3.646733	2.186864	-0.832369
C	-2.696500	1.305170	-0.386595
N	-5.017002	1.878092	1.127666
C	-2.921650	0.639346	0.855745
C	-4.785957	2.447353	-0.033149
C	-4.106654	0.964876	1.571556
C	-2.053342	-0.353934	1.371198
H	-5.529551	3.161964	-0.381658
H	-5.271682	0.561299	3.336032
C	-2.363488	-1.032854	2.530176
H	-1.169748	-0.652430	0.817742
C	-3.527668	-0.680569	3.264802
H	-3.737610	-1.217346	4.184377
C	-4.368654	0.292559	2.796896
H	3.497191	0.040888	0.844429
H	5.733399	-0.879852	0.417141
H	4.509562	-2.060445	-3.531080
H	2.244106	-1.165783	-3.090879
O	-1.616510	-2.050356	3.008571
H	-0.953414	-2.337594	2.324601
C	1.810677	5.151195	2.131826
H	0.404894	3.637541	1.796397
H	1.414309	5.423732	3.104685
H	2.674897	5.708109	1.776990

Ib2E-R (denoted as Ib2 in the main article)

H	2.483787	4.220709	-2.012552
C	1.468711	3.812426	-1.998092
C	-0.544362	3.388235	-0.623588
C	-0.273203	1.885380	-0.446321
C	0.779117	4.153804	-0.673572
C	1.501422	2.283706	-2.171882
H	-1.089742	3.543666	-1.560743
H	-0.295590	1.606258	0.614559
H	2.488679	1.926740	-2.466943
H	0.921182	4.255035	-2.834112
H	-1.183319	3.733140	0.192978
H	0.603970	5.229679	-0.596041
H	0.755834	1.919559	-2.877303
N	1.184211	1.612027	-0.852395
C	1.694834	3.694602	0.477684
H	2.617397	4.283630	0.433645
C	2.067988	2.217176	0.211730
H	3.092145	2.120009	-0.152323
H	1.959445	1.594410	1.104893
C	1.086901	3.891170	1.841468
C	-1.321406	1.017567	-1.184206
O	-1.369750	1.306437	-2.551212
C	1.425231	0.115989	-0.950489
H	0.811905	-0.216372	-1.788316
H	1.054993	-0.309268	-0.009884
C	3.250435	-0.585552	-2.506681
C	4.547501	-1.020084	-2.764514
C	2.851557	-0.293629	-1.198360
H	6.458705	-1.525378	-1.912107
C	3.756968	-0.464126	-0.148019
C	5.052263	-0.904243	-0.405721
C	5.449350	-1.178414	-1.713343
C	-2.694089	-1.885707	-2.618998

C	-2.578447	-3.097058	-0.128664
C	-3.867469	-2.133311	-1.913260
C	-1.448542	-2.264637	-2.111820
C	-1.391433	-2.846721	-0.828657
C	-3.812144	-2.757045	-0.668199
H	-4.824152	-1.838484	-2.334087
H	-4.722110	-2.956776	-0.110969
H	-2.518645	-3.546122	0.859092
C	-0.226240	-1.956410	-2.959198
O	-0.216165	-0.806151	-3.545322
H	-1.036363	0.477339	-3.021570
N	0.683060	-2.880621	-3.014385
H	1.429214	-2.535191	-3.626072
H	-2.726180	-1.385808	-3.582508
C	-0.097820	-3.112899	-0.159848
H	0.732146	-3.418023	-0.803175
N	0.047550	-2.960315	1.101893
C	1.348850	-3.299712	1.662325
H	2.025258	-3.688210	0.887692
H	1.191161	-4.108419	2.387648
C	2.028867	-2.142280	2.369224
C	3.408541	-0.059710	3.656721
C	1.376836	-0.950228	2.688476
C	3.376443	-2.284163	2.718294
C	4.061910	-1.256350	3.357376
C	2.064211	0.085494	3.326669
H	0.323873	-0.822879	2.457745
H	3.895908	-3.207407	2.472006
H	5.109092	-1.385135	3.614128
H	1.541289	1.008048	3.566029
H	3.941088	0.747357	4.149766
H	-1.078717	-0.038683	-1.039733
H	-3.389459	2.588847	-2.010428
C	-3.587635	2.107499	-1.058914
C	-2.661519	1.258416	-0.509996
N	-5.139219	1.769274	0.756549
C	-2.988854	0.597799	0.711455
C	-4.808258	2.339213	-0.379452
C	-4.252312	0.886412	1.297691
C	-2.150728	-0.368665	1.317806
H	-5.533135	3.029569	-0.806834
H	-5.585099	0.446776	2.929838
C	-2.567701	-1.067066	2.430273
H	-1.206178	-0.642619	0.860275
C	-3.810190	-0.748348	3.040872
H	-4.102139	-1.299647	3.929002
C	-4.622640	0.205011	2.489764
H	3.448346	-0.262227	0.875102
H	5.746567	-1.040969	0.417920
H	4.849678	-1.246457	-3.782074
H	2.524784	-0.483961	-3.312134
O	-1.855837	-2.081538	2.964995
H	-1.170187	-2.388964	2.308234
C	1.572932	4.734634	2.747641
H	0.201010	3.302151	2.084681
H	1.105850	4.858461	3.719378
H	2.457267	5.334026	2.543909

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H	0.332983	1.215963	4.926060
C	-0.318828	1.450203	4.078816
C	-2.016291	0.577425	2.507156
C	-1.046401	0.327165	1.346499
C	-1.296308	0.298528	3.827944
C	0.512553	1.680762	2.803082
H	-2.376317	1.612851	2.487502
H	-1.074820	-0.719055	1.037283
H	0.183358	2.544592	2.229232
H	-0.863219	2.366443	4.322074
H	-2.883347	-0.076270	2.373997
H	-2.012951	0.209483	4.648414
H	1.575010	1.777675	3.029292
N	0.388186	0.485275	1.885379
C	-0.475745	-1.004779	3.715656
H	-0.029379	-1.195122	4.698175
C	0.673482	-0.754237	2.712832
H	1.622538	-0.565162	3.218394
H	0.791268	-1.576329	2.003747
C	-1.318623	-2.201466	3.342444
H	-1.469781	-2.394869	2.278992
C	-1.864817	-3.013228	4.243397
H	-2.482005	-3.856264	3.950096
H	-1.710068	-2.861996	5.309966
C	-1.343511	1.175544	0.096703
O	-0.952465	2.503958	0.380986
C	1.358706	0.586893	0.720902
H	1.146928	1.552229	0.256354
H	1.075246	-0.233928	0.056262
C	2.922234	-3.605639	-1.134621
C	3.372418	-1.346653	-2.705795
C	4.211174	-3.305701	-1.574125
C	1.858064	-2.771298	-1.465786
C	2.078691	-1.628148	-2.255778
C	4.435831	-2.176243	-2.357473
H	5.039452	-3.955816	-1.308605
H	5.436273	-1.946642	-2.710010
H	3.549247	-0.494345	-3.354208
C	0.473663	-2.989902	-0.890261
O	0.177229	-2.250620	0.092442
H	-0.895137	2.994570	-0.457978
N	-0.337838	-3.851818	-1.448603
H	0.095049	-4.309714	-2.247830
H	2.741441	-4.483594	-0.520201
C	0.880396	-0.839091	-2.648870
H	-0.018976	-1.446983	-2.792280
N	0.726108	0.410845	-2.831990
C	1.807511	1.353218	-2.604321
H	2.351061	1.492440	-3.550012
H	2.544390	0.998583	-1.866344
C	1.251429	2.694596	-2.170133
C	0.261846	5.191548	-1.355844
C	0.010503	3.147830	-2.630218
C	1.991762	3.508409	-1.310401
C	1.499942	4.745199	-0.897892
C	-0.477653	4.393641	-2.231038
H	-0.573136	2.511203	-3.287402
H	2.958621	3.161379	-0.951674
H	2.082864	5.358512	-0.217527
H	-1.441764	4.735679	-2.595688
H	-0.125986	6.152786	-1.034073
H	-0.765209	0.783834	-0.753824
H	-3.162986	3.141937	0.245644
C	-3.603136	2.216871	-0.107955
C	-2.826400	1.092965	-0.253947
N	-5.601241	1.084689	-0.809210

C	-3.449695	-0.113148	-0.713109
C	-4.983008	2.168751	-0.406565
C	-4.855616	-0.045785	-0.956137
C	-2.766494	-1.343129	-0.912879
C	-5.587344	3.067412	-0.294662
H	-6.604718	-1.147825	-1.545604
C	-3.461033	-2.484150	-1.295334
H	-1.694923	-1.420843	-0.748814
C	-4.868139	-2.401711	-1.524267
H	-5.380933	-3.308504	-1.830211
C	-5.536217	-1.223168	-1.368267
O	-2.916302	-3.685152	-1.466218
H	-1.873760	-3.705733	-1.373559
C	2.816721	0.473500	1.078653
C	5.555965	0.236654	1.593183
C	3.448782	-0.770039	0.987379
C	3.574411	1.601335	1.413445
C	4.936847	1.482703	1.675785
C	4.811534	-0.888895	1.244307
H	2.863634	-1.639335	0.696696
H	3.097432	2.578469	1.457194
H	5.515643	2.363378	1.935332
H	5.291125	-1.859401	1.159869
H	6.619684	0.145903	1.790229

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H	1.279170	-5.104520	-0.321369
C	0.664495	-4.446186	0.299994
C	-1.420340	-3.136572	0.441909
C	-0.802638	-1.787521	0.048503
C	-0.720028	-4.261071	-0.324680
C	1.321336	-3.064082	0.440007
H	-1.310923	-3.299082	1.520675
H	-1.314279	-1.387266	-0.833903
H	1.258637	-2.654286	1.447985
H	0.580876	-4.903811	1.289147
H	-2.492615	-3.099884	0.231228
H	-1.299239	-5.186089	-0.274196
H	2.362782	-3.081938	0.122174
N	0.626438	-2.053191	-0.452410
C	-0.521936	-3.854068	-1.798315
H	-0.039995	-4.691847	-2.313944
C	0.470782	-2.664391	-1.827918
H	1.466732	-2.982439	-2.139616
C	0.140870	-1.864822	-2.497006
C	-1.817339	-3.566009	-2.511444
H	-2.391466	-2.696667	-2.187961
C	-2.292445	-4.324526	-3.494906
C	-3.237629	-4.102771	-3.979760
H	-1.749026	-5.198096	-3.847916
C	-0.907596	-0.689844	1.125701
O	0.039841	-0.892513	2.147222
C	1.456108	-0.767871	-0.509191
H	1.788664	-0.598634	0.518231
H	0.779310	0.041041	-0.808845
C	-0.059876	5.095444	-1.694459
C	1.099447	4.809287	0.810394
C	0.653547	6.151827	-1.136255
C	-0.181420	3.877162	-1.026008
C	0.404568	3.733951	0.245055
C	1.234077	6.010134	0.122338
H	0.745966	7.089266	-1.676322
H	1.773977	6.835486	0.575402
H	1.506162	4.718399	1.812665
C	-0.936739	2.763795	-1.723170
O	-2.015494	3.106476	-2.305369
H	0.415224	0.002466	2.318970
N	-0.374488	1.578311	-1.692349
H	-0.961687	0.966992	-2.273278
H	-0.536627	5.200840	-2.663876
C	0.133908	2.509241	1.039689
H	-0.904098	2.171552	0.985331
N	0.905663	1.827463	1.793594
C	2.322280	2.175571	1.913696
H	2.425175	2.905274	2.727928
H	2.707710	2.650290	1.002580
C	3.149347	0.958219	2.261530
C	4.692690	-1.280532	2.944316
C	2.788082	0.147453	3.343451
C	4.293552	0.638322	1.531813
C	5.068541	-0.469603	1.877626
C	3.546720	-0.969136	3.678081
H	1.907775	0.399831	3.930449
H	4.579223	1.254164	0.682524
H	5.957177	-0.705371	1.298770
H	3.251922	-1.590666	4.518038
H	5.290384	-2.147322	3.208853
H	-0.703229	0.257007	0.621571
H	-1.787990	-1.666855	3.480156
C	-2.597256	-1.258418	2.885021
C	-2.328919	-0.672288	1.673040
N	-4.965774	-0.879952	2.677662
C	-3.415652	-0.106807	0.937943
C	-3.931752	-1.334282	3.347183
C	-4.721021	-0.265221	1.486613
C	-3.253363	0.601297	-0.279872
H	-4.138651	-1.806839	4.305805
H	-6.818127	0.108922	1.188227
C	-4.345631	1.128690	-0.943663
H	-2.260943	0.771558	-0.683391
C	-5.653210	0.919630	-0.417083
H	-6.494598	1.331467	-0.965653
C	-5.829877	0.251515	0.762095
O	-4.255902	1.830744	-2.081056
H	-3.322144	2.197289	-2.216393
C	2.614427	-0.813074	-1.473310
C	4.727562	-0.813534	-3.312392
C	2.471000	-0.196300	-2.721200
C	3.840260	-1.402699	-1.146677
C	4.888785	-1.408497	-2.062490
C	3.519748	-0.199905	-3.636988
H	1.539606	0.316718	-2.950792
H	3.992267	-1.830799	-0.160308
H	5.835343	-1.867806	-1.794257
H	3.395796	0.283875	-4.600775
H	5.546732	-0.815286	-4.024869

Ia6E

H	-5.206682	-1.805827	2.155337
C	-4.576828	-1.129417	1.570848
C	-4.039191	-0.278937	-0.708420
C	-2.559828	-0.232751	-0.258983
C	-4.810851	-1.346942	0.073821
C	-3.102003	-1.417767	1.886035

H	-4.490302	0.697530	-0.517601
H	-1.888078	-0.364643	-1.113083
H	-2.962387	-2.397328	2.350501
H	-4.814537	-0.100244	1.841538
H	-4.099820	-0.464199	-1.784283
H	-5.876636	-1.286113	-0.161358
H	-2.644254	-0.656600	2.518234
N	-2.285059	-1.472299	0.609158
C	-4.274607	-2.745119	-0.282858
H	-4.657936	-3.456395	0.458139
C	-2.737984	-2.687444	-0.174682
H	-2.333089	-3.565761	0.331838
H	-2.263474	-2.614778	-1.156443
C	-4.686078	-3.224610	-1.647008
H	-4.360167	-2.620516	-2.494656
C	-5.410717	-4.318820	-1.860940
H	-5.697966	-4.623245	-2.862233
H	-5.743659	-4.947895	-1.038749
C	-2.213255	1.119388	0.426446
O	-3.162468	1.498088	1.374632
C	-0.810026	-1.616171	0.994800
H	-0.808430	-2.069121	1.987885
H	-0.406626	-0.613003	1.127606
C	-0.163182	3.261466	2.281735
C	2.245730	2.645062	1.061094
C	0.478897	4.214686	1.498515
C	0.381911	1.987081	2.471861
C	1.601753	1.677690	1.841986
C	1.693528	3.908528	0.889012
H	0.030898	5.194556	1.363414
H	2.202425	4.644445	0.274069
H	3.178912	2.382759	0.569874
C	-0.371876	0.953823	3.299486
O	0.246262	-0.080558	3.651502
H	-2.660972	1.530967	2.265417
N	-1.642847	1.254472	3.547399
H	-2.004502	0.514604	4.154594
H	-1.113982	3.483532	2.754521
C	2.237732	0.335721	1.901629
C	2.399709	-0.123225	2.876825
N	2.606996	-0.233733	0.820959
C	3.338303	-1.496496	0.926428
H	2.782128	-2.252965	0.363091
H	3.410429	-1.827354	1.971430
C	4.715366	-1.331483	0.324295
C	7.242102	-0.949810	-0.815595
C	5.835987	-1.153929	1.135442
C	4.869190	-1.311562	-1.064111
C	6.124943	-1.119304	-1.632643
C	7.096192	-0.967883	0.569425
H	5.720987	-1.164185	2.216766
H	3.993932	-1.440068	-1.697664
H	6.233851	-1.104799	-2.712895
H	7.962710	-0.836706	1.210642
H	8.222858	-0.804549	-1.258129
H	-1.237884	1.037263	0.911706
H	-3.997264	3.029348	-0.344227
C	-3.098799	3.032708	-0.951854
C	-2.078024	2.160968	-0.673434
N	-1.908932	4.012768	-2.807585
C	-0.888162	2.244659	-1.456395
C	-2.965658	3.940342	-2.031468
C	-0.865072	3.181539	-2.525828
C	0.260835	1.461615	-1.200594
H	-3.783167	4.622942	-2.256915
H	0.298550	3.975827	-4.152791
C	1.393488	1.583121	-1.977412
H	0.299045	0.795133	-0.347012
C	1.399462	2.486598	-3.074816
H	2.299456	2.556016	-3.677588
C	0.302834	3.264388	-3.332731
O	2.519298	0.884680	-1.739544
H	2.484975	0.458462	-0.834902
C	0.044845	-2.441462	0.064009
C	1.725499	-4.019557	-1.534286
C	0.451045	-3.709995	0.489302
C	0.492939	-1.971298	-1.175629
C	1.323739	-2.757378	-1.969959
C	1.286459	-4.495856	-0.301541
H	0.119933	-4.080513	1.456369
H	0.207596	-0.986522	-1.532200
H	1.665102	-2.375313	-2.927162
H	1.597996	-5.474185	0.049640
H	2.380642	-4.625819	-2.151669

Ib7E-R

H	-5.194386	-1.731122	2.170108
C	-4.563766	-1.066356	1.573166
C	-4.037834	-0.252370	-0.725498
C	-2.554141	-0.216074	-0.289211
C	-4.815355	-1.298470	0.081119
C	-3.087511	-1.362998	1.881089
H	-4.476913	0.731743	-0.548446
H	-1.890686	-0.364492	-1.147112
H	-2.956539	-2.340921	2.352036
H	-4.793213	-0.033236	1.835256
H	-4.109922	-0.455899	-1.797282
H	-5.882542	-1.225682	-0.144340
H	-2.621879	-0.599766	2.511269
N	-2.287687	-1.447238	0.591626
C	-4.302168	-2.708175	-0.262744
H	-4.686023	-3.404712	0.491830
C	-2.764615	-2.666872	-0.171342
H	-2.364847	-3.543394	0.342647
H	-2.299249	-2.612487	-1.158822
C	-4.734413	-3.201179	-1.615631
H	-4.413321	-2.611500	-2.475240
C	-5.471487	-4.291476	-1.806047
H	-5.773902	-4.606939	-2.799422
H	-5.799822	-4.906209	-0.971248
C	-2.190761	1.139937	0.380077
O	-3.146697	1.543854	1.315151
C	-0.811865	-1.612865	0.953284
H	-0.805102	-2.093455	1.933375
H	-0.398739	-0.616844	1.107560
C	-0.191107	3.184406	2.376465
C	2.237921	2.615295	1.180025
C	0.461864	4.167004	1.639198
C	0.356927	1.909332	2.545179
C	1.587938	1.622117	1.921993
C	1.686905	3.884257	1.041289
H	0.011659	5.148697	1.526735
H	2.202891	4.639770	0.456871
H	3.176287	2.369449	0.690010
C	-0.464324	0.889750	3.320147

O	-1.716899	1.150798	3.458230
H	-2.671509	1.523607	2.200239
N	0.170242	-0.158211	3.759557
H	-0.520361	-0.734117	4.253023
H	-1.157665	3.381519	2.828524
C	2.226536	0.279793	1.941139
H	2.364766	-0.214688	2.902918
N	2.608732	-0.251895	0.845894
C	3.326734	-1.525008	0.915602
H	2.766475	-2.255910	0.322907
H	3.386622	-1.890641	1.949663
C	4.709848	-1.356082	0.328813
C	7.248030	-0.965121	-0.781935
C	5.821361	-1.179971	1.152967
C	4.878719	-1.330095	-1.057563
C	6.140254	-1.133126	-1.611721
C	7.087161	-0.989209	0.601504
H	5.694559	-1.195233	2.232957
H	4.010525	-1.456840	-1.701046
H	6.260833	-1.113933	-2.690653
H	7.946411	-0.859427	1.252664
H	8.233257	-0.816550	-1.213302
H	-1.222325	1.054312	0.878102
H	-3.974510	3.028066	-0.444766
C	-3.063970	3.030863	-1.033964
C	-2.040879	2.171365	-0.726296
N	-1.845780	4.004388	-2.873867
C	-0.835428	2.259979	-1.483950
C	-2.917959	3.928724	-2.119672
C	-0.799619	3.187430	-2.561655
C	0.316383	1.491918	-1.196008
H	-3.737731	4.600113	-2.368974
H	0.390522	3.980531	-4.169916
C	1.463406	1.617902	-1.950993
H	0.344033	0.831277	-0.337223
C	1.483418	2.512699	-3.055635
H	2.395124	2.586295	-3.639992
C	0.384689	3.276416	-3.343636
O	2.589541	0.930842	-1.686958
H	2.530627	0.488568	-0.791629
C	0.029317	-2.425290	-0.001614
C	1.700578	-3.981950	-1.630974
C	0.424351	-3.706593	0.395790
C	0.484083	-1.931615	-1.229517
C	1.310073	-2.707180	-2.039328
C	1.254645	-4.481966	-0.410190
H	0.090034	-4.095170	1.354589
H	0.210113	-0.935732	-1.562960
H	1.657145	-2.307085	-2.987100
H	1.557123	-5.470378	-0.079970
H	2.352452	-4.579714	-2.260008

Ia14Z

H	4.061040	0.231609	3.198682
C	3.135977	0.528836	2.694496
C	0.929105	-0.218172	1.877362
C	1.359648	-0.458027	0.422923
C	2.073275	-0.566548	2.830135
C	3.394773	0.780763	1.199375
H	0.654905	0.829758	2.031580
H	1.136261	-1.491738	0.145299
H	2.861745	1.656116	0.822350
H	2.790696	1.457949	3.155396
H	0.035751	-0.824005	2.047851
H	1.714403	-0.632791	3.860244
H	4.457649	0.895565	0.986470
N	2.901135	-0.393533	0.385824
C	2.706189	-1.903795	2.410381
H	3.494988	-2.156772	3.128087
C	3.388423	-1.669361	1.041281
H	4.470109	-1.566822	1.145190
H	3.180701	-2.480707	0.339274
C	1.713443	-3.037837	2.384164
H	0.857488	-2.939756	1.712482
C	1.831750	-4.120059	3.148897
H	1.096880	-4.918636	3.119485
H	2.667644	-4.245555	3.834029
C	0.522581	0.357084	-0.602372
O	0.795971	-0.025108	-1.924162
C	3.426759	-0.330438	-1.038504
H	3.077328	0.617966	-1.438825
H	2.907483	-1.122183	-1.578914
-3	094921	-4.139603	-1.635878
C	-5.089146	-3.268755	0.086454
C	-4.340680	-4.760605	-1.649935
C	-2.823987	-3.090171	-0.756242
C	-3.834071	-2.655413	0.117481
C	-5.342843	-4.322116	-0.788203
H	-4.528475	-5.584110	-2.332043
H	-6.319325	-4.796187	-0.795979
H	-5.869815	-2.916825	0.756177
C	-1.461302	-2.418880	-0.713937
O	-1.037416	-2.126211	0.438759
H	0.259147	-0.883839	-2.025610
N	-0.829306	-2.158581	-1.841301
H	-1.391467	-2.438460	-2.643134
H	-2.310514	-4.480862	-2.306409
C	-3.598368	-1.539652	1.088165
H	-2.976790	-1.769867	1.951889
N	-4.071550	-0.358056	1.021544
C	-4.860198	0.075899	-0.137374
H	-5.775348	0.536807	0.248223
H	-5.142405	-0.763692	-0.781680
C	-4.061187	1.093487	-0.921667
C	-2.430383	2.946951	-2.236593
C	-4.326829	2.457111	-0.824301
C	-2.978005	0.662968	-1.692911
C	-2.164409	1.581415	-2.346540
C	-3.514068	3.382640	-1.479639
H	-5.155581	2.799048	-0.208567
H	-2.748098	-0.398565	-1.762844
H	-1.296030	1.230422	-2.897971
H	-3.718726	4.444842	-1.381565
H	-1.780749	3.669102	-2.723839
H	-0.481649	-0.000324	-0.340578
H	2.014596	2.216101	-1.950522
C	1.360523	2.656170	-1.205382
C	0.520091	1.867481	-0.455587
N	0.560437	4.695509	-0.208282
C	-0.422710	2.528292	0.398492
C	1.354017	4.060361	-1.038677
C	-0.340719	3.948414	0.490150
C	-1.471006	1.857687	1.081724
H	2.042799	4.670342	-1.620851
H	-1.168660	5.718020	1.389961

C	-2.405793	2.564126	1.806663
H	-1.591800	0.781453	1.000964
C	-2.276358	3.972452	1.955087
H	-3.013518	4.495963	2.556070
C	-1.269059	4.639536	1.316273
O	-3.472793	1.983332	2.390929
H	-3.617815	1.071681	2.009710
C	4.923345	-0.449657	-1.176058
C	7.693443	-0.655933	-1.535725
C	5.525837	-1.699389	-1.353654
C	5.723645	0.696842	-1.211630
C	7.101557	0.595708	-1.384325
C	6.902666	-1.803604	-1.525811
H	4.912667	-2.596956	-1.368183
H	5.262553	1.677412	-1.116364
H	7.709294	1.494405	-1.409260
H	7.356503	-2.779910	-1.662104
H	8.766989	-0.736722	-1.674249

Ib18Z-R

H	4.126453	0.025847	3.140918
C	3.162803	0.230289	2.664545
C	1.022676	-0.724032	1.894938
C	1.423059	-0.836308	0.415185
C	2.234413	-0.982259	2.792041
C	3.360780	0.553820	1.172779
H	0.646004	0.278947	2.108557
H	1.320156	-1.869621	0.069188
H	2.752126	1.396482	0.839948
H	2.724732	1.100106	3.160739
H	0.200028	-1.423041	2.079178
H	1.921524	-1.123687	3.829172
H	4.404556	0.760627	0.937137
N	2.946374	-0.632249	0.330894
C	2.997974	-2.224172	2.302913
H	3.840079	-2.398451	2.981679
C	3.585089	-1.877055	0.914794
H	4.654777	-1.669757	0.971402
H	3.425208	-2.678921	0.189465
C	2.151872	-3.470339	2.288494
H	1.284567	-3.485192	1.626317
C	2.403277	-4.532565	3.047668
H	1.766253	-5.410738	3.026017
H	3.257395	-4.557636	3.720356
C	0.485991	-0.038141	-0.546196
O	0.648832	-0.476295	-1.868185
C	3.396013	-0.481282	-1.114092
H	2.906336	0.415912	-1.477915
H	2.967185	-1.332189	-1.645872
C	-4.010597	-3.437217	-1.994172
C	-5.716922	-2.472630	-0.029817
C	-5.371462	-3.719449	-2.060310
C	-3.478716	-2.706224	-0.930697
C	-4.347829	-2.198694	0.046592
C	-6.228194	-3.242657	-1.069881
H	-5.764952	-4.306235	-2.884954
H	-7.291593	-3.456103	-1.113591
H	-6.383858	-2.071517	0.729348
C	-1.981157	-2.475846	-0.880385
O	-1.434245	-2.112154	-1.977128
H	-0.076201	-1.157665	-2.003947
N	-1.433230	-2.706355	0.285047
H	-0.424273	-2.594411	0.155118
H	-3.334042	-3.785609	-2.768603
C	-3.833712	-1.322652	1.143330
H	-3.214561	-1.796921	1.903434
N	-4.037000	-0.069760	1.267616
C	-4.792120	0.685251	0.259399
H	-5.461248	1.359102	0.803581
H	-5.402725	0.029853	-0.369401
C	-3.851892	1.497115	-0.608779
C	-2.056054	2.959794	-2.184010
C	-3.799755	2.886266	-0.514723
C	-2.990980	0.843512	-1.495905
C	-2.098168	1.568131	-2.277768
C	-2.904652	3.616269	-1.298202
H	-4.448430	3.401159	0.190594
H	-3.003832	-0.239881	-1.581149
H	-1.411885	1.037293	-2.932005
H	-2.863361	4.697681	-1.203768
H	-1.347550	3.526826	-2.781407
H	-0.506858	-0.352646	-0.193248
H	1.736959	1.735773	-2.208234
C	1.264435	2.217101	-1.359273
C	0.541869	1.480548	-0.449915
N	0.781701	4.303881	-0.260679
C	-0.220154	2.203766	0.524242
C	1.365210	3.620176	-1.217552
C	-0.031067	3.615955	0.588319
C	-1.211425	1.613480	1.348425
H	1.968870	4.185151	-1.925803
H	-0.571007	5.433033	1.604221
C	-1.980931	2.383383	2.194456
H	-1.445227	0.556832	1.265688
C	-1.710087	3.771280	2.335261
H	-2.307924	4.344188	3.037274
C	-0.761580	4.365637	1.551134
O	-3.017463	1.880531	2.893948
H	-3.339487	1.048803	2.437071
C	4.885697	-0.377967	-1.312544
C	7.634867	-0.143624	-1.777810
C	5.667131	-1.516991	-1.527818
C	5.492964	0.880897	-1.361135
C	6.861370	0.998939	-1.586355
C	7.035662	-1.401361	-1.753701
H	5.201834	-2.499527	-1.530817
H	4.885585	1.774821	-1.233329
H	7.319811	1.981870	-1.623056
H	7.631093	-2.293110	-1.921233
H	8.701394	-0.053576	-1.958120

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H	-5.267679	-1.130077	1.918122
C	-4.431666	-0.454063	1.718360
C	-3.772211	1.803981	0.892646
C	-2.537348	1.116862	0.262818
C	-4.932268	0.809711	1.011274
C	-3.409153	-1.168254	0.815477
H	-3.507790	2.166356	1.887821
H	-2.208303	1.659255	-0.628695
H	-3.841834	-2.037748	0.315614
H	-3.963709	-0.187171	2.667204
H	-4.060866	2.671380	0.293150
H	-5.756380	1.261856	1.569444

H	-2.495301	-1.473043	1.331260
N	-2.974347	-0.241651	-0.298514
C	-5.410644	0.400550	-0.393018
H	-6.049025	-0.485168	-0.290833
C	-4.156888	0.018027	-1.204577
H	-4.324285	-0.888902	-1.784786
H	-3.848658	0.817762	-1.886007
C	-6.198289	1.463244	-1.106950
H	-5.688501	2.410362	-1.287823
C	-7.453337	1.305211	-1.517080
H	-7.990879	2.102079	-2.020952
H	-7.987168	0.370840	-1.360487
C	-1.337688	1.069967	1.243317
O	-1.786116	0.741577	2.537464
C	-1.838411	-0.845510	-1.117131
H	-1.004203	-0.974980	-0.426566
H	-1.600187	-0.092254	-1.874235
C	2.251608	-2.676443	3.708352
C	3.864607	-2.484600	1.469622
C	3.587294	-3.052082	3.788554
C	1.693086	-2.210000	2.514403
C	2.518926	-2.103688	1.380708
C	4.399533	-2.962324	2.660112
H	3.992818	-3.419312	4.726512
H	5.442832	-3.258987	2.704721
H	4.497240	-2.399892	0.588464
C	0.209182	-1.891921	2.466797
O	-0.329735	-1.884119	1.310525
H	-1.097463	0.196403	2.967799
N	-0.372912	-1.691041	3.626104
H	-1.381488	-1.644336	3.441865
H	1.600693	-2.740270	4.573091
C	2.038057	-1.597236	0.058324
H	1.238844	-2.157768	-0.422513
N	2.505632	-0.597388	-0.584776
C	3.546699	0.251521	-0.012765
H	3.821542	-0.040931	1.006963
H	3.138568	1.267427	0.048184
C	4.779570	0.278044	-0.891982
C	7.113461	0.345473	-2.445617
C	5.633349	1.385018	-0.846402
C	5.102759	-0.787248	-1.732652
C	6.263183	-0.754871	-2.504842
C	6.794159	1.417672	-1.612822
H	5.381660	2.227555	-0.206138
H	4.435236	-1.642458	-1.793916
H	6.499847	-1.591579	-3.155390
H	7.446466	2.284627	-1.567372
H	8.016200	0.371527	-3.048065
H	-0.606561	0.323366	0.924298
H	-1.641549	3.168748	2.974109
C	-1.000246	3.407792	2.132647
C	-0.702882	2.452006	1.196727
N	0.342446	5.076488	1.020690
C	0.195760	2.796047	0.142137
C	-0.454451	4.708981	1.996580
C	0.687012	4.129819	0.100917
C	0.649720	1.863209	-0.820297
H	-0.704484	5.470012	2.733660
H	1.953619	5.515506	-0.950665
C	1.596878	2.219534	-1.755537
H	0.328790	0.829335	-0.789079
C	2.051128	3.562996	-1.830379
H	2.783069	3.818020	-2.590251
C	1.600057	4.489481	-0.927985
O	2.150397	1.313887	-2.592768
H	2.129869	0.435142	-2.134271
C	-2.147745	-2.173861	-1.758871
C	-2.635876	-4.652894	-2.954367
C	-1.882350	-3.356928	-1.059965
C	-2.630152	-2.244504	-3.069391
C	-2.878071	-3.478486	-3.664239
C	-2.133045	-4.590321	-1.656205
H	-1.458786	-3.291617	-0.059597
H	-2.802876	-1.329063	-3.631233
H	-3.251440	-3.522374	-4.682343
H	-1.924464	-5.504622	-1.109496
H	-2.825357	-5.616068	-3.418063

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H	5.495880	-0.266571	2.266986
C	4.516375	-0.596159	1.910237
C	3.265274	-2.267673	0.591509
C	2.332316	-1.137819	0.100044
C	4.663232	-1.723730	0.885827
C	3.794274	0.587337	1.252274
H	2.858154	-2.689503	1.513292
H	1.995466	-1.336335	-0.922919
H	4.490627	1.380385	0.972802
H	3.935291	-0.948909	2.765172
H	3.295190	-3.071561	-0.148927
H	5.298543	-2.521061	1.280537
H	3.000642	1.010756	1.866833
N	3.158021	0.149021	-0.052345
C	5.292869	-1.148050	-0.396437
H	6.191513	-0.587664	-0.112776
C	4.273641	-0.169865	-1.022200
H	4.744171	0.775975	-1.291085
H	3.797186	-0.586112	-1.915491
C	5.692099	-2.203570	-1.389924
H	4.886284	-2.815076	-1.798024
C	6.944342	-2.421821	-1.780110
H	7.189206	-3.205555	-2.489878
H	7.769412	-1.823590	-1.400671
C	1.070435	-1.001733	0.993683
O	1.402422	-0.805654	2.335311
C	2.278030	1.253078	-0.617815
H	1.510470	1.438110	0.132209
H	1.825793	0.835016	-1.522391
C	-1.521128	1.127898	3.485281
C	-3.695324	0.676946	1.835806
C	-2.695621	0.613924	4.023607
C	-1.417369	1.449685	2.130315
C	-2.504217	1.158549	1.267120
C	-3.797633	0.417650	3.197911
H	-2.756725	0.392002	5.084736
H	-4.736331	0.056829	3.606088
H	-4.574237	0.536992	1.219857
C	-0.136832	2.170694	1.736582
O	0.949793	1.746760	2.292029
H	1.170719	0.156252	2.517996
N	-0.267082	3.183711	0.934169
H	0.659188	3.606501	0.819034
H	-0.661597	1.319865	4.119393
C	-2.310857	1.317274	-0.198683

H	-1.486312	1.982605	-0.450437
N	-2.891910	0.761392	-1.196575
C	-3.990272	-0.184082	-1.057258
H	-3.869334	-0.831527	-0.177774
H	-3.951562	-0.838167	-1.936404
C	-5.359389	0.474136	-1.036977
C	-7.925370	1.604297	-1.018169
C	-6.481689	-0.311694	-0.753598
C	-5.536399	1.830900	-1.308030
C	-6.813287	2.391767	-1.299563
C	-7.755317	0.247434	-0.743449
H	-6.351330	-1.369654	-0.536093
H	-4.672783	2.450559	-1.527229
H	-6.935501	3.449796	-1.511532
H	-8.615821	-0.374716	-0.516241
H	-8.918447	2.042911	-1.007781
H	0.453294	-0.167193	0.637853
H	0.832804	-3.127557	2.672335
C	0.299787	-3.275601	1.739634
C	0.270282	-2.278280	0.799524
N	-1.025304	-4.758269	0.375871
C	-0.499631	-2.489014	-0.383599
C	-0.363493	-4.499208	1.479076
C	-1.114933	-3.761314	-0.550625
C	-0.716901	-1.485726	-1.360749
H	-0.321568	-5.295068	2.220558
H	-2.318631	-4.989118	-1.843963
C	-1.534875	-1.723294	-2.441748
H	-0.298577	-0.491201	-1.240904
C	-2.087820	-3.014353	-2.647125
H	-2.707164	-3.176791	-3.523713
C	-1.877744	-4.004511	-1.724767
O	-1.872672	-0.738807	-3.315413
H	-2.030480	0.080051	-2.782766
C	2.996601	2.541368	-0.923910
C	4.264868	4.966584	-1.494609
C	3.188549	3.493036	0.084468
C	3.429617	2.824070	-2.221803
C	4.063473	4.030632	-2.506779
C	3.824519	4.697972	-0.199769
H	2.824494	3.284233	1.088679
H	3.264339	2.098051	-3.014645
H	4.393919	4.240867	-3.518912
H	3.967929	5.430778	0.587679
H	4.756592	5.908609	-1.715963

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H	3.522028	-2.313926	-3.006952
C	3.015596	-1.445639	-2.576030
C	3.287003	0.725173	-1.412969
C	1.986747	0.413134	-0.631802
C	4.010386	-0.558473	-1.824662
C	1.948223	-1.925497	-1.585830
H	3.033552	1.280027	-2.317555
H	2.002268	0.884457	0.357203
H	2.127966	-2.950201	-1.248558
H	2.542576	-0.878836	-3.379893
H	3.934800	1.370910	-0.813680
H	4.866926	-0.315974	-2.459240
H	0.936084	-1.867830	-1.982386
N	1.980748	-1.091168	-0.318875
C	4.482678	-1.322762	-0.575840
H	4.766144	-2.337003	-0.881488
C	3.282372	-1.406334	0.389222
H	3.178157	-2.404302	0.818671
H	3.366275	-0.692856	1.212576
C	5.664293	-0.693132	0.107449
H	5.521862	0.317588	0.491781
C	6.840309	-1.294270	0.260951
H	7.671737	-0.799002	0.752079
H	7.011644	-2.305143	-0.101662
C	0.711953	0.922077	-1.361292
O	0.606128	0.371631	-2.651975
C	0.800271	-1.536582	0.547092
H	0.693155	-2.601858	0.330666
H	-0.095655	-1.025244	0.189731
C	-5.367748	0.274055	0.787091
C	-4.991973	-0.379237	-1.886551
C	-6.461062	-0.072499	-0.002713
C	-4.077684	0.295896	0.256624
C	-3.889076	-0.063747	-1.088943
C	-6.275103	-0.388165	-1.345867
H	-7.456584	-0.093823	0.429648
H	-7.124176	-0.642337	-1.972175
H	-4.843679	-0.605720	-2.939152
C	-2.868399	0.664802	1.101568
O	-1.793574	0.070254	0.813291
H	-0.236712	-0.151763	-2.679758
N	-2.987854	1.569772	2.048388
H	-3.915573	1.986564	2.060124
H	-5.514259	0.514364	1.836555
C	-2.521314	0.006851	-1.682222
H	-2.058048	0.997166	-1.633525
N	-1.839010	-0.899852	-2.262227
C	-2.339589	-2.275753	-2.348786
H	-2.083634	-2.650916	-3.343975
H	-3.427541	-2.321257	-2.241280
C	-1.712265	-3.167569	-1.296266
C	-0.630025	-4.859174	0.658507
C	-2.102094	-3.044746	0.042255
C	-0.769693	-4.136220	-1.641272
C	-0.226870	-4.979312	-0.669571
C	-1.565462	-3.884912	1.013228
H	-2.810704	-2.270702	0.324099
H	-0.462344	-4.238442	-2.679745
H	0.500404	-5.734114	-0.954258
H	-1.873544	-3.778259	2.048991
H	-0.217752	-5.520226	1.415311
H	-0.160315	0.651754	-0.757153
H	1.521663	2.460133	-3.456821
C	1.298569	3.049186	-2.573821
C	0.807265	2.443209	-1.443134
N	1.330901	5.226888	-1.540881
C	0.452402	3.277441	-0.339501
C	1.537330	4.444208	-2.575366
C	0.782660	4.660836	-0.429311
C	-0.223407	2.796180	0.804270
H	1.943472	4.913306	-3.469923
H	0.789340	6.540832	0.617648
C	-0.528341	3.636541	1.861200
H	-0.584094	1.772713	0.838704
C	-0.112398	4.999995	1.805258
H	-0.344659	5.639598	2.651539
C	0.509104	5.494158	0.690302
O	-1.210447	3.219361	2.931948

H	-1.861777	2.443057	2.634714
C	0.979397	-1.353011	2.032196
C	1.286130	-1.103919	4.807023
C	1.337734	-2.457370	2.812799
C	0.755198	-0.126791	2.663429
C	0.914609	-0.001279	4.040806
C	1.492751	-2.336453	4.190647
H	1.482026	-3.424497	2.335262
H	0.428575	0.728908	2.086020
H	0.727520	0.958696	4.511994
H	1.767796	-3.204255	4.781772
H	1.401875	-1.006410	5.882139

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H	3.728115	-2.072513	-2.925498
C	3.148316	-1.230786	-2.536692
C	3.222755	1.028325	-1.533080
C	1.990941	0.644269	-0.676698
C	4.067126	-0.201358	-1.874926
C	2.160187	-1.745256	-1.483198
H	2.882992	1.473233	-2.468388
H	2.012338	1.177493	0.277726
H	2.451475	-2.722521	-1.089080
H	2.603589	-0.767955	-3.361590
H	3.814258	1.786439	-1.013047
H	4.878982	0.081419	-2.550182
H	1.135772	-1.817896	-1.844359
N	2.143129	-0.830989	-0.272378
C	4.645839	-0.829270	-0.594785
H	5.025194	-1.827385	-0.845317
C	3.487437	-0.969482	0.412723
C	3.492881	-1.944218	0.905821
H	3.522130	-0.198909	1.186561
C	5.774712	-0.038963	0.006664
H	5.542582	0.979093	0.322202
C	7.007868	-0.510447	0.164232
H	7.798411	0.097695	0.592101
H	7.269194	-1.523819	-0.131229
C	0.637480	0.968839	-1.365872
O	0.562739	0.383579	-2.642617
C	1.048534	-1.337235	0.662931
H	1.108372	-2.426196	0.587655
H	0.076383	-1.036231	0.260781
C	-5.525684	-0.308287	0.486928
C	-4.740016	-1.199406	-2.023141
C	-6.474203	-0.811670	-0.398276
C	-4.173782	-0.267582	0.144571
C	-3.779909	-0.720951	-1.125528
C	-6.081580	-1.257975	-1.658465
H	-7.520555	-0.845683	-0.110281
H	-6.816800	-1.635776	-2.361875
H	-4.434812	-1.501583	-3.021574
C	-3.180259	0.241464	1.166057
O	-3.603184	1.145813	1.961226
H	-0.137922	-0.317851	-2.604000
N	-2.002021	-0.329358	1.143376
H	-1.473544	0.048370	1.937177
H	-5.818183	0.063757	1.463339
C	-2.376356	-0.519238	-1.576909
H	-2.044606	0.521817	-1.516777
N	-1.538985	-1.343203	-2.071293
C	-1.848563	-2.775133	-2.140845
H	-1.527699	-3.133614	-3.123460
H	-2.921787	-2.965273	-2.042674
C	-1.116288	-3.536090	-1.054029
C	0.200475	-4.933184	0.986366
C	-1.535979	-3.410136	0.274375
C	-0.034245	-4.365893	-1.349397
C	0.625848	-5.061219	-0.334480
C	-0.881173	-4.103289	1.288543
H	-2.348328	-2.730980	0.517366
H	0.296854	-4.470092	-2.380491
H	1.465039	-5.705848	-0.578741
H	-1.211036	-3.991335	2.317254
H	0.707925	-5.477179	1.777839
H	-0.166712	0.591463	-0.725510
H	1.380722	2.573310	-3.426495
C	1.007364	3.136624	-2.578403
C	0.507047	2.485343	-1.476153
N	0.636087	5.312092	-1.618485
C	-0.087738	3.279871	-0.446508
C	1.047331	4.549644	-2.605186
C	0.057325	4.694397	-0.551757
C	-0.833575	2.743359	0.633309
H	1.467569	5.054735	-3.472955
H	-0.299993	6.582550	0.413456
C	-1.363104	3.562360	1.614014
H	-1.056357	1.682504	0.671127
C	-1.120774	4.965800	1.555517
H	-1.527660	5.586771	2.347452
C	-0.447266	5.510217	0.498089
O	-2.096843	3.110849	2.640276
H	-2.585325	2.245694	2.405174
C	1.208457	-0.933496	2.107086
C	1.493799	-0.279848	4.819097
C	1.603813	-1.900463	3.035737
C	0.945485	0.364048	2.558930
C	1.089314	0.690242	3.904325
C	1.747065	-1.577831	4.383015
H	1.787168	-2.918608	2.698859
H	0.606036	1.129951	1.867983
H	0.870318	1.700726	4.234932
H	2.052440	-2.341993	5.090799
H	1.601257	-0.027191	5.869203

Ia22Z

H	4.355622	1.372765	2.906080
C	3.405705	1.415247	2.364191
C	1.318148	0.225823	1.811980
C	1.790654	-0.326437	0.459794
C	2.487150	0.267855	2.759707
C	3.648064	1.308727	0.848848
H	0.926550	1.240002	1.703431
H	1.707326	-1.414154	0.482704
H	3.020189	1.989577	0.270727
H	2.942913	2.381439	2.581161
H	0.500905	-0.418974	2.148248
H	2.125778	0.423107	3.817034
H	4.691253	1.491896	0.592810
N	3.311630	-0.087841	0.371659
C	3.285582	-1.044023	2.718784
H	4.091115	-1.004671	3.460778
C	3.950872	-1.081245	1.322532
H	5.008394	-0.815708	1.373781

H	3.861508	-2.065126	0.854642
C	2.444304	-2.262680	3.002461
H	1.579461	-2.441491	2.358431
C	2.704171	-3.098007	4.004738
H	2.078813	-3.963865	4.199056
H	3.551194	-2.943907	4.670102
C	0.873067	0.078020	-0.733815
O	1.186497	-0.614770	-1.915822
C	3.842910	-0.335717	-1.030970
H	3.346640	0.390389	-1.667572
H	3.479653	-1.324860	-1.314574
C	-2.104935	-4.019930	-1.672904
C	-4.331689	-2.795055	-0.581972
C	-3.371964	-4.354859	-2.137593
C	-1.923835	-3.078266	-0.654747
C	-3.058111	-2.446262	-0.115456
C	-4.495258	-3.746677	-1.582075
H	-3.484017	-5.096287	-2.922904
H	-5.492266	-4.008870	-1.922879
H	-5.201650	-2.310283	-0.146756
C	-0.522464	-2.833733	-0.116015
O	-0.429971	-2.364967	1.055136
H	0.877260	-1.551220	-1.780882
N	0.459611	-3.165828	-0.940082
H	1.324897	-3.126192	-0.391442
H	-1.218560	-4.490553	-2.083097
C	-2.988743	-1.398768	0.945393
H	-2.525864	-1.679107	1.888510
N	-3.456080	-0.212536	0.860293
C	-4.024835	0.295760	-0.393251
H	-3.802788	-0.349182	-1.249357
H	-3.541085	1.263540	-0.576399
C	-5.520511	0.508861	-0.276738
C	-8.284212	0.929042	-0.084288
C	-6.394529	-0.093497	-1.182811
C	-6.043871	1.331085	0.725772
C	-7.416726	1.536311	0.823456
C	-7.769827	0.116595	-1.090760
H	-5.994170	-0.734761	-1.965183
H	-5.366885	1.819948	1.421687
H	-7.811280	2.177904	1.605798
H	-8.437328	-0.356590	-1.804691
H	-9.354950	1.092034	-0.008022
H	-0.098760	-0.271637	-0.359268
H	2.137611	1.562673	-2.663708
C	1.495736	2.156386	-2.022461
C	0.750369	1.564283	-1.029941
N	0.619875	4.351517	-1.558382
C	-0.192910	2.387401	-0.334293
C	1.407664	3.551577	-2.238049
C	-0.197898	3.781268	-0.630231
C	-1.148132	1.883250	0.584647
H	2.027486	4.010747	-3.005833
H	-1.089796	5.685520	-0.178490
C	-2.069230	2.715378	1.181651
H	-1.187579	0.827033	0.822774
C	-2.033570	4.113715	0.929674
H	-2.759280	4.748010	1.428573
C	-1.119628	4.624994	0.050335
O	-3.030631	2.250375	2.008636
H	-3.149283	1.272574	1.842578
C	5.339145	-0.227723	-1.176639
C	8.105073	-0.020922	-1.551279
C	5.915304	0.987103	-1.561818
C	6.162170	-1.345540	-1.011092
C	7.538413	-1.241846	-1.191081
C	7.291302	1.093386	-1.742446
H	5.278598	1.852919	-1.732598
H	5.723374	-2.305754	-0.751576
H	8.166430	-2.117190	-1.059675
H	7.724645	2.042209	-2.041988
H	9.177945	0.058527	-1.695463

Ib21Z-R

H	4.590301	1.674115	2.636342
C	3.589146	1.636433	2.196144
C	1.524771	0.311157	1.939835
C	1.887877	-0.299326	0.576847
C	2.785466	0.473724	2.787600
C	3.679614	1.448959	0.671171
H	1.060195	1.293412	1.810820
H	1.865845	-1.393672	0.623456
H	2.956154	2.058974	0.127259
H	3.097459	2.589387	2.407463
H	0.785356	-0.337026	2.418786
H	2.528304	0.666785	3.831779
H	4.678871	1.668377	0.295437
N	3.375822	0.011538	0.315278
C	3.645005	-0.801705	2.690934
H	4.506146	-0.675567	3.356290
C	4.174243	-0.881958	1.245779
H	5.210428	-0.548424	1.170863
H	4.105004	-1.895194	0.841782
C	2.897446	-2.046652	3.109477
H	2.423112	-2.634407	2.321458
C	2.786293	-2.444397	4.373581
H	2.218988	-3.329782	4.641090
H	3.260425	-1.896159	5.185096
C	0.824948	0.006478	-0.520707
O	1.032382	-0.746647	-1.687382
C	3.766014	-0.306242	-1.119720
H	3.178195	0.360929	-1.742555
H	3.411437	-1.322225	-1.299351
C	-1.703791	-4.016372	-1.424168
C	-4.156821	-2.939464	-0.732390
C	-2.846345	-4.403513	-2.117327
C	-1.765788	-3.111230	-0.362254
C	-3.011820	-2.548670	-0.029266
C	-4.083126	-3.870016	-1.764195
H	-2.771769	-5.120464	-2.929492
H	-4.984100	-4.166679	-2.292382
H	-5.114926	-2.502294	-0.460827
C	-0.474222	-2.821880	0.383520
O	0.615763	-2.987352	-0.273733
H	0.868755	-1.684316	-1.397903
N	-0.612429	-2.467075	1.632502
H	0.326486	-2.381078	2.033062
H	-0.729325	-4.413773	-1.688152
C	-3.165651	-1.520420	1.041848
H	-2.857718	-1.807481	2.043218
N	-3.619374	-0.335931	0.894953
C	-4.007405	0.181180	-0.420436
H	-3.705553	-0.474782	-1.243020
H	-3.479699	1.134320	-0.547912
C	-5.499322	0.435086	-0.469294

C	-8.254513	0.930588	-0.553597
C	-6.295519	-0.159950	-1.447732
C	-6.094486	1.286939	0.466771
C	-7.463511	1.530404	0.426753
C	-7.667486	0.087839	-1.493008
H	-5.838381	-0.821974	-2.180113
H	-5.473153	1.761846	1.222810
H	-7.914794	2.194411	1.158084
H	-8.275112	-0.380421	-2.261601
H	-9.322617	1.122875	-0.585145
H	-0.079647	-0.360652	-0.016579
H	1.859827	1.476327	-2.597200
C	1.224682	2.056120	-1.936807
C	0.586422	1.464578	-0.871647
N	0.242544	4.210446	-1.504903
C	-0.370208	2.254261	-0.153336
C	1.036280	3.432113	-2.202203
C	-0.483543	3.630617	-0.509250
C	-1.255408	1.730965	0.827182
H	1.576776	3.894979	-3.025573
H	-1.476051	5.493885	-0.101553
C	-2.233653	2.522285	1.390447
H	-1.222602	0.684947	1.114484
C	-2.290797	3.909982	1.089926
H	-3.051170	4.512220	1.576851
C	-1.431384	4.444351	0.171336
O	-3.177531	2.023202	2.219995
H	-3.334578	1.065860	1.975875
C	5.234205	-0.164404	-1.428925
C	7.939050	0.091862	-2.102405
C	5.731994	1.045447	-1.923969
C	6.102103	-1.253562	-1.304545
C	7.448314	-1.125136	-1.633110
C	7.078139	1.176484	-2.252912
H	5.056663	1.886950	-2.063963
H	5.721660	-2.211639	-0.959435
H	8.111626	-1.978174	-1.532764
H	7.450868	2.120971	-2.635712
H	8.988187	0.190400	-2.362604

Ia3E

H	-4.417949	-3.230658	1.316600
C	-4.021421	-2.256590	1.017592
C	-4.031743	-0.480129	-0.721415
C	-2.521003	-0.298146	-0.460681
C	-4.457213	-1.917423	-0.410993
C	-2.485904	-2.290943	1.085269
H	-4.581807	0.201814	-0.068451
H	-2.002201	0.014862	-1.372206
H	-2.091728	-3.309260	1.122097
H	-4.396376	-1.496998	1.705644
H	-4.268183	-0.214594	-1.755215
H	-5.540992	-2.017622	-0.513105
H	-2.086271	-1.723046	1.926820
N	-1.902638	-1.678471	-0.167420
C	-3.754364	-2.892625	-1.373185
H	-3.909192	-3.910789	-0.997261
C	-2.243547	-2.574074	-1.335724
H	-1.652235	-3.483145	-1.227017
H	-1.911554	-2.045561	-2.235038
C	-4.275917	-2.828748	-2.781880
H	-4.150732	-1.879359	-3.304116
C	-4.871184	-3.844105	-3.400285
H	-5.248526	-3.748961	-4.413381
H	-5.004417	-4.806728	-2.912393
C	-2.255291	0.763060	0.639115
O	-3.078894	0.584397	1.747878
C	-0.395161	-1.534835	-0.048213
H	-0.227988	-0.855990	0.788582
H	-0.071227	-1.048705	-0.974341
C	0.759725	-3.134682	1.499794
C	1.561291	-4.251062	1.729955
C	0.386557	-2.799144	0.194240
H	2.630477	-5.896983	0.846534
C	0.847037	-3.576881	-0.874381
C	1.645551	-4.691984	-0.641267
C	2.000472	-5.032076	0.663337
C	-0.226654	2.499902	3.002157
C	1.902293	2.684329	1.235052
C	0.130956	3.736680	2.473283
C	0.482397	1.340392	2.675931
C	1.542726	1.434764	1.753177
C	1.212055	3.833387	1.599719
H	-0.430379	4.624592	2.748220
H	1.503478	4.794737	1.187966
H	2.721462	2.740701	0.523782
C	0.086756	0.023191	3.325605
O	1.004804	-0.755885	3.680332
H	-2.436373	0.369272	2.520165
N	-1.219738	-0.160149	3.459978
H	-1.357892	-1.042817	3.958250
H	-1.067819	2.413107	3.682393
C	2.216456	0.227929	1.219755
H	2.381657	-0.607038	1.906950
N	2.545916	0.166675	-0.012852
C	3.253600	-1.028203	-0.474102
H	2.722257	-1.406668	-1.355915
H	3.248098	-1.819789	0.288879
C	4.671536	-0.660254	-0.852820
C	7.283624	0.080810	-1.525801
C	5.749730	-1.106677	-0.090038
C	4.909681	0.167272	-1.953957
C	6.208478	0.537031	-2.288615
C	7.052611	-0.741597	-0.426622
H	5.567957	-1.743905	0.771933
H	4.070974	0.525738	-2.547058
H	6.384203	1.180173	-3.145695
H	7.885331	-1.097638	0.172368
H	8.297490	0.367070	-1.788210
H	-1.209907	0.715581	0.957374
H	-4.339836	2.499831	0.883134
C	-3.572300	2.867094	0.210564
C	-2.439585	2.127535	-0.004790
N	-2.823801	4.643371	-1.240776
C	-1.423861	2.672682	-0.848606
C	-3.719915	4.118911	-0.437552
C	-1.671516	3.940612	-1.442234
C	-0.180015	2.036303	-1.076315
H	-4.627017	4.698705	-0.274873
H	-0.876794	5.478375	-2.721438
C	0.799444	2.641938	-1.833330
H	0.058947	1.096711	-0.592341
C	0.536374	3.889059	-2.459997
H	1.318199	4.337510	-3.064774
C	-0.666464	4.514874	-2.267619

H	0.601336	-3.295386	-1.896182
H	2.000259	-5.285799	-1.477475
H	1.853440	-4.500357	2.745101
H	0.468628	-2.497986	2.335051
O	2.030709	2.111018	-1.989122
H	2.184347	1.405310	-1.301295

Ib3E-R

H	-4.591004	-3.026759	1.214421
C	-4.120836	-2.080234	0.933957
C	-4.003806	-0.267349	-0.755984
C	-2.486902	-0.184608	-0.479135
C	-4.517513	-1.685786	-0.491386
C	-2.594403	-2.234230	1.005708
H	-4.521285	0.427155	-0.089336
H	-1.945674	0.115991	-1.381775
H	-2.286900	-3.282123	0.975809
H	-4.444170	-1.307554	1.634303
H	-4.212279	0.044280	-1.783174
H	-5.603524	-1.718952	-0.611371
H	-2.149952	-1.762621	1.884353
N	-1.956940	-1.603627	-0.216102
C	-3.856943	-2.678886	-1.467077
H	-4.063269	-3.694533	-1.109258
C	-2.331638	-2.437010	-1.419053
H	-1.782675	-3.376320	-1.344992
H	-1.973569	-1.892009	-2.298182
C	-4.367920	-2.567229	-2.876471
H	-4.221924	-1.606687	-3.371981
C	-4.977389	-3.555158	-3.524769
H	-5.345795	-3.428440	-4.537688
H	-5.113336	-4.526763	-3.061451
C	-2.151107	0.838545	0.634029
O	-2.948055	0.665109	1.768124
C	-0.447944	-1.546473	-0.065893
H	-0.265586	-0.915863	0.804214
H	-0.076522	-1.043708	-0.965237
C	0.468224	-3.323031	1.442322
C	1.181768	-4.498502	1.658945
C	0.248380	-2.864220	0.140259
H	2.248432	-6.130168	0.747189
C	0.766112	-3.584423	-0.940565
C	1.479802	-4.759458	-0.723341
C	1.686125	-5.217410	0.576803
C	-0.191125	2.267642	3.176888
C	1.881636	2.586237	1.358901
C	0.131164	3.536398	2.706198
C	0.537377	1.143782	2.777045
C	1.560950	1.304621	1.824684
C	1.184049	3.699926	1.806001
H	-0.439444	4.398255	3.039066
H	1.441431	4.686948	1.434561
H	2.672062	2.694178	0.621257
C	0.129119	-0.205081	3.336661
O	-1.117819	-0.510836	3.223208
H	-2.319002	0.314881	2.465896
N	1.076754	-0.907635	3.879718
H	0.643914	-1.765808	4.239293
H	-1.018166	2.132668	3.868136
C	2.219317	0.127838	1.216202
H	2.353987	-0.753577	1.852704
N	2.564985	0.131981	-0.013336
C	3.235544	-1.057824	-0.537899
H	2.689680	-1.375359	-1.434944
H	3.210323	-1.885374	0.185315
C	4.661991	-0.711941	-0.904332
C	7.289399	0.002417	-1.543238
C	5.723030	-1.144135	-0.109475
C	4.924836	0.088369	-2.019403
C	6.231776	0.444808	-2.337592
C	7.033486	-0.792222	-0.428824
H	5.520915	-1.759000	0.764163
H	4.099043	0.437136	-2.635893
H	6.427416	1.065974	-3.206419
H	7.852941	-1.137127	0.194410
H	8.309554	0.277672	-1.792771
H	-1.099985	0.749270	0.918893
H	-4.194308	2.625513	0.944322
C	-3.421727	2.984900	0.273107
C	-2.311007	2.221109	0.028946
N	-2.637218	4.774540	-1.142163
C	-1.287859	2.758542	-0.810243
C	-3.541768	4.254367	-0.345633
C	-1.504244	4.048474	-1.367335
C	-0.061857	2.096142	-1.059999
H	-4.432402	4.853128	-0.162714
H	-0.670561	5.602566	-2.601531
C	0.937013	2.704590	-1.788286
H	0.152876	1.133658	-0.609901
C	0.706004	3.975763	-2.378775
H	1.501629	4.425146	-2.964542
C	-0.484058	4.621904	-2.174967
H	0.627147	-3.214368	-1.954224
H	1.883286	-5.310086	-1.566995
H	1.353365	-4.845996	2.672730
H	0.093860	-2.740130	2.281247
O	2.159168	2.152461	-1.944399
H	2.285715	1.427211	-1.272053

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H	-4.376637	3.433330	-1.466750
C	-3.947479	2.465771	-1.744595
C	-3.685603	0.093818	-1.121195
C	-2.293904	0.244082	-0.491525
C	-4.505731	1.357714	-0.850480
C	-2.417756	2.489411	-1.595502
H	-3.589991	-0.062127	-2.202390
H	-2.309022	-0.116246	0.542080
H	-1.900199	1.995186	-2.416669
H	-4.200209	2.278115	-2.791335
H	-4.158771	-0.800145	-0.706475
H	-5.564866	1.185203	-1.055565
H	-2.047741	3.506994	-1.484089
N	-2.000113	1.742724	-0.344247
C	-4.329839	1.803380	0.616161
H	-4.952331	2.691260	0.772417
C	-2.852139	2.234509	0.803600
H	-2.746267	3.320613	0.823590
H	-2.418445	1.827483	1.721055
C	-4.767558	0.756084	1.606315
H	-4.180553	-0.161515	1.662617
C	-5.831028	0.891670	2.393012
H	-6.129877	0.109664	3.083564
H	-6.440689	1.792071	2.372307

C	-1.182120	-0.550977	-1.199034
O	-0.898897	0.001805	-2.463852
C	-0.521253	1.961074	-0.057125
H	-0.007856	1.680737	-0.980031
H	-0.234723	1.237807	0.713639
C	4.329558	-2.206104	1.481458
C	4.214277	-2.471719	-1.278363
C	5.425996	-2.711093	0.787302
C	3.167367	-1.819875	0.811945
C	3.137714	-1.909292	-0.588417
C	5.359003	-2.872342	-0.594966
H	6.324286	-2.994168	1.327283
H	6.194730	-3.300918	-1.139240
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C	1.941339	-1.315211	1.563182
O	1.266164	-0.411614	1.001778
H	0.072481	-0.146149	-2.606169
N	1.641613	-1.877463	2.719397
H	2.297960	-2.626095	2.932975
H	4.378487	-2.097174	2.561680
C	1.93260	-1.451313	-1.344478
C	1.022102	-2.015234	-1.152235
N	1.863359	-0.515415	-2.206000
C	3.056974	0.305427	-2.506389
H	2.786249	0.939625	-3.355031
H	3.885192	-0.331899	-2.830800
C	3.511014	1.177047	-1.351317
C	4.298595	2.783325	0.810723
C	2.815695	2.348029	-1.040907
C	4.628540	0.840383	-0.582687
C	5.018390	1.634722	0.492286
C	3.197720	3.143797	0.036647
H	1.972097	2.645477	-1.660331
H	5.194735	-0.056383	-0.818694
H	5.884755	1.351013	1.082610
H	2.641659	4.047762	0.268607
H	4.597505	3.400136	1.652830
H	-0.290084	-0.508444	-0.564483
H	-2.106594	-1.889435	-3.373494
C	-2.140961	-2.494565	-2.474102
C	-1.660835	-1.993093	-1.290977
N	-2.811552	-4.570612	-1.449796
C	-1.690942	-2.829988	-0.133149
C	-2.701625	-3.793962	-2.503194
C	-2.308431	-4.107039	-0.270096
C	-1.131097	-2.452014	1.111210
H	-3.089565	-4.186764	-3.441425
H	-2.881297	-5.906971	0.760361
C	-1.175663	-3.309923	2.196164
H	-0.597682	-1.510862	1.218863
C	-1.851812	-4.559044	2.072412
H	-1.890272	-5.206381	2.943246
C	-2.393215	-4.943864	0.875803
O	-0.594177	-3.013975	3.363371
H	0.225512	-2.396191	3.166012
C	-0.169917	3.364197	0.365946
C	0.582650	5.933774	1.193536
C	-0.005721	3.654086	1.723066
C	0.070485	4.373576	-0.573907
C	0.435800	5.652677	-0.163858
C	0.367405	4.930582	2.136220
H	-0.150579	2.868773	2.460427
H	0.000404	4.154972	-1.636951
H	0.620430	6.423553	-0.905087
H	0.497828	5.137855	3.193462
H	0.876433	6.928211	1.514270

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H	-5.375602	1.782778	-1.241355
C	-4.661108	1.012129	-1.546793
C	-3.547609	-1.099744	-0.928379
C	-2.255562	-0.461228	-0.398762
C	-4.736788	-0.190853	-0.604960
C	-3.225985	1.561100	-1.519295
H	-3.476778	-1.242828	-2.012956
H	-2.086393	-0.769974	0.639025
H	-2.627778	1.240199	-2.371054
H	-4.908637	0.715789	-2.569354
H	-3.653252	-2.090906	-0.479612
H	-5.680586	-0.726875	-0.729060
H	-3.216324	2.648127	-1.452876
N	-2.491878	1.052609	-0.292893
C	-4.627466	0.335594	0.840886
H	-5.507827	0.956615	1.039237
C	-3.385114	1.260492	0.910115
H	-3.665773	2.314849	0.906538
H	-2.777310	1.067315	1.798378
C	-4.601993	-0.763729	1.870258
H	-3.734658	-1.425000	1.882430
C	-5.582056	-0.970109	2.744936
H	-5.539142	-1.781849	3.463919
H	-6.463277	-0.333260	2.770110
C	-0.974309	-0.849911	-1.161197
O	-0.915064	-0.204394	-2.412055
C	-1.173251	1.796864	-0.128846
H	-0.661692	1.685900	-1.086705
H	-0.594013	1.255425	0.622757
C	4.848483	-1.019585	1.416918
C	4.711630	-1.067577	-1.352726
C	6.010936	-1.179246	0.669588
C	3.608239	-0.848408	0.798477
C	3.550081	-0.854024	-0.603732
C	5.942456	-1.217855	-0.722201
H	6.967211	-1.295737	1.170663
H	6.839451	-1.376452	-1.312869
H	4.646191	-1.128163	-2.436027
C	2.391146	-0.665762	1.682588
O	2.412834	-1.307516	2.789497
H	0.052532	-0.037333	-2.566995
N	1.459743	0.140429	1.242468
H	0.752101	0.165655	1.988643
H	4.879743	-1.027536	2.501484
C	2.245937	-0.733592	-1.306895
H	1.541570	-1.541145	-1.091443
N	1.863727	0.147486	-2.144452
C	2.747963	1.290146	-2.456878
H	2.310689	1.791482	-3.324798
H	3.743579	0.942983	-2.747580
C	2.866952	2.273336	-1.310294
C	3.028105	4.059747	0.844462
C	1.855812	3.208830	-1.083122
C	3.976552	2.264086	-0.460836
C	4.055670	3.148636	0.611397
C	1.929437	4.095711	-0.011411
H	1.006566	3.250905	-1.762547

H	4.783618	1.557979	-0.636648
H	4.922416	3.124411	1.265213
H	1.132674	4.816576	0.151654
H	3.087945	4.747950	1.682320
H	-0.125551	-0.533814	-0.543494
H	-1.585908	-2.304422	-3.348220
C	-1.352346	-2.935435	-2.497963
C	-0.965169	-2.368426	-1.309104
N	-1.225171	-5.170402	-1.611028
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C	-1.463942	-4.341729	-2.601024
C	-0.798148	-4.634683	-0.433078
C	-0.101619	-2.776898	1.010867
H	-1.783084	-4.784388	-3.542975
H	-0.661204	-6.583681	0.466542
C	0.246024	-3.669167	2.007606
H	0.096749	-1.721222	1.161401
C	-0.000082	-5.059683	1.820483
H	0.256746	-5.735479	2.630172
C	-0.500414	-5.523443	0.635524
O	0.806852	-3.294867	3.166754
H	1.321964	-2.429783	3.043875
C	-1.315017	3.246649	0.254886
C	-1.453684	5.945431	0.989107
C	-1.227112	3.621898	1.598092
C	-1.450368	4.242357	-0.719019
C	-1.526181	5.583967	-0.355009
C	-1.299390	4.962651	1.965139
H	-1.080449	2.861134	2.360846
H	-1.470930	3.971196	-1.772260
H	-1.628374	6.345729	-1.121070
H	-1.225032	5.239851	3.011706
H	-1.504525	6.991521	1.274142

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H	2.218611	-3.404124	-2.789646
C	1.956460	-2.395877	-2.456928
C	2.681694	0.012576	-2.438976
C	2.048645	0.053968	-1.026909
C	3.095333	-1.424918	-2.792425
C	1.744603	-2.410097	-0.930612
H	1.950701	0.370902	-3.162819
H	2.502861	0.846883	-0.429448
H	2.177746	-3.297732	-0.461970
H	1.040144	-2.084754	-2.957053
H	3.548509	0.678321	-2.478256
H	3.355025	-1.492572	-3.852123
H	0.696126	-2.342427	-0.625798
N	2.461132	-1.233324	-0.303022
C	4.300921	-1.827625	-1.924253
H	4.413099	-2.917416	-1.972131
C	3.953504	-1.417465	-0.482778
H	4.274953	-2.169361	0.240508
H	4.413975	-0.464624	-0.208590
C	5.602832	-1.208084	-2.348331
H	5.649342	-0.118503	-2.346686
C	6.671175	-1.909184	-2.716145
H	7.590615	-1.423278	-3.026855
H	6.661466	-2.996544	-2.720855
C	0.502124	0.264500	-1.063774
O	0.008310	-0.161684	-2.310944
C	2.148433	-1.207843	1.189343
H	2.287350	-2.242826	1.514219
H	1.084120	-0.988692	1.293202
C	-3.779571	-3.592718	2.149377
C	-4.057663	-4.008504	-0.578219
C	-4.699816	-4.526923	1.681927
C	-2.992394	-2.849689	1.267249
C	-3.139430	-3.063383	-0.112003
C	-4.843205	-4.733991	0.312391
H	-5.295065	-5.100028	2.386012
H	-5.556255	-5.461377	-0.062198
H	-4.160787	-4.168744	-1.648450
C	-1.945984	-1.880873	1.795912
O	-0.840731	-1.853447	1.187212
H	-0.939614	-0.423792	-2.154824
N	-2.256511	-1.137319	2.837565
H	-3.224470	-1.280748	3.116134
H	-3.648972	-3.450220	3.218664
C	-2.336125	-2.321991	-1.124119
H	-1.688028	-2.934588	-1.759080
N	-2.348850	-1.077868	-1.855874
C	-3.63724	-0.148505	-0.603561
H	-2.670779	0.040440	0.359236
H	-4.146550	-0.587500	-0.377681
C	-3.313872	1.163302	-1.342878
C	-3.553790	3.604953	-2.698913
C	-3.434602	1.193351	-2.734290
C	-3.321274	2.368619	-0.638427
C	-3.436538	3.582879	-1.310568
C	-3.555145	2.405824	-3.409108
H	-3.417610	0.259297	-3.289628
H	-3.201734	2.358760	0.443650
H	-3.412589	4.511692	-0.747986
H	-3.643846	2.414399	-4.491585
H	-3.636308	4.551581	-3.224625
H	0.029064	-0.327631	-0.270621
H	0.705950	2.296694	-2.836219
C	0.390649	2.639125	-1.855874
C	0.195165	1.740492	-0.835270
N	-0.222053	4.519159	-0.484081
C	-0.296059	2.233273	0.412545
C	0.169331	4.017055	-1.632885
C	-0.467749	3.644549	0.529881
C	-0.649432	1.400090	1.505048
H	0.337076	4.724489	-2.443350
H	-1.071223	5.250208	1.827549
C	-1.151688	1.936561	2.679357
H	-0.569713	0.318573	1.439631
C	-1.285314	3.352056	2.800163
H	-1.672638	3.749996	3.733201
C	-0.954908	4.172685	1.757388
O	-1.517813	1.182508	3.716191
H	-1.685369	0.202584	3.385075
C	3.032398	-0.295113	2.002602
C	4.686093	1.350088	3.557148
C	2.757390	1.069777	2.132019
C	4.131228	-0.828089	2.685234
C	4.955543	-0.013130	3.454829
C	3.583263	1.888196	2.899028
H	1.881224	1.495685	1.652304
H	4.336251	-1.894240	2.624126
H	5.802431	-0.444584	3.978867
H	3.354043	2.945176	2.990288
H	5.325708	1.987574	4.159423

Id6Z-S

H	1.631134	-4.048984	-1.925792
C	1.570862	-2.963119	-1.812142
C	2.643129	-0.771421	-2.396655
C	2.045525	-0.308987	-1.049431
C	2.831276	-2.296477	-2.381264
C	1.469384	-2.626295	-0.314007
H	1.962424	-0.485166	-3.197348
H	2.600074	0.550632	-0.667799
H	1.878418	-3.422003	0.314822
H	0.689279	-2.601579	-2.343131
H	3.599455	-0.270094	-2.570695
H	3.040082	-2.664849	-3.388692
H	0.453757	-2.417183	0.038587
N	2.326470	-1.409990	-0.019357
C	3.997546	-2.643344	-1.435334
H	3.942947	-3.711804	-1.194486
C	3.777674	-1.822916	-0.150760
H	4.034705	-2.393385	0.743853
H	4.364061	-0.900507	-0.148028
C	5.358862	-2.365807	-2.008176
H	5.572659	-1.332175	-2.282137
C	6.287316	-3.299563	-2.192862
H	7.255408	-3.062047	-2.622130
H	6.108418	-4.337651	-1.922780
C	0.521945	0.057210	-1.135328
O	-0.009338	-0.417104	-2.344761
C	2.054332	-0.938890	1.400895
H	1.981393	-1.851552	1.998666
H	1.071349	-0.469629	1.379595
C	-4.578749	-2.700548	2.321721
C	-4.533490	-3.553496	-0.319681
C	-5.601968	-3.509395	1.836673
C	-3.510624	-2.324482	1.505161
C	-3.506948	-2.740118	0.167337
C	-5.577962	-3.944079	0.513146
H	-6.417922	-3.801909	2.490531
H	-6.371949	-4.575804	0.127497
H	-4.519304	-3.866923	-1.360414
C	-2.387179	-1.518367	2.119469
O	-2.758726	-0.608543	2.935605
H	-0.961668	-0.633789	-2.136108
N	-1.169818	-1.869921	1.786968
H	-0.547771	-1.300960	2.371484
H	-4.588010	-2.349390	3.348651
C	-2.471130	-2.269478	-0.790880
H	-1.777351	-3.013701	-1.193214
N	-2.355078	-1.086024	-1.238379
C	-3.235882	-0.014561	-0.769561
H	-3.011391	0.220124	0.279525
H	-4.281622	-0.351805	-0.798443
C	-3.045147	1.222793	-1.618832
C	-2.640805	3.507631	-3.190491
C	-2.885769	1.114589	-3.002496
C	-3.012906	2.489163	-1.034034
C	-2.807289	3.625623	-1.812824
C	-2.686301	2.247980	-3.785148
H	-2.905910	0.130972	-3.465605
H	-3.109289	2.584010	0.045775
H	-2.753067	4.600952	-1.337669
H	-2.557940	2.146932	-4.858952
H	-2.468572	4.392412	-3.796442
H	-0.014310	-0.419686	-0.305435
H	1.057456	1.903938	-3.016810
C	0.743625	2.357676	-2.081112
C	0.367475	1.568561	-1.021763
N	0.398708	4.391119	-0.844903
C	-0.107674	2.209038	0.163555
C	0.732733	3.764013	-1.949402
C	-0.025393	3.631829	0.202471
C	-0.662200	1.518525	1.274908
H	1.037801	4.383379	-2.791142
H	-0.346261	5.389261	1.400495
C	-1.078253	2.202263	2.403681
H	-0.828858	0.446457	1.235183
C	-0.928986	3.619801	2.457936
H	-1.251784	4.130797	3.359681
C	-0.432042	4.306921	1.387096
O	-1.619469	1.611319	3.472733
H	-1.944131	0.668784	3.254963
C	3.085862	-0.002409	1.977599
C	4.983843	1.719714	3.104224
C	2.995134	1.379030	1.780158
C	4.120295	-0.506991	2.772085
C	5.066891	0.347003	3.329124
C	3.943951	2.234502	2.334478
H	2.168965	1.794342	1.209079
H	4.178087	-1.574534	2.969613
H	5.862508	-0.058792	3.945603
H	3.859508	3.304466	2.173585
H	5.719774	2.388052	3.539941

Ic1E (denoted as Ic in the main article)

H	3.774699	2.692321	-1.303296
C	2.831494	2.236793	-1.620963
C	0.372869	2.496364	-1.758849
C	0.079628	1.494693	-0.629131
C	1.679994	3.233999	-1.468079
C	2.528883	0.982490	-0.783353
H	0.460205	1.955176	-2.706422
H	-0.584163	1.938490	0.119957
H	3.375191	0.692042	-0.160169
H	2.940931	1.941743	-2.668356
H	-0.469575	3.186998	-1.845749
H	1.805852	4.075099	-2.154532
H	2.222870	0.136721	-1.398890
N	1.375951	1.250380	0.158748
C	1.675773	3.751842	-0.017013
H	2.613816	4.292481	0.150276
C	1.669022	2.521905	0.922385
H	2.637914	2.375287	1.401060
H	0.909956	2.606485	1.705006
C	0.538510	4.696905	0.267893
H	-0.466064	4.272660	0.304438
C	0.699989	6.001722	0.466457
H	-0.143975	6.657333	0.655210
H	1.686509	6.459418	0.447081
C	-0.611180	0.223142	-1.163400
O	0.128319	-0.328983	-2.221304
C	1.195975	0.075523	1.114563
H	1.236988	-0.828789	0.502149
H	0.191181	0.168913	1.535937
C	-3.383796	-2.319900	1.376130

C	-2.349214	-3.150215	-1.057974
C	-4.242161	-2.581262	0.312355
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C	-1.485138	-2.928090	0.020705
C	-3.721785	-2.969967	-0.919101
H	-5.313313	-2.453925	0.438397
H	-4.380697	-3.149444	-1.763129
H	-1.931321	-3.491804	-2.000514
C	-1.055928	-1.987680	2.333195
O	0.125581	-2.415452	2.303334
H	0.213069	-1.299900	-2.041944
N	-1.559896	-1.104634	3.185247
H	-0.826262	-0.869994	3.856527
H	-3.780553	-1.958615	2.319204
C	-0.056880	-3.284500	-0.179220
H	0.388122	-3.965562	0.548532
N	0.586615	-2.904409	-1.213970
C	1.907948	-3.500287	-1.428330
H	1.783146	-4.280476	-2.190223
H	2.282087	-3.985120	-0.516756
C	2.905218	-2.482009	-1.929163
C	4.719183	-0.556094	-2.856541
C	4.071487	-2.204925	-1.215917
C	2.667974	-1.801756	-3.128342
C	3.564776	-0.842592	-3.587919
C	4.975501	-1.244978	-1.673898
H	4.277343	-2.749648	-0.297302
H	1.768441	-2.020968	-3.698505
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H	5.876928	-1.036503	-1.105118
H	5.418224	0.193789	-3.214376
H	-0.712672	-0.512173	-0.358125
H	-1.615132	0.579858	-3.680119
C	-2.348581	0.779430	-2.906425
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C	-4.312354	1.248285	-1.054041
C	-2.799968	0.675265	0.780951
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H	-6.314231	1.752469	-0.445021
C	-3.828338	0.785248	1.696743
H	-1.841905	0.337337	1.152063
C	-5.109705	1.213699	1.244827
H	-5.901845	1.325778	1.978883
C	-5.337183	1.442109	-0.087084
O	-3.671003	0.464183	2.985788
H	-2.824053	-0.140945	3.086929
C	2.190647	0.019925	2.243310
C	3.986812	-0.080981	4.387173
C	1.841581	0.553084	3.487598
C	3.439317	-0.586707	2.091819
C	4.335874	-0.631802	3.156670
C	2.733836	0.506715	4.553713
H	0.857306	0.995859	3.622847
H	3.703807	-1.042945	1.141856
H	5.302816	-1.107469	3.026523
H	2.447992	0.921385	5.515125
H	4.683599	-0.120869	5.218500

Id2E-S (denoted as Id in the main article)

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C	1.664873	3.268798	-1.487150
C	2.537805	1.013729	-0.841719
H	0.423960	2.018521	-2.733598
H	-0.574644	1.925976	0.104161
H	3.394159	0.736046	-0.227353
H	2.900151	1.992457	-2.728951
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H	2.239395	0.164478	-1.456117
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C	1.679029	3.763064	-0.027382
H	2.619298	4.300747	0.136600
C	1.679886	2.519999	0.894765
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C	0.544898	4.704689	0.281778
H	-0.456398	4.275732	0.344823
C	0.704652	6.011543	0.467876
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C	-0.594044	0.239384	-1.216477
O	0.138866	-0.272646	-2.297888
C	1.230548	0.065547	1.048631
H	1.298208	-0.826193	0.418806
H	0.222120	0.128454	1.467079
C	-3.330440	-2.317415	1.516271
C	-2.507367	-3.058163	-1.020152
C	-4.277442	-2.540722	0.521322
C	-1.965382	-2.458869	1.269522
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C	-3.863422	-2.879098	-0.763570
H	-5.333673	-2.416799	0.741543
H	-4.590053	-3.018596	-1.557904
H	-2.169330	-3.358983	-2.007618
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O	-1.354092	-1.032664	3.086984
H	0.154878	-1.257427	-2.177293
N	0.182877	-2.590399	2.319408
H	0.746242	-2.153081	3.055799
H	-3.646616	-1.980882	2.498162
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H	0.311232	-4.005741	0.327288
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C	1.691872	-3.522872	-1.742587
H	1.506835	-4.115096	-2.647212
H	2.010471	-4.214596	-0.951155
C	2.789977	-2.523845	-2.026258
C	4.846914	-0.691452	-2.550895
C	3.849688	-2.370654	-1.131404
C	2.773256	-1.752837	-3.193399
C	3.791587	-0.839104	-3.452558
C	4.877039	-1.463107	-1.391739
H	3.875044	-2.976644	-0.228494
H	1.956925	-1.869991	-3.902311
H	3.767554	-0.246577	-4.362258
H	5.700224	-1.362313	-0.689623
H	5.644191	0.016452	-2.756450
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H	-6.273788	1.772159	-0.342736
C	-3.737958	0.781544	1.718798
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C	-5.026003	1.224128	1.312692
H	-5.794083	1.346595	2.070002
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C	2.211946	0.017917	2.191380
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C	1.796713	0.461613	3.451602
C	3.501324	-0.500000	2.044167
C	4.375295	-0.534357	3.127873
C	2.668422	0.424649	4.535595
H	0.771424	0.797367	3.585262
H	3.818017	-0.898132	1.084776
H	5.373671	-0.940861	3.000749
H	2.332605	0.768218	5.508679
H	4.643367	-0.094860	5.218227

Ib14Z

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C	-3.368549	-1.321636	-1.373064
C	-2.339173	-0.707110	-0.391963
C	-4.312869	-0.247351	-1.919153
C	-2.712929	1.583938	-1.399852
H	-2.825819	-1.785274	-2.200569
H	-2.432202	-1.164054	0.595491
H	-1.665579	1.762571	-1.626684
H	-2.757736	0.455772	-3.242891
H	-3.944703	-2.099438	-0.864403
H	-4.969192	-0.675561	-2.681037
H	-3.178206	2.534348	-1.124472
N	-2.742341	0.749526	-0.133881
C	-5.140571	0.350307	-0.773157
H	-5.597399	1.280724	-1.137173
C	-4.166521	0.721430	0.370909
H	-4.380033	1.709252	0.786509
H	-4.196404	-0.007707	1.184312
C	-6.252000	-0.511973	-0.228519
H	-6.732478	-0.120602	0.668981
C	-6.686209	-1.660205	-0.739890
H	-7.505918	-2.199871	-0.276774
H	-6.254521	-2.104299	-1.632528
C	-0.882193	-0.867091	-0.874913
O	-0.747793	-0.483350	-2.220434
C	-1.848839	1.446756	0.880577
H	-2.204893	2.479959	0.900531
H	-0.843920	1.458981	0.449457
C	0.810272	5.080673	-0.599344
C	3.298978	4.210862	0.283327
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C	1.277612	3.830534	-1.001271
C	2.532626	3.390005	-0.549421
C	2.815646	5.450391	0.691936
H	1.186059	6.851086	0.564380
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H	4.288970	3.886014	0.592069
C	0.441064	2.931476	-1.881619
O	0.536581	1.672643	-1.602037
H	-0.241290	0.380444	-2.205168
N	-0.277856	3.516552	-2.789437
H	-0.766318	2.785709	-3.318295
H	-0.157408	5.411204	-0.963082
C	3.099184	2.123806	-1.081634
H	2.996141	1.982387	-2.159302
N	3.728210	1.205216	-0.464891
C	3.847397	1.180619	0.993883
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H	4.871962	1.468760	1.258157
C	3.571662	-0.232229	1.453834
C	2.990531	-2.900770	2.057585
C	4.559481	-1.218116	1.344537
C	2.297461	-0.595083	1.889647
C	2.006181	-1.924653	2.188665
C	4.270710	-2.540548	1.641041
H	5.550723	-0.934031	0.994064
H	1.531877	0.172734	1.984738
H	1.009176	-2.212108	2.512160
H	5.040775	-3.298739	1.534435
H	2.758884	-3.939618	2.272557
H	-0.222157	-0.240984	-0.258708
H	-2.236180	-3.200428	-0.040563
C	-1.195518	-3.343920	-0.306513
C	-0.392706	-2.303345	-0.709072
N	0.541135	-4.982259	-0.594187
C	0.977536	-2.599403	-1.014684
C	-0.683201	-4.662478	-0.256925
C	1.372929	-3.968013	-0.967587
C	1.946456	-1.610714	-1.328340
H	-1.336144	-5.474659	0.057893
H	2.971688	-5.367970	-1.295940
C	3.253739	-1.975707	-1.587038
H	1.678897	-0.556791	-1.350253
C	3.621123	-3.349886	-1.617887
H	4.652291	-3.595094	-1.853412
C	2.706047	-4.315545	-1.312690
O	4.239213	-1.089447	-1.828455
H	4.039794	-0.217325	-1.370507
C	-1.903841	0.861702	2.267883
C	-2.021856	-0.157760	4.874191
C	-1.171902	-0.278100	2.618989
C	-2.685293	1.488439	3.242505
C	-2.746880	0.982635	4.537944
C	-1.232499	-0.786269	3.913382
H	-0.547936	-0.774995	1.879317
H	-3.242075	2.386569	2.986891
H	-3.356410	1.482031	5.284035
H	-0.659054	-1.669812	4.175500
H	-2.066720	-0.553527	5.883728

Ia16Z-S

H	-4.653194	0.423635	-2.691158
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C	-2.760333	-2.151205	-1.393543

C	-1.938391	-1.272002	-0.420172
C	-4.070816	-1.457007	-1.778442
C	-3.186219	0.788705	-1.149490
H	-2.162013	-2.324932	-2.291101
H	-1.749272	-1.801809	0.515762
H	-2.288261	1.334913	-1.440804
H	-3.009001	-0.115775	-3.099146
H	-2.974179	-3.118250	-0.929880
H	-4.587700	-2.029963	-2.552323
H	-3.915342	1.499290	-0.750060
N	-2.817859	-0.100860	0.021174
C	-4.959680	-1.304148	-0.538191
H	-5.752744	-0.582143	-0.777077
C	-4.090418	-0.691982	0.585286
H	-4.609653	0.113032	1.110116
H	-3.783172	-1.441880	1.318678
C	-5.629134	-2.557871	-0.033040
H	-6.134130	-2.449362	0.927418
C	-5.663665	-3.737083	-0.647037
H	-6.185885	-4.579234	-0.204638
H	-5.184140	-3.912106	-1.606119
C	-0.586866	-0.829602	-1.021978
O	-0.729364	-0.404073	-2.345289
C	-2.166110	0.771243	1.081699
H	-2.899387	1.552800	1.291662
H	-1.309894	1.255097	0.608833
C	-2.009864	4.006122	-0.227316
C	0.137127	3.519617	1.463352
C	-2.153114	4.200038	1.143059
C	-0.812191	3.534591	-0.766802
C	0.287787	3.302303	0.084519
C	-1.077181	3.946490	1.992174
H	-3.096175	4.555663	1.547760
H	-1.171565	4.106375	3.061514
H	0.981806	3.399830	2.130490
C	-0.759450	3.326623	-2.272787
O	-1.217693	4.243906	-2.983579
H	-0.521989	0.596890	-2.389284
N	-0.241094	2.165485	-2.663164
H	-0.251463	2.170860	-3.687748
H	-2.828494	4.220715	-0.908321
C	1.601624	2.989593	-0.532896
H	1.716243	3.372032	-1.546902
N	2.612055	2.356597	-0.078543
C	2.619556	1.702409	1.227231
H	1.636565	1.276025	1.475527
H	2.842005	2.460130	1.990470
C	3.689492	0.635591	1.297377
C	5.692014	-1.314531	1.456505
C	5.025383	0.973433	1.070909
C	3.368192	-0.687945	1.594658
C	4.361708	-1.661464	1.674747
C	6.021670	0.004597	1.148344
H	5.279281	2.001274	0.822604
H	2.327456	-0.965187	1.747812
H	4.093052	-2.691143	1.892472
H	7.057076	0.278621	0.968528
H	6.468874	-2.071111	1.515055
H	-0.172876	-0.005440	-0.417495
H	-0.875102	-3.558432	-0.322535
C	0.126815	-3.257983	-0.606671
C	0.433369	-1.966091	-0.959899
N	2.380691	-4.035746	-0.943423
C	1.794091	-1.678449	-1.305281
C	1.131356	-4.256617	-0.618387
C	2.723677	-2.757820	-1.277114
C	2.260945	-0.377623	-1.617020
H	0.867052	-5.276829	-0.345777
H	4.767625	-3.350736	-1.575048
C	3.606694	-0.153951	-1.831971
H	1.575457	0.461498	-1.684133
C	4.520633	-1.238258	-1.854439
H	5.566766	-1.022215	-2.046047
C	4.084673	-2.507033	-1.592829
O	4.114497	1.087393	-2.017542
H	3.628763	1.699465	-1.400245
C	-1.775735	0.057693	2.349287
C	-1.034487	-1.193284	4.742797
C	-0.546196	-0.601982	2.457461
C	-2.622587	0.093007	3.460228
C	-2.256627	-0.531651	4.649829
C	-0.177149	-1.226070	3.644651
H	0.129799	-0.633379	1.605849
H	-3.569845	0.623354	3.398546
H	-2.923081	-0.494982	5.505396
H	0.781183	-1.731603	3.713953
H	-0.746745	-1.677079	5.670708

Ic3E

H	0.915944	4.020893	-2.996177
C	0.718034	2.947027	-2.928859
C	-1.025931	1.186396	-2.912790
C	-0.941727	0.938839	-1.396074
C	-0.759333	2.661635	-3.213617
C	1.071877	2.422171	-1.525752
H	-0.279208	0.567874	-3.421045
H	-1.934457	0.995172	-0.937436
H	1.622599	3.159329	-0.940613
H	1.350003	2.445648	-3.666181
H	-2.011164	0.873576	-3.266710
H	-1.001612	2.890784	-4.254130
H	1.626526	1.485215	-1.563806
N	-0.190768	2.115904	-0.751411
C	-1.606939	3.547681	-2.280796
H	-1.410272	4.593752	-2.539049
C	-1.104993	3.318197	-0.834682
H	-0.527264	4.167600	-0.468532
H	-1.928316	3.137025	-0.138569
C	-3.086491	3.305229	-2.420748
H	-3.472337	2.351463	-2.058366
C	-3.925805	4.182110	-2.963353
H	-4.985005	3.968666	-3.063186
C	-3.579334	5.146550	-3.327401
C	-0.363668	-0.455636	-1.080755
O	0.877734	-0.632330	-1.714327
C	0.137491	1.800965	0.703759
H	0.903041	1.023588	0.685995
H	-0.773808	1.382011	1.143360
C	-1.344491	-2.753375	2.814246
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C	-1.278730	-4.019548	2.240727
C	-0.329276	-1.816976	2.613203
C	0.795459	-2.190755	1.857218
C	-0.193065	-4.363626	1.438655
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H	1.703494	-3.711885	0.645688
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O	0.597012	0.293337	3.176163
H	1.485483	-0.995009	-1.014192
N	-1.692674	0.030465	3.343336
H	-1.639426	1.002086	3.654652
H	-2.212501	-2.463106	3.397034
C	1.979260	-1.309464	1.679290
H	2.517402	-0.993959	2.575038
N	2.397960	-1.009031	0.513063
C	3.635842	-0.239641	0.402938
H	4.053523	-0.002792	1.390706
H	3.393153	0.709306	-0.095440
C	4.640693	-0.995892	-0.436237
C	6.455262	-2.446208	-1.995866
C	4.422641	-1.158801	-1.807465
C	5.770905	-1.568336	0.145848
C	6.677871	-2.288547	-0.630590
C	5.323333	-1.881014	-2.583747
H	3.539746	-0.718093	-2.266795
H	5.942620	-1.449334	1.212634
H	7.556477	-2.726778	-0.167320
H	5.145510	-2.001212	-3.647972
H	7.160135	-3.007184	-2.601539
H	-0.241431	-0.571109	0.002535
H	-0.351106	-2.065961	-3.292549
C	-1.238058	-2.198994	-2.682704
C	-1.394216	-1.482508	-1.525212
N	-3.325054	-3.369676	-2.365176
C	-2.553686	-1.721428	-0.727191
C	-2.239920	-3.126434	-3.064129
C	-3.485061	-2.690039	-1.193914
C	-2.777735	-1.083236	0.511922
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H	-5.330545	-3.709152	-0.760506
C	-3.847871	-1.428705	1.315622
H	-2.067374	-0.371131	0.910746
C	-4.798759	-2.372666	0.828893
H	-5.647756	-2.616738	1.460131
C	-4.621843	-2.975738	-0.388056
O	-4.005131	-0.935240	2.547918
H	-3.097052	-0.528169	2.875961
C	0.604022	2.979686	1.517033
C	1.466189	5.136810	3.078357
C	-0.315210	3.739230	2.246713
C	1.962044	3.295185	1.602063
C	2.392232	4.371443	2.373792
C	0.111388	4.814836	3.019415
H	-1.370386	3.477533	2.220908
H	2.692478	2.681573	1.080127
H	3.450648	4.603297	2.433193
H	-0.612550	5.394624	3.582720
H	1.800429	5.973124	3.683928

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C	0.282458	3.018495	-3.027018
C	-1.173595	1.017279	-2.933214
C	-1.030373	0.816592	-1.415505
C	-1.143935	2.511423	-3.258433
C	0.760782	2.549513	-1.642613
H	-0.348676	0.510780	-3.445496
H	-2.014500	0.762689	-0.939529
H	1.241524	3.353236	-1.084705
H	0.957209	2.620558	-3.789216
H	-2.104624	0.549246	-3.262752
H	-1.453811	2.687117	-4.291425
H	1.425226	1.687625	-1.703097
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C	-2.082188	3.275191	-2.302803
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C	-3.510254	2.802514	-2.378865
H	-3.733382	1.815735	-1.970280
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H	-4.311011	4.506954	-3.334057
C	-0.282822	-0.487266	-1.075961
O	0.970252	-0.520475	-1.709447
C	-0.003150	1.845968	0.628756
H	0.846178	1.160517	0.588433
H	-0.844444	1.337303	1.113094
C	-1.061468	-2.695430	2.948265
C	1.163258	-3.290607	1.409170
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C	-0.130073	-1.687740	2.696599
C	1.017750	-2.007365	1.947559
C	0.215654	-4.278885	1.658439
H	-1.633296	-4.747803	2.659452
H	0.344108	-5.271592	1.238521
H	2.039779	-3.510315	0.806226
C	-0.440680	-0.267331	3.132102
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H	1.606578	-0.837128	-1.012505
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H	0.238994	1.418620	3.616033
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C	3.678871	0.089589	0.358221
H	4.091083	0.401145	1.327271
H	3.355827	0.992574	-0.177718
C	4.723122	-0.626486	-0.467561
C	6.602515	-2.018097	-2.002859
C	4.517500	-0.815426	-1.837057
C	5.874513	-1.142849	0.125572
C	6.813672	-1.833323	-0.639002
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H	3.618619	-0.416699	-2.303881
H	6.037587	-1.002677	1.191337
H	7.708850	-2.228227	-0.168326
H	5.281507	-1.649935	-3.664800
H	7.332698	-2.557087	-2.598653
H	-0.144781	-0.564983	0.009246
H	-0.063605	-2.156540	-3.234065
C	-0.934161	-2.371858	-2.623829
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C	-1.823292	-3.417761	-2.978345
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C	-3.656848	-1.756235	1.317075
C	-1.982078	-0.544872	0.914070
C	-4.503306	-2.803427	0.859770
H	-5.335159	-3.107413	1.487495
C	-4.245446	-3.429287	-0.332411
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C	1.991288	4.700595	2.168038
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C	2.665103	-0.911899	-2.385808
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C	2.835340	-2.429692	-2.298994
C	1.194853	-2.605080	-0.436531
H	1.951988	-0.673373	-3.179585
H	2.840475	0.372524	-0.627270
H	0.178002	-2.242506	-0.304254
H	0.704505	-2.681608	-2.540438
H	3.618651	-0.439357	-2.638794
H	3.152373	-2.825432	-3.267460
H	1.389177	-3.404075	0.284297
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C	3.882680	-2.785209	-1.225131
H	3.807891	-3.860732	-1.025264
C	3.517586	-2.011896	0.060986
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H	4.176316	-1.155565	0.225220
C	5.295955	-2.484227	-1.640001
H	5.531001	-1.438883	-1.844874
C	6.243749	-3.407878	-1.768141
H	7.249882	-3.150318	-2.083070
H	6.043461	-4.456798	-1.562761
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O	-0.139506	-0.356197	-1.978067
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H	1.680570	-1.908604	1.976752
H	0.614352	-0.696869	1.275062
C	-3.772589	-3.780093	-0.444692
C	-5.422346	-1.751677	-1.358024
C	-4.943069	-4.095647	-1.125999
C	-3.405482	-2.452952	-0.208936
C	-4.254420	-1.428682	-0.656438
C	-5.773414	-3.076487	-1.588799
H	-5.202075	-5.134642	-1.306436
H	-6.684313	-3.310962	-2.130346
H	-6.064772	-0.950565	-1.715365
C	-2.097000	-2.153149	0.487219
O	-1.479610	-1.080451	0.127084
H	-0.822875	-0.705743	-1.341459
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H	-0.856656	-2.669688	1.792576
H	-3.109736	-4.559719	-0.084322
C	-4.006952	0.024347	-0.451766
H	-4.080895	0.629559	-1.362938
N	-3.803888	0.681934	0.616494
C	-3.705599	0.053900	1.925833
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C	-2.392213	0.381987	2.608518
C	0.009759	0.959945	3.938982
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H	-2.241566	2.386716	1.830181
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H	-0.146430	-1.033051	4.741183
H	-0.116515	2.884578	2.980451
H	0.950920	1.179591	4.436303
H	0.337507	0.507747	-0.192851
H	2.939053	1.561871	-2.539680
C	2.072869	2.201347	-2.420336
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C	2.141733	3.507908	-2.959374
C	0.038708	4.000471	-2.218909
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H	3.045155	3.822102	-3.478910
H	-0.834681	5.939679	-2.538466
C	-2.338322	3.379479	-0.847515
H	-1.523936	1.424853	-0.541331
C	-2.149889	4.666556	-1.424549
H	-2.946261	5.395269	-1.311546
C	-0.997896	4.963157	-2.093558
O	-3.501227	3.200910	-0.196064
H	-3.575668	2.270550	0.191039
C	2.542512	0.051970	1.983920
C	4.127782	1.978379	3.261597
C	2.389319	1.411203	1.685958
C	3.493041	-0.324694	2.936316
C	4.281979	0.630273	3.573231
C	3.180103	2.366761	2.315971
H	1.625763	1.739516	0.984885
H	3.606999	-1.374399	3.196323
H	5.010294	0.319364	4.315414
H	3.044094	3.416945	2.077879
H	4.738109	2.725949	3.758449

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C	2.510950	-1.112834	-2.287156
C	2.139309	-0.444693	-0.939724
C	2.642648	-2.628965	-2.128224
C	1.269318	-2.654202	-0.054505
H	1.722182	-0.891670	-3.010534
H	2.901388	0.277424	-0.638517
H	0.269200	-2.301518	0.196585

H	0.490668	-2.797382	-2.060981
H	3.445508	-0.693608	-2.671416
H	2.818584	-3.092373	-3.102309
H	1.570021	-3.415361	0.670686
N	2.237788	-1.505823	0.160076
C	3.808755	-2.956693	-1.175228
H	3.723750	-4.011146	-0.887289
C	3.637918	-2.079595	0.083381
H	3.797993	-2.653898	0.998500
H	4.325015	-1.230041	0.086293
C	5.167642	-2.746895	-1.783647
H	5.420440	-1.726469	-2.074910
C	6.048827	-3.722852	-1.981124
H	7.014643	-3.533292	-2.438363
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C	0.779269	0.294955	-1.000292
O	-0.210460	-0.464523	-1.634153
C	2.004901	-0.934517	1.550969
H	2.085082	-1.790346	2.226333
H	0.972987	-0.583007	1.583443
C	-3.973350	-3.702807	-0.343173
C	-5.351419	-1.644119	-1.575974
C	-5.019833	-3.996763	-1.209286
C	-3.587064	-2.384850	-0.090652
C	-4.307270	-1.340660	-0.690780
C	-5.713000	-2.960351	-1.833318
H	-5.292339	-5.029937	-1.402643
H	-6.528533	-3.175805	-2.516375
H	-5.891224	-0.831555	-2.056158
C	-2.426859	-2.158495	0.855946
O	-2.398136	-2.867040	1.887503
H	-0.860088	-0.768901	-0.904434
N	-1.572993	-1.204887	0.505061
H	-0.958916	-1.079411	1.314048
H	-3.427437	-4.496488	0.156975
C	-4.057042	0.112057	-0.490744
H	-4.054247	0.686037	-1.425342
N	-3.927990	0.817054	0.559477
C	-3.926823	0.287495	1.914649
C	-4.119782	-0.789882	1.957436
H	-4.749579	0.791081	2.438899
C	-2.618159	0.601103	2.620741
C	-0.133509	1.070332	3.842853
C	-1.896877	1.764476	2.340338
C	-2.105424	-0.299965	3.556386
C	-0.871384	-0.068773	4.162269
C	-0.657955	1.991520	2.936217
H	-2.292710	2.493668	1.641329
H	-2.642168	-1.221798	3.756089
H	-0.478461	-0.790130	4.872972
H	-0.102201	2.892707	2.690950
H	0.838221	1.242570	4.297458
H	0.447154	0.531250	0.023524
H	2.961164	1.350455	-2.440209
C	2.099497	2.002749	-2.378201
C	0.952052	1.641319	-1.711703
N	1.243732	4.156232	-3.012231
C	-0.121535	2.593835	-1.685922
C	2.197595	3.259905	-3.018869
C	0.096975	3.839032	-2.347634
C	-1.354920	2.373725	-1.015525
H	3.112753	3.516069	-3.549398
H	-0.725948	5.765385	-2.828234
C	-2.321161	3.365502	-0.994746
H	-1.547123	1.423332	-0.524115
C	-2.092784	4.604172	-1.655874
H	-2.878752	5.351792	-1.615441
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O	-3.508330	3.261008	-0.372002
H	-3.634306	2.356326	0.063812
C	2.958213	0.160442	1.956422
C	4.707305	2.190068	2.768858
C	2.666086	1.501799	1.683117
C	4.126640	-0.148398	2.659145
C	4.999514	0.859494	3.059568
C	3.537109	2.510482	2.083400
H	1.745709	1.767876	1.168990
H	4.350440	-1.183439	2.905674
H	5.901356	0.604905	3.606635
H	3.297001	3.545986	1.864817
H	5.384958	2.976916	3.084624

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H	1.594413	-4.403588	-1.022305
C	1.699209	-3.320005	-1.124510
C	3.153070	-1.464587	-1.951156
C	2.668630	-0.661607	-0.717968
C	3.086427	-2.971719	-1.674838
C	1.530380	-2.660483	0.254555
H	2.508644	-1.223695	-2.797355
H	3.416627	0.074284	-0.417485
H	1.640161	-3.374647	1.075513
H	0.930619	-2.952439	-1.805910
H	4.174655	-1.169460	-2.209260
H	3.286064	-3.531356	-2.592334
H	0.575949	-2.141759	0.378781
N	2.611761	-1.625712	0.474498
C	4.121494	-3.340343	-0.596754
C	3.883076	-4.341689	-0.218267
C	3.955812	-2.319468	0.545240
H	4.025047	-2.798894	1.523362
H	4.709302	-1.528879	0.492581
C	5.540807	-3.353653	-1.091189
H	5.928307	-2.413822	-1.486208
C	6.322231	-4.429329	-1.072541
H	7.338766	-4.399651	-1.451425
H	5.969438	-5.379441	-0.678460
C	1.326540	0.073495	-0.941215
O	0.565333	-0.634761	-1.898929
C	2.331437	-0.938182	1.811381
H	2.534475	-1.705260	2.563297
H	1.262452	-0.712198	1.834567
C	-3.888035	-1.481371	2.746671
C	-4.019311	-2.779977	0.291594
C	-4.873680	-2.437490	2.518488
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C	-3.036122	-1.814722	0.516180
C	-4.940682	-3.087584	1.287623
H	-5.585180	-2.678786	3.302357
H	-5.710188	-3.830650	1.103164
H	-4.081778	-3.265729	-0.678676
C	-1.886330	-0.113592	1.972233
O	-0.729583	-0.398967	1.552083
H	-0.383180	-0.352997	-1.814916
N	-2.224469	1.034749	2.526439

H	-3.219652	1.032646	2.749382
H	-3.825832	-0.981886	3.710303
C	-2.098871	-1.444980	-0.583517
H	-1.337187	-2.186560	-0.847063
N	-2.077125	-0.367751	-1.259998
C	-3.064536	0.695338	-1.007234
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C	-4.500938	0.230206	-1.120701
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C	-4.935632	-0.429949	-2.273023
C	-5.400948	0.430523	-0.074615
C	-6.712527	-0.029373	-0.170286
C	-6.244749	-0.891082	-2.372340
H	-4.235441	-0.594452	-3.088629
H	-5.061781	0.930688	0.829980
H	-7.400541	0.123857	0.655931
H	-6.570103	-1.405666	-3.271810
H	-8.157464	-1.056775	-1.393622
H	0.782021	0.095989	0.007699
H	3.190726	1.027747	-2.735566
C	2.529807	1.796483	-2.346488
C	1.561815	1.504890	-1.414677
N	1.944522	4.128180	-2.423211
C	0.728208	2.574762	-0.959681
C	2.682038	3.118409	-2.822380
C	0.979400	3.872048	-1.496902
C	-0.293585	2.412511	0.010656
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H	0.394533	5.942195	-1.468124
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H	-0.508636	1.434800	0.435282
C	-0.768781	4.791783	-0.084439
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C	0.192858	4.965241	-1.039510
O	-1.946765	3.410135	1.422424
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C	4.553883	2.687947	2.444236
C	2.511171	1.545638	1.870450
C	4.470077	0.274533	2.474316
C	5.175831	1.459444	2.665022
C	3.217066	2.730962	2.055392
H	1.456824	1.573552	1.606937
H	4.955895	-0.677683	2.671102
H	6.209787	1.423918	2.993188
H	2.718020	3.683105	1.901654
H	5.107634	3.610056	2.590944

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C	3.144803	-2.921241	-1.719762
C	1.587982	-2.675380	0.215872
H	2.522082	-1.169018	-2.812578
H	3.418059	0.104637	-0.413074
H	1.707727	-3.398271	1.027246
H	0.988110	-2.949523	-1.846951
H	4.188818	-1.087163	-2.229941
H	3.354854	-3.461594	-2.646273
H	0.623867	-2.178155	0.343061
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C	5.608921	-3.255926	-1.148132
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C	1.325977	0.084772	-0.936162
O	0.571658	-0.623240	-1.895252
C	2.351811	-0.959698	1.796420
H	2.545784	-1.740962	2.535805
H	1.279208	-0.747814	1.816935
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H	-2.875152	1.435976	-1.741433
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C	-6.162852	-1.030450	-2.428205
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H	-8.092133	-1.244563	-1.493709
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C	0.111424	4.964377	-1.081971
O	-2.190482	3.388955	1.200039
H	-2.262705	2.483881	1.653597
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C	4.665568	2.591414	2.543803
C	2.631229	1.532685	1.803876
C	4.460409	0.186946	2.609492
C	5.204243	1.340763	2.841076
C	3.374289	2.687204	2.029966
H	1.616818	1.617760	1.422626
H	4.880208	-0.783918	2.860863
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H	2.938868	3.657306	1.810657
H	5.246934	3.489876	2.725402

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H	2.236835	1.420378	3.467898
C	1.506940	0.783718	2.960299
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C	1.651672	-0.667284	3.429868
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H	2.707810	1.284751	1.183852
H	0.504343	1.150195	3.186773
H	0.657947	-2.561986	3.078719
H	1.603149	-0.722243	4.520491
H	0.949789	1.410478	0.934911
N	1.751091	-0.542282	0.850859
C	3.013583	-1.190776	2.941189
H	3.778545	-0.457218	3.222303
C	2.956734	-1.275702	1.399888
H	3.839789	-0.826207	0.949101
H	2.878002	-2.307254	1.041969
C	3.403923	-2.516814	3.532707
H	2.761865	-3.366052	3.295789
C	4.466832	-2.696657	4.311235
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H	5.133700	-1.874194	4.558768
C	-0.804807	-0.754275	0.765053
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H	1.415327	-1.436357	-1.035001
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C	1.900169	4.290155	0.014772
H	1.946690	5.344796	1.895525
H	2.939343	4.496337	-0.226242
H	1.516997	3.190560	-1.801880
C	-2.253471	3.553164	0.956899
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H	-1.713100	1.011174	1.152530
N	-2.860160	4.515341	1.570445
H	-3.817462	4.195806	1.751492
H	-0.459690	4.930518	2.376989
C	-0.977092	2.424832	-1.531178
H	-2.058710	2.565821	-1.616181
N	-0.344882	1.566235	-2.227803
C	-1.093437	0.767751	-3.194015
H	-0.958444	1.226865	-4.181121
H	-2.171905	0.756053	-2.975669
C	-0.531488	-0.637137	-3.212581
C	0.614977	-3.193368	-3.099644
C	-1.214141	-1.693814	-2.610305
C	0.727982	-0.875400	-3.771342
C	1.294372	-2.145878	-3.725413
C	-0.640909	-2.964470	-2.540583
H	-2.200237	-1.520218	-2.186660
H	1.270079	-0.054052	-4.234478
H	2.271105	-2.317072	-4.168533
H	-1.181460	-3.772004	-2.055085
H	1.060117	-4.182928	-3.055986
H	-0.678986	-0.423575	-0.276313
H	-0.835861	-3.505544	1.603665
C	-1.771779	-3.114486	1.219490
C	-1.903520	-1.826806	0.760472
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C	-3.197142	-1.440005	0.294228
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C	-3.443719	-0.156124	-0.222739
H	-2.770674	-5.000698	1.587004
H	-6.391941	-2.633065	0.133991
C	-4.727332	0.291094	-0.432691
H	-2.636969	0.539462	-0.394236
C	-5.812540	-0.619532	-0.328346
H	-6.815951	-0.263897	-0.540469
C	-5.579849	-1.917313	0.052117
O	-4.962535	1.590767	-0.714485
H	-4.202263	2.092841	-0.308829
C	3.175638	-0.237925	-1.257274
C	5.706980	0.182288	-2.374936
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C	3.924159	-1.314525	-1.743788
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C	4.965367	1.261531	-1.900828
H	3.119681	1.898304	-0.998417
H	3.510339	-2.319205	-1.692294
H	5.752652	-1.951122	-2.675459
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C	0.579829	-1.460513	2.884186
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C	1.738969	-0.620494	3.427960
C	1.785585	0.824471	1.384215
H	-0.362110	-1.101177	3.303397
H	0.617128	-2.326126	0.867969
H	2.754996	1.224639	1.076588
H	0.619796	1.210059	3.156984
H	0.700742	-2.507228	3.178311
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H	0.991946	1.381680	0.884646
N	1.746845	-0.590350	0.844874
C	3.071802	-1.189633	2.910513

H	3.860866	-0.461431	3.132560
C	2.953170	-1.333519	1.377195
H	3.830210	-0.926697	0.876808
H	2.833507	-2.375979	1.064298
C	3.460550	-2.499719	3.537206
H	2.783983	-3.339259	3.372601
C	4.561156	-2.677412	4.261978
H	4.798688	-3.638089	4.707661
H	5.262735	-1.865159	4.436449
C	-0.812505	-0.726020	0.864647
O	-1.098386	0.382340	1.681196
C	1.750915	-0.580013	-0.684331
H	1.061491	0.209596	-0.997847
H	1.339839	-1.545603	-0.996516
C	0.208310	4.651519	1.307334
C	1.116510	3.538876	-1.051747
C	1.520357	4.870776	0.906605
C	-0.665854	3.852423	0.562318
C	-0.195405	3.273682	-0.630601
C	1.977209	4.317656	-0.289669
H	2.178740	5.484863	1.513677
H	2.990613	4.504710	-0.633689
H	1.440837	3.123474	-2.000920
C	-2.056187	3.663653	1.157317
O	-2.483735	4.567876	1.898245
H	-1.670586	1.097244	1.252537
N	-2.653210	2.503332	0.867524
H	-3.507962	2.475248	1.433962
H	-0.177211	5.093934	2.219408
C	-1.010386	2.389614	-1.500533
H	-2.091965	2.550480	-1.530672
N	-0.433549	1.491041	-2.194685
C	-1.239808	0.676409	-3.099254
H	-1.159952	1.121126	-4.099506
H	-2.304162	0.670616	-2.820149
C	-0.678054	-0.728819	-3.132000
O	0.473554	-3.284667	-3.059590
C	-1.350227	-1.791975	-2.529743
C	0.572473	-0.961316	-3.713918
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C	-0.773583	-3.062047	-2.479555
H	-2.330959	-1.624764	-2.093201
H	1.106489	-0.134907	-4.177554
H	2.111016	-2.397125	-4.147659
H	-1.305578	-3.874675	-1.993178
H	0.921088	-4.273700	-3.030450
H	-0.703724	-0.425517	-0.188130
H	-0.959677	-3.420851	1.872225
C	-1.872261	-3.021086	1.442571
C	-1.944343	-1.760596	0.904616
N	-4.211107	-3.486874	1.024147
C	-3.210273	-1.357331	0.380264
C	-3.030228	-3.845632	1.466493
C	-4.317964	-2.237088	0.485003
C	-3.391619	-0.099057	-0.220416
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H	-6.423280	-2.476647	0.104238
C	-4.641603	0.349863	-0.567022
H	-2.562369	0.576513	-0.356302
C	-5.757934	-0.519572	-0.469586
H	-6.733611	-0.159833	-0.780111
C	-5.586898	-1.789397	0.023917
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C	3.098569	-0.362654	-1.320287
C	5.579722	0.022614	-2.556632
C	3.607127	0.925866	-1.500140
C	3.839685	-1.456220	-1.779951
C	5.073638	-1.266406	-2.393899
C	4.844748	1.118030	-2.110250
H	3.026915	1.783171	-1.170833
H	3.439613	-2.460822	-1.661710
H	5.638391	-2.123259	-2.747347
H	5.229183	2.124226	-2.244175
H	6.541817	0.172005	-3.036382

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H	4.236194	1.386482	3.002780
C	3.753347	0.638576	2.367343
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C	4.681491	0.258184	1.210034
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H	4.039865	-1.785166	1.020055
H	2.431397	-0.608504	-1.053124
H	1.549878	0.779410	2.244084
H	3.526205	-0.243762	2.965028
H	4.628245	-1.097719	-0.492111
H	5.658532	-0.051475	1.590799
H	2.400327	2.307901	1.911277
N	2.366938	0.959095	0.314925
C	4.837443	1.494419	0.309224
H	5.060450	2.357471	0.947689
C	3.476467	1.719974	-0.376848
H	3.200779	2.773458	-0.363216
H	3.477784	1.373655	-1.415468
C	5.933254	1.374195	-0.712539
H	5.827561	0.578076	-1.450535
C	6.997025	2.170965	-0.756972
H	7.772765	2.041540	-1.504842
H	7.129389	2.980233	-0.042828
C	1.578380	-1.480504	0.736775
O	1.935175	-1.668310	2.072350
C	1.029521	1.408308	-0.264218
H	0.264665	0.784890	0.202086
H	1.094299	1.200241	-1.336723
C	-3.377445	-1.069576	3.912910
C	-4.889168	-1.563053	1.629494
C	-4.738987	-1.345177	4.025705
C	-2.766096	-1.022036	2.662333
C	-3.532038	-1.254740	1.508240
C	-5.494251	-1.598617	2.883731
H	-5.207419	-1.370094	5.004864
H	-6.550588	-1.833296	2.967082
H	-5.467981	-1.800129	0.740866
C	-1.292850	-0.700651	2.510391
O	-1.005786	0.203463	1.672073
H	1.065964	-1.565143	2.614011
N	-0.411691	-1.382126	3.205813
H	-0.861543	-2.098732	3.771275
H	-2.781358	-0.878288	4.801260
C	-2.828560	-1.314534	0.197851
H	-1.916840	-1.917873	0.203097
N	-3.142307	-0.795758	-0.921946
C	-4.284439	0.106204	-1.049002

H	-4.786046	0.275786	-0.089645
H	-5.006768	-0.354426	-1.731780
C	-3.821697	1.431914	-1.610223
C	-3.003136	3.927581	-2.565301
C	-2.839184	2.157492	-0.928283
C	-4.377587	1.957333	-2.775871
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C	-2.440074	3.403988	-1.401042
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H	-5.137299	1.392098	-3.310064
H	-4.406705	3.600571	-4.165570
H	-1.693530	3.973556	-0.858030
H	-2.685601	4.899598	-2.931186
H	0.568480	-1.058205	0.684593
H	2.935478	-3.744546	1.317284
C	2.403535	-3.823291	0.375650
C	1.608645	-2.787502	-0.046439
N	1.903508	-5.160876	-1.563548
C	0.856036	-2.963579	-1.248786
C	2.521007	-4.988157	-0.418408
C	1.062119	-4.170328	-1.976172
C	-0.103351	-2.030046	-1.721885
H	3.168541	-5.798195	-0.086874
H	0.536941	-5.289110	-3.735855
C	-0.853020	-2.299604	-2.849584
H	-0.304785	-1.111316	-1.177182
C	-0.588051	-3.468615	-3.613695
H	-1.169755	-3.635706	-4.514715
C	0.343592	-4.373593	-3.185553
O	-1.852048	-1.493563	-3.265524
H	-2.261677	-1.074120	-2.456342
C	0.702818	2.857537	-0.003704
C	0.064446	5.530869	0.520009
C	1.053788	3.860489	-0.912438
C	-0.005744	3.200588	1.153746
C	-0.316585	4.532771	1.415912
C	0.741664	5.192600	-0.650421
H	1.564641	3.598094	-1.836153
H	-0.330234	2.407104	1.823886
H	-0.867168	4.790650	2.315079
H	1.019963	5.962723	-1.362905
H	-0.179928	6.568513	0.725411

Ib20Z-s

H	5.863557	1.424203	0.797481
C	5.146216	0.632460	1.034312
C	3.905965	-1.325214	0.168217
C	2.576610	-0.581554	-0.044835
C	5.079894	-0.383078	-0.108685
C	3.743601	1.221256	1.256502
H	3.960728	-1.678828	1.203747
H	2.224177	-0.708142	-1.075674
H	3.231891	0.782715	2.112050
H	5.478977	0.148105	1.955886
H	3.927957	-2.204399	-0.480053
H	6.013731	-0.945392	-0.183381
H	3.765253	2.306479	1.359045
N	2.863854	0.923752	0.057283
C	4.837492	0.390445	-1.419945
H	5.708340	1.029594	-1.601520
C	3.616077	1.315545	-1.192284
H	3.918079	2.355040	-1.052977
H	2.904441	1.266059	-2.021231
C	4.669125	-0.512432	-2.613006
H	3.770845	-1.129955	-2.650329
C	5.556958	-0.600033	-3.598963
H	5.411794	-1.276226	-4.435230
H	6.462342	0.002482	-3.601516
C	1.451570	-1.090900	0.891196
O	1.777318	-0.879647	2.236064
C	1.556283	1.681797	0.165689
H	1.104275	1.344305	1.101388
H	0.946284	1.352172	-0.682422
C	-2.482898	-0.062865	4.120068
C	-4.132404	-1.449648	2.358424
C	-3.553666	-0.808636	4.609426
C	-2.244421	0.021265	2.750845
C	-3.071571	-0.688280	1.862723
C	-4.383709	-1.497210	3.728133
H	-3.737631	-0.856336	5.678507
H	-5.212220	-2.088904	4.104699
H	-4.739994	-2.035351	1.673425
C	-1.155615	0.940632	2.241002
O	-0.025427	0.932748	2.859862
H	1.058867	-0.292754	2.616418
N	-1.524564	1.687692	1.238742
H	-0.762437	2.337540	1.022891
H	-1.823976	0.474287	4.795656
C	-2.630119	-0.800054	0.448411
H	-1.571944	-1.042427	0.371584
N	-3.258225	-0.740927	-0.656974
C	-4.658028	-0.322572	-0.695718
H	-5.050827	-0.114933	0.307307
H	-5.249365	-1.136359	-1.129726
C	-4.782231	0.917713	-1.554964
C	-4.993673	3.241971	-3.096036
C	-4.005162	2.039640	-1.245440
C	-5.657328	0.967219	-2.638952
C	-5.765825	2.126130	-3.407260
C	-4.113634	3.194699	-2.014011
H	-3.312626	1.995584	-0.403369
H	-6.256663	0.094411	-2.886596
H	-6.449129	2.153340	-4.250887
H	-3.509719	4.063633	-1.768507
H	-5.073998	4.144741	-3.694343
H	0.521183	-0.562598	0.650556
H	2.408762	-3.221474	2.253430
C	1.860137	-3.518399	1.366594
C	1.261122	-2.568661	0.578159
N	1.093624	-5.327985	-0.026348
C	0.487414	-3.007334	-0.539977
C	1.757675	-4.884960	1.015643
C	0.437264	-4.409366	-0.789520
C	-0.291700	-2.142869	-1.351875
H	2.255834	-5.632325	1.630462
H	-0.362937	-5.957996	-2.048822
C	-1.161882	-2.650190	-2.292511
H	-0.281140	-1.066944	-1.201223
C	-1.152297	-4.039058	-2.588631
H	-1.814842	-4.404181	-3.366696
C	-0.362300	-4.888648	-1.863130
O	-2.055879	-1.862762	-2.937196
H	-2.450818	-1.256756	-2.251895
C	1.675814	3.183303	0.208561
C	1.802020	5.969714	0.388871

C	1.797917	3.959949	-0.947810
C	1.579741	3.817382	1.452437
C	1.648502	5.204972	1.542897
C	1.868561	5.346912	-0.856554
C	1.824670	3.483344	-1.924477
H	1.417038	3.208881	2.340279
H	1.569569	5.687296	2.511851
H	1.963126	5.941850	-1.759343
H	1.852665	7.051911	0.456783

Ij2Z

H	-5.570431	1.661583	-1.502608
C	-4.866231	0.855602	-1.730615
C	-3.660852	-1.109111	-0.849785
C	-2.359165	-0.373743	-0.503342
C	-4.851027	-0.177835	-0.601595
C	-3.442712	1.407138	-1.896252
H	-3.649792	-1.425580	-1.899708
H	-2.137617	-0.483864	0.563015
H	-2.894620	0.938663	-2.713699
H	-5.181856	0.395327	-2.670565
H	-3.713118	-2.018294	-0.244493
H	-5.787144	-0.740308	-0.572397
H	-3.439685	2.488806	-2.032131
N	-2.624227	1.132446	-0.653115
C	-4.661416	0.583276	0.727140
H	-5.542369	1.216859	0.878711
C	-3.440222	1.524998	0.557736
H	-3.748056	2.560396	0.402257
H	-2.764238	1.489621	1.416547
C	-4.545809	-0.330760	1.919080
C	-3.666538	-0.973217	1.980614
C	-5.463968	-0.400801	2.878494
H	-5.358790	-1.083557	3.715425
H	-6.354324	0.223554	2.858996
C	-1.096882	-0.887995	-1.229693
O	-1.001429	-0.385586	-2.544678
C	-1.317597	1.917272	-0.712981
H	-0.959390	1.783015	-1.733674
H	-0.635030	1.425360	-0.016007
C	3.715819	1.532263	2.361695
C	3.937086	2.511740	-0.214165
C	4.807925	2.320951	2.016893
C	2.726475	1.203397	1.430043
C	2.844800	1.705156	0.124054
C	4.923826	2.809551	0.718102
H	5.559724	2.560493	2.762577
H	5.771494	3.425125	0.434533
H	4.020359	2.890872	-1.229808
C	1.550197	0.343306	1.865102
O	0.411203	0.626053	1.397523
H	-0.073748	-0.065076	-2.613902
N	1.779233	-0.648309	2.700635
H	2.767891	-0.742825	2.918270
H	3.613757	1.174872	3.382566
C	1.874171	1.441689	-0.981022
H	1.376379	2.337526	-1.369321
N	1.609950	0.352835	-1.584217
C	2.251999	-0.897958	-1.137307
H	1.871319	-1.690305	-1.792877
H	1.923916	-1.147301	-0.119355
C	3.764042	-0.868678	-1.197947
C	6.559743	-0.788730	-1.308138
C	4.414506	-0.478764	-2.371284
C	4.525745	-1.223843	-0.084694
C	5.917611	-1.185172	-0.137471
C	5.804371	-0.436710	-2.426629
H	3.825391	-0.196073	-3.240282
H	4.016666	-1.510129	0.833220
H	6.498847	-1.456476	0.738676
H	6.300255	-0.129617	-3.342763
H	7.644106	-0.753094	-1.350210
H	-0.243905	-0.535421	-0.642577
H	-1.645658	-2.594349	-3.268111
C	-1.445790	-3.115008	-2.337865
C	-1.110248	-2.407392	-1.210931
N	-1.319495	-5.226632	-1.183857
C	-0.814845	-3.128426	-0.014524
C	-1.536314	-4.526050	-2.273234
C	-0.952821	-4.546234	-0.060871
C	-0.383700	-2.502501	1.179245
H	-1.812037	-5.084606	-3.166042
H	-0.806901	-6.368913	1.073516
C	-0.072820	-3.257248	2.299258
H	-0.250902	-1.424071	1.232954
C	-0.258527	-4.671182	2.262692
H	-0.026679	-5.238251	3.159227
C	-0.683140	-5.291084	1.119484
O	0.400805	-2.711007	3.419974
H	0.866528	-1.800760	3.171096
C	-1.425257	3.373574	-0.346857
C	-1.542578	6.064404	0.408077
C	-1.093168	3.758884	0.956896
C	-1.772847	4.355236	-1.279900
C	-1.839663	5.693859	-0.901904
C	-1.158546	5.096720	1.334696
H	-0.756554	2.998218	1.658491
H	-1.970991	4.079541	-2.312710
H	-2.111462	6.448121	-1.633695
H	-0.899097	5.384764	2.348499
H	-1.591581	7.108561	0.701000

Ig1Z-S

H	-5.652547	1.313972	-1.663957
C	-4.868444	0.577221	-1.863231
C	-3.584801	-1.331251	-0.971934
C	-2.367214	-0.518030	-0.510641
C	-4.855888	-0.499589	-0.776434
C	-3.486639	1.248461	-1.894426
H	-3.479192	-1.602721	-2.028898
H	-2.205680	-0.671239	0.562304
H	-2.847003	0.872848	-2.692605
H	-5.070481	0.133325	-2.841476
H	-3.610912	-2.265481	-0.404503
H	-5.745743	-1.130259	-0.838757
H	-3.566285	2.332767	-1.972949
N	-2.735707	0.970981	-0.608303
C	-4.821962	0.213136	0.590880
H	-5.756793	0.774076	0.698482
C	-3.665528	1.245566	0.552652
H	-4.036343	2.262647	0.416932
H	-3.056629	1.219457	1.460489
C	-4.724762	-0.739861	1.753330
H	-3.812530	-1.330490	1.846886

C	-5.691846	-0.901168	2.651530
H	-5.594496	-1.608339	3.468887
H	-6.616178	-0.330424	2.599189
C	-1.028832	-0.895950	-1.183489
O	-0.925942	-0.365925	-2.484734
C	-1.492458	1.850636	-0.536323
H	-1.016677	1.731555	-1.509699
H	-0.841186	1.429156	0.240504
C	3.886476	1.447814	2.363348
C	3.919891	2.637635	-0.134872
C	4.985768	2.204068	1.975151
C	2.784951	1.276215	1.519834
C	2.818030	1.864367	0.248511
C	5.002772	2.806835	0.718962
H	5.827015	2.324295	2.651170
H	5.856492	3.398492	0.403358
H	3.937468	3.079477	-1.128290
C	1.630337	0.459569	2.061128
O	1.974572	-0.548239	2.764957
H	-0.036920	0.061549	-2.501467
N	0.423288	0.895172	1.795024
H	-0.231386	0.291280	2.305671
H	3.862239	0.964189	3.334303
C	1.776639	1.651647	-0.798198
H	1.208041	2.538927	-1.096799
N	1.537188	0.583072	-1.448391
C	2.265687	-0.653350	-1.096249
H	1.860488	-1.442115	-1.741978
H	2.038245	-0.942213	-0.061727
C	3.765062	-0.562410	-1.278380
C	6.536586	-0.361750	-1.604553
C	4.305195	-0.171899	-2.505960
C	4.623400	-0.859907	-0.219501
C	6.003137	-0.757611	-0.380019
C	5.683874	-0.070102	-2.668801
H	3.639932	0.063281	-3.333546
H	4.199338	-1.139069	0.742819
H	6.660408	-0.979762	0.455547
H	6.093892	0.237766	-3.626237
H	7.611992	-0.278372	-1.730028
H	-0.238536	-0.469498	-0.557730
H	-1.434246	-2.615329	-3.240904
C	-1.189750	-3.129527	-2.317616
C	-0.899955	-2.410588	-1.184678
N	-0.917375	-5.238456	-1.184313
C	-0.533537	-3.123802	-0.003987
C	-1.181340	-4.543706	-2.267184
C	-0.585472	-4.545849	-0.058893
C	-0.110186	-2.487492	1.187149
H	-1.423380	-5.110885	-3.164025
H	-0.327580	-6.364020	1.062927
C	0.244746	-3.227366	2.299534
H	-0.016102	-1.408004	1.226583
C	0.129415	-4.647041	2.260939
H	0.395808	-5.205070	3.153118
C	-0.265312	-5.281433	1.115355
O	0.695144	-2.667594	3.429189
H	1.072537	-1.747513	3.214298
C	-1.752576	3.300800	-0.224649
C	-2.151400	5.994852	0.417448
C	-1.653395	3.735683	1.101542
C	-2.012326	4.237980	-1.230166
C	-2.217860	5.577820	-0.910037
C	-1.859107	5.074185	1.422161
H	-1.377858	3.020140	1.872846
H	-2.033277	3.924174	-2.271139
H	-2.417667	6.296496	-1.698436
H	-1.779050	5.401074	2.454033
H	-2.309423	7.039697	0.665991

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H	0.874164	-3.579187	-2.063887
C	1.136048	-2.550057	-1.803072
C	2.772194	-0.704528	-2.101995
C	2.569321	-0.330702	-0.614025
C	2.529830	-2.198918	-2.328461
C	1.139485	-2.399478	-0.276810
H	2.063320	-0.128912	-2.703074
H	3.486839	0.073612	-0.180107
H	0.273137	-1.863168	0.099197
H	0.392251	-1.877352	-2.234908
C	3.780045	-0.429984	-2.426145
H	1.610804	-2.432489	-3.393253
H	1.211329	-3.362736	0.235915
N	2.361522	-1.622745	0.180608
C	3.560326	-3.025549	-1.533804
H	3.219795	-4.067590	-1.520582
C	3.573264	-2.489063	-0.084526
H	3.550435	-3.303000	0.643265
H	4.452644	-1.872290	0.117571
C	4.943348	-2.993691	-2.121771
H	5.419642	-2.015196	-2.194345
C	5.593112	-4.072915	-2.547494
H	6.587130	-4.004135	-2.977644
H	5.150255	-5.063904	-2.481101
C	1.443676	0.701583	-0.419228
O	0.273385	0.304910	-1.093074
C	2.210342	-1.379991	1.678312
H	2.055030	-2.375126	2.104202
H	1.279843	-0.817871	1.804190
C	-2.709332	-3.015832	-0.100867
C	-3.676579	-1.155185	-1.917362
C	-3.401306	-3.445286	-1.228495
C	-2.492357	-1.656987	0.138544
C	-2.995160	-0.718953	-0.776864
C	-3.889155	-2.510984	-2.141232
H	-3.556863	-4.506307	-1.399127
H	-4.429560	-2.835833	-3.024835
H	-4.061071	-0.420909	-2.620722
C	-1.685546	-1.234303	1.344322
O	-0.862760	-0.253435	1.162035
H	-0.350953	0.046577	-0.349236
N	-1.884714	-1.912357	2.432296
H	-1.259210	-1.521107	3.144856
H	-2.321956	-3.727727	0.621132
C	-2.856188	0.753617	-0.591619
H	-2.326545	1.279310	-1.392995
N	-3.296036	1.483980	0.352621
C	-4.040611	0.916050	1.485082
H	-4.363796	1.768554	2.091242
H	-3.365050	0.318367	2.105826
C	-5.249462	0.093846	1.089446
C	-7.485550	-1.415399	0.344954
C	-6.236861	0.648835	0.271142
C	-5.391464	-1.221276	1.533349

C	-6.505646	-1.972626	1.163060
C	-7.347878	-0.101628	-0.102306
H	-6.127081	1.671683	-0.081843
H	-4.603872	-1.661728	2.142312
H	-6.602132	-2.998170	1.507533
H	-8.107972	0.338341	-0.741262
H	-8.351805	-2.001889	0.053862
H	1.210479	0.784478	0.649672
H	3.866885	1.613679	-1.545430
C	3.111303	2.377076	-1.401470
C	1.876544	2.094508	-0.869341
N	2.618014	4.714195	-1.685970
C	0.955911	3.184812	-0.714198
C	3.436121	3.697799	-1.794706
C	1.387553	4.471453	-1.149581
C	-0.336783	3.047759	-0.144931
H	4.417858	3.897670	-2.220258
H	0.859111	6.544381	-1.359186
C	-1.187007	4.134981	-0.065303
H	-0.672350	2.087651	0.231597
C	-0.749238	5.416339	-0.501653
H	-1.440015	6.248947	-0.412948
C	0.503547	5.576111	-1.021362
O	-2.440887	4.063673	0.415135
H	-2.750668	3.107374	0.446494
C	3.398401	-0.714795	2.326030
C	5.606105	0.482519	3.568775
C	4.410879	-1.497991	2.889528
C	3.496119	0.678234	2.413570
C	4.595298	1.273029	3.027100
C	5.510366	-0.905626	3.503663
H	4.332430	-2.581893	2.858176
H	2.707730	1.310801	2.014687
H	4.655751	2.354797	3.087857
H	6.286005	-1.528522	3.937388
H	6.460762	0.947381	4.049844

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H	0.313930	-3.489676	-1.596826
C	0.678049	-2.476211	-1.404737
C	2.330119	-0.726064	-2.058421
C	2.450523	-0.344861	-0.563301
C	1.949661	-2.202292	-2.213534
C	1.010323	-2.335733	0.086426
H	1.553153	-0.105455	-2.511368
H	3.456011	0.002453	-0.321425
H	0.267754	-1.762511	0.638069
H	-0.108754	-1.766052	-1.670249
H	3.269378	-0.513517	-2.577909
H	1.792253	-2.436777	-3.269586
H	1.143433	-3.306313	0.572963
N	2.341699	-1.627564	0.267914
C	3.072330	-3.093178	-1.645010
H	2.680104	-4.112599	-1.548512
C	3.422146	-2.558494	-0.239121
H	3.513780	-3.369229	0.486937
H	4.355181	-1.989394	-0.237925
C	4.300988	-3.144155	-2.509700
H	4.819729	-2.198787	-2.673809
C	4.769474	-4.255512	-3.069485
H	5.653924	-4.245350	-3.698278
H	4.281839	-5.215780	-2.919234
C	1.424893	0.739060	-0.175297
O	0.146330	0.360559	-0.595082
C	2.532880	-1.378372	1.756402
H	2.421341	-2.361008	2.221703
H	1.685859	-0.767082	2.074503
C	-2.507781	-2.915201	0.401261
C	-3.221473	-1.298987	-1.735578
C	-2.934024	-3.494586	-0.789377
C	-2.417562	-1.528546	0.538192
C	-2.801753	-0.711809	-0.536904
C	-3.293196	-2.681793	-1.863991
H	-2.988494	-4.575333	-0.880475
H	-3.631065	-3.122125	-2.796943
H	-3.513000	-0.660951	-2.566225
C	-1.900780	-0.983057	1.857122
O	-2.388871	-1.445362	2.911551
H	-0.367260	0.199175	0.289627
N	-0.950103	-0.066814	1.724911
H	-0.667927	0.266968	2.647234
H	-2.234776	-3.532203	1.252782
C	-2.779178	0.778966	-0.480541
H	-2.162270	1.256922	-1.246803
N	-3.379811	1.565402	0.320276
C	-4.269906	1.056644	1.375295
H	-4.733698	1.938793	1.828861
H	-3.681159	0.567314	2.157983
C	-5.352735	0.122296	0.876370
C	-7.348389	-1.593868	-0.074259
C	-6.224200	0.540697	-0.132600
C	-5.490791	-1.160445	1.408640
C	-6.485364	-2.014498	0.934852
C	-7.215645	-0.312320	-0.608183
H	-6.115933	1.537848	-0.553145
H	-4.784920	-1.495567	2.166604
H	-6.578990	-3.014304	1.348875
H	-7.886127	0.022369	-1.394323
H	-8.120015	-2.261551	-0.445796
H	1.412158	0.860601	0.939985
H	3.780817	1.568775	-1.473407
C	3.037492	2.345955	-1.339365
C	1.822292	2.105489	-0.742189
N	2.557593	4.667130	-1.746084
C	0.912198	3.213467	-0.632562
C	3.361298	3.636917	-1.820616
C	1.340321	4.466777	-1.163487
C	-0.372949	3.134873	-0.034105
H	4.330954	3.800050	-2.287561
H	0.826848	6.525475	-1.499221
C	-1.222830	4.223659	-0.036457
H	-0.715353	2.210862	0.413036
C	-0.784100	5.471582	-0.556002
H	-1.468826	6.313166	-0.522730
O	0.466719	5.585115	-1.093965
O	-2.482195	4.173185	0.441544
H	-2.806872	3.225713	0.451156
C	3.860586	-0.766716	2.127242
C	6.333345	0.336960	2.843702
C	4.936161	-1.592466	2.469932
C	4.034188	0.621001	2.169825
C	5.264191	1.169572	2.520968
C	6.166556	-1.045769	2.822457
H	4.807838	-2.672097	2.471739
H	3.205550	1.285026	1.938449

H	5.382914	2.247786	2.549472
H	6.991098	-1.699429	3.087767
H	7.291374	0.765069	3.121356

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H	-4.374030	0.448790	-2.536432
C	-3.341024	0.221213	-2.257825
C	-1.516394	-1.464880	-2.334895
C	-1.083553	-0.997938	-0.920104
C	-3.012485	-1.241152	-2.568199
C	-3.163538	0.456468	-0.752795
H	-0.962261	-0.891622	-3.079097
H	-0.627592	-1.819868	-0.356940
H	-4.113226	0.446538	-0.221528
H	-2.673493	0.881499	-2.813146
H	-1.248494	-2.515749	-2.476170
H	-3.265792	-1.481378	-3.604148
H	-2.637568	1.382558	-0.528828
N	-2.367095	-0.681222	-0.130523
C	-3.828220	-2.123418	-1.610075
H	-4.867101	-1.772755	-1.619983
C	-3.241423	-1.917218	-0.199610
H	-4.034319	-1.779763	0.537149
H	-2.619089	-2.758915	0.111383
C	-3.822813	-3.581729	-1.974828
H	-2.853417	-4.081690	-1.966364
C	-4.913739	-4.268125	-2.301084
H	-4.864863	-5.317635	-2.573065
H	-5.895891	-3.801160	-2.309694
O	-0.050508	0.154967	-0.988380
C	-0.631669	1.233806	-1.665229
C	-2.130357	-0.311566	1.328065
H	-3.105965	0.036532	1.677884
H	-1.455241	0.548438	1.323278
C	4.254668	0.780341	0.763064
C	3.216298	2.481684	-1.169206
C	4.917235	0.938381	-0.449539
C	3.050851	1.440239	1.014710
C	2.556722	2.338367	0.056277
C	4.382377	1.771397	-1.431619
H	5.837372	0.393428	-0.638120
H	4.879319	1.879067	-2.390973
H	2.810035	3.169105	-1.905716
C	2.202267	1.118262	2.227009
O	1.098636	1.726144	2.326535
H	-0.145533	2.063349	-1.386720
N	2.660155	0.179095	3.041168
H	1.983481	0.092571	3.803150
H	4.638986	0.098085	1.514819
C	1.420714	3.254019	0.325783
H	1.504918	3.895047	1.209218
N	0.465816	3.406040	-0.504023
C	-0.501144	4.465690	-0.236467
H	-0.674547	5.006305	-1.172452
H	-0.094878	5.182062	0.492382
C	-1.816660	3.926730	0.284240
C	-4.254936	3.057789	1.354158
C	-1.847832	3.245927	1.505969
C	-3.010303	4.146531	-0.404487
C	-4.225563	3.711078	0.124374
C	-3.063097	2.825840	2.041901
H	-0.915432	3.041441	2.031598
H	-2.990389	4.671899	-1.356075
H	-5.147648	3.891747	-0.419989
H	-3.079884	2.314557	3.000808
H	-5.200490	2.729632	1.775671
H	0.249132	0.455619	0.029933
H	0.674058	0.681107	-3.528797
C	1.375957	0.008847	-3.048038
C	1.189248	-0.353715	-1.735992
N	3.394931	-1.288588	-3.260544
C	2.180854	-1.182223	-1.130750
C	2.486524	-0.487313	-3.768026
C	3.264706	-1.619943	-1.946148
C	2.190589	-1.498339	0.245940
H	2.612270	-0.206530	-4.812593
H	5.088163	-2.760467	-1.999237
C	3.271983	-2.130121	0.824602
H	1.410354	-1.124556	0.892407
C	4.301266	-2.652293	-0.006988
H	5.117983	-3.190528	0.464430
C	4.288788	-2.409226	-1.353736
O	3.429519	-2.199468	2.161017
H	3.130229	-1.285183	2.549521
C	-1.596186	-1.400589	2.223975
C	-0.519771	-3.341661	3.932694
C	-0.269580	-1.320235	2.645825
C	-2.403732	-2.428417	2.729364
C	-1.866060	-3.395255	3.571759
C	0.276253	-2.294898	3.479494
H	0.319893	-0.454995	2.356037
H	-3.460723	-2.473244	2.485469
H	-2.502339	-4.187707	3.952696
H	1.322652	-2.234479	3.761431
H	-0.101470	-4.103381	4.583202

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H	4.469697	-0.357050	-2.422223
C	3.423976	-0.150510	-2.176789
C	1.569269	1.496926	-2.306657
C	1.102899	1.016893	-0.907459
C	3.076740	1.306288	-2.492217
C	3.200947	-0.396895	-0.679561
H	1.051529	0.913658	-3.069300
H	0.612998	1.827278	-0.356580
H	4.137702	-0.375432	-0.116101
H	2.788052	-0.821051	-2.756488
H	1.283053	2.541977	-2.454335
H	3.358059	1.555977	-3.518667
H	2.681960	-1.332615	-0.479596
N	2.364743	0.724015	-0.078601
C	3.842947	2.200863	-1.504916
H	4.888375	1.871025	-1.481324
C	3.214657	1.977593	-0.114936
H	3.985774	1.853920	0.647355
H	2.563383	2.804685	0.175744
C	3.820087	3.660469	-1.863648
H	2.838663	4.133960	-1.912197
C	4.910036	4.378007	-2.118654
H	4.849621	5.427904	-2.386807
H	5.903071	3.937455	-2.068850
C	0.094766	-0.154983	-1.008338
O	0.704811	-1.221935	-1.676595
C	2.086984	0.342953	1.367254

H	3.062360	0.032616	1.753588
H	1.453106	-0.546882	1.331841
C	-4.223176	-0.800114	0.703715
C	-3.166594	-2.458449	-1.245610
C	-4.864655	-0.915794	-0.524867
C	-3.042220	-1.491661	0.976166
C	-2.537375	-2.370895	0.001492
C	-4.318293	-1.727228	-1.516807
H	-5.772039	-0.351344	-0.718266
H	-4.790357	-1.799402	-2.492011
H	-2.747026	-3.122296	-1.996269
C	-2.287495	-1.174518	2.251029
O	-2.700480	-0.188439	2.957316
H	0.212484	-2.054194	-1.414062
N	-1.240354	-1.922024	2.491243
H	-0.838101	-1.597913	3.376432
H	-4.602614	-0.124942	1.464235
C	-1.413941	-3.309861	0.243334
H	-1.521164	-4.002556	1.083034
N	-0.430201	-3.399431	-0.561566
C	0.541943	-4.462624	-0.329412
C	0.726901	-4.965391	-1.284246
H	0.138090	-5.209268	0.369838
C	1.846125	-3.923924	0.219145
C	4.257808	-3.047251	1.340661
C	1.850497	-3.260060	1.450790
C	3.051982	-4.121029	-0.454478
C	4.254230	-3.682149	0.100983
C	3.052745	-2.835166	2.012042
H	0.903476	-3.075661	1.959247
H	3.052604	-4.630832	-1.414739
H	5.186790	-3.845228	-0.430960
H	3.049587	-2.337142	2.978186
H	5.193565	-2.716661	1.781742
H	-0.225029	-0.465151	0.001186
H	-0.583296	-0.670007	-3.570437
C	-1.293959	-0.002813	-3.095377
C	-1.132628	0.345407	-1.776780
N	-3.298261	1.314197	-3.333647
C	-2.131868	1.169779	-1.181320
C	-2.388670	0.507669	-3.830499
C	-3.191336	1.632544	-2.013566
C	-2.166441	1.466465	0.198803
H	-2.497137	0.237717	-4.879796
H	-4.993027	2.805402	-2.093369
C	-3.242011	2.123250	0.754487
H	-1.415331	1.064306	0.865005
C	-4.244367	2.673988	-0.087737
H	-5.057751	3.226863	0.372095
C	-4.212538	2.435492	-1.435506
O	-3.416494	2.192138	2.092020
H	-3.092849	1.313649	2.467415
C	1.471949	1.392045	2.263241
C	0.285236	3.172133	4.078598
C	0.171929	1.184030	2.724835
C	2.194885	2.482229	2.767765
C	1.599391	3.371911	3.655149
C	-0.424352	2.066455	3.623474
H	-0.369587	0.295829	2.415208
H	3.233160	2.636724	2.493230
H	2.171008	4.214867	4.030622
H	-1.434370	1.862672	3.961764
H	-0.170231	3.866354	4.777948

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H	3.672965	4.001263	-1.061745
C	2.742063	3.526344	-1.386822
C	0.352990	3.170481	-0.890404
C	0.519241	1.781521	-0.245783
C	1.561595	4.047720	-0.566737
C	2.823473	2.001858	-1.212249
H	0.254983	3.067752	-1.976843
H	0.075212	1.787993	0.754996
H	3.847726	1.671976	-1.032585
H	2.602660	3.757426	-2.446045
H	-0.577054	3.607154	-0.518222
H	1.353992	5.094210	-0.805121
H	2.413965	1.445506	-2.053825
N	2.018441	1.563037	0.005097
C	1.911800	3.904001	0.926874
H	2.748173	4.582454	1.136804
C	2.416571	2.468069	1.151751
C	3.508200	2.425820	1.198377
H	2.025058	2.031141	2.067574
C	0.755493	4.334613	1.799108
H	0.449998	5.366431	1.621827
C	0.089780	3.628578	2.709882
H	-0.732500	4.076394	3.258141
H	0.317085	2.594767	2.960388
C	-0.178757	0.659292	-1.047199
O	0.547912	0.354016	-2.212301
C	2.389764	0.109263	0.301425
H	3.458948	0.044776	0.094181
H	1.877799	-0.491458	-0.448198
C	-3.780392	-2.173063	0.045828
C	-2.231962	-1.955368	-2.241475
C	-4.344629	-1.682693	-1.128024
C	-2.445731	-2.578695	0.096325
C	-1.666451	-2.484794	-1.073264
C	-3.563150	-1.558015	-2.274344
H	-5.387186	-1.378805	-1.141423
H	-3.986017	-1.151828	-3.188311
H	-1.614780	-1.883135	-3.132961
C	-1.871780	-3.095764	1.404746
O	-1.056330	-4.044295	1.365547
H	0.526337	-0.633155	-2.307836
N	-2.318775	-2.475726	2.490990
H	-1.926618	-2.942751	3.309302
H	-4.368002	-2.225221	0.957510
C	-0.285425	-3.013513	-1.161019
H	-0.098347	-3.955501	-0.641145
N	0.618895	-2.444728	-1.863601
C	1.851578	-3.211880	-2.066217
H	1.871394	-3.490795	-3.126884
H	1.833907	-4.140961	-1.481356
C	3.106601	-2.433467	-1.746136
C	5.477406	-1.047604	-1.184875
C	3.846630	-2.729822	-0.599774
C	3.554210	-1.421039	-2.600067
C	4.732601	-0.732442	-2.323108
C	5.029115	-2.044612	-0.320342
H	3.498778	-3.508316	0.074477
H	2.982309	-1.181584	-3.493868
H	5.077291	0.043255	-3.000938
H	5.599381	-2.293219	0.569523

H	6.403104	-0.519825	-0.976304
H	-0.247619	-0.236282	-0.418645
H	-1.133351	1.540762	-3.403172
C	-1.889794	1.571257	-2.626600
C	-1.592109	1.126583	-1.363142
N	-4.158028	2.102678	-2.027199
C	-2.622950	1.124417	-0.376702
C	-3.187591	2.051552	-2.910750
C	-3.894594	1.633113	-0.775834
C	-2.476701	0.574018	0.920419
H	-3.418312	2.411419	-3.912231
H	-5.912846	2.037488	-0.152391
C	-3.564825	0.447177	1.767928
H	-1.538696	0.128806	1.237817
C	-4.806122	1.042570	1.392529
H	-5.631862	0.973107	2.094470
C	-4.961751	1.618583	0.162991
O	-3.516567	-0.254646	2.900814
H	-2.970729	-1.169514	2.720514
C	2.134426	-0.360438	1.707380
C	1.747221	-1.187911	4.354263
C	0.926951	-0.943030	2.095991
C	3.162001	-0.240320	2.651785
C	2.972437	-0.647133	3.967190
C	0.730614	-1.341727	3.416566
H	0.135083	-1.123671	1.372609
H	4.119327	0.177361	2.347174
H	3.778290	-0.545035	4.686926
H	-0.221992	-1.777204	3.693915
H	1.591011	-1.502514	5.381341

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H	4.682342	2.623391	-0.971137
C	3.741473	2.207458	-1.344507
C	1.297058	2.524439	-1.523475
C	0.925646	1.512857	-0.420676
C	2.610483	3.225293	-1.185855
C	3.373717	0.929048	-0.574429
H	1.402137	1.999212	-2.478276
H	0.263117	1.977249	0.318379
H	4.196194	0.586148	0.054698
H	3.883436	1.960599	-2.400038
H	0.470559	3.237049	-1.625950
H	2.768251	4.081996	-1.846843
H	3.057560	0.112102	-1.220185
N	2.207922	1.196780	0.370249
C	2.570083	3.690206	0.281266
H	3.503209	4.230131	0.485086
C	2.558647	2.433974	1.168368
C	3.543813	2.238145	1.600124
H	1.839906	2.513166	1.979896
C	1.431309	4.655017	0.513182
H	1.483288	5.539946	-0.121983
C	0.410854	4.547890	1.360518
H	-0.343322	5.326173	1.413984
H	0.270046	3.708253	2.037311
C	0.197894	0.281591	-1.000769
O	1.083523	-0.460240	-1.798356
C	2.097220	-0.016853	1.291134
H	3.126762	-0.222312	1.595170
H	1.774552	-0.844247	0.654349
C	-3.985065	-1.840036	-0.169012
C	-1.891104	-2.414260	-1.880631
C	-4.151270	-1.678011	-1.539672
C	-2.785900	-2.304474	0.377597
C	-1.721849	-2.604300	-0.500579
C	-3.093982	-1.958375	-2.402929
H	-5.096339	-1.313318	-1.931306
H	-3.203756	-1.816737	-3.473981
H	-1.059453	-2.643503	-2.541283
C	-2.710000	-2.374254	1.895792
O	-3.413415	-1.506577	2.534840
H	0.906476	-1.420631	-1.615044
N	-1.968956	-3.307535	2.415310
H	-2.040650	-3.207103	3.432930
H	-4.782093	-1.570255	0.517134
C	-0.423330	-3.144080	-0.033268
H	-0.449864	-3.740168	0.881629
N	0.659383	-2.938305	-0.682539
C	1.855358	-3.639195	-0.207599
H	1.853964	-4.634476	-0.671989
H	1.820877	-3.791664	0.879397
C	3.132760	-2.930541	-0.599800
C	5.540093	-1.703370	-1.351495
C	4.117822	-2.657154	0.350259
C	3.366197	-2.581550	-1.933922
C	4.558657	-1.968218	-2.307621
C	5.318161	-2.050992	-0.021190
H	3.945512	-2.926112	1.390192
H	2.605682	-2.792399	-2.682272
H	4.726778	-1.703124	-3.347149
H	6.077243	-1.852405	0.729689
H	6.472916	-1.231265	-1.644669
H	-0.171000	-0.340485	-0.178156
H	-0.004950	0.515100	-3.675018
C	-0.909975	0.839362	-3.173483
C	-1.003062	0.765196	-1.806108
N	-3.140413	1.714298	-3.398059
C	-2.236394	1.131037	-1.189805
C	-2.004395	1.322261	-3.926090
C	-3.271911	1.609957	-2.045610
C	-2.509178	0.969414	0.190290
H	-1.920003	1.388935	-5.009573
H	-5.284007	2.360666	-2.144076
C	-3.769993	1.213664	0.695531
H	-1.764835	0.561278	0.865942
C	-4.768587	1.778465	-0.144252
H	-5.738134	1.997188	0.292634
C	-4.522332	1.970879	-1.475806
O	-4.111798	0.897006	1.958421
H	-3.739888	-0.027859	2.171423
C	1.237009	0.141795	2.518763
C	-0.298055	0.397577	4.848383
C	-0.059427	-0.370541	2.576610
C	1.776942	0.732201	3.670326
C	1.014083	0.869704	4.823258
C	-0.832169	-0.235546	3.730559
H	-0.469658	-0.924142	1.734903
H	2.807779	1.077784	3.665938
H	1.447249	1.333692	5.703636
H	-1.843607	-0.634656	3.732515
H	-0.895543	0.505296	5.748489

Ia8E

H	-5.206287	1.805466	-2.155922
C	-4.576593	1.129029	-1.571291
C	-4.039214	0.278768	0.708135
C	-2.559812	0.232349	0.258811
C	-4.810712	1.346750	-0.074305
C	-3.101689	1.417124	-1.886375
H	-4.490422	-0.697669	0.517418
H	-1.888098	0.364245	1.112935
H	-2.643940	0.655812	-2.518385
H	-4.814446	0.099862	-1.841882
H	-4.099894	0.464174	1.783970
H	-5.876521	1.286046	0.160802
H	-2.961880	2.396595	-2.350972
N	-2.284879	1.471775	-0.609417
C	-4.274380	2.744925	0.282231
H	-4.657532	3.456132	-0.458924
C	-2.737767	2.687042	0.174257
H	-2.332703	3.565271	-0.332283
H	-2.263385	2.614395	1.156083
C	-4.685942	3.224705	1.646254
H	-4.360439	2.620561	2.494023
C	-5.410149	4.319251	1.859933
H	-5.697445	4.623919	2.861139
H	-5.742673	4.948371	1.037608
C	-2.213381	-1.119917	-0.426491
O	-3.162781	-1.498668	-1.374504
C	-0.809799	1.615585	-0.994831
H	-0.808042	2.068395	-1.987980
H	-0.406344	0.612400	-1.127367
C	-0.162457	-3.261507	-2.281981
C	2.246472	-2.644806	-1.061540
C	0.479894	-4.214696	-1.498952
C	0.382420	-1.987025	-2.472111
C	1.602197	-1.677440	-1.842217
C	1.694567	-3.908413	-0.889600
H	0.032111	-5.194677	-1.363925
H	2.203680	-4.644353	-0.274863
H	3.179666	-2.382391	-0.570454
C	-0.371591	-0.953876	-3.299719
O	0.246421	0.080454	-3.651984
H	-2.661477	-1.531492	-2.265240
N	-1.642554	-1.254765	-3.547408
H	-2.004431	-0.515089	-4.154709
H	-1.113267	-3.483694	-2.754683
C	2.237932	-0.335361	-1.901683
H	2.399677	0.123844	-2.876793
N	2.607040	0.233960	-0.820883
H	-1.238101	-1.037974	-0.911978
H	-3.997457	-3.029605	0.344786
C	-3.098997	-3.032788	0.952420
C	-2.078140	-2.161262	0.673609
N	-1.909343	-4.011889	2.808777
C	-0.888304	-2.244671	1.456634
C	-2.965982	-3.939882	2.032489
C	-0.865425	-3.180875	2.526660
C	0.260806	-1.461895	1.200434
H	-3.783534	-4.622331	2.258234
H	0.297894	-3.974042	4.154412
C	1.393333	-1.582934	1.977500
H	0.299149	-0.795994	0.346401
C	1.399027	-2.485616	3.075595
H	2.298905	-2.554624	3.678588
C	0.302346	-3.263196	3.333842
O	2.519292	-0.884926	1.739276
H	2.484966	-0.458866	0.834556
C	0.044740	2.441102	-0.063950
C	1.724416	4.019807	1.534770
C	0.492923	1.970986	1.175668
C	0.450388	3.709881	-0.489036
C	1.285321	4.496039	0.302016
C	1.323238	2.757362	1.970214
H	0.208081	0.985989	1.532029
H	0.119218	4.080365	-1.456097
H	1.596437	5.474561	-0.049005
H	1.664679	2.375322	2.927402
H	2.379171	4.626316	2.152322
C	3.338016	1.496934	-0.925892
C	4.715166	1.331809	-0.323987
H	3.409984	1.828278	-1.970753
H	2.781772	2.253055	-0.362149
C	5.835600	1.154003	-1.135349
C	7.095864	0.967714	-0.569564
C	7.242026	0.949641	0.815438
C	6.125057	1.119344	1.632691
C	4.869231	1.311833	1.064383
H	5.720390	1.164273	-2.216652
H	7.962244	0.836326	-1.210923
H	8.222843	0.804205	1.257780
H	6.234157	1.104810	2.712923
H	3.994090	1.440435	1.698071

Ib6E-R

H	-5.194339	-1.731304	2.170092
C	-4.563739	-1.066528	1.573141
C	-4.037815	-0.252569	-0.725533
C	-2.554128	-0.216200	-0.289227
C	-4.815302	-1.298685	0.081096
C	-3.087476	-1.363108	1.881084
H	-4.476938	0.731529	-0.548509
H	-1.890655	-0.364604	-1.147116
H	-2.621876	-0.599845	2.511251
H	-4.793228	-0.033410	1.835200
H	-4.109882	-0.456125	-1.797313
H	-5.882490	-1.225943	-0.144376
H	-2.956471	-2.341015	2.352053
N	-2.287636	-1.447339	0.591633
C	-4.302055	-2.708377	-0.262732
H	-4.685884	-3.404914	0.491855
C	-2.764505	-2.667007	-0.171321
H	-2.364706	-3.543504	0.342686
H	-2.299131	-2.612617	-1.158798
C	-4.734273	-3.201433	-1.615609
H	-4.413208	-2.611758	-2.475232
C	-5.471293	-4.291770	-1.805999
H	-5.773690	-4.607275	-2.799366
H	-5.799598	-4.906497	-0.971184
C	-2.190821	1.139836	0.380052
O	-3.146782	1.543710	1.315119
C	-0.811814	-1.612913	0.953311
H	-0.805053	-2.093546	1.933382
H	-0.398737	-0.616879	1.107639
C	-0.191253	3.184489	2.376437
C	2.237841	2.615506	1.180071
C	0.461687	4.167122	1.639189
C	0.356841	1.909444	2.545165

C	1.587886	1.622294	1.922017
C	1.686761	3.884439	1.041317
H	0.011433	5.148791	1.526713
H	2.202726	4.639979	0.456914
H	3.176236	2.369714	0.690088
C	-0.464380	0.889825	3.320116
O	-1.716962	1.150837	3.458215
H	-2.671588	1.523527	2.200205
N	0.170214	-0.158132	3.759496
H	-0.520373	-0.734069	4.252948
H	-1.157834	3.381552	2.828471
C	2.226552	0.280001	1.941195
H	2.364792	-0.214450	2.902988
N	2.608783	-0.251700	0.845969
H	-1.222382	1.054265	0.878084
H	-3.974695	3.027816	-0.444849
C	-3.064145	3.030675	-1.034030
C	-2.040991	2.171262	-0.726331
N	-1.846003	4.004265	-2.873929
C	-0.835533	2.259964	-1.483962
C	-2.918188	3.928530	-2.119751
C	-0.799779	3.187399	-2.561683
C	0.316339	1.492009	-1.195977
H	-3.738010	4.599848	-2.369078
H	0.390332	3.980566	-4.169936
C	1.463370	1.618082	-1.950934
H	0.344026	0.831390	-0.337175
C	1.483327	2.512857	-3.055595
H	2.395040	2.586521	-3.639935
C	0.384538	3.276469	-3.343639
O	2.589563	0.931135	-1.686856
H	2.530652	0.488813	-0.791550
C	0.029427	-2.425262	-0.001600
C	1.700868	-3.981751	-1.630942
C	0.484239	-1.931502	-1.229452
C	0.424500	-3.706568	0.395758
C	1.254862	-4.481856	-0.410213
C	1.310316	-2.706983	-2.039255
H	0.210250	-0.935612	-1.562856
H	0.090155	-4.095211	1.354520
H	1.557393	-5.470269	-0.080026
H	1.657425	-2.306821	-2.986985
H	2.352820	-4.579443	-2.259963
C	3.326789	-1.524809	0.915733
C	4.709873	-1.355979	0.328845
H	3.386735	-1.890359	1.949819
H	2.766486	-2.255758	0.323139
C	5.821468	-1.180071	1.152926
C	7.087255	-0.989444	0.601383
C	7.248025	-0.965304	-0.782066
C	6.140166	-1.133109	-1.611781
C	4.878643	-1.329939	-1.057544
H	5.694743	-1.195387	2.232923
H	7.946568	-0.859812	1.252490
H	8.233240	-0.816835	-1.213497
H	6.260671	-1.113862	-2.690719
H	4.010375	-1.456501	-1.700970

Table

H	2.173687	3.823644	-2.146718
C	1.896643	3.095363	-1.379574
C	2.252168	2.338631	0.960890
C	2.117056	0.880986	0.455559
C	2.787805	3.250331	-0.146096
C	2.069144	1.676525	-1.942364
H	1.266265	2.691024	1.274273
H	2.736836	0.201370	1.042029
H	2.718967	1.657841	-2.821798
H	0.851748	3.256172	-1.106603
H	2.907574	2.376268	1.835921
H	2.795823	4.288233	0.196568
H	1.113624	1.215231	-2.198186
N	2.763872	0.791674	-0.924598
C	4.214216	2.818631	-0.536349
H	4.474449	3.319816	-1.476039
C	4.184346	1.294130	-0.774042
H	4.715522	1.018576	-1.687373
H	4.624915	0.741809	0.059713
C	5.256543	3.172976	0.487286
H	5.145315	2.719633	1.473049
C	6.277188	3.992540	0.253561
H	7.001244	4.232028	1.025778
H	6.422356	4.454073	-0.720289
C	0.653156	0.379130	0.525755
O	-0.236659	1.319101	-0.021679
C	2.790447	-0.630844	-1.460127
H	3.246936	-0.554565	-2.450433
H	1.753776	-0.922924	-1.614540
C	2.850353	-2.364252	0.377679
C	3.529384	-3.301059	1.151706
C	3.526939	-1.625532	-0.599988
H	5.419113	-4.251663	1.549807
C	4.888722	-1.866857	-0.808079
C	5.568728	-2.803522	-0.035615
C	4.890388	-3.518218	0.949348
C	-2.786587	-3.154340	-1.227672
C	-0.077470	-3.058800	-1.863876
C	-1.943873	-4.187606	-0.828720
C	-2.272454	-2.057252	-1.922742
C	-0.906503	-2.000795	-2.237381
C	-0.588255	-4.141081	-1.149965
H	-2.346496	-5.032394	-0.278785
H	0.071276	-4.949098	-0.847435
H	0.974102	-3.024383	-2.136713
C	-3.160986	-0.952638	-2.344989
H	-0.514893	0.968057	-0.914505
H	-3.847960	-3.189301	-1.000644
C	-0.343918	-0.760848	-2.890822
H	0.553218	-0.566688	-0.030099
H	2.172934	0.595820	2.873186
C	1.167230	0.224566	3.019787
C	0.278049	0.071630	1.979963
N	-0.382419	-0.549647	4.678371
C	-1.033806	-0.421206	2.301756
C	0.797217	-0.092444	4.345694
C	-1.290325	-0.716873	3.676678
C	-2.066209	-0.643617	1.348443
H	1.521550	0.043572	5.146400
H	-2.721359	-1.437482	5.107229
C	-3.299040	-1.127591	1.754873
H	-1.899964	-0.411186	0.300896
C	-3.537100	-1.423523	3.126414
H	-4.516975	-1.802638	3.398874
C	-2.561575	-1.222675	4.055453
H	5.418723	-1.328569	-1.589858

H	6.624835	-2.981495	-0.210229
H	2.991641	-3.864963	1.906910
H	1.782490	-2.224103	0.530502
O	-4.342426	-1.355562	0.944422
O	-4.186566	-1.055672	-0.001463
N	-4.140138	-0.585659	-1.621985
H	-2.941476	-0.455240	-3.294645
C	-4.943440	0.549877	-2.051010
H	-5.997826	0.255500	-2.038108
H	-4.686867	0.843844	-3.079765
C	-4.726743	1.710353	-1.099473
C	-4.282625	3.843912	0.655314
C	-3.428247	2.045822	-0.708203
C	-5.799906	2.451657	-0.606766
C	-5.579147	3.519221	0.262088
C	-3.206367	3.102264	0.169718
H	-2.589251	1.471589	-1.093659
H	-6.814031	2.190389	-0.899201
H	-6.422457	4.089300	0.640589
H	-2.190200	3.333194	0.475669
H	-4.112817	4.666986	1.342974
O	-0.784266	0.361161	-2.419910
N	0.533778	-0.950110	-3.827291
H	0.824522	-0.024847	-4.162090

Ib11E-S

H	-2.376740	-3.721166	-2.306196
C	-2.073912	-3.027638	-1.517151
C	-2.363378	-2.363563	0.859431
C	-2.174314	-0.895267	0.405029
C	-2.947678	-3.209930	-0.274503
C	-2.230805	-1.587125	-2.021017
H	-1.389333	-2.764756	1.149937
H	-2.747562	-0.212562	1.032711
H	-2.902352	-1.513862	-2.880410
H	-1.028011	-3.217317	-1.266488
H	-3.014696	-2.407735	1.737278
H	-2.982928	-4.261066	0.022931
H	-1.286301	-1.121787	-2.288119
N	-2.858991	-0.723357	-0.949303
C	-4.366321	-2.714410	-0.615612
H	-4.659127	-3.155052	-1.575844
C	-4.291385	-1.180850	-0.772165
H	-4.844806	-0.840655	-1.649864
H	-4.680348	-0.659831	0.106476
C	-5.403433	-3.089767	0.405617
H	-5.262956	-2.692809	1.411634
C	-6.454153	-3.862143	0.145824
H	-7.174025	-4.119468	0.916230
H	-6.628486	-4.266968	-0.848273
C	-0.687323	-0.454050	0.468058
O	0.173821	-1.427722	-0.064310
C	-2.840277	0.718459	-1.433372
H	-3.391462	0.708850	-2.377364
H	-1.803753	0.943367	-1.677556
C	-2.583014	2.427649	0.404728
C	-3.111579	3.366219	1.286849
C	-3.418449	1.722058	-0.468440
H	-4.893981	4.349343	1.985994
C	-4.789195	2.000533	-0.464907
C	-5.319191	2.938209	0.416908
C	-4.481587	3.617270	1.299023
C	2.709472	3.107957	-1.385422
C	0.030524	2.910972	-2.099720
C	1.632739	4.142972	-1.076491
C	2.245783	1.955884	-2.028252
C	0.887237	1.841232	-2.362924
C	0.491180	4.049264	-1.443991
H	2.199710	5.029474	-0.568849
H	-0.193907	4.862665	-1.223711
H	-1.005811	2.837590	-2.418057
C	3.199545	0.879381	-2.382010
H	0.535089	-1.079033	-0.940382
H	3.762902	3.185306	-1.133535
C	0.326330	0.573163	-2.974167
H	-0.553619	0.482695	-0.095556
H	-2.186436	-0.762577	2.823366
C	-1.194565	-0.356975	2.970427
C	-0.317275	-0.152103	1.928589
N	0.325380	0.454448	4.638118
C	0.977713	0.378086	2.258773
C	-0.834382	-0.047417	4.300467
C	1.223537	0.668933	3.637144
C	2.004071	0.641936	1.310049
H	-1.551340	-0.224183	5.099968
H	2.622963	1.433672	5.075533
C	3.219126	1.166719	1.722287
H	1.849095	0.410523	0.259946
C	3.441464	1.465817	3.096030
H	4.406079	1.879828	3.372268
C	2.473354	1.221369	4.021749
H	-5.446313	1.491382	-1.165369
H	-6.384643	3.143994	0.407744
H	-2.450275	3.904586	1.958068
H	-1.508265	2.263210	0.386652
O	4.256291	1.434050	0.918423
H	4.132282	1.094063	-0.023048
N	4.147161	0.564728	-1.595073
H	3.064964	0.374823	-3.341025
C	5.026758	-0.537577	-1.952632
H	6.062471	-0.182756	-1.925522
H	4.817562	-0.889758	-2.973909
C	4.850559	-1.665659	-0.954555
C	4.488282	-3.735421	0.893798
C	3.564773	-2.033640	-0.548641
C	5.951019	-2.342588	-0.430003
C	5.771613	-3.378582	0.485355
C	3.384959	-3.058274	0.376006
H	2.702822	-1.510591	-0.958002
H	6.954643	-2.054501	-0.733547
H	6.636171	-3.896967	0.889391
H	2.378713	-3.316834	0.692953
H	4.349768	-4.532354	1.618211
O	-0.631845	0.676478	-3.772787
N	0.907321	-0.544218	-2.530722
H	0.533077	-1.321062	-3.085420

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H	-3.527956	-0.491685	3.548787
C	-2.604337	-0.057528	3.153142
C	-1.575313	1.980288	2.168765
C	-1.648846	1.482886	0.714412
C	-2.770799	1.452239	2.960605
C	-2.235584	-0.695365	1.803821

H	-0.638047	1.632765	2.610221
H	-2.194991	2.186833	0.081968
H	-2.795058	-1.612970	1.612621
H	-1.806290	-0.263978	3.870930
H	-1.564077	3.072765	2.173635
H	-2.843931	1.958021	3.927212
H	-1.167841	-0.913325	1.715651
N	-2.580709	0.259226	0.682123
C	-4.049165	1.700756	2.136202
H	-4.906128	1.383117	2.743142
C	-3.987033	0.775433	0.910444
H	-4.611462	-0.108488	1.046306
H	-4.300794	1.266674	-0.011567
C	-4.226761	3.172672	1.849969
H	-4.265815	3.780441	2.754648
C	-4.330653	3.788441	0.674397
H	-4.455850	4.865283	0.625761
H	-4.311479	3.270584	-0.281248
C	-0.234767	1.290875	0.098255
O	0.684437	0.758963	1.014118
C	-2.500088	-0.443867	-0.667155
H	-1.578832	-1.029490	-0.643628
H	-2.397978	0.353371	-1.408859
C	-0.338447	-2.950066	-2.172696
C	2.260878	-2.213471	-2.814816
C	0.039027	-2.830026	-3.506625
C	0.565539	-2.678910	-1.142825
C	1.883962	-2.315530	-1.470185
C	1.342489	-2.455689	-3.829511
H	-0.681833	-3.030696	-4.293531
H	1.646637	-2.367891	-4.867756
H	3.287547	-1.957901	-3.058174
C	0.103548	-2.716298	0.297730
O	0.624276	-1.840546	1.084575
H	0.710278	-0.241320	0.937212
N	-0.789431	-3.613920	0.597317
H	-0.995617	-3.497315	1.595333
H	-1.349063	-3.248794	-1.909237
C	2.892890	-2.095588	-0.408594
C	2.736153	-2.592025	0.549151
N	3.900009	-1.344684	-0.615372
C	4.905000	-1.147753	0.435472
H	5.325715	-0.149642	0.265627
H	5.719190	-1.862044	0.263890
C	4.392105	-1.255828	1.852945
C	3.395385	-1.421009	4.462064
C	3.359332	-0.410299	2.270713
C	4.915913	-2.185351	2.750030
C	4.424268	-2.264620	4.053504
C	2.860445	-0.495107	3.564950
H	2.929275	0.302409	1.570062
H	5.712769	-2.851842	2.428841
H	4.841136	-2.990605	4.745045
H	2.048862	0.158704	3.871094
H	3.006443	-1.487960	5.473705
H	-0.301551	0.639858	-0.785444
H	-1.291561	3.917641	0.281716
C	-0.346878	3.832608	-0.243145
C	0.302292	2.632299	-0.413418
N	1.312976	5.081760	-1.453646
C	1.539346	2.651009	-1.143000
C	0.199038	5.027778	-0.768579
C	1.977885	3.909074	-1.652895
C	2.315838	1.493131	-1.413442
H	-0.328969	5.966226	-0.609638
H	3.473542	4.938600	-2.803466
C	3.475199	1.584597	-2.163627
H	2.010809	0.530129	-1.018315
C	3.895182	2.841644	-2.680094
H	4.808290	2.871155	-3.265969
C	3.168004	3.967607	-2.426673
O	4.263665	0.536216	-2.455281
H	4.054634	-0.241506	-1.846055
C	-3.682475	-1.314372	-1.012311
C	-5.872458	-2.907805	-1.712155
C	-4.727551	-0.787475	-1.778778
C	-3.726581	-2.658161	-0.626786
C	-4.822884	-3.446822	-0.972751
C	-5.819688	-1.576923	-2.123478
H	-4.680978	0.244114	-2.120504
H	-2.880591	-3.097974	-0.097133
H	-4.847241	-4.489898	-0.673217
H	-6.623137	-1.155981	-2.719469
H	-6.722691	-3.525950	-1.982908

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H	-3.830135	-0.269130	3.405506
C	-2.857967	0.125319	3.093705
C	-1.677615	2.075798	2.106710
C	-1.674583	1.544983	0.661531
C	-2.951609	1.628891	2.826818
C	-2.372132	-0.562599	1.810632
H	-0.789953	1.695279	2.620213
H	-2.173307	2.239467	-0.017850
H	-2.889955	-1.503174	1.618518
H	-2.143625	-0.080699	3.894726
H	-1.610561	3.165031	2.092376
H	-3.080389	2.183067	3.760281
H	-1.299500	-0.742681	1.813046
N	-2.625050	0.334875	0.618852
C	-4.154925	1.875271	1.895024
H	-5.064579	1.613095	2.449650
C	-4.032825	0.883916	0.724246
H	-4.682674	0.019448	0.865333
H	-4.275772	1.330474	-0.240730
C	-4.263935	3.336181	1.528382
H	-4.329951	3.988689	2.399631
C	-4.288916	3.895635	0.320763
H	-4.376520	4.971899	0.213994
H	-4.238987	3.330178	-0.606264
C	-0.233480	1.319580	0.125277
O	0.597595	0.693725	1.064079
C	-2.457850	-0.440062	-0.680095
H	-1.506908	-0.967847	-0.581423
H	-2.369586	0.315667	-1.466296
C	-0.292543	-2.682731	-2.476095
C	2.315472	-1.820935	-2.925841
C	0.111475	-2.331882	-3.760565
C	0.587090	-2.569252	-1.398620
C	1.910513	-2.157348	-1.627642
C	1.417220	-1.892476	-3.983959
H	-0.586374	-2.406383	-4.589065
H	1.739268	-1.624896	-4.985295
H	3.342598	-1.515761	-3.101303
C	0.082645	-2.878089	-0.003759

O	-0.612657	-3.907334	0.158308
H	0.610835	-0.315646	0.908702
N	0.431527	-1.971170	0.900500
H	0.103620	-2.298884	1.813775
H	-1.301300	-3.041593	-2.287798
C	2.880397	-2.146687	-0.511775
H	2.660024	-2.787599	0.342719
N	3.923240	-1.416854	-0.539157
C	4.856908	-1.453740	0.593835
H	5.439444	-0.527281	0.537830
H	5.562946	-2.278489	0.440718
C	4.196367	-1.566409	1.950494
C	2.943934	-1.735816	4.448228
C	3.199829	-0.651612	2.306450
C	4.553453	-2.567569	2.852459
C	3.934190	-2.650166	4.100221
C	2.575200	-0.737466	3.545169
H	2.890109	0.115545	1.600204
H	5.318703	-3.289534	2.578052
H	4.221363	-3.434195	4.794317
H	1.794155	-0.026724	3.799517
H	2.456706	-1.803617	5.416268
H	-0.274206	0.721301	-0.797500
H	-1.286631	3.947110	0.263463
C	-0.292455	3.870475	-0.159288
C	0.370520	2.671226	-0.291059
N	1.475584	5.153738	-1.157940
C	1.669348	2.709214	-0.907039
C	0.299270	5.080073	-0.590587
C	2.153137	3.984341	-1.331267
C	2.465069	1.559045	-1.159346
H	-0.245304	6.012846	-0.456538
H	3.741232	5.053875	-2.304767
C	3.682157	1.676073	-1.810488
H	2.123393	0.582646	-0.832020
C	4.148473	2.951420	-2.234264
H	5.107617	2.398858	-2.739821
C	3.405985	4.063248	-1.994963
O	4.491402	0.641547	-2.089307
H	4.209762	-0.183184	-1.573573
C	-3.576171	-1.400478	-0.997730
C	-5.633414	-3.183889	-1.640608
C	-4.657405	-0.983935	-1.782271
C	-3.516642	-2.729844	-0.565499
C	-4.546505	-3.613690	-0.883626
C	-5.684270	-1.867830	-2.097446
H	-4.691264	0.034662	-2.161445
H	-2.644959	-3.089901	-0.019330
H	-4.488971	-4.644342	-0.548610
H	-6.517051	-1.532198	-2.706916
H	-6.431602	-3.876102	-1.889403