Synthesis and Molecular Modeling of Resorcin[4]arene-Capped Porphyrins

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Supporting information available:

Details on the new parameters added to heme29 (1 figure, 4 tables; 4 pages).

Cartesian Coordinate Files of lowest-energy conformations of **3**, **5** and **7** (benzene inside) on the molecular modeling studies (3.arc files; 12 pages).

Molecular modeling

All the computational work was carried out on Silicon Graphics workstations (Indigo Entry 4000 and O2). Molecular Mechanics (MM) and Dynamics (MD) calculations were performed using MSI Inc. softwares (version 95.0) InsightII and Discover. Heme29,[1S] a specific version of CVFF force field, developed to model the heme moiety of cytochromes and defining new special atom types and parameters, was considered as the starting force field. Heme29 was adapted to our systems, which lack the coordinated metal ion, keeping few original CVFF stretching, bending and torsional parameters to guarantee the planarity of the porphyrin system. CVFF force field parameters simulate the porphyrin systems as constituted by 4 pyrrole rings connected by 4 aromatic carbon atoms without any agreement with the experimental reality. The update of CVFF force field from Kemmritz[2S] was considered as the starting force field to describe the porphyrin ring. Figure 1S reports the atom types used by Kemmritz. The CVFF stretching and bending parameters and the Kemmritz stretching parameter, applied in the present study to describe the peculiar bonds h–c#, na–hn and c]–cp of the porphyrin moiety, are reported in Tables 1S and 2S. The CVFF torsional parameter, describing the rotation around the bond c[–c, which replaces the heme29 torsional parameter in order to maintain the planarity of the porphyrin moiety, is reported in Table 3S. Moreover, a further bending parameter[3S] was added to describe the carbamate moiety of **7**. Finally, a new torsional parameter was implemented to describe the rotation around the bond connecting the porphyrin methine bridges of **5** and **7** to the phenyl rings of the arms (c]–cp bond). The new parameter was derived and calibrated taking as reference a tetraphenylporphyrin,[4S] whose 3D structure was known by X-ray crystallography, showing an average value of *ca* 60° for the above dihedral angle. To evaluate the torsional barrier around the c]–cp bond (see figure 1S), an adiabatic torsional potential curve was calculated along the dihedral angle, using MOPAC-AM1 calculations (Table 4S). This curve was reproduced by adding the following torsional term to our force field to describe the torsion c]–cp: n=4, K_Φ=2.7500 kcal/mol, Φ_0=0.0000°.

This adapted Heme29 was employed in Discover for geometry optimizations.

Throughout all calculations a dielectric constant ε = 1.0 has and a scale factor = 0.5 for the 1-4 vdW and the 1-4 electrostatic interactions were used.

Partial atomic charges for MM and MD simulations were obtained through MOPAC calculations, using the MNDO-ESP method. The final charges used for compounds **3**, **5** and **7** are listed in the last column of the three Cartesian Coordinate Files, generated by InsightII. The three files (.arc format) describe the lowest energy conformation of **3** (**comp3.arc**), **5** (**comp5.arc**) and **7** (**comp7.arc**), the last containing also a minimized benzene molecule inside the cavity).

The conformational analysis of **3**, **5** and **7** was performed by the discontinuous method of simulated annealing,[3S,5S] which involves high-temperature molecular dynamics and subsequent energy minimizations of the collected structures, To secure a comprehensive sampling of the conformational space, different conformations of the calixarene moiety[6S] were used to generate few local minimum-energy geometries of every capped porphyrins, which, in turn, were considered as starting geometries in consecutive simulated annealing runs. Conformational changes of the calixarene macrocycle, in fact, are very low-frequency motions and occur with a very low probability during (single) molecular dynamics runs.[5S] One hundred geometries of each compound were generated at 2 ps intervals through a first 200 ps molecular dynamics sampling performed at 900 K. Each geometry was then minimized with the *Conjugate Gradients* algorithm of molecular mechanics till convergence (average derivative of 0.005 $kcalmol^{-1}Å^{-1}$). A second loop of MD/MM simulations, 2 ps for each conformer previously found followed by a further energy minimization, was performed at 600 K. A third loop of MD/MM simulations was performed at 300 K. The output geometries of the different runs were compared each other to evaluate the completeness of the search procedure on **3**, **5** and **7**. In all cases the same lowest energy conformation was obtained at least two times from different runs and was reasonably considered as the true global minimum.

Notably, the cone (flattened cone) was the unique geometry of the calixarene cap detected in conformations of **3**, **5** and **7** populated at room temperature.

The benzene molecule was manually located close to the center of the cavity of the lowest energy conformation of **7**, with the plane of the molecule roughly perpendicular to the plane of the porphyrin. The structure of the system was then refined by energy minimization until convergence (average derivative of 0.001 $kcalmol^{-1}Å^{-1}$).

References

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Table 1S. Stretching parameters adapted to describe the porphyrin bonds h–c#, c]–cp and na–hn.

Bond	K (kcal/mol)	R_0 (Å)	original definition
c# – h[a]	363.4164	1.0800	c5 – h

na – hn[a]	483.4512	1.0260	np – hn
c] – cp[b]	280.0000	1.5200	c= – cp

[a] Parameter adapted from CVFF force field. [b] Parameter adapted from heme29 force field.

Table 2S. Bending parameters adapted to describe the porphyrin bonds h–c#, c]–cp and na–hn and the carbammate moiety of **7**.

Angle	K_Θ (kcal/mol)	Θ_0 (°)	CVFF definition
cp – c] – c[[a]	90.0000	120.0000	cp – cp – c5
c] – cp – cp[a]	90.0000	120.0000	cp – cp – cp
h – c# – c[[a]	44.2000	124.8000	h – c5 – c5
h – c# – c#[a]	44.2000	128.1655	h – c5 – c5
c[– na – hn[a]	27.5000	120.0000	c5 – np – hn
o – c' – n[b]	80.0000	110.6000	//

[a] Parameter adapted from CVFF force field. [b] Ref. 2S.

Table 3S. CVFF torsional parameter adapted to guarantee the planarity of the porphyrin system in the absence of a central metal ion.

Torsion	K_Φ (kcal/mol)	Φ_0 (°)	n	CVFF definition
* – c[– c] – *	12.0000	180.0000	2	* – cp – cp – *

Table 4S. Adiabatic torsional potential curve (kcal/mol) calculated along the dihedral angle c]–cp using MOPAC-AM1.

	Dihedral angle (°)												
	330	345	0	15	30	45	60	75	90	105	120	135	150
E[a]	12.8	46.6	74.9	46.3	12.8	1.0	0.0	0.2	0.4	0.2	0.0	1.1	12.9

[a] With respect to the lowest energy value found at 60°.

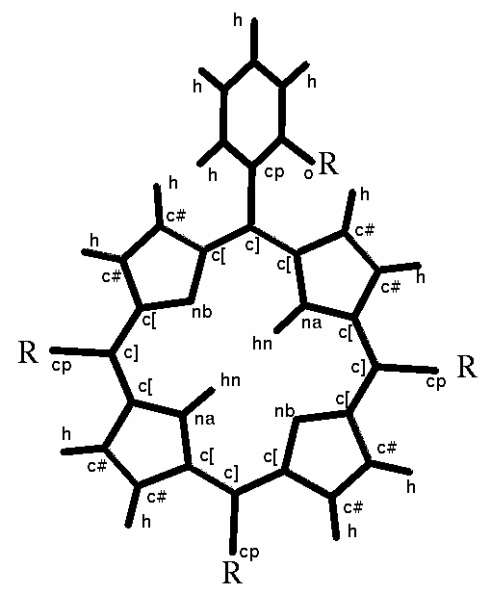

Figure 1S. Atom types used to describe the porphyrin ring of **3**, **5** and **7**. R's indicate the arms to the calixarene moiety.

File: comp3.arc

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CBB	9.953779221	8.208243370	-5.779032230	MOL	1B	c2	C	-0.010
CAB	9.621101379	7.258158207	-6.947474003	MOL	1B	c2	C	0.070
HAB1	10.473680496	7.273404121	-7.651546478	MOL	1B	h	H	0.010
HAB2	8.782624245	7.661548615	-7.546071529	MOL	1B	h	H	0.020
HBB1	10.665932655	7.732778072	-5.078515530	MOL	1B	h	H	0.030
HBB2	10.485019684	9.092505455	-6.175599098	MOL	1B	h	H	0.030
CBC	12.320784569	-1.232420683	-5.271371365	MOL	1B	c2	C	-0.010
HBC1	13.370718002	-1.355806112	-5.592440605	MOL	1B	h	H	0.030
HBC2	11.983201981	-2.249511003	-4.999465942	MOL	1B	h	H	0.030
CAC	11.479991913	-0.725033879	-6.460532188	MOL	1B	c2	C	0.070
HAC1	11.980297089	0.154870570	-6.902315617	MOL	1B	h	H	0.010
HAC2	11.517163277	-1.481687188	-7.265851021	MOL	1B	h	H	0.020
CBA	1.405778646	6.354598045	-3.880638123	MOL	1B	c2	C	-0.010
CAA	1.738275528	5.526158810	-5.139552593	MOL	1B	c2	C	0.070
HAA1	1.133191228	4.601504803	-5.152021408	MOL	1B	h	H	0.010
HAA2	1.383013368	6.085653305	-6.024679661	MOL	1B	h	H	0.020
HBA1	0.406628191	6.804346085	-4.027597904	MOL	1B	h	H	0.030
HBA2	2.090214968	7.218838692	-3.803597927	MOL	1B	h	H	0.030
CBD	4.102876663	-2.911131859	-2.679450274	MOL	1B	c2	C	-0.010
HBD1	3.504058361	-3.816171646	-2.470392227	MOL	1B	h	H	0.030
HBD2	3.802762747	-2.181600571	-1.903663397	MOL	1B	h	H	0.030
CAD	3.746843338	-2.390871048	-4.087526321	MOL	1B	c2	C	0.070
HAD1	4.226378441	-3.015680790	-4.864607811	MOL	1B	h	H	0.020
HAD2	2.666100264	-2.558892488	-4.250089645	MOL	1B	h	H	0.010
C4C	7.750946045	-0.548801064	-5.610194683	FRAG	1F	c[	C	0.060
NC	8.075400352	0.788680673	-5.754885674	FRAG	1F	na	N	-0.130
HC	7.420065880	1.563749313	-5.605353832	FRAG	1F	hn	H	0.240
C1C	9.415435791	0.942490935	-6.060739994	FRAG	1F	c[	C	0.060
C2C	9.987521172	-0.402295768	-6.162424088	FRAG	1F	c#	C	-0.100
C3C	8.958057404	-1.316934109	-5.917161465	FRAG	1F	c#	C	-0.090
CMC	9.076250076	-2.856592178	-5.922240257	FRAG	1F	c3	C	0.080
HMC1	9.725834846	-3.204952240	-6.745806217	FRAG	1F	h	H	0.010
HMC2	9.516028404	-3.220485449	-4.976319313	FRAG	1F	h	H	0.000
HMC3	8.097239494	-3.351721287	-6.051856518	FRAG	1F	h	H	0.000
CHC	10.072105408	2.185733080	-6.249595165	FRAG	1F	c]	C	-0.020
HHC	11.138222694	2.123337746	-6.460865498	FRAG	1F	h	H	0.050
C3D	3.159065008	0.177252620	-4.190190792	FRAG	1D	c#	C	-0.110
CMD	1.705554843	0.114895724	-3.672437429	FRAG	1D	c3	C	0.090
HMD1	1.528955579	-0.779352307	-3.047221184	FRAG	1D	h	H	-0.010
HMD2	1.460009575	0.995600939	-3.051176548	FRAG	1D	h	H	0.000
HMD3	0.989421189	0.085446395	-4.513444424	FRAG	1D	h	H	0.000
C4D	3.836976051	1.389537811	-4.642292023	FRAG	1D	c[	C	0.030
ND	5.140370846	1.043526649	-4.965349674	FRAG	1D	nb	N	-0.290
C1D	5.299880981	-0.331771851	-4.870475769	FRAG	1D	c[	C	0.040
C2D	4.043804169	-0.888538897	-4.359990597	FRAG	1D	c#	C	-0.110
CHD	6.482017994	-1.039824963	-5.209751606	FRAG	1D	c]	C	-0.020
HHD	6.415813446	-2.122072935	-5.108056545	FRAG	1D	h	H	0.050
C4A	5.495339394	5.361621857	-5.865575314	FRAG	1C	c[	C	0.060
C3A	4.231421947	6.096380234	-5.810402393	FRAG	1C	c#	C	-0.090
CMA	4.043968678	7.587321758	-6.168352127	FRAG	1C	c3	C	0.080
HMA1	4.148926735	8.222955704	-5.270941257	FRAG	1C	h	H	0.000
HMA2	4.783482552	7.930881977	-6.913941383	FRAG	1C	h	H	0.000
HMA3	3.043213844	7.779179573	-6.596080780	FRAG	1C	h	H	0.010

C2A	3.243971348	5.208381653	-5.364894867	FRAG	1C	c#	C	-0.100
C1A	3.882316113	3.902634382	-5.179278374	FRAG	1C	c[	C	0.060
NA	5.222206593	4.059336662	-5.486151218	FRAG	1C	na	N	-0.130
HA	5.919513226	3.308077574	-5.441453934	FRAG	1C	hn	H	0.240
CHA	3.279165030	2.688342571	-4.762842655	FRAG	1C	c]	C	-0.020
HHA	2.223298073	2.758190393	-4.504902840	FRAG	1C	h	H	0.050
C4B	9.547173500	3.503470898	-6.245411873	FRAG	1E	c[	C	0.030
C3B	10.274107933	4.741972446	-6.514799595	FRAG	1E	c#	C	-0.110
CMB	11.793085098	4.847300053	-6.773145199	FRAG	1E	c3	C	0.090
HMB1	12.362524986	4.122324944	-6.163789272	FRAG	1E	h	H	-0.010
HMB2	12.025545120	4.650043488	-7.835235119	FRAG	1E	h	H	0.000
HMB3	12.180998802	5.851921558	-6.523886681	FRAG	1E	h	H	0.000
C2B	9.337872505	5.774433613	-6.573783875	FRAG	1E	c#	C	-0.110
C1B	8.028918266	5.190788269	-6.264370441	FRAG	1E	c[	C	0.040
NB	8.220387459	3.838115692	-6.020339489	FRAG	1E	nb	N	-0.290
CHB	6.776763439	5.857049465	-6.219246864	FRAG	1E	c]	C	-0.020
HHB	6.810645580	6.917593479	-6.464981079	FRAG	1E	h	H	0.050
C	11.344510078	7.314203739	-1.687156796	MOL	1G	cp	C	-0.170
HC	12.023727417	8.149147034	-1.734043121	MOL	1G	h	H	0.060
C1	9.983264923	7.551150799	-1.483711123	MOL	1G	cp	C	0.180
C2	9.091181755	6.465598106	-1.433847070	MOL	1G	cp	C	-0.100
C3	9.587035179	5.168072224	-1.612591743	MOL	1G	cp	C	0.010
H3	8.902361870	4.331512928	-1.576469541	MOL	1G	h	H	0.060
C4	10.960927963	4.923946381	-1.726810813	MOL	1G	cp	C	-0.100
C5	11.843477249	6.015318394	-1.809803963	MOL	1G	cp	C	0.180
O	9.446820259	8.854256630	-1.321315765	MOL	1G	o	O	-0.310
C6	7.557665825	6.689505100	-1.169040680	MOL	1G	c1	C	0.080
C7	6.723043919	6.832627773	-2.483589411	MOL	1G	c2	C	-0.010
C8	7.058055878	8.028641701	-3.391380787	MOL	1G	c2	C	0.170
O1	8.279752731	7.757904530	-4.109311104	MOL	1G	o	O	-0.310
C9	8.724376678	8.700860977	-5.016513348	MOL	1G	c'	C	0.350
O2	8.207702637	9.801263809	-5.224907398	MOL	1G	o'	O	-0.350
H81	6.228924274	8.183213234	-4.107097149	MOL	1G	h	H	0.020
H82	7.137891293	8.960894585	-2.799281359	MOL	1G	h	H	0.020
H71	6.781812668	5.899583817	-3.075443506	MOL	1G	h	H	0.010
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H6	7.445536613	7.688491344	-0.704600930	MOL	1G	h	H	0.040
C12	11.514756203	3.456640720	-1.659211755	MOL	1G	c1	C	0.080
H12	12.541509628	3.564106226	-1.256098866	MOL	1G	h	H	0.040
C13	11.764388084	2.847377539	-3.074638605	MOL	1G	c2	C	-0.010
H131	10.833322525	2.410571337	-3.474977255	MOL	1G	h	H	0.010
H132	12.021813393	3.641705036	-3.800137758	MOL	1G	h	H	0.010
C14	12.911714554	1.812078834	-3.100627899	MOL	1G	c2	C	0.170
O3	12.806179047	0.912783384	-4.236338615	MOL	1G	o	O	-0.310
C15	12.297124863	-0.361061752	-4.010568619	MOL	1G	c'	C	0.350
O4	11.866955757	-0.785228610	-2.936134815	MOL	1G	o'	O	-0.350
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H142	12.977617264	1.262059093	-2.139936686	MOL	1G	h	H	0.020
O5	13.219860077	5.732065201	-2.008915663	MOL	1G	o	O	-0.310
C18	10.171814919	10.070731163	-1.611131310	MOL	1G	c3	C	0.220
C19	14.249691010	6.738998413	-2.131000519	MOL	1G	c3	C	0.220
C20	6.844657421	5.008755684	2.251428127	MOL	1G	cp	C	-0.170
H20	7.135569096	5.105801105	3.285262585	MOL	1G	h	H	0.070

C21	7.363033772	5.876664162	1.285785794	MOL	1G	cp	C	0.180
C22	6.963733673	5.741426945	-0.057592515	MOL	1G	cp	C	-0.110
C23	6.041395187	4.741863251	-0.389846981	MOL	1G	cp	C	0.010
H23	5.756036758	4.615353107	-1.422015309	MOL	1G	h	H	0.060
C24	5.493844986	3.892194748	0.576909006	MOL	1G	cp	C	-0.110
C25	5.932347298	4.015717506	1.904900908	MOL	1G	cp	C	0.180
O6	8.284481049	6.910197258	1.591470480	MOL	1G	o	O	-0.310
C26	4.446226597	2.779328585	0.184002236	MOL	1G	c1	C	0.080
C27	3.626490116	2.978083849	-1.129242063	MOL	1G	c2	C	-0.010
C28	2.646642447	4.169015884	-1.071957350	MOL	1G	c2	C	0.170
O7	2.378785610	4.673464298	-2.399954796	MOL	1G	o	O	-0.310
C29	1.382561564	5.632348061	-2.524827719	MOL	1G	c'	C	0.350
O8	0.564547300	5.931391716	-1.651800275	MOL	1G	o'	O	-0.350
H281	1.715819716	3.847842932	-0.563826203	MOL	1G	h	H	0.020
H282	3.062309980	4.991409302	-0.457870692	MOL	1G	h	H	0.020
H271	4.313677311	3.077949286	-1.989070058	MOL	1G	h	H	0.010
H272	3.035264969	2.071295023	-1.358842492	MOL	1G	h	H	0.010
H26	3.679237843	2.880282402	0.977301598	MOL	1G	h	H	0.040
O9	5.375344276	3.198856354	2.907294035	MOL	1G	o	O	-0.310
C32	8.611270905	7.331881046	2.934735775	MOL	1G	c3	C	0.220
C33	6.251036644	2.267380476	3.581711054	MOL	1G	c3	C	0.220
C34	4.839269161	-0.933971226	1.178151369	MOL	1G	cp	C	-0.170
H34	4.276412487	-1.696606040	1.690235734	MOL	1G	h	H	0.060
C35	4.255809307	0.315552711	0.951657951	MOL	1G	cp	C	0.180
C36	4.997244835	1.316372156	0.300926685	MOL	1G	cp	C	-0.100
C37	6.276446819	1.012705445	-0.178781256	MOL	1G	cp	C	0.010
H37	6.838918209	1.771576285	-0.705876589	MOL	1G	h	H	0.060
C38	6.881661892	-0.218669578	0.092395283	MOL	1G	cp	C	-0.100
C39	6.147098064	-1.207785726	0.769204378	MOL	1G	cp	C	0.180
O10	2.934088707	0.637472808	1.354653955	MOL	1G	o	O	-0.310
C40	8.364931107	-0.469500333	-0.362967849	MOL	1G	c1	C	0.080
H40	8.752811432	-1.325647593	0.222568870	MOL	1G	h	H	0.040
C41	8.452717781	-0.990467012	-1.833132148	MOL	1G	c2	C	-0.010
H411	8.068211555	-0.226558015	-2.535197973	MOL	1G	h	H	0.010
H412	9.518398285	-1.107597113	-2.094672441	MOL	1G	h	H	0.010
C42	7.780698776	-2.342736006	-2.131476879	MOL	1G	c2	C	0.170
H421	8.169356346	-2.736280918	-3.088885546	MOL	1G	h	H	0.020
H422	8.046091080	-3.089448929	-1.358050466	MOL	1G	h	H	0.020
O11	6.349570751	-2.167133093	-2.221385479	MOL	1G	o	O	-0.310
C43	5.577585697	-3.277536392	-2.510308266	MOL	1G	c'	C	0.350
O12	5.993973732	-4.431074142	-2.642513752	MOL	1G	o'	O	-0.350
O13	6.781246662	-2.454970598	1.000952005	MOL	1G	o	O	-0.310
C45	2.041496515	-0.280571699	2.025116205	MOL	1G	c3	C	0.220
C46	6.089675903	-3.645414352	1.440137506	MOL	1G	c3	C	0.220
C47	9.978766441	1.491697073	-0.920771480	MOL	1G	cp	C	0.010
H47	9.772789955	1.307253838	-1.962932825	MOL	1G	h	H	0.060
C48	10.834077835	2.543093204	-0.567550659	MOL	1G	cp	C	-0.110
C49	11.034871101	2.815826178	0.795385003	MOL	1G	cp	C	0.180
O14	11.912079811	3.846286535	1.186487079	MOL	1G	o	O	-0.310
C50	11.353687286	4.974038601	1.897564054	MOL	1G	c3	C	0.220
H501	10.927267075	4.676371098	2.873733044	MOL	1G	h	H	-0.020
H502	12.137347221	5.727371216	2.093658209	MOL	1G	h	H	-0.010
H503	10.560150146	5.471180916	1.309116602	MOL	1G	h	H	0.020

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C51     10.444106102    2.012333393    1.765214324 MOL  1G     cp      C  -0.170
H51     10.649052620    2.220778227    2.803121090 MOL  1G     h       H   0.070
C52      9.611435890    0.949124455    1.407727838 MOL  1G     cp      C   0.180
O15      8.994309425    0.102340087    2.363518476 MOL  1G     o       O  -0.310
C53      9.342061996    0.072721153    3.765875578 MOL  1G     c3      C   0.220
H531     9.115580559    1.036426902    4.258367538 MOL  1G     h       H   0.020
H532     8.762804031   -0.710528612    4.286697388 MOL  1G     h       H  -0.020
H533    10.415359497   -0.150714874    3.910701036 MOL  1G     h       H  -0.010
C54      9.356521606    0.689860404    0.046896804 MOL  1G     cp      C  -0.110
H181     9.510478020   10.948038101   -1.494971156 MOL  1G     h       H   0.020
H182    11.027458191   10.202743530   -0.923408151 MOL  1G     h       H  -0.020
H183    10.552414894   10.074551582   -2.649680614 MOL  1G     h       H  -0.020
H191    14.056097031    7.410898209   -2.987790346 MOL  1G     h       H  -0.020
H192    14.324260712    7.352578640   -1.213919640 MOL  1G     h       H   0.020
H193    15.232925415    6.263025284   -2.295358896 MOL  1G     h       H  -0.020
H321     9.306113243    8.190444946    2.907900810 MOL  1G     h       H   0.020
H322     9.104794502    6.521214962    3.502046108 MOL  1G     h       H  -0.020
H323     7.708279610    7.647919655    3.489361048 MOL  1G     h       H  -0.010
H331     7.042269707    2.785328150    4.155208111 MOL  1G     h       H   0.020
H332     6.736643314    1.577834010    2.866468906 MOL  1G     h       H  -0.010
H333     5.675277233    1.649946451    4.293967724 MOL  1G     h       H  -0.020
H451     1.072213173    0.208276927    2.229621887 MOL  1G     h       H  -0.020
H452     1.841053486   -1.173690915    1.404328465 MOL  1G     h       H   0.020
H453     2.459170103   -0.613283753    2.993473291 MOL  1G     h       H  -0.020
H461     5.260069847   -3.904157877    0.755804181 MOL  1G     h       H  -0.020
H462     6.783322334   -4.504963875    1.463608623 MOL  1G     h       H   0.020
H463     5.678040504   -3.519251823    2.458564520 MOL  1G     h       H  -0.020
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N1       1.516549349    2.088668585   -8.191767693 PYRO 1      na      N  -0.130
H1       0.799829125    2.558738470   -8.752102852 PYRO 1      hn      H   0.310
C2       2.684848309    2.701989174   -7.746034622 PYRO 1      c[      C   0.030
C3       3.404689074    1.667423844   -7.017878532 PYRO 1      c#      C  -0.140
H3       4.359533310    1.789911628   -6.526276112 PYRO 1      h       H   0.150
C4       2.646595478    0.536696017   -6.993868351 PYRO 1      c#      C  -0.140
H4       2.907335281   -0.381614208   -6.486671925 PYRO 1      h       H   0.150
C5       1.410659790    0.782313108   -7.722136497 PYRO 1      c[      C   0.030
C1       3.076448679    4.067291260   -7.953985691 PYRO 1      c]      C   0.020
C51      0.311016798   -0.119931854   -7.913074493 PYRO 1      c]      C   0.020
C1      -4.598205566   -0.517932057  -13.931571960 FRAG 1C     cp      C  -0.160
C2      -5.834358692    0.116229944  -13.998706818 FRAG 1C     cp      C  -0.090
C3      -6.059982300    1.281760812  -13.273349762 FRAG 1C     cp      C  -0.200
H3      -7.015043259    1.782379746  -13.328432083 FRAG 1C     h       H   0.130
C4      -5.054732323    1.814464569  -12.467465401 FRAG 1C     cp      C   0.110
C5      -3.794175386    1.189076304  -12.407153130 FRAG 1C     cp      C  -0.060
C6      -3.582633972    0.014145114  -13.142230034 FRAG 1C     cp      C  -0.080
H1      -4.423787117   -1.422452092  -14.496716499 FRAG 1C     h       H   0.130
H2      -6.619353771   -0.294203550  -14.618880272 FRAG 1C     h       H   0.130
H6      -2.622519493   -0.482660770  -13.100257874 FRAG 1C     h       H   0.140
C        0.274774492   -2.723214865   -5.023519516 FRAG 1I     cp      C  -0.200
C1       0.247912019   -1.504694939   -5.704730511 FRAG 1I     cp      C   0.110
C3       0.339836121   -1.484814644   -7.109827995 FRAG 1I     cp      C  -0.060
C4       0.434021175   -2.698377371   -7.804821014 FRAG 1I     cp      C  -0.080
C5       0.445703536   -3.907306433   -7.115418911 FRAG 1I     cp      C  -0.160
C6       0.366976053   -3.919817686   -5.726935387 FRAG 1I     cp      C  -0.090
HC       0.233538225   -2.729173660   -3.944774866 FRAG 1I     h       H   0.130
H4       0.495536685   -2.697823048   -8.884866714 FRAG 1I     h       H   0.140
H5       0.519525945   -4.837698936   -7.660287857 FRAG 1I     h       H   0.130
H6       0.385681748   -4.859966278   -5.192971230 FRAG 1I     h       H   0.130
C       -3.372488499    4.672362328   -2.401014328 MOL  1B     cp      C  -0.270
HC      -4.041712284    5.102795124   -1.673929691 MOL  1B     h       H   0.130
C1      -2.185764074    5.327525139   -2.716988802 MOL  1B     cp      C   0.140
C2      -1.274151564    4.745968819   -3.617390156 MOL  1B     cp      C  -0.110
C3      -1.609705448    3.521282196   -4.210403919 MOL  1B     cp      C  -0.050
H3      -0.937404633    3.087975025   -4.933930874 MOL  1B     h       H   0.140
C4      -2.805870771    2.857345343   -3.906497240 MOL  1B     cp      C  -0.110
C5      -3.699533224    3.461907387   -3.004631042 MOL  1B     cp      C   0.140
O       -1.866225958    6.535926342   -2.064613581 MOL  1B     o       O  -0.240
C6       0.063018329    5.498229504   -3.981838942 MOL  1B     c1      C   0.010
C7      -3.187978268    1.493160248   -4.600253105 MOL  1B     c1      C   0.010
O1      -4.894021988    2.806798220   -2.642189026 MOL  1B     o       O  -0.240
C8      -2.685525894    7.694980145   -2.350179195 MOL  1B     c3      C  -0.050
C9      -5.830535412    2.893103838  -10.424988747 MOL  1B     c2      C   0.010
H91     -6.927113533    3.037614822  -10.443388939 MOL  1B     h       H   0.080
H92     -5.658415318    1.887543201   -9.987818718 MOL  1B     h       H   0.080
O2      -5.315426826    3.006321669  -11.771379471 MOL  1B     o       O  -0.250
C10     -2.844489336    8.374520302  -10.073152542 MOL  1B     c2      C   0.010
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H101	-3.892698526	8.070676804	-9.896018028	MOL	1B	h	H	0.080
H102	-2.871423483	9.479020119	-10.147896767	MOL	1B	h	H	0.080
C11	-6.144998074	3.425331593	-3.027801037	MOL	1B	c3	C	-0.050
C12	0.203446075	9.241258621	-4.977460384	MOL	1B	cp	C	-0.260
H12	0.709995151	10.138628960	-4.669758320	MOL	1B	h	H	0.130
C13	0.493157715	8.036752701	-4.330565453	MOL	1B	cp	C	0.130
C14	-0.158282429	6.859134197	-4.738283634	MOL	1B	cp	C	-0.110
C15	-1.063124418	6.915750027	-5.804695129	MOL	1B	cp	C	-0.070
H15	-1.566948771	6.011626244	-6.118021965	MOL	1B	h	H	0.140
C16	-1.406503916	8.132473946	-6.404745579	MOL	1B	cp	C	-0.110
C17	-0.740340650	9.304437637	-6.006442547	MOL	1B	cp	C	0.130
O3	1.422482371	7.940169811	-3.261329412	MOL	1B	o	O	-0.230
C18	2.602552176	5.253433228	-4.622241497	MOL	1B	c2	C	0.010
H181	2.623072147	6.140499592	-5.288989067	MOL	1B	h	H	0.080
H182	2.868206024	5.620226383	-3.613061428	MOL	1B	h	H	0.080
C19	-2.545957327	8.172735214	-7.480269432	MOL	1B	c1	C	0.010
O4	-1.068592668	10.510996819	-6.680232525	MOL	1B	o	O	-0.230
C20	2.185366869	9.049370766	-2.731599331	MOL	1B	c3	C	-0.050
C21	-0.452709317	11.792814255	-6.414277077	MOL	1B	c3	C	-0.050
C22	-5.818145752	7.160202026	-5.668516636	MOL	1B	cp	C	-0.270
H22	-6.436865330	7.527440071	-4.868984222	MOL	1B	h	H	0.130
C23	-4.669577599	7.869746685	-6.027560234	MOL	1B	cp	C	0.140
C24	-3.852930784	7.388895035	-7.066981792	MOL	1B	cp	C	-0.110
C25	-4.209131241	6.198118210	-7.711301804	MOL	1B	cp	C	-0.050
H25	-3.566632748	5.805341721	-8.483559608	MOL	1B	h	H	0.140
C26	-5.370913982	5.494810581	-7.371920586	MOL	1B	cp	C	-0.110
C27	-6.181729794	5.985532284	-6.331621170	MOL	1B	cp	C	0.140
O5	-4.280216217	9.079239845	-5.393523216	MOL	1B	o	O	-0.240
C28	-5.762751579	4.164722919	-8.125751495	MOL	1B	c1	C	0.010
O6	-7.354199409	5.251347542	-6.011512756	MOL	1B	o	O	-0.240
C29	-5.073036194	9.781719208	-4.407997608	MOL	1B	c3	C	-0.050
C30	-8.369710922	5.689733028	-5.079071045	MOL	1B	c3	C	-0.050
C31	-6.591938972	0.838930190	-6.316513538	MOL	1B	cp	C	-0.260
H31	-7.394897461	0.125334889	-6.264987946	MOL	1B	h	H	0.130
C32	-5.459634304	0.651794493	-5.518904686	MOL	1B	cp	C	0.130
C33	-4.414341450	1.589836121	-5.573685646	MOL	1B	cp	C	-0.110
C34	-4.502319813	2.656839132	-6.475622177	MOL	1B	cp	C	-0.070
H34	-3.693345547	3.372668505	-6.526941776	MOL	1B	h	H	0.140
C35	-5.656483650	2.874318600	-7.235841751	MOL	1B	cp	C	-0.110
C36	-6.708283901	1.943700314	-7.164868832	MOL	1B	cp	C	0.130
O7	-5.308577061	-0.451405257	-4.637486458	MOL	1B	o	O	-0.230
O8	-7.854064941	2.179383755	-7.970128536	MOL	1B	o	O	-0.230
C37	-6.289770603	-1.499111652	-4.457555294	MOL	1B	c3	C	-0.050
C38	-8.969188690	1.266264081	-8.096915245	MOL	1B	c3	C	-0.050
C39	-0.998746693	0.092827335	-4.281688213	MOL	1B	c2	C	0.010
H391	-0.719506681	0.858005643	-3.533985853	MOL	1B	h	H	0.080
H392	-1.416414499	-0.747223258	-3.693376064	MOL	1B	h	H	0.080
O9	0.208611250	-0.295659542	-4.980391026	MOL	1B	o	O	-0.250
C40	-2.051794291	0.657530606	-5.261823654	MOL	1B	c2	C	-0.150
O10	3.551643133	4.237909794	-5.021842957	MOL	1B	o	O	-0.250
C41	1.194022655	4.637201309	-4.627815247	MOL	1B	c2	C	-0.150
C42	-5.151320457	3.958001614	-9.547816277	MOL	1B	c2	C	-0.150
O11	-2.419066429	7.768826485	-11.317434311	MOL	1B	o	O	-0.250

C43	-1.948697329	7.922686577	-8.897607803	MOL	1B	c2	C	-0.150
H6	0.466932774	5.745563984	-2.979631901	MOL	1B	h	H	0.110
H7	-3.516411304	0.868256092	-3.745598793	MOL	1B	h	H	0.110
H81	-2.271372080	8.588328362	-1.850184441	MOL	1B	h	H	0.060
H82	-2.716127872	7.911774158	-3.436022520	MOL	1B	h	H	0.110
H83	-3.724193335	7.562149525	-1.995479345	MOL	1B	h	H	0.060
H111	-6.993263245	2.769080639	-2.764394999	MOL	1B	h	H	0.060
H112	-6.298888206	4.394494534	-2.518476725	MOL	1B	h	H	0.060
H113	-6.191909313	3.598491430	-4.120891094	MOL	1B	h	H	0.110
H19	-2.893040657	9.224073410	-7.528677464	MOL	1B	h	H	0.110
H201	2.835349321	9.496987343	-3.506307125	MOL	1B	h	H	0.060
H202	2.835728168	8.707666397	-1.906343937	MOL	1B	h	H	0.110
H203	1.522459745	9.837911606	-2.329628944	MOL	1B	h	H	0.060
H211	-0.872490048	12.565994263	-7.082492352	MOL	1B	h	H	0.060
H212	0.639046311	11.758320808	-6.587570190	MOL	1B	h	H	0.060
H213	-0.633103549	12.117153168	-5.372650146	MOL	1B	h	H	0.110
H28	-6.838645458	4.326380730	-8.336964607	MOL	1B	h	H	0.110
H291	-6.059644699	10.069570541	-4.816272259	MOL	1B	h	H	0.060
H292	-5.234015942	9.164387703	-3.504997015	MOL	1B	h	H	0.060
H293	-4.558036327	10.706876755	-4.092488766	MOL	1B	h	H	0.110
H301	-8.806163788	6.658454418	-5.385668278	MOL	1B	h	H	0.060
H302	-9.190560341	4.951483727	-5.034286022	MOL	1B	h	H	0.110
H303	-7.960572243	5.796985149	-4.057589531	MOL	1B	h	H	0.060
H371	-5.931191444	-2.236737967	-3.717258930	MOL	1B	h	H	0.110
H372	-7.248793602	-1.092465401	-4.086338520	MOL	1B	h	H	0.060
H373	-6.479338646	-2.039722919	-5.403451443	MOL	1B	h	H	0.060
H381	-9.477930069	1.114770412	-7.126880646	MOL	1B	h	H	0.060
H382	-9.715004921	1.668054938	-8.806052208	MOL	1B	h	H	0.060
H383	-8.640892029	0.281681329	-8.479427338	MOL	1B	h	H	0.110
H401	-2.479552507	-0.202305093	-5.812598228	MOL	1B	h	H	0.090
H402	-1.557059646	1.257173896	-6.047597408	MOL	1B	h	H	0.090
H411	1.258351445	3.669616222	-4.094749451	MOL	1B	h	H	0.090
H412	0.925866246	4.376905918	-5.669156075	MOL	1B	h	H	0.090
H421	-4.074562550	3.716032743	-9.468898773	MOL	1B	h	H	0.090
H422	-5.192969322	4.915738583	-10.100584030	MOL	1B	h	H	0.090
H431	-1.682544112	6.855852604	-9.010438919	MOL	1B	h	H	0.090
H432	-0.981033087	8.450414658	-9.002273560	MOL	1B	h	H	0.090
C1	-0.119801022	7.480042458	-12.088304520	FRAG	1G	cp	C	-0.060
C2	-1.285517931	8.264477730	-11.993980408	FRAG	1G	cp	C	0.110
C3	-1.344929576	9.501712799	-12.638433456	FRAG	1G	cp	C	-0.200
C4	-0.249463007	9.975099564	-13.353302002	FRAG	1G	cp	C	-0.090
C5	0.908887744	9.210303307	-13.440199852	FRAG	1G	cp	C	-0.160
C6	0.975130141	7.969264984	-12.813830376	FRAG	1G	cp	C	-0.080
H3	-2.252051830	10.084556580	-12.586081505	FRAG	1G	h	H	0.130
H4	-0.301592410	10.935015678	-13.848460197	FRAG	1G	h	H	0.130
H5	1.758375168	9.578561783	-13.997644424	FRAG	1G	h	H	0.130
H6	1.880171061	7.381064415	-12.886280060	FRAG	1G	h	H	0.140
C1	4.430514812	4.554351807	-7.291650295	FRAG	1H	cp	C	-0.060
C2	5.504141331	4.928586483	-8.111967087	FRAG	1H	cp	C	-0.080
C3	6.708750725	5.345509529	-7.552853584	FRAG	1H	cp	C	-0.160
C4	6.857107162	5.391949654	-6.170638084	FRAG	1H	cp	C	-0.090
C5	5.799980164	5.025912762	-5.343618393	FRAG	1H	cp	C	-0.200
C6	4.584098339	4.621951103	-5.893183708	FRAG	1H	cp	C	0.110

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H2       5.399418354    4.890382290   -9.188037872 FRAG 1H     h        H   0.140
H3       7.531149864    5.628985405   -8.194129944 FRAG 1H     h        H   0.130
H4       7.796205044    5.708643436   -5.738121986 FRAG 1H     h        H   0.130
H5       5.912418842    5.052931786   -4.270101547 FRAG 1H     h        H   0.130
C4C     -0.818659723    0.126433671   -8.768047333 PORN 1D     c[       C  -0.020
C3      -2.028510332   -0.675774336   -8.867758751 PORN 1D     c#       C  -0.160
C4      -2.813456297   -0.166499227   -9.847313881 PORN 1D     c#       C  -0.160
C4A     -2.154171944    0.994944751  -10.420742035 PORN 1D     c[       C  -0.020
N4B     -0.991490185    1.182773709   -9.667351723 PORN 1D     nb       N  -0.230
CB      -2.616572857    1.783052683  -11.529685020 PORN 1D     c]       C   0.020
C6C     -2.079091549    3.058429241  -11.910526276 PORN 1D     c[       C   0.030
C5      -2.453466892    3.880447865  -13.052015305 PORN 1D     c#       C  -0.140
C6      -1.759221077    5.050372124  -12.999072075 PORN 1D     c#       C  -0.140
C6A     -0.890726030    5.030436516  -11.831363678 PORN 1D     c[       C   0.030
N6B     -1.089296341    3.781404734  -11.249400139 PORN 1D     na       N  -0.130
H6B     -0.609738886    3.457504272  -10.404500961 PORN 1D     hn       H   0.310
CC      -0.019730004    6.072771072  -11.368145943 PORN 1D     c]       C   0.020
C8C      0.926111937    5.939445972  -10.293264389 PORN 1D     c[       C  -0.020
C7       1.710193276    7.002923965   -9.683720589 PORN 1D     c#       C  -0.160
C8       2.550725460    6.460189819   -8.770391464 PORN 1D     c#       C  -0.160
H8       3.273160458    7.008253574   -8.182733536 PORN 1D     h        H   0.140
C8A      2.341360092    5.022379398   -8.736211777 PORN 1D     c[       C  -0.020
N8B      1.280422091    4.771558285   -9.611373901 PORN 1D     nb       N  -0.230
H3      -2.255337477   -1.555799842   -8.283425331 PORN 1D     h        H   0.140
H4      -3.762437820   -0.575379610  -10.163124084 PORN 1D     h        H   0.140
H5      -3.202923059    3.631676197  -13.790121078 PORN 1D     h        H   0.150
H6      -1.865457058    5.873695374  -13.691422462 PORN 1D     h        H   0.150
H7       1.662285447    8.051786423   -9.938494682 PORN 1D     h        H   0.140
end
end
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C1       5.258283185    1.841607885   -8.527492566 BENZ 1      cp      C  -0.100
H11      4.301954491    2.337926431   -8.498618222 BENZ 1      h       H   0.100
C2       6.449584424    2.567430586   -8.506359980 BENZ 1      cp      C  -0.100
H21      6.426539819    3.644943120   -8.460375142 BENZ 1      h       H   0.100
C3       7.670752567    1.893858270   -8.545764509 BENZ 1      cp      C  -0.100
H31      8.605145820    2.430802548   -8.530660600 BENZ 1      h       H   0.100
C4       7.701026427    0.508042110   -8.606347601 BENZ 1      cp      C  -0.100
H41      8.646933183   -0.011476675   -8.635679200 BENZ 1      h       H   0.100
C5       6.508753570   -0.205392794   -8.626780774 BENZ 1      cp      C  -0.100
H51      6.531697185   -1.275590856   -8.673419329 BENZ 1      h       H   0.100
C6       5.287123254    0.455681874   -8.587373662 BENZ 1      cp      C  -0.100
H61      4.364256429   -0.104291978   -8.605626020 BENZ 1      h       H   0.100
end
N1       8.523611519   -2.845995846   -9.726977302 PYRO 1      na      N  -0.170
H1       7.608164703   -2.909075228   -9.266697261 PYRO 1      hn      H   0.260
C2       8.694589853   -2.637516927  -11.095042878 PYRO 1      c[      C   0.040
C3      10.136251253   -2.598045881  -11.297741422 PYRO 1      c#      C  -0.070
H3      10.643158463   -2.473628488  -12.243563275 PYRO 1      h       H   0.090
C4      10.749626717   -2.630099443  -10.088594628 PYRO 1      c#      C  -0.070
H4      11.814350376   -2.532530712   -9.934092764 PYRO 1      h       H   0.090
C5       9.734929966   -2.721035703   -9.047377057 PYRO 1      c[      C   0.040
C1       7.676611117   -2.506462806  -12.097860566 PYRO 1      c]      C   0.000
C51      9.945312110   -2.655164646   -7.629000427 PYRO 1      c]      C   0.000
C1       4.720100534   -4.014675306   -1.767158696 FRAG 1C     cp      C  -0.080
C2       4.132010322   -2.908206257   -1.174963512 FRAG 1C     cp      C  -0.020
C3       3.955870430   -1.738888051   -1.902931107 FRAG 1C     cp      C  -0.070
H3       3.494897091   -0.905742768   -1.397068965 FRAG 1C     h       H   0.090
C4       4.367028491   -1.652183042   -3.244674138 FRAG 1C     cp      C   0.170
C5       4.962002786   -2.792637034   -3.846491817 FRAG 1C     cp      C  -0.100
C6       5.132453050   -3.960764866   -3.090319964 FRAG 1C     cp      C  -0.010
H1       4.857492872   -4.922240862   -1.197356504 FRAG 1C     h       H   0.060
H2       3.811715001   -2.955436486   -0.143886934 FRAG 1C     h       H   0.070
H6       5.587393853   -4.837214410   -3.532360326 FRAG 1C     h       H   0.070
C       13.382297948   -1.249205653   -6.388431528 FRAG 1I     cp      C  -0.070
C1      12.025571587   -1.272734098   -6.754838322 FRAG 1I     cp      C   0.170
C3      11.446473456   -2.511696324   -7.134753843 FRAG 1I     cp      C  -0.100
C4      12.234240314   -3.670716207   -7.132710557 FRAG 1I     cp      C  -0.010
C5      13.570673095   -3.617227661   -6.764019712 FRAG 1I     cp      C  -0.080
C6      14.144149165   -2.410425031   -6.393956463 FRAG 1I     cp      C  -0.020
HC      13.865816254   -0.335553284   -6.079528100 FRAG 1I     h       H   0.090
H4      11.809559913   -4.621713283   -7.425323885 FRAG 1I     h       H   0.070
H5      14.166208231   -4.518657189   -6.767189359 FRAG 1I     h       H   0.060
H6      15.185058073   -2.374268591   -6.105594083 FRAG 1I     h       H   0.070
C        9.389474514    8.427000142   -8.267924327 MOL  1B     cp      C  -0.200
HC       9.573912147    9.488034201   -8.210939509 MOL  1B     h       H   0.060
C1       9.288344385    7.795134648   -9.509768892 MOL  1B     cp      C   0.200
C2       9.077166618    6.404337862   -9.569526170 MOL  1B     cp      C  -0.130
C3       8.974007344    5.686981706   -8.369778996 MOL  1B     cp      C   0.020
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H3	8.779981564	4.630089659	-8.404994856	MOL	1B	h	H	0.060
C4	9.080354564	6.312634898	-7.122689298	MOL	1B	cp	C	-0.130
C5	9.267284014	7.704117568	-7.084245223	MOL	1B	cp	C	0.200
O	9.407414915	8.489660249	-10.740173092	MOL	1B	o	O	-0.300
C6	8.919970904	5.697410528	-10.971950794	MOL	1B	c1	C	0.090
C7	8.930674378	5.512732680	-5.771919915	MOL	1B	c1	C	0.090
O1	9.411833920	8.350246697	-5.839575373	MOL	1B	o	O	-0.300
C8	9.474078255	9.927665349	-10.858893621	MOL	1B	c3	C	0.220
C9	3.752780193	0.803597963	-3.708585548	MOL	1B	c'	C	0.500
O2	3.809794768	1.635658034	-4.810767268	MOL	1B	o	O	-0.350
CO	3.563031418	3.044995565	-4.576048016	MOL	1B	c2	C	0.240
HO1	4.277873176	3.424743530	-3.820708951	MOL	1B	h	H	0.010
HO2	2.548888421	3.209171093	-4.162826663	MOL	1B	h	H	0.010
O3	3.348782758	1.137034678	-2.592704380	MOL	1B	o'	O	-0.400
N	4.204929835	-0.410944953	-4.011576024	MOL	1B	n	N	-0.340
HN	4.536636499	-0.465222953	-4.978591333	MOL	1B	hn	H	0.180
C10	1.460356171	1.176644279	-10.593420449	MOL	1B	c'	C	0.500
O4	2.585994355	1.971558189	-10.672142052	MOL	1B	o	O	-0.350
C11	2.394318672	3.406425212	-10.731929224	MOL	1B	c2	C	0.240
H111	2.036017234	3.773216132	-9.751834819	MOL	1B	h	H	0.010
H112	1.623874914	3.684619612	-11.477934730	MOL	1B	h	H	0.010
O5	0.299404106	1.590186748	-10.598628383	MOL	1B	o'	O	-0.400
C12	8.495458239	9.416384833	-5.500828826	MOL	1B	c3	C	0.220
C13	6.365787675	6.913855310	-13.625848455	MOL	1B	cp	C	-0.190
H13	6.364728040	7.323738232	-14.622290949	MOL	1B	h	H	0.060
C14	7.586295349	6.656331700	-12.992471649	MOL	1B	cp	C	0.190
C15	7.589959007	6.112514489	-11.698252790	MOL	1B	cp	C	-0.120
C16	6.371290425	5.850802569	-11.065454986	MOL	1B	cp	C	0.020
H16	6.374322873	5.410282285	-10.077851434	MOL	1B	h	H	0.060
C17	5.149708527	6.073935568	-11.709032460	MOL	1B	cp	C	-0.120
C18	5.147906443	6.618147842	-13.003484266	MOL	1B	cp	C	0.190
O6	8.844128532	6.884613651	-13.604894584	MOL	1B	o	O	-0.300
C19	9.204742300	1.323444483	-13.440516729	MOL	1B	c'	C	0.500
O7	9.588415831	1.767077148	-14.524775617	MOL	1B	o'	O	-0.400
O8	9.112053526	2.057934129	-12.273252005	MOL	1B	o	O	-0.350
C20	9.292295464	3.491768892	-12.390165210	MOL	1B	c2	C	0.240
H201	10.295649773	3.736638663	-12.789582202	MOL	1B	h	H	0.010
H202	8.556691730	3.899442644	-13.110181774	MOL	1B	h	H	0.010
C21	3.828760625	5.616512612	-10.995901301	MOL	1B	c1	C	0.090
O9	3.889768097	6.819709133	-13.625102553	MOL	1B	o	O	-0.300
C22	9.014183408	7.448221520	-14.924551538	MOL	1B	c3	C	0.220
C23	3.715419258	7.401902762	-14.936233282	MOL	1B	c3	C	0.220
C24	3.238933513	8.297203395	-8.269039505	MOL	1B	cp	C	-0.200
H24	3.020089858	9.351127583	-8.220561744	MOL	1B	h	H	0.060
C25	3.368016016	7.681138413	-9.515738502	MOL	1B	cp	C	0.200
C26	3.639238702	6.303019527	-9.587202876	MOL	1B	cp	C	-0.130
C27	3.784281073	5.582334786	-8.396722487	MOL	1B	cp	C	0.020
H27	4.032337834	4.537344789	-8.448791450	MOL	1B	h	H	0.060
C28	3.652608076	6.190942016	-7.142155423	MOL	1B	cp	C	-0.130
C29	3.381123191	7.570175121	-7.085035578	MOL	1B	cp	C	0.200
O10	3.223257424	8.379955874	-10.740917803	MOL	1B	o	O	-0.300
C30	3.841083558	5.375650697	-5.803445301	MOL	1B	c1	C	0.090
O11	3.248390946	8.155427641	-5.800196337	MOL	1B	o	O	-0.300

C31	3.113081649	9.815746788	-10.851615410	MOL	1B	c3	C	0.220
C32	3.131653207	9.574874924	-5.559457558	MOL	1B	c3	C	0.220
C33	6.341903408	6.475000956	-3.049554540	MOL	1B	cp	C	-0.190
H33	6.326399356	6.801909563	-2.022940982	MOL	1B	h	H	0.060
C34	7.570781083	6.282008703	-3.689991951	MOL	1B	cp	C	0.190
C35	7.591576641	5.846817859	-5.024865707	MOL	1B	cp	C	-0.120
C36	6.380307660	5.625254909	-5.688053176	MOL	1B	cp	C	0.020
H36	6.395278769	5.268401910	-6.708764060	MOL	1B	h	H	0.060
C37	5.152121262	5.783807340	-5.040180183	MOL	1B	cp	C	-0.120
C38	5.133142324	6.219654968	-3.705859130	MOL	1B	cp	C	0.190
O12	8.819605066	6.490757427	-3.052818716	MOL	1B	o	O	-0.300
O13	3.866940745	6.345178881	-3.081345392	MOL	1B	o	O	-0.300
C39	8.970394683	6.982619204	-1.702314210	MOL	1B	c3	C	0.220
C40	3.673093365	6.804509313	-1.725033420	MOL	1B	c3	C	0.220
C41	11.497251058	1.231416184	-6.529502319	MOL	1B	c'	C	0.500
O14	10.337981783	1.967277940	-6.390157562	MOL	1B	o	O	-0.350
C42	10.466038258	3.399367000	-6.210737402	MOL	1B	c2	C	0.240
H421	11.224362884	3.648690436	-5.442450450	MOL	1B	h	H	0.010
H422	10.806234140	3.861876495	-7.156151264	MOL	1B	h	H	0.010
O15	12.639133646	1.692375276	-6.481070081	MOL	1B	o'	O	-0.400
N1	11.213475984	-0.052555385	-6.729791160	MOL	1B	n	N	-0.340
H1	10.212754772	-0.208126689	-6.879966306	MOL	1B	hn	H	0.180
C43	9.101128857	3.959042938	-5.779395108	MOL	1B	c2	C	-0.010
N2	8.809813718	0.068589770	-13.239043133	MOL	1B	n	N	-0.340
H2	8.482590272	-0.080116083	-12.280535671	MOL	1B	hn	H	0.180
C44	9.104982366	4.144472924	-11.008904460	MOL	1B	c2	C	-0.010
C45	3.721861104	3.818624483	-5.897218097	MOL	1B	c2	C	-0.010
N3	1.800848402	-0.105993355	-10.504452453	MOL	1B	n	N	-0.340
HN3	2.808068241	-0.230005729	-10.369615987	MOL	1B	hn	H	0.180
C46	3.731735176	4.060837529	-11.113068852	MOL	1B	c2	C	-0.010
H6	9.782175845	6.074100709	-11.555493204	MOL	1B	h	H	0.040
H7	9.776294951	5.864655869	-5.149993900	MOL	1B	h	H	0.040
H81	9.506482766	10.222201487	-11.923296696	MOL	1B	h	H	0.020
H82	8.588777760	10.410716812	-10.405015669	MOL	1B	h	H	-0.020
H83	10.381630850	10.330487524	-10.372363620	MOL	1B	h	H	-0.010
H121	8.651077716	10.307769428	-6.136307195	MOL	1B	h	H	-0.020
H122	7.441396097	9.094468502	-5.602810057	MOL	1B	h	H	-0.030
H123	8.644418797	9.726630739	-4.450934118	MOL	1B	h	H	0.030
H21	2.967052691	5.972838923	-11.592636494	MOL	1B	h	H	0.040
H221	8.543346714	6.812794510	-15.697437355	MOL	1B	h	H	-0.020
H222	10.088039323	7.532637408	-15.170220571	MOL	1B	h	H	0.020
H223	8.575567803	8.461375279	-14.988800730	MOL	1B	h	H	-0.020
H231	4.134325279	8.424410084	-14.981832565	MOL	1B	h	H	-0.010
H232	2.641277440	7.470078671	-15.185045504	MOL	1B	h	H	-0.020
H233	4.201248822	6.788589725	-15.717854661	MOL	1B	h	H	0.020
H30	2.963947128	5.664962717	-5.192892151	MOL	1B	h	H	0.040
H311	3.984310822	10.322693040	-10.396593622	MOL	1B	h	H	-0.020
H312	3.069430698	10.115127688	-11.914308864	MOL	1B	h	H	0.030
H313	2.194951687	10.188058898	-10.360723650	MOL	1B	h	H	-0.030
H321	3.103084924	9.776940036	-4.473668413	MOL	1B	h	H	-0.010
H322	3.993156135	10.126704682	-5.979518146	MOL	1B	h	H	-0.020
H323	2.203713391	9.983911934	-6.000385996	MOL	1B	h	H	0.020
H391	8.508541694	6.295464003	-0.969259311	MOL	1B	h	H	-0.010

H392	10.040850709	7.075203786	-1.445002195	MOL	1B	h	H	0.020
H393	8.510548353	7.981496820	-1.584542609	MOL	1B	h	H	-0.020
H401	4.069155131	7.827699976	-1.586361460	MOL	1B	h	H	-0.020
H402	2.596568052	6.826362145	-1.477539759	MOL	1B	h	H	0.020
H403	4.169645034	6.134973757	-0.998434826	MOL	1B	h	H	-0.020
H431	8.900334004	3.558941132	-4.766588639	MOL	1B	h	H	0.010
H432	8.309743981	3.515030628	-6.406295010	MOL	1B	h	H	0.010
H441	9.965929682	3.852082033	-10.379021754	MOL	1B	h	H	0.010
H442	8.225106679	3.680649390	-10.532932744	MOL	1B	h	H	0.010
H451	4.620664614	3.434239798	-6.407235936	MOL	1B	h	H	0.010
H452	2.874179226	3.543721368	-6.552456904	MOL	1B	h	H	0.010
H461	4.543501387	3.605298281	-10.521676925	MOL	1B	h	H	0.010
H462	3.950098444	3.753187395	-12.154138027	MOL	1B	h	H	0.010
C1	1.677579607	-2.598370487	-10.311021853	FRAG	1G	cp	C	-0.100
C2	1.043303157	-1.358326168	-10.584059435	FRAG	1G	cp	C	0.170
C3	-0.314079266	-1.363495095	-10.948469828	FRAG	1G	cp	C	-0.080
C4	-1.023921253	-2.553526348	-11.043435818	FRAG	1G	cp	C	-0.030
C5	-0.396598437	-3.761027930	-10.777681338	FRAG	1G	cp	C	-0.080
C6	0.941891642	-3.786695270	-10.413396038	FRAG	1G	cp	C	-0.010
H3	-0.838021242	-0.448857501	-11.178604336	FRAG	1G	h	H	0.090
H4	-2.066148509	-2.538906611	-11.328922868	FRAG	1G	h	H	0.070
H5	-0.951676509	-4.684865309	-10.852623647	FRAG	1G	h	H	0.060
H6	1.408924074	-4.739487465	-10.202842300	FRAG	1G	h	H	0.070
C1	8.161755046	-2.323460433	-13.599770526	FRAG	1H	cp	C	-0.100
C2	8.043247034	-3.432296615	-14.449358681	FRAG	1H	cp	C	-0.010
C3	8.455681296	-3.359060938	-15.771585290	FRAG	1H	cp	C	-0.080
C4	8.992160492	-2.182382739	-16.270014371	FRAG	1H	cp	C	-0.030
C5	9.116063843	-1.069708578	-15.448411683	FRAG	1H	cp	C	-0.080
C6	8.703266218	-1.111766438	-14.105110326	FRAG	1H	cp	C	0.170
H2	7.629151300	-4.361648928	-14.081578227	FRAG	1H	h	H	0.070
H3	8.358683592	-4.222209774	-16.414041586	FRAG	1H	h	H	0.060
H4	9.312725769	-2.130543290	-17.300787513	FRAG	1H	h	H	0.070
H5	9.537973329	-0.177777146	-15.883191727	FRAG	1H	h	H	0.090
C4C	8.920199390	-2.702656881	-6.624879755	PORN	1D	c[	C	0.020
C3	9.111598997	-2.575167604	-5.189363052	PORN	1D	c#	C	-0.090
C4	7.904539058	-2.608698414	-4.581594957	PORN	1D	c#	C	-0.090
C4A	6.870089243	-2.788650910	-5.589587607	PORN	1D	c[	C	0.020
N4B	7.545761697	-2.886751361	-6.810339958	PORN	1D	nb	N	-0.340
CB	5.452051077	-2.830000116	-5.357437689	PORN	1D	c]	C	0.000
C6C	4.439126951	-2.924560892	-6.369449235	PORN	1D	c[	C	0.040
C5	2.997447244	-2.966439957	-6.166909885	PORN	1D	c#	C	-0.070
C6	2.383980450	-2.927571648	-7.375809225	PORN	1D	c#	C	-0.070
C6A	3.399891909	-2.887967674	-8.418975598	PORN	1D	c[	C	0.040
N6B	4.616784436	-3.013476094	-7.749600894	PORN	1D	na	N	-0.170
H6B	5.532666876	-2.997907069	-8.213064898	PORN	1D	hn	H	0.260
CC	3.184356733	-2.716589735	-9.827645553	PORN	1D	c]	C	0.000
C8C	4.208698041	-2.637324958	-10.830483546	PORN	1D	c[	C	0.020
C7	4.009131191	-2.401387737	-12.251050302	PORN	1D	c#	C	-0.090
C8	5.215350422	-2.332151679	-12.857465785	PORN	1D	c#	C	-0.090
H8	5.366094558	-2.122842084	-13.906035578	PORN	1D	h	H	0.080
C8A	6.258597124	-2.547816281	-11.865689112	PORN	1D	c[	C	0.020
N8B	5.590232411	-2.775666154	-10.658278746	PORN	1D	nb	N	-0.340
H3	10.053450175	-2.428267409	-4.682041916	PORN	1D	h	H	0.080

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H4       7.746651706   -2.492943884   -3.519683359 PORN 1D     h       H   0.080
H5       2.486921944   -2.942240642   -5.215226642 PORN 1D     h       H   0.090
H6       1.315684411   -2.865646789   -7.524205780 PORN 1D     h       H   0.090
H7       3.060713402   -2.254740679  -12.746120367 PORN 1D     h       H   0.080
end
end
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