

Electronic Supporting Information

Cross-linking of aromatic phenolate groups by cytochrome P450 enzymes: A model for the biosynthesis of vancomycin by OxyB

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Methods:

Model set-up:

Our model set-up follows previously reported methods and will be briefly summarised here.¹ We started our work from the 1LG9 protein databank (pdb) file, which is a P450 monomer of the resting state structure of OxyB. The docking of the prepared substrate with the OxyB was carried out using AutoDock Vina 4.0v.² The UCSF Chimera software³ was used for visualizing the various docking poses and we selected the most stable substrate-bound structure. Subsequently, hydrogen atoms were added in Chimera. The model was based on the active site of the 1LG9 pdb structure with residues selected as highlighted in Scheme S1 below. We took the heme and replaced all side chains by hydrogen atoms except propionate group A, which was included in the model. The axial cysteinate (Cys₃₄₇) was abbreviated to methylmercaptate and the resting state iron(III)-(water)heme replaced by iron(IV)-oxo heme cation radical or Compound I. The substrate binding pocket was described through the chains Leu₂₃₅-Ala₂₃₆-Gly₂₃₇-Asp₂₃₈-Asp₂₃₉-Asn₂₄₀-Ile₂₄₁ with Asp₂₃₈ abbreviated to Gly. In addition, the following groups were part of the model: namely, dimethylsulfide for Met₅₅ and the small chain Gln₂₃₂-Val₂₃₃ and Pro₂₈₆. The complete model had a total number of atoms of 258 and was calculated in the doublet and quartet spin states.

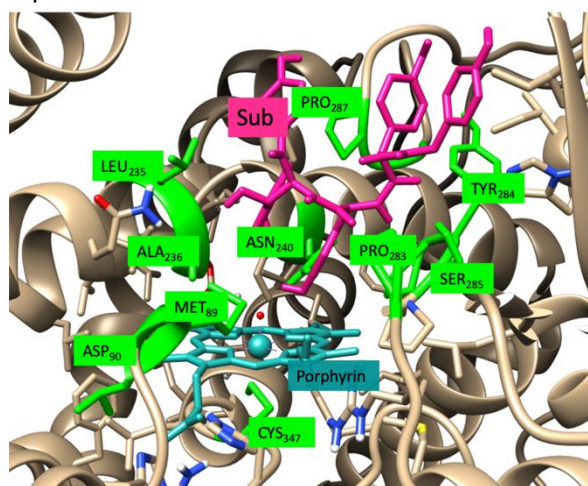


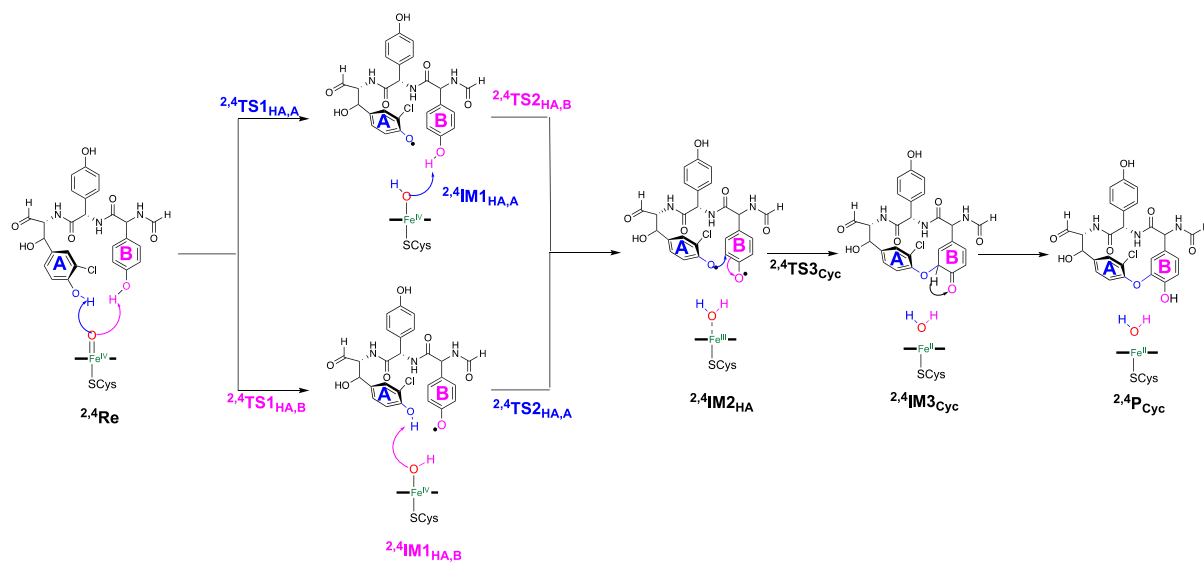
Fig. S1: Active site model of substrate bound complex of OxyB taken from the pdb file.

Computational methods:

All the quantum mechanical calculations were done using density functional theory (DFT) methods which are implemented in Gaussian-09.⁴ In previous work we extensively tested and benchmarked models and methods for P450 reaction mechanisms and reproduced experimental structures and rate constants well.^{5, 6} All calculations used the unrestricted B3LYP hybrid density functional method,⁷ in combination with a basis set containing an LANL2DZ + ECP on iron and 6-31G* on the rest of the atoms (basis set BS1).⁸ Full geometry optimizations, frequencies and scan calculations were run for all structures using UB3LYP/BS1 in the gas-phase. Subsequent single point calculations with the polarized continuum model (CPCM)⁹ were performed with a dielectric constant mimicking chlorobenzene, and a triple- ζ quality basis set (basis set BS2) containing LACV3P+ + ECP on iron and 6-311+G* on the rest of the atoms.

References:

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Scheme S1: Reaction mechanism and definition of structures studied in this work.

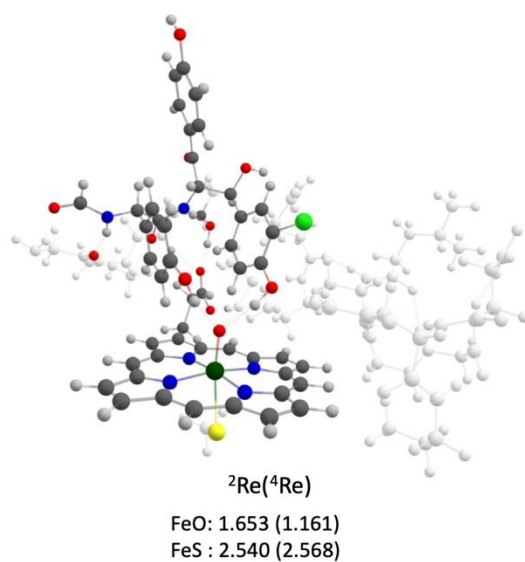


Fig. S2: The optimized structures of reactant complex calculated using UB3LYP/BS1/UB3LYP/BS2. The bond lengths are in angstroms.

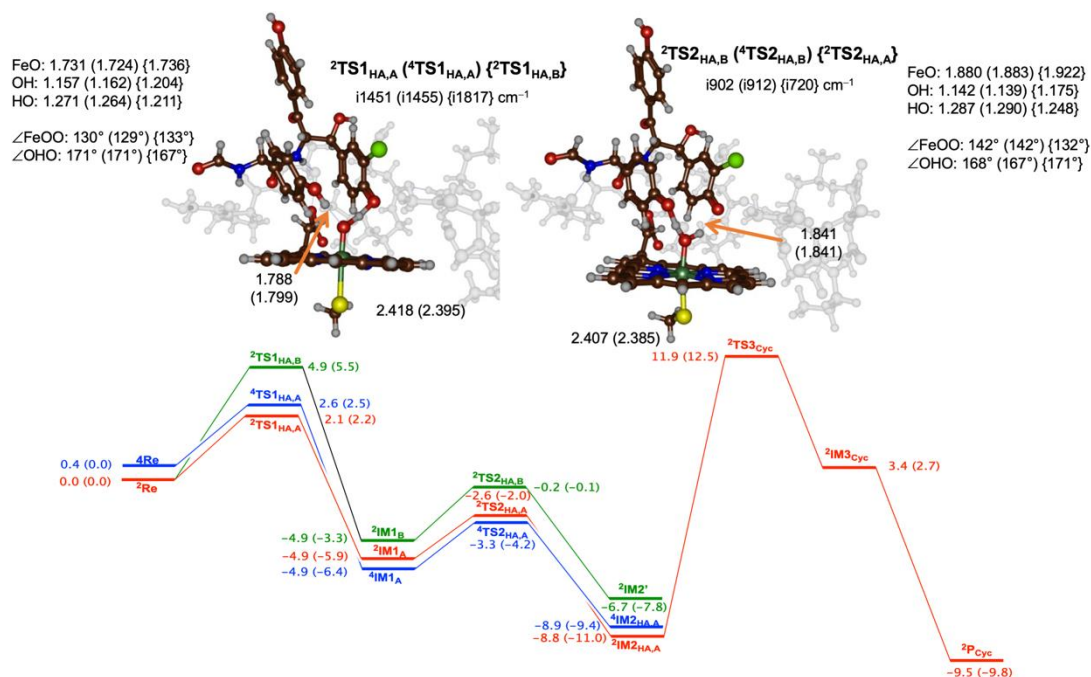
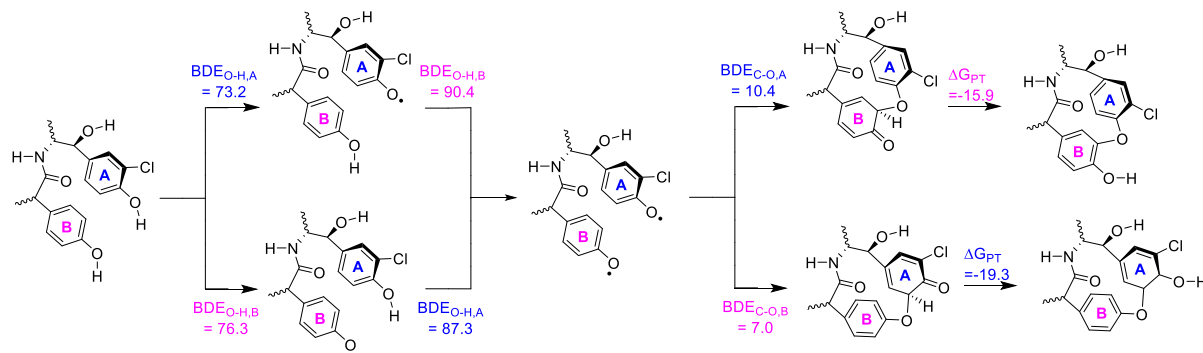


Fig. S3: Potential energy profile of substrate cyclization by iron(IV)-oxo of OxyB calculated using UB3LYP/BS1/UB3LYP/BS2. Data for $\Delta E + \text{ZPE}$ ($\Delta G^{298\text{K}}$) are given in kcal mol⁻¹. The optimized geometries of transition states have bond lengths in angstroms and imaginary frequencies in cm⁻¹.



Scheme S2: UB3LYP/BS2//UB3LYP/BS1 calculated bond dissociation free energies (BDE) for bonds broken or formed in each step. The last step represents an isomerization free energy. ΔG values in kcal mol⁻¹.

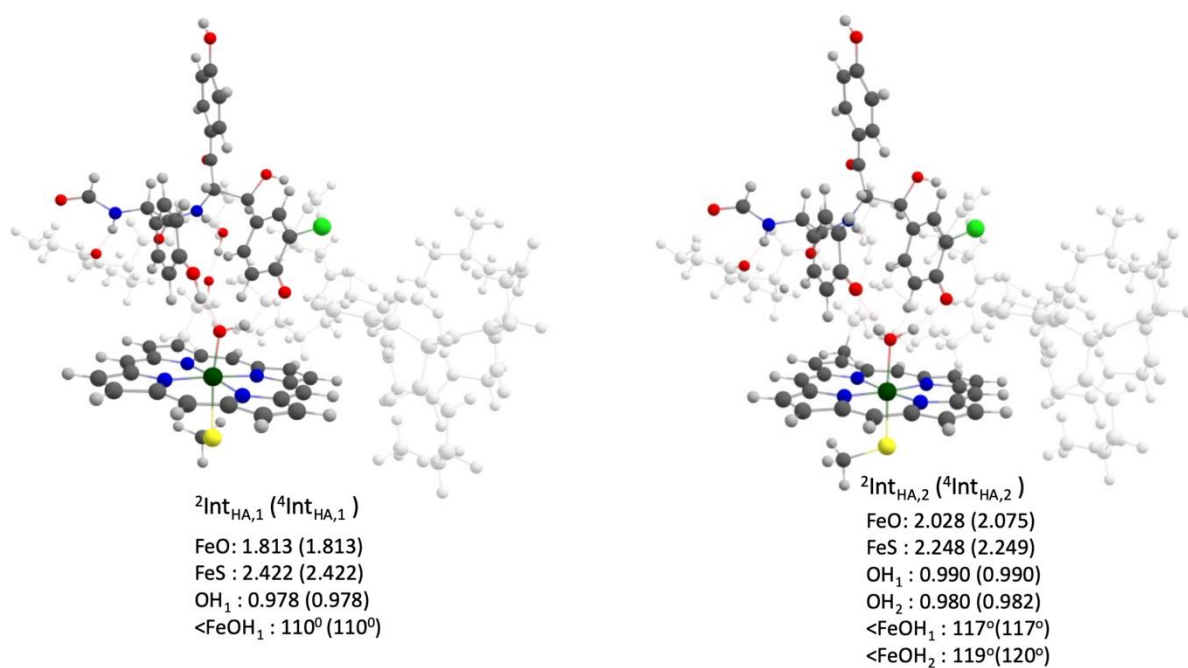


Fig. S4: The optimized structures of intermediates calculated using UB3LYP/BS1/UB3LYP/BS2. The bond lengths and bond angles are in angstroms.

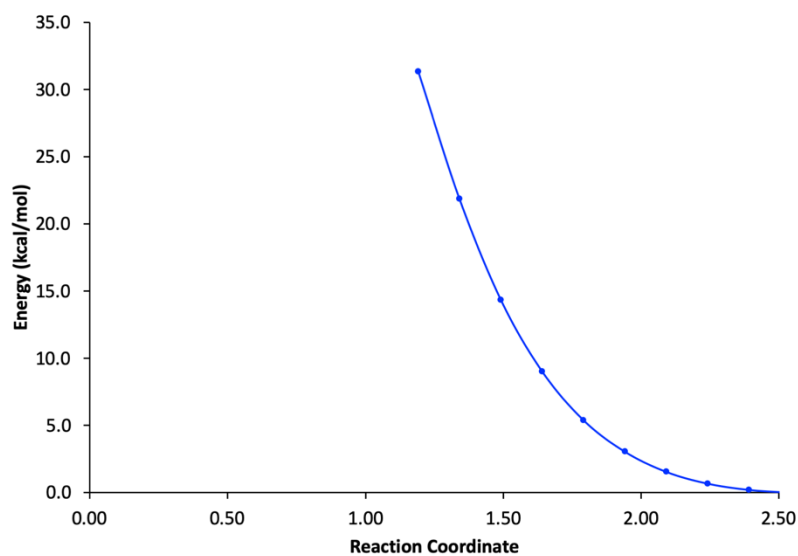


Fig. S5: UB3LYP/BS1 calculated geometry scan for direct ring-closure from $^2\text{IM1}_A$. As can be seen this is an unfavorable pathway that does not lead to a stable product.

Table S1: Absolute (free) energies (in au) of optimized geometries of the OxyB model with substrate in binding position A for the cyclization reaction as calculated at the UB3LYP level of theory in the doublet spin state.

System	BS1			BS2 + Solv		
	E	E+ZPE	G	E	E+ZPE	G
² Re	-7749.328659	-7747.223033	-7747.430764	-7751.422483	-7749.316857	-7749.524588
² TS1 _{HA,A}	-7749.315416	-7747.217109	-7747.424724	-7751.411862	-7749.313555	-7749.521170
² IM1 _A	-7749.332881	-7747.229071	-7747.438445	-7751.428400	-7749.324590	-7749.533963
² TS2 _{HA,B}	-7749.321752	-7747.223790	-7747.430533	-7751.418929	-7749.320967	-7749.527710
² IM2 _B	-7749.333152	-7747.231352	-7747.442562	-7751.432653	-7749.330853	-7749.542063
² TS3 _{Cyc}	-7749.312327	-7747.207609	-7747.414520	-7751.402555	-7749.297837	-7749.504748
² IM3 _{Cyc}	-7749.330201	-7747.223070	-7747.431964	-7751.418564	-7749.311433	-7749.520327
² P _{Cyc}	-7749.353495	-7747.245529	-7747.453735	-7751.439955	-7749.331989	-7749.540195

Table S2: Relative (free) energies (in kcal mol⁻¹) of optimized geometries of the OxyB model with substrate in binding position A for the cyclization reaction as calculated at the UB3LYP level of theory in the doublet spin state.

System	BS1			BS2 + Solv		
	ΔE	ΔE+ZPE	ΔG	ΔE	ΔE+ZPE	ΔG
² Re	0.00	0.00	0.00	0.00	0.00	0.00
² TS1 _{HA,A}	8.31	3.72	3.79	6.67	2.07	2.15
² IM1 _A	-2.65	-3.79	-4.82	-3.71	-4.85	-5.88
² TS2 _{HA,B}	4.33	-0.48	0.14	2.23	-2.58	-1.96
² IM2 _B	-2.82	-5.22	-7.40	-6.38	-8.78	-10.97
² TS3 _{Cyc}	10.25	9.68	10.19	12.51	11.94	12.45
² IM3 _{Cyc}	-0.97	-0.02	-0.75	2.46	3.40	2.67
² P _{Cyc}	-15.58	-14.12	-14.41	-10.96	-9.50	-9.79

Table S3: Absolute (free) energies (in au) of optimized geometries of the OxyB model with substrate in binding position A for the cyclization reaction as calculated at the UB3LYP level of theory in the quartet spin state.

System	BS1			BS2 + Solv		
	E	E+ZPE	G	E	E+ZPE	G
⁴ Re	-7749.328330	-7747.222680	-7747.431047	-7751.421956	-7749.316307	-7749.524673
⁴ TS1 _{HA,A}	-7749.315625	-7747.216945	-7747.424850	-7751.411364	-7749.312684	-7749.520589
⁴ IM1 _A	-7749.332892	-7747.229080	-7747.439158	-7751.428473	-7749.324661	-7749.534739
⁴ TS2 _{HA,B}	-7749.322312	-7747.223841	-7747.433143	-7751.420515	-7749.322044	-7749.531346
⁴ IM2 _B	-7749.333199	-7747.231781	-7747.440309	-7751.432434	-7749.331016	-7749.539544
⁴ IM3 _{Cyc}	-7749.336811	-7747.234184	-7747.446011	-7751.425650	-7749.323023	-7749.534850

Table S4: Relative (free) energies (in kcal mol⁻¹) of optimized geometries of the OxyB model with substrate in binding position A for the cyclization reaction as calculated at the UB3LYP level of theory in the quartet spin state.

System	BS1			BS2 + Solv		
	ΔE	ΔE+ZPE	ΔG	ΔE	ΔE+ZPE	ΔG
⁴ Re	0.21	0.22	-0.18	0.33	0.35	-0.05
⁴ TS1 _{HA,A}	8.18	3.82	3.71	6.98	2.62	2.51
⁴ IM1 _A	-2.66	-3.79	-5.27	-3.76	-4.90	-6.37
⁴ TS2 _{HA,B}	3.98	-0.51	-1.49	1.24	-3.25	-4.24
⁴ IM2 _B	-2.85	-5.49	-5.99	-6.24	-8.88	-9.38
⁴ IM3 _{Cyc}	-5.12	-7.00	-9.57	-1.99	-3.87	-6.44

Table S5: Group spin densities of optimized geometries of the OxyB model with substrate as calculated at the UB3LYP level of theory in the doublet spin state.

System		Fe	O	Porphyrin	Substrate	Amino Acids	Total
² Re	Gas	1.3992	0.7158	-0.3133	0.007	-0.8083	1.00
	Solvent	1.7694	0.6698	-0.7538	-0.0188	-0.6667	1.00
² TS1 _{HA,A}	Gas	1.7339	0.3988	-0.6508	-0.0256	-0.4562	1.00
	Solvent	2.1231	0.3766	-1.2289	-0.0515	-0.2193	1.00
² IM1 _A	Gas	0.9700	0.0601	0.5460	-0.7993	0.2233	1.00
	Solvent	1.0791	0.1268	0.1728	-1.0059	0.6271	1.00
² TS2 _{HA,B}	Gas	1.0843	0.0351	-0.4685	0.9899	-0.6408	1.00
	Solvent	1.3475	0.0316	-0.7631	0.9904	-0.6063	1.00
² IM2 _B	Gas	1.0002	-0.0075	-0.3084	0.4569	-0.1413	1.00
	Solvent	1.2209	-0.0073	-0.3951	0.1377	0.0437	1.00
² TS3 _{Cyc}	Gas	1.0163	-0.0036	-0.0679	0.0007	0.0545	1.00
	Solvent	1.2160	-0.0114	-0.2423	0.0033	0.0344	1.00
² IM3 _{Cyc}	Gas	1.0242	-0.0035	-0.0679	0.0008	0.0464	1.00
	Solvent	1.2193	-0.0120	-0.2419	0.0046	0.0300	1.00
² P _{Cyc}	Gas	1.0228	-0.0033	-0.0686	0.0049	0.0441	1.00
	Solvent	1.1635	-0.0034	-0.2138	0.0016	0.0520	1.00

Table S6: Group spin densities of optimized geometries of the OxyB model with substrate as calculated at the UB3LYP level of theory in the quartet spin state.

System		Fe	O	Porphyrin	Substrate	Amino Acids	Total
⁴ Re	Gas	1.2070	0.8131	0.2712	0.0043	0.7045	3.00
	Solvent	1.3688	0.7591	0.2406	-0.0051	0.6367	3.00
⁴ TS1 _{HA,A}	Gas	1.5453	0.4268	0.3529	0.1645	0.5105	3.00
	Solvent	1.6943	0.4635	0.4971	0.0919	0.2532	3.00
⁴ IM1 _A	Gas	1.6463	0.2271	-0.0936	0.8026	0.4176	3.00
	Solvent	1.0761	0.1318	0.1891	0.9903	0.6126	3.00
⁴ TS2 _{HA,B}	Gas	1.0409	0.0607	0.3531	1.0028	0.5426	3.00
	Solvent	1.1293	0.0593	0.3024	0.9951	0.5139	3.00
⁴ IM2 _B	Gas	0.9907	0.0105	0.1468	1.5642	0.2878	3.00
	Solvent	1.1293	0.0593	0.3024	0.9951	0.5139	3.00
⁴ IM3 _{Cyc}	Gas	1.1510	0.0039	0.1055	1.6671	0.0724	3.00
	Solvent	1.1942	0.0125	-0.0927	1.8383	0.0477	3.00

Table S7: Group charges of optimized geometries of the OxyB model with substrate as calculated at the UB3LYP level of theory in the doublet spin state.

System		Fe	O	Porphyrin	Substrate	Amino Acids	Total
² Re	Gas	0.4843	-0.5550	-0.8486	-0.1390	-0.9417	-2.00
	Solvent	-4.3476	0.1133	2.8297	-0.3311	-0.2641	-2.00
² TS1 _{HA,A}	Gas	0.4441	-0.7426	-0.6005	-0.1803	-0.9207	-2.00
	Solvent	-4.7728	0.0557	3.1265	-0.1849	-0.2245	-2.00
² IM1 _A	Gas	0.3422	-0.8224	-0.7775	0.2058	-0.9481	-2.00
	Solvent	-3.9243	0.0558	2.1800	0.0636	-0.3751	-2.00
² TS2 _{HA,B}	Gas	0.3749	-0.8643	-0.8295	0.2607	-0.9418	-2.00
	Solvent	-4.3177	0.0250	2.6434	-0.0871	-0.2636	-2.00
² IM2 _B	Gas	0.2356	-0.8198	-1.0398	0.5629	-0.9390	-2.00
	Solvent	-3.2828	0.2229	1.6146	0.1191	-0.6737	-2.00
² TS3 _{Cyc}	Gas	0.1947	-0.7972	-1.2190	0.9165	-1.0950	-2.00
	Solvent	-2.8341	0.1584	1.4848	0.0871	-0.8962	-2.00
² IM3 _{Cyc}	Gas	0.1964	-0.7808	-1.1921	0.9029	-1.1264	-2.00
	Solvent	-2.5247	0.2715	1.2944	-0.1185	-0.9227	-2.00
² P _{Cyc}	Gas	0.1777	-0.7824	-1.2228	0.7053	-0.8777	-2.00
	Solvent	-1.5205	-0.1834	-0.2376	0.7025	-0.7610	-2.00

Table S8: Group charges of optimized geometries of the OxyB model with substrate as calculated at the UB3LYP level of theory in the quartet spin state.

System		Fe	O	Porphyrin	Substrate	Amino Acids	Total
⁴ Re	Gas	0.4796	-0.4708	-0.8893	-0.0944	-1.0251	-2.00
	Solvent	-4.2089	0.2466	2.8430	-0.0033	-0.8773	-2.00
⁴ TS1 _{HA,A}	Gas	0.4227	-0.7400	-0.6755	-0.1318	-0.8755	-2.00
	Solvent	-4.7427	0.0645	3.0119	-0.1527	-0.1810	-2.00
⁴ IM1 _A	Gas	0.4073	-0.7747	-1.0039	0.2274	-0.8561	-2.00
	Solvent	-3.9193	0.0567	2.1733	0.0655	-0.3762	-2.00
⁴ TS2 _{HA,B}	Gas	0.3671	-0.8630	-0.8460	0.2607	-0.9189	-2.00
	Solvent	-4.5123	0.0338	2.7081	-0.0437	-0.1859	-2.00
⁴ IM2 _B	Gas	0.2347	-0.8175	-1.0629	0.5781	-0.9324	-2.00
	Solvent	-4.5123	0.0338	2.7081	-0.0437	-0.1859	-2.00
⁴ IM3 _{Cyc}	Gas	0.2780	-0.8236	-1.0494	0.6879	-1.0929	-2.00
	Solvent	-3.5127	0.1854	1.7238	0.5850	-0.9815	-2.00

Table S9: Absolute (free) energies (in au) of optimized geometries of the OxyB model with substrate in binding position B for the cyclization reaction as calculated at the UB3LYP level of theory in the doublet spin state.

System	BS1			BS2 + Solv		
	E	E+ZPE	G	E	E+ZPE	G
² Re	-7749.328659	-7747.223033	-7747.430764	-7751.422483	-7749.316857	-7749.524588
² TS1 _{HA,B}	-7749.311811	-7747.213208	-7747.420178	-7751.407693	-7749.309090	-7749.516060
² IM1 _B	-7749.332748	-7747.229918	-7747.435029	-7751.427488	-7749.324658	-7749.529769
² TS2 _{HA,A}	-7749.329838	-7747.232224	-7747.439677	-7751.414851	-7749.317237	-7749.524690
² IM2'	-7749.333762	-7747.232675	-7747.442066	-7751.428675	-7749.327588	-7749.536979
² IM3 _{Cyc}	-7749.330201	-7747.223070	-7747.431964	-7751.418564	-7749.311433	-7749.520327

Table S10: Relative (free) energies (in kcal mol⁻¹) of optimized geometries of the OxyB model with substrate in binding position B for the cyclization reaction as calculated at the UB3LYP level of theory in the doublet spin state.

System	BS1			BS2 + Solv		
	ΔE	ΔE+ZPE	ΔG	ΔE	ΔE+ZPE	ΔG
² Re	0.00	0.00	0.00	0.00	0.00	0.00
² TS1 _{HA,B}	10.57	6.17	6.64	9.28	4.87	5.35
² IM1 _B	-2.57	-4.32	-2.68	-3.14	-4.89	-3.25
² TS2 _{HA,A}	-0.74	-5.77	-5.59	4.79	-0.24	-0.06
² IM2'	-3.20	-6.05	-7.09	-3.89	-6.73	-7.78
² IM3 _{Cyc}	-0.97	-0.02	-0.75	2.46	3.40	2.67

Table S11: Group spin densities of optimized geometries of the OxyB model with substrate in binding position B as calculated at the UB3LYP level of theory in the doublet spin state.

System		Fe	O	Porphyrin	Substrate	Amino Acids	Total
² Re	Gas	1.3992	0.7158	-0.3133	0.0066	-0.8083	1.00
	Solvent	1.7694	0.6698	-0.7538	-0.0188	-0.6667	1.00
² TS1 _{HA,B}	Gas	1.8162	0.3873	-0.4966	-0.1528	-0.5541	1.00
	Solvent	2.1232	0.3713	-1.0403	-0.2318	-0.2224	1.00
² IM1 _B	Gas	0.9902	0.0955	-0.4745	0.9817	-0.5928	1.00
² TS2 _{HA,A}	Gas	0.9641	0.0409	0.5004	-0.9893	0.4840	1.00
² IM2'	Gas	-1.4383	0.0137	0.4826	1.1734	0.7686	1.00
	Solvent	-1.2365	0.0243	0.7629	1.4795	-0.0302	1.00
² IM3 _{Cyc}	Gas	1.0242	-0.0035	-0.0679	0.0008	0.0464	1.00
	Solvent	1.2193	-0.0120	-0.2419	0.0046	0.0300	1.00

Table S12: Group charges of optimized geometries of the OxyB model with substrate in binding position B as calculated at the UB3LYP level of theory in the doublet spin state.

System		Fe	O	Porphyrin	Substrate	Amino Acids	Total
² Re	Gas	0.4843	-0.5550	-0.8486	-0.1390	-0.9417	-2.00
	Solvent	-4.3476	0.1133	2.8297	-0.3311	-0.2641	-2.00
² TS1 _{HA,B}	Gas	0.5150	-0.7538	-0.7429	-0.0827	-0.9356	-2.00
	Solvent	-5.5169	-0.0326	3.7905	-0.0727	-0.1683	-2.00
² IM1 _B	Gas	0.3471	-0.7794	-0.8679	-0.1479	-0.5518	-2.00
² TS2 _{HA,A}	Gas	0.2962	-0.8449	-0.7170	-0.3220	-0.4123	-2.00
² IM2'	Gas	0.4768	-0.8344	-0.8061	-0.2668	-0.5694	-2.00
	Solvent	0.4768	-0.8344	-0.8061	-0.2668	-0.5694	-2.00
² IM3 _{Cyc}	Gas	0.1964	-0.7808	-1.1921	0.9029	-1.1264	-2.00
	Solvent	-2.5247	0.2715	1.2944	-0.1185	-0.9227	-2.00

Cartesian coordinates:

²Re

C	24.97738700	5.77869200	35.67742100
S	24.16990400	4.35159000	34.85881900
C	25.29048300	3.02055300	35.43227500
H	24.31852900	6.64346900	35.55293200
H	25.40446600	3.04994900	36.52233200
H	24.84653400	2.06794800	35.12902600
H	26.26984400	3.11957200	34.95265200
H	25.93597500	5.99659300	35.19470100
H	21.08936100	2.00473000	34.71908100
C	20.69882100	1.67818300	35.69103600
C	20.05621900	2.85088500	36.41718000
O	19.04095400	2.69077700	37.11114300
C	21.84648700	1.03520500	36.50019200
C	21.45995800	0.55605900	37.90183700
C	20.49288200	-0.61999400	37.89035700
H	22.37834500	0.25382700	38.42234800
H	19.91654900	0.93661100	35.51518200
H	21.02819000	1.37275500	38.49371500
H	22.67419000	1.74620000	36.60061100
H	22.22121300	0.17966600	35.92819400
H	19.88625300	-0.21952000	39.83347200
O	20.23699800	-1.28471900	36.89998100
N	19.95316500	-0.95337100	39.13484700
H	19.12879400	-1.54259800	39.07284200
N	20.68268400	4.04429600	36.27324600
C	20.28659100	5.26451400	36.96753400
H	19.86533600	5.97556000	36.24186600
C	21.45971100	5.91460300	37.71305900
H	21.10694500	6.86935300	38.12732100
C	22.05331900	5.03891800	38.81859600
H	19.48549200	4.98939500	37.65849900
H	22.33188700	4.05398600	38.43018100
H	22.24566700	6.16770500	36.98981000
H	21.56841300	4.06554100	35.77137800
H	22.97134900	5.48062800	39.21638200
H	21.33733800	4.88763900	39.63615400
C	15.45629600	3.06647200	36.76558500
C	15.58298000	3.70828100	38.13557900
O	14.63404000	4.27459300	38.68997300
C	14.66757500	1.73181600	36.82509000
C	13.21288600	1.82228800	37.32812600
C	12.30934300	2.65831100	36.41169300
C	12.61998400	0.41931400	37.53194200
H	13.26461200	-0.19707100	38.17304100
H	11.64154100	0.49208100	38.01870300
H	12.50244500	-0.10944900	36.57408700
H	12.19292600	2.18712200	35.42376700
H	11.32818000	2.76781600	36.88225700
H	12.70654300	3.66945800	36.26450200
H	14.93399500	3.77743400	36.11688200
H	13.21097700	2.32320800	38.30050200
H	15.22817700	1.03338900	37.46296000
H	14.68161900	1.29680200	35.81441300
N	16.79914300	3.61188700	38.75088600
C	16.92611800	3.90224600	40.17612800
C	16.71076700	5.38251100	40.53989600
O	16.47207600	5.70449200	41.70494400
C	18.27673500	3.40818100	40.70792200
H	17.58496000	3.18788200	38.25674800
H	16.12040300	3.38458000	40.70988700

H	19.11039800	3.88007700	40.17717600
H	18.36871200	3.64007500	41.77134500
H	18.35812900	2.32367100	40.58056100
N	16.82200000	6.28441400	39.52795700
C	16.46286600	7.68145500	39.69605000
C	14.96136000	8.02939900	39.78736800
O	14.65014400	9.20388900	39.97634100
H	16.89525700	5.90437600	38.59429500
H	16.90948300	8.05507000	40.62013000
H	16.88852400	8.25787300	38.86955100
N	14.08834600	7.00417300	39.65103600
C	12.66062500	7.16302200	39.89354000
C	12.24097000	6.45256300	41.19438000
O	12.06044600	7.08541500	42.24292300
H	14.42006200	6.06038900	39.45874100
H	12.45813400	8.22865900	39.99907400
N	12.15810900	5.10738400	41.08764400
C	11.55549700	4.27665100	42.13020100
C	12.26197900	4.33748700	43.49179200
O	11.63895700	4.08645700	44.51830600
C	11.51544800	2.80684800	41.64922400
C	10.87262800	2.55904600	40.24646900
O	11.05506400	3.44433700	39.35652300
O	10.28357100	1.46432200	40.11073000
H	11.99576100	4.66689900	40.15814800
H	10.53301900	4.61974200	42.33275200
H	10.99115500	2.20974400	42.39837400
H	12.54607400	2.42752500	41.59498700
N	13.60391300	4.61045100	43.47650800
C	14.38063500	4.71141900	44.70190200
C	14.74616200	6.16515700	45.06811600
O	15.72386700	6.40671400	45.78904500
C	15.62296100	3.80909600	44.68865600
C	16.08032100	3.43570700	46.10157000
H	13.72434100	4.35276200	45.50306000
H	14.04176800	4.86630500	42.59937400
H	16.43518700	4.25975700	44.10951700
H	15.34714200	2.87193900	44.18749600
O	15.31038700	3.39970800	47.05617500
N	17.39353100	3.09183200	46.21144000
H	17.70352000	2.73068600	47.10259800
H	18.02958300	2.99871900	45.42837000
N	13.90345000	7.11643400	44.60944400
C	14.03041600	8.52640800	44.94935500
H	13.07453600	8.86500900	45.37244900
C	14.40055800	9.40829900	43.74774100
C	15.81671000	9.16134300	43.22128400
H	14.79019300	8.59495100	45.73293500
H	13.67565300	9.23499900	42.94349100
H	15.94109600	8.11219600	42.93123400
H	16.00789500	9.77732800	42.33615800
H	13.17670500	6.86451900	43.94183200
N	31.78755500	0.55069800	44.37032700
C	31.94822800	0.68906700	42.93096800
C	30.65774900	1.21330500	42.30015100
O	29.58640300	1.14940400	42.90027000
H	30.88559600	0.11070500	44.56998000
H	32.77983400	1.37404100	42.71154700
N	30.74783100	1.72185800	41.03901600
C	29.54852700	1.97845900	40.24169600
C	29.02654500	0.65564400	39.62557000
O	29.73985700	-0.34861100	39.57551200
C	30.08831700	2.91742300	39.14598900

C	31.47876500	2.32080400	38.85699500	O	21.89702600	4.08260600	45.89422800
C	31.97117300	1.82107100	40.23401500	C	23.92161100	-1.71742400	41.95661000
H	31.38108000	1.47098000	38.17528900	N	24.95573200	-0.75097800	41.64149200
H	28.77457400	2.42978900	40.86516900	C	25.99407500	-0.31221100	42.40167400
H	32.67119000	2.53244800	40.69372300	O	26.73717700	0.58230200	42.00184500
H	32.47453100	0.85123400	40.15086100	C	26.21308000	-0.90786300	43.81172800
H	32.17122700	3.04065200	38.40825600	N	27.63276600	-0.73796700	44.11707300
H	30.17535200	3.93472300	39.54613000	C	28.28913700	-1.48924700	45.02256100
H	29.43692400	2.95062400	38.26889200	O	29.47497000	-1.39108600	45.32983800
N	27.78909300	0.72563000	39.08855300	C	25.26971000	-0.21876300	44.79438400
C	27.13614200	-0.47794600	38.58898300	C	25.22359400	1.18040000	44.85809800
C	25.77143100	-0.16836900	37.96193400	C	24.30684600	1.82833700	45.67431200
O	24.86167400	0.38460100	38.92380000	C	23.39904100	1.08988600	46.45051500
C	25.14190300	-1.43334900	37.38510700	C	23.47066500	-0.30922300	46.43604500
H	27.00411700	-1.20617200	39.40018000	C	24.39609200	-0.94913200	45.61001800
H	24.18146000	-1.19889100	36.91400400	O	22.45402500	1.68861300	47.21834600
H	25.79524400	-1.88253000	36.62762700	C	22.59562800	-1.22771200	41.28261900
H	27.19999100	1.54271700	39.26414700	C	21.88434100	-0.15369500	42.10180700
H	25.91574800	0.57144000	37.16142500	C	20.66169700	-0.43644600	42.72178200
H	24.97160000	-2.16775000	38.17871200	C	20.02517000	0.51779300	43.51506700
H	25.09245700	1.35193000	39.02303100	C	20.59989200	1.77806200	43.74075100
C	23.46764300	8.82321800	44.89458200	C	21.81041100	2.06555000	43.09100400
S	22.36377500	8.22818800	46.21417000	C	22.43695000	1.12330000	42.28240100
H	23.53269900	9.91411400	44.95727500	O	19.97590500	2.67711900	44.54097200
H	24.46493100	8.38313700	44.97829100	Cl	18.48987300	0.11767400	44.27215100
C	22.90295900	5.97810500	42.71756600	C	24.29314000	-3.12849700	41.43346500
H	23.09974400	6.00505100	41.65126100	O	24.96440200	-3.24098800	40.41760700
C	25.54331600	5.24826400	46.69513800	C	23.88967400	-4.33389800	42.21608700
H	26.59173800	5.05326200	46.89836600	O	21.77591000	-2.36602200	41.05865900
C	21.55110200	5.65195300	49.40979500	C	22.97173100	-4.30670900	43.28090000
H	21.33836700	5.58706200	50.47262600	C	22.64544900	-5.46682800	43.97465200
C	18.90885900	6.39452700	45.42747000	C	23.24119800	-6.68099400	43.61532000
H	17.84844400	6.53684300	45.24029600	C	24.15512400	-6.72750800	42.55400100
C	23.96291300	5.66385600	43.55839700	C	24.46730900	-5.56393300	41.86301900
C	25.31709500	5.37679000	43.10280600	O	22.89602700	-7.79228800	44.33160400
C	26.05117500	5.21220400	44.24293100	H	23.77911500	-1.74459000	43.03777700
C	25.16404300	5.37030200	45.36652100	H	24.95559200	-0.36097100	40.68974800
C	25.76372800	5.26927700	41.67361000	H	25.98563900	-1.98085600	43.80383600
H	26.85272300	5.39444700	41.63377700	H	28.14561200	-0.01201400	43.60701000
H	25.34502700	6.07941500	41.06669300	H	25.89921400	1.76606100	44.24094400
C	25.38701800	3.94002600	40.98255900	H	24.26077100	2.90995200	45.69196300
H	25.95320200	3.09758900	41.39364600	H	22.77587400	-0.87714200	47.04756400
H	24.32610500	3.71721100	41.17175400	H	24.42370800	-2.03800500	45.58867300
C	25.55553800	3.99788900	39.44288700	H	22.32842600	2.61604200	46.90878600
O	25.78311400	2.88304100	38.85121100	H	22.90538500	-0.80551300	40.31804000
O	25.42450900	5.10565100	38.88517800	H	20.21277400	-1.41565600	42.59955600
C	24.68201800	5.31287900	47.78509500	H	22.26075000	3.04096500	43.24406200
C	25.09687300	5.16386900	49.15592700	H	23.37481800	1.38393400	41.80337200
C	23.97278300	5.27276100	49.91961900	H	20.64313400	3.29577000	44.94044800
C	22.87515100	5.48976900	49.01348100	H	21.15475100	-2.11852100	40.34304700
C	20.48147500	5.87333600	48.55807200	H	22.47972300	-3.38152100	43.55876800
C	19.10469700	5.98856000	48.97672100	H	21.93060100	-5.45200400	44.79108200
C	18.36126200	6.18080500	47.85306200	H	24.61650000	-7.67405100	42.27482800
C	19.29024500	6.19751000	46.74900800	H	25.16787300	-5.58023300	41.03451100
C	19.78376000	6.41497500	44.35578300	H	23.37705800	-8.55413700	43.97213500
C	19.38328800	6.63404500	42.99046100	H	23.05476900	8.55770000	43.91442000
C	20.50926600	6.53685200	42.23062800	H	14.29276000	10.45976200	44.05277800
C	21.60023900	6.24219000	43.12586100	H	16.57279500	9.39292100	43.98272700
N	23.88916800	5.63968400	44.92981200	H	32.49782700	-0.08534700	44.72660600
N	23.32669800	5.51027700	47.71994500	H	32.17930200	-0.25111600	42.38889800
N	20.57353300	6.00921500	47.19286300	H	27.63868600	-2.25622100	45.49247900
N	21.14673000	6.19977900	44.42285000	H	20.61009400	6.63525200	41.15769800
Fe	22.20812000	5.69775400	46.05484800	H	18.36081800	6.79749900	42.67720500

H	17.29080600	6.28440100	47.73101000	N	16.85625800	3.65919000	38.84980500
H	18.76858700	5.91379200	50.00338200	C	17.02444100	4.03259100	40.25185300
H	23.87808200	5.20928300	50.99633800	C	16.76336600	5.52324000	40.53352100
H	26.11700100	4.98926900	49.47358100	O	16.53123300	5.91043100	41.67921300
H	27.10705200	4.98236900	44.32119700	C	18.41107900	3.61530300	40.75560800
H	27.78786300	-0.94689700	37.84171200	H	17.64519500	3.25482700	38.34372500
H	25.12895700	5.56913300	36.74325700	H	16.25756500	3.51750500	40.84187700
H	16.45022400	2.88149400	36.34262300	H	19.20521800	4.10092300	40.17897200
H	12.09918100	6.75728400	39.04310100	H	18.53599300	3.88211600	41.80745100
²Ts1_{HA,A}				H	18.53568400	2.53183900	40.66040800
C	25.04372300	5.76066500	35.72395100	N	16.82190300	6.36563100	39.46603200
S	24.21191700	4.35922700	34.88515600	C	16.42210700	7.75732900	39.56216400
C	25.29946800	2.99858700	35.45188000	C	14.91165000	8.06103700	39.65456200
H	24.40999100	6.64296500	35.59194800	O	14.56087200	9.23155800	39.78910000
H	25.41215400	3.02154500	36.54233100	H	16.90586600	5.93605300	38.55500000
H	24.83257400	2.05846800	35.14404000	H	16.86702500	8.19514900	40.45855800
H	26.28152800	3.07601200	34.97373300	H	16.81815300	8.30104400	38.69948300
H	26.01501800	5.95489200	35.25679800	N	14.07092400	7.00187900	39.57426000
H	21.07307500	1.99584200	34.77130500	C	12.63983300	7.13147400	39.81144000
C	20.67177100	1.69102700	35.74605800	C	12.24095900	6.46058600	41.13833700
C	20.07321100	2.89255600	36.46263700	O	12.05342900	7.12202000	42.16630200
O	19.04991800	2.77523700	37.15361600	H	14.43225500	6.05862200	39.43934200
C	21.79381700	1.00537300	36.55593600	H	12.40984300	8.19472300	39.87764500
C	21.39899200	0.55832500	37.96567400	N	12.18510600	5.10909300	41.08283900
C	20.37191500	-0.56714100	37.98518100	C	11.61984300	4.30931500	42.16891700
H	22.30792300	0.21946700	38.47872300	C	12.36945600	4.41845800	43.50717400
H	19.86091900	0.97932000	35.57761200	O	11.78214200	4.17458900	44.55585700
H	21.01551200	1.40086100	38.55458800	C	11.57867500	2.82315300	41.74614400
H	22.65370900	1.67901600	36.64460600	C	10.86825900	2.52837900	40.39273600
H	22.12636900	0.12877500	35.98945700	O	11.01632300	3.35059000	39.44672500
H	19.91743900	-0.18110800	39.97338700	O	10.24311900	1.43919900	40.34155900
O	20.03058300	-1.19709000	36.99653200	H	12.03566300	4.64149900	40.17285500
N	19.87706500	-0.88952300	39.24717700	H	10.60200400	4.65251900	42.39234300
H	19.01703600	-1.42736600	39.22668300	H	11.10350300	2.24875500	42.54409900
N	20.73865300	4.06368600	36.31180400	H	12.60964300	2.45501500	41.64739800
C	20.35935500	5.30831500	36.97162400	N	13.69989700	4.72658000	43.44038900
H	19.95470100	6.00640700	36.22394300	C	14.52099100	4.87805400	44.63295200
C	21.53632600	5.96087300	37.70838500	C	14.81716100	6.35390300	44.97507700
H	21.19648200	6.93535300	38.08614800	O	15.78282000	6.65388200	45.68934600
C	22.10086400	5.11312800	38.85024200	C	15.80756700	4.04106100	44.56232700
H	19.54899900	5.06476000	37.66349300	C	16.32526600	3.64531700	45.94886400
H	22.35547000	4.10710900	38.50105300	H	13.92289900	4.49057600	45.46543900
H	22.33418300	6.17539900	36.98597000	H	14.10128900	4.96870700	42.54227000
H	21.62481500	4.05798800	35.81017900	H	16.58089600	4.54803700	43.97774500
H	23.02761900	5.54568100	39.23777200	H	15.56662200	3.10716700	44.03729000
H	21.37556700	5.01148100	39.66720000	O	15.59875600	3.61946400	46.93938300
C	15.48515900	2.97960200	36.93045100	N	17.63273000	3.27704300	45.99133300
C	15.61893400	3.67199200	38.27572800	H	17.97407100	2.90639300	46.86730500
O	14.65881800	4.20965700	38.84297000	H	18.24937100	3.18152000	45.18698400
C	14.74612300	1.62143800	37.04642500	N	13.93198200	7.26036100	44.50463100
C	13.28557700	1.68101200	37.53683100	C	14.00277600	8.68064500	44.81709800
C	12.35640500	2.42031700	36.56426600	H	13.03868500	8.98723000	45.24589100
C	12.75164900	0.26821100	37.81988200	C	14.32089600	9.55425700	43.59430100
H	13.40776400	-0.27544200	38.51256400	C	15.73894200	9.35638200	43.05215300
H	11.75804200	0.32244400	38.27749800	H	14.76819100	8.79563500	45.58962500
H	12.68026000	-0.32568700	36.89661500	H	13.59290900	9.33621700	42.80377900
H	12.27377100	1.88634400	35.60560000	H	15.90525200	8.30741800	42.78356500
H	11.36366800	2.51414200	37.01364500	H	15.89183900	9.96006700	42.15109200
H	12.71066200	3.43720200	36.35901700	H	13.20939300	6.96688300	43.85075400
H	14.92659800	3.65076700	36.26930700	N	31.68420300	0.87937400	44.36283100
H	13.25922300	2.23937500	38.47724500	C	31.87885000	0.91963900	42.92165000
H	15.32782200	0.97321000	37.71731500	C	30.60556500	1.40177600	42.22458600
H	14.78148100	1.14157300	36.05697000	O	29.51678000	1.37229500	42.79536500

H	30.79692900	0.41417600	44.57119000	C	20.57575800	6.72551000	42.26754300
H	32.71716900	1.58784700	42.67871600	C	21.60969900	6.27136500	43.16233400
N	30.73529100	1.83168200	40.93698500	N	23.80138600	5.42309800	44.97892200
C	29.56361200	2.06251900	40.09219400	N	23.12423300	5.02815600	47.72866100
C	29.04631600	0.72220500	39.51244300	N	20.45540900	5.84905000	47.18975900
O	29.76863300	-0.27625000	39.47696000	N	21.12478500	6.19149600	44.44153400
C	30.14571200	2.94878300	38.97406700	Fe	22.09400200	5.53658500	46.06138200
C	31.54053300	2.33224100	38.75645800	O	21.64913400	3.89076600	45.76216200
C	31.98506700	1.89399600	40.16986500	C	23.89027300	-1.71068800	41.95260500
H	31.45776500	1.45237900	38.11229300	N	24.91926500	-0.75776300	41.58690700
H	28.77710600	2.54938500	40.67156000	C	26.00028600	-0.34400900	42.29762100
H	32.67090900	2.62523400	40.61989200	O	26.77372900	0.49633300	41.84188500
H	32.48898500	0.92113800	40.14792100	C	26.22057200	-0.88403900	43.72967100
H	32.25182900	3.02742500	38.29816600	N	27.61984600	-0.61726000	44.06416600
H	30.22612200	3.98264600	39.33085800	C	28.30102700	-1.30026000	45.00267200
H	29.52313300	2.94557700	38.07556200	O	29.47112200	-1.11899000	45.33443400
N	27.80434600	0.77327300	38.98250500	C	25.21337800	-0.23181400	44.67288000
C	27.14928000	-0.45026500	38.53710900	C	24.89577700	1.12355800	44.52278200
C	25.77280200	-0.17376100	37.91894700	C	23.93259100	1.72765600	45.31591800
O	24.86278700	0.39165700	38.87174200	C	23.26090200	0.99099600	46.30544200
C	25.15141800	-1.46249000	37.38721100	C	23.59596400	-0.35865700	46.49300900
H	27.03545900	-1.14859600	39.37672000	C	24.55496700	-0.95818800	45.67523000
H	24.18062600	-1.25172100	36.92601800	O	22.29964900	1.54526600	47.08028300
H	25.79811800	-1.92490700	36.63202000	C	22.55803100	-1.25970600	41.26795700
H	27.20637000	1.58110300	39.17256100	C	21.86234100	-0.12009500	41.99845900
H	25.90012500	0.54287800	37.09423300	C	20.85319100	-0.39879000	42.93163100
H	25.00150000	-2.17600200	38.20397700	C	20.24213800	0.62354700	43.64953500
H	25.10709400	1.35298300	38.98651600	C	20.60804500	1.98915300	43.49181000
C	23.47423800	8.59889000	45.18435300	C	21.60036400	2.24207700	42.50946600
S	22.57994700	7.84613400	46.58810600	C	22.21164700	1.22383200	41.78664500
H	23.61653600	9.65680200	45.43221300	O	20.05769700	2.96268400	44.19347600
H	24.45291600	8.13833300	45.02594000	Cl	18.98349300	0.20629800	44.80425600
C	22.90600500	5.94901500	42.76710200	C	24.25888500	-3.13941600	41.47917400
H	23.13502400	6.03503000	41.71029500	O	24.88282000	-3.28864800	40.43756000
C	25.36125100	4.76799800	46.75429800	C	23.90443300	-4.31704800	42.32635100
H	26.39028000	4.49588900	46.96745900	O	21.73089400	-2.41302900	41.16074200
C	21.30048300	5.10401800	49.36432500	C	23.07052300	-4.25024800	43.45643800
H	21.03636800	4.92296800	50.40189300	C	22.78641800	-5.38708800	44.20548300
C	18.91045200	6.59074400	45.43295800	C	23.33985200	-6.61772400	43.83592500
H	17.87826400	6.86475300	45.23643900	C	24.17058700	-6.70402100	42.71061300
C	23.92511600	5.54053500	43.61401700	C	24.44218800	-5.56334700	41.96658100
C	25.28122700	5.22797200	43.18373100	O	23.03863200	-7.70577400	44.60659400
C	25.96560700	4.94965200	44.33335700	H	23.75657600	-1.68854500	43.03517800
C	25.04338100	5.05837100	45.43313600	H	24.90445200	-0.38779100	40.62775500
C	25.76927700	5.18776400	41.76429700	H	26.06281800	-1.97015800	43.74420400
H	26.85700500	5.32820400	41.75976900	H	28.09682600	0.11871500	43.53363900
H	25.35503800	6.01481900	41.17796500	H	25.39412900	1.71104800	43.75739400
C	25.42773200	3.87929200	41.01758200	H	23.66033300	2.76220000	45.15504200
H	26.02625600	3.03926200	41.38515200	H	23.07610100	-0.92731300	47.25848100
H	24.37925200	3.60982500	41.21249300	H	24.78292000	-2.01453900	45.81228600
C	25.57536600	4.00002500	39.47943700	H	22.06416700	2.43454100	46.71205800
O	25.77604300	2.90462800	38.84295800	H	22.85132500	-0.92378000	40.26488300
O	25.45551700	5.12981800	38.96509900	H	20.54466900	-1.42615800	43.09277300
C	24.46328400	4.74352100	47.81351200	H	21.87798400	3.27845100	42.34311500
C	24.81180700	4.39226000	49.16624400	H	22.97634600	1.47233000	41.05515000
C	23.66463800	4.46618300	49.89772400	H	20.88113300	3.53582400	44.97304200
C	22.62081700	4.87147200	48.99193600	H	21.04981600	-2.18847600	40.49631500
C	20.29717600	5.55889500	48.52241000	H	22.61646100	-3.31116200	43.75113100
C	18.92923400	5.78995000	48.92067600	H	22.13735000	-5.34031700	45.07399600
C	18.25839800	6.21134300	47.81403000	H	24.59965300	-7.66351800	42.42387000
C	19.22379800	6.24259100	46.74232500	H	25.07892600	-5.60993800	41.08918400
C	19.80277000	6.56435600	44.37180700	H	23.48405400	-8.48206700	44.23248700
C	19.45211000	6.90361500	43.01744300	H	22.89228200	8.53792100	44.26011600

H	14.17316800	10.60585300	43.88153800	H	12.29497300	2.12843400	35.34977700
H	16.49407300	9.63869400	43.79738600	H	11.45991400	2.62217800	36.85767100
H	32.40903600	0.29795300	44.77896600	H	12.75221300	3.62178600	36.20744500
H	32.12206500	-0.05504600	42.44999400	H	14.98500700	3.84236500	35.88889000
H	27.69077200	-2.09504400	45.48000800	H	13.42123100	2.27062000	38.18388600
H	20.71077000	6.87474100	41.20428200	H	15.48104800	1.13460400	37.25063100
H	18.45979200	7.19494400	42.70104500	H	14.85303200	1.36473200	35.62566700
H	17.20916200	6.43671900	47.67795700	N	16.77862700	3.72228000	38.61264500
H	18.54501500	5.62263200	49.91902300	C	16.81833500	3.95516400	40.05527300
H	23.52066600	4.26710500	50.95212900	C	16.64214700	5.42445500	40.48243000
H	25.80616500	4.11458800	49.49164300	O	16.42757000	5.69594800	41.66488700
H	27.00421000	4.65713500	44.42974200	C	18.10641900	3.37796300	40.65355600
H	27.79223100	-0.94156100	37.79677500	H	17.56995700	3.25434500	38.16876100
H	25.17429500	5.54657900	36.79190600	H	15.95612100	3.45193000	40.51015000
H	16.47617300	2.81500100	36.49332000	H	18.99312100	3.82690400	40.19306400
H	12.08718200	6.68095500	38.97763100	H	18.13884800	3.57474000	41.72726400
²IM1A				H	18.14523700	2.29521800	40.49287200
C	24.90206500	5.86265600	35.75684100	N	16.74007500	6.36845400	39.50892600
S	24.13895300	4.43800100	34.89271600	C	16.35221000	7.74889200	39.74380800
C	25.28932600	3.12163700	35.44162200	C	14.84381400	8.04531100	39.89655100
H	24.21943500	6.71183700	35.65588500	O	14.50419600	9.19076500	40.18768500
H	25.38254900	3.11454400	36.53404100	H	16.78224000	6.02832700	38.55857400
H	24.88145100	2.16754300	35.09534000	H	16.81647800	8.09739500	40.66870500
H	26.27366200	3.26817400	34.98502900	H	16.73826700	8.36753500	38.92833000
H	25.85601900	6.12209900	35.28564900	N	13.99742400	7.00876500	39.69475300
H	21.10317900	2.07683200	34.66991400	C	12.57574400	7.09434800	40.00039500
C	20.74325400	1.70889800	35.63869400	C	12.23302900	6.31272900	41.28380400
C	20.05731200	2.83304100	36.40333100	O	12.00727700	6.90192000	42.34899800
O	19.05651800	2.61008900	37.10201300	H	14.35174300	6.09955600	39.40312900
C	21.93181000	1.10836100	36.41982200	H	12.33084700	8.14392200	40.16150500
C	21.56700000	0.53261300	37.79137700	N	12.26056500	4.96824900	41.14141500
C	20.74177100	-0.74129000	37.69420600	C	11.72016600	4.06900000	42.16232500
H	22.50362400	0.29219500	38.31354700	C	12.40549000	4.15905500	43.53175400
H	19.99297200	0.93638400	35.45015100	O	11.79208400	3.84639800	44.54747700
H	21.04504600	1.27450100	38.40707600	C	11.80375800	2.61102900	41.65099000
H	22.70601000	1.87048000	36.56041900	C	11.20413300	2.33582700	40.23218000
H	22.36838600	0.30869300	35.81267900	O	11.31274000	3.26512500	39.37108200
H	19.66589100	-0.28575400	39.39532800	O	10.72983100	1.19459400	40.05894400
O	20.75671000	-1.48968500	36.73234900	H	12.11855300	4.53427800	40.20135600
N	20.00635400	-1.06718800	38.84351700	H	10.67106700	4.32273700	42.36064100
H	19.29288000	-1.76784200	38.66206300	H	11.31756700	1.95848100	42.37947800
N	20.63856400	4.05119400	36.28576200	H	12.86238900	2.31488800	41.60983200
C	20.22602600	5.23635700	37.03019500	N	13.72500600	4.52595800	43.53672700
H	19.80535800	5.97408600	36.33172900	C	14.47858800	4.65805800	44.77344600
C	21.38879100	5.86263000	37.81225200	C	14.78128100	6.12629100	45.13811900
H	21.02281100	6.79158800	38.27089100	O	15.75526500	6.41538800	45.84555600
C	21.98974300	4.94210800	38.87667300	C	15.75346800	3.80332000	44.78258700
H	19.42134500	4.92731200	37.70184000	C	16.20423500	3.45186900	46.20382100
H	22.29027300	3.98360200	38.44116300	H	13.82353600	4.27586400	45.56461500
H	22.17488600	6.15973400	37.10591900	H	14.15609000	4.82551600	42.66979200
H	21.52038300	4.11110300	35.78013000	H	16.55929600	4.28340900	44.21809900
H	22.89627300	5.38103600	39.30246200	H	15.52163300	2.85652400	44.27747800
H	21.27262500	4.73828000	39.68154300	O	15.42724200	3.41393200	47.15280200
C	15.54588400	3.18035200	36.55563800	N	17.52094500	3.12778400	46.32365500
C	15.60744600	3.85025500	37.91636800	H	17.83753000	2.80558200	47.22731100
O	14.64151800	4.45442000	38.39281800	H	18.16272800	3.04331800	45.54262300
C	14.85019500	1.79515700	36.63847900	N	13.88652500	7.03609600	44.69150200
C	13.41495900	1.78789000	37.20179300	C	13.95707000	8.45089700	45.02650300
C	12.42412900	2.58512800	36.34306400	H	12.97469300	8.76015300	45.40878500
C	12.91608600	0.34870400	37.40395200	C	14.34798600	9.34166800	43.83801000
H	13.63006000	-0.24187900	37.99434100	C	15.78499000	9.12601100	43.35604900
H	11.96511200	0.35715500	37.94724700	H	14.68252700	8.54717900	45.83933300
H	12.77661300	-0.16590200	36.44122500	H	13.65355000	9.15781500	43.00973200

H	15.93709000	8.08492800	43.05053700	C	22.98509300	5.65061300	49.06956400
H	15.99484700	9.76213900	42.48959100	C	20.58830200	6.09217500	48.62249900
H	13.16618900	6.75051900	44.03034900	C	19.21974200	6.23015600	49.06088500
N	31.72164500	0.52254600	44.34630400	C	18.45559700	6.37418600	47.94198500
C	31.89116800	0.64877600	42.90703900	C	19.36390800	6.34163500	46.82277800
C	30.60734700	1.17515900	42.26455500	C	19.80814300	6.40825800	44.40585500
O	29.53030800	1.11301900	42.85451100	C	19.38948300	6.56435300	43.03458400
H	30.81710800	0.08808100	44.54580400	C	20.50981400	6.44390200	42.27009500
H	32.72770600	1.32754800	42.68757400	C	21.61038000	6.19346700	43.17209900
N	30.70981700	1.68382100	41.00418000	N	23.94807300	5.68776200	44.98529700
C	29.51797500	1.95139200	40.19918200	N	23.42542400	5.61566000	47.77405100
C	28.98575300	0.63411400	39.58100400	N	20.65644900	6.17445000	47.25389400
O	29.69294500	-0.37388200	39.52364300	N	21.16804500	6.18972900	44.46896500
C	30.07329800	2.88384200	39.10542200	Fe	22.29845300	5.85765200	46.12774900
C	31.46133400	2.27662700	38.82788400	O	21.96774100	4.07613700	46.05642300
C	31.94070700	1.78031200	40.21032300	C	23.82067200	-1.68373000	41.95887200
H	31.36201900	1.42418000	38.14971700	N	24.87031200	-0.74294700	41.63119400
H	28.74523200	2.41226800	40.81727900	C	25.93981600	-0.33994400	42.37411100
H	32.63682900	2.49273500	40.67434600	O	26.70991600	0.51630600	41.94734500
H	32.44451400	0.81010500	40.13467500	C	26.14902200	-0.92112800	43.79022600
H	32.16163200	2.98971500	38.38055700	N	27.56741300	-0.75391600	44.10135900
H	30.16450700	3.90141500	39.50385500	C	28.21469200	-1.49403000	45.02276200
H	29.42884900	2.91957100	38.22323600	O	29.40035700	-1.39953500	45.33100700
N	27.74597000	0.71218200	39.04853000	C	25.19980400	-0.22217100	44.75943600
C	27.08621200	-0.49183400	38.55961400	C	25.15245100	1.17823500	44.81061300
C	25.71290800	-0.18996900	37.94800600	C	24.23737700	1.83564500	45.62033600
O	24.81189100	0.36282100	38.92020000	C	23.33039500	1.10473700	46.41255800
C	25.08443900	-1.46198900	37.38471100	C	23.40340400	-0.29786800	46.40448200
H	26.96595300	-1.21806400	39.37471400	C	24.32504500	-0.94552600	45.58185200
H	24.11268400	-1.24440900	36.92926400	O	22.39931500	1.70500300	47.17925800
H	25.72987900	-1.90580700	36.61747600	C	22.49664300	-1.17304200	41.28540800
H	27.15820900	1.52744200	39.23813100	C	21.79610200	-0.11053000	42.11972800
H	25.84230200	0.54878300	37.14392100	C	20.55685800	-0.40479800	42.72275000
H	24.93611100	-2.19633600	38.18273700	C	19.89995300	0.54153400	43.48467500
H	25.05078000	1.32933300	39.02817400	C	20.46418900	1.86786800	43.71932800
C	23.51311500	8.82331600	44.82076400	C	21.74287300	2.11804200	43.08265400
S	22.41663400	8.27685300	46.16601700	C	22.36761800	1.17410100	42.30455800
H	23.54736600	9.91698700	44.81838700	O	19.88813700	2.74388800	44.41595000
H	24.51919900	8.41270200	44.94145700	Cl	18.36445500	0.16379800	44.20953400
C	22.92146000	5.94232900	42.77182400	C	24.15081100	-3.10912000	41.43718700
H	23.11409500	5.93972600	41.70398600	O	24.81595900	-3.23744500	40.42020700
C	25.61943200	5.29181300	46.73504500	C	23.71518600	-4.30058400	42.22123500
H	26.66697800	5.07869700	46.92622900	O	21.66158800	-2.28865700	41.02948100
C	21.66985600	5.87317100	49.46697000	C	22.83182700	-4.24235700	43.31373700
H	21.46616200	5.85346300	50.53390500	C	22.47051900	-5.39297700	44.00540300
C	18.95591300	6.45708900	45.49728000	C	22.99518400	-6.63034600	43.61507700
H	17.89127500	6.58555600	45.32394600	C	23.87479700	-6.70793600	42.52657700
C	23.99712000	5.67026600	43.61142800	C	24.22313000	-5.55296700	41.83923200
C	25.34199600	5.36067500	43.14228900	O	22.61710000	-7.73101400	44.32905500
C	26.09218800	5.20872900	44.27460800	H	23.68790500	-1.70343200	43.04139800
C	25.22561000	5.40489500	45.40806300	H	24.88937400	-0.37854100	40.66878600
C	25.77102400	5.23278600	41.70827100	H	25.91733100	-1.99380400	43.78858200
H	26.86118800	5.34341300	41.65587200	H	28.08808400	-0.04057900	43.58136800
H	25.35625100	6.04542500	41.10180900	H	25.83103200	1.75928800	44.19175400
C	25.37182200	3.90739200	41.02203900	H	24.18807400	2.91706100	45.62899300
H	25.94075600	3.05997700	41.41880100	H	22.71488100	-0.86001200	47.02869700
H	24.31293900	3.69275000	41.23137600	H	24.35591900	-2.03481900	45.57298400
C	25.50858000	3.96771000	39.47923200	H	22.29471600	2.65794700	46.88873000
O	25.72540700	2.85481300	38.87741500	H	22.81550200	-0.72335800	40.33611100
O	25.36532600	5.07576000	38.92649700	H	20.12461700	-1.38807900	42.57745600
C	24.77384700	5.39086800	47.83623600	H	22.18539200	3.09286600	43.25503600
C	25.19935800	5.26748700	49.21017500	H	23.32008800	1.40586000	41.83999000
C	24.08601700	5.43001000	49.97769600	H	21.16930100	3.90617700	45.51732100

N	13.86974000	6.96720600	44.76362400	H	24.33076000	3.70553500	41.25970100
C	13.87187400	8.37911700	45.11850200	C	25.49737100	3.95169700	39.48333400
H	12.86816100	8.63819800	45.48123400	O	25.73655500	2.83053400	38.90832500
C	14.25036300	9.30636500	43.95388700	O	25.31204400	5.04219700	38.90700200
C	15.69746400	9.14310800	43.48186100	C	24.74144800	5.41419000	47.80015100
H	14.57350000	8.49521900	45.94960700	C	25.15378000	5.26997000	49.17427200
H	13.57074500	9.12342500	43.11339200	C	24.03664700	5.44320900	49.93533200
H	15.87845600	8.11774000	43.14105900	C	22.94823900	5.68974100	49.02149600
H	15.89998000	9.81428900	42.64051700	C	20.56102800	6.16293000	48.56000600
H	13.15289500	6.65277100	44.11221700	C	19.19098600	6.30988700	48.98880900
N	31.58032300	0.51320300	44.48855100	C	18.43527400	6.46366600	47.86593500
C	31.78282200	0.61162600	43.05121500	C	19.35109600	6.43264200	46.75341200
C	30.51957200	1.14075400	42.37115000	C	19.81909000	6.53356200	44.34280600
O	29.42672900	1.08771200	42.93355200	C	19.41477200	6.70652500	42.96933900
H	30.66935400	0.08692400	44.67572200	C	20.54241100	6.59134000	42.21507700
H	32.63225600	1.27612500	42.83899000	C	21.63311300	6.32639000	43.12457000
N	30.65793400	1.63986200	41.11098500	N	23.94721200	5.76233400	44.94782700
C	29.49015400	1.91488200	40.27371900	N	23.39580900	5.65956200	47.72959500
C	28.97350200	0.60355000	39.62981100	N	20.63992000	6.25163200	47.19010700
O	29.68344500	-0.40325300	39.57847700	N	21.17733000	6.31172400	44.41887400
C	30.07910500	2.85261500	39.20240100	Fe	22.28190600	5.95651900	46.07447000
C	31.47241600	2.24219200	38.95959900	O	21.91920500	4.11769500	45.93249100
C	31.91053100	1.73170100	40.35090200	C	23.81435800	-1.83359400	41.88023400
H	31.38955700	1.39624400	38.27119700	N	24.86079500	-0.88673800	41.56006700
H	28.70113300	2.37363100	40.87259500	C	25.88238500	-0.42776900	42.33167500
H	32.59971200	2.43480300	40.83874300	O	26.65489500	0.43145500	41.91494300
H	32.40747100	0.75750800	40.28162000	C	26.03616700	-0.94822500	43.78008500
H	32.18788900	2.95668100	38.53922200	N	27.44530100	-0.78335500	44.13172900
H	30.16252300	3.86737200	39.60994800	C	28.05078600	-1.48505800	45.11124500
H	29.45958800	2.89603800	38.30277000	O	29.22267300	-1.37938600	45.46320900
N	27.74801100	0.68913500	39.06774600	C	25.07748300	-0.17493300	44.67748900
C	27.10012200	-0.50587200	38.54203100	C	25.10169800	1.23126700	44.67052000
C	25.73753500	-0.18841900	37.91392600	C	24.20438500	1.96184500	45.42202400
O	24.81377100	0.32608000	38.88417500	C	23.23458900	1.31897700	46.25875500
C	25.12050700	-1.43765600	37.29146100	C	23.24348900	-0.11055600	46.28133600
H	26.96829700	-1.25037600	39.33881700	C	24.14026800	-0.82630800	45.50388000
H	24.16621600	-1.18958800	36.81449900	O	22.38941000	1.99065700	46.97414400
H	25.78500300	-1.86297700	36.52984200	C	22.47607600	-1.30101200	41.26219400
H	27.15373800	1.49950100	39.26106800	C	21.82837900	-0.22481700	42.12024200
H	25.88334000	0.57753900	37.13893400	C	20.69138000	-0.53873700	42.89239300
H	24.93798000	-2.19486900	38.06067100	C	20.09245300	0.41427900	43.69541000
H	25.04160500	1.28817000	39.02372400	C	20.59830600	1.77318300	43.79723300
C	23.63988400	8.89090300	44.89369700	C	21.77202000	2.04225900	42.99729700
S	22.47703700	8.35295500	46.18893200	C	22.34570600	1.08823600	42.18034400
H	23.71338700	9.98231600	44.93256200	O	20.05010300	2.66204100	44.51619100
H	24.62825000	8.44570600	45.03748000	Cl	18.67112600	-0.00609000	44.62119000
C	22.94137500	6.05853600	42.73096400	C	24.14308900	-3.23623900	41.30363500
H	23.14109600	6.06245700	41.66438200	O	24.74514700	-3.32739900	40.24375400
C	25.59707700	5.31941800	46.70607800	C	23.79441500	-4.45467500	42.09096300
H	26.63968200	5.09002700	46.90501100	O	21.62310300	-2.41608100	41.05681300
C	21.63163100	5.92718800	49.41130000	C	22.90745100	-4.45601000	43.18218600
H	21.41913700	5.90191200	50.47619600	C	22.63215200	-5.62692300	43.87975100
C	18.95519700	6.56768500	45.42614200	C	23.25152000	-6.82300400	43.49929300
H	17.89246200	6.70036400	45.24622600	C	24.13480400	-6.84108000	42.41127600
C	24.00657200	5.75601500	43.57597900	C	24.39380100	-5.66767200	41.71493500
C	25.34720100	5.42303300	43.11264200	O	22.95921400	-7.94446400	44.22210300
C	26.08854500	5.25366100	44.24939000	H	23.69966000	-1.88989200	42.96284200
C	25.21760800	5.45520000	45.37701300	H	24.87797000	-0.51260300	40.60081700
C	25.77523300	5.27334000	41.68079200	H	25.78762400	-2.01528500	43.82920600
H	26.86427400	5.39294700	41.62226000	H	27.98582900	-0.08183100	43.61478400
H	25.34966900	6.06720900	41.05732300	H	25.82518200	1.74621100	44.04453800
C	25.38388500	3.92752200	41.02933500	H	24.21941200	3.04322000	45.39198700
H	25.96687400	3.09553900	41.43820500	H	22.51975400	-0.61216900	46.91650500

H	24.12143000	-1.91577600	45.53088400	H	22.26885500	6.11692800	36.83115600
H	22.21072100	3.17890600	46.51390100	H	21.54988500	4.00176700	35.64063900
H	22.76139800	-0.86985100	40.29340400	H	22.92824700	5.47386400	39.09424500
H	20.28290800	-1.54244400	42.84483700	H	21.27926700	4.91108700	39.48407900
H	22.17386600	3.04927000	43.04827500	C	15.58351200	3.47610500	36.37773700
H	23.21722100	1.34868300	41.58659200	C	15.60033600	4.05130500	37.78280300
H	21.14484100	3.86491200	45.37793500	O	14.60998600	4.59993900	38.27657100
H	20.95241600	-2.12490900	40.40388900	C	14.99370100	2.04109300	36.36129600
H	22.39834700	-3.54488700	43.47645700	C	13.57385400	1.88938900	36.94293500
H	21.94035000	-5.63468500	44.71593400	C	12.51419300	2.67129400	36.15489800
H	24.61453400	-7.77339500	42.11577600	C	13.18298500	0.40748200	37.04998600
H	25.06932600	-5.66334800	40.86560500	H	13.94807400	-0.16992300	37.58634700
H	23.45249800	-8.69180800	43.84891800	H	12.24388800	0.30793400	37.60445600
H	23.26908000	8.59848200	43.90455200	H	13.06138600	-0.04703500	36.05552000
H	14.07878600	10.34318400	44.28032700	H	12.41654900	2.28935900	35.12716200
H	16.40967700	9.36115200	44.28791100	H	11.55166600	2.58708900	36.66711400
H	32.27470200	-0.11820300	44.88231900	H	12.75591500	3.73869100	36.10722700
H	32.01192100	-0.34592000	42.53922300	H	14.97596700	4.14266000	35.75848500
H	27.37079900	-2.21667700	45.59546100	H	13.56498300	2.30250500	37.95674400
H	20.64507400	6.65851600	41.13972900	H	15.68381100	1.38579800	36.91119200
H	18.39238000	6.85906700	42.64872000	H	15.00746700	1.69000000	35.31844300
H	17.36336400	6.55896900	47.75170900	N	16.76139800	3.90078400	38.49061400
H	18.86364200	6.26820100	50.02024100	C	16.76896700	4.02279100	39.94818900
H	23.94037500	5.40484200	51.01315200	C	16.52566900	5.44798600	40.47680700
H	26.16590000	5.05847400	49.49525000	O	16.24070900	5.62365700	41.66259900
H	27.13641300	4.98706300	44.32016400	C	18.07610500	3.46333500	40.52228400
H	27.75610900	-0.95878100	37.78835800	H	17.55235900	3.43887600	38.03801400
H	25.08058600	5.51884600	36.76277600	H	15.92517000	3.44961400	40.35211200
H	16.57291200	3.29469100	36.05145200	H	18.94445500	4.00351300	40.13047500
H	11.89771600	6.67860900	39.26573000	H	18.07482100	3.56029900	41.61007600
2IM2_B				H	18.18108400	2.40490900	40.26022300
C	24.95462700	5.64986000	35.46687100	N	16.65426500	6.46554300	39.58536300
S	24.13199400	4.20584400	34.69440400	C	16.23352300	7.81929600	39.90434300
C	25.22939000	2.88064600	35.32350000	C	14.71678500	8.06469600	40.05993400
H	24.30570000	6.51742300	35.31379000	O	14.34044900	9.16777800	40.45054100
H	25.33496300	2.94620500	36.41276500	H	16.76534600	6.20067600	38.61674700
H	24.77471800	1.92421800	35.04930500	H	16.67987900	8.12250700	40.85385400
H	26.21409800	2.94943900	34.84951700	H	16.61312100	8.49557400	39.13281300
H	25.91618100	5.84079500	34.97877800	N	13.90020800	7.03090700	39.74556900
H	21.03741700	1.91496600	34.65244200	C	12.48284800	7.03595300	40.07694500
C	20.63577200	1.62954000	35.63267600	C	12.19308200	6.16125500	41.31316100
C	20.01186400	2.83810500	36.31593900	O	11.91501200	6.66897100	42.40522900
O	18.98932600	2.71538700	37.00817400	H	14.28542100	6.15765700	39.39047300
C	21.76698700	0.99498200	36.47035300	H	12.19472300	8.06074200	40.30992800
C	21.35990100	0.56388300	37.88222500	N	12.32350500	4.82876900	41.10148200
C	20.40682000	-0.62297200	37.89691000	C	11.83855000	3.84503900	42.07117700
H	22.27189800	0.28697000	38.42768500	C	12.49503500	3.92147200	43.45766000
H	19.83963300	0.89798600	35.47620600	O	11.87456400	3.53187700	44.44239800
H	20.91081600	1.39788000	38.43545700	C	12.03609600	2.42063000	41.50525300
H	22.60276700	1.69820900	36.55707200	C	11.42781400	2.15891200	40.09355700
H	22.13518200	0.11731200	35.92867400	O	11.44326200	3.10952800	39.25939500
H	19.69532000	-0.11551500	39.77377400	O	11.02547600	0.98828800	39.89128800
O	20.19928000	-1.34526600	36.93720300	H	12.22593900	4.45047300	40.14151900
N	19.82128200	-0.89836900	39.13935600	H	10.77125700	4.01085300	42.26417100
H	19.00399900	-1.49730000	39.06739700	H	11.62215500	1.70370500	42.21790400
N	20.66185700	4.01306900	36.13920900	H	13.11397300	2.21574500	41.43048200
C	20.28772300	5.26253600	36.79429600	N	13.78901600	4.36078400	43.50927900
H	19.90050500	5.96420900	36.04131500	C	14.50010300	4.48190300	44.77364400
C	21.46429900	5.89931100	37.54558900	C	14.74297300	5.94897000	45.18357600
H	21.12879600	6.87081100	37.93364300	O	15.70631000	6.25805800	45.89477700
C	22.01618900	5.03500900	38.68089400	C	15.79934800	3.66561500	44.81157700
H	19.46629000	5.02911200	37.47627800	C	16.20284000	3.30607400	46.24573600
H	22.28974500	4.03917200	38.31702400	H	13.83206500	4.05941400	45.53262200

H	14.23486000	4.71101500	42.66783600	C	26.08601600	5.31957800	44.01497100
H	16.61199400	4.17851600	44.28770400	C	25.24328700	5.51938100	45.16915100
H	15.61466000	2.72049600	44.28450800	C	25.70866900	5.34514700	41.46015300
O	15.38246700	3.21346400	47.15468900	H	26.79525100	5.47174100	41.37461500
N	17.52487500	3.04347100	46.42608600	H	25.26603000	6.13600700	40.84543100
H	17.80418800	2.71410600	47.33933100	C	25.31530300	3.99116200	40.82984800
H	18.20938200	2.98504400	45.67788900	H	25.86261000	3.16190700	41.29120200
N	13.80314000	6.83257300	44.77376400	H	24.24927400	3.79818500	41.02452900
C	13.81193700	8.23512900	45.16348900	C	25.49760700	3.95933300	39.29349500
H	12.80614600	8.49420300	45.52115500	O	25.69237800	2.80307800	38.76280000
C	14.21382900	9.18790000	44.02777100	O	25.41217400	5.03383200	38.67067200
C	15.66670800	9.02364600	43.57464000	C	24.85369200	5.58486400	47.60847100
H	14.50432000	8.32396400	46.00563200	C	25.31508100	5.52208100	48.97311100
H	13.54574600	9.03100900	43.17260100	C	24.22460400	5.73078300	49.76540600
H	15.84491400	8.00268900	43.21977600	C	23.09702900	5.91164800	48.88472700
H	15.88719200	9.70832600	42.74888000	C	20.67237900	6.21725300	48.48680200
H	13.09647100	6.53855000	44.10291800	C	19.30953300	6.32215900	48.96149600
N	31.72491100	0.33612000	44.33386200	C	18.50882600	6.37328600	47.86200300
C	31.85445300	0.52583900	42.89692500	C	19.38854200	6.31812900	46.71746000
C	30.54507300	1.05505700	42.31167700	C	19.79083100	6.37908700	44.29201700
O	29.49057600	0.96532200	42.94035100	C	19.33481800	6.52228000	42.92983100
H	30.81387400	-0.08086300	44.53720800	C	20.44560900	6.47175200	42.14394100
H	32.67292800	1.22796200	42.68274800	C	21.57575200	6.27690800	43.02482100
N	30.59743000	1.59853100	41.06610600	N	23.96037200	5.81161600	44.77284800
C	29.37556100	1.86143400	40.30548800	N	23.50358200	5.82222100	47.57458400
C	28.84266700	0.54079700	39.69201000	N	20.69755800	6.21328800	47.11762900
O	29.52568000	-0.48539300	39.68974700	N	21.15233900	6.23491900	44.32909200
C	29.87872700	2.82189400	39.21192500	Fe	22.33737400	6.09546800	45.94988900
C	31.26359500	2.23820200	38.87486700	O	22.05082600	4.03608800	45.84011900
C	31.79813300	1.72152400	40.22960100	C	23.77878300	-1.64296600	41.99605000
H	31.15265100	1.39859900	38.18190100	N	24.80883400	-0.67032900	41.68659900
H	28.61524500	2.29651200	40.95664400	C	25.84170400	-0.24029600	42.45315100
H	32.50351700	2.43186900	40.68201100	O	26.59224000	0.65931600	42.08882300
H	32.30751900	0.75758900	40.11853900	C	26.06473400	-0.87960500	43.85097900
H	31.93894500	2.96845600	38.41750700	N	27.48853300	-0.77130300	44.14467600
H	29.97184300	3.83249600	39.62685300	C	28.12208300	-1.59641200	45.00914100
H	29.20316600	2.86726000	38.35412600	O	29.31340600	-1.56964000	45.29422600
N	27.62516700	0.63251100	39.11541900	C	25.19536700	-0.16579700	44.87825700
C	26.96001200	-0.55944600	38.60502500	C	25.28247600	1.24206800	45.01239300
C	25.59306700	-0.22680900	37.99528600	C	24.46056100	1.91658800	45.88164200
O	24.71353300	0.36107000	38.96777600	C	23.49257400	1.20498100	46.69677800
C	24.92875900	-1.48085300	37.43466900	C	23.46750200	-0.24177400	46.58384700
H	26.83047900	-1.29626900	39.40851600	C	24.28910000	-0.89075900	45.68888200
H	23.97021800	-1.22970900	36.96903600	O	22.68960800	1.80917700	47.46087700
H	25.56561000	-1.94985300	36.67510900	C	22.45138900	-1.15520400	41.31588900
H	27.06217000	1.48120000	39.22199300	C	21.74768900	-0.09474900	42.14780300
H	25.74049300	0.50519200	37.18926700	C	20.61898400	-0.44086400	42.91175400
H	24.75001800	-2.20645000	38.23397400	C	20.00174900	0.49134200	43.72886200
H	24.95775100	1.33290300	39.02006400	C	20.49199200	1.84978600	43.86115800
C	24.27365300	8.75400200	46.40740300	C	21.63296000	2.16674600	43.03453000
S	22.55018000	8.33346900	45.95883000	C	22.22709800	1.23452900	42.21080500
H	24.36672500	9.84372700	46.34249700	O	19.96916500	2.70273300	44.64464700
H	24.51311500	8.43921600	47.42707500	Cl	18.60407600	0.02081300	44.66568100
C	22.88095400	6.07687900	42.59056700	C	24.16264000	-3.05809700	41.48984200
H	23.04858700	6.09606300	41.51877900	O	24.85275000	-3.17464900	40.48808800
C	25.66847900	5.42555600	46.48788800	C	23.75641600	-4.25521500	42.28178500
H	26.71943100	5.21164600	46.66053500	O	21.63804200	-2.29370700	41.08627800
C	21.78742300	6.10101100	49.31106100	C	22.81357100	-4.22505300	43.32513100
H	21.61529800	6.12927300	50.38341200	C	22.49174000	-5.37727000	44.03328600
C	18.95102900	6.39291700	45.40250500	C	23.11669200	-6.58758500	43.71044300
H	17.87991300	6.47833800	45.24595500	C	24.05448800	-6.63745800	42.67001100
C	23.98031400	5.81311500	43.40367600	C	24.36217700	-5.48183900	41.96420800
C	25.31392300	5.49255200	42.90220600	O	22.77493500	-7.68889900	44.44063700

N	14.85546700	4.05999000	44.31385100	H	26.60465500	5.85489900	46.81679200
C	15.43558300	4.56623800	45.54698800	C	21.88449000	8.06530000	49.05320700
C	15.14224000	6.06586100	45.75065900	H	21.73532800	8.38858700	50.07967400
O	15.94806800	6.79974800	46.33292300	C	19.03590200	7.54909400	45.17878500
C	16.93308500	4.26030400	45.69404600	H	17.96846700	7.62943900	45.00258800
C	17.36403000	4.24625500	47.16422000	C	24.01096700	6.24510100	43.40348200
H	14.92248200	4.03073500	46.35418800	C	25.34696600	5.82588800	42.99189200
H	15.13182100	4.46797400	43.42666900	C	26.06210500	5.70908300	44.15190000
H	17.54880400	4.95221400	45.11052500	C	25.19741900	6.08027600	45.24416000
H	17.10962700	3.25118600	45.30045900	C	25.80081700	5.57693100	41.57877000
O	16.58799500	3.96601800	48.07214800	H	26.81876400	5.97027700	41.45624300
N	18.69319400	4.45861700	47.38837500	H	25.18101900	6.12946200	40.86721800
H	18.97853800	4.52796900	48.35549900	C	25.78480000	4.09688700	41.14440000
H	19.31896400	4.87293100	46.70938900	H	26.63837900	3.54745200	41.55479500
N	13.93541600	6.48668400	45.29899300	H	24.89681900	3.59614400	41.55280800
C	13.45039700	7.84392800	45.50529900	C	25.72330300	3.88667700	39.61051400
H	12.41364100	7.78160800	45.86189500	O	26.12152100	2.74508400	39.19013500
C	13.50790800	8.72574200	44.24925700	O	25.25144000	4.80444700	38.90844800
C	14.92601700	8.98592900	43.73443600	C	24.80230300	6.64762700	47.61262500
H	14.05860500	8.27650400	46.30521200	C	25.25703000	6.83217400	48.96881900
H	12.91687800	8.26531700	43.44980500	C	24.22855000	7.40972200	49.65320200
H	15.41820600	8.04647100	43.45949900	C	23.13794700	7.56169900	48.72152700
H	14.89529500	9.61220000	42.83713700	C	20.78665000	8.11795900	48.20316900
H	13.35113000	5.84927200	44.76170600	C	19.44464200	8.46710000	48.61877500
N	29.95413900	-1.27781000	45.37231800	C	18.63262300	8.26881700	47.54506900
C	30.57983800	-0.90828400	44.11208400	C	19.48748400	7.83386800	46.46297300
C	29.62034100	-0.07787300	43.26132000	C	19.85461300	7.18404800	44.11730500
O	28.41372100	-0.04445600	43.50638700	C	19.39612900	6.98455200	42.76138800
H	29.01338400	-1.63607500	45.19578300	C	20.50375300	6.71980400	42.01547600
H	31.49659600	-0.33385700	44.30685800	C	21.63329800	6.72063200	42.91697800
N	30.14612700	0.59067100	42.20310000	N	23.94720900	6.39999000	44.76933700
C	29.27156000	1.15690700	41.17190600	N	23.50705200	7.08832300	47.48582700
C	28.76196100	0.02754100	40.24265800	N	20.78856700	7.74911600	46.88371500
O	29.38800300	-1.03231200	40.13523800	N	21.21555700	7.00086600	44.19223900
C	30.23150200	2.09850800	40.42072100	Fe	22.38368600	7.15008800	45.81527300
C	31.55435500	1.30958400	40.42804700	O	21.65011800	5.16913800	46.28160500
C	31.55520100	0.58272500	41.79065900	C	23.00354900	-1.67455200	41.15071500
H	31.54588900	0.56902200	39.62394000	N	24.19617500	-0.84205000	41.15843400
H	28.42854900	1.67277600	41.63523800	C	24.85779700	-0.25028800	42.19498900
H	32.16933700	1.11266600	42.53205000	O	25.70072700	0.62106100	42.00318900
H	31.93615700	-0.44019500	41.69740900	C	24.63972700	-0.73771800	43.64694400
H	32.43567000	1.94688200	40.30131300	N	25.92391900	-1.24223800	44.13008100
H	30.33304300	3.03695100	40.97901300	C	26.08952300	-2.44805400	44.72324400
H	29.87264800	2.33782800	39.41622600	O	27.14792200	-2.89845400	45.14431000
N	27.65852100	0.32828700	39.53324400	C	24.11634900	0.34136400	44.60244600
C	27.06305000	-0.64866000	38.63027500	C	24.34737500	1.68741400	44.45406300
C	25.97019500	-0.01659500	37.75967200	C	23.74343400	2.61090900	45.34978500
O	24.89166500	0.47863700	38.56307200	C	23.16287900	2.13635700	46.63535800
C	25.41211800	-1.02404700	36.75851000	C	22.96799800	0.68477700	46.75698800
H	26.63215000	-1.48407600	39.19950500	C	23.42217200	-0.14435900	45.78929200
H	24.66730900	-0.54138400	36.11638800	O	22.86266000	2.91896200	47.54161600
H	26.20914600	-1.42339700	36.11943600	C	21.79081300	-0.86748600	40.57156800
H	27.13990100	1.19468500	39.71477600	C	21.50495100	0.29158100	41.50325100
H	26.41163200	0.83420000	37.22165900	C	20.77209800	0.07460300	42.67549400
H	24.92931300	-1.85336000	37.28311000	C	20.82082600	1.00491800	43.71000200
H	25.17112300	1.39307300	38.84645000	C	21.61385000	2.18656700	43.59805100
C	24.69314800	9.49805800	45.52012200	C	22.19584100	2.45438500	42.33449900
S	22.88531800	9.27952600	45.34043900	C	22.15018200	1.52548900	41.31048300
H	24.91314100	10.55009800	45.30666100	O	21.88109900	2.94747000	44.63075900
H	25.02599600	9.26722200	46.53560500	Cl	19.91316100	0.72700800	45.17135000
C	22.93652900	6.41189500	42.53785100	C	23.26267000	-2.93645400	40.29250600
H	23.11218300	6.24319800	41.48053300	O	23.91309100	-2.82364100	39.26371600
C	25.58842800	6.15356600	46.57614800	C	22.77893600	-4.26777300	40.75116200

O	20.71358200	-1.77222000	40.43091400	H	22.67545300	1.65569100	35.94847400
C	21.78285300	-4.44771200	41.72696800	H	22.00381400	0.24328300	35.12525500
C	21.38121700	-5.72146400	42.11172800	H	19.17903100	0.44998800	38.53662100
C	21.98134700	-6.84379400	41.52905300	O	20.14298900	-1.37219400	36.21868700
C	22.97068500	-6.68262900	40.54921400	N	19.35187200	-0.48452900	38.17525800
C	23.35485500	-5.40575100	40.16251500	H	18.48923600	-0.99216800	37.99151200
O	21.56356800	-8.07335700	41.94965500	N	20.72208900	4.18620000	36.08886700
H	22.75254600	-1.96478000	42.17112000	C	20.39702500	5.31613000	36.95717900
H	24.48420300	-0.47261400	40.23849100	H	20.09645400	6.16416200	36.32687700
H	23.93883200	-1.57678600	43.68846900	C	21.56885000	5.72472400	37.85914900
H	26.76446800	-0.68088600	43.94502300	H	21.27849800	6.64193400	38.38978600
H	24.91236200	2.04944400	43.60444200	C	21.99471500	4.64710800	38.85807300
H	24.02351900	3.65656400	45.31235100	H	19.52620000	5.02383600	37.54764300
H	22.47553300	0.32355700	47.65351300	H	22.19142300	3.69905700	38.34463700
H	23.28062800	-1.21833700	45.89008000	H	22.42766300	5.99248900	37.23089700
H	22.19528700	4.65627100	46.91484500	H	21.57227600	4.26444200	35.53645600
H	22.11859900	-0.48721300	39.59716000	H	22.92769400	4.93478000	39.35013500
H	20.20247700	-0.84147100	42.79297300	H	21.21928300	4.47056900	39.61350400
H	22.74081700	3.38660000	42.22890300	C	15.79756900	3.12069200	36.06322600
H	22.68251800	1.71741000	40.38318800	C	15.64460700	3.84298500	37.39552800
H	21.62484200	4.60005100	45.48476400	O	14.58060100	4.40273000	37.70732700
H	20.10636600	-1.39486400	39.75849100	C	15.86678600	1.58308700	36.22142700
H	21.27761500	-3.58909200	42.15363900	C	14.73830000	0.94927700	37.05666100
H	20.60074600	-5.86652300	42.85166900	C	13.35256300	1.16462000	36.43049900
H	23.43340500	-7.55740200	40.09440600	C	15.00432300	-0.54459400	37.29225100
H	24.11264200	-5.26185400	39.39944800	H	16.03506600	-0.71114200	37.63596000
H	22.04812800	-8.75298100	41.45520400	H	14.34557900	-0.91936500	38.08163500
H	25.24413600	8.87260700	44.81256800	H	14.86076800	-1.13870600	36.37724300
H	13.01889600	9.68169200	44.49189000	H	13.29907200	0.74713300	35.41302600
H	15.54603400	9.48050900	44.49257900	H	12.58400700	0.67313600	37.03808500
H	30.47876300	-2.04015600	45.79583000	H	13.09710400	2.22882500	36.38217600
H	30.88558700	-1.75950000	43.46952600	H	14.94439500	3.41745200	35.44739800
H	25.14224600	-3.02222200	44.80269800	H	14.71512900	1.42129700	38.04756000
H	20.56515700	6.51060400	40.95504200	H	16.83457300	1.33398900	36.67450000
H	18.36223900	7.01637600	42.44181300	H	15.88266400	1.14100300	35.21243100
H	17.55712900	8.35160900	47.46389200	N	16.74068900	3.85270300	38.20011600
H	19.17309500	8.77842500	49.62029800	C	16.67957300	4.06559800	39.65437200
H	24.19179400	7.69916400	50.69653500	C	16.47401400	5.51814900	40.11930600
H	26.23925700	6.55595600	49.33257100	O	16.65308400	5.83131400	41.29718200
H	27.10024500	5.41723200	44.26224400	C	17.90866800	3.44202400	40.31884700
H	27.85481900	-1.06871600	37.99786700	H	17.59106100	3.42416500	37.83643400
H	25.01951200	5.74591400	36.89626800	H	15.78616600	3.52665200	40.01270400
H	16.73666800	3.43521300	35.62723000	H	18.84070400	3.82414700	39.88595600
H	11.54648200	5.05533900	40.21983200	H	17.90553000	3.68095600	41.38365900
				H	17.88745900	2.35382400	40.19882800
				N	15.99496700	6.40076000	39.18744100
C	25.05818000	5.99788000	35.83587900	C	15.29097000	7.58908100	39.63297500
S	24.35833700	4.59181300	34.89109700	C	13.88867400	7.34641900	40.22642800
C	25.43546300	3.25682900	35.53452700	O	13.30851200	8.26888900	40.79577500
H	24.38462200	6.85045800	35.70813100	H	15.64006400	5.97473600	38.33785500
H	25.45877300	3.27119100	36.62906600	H	15.86912900	8.07542000	40.42040100
H	25.02561800	2.30581200	35.18271000	H	15.20151200	8.29348300	38.79948800
H	26.45215900	3.36778200	35.14371600	N	13.37819600	6.09446300	40.08276900
H	26.04459300	6.26605700	35.44317100	C	12.18734100	5.67769700	40.80343800
H	21.02647000	2.37671400	34.27605100	C	12.47666100	4.86901100	42.08836300
C	20.65041500	1.91519800	35.19714900	O	11.95610400	5.19567100	43.16241600
C	20.11391900	2.97854400	36.14747500	H	13.85384400	5.41605500	39.49257800
O	19.18212700	2.71508200	36.92514600	H	11.63666800	6.57116200	41.09696400
C	21.76825900	1.05379800	35.82329300	N	13.29523200	3.80648100	41.93077600
C	21.41331200	0.44039500	37.18290700	C	13.38937100	2.73477300	42.92221000
C	20.25033400	-0.54220500	37.10546000	C	13.84888800	3.20277200	44.30829600
H	22.29238700	-0.10864500	37.54117900	O	13.42660600	2.66508200	45.32591200
H	19.80354600	1.27532400	34.93204400	C	14.35597600	1.62816400	42.42009100
H	21.21184900	1.22248000	37.92162900				

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C	14.21484900	1.19279000	40.92719000	C	24.71958800	9.25781000	45.71336300
O	14.19705100	2.16170400	40.07961300	S	22.90780700	9.14109100	45.48529200
O	14.19592700	-0.01989000	40.67664100	H	24.99523300	10.30855900	45.56956900
H	13.57659900	3.45484700	40.99107000	H	25.01626400	8.94902500	46.71943100
H	12.39590000	2.30053300	43.08946500	C	22.89778000	6.36971900	42.59500300
H	14.23584500	0.75543100	43.06595200	H	23.09567900	6.23189800	41.53704100
H	15.38654600	1.99024800	42.54515800	C	25.41665400	5.84334100	46.69194800
N	14.80286800	4.18600000	44.31563700	H	26.41003400	5.48680900	46.94903200
C	15.33665500	4.72283600	45.55638100	C	21.74956500	7.87310800	49.13024800
C	15.04782000	6.22977000	45.70144000	H	21.58961000	8.17542500	50.16150100
O	15.84396700	6.98154300	46.27337000	C	18.98471700	7.61153800	45.17073600
C	16.82345500	4.40585500	45.77220400	H	17.92808400	7.75177400	44.96893700
C	17.19895000	4.43337400	47.25733800	C	23.93872700	6.12330100	43.48246100
H	14.78546200	4.21651400	46.35711400	C	25.26570300	5.65708000	43.09266300
H	15.09423600	4.58523700	43.42973900	C	25.93860100	5.46094700	44.26724200
H	17.46949500	5.07531900	45.19499100	C	25.06004600	5.83287900	45.34836100
H	17.00304700	3.38452200	45.41305900	C	25.75722400	5.45601300	41.68430600
O	16.37658500	4.24258000	48.14740900	H	26.80788800	5.76978000	41.62721100
N	18.52963700	4.58039800	47.52152700	H	25.21573600	6.10247600	40.98790500
H	18.78251100	4.68108500	48.49484300	C	25.64364300	4.01313500	41.15082300
H	19.20839100	4.90871800	46.84488600	H	26.40203900	3.35772400	41.59036600
N	13.85209900	6.63843600	45.20965100	H	24.67970800	3.58204900	41.45260400
C	13.36460700	8.00125400	45.36803500	C	25.69038300	3.91024900	39.60465200
H	12.32200900	7.94952100	45.70908300	O	26.03812300	2.77355000	39.12659300
C	13.44376500	8.84754500	44.08906400	O	25.34416900	4.90913200	38.94258500
C	14.87044100	9.09343100	43.59112200	C	24.62865800	6.34661400	47.72300700
H	13.95978900	8.45606000	46.16539700	C	25.05450900	6.46610200	49.09570800
H	12.86575700	8.36624600	43.29249900	C	24.03861500	7.07626800	49.77081900
H	15.36758300	8.14730200	43.34998700	C	22.98352200	7.31311600	48.81639900
H	14.85447900	9.69542800	42.67689700	C	20.67976100	8.00850300	48.25391300
H	13.27636900	5.98410400	44.68337000	C	19.34796800	8.42012100	48.64356700
N	30.22793100	-1.20172300	45.18586000	C	18.55625100	8.29454800	47.54406300
C	30.77569700	-0.80778800	43.89679700	C	19.41513100	7.84066200	46.47314400
C	29.75715300	0.01536900	43.11000100	C	19.81236300	7.23322100	44.12096900
O	28.56903900	0.04232000	43.43203000	C	19.38247500	7.09901100	42.74817600
H	29.28815500	-1.58173400	45.05366500	C	20.49644600	6.80704100	42.02206100
H	31.69251000	-0.21976300	44.04614900	C	21.59980700	6.72441400	42.95134600
N	30.21206100	0.68542500	42.01867900	N	23.84071800	6.23090600	44.85111200
C	29.27379800	1.22839500	41.03315300	N	23.36188400	6.85837300	47.57613300
C	28.74109800	0.08308700	40.13574300	N	20.69808900	7.67412400	46.92514400
O	29.36037900	-0.98071500	40.03376700	N	21.16058800	6.98056900	44.22534900
C	30.17244700	2.18735200	40.23094400	Fe	22.28956400	7.02815100	45.88144400
C	31.50819600	1.42260100	40.16555300	O	21.43024400	5.05878500	46.26466600
C	31.59337300	0.68575900	41.52128300	C	23.05467300	-1.73602100	41.23761100
H	31.47434200	0.68849100	39.35592600	N	24.22702100	-0.87669300	41.21158100
H	28.44423300	1.72607500	41.53858900	C	24.96029300	-0.32607500	42.22253700
H	32.24983600	1.21198600	42.22814700	O	25.79232000	0.54964500	42.00171300
H	31.97115000	-0.33508400	41.39686100	C	24.81974500	-0.82760900	43.67958600
H	32.36967900	2.07753700	39.99869000	N	26.13716400	-1.26023600	44.13475800
H	30.28739800	3.12744300	40.78367800	C	26.39651000	-2.49081600	44.63562100
H	29.75486800	2.41941700	39.24773200	O	27.48984800	-2.90158000	45.00588700
N	27.62273700	0.37332800	39.44413800	C	24.22274800	0.22902500	44.61730900
C	26.99354700	-0.63028200	38.59492300	C	24.07115500	1.52837500	44.29855900
C	25.84797200	-0.03235300	37.76953000	C	23.32302000	2.48942300	45.18138600
O	24.80371800	0.46735700	38.61624000	C	23.01512800	1.97413700	46.60059800
C	25.25013800	-1.07211100	36.82628400	C	23.23770200	0.55422000	46.87388500
H	26.60674700	-1.45908600	39.20370000	C	23.79379000	-0.24678300	45.93830500
H	24.46917100	-0.61572500	36.20858600	O	22.59038400	2.74891900	47.45414100
H	26.01796200	-1.48327000	36.15968900	C	21.83165100	-0.98600400	40.60131900
H	27.10392600	1.23859800	39.62836000	C	21.48969000	0.19852500	41.48217200
H	26.24777800	0.81033500	37.18865900	C	20.79531800	-0.01107800	42.68043300
H	24.80492400	-1.89054700	37.39933600	C	20.84712400	0.94344900	43.69326500
H	25.09146000	1.38193200	38.88811200	C	21.61338400	2.10488700	43.51619100

C	22.09541900	2.40920600	42.24356100	O	19.05420400	1.92473000	37.46629400
C	22.05143400	1.45382300	41.23107900	C	21.72479800	0.35875300	36.25086500
O	22.01420200	2.88272600	44.58737200	C	21.49417600	-0.26781500	37.63146900
Cl	20.04698800	0.63561000	45.21968700	C	20.36403200	-1.28707200	37.64159900
C	23.34374400	-3.03776900	40.44972600	H	22.41067300	-0.78469700	37.93611400
O	24.00167100	-2.97041600	39.42160800	H	19.68961600	0.47902400	35.50055100
C	22.87857800	-4.35181800	40.97438900	H	21.31221100	0.51662900	38.37259200
O	20.78398400	-1.92802100	40.47046900	H	22.60640300	1.00555200	36.32215100
C	21.88452200	-4.49694200	41.95787600	H	21.95692200	-0.43712700	35.53449600
C	21.49788200	-5.75544700	42.40367900	H	19.16906800	-0.10048100	38.78553600
C	22.11139600	-6.89720000	41.87539900	O	20.32036300	-2.24438100	36.88840900
C	23.09973800	-6.77128400	40.88941400	N	19.40312100	-1.08195000	38.63987000
C	23.46907200	-5.50989300	40.44216700	H	18.57687400	-1.65771400	38.49645500
O	21.70765500	-8.11034600	42.35392200	N	20.59873200	3.40585300	36.65343200
H	22.79879900	-1.97169600	42.27125200	C	20.25784200	4.54010700	37.51115900
H	24.47350900	-0.48740100	40.28850900	H	20.19112600	5.42884200	36.87043000
H	24.16830000	-1.70769300	43.73564600	C	21.26795800	4.78966900	38.63792600
H	26.93973600	-0.65042300	43.93707900	H	20.96046500	5.71366800	39.14747800
H	24.45106000	1.90915900	43.36005800	C	21.36959200	3.64369400	39.64429300
H	23.87176900	3.43082500	45.28102700	H	19.26168600	4.35388000	37.91796000
H	22.93538100	0.18658300	47.84931300	H	21.71024500	2.72657500	39.15073400
H	23.95279000	-1.29907000	46.16668200	H	22.26531000	4.97983200	38.22815900
H	21.92903500	4.47987800	46.88134700	H	21.43261900	3.51304100	36.07813400
H	22.16992800	-0.63449000	39.61967200	H	22.10423900	3.88828700	40.41603900
H	20.27110100	-0.94682800	42.84474700	H	20.40955100	3.43509500	40.13113800
H	22.60579300	3.35634100	42.10424400	C	16.09165200	3.33894000	35.96737100
H	22.54566300	1.65172600	40.28432800	C	15.88019000	4.00803100	37.31772000
H	21.43513100	4.54716300	45.43225300	O	15.05764000	4.92302500	37.46688300
H	20.16020000	-1.56345400	39.80700900	C	15.50723600	1.90598900	35.92692400
H	21.36990100	-3.62525300	42.34489300	C	14.03453500	1.78115000	36.36404800
H	20.71926700	-5.87393300	43.15027600	C	13.08466800	2.56686400	35.44801900
H	23.57347200	-7.66128300	40.47743300	C	13.61157100	0.30765300	36.65410600
H	24.22597500	-5.39359500	39.67350700	H	14.34597100	-0.27930200	37.02255300
H	22.20046300	-8.80680600	41.89213700	H	12.66062200	0.22886800	36.99284600
H	25.25503400	8.64942500	44.97951200	H	13.50907700	-0.15334300	35.46184600
H	12.95164700	9.80999500	44.29702900	H	13.15702000	2.22697000	34.40311000
H	15.47770400	9.60881800	44.34575800	H	12.04769000	2.43024900	35.77570900
H	30.79180500	-1.95707400	45.56999200	H	13.29521900	3.64167700	35.47758900
H	31.05831300	-1.64695500	43.22877500	H	15.61801800	3.98031600	35.21958300
H	25.48831900	-3.12796800	44.69861900	H	13.92120800	2.19842400	37.37352400
H	20.57634200	6.63196300	40.95665500	H	16.12795600	1.26688100	36.56916000
H	18.36069900	7.18844800	42.40240800	H	15.63186200	1.52014300	34.90265800
H	17.48926900	8.43673500	47.43877700	N	16.65420800	3.54721200	38.34075500
H	19.06600000	8.71974400	49.64576400	C	16.28930600	3.69841900	39.75552800
H	23.98825300	7.33623700	50.82132800	C	16.50908200	5.09515000	40.35760100
H	26.01099300	6.12838600	49.47588900	O	16.35638500	5.28800400	41.56731800
H	26.95852200	5.11647300	44.39451400	C	16.99256700	2.62346200	40.58847100
H	27.75503200	-1.05374900	37.92827500	H	17.38352000	2.87121300	38.11670800
H	25.13422800	5.72750200	36.89475200	H	15.19998000	3.53336800	39.81734300
H	16.71293600	3.46436900	35.56424700	H	18.08087600	2.66346100	40.45775800
H	11.56175600	5.06875200	40.13870200	H	16.76800700	2.77873600	41.64531600
² P _{Cyc}				H	16.63853600	1.63056700	40.29337500
C	24.33453000	5.79698400	36.07444200	N	16.79779800	6.10805300	39.48639700
S	23.80856300	4.31791700	35.12903600	C	16.52863200	7.48576800	39.86273000
C	25.09158200	3.14323000	35.70102600	C	15.04020000	7.84175200	40.05595900
H	23.54456700	6.54755500	35.97786400	O	14.74398400	8.89521600	40.61532000
H	25.14004200	3.12260400	36.79494200	H	16.66586500	5.88309500	38.50917000
H	24.82187800	2.15369400	35.32107600	H	17.01581900	7.71089100	40.81278500
H	26.06887900	3.42126000	35.29302500	H	16.95870100	8.15010600	39.10646200
H	25.26091000	6.20302100	35.65491500	N	14.13468200	6.94428700	39.58584800
H	20.80453200	1.64067300	34.76641400	C	12.73436100	7.02291900	39.96896500
C	20.52059900	1.15955600	35.71037000	C	12.38929600	6.16113300	41.20500700
C	19.98929900	2.20178400	36.69158900	O	11.86893600	6.67207200	42.20538700

H	14.44175400	6.14557500	39.03327900	H	26.76737800	-1.28754900	39.28857500
H	12.50175600	8.05834800	40.21713000	H	24.45525500	-0.82412200	36.32476800
N	12.69207600	4.85106500	41.09173500	H	26.08019500	-1.53388300	36.24564700
C	12.17771900	3.84292100	42.01551400	H	27.06884000	1.37113300	39.62432600
C	12.58793900	4.06968400	43.47552200	H	26.12825000	0.80514300	37.16325600
O	11.84611300	3.74534100	44.39678800	H	24.95876800	-2.00613500	37.54778600
C	12.64483600	2.42463300	41.58252200	H	24.99043000	1.34426100	38.91387600
C	12.62568000	2.11041200	40.05212900	C	24.23044700	9.26944600	45.74819100
O	13.23328000	2.97914800	39.32039300	S	22.45238900	8.85073500	45.64559000
O	12.09923300	1.05419000	39.68006100	H	24.32230100	10.33535100	45.51240800
H	12.99263700	4.41549800	40.19410700	H	24.62740700	9.09561000	46.75240800
H	11.08140800	3.87749100	42.02321300	C	22.71477800	5.92543600	42.87952600
H	12.03528700	1.69130400	42.11512500	H	22.88438600	5.75609600	41.82074500
H	13.68471000	2.29035500	41.91296100	C	25.51649300	6.07181100	46.82300600
N	13.84634500	4.57771100	43.66597400	H	26.57400900	5.92491600	47.02647200
C	14.38330200	4.80055600	44.99457500	C	21.68281600	7.54057200	49.40854500
C	14.56960200	6.29689800	45.31849000	H	21.52630500	7.83941600	50.44130100
O	15.44140100	6.66082300	46.12044500	C	18.80343900	6.90197500	45.57066700
C	15.68401900	4.02153700	45.24857500	H	17.73363800	6.98177600	45.39790200
C	15.97911100	3.87926700	46.74193200	C	23.82131800	5.88368200	43.71607200
H	13.62653700	4.41534700	45.68814200	C	25.17816300	5.58644200	43.26307700
H	14.41640200	4.81662100	42.85944400	C	25.94621300	5.59740500	44.39100700
H	16.52292700	4.46531600	44.70250600	C	25.08761300	5.91972800	45.50593700
H	15.53937000	3.00580300	44.86198100	C	25.58603900	5.33496000	41.83985800
O	15.12849700	3.50126500	47.53672800	H	26.65537300	5.55857800	41.73291000
N	17.28682500	4.09133000	47.10722400	H	25.05665400	6.01897300	41.16784300
H	17.44198600	4.14564700	48.10672600	C	25.31753400	3.90276600	41.32357600
H	17.83445200	4.74513900	46.56178700	H	26.05765500	3.18949300	41.69546100
N	13.69861800	7.13861900	44.71941700	H	24.34586500	3.55820300	41.70548900
C	13.66259900	8.56874800	44.99643200	C	25.22408000	3.83828000	39.77680600
H	12.61304000	8.85433000	45.14476500	O	25.74678300	2.81681800	39.21008400
C	14.28004600	9.43185800	43.88602300	O	24.61714400	4.76968700	39.20598900
C	15.78355000	9.21563600	43.69924000	C	24.70974500	6.49740700	47.88229100
H	14.19314100	8.72018800	45.94117200	C	25.17632600	6.73083200	49.22820600
H	13.76913900	9.22783500	42.93849600	C	24.10085300	7.16584500	49.94461800
H	15.99139900	8.17152000	43.44214500	C	22.97549800	7.18670100	49.04185800
H	16.16056200	9.83368200	42.87868000	C	20.56539500	7.50676400	48.58209500
H	13.06459300	6.77669100	44.00908600	C	19.21457300	7.78652100	49.01978000
N	31.20219500	-0.76827300	44.49287400	C	18.40047200	7.58330800	47.94741900
C	31.54091400	-0.22324000	43.18666700	C	19.26143600	7.19434500	46.85273800
C	30.32893000	0.47346200	42.57172300	C	19.62125700	6.55096700	44.50473500
O	29.19536300	0.28602000	43.01864500	C	19.15328100	6.32549700	43.15752500
H	30.31043000	-1.26477900	44.43214100	C	20.25928000	6.08939000	42.39997200
H	32.37346700	0.48849900	43.28221900	C	21.39990900	6.14433200	43.28441000
N	30.54243200	1.27210500	41.49509000	N	23.79343900	6.08484100	45.07704500
C	29.41449500	1.69593400	40.65829200	N	23.37044700	6.77515600	47.79147600
C	28.92629300	0.49423500	39.81082200	N	20.56823300	7.15381300	47.25890200
O	29.67925900	-0.45797700	39.58113000	N	20.99027300	6.40977400	44.56676800
C	30.05842300	2.77952900	39.77402900	Fe	22.19349500	6.68780300	46.15915100
C	31.46758300	2.21387100	39.51770700	O	21.73528100	4.67734600	46.71056800
C	31.83527300	1.49997000	40.83645900	C	23.32548800	-1.77534500	41.60603800
H	31.42708400	1.47889500	38.70933600	N	24.40409400	-0.81654300	41.43360500
H	28.60111200	2.06973700	41.28275900	C	25.42191300	-0.41097500	42.25917000
H	32.47798500	2.12581300	41.47152600	O	26.20501500	0.45924900	41.89789200
H	32.35641600	0.55529500	40.64702200	C	25.66295000	-1.03023100	43.67202000
H	32.19826400	2.98355400	39.24831900	N	27.04730300	-1.47700500	43.68455100
H	30.11115300	3.72257900	40.33149800	C	27.48694600	-2.53293900	44.40647100
H	29.48690400	2.95743800	38.85934100	O	28.66093300	-2.84062900	44.58575300
N	27.68139500	0.61307400	39.31156400	C	25.34937600	0.03228500	44.73011500
C	27.06237500	-0.49077900	38.59106100	C	24.00929500	0.23388400	45.04505900
C	25.82896300	-0.03857100	37.80181300	C	23.57893000	1.33467100	45.78586900
O	24.77727200	0.40177400	38.66851900	C	24.53133800	2.18578800	46.35772300
C	25.30028000	-1.17295300	36.92722900	C	25.88762600	1.93780400	46.11362200

C	26.30158400	0.90085900	45.27262400	H	29.20152400	8.23724200	39.46349500
O	24.09054800	3.23414400	47.12704800	H	28.03368800	9.24537900	40.35178200
C	21.94566500	-1.12743000	41.18582200	H	28.21997900	7.51744500	40.79129700
C	21.50409700	-0.16596800	42.27185600	H	27.45074100	5.53412400	39.34880000
C	20.84066500	-0.65314800	43.40568800	H	21.18992400	3.15556700	34.74212700
C	20.88628300	0.06335300	44.60358300	C	20.71428300	2.58969800	35.55406300
C	21.61521900	1.25710300	44.66103500	C	20.64086800	3.44171500	36.81711900
C	22.02135400	1.86492700	43.47085800	O	19.64453100	3.42954700	37.54855700
C	21.97695500	1.15136900	42.27787900	C	21.49669100	1.27612600	35.77856400
O	22.21603800	1.67144000	45.85109900	C	20.90365700	0.37469100	36.86644800
Cl	20.25687800	-0.65540300	46.07149900	C	19.59342800	-0.28281900	36.43503200
C	23.57608600	-3.02842500	40.72810100	H	21.60741500	-0.44109300	37.08410600
O	24.04028000	-2.87924600	39.60743900	H	19.69083800	2.36063600	35.24766200
C	23.30850500	-4.39033400	41.27046900	H	20.76400300	0.91869300	37.80785200
O	21.03276900	-2.18752600	40.96517500	H	22.53707500	1.50697800	36.03867800
C	22.57283600	-4.63985900	42.44173300	H	21.50985800	0.71942700	34.83632800
C	22.35950900	-5.93765400	42.89168300	H	18.85547600	-0.29552400	38.36813800
C	22.88990300	-7.01586500	42.17422000	O	19.28451600	-0.44505300	35.26526300
C	23.62198800	-6.78645400	41.00125200	N	18.82503100	-0.78278900	37.47653600
C	23.82004000	-5.48638000	40.55653700	H	17.88624600	-1.06264600	37.20580900
O	22.66279400	-8.27148600	42.66019300	N	21.75798100	4.16212200	37.09511300
H	23.26571400	-2.05865600	42.65707300	C	21.99738400	4.88952600	38.34194600
H	24.50467400	-0.42889700	40.48389500	H	22.04015900	5.96626700	38.12895800
H	25.02586400	-1.90478000	43.84426700	C	23.28574600	4.44131100	39.04578500
H	27.75171100	-0.83594700	43.30549400	H	23.43976500	5.10681600	39.90374200
H	23.27363800	-0.43315300	44.61732700	C	23.27399800	2.98217500	39.50982300
H	26.62470600	2.60788200	46.54970700	H	21.12494600	4.71096600	38.97376300
H	27.35368600	0.78764400	45.03207600	H	23.12283500	2.29778800	38.66484400
H	22.51877500	4.09025600	46.80825100	H	24.14212000	4.61530500	38.37657100
H	22.14512000	-0.58093200	40.25699500	H	22.53923200	4.07714300	36.45795700
H	20.38605700	-1.63796200	43.38107000	H	24.21930600	2.70988700	39.99149200
H	22.53706400	2.81939400	43.52320100	H	22.45996500	2.80764800	40.22427400
H	22.42521500	1.57607700	41.38562500	C	16.10647000	3.26631100	36.90257300
H	21.21542100	4.30236500	45.98168200	C	15.96687700	3.95851200	38.24793000
H	20.36775900	-1.87160600	40.31620900	O	14.86278700	4.16509000	38.76005300
H	22.12917400	-3.82064300	42.99611800	C	15.97857200	1.72662900	37.02041900
H	21.78261500	-6.13518700	43.78937800	C	14.68346600	1.18779900	37.65857400
H	24.03165200	-7.62693800	40.44265100	C	13.41367900	1.59937800	36.90209900
H	24.37671500	-5.28980200	39.64626500	C	14.74960400	-0.33990800	37.80361300
H	23.07677300	-8.91511500	42.06393100	H	15.67517600	-0.65168000	38.30659700
H	24.82012200	8.69771800	45.02637500	H	13.92279200	-0.69063700	38.42966200
H	14.08189900	10.48564300	44.13434100	H	14.70502400	-0.83980400	36.82362600
H	16.34373600	9.45526800	44.61153400	H	13.39753500	1.18539900	35.88212400
H	31.89994900	-1.46034800	44.75745800	H	12.54175700	1.23681100	37.45402000
H	31.86431900	-0.97183200	42.43485200	H	13.32066000	2.68878900	36.83728900
H	26.65827200	-3.13972500	44.82752500	H	15.31748400	3.65906800	36.25350900
H	20.31310700	5.87850000	41.34051500	H	14.58670900	1.60263700	38.66631500
H	18.11564600	6.32739900	42.84726100	H	16.83904300	1.36558600	37.60069400
H	17.32348700	7.66201400	47.86669800	H	16.09770700	1.31051000	36.00816400
H	18.94303100	8.08122600	50.02623000	N	17.12776500	4.34849200	38.85764200
H	24.05607300	7.44210600	50.99106800	C	17.16646000	4.67987200	40.28483000
H	26.19532900	6.58103600	49.56388800	C	16.38277800	5.94271200	40.67998400
H	27.01273900	5.41913500	44.46536500	O	16.14162900	6.16960400	41.86631800
H	27.81198800	-0.91464300	37.91431200	C	18.62396900	4.81875300	40.74111400
H	24.47673400	5.53081000	37.12808900	H	18.00826700	4.06465200	38.43018500
H	17.16492200	3.29098800	35.74301300	H	16.69568600	3.87054200	40.85617400
H	12.11750000	6.70114100	39.12149600	H	19.13624400	5.61063700	40.18275400
H	24.73996900	3.96606000	47.11308300	H	18.65557500	5.07299700	41.80243300
4Re				H	19.16152700	3.87826800	40.58757900
C	27.31336200	6.10348800	38.42345100	N	16.00910300	6.78973800	39.68281100
S	26.88531000	7.84596400	38.78726000	C	15.08900200	7.88549600	39.93162600
C	28.22867100	8.23936200	39.96759900	C	13.60508600	7.52781500	40.17181300
H	26.48193300	5.67889800	37.85241300	O	12.82768400	8.43558000	40.46390400

H	16.13561900	6.46001300	38.73654100	H	31.17512700	4.95382400	39.51527400
H	15.41210000	8.42070300	40.82732800	H	29.81237200	3.91723900	39.08437700
H	15.13485800	8.58581200	39.09221300	N	29.37028500	1.62109900	40.82662200
N	13.26968100	6.22509800	40.03394800	C	28.42789500	0.51654400	40.70700400
C	11.95411700	5.71063000	40.38834700	C	27.11572100	0.93409000	40.01815700
C	11.98797300	4.96317400	41.73613300	O	26.38731600	1.87243800	40.79668500
O	11.55094600	5.49620400	42.76600800	C	26.21010600	-0.27582500	39.79799600
H	13.96637100	5.54131900	39.74257500	H	28.18241000	0.12465800	41.70334100
H	11.27476400	6.55741200	40.48571100	H	25.27438300	0.04435000	39.32603700
N	12.57272900	3.74751800	41.69030200	H	26.69305600	-1.01487400	39.14768100
C	12.50015100	2.79618700	42.80295300	H	28.99183100	2.52035400	41.14912300
C	13.07336800	3.32139700	44.12650100	H	27.37775700	1.37266900	39.03829800
O	12.63294800	2.93045900	45.20193500	H	25.96690400	-0.75507600	40.75311700
C	13.24875700	1.49928700	42.41149100	H	26.91718400	2.70338200	40.88624200
C	12.89348100	0.86760300	41.02734500	C	24.42788800	8.63817700	46.19208600
O	12.48323200	1.64812200	40.11177000	S	22.61419300	8.52413100	46.12622500
O	13.11055600	-0.36003100	40.92629200	H	24.70968700	9.63753800	46.53871300
H	12.62538500	3.21294100	40.79401600	H	24.85379500	7.87784800	46.85255900
H	11.45035900	2.56475600	43.02223300	C	24.95389600	6.25947600	43.61603900
H	13.08476700	0.75411200	43.19362700	H	25.90395800	6.27464100	43.08608400
H	14.32848700	1.70061400	42.39530700	C	23.36872200	4.40814000	47.79528500
N	14.13521800	4.17974800	44.02077800	H	23.79812100	3.77744700	48.56777800
C	14.80294800	4.74327300	45.17963500	C	19.11945300	6.63673700	47.15848600
C	14.29571400	6.15380000	45.58495600	H	18.20668900	6.74134200	47.73706700
O	14.93857600	6.83130800	46.39979600	C	20.52011700	8.00339200	42.73563900
C	16.31785100	4.80954500	44.98051100	H	20.04596700	8.51322400	41.90253000
C	17.06739700	3.52491900	45.27352500	C	24.89885400	5.56563300	44.82019700
H	14.57864200	4.07571200	46.01872700	C	26.01439400	4.81761600	45.38599600
H	14.40801100	4.50659700	43.10107500	C	25.53495700	4.28445800	46.54848900
H	16.70125200	5.55085500	45.68994100	C	24.16880900	4.71000100	46.70314400
H	16.55571000	5.18238200	43.97809900	C	27.40626600	4.69050400	44.82892600
O	16.66822100	2.63645800	46.00240400	H	28.02296400	4.22978800	45.60959500
N	18.32167800	3.44113900	44.64123300	H	27.81863400	5.68828100	44.63603300
H	19.00020100	2.87774100	45.16017500	C	27.55653400	3.88723900	43.51237300
H	18.73685200	4.32992700	44.37044500	H	28.39737300	3.18784000	43.60337500
N	13.13588900	6.55131300	45.02465300	H	26.68084600	3.25747300	43.31459300
C	12.53823900	7.85340100	45.27833800	C	27.82457600	4.74520000	42.24826400
H	11.49961400	7.70334000	45.60285200	O	28.00173900	4.08191400	41.16607000
C	12.56333100	8.76590900	44.04206100	O	27.85346800	5.98838100	42.35318700
C	13.97392600	9.16498400	43.59824600	C	22.06957800	4.86357600	47.99263800
H	13.09224200	8.29978900	46.10918700	C	21.27873300	4.59372300	49.16699700
H	12.05419200	8.25879800	43.21436500	C	20.09117100	5.23897600	48.99603200
H	14.57539800	8.27744100	43.37131500	C	20.15548800	5.89128300	47.71244100
H	13.92732100	9.77433900	42.68945200	C	19.13382200	7.20959600	45.89489000
H	12.67569400	5.95899900	44.33401100	C	18.00947900	7.89221000	45.29975300
N	35.91283200	1.43944200	41.55401900	C	18.39104700	8.23650800	44.03912800
C	35.06383300	2.02205900	40.51931500	C	19.75229400	7.78945700	43.87359500
C	33.61248000	2.26928400	40.97587800	C	21.85821100	7.66995600	42.60406000
O	33.27680100	2.03715900	42.13712300	C	22.67523300	7.98804000	41.46030400
H	35.73303400	1.96614400	42.41045300	C	23.93127900	7.52991700	41.72369200
H	35.50283500	2.97373400	40.18606100	C	23.87819300	6.90786500	43.02482600
N	32.76047900	2.78709300	40.05201100	N	23.79691900	5.49183600	45.63612700
C	31.33965000	2.96305100	40.34814800	N	21.36874300	5.65359500	47.12145000
C	30.59399600	1.60798200	40.24922700	N	20.18907800	7.16162000	45.01336400
O	31.09306200	0.64757100	39.65986800	N	22.61219800	7.01511300	43.55425900
C	30.89313200	3.93174200	39.23608700	Fe	21.94551800	6.19797600	45.26731600
C	31.71193100	3.44894200	38.02632700	O	21.43321300	4.79225700	44.59240000
C	33.06579600	3.02462800	38.63531100	C	21.81565000	-2.96263500	41.01094600
H	31.22867300	2.57766900	37.57407700	N	23.06141900	-2.32506100	41.41957300
H	31.21639100	3.38327200	41.34821700	C	23.69047500	-2.32649600	42.63531300
H	33.82035100	3.81806900	38.53373200	O	24.89754900	-2.10783300	42.71786400
H	33.45709300	2.12126800	38.15355300	C	22.87402000	-2.48554100	43.93045500
H	31.83110900	4.21371200	37.25190000	N	23.75332500	-3.14360200	44.89435800

C	23.36549000	-4.07499200	45.80084800	H	17.07627100	3.50776100	36.45273900
O	24.09419600	-4.61841900	46.61641900	H	11.60850200	5.04018300	39.59255800
C	22.34958800	-1.13157100	44.40971600	^a TS1 _{HA,A}			
C	23.09183100	0.04903800	44.26739300	C	25.03988600	5.78469500	35.73614200
C	22.59938500	1.26628300	44.73607500	S	24.21101600	4.38379500	34.89363300
C	21.34966500	1.31685500	45.36822400	C	25.30335600	3.02365700	35.45219800
C	20.60575800	0.14028500	45.53197700	H	24.39906400	6.66325900	35.61572700
C	21.10457800	-1.06430400	45.04912900	H	25.41992600	3.04321100	36.54193200
O	20.80793700	2.47098000	45.84357800	H	24.83697500	2.08384000	35.14318100
C	21.03058600	-2.01650400	40.04129500	H	26.28329200	3.10415300	34.97055300
C	20.14207600	-1.00067700	40.74690700	H	26.00593500	5.98948300	35.26304300
C	18.75688100	-1.21339700	40.80710000	H	21.09526800	2.02158100	34.77491800
C	17.90495100	-0.27846300	41.39090100	C	20.69100900	1.70966500	35.74615500
C	18.42119700	0.90080200	41.96576900	C	20.08733300	2.90376400	36.47005300
C	19.81299300	1.09497600	41.93250900	O	19.07238000	2.77344900	37.17115600
C	20.65832700	0.16730300	41.32394300	C	21.81190100	1.02209800	36.55595600
O	17.55504800	1.79632200	42.47725600	C	21.41602300	0.57041900	37.96372900
Cl	16.18201700	-0.55130600	41.37959000	C	20.39091500	-0.55598900	37.97745100
C	22.18122300	-4.27564100	40.26426400	H	22.32490800	0.22927800	38.47449400
O	23.20877300	-4.28812100	39.59881500	H	19.88232700	0.99709900	35.56953200
C	21.33946800	-5.48960100	40.41798300	H	21.03234500	1.41022500	38.55526400
O	20.29272300	-2.87119800	39.17933600	H	22.67093500	1.69580700	36.64734400
C	20.06259600	-5.48358300	41.00633600	H	22.14496400	0.14724500	35.98718600
C	19.32754800	-6.65591900	41.13264800	H	19.88945800	-0.14657200	39.94818800
C	19.86625500	-7.86426200	40.67452900	O	20.06778600	-1.19723100	36.99020300
C	21.13606000	-7.88791000	40.08069000	N	19.87582300	-0.86866600	39.23509200
C	21.85755200	-6.70886000	39.95182900	H	19.01878800	-1.41114100	39.20162200
O	19.11189000	-8.99037400	40.82982600	N	20.74037200	4.08079200	36.31667500
H	21.20397600	-3.16562600	41.88873800	C	20.36165500	5.31793300	36.99049900
H	23.74158600	-2.29810700	40.66251000	H	19.95110500	6.02204500	36.25172700
H	22.01661500	-3.14846300	43.77815300	C	21.54142000	5.96646700	37.72658100
H	24.73061800	-2.87235700	44.86025300	H	21.20081600	6.93534400	38.11721000
H	24.06197900	0.02519900	43.77939900	C	22.11775000	5.10801500	38.85450100
H	23.17686900	2.17789600	44.60816200	H	19.55584500	5.06577500	37.68424500
H	19.63350400	0.19530800	46.01276900	H	22.38021500	4.10994500	38.49039700
H	20.50754900	-1.96676300	45.16653300	H	22.33287600	6.19198300	37.00082000
H	21.23477200	3.27640700	45.45070000	H	21.62361500	4.08240500	35.81036100
H	21.80503900	-1.47857300	39.47069100	H	23.04144400	5.54375800	39.24432300
H	18.32939700	-2.11203200	40.37564400	H	21.39712000	4.98896700	39.67241600
H	20.23006900	1.99332100	42.37941200	C	15.49109000	2.97382200	36.91757500
H	21.72692600	0.36040800	41.30369100	C	15.62151500	3.66615100	38.26342700
H	17.97809500	2.39811100	43.14529800	O	14.66008100	4.20585900	38.82670400
H	19.82064500	-2.31799300	38.52338200	C	14.76527400	1.60863100	37.03545300
H	19.61715500	-4.55378000	41.34201900	C	13.30420300	1.65576100	37.52552500
H	18.33714000	-6.65480300	41.57595100	C	12.36696000	2.38150400	36.55024700
H	21.55181800	-8.82914000	39.72367000	C	12.78361700	0.23932700	37.81541800
H	22.83994500	-6.70647200	39.49109000	H	13.44718300	-0.29704100	38.50779700
H	19.60087900	-9.74652100	40.46889100	H	11.79006800	0.28761700	38.27745200
H	24.84417700	8.49083200	45.18803100	H	12.71254800	-0.35874700	36.89433300
H	11.97542700	9.66694400	44.27279200	H	12.28644300	1.84089600	35.59469000
H	14.49465800	9.73401600	44.37978100	H	11.37323800	2.46991200	37.00169100
H	35.53073900	0.51847800	41.77263400	H	12.71194300	3.40075800	36.33826800
H	35.06910200	1.36365500	39.64177800	H	14.92361900	3.63997900	36.25856000
H	22.28316200	-4.30949200	45.71968500	H	13.27199000	2.21870800	38.46452400
H	24.81727900	7.58107600	41.10102000	H	15.35282300	0.96684000	37.70810800
H	22.32058200	8.50874700	40.57945600	H	14.80505500	1.12713100	36.04662200
H	17.80625400	8.72982800	43.27399900	N	16.85674400	3.64985300	38.84290300
H	17.04245400	8.01335900	45.77316300	C	17.01996800	4.01718400	40.24723700
H	19.23470200	5.26877800	49.65726200	C	16.75477100	5.50596400	40.53532700
H	21.60371400	3.98525800	50.00135000	O	16.52123700	5.88660000	41.68297900
H	26.06781200	3.66230000	47.25791200	C	18.40639800	3.60090900	40.75281900
H	28.93053200	-0.27208900	40.14045500	H	17.64700600	3.24488900	38.33934900
H	28.22258000	6.04611700	37.81455100	H	16.25270200	3.49711600	40.83309800

H	19.20055800	4.07874800	40.17067800	C	31.51541900	2.32143000	38.76602900
H	18.53223100	3.87803200	41.80144000	C	31.97313100	1.84514000	40.16390300
H	18.52719700	2.51622800	40.66786400	H	31.42340200	1.45925900	38.09978300
N	16.81336100	6.35329700	39.47215400	H	28.77531700	2.51980400	40.71814100
C	16.41236400	7.74425500	39.57303600	H	32.68459400	2.54948600	40.61604100
C	14.90199900	8.04776500	39.66576100	H	32.45118400	0.86055200	40.11346800
O	14.55247300	9.21860800	39.80296500	H	32.22534500	3.02481400	38.31864900
H	16.89737000	5.92761000	38.55926300	H	30.21599800	3.96846400	39.38193100
H	16.85653100	8.17967600	40.47076600	H	29.49210400	2.95331700	38.12123800
H	16.80827400	8.29085100	38.71214100	N	27.79367900	0.77038900	38.99495800
N	14.05998700	6.98979300	39.58359200	C	27.13327800	-0.44686200	38.54048800
C	12.62945800	7.12078000	39.82384900	C	25.75897200	-0.15865600	37.92340500
C	12.23052100	6.44325600	41.14735300	O	24.85296400	0.40700700	38.88014900
O	12.04067300	7.10089300	42.17784800	C	25.13105000	-1.44071700	37.38346700
H	14.41997300	6.04637100	39.44431400	H	27.01474500	-1.15047900	39.37469300
H	12.40183200	8.18435500	39.89702400	H	24.15912300	-1.22335100	36.92824000
N	12.17687900	5.09130400	41.08664200	H	25.77301900	-1.89823700	36.62139300
C	11.60918300	4.28705200	42.16815000	H	27.20053200	1.58189000	39.18280500
C	12.35780200	4.38802200	43.50762400	H	25.89046500	0.56208000	37.10329900
O	11.76977500	4.13719100	44.55539100	H	24.98255000	-2.16101700	38.19420100
C	11.56262900	2.80376800	41.73580800	H	25.09974200	1.36788200	38.99418800
C	10.85269100	2.51844700	40.37991000	C	23.48316100	8.60080300	45.14881200
O	11.00542600	3.34878200	39.43689500	S	22.50399800	7.88876400	46.51302700
O	10.21813200	1.43047000	40.32099700	H	23.58113600	9.67365100	45.34189500
H	12.02204900	4.62661600	40.17404800	H	24.47723600	8.15305200	45.08413200
H	10.59075100	4.63138200	42.39264400	C	22.92451300	5.96106200	42.76084100
H	11.08144300	2.22532900	42.52911900	H	23.15729400	6.04486300	41.70569500
H	12.59293900	2.43038000	41.63696600	C	25.37919400	4.82103800	46.75797500
N	13.68753500	4.70048100	43.44459700	H	26.40842900	4.55733600	46.97510800
C	14.50601900	4.84778900	44.63937000	C	21.32111900	5.19716400	49.36234100
C	14.80421200	6.32266600	44.98355500	H	21.05939600	5.04043500	50.40382400
O	15.77592200	6.62133700	45.68935700	C	18.90987600	6.56439000	45.40076300
C	15.79177100	4.00990300	44.57112000	H	17.87457400	6.81966100	45.20004500
C	16.31496600	3.62887300	45.95953900	C	23.94188400	5.55945800	43.61228500
H	13.90415600	4.45942600	45.46896500	C	25.29831600	5.24829700	43.18617400
H	14.08933400	4.94721300	42.54751800	C	25.98254000	4.98006100	44.33724100
H	16.56113800	4.51050000	43.97618600	C	25.06070000	5.09525000	45.43553100
H	15.54671800	3.06979600	44.05856300	C	25.78712700	5.20059500	41.76737200
O	15.58729200	3.59277800	46.94860000	H	26.87535300	5.33374500	41.76282300
N	17.62756700	3.28044100	46.00550400	H	25.37934700	6.02851800	41.17879900
H	17.97557800	2.92316700	46.88397800	C	25.43692100	3.89328800	41.02246600
H	18.25096400	3.20733100	45.20536000	H	26.02781100	3.04938400	41.39194300
N	13.91325800	7.22943100	44.52406000	H	24.38684900	3.63250400	41.21586800
C	13.98751300	8.64931500	44.83741200	C	25.58749800	4.01105700	39.48463500
H	13.02477500	8.95699500	45.26874900	O	25.77353800	2.91256300	38.84928600
C	14.30435300	9.52412100	43.61512400	O	25.48336400	5.14135600	38.96930500
C	15.72086800	9.32527000	43.06925500	C	24.48030400	4.80333400	47.81550600
H	14.75475600	8.76205500	45.60824500	C	24.82969500	4.47616400	49.17314300
H	13.57394500	9.30830400	42.82601100	C	23.68370300	4.56468600	49.90425200
H	15.88567400	8.27666100	42.79903100	C	22.64019600	4.95314600	48.99207300
H	15.87165900	9.92986100	42.16850000	C	20.31569700	5.62690300	48.51310700
H	13.18938900	6.93768600	43.87051400	C	18.94584600	5.85109800	48.90640000
N	31.72030600	0.76769500	44.34471400	C	18.26719800	6.23143900	47.79035700
C	31.89460200	0.83165500	42.90184600	C	19.22883400	6.24896100	46.71603000
C	30.61835600	1.34329600	42.23248400	C	19.80502200	6.54201800	44.34586800
O	29.53803100	1.31694600	42.81811700	C	19.45898500	6.86941300	42.98773200
H	30.82107300	0.32893300	44.55769600	C	20.58937300	6.70855700	42.24675800
H	32.73857500	1.49200600	42.65747300	C	21.62528400	6.27283900	43.14828100
N	30.73563300	1.79807200	40.95213200	N	23.81897500	5.45182400	44.97612800
C	29.55488900	2.04092500	40.12388100	N	23.14231100	5.08199000	47.72742100
C	29.03120000	0.70751000	39.53368000	N	20.46676200	5.88556900	47.17143300
O	29.74498100	-0.29666300	39.49950700	N	21.13398500	6.19081500	44.42453600
C	30.12602400	2.94062700	39.01132900	Fe	22.11000200	5.56850000	46.05458600

O	21.69203700	3.91965700	45.77771800	H	17.21523200	6.43971800	47.65111400
C	23.88495100	-1.69413700	41.95162500	H	18.56555600	5.70623000	49.90940400
N	24.91928300	-0.74478800	41.59212800	H	23.54094100	4.38606700	50.96195600
C	25.99852200	-0.33637300	42.30873000	H	25.82365200	4.20507200	49.50312700
O	26.77203400	0.50862600	41.86344900	H	27.02153900	4.69269300	44.43556900
C	26.21482700	-0.89114100	43.73559900	H	27.77412400	-0.93686800	37.79759100
N	27.61712100	-0.64331400	44.07049000	H	25.18033800	5.56389100	36.80113600
C	28.28988100	-1.34103100	45.00380700	H	16.48266500	2.81900500	36.47749300
O	29.46326400	-1.17914300	45.33324300	H	12.07344300	6.67648600	38.98792400
C	25.21486200	-0.23400800	44.68311900				
C	24.93459600	1.13177600	44.56053300				
C	23.97565200	1.74107500	45.35333000				
C	23.27084200	0.99908300	46.31432800				
C	23.56816100	-0.36203000	46.47505500				
C	24.52445500	-0.96629100	45.65818500				
O	22.31226800	1.55932800	47.08828600				
C	22.55459900	-1.22734500	41.27377900				
C	21.87162800	-0.08836800	42.01625800				
C	20.86410500	-0.36631600	42.95006500				
C	20.26379600	0.65512100	43.67696000				
C	20.63706800	2.01918500	43.52109700				
C	21.63003400	2.27112500	42.53966400				
C	22.23184800	1.25301200	41.81165100				
O	20.08925900	2.99412500	44.22221400				
Cl	19.00682800	0.24116600	44.83272100				
C	24.24400100	-3.12159900	41.46562600				
O	24.87314000	-3.26555700	40.42682700				
C	23.87656500	-4.30393700	42.30012400				
O	21.71749600	-2.37194800	41.15861900				
C	23.02246500	-4.24371800	43.41503900				
C	22.72571700	-5.38464000	44.15253700				
C	23.28758100	-6.61263000	43.78699300				
C	24.13918100	-6.69209500	42.67701000				
C	24.42236800	-5.54739600	41.94361600				
O	22.97353900	-7.70495200	44.54629300				
H	23.75389500	-1.68146500	43.03436400				
H	24.90471800	-0.36774500	40.63611500				
H	26.04388200	-1.97500100	43.74166400				
H	28.10409900	0.08788300	43.54335500				
H	25.45865000	1.72243300	43.81598700				
H	23.73159500	2.78431500	45.21210300				
H	23.02268500	-0.93450600	47.21913700				
H	24.72358900	-2.03081100	45.77325500				
H	22.09804000	2.45799000	46.73424300				
H	22.84847700	-0.88434300	40.27394700				
H	20.54776900	-1.39204400	43.10444800				
H	21.91343100	3.30561500	42.37848200				
H	22.99631600	1.49876800	41.08019000				
H	20.91473100	3.56433600	44.99269200				
H	21.03877500	-2.13834700	40.49449900				
H	22.56146000	-3.30689400	43.70492300				
H	22.06034400	-5.34344000	45.00877700				
H	24.57509900	-7.64943300	42.39367700				
H	25.07467400	-5.58894800	41.07763000				
H	23.42686400	-8.47877700	44.17667100				
H	22.97220500	8.46824100	44.19111200				
H	14.15863400	10.57548600	43.90431200				
H	16.47798000	9.60587900	43.81263600				
H	32.43104200	0.15457600	44.73852700				
H	32.11637300	-0.13748700	42.40918400				
H	27.66875000	-2.12818600	45.47908600				
H	20.72843000	6.85747300	41.18460700				
H	18.46470900	7.14521700	42.66485700				
				⁴¹M1A			
				C	24.90542300	5.86338600	35.75899900
				S	24.13987600	4.44065800	34.89385800
				C	25.28862400	3.12226200	35.44126600
				H	24.22356400	6.71340900	35.65997300
				H	25.38219500	3.11433300	36.53364800
				H	24.87927100	2.16897800	35.09450800
				H	26.27297600	3.26775900	34.98437500
				H	25.85906200	6.12243400	35.28695500
				H	21.10437600	2.08013600	34.66951600
				C	20.74440600	1.71135400	35.63795200
				C	20.05830500	2.83484500	36.40340800
				O	19.05762400	2.61119700	37.10202500
				C	21.93297100	1.11004800	36.41845500
				C	21.56846600	0.53248600	37.78933700
				C	20.74205100	-0.74055100	37.69058300
				H	22.50526100	0.29040900	38.31041300
				H	19.99410600	0.93903600	35.44862600
				H	21.04770400	1.27387500	38.40662600
				H	22.70713800	1.87203800	36.55992700
				H	22.36955700	0.31113100	35.81033900
				H	19.66497200	-0.28522400	39.39099300
				O	20.75700600	-1.48810500	36.72808000
				N	20.00530500	-1.06655100	38.83896400
				H	19.29152100	-1.76662000	38.65649700
				N	20.63928600	4.05320700	36.28664100
				C	20.22614400	5.23800100	37.03136300
				H	19.80206900	5.97442200	36.33356600
				C	21.38963100	5.86701600	37.81010000
				H	21.02309700	6.79570000	38.26882300
				C	21.99458000	4.94831500	38.87389500
				H	19.42384800	4.92778600	37.70532100
				H	22.29552800	3.98987300	38.43850900
				H	22.17347800	6.16497200	37.10161000
				H	21.52121300	4.11349100	35.78129900
				H	22.90139900	5.38873800	39.29754900
				H	21.27948000	4.74396100	39.68042800
				C	15.54477600	3.17784900	36.56159400
				C	15.60819200	3.84789600	37.92218100
				O	14.64217900	4.45004500	38.40102500
				C	14.84684000	1.79385700	36.64460500
				C	13.41146800	1.78899000	37.20749300
				C	12.42204800	2.58762900	36.34842900
				C	12.91022000	0.35061800	37.40980700
				H	13.62321500	-0.24113300	38.00021100
				H	11.95932700	0.36072000	37.95322400
				H	12.76979100	-0.16381700	36.44713100
				H	12.29245600	2.13108500	35.35514000
				H	11.45781600	2.62615500	36.86289600
				H	12.75174100	3.62378500	36.21283500
				H	14.98457800	3.84071300	35.89505700
				H	13.41839400	2.27190200	38.18948100
				H	15.47637900	1.13243900	37.25718200
				H	14.84939300	1.36320500	35.63188200

N	16.78126500	3.72250500	38.61568800	H	30.81062900	0.08878900	44.55454800
C	16.82382500	3.95754900	40.05784000	H	32.72376500	1.32803300	42.69862000
C	16.64494600	5.42710200	40.48288300	N	30.70857100	1.68546600	41.01237900
O	16.43081900	5.69995200	41.66508300	C	29.51820200	1.95306800	40.20525200
C	18.11470000	3.38447400	40.65401800	C	28.98752500	0.63598300	39.58527300
H	17.57259000	3.25585600	38.17043000	O	29.69501800	-0.37184900	39.52886500
H	15.96388000	3.45304800	40.51558000	C	30.07535000	2.88624600	39.11307200
H	18.99925500	3.83484000	40.19079200	C	31.46398000	2.27935300	38.83772900
H	18.14923700	3.58290800	41.72735500	C	31.94088500	1.78225900	40.22076800
H	18.15587000	2.30157700	40.49493000	H	31.36604400	1.42732900	38.15882700
N	16.74069300	6.36984600	39.50794300	H	28.74413600	2.41338400	40.82211100
C	16.35235400	7.75032900	39.74143400	H	32.63623600	2.49439100	40.68638000
C	14.84386500	8.04672000	39.89325200	H	32.44473100	0.81204100	40.14550700
O	14.50396200	9.19276100	40.18165600	H	32.16499300	2.99282800	38.39215000
H	16.78349700	6.02862000	38.55800300	H	30.16566100	3.90362100	39.51221800
H	16.81605600	8.09951200	40.66637500	H	29.43251600	2.92234300	38.22972500
H	16.73865200	8.36854100	38.92575400	N	27.74884700	0.71408700	39.05016700
N	13.99775700	7.00939700	39.69428500	C	27.09033200	-0.48987800	38.55948800
C	12.57600900	7.09546800	39.99950700	C	25.71758100	-0.18830300	37.94644300
C	12.23305800	6.31556000	41.28385900	O	24.81484600	0.36275900	38.91801100
O	12.00947500	6.90605400	42.34880800	C	25.09064700	-1.46006000	37.38088500
H	14.35237600	6.09936000	39.40563700	H	26.96956000	-1.21682800	39.37387200
H	12.33124700	8.14528500	40.15925000	H	24.11938700	-1.24243800	36.92439000
N	12.25875900	4.97095800	41.14267900	H	25.73734800	-1.90265300	36.61400200
C	11.71857000	4.07318900	42.16494400	H	27.16039400	1.52898000	39.23925300
C	12.40582700	4.16314800	43.53345400	H	25.84748900	0.55142400	37.14334500
O	11.79329000	3.85203400	44.55017000	H	24.94154600	-2.19538000	38.17786600
C	11.79954600	2.61479900	41.65447700	H	25.05311600	1.32923000	39.02739700
C	11.19856400	2.33954000	40.23619900	C	23.51625400	8.82008300	44.82479000
O	11.30718800	3.26837400	39.37460300	S	22.42101800	8.27327500	46.17090100
O	10.72320800	1.19862800	40.06388400	H	23.55153800	9.91372300	44.82372000
H	12.11515800	4.53634200	40.20319900	H	24.52219400	8.40853200	44.94372800
H	10.67005900	4.32844500	42.36442700	C	22.92312100	5.94126600	42.77377100
H	11.31290300	1.96345700	42.38375300	H	23.11643400	5.93913700	41.70604400
H	12.85765200	2.31690100	41.61273600	C	25.61713800	5.28208100	46.73831200
N	13.72566600	4.52890800	43.53655000	H	26.66412700	5.06671400	46.93000800
C	14.48111500	4.66104300	44.77214200	C	21.66763000	5.86945700	49.46900700
C	14.78424200	6.12925600	45.13667800	H	21.46317300	5.84946600	50.53578300
O	15.75822700	6.41795200	45.84427000	C	18.95719100	6.46054700	45.49789700
C	15.75623100	3.80657700	44.77907000	H	17.89280500	6.59041700	45.32413300
C	16.20898300	3.45418300	46.19944200	C	23.99787300	5.66736900	43.61394200
H	13.82743600	4.27857300	45.56431400	C	25.34269000	5.35630300	43.14547700
H	14.15580000	4.82751600	42.66883700	C	26.09173600	5.20175800	44.27820400
H	16.56111400	4.28720400	44.21372500	C	25.22457500	5.39778100	45.41118900
H	15.52388800	2.86001100	44.27373500	C	25.77273400	5.22969700	41.71165400
O	15.43315000	3.41497400	47.14931000	H	26.86310100	5.33893100	41.66035700
N	17.52616800	3.13126500	46.31746600	H	25.35967000	6.04369400	41.10586700
H	17.84380600	2.80743200	47.22017300	C	25.37228000	3.90581300	41.02330800
H	18.16663600	3.04691000	45.53532900	H	25.93951000	3.05700700	41.41958000
N	13.88964400	7.03937300	44.69038600	H	24.31286900	3.69248500	41.23124700
C	13.96060000	8.45411800	45.02549300	C	25.51096600	3.96803400	39.48073100
H	12.97909700	8.76318300	45.41018800	O	25.72717200	2.85562300	38.87778300
C	14.34844600	9.34500600	43.83607700	O	25.36984200	5.07702700	38.92932800
C	15.78461900	9.13025400	43.35121800	C	24.77103700	5.38141900	47.83903500
H	14.68801700	8.55042200	45.83656300	C	25.19579100	5.25588800	49.21305500
H	13.65239100	9.16042500	43.00932100	C	24.08260100	5.42029000	49.98034700
H	15.93703900	8.08904400	43.04629500	C	22.98243100	5.64410000	49.07207600
H	15.99208000	9.76586300	42.48379200	C	20.58713100	6.09154200	48.62389000
H	13.16872400	6.75402500	44.02978000	C	19.21861400	6.23187000	49.06144700
N	31.71485800	0.52436900	44.35616200	C	18.45545200	6.37784400	47.94211000
C	31.88653300	0.64983000	42.91704000	C	19.36431400	6.34425900	46.82345600
C	30.60388000	1.17651600	42.27249300	C	19.80982900	6.41065400	44.40673200
O	29.52586100	1.11447700	42.86063300	C	19.39183200	6.56775000	43.03538400

C	20.51226500	6.44593600	42.27122600	H	14.20972400	10.39341200	44.13988100
C	21.61216400	6.19371200	43.17351800	H	16.51252600	9.35980500	44.13993700
N	23.94786700	5.68335600	44.98779000	H	32.42134400	-0.10929700	44.72391700
N	23.42312000	5.60908700	47.77662800	H	32.11599600	-0.29599700	42.38388600
N	20.65642700	6.17465200	47.25544500	H	27.55077900	-2.25222600	45.50293100
N	21.16922900	6.19017000	44.47024900	H	20.60398000	6.50641700	41.19452100
Fe	22.29785400	5.85521700	46.12992500	H	18.36729100	6.71943500	42.72184800
O	21.96347800	4.07472600	46.05719600	H	17.38244000	6.47309800	47.83652800
C	23.81885100	-1.68764200	41.95325000	H	18.89779200	6.19550900	50.09524400
N	24.86902900	-0.74698600	41.62705700	H	23.99529100	5.39100300	51.05940300
C	25.93765300	-0.34425100	42.37138400	H	26.21326800	5.06212500	49.52868400
O	26.70862200	0.51165500	41.94555400	H	27.14492900	4.95561400	44.34394300
C	26.14476300	-0.92539900	43.78780800	H	27.73366600	-0.96005800	37.80583800
N	27.56268400	-0.75787100	44.10097900	H	25.05958100	5.62257300	36.81762200
C	28.20889800	-1.49827300	45.02288500	H	16.55429100	3.04759700	36.15507900
O	29.39401500	-1.40332400	45.33310100	H	12.00042400	6.70001300	39.15381800
C	25.19398900	-0.22681200	44.75572900				
C	25.14568400	1.17358700	44.80643300	⁴ TS _{2HA,B}			
C	24.22966000	1.83061600	45.61535200	C	24.97157700	5.87197700	35.75213400
C	23.32277200	1.09930800	46.40739600	S	24.18463900	4.45336500	34.89947300
C	23.39651600	-0.30324000	46.39962400	C	25.31150800	3.12279600	35.46176300
C	24.31906400	-0.95049200	45.57766300	H	24.30229900	6.73119000	35.64650100
O	22.39120500	1.69937800	47.17372400	H	25.40807400	3.12854300	36.55379900
C	22.49552700	-1.17615600	41.27913900	H	24.88472100	2.17201400	35.12960400
C	21.79592100	-0.11241300	42.11255000	H	26.29734200	3.24439400	35.00100400
C	20.55839800	-0.40637400	42.71918200	H	25.92876700	6.11294400	35.27764400
C	19.90270900	0.54088700	43.48104300	H	21.11250700	2.12634000	34.66367000
C	20.46616100	1.86830200	43.71114500	C	20.72915400	1.75359600	35.62152100
C	21.74291500	2.11821500	43.07059200	C	20.08078100	2.88486700	36.40642000
C	22.36676400	1.17312100	42.29321300	O	19.08956400	2.67361800	37.12193400
O	19.89103300	2.74565100	44.40691100	C	21.88377700	1.08291600	36.39701400
Cl	18.36935100	0.16332900	44.21045500	C	21.50530800	0.55541200	37.78355400
C	24.14898600	-3.11272600	41.43065200	C	20.51362800	-0.59799900	37.73330400
O	24.81334900	-3.24027000	40.41306900	H	22.42481300	0.20632700	38.27212500
C	23.71408200	-4.30477300	42.21420200	H	19.95103300	1.01509500	35.41451600
O	21.65943300	-2.29118500	41.02400600	H	21.10780500	1.35779600	38.41616600
C	22.83090600	-4.24750500	43.30691000	H	22.71187100	1.79009600	36.51707200
C	22.47012800	-5.39867200	43.99794100	H	22.25324900	0.24714100	35.79339200
C	22.99519600	-6.63561500	43.60679400	H	19.71659000	-0.09625700	39.57360400
C	23.87466700	-6.71223900	42.51811600	O	20.32788300	-1.29388500	36.74964800
C	24.22242700	-5.55673700	41.83137000	N	19.86461200	-0.87720200	38.94191800
O	22.61762600	-7.73684500	44.32017600	H	19.04299300	-1.46257400	38.82276800
H	23.68516500	-1.70801600	43.03564500	N	20.67732900	4.09559900	36.28898400
H	24.88942600	-0.38220900	40.66482900	C	20.27914400	5.28361400	37.03652400
H	25.91344100	-1.99815800	43.78576800	H	19.84613000	6.01908100	36.34302600
H	28.08368100	-0.04372800	43.58243500	C	21.45512900	5.91298700	37.79546800
H	25.82433000	1.75489900	44.18789600	H	21.09909400	6.84829900	38.24937700
H	24.17967900	2.91200700	45.62381200	C	22.06797800	5.00127900	38.86069800
H	22.70804400	-0.86569600	47.02360500	H	19.48645700	4.97633300	37.72327200
H	24.35056800	-2.03976700	45.56904700	H	22.35191800	4.03438100	38.43247300
H	22.28854400	2.65289200	46.88467500	H	22.23139200	6.20019300	37.07430500
H	22.81501500	-0.72754200	40.32955000	H	21.55242000	4.14909500	35.77158300
H	20.12638700	-1.39018200	42.57671000	H	22.98646000	5.43650700	39.26437000
H	22.18472200	3.09400200	43.23951800	H	21.36402700	4.81429600	39.68103700
H	23.31789700	1.40471500	41.82581800	C	15.51631700	2.95443400	36.78703100
H	21.16760600	3.90504200	45.51411900	C	15.61900300	3.65057500	38.13228400
H	21.09345700	-2.04564100	40.26133700	O	14.65035500	4.20710100	38.66054900
H	22.39666600	-3.30343800	43.61608800	C	14.81240100	1.57681300	36.90818200
H	21.78323800	-5.35958200	44.83715600	C	13.37171400	1.59384900	37.45739600
H	24.28163700	-7.67600400	42.21476700	C	12.39189800	2.35762100	36.55658600
H	24.89774500	-5.59633300	40.98301200	C	12.86873500	0.16383400	37.70878300
H	23.05034600	-8.51739200	43.93987500	H	13.57059900	-0.40119700	38.33700100
H	23.11949600	8.48119400	43.86067300	H	11.90639900	0.19155300	38.23049200
				H	12.74814900	-0.39063800	36.76599000

H	12.27535400	1.86376800	35.57981000	H	15.91341300	8.13442100	42.92662900
H	11.42073400	2.41516200	37.05574900	H	15.90761000	9.79210800	42.30682300
H	12.72212000	3.38828200	36.38411800	H	13.20185500	6.77350900	44.00448800
H	14.94283800	3.60763800	36.12161600	N	31.54806900	0.41832800	44.55365900
H	13.37115600	2.11448200	38.41933500	C	31.77335800	0.59621200	43.12740800
H	15.43428600	0.93214900	37.54595000	C	30.51164700	1.13408200	42.45179500
H	14.82144500	1.11452400	35.90967700	O	29.41285100	1.04751700	42.99810300
N	16.83471600	3.60864800	38.75599900	H	30.63549600	-0.01928900	44.70231700
C	16.94902200	3.92484800	40.17775000	H	32.61088000	1.28967600	42.96481900
C	16.71565900	5.40710900	40.52433400	N	30.65951400	1.68175600	41.21314200
O	16.51747500	5.74184500	41.69289100	C	29.49937200	1.96436000	40.36812800
C	18.29874300	3.44898200	40.72720700	C	29.01127400	0.66347500	39.68128300
H	17.63223000	3.19260500	38.27411800	O	29.72715100	-0.33894100	39.63308100
H	16.14358200	3.40691600	40.71204900	C	30.08734200	2.94365300	39.33452800
H	19.13270000	3.91657900	40.19303000	C	31.49329200	2.36263200	39.09273500
H	18.38374000	3.69950500	41.78688200	C	31.92032200	1.81380500	40.47298700
H	18.38716300	2.36259500	40.61943900	H	31.43390600	1.53869400	38.37566200
N	16.75187500	6.29422400	39.49369800	H	28.69472800	2.39167800	40.96934200
C	16.33550000	7.67581700	39.65730600	H	32.59390000	2.50956400	40.99213100
C	14.82278300	9.95187400	39.79943600	H	32.43118100	0.84884800	40.37924700
O	14.46114500	9.10901800	40.00499200	H	32.20323100	3.10109200	38.70583500
H	16.79672300	5.90194100	38.56358600	H	30.14938000	3.94645700	39.77405200
H	16.79604000	8.08132400	40.56070800	H	29.47936000	3.00547300	38.42826100
H	16.70477800	8.25984400	38.80918100	N	27.80214400	0.75331500	39.08516000
N	13.99631200	6.88624200	39.68302800	C	27.17139000	-0.43834900	38.53206100
C	12.57156800	6.97242200	39.97462900	C	25.81766000	-0.12253500	37.88422000
C	12.23190400	6.25307700	41.29388300	O	24.87566800	0.38106200	38.84243500
O	12.02785100	6.88835100	42.33647100	C	25.21741100	-1.37211400	37.24600100
H	14.36795500	5.96175200	39.47143200	H	27.03090300	-1.19290200	39.31770900
H	12.31683000	8.02668600	40.08015200	H	24.27138700	-1.12855200	36.75079600
N	12.24113800	4.90367300	41.20813800	H	25.89844900	-1.79309000	36.49680000
C	11.71369000	4.05282000	42.27549300	H	27.19983500	1.55899900	39.27275500
C	12.44171200	4.17879800	43.62109600	H	25.97146700	0.64904100	37.11624000
O	11.85700200	3.90057200	44.66304400	H	25.02289700	-2.13158900	38.00987000
C	11.75669300	2.57609800	41.81617000	H	25.09899600	1.34180100	38.99675200
C	11.10408600	2.26518600	40.43003200	C	23.63869700	8.87633300	44.92676500
O	11.21252500	3.14898800	39.52568700	S	22.49944400	8.31478600	46.23365100
O	10.58668800	1.13350600	40.32016200	H	23.70464300	9.96767400	44.98009300
H	12.08362400	4.43815800	40.28904500	H	24.63195600	8.43636100	45.05111900
H	10.67610700	4.33433400	42.49468200	C	22.99037300	6.05047000	42.74026700
H	11.28637100	1.95914500	42.58450900	H	23.20002000	6.05623100	41.67567100
H	12.80802700	2.26153100	41.74711100	C	25.61526000	5.32528700	46.73914300
N	13.76138900	4.54072400	43.57424800	H	26.65907700	5.10914000	46.94660100
C	14.55554100	4.71446800	44.78077000	C	21.60999100	5.83764100	49.40436500
C	14.84204500	6.19642900	45.10180200	H	21.38391500	5.78530500	50.46558000
O	15.82160000	6.51780200	45.78739800	C	18.98699600	6.59131900	45.40346700
C	15.84509100	3.88067700	44.76264500	H	17.92799400	6.73901800	45.21329500
C	16.33933500	3.54579500	46.17389000	C	24.04631000	5.74883100	43.59460700
H	13.93645500	4.34040700	45.60405900	C	25.39429100	5.42887200	43.14417000
H	14.16302300	4.81194000	42.68459100	C	26.12761000	5.26956400	44.28724700
H	16.62751100	4.36882700	44.17298400	C	25.24540800	5.46168100	45.40772200
H	15.61613700	2.92618000	44.27082100	C	25.83859100	5.28805400	41.71652400
O	15.59275900	3.53792600	47.14858700	H	26.93021100	5.38967100	41.67499800
N	17.65514800	3.20928200	46.25844500	H	25.43619700	6.09778100	41.09788700
H	17.98487600	2.87771100	47.15434900	C	25.43311700	3.95926400	41.03977600
H	18.27075600	3.07179000	45.46170200	H	25.99466200	3.11088100	41.44501000
N	13.93001200	7.08368400	44.64532500	H	24.37294400	3.75237900	41.24951500
C	13.98530500	8.50704600	44.94571300	C	25.57350300	4.00596500	39.49646800
H	13.01152200	8.80811800	45.35573700	O	25.79206300	2.88883100	38.90606700
C	14.31670600	9.37576600	43.72309800	O	25.42963000	5.11066000	38.93559100
C	15.74260300	9.18122500	43.20086300	C	24.74593900	5.39435700	47.82402600
H	14.73720400	8.63521800	45.72953200	C	25.14239300	5.23145400	49.20095500
H	13.60046500	9.15294900	42.92342200	C	24.01206900	5.36923300	49.94947700

C	22.93178300	5.61753900	49.02610500	H	20.96855800	-2.02032300	40.22981900
C	20.55029000	6.09832900	48.54546000	H	22.31976800	-3.46155300	43.38715800
C	19.17588800	6.24181400	48.96110500	H	21.73484800	-5.55832300	44.55530900
C	18.43597200	6.43581800	47.83343900	H	24.26625000	-7.76975900	41.87477000
C	19.36603600	6.42794900	46.73252500	H	24.85373800	-5.64973300	40.69859700
C	19.86119700	6.55686800	44.32899100	H	23.04405600	-8.67375500	43.57353300
C	19.47036300	6.74525700	42.95392200	H	23.25568000	8.59499700	43.93933500
C	20.60116200	6.61318800	42.20706300	H	14.16206100	10.42824800	44.00410000
C	21.68003500	6.32660900	43.12390000	H	16.48744000	9.45665100	43.95873800
N	23.97456800	5.75359500	44.96753900	H	32.23795700	-0.23171500	44.92415500
N	23.39774200	5.61813100	47.73919700	H	32.03324200	-0.32792800	42.57101600
N	20.64716200	6.22515900	47.18111200	H	27.31365600	-2.34247700	45.50053700
N	21.21485800	6.31152200	44.41267900	H	20.71348300	6.68437600	41.13295100
Fe	22.30572200	5.94304100	46.07725400	H	18.45294700	6.91599200	42.62792600
O	21.92082400	4.10741500	45.90947500	H	17.36608800	6.54116200	47.70889700
C	23.77647200	-1.78412700	41.80498100	H	18.83453300	6.17196200	49.98654600
N	24.84748300	-0.85738900	41.50897600	H	23.90176300	5.30770400	51.02504900
C	25.86747800	-0.42756400	42.29887400	H	26.15368000	5.03067500	49.53175800
O	26.65745500	0.42617100	41.90408900	H	27.17786700	5.01511000	44.36730200
C	26.00144200	-0.97617300	43.73910000	H	27.84272700	-0.87811300	37.78423600
N	27.41121300	-0.84703800	44.10159700	H	25.12299600	5.63810400	36.81275400
C	28.00492200	-1.60047400	45.04911300	H	16.51428800	2.81356500	36.35676900
O	29.17805800	-1.52781900	45.40560600	H	12.00395500	6.53024500	39.14684000
C	25.05381100	-0.20026800	44.64602400				
C	25.12364200	1.20425900	44.68677100	41M2_B			
C	24.23468100	1.93890200	45.44501500	C	24.95771900	5.64908300	35.47196800
C	23.22370300	1.30071200	46.23469300	S	24.13832500	4.20544100	34.69526700
C	23.18905700	-0.12821600	46.21368500	C	25.22943800	2.87943200	35.33354700
C	24.08040300	-0.84739800	45.43257500	H	24.31102600	6.51738700	35.31368100
O	22.37666900	1.97648200	46.94841600	H	25.32823200	2.94653800	36.42331700
C	22.45705100	-1.21661300	41.17442800	H	24.77502100	1.92331800	35.05789400
C	21.81205700	-0.14320000	42.03800800	H	26.21733100	2.94582000	34.86592100
C	20.61501600	-0.42675100	42.72491100	H	25.92286800	5.83824700	34.99032500
C	20.01031800	0.52733400	43.52148500	H	21.03472000	1.91299500	34.64851000
C	20.57328600	1.85391400	43.70667900	C	20.63200600	1.63186100	35.62954900
C	21.80849700	2.09083900	42.99474500	C	20.01102100	2.84449600	36.30822700
C	22.38612700	1.13926800	42.17973500	O	18.98586100	2.72764400	36.99752100
O	20.02186000	2.74505600	44.41987300	C	21.76116000	0.99675700	36.46957800
Cl	18.51280600	0.14748800	44.33870100	C	21.35360300	0.57395300	37.88385300
C	24.07653100	-3.18791600	41.21633100	C	20.39192200	-0.60572500	37.90494900
O	24.70784300	-3.28132200	40.17395800	H	22.26481500	0.29216600	38.42829800
C	23.65590700	-4.40727200	41.96604800	H	19.83391100	0.90204100	35.47519200
O	21.58772300	-2.31098900	40.93225000	H	20.91214400	1.41340500	38.43502600
C	22.77141300	-4.39095600	43.05893400	H	22.59987300	1.69689900	36.55256000
C	22.42476900	-5.56529900	43.71764500	H	22.12539100	0.11501000	35.93189400
C	22.96655100	-6.78411600	43.29391400	H	19.68470500	-0.08461200	39.77970100
C	23.84682700	-6.81985000	42.20395300	O	20.17866000	-1.33121200	36.94891000
C	24.17917600	-5.64161700	41.54848600	N	19.80578000	-0.87146600	39.14928400
O	22.60345800	-7.90957900	43.97725800	H	18.98454100	-1.46538300	39.08050100
H	23.64730400	-1.84827300	42.88513500	N	20.66567900	4.01676000	36.12970500
H	24.88706600	-0.47412100	40.55446400	C	20.29445100	5.26930300	36.78057300
H	25.73130900	-2.03855400	43.76781800	H	19.92372100	5.97441900	36.02260300
H	27.96561900	-0.13678100	43.61242500	C	21.46635600	5.89552800	37.54805700
H	25.87718700	1.71512700	44.09373800	H	21.13330100	6.86851800	37.93452900
H	24.28728500	3.01967800	45.45662400	C	21.99744700	5.02423400	38.68771200
H	22.43589300	-0.62590200	46.81727200	H	19.46186600	5.04296800	37.45134400
H	24.02867200	-1.93605600	45.42592900	H	22.27130900	4.02851900	38.32385900
H	22.20454400	3.16969200	46.49022200	H	22.28169400	6.10872900	36.84469000
H	22.76832900	-0.77231400	40.22004200	H	21.55565200	4.00079000	35.63471400
H	20.16669300	-1.40821200	42.61792500	H	22.90579400	5.45724800	39.11506700
H	22.25565100	3.07234600	43.11132900	H	21.24856500	4.90103400	39.47991300
H	23.30347900	1.37856400	41.65087300	C	15.59724200	3.50083000	36.34412500
H	21.14500100	3.86783000	45.35021000	C	15.60238100	4.07713100	37.74875100
				O	14.60919400	4.62985000	38.23222300

C	15.03501600	2.05464300	36.33070000	N	13.80058300	6.82014200	44.78182800
C	13.62229600	1.87683800	36.92221600	C	13.79674800	8.22280500	45.17154300
C	12.54330100	2.64034100	36.14238600	H	12.78721300	8.47380700	45.52424300
C	13.25855900	0.38824700	37.03135000	C	14.19682400	9.17906100	44.03816100
H	14.03776500	-0.17585800	37.56148100	C	15.65231300	9.02440400	43.59017100
H	12.32554200	0.27207500	37.59281900	H	14.48428500	8.31688600	46.01709500
H	13.13728500	-0.06802100	36.03764700	H	13.53307100	9.01902400	43.18024700
H	12.44482800	2.25677400	35.11535400	H	15.83802400	8.00487300	43.23510300
H	11.58613400	2.53931200	36.66154400	H	15.87145600	9.71105500	42.76573600
H	12.76626100	3.71168500	36.09338300	H	13.09542100	6.51904300	44.11250900
H	14.97777500	4.15534300	35.72409000	N	31.71687400	0.30656400	44.33342700
H	13.61263900	2.28882700	37.93662300	C	31.84793800	0.50144300	42.89735000
H	15.74138400	1.41273300	36.87555300	C	30.53935900	1.03329200	42.31267100
H	15.04810900	1.70405500	35.28769500	O	29.48403800	0.94099100	42.93946800
N	16.75553300	3.92040200	38.46823400	H	30.80515200	-0.10997400	44.53488000
C	16.74909700	4.03159600	39.92678800	H	32.66685900	1.20409900	42.68647500
C	16.51819900	5.45482100	40.46629800	N	30.59316500	1.58229800	41.06951000
O	16.24187600	5.62375300	41.65525500	C	29.37195700	1.84944100	40.30924400
C	18.04167000	3.44897100	40.51050300	C	28.83894300	0.53236700	39.68850100
H	17.54934300	3.45764400	38.02150000	O	29.52435600	-0.49220300	39.67504100
H	15.89297100	3.46651900	40.31616900	C	29.87650100	2.81478000	39.22057500
H	18.92216700	3.97760400	40.13006600	C	31.26156800	2.23234900	38.88212200
H	18.03031400	3.54075500	41.59864200	C	31.79475500	1.70963200	40.23505800
H	18.13263800	2.39037300	40.24383700	H	31.15098300	1.39571400	38.18556800
N	16.64251800	6.47760500	39.58035600	H	28.61137100	2.28177000	40.96191300
C	16.21666500	7.82755100	39.90904300	H	32.49934200	2.41822200	40.69151800
C	14.69905500	8.06206800	40.07330500	H	32.30471600	0.74646700	40.12007800
O	14.31716000	9.15824000	40.47769600	H	31.93746800	2.96448400	38.42857100
H	16.74501800	6.21817100	38.60934600	H	29.96947600	3.82347200	39.64021400
H	16.66547800	8.12726400	40.85843900	H	29.20168700	2.86419000	38.36239100
H	16.58929300	8.51033100	39.13985400	N	27.61864000	0.62595900	39.11834400
N	13.88790000	7.02661300	39.75041600	C	26.95345900	-0.56300400	38.60110200
C	12.47258100	7.01725000	40.08963900	C	25.58730300	-0.22661600	37.99163400
C	12.19643300	6.13339000	41.32263900	O	24.70670900	0.35510700	38.96664800
O	11.90951900	6.63304900	42.41608300	C	24.92350600	-1.47722100	37.42279000
H	14.27687500	6.16173900	39.37922600	H	26.82249200	-1.30401000	39.40059900
H	12.17613100	8.03795800	40.32996900	H	23.96609200	-1.22288400	36.95654300
N	12.34666700	4.80347500	41.10683900	H	25.56170300	-1.94238800	36.66199300
C	11.87282300	3.81063300	42.07291900	H	27.05447100	1.47243000	39.23485000
C	12.52287800	3.89471300	43.46191700	H	25.73596000	0.51022200	37.19027600
O	11.90268500	3.49970700	44.44462500	H	24.74226700	-2.20678400	38.21785800
C	12.09376600	2.39016300	41.50578700	H	24.95038300	1.32630600	39.02560100
C	11.49527700	2.12192300	40.09111400	C	24.26815600	8.79442000	46.37209300
O	11.49972700	3.07445400	39.25907000	S	22.53817400	8.36152900	45.96267400
O	11.11199300	0.94563300	39.88481200	H	24.34915800	9.88542400	46.31324200
H	12.25603500	4.42636600	40.14567200	H	24.53522100	8.47466600	47.38329600
H	10.80245100	3.96007500	42.26203800	C	22.87048700	6.07939300	42.59596100
H	11.68737500	1.66614000	42.21560600	H	23.03416200	6.08915900	41.52343000
H	13.17484000	2.20113300	41.43528700	C	25.67577800	5.48027400	46.48823300
N	13.81223000	4.34698100	43.51793600	H	26.72851300	5.27372000	46.65908800
C	14.51700100	4.47550000	44.78504200	C	21.79836600	6.14229300	49.31923100
C	14.74798100	5.94511600	45.19243200	H	21.62934200	6.17367600	50.39199000
O	15.70945400	6.26376700	45.90206400	C	18.94901900	6.40315100	45.41839000
C	15.82099200	3.66735100	44.83137400	H	17.87696600	6.48219500	45.26457000
C	16.21992800	3.31480800	46.26874900	C	23.97502200	5.83032300	43.40745300
H	13.84825800	4.05051700	45.54200500	C	25.30844800	5.51295900	42.90354000
H	14.25818500	4.70038800	42.67774900	C	26.08573100	5.35535700	44.01498100
H	16.63339700	4.18336100	44.31005900	C	25.24593600	5.56053500	45.17028900
H	15.64464700	2.71952600	44.30630100	C	25.69876000	5.35570100	41.46137400
O	15.39656700	3.22649000	47.17537200	H	26.78438200	5.48704300	41.37118100
N	17.54171700	3.05498000	46.45489500	H	25.25034700	6.13971200	40.84201300
H	17.81764800	2.72803300	47.37009200	C	25.30996400	3.99553900	40.84137500
H	18.22749600	2.98767700	45.70851700	H	25.86401500	3.17177400	41.30460400

H	24.24598500	3.79735700	41.04213000	H	24.19070700	-1.96027400	45.56972600
C	25.48558700	3.95661300	39.30415300	H	22.25930600	3.51071700	46.64432600
O	25.68558900	2.79946300	38.77842400	H	22.74649600	-0.71169400	40.37129200
O	25.39055400	5.02794700	38.67687000	H	20.21610700	-1.44316200	42.86229400
C	24.86359100	5.64135600	47.61060600	H	22.05849100	3.16268600	43.16969000
C	25.32959400	5.58952400	48.97406300	H	23.11521100	1.50944100	41.66972700
C	24.23949500	5.79254200	49.76843100	H	21.21249000	3.74272900	45.47374100
C	23.10824000	5.95993000	48.88999800	H	20.97063000	-2.01033700	40.40481400
C	20.68050700	6.25132800	48.49820900	H	22.28366200	-3.32054400	43.56397500
C	19.31888900	6.35459700	48.97666300	H	21.73112500	-5.38374200	44.80575700
C	18.51473000	6.39906800	47.87952600	H	24.46851600	-7.60807100	42.34746600
C	19.39095900	6.34067000	46.73254500	H	25.02498500	-5.52243500	41.09850000
C	19.78513000	6.38179300	44.30498800	H	23.20615700	-8.48338300	44.03541700
C	19.32345500	6.50906200	42.94304500	H	24.97011600	8.35004400	45.66126300
C	20.43167500	6.45526500	42.15388500	H	14.02026000	10.20758800	44.38739800
C	21.56571100	6.27452600	43.03269000	H	16.35019200	9.22502100	44.41248500
N	23.95996500	5.84216800	44.77616500	H	32.41554200	-0.36258000	44.64871800
N	23.51168800	5.86768400	47.57937100	H	32.07771600	-0.41547800	42.31701200
N	20.70162800	6.24226600	47.12877200	H	27.42287800	-2.36353700	45.46701600
N	21.14709000	6.24348100	44.33898800	H	20.49541800	6.51945200	41.07518800
Fe	22.33824100	6.12176900	45.95644100	H	18.28390000	6.60041100	42.65610000
O	22.06540000	4.06689500	45.85835900	H	17.43600100	6.44782200	47.80558500
C	23.76880500	-1.65864200	41.99127200	H	19.03493600	6.36913100	50.02195200
N	24.80496700	-0.69310600	41.68138800	H	24.18833000	5.81501000	50.85016600
C	25.83473800	-0.26002600	42.45109600	H	26.35707400	5.41433400	49.26861100
O	26.58449200	0.64027200	42.08659700	H	27.14058500	5.10906600	44.05432400
C	26.05435800	-0.89577700	43.85059500	H	27.59152500	-1.02785900	37.83867300
N	27.47988500	-0.79691700	44.14059700	H	25.09783600	5.47113800	36.54497900
C	28.10917000	-1.61969000	45.00985400	H	16.61370400	3.48986600	35.93487800
O	29.30118900	-1.59805300	45.29362000	H	11.89789700	6.65273800	39.22942500
C	25.18965800	-0.17056900	44.87338200	⁴ IM3 _{Cyc}			
C	25.30468000	1.23442400	45.01624400	C	25.05818000	5.99788000	35.83587900
C	24.48974500	1.92107500	45.88247000	S	24.35833700	4.59181300	34.89109700
C	23.49683600	1.22826000	46.68184000	C	25.43546300	3.25682900	35.53452700
C	23.43901300	-0.21536600	46.55713600	H	24.38462200	6.85045800	35.70813100
C	24.25863600	-0.87826000	45.66918800	H	25.45877300	3.27119100	36.62906600
O	22.70197500	1.84750000	47.44464000	H	25.02561800	2.30581200	35.18271000
C	22.43924700	-1.15344000	41.32774100	H	26.45215900	3.36778200	35.14371600
C	21.75103400	-0.09619900	42.17673900	H	26.04459300	6.26605700	35.44317100
C	20.61577500	-0.43744400	42.93332900	H	21.02647000	2.37671400	34.27605100
C	20.00813900	0.49214800	43.76022900	C	20.65041500	1.91519800	35.19714900
C	20.51310700	1.84386500	43.90811600	C	20.11391900	2.97854400	36.14747500
C	21.66439100	2.15461700	43.09349300	O	19.18212700	2.71508200	36.92514600
C	22.24925800	1.22495900	42.26038600	C	21.76825900	1.05379800	35.82329300
O	19.99212600	2.69631600	44.69306300	C	21.41331200	0.44039500	37.18290700
Cl	18.60128400	0.02835200	44.68649100	C	20.25033400	-0.54220500	37.10546000
C	24.13537600	-3.07240200	41.46876900	H	22.29238700	-0.10864500	37.54117900
O	24.81731700	-3.18591000	40.46112900	H	19.80354600	1.27532400	34.93204400
C	23.72285300	-4.27319300	42.25187000	H	21.21184900	1.22248000	37.92162900
O	21.61463200	-2.28261500	41.09263400	H	22.67545300	1.65569100	35.94847400
C	22.78879200	-4.24368800	43.30304000	H	22.00381400	0.24328300	35.12525500
C	22.45970000	-5.39970100	44.00160300	H	19.17903100	0.44998800	38.53662100
C	23.06844000	-6.61333700	43.66092900	O	20.14298900	-1.37219400	36.21868700
C	23.99746800	-6.66250500	42.61265100	N	19.35187200	-0.48452900	38.17525800
C	24.31243700	-5.50293300	41.91660100	H	18.48923600	-0.99216800	37.99151200
O	22.72009900	-7.71867200	44.38204200	N	20.72208900	4.18620000	36.08886700
H	23.62389900	-1.69361400	43.07181600	C	20.39702500	5.31613000	36.95717900
H	24.81450400	-0.31045600	40.72333000	H	20.09645400	6.16416200	36.32687700
H	25.77023000	-1.95403200	43.83402700	C	21.56885000	5.72472400	37.85914900
H	28.03098800	-0.09535800	43.63229500	H	21.27849800	6.64193400	38.38978600
H	26.02653800	1.76714500	44.40432800	C	21.99471500	4.64710800	38.85807300
H	24.55041800	2.99913800	45.97266000	H	19.52620000	5.02383600	37.54764300
H	22.70734400	-0.73838000	47.16533600	H	22.19142300	3.69905700	38.34463700

H	22.42766300	5.99248900	37.23089700	H	15.09423600	4.58523700	43.42973900
H	21.57227600	4.26444200	35.53645600	H	17.46949500	5.07531900	45.19499100
H	22.92769400	4.93478000	39.35013500	H	17.00304700	3.38452200	45.41305900
H	21.21928300	4.47056900	39.61350400	O	16.37658500	4.24258000	48.14740900
C	15.79756900	3.12069200	36.06322600	N	18.52963700	4.58039800	47.52152700
C	15.64460700	3.84298500	37.39552800	H	18.78251100	4.68108500	48.49484300
O	14.58060100	4.40273000	37.70732700	H	19.20839100	4.90871800	46.84488600
C	15.86678600	1.58308700	36.22142700	N	13.85209900	6.63843600	45.20965100
C	14.73830000	0.94927700	37.05666100	C	13.36460700	8.00125400	45.36803500
C	13.35256300	1.16462000	36.43049900	H	12.32200900	7.94952100	45.70908300
C	15.00432300	-0.54459400	37.29225100	C	13.44376500	8.84754500	44.08906400
H	16.03506600	-0.71114200	37.63596000	C	14.87044100	9.09343100	43.59112200
H	14.34557900	-0.91936500	38.08163500	H	13.95978900	8.45606000	46.16539700
H	14.86076800	-1.13870600	36.37724300	H	12.86575700	8.36624600	43.29249900
H	13.29907200	0.74713300	35.41302600	H	15.36758300	8.14730200	43.34998700
H	12.58400700	0.67313600	37.03808500	H	14.85447900	9.69542800	42.67689700
H	13.09710400	2.22882500	36.38217600	H	13.27636900	5.98410400	44.68337000
H	14.94439500	3.41745200	35.44739800	N	30.22793100	-1.20172300	45.18586000
H	14.71512900	1.42129700	38.04756000	C	30.77569700	-0.80778800	43.89679700
H	16.83457300	1.33398900	36.67450000	C	29.75715300	0.01536900	43.11000100
H	15.88266400	1.14100300	35.21243100	O	28.56903900	0.04232000	43.43203000
N	16.74068900	3.85270300	38.20011600	H	29.28815500	-1.58173400	45.05366500
C	16.67957300	4.06559800	39.65437200	H	31.69251000	-0.21976300	44.04614900
C	16.47401400	5.51814900	40.11930600	N	30.21206100	0.68542500	42.01867900
O	16.65308400	5.83131400	41.29718200	C	29.27379800	1.22839500	41.03315300
C	17.90866800	3.44202400	40.31884700	C	28.74109800	0.08308700	40.13574300
H	17.59106100	3.42416500	37.83643400	O	29.36037900	-0.98071500	40.03376700
H	15.78616600	3.52665200	40.01270400	C	30.17244700	2.18735200	40.23094400
H	18.84070400	3.82414700	39.88595600	C	31.50819600	1.42260100	40.16555300
H	17.90553000	3.68095600	41.38365900	C	31.59337300	0.68575900	41.52128300
H	17.88745900	2.35382400	40.19882800	H	31.47434200	0.68849100	39.35592600
N	15.99496700	6.40076000	39.18744100	H	28.44423300	1.72607500	41.53858900
C	15.29097000	7.58908100	39.63297500	H	32.24983600	1.21198600	42.22814700
C	13.88867400	7.34641900	40.22642800	H	31.97115000	-0.33508400	41.39686100
O	13.30851200	8.26888900	40.79577500	H	32.36967900	2.07753700	39.99869000
H	15.64006400	5.97473600	38.33785500	H	30.28739800	3.12744300	40.78367800
H	15.86912900	8.07542000	40.42040100	H	29.75486800	2.41941700	39.24773200
H	15.20151200	8.29348300	38.79948800	N	27.62273700	0.37332800	39.44413800
N	13.37819600	6.09446300	40.08276900	C	26.99354700	-0.63028200	38.59492300
C	12.18734100	5.67769700	40.80343800	C	25.84797200	-0.03235300	37.76953000
C	12.47666100	4.86901100	42.08836300	O	24.80371800	0.46735700	38.61624000
O	11.95610400	5.19567100	43.16241600	C	25.25013800	-1.07211100	36.82628400
H	13.85384400	5.41605500	39.49257800	H	26.60674700	-1.45908600	39.20370000
H	11.63666800	6.57116200	41.09696400	H	24.46917100	-0.61572500	36.20858600
N	13.29523200	3.80648100	41.93077600	H	26.01796200	-1.48327000	36.15968900
C	13.38937100	2.73477300	42.92221000	H	27.10392600	1.23859800	39.62836000
C	13.84888800	3.20277200	44.30829600	H	26.24777800	0.81033500	37.18865900
O	13.42660600	2.66508200	45.32591200	H	24.80492400	-1.89054700	37.39933600
C	14.35597600	1.62816400	42.42009100	H	25.09146000	1.38193200	38.88811200
C	14.21484900	1.19279000	40.92719000	C	24.71958800	9.25781000	45.71336300
O	14.19705100	2.16170400	40.07961300	S	22.90780700	9.14109100	45.48529200
O	14.19592700	-0.01989000	40.67664100	H	24.99523300	10.30855900	45.56956900
H	13.57659900	3.45484700	40.99107000	H	25.01626400	8.94902500	46.71943100
H	12.39590000	2.30053300	43.08946500	C	22.89778000	6.36971900	42.59500300
H	14.23584500	0.75543100	43.06595200	H	23.09567900	6.23189800	41.53704100
H	15.38654600	1.99024800	42.54515800	C	25.41665400	5.84334100	46.69194800
N	14.80286800	4.18600000	44.31563700	H	26.41003400	5.48680900	46.94903200
C	15.33665500	4.72283600	45.55638100	C	21.74956500	7.87310800	49.13024800
C	15.04782000	6.22977000	45.70144000	H	21.58961000	8.17542500	50.16150100
O	15.84396700	6.98154300	46.27337000	C	18.98471700	7.61153800	45.17073600
C	16.82345500	4.40585500	45.77220400	H	17.92808400	7.75177400	44.96893700
C	17.19895000	4.43337400	47.25733800	C	23.93872700	6.12330100	43.48246100
H	14.78546200	4.21651400	46.35711400	C	25.26570300	5.65708000	43.09266300

C	25.93860100	5.46094700	44.26724200	H	22.79879900	-1.97169600	42.27125200	
C	25.06004600	5.83287900	45.34836100	H	24.47350900	-0.48740100	40.28850900	
C	25.75722400	5.45601300	41.68430600	H	24.16830000	-1.70769300	43.73564600	
H	26.80788800	5.76978000	41.62721100	H	26.93973600	-0.65042300	43.93707900	
H	25.21573600	6.10247600	40.98790500	H	24.45106000	1.90915900	43.36005800	
C	25.64364300	4.01313500	41.15082300	H	23.87176900	3.43082500	45.28102700	
H	26.40203900	3.35772400	41.59036600	H	22.93538100	0.18658300	47.84931300	
H	24.67970800	3.58204900	41.45260400	H	23.95279000	-1.29907000	46.16668200	
C	25.69038300	3.91024900	39.60465200	H	21.92903500	4.47987800	46.88134700	
O	26.03812300	2.77355000	39.12659300	H	22.16992800	-0.63449000	39.61967200	
O	25.34416900	4.90913200	38.94258500	H	20.27110100	-0.94682800	42.84474700	
C	24.62865800	6.34661400	47.72300700	H	22.60579300	3.35634100	42.10424400	
C	25.05450900	6.46610200	49.09570800	H	22.54566300	1.65172600	40.28432800	
C	24.03861500	7.07626800	49.77081900	H	21.43513100	4.54716300	45.43225300	
C	22.98352200	7.31311600	48.81639900	H	20.16020000	-1.56345400	39.80700900	
C	20.67976100	8.00850300	48.25391300	H	21.36990100	-3.62525300	42.34489300	
C	19.34796800	8.42012100	48.64356700	H	20.71926700	-5.87393300	43.15027600	
C	18.55625100	8.29454800	47.54406300	H	23.57347200	-7.66128300	40.47743300	
C	19.41513100	7.84066200	46.47314400	H	24.22597500	-5.39359500	39.67350700	
C	19.81236300	7.23322100	44.12096900	H	22.20046300	-8.80680600	41.89213700	
C	19.38247500	7.09901100	42.74817600	H	25.25503400	8.64942500	44.97951200	
C	20.49644600	6.80704100	42.02206100	H	12.95164700	9.80999500	44.29702900	
C	21.59980700	6.72441400	42.95134600	H	15.47770400	9.60881800	44.34575800	
N	23.84071800	6.23090600	44.85111200	H	30.79180500	-1.95707400	45.56999200	
N	23.36188400	6.85837300	47.57613300	H	31.05831300	-1.64695500	43.22877500	
N	20.69808900	7.67412400	46.92514400	H	25.48831900	-3.12796800	44.69861900	
N	21.16058800	6.98056900	44.22534900	H	20.57634200	6.63196300	40.95665500	
Fe	22.28956400	7.02815100	45.88144400	H	18.36069900	7.18844800	42.40240800	
O	21.43024400	5.05878500	46.26466600	H	17.48926900	8.43673500	47.43877700	
C	23.05467300	-1.73602100	41.23761100	H	19.06600000	8.71974400	49.64576400	
N	24.22702100	-0.87669300	41.21158100	H	23.98825300	7.33623700	50.82132800	
C	24.96029300	-0.32607500	42.22253700	H	26.01099300	6.12838600	49.47588900	
O	25.79232000	0.54964500	42.00171300	H	26.95852200	5.11647300	44.39451400	
C	24.81974500	-0.82760900	43.67958600	H	27.75503200	-1.05374900	37.92827500	
N	26.13716400	-1.26023600	44.13475800	H	25.13422800	5.72750200	36.89475200	
C	26.39651000	-2.49081600	44.63562100	H	16.71293600	3.46436900	35.56424700	
O	27.48984800	-2.90158000	45.00588700	H	11.56175600	5.06875200	40.13870200	
C	24.22274800	0.22902500	44.61730900					
C	24.07115500	1.52837500	44.29855900	²TS1_{HA,B}	C	24.97697000	5.76605100	35.63542200
C	23.32302000	2.48942300	45.18138600		S	24.16881000	4.32750900	34.83784200
C	23.01512800	1.97413700	46.60059800		C	25.28423300	3.00411700	35.43861500
C	23.23770200	0.55422000	46.87388500		H	24.31769300	6.62898000	35.50108400
C	23.79379000	-0.24678300	45.93830500		H	25.39491800	3.05125200	36.52823600
O	22.59038400	2.74891900	47.45414100		H	24.83975300	2.04733000	35.14981000
C	21.83165100	-0.98600400	40.60131900		H	26.26576500	3.09307900	34.96154600
C	21.48969000	0.19852500	41.48217200		H	25.93489900	5.97767100	35.14867900
C	20.79531800	-0.01107800	42.68043300		H	21.08023700	2.01637900	34.71243500
C	20.84712400	0.94344900	43.69326500		C	20.68890100	1.69112800	35.68441900
C	21.61338400	2.10488700	43.51619100		C	20.05692900	2.86674700	36.41500400
C	22.09541900	2.40920600	42.24356100		O	19.04942200	2.70940400	37.12126100
C	22.05143400	1.45382300	41.23107900		C	21.83266500	1.03687400	36.49012500
O	22.01420200	2.88272600	44.58737200		C	21.44630000	0.56461300	37.89412300
Cl	20.04698800	0.63561000	45.21968700		C	20.45483800	-0.59112500	37.88819400
C	23.34374400	-3.03776900	40.44972600		H	22.36184700	0.24400500	38.40845500
O	24.00167100	-2.97041600	39.42160800		H	19.90056300	0.95593100	35.50890700
C	22.87857800	-4.35181800	40.97438900		H	21.03590800	1.38956600	38.48943600
O	20.78398400	-1.92802100	40.47046900		H	22.66817700	1.73916700	36.58646800
C	21.88452200	-4.49694200	41.95787600		H	22.19572400	0.17640600	35.91793400
C	21.49788200	-5.75544700	42.40367900		H	19.85972200	-0.17150600	39.83123100
C	22.11139600	-6.89720000	41.87539900		O	20.18449200	-1.25416900	36.90046500
C	23.09973800	-6.77128400	40.88941400		N	19.90916200	-0.90814400	39.13399900
C	23.46907200	-5.50989300	40.44216700		H	19.07301200	-1.48083600	39.07547500
O	21.70765500	-8.11034600	42.35392200		N	20.68287900	4.05877600	36.26072400

C	20.29641800	5.28117300	36.95693100	N	13.65088600	4.61736800	43.48466000
H	19.88079200	5.99579000	36.23158900	C	14.42716200	4.73045100	44.71053400
C	21.47400500	5.92146100	37.70376300	C	14.76782200	6.19057700	45.07632300
H	21.12898700	6.87893100	38.11802400	O	15.73897800	6.44902000	45.79838500
C	22.05908100	5.04108500	38.80991800	C	15.68431600	3.84928400	44.69315300
H	19.49329800	5.01058600	37.64732300	C	16.14536900	3.47415500	46.10486600
H	22.32987000	4.05356300	38.42245600	H	13.77897300	4.35995100	45.51269700
H	22.26274400	6.16807900	36.98128300	H	14.08784100	4.87863800	42.60837800
H	21.56578700	4.07584700	35.75367300	H	16.49054500	4.31868800	44.12093300
H	22.98022100	5.47600800	39.20741500	H	15.42690600	2.91162000	44.18329900
H	21.34199300	4.89684300	39.62766500	O	15.37759500	3.43941900	47.06197700
C	15.47664100	3.04425900	36.78817800	N	17.45586000	3.12463400	46.20735600
C	15.59334600	3.69433500	38.15548500	H	17.78060100	2.79389200	47.10482500
O	14.63561900	4.25021100	38.70634100	H	18.09968600	3.05929500	45.42736700
C	14.72129200	1.69113900	36.85695700	N	13.90948300	7.12801000	44.61485100
C	13.26594500	1.74924600	37.36292600	C	14.01705000	8.54087100	44.94901400
C	12.33949000	2.55006700	36.43781000	H	13.05903000	8.86782400	45.37660600
C	12.71171900	0.33318100	37.58383000	C	14.36817900	9.42340000	43.74206200
H	13.36952000	-0.25587700	38.23686800	C	15.78298300	9.19058700	43.20567200
H	11.72810300	0.38324500	38.06288900	H	14.78028200	8.62282200	45.72788800
H	12.61403700	-0.21196100	36.63319800	H	13.63924800	9.23984100	42.94354500
H	12.23626000	2.06450400	35.45557200	H	15.91634200	8.14179000	42.91845000
H	11.35451500	2.63873100	36.90486400	H	15.96107500	9.80539900	42.31699900
H	12.70925300	3.56959200	36.27881700	H	13.18706600	6.86251500	43.94880600
H	14.93538300	3.73986100	36.13850700	N	31.76571200	0.35567200	44.42278400
H	13.25476700	2.26162200	38.32938700	C	31.92920000	0.55921300	42.99133000
H	15.30029500	1.01056400	37.49757700	C	30.63762400	1.10411500	42.38099600
H	14.74305400	1.25016400	35.84910000	O	29.56688400	1.01231400	42.97980000
N	16.80943600	3.61505900	38.77150600	H	30.85404200	-0.07190000	44.60243400
C	16.93431700	3.91706400	40.19502100	H	32.75758900	1.25754500	42.80394300
C	16.69070600	5.39587300	40.54591000	N	30.72541500	1.66338200	41.14244300
O	16.41930800	5.72224300	41.70203000	C	29.52602300	1.93789100	40.35107300
C	18.29598100	3.45322300	40.72553800	C	29.02010200	0.63176100	39.68638600
H	17.59968700	3.19818400	38.27823500	O	29.72915000	-0.37544200	39.63839100
H	16.14026000	3.38801800	40.73478000	C	30.05831300	2.92463800	39.29518900
H	19.11815300	3.93444300	40.18555900	C	31.45525400	2.35344700	38.98658700
H	18.39065500	3.69768000	41.78590200	C	31.94892000	1.79980700	40.34281200
H	18.39608100	2.36900500	40.60910000	H	31.36850800	1.53323200	38.26780500
N	16.81629600	6.29336500	39.53128300	H	28.74446500	2.35488900	40.98874900
C	16.44704400	7.68913000	39.68669200	H	32.64582000	2.49416700	40.83188200
C	14.94285400	8.02518700	39.77170100	H	32.45563800	0.83583900	40.22047600
O	14.61909400	9.19643900	39.95784500	H	32.14225700	3.09812100	38.57137900
H	16.91691100	5.91029500	38.60142400	H	30.13465300	3.92612500	39.73529400
H	16.88807500	8.07485800	40.60862800	H	29.40846900	2.98598500	38.41857100
H	16.87094300	8.26108100	38.85624400	N	27.80061700	0.72024100	39.11198100
N	14.07864400	6.99198400	39.63211000	C	27.15195900	-0.47424900	38.58600300
C	12.65190600	7.13724500	39.88507400	C	25.78830000	-0.15580200	37.96093200
C	12.24866200	6.42344400	41.18898600	O	24.87565600	0.38326700	38.92808500
O	12.05136900	7.05327700	42.23478300	C	25.15976400	-1.41264400	37.36562200
H	14.42022700	6.05003200	39.44900200	H	27.02053300	-1.21827900	39.38307400
H	12.44006000	8.20080000	39.99292500	H	24.20268600	-1.17039200	36.89159700
N	12.19643900	5.07404600	41.08993800	H	25.81649300	-1.85498300	36.60706000
C	11.60799500	4.24096900	42.13858600	H	27.21022700	1.53667700	39.28937500
C	12.31658700	4.31702400	43.50000900	H	25.93406700	0.59552400	37.17180400
O	11.69558500	4.05211000	44.52429200	H	24.98216300	-2.15555300	38.14980700
C	11.58668700	2.76724600	41.67193200	H	25.10570200	1.34893900	39.04050300
C	10.91555200	2.50380200	40.29018200	C	23.24658100	8.84654300	44.94976100
O	11.06863700	3.36780700	39.38059200	S	22.46836300	8.09750400	46.42408200
O	10.32107600	1.40355900	40.18382200	H	23.27915300	9.92833500	45.12174500
H	12.05017400	4.63424400	40.16356800	H	24.26508800	8.48080400	44.79499100
H	10.58177200	4.57138100	42.34256300	C	22.84934200	5.96447400	42.68762900
H	11.09205400	2.16750800	42.43891800	H	23.02206700	5.97810700	41.61714200
H	12.62227200	2.40666400	41.59374700	C	25.59356400	5.45038600	46.63281900

H	22.66685000	1.74377600	36.53227800	C	11.05246100	2.40950900	40.27748800
H	22.19072300	0.17454900	35.88086000	O	11.18428400	3.33463800	39.41459400
H	19.82852800	-0.11535800	39.78111100	O	10.52924300	1.28909200	40.11135000
O	20.18837000	-1.24982900	36.87588100	H	12.05186600	4.56597500	40.23345400
N	19.89105700	-0.86715700	39.10128800	H	10.62887800	4.40922000	42.41763300
H	19.05502100	-1.44036200	39.04247300	H	11.19087100	2.02269500	42.42186400
N	20.68836600	4.06608300	36.17997000	H	12.73372800	2.32642500	41.62499200
C	20.30026500	5.29622800	36.86176300	N	13.70641100	4.51234800	43.54222600
H	19.88905400	6.00380300	36.12716700	C	14.48150800	4.62616400	44.76731800
C	21.47540700	5.94317800	37.60680400	C	14.80778500	6.08700400	45.14141800
H	21.13052900	6.90686000	38.00638100	O	15.78772800	6.35402300	45.85016400
C	22.05111700	5.07636800	38.72867300	C	15.74741600	3.75733900	44.75191300
H	19.49325700	5.03450800	37.55094200	C	16.21333900	3.39494000	46.16505600
H	22.32209200	4.08333900	38.35560100	H	13.83473100	4.24497000	45.56583400
H	22.26927500	6.17802900	36.88572300	H	14.13049500	4.80147600	42.66843600
H	21.57073800	4.07725900	35.67226200	H	16.54828500	4.23030200	44.17463400
H	22.96985400	5.51497700	39.12811000	H	15.49650200	2.81440600	44.24884200
H	21.32772000	4.94461700	39.54297100	O	15.44094700	3.32901300	47.11654900
C	15.47824300	3.15980100	36.65513400	N	17.53688400	3.09693900	46.27996900
C	15.58834800	3.79976300	38.02734800	H	17.85337500	2.74659700	47.17312800
O	14.63204000	4.36570400	38.56713500	H	18.18003500	3.02040800	45.50005000
C	14.73742900	1.79743700	36.71838900	N	13.92834800	7.01492600	44.70305600
C	13.29794500	1.82975400	37.26997500	C	14.01895600	8.42527400	45.05170600
C	12.33856300	2.66086700	36.40760700	H	13.05168200	8.73801800	45.46861000
C	12.75429400	0.40482200	37.45777800	C	14.37793800	9.32459900	43.85951500
H	13.44338000	-0.20992100	38.05285100	C	15.80049400	9.10887100	43.33684300
H	11.79717000	0.43768600	37.98934000	H	14.77081700	8.50731100	45.84169600
H	12.61092400	-0.10023100	36.49050200	H	13.66015000	9.14642000	43.05005400
H	12.20292400	2.21315400	35.41105500	H	15.94261900	8.06713900	43.02883900
H	11.37210300	2.72565700	36.91531900	H	15.98596700	9.74370000	42.46387100
H	12.69911200	3.68775800	36.27794600	H	13.20117800	6.74619600	44.04207100
H	14.92701100	3.85367900	36.01238400	N	31.66893300	0.40086300	44.54703500
H	13.31147700	2.30597300	38.25470200	C	31.83714800	0.61087800	43.11699500
H	15.34199600	1.10992800	37.32737300	C	30.53596200	1.12401500	42.49996400
H	14.73437300	1.37805500	35.70092100	O	29.46598700	1.01000700	43.09751300
N	16.79577600	3.69607700	38.66099600	H	30.75854900	-0.03173400	44.71907700
C	16.89998100	3.94084000	40.09747000	H	32.64868900	1.33018900	42.93516300
C	16.67648900	5.40611200	40.51335800	N	30.61404700	1.68151000	41.26168300
O	16.44591000	5.68301800	41.69150600	C	29.41082000	1.93102900	40.46839800
C	18.24450700	3.43213800	40.63118500	C	28.93236000	0.61274800	39.80524900
H	17.58138800	3.26276300	38.17541600	O	29.63785500	-0.39796300	39.80687900
H	16.08826000	3.40317500	40.60219800	C	29.92364900	2.93033100	39.41504000
H	19.08382000	3.92287000	40.12690800	C	31.33187900	2.38715900	39.10724200
H	18.32188300	3.63134800	41.70220500	C	31.83583000	1.84373600	40.46386000
H	18.33003800	2.35228200	40.46980200	H	31.26225800	1.56575400	38.38761900
N	16.76698800	6.34463000	39.53330500	H	28.61884800	2.32881100	41.10550700
C	16.37980600	7.72692900	39.75560800	H	32.51668300	2.55274400	40.95419200
C	14.87254800	8.03494600	39.89187100	H	32.36322400	0.89064900	40.34323300
O	14.53876700	9.19202300	40.14182000	H	32.00422200	3.14496000	38.69218100
H	16.82540200	5.99808100	38.58582100	H	29.98027400	3.93199000	39.85762100
H	16.83763300	8.07999100	40.68218300	H	29.27378400	2.98213000	38.53797400
H	16.77514300	8.33954500	38.94006300	N	27.73654700	0.69281900	39.18366300
N	14.02114600	6.99678200	39.72439100	C	27.11833000	-0.49438200	38.60643000
C	12.59774200	7.10316900	40.01630400	C	25.76605400	-0.16405600	37.96296500
C	12.23860400	6.34234300	41.30732700	O	24.85002000	0.37863300	38.92661700
O	12.04493500	6.94480200	42.37198300	C	25.13676000	-1.40818700	37.34355900
H	14.37149000	6.07329300	39.47565300	H	26.97706200	-1.26263300	39.37777700
H	12.36539600	8.15806500	40.16052800	H	24.19112700	-1.15159800	36.85458300
N	12.21839100	4.99807400	41.17076100	H	25.80350800	-1.84776200	36.59195400
C	11.66469700	4.11839700	42.20109300	H	27.15589000	1.53021200	39.28089500
C	12.37629100	4.18446300	43.55858600	H	25.92728000	0.59543100	37.18535600
O	11.77097100	3.88980900	44.58455900	H	24.93922900	-2.15812000	38.11551700
C	11.68722400	2.65921300	41.68611000	H	25.06544400	1.35279500	39.00212100

O	19.00306100	3.86935100	37.37524600	H	14.71597900	5.37412000	39.35116900
C	21.47195900	1.76344000	36.55644600	H	12.73133800	7.58550600	39.29972100
C	21.12864600	1.28513500	37.97067700	N	12.33883600	4.74876100	40.96502200
C	19.97313400	0.29052000	38.02114900	C	11.72650800	4.14205100	42.14458200
H	22.02381500	0.82534800	38.40906200	C	12.46998100	4.39789900	43.46553300
H	19.48465600	1.99253700	35.72922400	O	11.85935100	4.33386300	44.52807000
H	20.88448700	2.13423500	38.62258400	C	11.60796500	2.61561700	41.92912500
H	22.40287500	2.33965200	36.61173200	C	10.89079500	2.17038300	40.61908400
H	21.67370100	0.88861100	35.92792500	O	11.09930500	2.84344700	39.56928700
H	19.93676100	0.36917700	40.09812000	O	10.20326100	1.12374300	40.71106900
O	19.37372900	-0.10983800	37.03400400	H	12.18043100	4.15770600	40.13114400
N	19.65827900	-0.18151700	39.29028400	H	10.72687400	4.56593100	42.30400000
H	18.73273400	-0.59210300	39.36033100	H	11.09778000	2.18190300	42.79186500
N	20.76980800	4.94144400	36.41086800	H	12.61942300	2.18655000	41.89434500
C	20.61394400	6.20360900	37.12837600	N	13.81531500	4.62873600	43.38302100
H	20.27738100	6.98022200	36.42702500	C	14.62099800	4.90137200	44.56441200
C	21.91091000	6.64357200	37.81921000	C	14.95438100	6.39763100	44.74329900
H	21.72393600	7.61967200	38.28760000	O	15.88657100	6.74835900	45.47921900
C	22.42292000	5.64335700	38.85670300	C	15.88541500	4.02960000	44.62320600
H	19.81744400	6.05228300	37.86086200	C	16.34774600	3.76533600	46.06201800
H	22.59610900	4.66177200	38.40404000	H	13.99781700	4.63207800	45.42464500
H	22.68661000	6.81068900	37.06080500	H	14.24506900	4.71542300	42.46906100
H	21.61376300	4.82910500	35.85377200	H	16.69177400	4.45659200	44.01887400
H	23.38396000	5.96407400	39.26763800	H	15.63790500	3.05279900	44.18684800
H	21.70118100	5.51258300	39.67229700	O	15.59204800	3.86165700	47.02471100
C	15.66444300	2.04397600	37.50321800	N	17.63871500	3.36095600	46.18579100
C	15.83963300	2.80318700	38.80856800	H	17.94832200	3.10713700	47.11336800
O	14.89697900	3.33390400	39.40782400	H	18.29547800	3.20702300	45.42370700
C	14.87453200	0.72410200	37.68718800	N	14.13663800	7.26834200	44.11158200
C	13.38844500	0.88241100	38.06708500	C	14.23884500	8.71255500	44.26082200
C	12.54362000	1.47118400	36.92831900	H	13.30815700	9.08560000	44.71270300
C	12.79593000	-0.45665300	38.53177400	C	14.48420000	9.43510700	42.92783200
H	13.38511700	-0.88958100	39.35107200	C	15.86501700	9.16054200	42.32561000
H	11.77391600	-0.31283200	38.89887600	H	15.05155300	8.89928900	44.96843000
H	12.77550100	-1.19147100	37.71293000	H	13.70790600	9.13129500	42.21523700
H	12.47873400	0.77532400	36.07819300	H	16.01575600	8.08525000	42.18222600
H	11.53732700	1.68552900	37.29998600	H	15.96211400	9.64233500	41.34643800
H	12.95681400	2.41735000	36.55715200	H	13.43399900	6.91935000	43.46263100
H	15.12987000	2.70322300	36.80991000	N	31.55831800	-0.02455500	44.37780600
H	13.32115900	1.58348000	38.90370000	C	31.72715500	0.21464100	42.95228100
H	15.38583500	0.12389600	38.45391500	C	30.45526200	0.82598300	42.36384500
H	14.95709700	0.15209900	36.75088800	O	29.38403100	0.75338800	42.96550900
N	17.10709900	2.84143500	39.31705700	H	30.62022900	-0.39369200	44.54886400
C	17.36634600	3.54918700	40.56696800	H	32.58055700	0.88653200	42.78176700
C	17.00056600	5.04358100	40.51902600	N	30.55976300	1.42308800	41.14646800
O	16.64177700	5.63677000	41.53762000	C	29.37041500	1.79517100	40.38040300
C	18.82466900	3.36434700	40.99715800	C	28.79223800	0.55144800	39.65702400
H	17.88136900	2.72125200	38.66965700	O	29.43286000	-0.49858200	39.57487400
H	16.70481000	3.13359000	41.33197600	C	29.94404600	2.80638800	39.37005600
H	19.50952300	3.75969500	40.23835200	C	31.30864700	2.18264100	39.02135300
H	19.01414700	3.88196900	41.94043800	C	31.78480100	1.54481400	40.34634600
H	19.04111200	2.30331300	41.15229700	H	31.17694000	1.40161900	38.26644000
N	17.11124100	5.65322500	39.30775500	H	28.61490200	2.21767600	41.04513600
C	16.72670800	7.03860100	39.11263400	H	32.51250900	2.18554400	40.86271300
C	15.21858800	7.36283500	39.09792100	H	32.24946000	0.56688200	40.17673900
O	14.87984500	8.53687900	38.96008600	H	32.02835200	2.91108000	38.63393600
H	17.48425200	5.12130900	38.52782300	H	30.07341700	3.77930100	39.85876600
H	17.14937700	7.65927100	39.90808600	H	29.29206300	2.94467900	38.50409100
H	17.14490000	7.38688800	38.16406400	N	27.58794600	0.74576900	39.07944900
N	14.36241900	6.32130700	39.23503500	C	26.87742200	-0.35588800	38.44262800
C	12.93022800	6.51998900	39.41472900	C	25.53746600	0.10821800	37.85660500
C	12.48463600	6.08431400	40.82243900	O	24.67841400	0.64302900	38.87472500
O	12.33490100	6.90413900	41.73759200	C	24.81166400	-1.04541400	37.17075600

H	25.41601100	3.24113400	36.58567600	H	17.26239900	5.24355100	38.50010000
H	24.72495000	2.34623100	35.19336500	H	17.06838800	7.72275300	40.04506600
H	26.26140900	3.22207100	35.00441500	H	17.05178300	7.56269400	38.28802100
H	26.27853000	6.11075100	35.27668200	N	14.25643900	6.47969000	39.33450000
H	20.76486800	2.69966100	34.78828700	C	12.82983500	6.69119400	39.54274100
C	20.42862600	2.42823600	35.79704200	C	12.39441800	6.18378000	40.92949800
C	19.98925600	3.68465600	36.53790100	O	12.23884000	6.95637100	41.88309600
O	18.98092100	3.69639700	37.26465300	H	14.59429900	5.52166200	39.39557000
C	21.56599800	1.66063600	36.50563300	H	12.64624000	7.76414200	39.48920300
C	21.22555600	1.13382300	37.90293700	N	12.26449200	4.84045800	41.00849400
C	20.18374800	0.01975300	37.88687800	C	11.66166200	4.17324200	42.16043500
H	22.14703300	0.75236800	38.36321500	C	12.40705800	4.37678400	43.48967600
H	19.55604400	1.77932700	35.69825100	O	11.80000200	4.26135600	44.54969700
H	20.87641900	1.94289600	38.55743800	C	11.56091900	2.65670000	41.87755300
H	22.45049800	2.30266600	36.58664600	C	10.84238400	2.26010900	40.55378300
H	21.84030100	0.81108400	35.87085800	O	11.02323100	2.98726800	39.53634100
H	19.83790900	0.23711400	39.92276700	O	10.18225500	1.19259200	40.59944700
O	19.77705300	-0.51688200	36.86872500	H	12.10909300	4.28985300	40.14798100
N	19.74985000	-0.40572200	39.14158500	H	10.65797300	4.57793500	42.34142000
H	18.87489200	-0.91979200	39.11868000	H	11.06202500	2.17864900	42.72321600
N	20.77179000	4.77444900	36.35834400	H	12.57731600	2.24242800	41.81866100
C	20.58076900	6.03773500	37.06603700	N	13.75057500	4.61826800	43.41233200
H	20.25277100	6.80680600	36.35229100	C	14.56214600	4.84308400	44.59990300
C	21.85362000	6.49879600	37.78752800	C	14.91692400	6.32852500	44.82320000
H	21.64100500	7.47414400	38.24632800	O	15.87270100	6.64254700	45.54302200
C	22.35580100	5.51263700	38.84329200	C	15.81648200	3.95632200	44.62817800
H	19.76665000	5.87944400	37.77752800	C	16.29146100	3.66803000	46.05647000
H	22.55097400	4.52972600	38.40218500	H	13.93738800	4.55368900	45.45230300
H	22.64540500	6.67431400	37.04791400	H	14.17491100	4.74582900	42.50090100
H	21.63372700	4.66938100	35.82767400	H	16.61983100	4.38458300	44.02069700
H	23.30394700	5.84992300	39.27065100	H	15.55115200	2.98898800	44.18118200
H	21.62022400	5.38063200	39.64627600	O	15.54182100	3.73821600	47.02720400
C	15.46681100	2.31122600	37.30897100	N	17.58515300	3.26590600	46.16236400
C	15.67060400	2.98806400	38.65459900	H	17.91315500	3.01722400	47.08488000
O	14.74446800	3.50801300	39.28843500	H	18.23344800	3.14526100	45.38844600
C	14.70864800	0.96616200	37.43633800	N	14.08903000	7.22898400	44.24647400
C	13.23348900	1.07896100	37.87207600	C	14.21241000	8.66587100	44.44255200
C	12.34136800	1.70079100	36.78821300	H	13.28863500	9.03651600	44.91001700
C	12.67896900	-0.28876200	38.29830200	C	14.46414800	9.42955500	43.13382100
H	13.30334500	-0.74636300	39.07706700	C	15.83689800	9.15130800	42.51520100
H	11.66909500	-0.17699400	38.70719000	H	15.03041900	8.81722400	45.15245400
H	12.64019500	-0.98815100	37.44968800	H	13.67849300	9.16494900	42.41567500
H	12.25516700	1.03819600	35.91388600	H	15.96716200	8.07921900	42.33240300
H	11.34663300	1.88689800	37.20308600	H	15.93884800	9.66762200	41.55430000
H	12.72907500	2.66658500	36.44127000	H	13.36751000	6.91003900	43.60345000
H	14.89356900	3.00154900	36.68037300	N	31.62476200	-0.00294500	44.39035900
H	13.18170400	1.74301200	38.73950100	C	31.79096100	0.23535900	42.96443300
H	15.25430500	0.33207900	38.15012100	C	30.51231400	0.83158700	42.37517100
H	14.76887100	0.45175000	36.46552000	O	29.44145400	0.74362400	42.97534900
N	16.93980100	2.96853100	39.15485000	H	30.68622100	-0.36938600	44.56438500
C	17.22203100	3.57924500	40.44974500	H	32.63706900	0.91597500	42.79203400
C	16.90270400	5.08508400	40.50457600	N	30.60977100	1.43284600	41.15947700
O	16.60075600	5.62582400	41.56832900	C	29.41486600	1.79403400	40.39658800
C	18.67605600	3.32273500	40.85829300	C	28.84083500	0.54310900	39.68306200
H	17.1558400	2.81115500	38.51550300	O	29.49060700	-0.50102700	39.59661900
H	16.55069900	3.13435900	41.18983200	C	29.97753700	2.80352000	39.37829600
H	19.36904400	3.73154900	40.11469000	C	31.34620100	2.18924400	39.02940300
H	18.88789500	3.78413800	41.82577600	C	31.83256200	1.56752900	40.35793300
H	18.85504300	2.24633200	40.95220100	H	31.21831600	1.40023500	38.28214300
N	16.99573000	5.76265500	39.32777800	H	28.65980600	2.21624100	41.06215000
C	16.63040200	7.16263600	39.21437400	H	32.55087600	2.22268200	40.86946400
C	15.12753000	7.51225600	39.22887800	H	32.31189700	0.59558000	40.19479700
O	14.80747300	8.69629500	39.14552000	H	32.05794700	2.92060300	38.63287200

H	30.09996100	3.78057100	39.86052400	C	27.91052300	-1.76849000	44.98818800
H	29.32175200	2.93089700	38.51345400	O	29.09269600	-1.78362500	45.31124400
N	27.62784900	0.72311700	39.11890600	C	25.01180200	-0.29338500	44.77224300
C	26.92406600	-0.38888700	38.49300100	C	25.12371800	1.10400300	44.97622300
C	25.58211600	0.05915900	37.89994500	C	24.26862000	1.76079000	45.82674500
O	24.71625100	0.59881600	38.91118500	C	23.23687900	1.04245500	46.55226900
C	24.86759400	-1.10699700	37.22346000	C	23.18052400	-0.39511500	46.36624900
H	26.75068100	-1.19019000	39.22278400	C	24.04033400	-1.02649000	45.49338900
H	23.92390600	-0.76938600	36.78158100	O	22.41170100	1.63359200	47.30489200
H	25.48798400	-1.53113900	36.42487900	C	22.43404600	-1.08250900	41.07662600
H	27.10046300	1.58428200	39.28787300	C	21.76617300	-0.01829300	41.93069200
H	25.77533000	0.85059900	37.16323100	C	20.65978000	-0.35004300	42.73192300
H	24.65293500	-1.89491000	37.95185700	C	20.06780300	0.59523800	43.55565100
H	25.00022000	1.54944200	39.05087100	C	20.55270100	1.95232700	43.65357400
C	23.02652400	9.01488200	44.98814200	C	21.67505600	2.25019400	42.80299200
S	22.79958700	8.14674400	46.58245800	C	22.25042700	1.30708300	41.97366400
H	23.29110300	10.05219200	45.22028200	O	20.02902800	2.83064800	44.41983500
H	23.83551500	8.56876500	44.40267300	Cl	18.68458100	0.13619900	44.52899900
C	23.02277100	6.11978100	42.80422700	C	24.10486000	-3.02069800	41.13475100
H	23.22898400	6.16315600	41.74005400	O	24.78441800	-3.06391300	40.11936700
C	25.60673800	5.25594500	46.79652200	C	23.69466100	-4.27446500	41.83152200
H	26.65087600	5.03527400	46.99987500	O	21.57901300	-2.18612900	40.81339400
C	21.60098200	5.56420800	49.49907500	C	22.73919800	-4.32417700	42.86234100
H	21.36911600	5.44559800	50.55368800	C	22.40975300	-5.52737000	43.47613800
C	19.04403600	6.59335900	45.52263000	C	23.04065600	-6.70907900	43.07017300
H	17.99097500	6.77646100	45.32783300	C	23.99156400	-6.67910200	42.04097700
C	24.07907100	5.79547800	43.65163600	C	24.30582200	-5.47300700	41.42862600
C	25.43227500	5.48343700	43.20413100	O	22.69113500	-7.86374000	43.70939600
C	26.14729800	5.27519900	44.34852400	H	23.54615700	-1.75383700	42.81729000
C	25.24828800	5.43623200	45.46641800	H	24.82291700	-0.21959200	40.61594600
C	25.89275800	5.38734600	41.77726300	H	25.62553000	-2.03445900	43.68093700
H	26.98620000	5.47238900	41.75061900	H	27.91711200	-0.21670900	43.64009000
H	25.51445200	6.22685300	41.18392200	H	25.87439400	1.65649000	44.41927400
C	25.47564200	4.08629900	41.05785100	H	24.32194200	2.83462000	45.95621000
H	25.98377300	3.21316600	41.48113200	H	22.41840700	-0.93820600	46.91658200
H	24.40030800	3.91194900	41.21341900	H	23.97249900	-2.10315100	45.34648900
C	25.69724300	4.13782300	39.52681800	H	22.76963800	-0.63843100	40.13033800
O	25.81700500	3.00540500	38.92930000	H	20.26231200	-1.35901400	42.69738000
O	25.71050200	5.25247500	38.97143000	H	22.05436200	3.26687100	42.83403300
C	24.74301000	5.29109600	47.89059800	H	23.09305900	1.59007200	41.34887000
C	25.14860400	5.06279300	49.25615800	H	20.91628400	-1.86042200	40.17144000
C	24.02021900	5.13639000	50.01779400	H	22.21579400	-3.42560200	43.16855900
C	22.92980900	5.41214600	49.11604700	H	21.66386900	-5.57244000	44.26316800
C	20.54488900	5.85592300	48.64226100	H	24.47994200	-7.59997100	41.72495600
C	19.16455600	5.98891700	49.04909800	H	25.03450700	-5.43128400	40.62569600
C	18.44873400	6.27790200	47.92740700	H	23.19442300	-8.59793300	43.32364900
C	19.39929000	6.32761300	46.84031800	H	22.10907700	9.00878600	44.39382300
C	19.92112200	6.59649000	44.44141500	H	14.35693300	10.50436200	43.34236800
C	19.51051500	6.82405300	43.07614000	H	16.64697600	9.48222600	43.17844000
C	20.63043100	6.69870100	42.31043000	H	32.27705200	-0.72252000	44.69314100
C	21.71775800	6.38509000	43.20724000	H	32.00127300	-0.66918400	42.35799600
N	23.98913500	5.74905000	45.01817100	H	27.19049300	-2.50212000	45.40845500
N	23.39086600	5.50018900	47.82680400	H	20.72801200	6.79603400	41.23718600
N	20.66502400	6.06044000	47.29245400	H	18.49098500	7.01056600	42.76488600
N	21.26627100	6.34228100	44.50242300	H	17.38229700	6.41179000	47.79958500
Fe	22.33483500	5.97881500	46.16354600	H	18.80585800	5.85695400	50.06246900
O	21.98024000	3.99008600	45.84360600	H	23.91902600	5.01201900	51.08888400
C	23.73173200	-1.64721100	41.74801200	H	26.16509100	4.86354300	49.57233200
N	24.78696700	-0.67458100	41.54003200	H	27.19617000	5.01577900	44.43374800
C	25.77129300	-0.27787600	42.38292600	H	27.55376400	-0.81229300	37.69973100
O	26.53749100	0.63958600	42.10406900	H	25.44301200	5.77766000	36.83328100
C	25.91880300	-0.98158000	43.75958400	H	16.43582800	2.14808300	36.82262100
N	27.33146500	-0.91195900	44.11670900	H	12.25947600	6.17823700	38.75771900

H	21.19514500	3.71418800	45.29062900
H	22.03277300	3.36941700	46.60282700