

Supplementary material

**Binding free energies in the SAMPL6 octa-acid host–guest
challenge calculated with MM and QM methods**

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Figure S1. The nine ligands involved in SAMPL4.

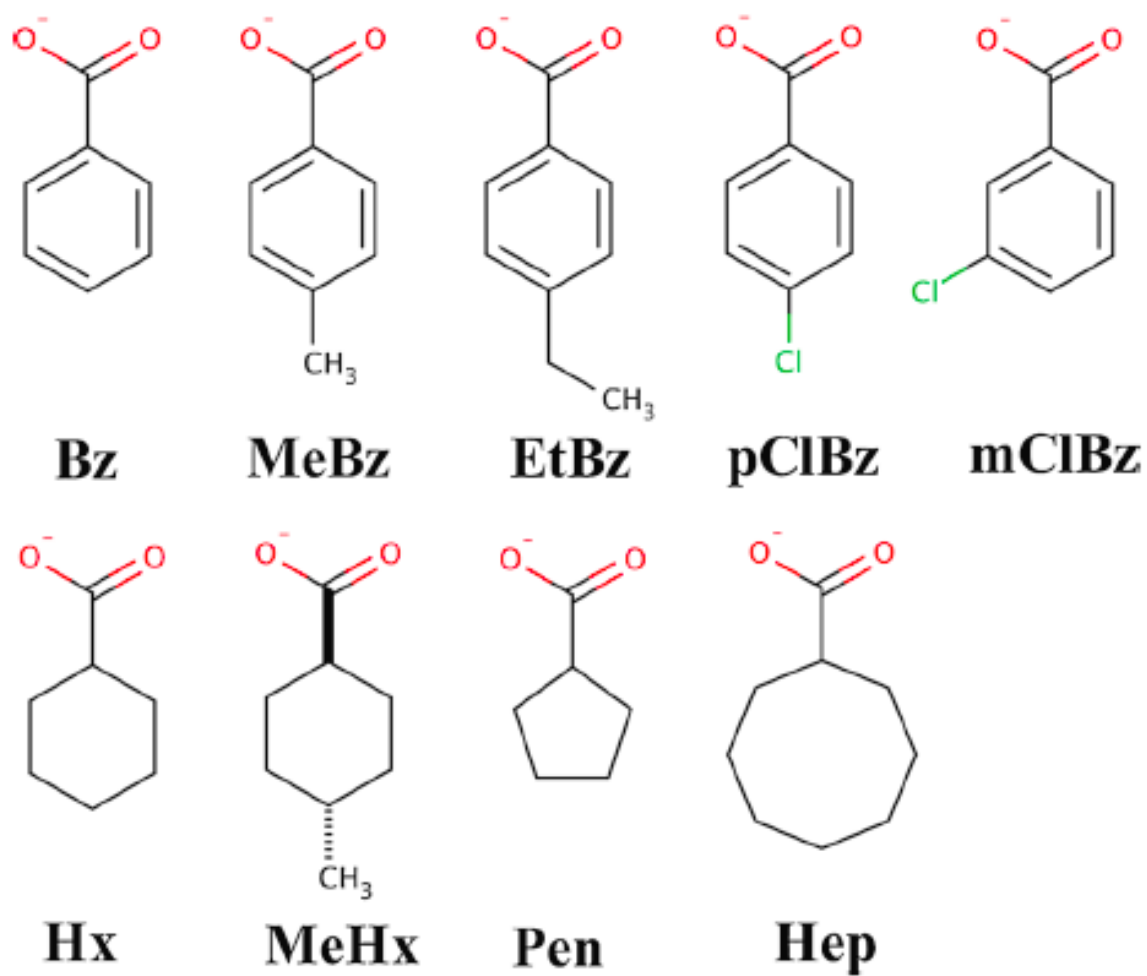


Figure S2. The six ligands involved in the SAMPL5 challenge. Only the carboxylate ligands G1, G2, G4 and G6 were considered in this study and they were called S5-G1 to S5-G6.

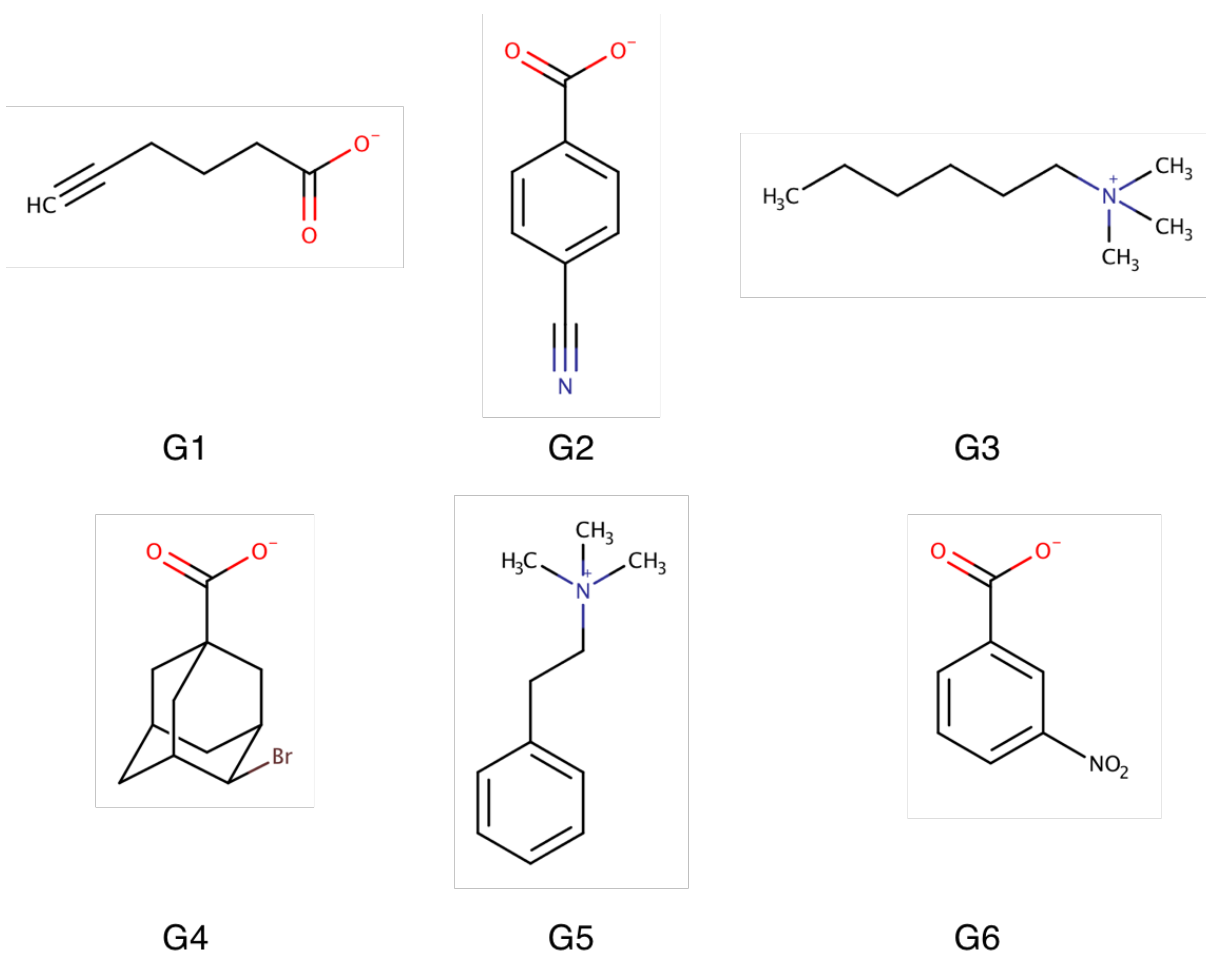


Figure S3. Atom names used in the geometric measure description.

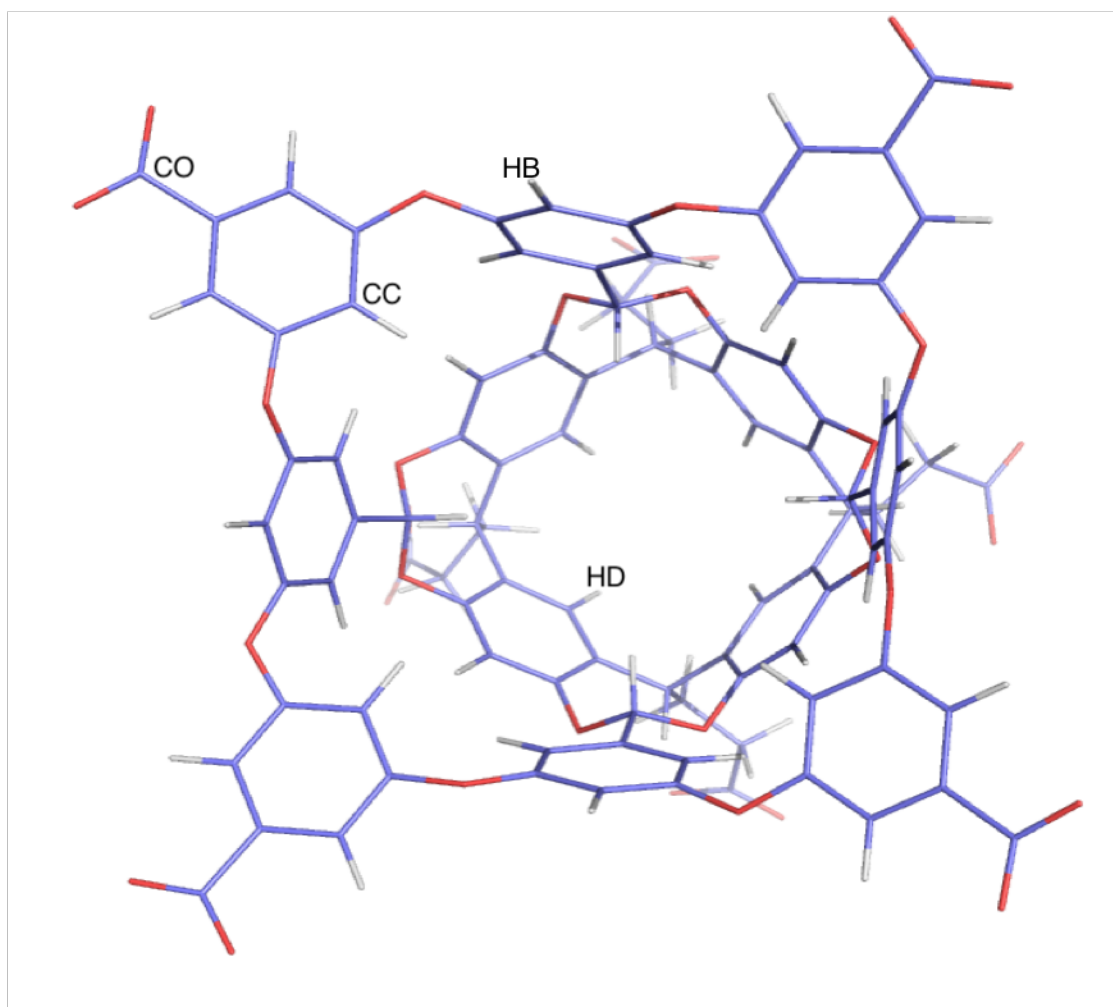
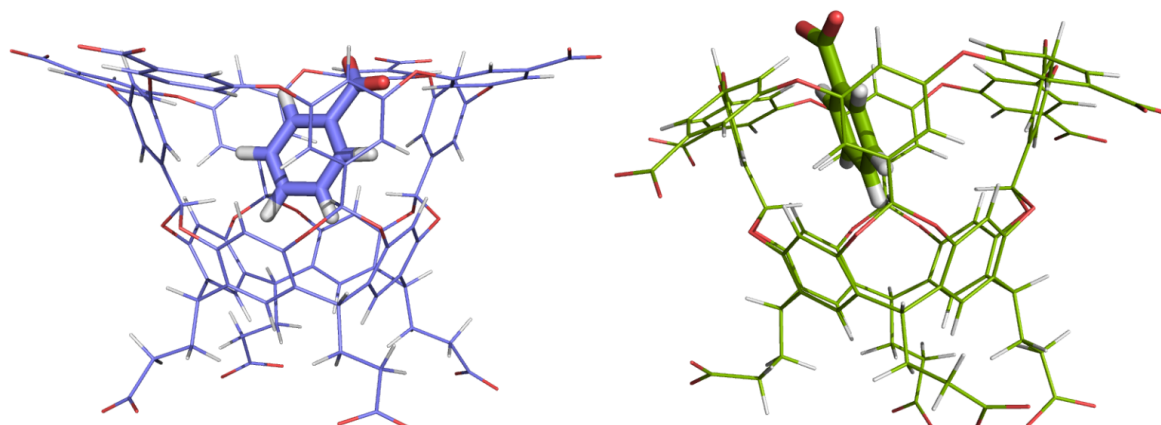
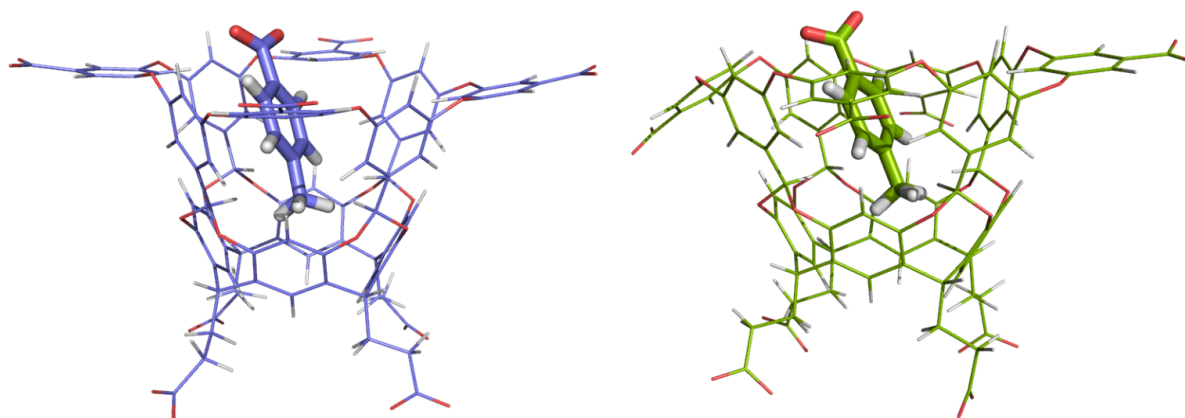


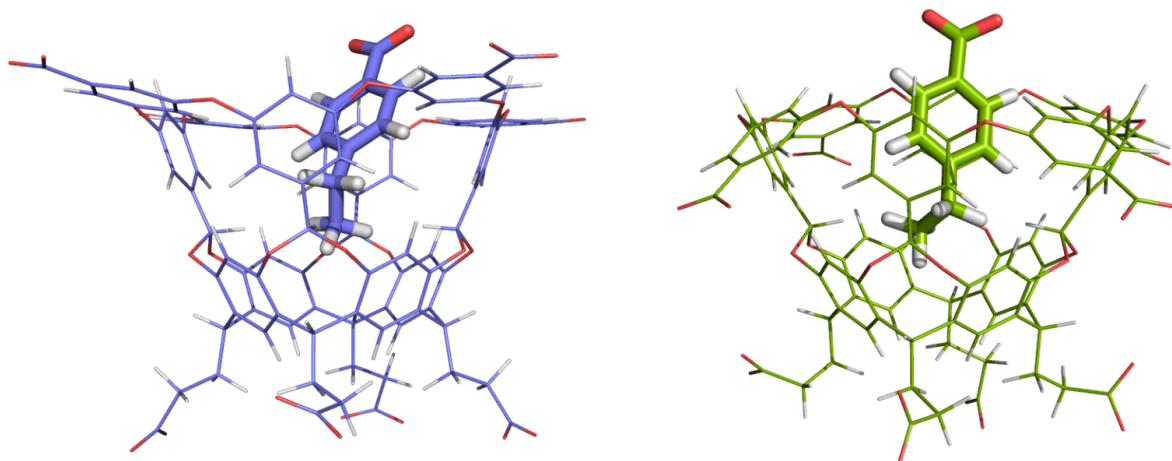
Figure S4. Comparison of the SAMPL4 and SAMPL5 optimised with DFT in vacuum (blue) or with PM6-DH+/MM (green). Water molecules were excluded for clarity.



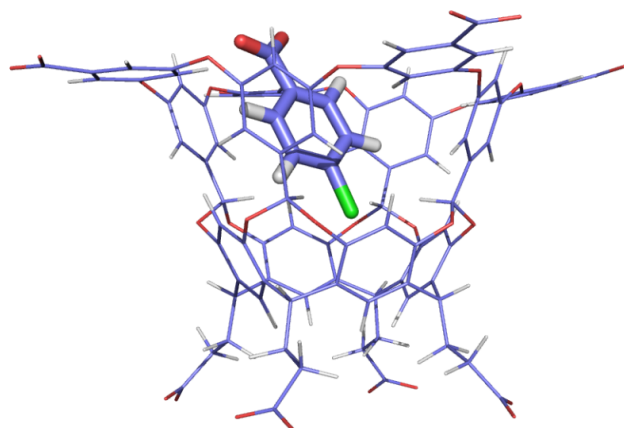
Bz in OAH



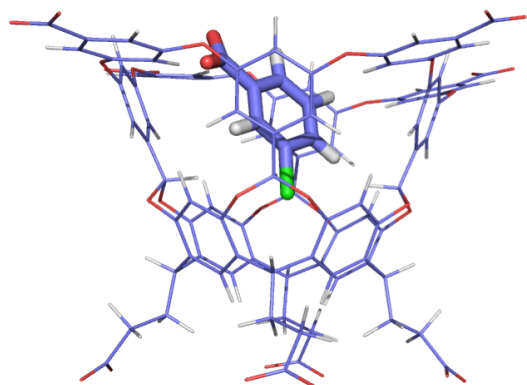
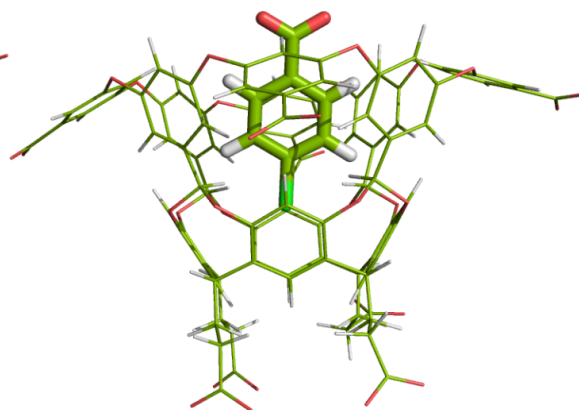
MeBz in OAH



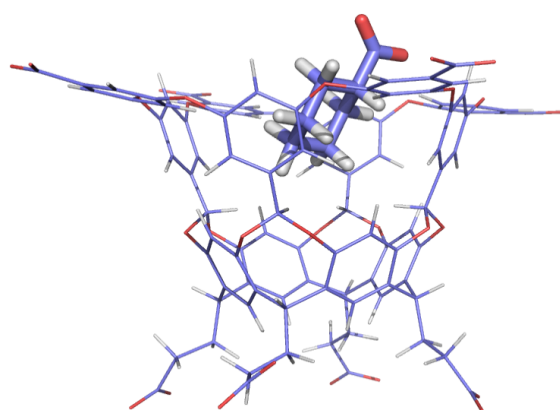
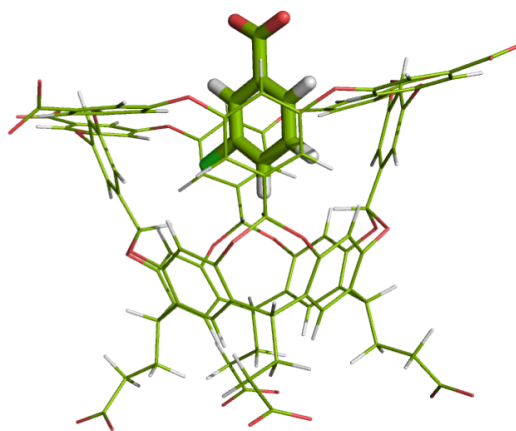
EtBz in OAH



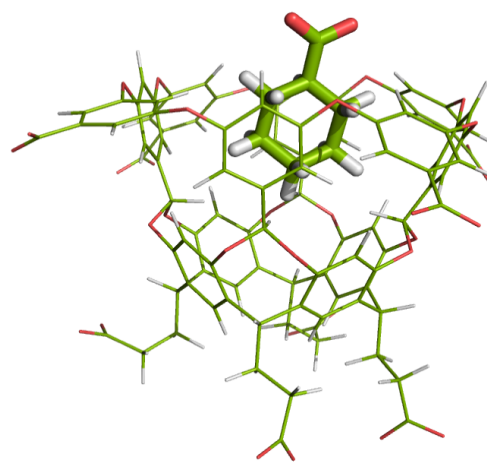
pClBz in OAH

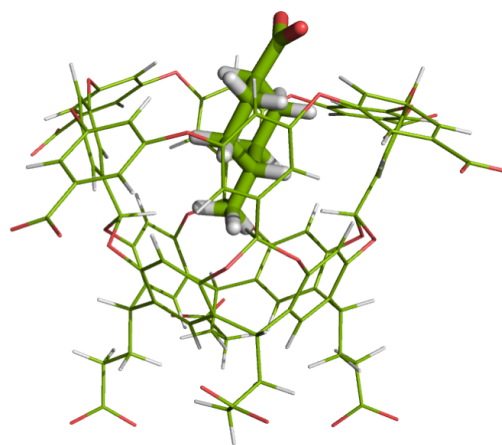
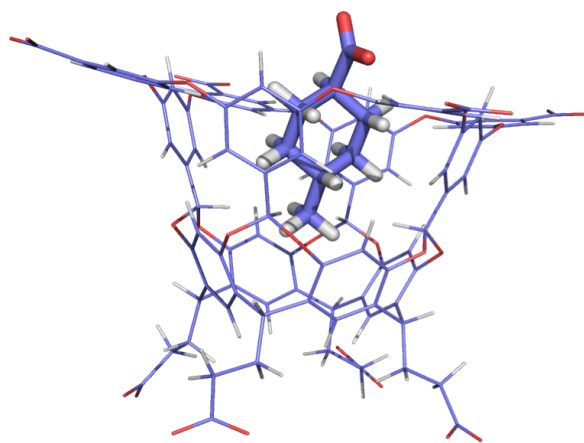


mClBz in OAH

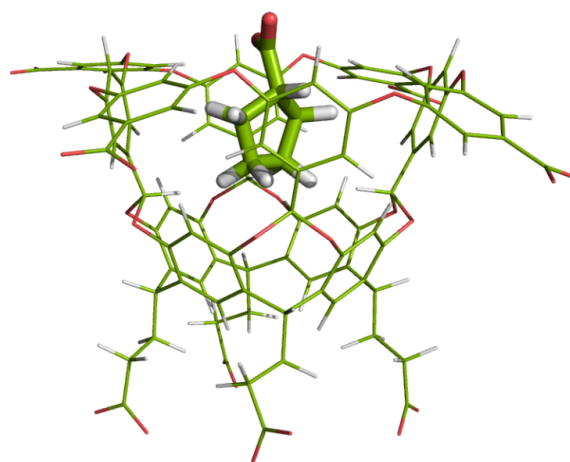
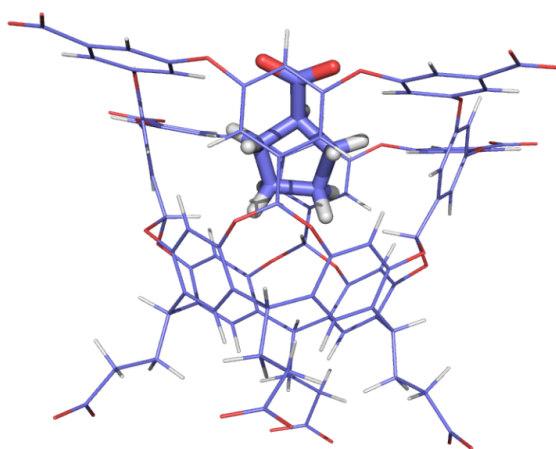


Hx in OAH

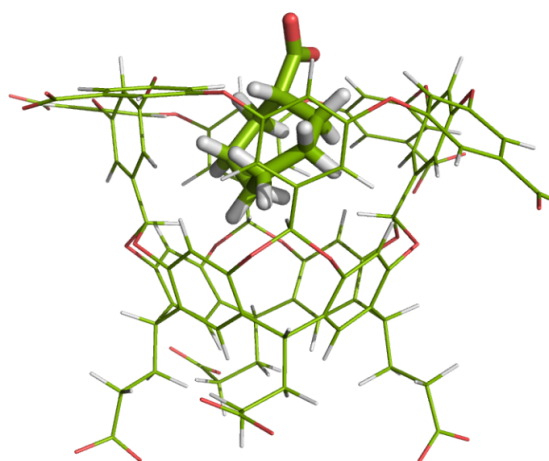
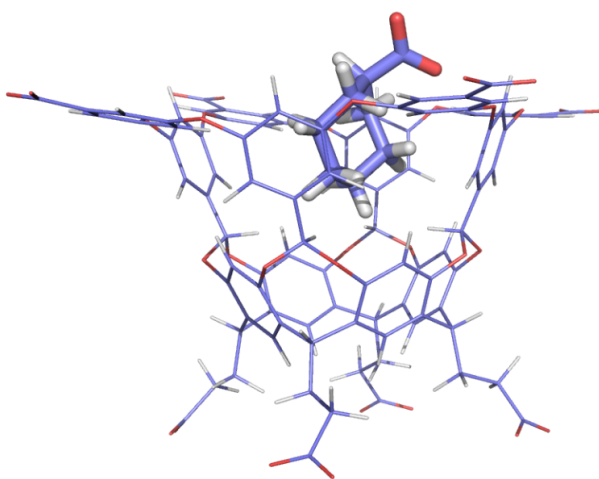




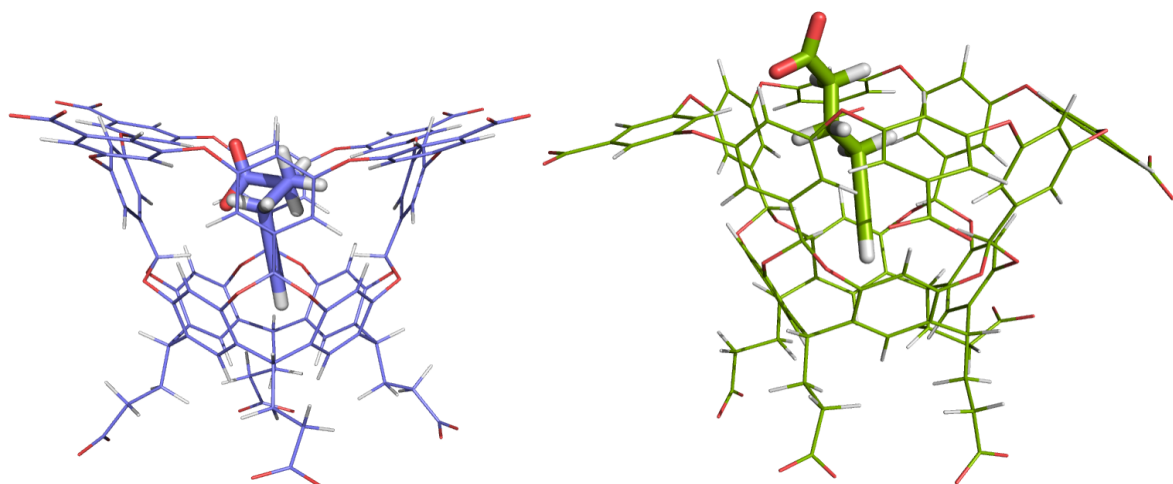
MeHx in OAH



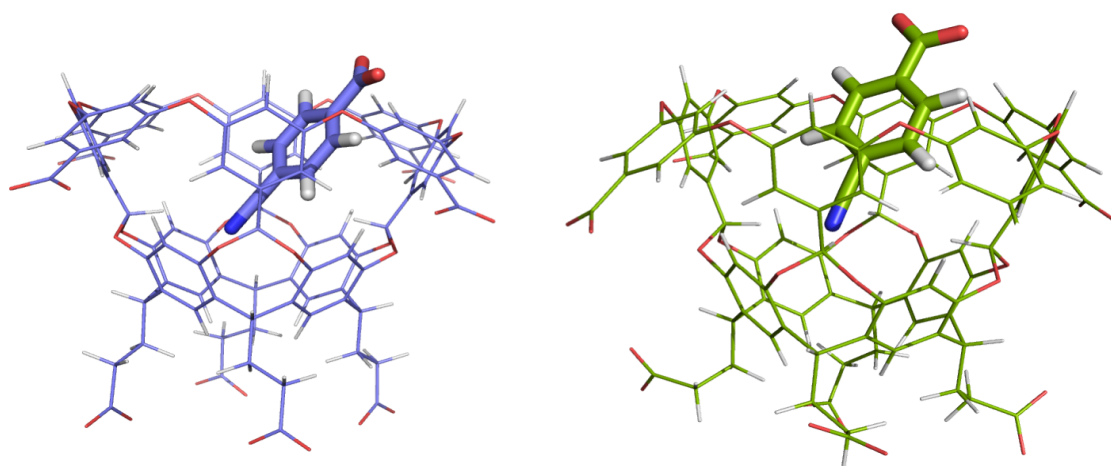
Pen in OAH



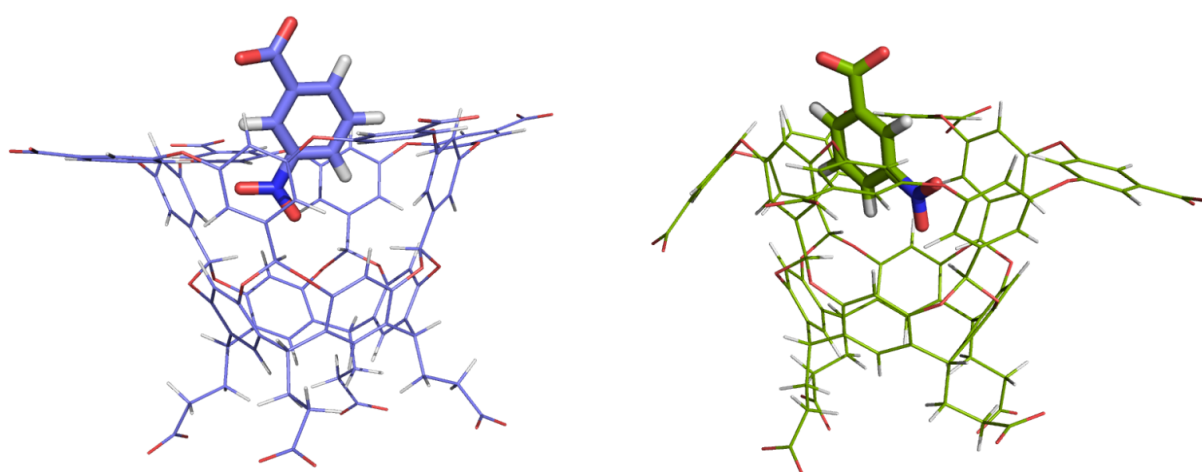
Hep in OAH



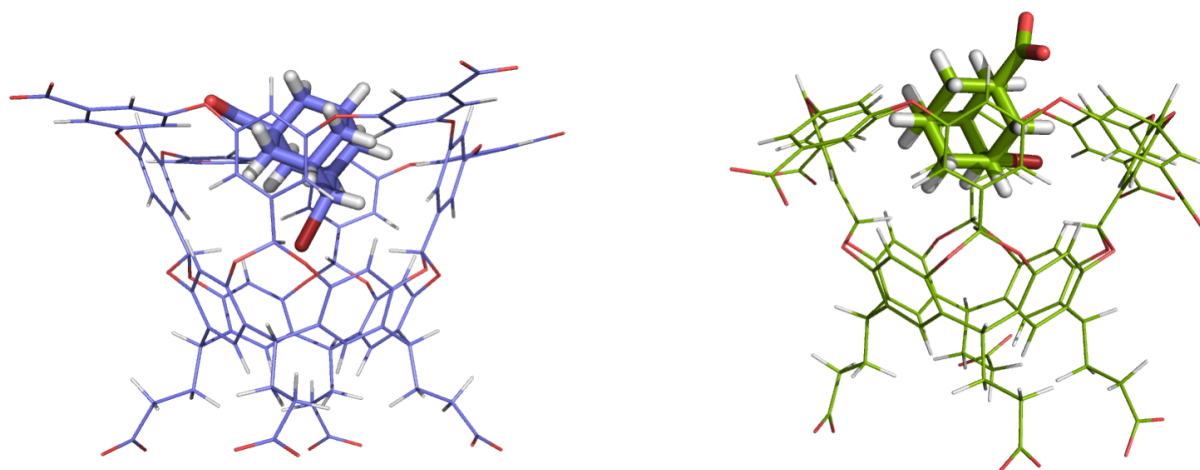
S5-G1 in OAH



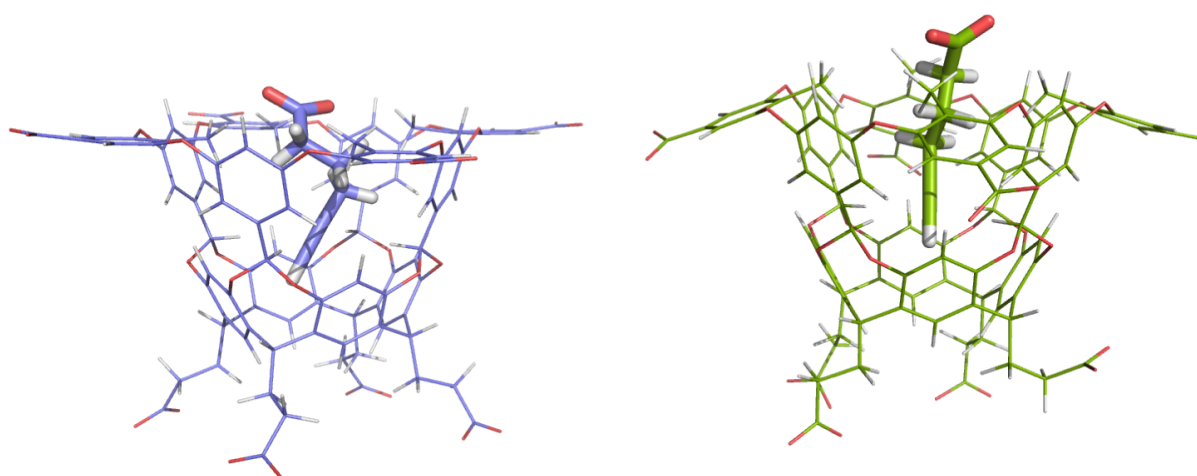
S5-G2 in OAH



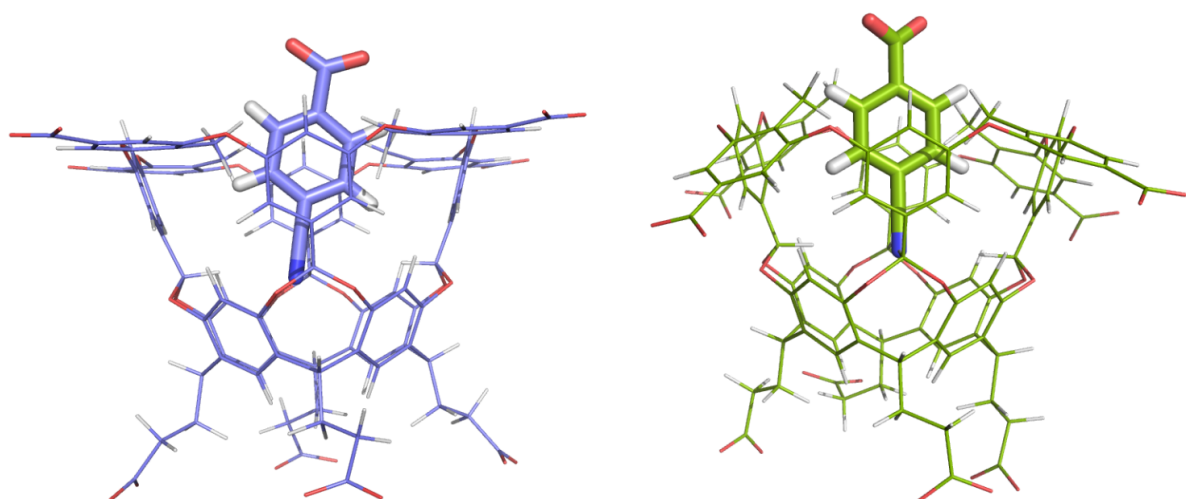
S5-G4 in OAH



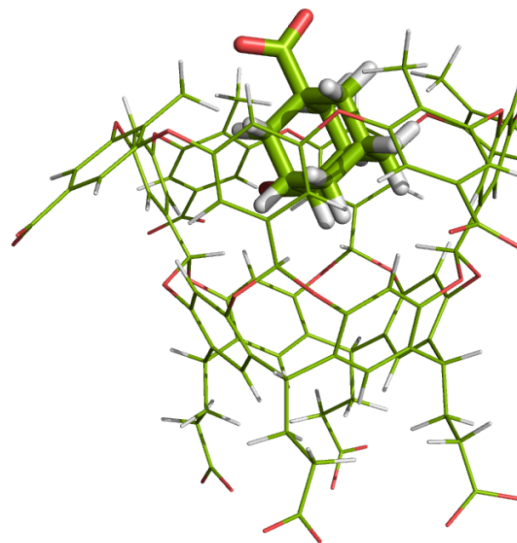
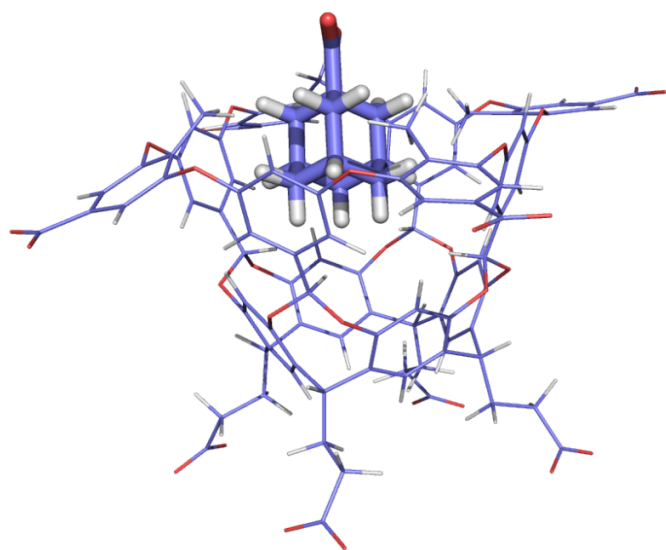
S5-G6 in OAH



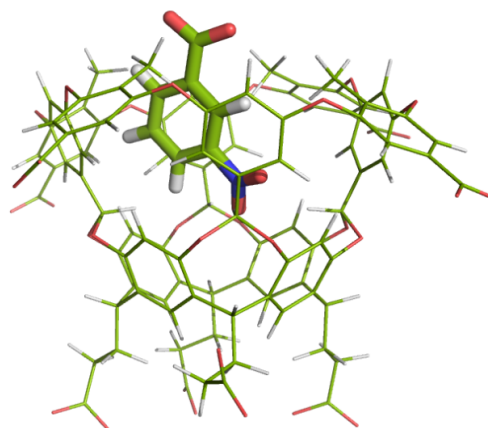
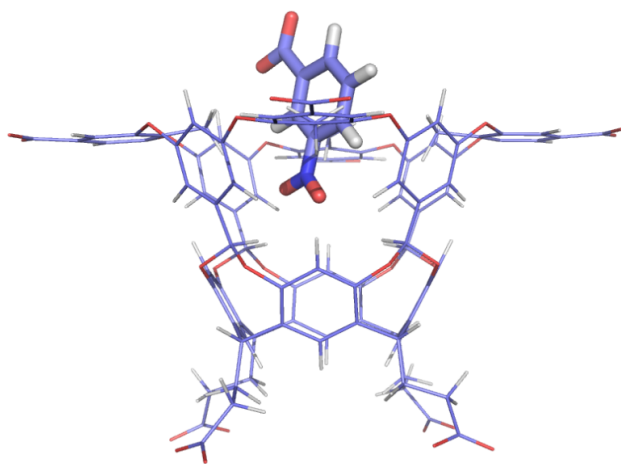
S5-G1 in OAM



S5-G2 in OAM



S5-G4 in OAM



S5-G6 in OAM

Figure S5. All SQM results for SAMPL6, together with the Boltzmann averages (crosses).

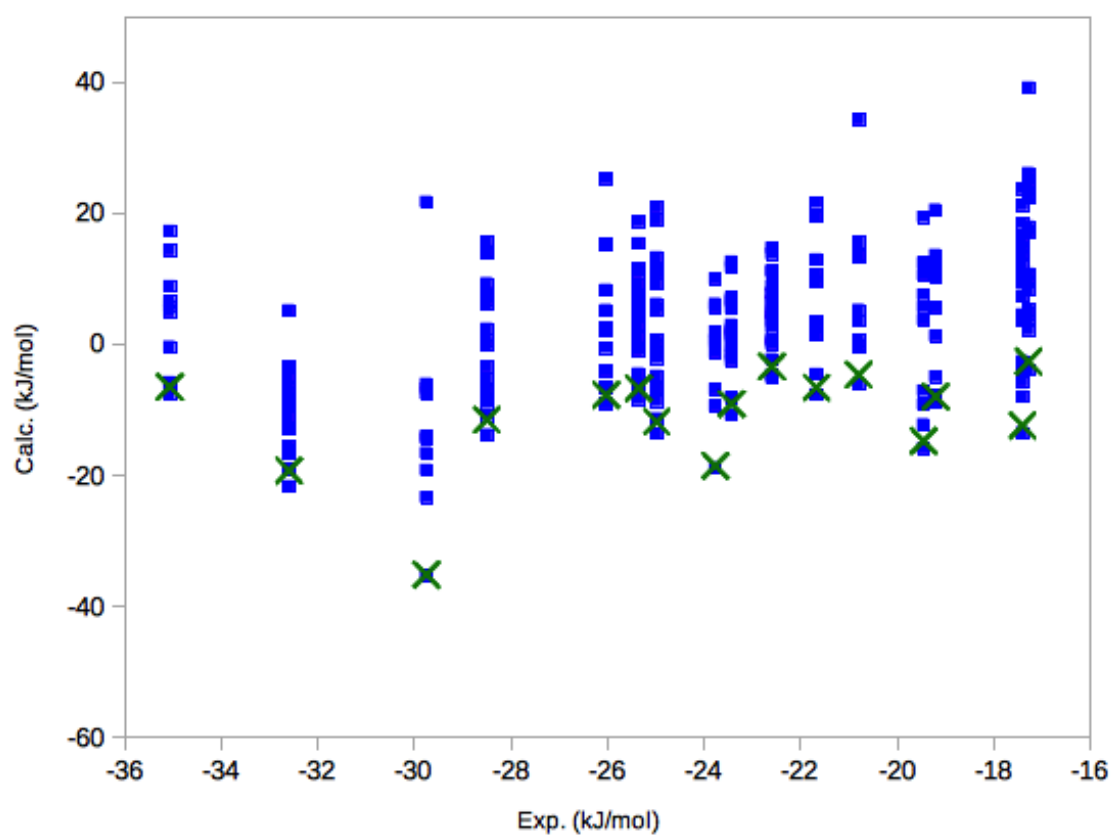
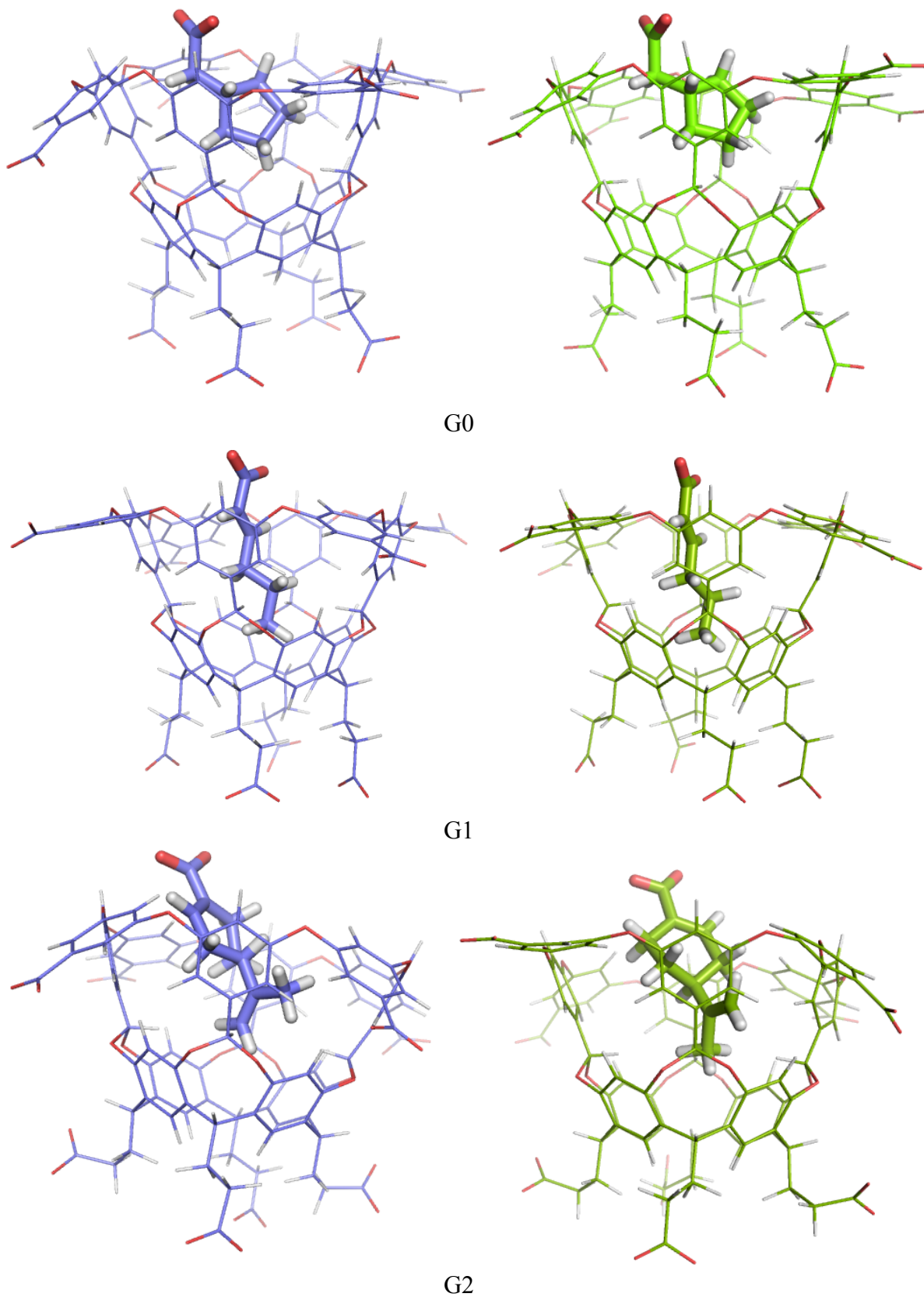
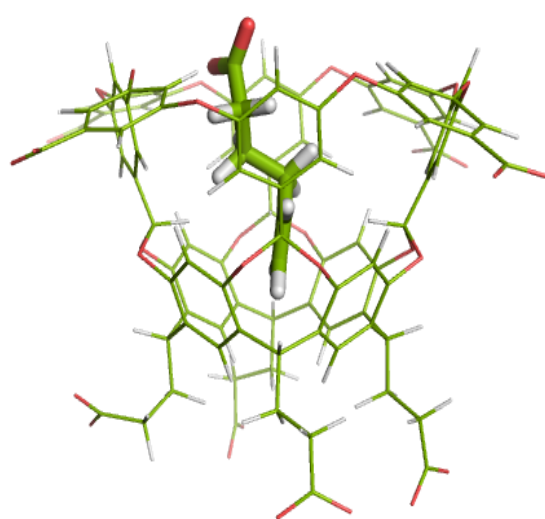
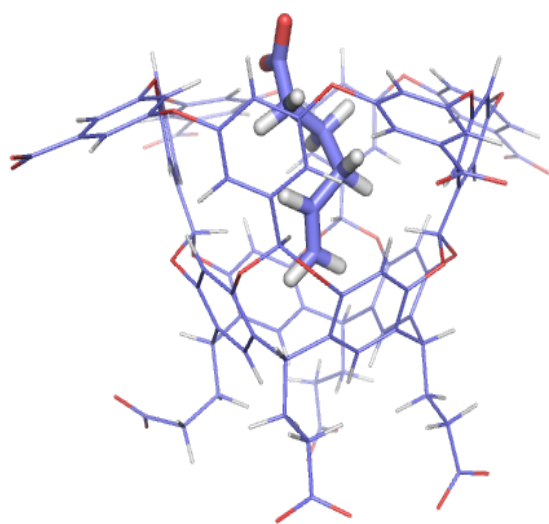
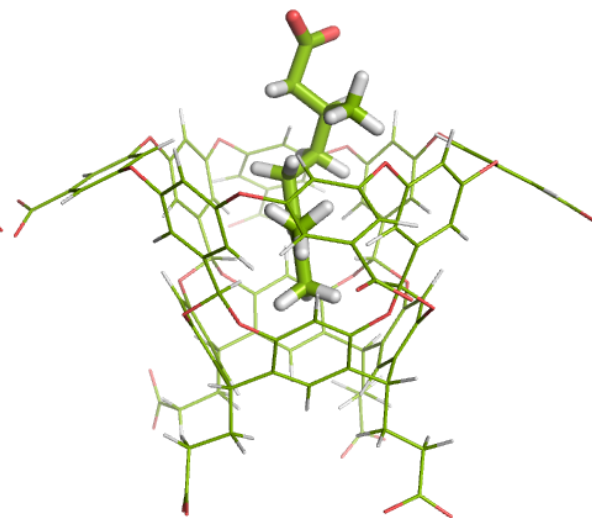
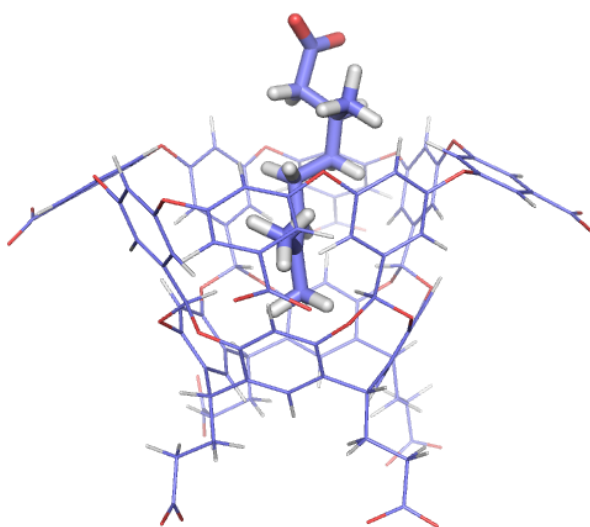


Figure S6. Comparison of the SAMPL6 host-guest complexes optimised with DFT/MM (blue) or with PM6-DH+/MM (green). Water molecules were excluded for clarity. Only complexes with the 8 guests in OAH hosts are shown. From top to bottom: G0 to G8.

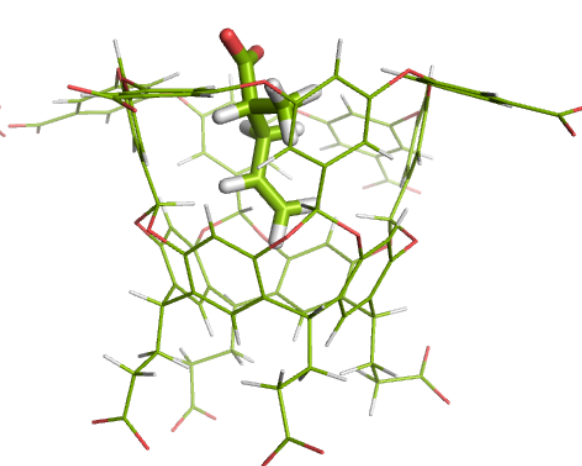
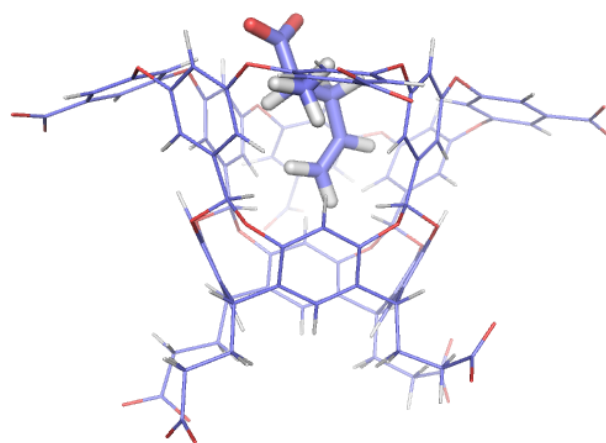




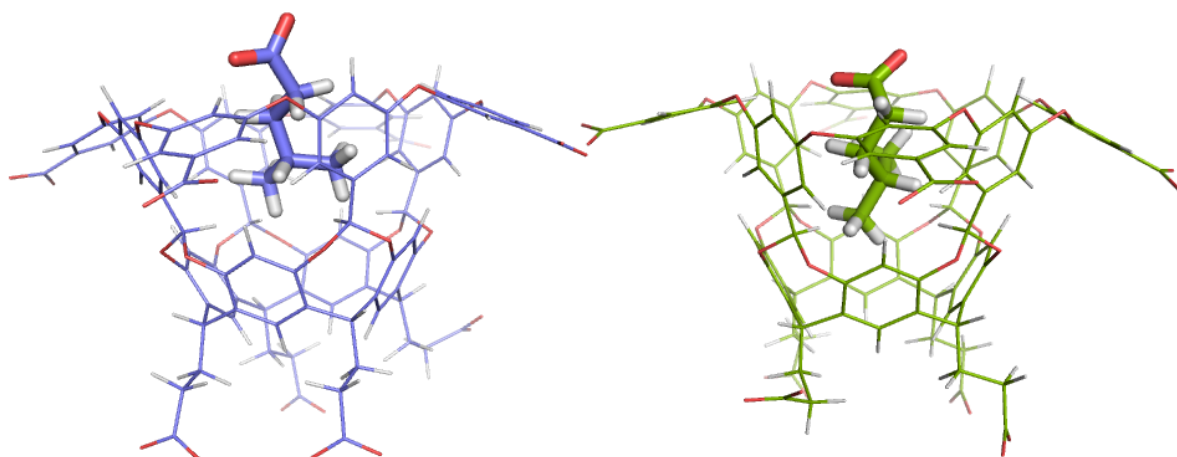
G3



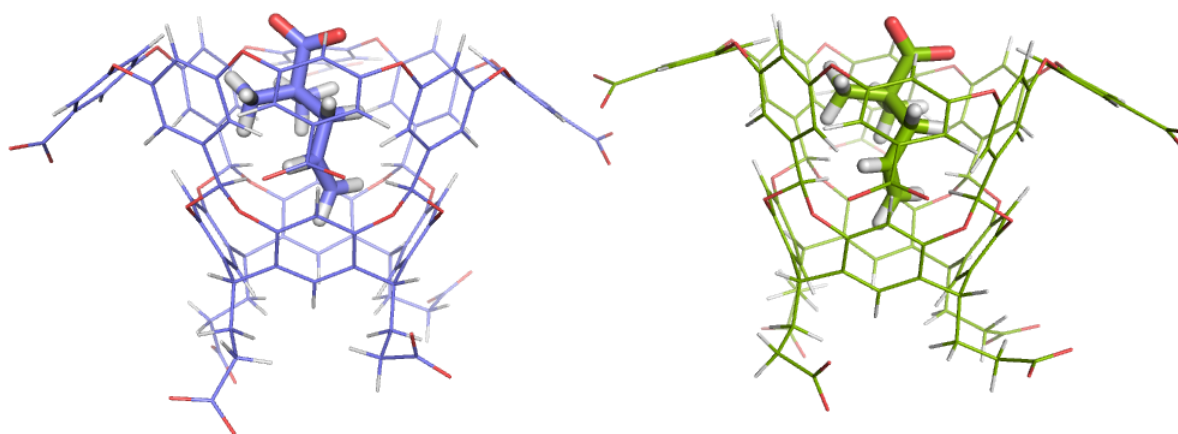
G4



G5



G6



G7

Table S1. Added dihedral parameters (needed for ligand G2). n is the periodicity, k the force constant (in kcal/mol) and φ the phase shift.

Atom types	n	k	φ
c2-ce-c3-hc	6	0.336	0
c -ce-c3-hc	6	0.550	0
c2-ce-c3-c3	6	0.588	0
c -ce-c3-c3	6	1.136	0

Table S2. Calculated relative binding free energies (kJ/mol) for the SAMPL6 ligands in the OAH host obtained with FEP at the MM and QM/MM levels. The relative affinities involving the SAMPL6 ligands, as well as the A6, A8 and MeHx ligands were obtained by using 1–2 perturbations from Table 1 and the intermediate ligands are specified in the last column. The experimental results are given in the “Exp.” column.

	Exp	MM-FEP	QM/MM-FEP	Via
G0 → G2	-11.3±0.15	-18.6±0.4	-8.2±0.6	A7
G1 → A6	-2.4±0.15	-5.8±0.1	-11.2±0.5	
G2 → MeHx	3.2±0.27	-4.2±1.5		
G3 → A6	-0.2±0.15	-8.7±0.1	-7.0±0.5	
G4 → A8	1.7±0.15	3.9±2.1	1.2±2.2	
G5 → G6	-1.6±0.12	-6.5±0.4	-6.3±0.6	A5
G6 → A6	-1.0±0.15	-5.0±0.3	-5.8±0.5	A5
G5 → G7	-6.8±0.12	-10.2±0.3	-6.4±0.5	
G0 → A6	1.9±0.18	-1.9±0.9	-0.3±1.0	A7
G0 → A8	-4.3±0.18	-8.9±0.5	-9.3±0.7	A7
G5 → A6	-2.6±0.15	-11.5±0.3	-12.1±0.6	A5
MAD		5.3±0.2	4.5±0.2	
MSD		-4.9±0.3	-3.8±0.3	
RMSD		5.7±0.2	5.3±0.2	
Max		8.9±0.5	9.5±0.5	
slope		1.6±0.0	1.1±0.0	
R^2		0.69±0.03	0.48±0.03	
τ		0.64±0.07	0.64±0.14	
τ_{90}		0.60±0.05	1.00±0.00	

Table S3. Geometric measures for the SAMPL4 and SAMPL5 guests from DFT structures optimised in vacuum (Vac) [15,31] or optimised with PM6-DH+/MM water molecules (SQM).

		Bz	MeBz	EtBz	pClBz	mClBz	Hx	MeHx	Pen	Hep
r_{Dm}	Vac	3.9	3.3	3.7	3.9	3.9	5.9	3.9	4.7	5.1
	SQM	3.9	3.0	2.9	3.7	6.6	4.9	3.3	4.9	4.7
α_T	Vac	38	32	35	32	54	30	36	46	58
	SQM	157	163	147	165	170	142	160	140	149
r_{O1}	Vac	-0.2	1.3	2.2	1.2	-0.1	1.8	1.7	0.9	1.5
	SQM	1.4	1.4	2.5	2.0	4.2	2.2	2.0	1.6	2.0
r_{O2}	Vac	0.9	1.6	2.8	1.8	1.5	3.0	3.0	1.0	3.2
	SQM	1.5	1.7	2.5	2.0	4.3	2.2	1.8	1.4	2.0
Δr_{BB}	Vac	0.2	0.4	0.3	0.4	0.2	0.3	0.1	0.1	0.0
	SQM	1.8	1.4	1.5	2.0	0.3	2.0	1.2	0.8	1.3
r_{Cav}	Vac	19.7	19.8	20.0	19.8	19.5	19.9	19.9	19.9	19.9
	SQM	18.6	18.6	18.3	18.3	19.7	18.4	18.5	18.6	18.5
		OAH				OAM				
		S5-G1	S5-G2	S5-G4	S5-G6	S5-G1	S5-G2	S5-G4	S5-G6	
r_{Dm}	Vac	2.6	3.2	4.5	5.9	3.1	4.1	5.2	6.0	
	SQM	2.9	4.0	3.3	3.0	3.4	3.7	2.7	2.9	
α_T	Vac	83	48	65	35	47	40	14	59	
	SQM	138	149	112	120	113	168	113	120	
r_{O1}	Vac	-2.0	1.6	1.2	4.6	0.6	3.3	3.5	2.7	
	SQM	1.5	2.1	2.2	2.5	2.3	2.8	2.7	2.7	
r_{O2}	Vac	0.2	0.0	1.3	3.1	1.5	2.8	3.0	4.3	
	SQM	1.8	2.0	2.6	2.3	2.4	2.9	2.8	2.8	
Δr_{BB}	Vac	0.5	2.9	0.5	0.6	0.5	1.0	1.2	0.5	
	SQM	2.1	2.3	0.8	1.7	1.5	1.3	1.2	1.3	
r_{Cav}	Vac	19.6	18.3	19.8	20.0	20.1	20.1	19.9	20.1	
	SQM	18.6	18.3	18.5	18.3	18.6	18.3	17.8	18.3	

Table S4. Energy components for the SQM results of SAMPL6, employing the snapshot with the minimum energy. The energy terms are defined in Eqn. 4. A negative sign of R^2 indicates that R is negative (anti-correlation).

	OAH					OAM				
	ΔE_{QM}	ΔG_{solv}	$\Delta E_{\text{QM}} + \Delta G_{\text{solv}}$	ΔG_{therm}	ΔG_{tot}	ΔE_{QM}	ΔG_{solv}	$\Delta E_{\text{QM}} + \Delta G_{\text{solv}}$	ΔG_{therm}	ΔG_{tot}
G0	868.6	-925.2	-56.6	45.6	-18.9	853.4	-921.9	-68.4	69.7	-6.6
G1	875.2	-932.4	-57.2	49.1	-15.9	834.8	-895.7	-60.9	57.4	-11.4
G2	868.3	-924.6	-56.4	58.5	-5.8	780.6	-859.1	-78.5	78.1	-8.3
G3	911.4	-959.7	-48.4	48.6	-7.7	864.5	-912.6	-48.0	54.5	-1.5
G4	797.6	-875.0	-77.4	50.1	-35.3	757.5	-843.0	-85.5	76.7	-16.8
G5	906.6	-954.5	-47.9	48.0	-7.8	857.2	-922.5	-65.3	65.3	-8.0
G6	880.4	-928.9	-48.5	56.1	-0.4	814.4	-874.7	-60.3	63.5	-4.8
G7	942.4	-995.5	-53.1	54.4	-6.6	859.7	-931.7	-71.9	75.9	-4.0
R^2	0.16	-0.12	0.28	-0.30	0.06	0.66	-0.68	0.24	-0.08	0.43

Table S5. Submitted SQM and DFT ΔG_{bind} results (kJ/mol) involving incorrect ΔG_{therm} estimates (the ligands had dissociated for SQM and the calculations did not involve any partial atomic charges for DFT). A constant offset of -20.9 kJ/mol was added to the DFT results to bring them to the same magnitude as the SQM results. Values in brackets for the quality measures of DFT are calculated with this offset.

	OAH		OAM	
	SQM	DFT	SQM	DFT
G0	-24.4	5.0	-35.3	18.6
G1	-25.9	5.8	-28.6	3.2
G2	-21.5	-20.5	-43.2	5.2
G3	-16.6	3.5	-19.3	17.8
G4	-44.1	-27.0	-48.0	-22.3
G5	-16.4	-1.0	-33.6	18.5
G6	-16.7	13.2	-27.8	16.9
G7	-20.4	2.0	-41.4	12.6
MAD	6.6	22 (8.0)	11.7	33 (14.6)
MADtr	6.3	7.7	7.0	7.5
MSD	-1.2	22 (1.2)	-10.7	33 (11.9)
RMSD	8.0	24 (9.3)	13.5	34 (15.5)
max	14.4	34 (18.2)	24.2	44 (23.1)
slope	0.3	2.0	0.7	2.0
R^2	0.18	0.66	0.14	0.57
τ	0.36	0.43	0.36	0.29
τ_{90}	0.36	0.43	0.41	0.33

Table S6. Geometric measures for the SAMPL6 ligands from MD simulations, as well as SQM and DFT optimisations. The MD and SQM results are averaged over 10 or 20 structures. Distances are in Å and angles in degrees.

		G0	G1	G2	G3	G4	G5	G6	G7
OAH									
r_{Dm}	MD	4.9±0.4	3.5±0.3	3.9±0.3	3.4±0.5	3.7±0.2	3.6±0.5	5.1±0.7	3.3±0.2
	SQM	4.7±0.4	3.2±0.3	3.3±0.3	2.9±0.5	3.3±0.2	3.3±0.5	4.8±0.8	2.8±0.2
	DFT	4.4	3.1	3.9	3.0	3.4	4.6	4.7	2.7
α_T	MD	156±15	161±12	123±15	149±15	159±11	161±6	155±15	156±9
	SQM	152±13	155±13	123±17	150±11	157±10	156±7	149±14	148±11
	DFT	174	164	126	147	161	158	149	170
r_{O1}	MD	2.4±0.5	2.6±0.4	2.8±0.8	1.6±0.4	4.1±0.6	1.6±0.4	2.0±0.6	1.5±0.2
	SQM	2.2±0.6	2.1±0.7	2.3±0.7	1.2±0.6	3.9±0.4	1.2±0.6	1.7±0.5	1.1±0.3
	DFT	1.9	2.1	3.3	1.0	4.8	2.2	1.9	0.9
r_{O2}	MD	2.5±0.4	2.4±0.3	2.7±0.7	1.3±0.5	4.5±0.4	1.5±0.5	1.9±0.6	1.3±0.4
	SQM	2.3±0.5	1.8±0.5	2.2±0.5	1.2±0.6	4.2±0.4	1.1±0.5	1.6±0.8	0.6±0.6
	DFT	2.1	1.8	3.1	2.1	4.1	1.0	2.9	0.7
Δr_O	MD	0.3±0.2	0.3±0.2	0.4±0.4	0.4±0.3	0.8±0.4	0.4±0.3	0.5±0.3	0.4±0.3
	SQM	0.5±0.4	0.5±0.3	0.3±0.2	0.5±0.4	0.7±0.4	0.7±0.3	0.7±0.3	0.9±0.4
	DFT	0.2	0.3	0.2	1.1	0.7	1.1	1.0	0.2
Δr_{BB}	MD	1.4±1.0	1.7±1.4	0.8±0.6	1.0±0.8	2.0±1.2	1.5±0.9	1.1±1.1	1.1±0.6
	SQM	1.6±0.9	1.7±0.5	1.0±0.7	1.3±1.0	2.0±1.0	1.5±1.2	1.1±1.2	1.2±1.1
	DFT	0.5	0.6	1.1	0.0	1.4	4.0	0.7	0.1
r_{Cav}	MD	18.7±0.8	18.7±0.5	18.5±0.7	18.5±0.8	18.5±0.7	18.7±0.9	18.9±0.6	18.6±0.4
	SQM	18.6±0.8	18.6±0.5	18.4±0.7	18.5±0.8	18.3±0.7	18.6±1.0	18.7±0.5	18.4±0.6
	DFT	18.8	19.3	18.1	18.8	18.1	18.6	18.9	18.3
OAM									
r_{Dm}	MD	4.8±0.3	3.8±0.4	4.1±0.5	3.9±0.3	3.7±0.3	4.1±0.5	5.3±0.3	3.4±0.6
	SQM	4.6±0.4	3.4±0.5	3.9±0.5	3.5±0.5	3.4±0.2	3.6±0.8	5.3±0.5	2.9±0.5
	DFT	4.0	3.4	3.9	3.4	3.4	4.2	6.1	3.4
α_T	MD	148±10	162±9	136±16	150±10	160±13	163±8	162±8	160±7
	SQM	144±12	157±8	136±16	147±13	160±11	157±10	156±10	154±7
	DFT	142	163	117	141	149	173	164	153
r_{O1}	MD	2.6±0.4	2.9±0.5	3.6±0.8	2.8±0.4	4.6±0.5	2.1±0.6	3.2±0.4	1.3±0.3
	SQM	2.2±0.6	2.3±0.6	3.4±0.7	2.7±0.6	4.2±0.7	1.7±0.6	2.8±0.6	1.0±0.5
	DFT	2.7	2.8	4.0	3.0	4.5	1.7	4.0	1.8
r_{O2}	MD	2.5±0.5	2.6±0.6	3.5±0.5	2.7±0.5	4.5±0.6	1.9±0.6	3.2±0.4	1.2±0.4
	SQM	2.1±0.7	2.2±0.6	3.3±0.8	2.4±0.6	4.3±0.7	1.5±0.8	3.0±0.7	0.8±0.6
	DFT	1.1	1.9	3.6	1.8	4.3	2.3	3.9	0.8
Δr_O	MD	0.5±0.2	0.5±0.3	0.4±0.3	0.4±0.3	0.4±0.4	0.5±0.3	0.3±0.2	0.4±0.3
	SQM	0.7±0.5	0.5±0.3	0.3±0.3	0.7±0.4	0.4±0.4	0.6±0.5	0.5±0.4	0.7±0.4
	DFT	1.6	0.9	0.4	1.2	0.2	0.6	0.1	1.0
Δr_{BB}	MD	1.3±0.9	0.8±0.8	1.7±1.1	1.3±0.9	1.0±0.9	1.2±0.9	1.4±1.1	1.1±0.7
	SQM	1.5±0.8	0.8±0.7	1.7±1.0	1.4±1.1	1.1±0.9	1.1±0.7	1.5±0.9	1.0±0.7
	DFT	2.8	1.7	2.1	0.2	2.5	1.4	0.9	1.5
r_{Cav}	MD	18.4±0.5	18.7±0.7	18.4±0.5	18.7±0.6	18.5±0.5	18.5±0.5	18.7±0.5	18.5±0.6
	SQM	18.2±0.6	18.5±0.5	18.2±0.5	18.4±0.6	18.3±0.4	18.4±0.4	18.4±0.5	18.3±0.6
	DFT	18.4	18.3	18.4	18.4	18.5	18.3	18.6	17.6

Table S7. Overlap measures for the various MM and QM/MM FEP simulations. For Ω , K_{AB} and Π , the minimum value over the 2×13 (MM) or 2×4 (MM $\rightarrow$ QM/MM) simulations (13 λ or 4 Λ values and simulations for both the free and the bound ligand) are listed, whereas for $w_{\max}$ and ΔG_{EA} the maximum value is given.

	simulation 1					simulation 2					simulation 3				
	Ω	K_{AB}	Π	$w_{\max}$	ΔG_{EA}	Ω	K_{AB}	Π	$w_{\max}$	ΔG_{EA}	Ω	K_{AB}	Π	$w_{\max}$	ΔG_{EA}
OAH															
A5 $\rightarrow$ A6	1.0	1.0	1.9	0.02	0.3	1.0	1.0	1.1	0.05	0.2	1.0	1.0	1.7	0.02	0.4
A6 $\rightarrow$ A7	1.0	1.0	1.7	0.07	0.3	1.0	1.0	1.9	0.07	0.3	1.0	1.0	1.6	0.17	0.7
A7 $\rightarrow$ A8	1.0	1.0	1.9	0.04	0.2	1.0	1.0	1.7	0.02	0.5	1.0	1.0	1.8	0.02	0.2
G0 $\rightarrow$ A7	1.0	1.0	1.0	0.14	1.9	1.0	1.0	0.9	0.24	0.8	1.0	1.0	1.0	0.30	1.7
G1 $\rightarrow$ A6	1.0	1.0	1.4	0.10	0.6	1.0	1.0	1.4	0.12	0.5	0.9	0.5	1.4	0.07	0.4
G2 $\rightarrow$ A7	1.0	1.0	1.0	0.16	1.1	1.0	1.0	1.0	0.12	2.1	1.0	1.0	0.9	0.17	0.6
G2 $\rightarrow$ MeHx	1.0	1.0	1.3	0.17	6.3	1.0	1.0	1.3	0.18	4.3	1.0	1.0	1.0	0.15	5.9
G3 $\rightarrow$ A6	1.0	1.0	1.2	0.14	1.0	1.0	0.9	1.5	0.15	0.6	1.0	1.0	1.4	0.10	0.9
G4 $\rightarrow$ A8	1.0	1.0	0.4	0.26	4.1	1.0	1.0	0.2	0.41	4.2	1.0	1.0	0.4	0.20	2.8
G5 $\rightarrow$ A5	1.0	1.0	1.6	0.10	0.7	1.0	1.0	1.6	0.16	1.1	1.0	1.0	1.6	0.06	0.8
G5 $\rightarrow$ G7	1.0	1.0	1.7	0.05	0.6	1.0	1.0	1.6	0.11	0.8	1.0	1.0	1.9	0.04	0.4
G6 $\rightarrow$ A5	1.0	1.0	1.7	0.04	0.2	1.0	1.0	1.7	0.02	0.2	1.0	1.0	1.7	0.09	0.3
OAM															
A5 $\rightarrow$ A6	1.0	1.0	1.9	0.02	0.2	1.0	1.0	1.9	0.05	0.2	1.0	1.0	1.7	0.02	0.3
A6 $\rightarrow$ A7	1.0	1.0	1.8	0.03	0.2	1.0	1.0	1.8	0.03	0.2	1.0	1.0	1.7	0.03	0.2
A7 $\rightarrow$ A8	1.0	1.0	1.8	0.05	0.2	1.0	1.0	1.9	0.02	0.2	1.0	1.0	1.8	0.04	0.4
G0 $\rightarrow$ A7	1.0	1.0	0.7	0.27	1.5	1.0	1.0	0.8	0.14	2.5	1.0	1.0	0.8	0.21	1.5
G1 $\rightarrow$ A6	1.0	1.0	1.7	0.07	0.7	0.6	0.5	1.6	0.07	0.5	0.8	0.4	1.3	0.34	2.0
G2 $\rightarrow$ A7	1.0	1.0	0.7	0.41	1.7	1.0	1.0	0.7	0.41	1.7	1.0	1.0	0.7	0.41	1.7
G2 $\rightarrow$ MeHx	1.0	1.0	1.2	0.14	5.6	1.0	1.0	0.9	0.42	5.8	1.0	1.0	1.3	0.20	5.5
G3 $\rightarrow$ A6	1.0	1.0	1.3	0.23	0.7	1.0	1.0	1.4	0.24	1.1	1.0	1.0	1.2	0.17	1.0
G4 $\rightarrow$ A8	1.0	1.0	0.4	0.15	4.4	1.0	1.0	0.3	0.30	2.6	1.0	1.0	0.5	0.28	3.1
G5 $\rightarrow$ A5	1.0	1.0	1.4	0.17	0.7	1.0	1.0	1.4	0.17	0.7	1.0	1.0	1.4	0.17	0.7
G5 $\rightarrow$ G7	1.0	1.0	1.5	0.03	0.8	1.0	1.0	1.5	0.22	0.7	1.0	1.0	1.7	0.09	0.6
G6 $\rightarrow$ A5	1.0	1.0	2.0	0.03	0.1	1.0	1.0	1.8	0.05	0.2	1.0	1.0	1.8	0.02	0.2
OAM $\rightarrow$ OAH	1.0	1.0	1.2	0.30	1.0	1.0	1.0	1.2	0.30	1.0	1.0	1.0	1.2	0.30	1.0
MM $\rightarrow$ QM/MM; OAH															
G0	1.0	1.2	0.8	0.2	0.5										
G1 ^a	1.0	1.1	1.0	0.2	0.8										
G2 ^a	1.0	1.1	0.8	0.2	1.3										
G3	1.0	1.1	0.8	0.3	1.2										
G4 ^a	1.0	1.2	0.7	0.5	2.3										
G5	1.0	1.2	0.9	0.5	0.6										
G6	1.0	1.2	0.8	0.2	1.3										
G7 ^a	1.0	1.1	0.8	0.2	0.7										
A5	1.0	1.2	0.9	0.2	0.9										
A6	1.0	1.2	1.0	0.4	1.1										
A7	1.0	1.1	0.8	0.2	0.5										
A8	1.0	1.2	0.6	0.3	0.3										
MM $\rightarrow$ QM/MM; OAM															
G0	1.0	1.2	0.8	0.2	0.9	1.0	1.2	0.8	0.1	0.7					
G1 ^a	1.0	1.1	0.9	0.2	0.5	1.0	1.1	0.9	0.2	0.5					
G2 ^b	1.0	1.1	0.5	0.1	2.2	1.0	1.1	0.5	0.1	2.2					
G3	1.0	1.2	0.9	0.2	0.8	1.0	1.2	0.9	0.2	0.8					
G4 ^c	1.0	1.1	1.1	0.2	0.9	1.0	1.1	1.1	0.2	0.9					
G5	1.0	1.2	0.9	0.2	1.1	1.0	1.2	0.9	0.2	1.1					
G6	1.0	1.2	0.7	0.2	0.8	1.0	1.2	0.7	0.2	0.8					
G7 ^a	1.0	1.2	0.4	0.3	1.4	1.0	1.2	0.4	0.3	1.4					
A5	1.0	1.2	0.8	0.3	0.4	1.0	1.2	0.8	0.3	0.4					
A6	1.0	1.2	1.0	0.2	1.2	1.0	1.2	1.0	0.2	1.2					
A7	1.0	1.1	0.7	0.2	1.0	1.0	1.1	0.7	0.2	1.0					
A8	1.0	1.2	0.6	0.2	0.7	1.0	1.2	0.6	0.2	0.7					

^a An extra $\Lambda = 0.8333$ value was added.

^b $\Lambda = 0.8333$ was added and also $\Lambda = 0.5$ for the first simulation.

^c $\Lambda = 0.8333$ was added and also $\Lambda = 0.1667$ for the first simulation.

Table S8. Amber topology files for the various ligands. Column 2 shows the atom names, column 3 the atom types and the last column the charges.

```
g0.in
0      0      2

This is a remark line
molecule.res
G00 INT 0
CORRECT      OMIT DU      BEG
0.0000
1  DUMM DU      M      0 -1 -2      0.000      .0      .0      .00000
2  DUMM DU      M      1  0 -1      1.449      .0      .0      .00000
3  DUMM DU      M      2  1  0      1.523      111.21      .0      .00000
4  C4    c3      M      3  2  1      1.540      111.208      -180.000      -0.207296
5  H5    hc      E      4  3  2      1.123      49.439      -139.756      0.029009
6  H6    hc      E      4  3  2      1.120      88.106      105.390      0.029009
7  C2    c3      M      4  3  2      1.521      158.523      -106.058      0.102479
8  H1    hc      E      7  4  3      1.119      110.134      -8.509      -0.044373
9  H2    hc      E      7  4  3      1.118      111.314      -127.435      -0.044373
10 C3    c3      M      7  4  3      1.522      106.958      111.109      0.102479
11 H3    hc      E     10  7  4      1.119      110.204      99.911      -0.044373
12 H4    hc      E     10  7  4      1.118      111.064      -141.412      -0.044373
13 C5    c3      M     10  7  4      1.522      106.923      -19.984      -0.207296
14 H7    hc      E     13 10  7      1.118      110.635      136.415      0.029009
15 H8    hc      E     13 10  7      1.118      110.154      -105.082      0.029009
16 C6    c3      M     13 10  7      1.534      107.783      15.312      0.341815
17 H9    hc      E     16 13 10      1.124      109.274      113.135      -0.066911
18 C7    c3      M     16 13 10      1.515      111.745      -127.765      -0.203906
19 H10   hc      E     18 16 13      1.119      110.000      62.587      0.001540
20 H11   hc      E     18 16 13      1.120      109.239      -56.229      0.001540
21 C1    c      M     18 16 13      1.539      111.358      -176.502      0.825718
22 O2    o      E     21 18 16      1.265      118.218      90.370      -0.814354
23 O1    o      M     21 18 16      1.267      118.036      -90.312      -0.814354
```

```
LOOP
C6    C4

IMPROPER
C7    O2    C1    O1

DONE
STOP
```

```
g1.in
0      0      2

This is a remark line
molecule.res
G01 INT 0
CORRECT      OMIT DU      BEG
0.0000
1  DUMM DU      M      0 -1 -2      0.000      .0      .0      .00000
2  DUMM DU      M      1  0 -1      1.449      .0      .0      .00000
3  DUMM DU      M      2  1  0      1.523      111.21      .0      .00000
4  C4    c3      M      3  2  1      1.540      111.208      -180.000      -0.337711
5  H3    hc      E      4  3  2      1.117      87.230      15.755      0.059021
6  H4    hc      E      4  3  2      1.117      49.596      132.809      0.059021
7  H5    hc      E      4  3  2      1.117      73.459      -94.070      0.059021
8  C6    c3      M      4  3  2      1.507      158.091      161.436      0.225997
9  H8    hc      E      8  4  3      1.121      109.655      35.465      -0.035338
10 H9    hc      E      8  4  3      1.122      109.712      -81.833      -0.035338
11 C5    c3      M      8  4  3      1.517      111.707      156.864      0.082550
12 H6    hc      E     11  8  4      1.124      109.233      57.949      -0.005284
13 H7    hc      E     11  8  4      1.124      109.053      -58.604      -0.005284
14 C2    c2      M     11  8  4      1.483      111.577      -179.269      -0.236852
15 H2    ha      E     14 11  8      1.102      115.904      49.076      0.127587
16 C1    ce      M     14 11  8      1.334      124.353      -131.783      -0.314259
17 H1    ha      E     16 14 11      1.101      122.077      1.096      0.116844
18 C3    c      M     16 14 11      1.512      123.418      -178.998      0.893864
19 O2    o      E     18 16 14      1.266      117.144      179.832      -0.826920
20 O1    o      M     18 16 14      1.265      119.317      -0.128      -0.826920
```

LOOP

IMPROPER

```
C5  C1  C2  H2
C3  C2  C1  H1
C1  O2  C3  O1
```

DONE

STOP

g2.in

```
0    0    2
```

This is a remark line

molecule.res

G02 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	C3	c2	M	3	2	1	1.540	111.208	-180.000	-0.550839
5	H2	ha	E	4	3	2	1.097	61.346	-84.396	0.179459
6	H3	ha	E	4	3	2	1.101	159.323	3.540	0.179459
7	C5	c2	M	4	3	2	1.336	65.166	117.833	0.300739
8	C10	c3	3	7	4	3	1.485	121.995	23.343	-0.539703
9	H11	hc	E	8	7	4	1.119	110.014	125.114	0.129148
10	H12	hc	E	8	7	4	1.119	110.246	-115.708	0.129148
11	H13	hc	E	8	7	4	1.117	111.560	4.727	0.129148
12	C9	c3	M	7	4	3	1.500	123.071	-157.337	-0.027487
13	C8	c3	3	12	7	4	1.526	111.215	-87.749	-0.117069
14	C7	c3	B	13	12	7	1.515	112.849	71.741	0.158321
15	H6	hc	E	14	13	12	1.124	109.623	-73.311	-0.015031
16	H7	hc	E	14	13	12	1.124	110.178	168.907	-0.015031
17	H8	hc	E	13	12	7	1.121	109.258	-50.661	0.023019
18	H9	hc	E	13	12	7	1.122	108.073	-167.508	0.023019
19	H10	hc	E	12	7	4	1.130	107.081	155.252	0.009293
20	C6	c3	M	12	7	4	1.527	112.863	37.606	0.062274
21	H4	hc	E	20	12	7	1.125	108.139	148.745	-0.006720
22	H5	hc	E	20	12	7	1.124	109.050	32.774	-0.006720
23	C1	c2	M	20	12	7	1.482	114.659	-90.332	-0.249086
24	H1	ha	E	23	20	12	1.103	115.822	170.930	0.118877
25	C2	ce	M	23	20	12	1.339	124.481	-9.784	-0.115043
26	C4	c	M	25	23	20	1.520	121.939	-178.117	0.806963
27	O2	o	E	26	25	23	1.265	118.003	160.667	-0.803070
28	O1	o	M	26	25	23	1.265	118.427	-19.171	-0.803070

LOOP

```
C2    C7
```

IMPROPER

```
C5  H2  C3  H3
C3  C9  C5  C10
C6  C2  C1  H1
C1  C4  C2  C7
C2  O2  C4  O1
```

DONE

STOP

g3.in

```
0    0    2
```

This is a remark line

molecule.res

G03 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	C1	c2	M	3	2	1	1.540	111.208	-180.000	-0.586692
5	H1	ha	E	4	3	2	1.096	33.502	90.284	0.208105
6	H2	ha	E	4	3	2	1.097	109.931	-163.902	0.208105
7	C2	c2	M	4	3	2	1.332	117.835	-17.081	-0.066049

8	H3	ha	E	7	4	3	1.103	120.627	39.003	0.106325
9	C4	c3	M	7	4	3	1.483	124.088	-140.587	-0.097402
10	H4	hc	E	9	7	4	1.125	107.742	102.781	0.061966
11	H5	hc	E	9	7	4	1.130	111.230	-15.135	0.061966
12	C6	c3	M	9	7	4	1.519	112.781	-136.562	0.178867
13	H8	hc	E	12	9	7	1.122	108.728	-152.662	-0.079111
14	H9	hc	E	12	9	7	1.123	109.912	-35.622	-0.079111
15	C5	c3	M	12	9	7	1.512	112.266	87.106	-0.045479
16	H6	hc	E	15	12	9	1.118	109.943	-47.976	-0.030069
17	H7	hc	E	15	12	9	1.120	109.294	-166.857	-0.030069
18	C3	c	M	15	12	9	1.539	111.611	72.819	0.822902
19	O2	o	E	18	15	12	1.265	117.958	105.830	-0.817128
20	O1	o	M	18	15	12	1.266	118.524	-74.776	-0.817128

LOOP

IMPROPER

C2	H1	C1	H2
C1	C4	C2	H3
C5	O2	C3	O1

DONE

STOP

g4.in

0 0 2

This is a remark line

molecule.res

G04 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	C4	c3	M	3	2	1	1.540	111.208	-180.000	-0.475421
5	H2	hc	E	4	3	2	1.118	143.324	-89.571	0.105535
6	H3	hc	E	4	3	2	1.118	75.437	169.075	0.105535
7	H4	hc	E	4	3	2	1.119	104.919	63.696	0.105535
8	C2	c2	M	4	3	2	1.482	41.308	-40.023	0.449210
9	C5	c3	3	8	4	3	1.482	116.013	152.280	-0.475421
10	H5	hc	E	9	8	4	1.120	110.404	-133.023	0.105535
11	H6	hc	E	9	8	4	1.120	110.156	108.109	0.105535
12	H7	hc	E	9	8	4	1.117	111.339	-12.137	0.105535
13	C1	c2	M	8	4	3	1.344	122.012	-27.552	-0.500131
14	H1	ha	E	13	8	4	1.103	120.200	0.223	0.168018
15	C7	c3	M	13	8	4	1.479	123.731	179.776	-0.016142
16	H11	hc	E	15	13	8	1.126	108.801	52.790	0.106301
17	H12	hc	E	15	13	8	1.132	110.482	-63.549	0.106301
18	C9	c3	M	15	13	8	1.514	113.916	174.422	-0.474484
19	H15	hc	E	18	15	13	1.125	107.909	-172.115	0.122028
20	H16	hc	E	18	15	13	1.122	109.689	-54.548	0.122028
21	C10	c3	M	18	15	13	1.522	113.933	68.102	0.468924
22	C6	c3	3	21	18	15	1.517	109.440	179.616	-0.650813
23	H8	hc	E	22	21	18	1.121	109.018	-72.480	0.138642
24	H9	hc	E	22	21	18	1.116	110.277	168.446	0.138642
25	H10	hc	E	22	21	18	1.116	110.993	48.228	0.138642
26	H17	hc	E	21	18	15	1.128	108.236	-62.327	-0.063160
27	C8	c3	M	21	18	15	1.520	112.356	57.210	-0.220767
28	H13	hc	E	27	21	18	1.119	109.447	-76.933	0.005765
29	H14	hc	E	27	21	18	1.120	109.188	165.026	0.005765
30	C3	c	M	27	21	18	1.539	112.977	44.318	0.935337
31	O2	o	E	30	27	21	1.265	118.762	73.047	-0.831236
32	O1	o	M	30	27	21	1.267	117.655	-107.365	-0.831236

LOOP

IMPROPER

C1	C4	C2	C5
C2	C7	C1	H1
C8	O2	C3	O1

DONE

STOP

```

g5.in
  0      0      2

This is a remark line
molecule.res
G05 INT 0
CORRECT      OMIT DU      BEG
0.0000
  1  DUMM  DU      M      0 -1 -2      0.000      .0      .0      .00000
  2  DUMM  DU      M      1  0 -1      1.449      .0      .0      .00000
  3  DUMM  DU      M      2  1  0      1.523     111.21      .0      .00000
  4  C1     c2      M      3  2  1      1.540     111.208    -180.000    -0.603726
  5  H1     ha      E      4  3  2      1.096      26.842     141.810     0.189486
  6  H2     ha      E      4  3  2      1.097      90.418     -14.898     0.189486
  7  C2     c2      M      4  3  2      1.332     145.417    -178.409    -0.007134
  8  H3     ha      E      7  4  3      1.104     120.458     -20.256     0.115498
  9  C5     c3      M      7  4  3      1.482     124.150     159.417    -0.199489
 10  H7     hc      E      9  7  4      1.123     110.106      30.508     0.094075
 11  H8     hc      E      9  7  4      1.125     109.271     -86.275     0.094075
 12  C6     c3      M      9  7  4      1.519     113.629     152.517     0.137407
 13  C4     c3      3     12  9  7      1.510     112.185      70.997    -0.147345
 14  H4     hc      E     13 12  9      1.117     109.887      63.053     0.013271
 15  H5     hc      E     13 12  9      1.118     111.584     -57.561     0.013271
 16  H6     hc      E     13 12  9      1.117     109.774    -177.777     0.013271
 17  H9     hc      E     12  9  7      1.122     109.272     -50.543    -0.050387
 18  C3     c      M     12  9  7      1.554     108.991    -168.406     0.795781
 19  O2     o      E     18 12  9      1.263     117.422     129.380    -0.823770
 20  O1     o      M     18 12  9      1.263     118.341     -50.719    -0.823770

```

LOOP

```

IMPROPER
  C2  H1  C1  H2
  C1  C5  C2  H3
  C6  O2  C3  O1

```

DONE
STOP

```

g6.in
  0      0      2

```

```

This is a remark line
molecule.res
G06 INT 0
CORRECT      OMIT DU      BEG
0.0000
  1  DUMM  DU      M      0 -1 -2      0.000      .0      .0      .00000
  2  DUMM  DU      M      1  0 -1      1.449      .0      .0      .00000
  3  DUMM  DU      M      2  1  0      1.523     111.21      .0      .00000
  4  C2     c3      M      3  2  1      1.540     111.208    -180.000    -0.542569
  5  H1     hc      E      4  3  2      1.118      52.737      71.321     0.095267
  6  H2     hc      E      4  3  2      1.117      55.716    -103.539     0.095267
  7  H3     hc      E      4  3  2      1.116     126.383     -14.964     0.095267
  8  C6     c3      M      4  3  2      1.514     123.432     163.301     0.563408
  9  C3     c3      3      8  4  3      1.514     110.065      1.918    -0.542569
 10  H4     hc      E      9  8  4      1.117     110.758     -64.581     0.095267
 11  H5     hc      E      9  8  4      1.117     110.196     175.419     0.095267
 12  H6     hc      E      9  8  4      1.116     110.501      55.583     0.095267
 13  H11    hc      E      8  4  3      1.134     108.666     121.243    -0.024633
 14  C5     c3      M      8  4  3      1.523     111.312    -121.183     0.026903
 15  H9     hc      E     14  8  4      1.123     109.300      41.951    -0.037058
 16  H10    hc      E     14  8  4      1.122     109.123     158.863    -0.037058
 17  C4     c3      M     14  8  4      1.511     112.519     -80.523    -0.160306
 18  H7     hc      E     17 14  8      1.119     110.222      49.917    -0.002250
 19  H8     hc      E     17 14  8      1.120     109.172     168.679    -0.002250
 20  C1     c      M     17 14  8      1.539     111.778     -71.085     0.816909
 21  O2     o      E     20 17 14      1.265     118.023    -101.558    -0.815063
 22  O1     o      M     20 17 14      1.267     118.382      79.028    -0.815063

```

LOOP

```

IMPROPER
  C4  O2  C1  O1

```

DONE
STOP

g7.in
0 0 2

This is a remark line
molecule.res

G07 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	C1	c2	M	3	2	1	1.540	111.208	-180.000	-0.480641
5	H1	ha	E	4	3	2	1.096	36.058	-106.665	0.186812
6	H2	ha	E	4	3	2	1.103	115.325	152.664	0.186812
7	C2	c2	M	4	3	2	1.333	113.015	7.496	-0.067282
8	H3	ha	E	7	4	3	1.102	121.189	-39.961	0.087590
9	C6	c3	M	7	4	3	1.484	123.299	140.057	-0.428011
10	H10	hc	E	9	7	4	1.125	109.403	-37.710	0.085055
11	H11	hc	E	9	7	4	1.124	108.752	-155.485	0.085055
12	C7	c3	M	9	7	4	1.527	114.127	82.438	0.626034
13	C4	c3	3	12	9	7	1.521	108.663	166.391	0.002087
14	H4	hc	E	13	12	9	1.117	111.087	-63.729	-0.066202
15	H5	hc	E	13	12	9	1.115	110.020	56.786	-0.066202
16	H6	hc	E	13	12	9	1.117	109.442	176.105	-0.066202
17	C5	c3	3	12	9	7	1.515	111.065	45.842	0.002087
18	H7	hc	E	17	12	9	1.118	110.900	62.048	-0.066202
19	H8	hc	E	17	12	9	1.116	110.250	-58.409	-0.066202
20	H9	hc	E	17	12	9	1.118	109.348	-177.355	-0.066202
21	C3	c	M	12	9	7	1.565	110.998	-76.539	0.723973
22	O2	o	E	21	12	9	1.264	118.565	-22.791	-0.806180
23	O1	o	M	21	12	9	1.263	117.624	158.853	-0.806180

LOOP

IMPROPER

C2	H1	C1	H2
C1	C6	C2	H3
C7	O2	C3	O1

DONE
STOP

g8.in
0 0 2

This is a remark line
molecule.res

G08 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.522	111.1	.0	.00000
4	C7	c3	M	3	2	1	1.540	111.208	180.000	0.04265
5	H71	hc	E	4	3	2	1.122	81.392	-93.306	-0.01316
6	H72	hc	E	4	3	2	1.122	65.058	152.730	-0.01316
7	C6	c3	M	4	3	2	1.515	168.542	90.000	-0.18845
8	H62	hc	E	7	4	3	1.121	109.650	2.551	0.02508
9	H61	hc	E	7	4	3	1.122	109.869	120.498	0.02508
10	C5	c3	M	7	4	3	1.522	111.189	-118.342	0.43052
11	C8	c3	3	10	7	4	1.512	110.777	179.271	-0.72383
12	H83	hc	E	11	10	7	1.117	110.594	-61.246	0.15067
13	H81	hc	E	11	10	7	1.117	110.481	178.740	0.15067
14	H82	hc	E	11	10	7	1.117	110.460	58.638	0.15067
15	H5	hc	E	10	7	4	1.127	108.166	-61.725	-0.02653
16	C4	c3	M	10	7	4	1.521	110.132	56.330	-0.18845
17	H41	hc	E	16	10	7	1.121	109.259	-177.858	0.02508
18	H42	hc	E	16	10	7	1.121	109.226	64.877	0.02508
19	C3	c3	M	16	10	7	1.515	111.225	-56.350	0.04265
20	H32	hc	E	19	16	10	1.121	109.290	176.998	-0.01316
21	H31	hc	E	19	16	10	1.122	110.054	-65.084	-0.01316
22	C2	c3	M	19	16	10	1.517	112.071	55.773	-0.01695
23	H2	hc	E	22	19	16	1.123	109.228	66.529	-0.02201

24	C1	c	M	22	19	16	1.550	109.607	-174.973	0.76956
25	O12	o	E	24	22	19	1.264	117.499	-119.255	-0.80942
26	O11	o	M	24	22	19	1.264	118.446	60.731	-0.80942

LOOP
C2 C7

IMPROPER
C2 O12 C1 O11

DONE
STOP

a5.in
0 0 2

This is a remark line
molecule.res

A05 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	O1	o	M	3	2	1	1.540	111.208	-180.000	-0.835855
5	C1	c	M	4	3	2	1.266	85.332	9.537	0.879052
6	O2	o	E	5	4	3	1.264	123.771	161.639	-0.835855
7	C2	c3	M	5	4	3	1.539	118.485	-19.484	-0.310310
8	H1	hc	E	7	5	4	1.118	109.343	169.841	0.027152
9	H2	hc	E	7	5	4	1.120	107.770	-73.105	0.027152
10	C3	c3	M	7	5	4	1.509	111.363	47.584	0.169956
11	H3	hc	E	10	7	5	1.122	109.458	65.864	-0.029916
12	H4	hc	E	10	7	5	1.124	108.669	-50.737	-0.029916
13	C4	c3	M	10	7	5	1.514	111.982	-172.563	0.237876
14	H5	hc	E	13	10	7	1.122	109.468	-57.479	-0.061104
15	H6	hc	E	13	10	7	1.122	109.365	59.448	-0.061104
16	C5	c3	M	13	10	7	1.507	111.836	-179.087	-0.360822
17	H7	hc	E	16	13	10	1.117	110.564	60.349	0.061231
18	H8	hc	E	16	13	10	1.117	110.518	-59.349	0.061231
19	H9	hc	E	16	13	10	1.117	110.746	-179.499	0.061231

LOOP

IMPROPER
C2 O1 C1 O2

DONE
STOP

a6.in
0 0 2

This is a remark line
molecule.res

A06 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	O1	o	M	3	2	1	1.540	111.208	-180.000	-0.829277
5	C1	c	M	4	3	2	1.266	84.287	10.337	0.841929
6	O2	o	E	5	4	3	1.265	123.658	163.300	-0.829277
7	C2	c3	M	5	4	3	1.539	118.560	-17.751	-0.169594
8	H1	hc	E	7	5	4	1.118	109.330	169.159	-0.002999
9	H2	hc	E	7	5	4	1.119	107.788	-73.813	-0.002999
10	C3	c3	M	7	5	4	1.509	111.347	46.906	0.079902
11	H3	hc	E	10	7	5	1.121	109.460	65.971	-0.021563
12	H4	hc	E	10	7	5	1.123	108.610	-50.653	-0.021563
13	C4	c3	M	10	7	5	1.514	111.900	-172.452	0.030050
14	H5	hc	E	13	10	7	1.122	109.656	-57.856	-0.018411
15	H6	hc	E	13	10	7	1.122	109.566	59.414	-0.018411
16	C5	c3	M	13	10	7	1.514	111.551	-179.240	0.195696
17	H7	hc	E	16	13	10	1.123	109.372	58.793	-0.045398
18	H8	hc	E	16	13	10	1.123	109.280	-58.034	-0.045398

19	C6	c3	M	16	13	10	1.507	111.877	-179.623	-0.280716
20	H9	hc	E	19	16	13	1.117	110.644	-59.741	0.046010
21	H10	hc	E	19	16	13	1.116	110.663	-179.931	0.046010
22	H11	hc	E	19	16	13	1.117	110.578	59.984	0.046010

LOOP

IMPROPER

C2 O1 C1 O2

DONE

STOP

a7.in

0 0 2

This is a remark line

molecule.res

A07 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	O1	o	M	3	2	1	1.540	111.208	-180.000	-0.826359
5	C1	c	M	4	3	2	1.265	86.873	15.335	0.834339
6	O2	o	E	5	4	3	1.265	123.724	160.957	-0.826359
7	C2	c3	M	5	4	3	1.539	118.584	-20.254	-0.220676
8	H1	hc	E	7	5	4	1.118	109.430	169.115	0.009323
9	H2	hc	E	7	5	4	1.120	107.800	-73.765	0.009323
10	C3	c3	M	7	5	4	1.509	111.309	46.842	0.222015
11	H3	hc	E	10	7	5	1.122	109.443	66.055	-0.047730
12	H4	hc	E	10	7	5	1.123	108.697	-50.567	-0.047730
13	C4	c3	M	10	7	5	1.514	111.954	-172.426	-0.064639
14	H5	hc	E	13	10	7	1.123	109.628	-57.690	-0.010939
15	H6	hc	E	13	10	7	1.122	109.502	59.471	-0.010939
16	C5	c3	M	13	10	7	1.513	111.566	-179.158	0.012635
17	H7	hc	E	16	13	10	1.122	109.513	58.891	-0.012572
18	H8	hc	E	16	13	10	1.122	109.472	-58.183	-0.012572
19	C6	c3	M	16	13	10	1.514	111.662	-179.609	0.270816
20	H9	hc	E	19	16	13	1.122	109.368	-58.385	-0.063250
21	H10	hc	E	19	16	13	1.121	109.376	58.493	-0.063250
22	C7	c3	M	19	16	13	1.507	111.762	-179.907	-0.321321
23	H11	hc	E	22	19	16	1.117	110.623	59.958	0.056629
24	H12	hc	E	22	19	16	1.116	110.558	-59.818	0.056629
25	H13	hc	E	22	19	16	1.116	110.586	-179.927	0.056629

LOOP

IMPROPER

C2 O1 C1 O2

DONE

STOP

a8.in

0 0 2

This is a remark line

molecule.res

A08 INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.523	111.21	.0	.00000
4	O1	o	M	3	2	1	1.540	111.208	-180.000	-0.833457
5	C1	c	M	4	3	2	1.265	104.840	3.892	0.863410
6	O2	o	E	5	4	3	1.266	123.703	16.901	-0.833457
7	C2	c3	M	5	4	3	1.539	118.588	-162.028	-0.212789
8	H1	hc	E	7	5	4	1.119	107.778	73.889	0.007998
9	H2	hc	E	7	5	4	1.118	109.414	-169.003	0.007998
10	C3	c3	M	7	5	4	1.509	111.323	-46.738	0.036860
11	H3	hc	E	10	7	5	1.123	108.616	50.593	0.002689
12	H4	hc	E	10	7	5	1.121	109.419	-65.978	0.002689

13	C4	c3	M	10	7	5	1.514	111.921	172.444	0.077496
14	H5	hc	E	13	10	7	1.122	109.485	-59.527	-0.002666
15	H6	hc	E	13	10	7	1.122	109.571	57.580	-0.002666
16	C5	c3	M	13	10	7	1.514	111.455	179.193	-0.158893
17	H7	hc	E	16	13	10	1.123	108.842	57.445	0.030075
18	H8	hc	E	16	13	10	1.122	109.418	-59.184	0.030075
19	C6	c3	M	16	13	10	1.514	112.849	178.460	-0.059096
20	H9	hc	E	19	16	13	1.123	109.255	-162.702	0.021808
21	H10	hc	E	19	16	13	1.122	109.568	-45.680	0.021808
22	C7	c3	M	19	16	13	1.514	112.472	76.220	0.144144
23	H11	hc	E	22	19	16	1.123	109.416	58.171	-0.012146
24	H12	hc	E	22	19	16	1.122	109.377	-58.823	-0.012146
25	C8	c3	M	22	19	16	1.507	111.636	179.644	-0.296338
26	H13	hc	E	25	22	19	1.116	110.483	-179.943	0.058869
27	H14	hc	E	25	22	19	1.117	110.604	60.059	0.058869
28	H15	hc	E	25	22	19	1.117	110.725	-59.826	0.058869

LOOP

IMPROPER

C2 O1 C1 O2

DONE

STOP