

*Supporting Information*

Chirality Amplification in Helical Block Copolymers.  
Synthesis and Chiroptical Properties of Block Copolymers of  
Chiral/Achiral Acetylene Monomers

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**Correction of the Degree of Polymerization of the Block Copolymer of 1a and 1b.** The molecular weight obtained by SEC using the calibration curve made with standard polystyrene samples is not the true one. One may correct this molecular weight to estimate the true molecular weight or degree of polymerization by the following procedure. It is well known that the elution volume  $V_E$  of a polymer fraction eluted from an SEC column is a universal function of the molecular weight multiplied by the intrinsic viscosity. Thus, when the molecular weight and the intrinsic viscosity of the block copolymer sample of **1a** and **1b** are denoted as  $M$  and  $[\eta]$ , respectively, and those of polystyrene with the same  $V_E$  as  $M_{PS}$  and  $[\eta]_{PS}$ , respectively, we have the relation  $M[\eta] = M_{PS}[\eta]_{PS}$ .

Tsimpris<sup>1</sup> demonstrated the Mark-Houwink-Sakurada relation for polystyrene in DMF

$$[\eta]_{PS} = K_{PS}M_{PS}^{a_{PS}} \quad (S1)$$

with  $K_{PS} = 0.0318 \text{ cm}^3/\text{g}$  and  $a_{PS} = 0.603$ . Hirao et al.<sup>2</sup> and Ashida et al.<sup>3</sup> reported the relation between  $[\eta]$  and the degree of polymerization  $N_0$  for poly(phenylacetylene) derivatives in good solvents, which is given in the form

$$[\eta]M = K'N_0^{1+a} \quad (S2)$$

with  $K' = 174 \text{ cm}^3/\text{g}$ , and  $a = 0.609$ . Assuming that the same relation holds for the block copolymer of 1a and 1b, we can calculate  $N_0$  of the copolymer by

$$N_0 = \left[ (K_{PS}/K')M_{PS}^{1+a_{PS}} \right]^{1/(1+a)} \quad (S3)$$

When we substitute weight average molecular weights  $M_w$  calculated from  $M_n$  and  $M_w/M_n$  listed in the fifth and sixth columns of Table 2 into  $M_{PS}$  in eq S3, we obtain values of  $N_{0,w}$  listed in the seventh column of Table 2.

## References

1. C. W. Tsimpris, B. Suryanarayanan, X. G. Mayhan, *J. Polym. Sci. Part A-2: Polym. Phys.* 1972, **10**, 1837–1839.
2. T. Hirao, T. Sato, T. Norisuye, A. Teramoto, T. Masuda, T. Higashimura, *Polym. J.* 1991, **23**, 925–932.
3. Y. Ashida, T. Sato, K. Morino, K. Maeda, Y. Okamoto, E. Yashima, *Macromolecules* 2003, **36**, 3345–3350.

**Table S1. Atomic Charges of Ethynyl Groups of Monomers 1a and 1b <sup>a</sup>**

monomer	Mulliken charge	
	$-C\equiv CH$	$-C\equiv CH$
<b>1a</b>	+0.364	-0.607
<b>1b</b>	+0.364	-0.606

<sup>a</sup> Calculated by the DFT (B3LYP/6-31G\*) method.

**Table S2. Interatomic Distances in the Optimized Geometry of the Most Stable 24-mer of 1b<sup>a</sup> ( $\phi = 137.5^\circ$ )**

unit number		interatomic distance ( $>N-H\cdots O=C<$ , Å)	
<i>n</i>	<i>n</i> +2	amide	carbamate
1	3	3.63793	2.10105
2	4	3.88109	2.04720
3	5	3.37643	2.10105
4	6	2.12001	2.01225
5	7	3.29120	2.02249
6	8	2.04345	1.96890
7	9	2.05384	2.03999
8	10	2.04345	1.92700
9	11	2.07886	1.96184
10	12	2.08103	1.99560
11	13	2.88233	2.00131
12	14	2.20309	1.97429
13	15	2.07750	1.97641
14	16	2.03388	1.98599
15	17	2.04999	1.95101
16	18	2.11358	1.98623
17	19	2.79057	2.02576
18	20	2.00546	1.98740
19	21	2.31798	1.96769
20	22	2.20127	1.96089
21	23	2.31798	1.99128
22	24	1.99060	1.98822
average		2.43598	1.99881

<sup>a</sup> Calculated by the PM6 method.

**Table S3. Energies for Various Conformers of 16-mer of 1b Calculated by the PM6 Method**<sup>a</sup>

conformer	solvent molecule <sup>b</sup>	$\Delta E^c$ (kJ/mol)	$\Delta\Delta E^d$ (kJ/mol)
<b>1b-16-mer<sub>RH</sub></b>	none	0.00	0.00
<b>1b-16-mer<sub>RH</sub>/16CHCl<sub>3</sub></b>	CHCl <sub>3</sub>	-32.27	0.00
<b>1b-16-mer<sub>RH</sub>/16THF</b>	THF	-28.85	0.00
<b>1b-8-mer<sub>RH</sub>-1b-8-mer<sub>LH</sub></b>	none	+0.47	+0.47
<b>1b-8-mer<sub>RH</sub>-1b-8-mer<sub>LH</sub>/16CHCl<sub>3</sub></b>	CHCl <sub>3</sub>	-27.43	+4.84
<b>1b-8-mer<sub>RH</sub>-1b-8-mer<sub>LH</sub>/16THF</b>	THF	-28.55	+0.30

<sup>a</sup> All geometries were fully optimized. <sup>b</sup> Total of sixteen solvent molecules were located at the side chains of one conformer. The distance between each solvent molecule and hydrogen atom of -CO<sub>2</sub>NH- was set to be 2 Å in the initial conformation. <sup>c</sup> Relative energy per monomer unit using the value of **1b-16-mer<sub>RH</sub>** as a standard. The value of a conformer with solvent molecules was adjusted using the energy values of CHCl<sub>3</sub> and THF molecules, respectively. <sup>d</sup> Energy difference between **1b-8-mer<sub>RH</sub>-1b-8-mer<sub>LH</sub>** series and **1b-16-mer<sub>RH</sub>** series accompanying no, 16 CHCl<sub>3</sub> and 16 THF molecules, respectively.

## Cartesian Coordinates of Optimized Geometries

### The most stable 24-mer of 1b ( $\phi = 137.5^\circ$ )

C	-26.79413800	-1.08084900	0.81239000
C	-25.56021000	-0.90396300	0.32003000
C	-24.86110600	0.38233800	0.49978400
C	-23.56395700	0.55790300	0.82871400
C	-22.62545600	-0.57059500	0.90648300
C	-21.35614400	-0.61248800	0.45071300
C	-20.60126900	0.58059800	0.04212700
C	-19.30874900	0.84700000	0.32945500
C	-18.42352700	-0.16782900	0.91632600
C	-17.14206800	-0.42807600	0.58038500
C	-16.30894900	0.51837500	-0.17019800
C	-15.01533200	0.82385700	0.07179200
C	-14.17556900	-0.01490700	0.93717100
C	-12.89593600	-0.37709900	0.70624800
C	-12.09969700	0.25343200	-0.35283700
C	-10.81059000	0.64752800	-0.27210400
C	-9.89734800	0.14104400	0.75526000
C	-8.61045600	-0.23911900	0.59774300
C	-7.82080100	0.19327800	-0.56200000
C	-6.53844800	0.61269700	-0.53634900
C	-5.69978500	0.44008700	0.65497600
C	-4.41105700	0.04141800	0.68356600
C	-3.57656400	0.02208400	-0.52036600
C	-2.29266300	0.42463000	-0.62975900
C	-1.43245300	0.58960600	0.54471500
C	-0.14242200	0.21421300	0.67721800
C	0.70604200	-0.08318100	-0.47969200
C	1.99050500	0.28758400	-0.66809200
C	2.85692100	0.69628500	0.44095900
C	4.14781700	0.34765500	0.63044500
C	4.94373800	-0.24351300	-0.45171700
C	6.22168800	0.06209100	-0.75819400
C	7.05492900	0.85642000	0.14968800
C	8.34721900	0.63282800	0.46782000
C	9.20671200	-0.23679400	-0.33881100
C	10.48768300	-0.00746100	-0.69614700
C	11.31744600	0.99051700	-0.01608500
C	12.60840200	0.84992500	0.35166800
C	13.44533400	-0.24086200	-0.15503700
C	14.72710600	-0.16263400	-0.57061400
C	15.58003500	0.98379300	-0.24907800
C	16.87208100	0.96298900	0.14171900
C	17.71581800	-0.22104200	-0.02836500
C	18.99681400	-0.26892100	-0.44918800
C	19.86616400	0.90938100	-0.49754600
C	21.16055700	0.98459000	-0.12262300
C	21.95237000	-0.21082300	0.17883400
C	23.21695600	-0.43494300	-0.20116500
C	-23.33124600	-4.06309700	-1.53349400
C	-24.84607700	-2.01372200	-0.36118100

C	-23.58484200	-2.88087300	-2.25043700
C	-23.88304600	-4.24519900	-0.24797800
C	-24.64391000	-3.22708800	0.32101300
C	-24.32980800	-1.86144800	-1.65648400
N	-22.49833100	-5.11104900	-2.04834600
C	-22.15159200	-5.28236700	-3.39415800
O	-22.53275400	-4.55180700	-4.28832600
C	-21.22527300	-6.47807000	-3.67219700
N	-21.87480800	-7.76796200	-3.40586100
C	-21.79202900	-8.35968800	-2.15447300
O	-21.16375700	-7.92977200	-1.19445200
O	-22.51890500	-9.51582800	-2.17098800
C	-22.66924600	-10.34328000	-0.92744700
C	-23.54947400	-11.45953300	-1.48093800
C	-21.29507000	-10.82361800	-0.49510000
C	-23.36921400	-9.49138300	0.12003700
H	-27.34265200	-2.00525500	0.71670200
H	-23.19529500	-2.75932800	-3.26610300
H	-23.71301700	-5.16710200	0.30245300
H	-25.07170300	-3.36455300	1.31410900
H	-24.50190900	-0.93255500	-2.20068300
H	-22.10024500	-5.75727200	-1.35055400
H	-20.27180600	-6.37239400	-3.07423800
H	-22.48974300	-8.15162300	-4.11976600
H	-23.03515400	-12.02029500	-2.27238200
H	-24.46897300	-11.05835900	-1.92809300
H	-23.83654900	-12.16659600	-0.69606000
H	-20.71910300	-10.02610700	0.00931500
H	-20.69762300	-11.16698600	-1.34842100
H	-21.36131100	-11.65504000	0.21517600
H	-22.72855600	-8.65660300	0.44753700
H	-23.62576500	-10.07731600	1.00847300
H	-24.29612600	-9.05159700	-0.26811800
H	-20.91088900	-6.43525400	-4.74334200
H	-25.51625800	1.25534800	0.41118500
C	-23.02732200	1.92075100	1.06769800
C	-23.09226700	2.89973700	0.06180300
C	-22.39013000	2.22416300	2.28177300
C	-22.46153200	4.13124000	0.22873600
H	-23.61929800	2.68564600	-0.86792200
C	-21.77415600	3.45937000	2.47289800
H	-22.36284100	1.47911700	3.07750100
C	-21.77276600	4.40299400	1.42954900
H	-22.49505600	4.86889300	-0.56964800
H	-21.28537100	3.68998500	3.42522700
N	-21.06063900	5.64283000	1.52268000
C	-20.57662800	6.21102600	2.70919500
H	-20.85560800	6.11760900	0.63006900
O	-20.74786600	5.72167800	3.80937400
C	-19.77905500	7.51158600	2.52557100
N	-20.60073600	8.61255900	2.01006700
H	-18.88799900	7.32149100	1.85556600
H	-19.34705900	7.79961400	3.51486100
C	-20.70963000	8.83722600	0.64461400

H	-21.15685000	9.14911600	2.67062600	O	-19.35855100	-9.36161800	1.78167400
O	-20.15808600	8.18475300	-0.23291900	N	-17.46175900	8.90193400	-1.50436900
O	-21.54556200	9.89754400	0.45037200	H	-15.45465300	8.14092000	-1.33301400
C	-21.82320200	10.42418500	-0.92861400	H	-16.08703100	9.02437100	0.10282400
C	-22.82016500	11.52307600	-0.57009100	C	-19.46992100	-9.58514500	3.26062300
C	-20.52233400	10.95985700	-1.49914200	C	-17.20510000	9.26589100	-2.82321000
C	-22.43778400	9.30693500	-1.75512400	H	-18.43171300	8.69222600	-1.20920200
H	-22.35417800	12.30013800	0.04936600	C	-20.67497100	-10.52251900	3.27808100
H	-23.66272000	11.12238000	0.00934900	C	-18.19353000	-10.24026100	3.75895300
H	-23.22504100	12.00064400	-1.46788100	C	-19.75146500	-8.23822300	3.90964800
H	-19.89991700	10.15986400	-1.94026900	O	-16.11375000	9.48863600	-3.31938100
H	-19.91147600	11.44550800	-0.72752500	O	-18.40718900	9.43748100	-3.46538200
H	-20.69678200	11.69631800	-2.29008300	H	-20.43432100	-11.49264100	2.82606600
H	-21.71743200	8.48614700	-1.91301000	H	-21.50959500	-10.10142300	2.70044500
H	-22.74653200	9.66195200	-2.74368200	H	-21.02544400	-10.70070500	4.29960500
H	-23.31619400	8.87184300	-1.26446900	H	-17.37623400	-9.50612300	3.88531200
H	-23.07225600	-1.49083100	1.30321700	H	-17.83074400	-11.00413800	3.06055800
C	-20.67063500	-1.92695300	0.34997900	H	-18.33836200	-10.72255800	4.73114200
C	-20.52369300	-2.76627400	1.46602200	H	-18.87877200	-7.56968000	3.82737500
C	-20.14600300	-2.32786100	-0.89021300	H	-19.98440100	-8.34376200	4.97379300
H	-21.19499300	1.33361500	-0.48868500	H	-20.59503000	-7.72679600	3.43062200
C	-19.81855900	-3.96435200	1.36246100	C	-18.44106000	9.95902300	-4.86661300
H	-20.94935800	-2.47195900	2.42489100	C	-19.94769400	9.93055300	-5.11753600
C	-19.45221100	-3.52943300	-1.01339200	C	-17.86175100	11.36563600	-4.86191000
H	-20.27732200	-1.68799100	-1.76414300	C	-17.67660100	8.99520100	-5.76001900
C	-18.75261500	2.18650700	0.01736700	H	-20.48470500	10.57371800	-4.40994800
C	-19.27007400	-4.34095200	0.11965100	H	-20.34925600	8.91664500	-4.98836300
H	-19.69099100	-4.59474900	2.23879800	H	-20.18614000	10.26397500	-6.13207500
H	-19.04435200	-3.83327400	-1.98247700	H	-16.78617600	11.34727400	-4.61555300
C	-18.72859700	2.66640000	-1.30320900	H	-18.34658900	12.00200400	-4.11336500
C	-18.22364700	2.97648900	1.05035800	H	-17.96590600	11.84936900	-5.83753000
N	-18.53234800	-5.56996000	0.06321500	H	-16.58859600	9.03592800	-5.56577200
C	-18.13606800	3.89215300	-1.59940600	H	-17.82641500	9.22147000	-6.81941600
H	-19.16401000	2.06873700	-2.10380900	H	-17.98275600	7.95641100	-5.58882500
C	-17.64606100	4.21435700	0.77198200	H	-18.92295800	-0.83811200	1.62703300
H	-18.25980200	2.61583500	2.07923300	C	-16.54263500	-1.72020300	1.00071700
C	-18.27563800	-6.29727800	-1.10154400	C	-16.45980600	-2.09455900	2.35111900
H	-18.15837000	-5.91756400	0.95732800	C	-16.05575700	-2.58974400	0.00996100
C	-17.58357800	4.66502900	-0.55765300	H	-16.85395600	1.09043200	-0.93093000
H	-18.10540200	4.24698100	-2.62733300	C	-15.85820100	-3.29865000	2.71562400
H	-17.23832800	4.82757200	1.58121300	H	-16.85555500	-1.43383300	3.12185800
O	-18.57062000	-5.90378700	-2.21937600	C	-15.46956000	-3.80419500	0.35742600
C	-17.60497300	-7.65824800	-0.88381800	H	-16.13576200	-2.30967000	-1.04138300
N	-16.97537800	5.91610400	-0.91084100	C	-14.42298200	2.03473300	-0.54953900
N	-18.44802000	-8.59661000	-0.12324200	C	-15.35385900	-4.15265800	1.71458200
H	-16.59782500	-7.52192000	-0.39038800	H	-15.77852200	-3.56841200	3.76601600
H	-17.38848600	-8.11090400	-1.88288800	H	-15.10108400	-4.48087800	-0.41984400
C	-16.84098700	7.00088000	-0.04903800	C	-14.65665800	2.35346100	-1.89740700
H	-16.57900700	5.98439700	-1.86537500	C	-13.63158900	2.89386000	0.23573000
C	-18.35389000	-8.59068800	1.27033500	H	-14.68965700	-0.42114900	1.81629800
H	-19.37195900	-8.81309200	-0.54360900	N	-14.72222600	-5.37217400	2.12922600
O	-17.10040400	6.95193200	1.14508100	C	-14.10704900	3.50662100	-2.45948200
C	-16.37258000	8.30627100	-0.70534500	H	-15.26940800	1.69584500	-2.51400100
O	-17.48583600	-8.04001400	1.93525100	C	-13.06825000	4.04335900	-0.31552900

H	-13.45695500	2.65469500	1.28532400	C	-14.43601000	-8.54179600	7.19993200
C	-12.30160600	-1.45047000	1.53991100	C	-15.97356300	-6.55784500	6.80985700
C	-14.57580900	-6.50557000	1.32685500	O	-11.96758300	7.80752400	-5.98536600
H	-14.33622000	-5.38736200	3.08640000	O	-14.05251200	8.64209900	-6.45928700
C	-13.30624800	4.34282700	-1.66718900	N	-11.04739400	-6.99813700	5.81412700
H	-14.30028500	3.75992100	-3.50101300	H	-9.11059300	-6.37579800	5.11522400
H	-12.45617100	4.70380700	0.29585500	H	-9.83884700	-7.78353600	4.25944000
C	-12.13125400	-1.28592800	2.92433600	C	-9.26887900	5.83061400	-4.03938300
C	-11.93180200	-2.66130200	0.93273100	H	-8.42529800	4.10749300	-4.89989000
H	-12.67867200	0.52451200	-1.24651600	H	-16.75614400	-9.96408700	6.77877500
O	-14.93955700	-6.55505700	0.16165300	H	-17.82920400	-8.61865000	6.39475700
C	-13.93098200	-7.71108700	2.02042000	H	-17.18521500	-8.79291800	8.04040500
N	-12.70498600	5.52862100	-2.23807200	H	-13.57810600	-7.91296200	6.89386500
C	-11.55857800	-2.29964800	3.69024900	H	-14.20548000	-9.56783500	6.89314900
H	-12.44259600	-0.35746400	3.40164900	H	-14.45343100	-8.50837600	8.29858500
C	-11.38322700	-3.69397500	1.69080200	H	-15.10313000	-5.96853800	6.47388900
H	-12.07919200	-2.79606400	-0.13954400	H	-16.13806500	-6.32138700	7.86557500
C	-10.31932500	1.61410000	-1.28685900	H	-16.84022800	-6.19882600	6.24331200
N	-14.78804900	-8.29799100	3.06489700	C	-13.79305600	8.74624100	-7.92905600
H	-12.92138300	-7.42540100	2.44067400	C	-10.65682700	-6.75129500	7.12296700
H	-13.72677600	-8.49609800	1.25174700	H	-12.04901700	-7.04080700	5.56227500
C	-13.47333500	6.58612700	-2.70007600	O	-9.98189900	6.31402500	-3.16526800
H	-11.66932400	5.54021300	-2.31115500	C	-8.60535700	6.68552400	-5.12683800
C	-11.18156900	-3.50681200	3.06898600	C	-15.15642100	9.24957700	-8.39819600
H	-11.41263400	-2.15910300	4.75902500	C	-12.68035100	9.76168000	-8.14425600
H	-11.11752400	-4.64496800	1.22044300	C	-13.45558500	7.36171400	-8.46080000
C	-10.30793400	1.30273900	-2.65628400	O	-9.51332400	-6.62572000	7.53085700
C	-9.90707300	2.88643600	-0.85822300	O	-11.77628000	-6.75230700	7.92087200
C	-14.72560600	-7.75101100	4.34777300	N	-9.31210200	6.59819200	-6.41243600
H	-15.69272000	-8.68109200	2.74051300	H	-7.52143900	6.38821600	-5.24682900
O	-14.69901700	6.58065900	-2.64289300	H	-8.60553100	7.75125100	-4.79135800
C	-12.68723900	7.78841200	-3.23090800	H	-15.45123500	10.15402900	-7.84884100
N	-10.59079900	-4.52462700	3.89128500	H	-15.93940600	8.50171200	-8.22174800
C	-9.86954800	2.24046500	-3.59087400	H	-15.14528500	9.48761800	-9.46605600
H	-10.63976400	0.31971100	-2.99072800	H	-11.72243100	9.39228900	-7.74406500
C	-9.49114800	3.84171000	-1.78306100	H	-12.89418700	10.70824000	-7.63333600
H	-9.91553400	3.12685500	0.20509700	H	-12.52917900	9.97814600	-9.20605100
O	-13.89586100	-6.94062800	4.74399700	H	-12.47631300	7.01570200	-8.08286500
O	-15.70661000	-8.30488000	5.11956600	H	-13.40914600	7.35043600	-9.55338000
N	-13.43035700	8.47569100	-4.29892100	H	-14.19401100	6.61698200	-8.14224800
H	-11.65599200	7.49999600	-3.58737300	C	-11.63055200	-6.63009500	9.40420600
H	-12.52434300	8.50925600	-2.39191400	C	-9.10165800	5.49665100	-7.23336100
C	-10.68442900	-5.88990800	3.63907400	H	-10.18754200	7.14350000	-6.50219500
H	-10.02008600	-4.19523600	4.69131400	C	-13.10152200	-6.64685700	9.81661600
C	-9.46418600	3.51303500	-3.14965200	C	-10.85773400	-7.84097700	9.90528300
H	-9.84991100	1.98988000	-4.64981500	C	-10.94744200	-5.30785800	9.71648700
H	-9.18456900	4.83598600	-1.45309600	O	-8.23733500	4.63872300	-7.08000500
C	-15.73785700	-8.04510600	6.59752900	O	-9.99080200	5.54081300	-8.26729200
C	-13.05169700	8.23782900	-5.61644800	H	-13.60554000	-7.56003100	9.46223000
H	-14.41482800	8.72612400	-4.08188300	H	-13.64429300	-5.79945500	9.37841000
O	-11.22173400	-6.35512700	2.64431700	H	-13.20802700	-6.59635800	10.90411700
C	-10.07806700	-6.79433100	4.72165200	H	-9.81760400	-7.82379000	9.53665200
N	-9.00569000	4.46810200	-4.12167800	H	-11.30161900	-8.77930800	9.55435100
C	-16.94312000	-8.90151800	6.97852000	H	-10.81705400	-7.87238500	10.99784500



H	-9.88284600	-5.32285300	9.41638500	N	-6.73959800	-5.33400300	7.70335300
H	-10.98364800	-5.07723300	10.78471600	H	-5.01091700	-4.80461900	6.54702600
H	-11.41098700	-4.47601300	9.17348800	H	-5.92617200	-6.23358500	5.97345800
C	-9.87904000	4.58424100	-9.41583900	C	-4.99270200	4.65429600	-5.50919000
C	-11.06399400	5.06369400	-10.25135100	H	-3.74140300	2.96000900	-5.60570400
C	-8.53924000	4.81151500	-10.09501500	C	-2.87681400	-1.32769900	4.43220700
C	-10.06002100	3.17204000	-8.88240900	H	-3.18393500	0.70085300	5.14709000
H	-10.93245500	6.10719900	-10.56512000	H	-2.68083100	-3.25703000	3.45933400
H	-11.99772200	5.02283700	-9.67438600	C	-1.59889900	-0.30665800	-2.94552800
H	-11.19222900	4.44994800	-11.14800900	C	-1.53898300	2.04750900	-2.34887900
H	-7.71525100	4.30247100	-9.56102200	H	-1.95703000	0.96368900	1.43385500
H	-8.28230700	5.87734400	-10.13359300	C	-6.28761800	-4.54966300	8.75906500
H	-8.53369600	4.43353800	-11.12185200	H	-7.72931600	-5.64687500	7.67485600
H	-9.22397400	2.89071900	-8.21948900	O	-5.78638100	5.31716600	-4.85701700
H	-10.10046200	2.43793300	-9.69270300	C	-4.47591700	5.11613800	-6.87989300
H	-10.97947300	3.07617000	-8.29290700	N	-2.36422200	-1.77830200	5.69642500
H	-10.38485500	-0.06006100	1.71830000	C	-1.15210100	0.00011100	-4.23129000
C	-7.97465700	-1.08496500	1.64022000	H	-1.80713900	-1.34211200	-2.67816400
C	-8.14723700	-0.81203600	3.00777600	C	-1.12527500	2.37087000	-3.63930600
C	-7.20972900	-2.20062900	1.25250100	H	-1.68903600	2.83773700	-1.61270100
H	-8.37424800	0.23741600	-1.50662900	C	0.41224700	0.12215500	2.05260500
C	-7.56396100	-1.63112500	3.97546000	O	-5.19116800	-4.01146400	8.83342800
H	-8.73963900	0.04769400	3.32047600	O	-7.22754500	-4.53347600	9.75437300
C	-6.61415700	-3.02224300	2.20900600	N	-5.34637500	4.59185900	-7.95055000
H	-7.08091500	-2.42182300	0.19243800	H	-3.40241100	4.81646500	-7.04439200
C	-5.99631800	1.31807600	-1.72503400	H	-4.50426900	6.23199900	-6.91575100
C	-6.79046800	-2.72997500	3.57146900	C	-2.61652500	-3.04197000	6.22054800
H	-7.70966600	-1.42405100	5.03472000	H	-1.76182100	-1.11961400	6.22238400
H	-6.02389500	-3.88400500	1.90289200	C	-0.91882500	1.34308700	-4.57597200
C	-5.79309900	0.65325400	-2.94481500	H	-0.99458600	-0.79182800	-4.96108200
C	-5.72752500	2.69307000	-1.62784100	H	-0.97256600	3.41218400	-3.92801300
H	-6.23433400	0.57362100	1.60497900	C	0.56181600	1.26199700	2.85939900
N	-6.15093800	-3.57004100	4.56212500	C	0.74586700	-1.14185400	2.56512100
C	-5.29045200	1.34199800	-4.04808800	H	0.17296600	-0.54954200	-1.31777600
H	-6.02609600	-0.40762000	-3.02950300	C	-6.88011700	-3.97481900	11.09823300
C	-5.25834200	3.40143600	-2.73323200	C	-4.85082500	3.58392600	-8.77588400
H	-5.89582000	3.21142200	-0.68381000	H	-6.36902100	4.63922100	-7.77302300
C	-3.84923500	-0.40223500	1.98348100	O	-3.35294700	-3.85166100	5.66730900
C	-6.88139900	-4.36665900	5.43138200	C	-1.90451200	-3.33800100	7.54750200
H	-5.11574700	-3.52267500	4.61566200	N	-0.45303600	1.64622000	-5.90350900
C	-5.02655800	2.72009700	-3.93941200	C	1.07852000	1.15070700	4.14953700
H	-5.11537500	0.81908300	-4.98602300	H	0.27700600	2.23999700	2.47259500
H	-5.08753100	4.47807700	-2.67367300	C	1.23171400	-1.27149100	3.86528400
C	-3.76120700	0.46963600	3.08089300	H	0.61793800	-2.02841600	1.94373900
C	-3.45042800	-1.74150900	2.12210400	C	2.53383900	0.25319300	-2.05124600
H	-4.11779400	-0.24760900	-1.43583900	C	-8.19979300	-4.21627100	11.82781000
O	-8.10563800	-4.42630300	5.39824100	C	-5.72962900	-4.78979400	11.67057300
C	-6.05462200	-5.21105400	6.40637600	C	-6.55187400	-2.49824200	10.93848600
N	-4.52639100	3.40838300	-5.10033700	O	-3.67503800	3.33080400	-8.98388200
C	-3.26364400	0.01871100	4.30277900	O	-5.90157700	2.96530900	-9.40413800
H	-4.08057700	1.50642800	2.97578700	N	-2.57356800	-2.69942600	8.69079500
C	-2.97638000	-2.21250800	3.34438700	H	-0.82328400	-3.01660100	7.48879200
H	-3.51672100	-2.41588900	1.26808400	H	-1.89917300	-4.44327200	7.71078000
C	-1.77828100	0.70957100	-1.99405100	C	-0.92514000	2.71720100	-6.65250700

H	0.33084000	1.07260000	-6.26824100	H	-1.86229800	2.59234800	-9.37255200
C	1.41398600	-0.12106800	4.65124600	O	0.89994400	-2.16212100	6.59121200
H	1.20984000	2.03863800	4.76449800	C	2.21365100	-1.05328400	8.28802600
H	1.45773300	-2.25688100	4.27863500	N	4.00624500	0.24845800	-6.02582000
C	2.59820300	-0.94360800	-2.78397600	C	5.13420700	1.90133500	3.95305500
C	2.94838100	1.45682300	-2.64473800	H	3.99135400	2.55326800	2.24947300
H	2.34280900	1.26096400	1.22767200	C	6.09527000	-0.33810900	3.79792500
H	-8.49525600	-5.27249600	11.76557600	H	5.67153600	-1.41432500	1.97966800
H	-9.01420200	-3.63234300	11.38106600	C	6.74909600	-0.39168500	-2.06952400
H	-8.12411300	-3.94482700	12.88497900	C	-4.31798800	0.39945000	11.44572700
H	-4.80657700	-4.63892500	11.08819900	C	-1.79964900	0.57361100	11.15489300
H	-5.94684400	-5.86454800	11.64842600	C	-3.35080300	1.46149400	9.34895500
H	-5.51190200	-4.51110400	12.70604100	O	0.19420600	0.17629800	-8.78604400
H	-5.60004300	-2.35374800	10.39587600	O	-1.62256300	0.34992600	-10.18205000
H	-6.45544900	-2.00061100	11.90764300	N	1.36141700	-0.15260000	9.08619500
H	-7.32289300	-1.97511500	10.36115900	H	3.27192300	-0.67620000	8.25096300
C	-5.64436200	1.90842300	-10.43254000	H	2.24390400	-2.05700500	8.77871300
C	-2.37809800	-1.34268000	8.92291800	C	3.37136400	0.93194900	-7.05225400
H	-3.43768200	-3.15500500	9.03490700	H	4.89096900	-0.26688400	-6.19264800
O	-1.82928700	3.44845400	-6.26593200	C	5.89738200	0.86057800	4.50290000
C	-0.23575200	2.89735000	-8.01274600	H	4.97697900	2.82097600	4.51464500
N	1.94868900	-0.20629600	5.98359400	H	6.68087900	-1.14385800	4.23693800
C	3.09416100	-0.94688400	-4.08783100	C	6.95071200	-1.75244600	-2.34997600
H	2.26223000	-1.87546200	-2.33034100	C	6.98488300	0.56908500	-3.06636300
C	3.42279600	1.47022300	-3.95637500	H	-4.20302000	-0.42896600	12.15703800
H	2.89099400	2.38640900	-2.07839400	H	-5.26889800	0.23633200	10.92178100
C	4.76672800	0.55151600	1.96374900	H	-4.39898800	1.32976300	12.01626700
C	-7.08140800	1.53272100	-10.78669900	H	-0.96744400	0.55572600	10.42714600
C	-4.88802700	2.54339300	-11.58914900	H	-1.62396300	-0.24331400	11.86319800
C	-4.88493900	0.76990600	-9.77034300	H	-1.69913000	1.52541800	11.69714100
O	-1.53526700	-0.63351500	8.38011200	H	-2.50976800	1.43714000	8.63549800
O	-3.25105100	-0.92681700	9.88567200	H	-3.42394500	2.48249600	9.73555100
N	-0.95442200	2.18928200	-9.08321400	H	-4.26106900	1.25209700	8.77477300
H	0.83873500	2.55639300	-7.96928500	C	-1.43830000	-1.01276700	-10.77665400
H	-0.21806300	3.98655000	-8.25881900	C	1.93625900	0.94141900	9.71827000
C	1.62034700	-1.21800100	6.88090900	H	0.33987500	-0.19259800	8.92293900
H	2.63106300	0.52466500	6.25536900	O	2.37829400	1.62519800	-6.86503400
C	3.50338700	0.26428400	-4.67056900	C	3.97468800	0.73769900	-8.45021000
H	3.15436400	-1.87639500	-4.65112500	N	6.50797500	1.01965400	5.80511000
H	3.71510900	2.40681900	-4.43032100	C	7.41580300	-2.15404200	-3.60238700
C	4.57689700	1.74294800	2.68325500	H	6.74494700	-2.49998400	-1.58446700
C	5.52688100	-0.48645800	2.53391900	C	7.41763900	0.17854900	-4.33192100
H	4.39731600	-0.94556200	-1.09176100	H	6.81871500	1.62469100	-2.85027200
H	-7.59400400	2.34547400	-11.31478000	C	-2.58188800	-1.01177900	-11.78865800
H	-7.66677700	1.32895900	-9.87887200	C	-0.07001300	-1.08121500	-11.43423300
H	-7.11398200	0.64039300	-11.41913400	C	-1.62775500	-2.03132000	-9.66245300
H	-3.86189700	2.81494700	-11.29028900	O	3.12184900	1.09727200	9.96276600
H	-5.37180100	3.46538800	-11.93185500	O	0.93668700	1.79749000	10.11111400
H	-4.81036800	1.86401200	-12.44330500	N	3.14455100	-0.20340500	-9.22565900
H	-3.88156700	1.09376500	-9.43732000	H	5.04655300	0.39118600	-8.41093700
H	-4.71482000	-0.06628100	-10.46633300	H	3.98039000	1.72319900	-8.97565600
H	-5.40997000	0.38480200	-8.89046000	C	5.76145800	1.02117500	6.97580000
C	-3.14736500	0.45172500	10.46726700	H	7.53815900	1.14681700	5.82104100
C	-0.70965100	0.83426300	-9.28241700	C	7.64614600	-1.18358400	-4.59301700

H	7.58961800	-3.20805300	-3.81186500	H	3.89537300	-4.66473600	-11.97425500
H	7.57058200	0.91879100	-5.11846700	H	4.58312000	-3.97134200	-8.87595700
H	-2.42151400	-0.25785300	-12.56952900	H	3.79463200	-5.47967900	-9.32980600
H	-3.54218900	-0.76217800	-11.30342700	H	2.99654600	-4.36569900	-8.19256000
H	-2.68715900	-1.98785400	-12.27081800	C	5.89954100	5.29204400	10.85384600
H	0.73646300	-1.23352600	-10.69155000	C	7.86010600	-4.05190900	-8.57190700
H	0.16719900	-0.15491000	-11.97144000	H	6.68571000	-2.50412900	-9.38801800
H	-0.00402600	-1.90577200	-12.15030400	C	4.66154800	5.59570700	11.69391000
H	-0.82716400	-1.93814500	-8.90865000	C	7.14166400	5.06772300	11.70356000
H	-1.60536200	-3.05625600	-10.04385900	C	6.11398600	6.28768300	9.72384800
H	-2.57780600	-1.88430800	-9.13642600	O	8.77876900	-4.42904900	-7.85855400
C	1.27699400	3.04716000	10.86105800	O	6.94876000	-4.88196200	-9.17193100
C	3.65628500	-1.47110700	-9.49147500	H	4.48715500	4.80826000	12.43928100
H	2.11618000	-0.06965200	-9.16467700	H	3.75386500	5.64042200	11.07051300
O	4.54492400	0.87916900	6.98163400	H	4.76352200	6.54910800	12.22044100
C	6.58589900	1.15827900	8.26116800	H	8.01450000	4.81740600	11.07943400
N	8.13307600	-1.60783300	-5.87962700	H	7.00549500	4.23627100	12.40579400
C	-0.11961000	3.64304600	11.02575500	H	7.39991800	5.95874600	12.28416400
C	1.91452300	2.65034800	12.18387700	H	6.99900000	6.01971500	9.11882400
C	2.18377200	3.89568800	9.98504900	H	6.27288900	7.30084500	10.10424300
O	4.83498600	-1.78963000	-9.48003500	H	5.25881400	6.30922900	9.03908900
O	2.63096700	-2.30356900	-9.86102400	C	7.13742300	-6.36610100	-9.10663500
N	5.89813200	2.01140600	9.24140600	C	6.01650300	-6.81578700	-10.04081000
H	7.62639100	1.54774700	8.06094000	C	8.51826100	-6.71491900	-9.63797200
H	6.71939900	0.13989500	8.70318300	C	6.91849200	-6.79016100	-7.66168600
C	7.63296100	-1.11731700	-7.07922400	H	6.18296500	-6.45366200	-11.06326900
H	8.94360200	-2.25640100	-5.88284000	H	5.04137300	-6.40947800	-9.71931400
H	-0.79489100	2.93846500	11.53904700	H	5.93801300	-7.90623400	-10.07173600
H	-0.57639800	3.85902200	10.05145700	H	9.30903800	-6.50202200	-8.89346200
H	-0.08921200	4.57161600	11.60286000	H	8.76439600	-6.13456600	-10.53518600
H	2.90009200	2.18052900	12.01984900	H	8.59786000	-7.77554500	-9.89512400
H	1.30320600	1.91987600	12.72564000	H	7.71586600	-6.38959600	-7.01272200
H	2.06818800	3.51497800	12.83562700	H	6.91748200	-7.87859300	-7.55498200
H	3.17924100	3.42692100	9.86142400	H	5.96869000	-6.40929300	-7.26892200
H	2.36531400	4.88710300	10.42183200	H	6.50595200	1.63879600	0.69171300
H	1.76933700	4.03335100	8.98086900	C	8.88698900	1.29581900	1.68192700
C	2.92754300	-3.71234200	-10.27209500	C	8.95662900	2.69407900	1.79027700
C	6.37998600	3.29033800	9.47048000	C	9.27652000	0.49332600	2.76675100
H	4.92475100	1.75450500	9.48970400	H	8.69009200	-1.10053500	-0.77491200
O	6.69558100	-0.32851500	-7.12871700	C	9.42660500	3.29031100	2.96025700
C	8.34449800	-1.64299000	-8.33405600	H	8.64403100	3.31813600	0.95317300
C	1.50873100	-4.21375800	-10.53132500	C	9.72185600	1.07578900	3.95138900
C	3.78827500	-3.67290800	-11.52524300	H	9.22440100	-0.59229300	2.68143000
C	3.59830100	-4.42012600	-9.10511200	C	11.04837100	-0.79451500	-1.82463300
O	7.45920600	3.72948100	9.09475900	C	9.80401900	2.47623400	4.04374800
O	5.49040000	3.98459900	10.24942200	H	9.49197400	4.37404800	3.03369300
N	7.59648800	-2.74310700	-8.95946100	H	10.00650600	0.45327900	4.80171100
H	9.39873400	-1.96894800	-8.09939200	C	11.19246500	-2.18917300	-1.74777800
H	8.42339200	-0.80519500	-9.06900000	C	11.38250300	-0.12189000	-3.01146200
H	1.07334600	-3.75196700	-11.42543300	H	10.77919300	1.89584800	0.28952300
H	0.84626500	-3.95964700	-9.69152000	N	10.29106700	3.10324100	5.24203200
H	1.48907500	-5.29964100	-10.66355400	C	11.68770100	-2.90784100	-2.83601000
H	4.80213700	-3.30282800	-11.29755100	H	10.91810200	-2.71298200	-0.83275400
H	3.36940100	-3.00041400	-12.28283700	C	11.85154900	-0.83228700	-4.11573900

H	11.26453900	0.96017500	-3.07122100	H	10.72118400	-4.84153100	-7.90302400
C	13.15673800	1.81936000	1.33333300	O	13.49113300	3.65180300	6.09616900
C	10.03425300	2.62149200	6.52221900	C	14.68606800	5.73822800	6.39624100
H	10.89062900	3.93853500	5.12536200	N	16.49797600	-4.50144200	-3.84308200
C	12.01182100	-2.22404200	-4.01991400	C	18.09772300	4.50824200	0.74660100
H	11.81212800	-3.98723300	-2.77150800	H	17.54455100	3.37295100	-0.99918400
H	12.07914000	-0.31884200	-5.04975800	C	17.93531800	3.32423800	2.87908500
C	13.33723300	3.17276500	1.00749900	H	17.32576100	1.26141100	2.75786100
C	13.43017600	1.37225500	2.63601300	C	19.50244200	-1.58950100	-0.90892900
H	12.91012600	-1.18950800	-0.28867000	C	8.11386800	8.68512600	7.74328800
O	9.30045800	1.66224800	6.73268500	C	10.60681900	8.72492600	7.25361100
C	10.73929700	3.39007300	7.64861900	C	8.97575000	7.89458000	5.48625300
N	12.51913900	-2.98005500	-5.14043400	O	13.27760100	-6.56152100	-6.91999300
C	13.80545000	4.07167000	1.96439400	O	11.13164800	-7.17025000	-7.46776600
H	13.11080600	3.52264600	0.00079700	N	13.82298000	6.92032700	6.21491800
C	13.86690900	2.26600800	3.61176500	H	15.75107000	5.97514400	6.11491400
H	13.28756100	0.32136300	2.88848400	H	14.69373300	5.47265500	7.48032100
C	15.24620700	-1.28822500	-1.39009300	C	16.04290300	-4.72362600	-5.13628900
N	10.02752400	4.62661900	8.00342100	H	17.22146200	-5.13000900	-3.44389700
H	11.80838700	3.61393100	7.36165000	C	18.21907600	4.48985000	2.14857300
H	10.78363900	2.73413300	8.55231000	H	18.32092500	5.41147200	0.18322600
C	11.91648600	-2.95572600	-6.38968500	H	18.00238400	3.33046300	3.96916300
H	13.39928300	-3.50746900	-4.98560600	C	19.72942400	-2.64220500	-0.00871600
C	14.05972600	3.61592500	3.27232100	C	19.66184700	-1.80210600	-2.28750900
H	13.96133900	5.11624900	1.70323000	H	19.35309600	1.82950500	-0.80391100
H	14.04268200	1.92902100	4.63618300	H	8.32702100	8.71757300	8.81958500
C	15.43057600	-2.56982300	-0.84689600	H	7.19200900	8.10057400	7.62124100
C	15.47611200	-1.07126000	-2.75811900	H	7.91465900	9.70632400	7.40405000
H	15.04787700	1.94378500	-0.23182400	H	11.39803500	8.36958100	6.56813300
C	10.18621100	5.75626800	7.20889500	H	10.95040000	8.52033500	8.27492900
H	9.16336400	4.51794500	8.56504900	H	10.55183400	9.81180300	7.13585500
O	10.92144700	-2.28056000	-6.62767100	H	9.81116800	7.39335200	4.96994500
C	12.57439600	-3.84493700	-7.45336000	H	8.81167700	8.85996200	4.99822400
N	14.51119500	4.57124200	4.24358600	H	8.08323000	7.27906300	5.31917200
C	15.85920500	-3.62383900	-1.65299300	C	11.37507900	-8.62732800	-7.22714000
H	15.23761200	-2.74217600	0.21175100	C	14.05804600	7.74423500	5.11075100
C	15.87300300	-2.12312000	-3.58202600	H	12.84116700	6.80966900	6.53670000
H	15.33044100	-0.07655200	-3.18017600	O	15.21288900	-4.00496000	-5.68218400
C	17.40252300	2.18371600	0.80169500	C	16.63907700	-5.96433300	-5.81739800
O	11.03532900	5.91366400	6.33712600	N	18.64782900	5.69562200	2.80528100
O	9.27438200	6.69683200	7.59357400	C	20.13043600	-3.89344300	-0.47431900
N	11.72885300	-5.01866400	-7.73064900	H	19.58918300	-2.48174600	1.06008300
H	13.61670200	-4.16149600	-7.16099100	C	20.02944600	-3.05774300	-2.76978100
H	12.67970900	-3.24999200	-8.39329600	H	19.48103600	-0.98468600	-2.98606400
C	14.16874300	4.53526400	5.59335200	C	21.72837200	2.34026700	0.08379300
H	15.16491800	5.30329100	3.91155700	C	9.98645900	-9.17946900	-7.54144500
C	16.07101100	-3.39810600	-3.02542300	C	12.44052400	-9.10423700	-8.20196400
H	16.01818500	-4.61187800	-1.22486800	C	11.76281100	-8.81428900	-5.76816000
H	16.01833100	-1.96467900	-4.65226700	O	15.04743200	7.72840000	4.39031700
C	17.67178900	3.35793800	0.08301500	O	13.03053900	8.63792000	4.99910900
C	17.54276800	2.17259200	2.19931700	N	15.83227500	-7.16332400	-5.53797800
H	17.18202700	-1.16979100	0.11558300	H	17.70766500	-6.12459700	-5.49774300
C	9.27133000	8.05899100	6.96939000	H	16.65182600	-5.79478300	-6.92136800
C	12.15448000	-6.27155100	-7.30693900	C	18.16478600	6.13051100	4.03534000

H	19.41343900	6.21779900	2.34464000	O	19.27344500	-5.53014800	-4.13299000
C	20.26926700	-4.09928500	-1.85928600	C	20.65234200	-7.46518700	-3.66501500
H	20.32192200	-4.70219100	0.22764000	N	22.53227300	6.44765100	0.68738500
H	20.11190600	-3.23878100	-3.84298200	C	24.34244200	-3.81512100	1.10555700
C	22.21129300	3.13035900	-0.96663800	H	24.11027500	-1.86438300	1.99603800
C	21.63388700	2.88365500	1.37753900	C	24.00077300	-3.92786900	-1.31007700
H	21.39780200	-0.99462400	0.70981000	H	23.51910400	-2.06564500	-2.27259000
H	9.74094000	-9.07112200	-8.60517900	C	13.78582700	-10.52645700	-3.34475900
H	9.21333800	-8.63381800	-6.98236000	C	16.32052500	-10.55003000	-3.18710100
H	9.91211900	-10.23961100	-7.28119600	C	14.96882500	-8.95571100	-1.73591100
H	13.42070500	-8.65548700	-7.97237200	O	19.40130100	9.41541000	2.50776000
H	12.19963000	-8.82394300	-9.23425000	O	17.21644600	10.12173900	2.53523100
H	12.56127900	-10.19142200	-8.16738500	N	19.74233200	-8.45730400	-3.06484300
H	12.77235300	-8.41717600	-5.56057600	H	21.70158100	-7.59583800	-3.27942700
H	11.76779800	-9.87175700	-5.48737200	H	20.69359900	-7.64285200	-4.76747100
H	11.07266500	-8.28724300	-5.09916000	C	21.98186900	7.21781200	1.71164400
C	13.09900900	9.74702300	3.99201500	H	23.00706100	6.93408200	-0.10067900
C	16.00161600	-7.82156800	-4.32400800	C	24.25839200	-4.56490700	-0.08349300
H	14.92601200	-7.23187900	-6.03506000	H	24.59210000	-4.29674000	2.04924800
O	17.33874600	5.51057700	4.68908000	H	23.97350800	-4.50399600	-2.23917500
C	18.73131800	7.48216700	4.49942300	H	13.82906600	-10.97377900	-4.34638700
N	20.66942300	-5.40613800	-2.31104900	H	12.89458200	-9.88599200	-3.31847500
C	22.51486600	4.47654200	-0.75150500	H	13.64375200	-11.33256600	-2.61812300
H	22.32736300	2.70034500	-1.96094900	H	17.20740800	-10.00327500	-2.81765200
C	21.92824300	4.22469400	1.60610500	H	16.51739000	-10.80847500	-4.23472400
H	21.29634300	2.25643200	2.20429900	H	16.26380900	-11.48471800	-2.62040500
C	23.73459700	-1.81780700	-0.13128100	H	15.87840000	-8.35238700	-1.57537900
C	11.78387900	10.45624700	4.30480600	H	14.85820400	-9.62675500	-0.87906600
C	14.32113200	10.59843600	4.29290300	H	14.12201500	-8.25912100	-1.72995600
C	13.12003800	9.11951100	2.60655000	C	17.43597500	11.17311100	1.48955700
O	16.92124400	-7.65528400	-3.53219900	C	20.12083300	-9.09138000	-1.88789900
O	14.99840800	-8.73861300	-4.17085500	H	18.73480000	-8.36361800	-3.29903600
N	17.86427700	8.58661500	4.05089900	O	21.34623700	6.74559000	2.64408000
H	19.78953600	7.63179300	4.14740500	C	22.23886300	8.73163600	1.60627600
H	18.76273200	7.48837500	5.61642300	N	24.42750600	-5.99013300	-0.00226400
C	20.12512900	-6.04277500	-3.41926800	C	16.01961900	11.73104800	1.38062400
H	21.44938400	-5.84940000	-1.79267400	C	18.43616200	12.18367300	2.02725700
C	22.32616400	5.03510900	0.52811200	C	17.89537700	10.48766500	0.21125400
H	22.87292300	5.08877000	-1.57720200	O	21.25225500	-9.12734500	-1.42049600
H	21.82364700	4.64659900	2.61010900	O	19.04240200	-9.74946300	-1.35948400
C	24.07488300	-2.44487700	1.07478900	N	21.41494300	9.36199400	0.56569500
C	23.74612600	-2.55942200	-1.32691100	H	23.32096500	8.93938800	1.43233500
H	11.81319400	10.94229000	5.28758400	H	21.95830600	9.19376800	2.59074200
H	10.94859900	9.74183600	4.32859000	C	23.89274600	-6.89824700	-0.91348800
H	11.55509500	11.21942000	3.55437600	H	24.85952000	-6.35321900	0.87169200
H	15.24862200	10.13739500	3.90702100	H	15.73011900	12.27716000	2.28689300
H	14.46057300	10.73628000	5.37222500	H	15.28754900	10.92141500	1.25057900
H	14.24333000	11.59154200	3.83931400	H	15.92570900	12.41393600	0.53002500
H	14.05723100	8.56286200	2.43886600	H	19.43668700	11.73862800	2.14638400
H	13.03894300	9.87492900	1.81937200	H	18.14106600	12.56030200	3.01444200
H	12.29806100	8.40559100	2.47457900	H	18.53815700	13.04465300	1.35811500
C	15.05082500	-9.72661300	-3.04443600	H	18.91281300	10.07144400	0.30896800
C	18.26796900	9.35915900	2.96871000	H	17.92212800	11.18342000	-0.63469800
H	16.85406500	8.49896400	4.27156000	H	17.23609700	9.65433800	-0.05953600

C	19.22032800	-10.64879000	-0.17382700
C	21.71849700	9.17412900	-0.77731000
H	20.47350800	9.69393100	0.85307500
O	23.30276200	-6.56215900	-1.93216400
C	24.10584000	-8.38258200	-0.56805400
C	17.78471500	-11.13658600	0.00025500
C	20.18666600	-11.75909900	-0.55345500
C	19.69734000	-9.80487200	0.99871600
O	22.70799600	8.59905300	-1.21351200
O	20.73798600	9.75495300	-1.52976600
N	23.23895700	-8.82733300	0.53183600
H	25.17731800	-8.58391800	-0.33141300
H	23.84008800	-8.98524100	-1.47765500
H	17.47587000	-11.78757100	-0.82707200
H	17.08218300	-10.29121700	0.01599600
H	17.66524400	-11.69561100	0.93388500
H	21.20217700	-11.36920900	-0.72731100
H	19.88181900	-12.26313500	-1.47881000
H	20.25724600	-12.51803200	0.23291600
H	20.72923500	-9.44158400	0.85359100
H	19.69535900	-10.37381800	1.93502300
H	19.06653300	-8.91942600	1.14201400
C	20.87097000	9.81864400	-3.02498400
C	23.51149700	-8.44098000	1.83848800
H	22.29627800	-9.17787700	0.27079700
C	19.58684200	10.57182200	-3.35909600
C	22.12978500	10.60148700	-3.35718100
C	20.88568600	8.39508600	-3.55715200
O	24.50244200	-7.82493400	2.21091200
O	22.49828100	-8.87990000	2.64231300
H	19.57027500	11.56295600	-2.88831400
H	18.70143000	10.03210800	-2.99953200
H	19.48147800	10.71032700	-4.44075600
H	23.03509800	10.05633500	-3.04067000
H	22.15178600	11.57344700	-2.85008500
H	22.22024400	10.78394900	-4.43325700
H	21.79506400	7.86004900	-3.23727100
H	20.86403300	8.37376300	-4.65206900
H	20.02920600	7.81484100	-3.19471100
C	22.59201800	-8.71569400	4.13279000
C	21.28244600	-9.38316400	4.54195600
C	23.82313800	-9.46268700	4.61677100
C	22.62708100	-7.22780500	4.44112500
H	21.25469600	-10.43479800	4.22967500
H	20.41945600	-8.88862200	4.07797600
H	21.14624900	-9.35023700	5.62852900
H	24.74883700	-8.99018200	4.24687000
H	23.83508900	-10.50110800	4.26483400
H	23.88183000	-9.47971300	5.71022400
H	23.55714400	-6.76643700	4.07010200
H	22.57752000	-7.03818000	5.51879100
H	21.79439700	-6.69345600	3.96925000
H	-27.34343100	-0.31268100	1.33402700
H	23.85237100	0.31073300	-0.67387400

### CHCl<sub>3</sub>

C	0.00018500	0.00007600	0.45569300
H	0.00031000	-0.00040200	1.54127000
Cl	-0.98611000	-1.36839100	-0.08402700
Cl	1.67834300	-0.16958400	-0.08379000
Cl	-0.69231700	1.53797200	-0.08367800

### THF

C	1.17624200	0.46314600	-0.00000100
O	-0.00000100	1.24964900	0.00000300
C	-1.17624300	0.46314300	0.00000000
C	-0.77078500	-1.02362200	-0.00000200
C	0.77078700	-1.02362100	0.00000100
H	1.77065900	0.71922100	-0.88516300
H	1.77066500	0.71922100	0.88515600
H	-1.77066400	0.71921600	0.88516000
H	-1.77066300	0.71921900	-0.88515900
H	-1.16638000	-1.53709000	0.87920500
H	-1.16637700	-1.53708600	-0.87921300
H	1.16638000	-1.53708400	0.87921100
H	1.16638300	-1.53708700	-0.87920700

### 1b-16-mer<sub>RH</sub>

C	-14.32235100	-1.20319300	0.57756300
C	-12.98111900	-1.22461900	0.61657600
C	-12.21150500	-1.55611000	-0.59742300
C	-10.90600200	-1.30195100	-0.87130300
C	-10.03760300	-0.53563400	0.03762000
C	-8.70111600	-0.65359400	0.24422000
C	-7.86169800	-1.61735800	-0.48763000
C	-6.58901400	-1.42677900	-0.91535000
C	-5.84360500	-0.20712400	-0.56884100
C	-4.52179900	-0.09803100	-0.29161900
C	-3.58705200	-1.22358100	-0.47401300
C	-2.31156500	-1.13294400	-0.91864700
C	-1.69421200	0.18752100	-1.12363700
C	-0.42716400	0.55137000	-0.81610200
C	0.56935900	-0.45012500	-0.41621300
C	1.90180000	-0.44964800	-0.65897000
C	2.56099600	0.73015300	-1.23294200
C	3.79649100	1.23740800	-0.98321800
C	4.77982800	0.48026700	-0.21132000
C	6.12854200	0.59943700	-0.03933000
C	6.84418200	1.73534300	-0.61356900
C	8.12295000	2.19555500	-0.60951500
C	9.27382600	1.52623100	0.00664200
C	9.54417500	0.22029000	-0.13833400
H	-14.90625600	-0.97942200	1.46481300
C	-12.24852200	-0.90997400	1.87762200
C	-12.31632300	0.36200200	2.45041200
C	-11.35307300	-1.83318800	2.42353600
H	-12.78982900	-2.04866700	-1.37875600
C	-11.45617300	0.72182400	3.48196000

H	-13.00386900	1.09514400	2.03734000	H	-5.74570600	0.21398900	3.76383500
C	-10.50161300	-1.49634200	3.46650200	C	-5.97422100	-3.81759600	-1.43824100
H	-11.27943700	-2.82265200	1.97988700	C	-5.20664100	-2.07580900	-2.89467700
C	-10.29990000	-1.81136400	-2.13227700	H	-6.44149900	0.67823000	-0.38490200
C	-10.52226600	-0.19308300	3.97759700	N	-6.22230700	2.88700500	3.97069700
H	-11.48792200	1.72741200	3.89415200	C	-5.25048300	-4.74407900	-2.17639300
H	-9.79829000	-2.21542200	3.86172600	H	-6.53004700	-4.14181100	-0.56240200
C	-10.39783500	-3.15918200	-2.48780500	C	-4.47648600	-2.98863100	-3.64418700
C	-9.47749300	-0.98820800	-2.90969700	H	-5.17756100	-1.02633200	-3.17414800
N	-9.60993600	0.25403300	4.95556300	C	-4.04495900	1.18888200	0.28955900
C	-9.63386300	-3.67664800	-3.52574600	C	-5.59373900	2.65053600	5.15538200
H	-11.02125200	-3.82231600	-1.89423400	H	-6.47849700	3.85165900	3.80751200
C	-8.71736500	-1.48380900	-3.95906700	C	-4.47341200	-4.33821800	-3.26812300
H	-9.38692800	0.06187800	-2.64513100	H	-5.25954700	-5.79246900	-1.88648900
C	-8.90211700	-0.53031300	5.82394400	H	-3.89359800	-2.66422500	-4.49504600
H	-9.39487100	1.24783600	4.96013800	C	-4.39667700	2.42775000	-0.25299200
C	-8.75756900	-2.85493100	-4.24188200	C	-3.23666100	1.17402400	1.43325500
H	-9.68133000	-4.73915200	-3.75373600	H	-3.99451900	-2.22185200	-0.35267100
H	-8.06018300	-0.83849500	-4.52450400	O	-5.25397000	1.55033100	5.55723000
O	-8.95141000	-1.74482500	5.87030700	C	-5.34574300	3.90066600	5.99783300
C	-8.00143300	0.25546200	6.77916800	N	-3.70871800	-5.31887800	-3.91991000
N	-7.93961700	-3.46565100	-5.20863200	C	-3.95262300	3.61156800	0.32711900
N	-8.70122200	1.26707200	7.55512400	H	-5.00395500	2.46180200	-1.15359900
H	-7.18998700	0.73384300	6.22066900	C	-2.80114600	2.34806700	2.02962000
H	-7.56363300	-0.47061600	7.46412900	H	-2.93859000	0.21745500	1.85426800
C	-6.93265700	-2.90428300	-5.94191000	C	-1.54933300	-2.37516200	-1.21704700
H	-8.03122900	-4.46951700	-5.29892300	N	-6.37564900	4.90106600	5.80569500
C	-8.84048000	2.53685200	7.13799300	H	-4.37660900	4.32880100	5.71942700
H	-9.10554500	1.02478100	8.44822100	H	-5.30051400	3.56239700	7.03728500
O	-6.62914400	-1.72713600	-5.94432900	C	-3.05641000	-5.22675600	-5.11427900
C	-6.14175100	-3.89396100	-6.79824200	H	-3.72613600	-6.24396300	-3.51060000
O	-8.48367800	2.95342900	6.03836300	C	-3.15601400	3.58040900	1.47223700
O	-9.43277100	3.30224100	8.06847900	H	-4.22286500	4.57100300	-0.10718200
N	-6.85426000	-5.11636500	-7.12169300	H	-2.18941600	2.32321000	2.92194100
H	-5.22374300	-4.15508100	-6.26006000	C	-1.45582500	-3.42801600	-0.30200900
H	-5.84197100	-3.35743500	-7.70238700	C	-0.86211900	-2.49252400	-2.43072000
C	-9.64409800	4.66308100	7.69531400	H	-2.37058500	0.98974900	-1.39568100
C	-6.32595300	-6.35081100	-6.90128200	C	-6.10841100	6.20504000	5.58941300
H	-7.59466000	-5.07766100	-7.81033800	H	-7.34423900	4.60126300	5.88253100
O	-5.33687800	-6.59222100	-6.23497300	O	-2.98707800	-4.21744200	-5.79499800
O	-7.07425400	-7.29408500	-7.50162500	C	-2.37461800	-6.51330500	-5.57036800
C	-6.61900600	-8.63131500	-7.31160900	N	-2.71809900	4.80155900	2.03553700
H	-10.54392400	0.18735600	0.66457900	C	-0.67832300	-4.54598300	-0.58190100
C	-8.09123200	0.23546600	1.27236000	H	-1.96445000	-3.34841800	0.65528000
C	-8.43035800	1.59093300	1.33732800	C	-0.09970100	-3.61272800	-2.73109800
C	-7.13559800	-0.24222100	2.17762400	H	-0.91509300	-1.67690300	-3.14688600
H	-8.35317600	-2.52847700	-0.81468900	C	-0.12057500	2.00638600	-0.78061600
C	-7.81619100	2.43669700	2.24753300	O	-4.99883300	6.70318400	5.49528600
H	-9.15595300	1.99377300	0.63631600	O	-7.25411700	6.91291800	5.47776000
C	-6.50555400	0.59308900	3.09369000	N	-3.03242500	-7.70668300	-5.07759600
H	-6.85168200	-1.29048100	2.13648100	H	-1.33690800	-6.50934200	-5.21642300
C	-5.93984700	-2.45881200	-1.76596800	H	-2.37182500	-6.48059800	-6.66332100
C	-6.83397400	1.95389900	3.11887000	C	-2.61968900	5.04971300	3.37196700
H	-8.07778500	3.49235500	2.26825300	H	-2.49600400	5.57025500	1.40810100

C	0.00588900	-4.64805200	-1.79560500	C	-4.72664000	9.30699000	0.71279700
H	-0.59535700	-5.35138800	0.14387800	C	0.96079300	-8.83571300	-1.08904800
H	0.41892500	-3.69158700	-3.67698100	H	0.08737800	-9.14061300	-2.90088000
C	-0.42043500	2.86444400	-1.84092300	O	0.20617900	6.46887300	1.76410600
C	0.42654500	2.55558100	0.38468500	C	0.33170300	8.42912800	0.37167400
H	0.17301800	-1.35950600	0.01889000	N	4.34217500	-5.48729900	0.41891500
C	-7.06998100	8.29745100	5.18835300	C	4.17442300	4.37934000	-3.10832700
C	-2.34830000	-8.74522100	-4.54840700	H	4.24149300	2.27136800	-3.51733000
H	-3.99155100	-7.85653200	-5.37290200	C	3.86106300	5.01420700	-0.79808000
O	-2.81433100	4.21311000	4.24046400	H	3.71529100	3.38364900	0.58416900
C	-2.27534000	6.50163600	3.70809400	C	6.72527900	-0.57922900	0.67261400
N	0.78808000	-5.79899800	-2.03293400	O	1.71551600	-8.18741200	-0.36605200
C	-0.18881100	4.23085500	-1.73302100	O	0.09411100	-9.75057100	-0.60671000
H	-0.82741000	2.45382400	-2.76106700	N	-0.72884800	8.80378300	-0.54822900
C	0.64033200	3.91980200	0.51304400	H	1.29284800	8.74179100	-0.04610500
H	0.68125300	1.89406300	1.20873500	H	0.15984500	8.92176100	1.32903500
C	2.61150200	-1.72675100	-0.36263200	C	4.43548500	-6.56484200	-0.40819300
O	-1.15259100	-8.76554600	-4.31338900	H	4.75867400	-5.59346000	1.34018600
O	-3.17626100	-9.77819200	-4.28216400	C	4.02471600	5.37676000	-2.13964800
N	-3.34546000	7.41399000	3.34036000	H	4.30581300	4.66465200	-4.14967600
H	-1.35658200	6.79533300	3.19177200	H	3.73648900	5.77884300	-0.04309100
H	-2.13940000	6.55713400	4.78798400	C	7.36596000	-0.54418400	1.91545800
C	0.96610700	-6.39890700	-3.24742700	C	6.52563900	-1.83254800	0.08672500
H	1.20440400	-6.26351000	-1.22951400	C	0.11443800	-9.90171200	0.81006400
C	0.32835000	4.76918400	-0.55363800	C	-0.53053700	8.80968400	-1.87640500
H	-0.42386500	4.89288100	-2.56298000	H	-1.68098800	8.71162800	-0.20346700
H	1.04556000	4.33487300	1.42626300	O	4.13225100	-6.56117400	-1.59093700
C	2.64057800	-2.26398000	0.92660800	C	4.91292200	-7.82678000	0.31201800
C	3.17517300	-2.46580500	-1.40608300	N	4.06015000	6.71610800	-2.57575000
H	1.90901800	1.37223400	-1.81415600	C	7.76011000	-1.71846800	2.54641100
C	-2.54218300	-10.90259500	-3.67733700	H	7.55522000	0.41110500	2.39765700
C	-3.45389000	7.93105000	2.11179800	C	6.92774000	-3.01631100	0.69263300
H	-4.11143300	7.51978300	3.99978300	H	6.02685200	-1.88649100	-0.87685100
O	0.58691300	-5.93104600	-4.30816200	O	0.54363500	8.59656900	-2.43328000
C	1.66586500	-7.75710300	-3.16444900	O	-1.66457600	9.08528100	-2.54766400
N	0.51805000	6.16587800	-0.47903500	N	3.97256500	-8.24456100	1.33857000
C	3.22342100	-3.50033200	1.16510300	H	5.88245200	-7.63467800	0.78088800
H	2.21046200	-1.69756900	1.74802300	H	5.00325000	-8.61643300	-0.43464400
C	3.73770200	-3.71792100	-1.18611900	C	3.59943600	7.81579600	-1.91522700
H	3.15394000	-2.05771000	-2.41319700	H	4.50950200	6.89395500	-3.47049800
C	3.97538100	2.65948200	-1.41874000	C	7.54014600	-2.96679800	1.94709400
O	-2.67434400	7.73130700	1.18165800	H	8.25760400	-1.67133600	3.51304100
O	-4.54640000	8.71661400	1.99645300	H	6.76197500	-3.96437800	0.20167300
N	0.88593900	-8.73403100	-2.42151000	C	-1.53201400	9.10654200	-3.96563600
H	2.64441000	-7.64412900	-2.68824500	C	4.06867900	-7.78523000	2.59993200
H	1.78225700	-8.11666300	-4.18665400	H	3.04744700	-8.51926900	1.01510900
C	0.36002100	6.92466500	0.64276700	O	3.16873600	7.81242300	-0.77270800
H	0.73298800	6.66273100	-1.33947100	C	3.63562500	9.08984200	-2.76149800
C	3.76542100	-4.23912000	0.11152200	N	7.94071500	-4.12277200	2.64709200
H	3.25418200	-3.90901500	2.17206700	O	4.99081100	-7.11034400	3.04619800
H	4.14965100	-4.29417800	-2.00373000	O	3.01195200	-8.17068400	3.34179400
C	4.13895100	3.03666000	-2.75297200	N	2.85570500	8.97486700	-3.98104500
C	3.84733600	3.66651100	-0.45727800	H	4.67347800	9.31427900	-3.02375400
H	4.35401600	-0.39565600	0.25989600	H	3.21800500	9.89170300	-2.15225800





C	0.94028600	-12.67144100	-0.94752400	H	-3.68126600	-9.13110200	2.95017500
C	0.96581000	-11.48803700	-0.28308200	C	7.19133500	-6.20939600	-7.24642300
C	1.96759400	-10.43988300	-0.53719800	H	5.26502900	-6.93067400	-7.23599500
C	1.87184200	-9.08981900	-0.39854200	O	-1.75026600	-9.46169900	5.42873000
C	0.65979700	-8.41791300	0.08922200	C	-3.97678300	-8.57797500	5.35788000
C	0.52120700	-7.20995500	0.68975800	O	8.26054400	-6.07461900	-6.67003200
C	1.64906900	-6.26706600	0.81398500	O	6.99469400	-5.91940600	-8.54231000
C	1.60848600	-4.93768100	0.55568100	N	-5.19071500	-9.33918500	5.11209800
C	0.33418300	-4.25260000	0.29055100	H	-4.10791300	-7.56456600	4.96474100
C	-0.03367800	-2.97366000	0.56069600	H	-3.81461700	-8.51063300	6.43358700
C	0.90421600	-1.97900800	1.06845400	C	8.16988500	-5.53477800	-9.25833900
C	0.82210200	-0.63020700	1.25877500	C	-5.96069200	-9.14270000	4.03106700
C	-0.41045300	0.13596800	1.10641500	H	-5.43798500	-10.09341100	5.73746500
C	-0.68267600	1.47503500	1.03735500	O	-5.68973200	-8.37697300	3.10900300
C	0.33646700	2.50615700	1.19174300	O	-7.07701200	-9.89505400	4.07210200
C	0.30405100	3.86347000	1.05508700	C	-7.75793100	-10.04155300	2.82185600
C	-0.89164500	4.57093500	0.59952300	H	2.91123800	-10.78938400	-0.93503900
C	-1.32395100	5.82194900	0.90108200	C	3.07480800	-8.31311600	-0.81609200
C	-0.48298600	6.72216600	1.71026700	C	4.35003900	-8.69815600	-0.38873700
C	-0.23752400	8.02901900	1.46758000	C	2.96598900	-7.21192500	-1.67520700
C	-0.97025500	8.74411700	0.40845600	H	-0.24839800	-9.00475100	0.02898200
C	-1.54079000	9.94525900	0.57608200	C	5.48517600	-8.00357600	-0.78932300
H	2.41227300	-14.84928200	-3.16002300	H	4.44844900	-9.54263200	0.28746600
C	2.70501800	-12.21103000	-2.75441300	C	4.09441800	-6.50974400	-2.08040300
C	4.08775700	-12.26285600	-2.56614400	H	1.98304400	-6.90072000	-2.01948200
C	2.17567200	-11.16420900	-3.51411400	C	-0.82729000	-6.83314100	1.20325000
H	0.19016900	-13.39091500	-0.61917200	C	5.35582000	-6.89931000	-1.62836900
C	4.90863200	-11.25417300	-3.06004300	H	6.46974000	-8.30356300	-0.44812700
H	4.51525200	-13.06940000	-1.97679100	H	4.00801800	-5.65803000	-2.75029500
C	2.98524500	-10.16122600	-4.03073500	C	-1.97774400	-6.97795400	0.41876200
H	1.10038700	-11.10874900	-3.66171700	C	-0.97414300	-6.28835700	2.48346700
C	-0.05418200	-11.20061800	0.76395600	H	2.63085000	-6.70516700	0.96445600
C	4.36031400	-10.18582900	-3.77313300	N	6.50319200	-6.16848500	-2.04078200
H	5.98000100	-11.27897100	-2.87877900	C	-3.21318600	-6.53608700	0.87312500
H	2.56178600	-9.34756900	-4.60495100	H	-1.89181700	-7.39611500	-0.58068700
C	-1.41990500	-11.18269800	0.46841200	C	-2.20951900	-5.86359700	2.96225900
C	0.35510800	-10.74221400	2.02018800	H	-0.09449100	-6.17122100	3.11098200
N	5.22076100	-9.13853900	-4.16736500	C	2.89400100	-4.20852000	0.37842800
C	-2.32980800	-10.63792800	1.36745700	C	7.56925500	-6.75615100	-2.62425300
H	-1.76014100	-11.52611600	-0.50484000	H	6.50473800	-5.15064000	-1.94051400
C	-0.54077500	-10.20936000	2.93458600	C	-3.33753000	-5.95213900	2.13779000
H	1.41510300	-10.74256500	2.25934200	H	-4.09058700	-6.61795100	0.23688500
C	5.04212000	-8.31645300	-5.23407600	H	-2.30040400	-5.43420500	3.95159800
H	6.04249200	-8.96837200	-3.58450800	C	3.90012600	-4.18131400	1.34468600
C	-1.89465200	-10.11520800	2.58976600	C	3.10125800	-3.53065100	-0.83208800
H	-3.38541600	-10.58390300	1.11156500	H	-0.45761000	-4.88631700	-0.09254600
H	-0.20299000	-9.83222500	3.88921200	O	7.69144200	-7.97224500	-2.78535400
O	4.13536300	-8.39100000	-6.04799100	C	8.60842300	-5.80250500	-3.19179700
C	6.10261200	-7.22614800	-5.33986800	N	-4.59801100	-5.42914700	2.49497800
N	-2.84700300	-9.48485300	3.41151400	C	5.07538300	-3.46206600	1.12570200
N	6.05006700	-6.64174600	-6.65871000	H	3.74723500	-4.69789400	2.28790200
H	7.10148200	-7.62811100	-5.14715500	C	4.27173800	-2.82716500	-1.06024200
H	5.88780400	-6.47693900	-4.56389600	H	2.32197500	-3.54973200	-1.59008600
C	-2.72917200	-9.21991300	4.74927100	C	-1.48292000	-2.66906000	0.35950300

N	9.92445000	-6.37753300	-3.05627700	H	5.01074300	0.70833600	-0.20652500
H	8.58857600	-4.82933100	-2.70207500	C	-2.70464400	1.28039300	-0.40906000
H	8.35420700	-5.65939400	-4.25351900	C	-2.90371200	2.61846600	1.57045800
C	-5.08671400	-5.27678300	3.75652700	H	1.30684800	2.11934600	1.46461700
H	-5.20985200	-5.13821100	1.73341300	C	-10.01845100	-6.28111800	0.83481800
C	5.25401200	-2.77567900	-0.06982200	C	10.63533100	-1.31991300	-0.56224400
H	5.85065200	-3.42215800	1.88468000	H	9.91863200	-2.89292600	-1.66066800
H	4.43116100	-2.29655900	-1.99450300	O	-6.51977100	-3.55461500	0.96284100
C	-2.00321000	-2.30016600	-0.88059300	C	-7.93396200	-1.71087900	0.31488200
C	-2.34671900	-2.78249000	1.45306100	N	5.86977400	1.94496200	2.01758700
H	1.89080400	-2.38069200	1.26015900	C	-4.02732000	1.55571400	-0.74932400
C	10.91951700	-5.72337400	-2.42838600	H	-2.10528700	0.65827300	-1.06714100
H	10.01833600	-7.37481900	-3.20291200	C	-4.21971000	2.90922500	1.23769000
O	-4.44438000	-5.44053700	4.78134100	H	-2.47154500	3.04541100	2.47110800
C	-6.56826800	-4.91400400	3.79886000	C	1.56493300	4.58243500	1.39671300
N	6.42361000	-1.99153700	-0.30192400	O	10.49135000	-0.21236000	-0.05464500
C	-3.35999800	-2.02101100	-1.01988100	O	11.76042400	-2.04157700	-0.41562600
H	-1.33967000	-2.22176400	-1.73759500	N	-9.02479800	-2.64372600	0.33203500
C	-3.69823300	-2.49637900	1.32434900	H	-7.96142600	-1.12884600	-0.60664500
H	-1.94372800	-3.07797600	2.41728100	H	-7.99421900	-0.99360000	1.14891300
C	2.15202400	0.01005100	1.52362200	C	7.06878700	1.57218900	1.51859000
O	10.88308200	-4.55038700	-2.07311400	H	5.82334900	2.85053500	2.49011100
O	11.97502500	-6.52959100	-2.23322200	C	-4.79354800	2.37593700	0.07697600
N	-7.32750600	-5.92885700	3.08485100	H	-4.45730600	1.15405200	-1.65910900
H	-6.74804200	-3.95206200	3.30855100	H	-4.81759000	3.55082500	1.87941100
H	-6.85664400	-4.84216000	4.85035900	C	2.29225000	4.22123800	2.53678500
C	7.31090400	-2.33053100	-1.25477000	C	2.06857600	5.62002700	0.60079900
H	6.58331900	-1.14683900	0.25256500	H	-1.55951000	3.96153300	0.00881900
C	-4.20503700	-2.10562400	0.08505700	C	12.79987500	-1.36493400	0.29848300
H	-3.77133800	-1.72973800	-1.98286600	C	-10.21252400	-2.29988900	-0.19248700
H	-4.36353700	-2.56342500	2.17862900	H	-8.96253100	-3.44062800	0.96511000
C	2.51917300	0.55587800	2.75676000	O	7.29310100	0.51614300	0.93167400
C	3.07899100	0.04522200	0.47822600	C	8.16087100	2.60783300	1.73001600
H	-1.29034000	-0.48697000	1.01135400	N	-6.14404000	2.69296800	-0.22199300
C	13.11582400	-5.93908500	-1.61412100	C	3.49519400	4.83678100	2.86047400
C	-8.45236800	-5.59861500	2.42997900	H	1.89496600	3.45433800	3.19497700
H	-6.89133500	-6.83330200	2.90458600	C	3.26899100	6.24328600	0.91334500
O	7.24493700	-3.37403800	-1.90836000	H	1.51034900	5.93345000	-0.27729800
C	8.42417400	-1.33694200	-1.53175400	C	-2.68623500	6.22671400	0.46046100
N	-5.56555200	-1.73514000	-0.05083400	O	-10.45441900	-1.25152100	-0.78205000
C	3.76160100	1.15980900	2.92031400	O	-11.12178800	-3.28021000	-0.01022000
H	1.81724600	0.52696800	3.58637400	N	9.45132600	2.05278100	1.42335200
C	4.31904800	0.65414100	0.62756300	H	8.12579500	2.98262900	2.75784000
H	2.80528200	-0.38947700	-0.47822300	H	7.93837600	3.47024500	1.08462800
C	-2.11636300	1.80196600	0.74576000	C	-7.05049900	1.81039200	-0.70890300
O	-8.99534000	-4.50374000	2.48936800	H	-6.45967800	3.65049500	-0.05951400
O	-8.93380400	-6.62911500	1.70441200	C	3.99881700	5.84315500	2.03720400
N	9.71520600	-1.95514600	-1.31061400	H	4.03867300	4.55142000	3.75331900
H	8.35567000	-0.45589200	-0.89257100	H	3.65694500	7.03524400	0.27862100
H	8.31517200	-1.02465000	-2.57813900	C	-3.30722100	5.63539700	-0.65006300
C	-6.60605700	-2.44693400	0.43724500	C	-3.41760100	7.17622300	1.18733800
H	-5.77518500	-0.84493300	-0.50727400	C	-12.40647900	-3.04429000	-0.58788700
C	4.65689500	1.23065400	1.85055300	C	10.53463900	2.81797100	1.63418300
H	4.04520500	1.58995700	3.87734800	H	9.53574000	1.12084700	1.01576700

O	-6.77094800	0.68333700	-1.10929100	H	1.64297700	9.63658700	0.44874400
C	-8.50114100	2.27539400	-0.61680500	C	-2.59145400	10.41997800	-0.34089600
N	5.24148000	6.46736300	2.31417300	C	3.20594400	9.57649000	3.45569100
C	-4.60166500	5.96963600	-1.01469700	H	2.41251100	8.70275500	5.24983600
H	-2.76744600	4.91687700	-1.25900200	H	3.73663600	10.40203400	1.54450000
C	-4.71045900	7.52965200	0.81883400	C	-2.49261800	10.27772000	-1.72869700
H	-2.96121900	7.64405500	2.05421400	C	-3.80368000	10.86568400	0.20075500
O	10.49550900	3.95774600	2.09183300	N	4.39803800	9.98191200	4.10124800
O	11.67418500	2.20618100	1.28017500	C	-3.59016700	10.51579900	-2.54490500
N	-9.36756900	1.55470500	-1.50988200	H	-1.55017300	9.96117400	-2.16642400
H	-8.57893400	3.34277600	-0.83125600	C	-4.91235800	11.08816100	-0.60475100
H	-8.80892300	2.12507600	0.42824800	H	-3.88926100	10.99382700	1.27727900
C	6.34643300	5.80163000	2.73002100	C	5.64165500	9.77364600	3.60129300
H	5.33437400	7.46273100	2.09929800	H	4.35298000	10.18859700	5.10001100
C	-5.30761900	6.92674300	-0.28462200	C	-4.81051900	10.89097600	-1.98252000
H	-5.06716600	5.50395600	-1.87703300	H	-3.51713000	10.38819300	-3.62174900
H	-5.26350500	8.27130700	1.38774400	H	-5.85865000	11.40009200	-0.17773500
C	12.85771200	2.98686800	1.45910500	O	5.87826500	9.32500000	2.48237300
C	-10.18738400	2.20648900	-2.35831500	C	6.75974100	10.07608200	4.59929000
H	-9.49832000	0.55011600	-1.40454200	N	-5.92896200	11.07473900	-2.83194200
O	6.36809700	4.61586300	3.04508800	N	6.85169700	9.02385300	5.58928500
C	7.62961100	6.63948300	2.72132800	H	6.58455300	11.03017200	5.10649300
N	-6.61160000	7.31292600	-0.69774400	H	7.70243600	10.12380400	4.05179000
O	-10.25842000	3.42463900	-2.49266200	C	-7.14831200	10.52632400	-2.61139100
O	-10.93558400	1.34763100	-3.06343200	H	-5.77532100	11.47424300	-3.75926600
N	8.76001000	5.93619000	3.25712100	C	6.02668900	9.00521400	6.65896800
H	7.47326500	7.56564800	3.27762900	H	7.48221000	8.23495000	5.43421500
H	7.83527500	6.93686300	1.68649300	O	-7.46528200	9.93003900	-1.58411300
C	-7.58037100	6.41518700	-0.96636300	C	-8.12774300	10.69009800	-3.77378200
H	-6.79658600	8.30441300	-0.86826600	O	5.13279400	9.81138600	6.87527700
C	-11.81619100	1.95713500	-4.00479100	O	6.32464500	7.97954100	7.47655300
C	9.22011700	6.17325700	4.50071700	N	-7.70849400	9.96735300	-4.95637600
H	9.19365500	5.17011600	2.73839400	H	-8.23829300	11.74987600	-4.02541200
O	-7.46582200	5.20339200	-0.78629300	H	-9.08855800	10.29017500	-3.44887500
C	-8.88249400	6.97726100	-1.52810600	C	5.55956000	7.93468300	8.68018200
O	8.75509100	6.98070500	5.29857900	C	-6.78981800	10.47877600	-5.80280400
O	10.30195100	5.42741000	4.77084600	H	-8.03869700	9.01452400	-5.07463100
N	-9.33243300	6.13964900	-2.61594700	O	-6.22078300	11.55254100	-5.64912100
H	-8.76168700	8.00041700	-1.88855600	O	-6.56204600	9.65856500	-6.84037800
H	-9.62716900	6.97665900	-0.72281000	C	-5.60632900	10.14460200	-7.78090400
C	10.93685500	5.72150400	6.01691700	H	1.15435000	-15.16984700	-1.83274100
C	-9.45138800	6.60869200	-3.86677400	H	-1.38163300	10.49579800	1.50361100
H	-9.46634000	5.13939500	-2.45854000	H	8.93771800	-6.30602000	-9.16975100
O	-9.24268900	7.76899400	-4.21825600	H	8.56218900	-4.58870000	-8.87970300
O	-9.85877400	5.64673700	-4.71291600	H	7.85363000	-5.42500400	-10.29421800
C	-10.01279700	6.05594600	-6.07178900	H	13.66391600	-6.76028800	-1.15327600
H	0.11131200	6.24439400	2.48245500	H	12.81099400	-5.20856000	-0.86142600
C	0.85698100	8.69333600	2.21372700	H	13.74099600	-5.45570400	-2.36909000
C	1.07447200	8.45922000	3.57585400	H	13.58188100	-2.10801400	0.44580000
C	1.81158300	9.43157500	1.50222800	H	12.42554200	-0.99109800	1.25284100
H	-1.23028900	8.17178100	-0.47988700	H	13.17744400	-0.52745800	-0.29671700
C	2.23630200	8.89934600	4.19541900	H	13.67753500	2.34656500	1.13624400
H	0.33109600	7.91211700	4.14842000	H	12.97366300	3.26485900	2.50928600
C	2.98462900	9.86123700	2.10734800	H	12.81706700	3.88895100	0.84239700



C	-7.61467200	3.05800300	0.36759000	H	8.14037500	-4.76091200	0.84923700
C	-8.94126900	2.87826100	0.35528800	C	9.26973800	0.64139600	-0.89560500
H	15.22794100	-5.01428400	-0.76778600	H	10.33584500	-0.53367200	0.54778100
C	12.84209300	-3.84066800	-1.22709100	C	7.76984000	-0.56480400	-2.36019200
C	13.35619300	-2.54418800	-1.29666300	H	7.68617100	-2.67967900	-2.04409300
C	11.80628000	-4.18804200	-2.09765900	C	5.75089800	-4.05170700	1.51476900
H	12.50920600	-5.93150000	1.54865600	C	8.29269200	0.64988200	-1.89884900
C	12.77219200	-1.59579400	-2.12840800	H	9.70573500	1.58416100	-0.57320400
H	14.16596400	-2.25595700	-0.63203500	H	7.04909800	-0.56714200	-3.16747000
C	11.22092600	-3.25814200	-2.94674200	C	5.31283200	-5.21913200	0.88146900
H	11.39400100	-5.19260000	-2.05100600	C	5.04250400	-3.60916000	2.63632900
C	10.11315700	-5.14477900	2.17837800	H	7.26773000	-1.04692900	0.73983300
C	11.66857200	-1.93125000	-2.91995800	N	7.89387000	1.90577400	-2.37737800
H	13.13941300	-0.57230500	-2.13382200	C	4.13096200	-5.83793200	1.27602700
H	10.38641600	-3.53022400	-3.57748600	H	5.85183400	-5.58832300	0.01283300
C	9.72164500	-6.48228900	2.07032700	C	3.86695400	-4.21986500	3.04924900
C	9.47256400	-4.34994300	3.13473000	H	5.38361100	-2.71951100	3.15790300
N	11.02258300	-0.88800800	-3.60947900	C	5.16633000	0.18556100	-0.07697200
C	8.64647700	-6.96711400	2.80298900	C	7.13788900	2.20548100	-3.47422500
H	10.20494300	-7.12158500	1.33628500	H	8.30490700	2.70817300	-1.90214600
C	8.40732400	-4.82099300	3.88910600	C	3.37027200	-5.30978300	2.32571700
H	9.76883400	-3.30899900	3.23470300	H	3.75940200	-6.70502000	0.73512600
C	10.05692300	-0.99496600	-4.57063200	H	3.31375000	-3.83223800	3.89415800
H	11.22391000	0.05696900	-3.28917200	C	5.31295700	1.22599200	0.84250600
C	7.94242600	-6.12517200	3.67195200	C	4.75235300	0.50348100	-1.37476900
H	8.30615200	-7.98975600	2.65888800	H	4.16790500	-3.12770600	0.16870100
H	7.89184900	-4.17780900	4.58836100	O	6.61268000	1.38818400	-4.21311000
O	9.66278800	-2.04290800	-5.05644100	C	7.08219800	3.71349100	-3.74162800
C	9.53982300	0.36160900	-5.05204100	N	2.09648900	-5.86915600	2.57151600
N	6.75524700	-6.62566900	4.22708100	C	4.92695300	2.52253900	0.50786600
N	10.54056600	1.09061700	-5.80594600	H	5.64621100	1.00375100	1.85282400
H	9.25459300	0.98188700	-4.20054800	C	4.38018000	1.79176400	-1.72780300
H	8.65646700	0.18519200	-5.66914600	H	4.64679400	-0.29373200	-2.10537400
C	5.82435100	-5.95765900	4.97000300	C	1.69434600	-2.73691400	0.40122900
H	6.51688600	-7.58828400	4.00197400	N	8.37791100	4.22732400	-4.16153400
C	11.40287500	1.90699100	-5.16733600	H	6.74262300	4.23994000	-2.84301500
H	10.72715900	0.83200100	-6.77947400	H	6.35423000	3.88549700	-4.53447000
O	5.97762300	-4.84804700	5.45501600	C	1.35126900	-5.74628200	3.70489600
C	4.53076800	-6.75242600	5.17233300	H	1.63119700	-6.31031500	1.77907600
O	11.39784100	2.15063100	-3.96836300	C	4.40957200	2.80272200	-0.75987500
O	12.29066600	2.43850200	-6.03834200	H	4.98296000	3.31827700	1.24658500
N	4.64859100	-7.70629400	6.25766200	H	4.02660700	2.00476600	-2.72756100
H	4.25356700	-7.27443500	4.24894600	C	1.57631300	-3.75996300	-0.54272800
H	3.74115300	-6.03853900	5.41441900	C	0.75422500	-2.68448100	1.43660100
C	13.13699600	3.44891100	-5.49862600	H	3.01776400	0.46281600	0.59415800
C	5.24839400	-8.89583600	6.05824000	C	9.33870100	4.53500900	-3.26933400
H	4.16223700	-7.49483000	7.12787000	H	8.52110300	4.41625200	-5.15346300
O	5.74969800	-9.26525400	5.00641200	O	1.72832700	-5.20465900	4.73628100
O	5.22356600	-9.65334800	7.17617200	C	-0.02489900	-6.40374500	3.60879400
C	5.81212100	-10.94227100	7.03049400	N	3.86767200	4.08642000	-1.00384400
H	11.25380900	-2.68807800	0.04141500	C	0.49126900	-4.62712500	-0.51285300
C	9.03224900	-1.75604700	-0.64922000	H	2.30903200	-3.83686500	-1.34191200
C	9.63307800	-0.54814600	-0.28120500	C	-0.33768600	-3.54153100	1.48328000
C	8.14619200	-1.74586700	-1.73137600	H	0.84695100	-1.90454600	2.18796300

C	0.94123700	1.72843400	-0.02779500	C	-0.30545500	6.72744300	-0.46895700
O	9.24442100	4.39512700	-2.05669700	H	-0.49175700	5.97228000	1.41067100
O	10.43107800	5.05685600	-3.86943000	C	-4.74912700	-2.82968600	-0.91717800
N	0.06660900	-7.84359200	3.48315700	H	-4.21969400	-2.64743100	-2.99197900
H	-0.57981000	-5.99903700	2.75782600	H	-4.96698100	-2.92470900	1.22429700
H	-0.56824000	-6.15832400	4.52354700	C	-2.59606100	3.15945500	2.48301900
C	3.76324000	4.69086400	-2.22171200	C	-3.62652800	3.95588400	0.46844200
H	3.41762000	4.55638900	-0.22031700	H	-3.99086300	0.39441400	-0.98873500
C	-0.50479300	-4.48550000	0.46202700	C	4.18137100	8.43130600	1.80446100
H	0.37544000	-5.39346700	-1.27565000	C	-2.46969200	-8.10247300	-0.67841800
H	-1.08741300	-3.45129500	2.25856300	H	-3.21443100	-8.48598600	1.19856800
C	1.34007600	2.47052300	1.09023900	O	-0.03193400	6.59270300	-1.65508400
C	0.28549900	2.39905700	-1.06594000	C	-0.73331200	8.06826300	0.11649600
H	0.10647600	-1.50024000	-0.96588600	N	-5.98318400	-3.44810700	-1.22222600
C	11.52463700	5.28343800	-2.97965400	C	-2.78812600	4.40613800	3.06737400
C	0.19404700	-8.43627200	2.27977300	H	-2.13752300	2.35833800	3.05716200
H	0.16389500	-8.40333100	4.33534900	C	-3.81432800	5.20893200	1.03301800
O	4.19478900	4.21920000	-3.26482300	H	-3.97877400	3.76991500	-0.54298100
C	3.08697200	6.05853500	-2.18075100	C	-6.51295600	0.47978200	-0.44536300
N	-1.64892100	-5.28096000	0.31450700	O	-2.24375800	-7.32940600	-1.60030900
C	0.99175700	3.81027700	1.21487100	O	-2.07559800	-9.39689200	-0.69792700
H	1.85868000	1.96972200	1.90354100	N	0.21243400	8.57258400	1.09171000
C	-0.06211200	3.73826000	-0.95803400	H	-1.71686500	7.96440000	0.58783600
H	-0.02355600	1.83663000	-1.94260900	H	-0.80864400	8.77846600	-0.71058400
C	-2.43628300	-1.32108600	-0.41125500	C	-6.64087900	-4.34575100	-0.43563500
O	0.20377200	-7.86694400	1.19721200	H	-6.46543600	-3.13803900	-2.06394900
O	0.31910700	-9.77643700	2.42476000	C	-3.42807600	5.42652300	2.35922700
N	3.83592100	7.01791600	-1.39730900	H	-2.47301500	4.59157900	4.09124700
H	2.07476600	5.97042700	-1.77102600	H	-4.29147100	6.00597400	0.47748800
H	3.01277300	6.41082100	-3.21262000	C	-6.58993500	0.55005900	-1.83934900
C	-2.65858500	-5.49738000	1.20211500	C	-7.49780300	-0.24320200	0.23562200
H	-1.72227800	-5.78697200	-0.56652600	C	-1.21574700	-9.72171000	-1.78799600
C	0.24284100	4.43499500	0.21468500	C	0.12832500	8.22339400	2.39033200
H	1.25810800	4.37521300	2.10419500	H	1.10902100	8.90785800	0.74388000
H	-0.61284300	4.23687300	-1.74564300	O	-6.21886000	-4.77157500	0.63067400
C	-2.77423200	-1.68149600	-1.71746700	C	-7.96418100	-4.82617000	-1.02701900
C	-3.22092200	-1.81560500	0.63608800	N	-3.72940200	6.61802300	3.04151400
H	-0.99038500	1.40572500	1.16336400	C	-7.64157400	-0.04189100	-2.52401300
C	0.41191200	-10.51161900	1.20761800	H	-5.83804100	1.11389500	-2.38556500
C	3.57225800	7.21551200	-0.08928200	C	-8.55266900	-0.84919300	-0.43490700
H	4.67970300	7.41730300	-1.80744500	H	-7.45113500	-0.30205800	1.31991400
O	-2.72860600	-5.00954100	2.32070700	O	-0.76560100	7.55848100	2.89586700
C	-3.70707300	-6.48240800	0.67023600	O	1.17398700	8.71653200	3.09127700
N	-0.25249700	5.73095700	0.45139500	N	-7.78448600	-5.52088300	-2.28532400
C	-3.92909100	-2.41660000	-1.97037900	H	-8.64014000	-3.97743200	-1.17716800
H	-2.17238700	-1.31572500	-2.54527800	H	-8.41604100	-5.50568900	-0.30081200
C	-4.35991100	-2.57132000	0.40166500	C	-3.79680000	7.86349700	2.50706500
H	-2.96418900	-1.54955800	1.65796000	H	-3.82324100	6.55456700	4.05291600
C	-3.04770700	2.90232900	1.18626600	C	-8.64118900	-0.72381700	-1.82589700
O	2.67393200	6.67707200	0.54169000	H	-7.71897100	0.04564200	-3.60508600
O	4.45739400	8.07912900	0.45393400	H	-9.32163900	-1.38831700	0.10343700
N	-3.15792100	-7.80864400	0.43761700	C	1.11486100	8.47432100	4.49179300
H	-4.13501300	-6.09392200	-0.26025300	C	-7.79408000	-4.85561700	-3.45740200
H	-4.50533400	-6.55188900	1.41004300	H	-7.46990800	-6.49117600	-2.26110000

O	-3.70285200	8.12668100	1.31471000	N	-5.41417300	8.01525000	8.25237500
C	-4.01164000	8.95095700	3.55555600	H	-7.47469800	7.82941400	8.15055400
N	-9.73667400	-1.19199200	-2.56800400	H	-6.81256500	9.35180500	7.51096400
O	-8.00993000	-3.65827300	-3.58976900	C	-12.76384600	0.95856300	-4.74667800
O	-7.50372100	-5.68368200	-4.48399000	H	-11.52570300	2.47012100	-5.24148600
N	-2.90630000	9.05567500	4.48722500	C	-5.14935900	6.78863100	8.74463200
H	-4.93171000	8.74157100	4.11207000	H	-4.62883900	8.63383600	8.05519300
H	-4.12171900	9.90021100	3.02613500	O	-13.22422500	0.14394100	-3.95761700
C	-10.54112200	-2.24387000	-2.28010400	C	-13.25699400	1.01883900	-6.19944100
H	-9.88550200	-0.75245300	-3.47438000	O	-5.92313700	5.83981600	8.74931500
C	-7.57549900	-5.07803600	-5.76953400	O	-3.91645900	6.73100100	9.28571900
C	-2.82024500	8.24062600	5.55665400	N	-12.27030200	0.64705400	-7.19111300
H	-2.04101000	9.46507100	4.13904300	H	-13.60338300	2.03318500	-6.42311800
O	-10.51094600	-2.89717600	-1.24382800	H	-14.10063800	0.33114400	-6.27447900
C	-11.52024000	-2.55803400	-3.40901400	C	-3.54226500	5.44356600	9.76515400
O	-3.67505500	7.44206000	5.91951600	C	-11.30415700	1.51694800	-7.54661100
O	-1.64896400	8.41770300	6.20368200	H	-12.10991600	-0.34638600	-7.35142700
N	-10.85263900	-2.98314800	-4.62451700	O	-11.21068300	2.67427700	-7.15817500
H	-12.12233000	-1.66839500	-3.62299900	O	-10.44966600	0.96915400	-8.43296300
H	-12.17417900	-3.36255000	-3.06513600	C	-9.37036900	1.81659800	-8.81414900
C	-1.49356700	7.63609900	7.38202200	H	14.77039400	-5.88408600	0.80710900
C	-10.33313300	-2.08677800	-5.48664900	H	-9.45900700	2.69065200	1.29628000
H	-10.46475800	-3.92536900	-4.63329100	H	13.58861300	3.11508700	-4.56238600
O	-10.45193500	-0.86933000	-5.41203600	H	12.55704300	4.35887900	-5.32047900
O	-9.65710000	-2.70408300	-6.47674800	H	13.90163700	3.62900000	-6.25345700
C	-9.12267100	-1.83233500	-7.46608500	H	12.25887600	5.85075200	-3.55205400
H	-5.07381000	1.89455800	2.33974900	H	11.93965400	4.32423800	-2.66109400
C	-6.86577200	3.76786100	2.73768800	H	11.19744900	5.85506000	-2.11000100
C	-6.52513200	3.33076200	4.02469600	H	5.02906500	9.03600300	2.12838900
C	-7.18629400	5.12107700	2.57370700	H	4.08553100	7.53834200	2.42659100
H	-7.09225100	3.14735200	-0.58430400	H	3.25087400	9.00187900	1.86942800
C	-6.48246800	4.21399300	5.09027700	H	2.07485900	8.80844000	4.88743300
H	-6.29963500	2.28135500	4.19105800	H	0.96283000	7.41185300	4.69477600
C	-7.13716000	6.02422400	3.63116100	H	0.29343000	9.03667300	4.94404100
H	-7.46011500	5.47896500	1.58509200	H	-0.46402400	7.79602500	7.70523400
C	-9.73054100	2.70757900	-0.87564300	H	-1.66948700	6.57896300	7.16948200
C	-6.77872000	5.57068300	4.90515600	H	-2.19598800	7.96042200	8.15346500
H	-6.22034000	3.86031000	6.08486300	H	-3.54758700	4.71496000	8.95074600
H	-7.37237600	7.06916400	3.47850200	H	-4.22821200	5.10911300	10.54591500
C	-9.34810000	3.26033400	-2.10495300	H	-2.53553400	5.56096100	10.16586800
C	-10.85453900	1.87362400	-0.86074300	H	5.71355200	-11.42040400	8.00423100
N	-6.74849100	6.38610600	6.05064500	H	6.86391200	-10.85476400	6.74989100
C	-10.04627600	2.96822700	-3.26522300	H	5.28688600	-11.51962600	6.26549100
H	-8.49536700	3.93176400	-2.15090000	H	0.65508200	-11.53331200	1.49908900
C	-11.56561700	1.56632500	-2.01558900	H	-0.54295800	-10.47678800	0.67935900
H	-11.16739500	1.42863100	0.08079600	H	1.19689700	-10.09894600	0.56956000
C	-6.72716000	7.74169800	6.12495200	H	-1.02777700	-10.79263900	-1.70688700
H	-6.62667900	5.90221300	6.93953100	H	-0.28132800	-9.16038400	-1.70613600
C	-11.15819500	2.11553000	-3.23588600	H	-1.69680600	-9.48912600	-2.73941500
H	-9.73852900	3.40487600	-4.21268500	H	-7.18653100	-5.82135400	-6.46609200
H	-12.42412900	0.90952500	-1.98124100	H	-6.97388700	-4.16683500	-5.80218300
O	-6.79207400	8.50606200	5.17076400	H	-8.60949700	-4.82090500	-6.01530400
C	-6.66231400	8.27253200	7.56509700	H	-8.52005800	-2.46533200	-8.11867100
N	-11.83429200	1.90478800	-4.45134600	H	-8.50406500	-1.05856300	-7.00494800



H	-9.92651500	-1.35072300	-8.02775500	H	4.82448600	9.69554200	-1.61529500
H	-8.77039700	1.23138400	-9.51068200	H	4.53836400	11.30940100	-2.29160200
H	-8.77721400	2.09838900	-7.94114200	O	-1.00564900	10.72943900	3.09268300
H	-9.74419200	2.72169200	-9.29704100	C	-1.62140200	11.03064400	1.83786300
O	11.11622600	-0.11493900	-8.31863300	C	0.04947500	11.66083700	3.27396300
C	10.35925800	-1.33597700	-8.21389600	C	-0.51620700	11.63452000	0.94207900
C	12.49867400	-0.39673000	-8.08232900	H	-2.42765400	11.76028100	2.00239200
C	11.33787400	-2.43100000	-7.77264000	H	-2.06115100	10.10458800	1.45609800
H	9.88795800	-1.54202200	-9.17924900	C	0.68795400	11.78753100	1.89242000
H	9.57724300	-1.18990800	-7.46153300	H	0.72109700	11.26380300	4.03925900
C	12.49546900	-1.62284100	-7.17857800	H	-0.35871300	12.62436700	3.61825000
H	12.94362300	0.49606300	-7.63330400	H	-0.26618500	10.98137200	0.10279600
H	12.99993300	-0.60554900	-9.03769300	H	-0.83566800	12.59956100	0.53963200
H	10.88107700	-3.10717800	-7.04839600	H	1.39415100	10.96650900	1.74219700
H	11.68517900	-3.00910600	-8.63482200	H	1.21755900	12.73469700	1.76134700
H	12.26862200	-1.32922900	-6.14730400	O	-3.69269700	10.20274600	7.34558400
H	13.44591400	-2.16091900	-7.18411200	C	-4.51491300	10.94068300	6.43955500
O	8.34917100	4.25399100	-7.01496200	C	-2.59295800	11.03431200	7.68023000
C	7.87306100	2.90734800	-7.07453300	C	-3.57124400	11.88899900	5.66577800
C	9.73871600	4.19843700	-7.33072600	H	-5.25470700	11.51584700	7.01524700
C	8.60821100	2.26262400	-8.25607800	H	-5.04627100	10.21745700	5.81410500
H	6.78791500	2.94596500	-7.18429700	C	-2.20874300	11.70286200	6.36259900
H	8.10623900	2.39236300	-6.13285200	H	-1.80982100	10.40171200	8.10424700
C	9.87929900	3.12656000	-8.42047600	H	-2.90041700	11.77854400	8.43148500
H	10.30878700	3.92365000	-6.43131100	H	-3.50476500	11.62583600	4.60774600
H	10.04273200	5.19973200	-7.64377400	H	-3.92206200	12.92188000	5.73928800
H	8.84461000	1.21330800	-8.05968900	H	-1.57776900	11.02505200	5.78162300
H	7.99566200	2.29959900	-9.15950200	H	-1.67271200	12.64380800	6.51083900
H	10.79718800	2.54648900	-8.29729500	O	3.11399400	-6.56223500	8.38423500
H	9.90409400	3.58687000	-9.41139900	C	2.54583100	-5.31203700	7.97686800
O	5.97148500	7.79793600	-3.18266200	C	4.16717200	-6.23371400	9.28634900
C	5.65370400	7.15024800	-4.41871500	C	3.72075200	-4.31905200	7.88986300
C	7.33257900	7.48001100	-2.91446300	H	1.81759900	-4.99779600	8.73769600
C	6.93927200	7.20314900	-5.27116400	H	2.02732800	-5.46676500	7.02793500
H	4.81338400	7.69140800	-4.86220300	C	4.86639900	-5.03535700	8.64115200
H	5.34164100	6.11608300	-4.21948800	H	4.79844600	-7.12071800	9.39584900
C	8.02846700	7.64203200	-4.26671800	H	3.74103700	-5.97603900	10.26727700
H	7.41854400	6.44707900	-2.54331100	H	4.01491900	-4.12599700	6.85517600
H	7.68733600	8.16308300	-2.13951500	H	3.45658800	-3.36511800	8.35267400
H	7.15813700	6.22873500	-5.71579500	H	5.61842400	-5.37269700	7.92259300
H	6.84708800	7.92263700	-6.08774900	H	5.36017700	-4.39832900	9.37846800
H	8.94204300	7.04737800	-4.34136800	O	0.31197100	-9.13482600	6.00120200
H	8.28765100	8.69308400	-4.42119700	C	1.20323500	-8.40956600	6.86684700
O	2.25384800	9.72258300	-0.56631800	C	0.76217500	-10.49152400	5.85855900
C	1.80225200	9.50683800	-1.90601900	C	2.00243500	-9.48066600	7.59574400
C	3.22616400	10.75462500	-0.62615000	H	0.60457300	-7.77555800	7.52587700
C	3.01103900	9.80139600	-2.81937000	H	1.85432000	-7.76474700	6.25707300
H	0.97674900	10.20261900	-2.11919400	C	2.14619100	-10.53831800	6.50034200
H	1.42250500	8.48309900	-1.96910200	H	0.75687800	-10.74496500	4.79412500
C	4.05323400	10.42680200	-1.86826300	H	0.05718700	-11.14862800	6.38386500
H	3.79523600	10.73730000	0.30644700	H	2.95300000	-9.11700300	7.98170900
H	2.72436200	11.73094600	-0.72287100	H	1.41585600	-9.88008800	8.43128500
H	3.40235800	8.88907700	-3.27544300	H	2.91206100	-10.23301500	5.77664800
H	2.73020100	10.48723800	-3.62274600	H	2.40134200	-11.53212100	6.87912900

O	-3.79373900	-8.97785200	2.90453200
C	-3.35374000	-7.95107600	3.81510900
C	-3.56282700	-10.27004100	3.46552400
C	-2.86998600	-8.67655300	5.07184900
H	-4.18452300	-7.26388500	3.99918500
H	-2.54903600	-7.38894400	3.32911400
C	-2.49112800	-10.05689900	4.52957500
H	-3.25795500	-10.94044300	2.65497200
H	-4.49645000	-10.65029200	3.90465000
H	-2.02650400	-8.17501800	5.55257400
H	-3.68283400	-8.76497800	5.80120800
H	-1.50331900	-10.02255500	4.05809500
H	-2.49051700	-10.83740200	5.29508900
O	-7.03903400	-8.18531100	-1.51347400
C	-7.05945600	-8.10462000	-0.08523700
C	-5.75990500	-8.71030100	-1.85253900
C	-6.25260100	-9.31730900	0.42223300
H	-8.10747600	-8.11275900	0.22473400
H	-6.60468300	-7.15788200	0.23587800
C	-5.54030000	-9.84027800	-0.84571400
H	-4.99072400	-7.92929700	-1.75110200
H	-5.79998200	-9.03375000	-2.89469200
H	-5.54265000	-9.01609500	1.19650800
H	-6.90680200	-10.08160400	0.84805900
H	-4.48103300	-10.05153300	-0.68300600
H	-6.02445200	-10.75122000	-1.20847100
O	-10.42129900	-5.77096300	-4.11547600
C	-10.92157500	-6.00716000	-2.79578900
C	-10.31248300	-7.03811000	-4.74670300
C	-10.39734300	-7.39718300	-2.37579500
H	-12.02125100	-6.00003800	-2.82660800
H	-10.58581100	-5.18201100	-2.16100200
C	-9.75559200	-7.95703400	-3.66158200
H	-9.65756100	-6.92636300	-5.61447600
H	-11.30635900	-7.37107200	-5.08624000
H	-9.66038600	-7.32931200	-1.57209700
H	-11.21901200	-8.02831400	-2.02715800
H	-8.66881000	-7.85611000	-3.61805900
H	-9.99973800	-9.00763300	-3.83608400
O	-12.45593900	-2.27713500	-7.28293100
C	-13.48198500	-2.60427100	-6.34497900
C	-12.25619700	-3.42283700	-8.09569100
C	-13.38149100	-4.12664500	-6.09857600
H	-14.45933200	-2.34605500	-6.77844400
H	-13.32173500	-1.98726300	-5.45584000
C	-12.32857100	-4.59736600	-7.12203300
H	-11.28996900	-3.31644300	-8.59428700
H	-13.04963900	-3.48602500	-8.85663800
H	-13.06330800	-4.35539400	-5.07923100
H	-14.34897100	-4.60637900	-6.26906800
H	-11.35829000	-4.72649000	-6.63539700
H	-12.60190900	-5.53360900	-7.61510100

### 1b-8-mer<sub>RH</sub>-1b-8-mer<sub>LH</sub>

C	13.53795100	1.46286200	-1.91203400
C	12.24961400	1.14658200	-1.71055300
C	11.87141600	0.21686400	-0.62760300
C	10.66411000	0.08976100	-0.02182300
C	9.53193900	0.98300800	-0.32756700
C	8.21274600	0.67249400	-0.36325600
C	7.71340400	-0.67861400	-0.05959600
C	6.55563500	-0.98794100	0.57073100
C	5.60043400	0.06675300	0.95878400
C	4.26279500	0.01817400	0.75959600
C	3.65268700	-1.21341400	0.23335900
C	2.50587800	-1.79133700	0.65298600
H	13.83474000	2.12492200	-2.71951900
C	11.17559200	1.72120900	-2.57206400
C	10.94385500	3.09795300	-2.62051300
C	10.27820000	0.87936800	-3.23287200
H	12.67810900	-0.42082800	-0.26745100
C	9.80628900	3.60414300	-3.23875300
H	11.62693100	3.77093800	-2.10879100
C	9.14904600	1.36895600	-3.87409500
H	10.43797000	-0.19496300	-3.19270500
C	10.43515700	-0.97658500	0.99144000
C	8.88424600	2.74362300	-3.84307500
H	9.61238000	4.67402500	-3.23175300
H	8.45290200	0.69909900	-4.35808300
C	10.73737700	-2.31549700	0.72394900
C	9.75957600	-0.68434800	2.18080900
H	9.79247800	1.99263200	-0.62235400
N	7.70296000	3.30748800	-4.36686300
C	10.31993500	-3.32442000	1.58336000
H	11.24695600	-2.57179000	-0.20118100
C	9.34959700	-1.67670600	3.05824200
H	9.50283100	0.34899300	2.39831200
C	7.25815200	1.73928100	-0.76988300
C	6.81272300	2.70558500	-5.21244600
H	7.42150700	4.20369300	-3.97837400
C	9.59983900	-3.01848800	2.74328400
H	10.52782700	-4.36441800	1.34336300
H	8.81155200	-1.42938000	3.96169700
C	7.38726000	3.04471600	-0.28515200
C	6.18665000	1.46421900	-1.62949000
H	8.38922500	-1.49984000	-0.27581500
O	6.91862400	1.57936000	-5.65932600
C	5.61276200	3.58085600	-5.58387100
N	9.13526100	-4.08872900	3.53079800
C	6.46746400	4.02503200	-0.62442300
H	8.19828500	3.28346000	0.39815900
C	5.25157500	2.43266900	-1.97569000
H	6.06512800	0.45400300	-2.01273900
C	6.27047500	-2.41145200	0.89190300
N	5.97263700	4.88655200	-6.11139000
H	4.96463000	3.71670100	-4.71144400
H	5.05182600	3.03513100	-6.34300200

C	8.64764200	-4.02358100	4.80797900	C	10.60907500	-9.01244000	3.37051300
H	9.06933600	-4.99287600	3.07100700	C	3.64973300	8.32418700	-1.84128100
C	5.38243400	3.72699600	-1.45689800	H	4.87064300	7.20801500	-3.04632600
H	6.57274500	5.02880900	-0.21775700	O	5.52492300	-6.53863800	4.06040200
H	4.41075700	2.19051200	-2.61292300	C	5.58142200	-8.61765600	2.84839200
C	6.47936000	-3.42563900	-0.04888400	N	1.55408600	5.01252300	1.22511700
C	5.77586200	-2.77266300	2.14947600	C	2.39374500	-4.94554400	-1.44378700
H	6.02675200	1.01247900	1.28006700	H	2.52036900	-2.84753300	-1.88475300
C	6.12431500	5.97079900	-5.33298200	C	2.09171600	-5.53080700	0.88233300
H	6.15617000	4.99604300	-7.09847600	H	1.97151200	-3.87461500	2.23692700
O	8.53430500	-3.00649500	5.46534800	O	2.55902800	8.55388000	-1.34342800
C	8.23154500	-5.38115500	5.37788600	O	4.73753700	9.09911200	-1.65527300
N	4.48093300	4.77123800	-1.72576000	N	6.80964900	-9.01709500	2.17598400
C	6.20470200	-4.74991200	0.25882000	H	4.72938000	-8.99605000	2.27695700
H	6.83223400	-3.16545500	-1.04326600	H	5.56898700	-9.03082800	3.85765800
C	5.50768800	-4.09651900	2.47731700	C	0.90049800	5.74458900	0.28125700
H	5.58862700	-1.99508000	2.88534500	H	1.62851800	5.44127100	2.14533000
C	3.47594200	1.26354300	0.93960900	C	2.26889800	-5.91996900	-0.44894600
O	6.02802300	5.96848700	-4.10985400	H	2.50471500	-5.25409200	-2.48079800
O	6.40032100	7.06626900	-6.05681400	H	1.98775300	-6.28074900	1.65423100
N	9.27694500	-6.39025100	5.31848300	C	4.54111300	10.19946200	-0.76437300
H	7.35510300	-5.75503400	4.83695800	C	6.83409600	-9.14922700	0.83376100
H	7.95649400	-5.21518100	6.41957800	H	7.68048300	-8.69056300	2.59115900
C	3.54137700	4.83654100	-2.70822400	O	0.70512000	5.39159100	-0.87156200
H	4.73392900	5.66208900	-1.32190300	C	0.40689000	7.10242100	0.79724600
C	5.72111300	-5.09833200	1.52333700	N	2.32437500	-7.27164800	-0.85009000
H	6.35930500	-5.52794900	-0.48531300	O	5.85131700	-9.11281100	0.10111900
H	5.12271700	-4.35934400	3.45351700	O	8.08495900	-9.34158000	0.37860400
C	3.69457800	2.12729100	2.01770500	N	1.48328300	7.98855000	1.20168100
C	2.57265900	1.66441000	-0.05292800	H	-0.26892800	6.96214900	1.64832000
H	4.27225700	-1.79273800	-0.44379200	H	-0.13946800	7.57652900	-0.02047600
C	6.60194700	8.26186700	-5.30576800	C	2.73366500	-8.32770900	-0.09256600
C	9.41214700	-7.21840700	4.26857600	H	2.18404100	-7.46067300	-1.84101600
H	9.95262200	-6.46634400	6.06531600	C	8.19046800	-9.48718200	-1.03558800
O	3.15064300	3.88967600	-3.36416000	C	2.05793700	7.88659700	2.41640800
C	2.98822200	6.23984100	-2.96481900	H	1.97889000	8.48559600	0.46067900
N	5.46744200	-6.46039700	1.76967700	O	2.95640800	-8.28124600	1.10733300
C	3.04894700	3.35377600	2.08749300	C	2.91776500	-9.61855400	-0.89685100
H	4.36934200	1.82694200	2.81447700	O	1.71577800	7.11083800	3.30406000
C	1.93639900	2.90013200	-0.01115300	O	3.08129600	8.75680700	2.54961400
H	2.37841000	0.99697000	-0.88839100	N	3.95766100	-9.52039900	-1.90178500
C	2.27166000	-3.19472700	0.22243700	H	1.98183000	-9.88621300	-1.39660700
O	8.73441900	-7.16015000	3.24570500	H	3.18966200	-10.40030900	-0.18750500
O	10.39229400	-8.11536100	4.45971200	C	3.74213500	8.70186800	3.81437500
N	3.94063800	7.28004500	-2.63980100	C	3.71612400	-8.94020900	-3.09787200
H	2.08564300	6.38094100	-2.36208200	H	4.91466500	-9.55143000	-1.56534300
H	2.70715900	6.26538400	-4.02115400	O	2.62778600	-8.53460200	-3.48011000
C	5.49801500	-7.09589300	2.97474700	O	4.83875300	-8.86617200	-3.83761600
H	5.33962400	-7.05741700	0.95750700	C	4.66501000	-8.25269000	-5.11342900
C	2.17645600	3.75618000	1.07074000	H	11.51330200	-9.56400900	3.62293400
H	3.21928500	4.01267000	2.93631600	H	10.73646500	-8.46239500	2.43585200
H	1.26744300	3.20217700	-0.80557600	H	9.76666200	-9.70231100	3.26688700
C	2.40201700	-3.59877700	-1.10919400	H	9.25691600	-9.55616500	-1.24487600
C	2.08473700	-4.17838800	1.19970100	H	7.75480600	-8.62567900	-1.54707800

H	7.68096500	-10.39550500	-1.36714400	C	-3.03527700	4.31405900	0.53746200
H	5.64814800	-8.26806100	-5.58217700	H	-1.96716200	2.77279700	-0.48959000
H	4.30975500	-7.22572900	-5.00128000	C	-4.93795800	3.62045400	1.85356800
H	3.94535800	-8.81372800	-5.71332300	H	-5.32294900	1.51531700	1.86433300
H	6.92725400	9.00884000	-6.02915800	N	-4.96021100	-4.35906600	-3.48553600
H	5.66914900	8.58071800	-4.83192300	O	-4.25356400	1.85019600	5.61275800
H	7.36557900	8.11028100	-4.53989700	C	-4.24840400	4.25003600	5.63450200
H	5.48108500	10.74952800	-0.76599800	C	-7.04622300	1.92764500	-0.90952100
H	4.31774000	9.83925300	0.24262500	H	-5.02686700	1.82485400	-1.45608600
H	3.72300600	10.83625900	-1.11110400	C	-7.03520800	-2.06673800	0.12753300
H	4.56560400	9.41437100	3.74515300	C	-7.06405100	-1.40211400	-2.17481900
H	4.12027700	7.69375700	4.01053800	C	-4.11136400	4.64102900	1.36973700
H	3.05407300	8.98682400	4.61568300	H	-2.39526400	5.10094300	0.14237700
H	14.32392700	1.06417700	-1.27656900	H	-5.78260500	3.86772000	2.48224900
C	1.63386600	-1.13486800	1.63910800	C	-5.24311000	-4.18315500	-4.81125600
C	0.28214900	-1.06520400	1.60853600	H	-5.46815900	-5.10018500	-3.01043600
H	2.14058500	-0.54213900	2.39815500	N	-3.23802600	5.13094500	6.20057300
C	-0.53308300	-1.77847300	0.60367300	H	-4.70340800	4.74522800	4.76913500
C	-0.40095000	-0.11454600	2.53196400	H	-5.02449000	4.08201000	6.38129700
C	-1.62770100	-1.28104000	-0.02527100	C	-8.18003700	1.19599400	-0.29483300
H	-0.19370700	-2.76905000	0.31121100	C	-7.09427100	3.38776500	-1.13620600
C	0.08162600	1.19532700	2.64165200	C	-7.89530500	-3.11698700	-0.16723400
C	-1.60872400	-0.42257500	3.16307800	H	-6.71047500	-1.90646800	1.15258300
C	-2.07946100	0.10372100	0.20601900	C	-7.90829500	-2.45912600	-2.49050300
C	-2.39332700	-2.12319500	-0.98358900	H	-6.75140300	-0.71966000	-2.96120700
C	-0.65747600	2.17372500	3.28566400	N	-4.28716500	5.99950400	1.68642900
H	1.00809900	1.46543900	2.14577800	O	-4.81368100	-3.28415400	-5.50957100
C	-2.34853600	0.54034700	3.84028000	C	-6.18197300	-5.24785200	-5.38766600
H	-2.00948800	-1.42919000	3.07361900	C	-2.45375600	5.92508000	5.44957500
C	-3.35804100	0.54219700	0.28673800	H	-3.03989900	5.09407900	7.19077300
H	-1.29579000	0.82187500	0.42482500	C	-9.33169100	0.93800600	-0.92362800
C	-2.77536000	-3.43001600	-0.66391700	H	-7.96172300	0.66218000	0.63027200
C	-2.84967700	-1.58593700	-2.19245000	C	-6.40461300	3.99781000	-2.19037400
C	-1.89097100	1.86340400	3.86534600	C	-7.67565500	4.21020800	-0.16412400
H	-0.29557400	3.19980100	3.30972000	C	-8.32273100	-3.33489600	-1.47918500
H	-3.29168500	0.29154900	4.30624000	H	-8.23387000	-3.78436200	0.62237800
C	-4.49215000	-0.37949600	0.07969300	H	-8.25060500	-2.61061500	-3.50490800
C	-3.60674300	1.96177400	0.65383800	C	-5.02297600	6.53377700	2.70015700
C	-3.61234300	-4.15347500	-1.50430700	H	-3.59243800	6.61946100	1.29390100
H	-2.45188700	-3.86315200	0.27891600	N	-5.70452900	-6.61123900	-5.21115600
C	-3.67156300	-2.30077800	-3.05125300	H	-7.17041300	-5.15949400	-4.92381300
H	-2.58216200	-0.56365500	-2.44627100	H	-6.27149800	-5.04260000	-6.45443300
N	-2.62402800	2.93360400	4.41066200	O	-2.48072300	5.96951300	4.21936000
C	-5.62878700	-0.10029700	-0.59640500	O	-1.62441200	6.65989400	6.20216400
H	-4.34239200	-1.40757400	0.39654200	C	-10.25076000	-0.12559900	-0.48804100
C	-2.79015000	2.99602500	0.18372100	H	-9.51538800	1.38247900	-1.90173300
C	-4.67249200	2.30433400	1.49519300	C	-6.26097000	5.37553400	-2.23923500
C	-4.07794800	-3.59331000	-2.69761200	H	-5.96826500	3.38156700	-2.97146900
H	-3.92329700	-5.15861700	-1.22984100	C	-7.52147900	5.59066200	-0.18637100
H	-4.01765900	-1.86593600	-3.97819900	H	-8.22386900	3.75165900	0.65457500
C	-3.71732500	2.87170800	5.22487400	N	-9.15574000	-4.44565200	-1.71732800
H	-2.37435000	3.85666200	4.06545700	O	-5.87839200	5.94120500	3.33292700
C	-5.88500900	1.26575900	-1.09343600	C	-4.68044700	7.98736600	3.03013500
C	-6.59495000	-1.19691300	-0.87322500	C	-5.99234200	-7.33229100	-4.11478400

H	-5.08711900	-7.02519500	-5.89470600
C	-0.69496400	7.46861400	5.47569000
C	-10.44210200	-0.45991900	0.85800000
C	-10.83851400	-0.94370700	-1.45794300
C	-6.79313200	6.17851400	-1.22515200
H	-5.71589000	5.84269700	-3.05649400
H	-7.93410400	6.20488500	0.60238200
C	-9.35442600	-5.08972300	-2.90088600
H	-9.59421400	-4.86985900	-0.90455900
N	-3.28610100	8.29521600	2.79020500
H	-5.30163800	8.64386500	2.41490600
H	-4.94631200	8.13052500	4.08113700
O	-6.61806300	-6.90548800	-3.14789700
O	-5.50437400	-8.57996100	-4.18941500
H	-0.01509500	7.87129300	6.22510500
H	-1.21430700	8.28730100	4.96876600
H	-0.14403800	6.87634300	4.74417100
C	-11.14354500	-1.60222000	1.21082200
H	-10.02720000	0.17777800	1.63354800
C	-11.53589900	-2.09736600	-1.12250200
H	-10.70275800	-0.69829000	-2.50816900
N	-6.58157800	7.56860000	-1.32469900
O	-9.01522700	-4.66548600	-3.99454300
C	-10.00312500	-6.46645000	-2.74268800
C	-2.87782300	9.32933700	2.02724500
H	-2.59516700	7.68315600	3.21758900
C	-5.73692500	-9.38661600	-3.03523800
C	-11.67082900	-2.44386200	0.22469900
H	-11.27613000	-1.86256400	2.25854300
H	-11.94689000	-2.73938100	-1.88914200
C	-6.57381900	8.47097800	-0.30498800
H	-6.24299600	7.91352300	-2.22185500
N	-9.17236900	-7.36294200	-1.95441100
H	-10.97581600	-6.36771900	-2.25320400
H	-10.12991200	-6.88010400	-3.74377500
O	-3.60299600	10.13794500	1.47466300
O	-1.53029400	9.34735800	1.92620900
H	-5.19635800	-10.31441200	-3.21489200
H	-5.36577700	-8.88948400	-2.13685100
H	-6.80458000	-9.58933000	-2.91651200
N	-12.33213100	-3.61239300	0.65611700
O	-6.86564200	8.22462600	0.85521200
C	-6.13187400	9.87299900	-0.74153500
C	-9.30721400	-7.41890200	-0.61587300
H	-8.24669000	-7.57386400	-2.32201700
C	-1.01584000	10.36146800	1.06159900
C	-12.53226500	-4.75414800	-0.06006900
H	-12.59695600	-3.65039100	1.63882200
N	-4.72902400	9.92985400	-1.10007200
H	-6.72821400	10.20778200	-1.59582700
H	-6.29529900	10.53964600	0.10443800
O	-10.18427600	-6.85430700	0.03091000
O	-8.35770700	-8.18747800	-0.05342800
H	0.06790500	10.26117400	1.11724100

H	-1.36271400	10.20284100	0.03444400
H	-1.33634900	11.35000100	1.40106600
O	-12.28833300	-4.88494200	-1.24943100
C	-13.09735600	-5.90682100	0.77668900
C	-4.29550800	9.52938700	-2.30956500
H	-4.06113500	10.13275800	-0.36221300
C	-8.43499200	-8.29048000	1.36612600
N	-12.21823200	-6.32782500	1.84955800
H	-14.05682400	-5.61508500	1.21475500
H	-13.24884800	-6.74554500	0.09692600
O	-5.00556500	9.12033300	-3.21753000
O	-2.95378800	9.63724000	-2.40865800
H	-7.55814400	-8.86197000	1.66643600
H	-8.42406800	-7.30067600	1.82832000
H	-9.34682100	-8.81457300	1.66413100
C	-12.17965800	-5.65284500	3.01996800
H	-11.38872900	-6.84348200	1.57284000
C	-2.42199600	9.22222500	-3.66515100
O	-12.90970500	-4.72025800	3.32408100
O	-11.22697800	-6.14677400	3.83367700
H	-1.34116000	9.31565100	-3.57104100
H	-2.70027100	8.18811900	-3.87789700
H	-2.79481000	9.86302900	-4.46729100
C	-11.11874300	-5.47496900	5.08673200
H	-10.31359400	-5.97799100	5.62017000
H	-10.87918200	-4.41983200	4.93664500
H	-12.05492400	-5.55031000	5.64344500

### 1b-8-mer<sub>RH</sub>-1b-8-mer<sub>LH</sub>/16CHCl<sub>3</sub>

C	-4.46361100	12.76077400	-1.15648800
C	-4.01322400	11.54351700	-1.49397200
C	-2.57815100	11.23474500	-1.34356700
C	-1.92599200	10.05010000	-1.19882500
C	-2.61162700	8.74785400	-1.17943200
C	-2.28530500	7.56153600	-0.59122400
C	-1.03527300	7.31535100	0.11655600
C	-0.62842300	6.26949100	0.88743900
C	-1.52938300	5.18746100	1.29733500
C	-1.23289500	3.87595000	1.46795000
C	0.15862100	3.39767800	1.38780100
C	0.77014300	2.54939000	2.24331500
H	-5.51209300	13.02025900	-1.26438300
C	-4.94626100	10.51323100	-2.03141700
C	-5.91460900	9.92224800	-1.21990400
C	-4.78776400	10.04019700	-3.33833700
H	-1.94968900	12.12369600	-1.29290300
C	-6.64459300	8.82701600	-1.67262700
H	-6.05612800	10.28985100	-0.20708400
C	-5.50979500	8.94991800	-3.80118100
H	-4.04336200	10.50089300	-3.98223000
C	-0.44351200	10.11867100	-1.00953300
C	-6.41348300	8.30788300	-2.94672200
H	-7.37506100	8.34548800	-1.02704200
H	-5.36554900	8.57533800	-4.80637800

C	0.42942600	9.42146200	-1.85410100	H	3.76294700	6.53373000	-0.54957000
C	0.10732300	10.83834100	0.05304100	H	3.16171200	5.91085500	3.64959500
H	-3.56908200	8.73336500	-1.68216000	C	-3.50046000	3.18710600	2.35658800
N	-7.06120000	7.11102900	-3.32438300	C	-2.37069200	1.76289000	0.78302900
C	1.79778800	9.41965600	-1.61833700	H	0.79214200	3.88154500	0.65151800
H	0.02435000	8.85098400	-2.68614500	C	-12.82273700	6.03423500	-4.50185700
C	1.47618800	10.83745400	0.30606200	C	7.96212300	11.78285400	1.16473500
H	-0.55614500	11.37416500	0.72616200	H	6.15813100	12.70645900	0.81114300
C	-3.30841900	6.47579900	-0.71449600	O	-7.99309600	4.80395000	-1.57746200
C	-7.47659600	6.82594800	-4.58804800	C	-8.51151700	2.53380600	-1.04083600
H	-7.26314300	6.42987200	-2.59171500	N	5.01340000	6.25978100	1.81093500
C	2.33051600	10.11231200	-0.52571300	C	-4.60688000	2.34087900	2.33281600
H	2.46620800	8.87307500	-2.27912900	H	-3.51257100	4.06616000	2.99432100
H	1.87793600	11.38392200	1.14896000	C	-3.47969100	0.92784800	0.73636600
C	-4.59750800	6.69713900	-0.22531000	H	-1.49197900	1.52917600	0.18794500
C	-3.02014000	5.22362600	-1.27145400	C	2.24788800	2.42475700	2.13020500
H	-0.27903200	8.07219200	-0.02828300	O	8.61978800	10.74972700	1.23685400
O	-7.39607600	7.57996600	-5.54342100	O	8.44544300	12.99502500	1.45945900
C	-8.11263800	5.44990800	-4.76560300	N	-9.74119300	2.82191900	-1.73814700
N	3.72680900	10.02837200	-0.29645900	H	-8.69452200	2.41388300	0.03755000
C	-5.57454600	5.71141600	-0.28544800	H	-8.05168000	1.60622100	-1.39812200
H	-4.82752900	7.65458400	0.23179300	C	5.88081000	7.09512900	1.18286600
C	-3.99105400	4.23028000	-1.34328800	H	5.38744400	5.65936000	2.54512200
H	-2.01779900	5.02295800	-1.64035600	C	-4.60439700	1.21204100	1.51552900
C	0.83298300	6.25203000	1.18529900	H	-5.47925500	2.55878000	2.94228000
N	-9.41868900	5.61619300	-5.37847600	H	-3.48815100	0.05142600	0.09536400
H	-8.23634600	4.92348700	-3.81815200	C	2.87929800	1.94481300	0.98229800
H	-7.46581600	4.85981300	-5.42396600	C	3.03585700	2.84594600	3.20554500
C	4.48291700	10.98520600	0.28965300	C	9.80465700	13.01527400	1.89737600
H	4.18556900	9.13620100	-0.47883000	C	-10.83195000	2.07723600	-1.49264000
C	-5.27686600	4.47371500	-0.85502400	H	-9.86234500	3.74690400	-2.15764600
H	-6.56539200	5.89561100	0.11465000	O	5.60510900	7.76615700	0.19384100
H	-3.75900400	3.26228000	-1.77943500	C	7.23722000	7.22510100	1.88048000
C	1.71943100	6.44270900	0.11890000	N	-5.72855000	0.33724300	1.47909300
C	1.37233300	6.03631200	2.45805100	C	4.26654800	1.90361500	0.89771000
H	-2.57871100	5.45641800	1.34620300	H	2.27656800	1.58080700	0.15489200
C	-10.53500500	5.52356000	-4.60675700	C	4.42039400	2.82632300	3.13074500
H	-9.45485300	6.27952900	-6.14540000	H	2.54826600	3.19241000	4.11372700
O	4.06288300	12.06307600	0.69763900	O	-10.85539300	1.06875100	-0.78882800
C	5.96192400	10.63533600	0.43382200	O	-11.92056200	2.57306900	-2.11337400
N	-6.26746900	3.45779100	-0.91232000	N	8.21150100	7.89919800	1.06870600
C	3.09538400	6.42714600	0.29521500	H	7.60386600	6.24179100	2.18455800
H	1.31419000	6.56938800	-0.88049100	H	7.07397300	7.81175300	2.79252600
C	2.74847100	6.04937900	2.65384000	C	-6.38457900	0.03225000	0.33077100
H	0.70707100	5.86284400	3.29990400	H	-6.15347800	0.01108000	2.34786600
C	-2.36879100	2.92040400	1.57755800	C	5.03766700	2.36947300	1.96213900
O	-10.59913300	4.92200500	-3.54587700	H	4.75296500	1.50282400	0.01084900
O	-11.57541000	6.13213100	-5.18982900	H	5.02706000	3.15947500	3.96338500
N	6.67617300	11.83666500	0.77569500	C	-13.17869700	2.07848400	-1.65595900
H	6.34970700	10.17087200	-0.47944700	C	8.82848800	7.22089700	0.07612900
H	6.06523000	9.88487800	1.22673700	H	8.18278500	8.91643900	0.99588900
C	-7.56078300	3.70889900	-1.22253900	O	-6.08765000	0.50891200	-0.76588000
H	-5.97808400	2.48198600	-0.80035100	C	-7.56538700	-0.92024800	0.50973700
C	3.61936900	6.24151700	1.57477100	N	6.44588100	2.35729800	1.83882800

O	8.79093500	6.00941700	-0.07458500	H	-2.36261100	0.79794700	3.25503800
O	9.52533700	8.05183300	-0.71637400	C	-1.51882400	-2.32789300	5.37404300
N	-8.74552000	-0.20486500	0.95176900	H	0.49356900	-1.59831300	5.38239100
H	-7.31421900	-1.67565300	1.26267400	C	0.18670800	-3.08220100	1.45242800
H	-7.77601000	-1.40368500	-0.44453000	H	-0.52112700	-1.33697500	2.30110700
C	7.26392100	3.33649500	2.29608200	C	4.06847500	-1.73998200	2.42496800
H	6.86399100	1.65439700	1.22955700	C	2.97565500	-1.42030700	0.30764000
C	10.27785200	7.41466600	-1.74617100	C	-2.81492900	-2.13501400	4.88325700
C	-8.91286100	0.05286500	2.26799900	H	-4.11638400	-0.83294300	3.77091100
H	-9.43234200	0.14873200	0.28387200	H	-1.29135100	-3.21257000	5.95318600
O	6.90152400	4.28005800	2.99332200	C	1.33447300	-3.88912300	1.02875500
C	8.72416200	3.18810700	1.86621300	C	-1.22284800	-3.55907100	1.41026600
O	-8.12572000	-0.26910900	3.14855100	C	5.26355200	-2.00603200	1.75881800
O	-10.06222400	0.71429000	2.48784900	H	4.03195200	-1.77605200	3.51039800
N	8.90674600	3.24948100	0.43155800	C	4.15897200	-1.67736300	-0.36398600
H	9.12640100	2.23597200	2.22807600	H	2.06967100	-1.21438700	-0.25709500
H	9.28182200	4.00885900	2.31881700	N	-3.86233500	-3.05770200	5.04440800
C	-10.40341600	0.88786200	3.85979300	C	1.44089800	-4.75611600	-0.00753400
C	8.76263800	2.15993700	-0.34362500	H	2.25107400	-3.64809800	1.54699200
H	8.97340500	4.17195000	0.00234500	C	-2.26866300	-2.64719900	1.21748700
O	8.39078100	1.05986400	0.06332900	C	-1.55474500	-4.89607900	1.66269200
O	9.10439600	2.41912400	-1.61250400	C	5.31301900	-1.97876100	0.36603000
C	8.98469200	1.32422400	-2.52935900	H	6.16577000	-2.23732400	2.31833400
H	10.05345500	14.06849200	2.02063900	H	4.20253700	-1.65640500	-1.44572200
H	10.45578100	12.55079800	1.15287900	C	-3.99534400	-3.96914300	6.04901200
H	9.90647100	12.48418200	2.84619400	H	-4.63978500	-2.95505500	4.38830000
H	10.77523800	8.22122900	-2.28170000	C	0.23240700	-5.09896000	-0.77456800
H	9.61443100	6.85667400	-2.41052800	C	2.79865400	-5.24022900	-0.38097100
H	11.01715400	6.73625900	-1.31295100	C	-3.59369200	-3.03291500	1.32373000
H	9.11515200	1.76155300	-3.51809700	H	-2.04083000	-1.61150700	0.98470800
H	8.00578800	0.84787200	-2.43619300	C	-2.88198900	-5.29817900	1.75469600
H	9.77895300	0.59669000	-2.33316200	H	-0.76078200	-5.62384100	1.80351700
H	-12.91525200	6.86659000	-3.79813400	N	6.53117100	-2.28106300	-0.28669700
H	-13.59638400	6.09669300	-5.26805200	O	-3.14406800	-4.24139000	6.87626500
H	-12.88821300	5.08709900	-3.96335600	C	-5.40974600	-4.54761900	6.14629500
H	-13.91683300	2.81246300	-1.97574500	C	-0.14160700	-6.31466300	-1.23247300
H	-13.18163300	1.97869200	-0.56951700	H	-0.50967500	-4.30937200	-0.83559600
H	-13.41022200	1.11417300	-2.11647100	C	3.83536600	-5.31647200	0.56081800
H	-11.25019300	1.57321000	3.86933700	C	3.10946300	-5.54402400	-1.71367000
H	-9.56300000	1.30474000	4.41851700	C	-3.90429400	-4.36325200	1.60286500
H	-10.69206100	-0.07450100	4.29522500	H	-4.38886000	-2.30608000	1.18828600
H	-3.79591000	13.52346200	-0.76500600	H	-3.13156800	-6.33522800	1.95987800
C	0.03098800	1.82111300	3.28183500	C	7.00791000	-1.59240700	-1.35643600
C	0.28582800	0.55108500	3.68049900	H	7.06468300	-3.08738000	0.03689900
H	-0.90198400	2.27349600	3.60788600	N	-6.24728700	-3.55572400	6.79782800
C	1.53934600	-0.11410600	3.23101500	H	-5.83501900	-4.73887800	5.15760100
C	-0.79502000	-0.26209400	4.29960100	H	-5.36829600	-5.47787500	6.71778800
C	1.60388200	-1.14739900	2.35814300	C	0.79672800	-7.44588300	-1.17855000
H	2.47404800	0.37434000	3.48669500	C	-1.54310600	-6.46752700	-1.69585700
C	-2.11942200	-0.05319300	3.88121200	C	5.13314800	-5.64073100	0.19224300
C	-0.52760800	-1.40072000	5.06718800	H	3.62771600	-5.12859300	1.60980900
C	0.37681700	-1.84927200	1.98895100	C	4.40057800	-5.88951000	-2.09148600
C	2.90796400	-1.45055700	1.70799300	H	2.32697100	-5.49604100	-2.46538900
C	-3.10977700	-0.97627800	4.15857900	N	-5.26059100	-4.77564100	1.67584300

O	6.40908300	-0.69578400	-1.93030700	C	12.29549100	-2.29075300	1.04719900
C	8.43024000	-1.98688700	-1.76112800	C	4.92409900	-10.01533400	-2.32828000
C	-7.40150800	-3.09809600	6.27753000	H	4.59775600	-10.59024400	-0.28503800
H	-5.86667000	-3.04272200	7.58280400	H	4.96227500	-9.38877700	-4.38117400
C	1.04844900	-8.26431300	-2.21035500	C	-6.63444100	-6.43714100	-1.27662800
H	1.48199400	-7.46263800	-0.33415500	H	-6.03069400	-5.92645100	-3.11816800
C	-2.15121400	-5.49880500	-2.50176400	N	10.30305900	-6.02106100	-0.97164300
C	-2.34286500	-7.47876700	-1.14855100	H	9.06323200	-7.37967900	-1.94395400
C	5.42289000	-5.92572400	-1.14321900	H	9.25197200	-5.82638400	-2.75536000
H	5.92116600	-5.69126000	0.93496500	O	-9.78037300	-3.43016400	0.63349300
H	4.62502900	-6.12356800	-3.12857900	O	-10.37482500	-2.30732800	2.50697500
C	-6.22249700	-4.06356700	2.29506300	H	12.61393900	-1.75849800	1.94231600
H	-5.53820800	-5.59899100	1.13498200	H	12.11504500	-3.34447400	1.27516500
N	9.34495200	-1.55620200	-0.72235000	H	13.05644600	-2.20079900	0.26813000
H	8.52599500	-3.07056200	-1.86928100	N	6.26668000	-10.47094300	-2.32232400
H	8.64259100	-1.51202500	-2.72294600	O	-6.39364700	-6.73239700	-0.10923100
O	-8.00781800	-3.61250500	5.34002000	C	-8.03367900	-5.99975400	-1.71452500
O	-7.81858600	-2.00379700	6.92094800	C	10.86249000	-6.95079700	-0.18380700
C	2.30108700	-9.03655500	-2.26944600	H	10.51405000	-5.03961400	-0.79214100
H	0.44424700	-8.20059400	-3.11536500	C	-11.52683000	-1.84375100	1.79549200
C	-3.52395100	-5.50037200	-2.70078200	C	7.31922500	-9.71349200	-2.71492200
H	-1.54038100	-4.72319400	-2.95471400	H	6.49313300	-11.32100900	-1.80458100
C	-3.72189600	-7.47956800	-1.32543000	N	-8.13785500	-4.55260600	-1.64935800
H	-1.87820300	-8.24703800	-0.53618900	H	-8.25867000	-6.34131800	-2.73000900
N	6.72555100	-6.30305300	-1.55490400	H	-8.75149900	-6.43287100	-1.01979600
O	-6.02493200	-3.06674300	2.99347100	O	10.60207100	-8.15174500	-0.18708500
C	-7.63735300	-4.58491900	2.05917500	O	11.79319100	-6.41636300	0.63048600
C	10.47050700	-2.21589200	-0.42022600	H	-12.02055700	-1.14147900	2.46644500
H	9.13826600	-0.68786600	-0.22718200	H	-11.22365500	-1.34229800	0.87167700
C	-9.04699400	-1.44904800	6.45209100	H	-12.18923100	-2.68500800	1.57036300
C	2.85867400	-9.64838400	-1.14143100	O	7.22306100	-8.60008900	-3.22723700
C	3.05919000	-8.99008800	-3.44681900	C	8.68216400	-10.34516400	-2.43473700
C	-4.31448400	-6.47163800	-2.08581900	C	-7.55619900	-3.79484700	-2.60891300
H	-4.00058700	-4.73266200	-3.30543200	H	-8.67826300	-4.10522800	-0.90884000
H	-4.34333900	-8.24030600	-0.86643600	C	12.48918900	-7.36418100	1.44444700
C	7.87587900	-5.75311700	-1.10755000	N	8.98873600	-10.36787700	-1.01828500
H	6.79048400	-7.03577300	-2.26557800	H	8.71469000	-11.36991900	-2.81733800
N	-8.60905800	-3.66176200	2.58493100	H	9.43416200	-9.74776500	-2.95270400
H	-7.79963500	-4.72147700	0.98724400	O	-6.95840500	-4.22900000	-3.58149400
H	-7.74285300	-5.58130900	2.50978400	O	-7.70518500	-2.48427300	-2.35158800
O	10.91331100	-3.19933000	-1.01922900	H	13.11964900	-6.77159100	2.10400300
O	11.08515000	-1.65913800	0.63571200	H	11.78029800	-7.96477300	2.01605100
H	-9.15541000	-0.50034300	6.97633500	H	13.10741400	-8.01513800	0.82043200
H	-9.87741600	-2.11073700	6.70664700	C	8.50258600	-11.35594900	-0.23398300
H	-9.00072200	-1.28412900	5.37176800	H	9.47118400	-9.57796500	-0.59224400
C	4.15820500	-10.13622700	-1.16908600	C	-7.16409000	-1.58143800	-3.32192400
H	2.27372600	-9.72053900	-0.22901300	O	7.76147800	-12.25120000	-0.61882800
C	4.36472900	-9.46099400	-3.47922400	O	8.93556700	-11.24223500	1.03084900
H	2.63347100	-8.53109800	-4.33570000	H	-7.19307700	-0.60099800	-2.84738900
N	-5.71667700	-6.40464900	-2.27513400	H	-6.13713900	-1.86014000	-3.56237000
O	7.95626900	-4.85516100	-0.27184100	H	-7.77484400	-1.59465600	-4.22725400
C	9.14222000	-6.30350300	-1.77274800	C	8.45213100	-12.25211400	1.91507600
C	-9.58680900	-3.15445100	1.81406300	H	8.87834700	-12.01580800	2.88890800
H	-8.38808200	-3.21440500	3.47409900	H	7.36089300	-12.23351500	1.95892500



H	8.77808800	-13.23943400	1.58216300
H	-9.46816300	3.08214300	-4.53075100
C	-8.94193800	2.20692500	-4.91391100
Cl	-7.36874100	2.09869600	-4.08701700
Cl	-8.70055700	2.38707700	-6.65455800
Cl	-9.93575600	0.78298300	-4.54238200
H	-12.59810500	1.68569200	-4.46987300
C	-13.11906100	2.00014300	-5.37251800
Cl	-12.11182100	3.21072800	-6.17750100
Cl	-14.68133600	2.69335300	-4.88559700
Cl	-13.35571600	0.58842700	-6.41152400
H	-12.15658800	-0.55055000	-1.38563000
C	-12.12272400	-1.44430100	-2.00513700
Cl	-13.11659800	-2.70731800	-1.25274100
Cl	-10.43022400	-1.92314300	-2.11581100
Cl	-12.76563400	-1.03133100	-3.61185100
H	-8.04045700	-5.63930200	4.94682900
C	-8.03253300	-6.71719100	5.10097000
Cl	-6.55564600	-7.37963400	4.35802000
Cl	-9.47212800	-7.40129800	4.33595000
Cl	-8.02881200	-6.98596100	6.85069400
H	-10.26866100	-3.52520900	4.61240800
C	-11.24957800	-3.86249000	4.93749300
Cl	-12.25497800	-2.41980500	5.23239600
Cl	-11.02404200	-4.79192300	6.42511400
Cl	-11.96253700	-4.84737700	3.65559300
H	-11.34202300	-4.57417700	-0.03824500
C	-11.68476900	-5.60520100	-0.09846000
Cl	-13.34563200	-5.68151100	0.52007300
Cl	-10.59558600	-6.57886400	0.91137000
Cl	-11.61232600	-6.11753700	-1.79259900
H	4.62966000	11.55478700	2.83665700
C	4.72918000	10.82950600	3.64368900
Cl	3.98817100	9.30832100	3.09722300
Cl	3.89219100	11.46350600	5.06700300
Cl	6.46162400	10.60363300	3.97143200
H	10.29310400	9.40025600	1.34776600
C	11.37542200	9.33199000	1.37870200
Cl	11.93117400	10.17210600	2.83993900
Cl	12.00009800	10.12723900	-0.07836600
Cl	11.84472000	7.62273300	1.42581800
H	11.17855800	3.26675200	-0.93629200
C	12.03459500	2.93013900	-0.35720000
Cl	12.15366400	3.94264300	1.09248500
Cl	13.48301100	3.09249200	-1.36312600
Cl	11.74246600	1.23225700	0.07618800
H	11.80086100	-2.87010200	-2.99588300
C	11.77107100	-3.34290000	-3.97468000
Cl	11.96737400	-5.08218100	-3.70849100
Cl	13.07130300	-2.68981600	-4.98127100
Cl	10.18532500	-2.99464800	-4.69726900
H	12.89495300	-4.64203800	-0.63130800
C	13.97198700	-4.76826600	-0.73520300
Cl	14.56363100	-3.48871100	-1.81056300

Cl	14.29439600	-6.37316900	-1.39931500
Cl	14.71151600	-4.61541100	0.87849600
H	11.78964600	-9.70002400	-1.04677300
C	12.37474900	-9.88579500	-1.94443300
Cl	14.09260700	-9.82076000	-1.50826100
Cl	11.96593700	-8.60175200	-3.10172700
Cl	11.95153800	-11.48176800	-2.58828700

### 1b-8-mer<sub>RH</sub>-1b-8-mer<sub>LH</sub>/16THF

C	-13.89186400	3.74775100	-0.40292800
C	-12.56290000	3.61084500	-0.52539100
C	-11.65133000	4.49581600	0.22935900
C	-10.35256800	4.28514900	0.56380300
C	-9.64909600	3.02952500	0.26098200
C	-8.32691000	2.80777400	0.04904600
C	-7.26722200	3.82828200	0.15910200
C	-6.01823900	3.62664000	0.64794100
C	-5.56219500	2.29628000	1.09021000
C	-4.31988900	1.76622800	0.96506900
C	-3.20257100	2.55982300	0.42327900
C	-1.92384300	2.59610300	0.86645500
H	-14.57550500	3.12444100	-0.97098000
C	-11.97970300	2.57294100	-1.42551300
C	-12.20136700	1.21238100	-1.19964500
C	-11.06323100	2.93712200	-2.41574100
H	-12.09990800	5.42899400	0.56875400
C	-11.45864800	0.25057200	-1.87775700
H	-12.90786600	0.90885900	-0.43161900
C	-10.32864200	1.98932200	-3.11371400
H	-10.87406100	3.99190400	-2.59644000
C	-9.54863100	5.36048600	1.20840700
C	-10.49081200	0.63240400	-2.81023700
H	-11.59954400	-0.80520600	-1.66014400
H	-9.60063400	2.28970200	-3.85501600
C	-9.35035500	6.58436200	0.56231800
C	-8.78690200	5.09017000	2.34989700
H	-10.28437100	2.16353500	0.12443200
N	-9.66351300	-0.36729800	-3.36604400
C	-8.34121700	7.44542000	0.97299300
H	-9.93227300	6.81872100	-0.32500800
C	-7.78454200	5.94625200	2.78606200
H	-8.92797600	4.14149500	2.86124800
C	-7.91979000	1.43394200	-0.35623800
C	-8.99968300	-0.29302700	-4.55848900
H	-9.46179700	-1.17741300	-2.78257400
C	-7.51317800	7.10649900	2.05010800
H	-8.15211500	8.36700200	0.42732000
H	-7.16972400	5.69620500	3.63955500
C	-8.38548000	0.29614000	0.31027300
C	-6.99242200	1.25865500	-1.38860800
H	-7.52991100	4.85001400	-0.09793900
O	-9.09482300	0.63201800	-5.34873400
C	-8.14225400	-1.52132700	-4.85689300
N	-6.40910500	7.93949700	2.29135600

C	-7.88362200	-0.96116500	0.00312500	H	-4.82421000	-4.61460300	-3.06640100
H	-9.10616800	0.40688400	1.11619500	C	-1.22468000	8.07238200	1.90756900
C	-6.48312900	0.00916400	-1.71210600	H	-1.61817100	7.85616000	-0.06743500
H	-6.62113800	2.13385500	-1.91474200	C	-3.98363500	-2.47107200	1.69379700
C	-5.08289400	4.77741200	0.75737500	H	-5.16314000	-2.09618000	3.45509300
N	-8.93934900	-2.72220500	-5.00577000	H	-2.79917900	-2.51421100	-0.10469300
H	-7.40412500	-1.67069500	-4.06238700	C	-0.91988200	3.77232500	-1.11811800
H	-7.60996100	-1.32661700	-5.79046400	C	-0.25808100	4.45883200	1.08133600
C	-5.49828700	7.87698800	3.30754300	C	-6.92089300	12.88702600	2.35521100
H	-6.23620600	8.66215400	1.59680800	C	-7.06195500	-5.42113700	-0.80064400
C	-6.90328700	-1.10956600	-0.98321000	H	-7.08550500	-5.34607400	-2.83676700
H	-8.21820500	-1.83726200	0.55354200	O	-1.43409500	7.81361200	3.08359700
H	-5.73515800	-0.10353000	-2.48523800	C	-0.07800900	8.98699800	1.48038000
C	-4.82716700	5.62412000	-0.32639200	N	-3.90537900	-3.83876400	2.02110800
C	-4.35406700	4.97640200	1.93303700	C	-0.07063300	4.72085300	-1.66611000
H	-6.33917500	1.62629100	1.44067100	H	-1.49365300	3.12058500	-1.77084600
C	-9.23666000	-3.50305100	-3.95157600	C	0.61031400	5.40666700	0.54857800
H	-9.39050200	-2.90712200	-5.90476900	H	-0.32838700	4.35318200	2.16150100
O	-5.55842400	7.11430400	4.25897600	O	-6.59830600	-5.04733900	0.27434200
C	-4.39699200	8.93599000	3.18221600	O	-8.18242300	-6.16586600	-0.89306600
N	-6.34029600	-2.38376300	-1.15421900	N	-0.51748800	10.12678100	0.70509800
C	-3.81942500	6.57692100	-0.25947300	H	0.64991900	8.40916500	0.90000700
H	-5.38079900	5.48802600	-1.25180800	H	0.40786800	9.33876600	2.39351900
C	-3.34993700	5.93161800	2.02158700	C	-3.49288600	-4.87947600	1.24372700
H	-4.54897700	4.33708800	2.78993500	H	-4.26961400	-4.09482700	2.93677600
C	-4.15372000	0.31622400	1.26516900	C	0.71769600	5.53408500	-0.84318300
O	-8.84679900	-3.33115000	-2.80422900	H	0.01307400	4.81991900	-2.74585500
O	-10.06719200	-4.50816500	-4.31652800	H	1.21735400	6.02520900	1.19633700
N	-4.89980000	10.25174800	3.54568100	C	-8.84857800	-6.40243600	0.34585500
H	-4.01088800	8.97669800	2.15796600	C	-0.63850700	10.06852400	-0.63498600
H	-3.57937400	8.65662600	3.84794700	H	-0.79557400	10.97475500	1.20038200
C	-5.71464000	-2.86091800	-2.26024400	O	-3.03357900	-4.77165200	0.11548600
H	-6.46727200	-3.04221200	-0.38956400	C	-3.66763100	-6.24825500	1.91483300
C	-3.04779700	6.71324700	0.89990100	N	1.60171500	6.41177900	-1.49147400
H	-3.59400000	7.19758400	-1.12326400	O	-0.41480400	9.07886100	-1.32184800
H	-2.78464600	6.05257400	2.93544900	O	-1.08723000	11.24054400	-1.12827000
C	-4.77537300	-0.28245800	2.36785100	N	-5.06016800	-6.57697400	2.18015300
C	-3.44327400	-0.51572200	0.38857000	H	-3.10447500	-6.28428600	2.85376000
H	-3.46696900	3.28287400	-0.34196700	H	-3.26790800	-6.99845600	1.23101900
C	-10.35536800	-5.43946500	-3.27930100	C	2.41954900	7.35109200	-0.95299600
C	-5.64121000	10.95443800	2.66347900	H	1.59125100	6.38258600	-2.51012800
H	-4.95716000	10.48783700	4.54098900	C	-1.20217900	11.28222500	-2.54690000
O	-5.45658700	-2.20783800	-3.26252800	C	-5.71398000	-6.04322900	3.23778900
C	-5.35297800	-4.33758200	-2.15202300	H	-5.64501700	-6.73860900	1.36869200
N	-1.97042200	7.61892700	0.85882000	O	2.55975700	7.56450600	0.24619500
C	-4.69032700	-1.65089300	2.58210300	C	3.19030100	8.15112100	-2.00822300
H	-5.31559500	0.33801400	3.07805800	O	-5.20097200	-5.39653500	4.14130400
C	-3.35987300	-1.89239700	0.58104200	O	-7.02584600	-6.33715000	3.20249700
H	-2.94464100	-0.07095800	-0.46864500	N	2.34203300	9.03723800	-2.78445500
C	-1.01854300	3.61205400	0.26668400	H	3.70070700	7.45988600	-2.68824000
O	-5.78453300	10.68681900	1.47999500	H	3.92826000	8.75627400	-1.47862200
O	-6.20913700	12.03393000	3.24942300	C	-7.79037500	-5.76346100	4.25983100
N	-6.51969100	-5.18612200	-2.00389800	C	1.58348900	8.55229500	-3.78679900
H	-4.68164600	-4.48248200	-1.29901200	H	2.04709200	9.91269700	-2.35216700

O	1.59950000	7.39982600	-4.20297400	C	3.10530700	-4.05044600	1.85779000
O	0.81120800	9.51412300	-4.32796500	C	4.98324800	1.79493400	-1.90994200
C	-0.13056600	9.04768700	-5.28767000	H	5.47346600	3.06089700	-0.24671000
H	-7.35750700	13.66594400	2.97851000	H	4.24514400	0.45800900	-3.41976700
H	-7.69958700	12.33006600	1.83148400	C	1.75873100	-4.57924700	4.81676700
H	-6.23843300	13.32268600	1.62130400	H	-0.07774900	-4.61636200	3.97323300
H	-1.64845400	12.25054900	-2.77486400	C	4.56817700	-3.42387200	-0.75998300
H	-1.84424500	10.47290200	-2.90429600	C	6.18177300	-1.48162300	-0.35935100
H	-0.21952700	11.18384000	-3.01408300	C	1.19216000	-5.42918700	0.40863400
H	-0.67602000	9.93204500	-5.61768500	H	0.57212400	-3.51206000	-0.32618600
H	-0.81331800	8.32673800	-4.83114600	C	3.05271600	-5.43356400	1.94948500
H	0.37777800	8.57603900	-6.13106200	H	3.86831600	-3.51669000	2.41752600
H	-11.08445000	-6.13165000	-3.70086600	N	6.11657800	2.22932300	-2.63240000
H	-9.44905700	-5.97097600	-2.97677300	O	2.77361900	-3.99729700	5.16398500
H	-10.76911600	-4.93019500	-2.40565400	C	1.58430700	-6.09310500	4.97999300
H	-9.76442600	-6.93276100	0.08589900	C	5.42425400	-4.45902200	-0.90714300
H	-9.07723500	-5.45669300	0.84270900	H	3.53158000	-3.59142600	-1.02865100
H	-8.23051300	-7.00857800	1.01282500	C	7.01122900	-1.03665900	0.67035400
H	-8.82125000	-6.06047000	4.07220700	C	6.60242800	-1.29844300	-1.68180700
H	-7.69803600	-4.67597000	4.25114500	C	2.12178900	-6.13845300	1.17768600
H	-7.45413000	-6.14188900	5.22646600	H	0.44169700	-5.97293300	-0.16037500
H	-14.32491800	4.48721900	0.26498200	H	3.75235200	-5.96972000	2.57726300
C	-1.45046200	1.70930300	1.94085100	C	6.10698000	2.59306000	-3.94837000
C	-0.24813100	1.08449200	2.01423200	H	6.92250100	2.53221100	-2.09063100
H	-2.20379900	1.41285300	2.66763100	N	0.46964300	-6.43155000	5.85157100
C	0.86369100	1.36684400	1.08257800	H	1.42338800	-6.55787500	4.00314900
C	-0.07075900	-0.06906800	2.94213600	H	2.50820700	-6.49666200	5.39477400
C	1.67493000	0.46042200	0.48530300	C	6.83241200	-4.30658600	-0.47537700
H	1.03621700	2.40584500	0.82487900	C	4.91490400	-5.75756600	-1.40640600
C	-1.09681100	-1.01742400	3.05016000	C	8.23982500	-0.44592800	0.38618700
C	1.16900400	-0.38758700	3.50545500	H	6.70470100	-1.18300200	1.70301100
C	1.51414400	-0.99525700	0.66166100	C	7.81189800	-0.69307500	-1.97843000
C	2.78150000	0.96965700	-0.37473200	H	5.96842200	-1.65734200	-2.48810400
C	-0.84767300	-2.27948300	3.56023200	N	2.12232800	-7.54490000	1.09325400
H	-2.07316800	-0.79809900	2.63369600	O	5.22233000	2.31454200	-4.74219500
C	1.43588700	-1.64582100	4.03470000	C	7.25464200	3.53583200	-4.30813400
H	1.97976200	0.33365500	3.43952300	C	-0.79176900	-6.47961400	5.37510900
C	2.52071500	-1.89407000	0.75665100	H	0.57501000	-6.28432800	6.85984100
H	0.50209100	-1.35452400	0.83613800	C	7.88746000	-4.45993600	-1.28518000
C	3.67280100	1.93148300	0.11252300	H	6.98921100	-3.85595000	0.50263800
C	3.00475600	0.44837700	-1.65352900	C	3.84168100	-5.82534300	-2.30607200
C	0.43832700	-2.62702400	3.99083300	C	5.41358500	-6.96305900	-0.89864300
H	-1.63414800	-3.03259900	3.55878400	C	8.64527100	-0.27488900	-0.93582900
H	2.42257300	-1.89946100	4.39903900	H	8.89800700	-0.12528200	1.18950800
C	3.93288000	-1.48134000	0.61125500	H	8.12632500	-0.54997400	-3.00479500
C	2.25033600	-3.33251800	1.01429000	C	2.66697900	-8.41917900	1.98678500
C	4.77028800	2.33007900	-0.63899900	H	1.69734100	-7.95723000	0.26453400
H	3.52461000	2.33591100	1.11030200	N	6.96979400	4.85073800	-3.74367700
C	4.08221500	0.86073400	-2.42778400	H	8.20453000	3.16781000	-3.91123000
H	2.33264800	-0.31637000	-2.03421900	H	7.31299800	3.61357600	-5.39537900
N	0.64704300	-3.98016600	4.29961900	O	-1.11897200	-6.31569500	4.20377000
C	4.86729500	-2.13492800	-0.11520900	O	-1.67628200	-6.75003300	6.35407500
H	4.20950400	-0.51383500	1.01831900	C	9.23796200	-3.97681700	-0.95674700
C	1.25694700	-4.04318800	0.33010100	H	7.72919700	-4.81783900	-2.30286900

C	3.28468600	-7.03991800	-2.66374100	C	13.87115000	-1.58387800	-0.77846300
H	3.44692500	-4.91169700	-2.74015400	H	13.31713800	-2.52148700	0.91826500
C	4.86434100	-8.19416200	-1.24582000	N	1.09397000	-11.62984100	-2.70347000
H	6.24855200	-6.93428500	-0.20436800	H	2.72186400	-11.60849000	-3.99074900
N	9.92783800	0.25573600	-1.19634700	H	2.86143200	-12.70777000	-2.59591400
O	3.17421200	-8.10390700	3.05406600	O	12.37635500	0.83318200	0.41034600
C	2.53998500	-9.88179000	1.56133500	O	12.55097400	3.06033600	0.82052300
C	7.33664000	5.11285100	-2.46257600	H	-1.88451400	-9.20877200	-0.33372200
H	6.08810500	5.29544000	-4.02230200	H	-1.91082300	-10.92908100	-0.79251500
C	-3.04598200	-6.67358300	5.95489800	H	-2.91640800	-10.34090200	0.57845700
C	9.72047600	-3.91210200	0.35642100	O	13.67418700	-1.20958800	-1.92745800
C	10.04686700	-3.45993500	-1.97507900	C	15.18400800	-1.26357000	-0.04990200
C	3.78967500	-8.23776900	-2.14027900	C	0.37524800	-10.64570300	-3.28318500
H	2.45677400	-7.07717700	-3.36805700	H	0.71429600	-12.04908400	-1.85333200
H	5.26407500	-9.11368800	-0.83948900	C	12.92564800	2.73447600	2.15366100
C	10.25220200	1.05402600	-2.24680200	N	15.04294800	-0.38622100	1.09206000
H	10.67309200	0.04071800	-0.53579600	H	15.64596600	-2.19738400	0.28728900
N	1.16787500	-10.34094900	1.63749000	H	15.84272200	-0.78467800	-0.77588300
H	2.91983300	-10.02494400	0.54424800	O	0.80145500	-9.82261300	-4.08344400
H	3.14679600	-10.47279000	2.25057600	O	-0.91449000	-10.70289600	-2.90316600
O	8.08085900	4.42967200	-1.77493000	H	12.92857000	3.67965900	2.69697000
O	6.78316500	6.26898200	-2.03603000	H	12.21132900	2.03711200	2.59692600
H	-3.62388100	-6.86420800	6.85874900	H	13.91770500	2.27686900	2.17455400
H	-3.26884300	-7.42865000	5.19593900	C	14.58070900	-0.86098200	2.26554400
H	-3.28106700	-5.68887700	5.54927700	H	14.97698600	0.61215200	0.90210100
C	10.95457400	-3.34673300	0.63313700	C	-1.68228400	-9.56223200	-3.25146800
H	9.12561400	-4.32139800	1.16819200	O	14.31971800	-2.03359500	2.50436300
C	11.28337600	-2.88062900	-1.71555200	O	14.47181200	0.11639400	3.18568500
H	9.68635900	-3.49170000	-3.00040400	H	-2.64373600	-9.69519500	-2.75438900
N	3.20459100	-9.42376800	-2.61418500	H	-1.19014600	-8.65312200	-2.89483200
O	9.45907000	1.45582700	-3.08883700	H	-1.81165200	-9.49964200	-4.33191300
C	11.73465000	1.42768500	-2.27327100	C	13.93498500	-0.30586400	4.43546600
C	0.29458200	-10.10799100	0.63827700	H	13.89774200	0.58916000	5.05573100
H	0.80330800	-10.65463400	2.54022500	H	12.93392800	-0.72192700	4.30177200
C	7.00554400	6.56431400	-0.66004200	H	14.57636700	-1.06187800	4.89282300
C	11.74986100	-2.82870900	-0.39741300	O	-5.12250800	10.54235900	6.37097400
H	11.32455300	-3.31167200	1.65525300	C	-5.34217100	9.18492200	6.79169000
H	11.88981400	-2.48057900	-2.51661200	C	-6.35518000	11.24303800	6.51866700
C	3.33616900	-10.68624700	-2.13104600	C	-6.85932500	8.92539000	6.68796100
H	2.50065300	-9.31397500	-3.34391000	H	-4.97484200	9.07003500	7.81787800
N	12.07068400	2.38578200	-1.23882100	H	-4.76608500	8.53244000	6.13114000
H	12.34516800	0.52562200	-2.14996300	C	-7.40824200	10.22997500	6.08548300
H	11.94513800	1.87502000	-3.24659800	H	-6.30367100	12.13710900	5.89271700
O	0.56376700	-9.58307600	-0.43570000	H	-6.49230300	11.53933700	7.56921600
O	-0.94513400	-10.50671700	0.99190300	H	-7.06879200	8.05596800	6.06234500
H	6.47137000	7.49468300	-0.46911300	H	-7.28850000	8.75125400	7.67876600
H	6.61219300	5.76557500	-0.02666700	H	-7.43036600	10.17414300	4.99158300
H	8.07278200	6.68750000	-0.45655000	H	-8.41249900	10.47691900	6.43742000
N	13.01760200	-2.33800900	-0.03892400	O	-1.22024300	12.13528700	2.59296200
O	4.02944400	-11.00857100	-1.17442800	C	-1.37936000	11.34709000	3.77349000
C	2.52259600	-11.72194600	-2.91982200	C	-2.51177000	12.67892000	2.33182700
C	12.34106500	1.99421300	0.02020800	C	-2.29291600	12.17521800	4.69047600
H	12.01295800	3.38161500	-1.45526300	H	-0.38342900	11.16137500	4.18347200
C	-1.97458900	-10.22983600	0.04421100	H	-1.83910400	10.38153000	3.51391400

C	-3.03472200	13.11468500	3.70732000	H	16.22886200	1.55237700	-1.88664700
H	-3.15391200	11.90354700	1.88371900	H	13.90455800	4.55303400	-0.94033600
H	-2.38907200	13.49339600	1.61455500	H	15.47363000	5.20581600	-1.44505700
H	-2.97621800	11.54266800	5.26178800	H	13.98919800	3.26158100	-2.88278700
H	-1.69904800	12.75469100	5.40135400	H	15.73147500	3.48090200	-3.08030300
H	-4.12002800	13.02039500	3.77828200	O	-10.21607800	-2.80403400	-7.54716100
H	-2.76774600	14.15718700	3.89807800	C	-10.45601500	-1.39751200	-7.68647300
O	1.85358700	11.30861500	-1.03445500	C	-11.49450600	-3.40364400	-7.34656000
C	2.52200000	11.00507800	0.19098700	C	-11.68742100	-1.07299100	-6.81077800
C	1.66857500	12.71600800	-1.05729900	H	-10.64696000	-1.17780900	-8.74581000
C	2.02740400	12.04369000	1.22066500	H	-9.55370300	-0.86536100	-7.37069100
H	3.60727900	11.10033900	0.03808400	C	-12.20809800	-2.45999900	-6.37974000
H	2.29905900	9.96502300	0.44199200	H	-11.33469900	-4.40974100	-6.95010100
C	1.24903000	13.06821700	0.36876400	H	-12.02123400	-3.47236000	-8.31082800
H	0.91405400	12.94375300	-1.81330200	H	-11.41565500	-0.45259200	-5.95440400
H	2.61328700	13.21155100	-1.33041300	H	-12.43725500	-0.52780000	-7.39096000
H	1.37738200	11.59843200	1.97790700	H	-11.89657100	-2.69008600	-5.35462700
H	2.87260400	12.50628000	1.73664800	H	-13.29825100	-2.54559500	-6.43421900
H	0.17250200	12.92043000	0.48373300	O	-7.27837400	-5.47158200	-4.72333000
H	1.48447700	14.10283900	0.62911800	C	-6.40912900	-4.65185000	-5.51252400
O	4.41484600	6.06261800	-4.32350200	C	-7.86802100	-6.41313600	-5.60899800
C	4.83392400	7.13669800	-5.15618300	C	-7.04344100	-4.57842400	-6.91768700
C	3.67854200	5.18590900	-5.18387700	H	-5.41847300	-5.12744800	-5.55762500
C	5.30699500	6.46447000	-6.45450800	H	-6.31059100	-3.68865200	-5.00522500
H	5.61532000	7.68394200	-4.62137300	C	-8.19888900	-5.59759200	-6.85640200
H	3.97855300	7.80267500	-5.33731200	H	-8.74040000	-6.84399000	-5.11189600
C	4.49403000	5.14468200	-6.48626900	H	-7.14767600	-7.21644500	-5.82916600
H	2.68090000	5.61300400	-5.33707700	H	-7.41868000	-3.57892200	-7.14979500
H	3.60436300	4.21631500	-4.68857500	H	-6.31113500	-4.84660600	-7.68336500
H	5.12656400	7.09671100	-7.32650900	H	-9.14995700	-5.08079600	-6.70876300
H	6.38172900	6.26141700	-6.40773200	H	-8.27313700	-6.21328700	-7.75562300
H	3.84564800	5.07657100	-7.36201300	O	-4.44820500	-8.58659800	-0.82022400
H	5.14515600	4.26710000	-6.48354400	C	-4.13210400	-7.49019500	-1.67054700
O	11.83252300	4.97727000	-2.41732000	C	-5.84876600	-8.76041700	-0.95384400
C	11.04066200	5.87432700	-1.63916900	C	-4.92424800	-7.76118800	-2.95698000
C	10.99714400	4.59737500	-3.51333200	H	-3.04653400	-7.45756600	-1.79690100
C	10.29840500	6.74946900	-2.66434500	H	-4.44735100	-6.55438200	-1.18848100
H	11.71968700	6.42759800	-0.98609100	C	-6.17335000	-8.51276000	-2.44109100
H	10.32781900	5.29999200	-1.03243900	H	-6.38011600	-8.02247500	-0.32693200
C	10.32571100	5.90055200	-3.95861300	H	-6.10163900	-9.76130800	-0.59549500
H	10.25711700	3.85895500	-3.17361300	H	-5.18789900	-6.84804300	-3.49583800
H	11.63831600	4.14604100	-4.27522300	H	-4.34243000	-8.39798100	-3.63039600
H	9.27840400	6.97194300	-2.34216400	H	-7.08315200	-7.91552500	-2.54665200
H	10.81477500	7.70060600	-2.81416700	H	-6.31930500	-9.45449200	-2.97596800
H	9.32770200	5.72569300	-4.36766400	O	0.60124000	-12.84436200	-0.17519000
H	10.92786600	6.39444300	-4.72540800	C	-0.39083700	-13.61039900	0.48938100
O	15.14100200	2.17652100	-0.24362100	C	1.85627700	-13.20959700	0.39979200
C	15.57224000	3.51582700	-0.05190500	C	0.02944800	-13.57474400	1.95732600
C	15.21892200	1.91637800	-1.64648500	H	-0.39609500	-14.63851200	0.09483400
C	14.93165900	4.28869100	-1.20204600	H	-1.35912800	-13.14446600	0.29340900
H	16.67144000	3.56403800	-0.09905400	C	1.57014000	-13.52729400	1.88245300
H	15.24308100	3.83737600	0.93904200	H	2.55174500	-12.38304100	0.23192700
C	14.94470900	3.26223600	-2.35341000	H	2.24128200	-14.09981800	-0.11948500
H	14.50148300	1.12324200	-1.87448600	H	-0.34997300	-12.66011900	2.41584700

H	-0.34585600	-14.43022200	2.52410200
H	1.96144200	-12.75613200	2.54962100
H	2.02208000	-14.48063200	2.16781000
O	0.31387700	-11.12292300	4.25040500
C	-1.11094500	-11.00442900	4.37666900
C	0.96547900	-10.24275800	5.18351800
C	-1.34486300	-9.76711700	5.23608800
H	-1.49566400	-11.91098500	4.86179500
H	-1.53862500	-10.92639000	3.37283600
C	-0.12358300	-9.80693900	6.15724300
H	1.38761800	-9.38658900	4.63797000
H	1.78418900	-10.79377200	5.65374400
H	-1.32227300	-8.86964800	4.60736400
H	-2.29730000	-9.79580800	5.77157600
H	0.09217600	-8.85003800	6.63359800
H	-0.26394800	-10.56674500	6.93365000
O	0.68434800	-5.29419900	8.48615600
C	-0.59159500	-4.68491400	8.65525600
C	1.63231700	-4.23872000	8.27354800
C	-0.60123800	-3.54874400	7.63845500
H	-0.68498000	-4.29551900	9.68072000
H	-1.34902000	-5.45327000	8.48983100
C	0.84021700	-3.02261700	7.74447500
H	2.37935800	-4.59610000	7.56020300
H	2.13254100	-4.01404200	9.22343400
H	-0.79128300	-3.94603200	6.63482900
H	-1.35259800	-2.78517700	7.85252300
H	1.23096300	-2.66906000	6.78752400
H	0.89331100	-2.19331300	8.45556100