Supporting Information

Dimers of Glycoluril Based Molecular Clips

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Table of contents

NMR spectra S2
NMR titration experiments S11
Determination of activation Gibbs energies of the conformer interconversions S15
Computational details S18

NMR spectra

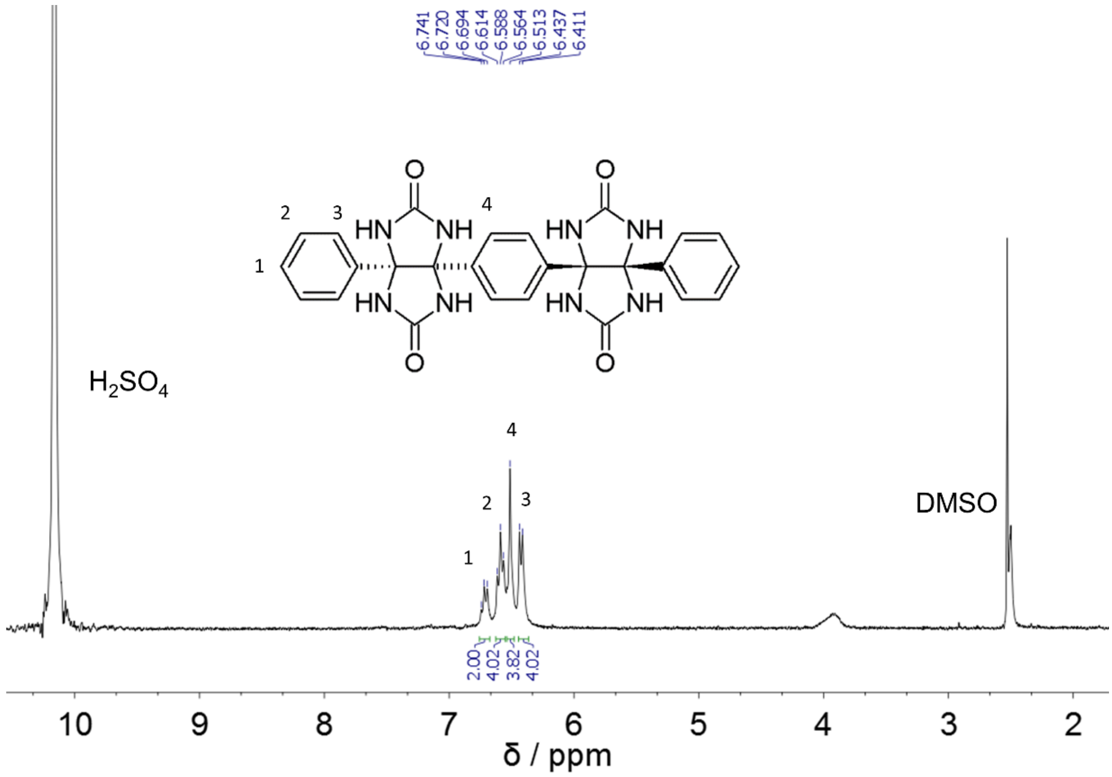

Figure S1. ^{1}H NMR spectrum (300 MHz, 96% D_2SO_4, DMSO–d_6 as external reference) of **4a**

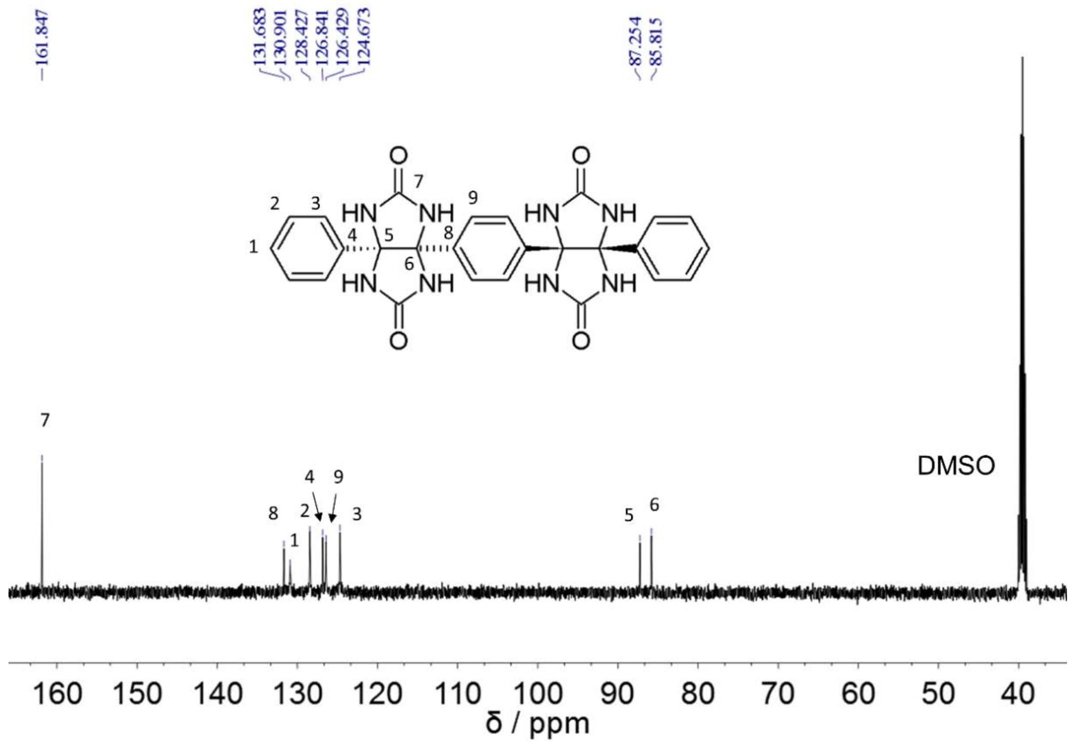

Figure S2. ^{13}C NMR spectrum (125 MHz, 96% D_2SO_4, DMSO–d_6 as external reference) of **4a**

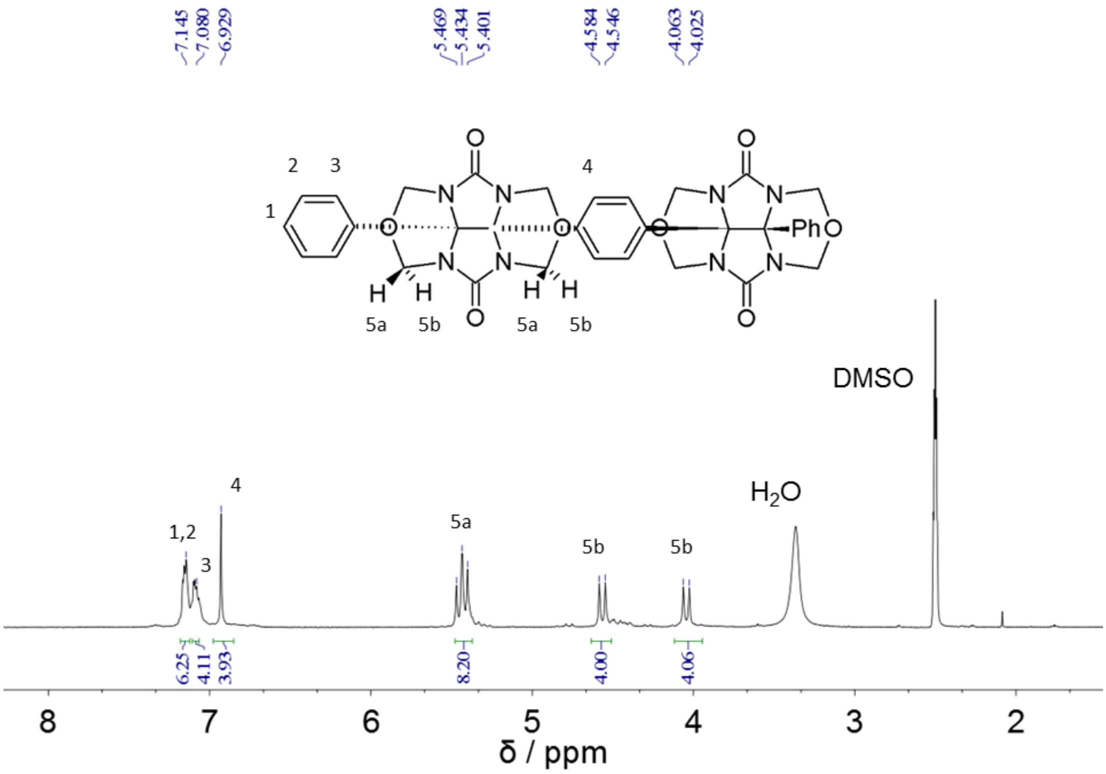

Figure S3. [1]H NMR spectrum (300 MHz, DMSO-d_6) of **5a**

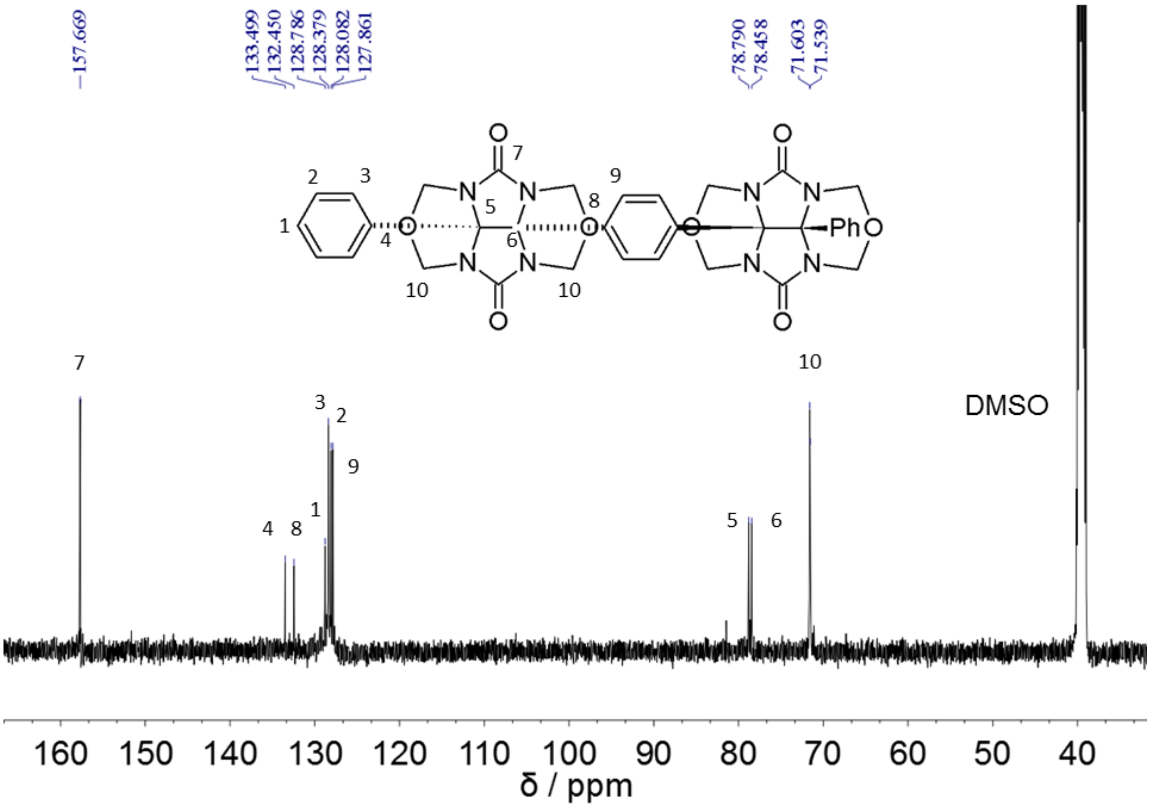

Figure S4. [13]C NMR spectrum (125 MHz, DMSO-d_6) of **5a**

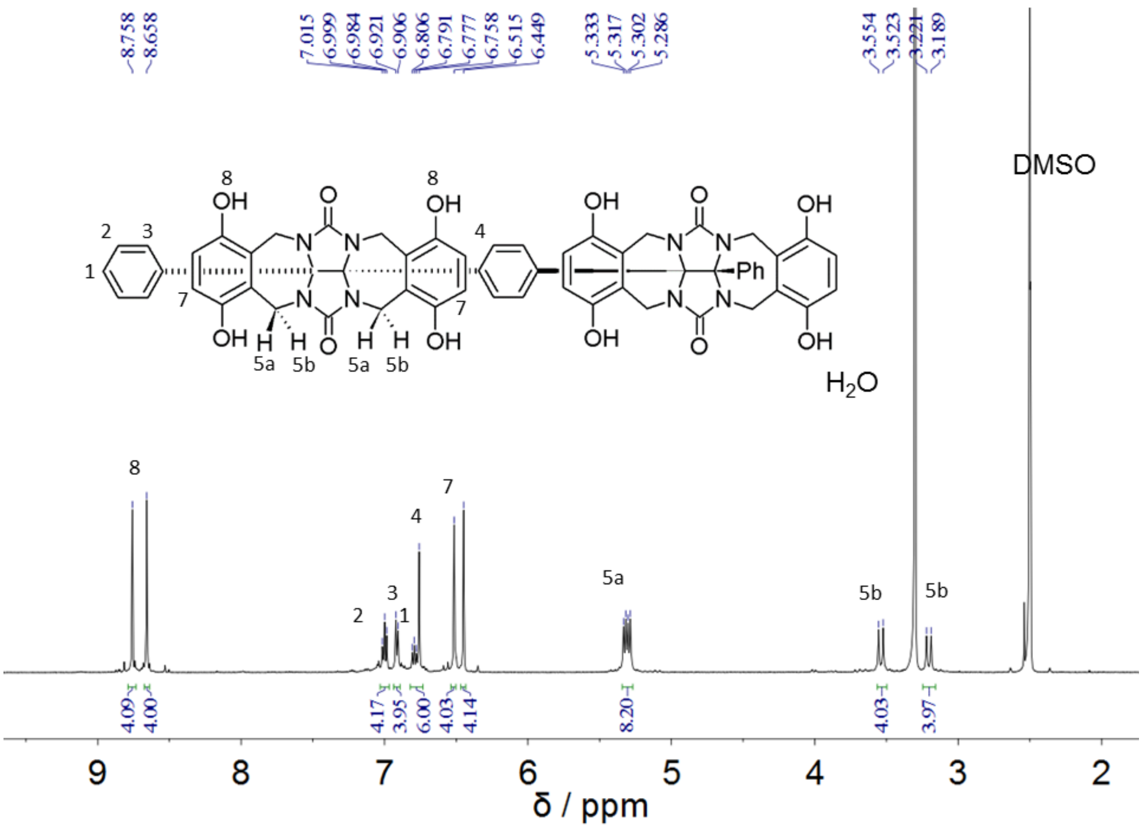

Figure S5. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of **6**

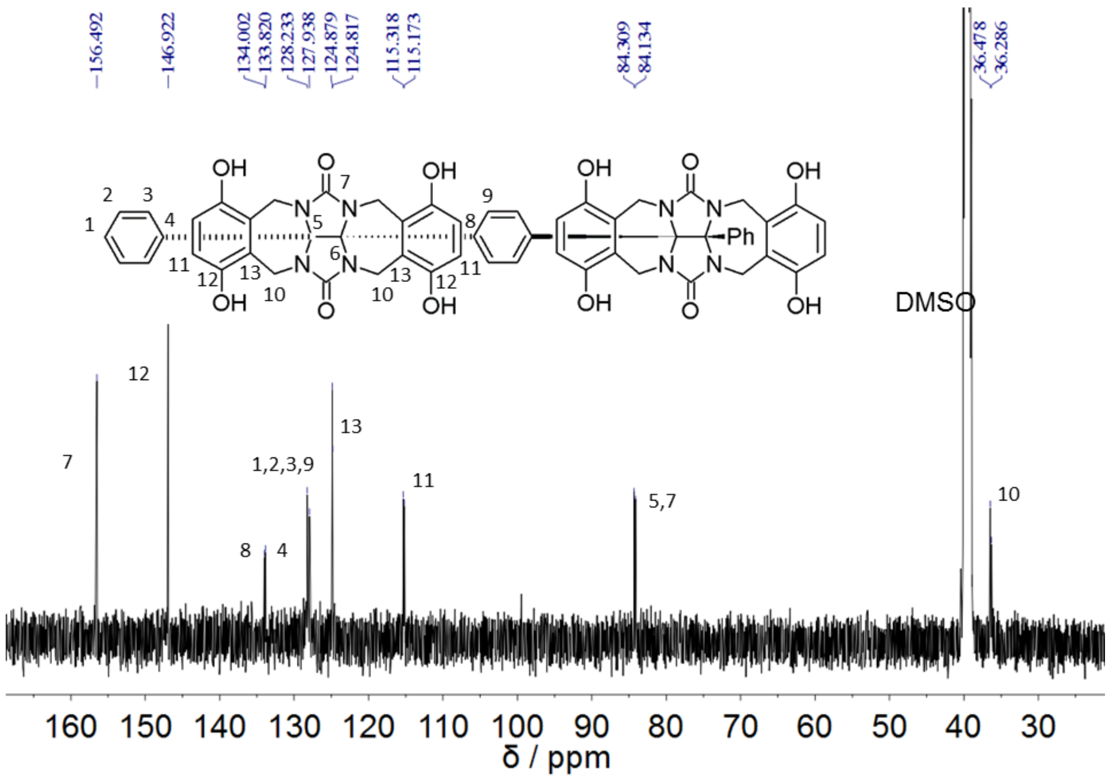

Figure S6. ^{13}C NMR spectrum (125 MHz, DMSO-d_6) of **6**

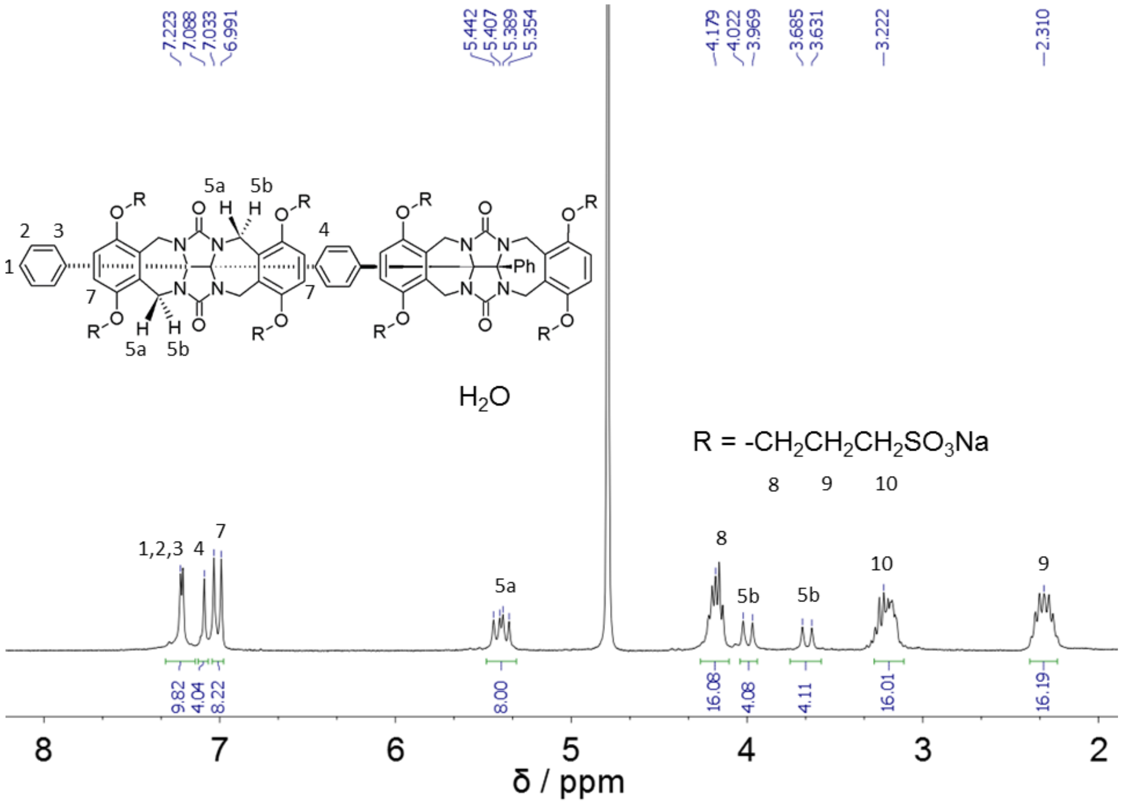

Figure S7. ^{1}H NMR spectrum (300 MHz, D_2O) of **7a**

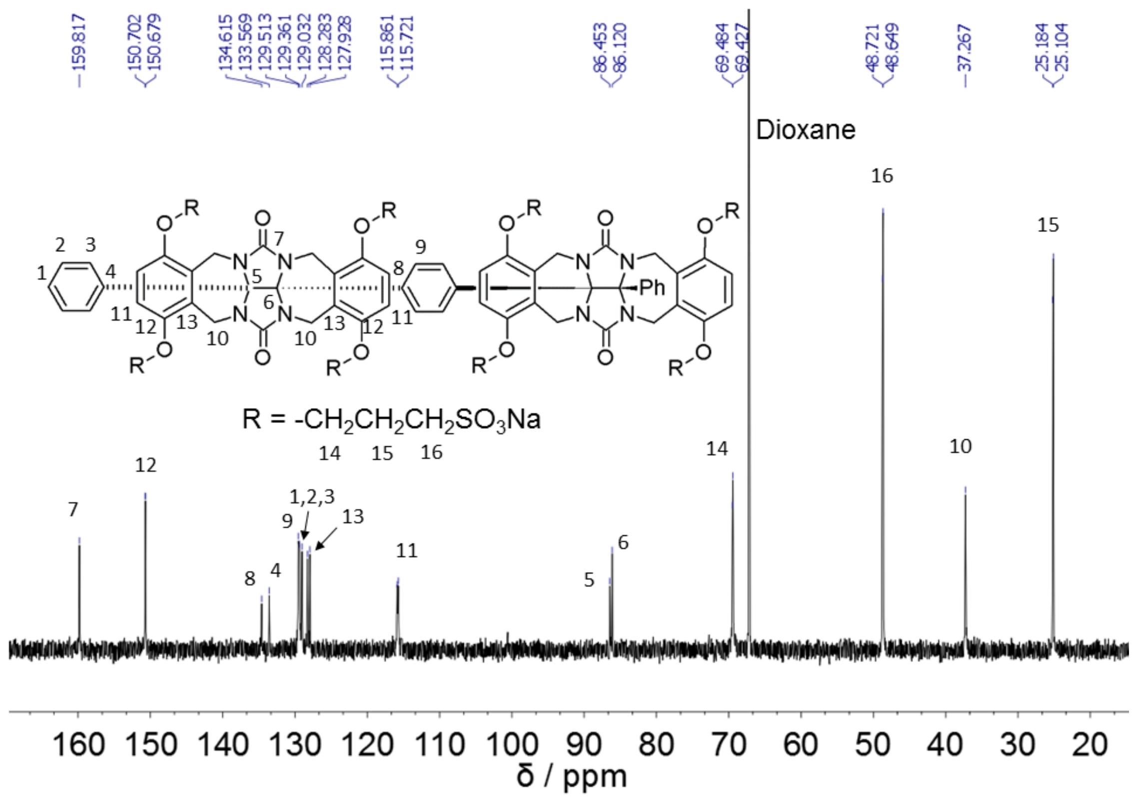

Figure S8. ^{13}C NMR spectrum (125 MHz, D_2O, 1,4-dioxane as internal reference) of **7a**

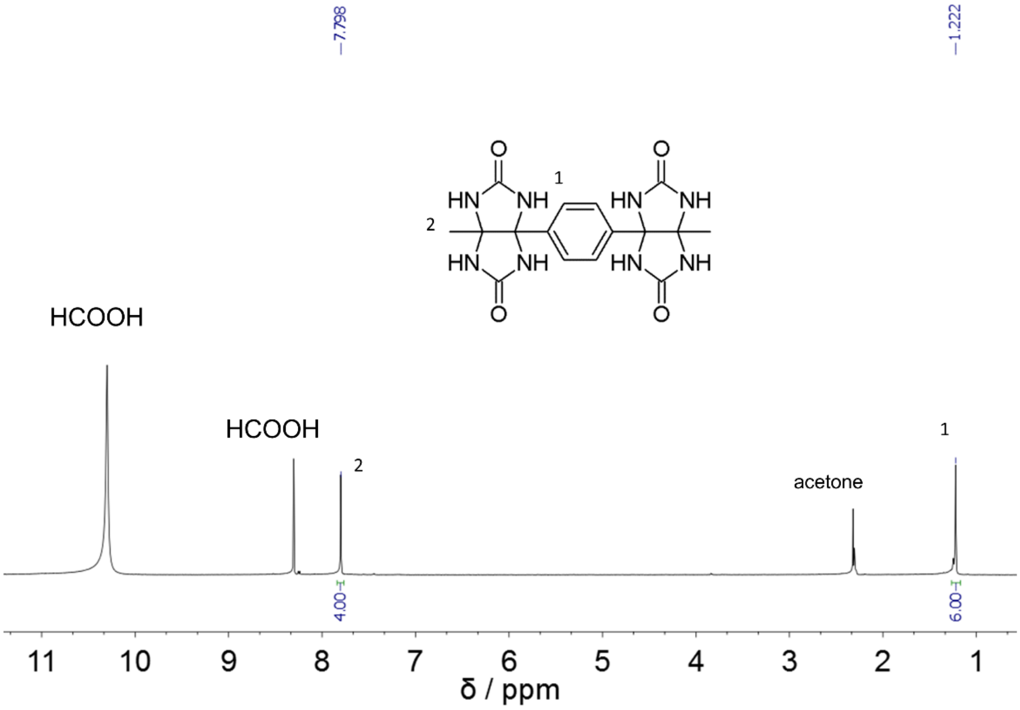

Figure S9. ^{1}H NMR spectrum (500 MHz, 95 % DCOOD) of **4b**

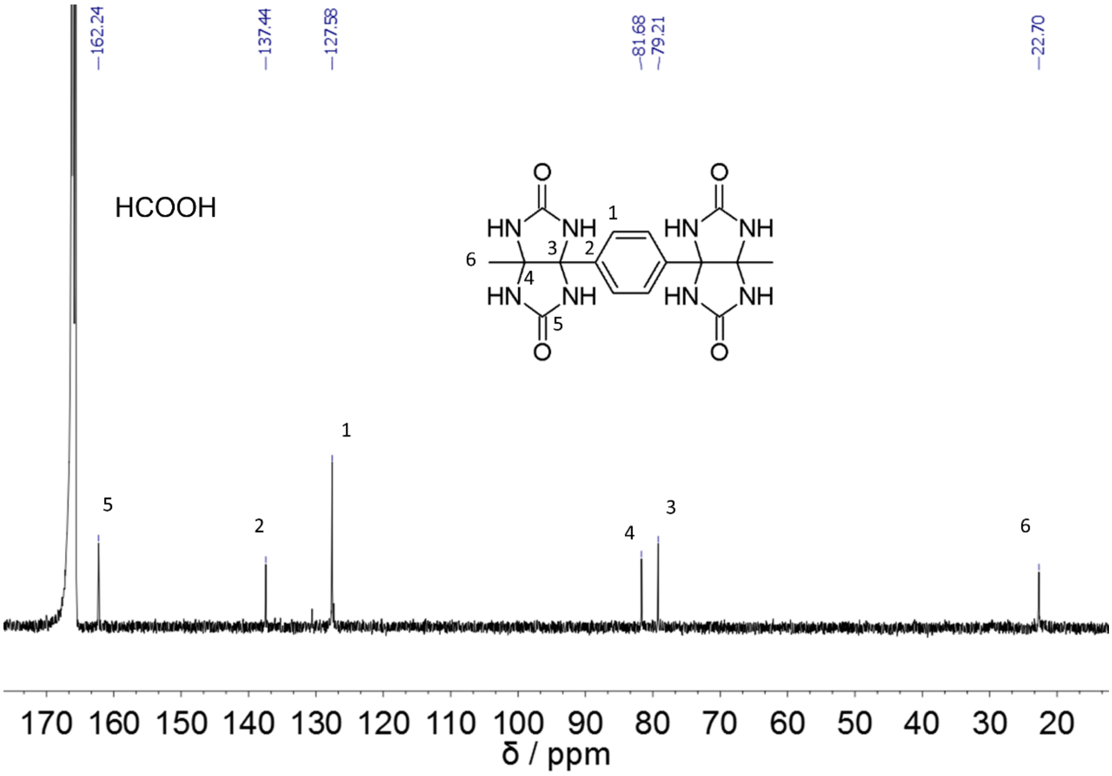

Figure S10. ^{13}C NMR (125 MHz, 95% DCOOD) spectrum of **4b**

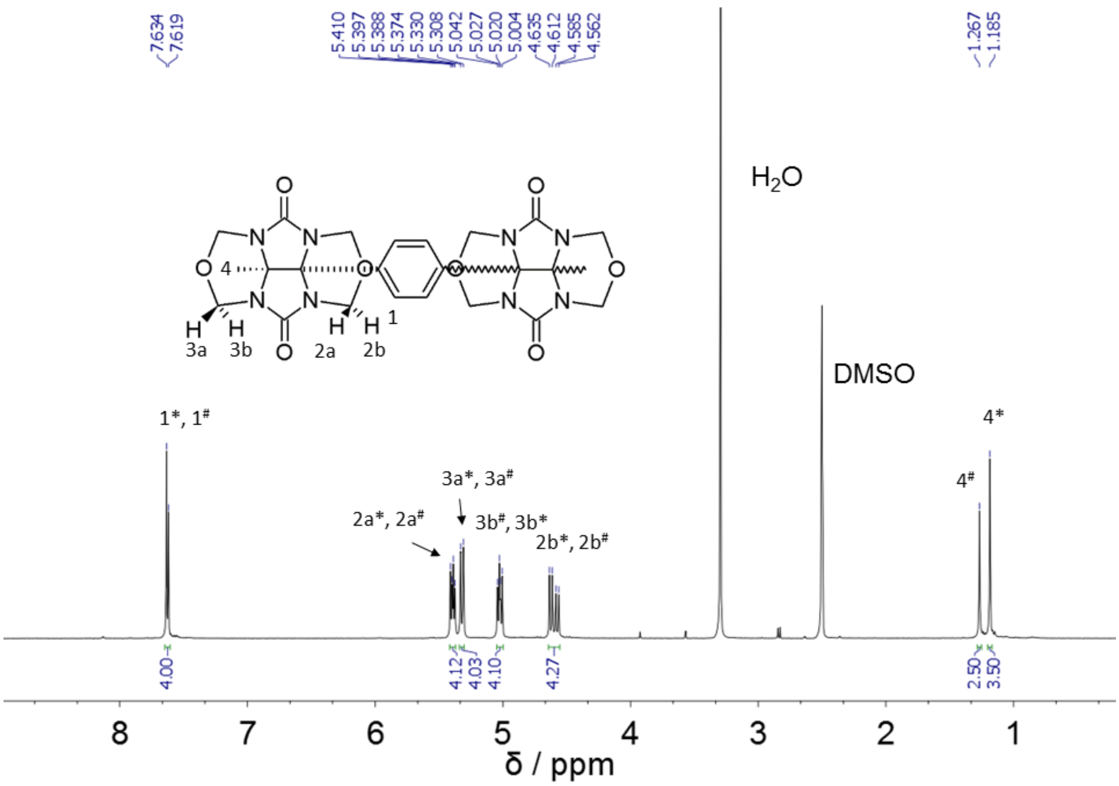

Figure S11. [1]H NMR spectrum (500 MHz, DMSO-d_6) of **5b**. Symbols * and # mark signals of different conformers.

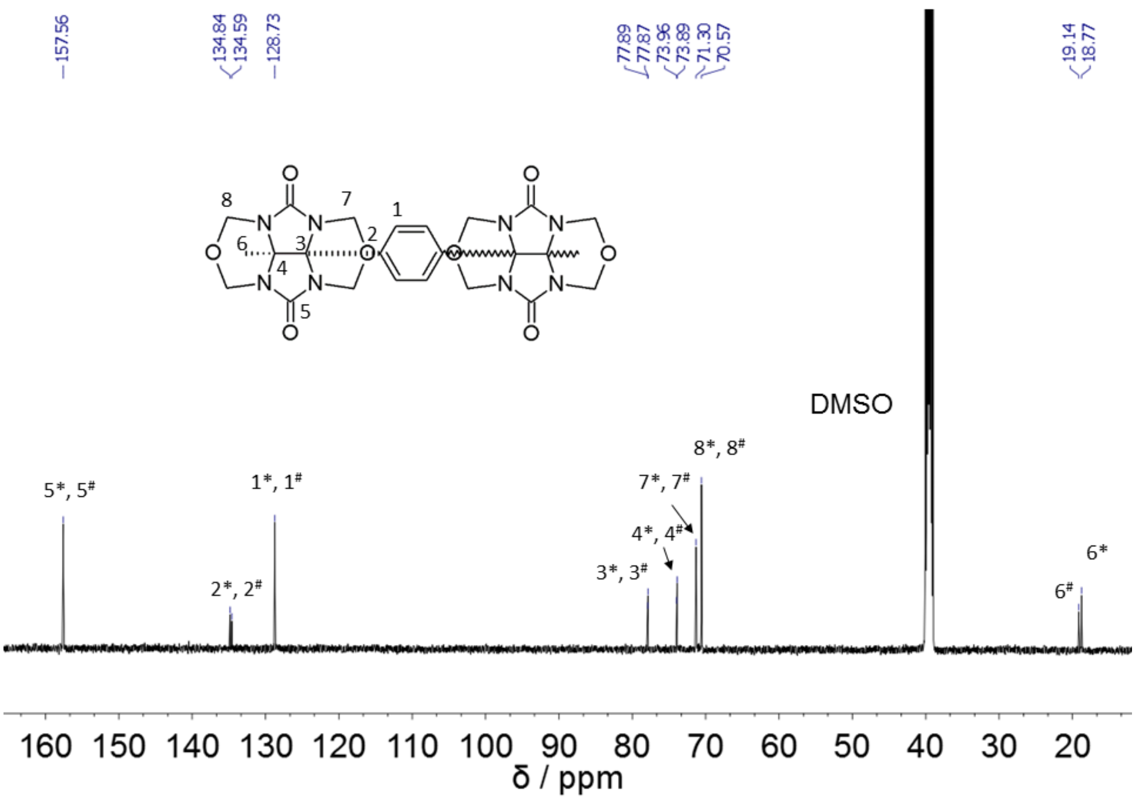

Figure s12. [13]C NMR spectrum (125 MHz, DMSO-d_6) of **5b**. Symbols * and # mark signals of different conformers.

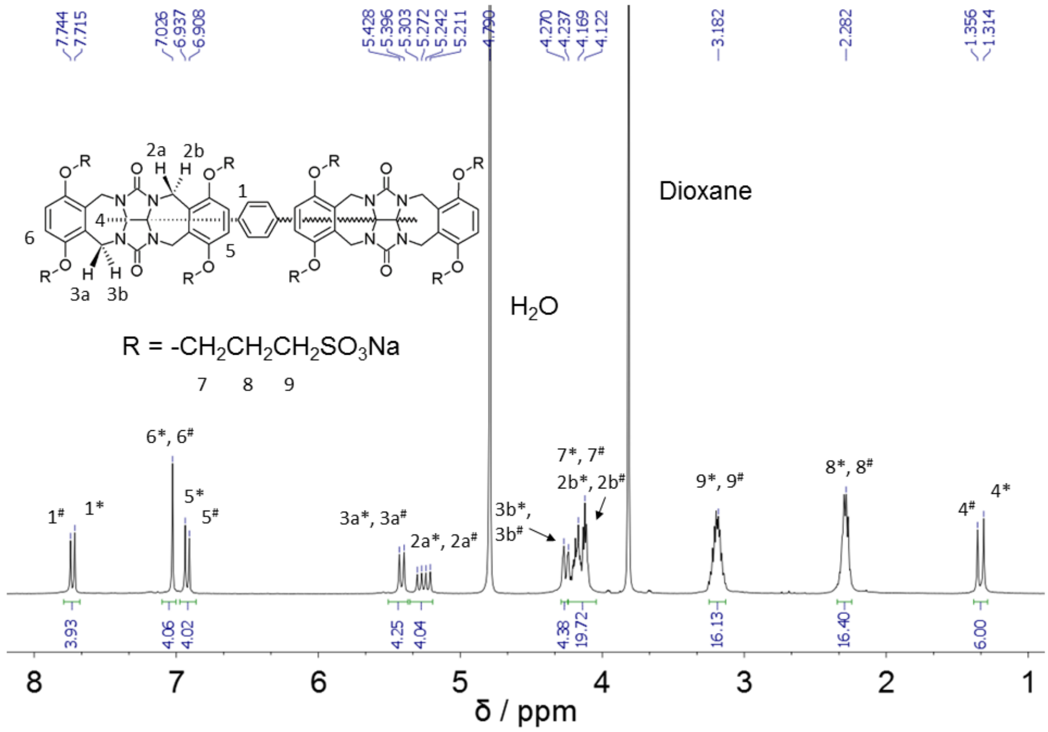

Figure S13. ^{1}H NMR spectrum (500 MHz, D_2O) of **7b**. Symbols * and # mark signals of different conformers.

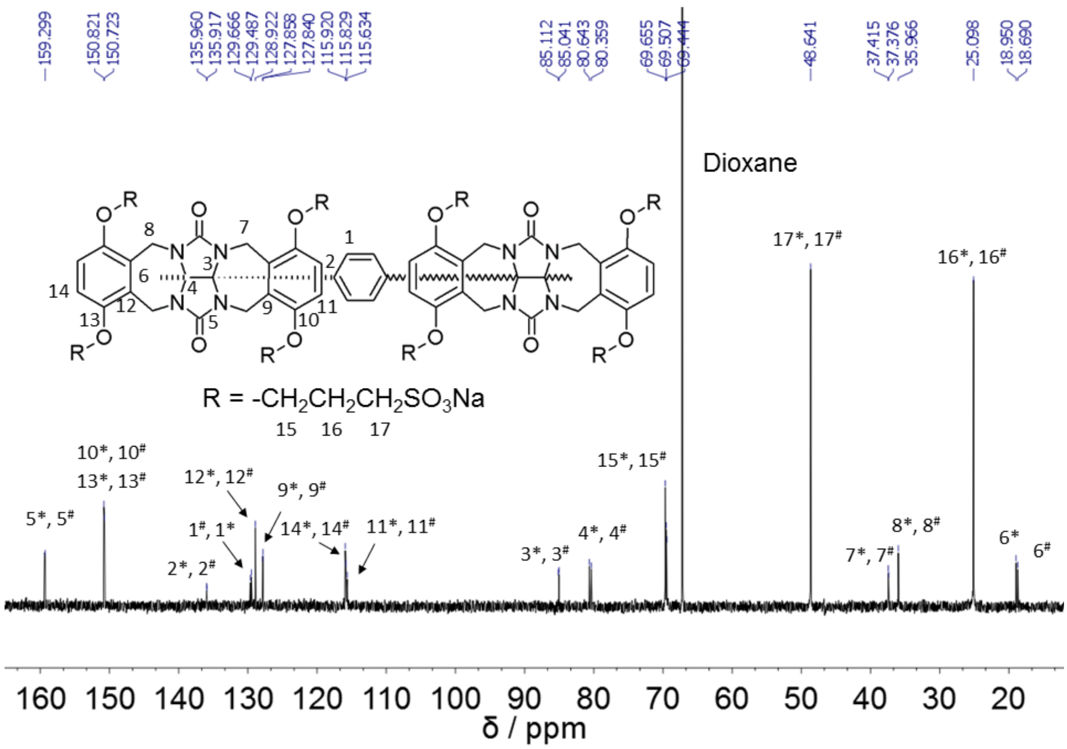

Figure S14. ^{13}C NMR spectrum (125 MHz, D_2O, 1,4-dioxane as internal reference) of **7b**. Symbols * and # mark signals of different conformers.

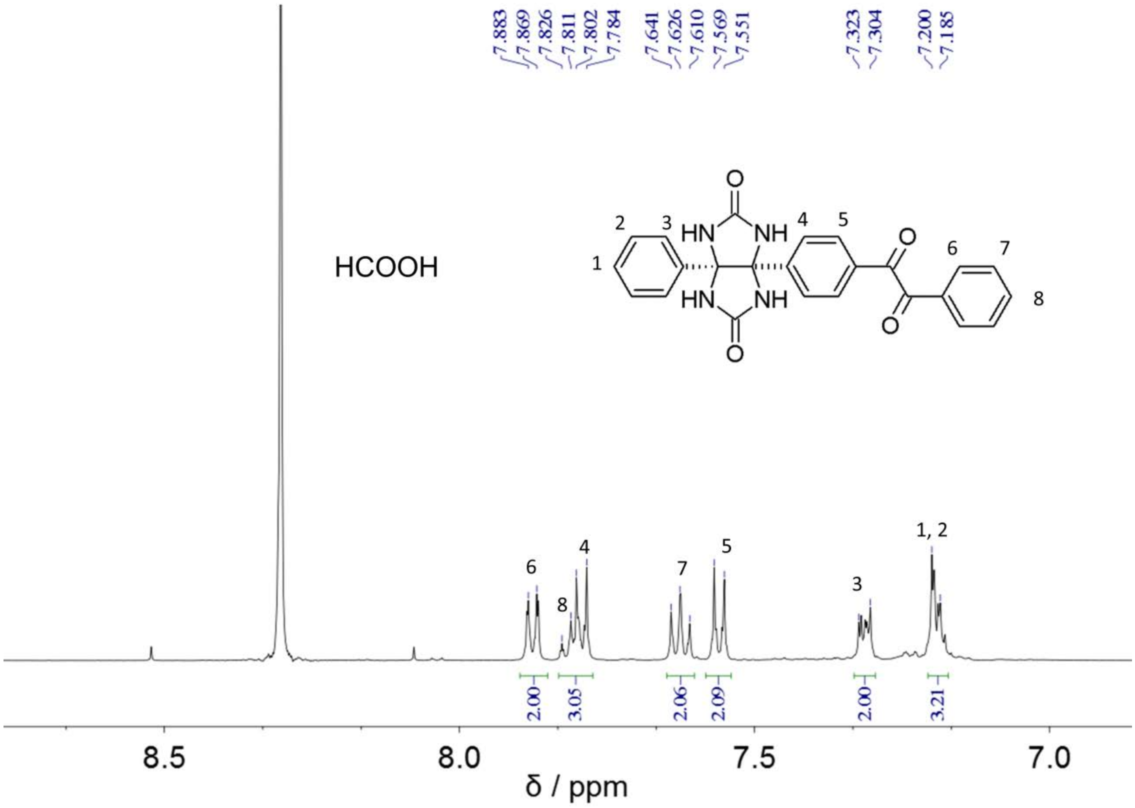

Figure S15. [1]H NMR spectrum (500 MHz, 95% DCOOD) of **9**

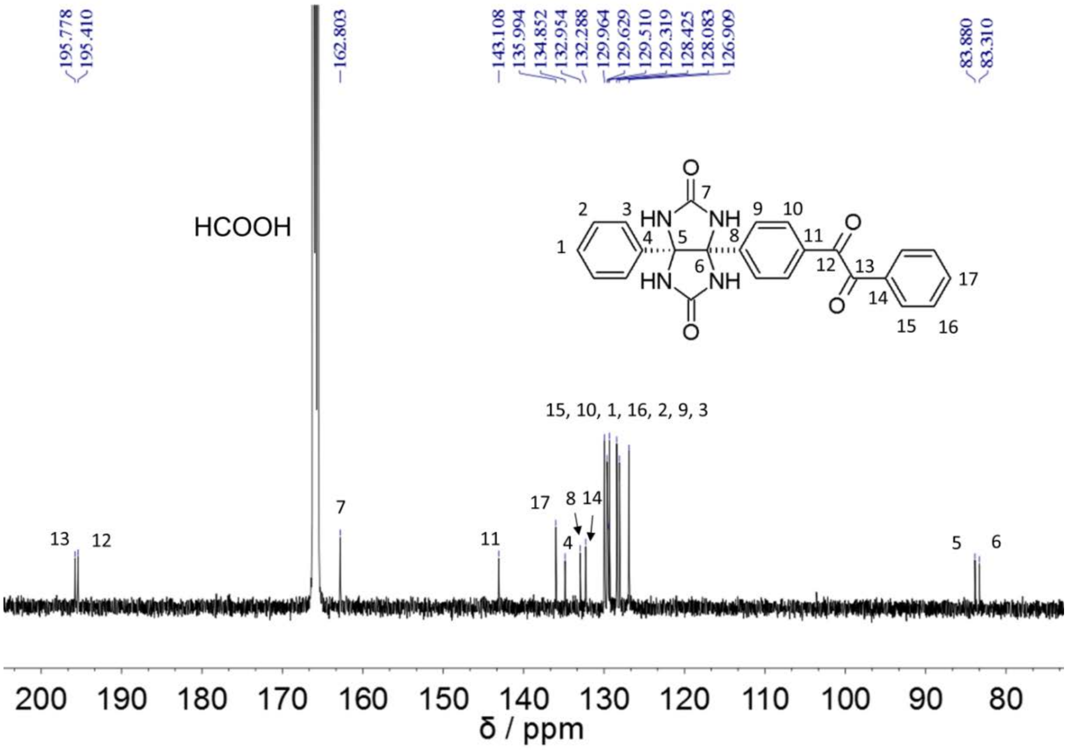

Figure S16. [13]C NMR (125 MHz, 95% DCOOD) spectrum of **9**

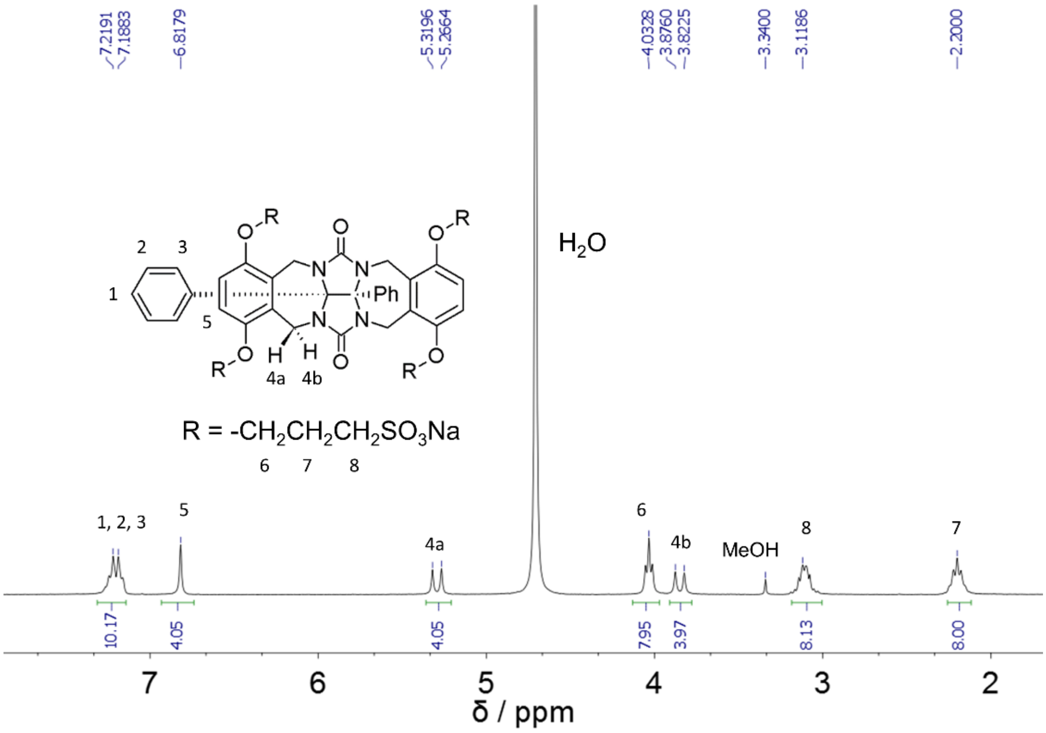

Figure S17. [1]H NMR spectrum (500 MHz, D_2O) of **12**

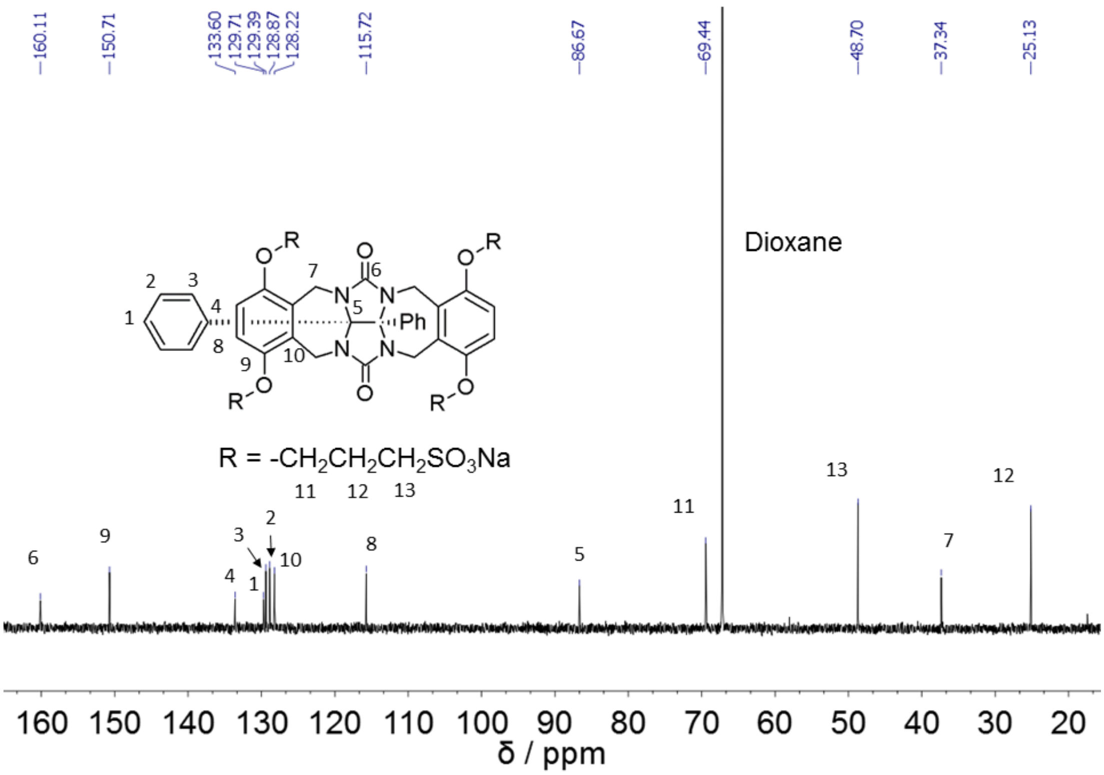

Figure S18. [13]C NMR spectrum (125 MHz, D_2O, 1,4-dioxane as internal reference) of **12**

NMR titration experiments

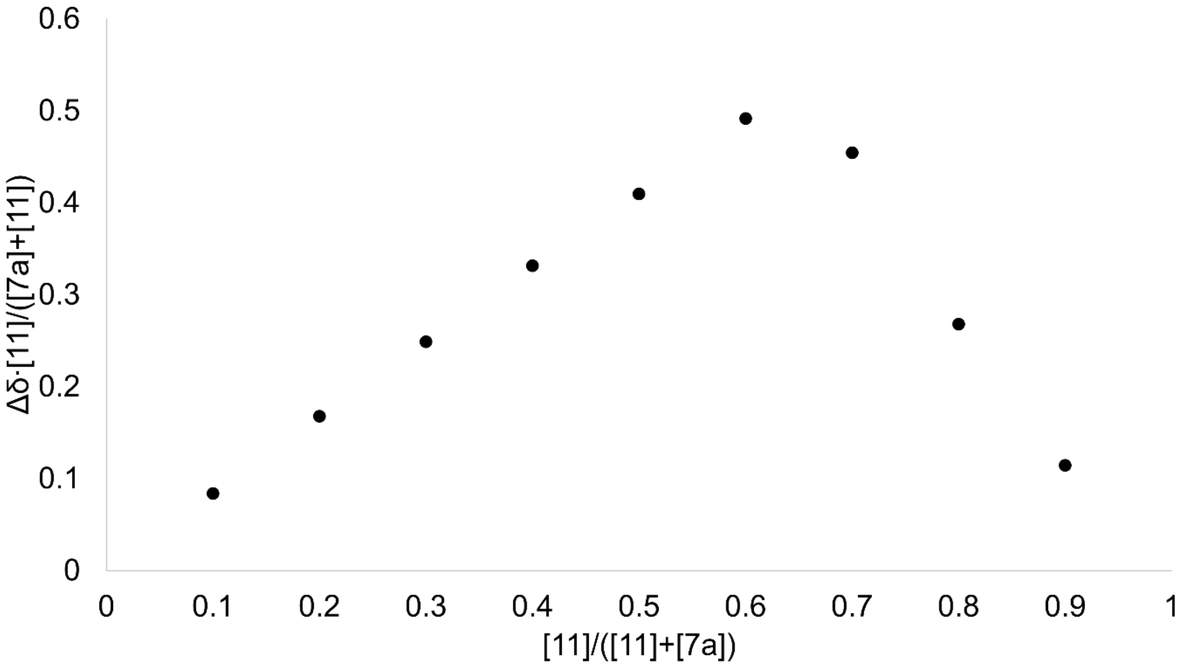

Figure S19. Job's plot of complexation of **11** by clip **7a**

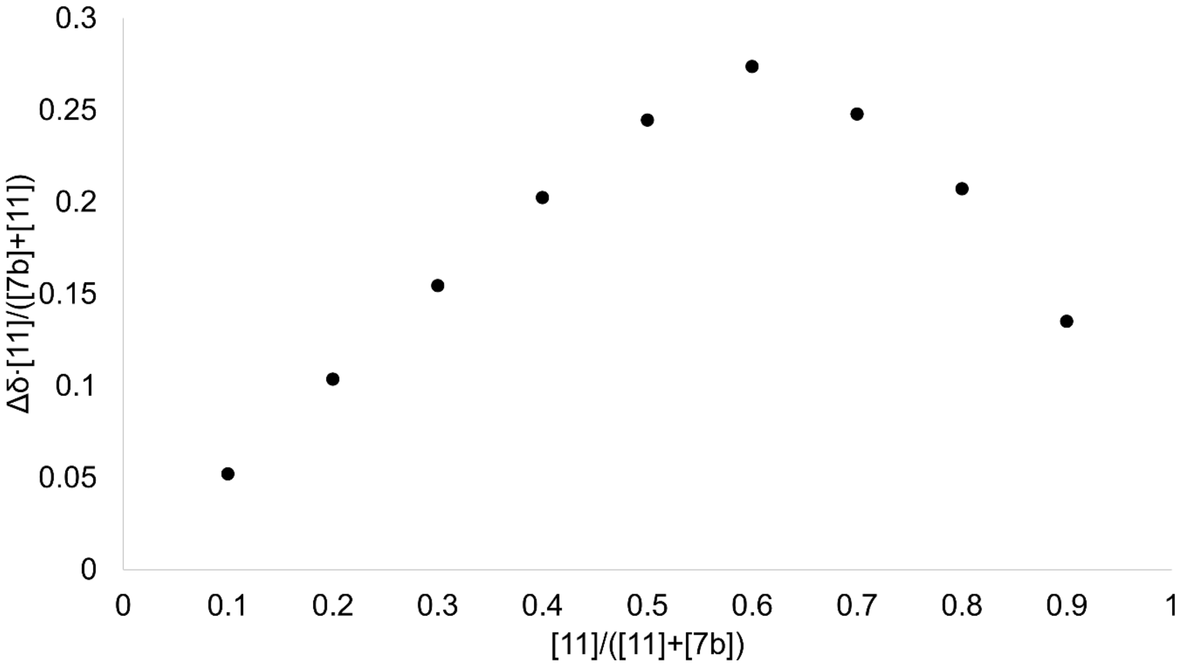

Figure S20. Job's plot of complexation of **11** by clip **7b**

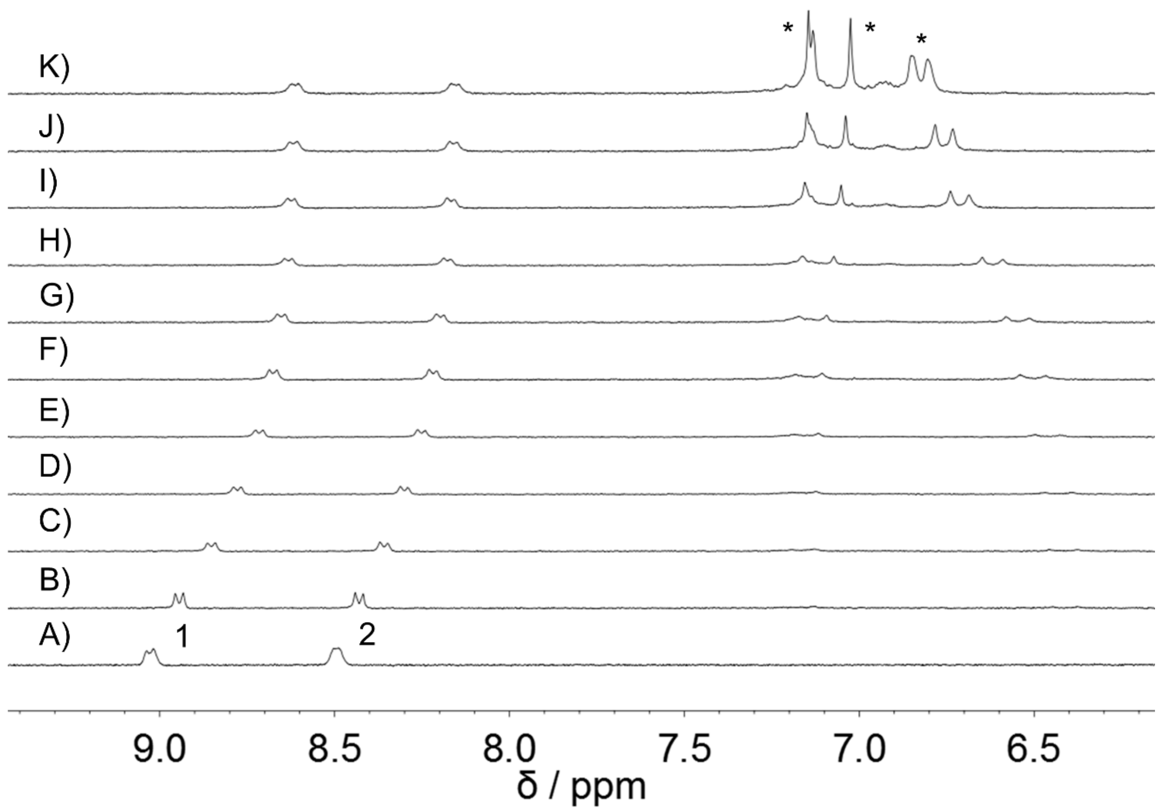

Figure S21. [1]H NMR (300 MHz, D_2O) spectra **11** in the absence (A) and in the presence of 0.13 equiv. (B), 0.25 equiv. (C), 0.38 equiv. (D), 0.50 equiv. (E), 0.63 equiv. (F), 0.75 equiv. (G), 1.00 equiv. (H), 1.50 equiv. (I), 2.00 equiv. (J), and 3.00 equiv. (K) of **7a**. *Signals of **7a**.

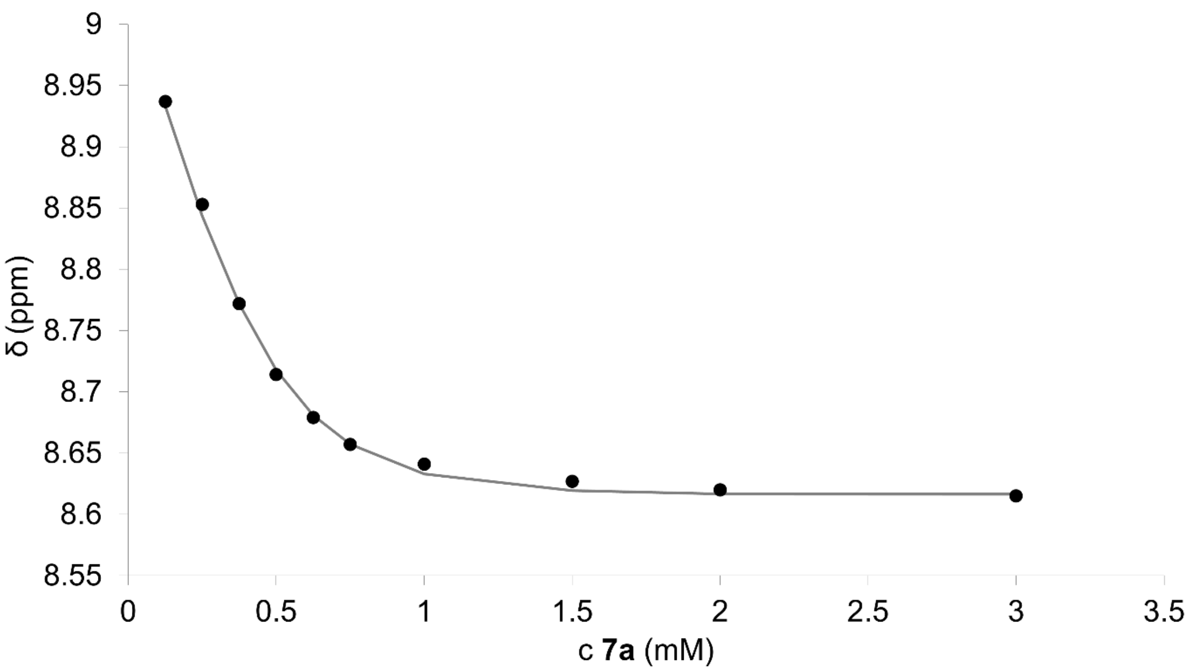

Figure S22. Plot of chemical shift of **11** (signal *1*) vs. analytical concentration of **7a**

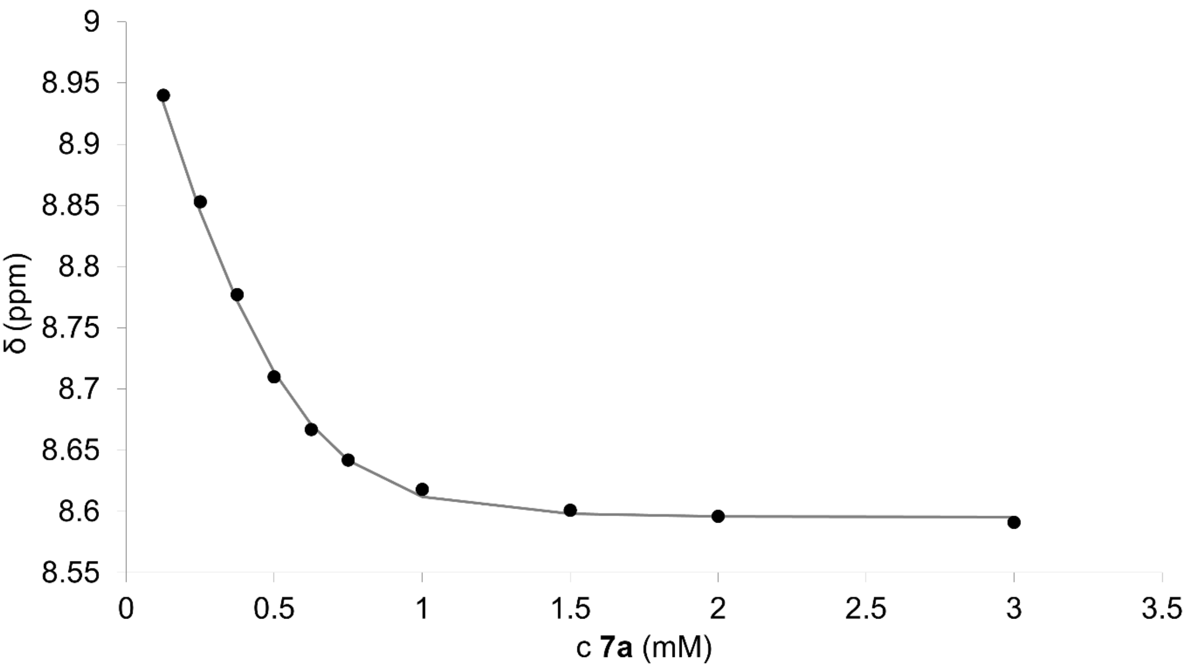

Figure S23. Plot of chemical shift of **11** (signal *1*) vs. analytical concentration of **7b**

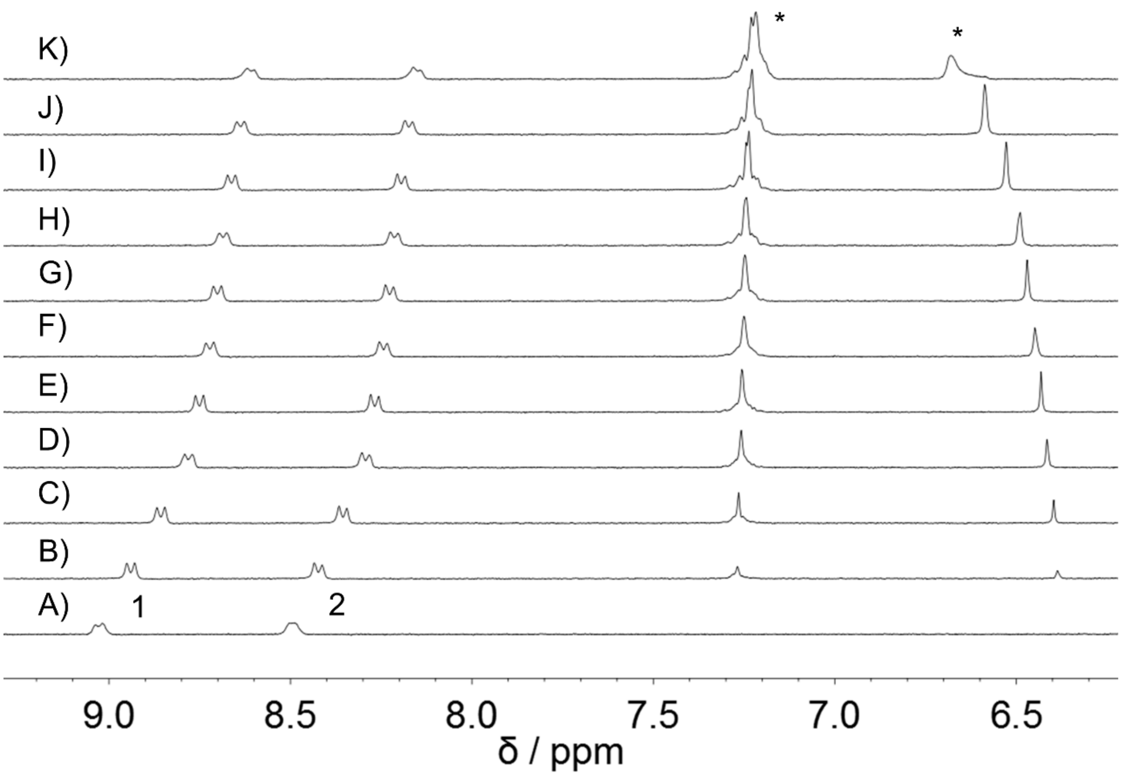

Figure S24. [1]H NMR (300 MHz, D_2O) spectra **11** in the absence (A) and in the presence of 0.25 equiv. (B), 0.5 equiv. (C), 0.75 equiv. (D), 0.86 equiv. (E), 1.00 equiv. (F), 1.16 equiv. (G), 1.25 equiv. (H), 1.50 equiv. (I), 2.00 equiv. (J), and 3.00 equiv. (K) of **7a**. *Signals of **12**.

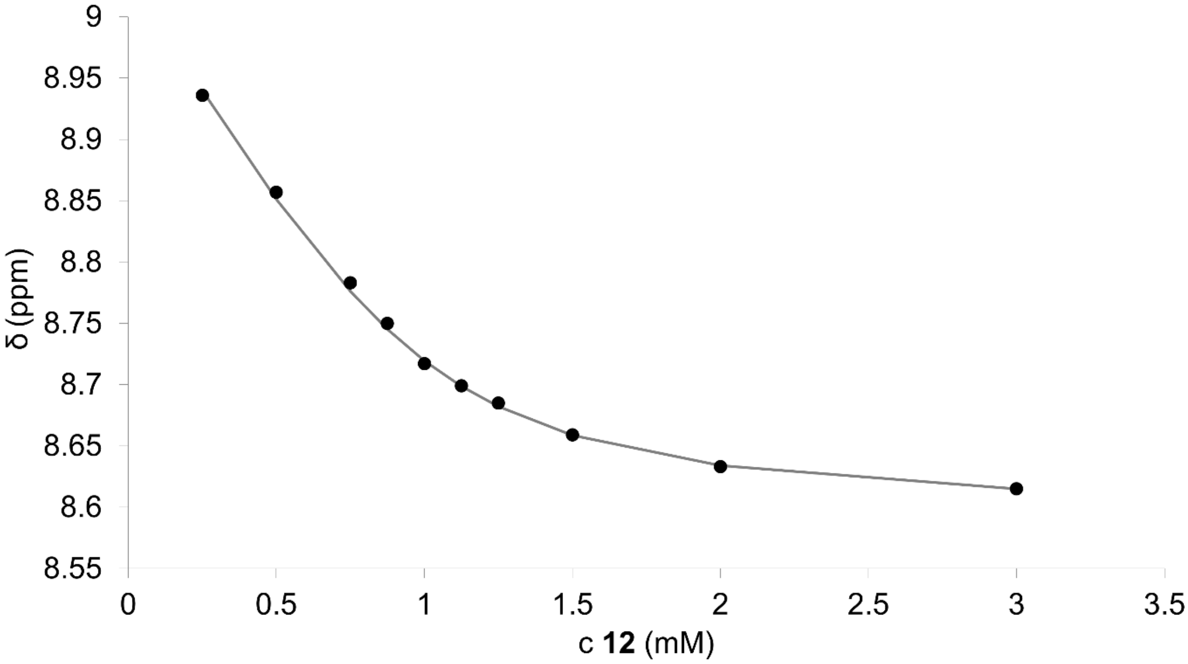

Figure S25. Plot of chemical shift of **11** (signal *1*) vs. analytical concentration of **12**

Determination of activation Gibbs energies of the conformer interconversions

^{1}H NMR spectra (500 MHz, DMSO–*d6*) of compounds **5b** and **7b** were recorded at temperatures varying from 30 °C to 140 °C (*Figures S26 and S27*).

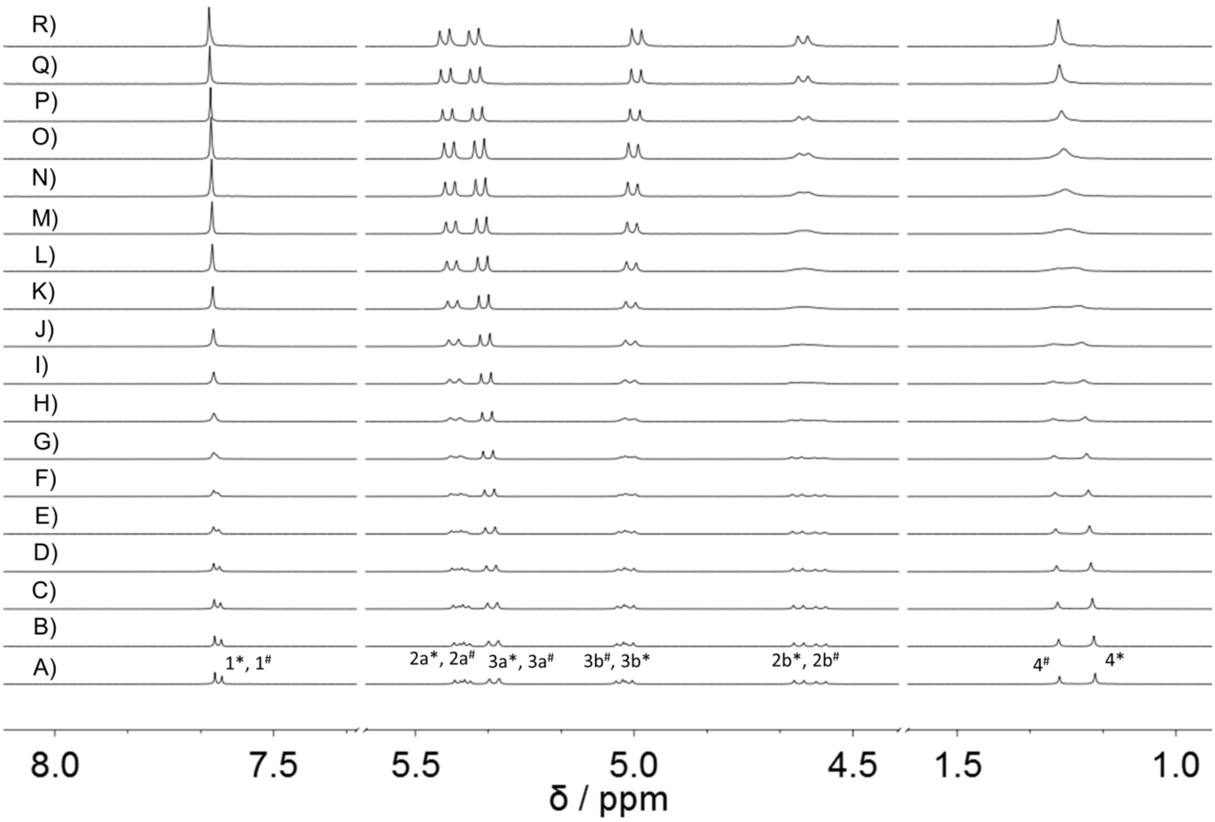

Figure S26. Temperature dependent ^{1}H NMR spectrum of compound **5b** (500 MHz, DMSO–*d6*). 30 °C (A), 35 °C (B), 40 °C (C), 45 °C (D), 50 °C (E), 55 °C (F), 60 °C (G), 65 °C (H), 70 °C (I), 75 °C (J), 80 °C (K), 85 °C (L), 90 °C (M), 95 °C (N), 100 °C (O), 110 °C, (P) 120 °C (Q), 130 °C (R).

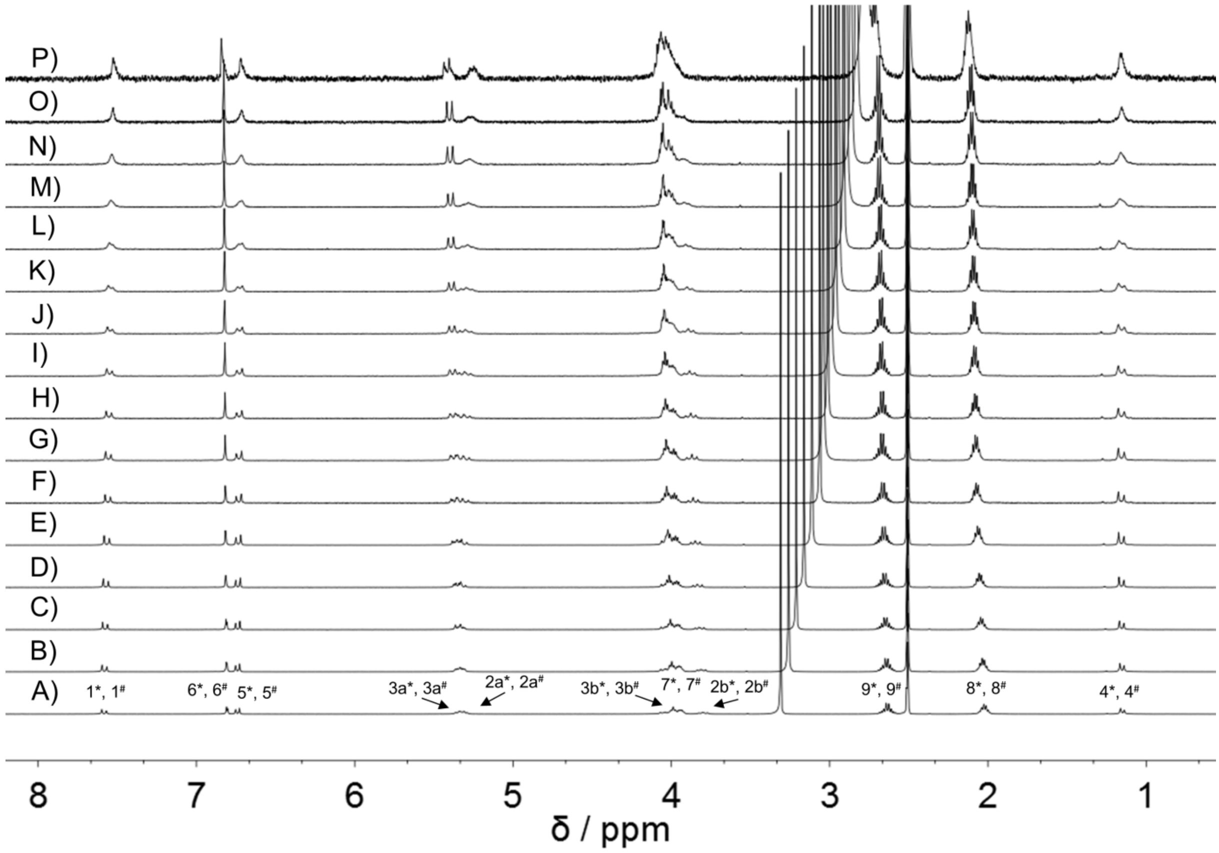

Figure S26. Temperature dependent ^{1}H NMR spectrum of compound **7b** (500 MHz, DMSO–*d6*). 30 °C (A), 40 °C (B), 50 °C (C), 60 °C (D), 70 °C (E), 80 °C (F), 85 °C (G), 90 °C (H), 95 °C (I), 100 °C (J), 105 °C (K), 110 °C (L), 115 °C (M), 120 °C (N), 130 °C (O), 140 °C, (P).

The rate constants of the interconversion at the coalescence temperature were calculated using equation (1),[1]

$$\frac{k_1}{p_{major}} = \frac{k_{-1}}{p_{minor}} = \frac{\pi\Delta\nu_0}{X} \qquad (1)$$

where k_1 is the rate constant of the major to minor conformer interconversion, p_{major} is the population of the major conformer, k_{-1} is the rate constant of the minor to major conformer interconversion, p_{minor} is the population of the minor conformer, $\Delta\nu_0$ is the frequency difference between selected signals of conformers in the slow exchange regime at the NMR timescale, X is given by equation (2),[1]

$$X^6 - 6X^4 + [12 - 27(\Delta p)^2]X^2 - 8 = 0 \qquad (2)$$

where Δp is the population difference $p_{major} - p_{minor}$. The activation Gibbs energies of the interconversion $\Delta G^{\ddagger}$was then calculated using Eyring equation (3),

$$k = \frac{k_B T_c}{h} e^{\frac{\Delta G^{\ddagger}}{RT_c}} \qquad (3)$$

where k_B is Boltzmann constant, h is Planck constant, R is gas constant and T_c is the coalescence temperature. Results are summarized in *Table S1*.

Table S1. Conformer populations, coalescence temperatures, frequency differences, rate constants and determined values of activation Gibbs energy of the interconversion of conformers.

Compound:		**5b**		**7b**	
p_{major}		0.58		0.58	
p_{minor}		0.42		0.42	
X		1.82		1.82	
Signal:		*1*	*4*	*1*	*4*
$T_C\ (K)$		333	363	388	388
$\Delta\nu_0\ (Hz)$		7.83	40.78	14.37	11.83
$k_1\ (s^{-1})$		5.68	29.56	10.42	8.58
$k_{-1}\ (s^{-1})$		7.84	40.83	14.39	11.84
$\Delta G^{\ddagger}$ (kcal mol^{-1})	**Major → minor**	18.42	18.95	21.05	21.14
	Minor → major	18.20	18.71	20.81	20.89

Computational details

Geometry optimizations of glycoluril-based clips were performed using Spartan ’14 software.[2] All structures were built *in silico.* Structures of syn and anti conformers of compound **5b** were first pre-optimized at the PM6 semi-empirical level of theory[3] and further optimized at the RB3LYP/6-311G* level of theory[4–6]. Structure of the **7a**·$\mathbf{11}_2$ complex was optimized at the PM6 semi-empirical level of theory.

Table S2. Geometry of syn conformer of clip **5b** optimized at the RB3LYP/6-311G* level of theory. The predicted absolute energy value for this structure was found to be of −5173610.98 kJ/mol.

s	x [Å]	y[Å]	z[Å]	s	x [Å]	y[Å]	z[Å]
C	5.642172	1.187808	1.94451	H	5.615629	2.002058	2.668102
N	4.447316	1.196673	1.084077	H	1.46	2.141138	-0.378871
C	4.539949	1.733585	-0.188231	H	1.46	-2.141138	-0.378871
C	3.598842	0	1.116462	H	-1.2346	2.141138	-0.378871
N	3.491919	1.205239	-0.95364	H	-1.2346	-2.141138	-0.378871
C	2.933377	0	-0.330592	H	5.615629	-2.002058	2.668102
N	4.447316	-1.196673	1.084077	H	6.531672	-1.29225	1.311383
C	4.539949	-1.733585	-0.188231	H	-6.531672	-1.29225	1.311383
N	3.491919	-1.205239	-0.95364	H	-5.615629	-2.002058	2.668102
O	5.36156	2.539016	-0.562387	H	-5.615629	2.002058	2.668102
O	5.36156	-2.539016	-0.562387	H	-6.531672	1.29225	1.311383
C	1.408881	0	-0.363101	H	2.014083	0.888152	2.293743
C	0.695806	1.201133	-0.363998	H	2.014083	-0.888152	2.293743
C	0.695806	-1.201133	-0.363998	H	3.227735	0	3.227601
C	-0.695806	1.201133	-0.363998	H	-2.014083	-0.888152	2.293743
C	-0.695806	-1.201133	-0.363998	H	-2.014083	0.888152	2.293743
C	-1.408881	0	-0.363101	H	-3.227735	0	3.227601
N	-3.491919	-1.205239	-0.95364	H	2.626671	1.24	-2.84994
C	-4.539949	-1.733585	-0.188231	H	4.225589	2.022693	-2.703908
C	-2.933377	0	-0.330592	H	4.225589	-2.022693	-2.703908
N	-4.447316	-1.196673	1.084077	H	2.626671	-1.2224	-2.84994
C	-3.598842	0	1.116462	H	-4.225589	-2.022693	-2.703908
N	-3.491919	1.205239	-0.95364	H	-2.626671	1.24	-2.84994
C	-4.539949	1.733585	-0.188231	H	-4.225589	2.022693	-2.703908
N	-4.447316	1.196673	1.084077	O	4.296975	0	-2.836141
O	-5.36156	-2.539016	-0.562387	O	-4.296975	0	-2.836141
O	-5.36156	2.539016	-0.562387	H	-2.626671	-1.2224	-2.84994
C	5.642172	-1.187808	1.94451				
C	-5.642172	-1.187808	1.94451				
C	-5.642172	1.187808	1.94451				
C	2.647168	0	2.305384				
C	-2.647168	0	2.305384				
C	3.624958	1.170166	-2.397959				
C	3.624958	-1.170166	-2.397959				
C	-3.624958	-1.170166	-2.397959				
C	-3.624958	1.170166	-2.397959				
O	-5.668894	0	2.706476				
O	5.668894	0	2.706476				
H	6.531672	1.29225	1.311383				

Table S3. Geometry of anti conformer of clip **5b** optimized at the RB3LYP/6-311G* level of theory. The predicted absolute energy value for this structure was found to be of −5173655.61 kJ/mol.

s	x [Å]	y[Å]	z[Å]	s	x [Å]	y[Å]	z[Å]
C	5.845576	-1.612931	1.172337	H	5.668027	-2.693778	1.231599
N	4.572864	-0.915929	1.204216	H	1.223925	0.165827	-2.141597
C	4.517259	0.367666	1.748321	H	1.223925	0.165827	2.141597
C	3.740580	-1.032352	0.000000	H	-1.223925	-0.165827	-2.141597
N	3.400260	1.007839	1.202618	H	-1.223925	-0.165827	2.141597
C	2.915965	0.324647	0.000000	H	5.668027	-2.693778	-1.231599
N	4.572864	-0.915929	-1.204216	H	6.435475	-1.281050	-2.022541
C	4.517259	0.367666	-1.748321	H	-6.435475	1.281050	2.022541
N	3.400260	1.007839	-1.202618	H	-5.668027	2.693778	1.231599
O	5.260168	0.824657	2.582300	H	-5.668027	2.693778	-1.231599
O	5.260168	0.824657	-2.582300	H	-6.435475	1.281050	-2.022541
C	1.396949	0.181959	0.000000	H	2.298573	-2.379270	0.888258
C	0.690191	0.089593	-1.201381	H	2.298573	-2.379270	-0.888258
C	0.690191	0.089593	1.201381	H	3.591157	-3.187816	0.000000
C	-0.690191	-0.089593	-1.201381	H	-2.298573	2.379270	0.888258
C	-0.690191	-0.089593	1.201381	H	-2.298573	2.379270	-0.888258
C	-1.396949	-0.181959	0.000000	H	-3.591157	3.187816	0.000000
N	-3.400260	-1.007839	1.202618	H	2.304919	2.780182	1.226640
C	-4.517259	-0.367666	1.748321	H	3.912886	2.834480	2.022674
C	-2.915965	-0.324647	0.000000	H	3.912886	2.834480	-2.022674
N	-4.572864	0.915929	1.204216	H	2.304919	2.780182	-1.226640
C	-3.740580	1.032352	0.000000	H	-3.912886	-2.834480	2.022674
N	-3.400260	-1.007839	-1.202618	H	-2.304919	-2.780182	-1.226640
C	-4.517259	-0.367666	-1.748321	H	-3.912886	-2.834480	-2.022674
N	-4.572864	0.915929	-1.204216	O	3.959589	2.978251	0.000000
O	-5.260168	-0.824657	2.582300	O	-3.959589	-2.978251	0.000000
O	-5.260168	-0.824657	-2.582300	H	-2.304919	-2.780182	1.226640
C	5.845576	-1.612931	-1.172337				
C	-5.845576	1.612931	1.172337				
C	-5.845576	1.612931	-1.172337				
C	2.927824	-2.320685	0.000000				
C	-2.927824	2.320685	0.000000				
C	3.351964	2.458000	1.171436				
C	3.351964	2.458000	-1.171436				
C	-3.351964	-2.458000	1.171436				
C	-3.351964	-2.458000	-1.171436				
O	-6.582479	1.305480	0.000000				
O	6.582479	-1.305480	0.000000				
H	6.435475	-1.281050	2.022541				

Table S4. Geometry of **7a·11**$_2$ complex optimized at PM6 semi-empirical level of theory.

s	x [Å]	y[Å]	z[Å]	s	x [Å]	y[Å]	z[Å]
C	-5.157315	-0.790813	8.730569	H	0.227946	2.335374	7.784461
S	-4.240323	-1.681232	9.990063	H	1.648746	1.124248	-1.240950
O	-5.238933	-2.106100	10.975932	H	-2.008810	-1.176980	-1.101985
O	-3.592170	-2.843779	9.246640	H	2.389070	0.073984	0.860694
O	-3.166663	-0.793201	10.473417	H	-1.271247	-2.219046	1.005514
C	-4.221978	-0.095598	7.754492	H	2.405607	1.196058	3.873798
C	-3.389206	-1.103105	6.960116	H	1.014765	1.128505	2.719446
S	4.004597	4.077580	10.034647	H	-0.872466	-1.783137	-3.363031
O	2.793612	3.985477	10.865986	H	-2.409113	-1.614488	-4.301577
O	4.938507	5.162317	10.365498	H	2.103224	1.099125	-4.366906
O	4.681074	2.726481	9.916066	H	1.531352	-0.299131	-3.378695
C	-0.711841	-0.037366	4.802540	H	-4.956097	2.521911	-2.805956
C	0.484482	0.684328	4.756151	H	-4.059282	3.378088	-1.490046
C	-1.576069	0.148604	5.913945	H	3.117993	-7.217233	7.476299
C	0.778668	1.572090	5.829190	H	5.272418	-5.982746	7.344813
C	-1.239109	0.964436	6.994014	H	-0.821141	-1.636400	-8.645636
C	-0.046174	1.688813	6.949930	H	1.322721	-0.376539	-8.664119
O	-2.810527	-0.468834	5.782762	H	-1.508739	4.948669	-1.619577
O	1.945775	2.284891	5.642851	H	-0.478909	5.319978	-3.057465
N	-2.930656	1.992256	-2.628118	H	-5.647506	6.054902	-5.688930
C	-3.062333	0.763046	-3.330743	H	-3.587982	7.420472	-5.711075
C	-1.593826	2.199103	-2.030307	H	3.891157	-2.436230	0.747219
N	-1.791168	0.125930	-3.290173	H	0.211812	-4.703098	0.947773
C	-0.787178	0.859232	-2.487147	H	4.232592	-3.215094	-1.576990
N	-0.877610	3.276006	-2.757468	H	0.570717	-5.474905	-1.374092
C	0.200839	2.808719	-3.549250	H	2.578745	-4.737527	-2.646964
N	0.261157	1.400326	-3.381487	H	-3.448850	1.263168	-0.236757
C	-0.250856	0.078358	-1.301299	H	0.230894	3.524193	-0.461890
C	0.998944	0.397065	-0.749860	H	-3.418224	1.476598	2.229665
C	-1.047594	-0.888473	-0.670834	H	0.246846	3.726401	2.004334
C	1.412511	-0.187771	0.448408	H	-1.562712	2.686094	3.363449
C	-0.634752	-1.471001	0.529236	H	-2.842787	-1.835694	-8.403645
C	0.575783	-1.087671	1.124905	H	-2.473813	-3.531584	-7.865457
O	-4.078245	0.307954	-3.802702	H	-4.435117	-3.276436	-6.170201
O	0.965824	3.478927	-4.212459	H	-4.834941	-1.731302	-6.914746
C	0.976375	-1.637504	2.480868	H	-4.771964	-4.432742	-8.445816
N	-0.188217	-1.986488	3.338395	H	-6.216834	-3.722889	-7.756522
C	-0.173596	-3.324533	3.791088	H	2.882015	4.022755	5.728152
N	0.988675	-3.937407	3.269836	H	1.226921	4.089044	6.455804
C	1.811389	-3.028151	2.427942	H	-0.040491	-10.478838	7.098432
N	1.878762	-0.740114	3.239529	H	1.596085	-10.459776	7.747391
C	3.105685	-1.351628	3.617315	H	2.453186	-9.169019	5.811335
N	3.055617	-2.696609	3.160538	H	0.949208	-9.398685	4.916629
O	-1.013111	-3.862125	4.494786	H	-0.324186	-7.982275	6.563071

O	4.037962	-0.812530	4.168666	H	1.156259	-7.801545	7.589861
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C	-1.444681	-1.099818	-4.033340	H	3.516713	2.386445	7.657499
C	1.196474	0.501630	-4.079281	H	4.269004	4.782783	7.746831
C	-3.981022	3.021368	-2.544764	H	2.718921	5.286900	8.403438
C	3.285380	-6.502058	6.671212	H	-7.904487	3.483624	-4.195437
C	4.496466	-5.815151	6.591042	H	-7.485411	5.243892	-4.305610
C	2.310612	-6.275289	5.698425	H	-6.607313	4.927651	-6.628041
C	4.709191	-4.919960	5.539015	H	-6.806565	3.172446	-6.517683
C	2.517987	-5.384548	4.610268	H	-9.216176	3.298876	-6.665442
C	3.724127	-4.680281	4.539362	H	-9.276298	4.976525	-6.152183
O	1.038607	-6.815496	5.737513	H	6.688749	-4.815960	7.238182
O	5.864596	-4.194711	5.362861	H	7.550318	-5.330305	5.727193
C	-0.426508	-1.224393	-7.716844	H	8.090947	-2.914621	5.206882
C	0.779156	-0.520755	-7.728706	H	7.148272	-2.366996	6.591146
C	-1.110861	-1.390664	-6.508466	H	9.656266	-4.178899	6.835195
C	1.271322	-0.000027	-6.532565	H	9.701872	-2.433815	6.954994
C	-0.633263	-0.837985	-5.285928	H	-2.065895	8.679178	-4.987674
C	0.571426	-0.130677	-5.304523	H	-0.340732	8.522843	-4.472591
O	-2.265000	-2.120254	-6.367928	H	0.233971	7.138646	-6.403886
O	2.450085	0.720861	-6.434611	H	-1.457512	6.794114	-6.779030
C	-3.755722	4.219781	-3.443252	H	-1.837870	9.151319	-7.526587
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C	-4.859948	4.638619	-4.240986	H	4.416364	0.618080	-6.689212
C	-2.555120	6.148106	-4.287962	H	3.539553	-0.721911	-7.525707
O	-5.964427	3.818814	-4.112148	H	2.684159	0.851029	-9.267871
O	-1.386285	6.876018	-4.153904	H	3.171818	2.249813	-8.310014
C	-1.327068	4.678326	-2.687043	H	5.660962	1.366089	-8.608749
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C	-3.637249	6.537553	-5.075422	C	-1.190613	-0.972692	3.712412
C	2.040852	-3.536180	1.019012	C	1.433730	-5.314226	3.555978
C	3.164752	-3.112373	0.293371	C	4.087346	-3.716663	3.428744
C	1.103280	-4.381495	0.406771	H	-2.119533	-1.510254	4.047316
C	3.357270	-3.546725	-1.020543	H	-1.461433	-0.370490	2.810257
C	1.300577	-4.814364	-0.907168	H	1.820674	-5.777098	2.614677
C	2.427903	-4.400243	-1.622566	H	0.538232	-5.916504	3.867473
C	-1.619536	2.393646	-0.524463	H	4.276848	-4.298500	2.494848
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C	-2.621411	1.927260	1.638747	N	1.345989	4.521096	-8.139101
C	-0.563998	3.190709	1.512792	C	-0.424562	2.978169	-7.635546
C	-1.582064	2.611389	2.275861	C	-0.657969	4.532231	-9.469377
C	-2.948889	-2.579687	-7.584041	C	0.628840	5.017684	-9.195739
C	-4.402726	-2.732142	-7.136915	C	0.831147	3.509226	-7.355550
C	-5.229149	-3.463006	-8.181966	H	-0.813060	2.168358	-7.008967
S	-5.485635	-2.489575	-9.670578	H	-1.233582	5.037262	-10.262269

O	-5.807368	-3.474922	-10.712185	H	1.079260	5.853480	-9.788560
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C	1.021138	-10.459877	6.810117	C	-3.656862	3.793276	-9.039612
S	1.381201	-12.008878	5.911297	C	-2.707191	1.582869	-9.252666
O	0.525029	-13.006073	6.599289	C	-3.971953	1.082799	-9.558866
O	0.987827	-11.746824	4.506940	C	-4.913824	3.264547	-9.329055
O	2.831019	-12.235075	6.100868	H	-3.557601	4.869331	-8.847387
C	1.355641	-9.258421	5.947031	H	-1.858912	0.892011	-9.220409
C	0.782282	-7.989767	6.571677	H	-4.128525	-0.037829	-9.780410
C	2.768150	3.204158	7.766514	H	-5.861008	3.906031	-9.340336
C	3.421847	4.438444	8.363603	C	2.674298	5.093437	-7.861923
C	-7.243656	4.233536	-4.671731	H	3.418215	4.708506	-8.638522
C	-7.261915	4.133650	-6.196112	H	3.048414	4.847305	-6.862148
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S	-8.626701	4.813580	-8.453412	C	-6.388220	1.384033	-9.930070
O	-8.165897	6.213000	-8.395148	H	-6.505876	1.251051	-11.016832
O	-7.612296	3.918062	-9.117191	H	-7.207979	2.071744	-9.583988
O	-9.995467	4.618496	-8.959561	H	-6.566872	0.371436	-9.463909
S	8.609563	-3.402558	8.860316	C	2.688151	-1.882032	8.865684
O	9.886255	-3.481935	9.579762	N	5.032731	-0.474376	9.396175
O	7.706661	-4.570897	8.997973	C	3.931932	-2.533256	8.846584
O	7.828292	-2.138295	9.143571	C	2.643515	-0.518669	9.199239
C	7.016797	-4.502974	6.219449	C	3.824150	0.170326	9.468608
C	7.806125	-3.194054	6.241470	C	5.096089	-1.816061	9.114922
C	9.043811	-3.306005	7.118452	H	4.015063	-3.600876	8.616065
S	-0.120265	8.285057	-8.971139	H	1.693911	0.024588	9.236152
O	0.021363	9.541134	-9.722143	H	3.848083	1.295250	9.749418
O	-1.064005	7.291288	-9.549844	H	6.147097	-2.298635	9.104255
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C	-1.173448	8.033500	-5.011754	N	-0.902954	-3.907474	7.766793
C	-0.780068	7.600154	-6.422335	C	1.424386	-3.459717	7.393999
C	-0.810673	8.778428	-7.379381	C	0.272344	-2.444745	9.259592
C	3.549553	0.359148	-7.326857	C	-0.897931	-3.099462	8.872598
C	3.483483	1.214381	-8.588875	C	0.248388	-4.108601	7.035029
C	4.818224	1.241295	-9.307489	H	2.324456	-3.608903	6.779747
S	4.861361	2.620358	-10.495486	H	0.237074	-1.794432	10.142842
O	6.229307	3.161662	-10.360897	H	-1.906499	-2.949576	9.425624
O	4.562563	2.012647	-11.804533	H	0.194788	-4.784008	6.149524
O	3.804160	3.565082	-10.012964	C	6.282332	0.286776	9.612075
H	-5.840519	-1.480875	8.205222	H	7.074551	-0.355223	10.066241
H	-5.822119	-0.051412	9.212373	H	6.099888	1.202884	10.227030
H	-4.799559	0.536705	7.050273	H	6.689217	0.636628	8.643594
H	-3.546633	0.603645	8.303180	C	-2.153792	-4.568624	7.336231
H	-2.595010	-1.573139	7.564118	H	-2.115232	-5.655311	7.515311

H	-4.009482	-1.888130	6.487709	H	-2.332666	-4.394766	6.251963
H	-1.902817	1.042965	7.861431	H	-3.039202	-4.158716	7.902753

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