

Electronic Supplementary Information

Isatoic anhydride as a masked directing group and internal oxidant for
Rh(III)-catalyzed decarbonylative annulation through C–H activation:
insights from DFT calculations

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1. Computational Details

All DFT calculations were carried out with the Gaussian 09 suite of computational programs.^[1] The geometries of all stationary points were optimized using the B3LYP hybrid functional^[2] at the basis set level of 6-31G(d) (Lanl2dz for Rh).^[3] Frequencies were analytically computed at the same level of theory to obtain the Gibbs free energies and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). A thorough conformational search of key transition states and intermediates was performed with the Conformer-Rotamer Ensemble Sampling Tool (CREST) developed by Grimme and co-workers.^[4] The solvent effect was evaluated by using the SMD polarizable continuum model by carrying out single point calculations at the M06/6-311+G(d,p) (SDD for Rh) level.^[5,6] All transition state structures were confirmed to connect the proposed reactants and products by intrinsic reaction coordinate (IRC) calculations. The final free energies given in the paper (ΔG_{sol}) are the large basis set single-point energies with Gibbs free energy correction (at 298.15 K, 1 atm and 1 mol/L).

[1] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

[2] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.

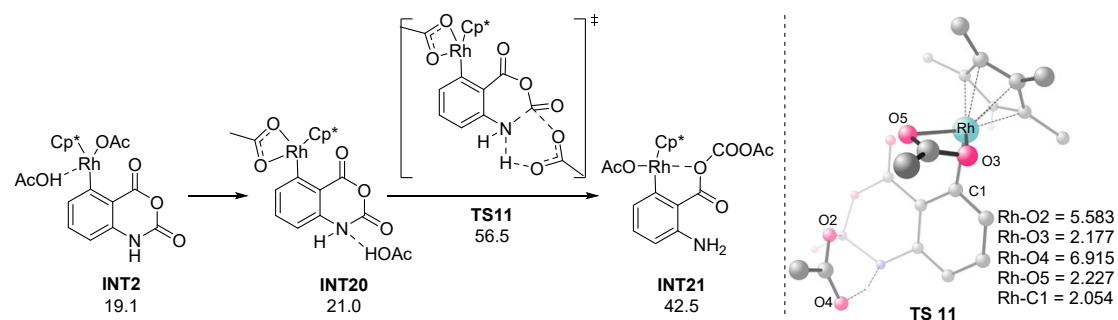
[3] (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270. (b) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284. (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

[4] (a) P. Pracht, F. Bohle and S. Grimme. *Phys. Chem. Chem. Phys.* **2020**, *22*, 7169. (b) S. Grimme. *J. Chem. Theory Comput.* **2019**, *15*, 2847.

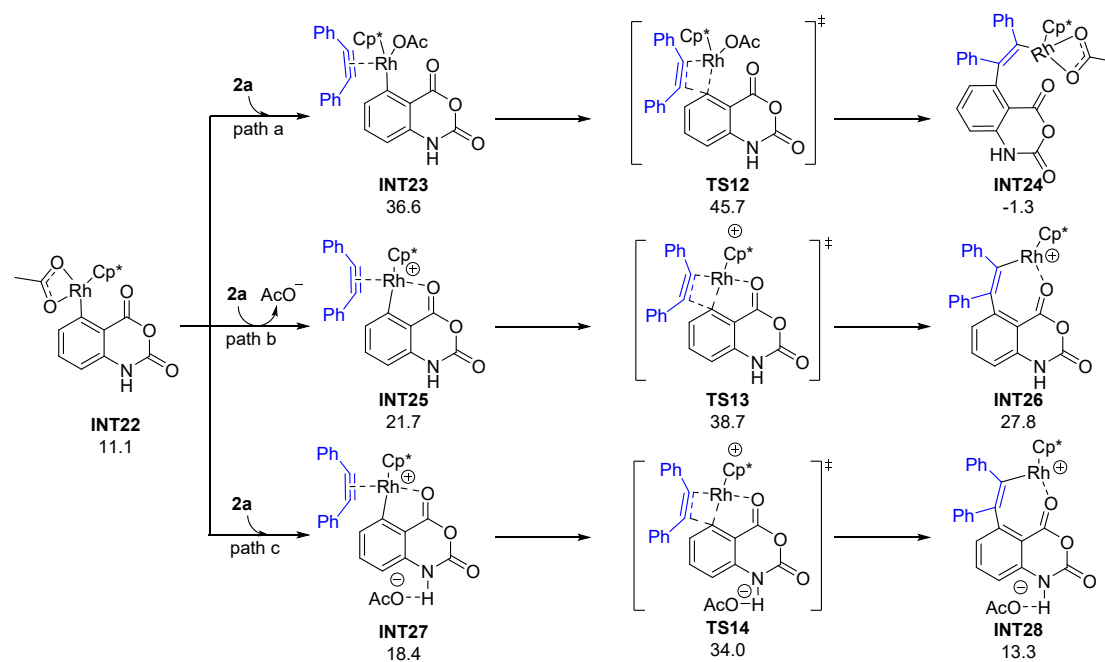
[5] (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.

[6] (a) Szentpály, L.; Fuentealba, P.; Preuss, H.; Stoll, H. *Chem. Phys. Lett.* **1982**, *93*, 555. (b) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866. (c) Schwerdtfeger, P.; Dolg, M.; Schwarz, W. H. E.; Bowmaker, G. A.; Boyd, P. D. W. *J. Chem. Phys.* **1989**, *91*, 1762.

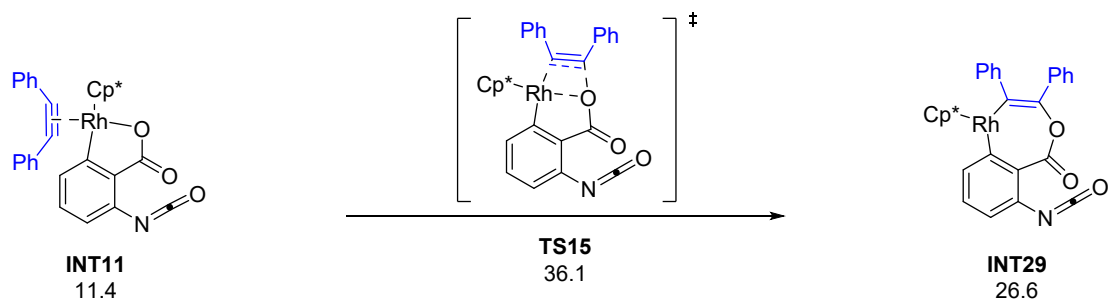
2. Additional Computational Results



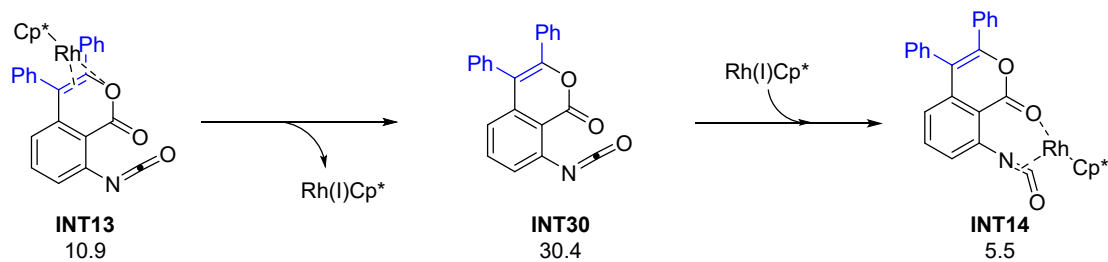
Scheme S1 Protonation of **INT2** by HOAc. Energies and key distances are in kcal/mol and Å, respectively. Irrelevant hydrogens have been omitted for clarity.



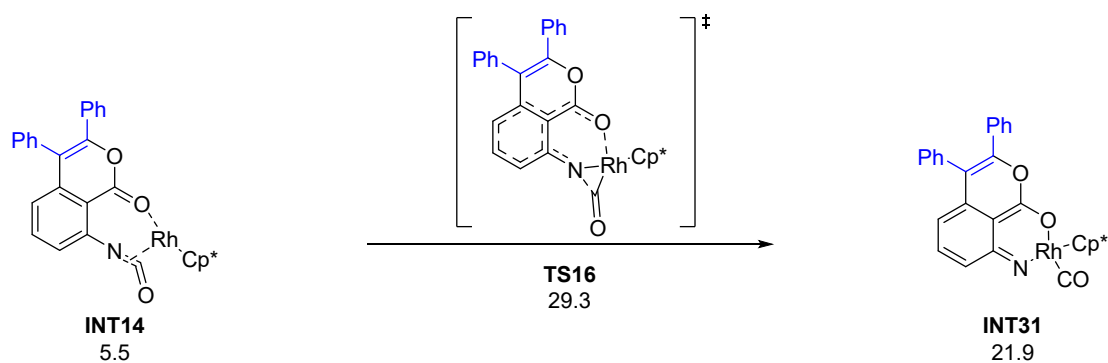
Scheme S2 Possible reactions involving alkyne insertion starting with **INT22**. Energies are given in kcal/mol.



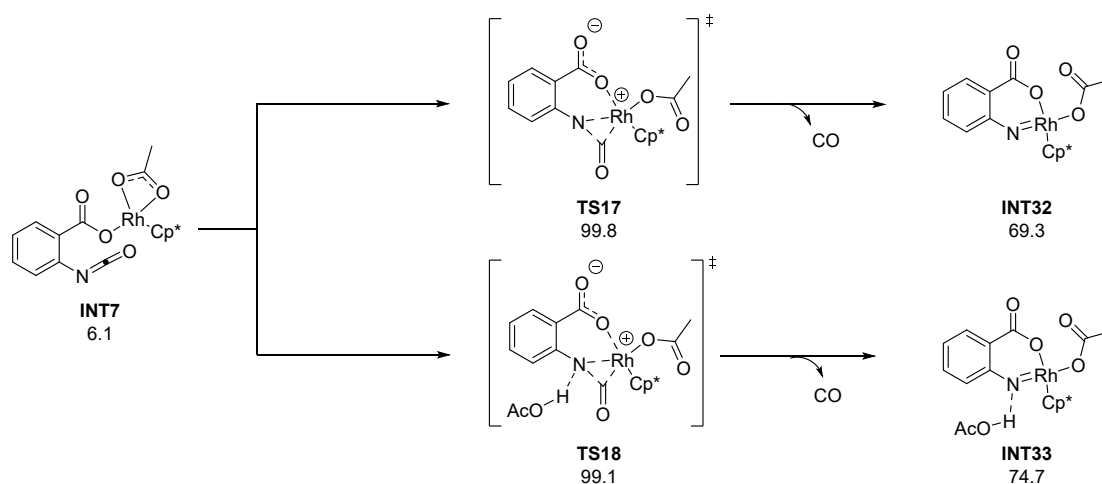
Scheme S3 The energy of alkyne insertion into the Rh-O bond. Energies are given in kcal/mol.



Scheme S4 The energy of extramolecular migration pathways from **INT13** to **INT15**. Energies are given in kcal/mol.



Scheme S5 The energy of direct decarbonylation from **INT15**. Energies are given in kcal/mol.



Scheme S6 Possible decarbonylation of isocyanate moiety from INT7. Energies are given in kcal/mol.

To validate the computational method, selected key transition states and intermediates were calculated with different functionals. It was found that the structures changed only marginally, and the obtained energy profile was consistent with the reported pathway in our research.

Table S1. Energies for key transition states and intermediates with different methods.

Entry	Method	Energies (kcal/mol)				
		TS1	TS2	TS5	TS6	INT12
1	(SMD)M06/6-311+G(d,p)/SDD//B3LYP/6-31G(d)/LANL2DZ (reported)	32.0	41.2	26.4	27.4	-2.0
2	(SMD)B3LYP-D3(BJ)/6-311+G(d,p)/SDD//B3LYP-D3(BJ)/6-31G(d)/LANL2DZ	28.8	34.1	24.8	23.9	-1.8
3	(SMD)B3LYP-D3(BJ)/6-311+G(d,p)/SDD// ω B97X-D/6-31G(d)/LANL2DZ	28.7	35.6	24.7	26.6	-2.2
4	(SMD) ω B97X-D/6-311+G(d,p)/SDD// ω B97X-D/6-31G(d)/LANL2DZ	31.0	38.3	29.6	28.4	-3.1
5	(SMD)B3LYP-D3(BJ)/6-311+G(d,p)// (SMD)B3LYP-D3(BJ)/6-31+G(d)	28.7	35.9	26.1	25.6	-7.0

3. Calculated Energy Values

Table S2. Energies (in Hartree) calculated by (SMD)M06/6-311+G(d,p)/SDD//B3LYP/6-31G(d)/Lanl2dz level.

Species	G ₂₉₈ ^a	E ₂₉₈ ^b	E _{sol} ^c	Imaginary Frequency
1a	-588.236406	-588.323394	-588.14482836	
2a	-539.309830	-539.462233	-539.17078022	
AcOH	-229.046872	-229.081789	-229.04076369	
Cp[*]Rh(OAc)₂	-956.353928	-956.627414	-957.38121781	
CO	-113.323559	-113.309452	-113.28106447	
3a	-1014.235906	-1014.494360	-1014.04479356	
AcO⁻	-228.477332	-228.497911	-228.56120994	
INT1	-1544.554768	-1544.933852	-1545.52303702	
TS1	-1544.521246	-1544.901001	-1545.49438403	-1194.8882
INT2	-1544.547095	-1544.929889	-1545.51790513	
INT3	-1315.933030	-1316.270277	-1316.93506956	
TS2	-1315.880370	-1316.215258	-1316.89416155	-961.5781
INT4	-1315.907022	-1316.245523	-1316.92150974	
INT5	-1544.573289	-1544.953988	-1545.53174490	
TS3	-1544.563970	-1544.940796	-1545.52039594	-220.7324
INT6	-1315.524438	-1315.848045	-1316.47546987	
TS4	-1315.502113	-1315.824809	-1316.45147468	-215.8713
INT7	-1315.523161	-1315.845727	-1316.47249242	
INT8	-1315.525430	-1315.846532	-1316.47248281	
TS5	-1315.480211	-1315.797648	-1316.43513163	-1033.2322
INT9	-1315.499272	-1315.822143	-1316.45878035	
INT10	-1086.452086	-1086.718978	-1087.40328627	
INT11	-1625.740088	-1626.184254	-1626.59825836	
TS6	-1625.713688	-1626.157405	-1626.57224954	-294.0378
INT12	-1625.757197	-1626.202007	-1626.62032754	
TS7	-1625.724404	-1626.170042	-1626.58197437	-216.7656
INT13	-1625.746917	-1626.194497	-1626.60254549	
INT14	-1625.774840	-1626.223001	-1626.61172705	
INT15	-1854.816679	-1855.319466	-1855.66250245	
TS8	-1854.790149	-1855.293009	-1855.64088623	-324.6920
INT16	-1854.809906	-1855.312834	-1855.66157477	
TS9	-1854.797251	-1855.297411	-1855.64848933	-130.3769
INT17	-1741.508723	-1742.008005	-1742.37154774	
INT18	-1970.560648	-1971.114223	-1971.43253770	
TS10	-1970.532870	-1971.087519	-1971.41388535	-669.4845
INT19	-1970.560154	-1971.116405	-1971.44167029	
INT20	-1544.541394	-1544.919716	-1545.51048234	

TS11	-1544.483501	-1544.865220	-1545.45718868	-291.4060
INT21	-1544.512510	-1544.894421	-1545.47982916	
INT22	-1315.511583	-1315.837619	-1316.46813596	
INT23	-1854.745819	-1855.250153	-1855.62412243	
TS12	-1854.731370	-1855.236632	-1855.61056221	-260.9483
INT24	-1854.813966	-1855.322727	-1855.68887429	
INT25	-1626.152973	-1626.611639	-1627.06148452	
TS13	-1626.124086	-1626.584492	-1627.03615428	-314.5244
INT26	-1626.147895	-1626.609937	-1627.05520208	
INT27	-1854.775758	-1855.274480	-1855.64746179	
TS14	-1854.752617	-1855.252360	-1855.62361940	-282.6167
INT28	-1854.788390	-1855.290311	-1855.65875735	
TS15	-1625.712064	-1626.154584	-1626.55726784	-251.8964
INT29	-1625.733493	-1626.179757	-1626.57611454	
INT30	-1126.371141	-1126.613685	-1126.14067410	
TS16	-1625.741352	-1626.188813	-1626.57304607	-330.6079
INT31	-1625.752159	-1626.198718	-1626.58388653	
TS17	-1315.372771	-1315.692836	-1316.32070103	-85.8721
INT32	-1202.115400	-1202.431483	-1203.07017201	
TS18	-1544.414119	-1544.793210	-1545.38680326	-380.7394
INT33	-1431.156782	-1431.527313	-1432.12196404	

^a Sum of electronic and thermal free energies

^b Sum of electronic energies

^c Single point energies calculated in DMF solution

4. Cartesian Coordinates for All Species

1a				H	2.45169400	-3.75498800	1.50260400
C	-7.86157500	4.44964400	4.20651700	H	1.95435700	-5.54538300	-0.15009100
C	-6.86945500	3.90967100	5.01788200				
C	-5.85032500	3.14431200	4.43647800	AcOH			
C	-5.83846800	2.92940100	3.04932900	C	-3.46646700	0.42077600	0.03210000
C	-6.84593400	3.48126500	2.24630200	H	-3.07411000	-0.46587500	0.54090400
C	-7.85705700	4.24032600	2.81977400	H	-3.17496600	1.32080400	0.57368900
H	-8.65051400	5.04252800	4.66072100	H	-3.03767200	0.43498000	-0.97534400
H	-6.87932100	4.07602800	6.09168900	C	-4.97062800	0.34629100	-0.04831500
H	-6.80728200	3.29664000	1.17782600	O	-5.75123100	1.15033300	0.40821200
H	-8.63862600	4.66898400	2.20082100	O	-5.37596700	-0.76579000	-0.71569000
C	-4.76673500	2.12577500	2.45024000	H	-6.35113900	-0.73365900	-0.72027000
N	-4.83447300	2.58164700	5.19725600				
H	-4.81089600	2.72078300	6.19884000	Cp⁺Rh(OAc)₂			
C	-3.79684600	1.81943800	4.70101400	C	-4.93864700	3.17807100	2.54102600
O	-3.81040700	1.62012900	3.34138400	C	-3.48628800	3.18103000	2.68810900
O	-4.63684200	1.86601200	1.28318000	C	-3.06562000	4.54200300	2.87666300
O	-2.92633500	1.34817000	5.38648500	C	-4.24130300	5.36693400	2.94260500
				C	-5.40125700	4.51486300	2.69350800
2a				C	-6.81768600	5.00163500	2.63929000
C	-3.49941300	1.27344100	-0.92193500	H	-7.03168800	5.68412700	3.46737700
C	-2.43587900	1.09775800	-0.01360100	H	-7.00166500	5.54105400	1.70072100
C	-2.16363700	2.11892600	0.91918400	H	-7.53048900	4.17586400	2.69824500
C	-2.93399500	3.27816200	0.93936300	C	-5.76577600	1.95260000	2.29600700
C	-3.98594100	3.44188300	0.03447100	H	-6.82912900	2.14369300	2.45900200
C	-4.26440500	2.43606100	-0.89445400	H	-5.63870300	1.60501900	1.26246400
H	-3.71350700	0.48989800	-1.64233700	H	-5.46687600	1.13930200	2.96401600
H	-1.34536400	1.98863900	1.62076900	C	-2.58155600	1.99472000	2.55992200
H	-2.71282100	4.05740600	1.66381200	H	-3.14267200	1.05982900	2.64013700
H	-4.58521100	4.34808400	0.05313400	H	-2.07444400	2.00085000	1.58514600
H	-5.08152300	2.55819100	-1.60041000	H	-1.83306200	2.01317100	3.35612900
C	-1.65029300	-0.09091300	-0.03792300	C	-1.64557700	5.00297400	2.99016300
C	-0.97996400	-1.10588600	-0.05906000	H	-1.05277800	4.28281900	3.55713600
C	-0.19453700	-2.29473700	-0.08340500	H	-1.21190800	5.11205200	1.98651900
C	-0.46734600	-3.31619500	-1.01571000	H	-1.57740500	5.97221200	3.49099600
C	0.86941400	-2.47026800	0.82446400	C	-4.28519600	6.85629900	3.10317600
C	0.30285100	-4.47553900	-1.03587900	H	-4.30355200	7.35084200	2.12197300
H	-1.28593100	-3.18604800	-1.71694600	H	-5.17842300	7.17031900	3.65101900
C	1.63424700	-3.63299500	0.79700300	H	-3.41296900	7.22551400	3.64836200
H	1.08396700	-1.68651400	1.54449800	Rh	-4.37884900	3.90890900	4.55261400
C	1.35521400	-4.63909700	-0.13144500	C	-5.89846300	3.16929400	6.45400000
H	0.08122600	-5.25499800	-1.75996100	C	-6.65759800	2.76515700	7.69161900

H	-7.55680300	3.37564800	7.80493300	H	-5.14988500	8.59380200	2.44981400
H	-6.91622300	1.70425000	7.65318800	C	-3.10521200	2.75912900	2.83368200
H	-6.01769300	2.93208200	8.56602400	C	-2.17944000	2.00691600	3.58019700
C	-1.31734500	3.92662300	7.61882500	C	-2.62215300	3.77963100	1.99727200
H	-0.27507800	3.60232300	7.58360600	C	-0.81715900	2.28841800	3.51416400
H	-1.83871700	3.36549000	8.40310500	H	-2.53677000	1.19895000	4.20906800
H	-1.37743800	4.98725200	7.88065100	C	-1.25744400	4.05262600	1.92952600
C	-1.99443000	3.65737900	6.27583400	H	-3.31088100	4.35183200	1.38780800
O	-3.13782000	4.27507000	6.16265500	C	-0.34972400	3.31433000	2.69067800
O	-1.47296300	2.91717700	5.43882000	H	-0.11931600	1.70138300	4.10512400
O	-5.93833600	4.36944600	6.03363700	H	-0.90320800	4.84159800	1.27161000
O	-5.17900900	2.32184200	5.83301800	H	0.71372200	3.53130200	2.63632300
				H	-7.69209000	-1.27887100	3.45676900
CO							
C	-4.75769800	2.10770200	2.36904200	AcO			
O	-4.63479200	1.86191200	1.26476100	C	-3.46778600	0.42209800	0.03285000
				H	-3.04524400	-0.45359400	0.54730200
3a				H	-3.18099000	1.33011000	0.57886000
C	-9.37748400	2.83893600	3.03546400	H	-3.00883800	0.44559700	-0.96661400
C	-9.51792100	1.46942500	3.20255700	C	-5.03093500	0.27098100	-0.09440300
C	-8.38213300	0.63813100	3.27989900	O	-5.71450400	1.18554600	0.43022400
C	-7.09088400	1.24335500	3.15807800	O	-5.40274400	-0.75921900	-0.71266300
C	-6.96651900	2.65129000	2.97390900				
C	-8.12370500	3.44081800	2.92679700	INT1			
H	-10.26937800	3.45922900	2.99168900	C	-3.18592200	0.54060700	-2.21696200
H	-10.50499500	1.02261200	3.29118700	C	-1.84199800	1.02608000	-1.92862200
H	-8.04589800	4.51385300	2.80918700	C	-1.94071500	2.45395500	-1.64821400
C	-5.90202100	0.41744000	3.23004000	C	-3.31762500	2.79751800	-1.62273300
N	-8.52286300	-0.69913600	3.49013900	C	-4.09539900	1.60435300	-1.97790900
H	-9.43756100	-1.11753500	3.42985000	C	-5.58629700	1.50577500	-2.09059200
O	-5.84856200	-0.79457700	3.38265100	H	-6.07844000	2.36702300	-1.63140500
O	-4.68830400	1.06264500	3.10914500	H	-5.89587400	1.46773000	-3.14379300
C	-5.63012600	3.23545800	2.86042000	H	-5.93578000	0.60227000	-1.58225700
C	-4.54343600	2.41593400	2.92276000	C	-3.55117000	-0.84281300	-2.65861800
C	-5.49001700	4.71897700	2.74048900	H	-4.45727900	-1.18201200	-2.15240400
C	-4.99415900	5.47659700	3.81109500	H	-3.72202000	-0.85453500	-3.74396900
C	-5.87336700	5.38626900	1.56583700	H	-2.75250800	-1.55554500	-2.43860900
C	-4.87012000	6.86246200	3.70658800	C	-0.56921300	0.25294100	-2.09140000
H	-4.70051800	4.97125300	4.72668200	H	-0.72375900	-0.80939900	-1.88591800
C	-5.75004800	6.77226400	1.46082600	H	-0.18209500	0.34995700	-3.11536700
H	-6.26446000	4.81119000	0.73057600	H	0.19852500	0.61295600	-1.40159900
C	-5.24633000	7.51445700	2.53119100	C	-0.79345700	3.38076200	-1.38852200
H	-4.48077400	7.43269400	4.54582500	H	0.07229200	2.83856200	-1.00062700
H	-6.04600200	7.27155300	0.54189400	H	-0.49162700	3.87654500	-2.32146400

H	-1.06526800	4.14382900	-0.65630900	C	-2.34507600	3.40493000	-0.15360300
C	-3.86240800	4.15410700	-1.29246900	H	-2.78357300	2.92152300	-1.03105400
H	-3.71356200	4.84765800	-2.13078700	H	-1.38896200	3.85473400	-0.45249700
H	-4.93370900	4.11219900	-1.08093000	H	-2.14861300	2.62432100	0.58388200
H	-3.35839900	4.55370500	-0.40773100	C	-2.88692000	4.10554400	2.93968500
Rh	-2.93022900	1.21170800	-0.11121600	H	-2.48910300	3.11328500	2.71915200
C	-4.17457900	-1.30470500	0.74373300	H	-2.04356200	4.74228500	3.24120600
C	-4.13836000	-2.60387400	1.54946400	H	-3.55967200	4.02791000	3.79698400
H	-5.08800600	-3.13459400	1.45238900	C	-5.05970700	6.43358100	3.06107000
H	-3.31904000	-3.24148800	1.20012700	H	-5.16577200	5.70909300	3.87283500
H	-3.94260500	-2.38069400	2.60371600	H	-4.36988900	7.21928200	3.39967500
C	-0.35320800	2.76334100	3.01802800	H	-6.03761700	6.89534900	2.90137900
H	-0.15600100	3.80337800	3.28965600	C	-5.63744000	7.39002300	0.04813200
H	0.57114100	2.27162000	2.70095300	H	-6.39192800	7.62529800	0.80346600
H	-0.72529900	2.22507100	3.89750100	H	-5.00563500	8.28001500	-0.08157900
C	-1.41165900	2.69746600	1.91862900	H	-6.14606600	7.17878700	-0.89395700
O	-1.45435700	1.54148700	1.32956600	C	-3.97606400	5.51678800	-1.91938600
O	-2.14664300	3.66825700	1.68327800	H	-3.38164800	6.39749900	-2.19992300
O	-5.19083100	-0.96768800	0.12423900	H	-3.50995600	4.63877500	-2.37316300
O	-3.05230300	-0.65028300	0.80718100	H	-4.98524900	5.61827200	-2.32603200
C	-7.88550000	4.40932400	4.21207300	Rh	-5.46634300	4.11938900	0.66496500
C	-6.88539200	3.88323200	5.02256900	C	-6.27202400	1.53925000	-0.59191800
C	-5.85712100	3.13255800	4.43889800	C	-6.25399800	0.45640700	-1.64851200
C	-5.83986800	2.92104000	3.05076500	H	-7.24490500	0.00580000	-1.74344400
C	-6.85659500	3.45877700	2.24857700	H	-5.92226900	0.86011200	-2.60683200
C	-7.87887700	4.19992600	2.82467300	H	-5.55454500	-0.32541900	-1.33034000
H	-8.68317000	4.98996600	4.66659100	C	-9.40257600	4.83678800	-1.09459700
H	-6.89611900	4.04826800	6.09639300	H	-9.70316900	5.25903900	-2.05553500
H	-6.82042900	3.27480900	1.18056600	H	-9.87441100	5.39709400	-0.27998300
H	-8.66881400	4.61508900	2.20730000	H	-9.75145300	3.80112900	-1.02030300
C	-4.74795500	2.14058200	2.46961900	C	-7.88042700	4.87912800	-0.95723500
N	-4.83236600	2.58323700	5.19720200	O	-7.47964400	4.43542100	0.20424300
H	-4.79333800	2.74336000	6.19530400	O	-7.17023500	5.29879000	-1.87103500
C	-3.79938000	1.82124200	4.69984800	O	-6.99973700	1.35215900	0.43324900
O	-3.83824000	1.59454400	3.33803700	O	-5.54186000	2.55663900	-0.77558900
O	-4.61919100	1.93057900	1.27853000	C	-7.72127500	3.61134300	4.37169100
O	-2.91352300	1.36103800	5.37081900	C	-6.94716600	2.84902000	5.23860500
				C	-5.90712000	2.07028700	4.71404700
TSI				C	-5.62564700	2.09234700	3.33557900
C	-3.56450400	4.71481000	1.75155600	C	-6.39816700	2.88669300	2.44329400
C	-4.55096800	5.78468400	1.80862500	C	-7.45794800	3.62172400	2.99555900
C	-4.78450900	6.23186800	0.46281700	H	-8.54266500	4.20032000	4.77260000
C	-4.03849200	5.38425600	-0.42949700	H	-7.15283400	2.83153200	6.30604200
C	-3.27254500	4.45047200	0.38487600	H	-6.66397500	2.23864700	1.29762200

H	-8.08515200	4.19980200	2.32557200	H	-9.73893600	3.62239600	-0.82725900
C	-4.54624300	1.22628600	2.84048400	C	-7.91423200	4.76674800	-0.67607700
N	-5.14358300	1.26308000	5.55320800	O	-7.47446300	4.28764400	0.47543200
H	-5.35009800	1.22427900	6.54264200	O	-7.21530000	5.23044000	-1.56901400
C	-4.12200300	0.43732100	5.14684400	O	-7.59543100	1.70000600	0.17841300
O	-3.86121900	0.46341800	3.79963400	O	-5.46541200	2.29146300	-0.27467200
O	-4.16779100	1.11095500	1.70116500	C	-7.56897000	3.50691500	4.50197000
O	-3.48003100	-0.26240400	5.88976100	C	-7.08293300	2.35212200	5.10385700
				C	-6.03848600	1.66807300	4.48272100
INT2				C	-5.46233500	2.14135200	3.27670900
C	-3.48224200	5.05085500	1.72886000	C	-5.97248500	3.31259500	2.64973900
C	-4.51898600	6.05936500	1.65735400	C	-7.03066400	3.96873500	3.29798100
C	-4.73934100	6.36606200	0.24516300	H	-8.38645800	4.04984200	4.97086000
C	-3.96569900	5.48354600	-0.53085200	H	-7.50583600	1.97772800	6.03244000
C	-3.20442200	4.64145900	0.38723600	H	-7.65012000	2.67237100	0.45990200
C	-2.21329600	3.61222800	-0.05968600	H	-7.46794500	4.84663000	2.83634600
H	-2.67935000	2.89729100	-0.74505400	C	-4.32634800	1.37919800	2.73936500
H	-1.38612800	4.10155600	-0.59142100	N	-5.55142600	0.49736800	5.06156600
H	-1.80904600	3.04383700	0.77685400	H	-5.97763400	0.14615200	5.90883800
C	-2.76502800	4.61493300	2.97134100	C	-4.57100100	-0.30478900	4.53690600
H	-2.36126500	3.60651900	2.86714200	O	-4.00097200	0.17366100	3.38710500
H	-1.92921100	5.29726500	3.17978200	O	-3.62163600	1.66149000	1.80171500
H	-3.42640800	4.62650700	3.84200500	O	-4.20767100	-1.34707100	5.02547900
C	-5.02488900	6.88035000	2.80645200				
H	-5.07815600	6.29284400	3.72674300	INT3			
H	-4.36132600	7.73706800	2.99121200	C	-3.55962900	0.91049800	-1.37720000
H	-6.02489500	7.27653400	2.60635600	C	-2.17114100	0.86490300	-1.04493600
C	-5.62369200	7.46603600	-0.25242000	C	-1.52766200	2.02559500	-1.65215600
H	-6.52948200	7.55807300	0.35421100	C	-2.53539200	2.75020300	-2.39505800
H	-5.08595200	8.42292300	-0.18597100	C	-3.80055300	2.09601300	-2.18613600
H	-5.92962700	7.30112500	-1.28478000	C	-5.11302700	2.49087100	-2.79030700
C	-3.91408500	5.41547400	-2.02842500	H	-5.18161700	3.57197400	-2.93524200
H	-3.23980900	6.18033600	-2.43821000	H	-5.23624700	2.01359300	-3.77162000
H	-3.54814400	4.44116400	-2.36458000	H	-5.95367200	2.18146600	-2.16401600
H	-4.91099200	5.56306300	-2.45066500	C	-4.59182200	-0.11019800	-1.01447000
Rh	-5.35674200	4.20948000	0.88327600	H	-5.56792200	0.34760200	-0.83119800
C	-6.39304600	1.47623600	-0.31417700	H	-4.71326700	-0.81137300	-1.85116800
C	-6.22899800	0.12185500	-0.95043500	H	-4.30548600	-0.68654600	-0.13302200
H	-6.82252000	0.07775000	-1.87049300	C	-1.48325600	-0.17906000	-0.22343000
H	-5.17860600	-0.05823100	-1.17942800	H	-2.15177900	-0.62337300	0.51800400
H	-6.60859100	-0.65305600	-0.27752900	H	-1.11623800	-0.98220000	-0.87681800
C	-9.43137000	4.67472300	-0.81097500	H	-0.62210300	0.23745500	0.30540700
H	-9.75632500	5.15900100	-1.73372000	C	-0.06104000	2.32400100	-1.62420700
H	-9.92051900	5.14112200	0.05044900	H	0.38012300	2.07681500	-0.65517400

H	0.45512700	1.72884300	-2.38922600	H	-1.21115300	5.20443100	2.81136100
H	0.13857100	3.37796000	-1.83107200	H	-2.51422000	4.58240300	3.83159500
C	-2.30201500	3.98733300	-3.20136600	C	-4.78187900	6.22059800	3.16823400
H	-1.95140600	3.71024400	-4.20452100	H	-4.43842300	5.68376200	4.05556900
H	-3.21579100	4.57445400	-3.31551000	H	-4.42787000	7.25690000	3.24901600
H	-1.54293800	4.62764600	-2.74514400	H	-5.87344700	6.24035000	3.18574200
Rh	-2.98485400	2.75726800	-0.25743600	C	-6.09987500	6.51727400	0.26186100
C	-1.49551500	5.55532200	2.24254900	H	-6.80032100	6.52760900	1.10030300
H	-1.17027100	6.44118000	1.69149300	H	-5.83760900	7.56018600	0.03844500
H	-0.68013200	5.16359200	2.85417900	H	-6.61843400	6.11098500	-0.61010700
H	-2.31662100	5.85484800	2.90460600	C	-4.13340800	5.10835700	-1.86160500
C	-1.98868600	4.50475300	1.29029400	H	-5.08488000	5.54594100	-2.16970300
O	-1.83025400	3.26133600	1.53046100	H	-3.32729600	5.66655300	-2.35322300
O	-2.60954000	4.82644900	0.22146000	H	-4.10050000	4.07491600	-2.22071400
C	-7.24690500	2.91773200	5.54711700	Rh	-4.70770800	3.60644200	1.00750000
C	-6.57065400	1.70957100	5.41254700	C	-6.36444500	1.75644500	-0.63678600
C	-5.78751900	1.49100400	4.27455700	C	-6.65213300	0.90724000	-1.85281700
C	-5.69004900	2.48942600	3.28425900	H	-7.72884600	0.85461200	-2.02617900
C	-6.38049600	3.70614000	3.43798000	H	-6.13504400	1.29601500	-2.73151700
C	-7.15735400	3.91895500	4.56512800	H	-6.28944700	-0.10887700	-1.65785200
H	-7.85465000	3.08503200	6.43122300	O	-7.18538900	1.75706700	0.31958500
H	-6.64717100	0.94334700	6.17841700	O	-5.27003700	2.42328500	-0.63332400
H	-6.28830100	4.45920500	2.66265800	C	-7.99081000	3.67739500	4.23967400
H	-7.69360400	4.85326200	4.69153100	C	-7.39393200	2.80377200	5.14376400
C	-4.85684500	2.23206500	2.12862900	C	-6.29453100	2.04059500	4.72174200
N	-5.09442600	0.29770600	4.08856400	C	-5.81293200	2.20034400	3.41634700
H	-5.16364500	-0.44133800	4.77858500	C	-6.42979300	3.05871500	2.46984800
C	-4.32166700	-0.00052600	3.00047000	C	-7.52902400	3.79898900	2.91627200
O	-4.22188700	1.02818300	2.06225100	H	-8.85243600	4.25526100	4.56191900
O	-4.67531400	3.01087100	1.19200400	H	-7.78015500	2.70118100	6.15364900
O	-3.74929800	-1.03597400	2.79100600	H	-6.65891100	2.55103700	1.31008400
				H	-8.07839600	4.42782600	2.22120200
TS2				C	-4.61618000	1.48820700	3.03247600
C	-3.03739100	4.88666800	1.75932800	N	-5.64869100	1.12886600	5.54506200
C	-4.25497100	5.60965700	1.90710200	H	-5.98870200	0.95568400	6.48403600
C	-4.86088400	5.73910800	0.58297200	C	-4.60083100	0.31694000	5.16537200
C	-3.95152300	5.16176800	-0.37844700	O	-4.10506900	0.56245000	3.87117300
C	-2.85973400	4.57020800	0.34310700	O	-4.00654500	1.70975600	1.97793600
C	-1.68072100	3.87066100	-0.25739700	O	-4.09002700	-0.52489500	5.84157000
H	-1.93242600	3.42293600	-1.22178300				
H	-0.86240000	4.58511700	-0.42080700	INT4			
H	-1.30541500	3.07899400	0.39649100	C	-3.10081800	5.12791100	1.80083900
C	-2.06778000	4.51774500	2.83669300	C	-4.32142900	5.87953600	1.66248800
H	-1.67949200	3.50489100	2.69580800	C	-4.76119900	5.72006000	0.30258500

C	-3.69333400	5.03808200	-0.44846000	O	-3.97484200	0.25849900	3.49826600
C	-2.68793100	4.67690300	0.45898000	O	-3.78149300	1.80601200	1.91276200
C	-1.42611500	3.91791600	0.18910800	O	-4.15734800	-1.31266600	5.09858900
H	-1.38960500	3.53716000	-0.83345200				
H	-0.55391700	4.56647400	0.34087300	INT5			
H	-1.32546600	3.06579400	0.86950700	C	-2.69368400	8.60856000	0.22476600
C	-2.24326300	5.03562500	3.02577200	C	-1.65155000	8.90184200	1.15105700
H	-1.71579500	4.07867800	3.07218000	C	-2.19200100	9.80249300	2.15686400
H	-1.48458100	5.82991000	3.01421800	C	-3.54400200	10.17424000	1.74242400
H	-2.82941700	5.14939700	3.94119700	C	-3.86411900	9.41592300	0.58813700
C	-4.96643600	6.72194600	2.71816100	C	-5.15222600	9.42611200	-0.17467700
H	-4.83814000	6.29922400	3.71725700	H	-5.96238100	9.86454100	0.41267100
H	-4.50396400	7.71796800	2.71518300	H	-5.04458100	10.01170700	-1.09787200
H	-6.03525300	6.85958800	2.53788400	H	-5.44549200	8.40992300	-0.45316200
C	-5.96088500	6.35865300	-0.32820100	C	-2.63979600	7.68506900	-0.95353000
H	-6.76685800	6.51469100	0.39334700	H	-3.45616900	6.95757300	-0.90590500
H	-5.69160200	7.34016200	-0.74160600	H	-2.73421000	8.24752500	-1.89147000
H	-6.35010900	5.75266800	-1.15091300	H	-1.70091100	7.12736000	-0.98372600
C	-3.75681700	4.75186600	-1.91664600	C	-0.28769600	8.28747200	1.20877200
H	-4.67158600	4.20600600	-2.17185200	H	-0.24836000	7.55749100	2.02770500
H	-3.75799200	5.68791100	-2.48886700	H	-0.04217900	7.76817100	0.27935300
H	-2.90631700	4.15408700	-2.25039500	H	0.47532700	9.05354500	1.38542100
Rh	-4.66178600	3.74302100	1.22556300	C	-1.43401200	10.39015100	3.30725700
C	-6.91437800	1.97923800	-0.28403700	H	-0.60246000	9.74370900	3.59952700
C	-7.38841600	1.17831600	-1.46029500	H	-1.02607400	11.37581900	3.04410500
H	-8.35939100	1.55293900	-1.79922600	H	-2.08220600	10.51015000	4.17955700
H	-6.65758000	1.22671400	-2.26701300	C	-4.42855700	11.15866300	2.44395700
H	-7.53156000	0.13636600	-1.15342100	H	-4.31448900	12.15657100	1.99947400
O	-7.78930400	2.04378200	0.70599600	H	-5.47958300	10.86756700	2.37898400
O	-5.80354500	2.52171800	-0.25032900	H	-4.16984300	11.23189200	3.50304300
C	-7.66703000	3.45493600	4.49359600	Rh	-3.36864800	8.02902200	2.25659900
C	-7.25454400	2.28603900	5.12846900	C	-5.33981500	8.48039100	4.53618300
C	-6.15100100	1.60208000	4.60454800	C	-5.59076000	8.76909500	6.01210100
C	-5.50169700	2.12108700	3.47445100	H	-5.83817700	7.82491900	6.51226800
C	-5.89576900	3.31616300	2.82343800	H	-4.70606100	9.18853000	6.49620400
C	-7.00873100	3.97099400	3.35650200	H	-6.44518000	9.44251600	6.12167400
H	-8.52748800	3.98673500	4.89083300	C	-1.50123200	4.75255000	4.41935100
H	-7.77926400	1.91149700	6.00199500	H	-0.72213500	4.49442900	3.69459700
H	-7.41073600	2.56930000	1.44728100	H	-1.91913100	3.84275100	4.85491200
H	-7.38094400	4.88915400	2.91147400	H	-1.03125500	5.35178800	5.20760100
C	-4.38519800	1.40652300	2.91954800	C	-2.60887700	5.56306400	3.74871800
N	-5.65597500	0.41949500	5.13557300	O	-3.79033700	5.24173900	3.85243500
H	-6.08745300	0.00344300	5.95283500	O	-2.13840900	6.59384500	3.08934600
C	-4.58396300	-0.29463400	4.64059300	O	-6.31753200	8.41433500	3.75477800

O	-4.10979400	8.30045900	4.22744900	H	-5.07974500	10.60048600	3.20243200
C	-9.00885700	4.55076400	4.82455200	Rh	-3.25215600	7.86918900	2.48032400
C	-8.18056500	5.48891800	4.22077100	C	-4.65288200	7.89731200	5.36755500
C	-7.26151500	5.05990900	3.25206700	C	-4.34965700	8.32433600	6.78387800
C	-7.18252800	3.70223800	2.90429700	H	-3.54940100	7.66602400	7.14104300
C	-8.02722400	2.76912000	3.52371400	H	-3.99142700	9.35566500	6.81024400
C	-8.93992800	3.19014900	4.48068700	H	-5.22110600	8.19636800	7.42951900
H	-9.72071900	4.87955900	5.57693200	C	-0.34988800	5.50631100	4.72201800
H	-8.21823700	6.54161400	4.48357500	H	-0.10084200	4.79556300	3.92581300
H	-7.94276800	1.72652000	3.23529500	H	-0.40604700	4.97499800	5.67424900
H	-9.59619500	2.47275000	4.96354200	H	0.44910300	6.25424000	4.75684000
C	-6.21593700	3.27835000	1.89129100	C	-1.69698200	6.16343400	4.41789800
N	-6.42691600	5.96486700	2.61664800	O	-2.69034400	5.93514700	5.09754800
H	-6.38478000	6.95184600	2.95381400	O	-1.62681800	6.95521000	3.37091400
C	-5.45406100	5.59753000	1.76369800	O	-5.55470100	6.99553200	5.24835700
O	-5.41156200	4.30438000	1.35791500	O	-4.02197100	8.45443500	4.43405400
O	-6.04832400	2.16649300	1.46348400	C	-9.62124300	5.07496800	4.11058900
O	-4.64889600	6.38590200	1.25711900	C	-8.35450700	5.64226100	4.10763100
				C	-7.41752200	5.26194100	3.12611700
TS3				C	-7.79589800	4.30189900	2.16477600
C	-2.78669800	8.14867900	0.37054100	C	-9.08205700	3.73872700	2.17816300
C	-1.85652400	8.93892400	1.12801400	C	-9.99656100	4.12237200	3.14685000
C	-2.61867400	9.85879000	1.93702900	H	-10.33342500	5.37346400	4.87567600
C	-4.02416800	9.73684500	1.54917800	H	-8.06336300	6.36805400	4.85983300
C	-4.12920400	8.68801300	0.60044000	H	-9.32920400	3.00345100	1.41900000
C	-5.36921400	8.19762900	-0.08148400	H	-10.99199600	3.68917200	3.16523900
H	-6.26585600	8.41281400	0.50535400	C	-6.82720200	3.90015900	1.14962700
H	-5.48136100	8.68350700	-1.06020900	N	-6.15312800	5.82899000	3.11950400
H	-5.32590500	7.11852700	-0.25210500	H	-5.72862500	6.54343000	4.23292700
C	-2.46846000	7.02770700	-0.57055000	C	-5.25953500	5.44963100	2.21843700
H	-3.08967800	6.15478700	-0.34624000	O	-5.57808600	4.52459900	1.24659900
H	-2.65516600	7.32643900	-1.61032100	O	-6.98951100	3.11211500	0.25003200
H	-1.42344400	6.72099200	-0.48458300	O	-4.08444300	5.87078500	2.12977600
C	-0.37654300	8.73257300	1.20056600				
H	-0.15001900	8.01504900	2.00123900	INT6			
H	0.01388400	8.33650700	0.25909300	C	-2.69453500	8.30469300	0.37287400
H	0.14032800	9.67191500	1.41767800	C	-2.06917600	9.12694400	1.39957500
C	-2.07532800	10.87359400	2.89576900	C	-3.10418600	9.73967500	2.16994300
H	-1.07285600	10.60053700	3.23434500	C	-4.38566600	9.31770300	1.61480900
H	-2.02098800	11.86583000	2.42743000	C	-4.12154600	8.47060700	0.48739000
H	-2.71517200	10.94860900	3.77972900	C	-5.16013400	7.85105600	-0.39433500
C	-5.13035000	10.57584000	2.10961600	H	-6.04413400	7.57358900	0.18385300
H	-5.04861700	11.60728000	1.74260900	H	-5.45631200	8.56542800	-1.17461400
H	-6.11292600	10.19295300	1.82395200	H	-4.78276800	6.95212200	-0.88775800

C	-1.96906000	7.52632000	-0.68253700	C	-1.38252300	5.40756700	0.32071000
H	-2.55930800	6.67270700	-1.02507700	C	-2.41342500	4.64927100	-0.38316400
H	-1.75686200	8.16140200	-1.55360400	C	-2.47723800	3.35692100	0.20956900
H	-1.01567500	7.14212600	-0.30936600	C	-3.39138500	2.23003700	-0.15759400
C	-0.59154800	9.26511000	1.60013700	H	-4.15958600	2.54858400	-0.86544800
H	-0.08496800	8.30276800	1.48362200	H	-2.81244400	1.42123300	-0.62262900
H	-0.17299800	9.95890900	0.85903900	H	-3.89007000	1.83355000	0.73169600
H	-0.35253300	9.64856500	2.59451200	C	-1.24506700	2.12762300	2.17879800
C	-2.93665900	10.67121300	3.33181500	H	-2.13175900	1.49420300	2.26104500
H	-1.92983200	10.61471300	3.75235100	H	-0.42752500	1.53004900	1.75038200
H	-3.11331900	11.70829100	3.01730900	H	-0.96859000	2.45528000	3.18289100
H	-3.64517400	10.43716000	4.13142100	C	0.39083400	4.89328800	2.17803200
C	-5.74102700	9.73524400	2.09356300	H	0.23362600	4.53144000	3.19519700
H	-6.18949200	10.45995700	1.40082300	H	1.28692600	4.41634200	1.75732600
H	-6.39297200	8.85994000	2.16556900	H	0.57569600	5.96998100	2.21974900
H	-5.68796400	10.20032400	3.08106500	C	-0.99644000	6.81630800	-0.00633100
Rh	-3.29405200	7.55716300	2.32720500	H	-0.47836000	7.29620300	0.82688700
C	-2.11271600	5.72160300	5.71263500	H	-0.32436300	6.82804100	-0.87538600
H	-2.58125600	4.73275500	5.64451400	H	-1.87357100	7.42027500	-0.25531000
H	-2.48291700	6.21645700	6.61363200	C	-3.23607800	5.17126700	-1.52193900
H	-1.03001000	5.58465800	5.76565700	H	-3.57098800	6.19519700	-1.33157600
C	-2.48377900	6.51112200	4.48742000	H	-2.65069800	5.17425700	-2.45102900
O	-3.53912800	7.22568000	4.46718600	H	-4.12510300	4.55821400	-1.68548000
O	-1.77369000	6.45036700	3.43160900	Rh	-2.94436400	4.84620600	1.75197600
C	-10.00821300	6.28157000	3.00699300	C	-2.80831500	5.54847700	6.03985200
C	-8.72066700	6.73031500	2.75308600	H	-3.79343300	5.14302900	6.29572900
C	-7.64250200	5.82098800	2.68284400	H	-2.91276500	6.63590800	5.97105000
C	-7.92555500	4.44905700	2.87937200	H	-2.09289100	5.28663800	6.82176700
C	-9.23232300	4.00446800	3.13605300	C	-2.35484500	4.97199100	4.70317000
C	-10.27616900	4.91428600	3.20096000	O	-3.10839400	5.37673600	3.71038000
H	-10.82256700	7.00047300	3.05819700	O	-1.39682200	4.20422100	4.62364100
H	-8.51819100	7.78739600	2.60903700	C	-9.39135600	4.39483700	4.36539800
H	-9.39363300	2.94045800	3.27921800	C	-8.62105200	5.39599800	3.78415300
H	-11.28939300	4.57764600	3.39942700	C	-7.36082200	5.10731000	3.23518600
C	-6.82661700	3.49183300	2.80735200	C	-6.88152600	3.77340100	3.28868300
N	-6.36874200	6.28928700	2.42377700	C	-7.66943700	2.78126900	3.88892300
C	-5.39437400	5.41518100	2.38352400	C	-8.91798100	3.07852000	4.42258800
O	-5.57779300	4.05745300	2.55899400	H	-10.36512900	4.64220700	4.78016800
O	-6.88731400	2.29158500	2.94023500	H	-8.97174400	6.42219300	3.74268100
O	-4.16156800	5.66615800	2.16266200	H	-7.26808600	1.77348100	3.92090400
				H	-9.51774700	2.29748300	4.88083600
TS4				C	-5.55668200	3.37824200	2.73280400
C	-1.52020000	3.31388700	1.31277700	N	-6.64932700	6.18120300	2.69721700
C	-0.79267400	4.57063900	1.32026400	C	-5.55290100	6.12713500	2.11359400

O	-5.00375600	4.33185200	1.98816400	H	-10.35771100	7.16106900	4.33492300
O	-5.04399600	2.27908600	2.90126300	H	-8.35904000	8.02111200	3.12916200
O	-4.62330900	6.66865100	1.56407500	H	-9.04632000	3.14217400	3.50909200
				H	-10.71525200	4.69449100	4.52493700
INT7				C	-6.80891100	3.62774100	2.27863800
C	-4.55298300	0.92845500	0.51107500	N	-6.52128400	6.68873600	2.00270900
C	-3.17135200	0.80501800	0.96199000	C	-5.51916900	6.42140600	1.37759600
C	-2.43814400	1.91640900	0.45175600	O	-5.57449000	4.02960800	2.17513600
C	-3.35626300	2.74926300	-0.31729800	O	-7.22965400	2.49565700	2.02468400
C	-4.64285100	2.10538700	-0.30866900	O	-4.54423400	6.38922500	0.71367100
C	-5.87579700	2.58331100	-1.01036200				
H	-5.83384400	3.65924500	-1.19773200	INT8			
H	-5.97239800	2.07607000	-1.98008400	C	-4.29109400	6.43622200	0.99914200
H	-6.76518800	2.37236700	-0.41315900	C	-4.76442100	6.39954300	-0.38091600
C	-5.66141500	-0.04390600	0.77365400	C	-4.11387200	5.31569300	-1.03952500
H	-6.56952700	0.49195500	1.05998000	C	-3.22176800	4.67187300	-0.08023300
H	-5.86385100	-0.64512600	-0.12331200	C	-3.30205700	5.40292600	1.15336200
H	-5.40312800	-0.72939600	1.58503600	C	-2.49114500	5.13399900	2.38249500
C	-2.64779000	-0.30812500	1.81766700	H	-1.54538500	5.69032400	2.32561800
H	-3.35309300	-0.55633500	2.61583400	H	-3.01332000	5.45700400	3.28707800
H	-2.49057800	-1.21163300	1.21381500	H	-2.26768100	4.07111500	2.47907300
H	-1.69596400	-0.04451800	2.28468000	C	-4.67800600	7.46367200	2.01902000
C	-0.98688300	2.22345900	0.66330100	H	-4.52203100	7.09621700	3.03629300
H	-0.54901400	1.59143100	1.43936900	H	-4.07634400	8.37475000	1.89497000
H	-0.42337500	2.05929000	-0.26447900	H	-5.73084900	7.74399500	1.92249300
H	-0.84646000	3.26643800	0.96304300	C	-5.77530700	7.34168200	-0.95956700
C	-2.97844300	3.98335300	-1.07829000	H	-6.60424800	7.50364100	-0.26433200
H	-2.70771300	3.72570700	-2.11177500	H	-5.31332300	8.31571900	-1.16835800
H	-3.79598400	4.70661300	-1.10496200	H	-6.19499100	6.95992900	-1.89315300
H	-2.12032700	4.48255700	-0.62061400	C	-4.29191500	4.87891100	-2.46181200
Rh	-4.05090100	2.66871000	1.74545200	H	-5.17153300	5.33826600	-2.91904800
C	-3.15512000	3.79957600	5.51977400	H	-3.41453900	5.15983500	-3.05896000
H	-3.94889600	4.50801500	5.78437000	H	-4.40928900	3.79320100	-2.52738900
H	-2.19653400	4.31986400	5.58675500	C	-2.30216200	3.52721100	-0.37072400
H	-3.18998500	2.96593800	6.22518600	H	-1.30364800	3.90184200	-0.63635800
C	-3.39252200	3.31209700	4.11458100	H	-2.21553800	2.86913400	0.49547400
O	-2.91756200	3.94655100	3.11853200	H	-2.66892800	2.93013200	-1.20998300
O	-4.10358300	2.27768900	3.89871100	Rh	-5.28931500	4.53312700	0.64869700
C	-9.64104300	6.46539600	3.90664800	C	-7.53615200	3.51640100	0.02538100
C	-8.52273000	6.95390400	3.23958200	C	-8.85670400	2.82335800	-0.18774700
C	-7.57496300	6.07992300	2.68292800	H	-9.66568800	3.55379300	-0.26297200
C	-7.76179900	4.68211200	2.79714500	H	-8.81905700	2.19830900	-1.08330400
C	-8.91035400	4.21692100	3.45334500	H	-9.05593900	2.17377900	0.67267100
C	-9.84115300	5.08704700	4.01309600	O	-7.48337400	4.65233900	0.59771900

O	-6.44926000	2.95831300	-0.33268900	Rh	-4.89588300	3.73781700	0.90901700
C	-6.33935100	0.19538000	6.09108700	C	-6.98368800	2.02555300	-0.39269200
C	-5.01638000	0.05234100	5.68985600	C	-7.62309800	1.26434500	-1.53591700
C	-4.50303900	0.78423700	4.60565800	H	-8.70180100	1.18591400	-1.38151600
C	-5.35008800	1.68719800	3.91586700	H	-7.40269400	1.74210400	-2.49246300
C	-6.67949700	1.81894700	4.34720400	H	-7.20887300	0.24947600	-1.54818600
C	-7.18051700	1.08508900	5.41746500	O	-7.46267000	1.86407600	0.76818200
H	-6.71203200	-0.38599700	6.93033200	O	-5.98838900	2.76683900	-0.66106500
H	-4.34555100	-0.62804000	6.20451500	C	-7.17140400	3.92092000	4.71560000
H	-7.31101500	2.51977400	3.81296500	C	-6.35582200	3.05995400	5.44558900
H	-8.21550500	1.20589300	5.72468500	C	-5.43182300	2.21141800	4.80552600
C	-4.88399600	2.48930000	2.73177600	C	-5.32183500	2.27320300	3.40190300
N	-3.15718600	0.56316000	4.32298600	C	-6.14790000	3.14754700	2.65395400
C	-2.32715300	0.92220300	3.50503700	C	-7.07361100	3.96492700	3.32351500
O	-3.81063900	2.21605300	2.16903900	H	-7.89322600	4.54466600	5.23705200
O	-5.68453700	3.44652800	2.38102900	H	-6.42375800	3.01135500	6.52796600
O	-1.34064400	1.11023600	2.88836300	H	-6.71463500	2.58957400	1.61613900
				H	-7.74399800	4.60207300	2.75164400
TSS				C	-4.33535600	1.45719100	2.61632800
C	-3.57121900	5.24249900	1.80867000	N	-4.67379000	1.39916000	5.63825600
C	-4.72941700	5.95590100	1.29659500	C	-3.86931900	0.48260700	5.52589900
C	-4.80241800	5.72851700	-0.10704800	O	-3.76704800	0.47568400	3.09391800
C	-3.64660600	4.92604800	-0.49717800	O	-4.12671800	1.87643400	1.39147800
C	-2.87171400	4.67346600	0.67549200	O	-3.10219300	-0.38159300	5.72815600
C	-1.61258000	3.86368500	0.76312500				
H	-1.14118300	3.75250500	-0.21656100	INT9			
H	-0.89161800	4.34239200	1.43446000	C	-3.27432800	5.34634000	1.64621300
H	-1.82944300	2.85999800	1.14885300	C	-4.48524300	6.09552100	1.36979700
C	-3.06298300	5.27708700	3.21998800	C	-4.82301900	5.86018200	0.00852700
H	-2.47963700	4.38199500	3.45326600	C	-3.72135700	5.11278300	-0.61877300
H	-2.41525500	6.15025800	3.38031800	C	-2.76805600	4.82644600	0.36705900
H	-3.88389000	5.33377100	3.94003000	C	-1.51035500	4.02132600	0.24001100
C	-5.62970800	6.84082900	2.10407800	H	-1.32750600	3.71716100	-0.79377200
H	-5.74532600	6.47532100	3.12667700	H	-0.64185500	4.59794500	0.58189300
H	-5.20330200	7.85218300	2.15537700	H	-1.57691000	3.11352800	0.85184000
H	-6.62498000	6.92478900	1.65938600	C	-2.49528000	5.35380700	2.92825900
C	-5.82459300	6.25865900	-1.06714000	H	-1.98545000	4.39841800	3.08180900
H	-6.71113400	6.63399100	-0.54932900	H	-1.73221600	6.14482200	2.91668700
H	-5.40778700	7.08456000	-1.65904400	H	-3.14585900	5.52771900	3.78958000
H	-6.14543500	5.47746200	-1.76312600	C	-5.19717100	6.98965000	2.33926000
C	-3.34416700	4.49951200	-1.90170300	H	-5.21390100	6.56576400	3.34647400
H	-3.02369200	5.35740400	-2.50806700	H	-4.68839600	7.96191500	2.39217500
H	-2.55239300	3.74733700	-1.93103500	H	-6.23117700	7.17640300	2.03722500
H	-4.23100000	4.06474100	-2.37328600	C	-5.99266500	6.42330100	-0.74414600

H	-6.81557400	6.68656600	-0.07373500	H	-1.61423500	6.78111100	2.60360200
H	-5.70446100	7.33181700	-1.29138900	H	-2.84466900	6.09593000	3.68065400
H	-6.37501500	5.70641200	-1.47753300	C	-5.11692600	7.22146900	2.22631200
C	-3.71146300	4.70526100	-2.06216400	H	-5.02721000	6.95085300	3.28195100
H	-3.70574700	5.58447200	-2.71955500	H	-4.67949900	8.22100800	2.09839400
H	-2.83480300	4.09922800	-2.30370200	H	-6.18152600	7.29774200	1.98974200
H	-4.60201100	4.11450300	-2.30637400	C	-6.12401900	6.08122600	-0.63440400
Rh	-4.74759600	3.88657600	1.10636300	H	-6.90223900	6.39644500	0.06525800
C	-6.70990500	1.65751200	-0.12739300	H	-5.97205500	6.89507200	-1.35716000
C	-7.17910700	0.78137200	-1.25618900	H	-6.50346500	5.21769800	-1.18941200
H	-8.24652200	0.56697400	-1.15294900	C	-3.79419000	4.38631000	-1.90432400
H	-6.97411900	1.26239400	-2.21282000	H	-3.77654000	5.16183600	-2.68210200
H	-6.64354600	-0.17366900	-1.20743200	H	-2.95603400	3.70925900	-2.08373900
O	-7.12826000	1.25025300	1.05871600	H	-4.71876100	3.81438300	-2.03916800
O	-6.00087100	2.64933500	-0.30873800	Rh	-4.47884400	4.02245400	1.44800300
C	-7.64888900	3.84805200	4.38173900	C	-7.57245600	3.88123000	4.52392100
C	-7.16323900	2.79772200	5.15443600	C	-7.31219500	2.63800100	5.08961300
C	-6.03564700	2.06822300	4.74081900	C	-6.25068700	1.84394700	4.61860300
C	-5.40041500	2.42959700	3.52829700	C	-5.45099600	2.33921800	3.56727800
C	-5.88149200	3.51397700	2.76076500	C	-5.71391800	3.60365500	3.00058300
C	-7.01710800	4.21245300	3.18577000	C	-6.77596800	4.37327000	3.48220800
H	-8.53134800	4.39020300	4.71409000	H	-8.40309400	4.47474000	4.89902600
H	-7.64666000	2.51349200	6.08345900	H	-7.91982700	2.25254900	5.90202300
H	-6.76247000	1.84318800	1.75839100	H	-7.00209200	5.34560300	3.05465500
H	-7.41509900	5.03542700	2.59806000	C	-4.31628400	1.58603900	2.95334300
C	-4.22927100	1.69816400	2.94713100	N	-6.07962100	0.61518800	5.24228200
N	-5.63474700	1.03013700	5.56951300	C	-5.34024800	-0.35567500	5.18522200
C	-4.75331000	0.18046900	5.60569500	O	-3.94411500	0.47938000	3.32697900
O	-3.67505200	0.75441500	3.51066000	O	-3.73953500	2.21921100	1.94169300
O	-3.86683800	2.13715400	1.76370100	O	-4.79950700	-1.38490300	5.34995700
O	-4.05468100	-0.71095600	5.91412900				

INT11

INT10

C	-3.11553600	5.63991400	1.59301800	C	-5.33317400	3.76204900	0.60020800
C	-4.42000700	6.23679000	1.33621300	C	-6.65021200	4.31195200	0.64153900
C	-4.84149900	5.75868900	0.07176100	C	-7.58591500	3.30109800	0.15495200
C	-3.72793000	5.00475200	-0.54081400	C	-6.85839600	2.12041000	-0.09191700
C	-2.66551600	4.96670600	0.36741800	C	-5.45740200	2.37146300	0.24564900
C	-1.34560300	4.26819200	0.23066100	C	-4.33556300	1.40510400	0.00389800
H	-1.24749200	3.78085700	-0.74232600	H	-4.62995600	0.38651300	0.27252600
H	-0.51473900	4.97682100	0.33740500	H	-4.04570600	1.40125300	-1.05617100
H	-1.23254700	3.49554400	0.99956600	H	-3.45114300	1.66278700	0.59248500
C	-2.24869700	5.90142800	2.78547700	C	-4.04810800	4.51179400	0.78156300
H	-1.59088900	5.05245500	2.99091700	H	-3.27776000	3.89527300	1.25059000
				H	-3.66858000	4.83762800	-0.19690800

H	-4.18092300	5.40698000	1.39518100	C	-9.68505900	0.62750600	2.76910700
C	-7.00208700	5.74694700	0.90481600	C	-12.07626600	2.08444700	2.88590200
H	-6.31286000	6.21052600	1.61632100	H	-10.84086600	3.77817100	3.39005800
H	-6.96537300	6.33282200	-0.02441600	C	-10.90529400	0.00191600	2.51763100
H	-8.01453100	5.84182000	1.30810700	H	-8.75013500	0.07977800	2.72977400
C	-9.04964000	3.53153600	-0.07890200	C	-12.10098400	0.72278800	2.57285400
H	-9.49153100	4.15298800	0.70554800	H	-13.00205000	2.65147600	2.93480800
H	-9.21154900	4.04725500	-1.03549700	H	-10.92028100	-1.05875200	2.28199400
H	-9.60865200	2.59332200	-0.10382500	H	-13.04762300	0.22651500	2.37669100
C	-7.37831400	0.79777500	-0.56752900				
H	-6.96833200	0.55236500	-1.55590100	TS6			
H	-7.08737900	0.00071400	0.12573200	C	-5.09808000	3.41093100	0.22406000
H	-8.46837200	0.79544300	-0.64434000	C	-6.32426700	4.17770000	0.38074200
Rh	-6.52218700	2.57973700	2.16369500	C	-7.43429200	3.33686600	0.00118800
C	-3.12106800	3.23133900	4.83186500	C	-6.92142700	2.02945000	-0.23595800
C	-2.88771900	1.94199500	5.29860300	C	-5.45911100	2.08840800	-0.11550300
C	-3.71425000	0.88117500	4.89449200	C	-4.55450300	0.91657500	-0.35377400
C	-4.77412600	1.14653300	3.99540300	H	-4.88251200	0.04838600	0.22756000
C	-4.99403700	2.45153000	3.52305300	H	-4.55897100	0.63091600	-1.41416900
C	-4.17698600	3.49757300	3.95106200	H	-3.52216900	1.13745400	-0.07072000
H	-2.47876500	4.04429400	5.16321000	C	-3.71388500	3.96177200	0.39687300
H	-2.07360000	1.72951900	5.98392900	H	-2.96690800	3.16545500	0.44351000
H	-4.35669000	4.51779500	3.62703000	H	-3.45061300	4.61907900	-0.44283700
C	-5.71210400	0.10803600	3.49189300	H	-3.62316900	4.54791700	1.31719500
N	-3.41558400	-0.36941300	5.42026000	C	-6.38756400	5.65549600	0.63907200
C	-3.83169200	-1.51747300	5.35832300	H	-5.57519300	5.98287200	1.29464900
O	-5.66535900	-1.08057100	3.80669400	H	-6.29740200	6.21982700	-0.29996800
O	-6.62102200	0.57301600	2.65889400	H	-7.33361400	5.94596100	1.10546900
O	-3.99838400	-2.67230200	5.49474000	C	-8.86578900	3.76982400	-0.11747200
C	-7.70127000	3.53700100	3.95426800	H	-9.10107800	4.58068800	0.57826800
C	-8.42630300	2.70097000	3.38002200	H	-9.07489800	4.13446400	-1.13245900
C	-7.25694200	4.51751500	4.91014400	H	-9.55528700	2.94811400	0.09185400
C	-6.57377300	4.12939600	6.07845800	C	-7.68516200	0.81640800	-0.67759400
C	-7.55136800	5.88050700	4.71089900	H	-7.61144200	0.68325900	-1.76603600
C	-6.20702400	5.08390400	7.02445900	H	-7.29048800	-0.08689200	-0.20295200
H	-6.33788100	3.08219000	6.23192500	H	-8.74507900	0.89106800	-0.42004600
C	-7.17663400	6.82872600	5.66047100	Rh	-6.46000900	2.50766500	1.89683900
H	-8.08379600	6.18423300	3.81493500	C	-3.30594500	3.82662700	4.63465500
C	-6.50398400	6.43373900	6.81968300	C	-2.89904400	2.59617200	5.14208700
H	-5.68490600	4.77097100	7.92426200	C	-3.66100600	1.43579200	4.91104100
H	-7.41496000	7.87638400	5.49766300	C	-4.83857400	1.53109900	4.13484900
H	-6.21458700	7.17404100	7.56048200	C	-5.26282900	2.79171800	3.66035000
C	-9.65436300	1.99851400	3.08421900	C	-4.49522100	3.93677000	3.91284000
C	-10.86394200	2.72154800	3.13941500	H	-2.70235300	4.71107400	4.82276500

H	-1.98900300	2.50237100	5.72554800	H	-3.50694900	-0.14022400	1.60213100
H	-4.84151000	4.91176700	3.58112000	H	-3.84888100	-1.49126300	0.51777800
C	-5.61282600	0.33001500	3.68380100	H	-3.19418500	0.01909200	-0.13462900
N	-3.15837600	0.26048100	5.45202700	C	-4.65469200	2.66554800	0.67261900
C	-3.50152700	-0.91264400	5.54764300	H	-3.77040200	2.37257900	1.24284800
O	-5.50778100	-0.76719800	4.23693100	H	-4.31955500	2.95655700	-0.33408600
O	-6.37314200	0.53877400	2.64215900	H	-5.08578400	3.54741400	1.15211600
O	-3.54793100	-2.05640000	5.80638900	C	-7.78531000	2.97837200	0.08334900
C	-7.19531700	3.19080900	4.00722200	H	-7.41561900	3.73766600	0.77782200
C	-8.02714200	2.59241300	3.22675400	H	-7.65820000	3.36598700	-0.93688600
C	-7.21318600	4.10262400	5.15483400	H	-8.85773400	2.85827700	0.25994400
C	-6.61033100	3.75640600	6.37667400	C	-8.96525700	-0.01537500	-0.28832700
C	-7.91306900	5.31826900	5.06073900	H	-9.02402900	-0.23912500	-1.36264900
C	-6.72595300	4.59762900	7.48003100	H	-9.30201000	-0.90554300	0.25223800
H	-6.06200800	2.82318300	6.45283700	H	-9.67418800	0.78797000	-0.07545300
C	-8.01529000	6.16436800	6.16559100	Rh	-6.73638200	0.61898300	2.17494900
H	-8.36816300	5.59539400	4.11411100	C	-4.91181000	5.48050000	3.63617100
C	-7.42500300	5.80458400	7.37800800	C	-3.71284600	4.77970000	3.73017300
H	-6.26864100	4.31155700	8.42313700	C	-3.71843200	3.40737900	4.01039500
H	-8.55755800	7.10206100	6.07831400	C	-4.94036700	2.70522800	4.14018100
H	-7.50780200	6.46051900	8.24033300	C	-6.14945200	3.42682700	4.04111000
C	-9.39667700	2.13127700	3.07169500	C	-6.12115100	4.81102400	3.80813500
C	-10.48378300	2.99529100	3.30004900	H	-4.90092600	6.54917700	3.43992300
C	-9.64807700	0.79936800	2.68869700	H	-2.75659000	5.27909200	3.61284900
C	-11.79198400	2.53707900	3.14565200	H	-7.05978200	5.35644700	3.76899000
H	-10.29741000	4.02083000	3.60391900	C	-4.88849400	1.23421600	4.52375100
C	-10.95899400	0.34907500	2.54436500	N	-2.46912600	2.78887200	4.09417000
H	-8.80341300	0.13567600	2.53294800	C	-1.95006900	1.81341100	4.60372100
C	-12.03388800	1.21495100	2.76638800	O	-4.25111500	0.92992700	5.53064500
H	-12.62297900	3.21420400	3.32517600	O	-5.45840400	0.34366900	3.75907400
H	-11.14203600	-0.68404300	2.26116400	O	-1.25294300	0.95060300	4.99174500
H	-13.05423700	0.86008300	2.64864500	C	-7.46990500	2.75097600	4.24349000
				C	-7.80224500	1.68542300	3.49947100
				C	-8.33031200	3.28643800	5.34299600
INT12				C	-7.76180800	3.56490700	6.59964500
C	-5.27303700	0.12474400	0.40840000	C	-9.70188500	3.52845100	5.16635900
C	-5.64136800	1.54439700	0.56777100	C	-8.54527400	4.04499000	7.64740200
C	-7.04937900	1.68139300	0.24678400	C	-6.70155500	3.38659000	6.75500200
C	-7.56472000	0.36637500	0.08846800	H	-10.48555000	4.01336200	6.21465700
C	-6.44016900	-0.58763700	0.13563800	C	-10.15256000	3.35150900	4.19532100
C	-6.59563200	-2.06606900	-0.06092300	H	-9.91140100	4.27160400	7.46000700
H	-7.42096900	-2.46648200	0.53808900	C	-8.08728800	4.24176500	8.61327000
H	-6.81908400	-2.29569500	-1.11194000	H	-11.54471700	4.19784600	6.05335700
H	-5.68899100	-2.60958700	0.21543200	H	-10.52063900	4.65116100	8.27601000
C	-3.88409200	-0.40267700	0.60736500	H			

C	-8.84802100	0.66273100	3.62827100	C	-4.94365600	4.12139100	4.87995500
C	-10.11797400	0.75868500	3.00849000	H	-3.33519900	5.26752900	5.71992000
C	-8.51791700	-0.54588300	4.29322000	H	-1.67999400	3.40332800	5.54342600
C	-11.02295000	-0.29178800	3.07623000	H	-5.65910200	4.92928800	4.98008900
H	-10.38185200	1.67344800	2.48535200	C	-4.76501200	0.60215200	3.45493300
C	-9.43240500	-1.60425400	4.33995000	N	-2.06691200	1.09681100	4.58766400
H	-7.55487300	-0.62635300	4.78750900	C	-1.91697900	-0.09184100	4.35388700
C	-10.68203200	-1.48207400	3.73744400	O	-4.21036600	-0.47530600	3.66319500
H	-12.00264100	-0.19012000	2.61617000	O	-5.71868800	0.71312900	2.54661100
H	-9.16507900	-2.51701000	4.86545900	O	-1.49412000	-1.17611200	4.19545300
H	-11.39573500	-2.29997600	3.78545300	C	-6.80600100	2.72714000	4.00920500
				C	-7.40847200	1.73680700	3.19516500
TS7				C	-7.79871200	3.52084600	4.81415000
C	-5.25794800	3.09680500	-0.15675600	C	-7.68049100	3.60957000	6.21493100
C	-5.65954300	4.32947100	0.37999300	C	-8.91408600	4.11664300	4.20531600
C	-7.11648900	4.30815400	0.44996100	C	-8.64401100	4.27231300	6.97207100
C	-7.59698000	3.12567700	-0.23708900	H	-6.82829100	3.15240000	6.70861500
C	-6.46023000	2.33303500	-0.53470800	C	-9.87981900	4.78077200	4.96400400
C	-6.42844400	1.01077500	-1.24308900	H	-9.01581600	4.05500100	3.12707400
H	-7.39829600	0.50669500	-1.20191600	C	-9.74854800	4.86248600	6.35012500
H	-6.16445900	1.13739100	-2.30280700	H	-8.53449800	4.32431900	8.05216400
H	-5.68875100	0.33824900	-0.79796000	H	-10.73295800	5.23703900	4.46863300
C	-3.85764200	2.60129100	-0.37436700	H	-10.49757200	5.38086600	6.94251400
H	-3.74385300	1.56709300	-0.03234300	C	-8.46356700	0.77094300	3.40404700
H	-3.59738900	2.62311900	-1.44151200	C	-9.12642600	0.20255900	2.29868300
H	-3.12412700	3.21063000	0.16023900	C	-8.79807000	0.32754900	4.70143000
C	-4.79296900	5.45491500	0.86476500	C	-10.10588000	-0.76738300	2.48312500
H	-3.74458900	5.15248800	0.93433600	H	-8.84475500	0.52816900	1.30323700
H	-4.84467100	6.31630100	0.18406800	C	-9.78232200	-0.63782900	4.88263000
H	-5.09805600	5.80439500	1.85754000	H	-8.28253500	0.75078300	5.55695200
C	-7.95301100	5.48846400	0.85318100	C	-10.43810800	-1.18603600	3.77540000
H	-7.56608300	5.96645600	1.75840400	H	-10.60900000	-1.20213800	1.62402200
H	-7.95493100	6.24594900	0.05643000	H	-10.03483700	-0.97137000	5.88509300
H	-8.99367400	5.20741400	1.03816300	H	-11.20272700	-1.94462600	3.91982900
C	-9.02682600	2.84215200	-0.59646300				
H	-9.32084100	3.39978000	-1.49706000	INT13			
H	-9.18848200	1.78098300	-0.80686200	C	-5.34222300	3.27437800	-0.19988200
H	-9.71647900	3.13073000	0.20317000	C	-5.79540700	4.43654300	0.44677700
Rh	-6.50064800	2.60704800	1.73537100	C	-7.23698500	4.28984400	0.59756700
C	-3.63209700	4.30886900	5.30265800	C	-7.67034300	3.11991800	-0.16573300
C	-2.70329300	3.28027500	5.20617400	C	-6.50595100	2.46254100	-0.60009500
C	-3.07980300	2.04596500	4.65420400	C	-6.41251800	1.20197500	-1.40996200
C	-4.39741900	1.85339200	4.17211700	H	-7.35213200	0.64205500	-1.39722000
C	-5.36088700	2.89193500	4.32755700	H	-6.17323000	1.42205500	-2.46035200

H	-5.62747800	0.53676600	-1.03422900	H	-10.78683600	4.79401300	4.09410200
C	-3.92273300	2.92290000	-0.54042500	H	-10.53620800	5.40975300	6.49616300
H	-3.72201700	1.85724100	-0.38597400	C	-8.28995100	0.65153000	3.49426200
H	-3.70813600	3.14123900	-1.59611400	C	-8.85967600	-0.03026800	2.40816600
H	-3.20969100	3.48786600	0.06646100	C	-8.87273200	0.50786500	4.76221500
C	-4.98713700	5.61068000	0.91659800	C	-9.98652100	-0.83117400	2.58222600
H	-3.93327700	5.34894700	1.05114300	H	-8.40568000	0.07556500	1.42722600
H	-5.02999800	6.43860200	0.19359700	C	-10.00674600	-0.28687600	4.93474700
H	-5.35364000	5.99692400	1.87346100	H	-8.44081700	1.02283700	5.61395700
C	-8.13722100	5.39277600	1.07395700	C	-10.56721800	-0.95798100	3.84693400
H	-7.79805300	5.81813400	2.02299000	H	-10.41416500	-1.35440400	1.73095100
H	-8.15178200	6.20466000	0.33258600	H	-10.44821200	-0.38481700	5.92297100
H	-9.16764100	5.05450100	1.20748200	H	-11.44959900	-1.57763800	3.98308300
C	-9.09633600	2.73744100	-0.43540700				
H	-9.52710900	3.35279500	-1.23833400	INT14			
H	-9.18016300	1.69158800	-0.74444000	C	-3.33119700	-2.78914300	5.75729900
H	-9.72835400	2.86738700	0.44924500	C	-2.13716800	-2.08376000	5.85520400
Rh	-6.41662000	2.59387300	1.72741000	C	-1.31358400	-2.41186400	4.67407600
C	-3.41918000	4.12852000	5.35480700	C	-1.97797600	-3.42835900	3.92650400
C	-2.55646500	3.03526200	5.33903200	C	-3.30186100	-3.54613300	4.49172600
C	-2.99176400	1.80923500	4.82176200	C	-4.35035100	-4.54089400	4.08072000
C	-4.31858500	1.68952800	4.32334800	H	-4.27227500	-4.78723100	3.01795600
C	-5.21352700	2.79799000	4.38887300	H	-4.24918700	-5.47667600	4.64923400
C	-4.72529100	4.01899600	4.89412900	H	-5.35869500	-4.15335800	4.25679600
H	-3.06624400	5.08160400	5.74013500	C	-4.49159000	-2.78720200	6.70750500
H	-1.54012700	3.10787400	5.70911900	H	-5.44117100	-2.64307800	6.18030000
H	-5.38214900	4.88028100	4.92392200	H	-4.56368000	-3.74372600	7.24462800
C	-4.74891900	0.48272100	3.61968000	H	-4.40281400	-1.99460000	7.45603100
N	-2.04996200	0.79355200	4.82984300	C	-1.70592700	-1.13152200	6.93177500
C	-1.89129200	-0.38114500	4.55822100	H	-2.53345500	-0.86819800	7.59688900
O	-4.13989200	-0.55804300	3.50203800	H	-0.90825500	-1.56712500	7.55023800
O	-5.94555200	0.57825400	2.90957000	H	-1.31091000	-0.20088900	6.50894600
O	-1.51303100	-1.47921400	4.38672900	C	0.08824000	-1.91510100	4.46663600
C	-6.61565800	2.66260800	3.94721000	H	0.16545000	-0.84169800	4.66889300
C	-7.04260800	1.44488000	3.29476000	H	0.79251600	-2.42757600	5.13807000
C	-7.67438700	3.48355800	4.63090000	H	0.42411100	-2.08274300	3.43964800
C	-7.56407400	3.81850500	5.99481100	C	-1.42995200	-4.21148100	2.76819300
C	-8.86168300	3.84614300	3.97369500	H	-1.03081800	-5.17872100	3.10560100
C	-8.58018100	4.50709600	6.65774000	H	-2.19678100	-4.41057900	2.01415900
H	-6.67821400	3.52624100	6.54925400	H	-0.61912700	-3.67361800	2.26889200
C	-9.88192400	4.52889300	4.63514600	Rh	-3.11717400	-1.53909000	3.67862800
H	-8.98433000	3.57306600	2.93250200	C	-7.53034600	1.43299500	2.08428400
C	-9.74503500	4.87189000	5.98092100	C	-6.87594900	0.22212700	2.28605000
H	-8.46133200	4.74975900	7.71069200	C	-5.48075200	0.17106100	2.43112400

C	-4.76145000	1.40887300	2.46732300	H	-4.09920600	-4.96984800	3.09316300
C	-5.43915200	2.64671000	2.24026200	H	-3.87995800	-5.64906900	4.71239700
C	-6.82708400	2.63378000	2.03520400	H	-5.17720600	-4.47866400	4.40600800
H	-8.60758500	1.44014900	1.93864400	C	-4.28011600	-3.05032400	6.83589200
H	-7.41650200	-0.71825800	2.28613000	H	-5.27373600	-2.96999300	6.38293800
H	-7.35045800	3.56179500	1.84280000	H	-4.22108000	-4.03480100	7.32163300
C	-3.36069600	1.45342900	2.82344400	H	-4.19913600	-2.29008200	7.61814700
N	-4.90241000	-1.08728800	2.52401000	C	-1.64854200	-1.13941900	6.92302900
O	-2.64221200	0.54134700	3.25137400	H	-2.43104600	-1.00086100	7.67456500
O	-2.72220100	2.65578100	2.74666600	H	-0.75341100	-1.51139200	7.44163400
C	-4.67427500	3.89134900	2.19615500	H	-1.39739900	-0.15161700	6.52011700
C	-3.33469300	3.84827100	2.43378400	C	-0.02728800	-1.61715200	4.27240300
C	-5.36490900	5.16300600	1.81960000	H	-0.07726600	-0.53752600	4.44904900
C	-6.23529800	5.80202400	2.71752000	H	0.77132200	-2.01958400	4.91160900
C	-5.17247800	5.72676100	0.55017600	H	0.26850500	-1.76970300	3.23112200
C	-6.88618700	6.98328700	2.35806800	C	-1.44476700	-4.01089400	2.60117900
H	-6.39568300	5.37122200	3.70253800	H	-1.02211500	-4.99766200	2.83686900
C	-5.82334000	6.90790700	0.19087100	H	-2.23889500	-4.15068600	1.86190100
H	-4.50577700	5.23625200	-0.15323300	H	-0.65890400	-3.41966400	2.12283200
C	-6.68053400	7.54001500	1.09359600	Rh	-3.27193700	-1.54863300	3.76124900
H	-7.55248100	7.46850400	3.06636100	C	-7.64447100	1.55286700	2.00527800
H	-5.66104300	7.33284700	-0.79598400	C	-7.06425200	0.32938600	2.33223600
H	-7.18705200	8.45961300	0.81345000	C	-5.69209900	0.23397600	2.59711400
C	-2.33295300	4.93710500	2.40954100	C	-4.90916500	1.43286500	2.58092400
C	-2.62617900	6.24170300	2.84238500	C	-5.51818000	2.68438900	2.24373800
C	-1.02622100	4.64919300	1.97296500	C	-6.88870700	2.71684700	1.94446000
C	-1.64504200	7.23126000	2.81892100	H	-8.70631400	1.59050700	1.77626200
H	-3.61613800	6.48081800	3.21087300	H	-7.65791600	-0.57918500	2.35042500
C	-0.05159900	5.64392300	1.94537600	H	-7.35425500	3.65357700	1.66556200
H	-0.78072100	3.64186100	1.65464300	C	-3.50719300	1.44138100	2.94010500
C	-0.35684500	6.93991800	2.36624800	N	-5.19744900	-1.06233000	2.84777400
H	-1.88877400	8.23230200	3.16404200	H	-6.35997500	-2.14400700	3.72114200
H	0.94899900	5.40409300	1.59634600	O	-2.80318800	0.50922600	3.34959900
H	0.40473900	7.71476400	2.34804700	O	-2.83287100	2.62094500	2.86618000
C	-3.83259400	-1.50813500	1.83197500	C	-4.71049000	3.90061500	2.18982700
O	-3.51136900	-1.75193900	0.69656600	C	-3.38861200	3.82614500	2.50207300
				C	-5.33332100	5.18062000	1.73192800
INT15				C	-6.23700800	5.87653300	2.55127600
C	-3.20309300	-2.90242500	5.80308200	C	-5.03862100	5.69736100	0.46211000
C	-2.07976900	-2.08421200	5.83963500	C	-6.82022500	7.06715900	2.11495700
C	-1.33847800	-2.28149000	4.57770100	H	-6.47757500	5.48264700	3.53542500
C	-1.95585100	-3.33834700	3.84356800	C	-5.62207000	6.88784800	0.02599100
C	-3.20223700	-3.61748000	4.51182800	H	-4.34591000	5.16286100	-0.18161400
C	-4.14389200	-4.73482300	4.16086500	C	-6.51279000	7.57672100	0.85122000

H	-7.51377400	7.59637000	2.76295200	H	0.40511700	-1.32768600	5.51590300
H	-5.38104400	7.27530100	-0.96016800	H	0.29471000	-1.47102200	3.75300800
H	-6.96710800	8.50342400	0.51145200	C	-1.03016500	-3.87455300	2.99426800
C	-2.35419800	4.88352400	2.51395500	H	-0.42840700	-4.68976300	3.41874600
C	-2.63270600	6.20273800	2.91088500	H	-1.66814900	-4.30269300	2.21677600
C	-1.03476800	4.55173800	2.15371400	H	-0.34461200	-3.17321700	2.51102400
C	-1.62350200	7.16368400	2.92703800	Rh	-3.39489900	-1.61082300	3.73746100
H	-3.63431100	6.47539500	3.22009000	C	-7.71750900	1.81807700	3.15714200
C	-0.03153900	5.51795600	2.16557700	C	-7.17650100	0.56193000	3.37166200
H	-0.80178600	3.53304600	1.86312400	C	-5.78439200	0.34344100	3.24395400
C	-0.32149900	6.82860300	2.55035200	C	-4.94860100	1.47275600	2.94885700
H	-1.85654800	8.17668300	3.24336800	C	-5.53364700	2.76747100	2.72967900
H	0.97920400	5.24465500	1.87536900	C	-6.91961900	2.91499100	2.82123600
H	0.46216300	7.58118400	2.56285200	H	-8.79317500	1.95046800	3.24198900
C	-8.83384600	-3.92718100	4.88255100	H	-7.79773400	-0.29171700	3.62497700
H	-9.86979400	-4.03942800	4.56081300	H	-7.37368000	3.87997000	2.63698300
H	-8.79845100	-3.55687800	5.91238400	C	-3.51985200	1.36363000	2.90021800
H	-8.33639700	-4.90328000	4.86961800	N	-5.35138600	-0.95163600	3.38362600
C	-8.11415900	-2.96979200	3.95741400	H	-6.09655700	-1.63562700	3.74072800
O	-8.61588300	-2.47265900	2.96691000	O	-2.79889400	0.36759600	3.12071700
O	-6.85671700	-2.73866100	4.36354800	O	-2.79144400	2.46723800	2.60383900
C	-4.22514500	-1.59980800	2.04739000	C	-4.67265300	3.90027500	2.40050500
O	-4.09413100	-1.92504700	0.89748000	C	-3.32650900	3.71382600	2.34836200
				C	-5.28810900	5.22341600	2.07479000
TS8				C	-5.87357000	6.01044900	3.07967900
C	-3.49520000	-2.81917100	5.69227000	C	-5.30599200	5.69197600	0.75347300
C	-2.49819500	-1.82173100	5.84920100	C	-6.45028500	7.24326300	2.77073400
C	-1.48836500	-2.04992800	4.82300600	H	-5.87097300	5.65385700	4.10641600
C	-1.84442300	-3.20704200	4.06472200	C	-5.88336700	6.92460600	0.44488500
C	-3.12768000	-3.65946700	4.55958800	H	-4.86162200	5.08685900	-0.03150100
C	-3.84807400	-4.90870300	4.15217400	C	-6.45497100	7.70415800	1.45212300
H	-3.30674600	-5.43322900	3.36004000	H	-6.89496100	7.84313100	3.56025200
H	-3.92921200	-5.58897200	5.01064400	H	-5.88775300	7.27401400	-0.58398900
H	-4.85614100	-4.68850600	3.77748800	H	-6.90418700	8.66374900	1.21129300
C	-4.73512600	-3.01472800	6.50950200	C	-2.24333000	4.67026700	2.03381400
H	-5.63720200	-2.99487000	5.88384300	C	-2.29060900	6.01651500	2.43505400
H	-4.69712700	-3.99024400	7.01291200	C	-1.10633300	4.21219400	1.34208500
H	-4.83522300	-2.24457000	7.27884500	C	-1.23891900	6.88031800	2.13525800
C	-2.42989500	-0.75422900	6.90268700	H	-3.14267700	6.38591400	2.99247500
H	-3.42096500	-0.52097400	7.30122800	C	-0.06095500	5.08172100	1.03982100
H	-1.79786800	-1.06866100	7.74504900	H	-1.04886100	3.17181000	1.04060900
H	-2.00540400	0.17299600	6.50472900	C	-0.12314300	6.42009800	1.43327800
C	-0.26299200	-1.20386300	4.65356100	H	-1.29058500	7.91611200	2.45924000
H	-0.52405900	-0.14251100	4.58296200	H	0.80408600	4.71151000	0.49650400

H	0.69371700	7.09750600	1.19987800	H	-8.82599400	2.00546100	3.41784600
C	-8.65947800	-4.32640200	3.57109700	H	-7.85810800	-0.21149700	3.92668300
H	-8.64947800	-5.13385000	2.83519600	H	-7.38875000	3.91523600	2.77598900
H	-9.51272800	-3.66479100	3.38338200	C	-3.60601900	1.30225200	2.85829000
H	-8.79934400	-4.74779000	4.57399300	N	-5.36019200	-0.79762800	3.98290300
C	-7.35427000	-3.52308000	3.52501000	H	-6.09269000	-1.53820000	4.10398700
O	-6.44113900	-3.88928900	2.75261700	O	-2.91192400	0.24834500	2.91302700
O	-7.29674900	-2.51229700	4.31550000	O	-2.84898200	2.36912500	2.49178500
C	-4.39143600	-1.74092400	2.07492500	C	-4.68625800	3.87951900	2.46644200
O	-4.72972000	-1.79547700	0.96347000	C	-3.35479000	3.64393900	2.32193100
INT16				C	-5.27061700	5.22665800	2.18906900
C	-3.56444800	-2.69997200	5.69022100	C	-5.81194400	6.00321700	3.22661100
C	-2.61799300	-1.62439600	5.70761200	C	-5.30604100	5.73114100	0.88118200
C	-1.55275200	-1.95403000	4.76441400	C	-6.35955500	7.25943600	2.96312800
C	-1.88273400	-3.17082600	4.11837800	H	-5.79878400	5.61780500	4.24255200
C	-3.16107300	-3.62618200	4.66526400	C	-5.85572200	6.98651300	0.61740300
C	-3.84977700	-4.91925900	4.35234900	H	-4.89746400	5.13444900	0.07074300
H	-3.20511600	-5.57858500	3.76390500	C	-6.38157100	7.75523900	1.65736500
H	-4.11337000	-5.44150700	5.27983300	H	-6.76911400	7.85032300	3.77814700
H	-4.77212800	-4.73570600	3.78212200	H	-5.87437800	7.36232700	-0.40206900
C	-4.78800900	-2.85291900	6.53871600	H	-6.80903200	8.73294500	1.45198300
H	-5.68368300	-3.01228500	5.92438900	C	-2.26041600	4.57392200	1.96786300
H	-4.66867700	-3.71954700	7.20324100	C	-2.23014800	5.90231200	2.42627400
H	-4.95559100	-1.97169100	7.16205500	C	-1.18974600	4.10836100	1.18201300
C	-2.60911300	-0.44784900	6.63862300	C	-1.17053200	6.74277100	2.09021700
H	-3.62478800	-0.15178000	6.91291900	H	-3.03014900	6.27494900	3.05468700
H	-2.06491100	-0.68390400	7.56349600	C	-0.13534600	4.95423900	0.84477500
H	-2.12073800	0.41654400	6.17929200	H	-1.19199400	3.08046700	0.83549400
C	-0.35536100	-1.08831200	4.51721800	C	-0.12168200	6.27587900	1.29534300
H	-0.66126300	-0.09241800	4.17714300	H	-1.16268600	7.76504100	2.45845900
H	0.22452100	-0.96646100	5.44054000	H	0.67734500	4.57887100	0.22874400
H	0.30316800	-1.51516300	3.75735200	H	0.70193500	6.93482000	1.03411800
C	-1.04745200	-3.93084000	3.12803100	C	-8.41940100	-4.44058900	3.08764900
H	-0.46135400	-4.70828500	3.63651300	H	-8.27452800	-5.09455300	2.22462700
H	-1.66721500	-4.42697200	2.37626200	H	-9.29345000	-3.80010700	2.92448300
H	-0.34686200	-3.27646500	2.60277500	H	-8.63245000	-5.04835500	3.97535100
Rh	-3.53705300	-1.64581500	3.66629900	C	-7.18137800	-3.56969600	3.34561700
C	-7.74970600	1.86172500	3.35569100	O	-6.17175400	-3.75478000	2.61064700
C	-7.22684300	0.62355100	3.63858300	O	-7.27694300	-2.73495600	4.29983100
C	-5.81300100	0.38416600	3.57031600	C	-4.18121200	-2.21414700	1.89623800
C	-4.98626200	1.48143900	3.10719000	O	-4.39153900	-2.42805700	0.79495600
C	-5.56637600	2.78135400	2.86122700	TS9			
C	-6.93832800	2.95336400	2.98352300	C	-3.32062000	-2.64155100	6.19102300

C	-2.31042800	-1.59689600	6.24758300	C	-6.36887100	7.32912500	2.64610700
C	-1.33425700	-1.86012400	5.19284600	H	-5.67424600	5.90400300	4.10614000
C	-1.78617900	-2.97646500	4.44905300	C	-6.04743300	6.71074400	0.33424800
C	-3.02020700	-3.46760300	5.06634600	H	-5.09891200	4.80499300	-0.00654400
C	-3.80461900	-4.66714300	4.64571600	C	-6.50460300	7.62275600	1.28720600
H	-3.28607200	-5.23096400	3.86570800	H	-6.72414700	8.03248600	3.39455400
H	-3.95721000	-5.33296300	5.50473700	H	-6.15410600	6.92907900	-0.72492600
H	-4.79591600	-4.36872800	4.26457900	H	-6.96681100	8.55487600	0.97369000
C	-4.45323400	-2.85643900	7.14923100	C	-2.30465600	4.56076300	1.75738500
H	-4.31169300	-3.80758600	7.68019900	C	-2.27341600	5.94392500	2.00556800
H	-4.49698600	-2.06080700	7.89765400	C	-1.27936200	3.99324400	0.97805400
H	-5.42082900	-2.88782600	6.63119100	C	-1.25846200	6.73581700	1.47189400
C	-2.16466800	-0.56371100	7.32232700	H	-3.03668200	6.39897700	2.62517200
H	-3.13595400	-0.26792100	7.72614100	C	-0.27003100	4.79026200	0.44255000
H	-1.56166800	-0.96147100	8.15099800	H	-1.28154600	2.92443600	0.79322100
H	-1.66383500	0.33360300	6.94823600	C	-0.25594000	6.16542800	0.68487200
C	-0.10898500	-1.03322000	4.94239300	H	-1.24866500	7.80234000	1.67950900
H	0.64220700	-1.21517600	5.72208400	H	0.50750700	4.33490700	-0.16485800
H	0.34537800	-1.26905200	3.97723700	H	0.53284700	6.78639000	0.26893300
H	-0.34383900	0.03587800	4.94498600	C	-8.67764000	-3.79828200	4.30099300
C	-1.11860600	-3.60221000	3.26134600	H	-8.95371800	-4.21964200	5.27417900
H	-0.51621400	-4.46730600	3.57031000	H	-8.70487700	-4.57771000	3.53550900
H	-1.85419000	-3.95356300	2.53311000	H	-9.42625400	-3.03312300	4.06163400
H	-0.45536500	-2.89634900	2.75472900	C	-7.28829500	-3.14794400	4.38309200
Rh	-3.35737800	-1.33961700	4.40459300	O	-7.12386100	-2.31878600	5.34162500
C	-7.63617200	2.02812000	3.90655200	O	-6.43462300	-3.46561600	3.51771100
C	-7.07438700	0.83728400	4.30259100	C	-4.47182100	-2.03882900	2.11599500
C	-5.67484300	0.58920600	4.12410700	O	-5.15261900	-1.72982300	1.25772500
C	-4.89578600	1.63208200	3.49095100				
C	-5.50815100	2.88442800	3.12541100	INT17			
C	-6.87190800	3.06030800	3.32764000	C	-3.95253800	-3.99858000	4.79859400
H	-8.70341500	2.18171100	4.04761000	C	-2.84536800	-3.05805900	4.79436400
H	-7.66507400	0.04454100	4.75160600	C	-2.38054700	-2.94728300	3.44997600
H	-7.35066700	3.98508400	3.03235800	C	-3.15507000	-3.84838600	2.61081300
C	-3.52442200	1.43864300	3.19788500	C	-4.09928600	-4.51080900	3.45429500
N	-5.17664500	-0.57500800	4.55138100	C	-5.09328100	-5.55317500	3.04284800
H	-5.89251000	-1.24250700	4.93861000	H	-5.32660300	-5.48801800	1.97706700
O	-2.81956700	0.40980400	3.37533900	H	-4.68799400	-6.55541300	3.23951000
O	-2.80919400	2.45299900	2.64257600	H	-6.02385300	-5.44126600	3.60397500
C	-4.67504300	3.92496600	2.52444900	C	-4.70174400	-4.48174000	6.00449700
C	-3.35218000	3.68209800	2.32213400	H	-5.77315900	-4.52805900	5.79264000
C	-5.30423000	5.21173600	2.09772700	H	-4.35275400	-5.47862500	6.30715200
C	-5.77663000	6.13116500	3.04832400	H	-4.55359400	-3.80872600	6.85428700
C	-5.45372900	5.51343200	0.73647400	C	-2.31612900	-2.34923900	6.00523000

H	-3.12809000	-1.88736500	6.57575300	C	-2.94395400	3.27242900	-1.88399000
H	-1.79282200	-3.05102300	6.66762300	H	-3.96933400	1.69725800	-0.83663800
H	-1.61231300	-1.55806500	5.73449400	C	-2.42572300	4.56716900	-1.81211100
C	-1.28665800	-2.05980500	2.93709800	H	-2.12841300	6.29163300	-0.55031900
H	-0.91774200	-1.38117200	3.70988600	H	-2.85577100	2.69917500	-2.80300000
H	-0.43991400	-2.66147600	2.58224700	H	-1.93075200	5.00743100	-2.67356900
H	-1.64246900	-1.45135500	2.09895800	C	-8.74626900	-2.79747800	2.56680200
C	-2.92700300	-4.07819400	1.14601700	H	-9.13095000	-1.77545000	2.66769400
H	-2.11368300	-4.79834700	0.97876700	H	-8.62143100	-2.99886700	1.49919300
H	-3.82431800	-4.47093100	0.66031800	H	-9.47167100	-3.48790700	3.00345100
H	-2.65651400	-3.14819700	0.63643300	C	-7.41402800	-2.90128800	3.30780700
Rh	-4.53647400	-2.32350000	3.51503000	O	-7.36321700	-3.36964400	4.45235400
C	-7.08568800	2.13354300	5.54652600	O	-6.41310600	-2.43730000	2.61906600
C	-6.73349700	0.80542400	5.60905400				
C	-5.82171000	0.22365600	4.67161600	INT18			
C	-5.35257500	1.08845700	3.60779700	C	-3.19845900	-2.48630100	5.83008200
C	-5.70729000	2.48467800	3.59199100	C	-2.08218800	-1.59507200	5.78741400
C	-6.57152000	2.99068500	4.55894200	C	-1.11013300	-2.12511600	4.82982200
H	-7.78065700	2.53225800	6.28218500	C	-1.65878100	-3.30658700	4.26843400
H	-7.13517900	0.16528600	6.39058000	C	-2.97936400	-3.52080600	4.84492200
H	-6.86409300	4.03212600	4.53983400	C	-3.83775400	-4.73333700	4.65002700
C	-4.58384800	0.57351700	2.52499700	H	-3.74273900	-5.12389400	3.63625400
N	-5.42596400	-1.04233800	4.84354200	H	-3.54729700	-5.51853400	5.36360700
H	-6.01780700	-1.55705900	5.48942500	H	-4.89324600	-4.49866200	4.80759800
O	-4.24902400	-0.60414000	2.27362700	C	-4.40886100	-2.37987700	6.70786500
O	-4.11877200	1.44115300	1.57829000	H	-5.32009500	-2.63707800	6.16043800
C	-5.17472300	3.34124700	2.53342200	H	-4.31988800	-3.07088400	7.55683100
C	-4.38120800	2.79255700	1.57500000	H	-4.53176000	-1.37047300	7.10825400
C	-5.55511400	4.78617200	2.49723100	C	-1.86871400	-0.36878500	6.62207700
C	-5.07034400	5.68121300	3.46488600	H	-2.80932500	0.00332900	7.03613600
C	-6.42138800	5.27101000	1.50691300	H	-1.19280400	-0.58444900	7.46078300
C	-5.43030900	7.02914400	3.43191600	H	-1.42119900	0.43474600	6.02930700
H	-4.40651800	5.31450700	4.24325400	C	0.21660600	-1.49389100	4.52950300
C	-6.78275200	6.61877500	1.47440300	H	0.11254800	-0.41571600	4.36858500
H	-6.80874100	4.58517900	0.75891200	H	0.91786700	-1.64318800	5.36174000
C	-6.28679100	7.50222400	2.43492000	H	0.66908000	-1.92019200	3.63055900
H	-5.04144800	7.70940400	4.18514300	C	-1.03876000	-4.19272200	3.23168800
H	-7.45393000	6.97729700	0.69847000	H	-0.59873000	-5.08077400	3.70538200
H	-6.56804500	8.55160000	2.40935300	H	-1.79315900	-4.53032800	2.51663700
C	-3.71449000	3.43228300	0.41885100	H	-0.24935800	-3.67902800	2.67745000
C	-3.17736700	4.72956400	0.48414100	Rh	-3.03510800	-1.58751100	3.79831100
C	-3.57594900	2.70635900	-0.77899600	C	-7.52535100	1.42528100	2.70230900
C	-2.54139900	5.28910700	-0.62254100	C	-6.92001600	0.24912800	3.07012000
H	-3.24620200	5.29738500	1.40404700	C	-5.49435800	0.14764400	3.20791900

C	-4.72770600	1.34113000	2.90003100	H	-8.89121400	-5.65693200	3.05971400
C	-5.39822900	2.56006200	2.51673000	H	-9.50556800	-4.21143700	2.26028200
C	-6.78501200	2.59151400	2.43013700	H	-9.36316700	-4.23588800	4.04341100
H	-8.60981600	1.45963700	2.62241100	C	-7.49886000	-4.01840100	3.00035000
H	-7.50876300	-0.63709700	3.28852700	O	-6.89387000	-4.42100300	1.89314000
H	-7.29604500	3.50585200	2.15926800	O	-7.00031500	-3.28895600	3.85187900
C	-3.31093300	1.35153700	3.00303800				
N	-4.97337400	-1.00237400	3.63010200	TS10			
H	-5.64801500	-1.76322900	3.70477600	C	-3.80800600	-2.39893800	5.61794600
O	-2.52494900	0.42310900	3.30063200	C	-2.86293900	-1.31472700	5.61812200
O	-2.63715500	2.51603200	2.76442300	C	-1.64033500	-1.78582300	4.96091000
C	-4.59718900	3.75459500	2.24917900	C	-1.86622200	-3.10621300	4.50212100
C	-3.24562500	3.68958700	2.38018600	C	-3.23348000	-3.48182200	4.86167700
C	-5.28376300	5.03665700	1.90339900	C	-3.88065900	-4.80731800	4.60954300
C	-5.32460400	6.09441300	2.82292000	H	-3.16932800	-5.51409000	4.17371900
C	-5.91660100	5.20060800	0.66040200	H	-4.25112500	-5.23302200	5.55090100
C	-5.96760100	7.29148200	2.50433000	H	-4.73264200	-4.70329600	3.91741300
H	-4.84402800	5.97504100	3.78976000	C	-5.15627000	-2.43711400	6.26553400
C	-6.55926000	6.39763700	0.34102500	H	-5.93421500	-2.75486100	5.55655000
H	-5.89897400	4.38446000	-0.05690000	H	-5.13541600	-3.15536500	7.09696700
C	-6.58519600	7.44760400	1.26208200	H	-5.43671300	-1.46263900	6.67439300
H	-5.98679500	8.10152900	3.22866800	C	-3.00263200	-0.00115700	6.32852400
H	-7.03876200	6.50991200	-0.62791200	H	-4.04847300	0.31065900	6.39330300
H	-7.08554900	8.37975900	1.01362200	H	-2.60883100	-0.06951600	7.35207500
C	-2.22633900	4.74565400	2.18677900	H	-2.44690600	0.78860200	5.81378300
C	-1.08719500	4.75775000	3.01303800	C	-0.40830900	-0.95147800	4.78375300
C	-2.33343200	5.71876400	1.17836200	H	-0.64826200	-0.00137900	4.29381300
C	-0.10275700	5.73060900	2.85448000	H	0.04451600	-0.72306900	5.75706900
H	-0.98027400	3.99853000	3.78031200	H	0.34054100	-1.46063600	4.17286000
C	-1.34308200	6.68659300	1.01982500	C	-0.94076500	-3.98144000	3.71520200
H	-3.18545000	5.71204700	0.50936600	H	-0.66921700	-4.87397100	4.29287600
C	-0.22712200	6.70174300	1.85879100	H	-1.42983600	-4.30861500	2.79154500
H	0.76487700	5.72762100	3.50899000	H	-0.01979900	-3.45926900	3.44468700
H	-1.44220000	7.42679000	0.23043200	Rh	-3.36806100	-1.74125700	3.54141200
H	0.54241400	7.45865000	1.73284000	C	-7.53724500	1.70403500	3.67023300
C	-3.83602200	-2.69560100	1.15473200	C	-7.03778000	0.41087100	3.60477400
C	-4.01568300	-2.57816700	-0.35446000	C	-5.71096300	0.17611900	3.18234800
H	-3.88773800	-3.56015200	-0.82032700	C	-4.88991800	1.31088000	2.87906000
H	-5.04106400	-2.24814100	-0.56110600	C	-5.42660300	2.63752900	2.93625100
H	-3.31920000	-1.85872500	-0.78913500	C	-6.75760900	2.81289300	3.33162800
O	-3.09459100	-1.79854900	1.68900200	H	-8.56759600	1.85773400	3.98156500
O	-4.39980300	-3.62764600	1.77248900	H	-7.65428900	-0.45388700	3.83454100
H	-5.94547900	-4.07411800	1.83761200	H	-7.18433600	3.80720400	3.36745500
C	-8.90742400	-4.56305800	3.10809500	C	-3.51213800	1.14398100	2.51052100

N	-5.28837200	-1.12414400	2.99742100	INT19			
H	-5.99591300	-1.80931300	3.37044400	C	-3.98235500	-1.45467700	6.47384000
O	-2.82679500	0.10350300	2.51384400	C	-2.95855000	-0.71382800	5.80518200
O	-2.80864300	2.24307600	2.13177000	C	-1.93431900	-1.63359500	5.36553700
C	-4.58699100	3.76648900	2.54437100	C	-2.28364600	-2.94453700	5.88240500
C	-3.30913700	3.52946100	2.13997900	C	-3.55252000	-2.84579800	6.53267800
C	-5.17156600	5.14222900	2.52242900	C	-4.35053800	-3.94967800	7.15546200
C	-5.45832500	5.81799700	3.71944300	H	-5.30235200	-4.06463100	6.62297400
C	-5.46682500	5.77154200	1.30464900	H	-3.82187000	-4.90497300	7.10774600
C	-6.01212800	7.09889400	3.69753200	H	-4.56536400	-3.72849300	8.20835300
H	-5.24075100	5.33641600	4.66926600	C	-5.22881900	-0.91378100	7.10737400
C	-6.02141000	7.05203300	1.28305200	H	-6.06689900	-1.60224500	6.96274200
H	-5.25629700	5.25331100	0.37358000	H	-5.09096600	-0.77152400	8.18836400
C	-6.29338400	7.72001300	2.47846400	H	-5.51056500	0.05120000	6.67693600
H	-6.22314800	7.61098800	4.63253400	C	-2.92089300	0.77255400	5.64088600
H	-6.24270000	7.52636600	0.33082200	H	-3.91275100	1.18809400	5.44242300
H	-6.72463300	8.71718100	2.46099700	H	-2.54850300	1.23199700	6.56677400
C	-2.27436200	4.47279200	1.66294000	H	-2.25337400	1.06502500	4.82954500
C	-2.13248800	5.76502000	2.19726600	C	-0.66193000	-1.27403800	4.65606600
C	-1.37356900	4.05182400	0.66677000	H	-0.83085000	-0.48631800	3.91779700
C	-1.13094700	6.61562900	1.73284700	H	0.10156800	-0.93076200	5.36871100
H	-2.79650600	6.10112400	2.98430800	H	-0.26030000	-2.13476200	4.11584800
C	-0.37866800	4.90881300	0.20186400	C	-1.47939300	-4.19295300	5.67997300
H	-1.45956900	3.05059600	0.25846800	H	-0.40882300	-3.98277900	5.77097800
C	-0.25391400	6.19503300	0.73111500	H	-1.73966100	-4.95841800	6.41621400
H	-1.03295600	7.60888700	2.16224900	H	-1.66904700	-4.60146200	4.68026700
H	0.30126000	4.56917300	-0.57459500	Rh	-3.82014500	-2.26814200	4.41539900
H	0.52429100	6.86194000	0.37014400	C	-7.27250300	1.20804600	3.13380300
C	-4.16437800	-2.88558100	0.79281800	C	-6.48521800	0.06284100	3.05344600
C	-4.19818500	-4.02389200	-0.19089300	C	-5.11514600	0.15881900	2.77742300
H	-4.93034500	-4.73738400	0.20717200	C	-4.54210300	1.44807800	2.59220300
H	-4.54412100	-3.67878500	-1.16826800	C	-5.35509700	2.61680100	2.67936300
H	-3.22283300	-4.50780000	-0.27111600	C	-6.72632100	2.47300500	2.94991200
O	-3.27644400	-2.87584200	1.69016900	H	-8.33645900	1.10799100	3.33171100
O	-5.07884000	-1.99338500	0.67690300	H	-6.92195800	-0.92165400	3.16598000
H	-5.18335600	-1.47698900	1.70011000	H	-7.35943000	3.34991900	3.00116000
C	-8.59909100	-4.50300400	2.79798200	C	-3.12268000	1.59393100	2.28693900
H	-9.05679600	-4.82449100	3.74125000	N	-4.38578500	-1.04961500	2.66127000
H	-8.50632800	-5.36013000	2.12635900	H	-4.99054500	-1.79448800	2.25121200
H	-9.27346300	-3.76081000	2.35492100	O	-2.29329900	0.70691300	2.21883300
C	-7.23114600	-3.86317100	3.07655300	O	-2.66295000	2.87738000	2.07414400
O	-6.21336900	-4.36708500	2.54458800	C	-4.75903600	3.93293800	2.45166200
O	-7.24753000	-2.84673100	3.85485800	C	-3.43115400	4.01238000	2.15841200
				C	-5.63365900	5.14550700	2.47091200

C	-6.16858500	5.63072200	3.67546600	H	-1.73646800	3.60881300	-0.23208200
C	-5.95683900	5.80751300	1.27740000	H	-1.07623100	5.25459900	-0.19705800
C	-6.99276400	6.75711100	3.68681800	H	-1.22835900	4.30579400	1.29896100
H	-5.92951600	5.12417600	4.60710700	C	-2.88241700	5.94471700	2.99680000
C	-6.78025300	6.93422400	1.28824300	H	-2.16019500	5.14465200	3.17782700
H	-5.55407900	5.43658100	0.33930100	H	-2.33460900	6.89694300	2.98581300
C	-7.29945500	7.41329200	2.49248500	H	-3.57583000	5.96830800	3.84187000
H	-7.39330900	7.12259900	4.62870700	C	-5.83399200	7.01378300	2.25662600
H	-7.01738300	7.43619700	0.35410200	H	-5.70076800	6.76027300	3.31196200
H	-7.94076700	8.29040700	2.50071200	H	-5.62393100	8.08658200	2.14112000
C	-2.60244900	5.20585500	1.87361800	H	-6.88806500	6.85702200	2.00621200
C	-2.80384700	6.43704300	2.52103100	C	-6.41390900	6.32259500	-0.77699700
C	-1.54556300	5.09425600	0.95084500	H	-7.29633100	5.93987500	-0.25295000
C	-1.98516400	7.52821400	2.23564900	H	-6.51416300	7.41389800	-0.84488800
H	-3.59168700	6.53935600	3.25729200	H	-6.42967300	5.91917000	-1.79221700
C	-0.73546300	6.19039400	0.66360900	C	-3.80227600	4.79390100	-1.96645400
H	-1.36406700	4.14302400	0.46275900	H	-3.01233500	5.37608200	-2.45976600
C	-0.95271900	7.41282000	1.30276200	H	-3.48882200	3.74450300	-1.97168200
H	-2.15217000	8.47006800	2.75112000	H	-4.70526500	4.87445400	-2.57727600
H	0.06964100	6.08698800	-0.05866300	Rh	-4.92475000	4.02771200	1.19577400
H	-0.31793100	8.26650200	1.08125100	C	-6.73732800	-1.45610500	4.07787200
C	-2.61180900	-3.53038400	1.94998400	C	-7.95097100	-2.34608000	4.18751300
C	-2.36727300	-4.78930900	1.12084700	H	-8.57659500	-2.02786600	5.02789000
H	-1.64801500	-4.57921600	0.32639600	H	-8.52214000	-2.30289900	3.25983600
H	-2.01051100	-5.61223900	1.74793000	H	-7.63929100	-3.37720700	4.38507700
H	-3.31552100	-5.10658200	0.67171500	C	-7.04551000	0.74711200	0.11072500
O	-3.24732300	-3.77287300	3.06364100	H	-8.06818600	1.01953500	-0.16093900
O	-2.24396900	-2.42411200	1.54696600	H	-7.06518400	0.08925100	0.98759700
H	-3.47998200	-0.98729600	2.17981900	H	-6.56519100	0.20463200	-0.70842900
C	-7.33094500	-4.72931700	3.46578100	C	-6.24421800	1.97248700	0.45582300
H	-8.00758800	-4.79313500	2.61103000	O	-6.82830300	3.05878900	0.79980100
H	-7.89963600	-4.60006800	4.39175500	O	-4.97560400	1.94649500	0.45242800
H	-6.77332800	-5.66974300	3.54951000	O	-6.01476700	-1.45639500	5.22100700
C	-6.33986900	-3.58574000	3.27314800	O	-6.41668300	-0.81127700	3.10217800
O	-5.72062100	-3.23680500	4.35464300	C	-6.65954100	3.19630800	5.02893600
O	-6.19563100	-3.07632200	2.14755200	C	-5.85424000	2.25095100	5.65769500
				C	-4.69752200	1.82854800	5.00674100
INT20				C	-4.32501000	2.35581500	3.74999600
C	-3.60341800	5.74283000	1.69689900	C	-5.16026600	3.29503200	3.09461400
C	-4.93596600	6.19443100	1.37750200	C	-6.32594600	3.69415600	3.76727800
C	-5.15499800	5.95380600	-0.05195700	H	-7.56986700	3.53279600	5.51957800
C	-4.03247400	5.28209800	-0.56630900	H	-6.12324600	1.83329500	6.62438200
C	-3.07693200	5.10909600	0.52738000	H	-5.24740600	-0.86528000	5.07333000
C	-1.70592800	4.53582800	0.34687400	H	-7.01035700	4.38610600	3.28725100

C	-3.04351900	1.92104100	3.18029900	C	-6.72213900	2.21873500	0.45561300
N	-3.90206500	0.82994500	5.59255000	O	-7.12918200	3.38133900	0.80139100
H	-4.06262800	0.58749800	6.56333900	O	-5.47848100	1.98017900	0.46116400
C	-2.66681000	0.42750800	5.11634800	O	-6.08635600	-1.16228600	5.64865000
O	-2.32819500	0.93531000	3.89904600	O	-4.73381400	-0.84802700	3.87278400
O	-2.50027200	2.32472400	2.18599800	C	-6.94399600	3.49102900	5.03709800
O	-1.94018300	-0.33208100	5.70846300	C	-6.25520400	2.47014100	5.69211600

TS11

C	-3.51209400	5.52800000	1.69176200	C	-5.43007000	3.34591600	3.10943000
C	-4.76909700	6.17862400	1.40808900	C	-6.54169400	3.90288900	3.76732900
C	-5.05590000	5.98682600	-0.01707800	H	-7.81008600	3.94698900	5.51012600
C	-4.05848200	5.15975200	-0.56380800	H	-6.57450800	2.10657200	6.66469600
C	-3.11264800	4.83923200	0.50338500	H	-5.22581100	0.01170600	5.96816700
C	-1.84960300	4.06670200	0.28359500	H	-7.12468000	4.66692600	3.26282300
H	-2.04571400	3.12258400	-0.23245300	C	-3.47744100	1.73686500	3.22218500
H	-1.16460800	4.65823300	-0.34042700	N	-4.48195600	0.79916900	5.72773100
H	-1.34906800	3.82486400	1.22032500	H	-3.97515800	1.08864000	6.56960900
C	-2.73960200	5.59648600	2.97531800	C	-3.47881100	-0.05241800	4.90115300
H	-2.20855700	4.66050100	3.16410400	O	-2.86906300	0.71354200	3.91630100
H	-1.99863000	6.40640700	2.93392700	O	-2.89604300	2.14944600	2.24762300
H	-3.39616100	5.79009700	3.82779800	O	-2.83856300	-0.85096200	5.53566500
C	-5.51346000	7.11679200	2.31184000				
H	-5.40412400	6.83378900	3.36237300				

INT21

H	-5.14002700	8.14472900	2.20229700	C	-3.08140400	4.37962000	1.40650200
H	-6.58306300	7.13003000	2.07906200	C	-3.76868000	5.38928600	2.13843900
C	-6.26027700	6.54781200	-0.71059600	C	-4.63598600	6.07215500	1.19689900
H	-7.17787600	6.31471700	-0.15997800	C	-4.30546100	5.58371300	-0.15102700
H	-6.18567500	7.64070400	-0.78546800	C	-3.36864300	4.55195100	-0.02622400
H	-6.36875000	6.14793100	-1.72154100	C	-2.73897200	3.73951000	-1.11801200
C	-3.93747300	4.65684600	-1.97199400	H	-3.20806700	3.93852300	-2.08474600
H	-3.12684600	5.17157700	-2.50540400	H	-1.67042000	3.97869500	-1.20881100
H	-3.71246900	3.58548300	-1.98755300	H	-2.82298000	2.66585400	-0.92319000
H	-4.85937500	4.81154100	-2.53864700	C	-2.10131100	3.37766300	1.93939800
Rh	-5.09479700	4.04332300	1.20623600	H	-2.24658600	2.40074700	1.46857800
C	-5.71233200	-1.43356200	4.47986300	H	-1.07270000	3.69980800	1.72606200
C	-6.41528200	-2.51791400	3.69404000	H	-2.19519700	3.25198700	3.02109800
H	-7.40884900	-2.70338700	4.10694400	C	-3.61409000	5.71729300	3.59338300
H	-6.47701100	-2.24562100	2.63720200	H	-3.19282200	4.87737400	4.15222900
H	-5.82442300	-3.43889800	3.76489200	H	-2.94111600	6.57604600	3.71991400
C	-7.71825100	1.14652500	0.09292600	H	-4.57308300	5.96987600	4.05300900
H	-8.60697800	1.58781100	-0.36530200	C	-5.46907200	7.28844100	1.46449500
H	-8.02883700	0.62568700	1.00650600	H	-5.60508700	7.45256500	2.53697000
H	-7.26253500	0.41665600	-0.58012200	H	-4.97861300	8.18263500	1.05412000

H	-6.45131400	7.17721700	0.99770900	C	-2.14293100	3.67853500	0.09985000
C	-4.92238300	6.12630800	-1.40337400	H	-2.53053400	2.97047700	-0.63804800
H	-4.48818200	7.10704300	-1.64322200	H	-1.27142800	4.18357100	-0.34073600
H	-4.75342600	5.46680900	-2.25849000	H	-1.81311600	3.09878800	0.96100500
H	-5.99949700	6.25618000	-1.26945100	C	-2.77713500	4.81299900	3.04914000
Rh	-5.27790000	4.01160200	1.26779100	H	-2.47674700	3.76280200	3.02646900
C	-6.66170500	0.29377200	-1.32397000	H	-1.87463000	5.42029600	3.20264100
C	-7.96562400	-0.44644200	-1.42598400	H	-3.42786400	4.95842200	3.91556500
H	-8.21128200	-0.59975900	-2.47717200	C	-5.02769400	7.10083900	2.70714000
H	-7.89756300	-1.40652900	-0.90498900	H	-5.06756200	6.58272700	3.66917200
H	-8.75383600	0.13804400	-0.93972100	H	-4.39656900	7.99210000	2.83169800
C	-9.09792600	3.76876400	-0.85272000	H	-6.04007900	7.44479000	2.47276000
H	-9.59926200	3.04632800	-0.19853000	C	-5.69345400	7.38871900	-0.37564500
H	-8.74879700	3.22627500	-1.73846400	H	-6.68107900	7.27479800	0.08405600
H	-9.80809200	4.54198300	-1.15238700	H	-5.35469100	8.41593500	-0.18738400
C	-7.91206600	4.39723700	-0.11904000	H	-5.81357100	7.26577400	-1.45458700
O	-7.87008700	5.61088400	0.09297700	C	-3.84048900	5.26913200	-1.99685400
O	-7.01163700	3.51858200	0.22021100	H	-2.87207800	5.61468000	-2.38340900
O	-6.00301300	0.75138900	-2.20911700	H	-3.93747800	4.20966400	-2.25616800
O	-6.33172800	0.42431500	0.04101900	H	-4.62372700	5.81480000	-2.52964300
C	-7.79281900	4.46234300	4.77262400	Rh	-5.33455100	4.32655300	0.96931500
C	-7.93453100	3.17282000	5.25889200	C	-8.54639300	2.50437800	-0.73001300
C	-7.33487100	2.09073000	4.58566800	H	-8.25378300	1.78223500	-1.49545800
C	-6.57347600	2.37145100	3.40051800	H	-9.23225000	3.24676100	-1.14657200
C	-6.40150600	3.70909800	2.93699200	H	-9.07255400	1.96920600	0.06940700
C	-7.03471800	4.73907600	3.62343300	C	-7.32873700	3.17939300	-0.15010800
H	-8.28627400	5.27944200	5.29509300	O	-7.44025200	4.31995300	0.41772800
H	-8.51669600	2.97921100	6.15655100	O	-6.19307400	2.61957100	-0.18190600
H	-7.19874400	0.04970400	4.48618100	C	-7.49769400	3.50728100	4.57828800
H	-6.97982800	5.75777600	3.25784200	C	-7.08071600	2.26800400	5.05206200
C	-6.05189800	1.25714000	2.64658300	C	-6.09631900	1.57906100	4.34217500
N	-7.46505700	0.82235800	5.08286900	C	-5.51497000	2.12959900	3.17519500
H	-8.18217200	0.65722300	5.77351200	C	-5.94825200	3.38851200	2.68691900
C	-5.12695600	0.92046900	0.40866900	C	-6.94910600	4.05095400	3.41297600
O	-5.24927900	1.70039700	1.53793500	H	-8.27004200	4.05180700	5.11663800
O	-6.15809000	0.06112600	2.82353900	H	-7.51258300	1.83283400	5.94955600
O	-4.07542300	0.76638600	-0.13823600	H	-7.32917400	5.00108500	3.05223900
				C	-4.44993000	1.35742400	2.52174600
INT22				N	-5.67476100	0.32716600	4.78533600
C	-3.46059000	5.20856500	1.77419500	H	-6.10168600	-0.08314800	5.60512400
C	-4.48845100	6.21109300	1.62626500	C	-4.75350200	-0.47323300	4.15675200
C	-4.71833500	6.40131600	0.19040900	O	-4.17904900	0.08024000	3.04387600
C	-3.92960700	5.47451300	-0.51330100	O	-3.76005600	1.69350600	1.59178500
C	-3.17507400	4.69780500	0.46857900	O	-4.44276100	-1.57659700	4.53518500

INT23

				C	-7.84444000	3.26747300	3.70068500
				C	-8.39254800	2.30559100	3.11026700
C	-4.85204500	3.12863500	0.62269700	C	-7.67142300	4.30542000	4.68667600
C	-5.82984900	4.14397400	0.88964800	C	-7.39003000	3.96152800	6.02390200
C	-7.11405400	3.63605300	0.45175800	C	-7.85377300	5.66165000	4.35627800
C	-6.93801700	2.32658800	-0.07963900	C	-7.28074500	4.95426800	6.99419400
C	-5.53928700	2.00487500	0.04838500	H	-7.27447700	2.91455300	6.27954400
C	-4.86603400	0.77788000	-0.48375000	C	-7.74308500	6.64952000	5.33373400
H	-5.56504100	-0.05321400	-0.57016700	H	-8.10837400	5.93141000	3.33626400
H	-4.44213700	0.99413600	-1.47498500	C	-7.45060900	6.29933200	6.65355300
H	-4.04312300	0.46238000	0.16438100	H	-7.06685100	4.67640500	8.02264700
C	-3.36115000	3.25315900	0.73520900	H	-7.89290600	7.69191100	5.06564600
H	-2.89367100	2.27804100	0.89564000	H	-7.36416600	7.06967500	7.41500100
H	-2.94149800	3.67377100	-0.18945200	C	-9.62443200	1.58025900	2.86627600
H	-3.06110900	3.89885800	1.56307000	C	-10.80950800	2.14088800	3.39293600
C	-5.55768400	5.57488100	1.26442300	C	-9.69915000	0.37618200	2.15104100
H	-4.49259600	5.74452800	1.44233000	C	-12.03309300	1.50539800	3.21006400
H	-5.85780300	6.24362800	0.44683200	H	-10.75502100	3.07191000	3.94973100
H	-6.10041200	5.88936800	2.16142500	C	-10.93254100	-0.25362700	1.97508400
C	-8.39228400	4.41855600	0.43502700	H	-8.79729400	-0.06435500	1.74059000
H	-8.36173000	5.25834100	1.13357000	C	-12.09962600	0.30310100	2.49870300
H	-8.56527000	4.82886300	-0.56940200	H	-12.93533400	1.94747100	3.62460700
H	-9.25354600	3.79556500	0.69134900	H	-10.97427800	-1.18943000	1.42421400
C	-7.97209000	1.50806200	-0.79432700	H	-13.05572100	-0.19384800	2.35663800
H	-7.90201500	1.66924000	-1.87969300	C	-6.27900800	-0.79417900	2.04789900
H	-7.83417200	0.44694800	-0.58253400	C	-5.69244700	-2.06026300	2.67177900
H	-8.98363500	1.78361200	-0.48380500	H	-5.90987500	-2.92155800	2.03685300
Rh	-6.35381200	2.32288700	2.21723800	H	-4.61163800	-1.95844400	2.81111300
C	-3.24158100	3.80866000	4.87151800	H	-6.13213300	-2.21630800	3.66259600
C	-2.97097400	2.78242400	5.76530000	O	-7.03395900	-0.86748800	1.07155300
C	-3.82092500	1.67370900	5.77208800	O	-5.89307900	0.28468500	2.66028000
C	-4.93375400	1.59427700	4.90551300				
C	-5.12127700	2.57245200	3.89667400	TS12			
C	-4.28780900	3.69642900	3.94852900	C	-4.79754400	3.04843400	0.47675500
H	-2.61661900	4.69865600	4.86862100	C	-5.84031400	4.02092000	0.67105500
H	-2.13135800	2.83506700	6.45333900	C	-7.09298500	3.44137200	0.24357200
H	-4.44253200	4.51655000	3.26193400	C	-6.84326000	2.10631000	-0.17978300
C	-5.90188400	0.53248600	5.24989200	C	-5.41749900	1.85849600	-0.00365100
N	-3.58031500	0.61897300	6.65773600	C	-4.71309400	0.59817600	-0.40376800
H	-2.73530100	0.62864900	7.21321200	H	-5.38089400	-0.26178700	-0.33445900
C	-4.20144600	-0.60934700	6.59468200	H	-4.36168600	0.68137500	-1.44192200
O	-5.34544300	-0.62042400	5.84872100	H	-3.84227100	0.40637200	0.22917800
O	-7.10046700	0.56640000	5.17642700	C	-3.32829300	3.27073100	0.68546900
O	-3.81357200	-1.59592600	7.17254600	H	-2.78982200	2.32087100	0.74148600

H	-2.89464900	3.84795400	-0.14301700	C	-9.47792000	1.84010300	2.89568700
H	-3.12650800	3.81688100	1.61263500	C	-10.54297200	2.57616900	3.45671000
C	-5.63692000	5.47748900	0.97562700	C	-9.76650100	0.70962500	2.11287300
H	-4.65529800	5.67071100	1.41486600	C	-11.86166400	2.19129900	3.23201700
H	-5.69514600	6.06104700	0.04614200	H	-10.32653900	3.44814300	4.06678400
H	-6.40080500	5.87567000	1.65076800	C	-11.09226200	0.32860900	1.89962100
C	-8.40268300	4.16922200	0.16205600	H	-8.94813500	0.12747100	1.70003200
H	-8.48035000	4.94989800	0.92474600	C	-12.14166500	1.06571100	2.45089600
H	-8.51259400	4.65413400	-0.81789000	H	-12.67213800	2.76920400	3.66871900
H	-9.24826600	3.48987600	0.29497800	H	-11.30210000	-0.55406400	1.30121000
C	-7.80653900	1.20429300	-0.89170400	H	-13.17189100	0.76536200	2.27809200
H	-7.67899600	1.30342800	-1.97958400	C	-6.33764400	-0.83975300	2.19267400
H	-7.64988700	0.16376700	-0.60617800	C	-5.79750900	-2.09636600	2.87143100
H	-8.84236300	1.46185800	-0.65464500	H	-6.05326000	-2.97641900	2.27765600
Rh	-6.33792100	2.23377100	2.06296000	H	-4.71417100	-2.03478000	3.01060700
C	-3.47754800	4.07720100	4.68815400	H	-6.24719700	-2.18839000	3.86597600
C	-2.98866400	3.05412800	5.48985100	O	-7.15958000	-0.92759800	1.27424600
C	-3.72522600	1.86869700	5.58213700	O	-5.84668700	0.25765600	2.69035700
C	-4.94188900	1.69722200	4.88685000				
C	-5.36102400	2.69212600	3.96431100	INT24			
C	-4.64233300	3.89697800	3.94002100	C	-0.85882300	3.06979500	6.75759600
H	-2.93879200	5.01960400	4.62803700	C	-1.61184500	4.28255100	6.41678800
H	-2.06542700	3.16783900	6.05137300	C	-1.01351500	4.87611400	5.25777200
H	-4.99772700	4.71508400	3.32841700	C	-0.01740700	3.95772200	4.77849300
C	-5.73907000	0.52039000	5.29251400	C	0.10960100	2.87558200	5.76553500
N	-3.25418200	0.82880800	6.38457500	C	1.07753200	1.73987500	5.62692400
H	-2.34555200	0.91551900	6.81997600	H	0.92464800	1.21369700	4.67796800
C	-3.76604000	-0.45043400	6.38912400	H	2.11167000	2.10720000	5.64086300
O	-4.99539800	-0.56405200	5.80720200	H	0.96730900	1.01061300	6.43334400
O	-6.93416200	0.40474500	5.33096600	C	-1.16732700	2.20108600	7.94100000
O	-3.21331500	-1.39817600	6.89173900	H	-0.53288700	1.31132500	7.96523400
C	-7.44939600	3.02039700	3.95571800	H	-1.01352600	2.74711700	8.88099000
C	-8.11100000	2.27310500	3.14941800	H	-2.21017200	1.86440900	7.92009100
C	-7.57299900	4.01117200	5.02203900	C	-2.64154300	4.88830900	7.32101400
C	-7.61630800	3.59073200	6.36351700	H	-3.39051700	4.15031900	7.62376500
C	-7.71746000	5.37848100	4.72856600	H	-2.16256000	5.27102300	8.23345900
C	-7.80367200	4.52262100	7.38309200	H	-3.16417800	5.71910000	6.84474400
H	-7.51888400	2.53333600	6.58418700	C	-1.29768300	6.23492300	4.69315000
C	-7.89310400	6.30642100	5.75426800	H	-2.30618700	6.57610400	4.94146100
H	-7.70052900	5.70585600	3.69295600	H	-0.58882900	6.96770400	5.10299400
C	-7.93542400	5.88117000	7.08412700	H	-1.19665200	6.24623500	3.60522900
H	-7.84655400	4.18577800	8.41537300	C	0.94094300	4.18926300	3.64910000
H	-8.00468800	7.36054600	5.51444700	H	1.85180300	4.68459200	4.01580300
H	-8.07559600	6.60433500	7.88297000	H	1.24019200	3.24684800	3.18200700

H	0.50405800	4.81660600	2.86897100	H	-2.66574300	-1.50198200	3.84468300
Rh	-1.95555000	2.93067900	4.68566200	H	-3.94562300	-1.17888000	5.06120900
C	-6.13243100	5.06751000	6.02985400	C	-2.91092000	0.56774300	4.36240300
C	-7.03561000	4.06100500	6.34125300	O	-3.48716500	1.39029800	5.14381000
C	-7.04910400	2.90177200	5.55738200	O	-1.86225500	0.94787100	3.74267100
C	-6.18053400	2.75443000	4.45847300				
C	-5.25133400	3.78081400	4.15056000	INT25			
C	-5.25022300	4.92562300	4.95448200	C	-5.11814500	3.46170000	0.70499100
H	-6.11703500	5.97572900	6.62673900	C	-6.39514300	4.13175900	0.73540900
H	-7.72325900	4.16139100	7.17669100	C	-7.41181300	3.19282900	0.24797000
H	-4.55947600	5.72537500	4.71021900	C	-6.79482800	1.94308600	0.06924200
C	-6.24056300	1.50157500	3.69353400	C	-5.36908500	2.08531800	0.40252700
N	-7.93244400	1.87269600	5.86283200	C	-4.34607100	1.00480500	0.22592600
H	-8.55533300	1.96391100	6.65400900	H	-4.71331700	0.04214200	0.59350300
C	-8.00718100	0.66491000	5.20947300	H	-4.11018500	0.88033200	-0.83952400
O	-7.15334000	0.53319100	4.14891500	H	-3.41356700	1.23758200	0.74612200
O	-5.59494500	1.19906900	2.72387900	C	-3.77750600	4.10656700	0.87311700
O	-8.75875700	-0.22551600	5.52176800	H	-3.04546500	3.42695400	1.31470000
C	-4.35508300	3.76505600	2.94675300	H	-3.39925200	4.41358600	-0.11121500
C	-3.01698000	3.57543000	3.02106300	H	-3.82913300	5.00199300	1.49638500
C	-5.08408900	4.06534300	1.66436200	C	-6.60667000	5.60514700	0.90568000
C	-5.99231400	5.13553600	1.58845600	H	-5.90110400	6.03848500	1.61935500
C	-4.90287000	3.27177000	0.51881400	H	-6.46477300	6.11917100	-0.05491400
C	-6.67221400	5.42221100	0.40366600	H	-7.62057000	5.82677400	1.24818700
H	-6.16615600	5.75529900	2.46394200	C	-8.83442200	3.55468900	-0.04519300
C	-5.58235100	3.55627400	-0.66404300	H	-9.24341100	4.23893500	0.70328300
H	-4.23608700	2.41937500	0.56987400	H	-8.89402700	4.05996100	-1.01860000
C	-6.46815800	4.63460600	-0.72990700	H	-9.48135100	2.67632900	-0.08419300
H	-7.36245700	6.26171500	0.36912000	C	-7.42777300	0.67205100	-0.40692900
H	-5.42744900	2.92487000	-1.53526400	H	-7.22431900	0.52560000	-1.47612900
H	-6.99954200	4.85283000	-1.65269300	H	-7.02758600	-0.19646000	0.12430300
C	-2.12817400	3.80933000	1.85078600	H	-8.51099900	0.68195500	-0.26868700
C	-2.03951900	5.09743800	1.28398300	Rh	-6.43298600	2.55606200	2.28819500
C	-1.32915300	2.79135500	1.29273100	C	-3.33118800	3.64791800	5.25630200
C	-1.18802000	5.35964900	0.20955600	C	-3.13063100	2.42716700	5.90420900
H	-2.66795000	5.89001600	1.67976500	C	-3.90000900	1.33667400	5.49899600
C	-0.48975200	3.05294800	0.21004400	C	-4.82700900	1.50435500	4.45537700
H	-1.38252700	1.79448100	1.71570600	C	-5.03351000	2.73142900	3.78772400
C	-0.40760300	4.33757300	-0.33446900	C	-4.26710900	3.81197300	4.21987100
H	-1.14463500	6.36206700	-0.20970400	H	-2.74174400	4.50465100	5.57233300
H	0.10444300	2.24572600	-0.21200200	H	-2.40171500	2.33254000	6.70322500
H	0.25122500	4.53763000	-1.17544900	H	-4.38995500	4.79808400	3.78431100
C	-3.46058200	-0.81758300	4.15058000	C	-5.61491000	0.38697400	4.03860300
H	-4.21508700	-0.77200200	3.35765200	N	-3.81132000	0.07062500	6.06827700

H	-3.15958400	-0.10570800	6.82377500	C	-6.30669200	5.48394500	0.81428600
C	-4.55454400	-1.02848700	5.70020200	H	-5.61876200	5.85597900	1.57865600
O	-5.46765100	-0.80692300	4.64985000	H	-6.08586800	6.02511600	-0.11601500
O	-6.44487200	0.47248800	3.11668400	H	-7.32489800	5.74624800	1.11224300
O	-4.48145800	-2.11695400	6.19081700	C	-8.59732900	3.50716100	-0.23086000
C	-7.83152100	3.59130500	4.00689700	H	-8.96870100	4.27427400	0.45395400
C	-8.45703800	2.71254800	3.38603400	H	-8.65873100	3.91533500	-1.24834500
C	-7.42952000	4.55274200	4.99550900	H	-9.27590600	2.65353800	-0.16940400
C	-7.19434600	4.13335500	6.31998700	C	-7.23308600	0.60352700	-0.62486900
C	-7.33016200	5.92090700	4.67856300	H	-6.95929500	0.46830500	-1.67995400
C	-6.86908700	5.06622500	7.30097900	H	-6.90410200	-0.29006200	-0.08598900
H	-7.28039400	3.08029000	6.56818700	H	-8.32267100	0.65421600	-0.56970700
C	-7.00355700	6.84692100	5.66648700	Rh	-6.37150700	2.42177100	2.08831000
H	-7.52641200	6.25167100	3.66417700	C	-3.46182200	3.67026800	5.20582000
C	-6.77066900	6.42252500	6.97748000	C	-3.17604300	2.43921300	5.79866300
H	-6.69903200	4.73587600	8.32143700	C	-3.96660700	1.33842600	5.45362900
H	-6.93909100	7.90169800	5.41588100	C	-5.00302500	1.49610900	4.51888300
H	-6.52066800	7.14759500	7.74639800	C	-5.34827300	2.75825400	3.96350600
C	-9.63232800	1.98386400	2.96389400	C	-4.53704200	3.84275700	4.32462000
C	-10.84941500	2.68955900	2.86063500	H	-2.84394800	4.52745600	5.45852400
C	-9.60960600	0.60357100	2.69159000	H	-2.35627500	2.33648700	6.50293300
C	-12.01552500	2.02375300	2.49165400	H	-4.76890600	4.83955700	3.96312500
H	-10.87108500	3.75252500	3.08117100	C	-5.65501100	0.31803000	4.01738100
C	-10.78363100	-0.05178700	2.32389200	N	-3.76385600	0.06509300	5.97128900
H	-8.67861400	0.05657400	2.78322000	H	-3.05267500	-0.09228100	6.67551500
C	-11.98571000	0.65315900	2.22000000	C	-4.50932700	-1.05301000	5.66171100
H	-12.94850400	2.57499400	2.41990700	O	-5.45110400	-0.86764600	4.63709500
H	-10.76052400	-1.11933800	2.12523400	O	-6.37714000	0.33433700	3.01340500
H	-12.89699400	0.13604200	1.93437800	O	-4.39027700	-2.12951900	6.16846400
				C	-7.25458300	3.22630200	4.09459600
TS13				C	-8.03530500	2.56834600	3.29364100
C	-4.87629600	3.29926800	0.56566100	C	-7.36583200	4.32868400	5.05709800
C	-6.15196800	4.00958800	0.59333200	C	-6.92723200	4.18640400	6.38549400
C	-7.18273900	3.12001300	0.07944000	C	-8.00092600	5.52260500	4.66918800
C	-6.58878800	1.84408200	-0.08494700	C	-7.13435800	5.21035200	7.30595200
C	-5.14733800	1.96216500	0.21216000	H	-6.44223500	3.26586100	6.69470600
C	-4.16837400	0.83790400	0.05903600	C	-8.19279400	6.55107400	5.59175000
H	-4.55882000	-0.09299900	0.48192600	H	-8.34462500	5.63490300	3.64526500
H	-3.96678800	0.65279100	-1.00441700	C	-7.76174300	6.39612900	6.91079800
H	-3.21407000	1.05858100	0.54340000	H	-6.80966400	5.08372800	8.33451300
C	-3.54191100	3.91334700	0.85819700	H	-8.68167300	7.46972600	5.28093200
H	-2.78259600	3.15490400	1.06293900	H	-7.91633200	7.19463700	7.63042700
H	-3.20015100	4.50356200	-0.00202000	C	-9.41191600	2.14766700	3.10905600
H	-3.58394400	4.58546400	1.72035400	C	-10.45824400	2.84432400	3.74853000

C	-9.72223400	1.03044800	2.31200900	H	-2.29572300	1.77137600	6.84260400
C	-11.77835400	2.43612300	3.57671000	H	-4.90992900	4.74125300	5.17475600
H	-10.23046000	3.70247500	4.37256700	C	-5.48542200	0.30257000	3.93368800
C	-11.04494000	0.62313200	2.15215400	N	-3.59475000	-0.30678900	5.77204200
H	-8.91451900	0.47174200	1.85160700	H	-2.86215400	-0.57164400	6.41955000
C	-12.07612200	1.32781400	2.77844500	C	-4.29067000	-1.36346800	5.23468400
H	-12.57710300	2.98235300	4.06996300	O	-5.22812900	-0.98677800	4.27028400
H	-11.27133900	-0.24912600	1.54579900	O	-6.07940900	0.46295900	2.86028700
H	-13.10714800	1.01127500	2.65112700	O	-4.12395300	-2.52003400	5.49181400
				C	-6.82447800	3.15002000	4.21445100
INT26				C	-7.72537600	2.52014800	3.34622900
C	-4.89131500	3.33549400	0.38900100	C	-7.36067000	4.40003000	4.86796500
C	-6.19438500	4.00343900	0.38925600	C	-7.37841500	4.52479500	6.27070200
C	-7.18758900	3.08319100	-0.10913800	C	-7.92258800	5.42720000	4.09560500
C	-6.54720100	1.80926000	-0.22583600	C	-7.94713500	5.64370400	6.87526700
C	-5.11083100	1.99203700	0.04679400	H	-6.95406200	3.73840200	6.88808500
C	-4.09799300	0.89150600	-0.05347100	C	-8.48237800	6.55268500	4.70256600
H	-4.44331800	-0.01793100	0.44900900	H	-7.91800800	5.34107800	3.01420500
H	-3.91940400	0.63395800	-1.10553000	C	-8.49876700	6.66322100	6.09317100
H	-3.13890900	1.17908000	0.38417100	H	-7.96155100	5.71939500	7.95874300
C	-3.59201400	4.00377600	0.72616800	H	-8.90558800	7.34191900	4.08780800
H	-2.81027000	3.27694200	0.96037000	H	-8.93694400	7.53675700	6.56668200
H	-3.23842000	4.60925000	-0.11902200	C	-9.13636100	2.26361900	3.45100500
H	-3.69491000	4.67431200	1.58563100	C	-9.82144200	2.34183500	4.69139600
C	-6.38495500	5.47922500	0.57272200	C	-9.85384200	1.80058400	2.32354400
H	-5.80244500	5.86668800	1.41376500	C	-11.16450500	2.00409000	4.78028600
H	-6.04881900	6.01009700	-0.32857500	H	-9.29168400	2.67800200	5.57496000
H	-7.43476900	5.73729700	0.73218400	C	-11.19886800	1.46592800	2.41639500
C	-8.57561600	3.45268300	-0.54279800	H	-9.32272900	1.68533500	1.38718400
H	-9.07600200	4.10812400	0.17558000	C	-11.86009900	1.57200500	3.64418100
H	-8.53103700	3.98819900	-1.50065600	H	-11.67523700	2.07253900	5.73608000
H	-9.20563600	2.57342300	-0.69446300	H	-11.73265400	1.11026800	1.54018000
C	-7.15079400	0.53593400	-0.73332500	H	-12.91057100	1.30670000	3.72006700
H	-6.92132300	0.40537300	-1.79990900				
H	-6.75276200	-0.33428300	-0.20361700	INT27			
H	-8.23842100	0.52694400	-0.62569000	C	-5.39534000	3.80571200	0.51953000
Rh	-6.37572300	2.42368800	1.92260800	C	-6.74355000	4.28655500	0.60987400
C	-3.50420300	3.35682100	5.99657900	C	-7.64197900	3.22538800	0.15097000
C	-3.14860100	2.03050400	6.22337100	C	-6.86433700	2.07851800	-0.08676700
C	-3.90929700	1.03710500	5.60541000	C	-5.46246300	2.40773600	0.19996800
C	-5.00192200	1.36582200	4.77104700	C	-4.30109600	1.49145900	-0.04797000
C	-5.46684600	2.72211700	4.66293100	H	-4.54229000	0.46225200	0.23278900
C	-4.63729600	3.69702400	5.25722000	H	-4.02811300	1.49080300	-1.11235600
H	-2.90343000	4.14952800	6.43260400	H	-3.42156100	1.79650900	0.52481100

C	-4.14793800	4.62604400	0.63990300	H	-7.67946200	7.97327000	5.40406300
H	-3.33349400	4.06590300	1.10411600	H	-6.29880900	7.42725500	7.40003100
H	-3.81895800	4.93932100	-0.36059200	C	-9.55186600	1.93756600	3.14861600
H	-4.31141800	5.53110500	1.23026300	C	-10.79490300	2.60184300	3.19900300
C	-7.15527000	5.70788600	0.85604200	C	-9.52077000	0.55814300	2.87416600
H	-6.49168800	6.20461900	1.56898700	C	-11.97752100	1.89969900	2.97908100
H	-7.13120400	6.28275900	-0.08025200	H	-10.82093900	3.66467400	3.42118100
H	-8.17424500	5.76561100	1.24852100	C	-10.71134300	-0.13392600	2.65721700
C	-9.11925800	3.38579000	-0.04780100	H	-8.56521300	0.04797400	2.84408900
H	-9.58307700	3.93264900	0.77852900	C	-11.93975200	0.52996900	2.70552000
H	-9.32246000	3.94793000	-0.96943900	H	-12.92897400	2.42253100	3.02449800
H	-9.62542000	2.42094900	-0.12425800	H	-10.67737000	-1.20095700	2.45529400
C	-7.32769400	0.72143100	-0.52154400	H	-12.86310200	-0.01704700	2.53611000
H	-6.96875300	0.49667300	-1.53440900	C	-0.56582500	-0.05926600	7.69205400
H	-6.93853600	-0.05227800	0.14891300	C	0.42315200	-0.69429600	8.65002900
H	-8.41755700	0.64548600	-0.52403600	H	1.10826300	0.06365500	9.03243500
Rh	-6.47571700	2.64650600	2.14043800	H	-0.11223800	-1.16745700	9.48015400
C	-3.03637000	3.54687600	4.76304700	H	0.98561500	-1.48239200	8.13797200
C	-2.76565900	2.29575100	5.29246300	O	-0.56222700	1.13058700	7.41633500
C	-3.58005700	1.19733800	4.92097800	O	-1.41784400	-0.95545100	7.20478500
C	-4.63145700	1.46301300	4.00840100				
C	-4.90376800	2.73729300	3.46689900	TS14			
C	-4.10004900	3.79353000	3.85703700	C	-5.10550800	3.39656500	0.21403200
H	-2.40782300	4.38444900	5.05993400	C	-6.35081500	4.13204200	0.39781000
H	-1.94920000	2.13022200	5.98955100	C	-7.44903500	3.27247700	-0.00197200
H	-4.27235300	4.80691000	3.50856800	C	-6.90977000	1.98346200	-0.24718900
C	-5.46659300	0.38677200	3.60465800	C	-5.44414200	2.07047000	-0.12415800
N	-3.35947600	-0.05415500	5.41974900	C	-4.51786000	0.91801700	-0.37165200
H	-2.07787200	-0.53477700	6.56965200	H	-4.84186100	0.02911300	0.17965800
C	-4.11284900	-1.09565700	5.07852000	H	-4.50051400	0.65822300	-1.43850900
O	-5.26972800	-0.81567100	4.07023200	H	-3.49459900	1.14678100	-0.06447000
O	-6.41575800	0.59058700	2.77548600	C	-3.73466700	3.98022500	0.38060100
O	-4.08502400	-2.25146900	5.39720700	H	-2.95912600	3.21393700	0.30812300
C	-7.67985800	3.59446800	3.96632900	H	-3.53852400	4.72885300	-0.39825800
C	-8.35702100	2.70929500	3.40977800	H	-3.61986000	4.47136300	1.35274800
C	-7.26081600	4.62774300	4.87362200	C	-6.43990000	5.60653200	0.66197500
C	-6.47741900	4.32736900	6.00438500	H	-5.64514800	5.94016000	1.33519600
C	-7.68702200	5.95457100	4.66559500	H	-6.33655800	6.17184700	-0.27497400
C	-6.14028700	5.33346500	6.90666500	H	-7.39960700	5.88281900	1.10770300
H	-6.14066300	3.30954700	6.16544000	C	-8.88643300	3.68234500	-0.12347100
C	-7.34082100	6.95450300	5.57140300	H	-9.14440000	4.46859000	0.59169400
H	-8.29803200	6.18826800	3.79911600	H	-9.08848000	4.07179000	-1.13051100
C	-6.56697400	6.64668400	6.69350500	H	-9.56298700	2.84251500	0.05353600
H	-5.53791100	5.08955400	7.77685400	C	-7.64963300	0.75953900	-0.69875000

H	-7.59563100	0.65567600	-1.79139200	C	-0.41864200	0.50463000	7.57190300
H	-7.22071200	-0.14570100	-0.25919300	C	0.66021000	-0.00947100	8.50452400
H	-8.70536700	0.80001200	-0.41788200	H	1.31747400	0.80962800	8.79969500
Rh	-6.44864400	2.49996800	1.88863900	H	0.20272900	-0.46028500	9.39170900
C	-3.29820500	3.81919100	4.72187000	H	1.24055200	-0.79396700	8.00716400
C	-2.91410200	2.59920700	5.25251500	O	-0.50406600	1.67337600	7.22560700
C	-3.67953800	1.43430200	4.96688200	O	-1.24028500	-0.46761500	7.19153300
C	-4.80856300	1.59725100	4.12503700				
C	-5.22832100	2.85628300	3.62610100	INT28			
C	-4.45854300	3.97326300	3.92868700	C	-4.61808600	2.39300500	0.55722700
H	-2.70039000	4.69968900	4.94711200	C	-5.49476200	3.58010800	0.53877600
H	-2.03872700	2.49885400	5.88872400	C	-6.80050000	3.17652000	0.11690700
H	-4.77195100	4.96736800	3.62195900	C	-6.80056300	1.73229600	0.10448900
C	-5.45592500	0.41583200	3.64693100	C	-5.40791000	1.27332000	0.29131100
N	-3.31855400	0.22309300	5.46897300	C	-5.00247000	-0.16906800	0.27907700
H	-1.95852600	-0.12669500	6.57164900	H	-5.57790500	-0.74223400	1.01517900
C	-4.01621800	-0.88333300	5.18902200	H	-5.18628200	-0.61547700	-0.70650900
O	-5.13102100	-0.74939800	4.15904900	H	-3.94293600	-0.29486300	0.51390100
O	-6.30419700	0.46452200	2.70873700	C	-3.15399900	2.44394300	0.87521800
O	-3.90120300	-2.00814000	5.59346900	H	-2.72264800	1.44426700	0.96410600
C	-7.19752300	3.23125200	4.00915400	H	-2.60593700	2.97873000	0.08834500
C	-8.00914000	2.60871300	3.22957100	H	-2.96396500	2.97036700	1.81765400
C	-7.20306600	4.13989800	5.15492700	C	-4.99837400	4.98538100	0.70189800
C	-6.59361900	3.78922400	6.37272500	H	-4.27655800	5.05833100	1.52076100
C	-7.90133000	5.35708200	5.06424100	H	-4.49435900	5.32112400	-0.21516000
C	-6.70007400	4.63048200	7.47635800	H	-5.81537100	5.68102600	0.90970200
H	-6.04463700	2.85639500	6.44517900	C	-7.92879900	4.06288600	-0.30827400
C	-7.99451700	6.20201100	6.17062300	H	-7.81302700	5.07902600	0.07807700
H	-8.36137800	5.63654500	4.12071900	H	-7.95486000	4.12644600	-1.40490400
C	-7.39719100	5.83924900	7.37868700	H	-8.89752500	3.68554800	0.02819100
H	-6.23530400	4.34381600	8.41532700	C	-7.93992600	0.85187000	-0.30783000
H	-8.53466700	7.14121000	6.08772800	H	-7.95138800	0.72557600	-1.39999700
H	-7.47221100	6.49501600	8.24170600	H	-7.85381500	-0.14154300	0.14130100
C	-9.37938300	2.14182900	3.08318400	H	-8.90152400	1.27519300	-0.00553000
C	-10.46388400	2.99891800	3.34812400	Rh	-6.38893000	2.34094700	2.12683500
C	-9.63717100	0.81889400	2.67563800	C	-3.72724100	4.31941800	4.85259500
C	-11.77378900	2.54258800	3.20484700	C	-3.05389900	3.12396500	5.04132100
H	-10.27332100	4.01709400	3.67302700	C	-3.75369000	1.89181300	4.95752600
C	-10.94959300	0.36932500	2.54200400	C	-5.13083300	1.93019800	4.58547300
H	-8.79908200	0.15372800	2.49433000	C	-5.84661400	3.17387500	4.47861600
C	-12.02110400	1.22904700	2.79990200	C	-5.11104000	4.35617200	4.60841400
H	-12.60214800	3.21436000	3.41343200	H	-3.17944400	5.25427400	4.94305000
H	-11.13611100	-0.65786100	2.24047900	H	-1.99309000	3.09324100	5.27811600
H	-13.04276700	0.87565200	2.69094100	H	-5.63659100	5.30613300	4.58273700

C	-5.69571300	0.64556100	4.20101700	C	-5.46590200	2.00518100	-0.15421600
N	-3.09122300	0.73331400	5.23023900	C	-4.53129100	0.86284000	-0.42356000
H	-1.38108000	0.54734500	5.74461000	H	-4.83645000	-0.03432200	0.12653200
C	-3.72305300	-0.44079400	5.24752900	H	-4.52120900	0.60738400	-1.49220900
O	-5.12276400	-0.44847800	4.64161400	H	-3.50581200	1.09990600	-0.12877500
O	-6.64215200	0.54463300	3.37361700	C	-3.73910400	3.93804200	0.17524400
O	-3.37189100	-1.52926700	5.60941000	H	-2.97972900	3.17205200	0.35307400
C	-7.36909200	3.27083400	4.47216100	H	-3.51059100	4.41960600	-0.78562600
C	-7.93571300	2.99758700	3.28495400	H	-3.62943900	4.69261200	0.95846600
C	-8.01765500	3.63979200	5.76121200	C	-6.47611000	5.57004800	0.53409000
C	-7.35533300	3.37887100	6.97649200	H	-5.59339000	5.98829200	1.02784000
C	-9.29047400	4.23771400	5.82367700	H	-6.57797500	6.07831500	-0.43590800
C	-7.94797000	3.68236600	8.20095000	H	-7.35004100	5.83313200	1.13783900
H	-6.36959300	2.92445300	6.96689700	C	-8.89504700	3.60160800	-0.03652100
C	-9.87913200	4.54461700	7.04904300	H	-9.17707100	4.21014400	0.82812400
H	-9.82231100	4.47055900	4.90962100	H	-9.08738000	4.20185800	-0.93663100
C	-9.21411700	4.26798100	8.24518800	H	-9.56384800	2.73692000	-0.06775400
H	-7.41549200	3.46020300	9.12191300	C	-7.65701500	0.66313900	-0.63523800
H	-10.86183200	5.00904500	7.06664200	H	-7.50824300	0.41414100	-1.69495800
H	-9.67481900	4.51001900	9.19906100	H	-7.30696200	-0.19152300	-0.04597000
C	-9.33719300	2.91061700	2.86102600	H	-8.73313700	0.76373600	-0.46847200
C	-10.04348100	4.03155000	2.38317400	Rh	-6.26511900	2.50571300	1.92353000
C	-9.99996100	1.66701200	2.89332500	C	-3.30484400	4.27583400	4.58790500
C	-11.37155700	3.91743900	1.96821000	C	-2.87594300	3.16229100	5.30460600
H	-9.54658900	4.99792600	2.35607000	C	-3.45296200	1.90600100	5.07037800
C	-11.32688200	1.55800100	2.47861000	C	-4.47408600	1.78763600	4.09263200
H	-9.46238500	0.79626300	3.25676000	C	-4.88938300	2.91784000	3.35245600
C	-12.01843400	2.68049400	2.01376600	C	-4.30422900	4.16088200	3.61632200
H	-11.90186000	4.79751300	1.61340800	H	-2.85500700	5.24554300	4.79029300
H	-11.82498400	0.59299500	2.52411900	H	-2.09822200	3.24098100	6.05705800
H	-13.05285600	2.59233300	1.69328600	H	-4.62276400	5.04751100	3.07365000
C	0.36736600	1.34089800	6.01386200	C	-5.18830800	0.51617900	3.81988500
C	1.76682600	0.96669600	6.45795600	N	-2.96465100	0.85797300	5.84290100
H	2.42036800	1.83812800	6.39978700	C	-3.11674700	-0.34075100	6.00316300
H	1.74106100	0.58865100	7.48572000	O	-4.94469100	-0.55890600	4.35809000
H	2.15767200	0.16092700	5.82775600	O	-6.19934400	0.62919100	2.94140100
O	0.04921700	2.47245900	5.67894700	O	-3.06162200	-1.46200200	6.35285300
O	-0.45226200	0.29510500	6.03991400	C	-7.80126200	1.46962600	3.94681200
				C	-7.75307000	2.63471100	3.40682000
TS15				C	-8.20553600	0.38436100	4.77376900
C	-5.12067900	3.35468600	0.14608700	C	-9.17712400	-0.53321200	4.31781400
C	-6.35150000	4.08400600	0.35360000	C	-7.66227000	0.23223700	6.06774800
C	-7.45383200	3.18851000	0.01700600	C	-9.60234700	-1.56690100	5.14359400
C	-6.91778200	1.91634200	-0.26545600	H	-9.57921800	-0.42093800	3.31586900

C	-8.09456000	-0.80519500	6.88754200	Rh	-6.21742500	2.46849600	1.79640600
H	-6.90959100	0.93361200	6.41154600	C	-3.24076400	4.01921400	4.58775700
C	-9.06134100	-1.70307600	6.42704500	C	-2.85457600	2.87189100	5.27549300
H	-10.35043500	-2.27089700	4.79073900	C	-3.47014300	1.64642400	4.99596000
H	-7.67304600	-0.92006200	7.88155500	C	-4.50398200	1.60059800	4.01878900
H	-9.39276500	-2.51504400	7.06863300	C	-4.87272700	2.76395600	3.29270300
C	-8.63504500	3.78824500	3.67036500	C	-4.23255500	3.96869100	3.60407400
C	-8.08598200	5.05348900	3.94049000	H	-2.76053400	4.96638400	4.82331600
C	-10.03401100	3.64705900	3.65694200	H	-2.08080800	2.90100500	6.03491700
C	-8.91605000	6.14209800	4.20657600	H	-4.51194500	4.88261800	3.08804400
H	-7.00675000	5.16449900	3.95570700	C	-5.20696600	0.34881300	3.71296700
C	-10.86010700	4.74317600	3.90767300	N	-3.02688500	0.55607100	5.72968600
H	-10.46825800	2.67403000	3.44566900	C	-3.11754900	-0.64887100	5.83904000
C	-10.30544300	5.99389600	4.18632300	O	-4.86225700	-0.78525800	3.93861600
H	-8.47517900	7.11087300	4.42688800	O	-6.43608800	0.54648400	3.01289800
H	-11.93947200	4.61647600	3.89000500	O	-3.05919600	-1.79164200	6.10758600
H	-10.94972300	6.84593900	4.38504900	C	-7.47070300	1.24642000	3.78991600
				C	-7.61629100	2.48219000	3.29634900
INT29				C	-8.07937000	0.45704700	4.86692000
C	-5.03739000	3.38683700	0.01903300	C	-8.05068300	-0.94984900	4.83446000
C	-6.21983900	4.14566100	0.42242500	C	-8.70539400	1.09348000	5.95688600
C	-7.39516100	3.37659700	0.01648500	C	-8.64027000	-1.69337400	5.85583700
C	-6.94584800	2.12237400	-0.43123400	H	-7.55222000	-1.45357500	4.01415000
C	-5.47880200	2.12752900	-0.42654100	C	-9.29915100	0.34367300	6.96841000
C	-4.63764100	0.97966500	-0.90447100	H	-8.71611600	2.17660400	6.01071500
H	-4.99102200	0.02654400	-0.49601800	C	-9.27124400	-1.05318200	6.92369100
H	-4.67501800	0.89568300	-1.99949800	H	-8.60358100	-2.77874800	5.81520400
H	-3.58945000	1.09555400	-0.61656600	H	-9.77442500	0.85298400	7.80274800
C	-3.62661200	3.89307800	0.06849400	H	-9.72933700	-1.63550900	7.71861600
H	-2.90289300	3.07950200	-0.02985100	C	-8.59327500	3.51305600	3.65397200
H	-3.44351300	4.60286900	-0.74993000	C	-8.16962200	4.79134900	4.06836200
H	-3.41149600	4.41033100	1.00838700	C	-9.97794400	3.27189200	3.55297200
C	-6.24131500	5.60507600	0.77392000	C	-9.09707500	5.78321800	4.38676300
H	-5.30630400	5.92029500	1.24616000	H	-7.10504900	4.98923700	4.15279700
H	-6.37352700	6.22077100	-0.12770800	C	-10.90201700	4.26914800	3.86384200
H	-7.06131100	5.83984000	1.45924800	H	-10.32055900	2.29261100	3.23115800
C	-8.80591900	3.88147300	0.06546400	C	-10.46733100	5.52896800	4.28300900
H	-8.99809300	4.46292100	0.97121600	H	-8.74828900	6.75855100	4.71696500
H	-9.00754600	4.53345400	-0.79612200	H	-11.96546600	4.06041000	3.77859100
H	-9.53138400	3.06381600	0.03843700	H	-11.18849300	6.30483900	4.52523700
C	-7.77965400	0.97206200	-0.91636000				
H	-7.74371200	0.89435400	-2.01192800	INT30			
H	-7.42175500	0.01904200	-0.51215400	C	-3.48140100	4.14035000	5.32091300
H	-8.82803600	1.08213600	-0.62650600	C	-2.50489400	3.22613600	4.93451700

C	-2.86563500	1.97036900	4.43468800	C	-4.28368400	-4.59343100	4.31363500
C	-4.24595700	1.63298000	4.33425800	H	-4.13390100	-5.01044100	3.31360100
C	-5.23680100	2.56630300	4.75160400	H	-4.19143100	-5.41782200	5.03448100
C	-4.83027200	3.82445300	5.23243400	H	-5.30830000	-4.21314600	4.36579000
H	-3.18180400	5.11515100	5.69584900	C	-4.64255100	-2.42824900	6.56142600
H	-1.44947500	3.46511300	5.00385000	H	-5.50095700	-2.15882700	5.93190000
H	-5.57660400	4.54888000	5.53309500	H	-4.87896300	-3.36936700	7.07350700
C	-4.66537000	0.35082400	3.78004800	H	-4.52502100	-1.65271300	7.32285400
N	-1.81208900	1.14967600	4.07546000	C	-1.92740000	-0.61791600	6.62655400
C	-1.57410100	0.04875400	3.61011800	H	-2.78800300	-0.32512900	7.23357800
O	-3.95052100	-0.53161600	3.34747800	H	-1.10677400	-0.87657500	7.30946800
O	-6.02211800	0.11166900	3.73916600	H	-1.61066600	0.25966300	6.05181400
O	-1.09303500	-0.93563900	3.19356900	C	0.03595400	-1.72143000	4.44515600
C	-6.65201900	2.21286000	4.65344100	H	0.00878600	-0.62960300	4.36164500
C	-6.99057700	0.98811500	4.16158000	H	0.71615100	-1.97260700	5.27073300
C	-7.68622800	3.22134800	5.03944200	H	0.47220200	-2.11470300	3.52296800
C	-7.88667500	3.56802100	6.38553700	C	-1.34792200	-4.28069700	3.01700800
C	-8.45902300	3.85905600	4.05850100	H	-0.91490300	-5.17714300	3.48197500
C	-8.84506500	4.51784400	6.74106600	H	-2.09866700	-4.61589800	2.29556500
H	-7.29164300	3.08306700	7.15525000	H	-0.55294700	-3.77868500	2.45864500
C	-9.41786900	4.80843700	4.41385800	Rh	-3.25824000	-1.54197800	3.61951300
H	-8.30807800	3.60229300	3.01386200	C	-7.66178400	1.61659100	2.93584300
C	-9.61461700	5.13964700	5.75541900	C	-7.07716100	0.40456100	3.20294500
H	-8.99165100	4.76987300	7.78798000	C	-5.64905600	0.22079800	3.19630100
H	-10.01011400	5.29044200	3.64071200	C	-4.86014800	1.42376500	2.94458400
H	-10.36143200	5.87897600	6.03169300	C	-5.50947600	2.68944200	2.67722700
C	-8.33108500	0.39062400	3.96872100	C	-6.89498100	2.76590100	2.65823300
C	-8.53429700	-0.48866400	2.88892900	H	-8.74699200	1.69340400	2.93051000
C	-9.39891400	0.63300100	4.84959900	H	-7.67503600	-0.47828100	3.40391400
C	-9.77663600	-1.08255700	2.68165000	H	-7.38803500	3.70289100	2.43499400
H	-7.71138100	-0.70451300	2.21658300	C	-3.44311400	1.40105400	2.98264000
C	-10.63742000	0.02979700	4.64164800	N	-5.26858000	-1.04451100	3.42942900
H	-9.25910900	1.27973500	5.70701200	O	-2.66571600	0.44000600	3.21668900
C	-10.83450300	-0.82425300	3.55528700	O	-2.74494500	2.54966200	2.76190100
H	-9.91609800	-1.75212900	1.83743300	C	-4.68581100	3.87017800	2.41526600
H	-11.44872400	0.22338100	5.33799000	C	-3.33208700	3.76291400	2.47333400
H	-11.80253000	-1.29134400	3.39560000	C	-5.34821500	5.15640100	2.03864000
				C	-6.05691800	5.90716100	2.99065100
				C	-5.28901500	5.62711000	0.71923700
TS16				C	-6.67683800	7.10571700	2.63417600
C	-3.41200900	-2.57149200	5.71938000	C	-6.11627700	5.54750700	4.01444500
C	-2.25347700	-1.76840000	5.71990400	H	-5.90935400	6.82536900	0.36218900
C	-1.33511400	-2.27818600	4.69112000	C	-4.74937300	5.04989100	-0.02609700
C	-1.94660600	-3.38054200	4.05872300	H	-6.60317400	7.56916900	1.31842100
C	-3.29396900	-3.50427300	4.61326000	C			

H	-7.21657700	7.67733300	3.38467700	C	-7.61122500	1.79568400	3.53473700
H	-5.85132100	7.17630600	-0.66473500	C	-7.04908500	0.58001200	3.78969100
H	-7.08584600	8.50224900	1.04032300	C	-5.63017000	0.32046000	3.56821600
C	-2.28540900	4.78495100	2.24840600	C	-4.84224100	1.49432600	3.15366700
C	-2.45079900	6.13109900	2.61846200	C	-5.48481700	2.77425900	2.91344200
C	-1.06054600	4.39221800	1.67622400	C	-6.84926100	2.90453700	3.07681300
C	-1.43065900	7.05580100	2.40224100	H	-8.68183500	1.92423500	3.68205800
H	-3.37232000	6.45415200	3.08677300	H	-7.64607600	-0.26111400	4.12700300
C	-0.04615800	5.32160200	1.45761400	H	-7.34177300	3.84596700	2.87154700
H	-0.91100100	3.35332800	1.40331600	C	-3.45052100	1.41520900	3.04329400
C	-0.22671500	6.65871300	1.81716600	N	-5.25951400	-0.91669200	3.77461700
H	-1.57698900	8.09038000	2.70078600	O	-2.68041300	0.42131500	3.23807200
H	0.88819500	4.99875000	1.00618100	O	-2.72159000	2.51907700	2.70662300
H	0.56566100	7.38316400	1.64906000	C	-4.64674200	3.90083600	2.49685800
C	-4.16548100	-1.77979000	1.95969400	C	-3.29914400	3.73988100	2.42229200
O	-4.59999000	-2.03016900	0.91408500	C	-5.29602200	5.19480300	2.12493200
				C	-5.87573800	6.01714400	3.10476800
INT31				C	-5.35460400	5.60310500	0.78487900
C	-3.62481300	-2.76616300	5.53178600	C	-6.48296600	7.22383400	2.75385300
C	-2.60169800	-1.79296300	5.70369900	H	-5.84431400	5.70599300	4.14542900
C	-1.46518200	-2.16125600	4.85179500	C	-5.96257900	6.80932200	0.43319400
C	-1.83577300	-3.28158600	4.08978900	H	-4.91538900	4.97069800	0.01866100
C	-3.22977800	-3.60456900	4.43210300	C	-6.52650400	7.62439400	1.41630900
C	-3.99160200	-4.80432300	3.94462600	H	-6.92135500	7.85110000	3.52576200
H	-3.70877900	-5.07564500	2.92331400	H	-5.99619100	7.11095000	-0.61043900
H	-3.79500600	-5.67684000	4.58341000	H	-6.99929900	8.56387600	1.14255800
H	-5.06867700	-4.61682500	3.95439600	C	-2.24842700	4.71085500	2.04143300
C	-4.95946800	-2.79074400	6.19888400	C	-2.32144000	6.07453800	2.37503500
H	-5.67089400	-2.21665600	5.57902600	C	-1.11035000	4.25021100	1.35262700
H	-5.33270800	-3.81407500	6.30775600	C	-1.29958700	6.94956200	2.01058300
H	-4.91952500	-2.33444000	7.19216300	H	-3.17208200	6.45026200	2.93032200
C	-2.58525100	-0.66864600	6.69742300	C	-0.09389800	5.12962400	0.98631800
H	-3.59765000	-0.39801000	7.00788100	H	-1.03051000	3.19700300	1.10634300
H	-2.01591600	-0.94469900	7.59597900	C	-0.18419100	6.48469000	1.31105100
H	-2.11754600	0.22458700	6.27139300	H	-1.37401900	7.99897800	2.28308400
C	-0.16999000	-1.40741500	4.81813700	H	0.77142200	4.75381400	0.44663900
H	-0.34413400	-0.34889500	4.59177000	H	0.60974800	7.17054800	1.02766100
H	0.33932800	-1.46052300	5.78916900	C	-3.70677000	-1.84753200	1.69972800
H	0.51064100	-1.80474500	4.06065100	O	-3.94173400	-2.05852500	0.59500700
C	-0.97961700	-4.05965700	3.13251200				
H	-0.52910400	-4.92714500	3.63436300	TS17			
H	-1.55969300	-4.44225900	2.28723500	C	-3.67169700	-2.51215000	5.84086400
H	-0.16624200	-3.45047600	2.72905400	C	-2.57217200	-1.65530200	5.97643300
Rh	-3.32836900	-1.54447900	3.53796500	C	-1.46468000	-2.21758000	5.21992200

C	-1.88884200	-3.48453000	4.67598700	H	-1.67456500	0.21632500	1.07143200
C	-3.28888200	-3.59514800	4.93557400	H	-0.33432100	-0.01333400	-0.08840200
C	-4.19241900	-4.73537200	4.57749900				
H	-3.76668800	-5.36191900	3.79004200	INT32			
H	-4.36902100	-5.37173300	5.45557400	C	-3.60165000	-2.81202800	5.87650400
H	-5.16644600	-4.36854500	4.23745400	C	-2.49039800	-1.92315400	6.09385800
C	-5.07219500	-2.25072200	6.21386500	C	-1.39607700	-2.33713300	5.21060300
H	-5.56388900	-1.89530400	5.27700900	C	-1.87396000	-3.38570000	4.40473600
H	-5.60526100	-3.15289600	6.53224500	C	-3.26161000	-3.66266900	4.77940000
H	-5.17999300	-1.47795700	6.97835300	C	-4.09358100	-4.78287300	4.23519500
C	-2.49932500	-0.36199200	6.72367400	H	-4.06248900	-4.78601200	3.14372300
H	-3.45246800	-0.10989700	7.19464900	H	-3.72322600	-5.74952100	4.60554300
H	-1.73421000	-0.41159700	7.50914900	H	-5.13802200	-4.68220000	4.54224300
H	-2.22066700	0.46272900	6.05643300	C	-4.91629700	-2.80337400	6.59817300
C	-0.06904200	-1.68705200	5.21057600	H	-5.69404000	-2.33907400	5.97813100
H	-0.06057200	-0.59998400	5.32581700	H	-5.23332200	-3.82356100	6.83861100
H	0.50205900	-2.12043600	6.04537100	H	-4.85318200	-2.24258500	7.53471400
H	0.43772600	-1.93583400	4.27514300	C	-2.36030000	-0.86553400	7.14852600
C	-0.99314900	-4.49840000	4.04407300	H	-3.32967400	-0.60648000	7.58195700
H	-0.31611600	-4.91758900	4.80097800	H	-1.70529400	-1.20991800	7.96028100
H	-1.55843700	-5.32445400	3.60437100	H	-1.92535100	0.04606100	6.72741300
H	-0.38725300	-4.02625400	3.26532400	C	-0.05741500	-1.66366500	5.16898000
Rh	-2.89109400	-1.77082900	3.39422300	H	-0.17149800	-0.60408200	4.90858600
C	-7.41507800	1.14909000	2.83732800	H	0.44104500	-1.72029300	6.14495800
C	-6.74471700	-0.05456700	2.94906300	H	0.60114600	-2.12451500	4.42862100
C	-5.33674500	-0.10877000	3.21007000	C	-1.13387800	-4.13164300	3.33636700
C	-4.63275800	1.13371200	3.30701900	H	-0.23758100	-3.59568900	3.01439600
C	-5.33493800	2.33510800	3.16865500	H	-0.82107400	-5.11624700	3.71075700
C	-6.70862900	2.35791500	2.94134400	H	-1.77420800	-4.29157500	2.46488000
H	-8.48592300	1.15592100	2.65201000	Rh	-3.23839900	-1.45226700	4.06272100
H	-7.26838100	-1.00131300	2.85995300	C	-7.07561100	1.50648700	2.16342500
H	-7.22773600	3.30667600	2.84151600	C	-6.66157500	0.50982700	3.02626300
C	-3.15773600	1.24623100	3.54074000	C	-5.27298000	0.32799100	3.32867100
N	-4.85694700	-1.36578100	3.40320700	C	-4.31829400	1.27828600	2.81700400
O	-2.38322800	0.21286500	3.28209700	C	-4.77710500	2.29701300	1.98768000
O	-2.66931300	2.30608700	3.92264500	C	-6.12589000	2.39721400	1.63661000
C	-3.68718400	-2.34591800	1.75074300	H	-8.12512300	1.60843700	1.90356600
O	-4.08882600	-2.71843500	0.74415300	H	-7.35850900	-0.20043700	3.45901400
H	-4.76613300	3.25467400	3.25870400	H	-6.44637600	3.19117500	0.96720000
C	-0.33078200	-1.39892400	1.54396600	C	-2.86664400	1.35938100	3.26478200
O	0.88787800	-1.50394300	1.54822100	N	-4.99025800	-0.77529700	4.04633500
O	-1.03814600	-2.13785600	2.39232900	O	-2.40719900	0.42438200	4.05350000
C	-1.06287600	-0.52074600	0.54637900	O	-2.20747300	2.34100100	2.94115300
H	-1.72258000	-1.12994900	-0.08319300	H	-4.04748400	3.01984600	1.63806000

C	-3.39731500	-2.16489100	1.17122100	C	-2.88366700	1.30882700	3.84045600
O	-3.85587800	-3.26845600	1.45676000	N	-5.07382000	-0.78369000	3.81817600
O	-3.00235900	-1.24846700	2.02125900	H	-5.78435300	-1.04783600	4.57713400
C	-3.21517600	-1.71743700	-0.27663400	O	-2.49506000	0.16703100	4.38961000
H	-3.76808100	-0.78936200	-0.45458800	O	-2.18280400	2.30028100	4.00260300
H	-2.15858200	-1.50636000	-0.47278000	C	-8.79625700	-1.82775500	6.29305300
H	-3.56915200	-2.49805800	-0.95279100	H	-8.76304700	-1.01501400	7.02714300
				H	-8.50135400	-2.74504700	6.81674500
TS18				H	-9.81276800	-1.93841700	5.91036300
C	-3.62747900	-3.43582900	5.39382200	C	-7.82680600	-1.53487200	5.14993800
C	-3.08349000	-2.32922700	6.12743800	O	-8.21835400	-1.47544100	3.98350400
C	-1.68762900	-2.18674200	5.73429100	O	-6.58487600	-1.36572700	5.53272700
C	-1.42011400	-3.10490000	4.67325900	C	-4.72854500	-2.29181300	2.88892300
C	-2.61360500	-3.88235600	4.44655800	O	-5.30906600	-2.98479900	2.16047600
C	-2.71655600	-5.06624200	3.53971700	H	-3.62729800	3.34699900	2.40881500
H	-2.26532300	-4.83848500	2.57263100	C	-2.10041600	-1.86667600	1.15739600
H	-2.19139900	-5.91914500	3.99153900	O	-1.83081400	-3.05289400	1.33192000
H	-3.75564200	-5.35960600	3.37575100	O	-2.68903800	-1.07176400	2.01600100
C	-4.95334500	-4.07888400	5.64983700	C	-1.75693700	-1.15994000	-0.15021900
H	-5.72016000	-3.32135700	5.84457100	H	-2.06052000	-0.11236600	-0.14500600
H	-5.27502400	-4.70118700	4.81144600	H	-0.67703100	-1.23244900	-0.31534100
H	-4.86799200	-4.72508400	6.53437400	H	-2.25280300	-1.68664700	-0.97210300
C	-3.76464000	-1.56085200	7.21765400				
H	-4.84317700	-1.50201200	7.04254600	INT33			
H	-3.58976400	-2.04671000	8.18782500	C	-3.54985300	-2.73720200	6.13334900
H	-3.37121600	-0.54227900	7.27271400	C	-2.44464200	-1.88152300	6.48723000
C	-0.75785700	-1.16986800	6.28301100	C	-1.30863000	-2.22761800	5.64104100
H	-0.97537100	-0.20701000	5.78537200	C	-1.74691300	-3.21213200	4.72926700
H	-0.91399400	-1.03110300	7.35730800	C	-3.14973400	-3.51575000	5.00256600
H	0.28739700	-1.43046800	6.10201500	C	-3.93771600	-4.58979700	4.31777800
C	-0.10567200	-3.30167100	3.98314600	H	-3.79983900	-4.52548500	3.23612100
H	0.44887500	-4.12146800	4.46072300	H	-3.60966000	-5.58215300	4.65881700
H	-0.25894400	-3.54702000	2.93095500	H	-5.00530800	-4.49000900	4.52156800
H	0.51156100	-2.40148200	4.03889900	C	-4.85296700	-2.82646800	6.86867100
Rh	-3.20744300	-1.72456100	3.95593700	H	-5.10745500	-1.87815300	7.35046700
C	-6.57800500	1.81263900	1.67475900	H	-5.67504600	-3.09732000	6.20426100
C	-6.37535900	0.61457000	2.35624800	H	-4.78412500	-3.58948300	7.65607700
C	-5.17616600	0.40401400	3.05778900	C	-2.37683200	-0.90745300	7.62363300
C	-4.17563100	1.39879400	3.07726600	H	-3.37007500	-0.66188600	8.00767200
C	-4.40253700	2.58916100	2.37729200	H	-1.78950600	-1.32767400	8.45142100
C	-5.58832100	2.79844800	1.67565700	H	-1.89576800	0.02203500	7.30417100
H	-7.51123800	1.97202300	1.14156800	C	0.03731400	-1.57407100	5.73479300
H	-7.14198500	-0.15244600	2.40998800	H	-0.05587600	-0.48925800	5.60536600
H	-5.74153300	3.72987600	1.13784700	H	0.49540000	-1.76121600	6.71443100

H	0.72048900	-1.94838700	4.96848800
C	-0.93654200	-3.87751500	3.65973400
H	-0.61331900	-4.87114000	3.99985600
H	-1.52721600	-4.00649000	2.75005600
H	-0.04200200	-3.30041900	3.41293000
Rh	-3.02864300	-1.25113300	4.43469600
C	-6.41027100	2.01809100	2.10733500
C	-6.19157800	0.91144200	2.90574600
C	-4.88917400	0.64069300	3.45187300
C	-3.83744300	1.61418300	3.24626100
C	-4.10702000	2.72708800	2.45935100
C	-5.36158500	2.91955800	1.87192900
H	-7.39027500	2.18895200	1.67186600
H	-6.98749300	0.19786900	3.10133700
H	-5.52999900	3.79405300	1.24862000
C	-2.49917400	1.61472700	3.96504500
N	-4.75856900	-0.54242500	4.07686000
H	-6.15459900	-1.79076100	4.13049300
O	-2.21104600	0.60214800	4.73694600
O	-1.77552200	2.59946900	3.86645100
C	-8.79657100	-3.68461200	3.86704600
H	-8.77996600	-4.09249300	4.88321500
H	-8.36489400	-4.44188500	3.20375500
H	-9.82355200	-3.47315000	3.56776700
C	-7.97493300	-2.41758700	3.79809800
O	-8.40621800	-1.34280300	3.42307400
O	-6.71102500	-2.62208400	4.19633000
H	-3.31158000	3.45493000	2.34015800
C	-2.78819100	-1.73431000	1.52411500
O	-3.39296500	-2.79416300	1.66493100
O	-2.43478900	-0.91410400	2.48680200
C	-2.35243700	-1.22365800	0.15378400
H	-2.83243200	-0.26126300	-0.05290500
H	-1.27079000	-1.05471500	0.13947200
H	-2.62824500	-1.94735600	-0.61554500