

Supplementary Information

Title: Effect of “Magic Chloro” in drug discovery: An *in silico* Approach

Submitted by: Sravani Joshi, Ruby Srivastava*

CSIR-Centre for Cellular and Molecular Biology,

Hyderabad.

Formulas Used

The ionization potential (IP) and electron affinity (EA) values were calculated by:

$$\text{IP (I)} = E(\text{N}-1) - E(\text{N})$$

$$\text{EA (A)} = E(\text{N}) - E(\text{N}+1),$$

Where $E(\text{N})$ =energy of complex and $E(\text{N}-1)$ and $E(\text{N}+1)$ are the cationic and anionic energies.

The HOMO-LUMO Gap

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$$

where E_{HOMO} is the energy of the highest occupied molecular orbital and E_{LUMO} is the energy of the lowest unoccupied molecular orbital.

The chemical descriptors are calculated using CDFT.¹

The chemical potential μ_p is defined as:

$$\mu_p = (\partial E / \partial N)_{v(r)} = -\chi$$

where μ_p is the chemical potential, E is the total energy, N is the number of electrons, $v(r)$ is the external potential of the system and χ is the global electronegativity.

The global hardness is given by:

$$\eta = (\partial^2 E / \partial N^2)_{(r)}$$

Using the finite difference approximation and the Koopmans theorem, the global electronegativity (χ) and the global hardness (η) are given by:

$$\chi = (I+A)/2 \approx -(E_{\text{HOMO}}+E_{\text{LUMO}})/2$$

$$\eta = (I-A)/2 \approx (E_{\text{LUMO}}-E_{\text{HOMO}})/2 \text{ respectively.}$$

The global softness which is the reciprocal of the global hardness can be obtained by:

$$S = 1/\eta$$

The electrophilicity index (ω) is defined as:

$$\omega = \mu_p^2/2\eta$$

$$\text{Electrodonating Power as } \omega^- \approx (3\varepsilon_{\text{H}} + \varepsilon_{\text{L}})^2/16\eta \approx -\frac{1}{4}(3I + A)$$

$$\text{Electroaccepting Power as } \omega^+ \approx (\varepsilon_{\text{H}} + 3\varepsilon_{\text{L}})^2/16\eta \approx -\frac{1}{4}(I + 3A)$$

while the Net Electrophilicity is $\Delta\omega_{\pm} = \omega^+ + \omega^-$, being ε_{H} and ε_{L} the frontier orbital energies related to the studied antagonists considered in this research.²

References:

- (1) Ángel Ulises Orozco-Valencia and Alberto Vela, The Electrodonating and Electroaccepting Powers in Atoms, *J. Mex. Chem. Soc.* 2012, 56(3), 294-301.
- (2) Chattaraj PK, Chakraborty A, Giri S. Net electrophilicity. *J Phys Chem A.* 2009 113(37):10068-74.

Complexes	cLopP	MW	TPSA	HBD	HBA	nrotb
	≤5	<500		<5	<10	
Ref 1	2.68	284.74	32.67	0	2	1
Ref 2	0.95	323.13	115.38	3	5	7
Ref 3	3.95	319.87	28.16	1	2	8
Ref 4	2.66	358.26	58.36	1	3	9
1a	3.15	425.43	167.66	5	11	7
1b	3.83	459.88	167.66	5	11	7
2a	1.05	323.35	72.73	1	5	5
2b	1.70	357.79	72.73	1	5	5
3-1a	0.97	284.33	91.28	2	3	3
3-1b	3.84	318.79	65.98	2	4	3
3-2a	3.25	298.37	55.12	1	4	3
3-2b	3.91	332.81	55.12	1	4	3
3-3a	3.52	364.43	72.95	1	6	4
3-3b	4.18	398.88	72.95	1	6	4
3-4a	4.50	363.44	60.06	1	5	4
3-4b	5.16	397.89	60.06	1	5	4
4a	3.79	317.73	97.37	5	6	3
4b	3.79	317.73	97.37	5	6	3
4c	4.44	352.18	97.37	5	6	3
5a	4.00	428.57	52.57	2	3	9
5b	4.69	463.01	52.57	2	3	9
6a	1.52	195.24	43.69	2	3	1
6b	2.10	229.69	43.69	2	3	1
7a	1.89	444.49	117.61	4	6	5
7b	2.35	513.38	117.61	4	6	5
8a	4.33	291.35	42.35	1	3	4
8b	5.87	360.24	42.35	1	3	4
9a	1.28	248.33	41.57	1	4	5
9b	1.96	282.77	41.57	1	4	5
9c	2.56	317.22	41.57	1	4	5
10a	2.16	247.68	49.33	2	2	3
10b	2.16	247.68	49.33	2	2	3
10c	5.25	316.57	49.33	2	3	2
11a	2.55	254.33	34.15	1	3	3
11b	3.18	288.78	34.15	1	3	3
11c	3.18	323.22	34.15	1	3	3
12a	3.41	388.38	122.64	5	7	4
12b	4.07	422.82	122.64	5	7	4
12c	4.75	457.27	122.64	5	7	4

Supplementary Table 1: CLP-clog P, MW-Molecular Weight (g/mol), TPSA-Topological Polar Surface Area (\AA^2), HBD-Number of Hydrogen Bond Donors, HBA-Number of Hydrogen Bond Acceptors, and nrotb- Number of Rotatable Bonds for the reference drugs Ref (1-4) and studied 12 inhibitors. These physicochemical parameters are taken by Molinspiration Chemoinformatics software.

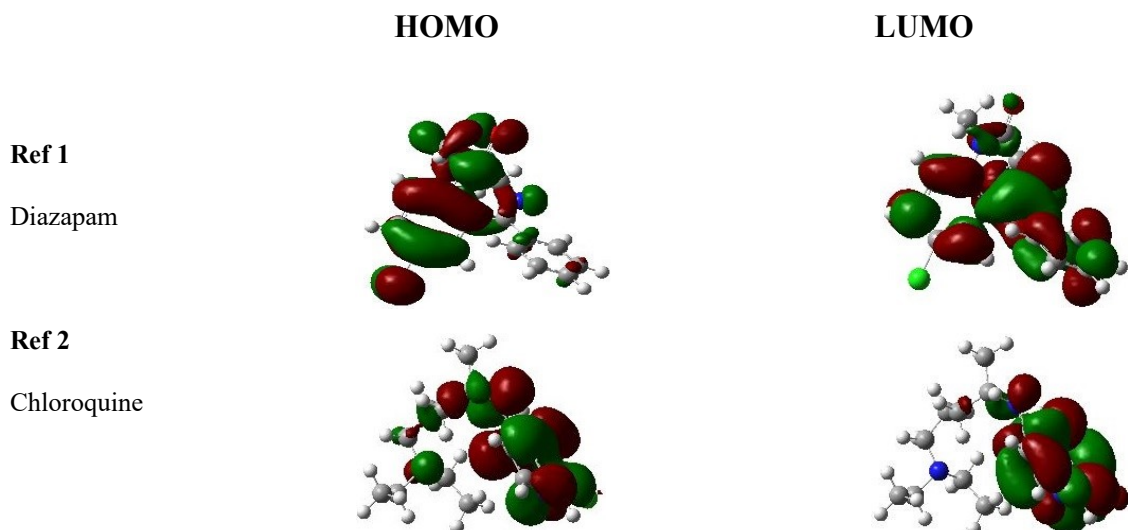
Complexes	DL	DS	S	MUT	TUM	IRR	REP
Ref 1	5.98	0.15	-4.67	✓	✓	✓	✓
Ref 2	-4.61	0.06	-2.37	✓	✓	✓	✓
Ref 3	7.39	0.25	-4.06	✓	✓	✓	✓
Ref 4	-1.23	0.11	-2.73	✓	✓	✓	✓
1a	-1.65	0.23	-4.69	✓	✓	✓	✓
1b	0.16	0.33	-5.43	✓	✓	✓	✓
2a	-4.26	0.36	-4.26	✓	✓	✓	✓
2b	-4.29	0.3	-5.0	✓	✓	✓	✓
3-1a	2.48	0.82	-3.3	✓	✓	✓	✓
3-1b	2.90	0.74	-4.04	✓	✓	✓	✓
3-2a	3.90	0.85	-2.96	✓	✓	✓	✓
3-2b	4.28	0.77	-3.7	✓	✓	✓	✓
3-3a	5.2	0.67	-4.47	✓	✓	✓	✓
3-3b	5.55	0.54	-5.21	✓	✓	✓	✓
3-4a	2.19	0.49	-5.48	✓	✓	✓	✓
3-4b	2.53	0.39	-6.22	✓	✓	✓	✓
4a	4.35	0.74	-3.93	✓	✓	✓	✓
4b	4.35	0.74	-3.93	✓	✓	✓	✓
4c	4.3	0.62	-4.67	✓	✓	✓	✓
5a	3.75	0.42	-5.66	✓	✓	✓	✓
5b	4.89	0.32	-6.4	✓	✓	✓	✓
6a	0.84	0.38	-4.85	✓	✓	✓	✓
6b	1.29	0.52	-5.14	✓	✓	✓	✓
7a	6.79	0.54	-4.57	✓	✓	✓	✓
7b	9.02	0.15	-6.04	✓	✓	✓	✓
8a	-2.72	0.35	-4.5	✓	✓	✓	✓
8b	-1.35	0.05	-5.98	✓	✓	✓	✓
9a	3.32	0.94	-1.38	✓	✓	✓	✓
9b	5.18	0.92	-2.12	✓	✓	✓	✓
9c	3.57	0.86	-2.85	✓	✓	✓	✓
10a	1.18	0.73	-3.57	✓	✓	✓	✓
10b	1.18	0.73	-3.57	✓	✓	✓	✓
10c	1.64	0.54	-5.04	✓	✓	✓	✓
11a	0.45	0.6	-4.39	✓	✓	✓	✓
11b	0.92	0.43	-5.12	✓	✓	✓	✓
11c	1.09	0.16	-5.86	✓	✓	✓	✓
12a	5.0	0.64	-4.89	✓	✓	✓	✓
12b	5.35	0.54	-5.52	✓	✓	✓	✓
12c	7.27	0.41	-6.36	✓	✓	✓	✓

Supplementary Table 2: Estimated physicochemical parameters as Druglikeness (DL), Drug Score (DS), Solubility (S) and Toxicity effects (Mutagenicity (MUT), Tumorigenicity (TUM), Irritant Effect (IRR), and Reproductive effect (REP)) for the reference drugs Ref (1-4) and studied 12 inhibitors. Osiris property explorer is used to estimate these properties. The color of tick indicates safe usage (green); mild toxicity (yellow) and high toxicity (red).

Complexes	arrhythmia	Cardiac failure	Heart block	herG Toxicity	hypertension	Myocardial Infarction
Ref 1	toxic	safe	toxic	safe	safe	toxic
Ref 2	safe	toxic	safe	safe	safe	safe
Ref 3	toxic	toxic	toxic	toxic	toxic	toxic
Ref 4	toxic	safe	safe	toxic	toxic	toxic
1a	safe	safe	safe	safe	safe	safe
1b	safe	safe	safe	safe	safe	safe
2a	safe	safe	safe	safe	toxic	safe
2b	safe	safe	safe	safe	toxic	safe
3-1a	safe	safe	safe	safe	safe	safe
3-1b	safe	safe	safe	safe	toxic	safe
3-2a	safe	safe	safe	safe	toxic	safe
3-2b	safe	safe	safe	safe	toxic	safe
3-3a	safe	safe	safe	safe	safe	safe
3-3b	safe	safe	safe	safe	safe	safe
3-4a	safe	safe	safe	safe	safe	safe
3-4b	safe	safe	safe	toxic	safe	safe
4a	safe	safe	safe	toxic	safe	safe
4b	safe	safe	safe	toxic	safe	safe
4c	safe	safe	safe	safe	toxic	safe
5a	safe	safe	safe	toxic	safe	safe
5b	safe	safe	safe	safe	toxic	toxic
6a	toxic	safe	safe	safe	safe	toxic
6b	toxic	safe	toxic	safe	safe	safe
7a	toxic	safe	toxic	safe	safe	safe
7b	toxic	safe	toxic	safe	safe	safe

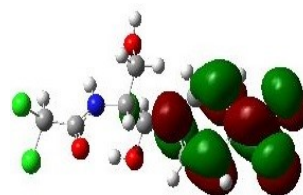
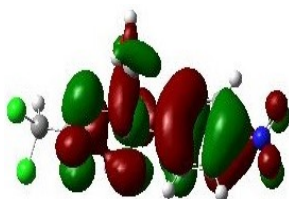
8a	safe	safe	safe	safe	safe	toxic
8b	safe	safe	safe	safe	toxic	safe
9a	toxic	safe	toxic	safe	safe	toxic
9b	toxic	toxic	safe	toxic	toxic	toxic
9c	toxic	safe	toxic	safe	toxic	toxic
10a	safe	safe	safe	safe	safe	safe
10b	safe	safe	safe	safe	safe	safe
10c	safe	safe	safe	safe	safe	safe
11a	safe	safe	safe	safe	safe	toxic
11b	safe	safe	safe	safe	safe	toxic
11c	safe	safe	safe	toxic	safe	toxic
12a	safe	safe	safe	safe	safe	toxic
12b	safe	safe	safe	safe	safe	safe
12c	safe	safe	safe	safe	safe	safe

Supplementary Table 3: *cardioToxCSM* web server is used to evaluate the cardiac toxicity outcomes (Arrhythmia, Cardiac Failure, Heart Block, hERG toxicity, Hypertension, and Myocardial Infarction) for the reference drugs Ref (1-4) and studied 12 inhibitors.



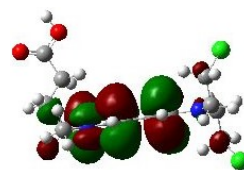
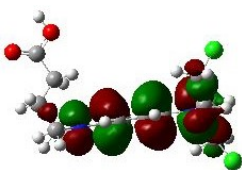
Ref 3

Chlororamphinicol

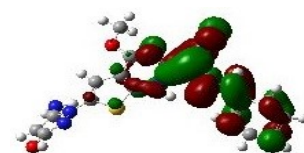
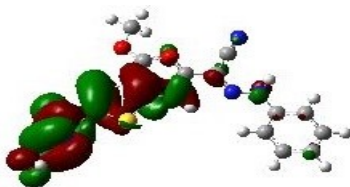


Ref 4

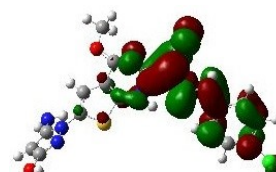
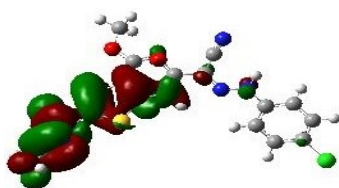
Bendamustine



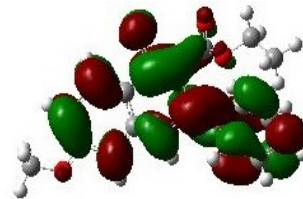
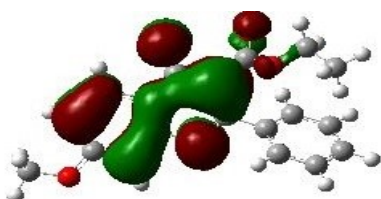
1a



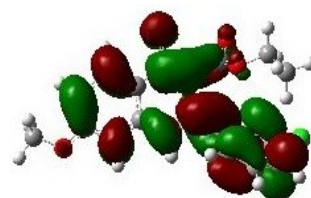
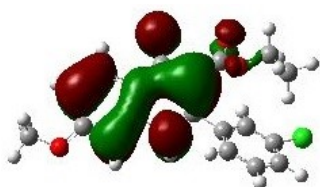
1b



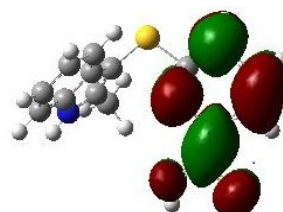
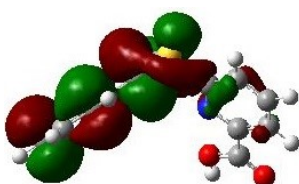
2a



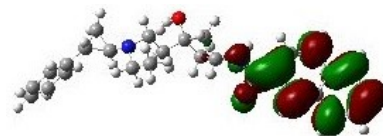
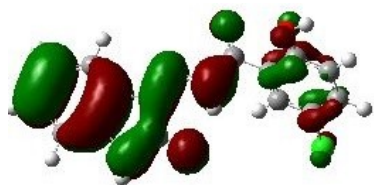
2b



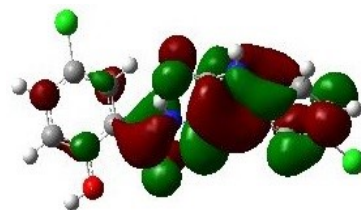
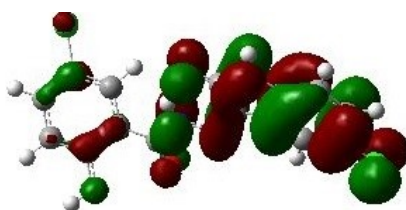
3-1a



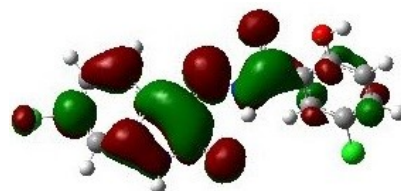
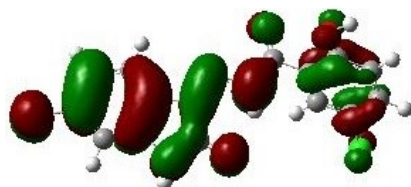
4a



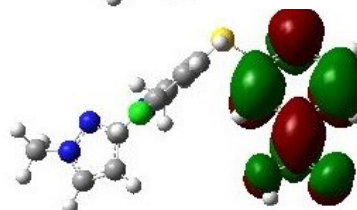
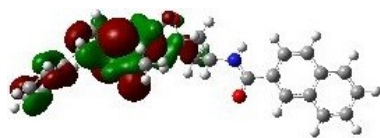
4b



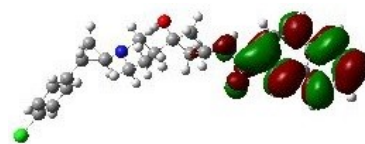
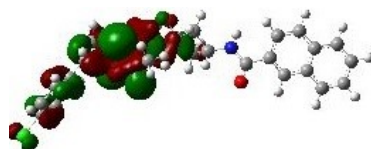
4c



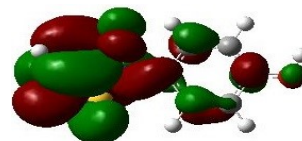
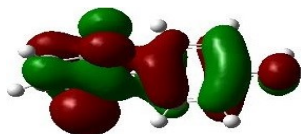
5a



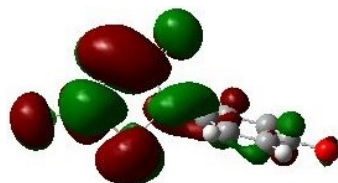
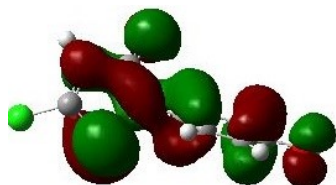
5b



6a



6b



7a



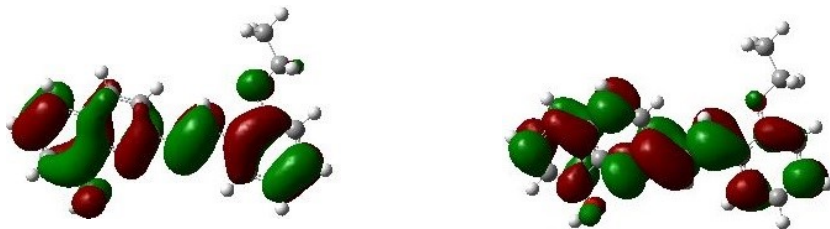
7b



8a



8b



9a



9b



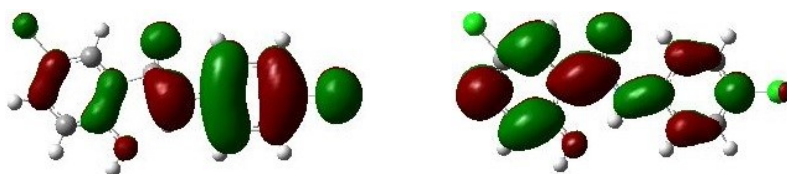
9c



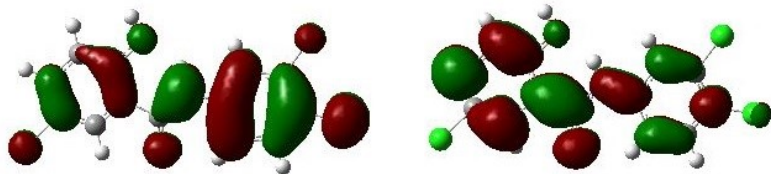
10a



10b



10c



11a



11b



11c



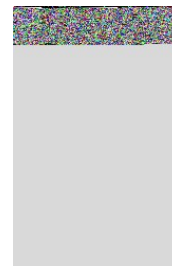
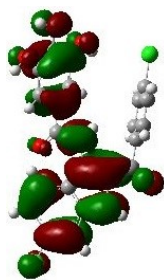
12a



12b



12c



Supplementary Figure 1: The Frontier Molecular Orbitals (FMOs) Highest occupied molecular orbital (HOMO) and Least unoccupied molecular orbital (LUMO) diagram for the reference drugs Ref (1-4) and studied 12 inhibitors.

Optimized coordinates of for the reference drugs Ref (1-4) and studied 12 inhibitors with wb97xd/6-31g(d,p) method and water as a solvent.

Ref 1 (Diazepam)

C1	0.52790300	4.22270300	-0.55491300
O	2.43290500	-3.54623400	-0.13991800
N	2.10193100	-1.40776000	0.54794800
N	-0.31617000	-1.94619500	-1.09964000
C	0.41530000	0.21552900	-0.22866900
C	1.69965400	-0.08281600	0.26222900
C	-0.58942400	-0.84745700	-0.50044500
C	1.05327200	-2.15150300	-1.54121500
C	1.93337900	-2.45012300	-0.33642900
C	-1.99627600	-0.62175800	-0.06418700
C	0.06958700	1.55017200	-0.47386800
C	2.59179100	0.96426900	0.52371000
C	2.95108300	-1.65417000	1.71161900
C	0.97727200	2.56354300	-0.22691700
C	2.24063500	2.28207600	0.28400700
C	-2.28951600	0.12658600	1.08087200
C	-3.04498900	-1.20262400	-0.78586100
C	-3.60742200	0.28679900	1.49812600
C	-4.36071200	-1.03432500	-0.37302000
C	-4.64515500	-0.29052300	0.77153300
H	1.45294800	-1.28519300	-2.08657900
H	1.09522400	-3.02470000	-2.19126700
H	-0.91782800	1.78323000	-0.85556900
H	3.58085300	0.74588200	0.90811100
H	2.68193200	-0.95520700	2.50321200
H	4.01337400	-1.54413800	1.47272900
H	2.77854800	-2.67441000	2.05015800
H	2.94702300	3.07964900	0.48146300
H	-1.48528900	0.57454700	1.65567300
H	-2.81320200	-1.77966600	-1.67441600
H	-3.82201600	0.86044100	2.39373800
H	-5.16721000	-1.48141500	-0.94503000
H	-5.67316000	-0.15945800	1.09357700

Ref 2 (Chloroquine)

Cl	5.25008900	-0.97342100	-0.99081900
N	-2.39921800	-1.68931900	-0.41924300
N	-0.66968000	2.29083800	-0.13598400
N	1.73220100	0.04909300	2.51755500
C	-2.91846600	1.25083100	-0.07773700
C	-2.79775700	0.56338200	-1.43870100
C	-2.09984600	2.54714700	0.04026300
C	-3.17625900	-0.91794800	-1.38793900
C	-2.52629000	3.61549200	-0.96140800
C	-1.02983600	-1.92141700	-0.87592300
C	-3.08710800	-2.93189900	-0.06818000
C	0.08195000	1.53481500	0.70766400
C	1.33074300	0.96027900	0.26848300
C	-0.07906800	-2.29168000	0.25677400
C	-4.17687700	-2.72241700	0.97806600
C	-0.28792800	1.28885700	2.02625700
C	2.10392200	0.23973900	1.21914000
C	1.80137800	1.04567900	-1.06452600
C	0.56841100	0.56384200	2.86467400
C	3.32875000	-0.34825400	0.80986700
C	2.98135200	0.46110700	-1.45021900
C	3.74185600	-0.23394800	-0.48921100
H	-2.57720300	0.54645900	0.68687700
H	-3.96896100	1.47546700	0.14228300
H	-1.77277100	0.66526600	-1.81369400
H	-3.43845200	1.05173400	-2.18114700
H	-2.24376100	2.95835100	1.04565000
H	-4.23188800	-0.99279900	-1.10746200
H	-3.09277900	-1.35458400	-2.40111000
H	-0.34100800	2.37867400	-1.08398700
H	-1.96978900	4.54286400	-0.80410300
H	-3.59246300	3.82546100	-0.84783700
H	-2.35812100	3.28384800	-1.99152200
H	-0.99676500	-2.68949600	-1.67177000
H	-0.66233300	-0.99514800	-1.32658000
H	-3.50940300	-3.41730100	-0.96730600
H	-2.35196200	-3.63209400	0.33695800
H	-0.13674000	-1.54154800	1.04968100
H	-0.30339700	-3.26929200	0.69320000
H	0.95067200	-2.32231900	-0.11222000
H	-3.74387700	-2.31343900	1.89529600
H	-4.94988500	-2.02929600	0.63293300
H	-4.66566100	-3.67191200	1.21560600
H	-1.21887900	1.66589700	2.42945600
H	1.23084000	1.56668200	-1.82585400
H	0.26330900	0.40417800	3.89760900
H	3.90725900	-0.89147500	1.54769000
H	3.32581100	0.52805600	-2.47508100

Ref 3 (Chloramphenicol)

Cl	-5.35776900	0.59176800	1.20091500
Cl	-4.90861300	-1.45832800	-0.86497200
O	-0.18469100	-1.36315600	-1.23311000
O	-0.26960600	2.77203900	-0.67249700

O	-2.65747400	-0.99415000	1.26955700
O	6.54862900	0.59681100	0.16548300
O	6.21880000	-1.33600700	1.06675200
N	-1.94983300	0.58780600	-0.21393600
N	5.82568700	-0.34215000	0.47083300
C	-0.54615000	0.58338900	0.17514000
C	0.28305400	-0.05872900	-0.96655200
C	1.74628000	-0.14551600	-0.60130600
C	-0.12471900	2.00631100	0.51142400
C	2.60735600	0.90903800	-0.91560200
C	2.24022900	-1.26354000	0.07370300
C	-2.88040900	-0.17485200	0.39617200
C	3.94810000	0.85547600	-0.56376800
C	3.57941000	-1.33569700	0.43034200
C	4.41201700	-0.27215800	0.10312300
C	-4.30825300	0.05713500	-0.13818100
H	-0.45817700	-0.04611000	1.06399400
H	0.18195500	0.57851000	-1.85487300
H	0.90999100	2.01199000	0.87456000
H	-0.77097200	2.38172300	1.31386400
H	-2.22564900	1.31793900	-0.85754500
H	2.21790000	1.78267200	-1.42890600
H	1.57102500	-2.08260900	0.30859900
H	-1.10439800	-1.28911500	-1.50901600
H	4.62736500	1.66304000	-0.80341800
H	3.97852800	-2.19734500	0.94940200
H	-0.15415000	3.70054100	-0.45216400
H	-4.36265500	0.82124500	-0.91027300

Ref 4 (Bendamustine)

Cl	3.89105000	3.28464300	0.23014300
Cl	5.04096900	-2.06063000	-1.20260700
O	-5.34248700	2.67418700	-1.57778300
O	-6.61706400	1.56683000	-0.10619200
N	-2.12376200	-1.36852000	1.25962700
N	3.04119000	0.18264900	-0.02911700
N	-1.61825800	-1.20630400	-0.92136100
C	-0.80270400	-0.96127000	1.19547300
C	-2.55065100	-1.49516700	-0.03569600
C	-0.50488900	-0.86765100	-0.17034800
C	-3.95129800	-1.87438200	-0.39837400
C	1.75120700	-0.19485600	0.35519900
C	0.76754900	-0.48393400	-0.60085100
C	-4.96584800	-0.74085300	-0.17998400
C	0.15156600	-0.67638900	2.16516200
C	1.41387800	-0.29926200	1.73379700
C	4.01872000	0.61771500	0.94390400
C	3.42453100	0.16897600	-1.42324000
C	-2.86206300	-1.59069600	2.48616100
C	-4.63623600	0.49788300	-1.00406200
C	3.77703600	2.01165500	1.51234600
C	3.64946300	-1.22325800	-2.00305200
C	-5.64409400	1.60324800	-0.82766000
H	-4.26497000	-2.75794100	0.16694700
H	-3.93643600	-2.15816400	-1.45375000
H	0.95503900	-0.42148300	-1.66504900
H	-5.01161600	-0.47054900	0.87985000

H	-5.96054500	-1.10666800	-0.44950100
H	-0.06538300	-0.74286800	3.22607000
H	2.15444900	-0.08465700	2.49290500
H	4.06944100	-0.07740100	1.79100400
H	5.00456000	0.58467300	0.47767100
H	2.66813700	0.66520900	-2.04468500
H	4.33560600	0.75787100	-1.53833900
H	-3.09294500	-0.64136400	2.97670400
H	-2.26731200	-2.20776100	3.16329600
H	-3.79251900	-2.11420000	2.27126500
H	-4.58327900	0.25918600	-2.07250700
H	-3.65096700	0.90077100	-0.74398400
H	4.52819800	2.25602900	2.26325800
H	2.78240900	2.11121400	1.94585700
H	3.88689300	-1.16399500	-3.06516200
H	2.78665900	-1.87198600	-1.85719000
H	-6.02452000	3.34238600	-1.41767100

1a

C	-5.50304700	0.84239300	-0.61878800
C	-6.72738100	0.23302900	-0.42257600
C	-6.42380900	-0.88516000	0.38240300
N	-4.57766900	0.11109400	0.07427000
H	-7.68485200	0.53954300	-0.81107500
N	-5.14594900	-0.98773300	0.68853900
N	-5.17176800	1.99539800	-1.29293700
H	-5.87569400	2.27566200	-1.96121400
H	-4.24880200	1.99145900	-1.70995000
O	-7.32836800	-1.77884000	0.81575000
H	-6.86552200	-2.44234900	1.34200500
C	-3.19491300	0.26922100	0.10319300
C	-2.47475800	1.41744800	0.15951300
S	-2.19164100	-1.16615200	0.00040500
C	-1.06447600	1.17076800	0.10856600
H	-2.90842900	2.40414000	0.24694000
C	-0.76739200	-0.17586700	0.03458600
C	-0.01704200	2.19217000	0.16350300
O	1.18487900	1.95299100	0.15277300
O	-0.50810600	3.42834500	0.22772200
C	0.45588000	4.48676100	0.28888000
H	1.08054700	4.38164900	1.17758700
H	1.08620800	4.47947700	-0.60200600
H	-0.12373700	5.40595000	0.33748400
N	0.50849900	-0.68431800	0.01779200
H	1.24394700	0.02199600	0.06551000
C	0.83509100	-2.00330700	-0.09188500
C	2.29402000	-2.26635900	-0.11817900
O	0.00959900	-2.90445000	-0.16179400
C	2.73620400	-3.62473700	-0.20994800
N	3.18117500	-4.69399400	-0.28257600
N	3.11015200	-1.25468300	-0.06071700

N	4.39623800	-1.39289600	-0.08038000
C	5.25152900	-0.27126300	-0.01969900
C	6.62662100	-0.50084400	-0.03589800
C	4.74077900	1.02520900	0.05328900
C	7.49917000	0.58038900	0.02212600
H	7.01251000	-1.51424100	-0.09250900
C	5.62841900	2.09334000	0.11085200
H	3.67036400	1.19479000	0.06465200
C	7.00566200	1.88014900	0.09569800
H	8.56882200	0.40103100	0.00971400
H	5.23530600	3.10296600	0.16784100
H	7.68858300	2.72140400	0.14087500
H	4.81486900	-2.31950600	-0.13968300

1b

C	-5.95603200	-1.22542500	0.59979600
C	-7.23424500	-0.74883000	0.38178700
C	-7.03842100	0.38373500	-0.43644900
N	-5.10297000	-0.41182200	-0.09438000
H	-8.15954900	-1.14725600	0.76468600
N	-5.77448600	0.61390400	-0.73083200
N	-5.51529000	-2.32844000	1.29458700
H	-6.19409200	-2.66995200	1.96038200
H	-4.60241500	-2.22321100	1.72052000
O	-8.02548900	1.17287800	-0.89200200
H	-7.62798100	1.87364300	-1.42334900
C	-3.71115100	-0.42584000	-0.10595900
C	-2.87493200	-1.49360000	-0.14065600
S	-2.86389700	1.10703400	-0.00808800
C	-1.49867400	-1.10081400	-0.07812400
H	-3.20258700	-2.52094200	-0.22103900
C	-1.34464400	0.27013600	-0.01730800
C	-0.34950800	-2.00772700	-0.10927700
O	0.82076900	-1.64365900	-0.09252000
O	-0.70781100	-3.28898600	-0.15803800
C	0.36184600	-4.24199900	-0.19460500
H	0.98004200	-4.08612200	-1.08036800
H	0.97963300	-4.15509500	0.70083900
H	-0.11844200	-5.21722400	-0.23251700
N	-0.12834100	0.90821700	0.00401900
H	0.67625300	0.28108000	-0.03253100
C	0.06070400	2.25360000	0.10516100
C	1.48740200	2.66295500	0.13502600
O	-0.85060600	3.06801600	0.16479700
C	1.78782800	4.05993400	0.22878000
N	2.11462800	5.17060100	0.30388600
N	2.39851500	1.73869200	0.07756000
N	3.66717500	2.00146300	0.09675300
C	4.61888500	0.96438700	0.03753100
C	5.96809000	1.31347100	0.05780200

C	4.22966100	-0.37336300	-0.03842600
C	6.93952300	0.32230800	0.00116800
H	6.26604300	2.35521300	0.11726700
C	5.20246700	-1.36238900	-0.09506000
H	3.18063900	-0.64446800	-0.05313000
C	6.54775600	-1.00880900	-0.07496400
H	7.98967400	0.58827300	0.01642900
H	4.91048200	-2.40430200	-0.15426900
H	3.99814200	2.96280700	0.15541900
C1	7.76809900	-2.26292200	-0.14619600

2a

C	-4.33415100	-0.61788200	0.09969700
C	-3.09246500	-1.24110900	0.04233800
C	-1.93673800	-0.46340700	-0.03667000
C	-2.00659100	0.93926400	-0.06258400
C	-3.27098300	1.53823500	-0.00075000
C	-4.42660100	0.78857200	0.07929800
H	-0.64720500	-2.07321200	-0.16298800
H	-3.04025700	-2.32417700	0.06068400
C	-0.78881900	1.76107700	-0.15224000
H	-3.31779900	2.62153700	-0.01826700
H	-5.38695100	1.28565400	0.12527300
C	0.46060000	1.00739600	-0.19348400
C	0.46622400	-0.36733900	-0.17220700
N	-0.69421200	-1.06618900	-0.09725600
O	-5.39789900	-1.44353000	0.17476400
O	-0.83564600	2.99479600	-0.15447500
C	-6.69731100	-0.87355400	0.23715500
H	-7.38794300	-1.71379400	0.29021000
H	-6.81601000	-0.24980300	1.12910100
H	-6.91540400	-0.28089700	-0.65720500
C	1.74261000	1.76272200	-0.24241500
O	2.01356200	2.62118300	-1.05551600
O	2.58088600	1.36694700	0.72191100
C	3.94802000	1.80040300	0.61867500
H	4.25201900	1.75528200	-0.43067500
H	4.01635900	2.84099100	0.94884200
C	1.69653700	-1.19617600	-0.25518900
C	2.62301100	-0.98281400	-1.27986200
C	1.93163200	-2.19319500	0.69446500
C	3.78048300	-1.74900500	-1.34285900
H	2.43590400	-0.21689800	-2.02600500
C	3.09355400	-2.95633400	0.62949400
H	1.22180800	-2.35401400	1.50024800
C	4.01936400	-2.73460200	-0.38650400

H	4.49517800	-1.57875000	-2.14083700
H	3.27703200	-3.72015200	1.37747100
H	4.92506500	-3.32985600	-0.43497700
C	4.77486100	0.87192100	1.48094400
H	4.68114000	-0.15850600	1.12634800
H	5.82700400	1.16376000	1.43182600
H	4.45290200	0.91595700	2.52446300

2b

C	-4.73377300	-0.79012500	-0.01034000
C	-3.45636000	-1.32593100	0.11170400
C	-2.34829800	-0.48157800	0.03836800
C	-2.50058300	0.90061000	-0.16001300
C	-3.79948300	1.41138700	-0.27681600
C	-4.90930200	0.59485300	-0.20586400
H	-0.95814900	-2.00009500	0.21625100
H	-3.33980100	-2.39333600	0.26376100
C	-1.33256500	1.79166300	-0.24461600
H	-3.91077700	2.47960400	-0.42704400
H	-5.89840400	1.02386300	-0.30067900
C	-0.03920500	1.12848000	-0.09536400
C	0.04513300	-0.23008000	0.09176500
N	-1.07081600	-0.99787100	0.15520400
O	-5.74775000	-1.67489400	0.07268700
O	-1.45261700	3.01032400	-0.39525500
C	-7.07971100	-1.19489500	-0.04287800
H	-7.72008100	-2.07044300	0.05227900
H	-7.31702200	-0.48370700	0.75494900
H	-7.25028500	-0.72507800	-1.01697000
C	1.19408100	1.96142700	-0.13816200
O	1.47149000	2.74655400	-1.01980300
O	1.98268100	1.72347900	0.91594100
C	3.32559900	2.23539300	0.85509300
H	3.71605600	2.07621000	-0.15406300
H	3.30458400	3.31198900	1.04629200
C	1.32669600	-0.97395800	0.21412700
C	2.31824600	-0.81216400	-0.75589700
C	1.54031600	-1.82784900	1.29692600
C	3.51787600	-1.49322200	-0.61173500
H	2.15740100	-0.15968000	-1.60690800
C	2.75027000	-2.50350600	1.41918700
H	0.77574500	-1.94310700	2.05809600
C	3.75112000	-2.34041600	0.46712600
H	2.92105600	-3.15736800	2.26684600
H	4.69671300	-2.86139900	0.55980600
C	4.13367400	1.48696700	1.89227900
H	4.12746700	0.41423800	1.67892800
H	5.16820300	1.83886200	1.87663100
H	3.72911400	1.64753000	2.89470400
C1	4.76712200	-1.27523700	-1.81807100

3-1a

C	-2.27598200	-0.45545700	-0.10516100
C	-2.86312500	0.80182600	0.15835900
C	-3.96429900	1.27664900	-0.55661200
C	-4.47159800	0.46379300	-1.55872600
C	-3.89782200	-0.79042300	-1.84049100
C	-2.80801900	-1.25777800	-1.12325700
C	-1.18915800	-0.59773000	0.82923600
C	-1.14531300	0.54694400	1.59623900
H	-4.40254200	2.24458900	-0.33660100
H	-4.31907600	-1.39974500	-2.63382400
H	-2.36921600	-2.22649000	-1.34292300
H	-2.33414800	2.29030200	1.58165100
N	-2.15137200	1.38095400	1.18785800
C	-0.18089200	0.95232400	2.65448400
H	0.58961900	1.60106300	2.22707200
H	-0.68102500	1.48744400	3.46591400
H	0.31466700	0.07016800	3.06426300
S	-0.11437200	-1.97355600	0.95704900
C	1.41151600	-1.38375700	0.22600800
C	2.39533900	-2.33490900	-0.08303600
C	2.74281300	0.33073500	-0.46810500
C	3.59623000	-1.88875300	-0.60714800
H	2.21261600	-3.39141200	0.07955600
C	3.78331600	-0.52193600	-0.80964500
H	4.37856000	-2.59524000	-0.86130700
H	4.70281300	-0.12159100	-1.21700300
N	1.57740000	-0.08478400	0.04194600
C	2.92987900	1.80545700	-0.66677100
O	3.93331500	2.28883800	-1.14787800
O	1.89052500	2.53589600	-0.25940600
H	2.11324900	3.46346900	-0.42538400
H	-5.32580400	0.80134400	-2.13680100

3-1b

C	-1.62390600	-0.72238900	0.29016300
C	-2.24299500	0.42690300	0.83013800
C	-3.47599600	0.89978900	0.37950500
C	-4.06924800	0.18076900	-0.64280200
C	-3.48449100	-0.96297000	-1.21015000
C	-2.26221000	-1.41738400	-0.74354800
C	-0.39128300	-0.89449500	1.01229500
C	-0.29978200	0.13061400	1.92898400
H	-3.94327300	1.78091300	0.80317200
H	-3.99555000	-1.48377100	-2.01146300
H	-1.80574800	-2.30129000	-1.17723000
H	-1.59157800	1.74229800	2.36574700
N	-1.41434200	0.91905000	1.81210300
C	0.79500400	0.47255500	2.87592200

H	1.44263500	1.23392900	2.43093900
H	0.39956900	0.85206000	3.82151500
H	1.40471300	-0.41087300	3.07451800
S	0.77669000	-2.17396900	0.76005000
C	2.12723100	-1.34583400	-0.07762000
C	3.10349200	-2.14781400	-0.68659700
C	3.22606100	0.56515600	-0.65385600
C	4.17662500	-1.52211800	-1.29741000
H	3.01203600	-3.22835500	-0.68299400
C	4.24740200	-0.12969600	-1.28668500
H	4.94894200	-2.10906900	-1.78191000
H	5.06500400	0.40780900	-1.74963700
N	2.18331400	-0.02496500	-0.05769500
C	3.29191900	2.06298000	-0.61808000
O	4.17215200	2.70243400	-1.15471400
O	2.29378000	2.62471800	0.06580500
H	2.43049600	3.58271200	0.03316900
Cl	-5.62420500	0.72146800	-1.26222100

3-2a

C	-2.02956800	-0.81936900	-0.18704300
C	-2.74831800	0.39341500	-0.11930600
C	-3.82421100	0.67146600	-0.96563400
C	-4.16703300	-0.29533800	-1.89910100
C	-3.45809000	-1.50785800	-1.98636700
C	-2.39487100	-1.77916900	-1.13939400
C	-1.02185300	-0.74206000	0.83458300
C	-1.15148000	0.48243600	1.45779700
H	-4.37204400	1.60566400	-0.89761700
H	-3.75192000	-2.24149500	-2.73039600
H	-1.85128000	-2.71669700	-1.20866900
N	-2.19107700	1.16840800	0.87918600
C	-0.32131900	1.06804500	2.54614000
H	0.25429600	1.92339100	2.17927600
H	-0.93285300	1.40103100	3.38973800
H	0.38459300	0.31786100	2.90498400
S	0.17212300	-1.96806100	1.19778200
C	1.66440200	-1.33295900	0.43501400
C	2.76511900	-2.19806600	0.34270400
C	2.83444600	0.37924400	-0.50922400
C	3.93797000	-1.70997000	-0.20619700
H	2.69233900	-3.22305400	0.68941100
C	3.98264500	-0.38786400	-0.64742400
H	4.80867700	-2.35007200	-0.29524400
H	4.87443500	0.04242300	-1.08470500
N	1.69389900	-0.07668100	0.02323700
C	2.86660600	1.80565600	-0.97201200
O	3.84285300	2.31731600	-1.47927600
O	1.72135900	2.45882500	-0.77041600
H	1.84766700	3.36070100	-1.09932700
H	-4.99699500	-0.11307300	-2.57415500

C	-2.66600400	2.49206200	1.22973700
H	-2.70210500	3.12333500	0.33842200
H	-3.66530500	2.44080200	1.67075000
H	-1.98758500	2.94892100	1.94795900

3-2b

C	1.44805300	-0.84714500	-0.35971700
C	2.14271400	0.35525800	-0.61298800
C	3.35474800	0.66809600	0.00524500
C	3.84460300	-0.26857000	0.89848000
C	3.18027300	-1.47238200	1.18204300
C	1.98139300	-1.76423800	0.55221500
C	0.27095400	-0.80681100	-1.18035200
C	0.28499000	0.38810200	-1.86975000
H	3.88730900	1.58991700	-0.19704800
H	3.61151500	-2.16717500	1.89321800
H	1.46329600	-2.69357000	0.76599700
N	1.41547500	1.08989100	-1.52437700
C	-0.72943400	0.93543700	-2.81125900
H	-1.21482300	1.82004800	-2.38800800
H	-0.28375700	1.21326700	-3.77071300
H	-1.49822400	0.18311400	-2.99129900
S	-0.97714100	-2.03049600	-1.24996700
C	-2.27866500	-1.33602000	-0.23115500
C	-3.35446900	-2.16973300	0.10817000
C	-3.20282200	0.43382600	0.86616500
C	-4.38422200	-1.63466200	0.86238300
H	-3.37259800	-3.20628500	-0.21032000
C	-4.31460300	-0.29901000	1.25706900
H	-5.23176700	-2.24899500	1.14527300
H	-5.09270800	0.16708700	1.84779800
N	-2.20090100	-0.06775300	0.13392100
C	-3.11192000	1.87414800	1.27403700
O	-3.95663500	2.42940300	1.94496400
O	-2.01496200	2.48650500	0.82603800
H	-2.05305600	3.40173400	1.13972600
C	1.81885200	2.39435200	-2.01303100
H	2.00646100	3.06560400	-1.17150600
H	2.72581100	2.31589200	-2.61823900
H	1.02447200	2.82017800	-2.62287700
Cl	5.36649400	0.06123600	1.71631200

3-3a

C	-0.32669500	2.22256700	0.03307800
C	-1.52703900	1.60664000	0.43909500
C	-2.38385400	2.18183000	1.37792500
C	-2.00532300	3.40103600	1.91982100
C	-0.80736500	4.02970200	1.53380300
C	0.03370000	3.45383300	0.59445900

C	0.26772200	1.34695900	-0.94334000
C	-0.55435900	0.25424600	-1.08911300
H	-3.30487300	1.69034500	1.67288800
H	-0.54032900	4.98217500	1.98040400
H	0.95620000	3.94259600	0.29610700
N	-1.64564600	0.41071600	-0.25680000
C	-0.35912100	-0.98063200	-1.89447700
H	-0.12535100	-1.82069800	-1.23278600
H	-1.25566100	-1.23007000	-2.46550100
H	0.48081700	-0.84253700	-2.57671100
S	1.80981600	1.58887400	-1.73676300
C	2.88714100	0.44895200	-0.86753300
C	4.26746600	0.55396900	-1.09398000
C	3.17251500	-1.33066500	0.52724300
C	5.10476300	-0.34728300	-0.45939300
H	4.66402000	1.32520000	-1.74515600
C	4.55200000	-1.31790100	0.37552900
H	6.17758400	-0.29530400	-0.60804600
H	5.16287000	-2.04572100	0.89403200
N	2.35042100	-0.46715100	-0.08005400
C	2.55598700	-2.37464500	1.41047600
O	3.20788200	-3.18854200	2.03060300
O	1.22315300	-2.32709700	1.44466400
H	0.92851100	-3.03732100	2.03311500
C	-2.67870100	-0.52599700	-0.06347900
C	-2.99820100	-1.20309200	1.12596800
N	-3.48295800	-0.85986100	-1.06875500
C	-4.07214600	-1.99257900	0.77114800
H	-2.51200600	-1.12653700	2.08532100
H	-4.66477400	-2.69248900	1.34033600
N	-4.31793900	-1.76412300	-0.53802800
C	-5.33916600	-2.37307400	-1.36789100
H	-4.87286600	-2.93072500	-2.18155400
H	-5.92707700	-3.05253900	-0.75217400
H	-5.99039500	-1.60114000	-1.78023700
H	-2.64509000	3.87762300	2.65545400

3-3b

C	0.52020900	-1.69375100	-0.72737000
C	1.56970600	-0.88756000	-0.24349000
C	2.65917700	-1.40572400	0.45547000
C	2.65428800	-2.77374200	0.66401600
C	1.62500800	-3.61086700	0.20549900
C	0.55702700	-3.07246900	-0.49348600
C	-0.39554800	-0.80809900	-1.39528300
C	0.10056200	0.46981300	-1.28943100
H	3.46032400	-0.77344200	0.81944200
H	1.67311900	-4.67552800	0.40198800
H	-0.24117600	-3.71371400	-0.85286500
N	1.29558900	0.42351700	-0.59631100

C	-0.49873400	1.76057400	-1.71894200
H	-0.84898000	2.31379900	-0.84185300
H	0.22670400	2.37878900	-2.25142800
H	-1.35673700	1.56777100	-2.36432900
S	-1.92183600	-1.26494500	-2.12146200
C	-3.11354600	-0.69765900	-0.90661900
C	-4.44783000	-1.10076200	-1.06106900
C	-3.61860100	0.54408000	0.93611100
C	-5.38044900	-0.63459000	-0.15036000
H	-4.73613900	-1.76322000	-1.86978700
C	-4.96431400	0.20973800	0.87856700
H	-6.42122400	-0.92643800	-0.23581500
H	-5.65418900	0.60152400	1.61495300
N	-2.70610400	0.10259000	0.06301100
C	-3.14915400	1.46007800	2.02703800
O	-3.88444600	1.90412200	2.88369100
O	-1.84706100	1.74329700	1.96204100
H	-1.64822300	2.33864700	2.69927200
Cl	3.99433400	-3.49672900	1.54302900
C	2.07699700	1.53286400	-0.21781200
C	2.34916700	1.97181600	1.08879300
N	2.65079200	2.29811500	-1.14151400
C	3.14279100	3.08366800	0.89703200
H	2.00804300	1.54517100	2.01846500
H	3.60180600	3.76392200	1.59810900
N	3.28586400	3.24463500	-0.43730800
C	4.03016300	4.27747600	-1.13211900
H	3.36530000	4.81975000	-1.80564000
H	4.44041400	4.96629100	-0.39489400
H	4.84421100	3.82953800	-1.70401500

3-4a

C	-0.18512900	1.77508300	0.12100200
C	-1.39185100	1.29658700	0.66545700
C	-1.94020700	1.81766800	1.83805800
C	-1.23771500	2.83292800	2.46976300
C	-0.02431500	3.31703700	1.94738100
C	0.50890700	2.79758000	0.77833800
C	0.05612100	1.00773100	-1.07444400
C	-0.97646900	0.10727100	-1.21308800
H	-2.87479300	1.44012100	2.23864500
H	0.49990900	4.10994400	2.47103100
H	1.44534600	3.17055000	0.37463800
N	-1.86156000	0.28880200	-0.16764000
C	-1.19461400	-0.94625200	-2.24184700
H	-1.33198900	-1.92283500	-1.76787100
H	-2.08908400	-0.74051700	-2.83471500
H	-0.32992500	-0.99413000	-2.90451400
S	1.41873700	1.19075900	-2.16124100
C	2.73331000	0.32330600	-1.31393900

C	4.02544800	0.44777800	-1.83382500
C	3.59171300	-1.11300700	0.42177100
C	5.09023400	-0.21137300	-1.22843500
H	4.20084700	1.06265700	-2.71171700
C	4.88054700	-0.99193200	-0.09783600
H	6.08814100	-0.10846800	-1.64077300
H	5.70078600	-1.50694100	0.38858500
C	3.39848100	-1.95396200	1.63482900
O	4.29046000	-2.54679000	2.20651700
O	2.12495000	-1.99873800	2.04876800
H	2.09601100	-2.56209700	2.83505500
C	-3.04226000	-0.44566400	0.05192400
C	-3.36256000	-1.22359300	1.17782900
N	-4.00947100	-0.45112400	-0.86060700
C	-4.61611900	-1.71823600	0.88342300
H	-2.76525900	-1.39785400	2.05843300
H	-5.27665600	-2.36700200	1.43827600
N	-4.95462600	-1.24363800	-0.33577300
C	-6.17250800	-1.49712800	-1.08091600
H	-5.93351000	-1.98815500	-2.02542600
H	-6.81509100	-2.14579900	-0.48710900
H	-6.68882200	-0.55666300	-1.27852400
C	2.51628900	-0.46101900	-0.18517400
H	-1.63198900	3.26083400	3.38571100
H	1.51877900	-0.56465900	0.22436900

3-4b

C	0.14611700	-0.92312900	-1.17127200
C	1.35391800	-0.81333500	-0.45657500
C	2.05141700	-1.92381300	0.01770100
C	1.48051300	-3.15736500	-0.24209600
C	0.27231400	-3.30785600	-0.94105000
C	-0.39793700	-2.18930200	-1.40786300
C	-0.26310500	0.41980900	-1.48974400
C	0.67683300	1.27974400	-0.96780500
H	2.98375500	-1.82780600	0.56113200
H	-0.12823300	-4.30039900	-1.11032300
H	-1.33253700	-2.29473100	-1.94913300
N	1.66436000	0.53316300	-0.35161300
C	0.71947500	2.76712100	-0.97258600
H	0.81676900	3.15093600	0.04735200
H	1.57435900	3.13445100	-1.54533200
H	-0.19962300	3.15702500	-1.41103100
S	-1.69430200	0.87577700	-2.39214200
C	-3.00102700	0.72669800	-1.17991600
C	-4.31772400	0.80750800	-1.64347900
C	-3.82934500	0.44479800	1.06623900
C	-5.38066300	0.71300300	-0.75139200
H	-4.51332300	0.94159400	-2.70329500
C	-5.14324400	0.52848400	0.60543100

H	-6.39805100	0.77777000	-1.12158500
H	-5.96100200	0.44657900	1.31193100
C	-3.60641400	0.24547500	2.52464200
O	-4.49475700	0.15564400	3.34711500
O	-2.31006800	0.17177400	2.85496700
H	-2.26238400	0.04314400	3.81289900
C	2.80109600	1.04481700	0.30429300
C	3.15853300	0.86575000	1.65133000
N	3.68115100	1.78624900	-0.36167900
C	4.34129200	1.56651000	1.76666200
H	2.62867600	0.31869700	2.41462700
H	4.99799500	1.72677900	2.60814600
N	4.60600100	2.10233700	0.55480600
C	5.73337400	2.93361000	0.17895100
H	5.37707700	3.90393100	-0.16978500
H	6.36880400	3.07234700	1.05249000
H	6.30476700	2.44751200	-0.61304300
C	-2.75662100	0.54786500	0.17817300
Cl	2.30219700	-4.60156100	0.33034200
H	-1.74037500	0.48632400	0.54828800

4a

C	0.22912	2.9193	-0.00071
C	-1.06639	3.64529	0.00511
C	-1.05257	5.07991	0.00461
C	0.13161	5.74044	-0.00113
C	1.39068	5.03488	-0.00679
C	1.44551	3.68004	-0.00663
C	-0.0159	1.57611	0.00085
C	-1.50439	1.34473	0.00787
H	-2.0155	5.61084	0.00894
H	2.40103	3.13589	-0.01093
N	0.95343	0.47099	-0.00334
N	-2.08411	2.73509	0.01015
O	-2.20344	0.09724	0.01152
N	0.50354	-0.85475	-0.00083
H	-0.47722	-1.04993	0.00381

C	1.47287	-1.95987	-0.00502
O	2.68496	-1.76724	-0.01074
C	0.86634	-3.37539	-0.00169
C	1.70175	-4.49234	0.00615
C	-0.519	-3.54035	-0.00626
C	1.15177	-5.77481	0.00915
C	-1.06872	-4.82228	-0.00377
H	-1.1774	-2.65967	-0.01224
C	-0.23316	-5.93954	0.00359
H	-0.66686	-6.95006	0.00632
H	2.30274	5.59436	-0.01123
H	-3.05932	2.95629	0.01464
Cl	-2.81634	-5.03051	-0.01007
H	1.7925	-6.63174	0.01572
O	3.12177	-4.32376	0.01178
H	3.54666	-5.1846	0.01487
H	0.13266	6.81044	-0.00147
4b			
C	0.22912	2.9193	-0.00071
C	-1.06639	3.64529	0.00511
C	-1.05257	5.07991	0.00461
C	0.13161	5.74044	-0.00113
C	1.39068	5.03488	-0.00679
C	1.44551	3.68004	-0.00663
C	-0.0159	1.57611	0.00085
C	-1.50439	1.34473	0.00787
H	-2.0155	5.61084	0.00894
H	2.40103	3.13589	-0.01093
N	0.95343	0.47099	-0.00334

N	-2.08411	2.73509	0.01015
O	-2.20344	0.09724	0.01152
N	0.50354	-0.85475	-0.00083
H	-0.47722	-1.04993	0.00381
C	1.47287	-1.95987	-0.00502
O	2.68496	-1.76724	-0.01074
C	0.86634	-3.37539	-0.00169
C	1.70175	-4.49234	0.00615
C	-0.519	-3.54035	-0.00626
C	1.15177	-5.77481	0.00915
C	-1.06872	-4.82228	-0.00377
H	-1.1774	-2.65967	-0.01224
C	-0.23316	-5.93954	0.00359
H	-0.66686	-6.95006	0.00632
H	-3.05932	2.95629	0.01464
Cl	-2.81634	-5.03051	-0.01007
H	1.7925	-6.63174	0.01572
O	3.12177	-4.32376	0.01178
H	3.54666	-5.1846	0.01487
H	0.13266	6.81044	-0.00147
Cl	2.89089	5.95515	-0.01409
4c			
C	0.22912	2.9193	-0.00071
C	-1.06639	3.64529	0.00511
C	-1.05257	5.07991	0.00461
C	0.13161	5.74044	-0.00113
C	1.39068	5.03488	-0.00679
C	1.44551	3.68004	-0.00663
C	-0.0159	1.57611	0.00085

C	-1.50439	1.34473	0.00787
H	-2.0155	5.61084	0.00894
H	2.40103	3.13589	-0.01093
N	0.95343	0.47099	-0.00334
N	-2.08411	2.73509	0.01015
O	-2.20344	0.09724	0.01152
N	0.50354	-0.85475	-0.00083
H	-0.47722	-1.04993	0.00381
C	1.47287	-1.95987	-0.00502
O	2.68496	-1.76724	-0.01074
C	0.86634	-3.37539	-0.00169
C	1.70175	-4.49234	0.00615
C	-0.519	-3.54035	-0.00626
C	1.15177	-5.77481	0.00915
C	-1.06872	-4.82228	-0.00377
H	-1.1774	-2.65967	-0.01224
C	-0.23316	-5.93954	0.00359
H	-0.66686	-6.95006	0.00632
Cl	0.18928	7.49949	-0.00194
H	2.30274	5.59436	-0.01123
H	-3.05932	2.95629	0.01464
Cl	-2.81634	-5.03051	-0.01007
H	1.7925	-6.63174	0.01572
O	3.12177	-4.32376	0.01178
H	3.54666	-5.1846	0.01487
5a			
C	-3.58035	0.21616	0.43579
O	-3.03145	1.27919	0.79645

N	-2.78387	-0.91873	0.22677
H	-3.15366	-1.60096	-0.4195
C	-1.3568	-0.77436	0.17301
C	-0.52396	-2.07105	0.22393
C	-0.65142	-0.41733	-1.16424
H	-1.06852	-0.07111	0.95506
C	0.44452	-1.44927	-0.80657
H	-1.05761	-2.90385	-0.24331
H	-0.13094	-2.39194	1.19222
H	-1.23046	-0.77591	-2.02036
H	-0.34731	0.61974	-1.32897
O	0.81572	-2.36872	-1.8128
C	1.68286	-0.7901	-0.18511
H	2.15639	-0.16261	-0.94885
H	1.36412	-0.1319	0.62877
C	2.65377	-1.84965	0.30821
H	2.93362	-2.50961	-0.51227
H	2.21638	-2.45576	1.10378
N	3.93944	-1.29029	0.86622
C	4.71585	-0.5369	-0.14279
C	6.21263	-0.68536	-0.2008
C	5.33553	-1.25453	-1.29368
H	4.30118	0.45214	-0.30163
H	6.63311	-1.43243	0.46818
H	5.29658	-0.76065	-2.25815
H	5.25651	-2.33604	-1.3363
H	1.23285	-1.87457	-2.52753
C	-5.0045	0.08079	0.24552
C	-5.83479	1.24329	0.31742

C	-5.65683	-1.16416	0.00132
C	-7.22106	1.18307	0.12791
H	-5.36432	2.20207	0.51412
C	-7.00751	-1.25566	-0.18083
H	-5.07984	-2.08665	-0.01263
C	-8.0676	2.33529	0.18082
C	-7.85504	-0.08677	-0.13656
H	-7.46984	-2.22504	-0.35267
C	-9.4343	2.23618	-0.01515
H	-7.61409	3.30398	0.37958
C	-9.23715	-0.14799	-0.32842
C	-10.0383	0.99803	-0.27211
H	-10.04637	3.1341	0.03168
H	-9.69217	-1.11722	-0.52578
H	-11.11093	0.92815	-0.42452
C	7.06932	0.52452	-0.36823
C	6.77639	1.51972	-1.30584
C	8.18427	0.68536	0.45859
C	7.58123	2.6493	-1.41142
H	5.91731	1.42181	-1.96389
C	8.99113	1.8148	0.35164
H	8.42211	-0.08052	1.19145
C	8.69165	2.80096	-0.58375
H	7.34031	3.4124	-2.14435
H	9.85374	1.92224	1.00125
H	9.31907	3.68209	-0.66873
C	4.37261	-1.47379	2.25892
C	4.78267	-2.89594	2.50406
H	3.526	-1.18546	2.92834

H	5.22419	-0.77753	2.45393
H	5.11196	-3.03581	3.56225
H	3.93084	-3.59192	2.30886
H	5.62913	-3.18406	1.83431
5b			
C	-4.17606	0.22353	0.42247
O	-3.54311	1.23487	0.79362
N	-3.47141	-0.9657	0.18573
H	-3.89376	-1.59857	-0.47858
C	-2.0372	-0.93013	0.13005
C	-1.31333	-2.29033	0.07299
C	-1.30754	-0.52853	-1.18122
H	-1.68655	-0.31721	0.9615
C	-0.29861	-1.67037	-0.91312
H	-1.91317	-3.03784	-0.45435
H	-0.94668	-2.71774	1.00983
H	-1.91598	-0.77184	-2.05715
H	-0.92057	0.49013	-1.26756
O	-0.00354	-2.53546	-1.99028
C	0.98966	-1.16428	-0.25083
H	1.51098	-0.51777	-0.9657
H	0.72547	-0.54972	0.61489
C	1.87378	-2.33439	0.14653
H	2.11229	-2.93535	-0.7303
H	1.3857	-2.97712	0.88168
N	3.19289	-1.92681	0.75883
C	4.00584	-1.09526	-0.15525
C	5.49006	-1.32403	-0.25854
C	4.56899	-1.6896	-1.40098

H	3.65073	-0.07097	-0.17547
H	5.87172	-2.17623	0.29734
H	4.5513	-1.07306	-2.29258
H	4.42576	-2.74966	-1.58217
H	0.44839	-2.02145	-2.66896
C	-5.60817	0.20017	0.24716
C	-6.34835	1.41987	0.34906
C	-6.35412	-0.98835	-0.00965
C	-7.73754	1.46589	0.17719
H	-5.80578	2.33752	0.55651
C	-7.70979	-0.97603	-0.17609
H	-5.8471	-1.9504	-0.04631
C	-8.49562	2.67634	0.26137
C	-8.46728	0.25149	-0.10037
H	-8.24514	-1.90515	-0.35822
C	-9.86824	2.68226	0.08247
H	-7.96903	3.60516	0.47019
C	-9.85242	0.2961	-0.27408
C	-10.56557	1.49694	-0.18714
H	-10.41131	3.62204	0.1529
H	-10.38056	-0.63312	-0.48151
H	-11.64224	1.50937	-0.32594
C	6.4177	-0.15726	-0.28374
C	6.18206	0.96444	-1.08348
C	7.54689	-0.16879	0.53818
C	7.04964	2.04987	-1.06633
H	5.31537	1.00806	-1.73613
C	8.4267	0.9081	0.56593
H	7.74714	-1.0303	1.16775

C	8.16658	2.0093	-0.23953
H	6.85919	2.91505	-1.6905
H	9.30094	0.88836	1.20606
Cl	9.26747	3.37349	-0.21518
C	3.62074	-2.31307	2.1111
C	3.83885	-3.79497	2.19561
H	2.83231	-1.98773	2.8326
H	4.5618	-1.76063	2.35029
H	4.16404	-4.08891	3.22305
H	2.89758	-4.34707	1.95628
H	4.62716	-4.12004	1.47383

6a

C	1.03263500	-0.90337200	0.83936000
C	2.41971900	-0.92619200	0.83350300
C	3.12607800	-0.06204900	-0.00666300
C	2.43511800	0.81484100	-0.84707000
C	1.04642500	0.81746200	-0.85275100
C	0.34207700	-0.03549800	-0.00617400
H	0.48124200	-1.55995100	1.50466600
H	2.96810700	-1.59973000	1.48237000
H	2.98131400	1.48646000	-1.50268500
H	0.50469600	1.48817500	-1.50981700
O	4.47899100	-0.11994500	0.03761200
H	4.85473500	0.51882200	-0.57733800
N	-1.08170500	-0.01719400	-0.00689900
C	-1.85517200	1.08634100	0.34282700
C	-3.26407500	0.70899600	0.22442200
C	-3.45086200	-0.55941600	-0.18043100
H	-4.05651300	1.40757400	0.45319000
H	-4.38756800	-1.07585400	-0.34241400
S	-1.97273500	-1.40852400	-0.45883800
O	-1.37923700	2.16301600	0.68733800

6b

C	1.68477700	-0.63921100	1.05298200
C	3.05973200	-0.81586600	1.01784600
C	3.80008500	-0.29681200	-0.04804300
C	3.15567300	0.39226800	-1.07946900
C	1.77677000	0.55141200	-1.04646800
C	1.04119100	0.04254100	0.02077000
H	1.10482400	-1.02801100	1.88354700

H	3.57436800	-1.34599400	1.81115400
H	3.72923900	0.79549200	-1.90845400
H	1.26727900	1.07628900	-1.84703900
O	5.13896600	-0.49379000	-0.02610500
H	5.54319500	-0.09540800	-0.80422900
N	-0.37330000	0.21999800	0.05506900
C	-1.00754300	1.43024800	0.31089500
C	-2.45650600	1.21848200	0.25664700
C	-2.78475800	-0.05297600	-0.02181100
H	-3.15983900	2.01985800	0.43065600
S	-1.41928300	-1.10576300	-0.24783600
O	-0.40618700	2.47076700	0.54106100
Cl	-4.36565900	-0.70978400	-0.16973500

7a

C	-5.82726200	-0.52518100	-0.33542000
C	-4.55778900	-1.05849300	-0.36591500
C	-3.42835600	-0.23371300	-0.06016600
C	-3.65683600	1.12697800	0.27357100
C	-4.97283900	1.64984100	0.29953500
C	-6.03124400	0.83143100	-0.00165400
H	-6.68048300	-1.15512900	-0.57078500
C	-2.51019800	1.90746800	0.57486800
H	-5.12552700	2.69293400	0.55742800
H	-7.04427600	1.21961800	0.01353700
C	-1.26918100	1.34251300	0.53104200
C	-1.13970500	-0.03228600	0.17643300
H	-2.63496800	2.95274700	0.84182000
H	-0.39279600	1.93384700	0.76791500
N	-2.18864400	-0.78804200	-0.10410500
C	0.16179700	-0.71100800	0.09533000
H	0.08027300	-1.76780100	-0.14671200
C	1.36387400	-0.14102100	0.26615400
H	1.43548600	0.92656300	0.45126200
C	2.65158200	-0.84376400	0.20086300
C	3.83070200	-0.10175400	-0.03919900
C	2.76765100	-2.22454500	0.38718300
C	5.06966300	-0.74231900	-0.09866500
C	3.99849100	-2.86818000	0.32317300
H	1.87557700	-2.80233200	0.60790200
C	5.14603500	-2.12170400	0.07918400
H	5.97547500	-0.17933300	-0.28627900
H	4.06055100	-3.94027600	0.47446300
H	6.11502600	-2.60806100	0.03088000
O	3.66375000	1.23180800	-0.21208700
C	4.81152900	2.05461300	-0.39704500
C	4.33036300	3.48554400	-0.50746100
H	5.34249100	1.74979600	-1.30747900
H	5.49411900	1.93515600	0.45359100
H	5.18416100	4.15162900	-0.65371200
H	3.65199500	3.59960900	-1.35662400
H	3.80657200	3.78728400	0.40298800
O	-4.30339600	-2.34996800	-0.67643400

H	-5.13567800	-2.80118900	-0.85415700
---	-------------	-------------	-------------

7b

C	-4.70746500	-0.82556700	0.26677200
C	-3.42578600	-1.33383000	0.26272500
C	-2.33846900	-0.43771000	0.00134200
C	-2.59964300	0.93604600	-0.24454700
C	-3.94404600	1.39153600	-0.22603200
C	-4.97978400	0.53457300	0.02374400
C	-1.47442900	1.76071700	-0.49951200
H	-6.00411600	0.88563300	0.03776600
C	-0.22214500	1.22088400	-0.49541700
C	-0.05633600	-0.16851200	-0.22994000
H	-1.61712100	2.81598300	-0.70110200
H	0.63625000	1.84812300	-0.70170100
N	-1.08898200	-0.96163400	0.00358200
C	1.25847400	-0.82108000	-0.19993100
H	1.20384100	-1.89856100	-0.06781100
C	2.44471200	-0.20083700	-0.28985100
H	2.48570100	0.88240200	-0.35521700
C	3.75120500	-0.86883600	-0.28358000
C	4.90322700	-0.12659500	0.06326500
C	3.91021900	-2.21385900	-0.63117100
C	6.16025600	-0.73408100	0.06486300
C	5.15898200	-2.82452500	-0.62534800
H	3.03848400	-2.78557600	-0.93374700
C	6.27999700	-2.07911700	-0.27601900
H	7.04658700	-0.17278900	0.33270500
H	5.25607900	-3.86828600	-0.90294700
H	7.26270900	-2.53955900	-0.27155000
O	4.69224300	1.16980100	0.39326600
C	5.81043800	1.99670700	0.70312400
C	5.28181600	3.38667400	0.98509500
H	6.50903100	2.00683000	-0.14272900
H	6.33643400	1.59402800	1.57759200
H	6.11173100	4.05378100	1.23051100
H	4.76203400	3.78621200	0.11074200
H	4.58794900	3.37125700	1.82921600
O	-3.12432200	-2.62047300	0.48967100
H	-3.93682200	-3.11838100	0.65004600
Cl	-6.04476800	-1.90727600	0.58530300
Cl	-4.30032700	3.07905100	-0.52635300

8a

C	-6.08437800	-0.80655800	-0.75627600
C	-5.60082000	0.46648400	-1.04762200
C	-4.34568000	0.85803500	-0.59084400
C	-3.56708000	-0.02377900	0.16389500
C	-4.06587100	-1.29217800	0.46871800
C	-5.31544300	-1.68559700	0.00446300
H	-7.06191800	-1.11108400	-1.11592300

H	-6.20348700	1.15936800	-1.62538700
H	-3.99348200	1.86320800	-0.80164600
H	-3.46010300	-1.96127000	1.07008900
H	-5.69141200	-2.67656300	0.23687700
C	-2.21071700	0.33931300	0.69698500
O	-1.76375100	-0.18134100	1.71883200
N	-1.51961200	1.26932600	-0.00560400
C	-0.17553000	1.66525200	0.37442800
C	0.89407000	0.68763300	-0.11486700
C	2.28735200	1.12413100	0.32866900
C	4.65855900	0.93609500	-0.00585000
C	3.36676300	-1.04697800	0.24216800
C	5.75931600	0.10848600	-0.65152300
H	4.67031000	1.94635200	-0.42859000
H	4.86256600	1.02238700	1.07874900
C	4.50086200	-1.82945600	-0.40374700
H	2.42112800	-1.53909300	-0.00098900
H	3.48692600	-1.07180400	1.34260500
H	5.62242200	0.10837700	-1.74436500
H	6.74032200	0.53049500	-0.42116100
H	4.32014200	-1.90303600	-1.48773900
H	4.55152000	-2.83849800	0.01184200
O	5.75614900	-1.22064400	-0.16303300
N	3.35689900	0.32508900	-0.25714000
H	0.00517500	2.66562900	-0.02905800
H	-0.14661200	1.73568400	1.46500700
H	0.64830000	-0.30311100	0.27932400
H	0.86778100	0.62560500	-1.20840000
H	2.44728700	2.16294200	0.01438400
H	2.34266000	1.11802900	1.43527100
H	-1.83813100	1.51605000	-0.92965200

8b

C	-5.32211100	-0.51381300	-0.14297900
C	-4.36146200	-1.17647000	0.61179800
C	-3.06975800	-0.66300600	0.65758900
C	-2.74135600	0.49816600	-0.04496900
C	-3.71975800	1.13222800	-0.81240700
C	-5.01643100	0.63828200	-0.86058700
H	-4.61387600	-2.08258500	1.14966900
H	-2.31810000	-1.20201400	1.22519500
H	-3.45363900	2.02134600	-1.37268000
H	-5.77814000	1.13754000	-1.44789100
C	-1.35924500	1.08907000	-0.05034900
O	-0.95269400	1.74363300	-1.00963000
N	-0.61086200	0.87463900	1.05479800
C	0.75852600	1.34644400	1.15712100
C	1.76116000	0.38162000	0.52294000
C	3.19104400	0.89329400	0.67372700
C	5.46062900	0.79902900	-0.10453300
C	4.32945400	-1.23275900	0.40253600
C	6.45504700	0.00806600	-0.94050500
H	5.34592700	1.80136600	-0.53069300

H	5.86292400	0.91279300	0.92048800
C	5.35481400	-1.97686500	-0.44054500
H	3.37797800	-1.76866600	0.34637100
H	4.65631600	-1.23447900	1.46048100
H	6.11378500	-0.01697200	-1.98737400
H	7.44190700	0.47531700	-0.90448600
H	4.97516400	-2.07603400	-1.46967100
H	5.52859000	-2.97574100	-0.03376500
O	6.60426900	-1.31129200	-0.44809600
N	4.16383900	0.12898300	-0.09739900
H	0.81703900	2.32264100	0.66703400
H	0.98373100	1.49031800	2.21723000
H	1.64259800	-0.60055900	0.99227100
H	1.52799500	0.26965200	-0.54090500
H	3.23282100	1.92877700	0.31404100
H	3.46340300	0.92173100	1.74748700
H	-1.01503400	0.40068200	1.84605900
Cl	-6.95283200	-1.14993500	-0.20069800

8c

C	-4.70136600	0.88029300	0.01067900
C	-3.67278900	1.67360700	-0.48826000
C	-2.39976600	1.14382600	-0.65013100
C	-2.14362600	-0.18521500	-0.31207000
C	-3.16899600	-0.97081800	0.20825300
C	-4.44571700	-0.44804200	0.36253100
H	-3.87382700	2.70755800	-0.74180800
H	-1.60922800	1.79155900	-1.01302600
H	-2.96154300	-1.99558000	0.49259000
C	-0.78733500	-0.82500600	-0.43883500
O	-0.45718400	-1.75339300	0.29674500
N	0.01734700	-0.33255200	-1.40481700
C	1.37148400	-0.82238200	-1.59622200
C	2.37641100	-0.14338000	-0.66505300
C	3.79024700	-0.66664200	-0.90237900
C	6.01439800	-0.92655000	-0.03466900
C	5.00624600	1.22925100	0.00045500
C	6.99446100	-0.45805800	1.03000500
H	5.83086300	-1.99910800	0.08911300
H	6.46849900	-0.77531800	-1.03282300
C	6.01464700	1.64897700	1.06001300
H	4.07818600	1.78382000	0.16423000
H	5.39225500	1.50470200	-1.00010200
H	6.59605200	-0.70399700	2.02687600
H	7.95979300	-0.95431700	0.90613600
H	5.58252800	1.48153900	2.05915000
H	6.25586200	2.70940200	0.95624400
O	7.23045400	0.93491300	0.93301100
N	4.75143800	-0.20551500	0.09186100
H	1.36819900	-1.90214600	-1.42152500
H	1.64190600	-0.65327700	-2.64178800
H	2.32372000	0.93825700	-0.82683200
H	2.09051000	-0.33633100	0.37399100

H	3.77125300	-1.76223800	-0.85270600
H	4.11660000	-0.40347700	-1.92806300
H	-0.33044100	0.37307600	-2.03372200
Cl	-6.28543500	1.57496200	0.19240200
Cl	-5.70036700	-1.47313800	0.99999900

9a

C	-6.17387	-1.27575	-0.0979
C	-5.25917	-1.34598	-1.14529
C	-4.06183	-0.63924	-1.07529
C	-3.77379	0.14674	0.04375
C	-4.70587	0.23072	1.0809
C	-5.89536	-0.48539	1.01615
H	-7.10675	-1.82727	-0.15397
H	-5.48236	-1.94067	-2.02483
H	-3.37321	-0.6795	-1.91379
H	-4.48198	0.86153	1.93424
H	-6.60954	-0.42511	1.83083
C	-2.51468	0.95866	0.1674
O	-2.49376	1.99887	0.82438
N	-1.4227	0.46709	-0.46375
C	-0.14477	1.15343	-0.48037
C	1.01522	0.17947	-0.29602
C	2.34836	0.92287	-0.29379
C	4.72585	0.80477	-0.58132
C	3.66422	-0.71936	0.9078
C	5.93002	-0.12254	-0.63083
H	4.63044	1.32501	-1.54027
H	4.89186	1.56914	0.20198
C	4.89857	-1.60584	0.82974
H	2.78882	-1.35464	1.06768
H	3.75541	-0.04429	1.78072
H	5.82149	-0.81901	-1.47699
H	6.84986	0.45083	-0.76539
H	4.75778	-2.35882	0.0381
H	5.05266	-2.12315	1.77948
O	6.06805	-0.84922	0.57638
N	3.50807	0.04006	-0.32956
H	-0.02715	1.70964	-1.41982
H	-0.16516	1.88334	0.33121
H	0.86299	-0.36306	0.64237
H	1.02526	-0.55972	-1.10567
H	2.39416	1.5594	-1.1854
H	2.38831	1.60173	0.58103
H	-1.48219	-0.42804	-0.92397

9b

C	-6.48149	-1.28447	0.04249
C	-5.25829	-1.94974	0.13015
C	-4.06698	-1.22474	0.11068
C	-4.0985	0.16612	0.00232
C	-5.32142	0.83112	-0.0858
C	-6.51303	0.10582	-0.06532
H	-5.23378	-3.04577	0.21591
H	-3.10283	-1.74899	0.18041

H	-5.34659	1.92727	-0.17122
H	-7.47701	0.6303	-0.1346
C	-2.78291	0.96634	-0.01924
O	-2.76227	2.18912	-0.12259
N	-1.55347	0.16824	0.09226
C	-0.24167	0.81406	-0.05935
C	1.04631	-0.02204	0.05745
C	2.42059	0.65453	-0.10138
C	4.49083	-0.09196	-1.27888
C	4.52917	0.31172	1.18961
C	5.80991	-0.83036	-1.17724
H	3.88258	-0.52308	-2.11593
H	4.68475	0.98553	-1.52338
C	5.8479	-0.42737	1.29101
H	3.94786	0.17395	2.13811
H	4.72585	1.40982	1.07143
H	5.61396	-1.92843	-1.05809
H	6.391	-0.69294	-2.12596
H	5.65374	-1.50525	1.53358
H	6.45585	0.00246	2.12891
O	6.63042	-0.33551	-0.0035
N	3.70857	-0.18156	0.01542
H	-0.22883	1.28178	-1.02163
H	-0.18363	1.58865	0.67654
H	1.03348	-0.48976	1.01973
H	0.98828	-0.79663	-0.67844
H	2.43342	1.12226	-1.06366
H	2.47862	1.42912	0.63451
H	-1.6095	-0.81401	0.27125
Cl	-7.98465	-2.1996	0.06781

9c

C	-6.48149	-1.28447	0.04249
C	-5.25829	-1.94974	0.13015
C	-4.06698	-1.22474	0.11068
C	-4.0985	0.16612	0.00232
C	-5.32142	0.83112	-0.0858
C	-6.51303	0.10582	-0.06532
H	-5.23378	-3.04577	0.21591
H	-3.10283	-1.74899	0.18041
H	-5.34659	1.92727	-0.17122
C	-2.78291	0.96634	-0.01924
O	-2.76227	2.18912	-0.12259
N	-1.55347	0.16824	0.09226
C	-0.24167	0.81406	-0.05935
C	1.04631	-0.02204	0.05745
C	2.42059	0.65453	-0.10138
C	4.49083	-0.09196	-1.27888
C	4.52917	0.31172	1.18961
C	5.80991	-0.83036	-1.17724
H	3.88258	-0.52308	-2.11593
H	4.68475	0.98553	-1.52338
C	5.8479	-0.42737	1.29101
H	3.94786	0.17395	2.13811
H	4.72585	1.40982	1.07143
H	5.61396	-1.92843	-1.05809

H	6.391	-0.69294	-2.12596
H	5.65374	-1.50525	1.53358
H	6.45585	0.00246	2.12891
O	6.63042	-0.33551	-0.0035
N	3.70857	-0.18156	0.01542
H	-0.22883	1.28178	-1.02163
H	-0.18363	1.58865	0.67654
H	1.03348	-0.48976	1.01973
H	0.98828	-0.79663	-0.67844
H	2.43342	1.12226	-1.06366
H	2.47862	1.42912	0.63451
H	-1.6095	-0.81401	0.27125
Cl	-7.98465	-2.1996	0.06781
Cl	-8.05595	0.94529	-0.1762

10a

C	3.77814600	1.07921400	-0.00000800
C	2.72383000	1.97805600	0.00035500
C	1.40141700	1.52902500	0.00051200
C	1.12062600	0.15067500	0.00024200
C	2.19718000	-0.74159200	-0.00012700
C	3.50169000	-0.28394200	-0.00023800
H	4.80081100	1.43767700	-0.00011700
H	2.92646800	3.04452200	0.00052300
H	1.97399100	-1.80147700	-0.00030600
C	-0.24367700	-0.49996100	0.00027800
O	-0.33225100	-1.72500000	0.00012600
C	-2.68622000	-0.00193800	0.00012600
C	-3.17556600	-1.31289600	0.00120300
C	-3.59078600	1.06880400	-0.00125500
C	-4.55172100	-1.53039000	0.00088800
H	-2.48377300	-2.14181200	0.00223500
C	-4.95895700	0.83530900	-0.00153600
H	-3.21648600	2.08873700	-0.00214500
C	-5.45036700	-0.46881800	-0.00046900
H	-4.91968600	-2.55171200	0.00173500
H	-5.64243100	1.67823700	-0.00260600
H	-6.51942800	-0.65285700	-0.00070400
H	-1.11125200	1.32436300	0.00046100
O	0.37371700	2.41401900	0.00088600
H	0.69522900	3.32156700	0.00156400
Cl	4.82368200	-1.43537400	-0.00067000
N	-1.31876100	0.33324000	0.00040500

10b

C	4.62168400	0.97079400	-0.00006100
C	3.60863000	1.91581600	0.00014000
C	2.26746100	1.52667600	0.00025900
C	1.92659500	0.16202200	0.00013700
C	2.96199500	-0.77793400	-0.00005400

C	4.28544000	-0.37902100	-0.00014300
H	5.65916900	1.28380300	-0.00015400
H	3.85897200	2.97183100	0.00020900
H	2.69116900	-1.82666900	-0.00013400
C	0.53640000	-0.42682100	0.00014100
O	0.39083100	-1.64572100	0.00001100
C	-1.87900300	0.17100800	0.00013700
C	-2.41669000	-1.12086800	0.00072800
C	-2.74650400	1.27154300	-0.00060300
C	-3.79689400	-1.29873200	0.00061100
H	-1.75860300	-1.97638800	0.00122900
C	-4.12187400	1.09492300	-0.00069800
H	-2.34266000	2.27932400	-0.00114000
C	-4.63892500	-0.19579700	-0.00008100
H	-4.20897500	-2.30139500	0.00107700
H	-4.78212000	1.95429900	-0.00126100
H	-0.25367700	1.43527200	0.00034600
O	1.27948400	2.45553700	0.00048600
H	1.63923100	3.34885500	0.00057100
Cl	5.55490000	-1.58745300	-0.00036300
Cl	-6.37801900	-0.43041900	-0.00020400
N	-0.50312800	0.45353100	0.00026400

10c

C	5.05841100	1.14165200	0.00010600
C	3.97034500	1.99915300	0.00077100
C	2.66681100	1.49824100	0.00090400
C	2.44126400	0.10985900	0.00032500
C	3.55137100	-0.74074400	-0.00033900
C	4.83648400	-0.23179100	-0.00044200
H	6.06628700	1.53972600	0.00001400
H	4.13110000	3.07269300	0.00120000
H	3.37110900	-1.80872700	-0.00076600
C	1.10479200	-0.59001100	0.00031400
O	1.05514500	-1.81547900	-0.00006300
C	-1.34814300	-0.19006800	0.00053900
C	-1.78048400	-1.52084000	0.00129400
C	-2.29961500	0.83616000	-0.00035600
C	-3.14002600	-1.80205900	0.00112800
H	-1.05825800	-2.32241300	0.00198100
C	-3.65513400	0.54217700	-0.00048400
H	-1.98663000	1.87454500	-0.00098500
C	-4.08747100	-0.78500000	0.00024800
H	-3.47240300	-2.83373800	0.00171600
H	0.16674000	1.20457400	0.00093600
O	1.60392100	2.33990000	0.00157600
H	1.88578200	3.26049700	0.00219600
Cl	6.20272100	-1.32948800	-0.00127800
N	-0.00410800	0.20571500	0.00071000
Cl	-5.78107900	-1.19529200	0.00008900
Cl	-4.78982600	1.86460900	-0.00160100

11a

C	-0.41581800	0.81994400	-0.00008600
C	0.98541300	0.95344300	-0.00003400
C	1.46176800	2.25770900	-0.00001100
C	0.57972700	3.33923000	-0.00003200
C	-0.77659200	3.06805600	-0.00007000
N	-1.27452300	1.82322400	-0.00010300
H	2.53348800	2.43490800	0.00002200
H	0.94109000	4.36069400	-0.00001700
H	-1.50762000	3.87222100	-0.00009100
O	-0.90344000	-0.45381400	-0.00013000
C	-2.27556400	-0.64891600	-0.00004300
C	-2.94069100	-0.78946500	1.21136600
C	-2.94076500	-0.78980600	-1.21137300
C	-4.30375500	-1.07361400	1.20611500
H	-2.39156600	-0.67719400	2.13991000
C	-4.30382800	-1.07395800	-1.20596100
H	-2.39169000	-0.67779200	-2.13997700
C	-4.98714600	-1.21550600	0.00011800
H	-4.83007200	-1.18697600	2.14821100
H	-4.83020300	-1.18758400	-2.14799300
H	-6.04904600	-1.43787400	0.00018200
C	1.90921400	-0.24354100	-0.00000400
C	2.79386700	-0.29334500	-1.25771000
C	2.79381200	-0.29331800	1.25774400
H	1.28926000	-1.14624900	-0.00000700
C	3.72777000	-1.50018600	-1.20655900
H	2.16769200	-0.34092300	-2.15478200
H	3.39689600	0.62032000	-1.32333100
C	3.72772000	-1.50015700	1.20665800
H	2.16759200	-0.34088400	2.15478600
H	3.39682900	0.62035300	1.32337900
H	3.11753500	-2.42220900	-1.25017900
H	4.38650100	-1.50384400	-2.08038400
H	3.11748500	-2.42217900	1.25027800
H	4.38641500	-1.50379000	2.08051100
N	4.54852700	-1.43913900	0.00006600
H	5.19811300	-2.21849700	0.00008800

11b

C	0.11453700	1.03592400	-0.20615000
C	-1.28655300	1.14928300	-0.12276600
C	-1.75571800	2.40065200	0.24926800
C	-0.86440300	3.44435300	0.51406000
C	0.48904900	3.19501900	0.39165700
N	0.98039000	1.99888800	0.03076400
H	-2.82308300	2.57373000	0.33452300
H	-1.22175100	4.42495300	0.80514800
H	1.22286500	3.97288900	0.58380400
O	0.59197500	-0.19130800	-0.58217300
C	1.95191600	-0.39150500	-0.61551500
C	2.62011300	-0.31830200	-1.83091100
C	2.64853300	-0.75744700	0.53625700
C	3.97937200	-0.60504200	-1.89636800
H	2.05817200	-0.03701400	-2.71455300

C	4.00773200	-1.04300300	0.47647900
C	4.67228100	-0.96474900	-0.74375000
H	4.49496100	-0.54627500	-2.84842400
H	4.53568000	-1.32556200	1.38004000
H	5.73228100	-1.18837700	-0.78935000
C	-2.16732600	-0.04581200	-0.40738800
C	-2.14622600	-1.05383700	0.75866800
C	-3.62121900	0.30387100	-0.74544600
H	-1.74193700	-0.55786200	-1.28123700
C	-2.99993700	-2.27345600	0.42025700
H	-1.11893700	-1.36386500	0.96971400
H	-2.54347400	-0.56825200	1.65823900
C	-4.41010700	-0.97036600	-1.04143000
H	-3.66385100	0.98155800	-1.60491600
H	-4.09613600	0.80962600	0.10367900
H	-2.52855700	-2.80574300	-0.42755800
H	-3.02128600	-2.96564300	1.26758100
H	-3.99007200	-1.44469600	-1.94838400
H	-5.45450700	-0.72449700	-1.25577200
N	-4.36653800	-1.85687200	0.11826800
H	-4.93208200	-2.67805300	-0.06921200
Cl	1.80392300	-0.86200400	2.06054700

11c

C	0.44255100	1.10873000	0.09151900
C	1.81988700	1.00754700	-0.16270600
C	2.37542500	2.08348300	-0.84400700
C	1.58777700	3.17035800	-1.22471100
C	0.24140200	3.14053900	-0.90756700
N	-0.33014600	2.11906900	-0.25393600
H	3.43430300	2.07414900	-1.08470800
H	2.01277400	4.01450700	-1.75421500
H	-0.41799500	3.95901600	-1.18279900
O	-0.13153200	0.05882400	0.76308400
C	-1.49062400	0.06260000	0.94829900
C	-2.01293900	0.51074600	2.15268100
C	-2.32729900	-0.46720700	-0.03877000
C	-3.38119000	0.43569800	2.38099400
H	-1.33365700	0.91110500	2.89601700
C	-3.70073800	-0.53598500	0.20464500
C	-4.22861200	-0.08477200	1.41060400
H	-3.79412000	0.78564200	3.31995500
H	-5.29643600	-0.14928100	1.58110200
C	2.62671800	-0.20591300	0.23865800
C	3.00436500	-1.05659100	-0.98724300
C	3.89282300	0.15294100	1.03255900
H	2.00054000	-0.82756900	0.88741900
C	3.83447200	-2.26669000	-0.56620100
H	2.09819500	-1.38501600	-1.50712200
H	3.58714400	-0.44604500	-1.68775800
C	4.67846600	-1.11076300	1.37607700
H	3.62368600	0.68846600	1.94880100
H	4.53590800	0.81274000	0.43859100
H	3.20067400	-2.93120200	0.05101400
H	4.14263800	-2.83636100	-1.44820400
H	4.06922300	-1.73180200	2.05974100

H	5.59933900	-0.84903600	1.90577800
N	5.02802200	-1.82290100	0.14950800
H	5.59537200	-2.63064800	0.38367700
Cl	-1.63093900	-1.02561800	-1.52609400
Cl	-4.78467200	-1.19030900	-0.99213900

12a

C	-2.99218700	-1.11605300	0.28319400
C	-4.21342100	-0.45885300	-0.00412900
C	-5.45260200	-1.10744000	0.11651100
C	-5.44048500	-2.42185200	0.53381700
C	-4.23135400	-3.09343100	0.83148600
C	-3.01393800	-2.45883200	0.70884100
C	-1.95517600	-0.14968800	0.08195400
C	-2.56950000	1.03624900	-0.30070300
H	-6.37890100	-0.59002400	-0.10813500
H	-4.26883900	-4.12680600	1.15998500
H	-2.08699600	-2.97725400	0.92103500
H	-4.58978800	1.54190700	-0.62171800
N	-3.93170600	0.82392200	-0.36340200
N	-0.57850900	-0.34032900	0.24331000
H	-0.04766800	0.49180900	0.45503400
C	0.13781100	-1.39723800	-0.26144200
O	-0.38107900	-2.34770500	-0.83185200
C	1.61885800	-1.28452800	-0.08206000
C	2.41988500	-2.04649800	-0.93238000
C	2.20505700	-0.44998200	0.87355000
C	3.80022200	-1.94879200	-0.83640800
H	1.95570200	-2.69908600	-1.66370200
C	3.59117500	-0.35359800	0.96536600
H	1.60100100	0.11309800	1.57819000
C	4.39840800	-1.10290100	0.10403300
O	4.23026700	0.43395900	1.86626700
H	3.58185100	0.90425400	2.40025900
O	5.74505000	-1.00313000	0.19777000
H	6.12823600	-1.59045600	-0.46683700
O	4.68171400	-2.63113700	-1.61720300
H	4.21554300	-3.19041200	-2.24646300
C	-2.04152700	2.33597300	-0.72211300
O	-2.72624400	3.08948600	-1.40485300
C	-0.66081400	2.72186700	-0.29309100
C	-0.29085800	2.64270000	1.05470600
C	0.25244300	3.19335700	-1.23773500
C	0.99228000	3.01392200	1.44748300
H	-1.00901200	2.29578200	1.79261000
C	1.54127600	3.53871800	-0.84461700
H	-0.04484900	3.26691200	-2.27860800
C	1.91275100	3.44736700	0.49553100
H	1.27094500	2.96048700	2.49471600
H	2.25778500	3.87942500	-1.58419700
H	2.91972100	3.71433200	0.79844100
H	-6.38070600	-2.95370100	0.63825000

12b

C	-2.59639500	-0.42050600	0.13619800
C	-3.67239400	0.46170000	-0.12709600
C	-5.01244900	0.05219000	-0.05591300
C	-5.22870500	-1.26213700	0.29107200
C	-4.18333000	-2.17024300	0.56601400
C	-2.87197700	-1.75465200	0.48753300
C	-1.39713300	0.34991000	-0.00516400
C	-1.78155100	1.64373000	-0.33135700
H	-5.82857200	0.73419500	-0.26076200
H	-4.42158600	-3.19275200	0.83352000
H	-2.06435300	-2.44940800	0.67927400
H	-3.67041700	2.52303600	-0.64785200
N	-3.15902800	1.68638500	-0.41454700
N	-0.08250300	-0.09325500	0.16445000
H	0.58953400	0.61950100	0.41001100
C	0.43762500	-1.25520700	-0.35235000
O	-0.23316300	-2.07689400	-0.96251800
C	1.90612400	-1.42413500	-0.12898600
C	2.59572700	-2.25478100	-1.01211300
C	2.58764300	-0.77724700	0.90539400
C	3.96689200	-2.40985400	-0.86805200
H	2.05725700	-2.76143100	-1.80581200
C	3.96354500	-0.93730500	1.04682100
H	2.05879800	-0.17124500	1.63443100
C	4.66321600	-1.75321000	0.15293700
O	4.69081300	-0.34557100	2.02675300
H	4.11353400	0.19667200	2.57392300
O	6.00116700	-1.90151200	0.29365700
H	6.30341000	-2.49794700	-0.40386200
O	4.74927100	-3.17903600	-1.67314100
H	4.22309700	-3.59269600	-2.36445100
C	-1.02682800	2.85011300	-0.68579500
O	-1.56643500	3.74275300	-1.32896400
C	0.39667100	2.96759600	-0.24428800
C	0.74632100	2.75031400	1.09355300
C	1.37578600	3.33607600	-1.16858500
C	2.07290300	2.88181300	1.49521000
H	-0.01952300	2.48769000	1.81823700
C	2.70325700	3.44232900	-0.76744900
H	1.09547100	3.51722100	-2.20087400
C	3.05291400	3.21296800	0.56200700
H	2.33816200	2.72324800	2.53516300
H	3.46588700	3.70507600	-1.49250700
H	4.08906700	3.29745600	0.87204100
C1	-6.87996700	-1.84618900	0.39919800

12c

C	2.97254600	-0.29641100	-0.19878700
C	3.95047800	0.66845700	0.14230200
C	5.32579200	0.40826100	0.04528200
C	5.67648400	-0.84312300	-0.40846500
C	4.73040600	-1.82862500	-0.76605000
C	3.38353900	-1.56028700	-0.65996600
C	1.69957100	0.32567100	0.00331900
C	1.94602400	1.62077600	0.44021300

H	6.06691100	1.15132300	0.31274800
H	5.07496100	-2.79270000	-1.12070100
H	2.65133400	-2.31506000	-0.91721600
H	3.73276600	2.66643500	0.83564200
N	3.31128700	1.80348100	0.52972000
N	0.44127900	-0.25264000	-0.19486100
H	-0.30684800	0.38801800	-0.41416600
C	0.05872900	-1.47604200	0.30207700
O	0.83230200	-2.23502000	0.86965300
C	-1.39027200	-1.79868200	0.12286600
C	-1.93169000	-2.74784700	0.98978200
C	-2.19573500	-1.18655600	-0.84212000
C	-3.27952700	-3.06173400	0.89987200
H	-1.29599600	-3.22281000	1.72895900
C	-3.54874300	-1.50672000	-0.92974500
H	-1.78222200	-0.48591200	-1.56156600
C	-4.09956100	-2.44453500	-0.05054700
O	-4.39373900	-0.96648100	-1.84271200
H	-3.92671900	-0.31102600	-2.37064900
O	-5.41571900	-2.74656500	-0.13960000
H	-5.60865400	-3.41146500	0.53435000
O	-3.92234000	-3.95830900	1.69641700
H	-3.31057200	-4.35712600	2.32299100
C	1.06779700	2.69871900	0.90173600
O	1.50552500	3.58779000	1.62124600
C	-0.36565000	2.68712000	0.47439100
C	-0.70300500	2.55851100	-0.87649400
C	-1.37193800	2.83581500	1.42885300
C	-2.03662400	2.55190200	-1.27063600
H	0.07649200	2.46791900	-1.62739600
C	-2.70849000	2.80636600	1.04976800
H	-1.10971900	2.95303300	2.47455500
C	-3.02460600	2.65861400	-0.29706300
H	-2.30156800	2.45730400	-2.31710700
H	-3.49394900	2.89324600	1.79102300
Cl	7.37892200	-1.24206000	-0.55263900
Cl	-4.70336700	2.60639500	-0.78024600

