

Solvent and substituent size influence on the cyclochiral rigidity of aminomethylene  
derivatives of resorcin[4]arene

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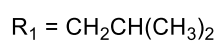
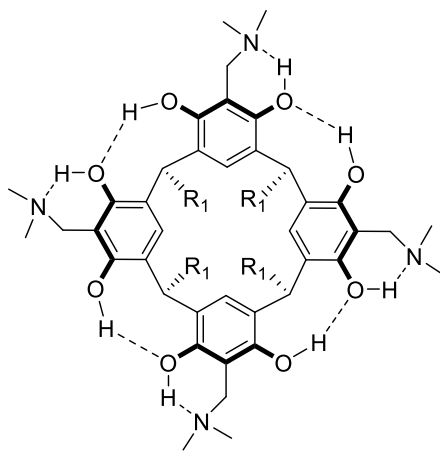
E-mail: Waldemar.Iwanek@pbs.edu.pl

Supporting information

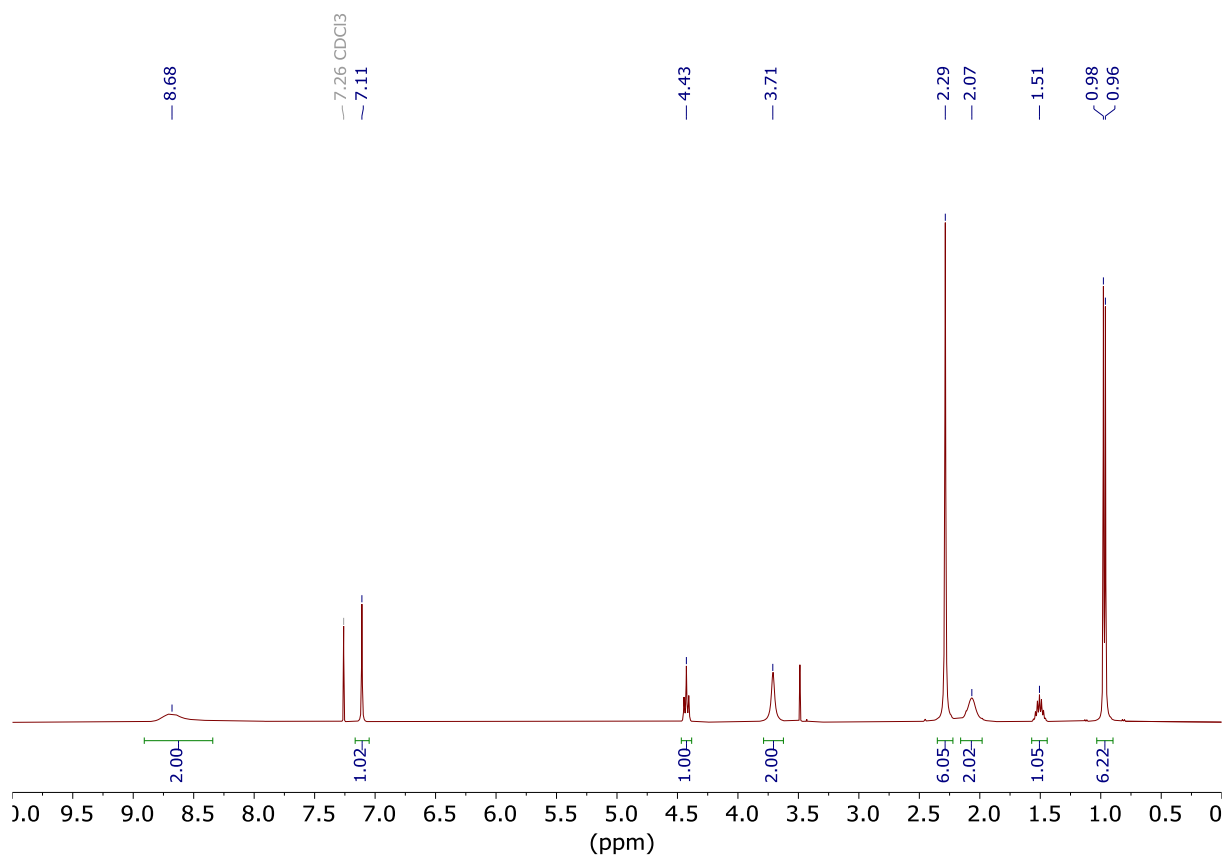
1. NMR spectra of AMD-R[4]A.
2. The xyz coordinates of the optimized structures in  $\text{CHCl}_3$ .

1. NMR spectra of AMD-R[4]A.

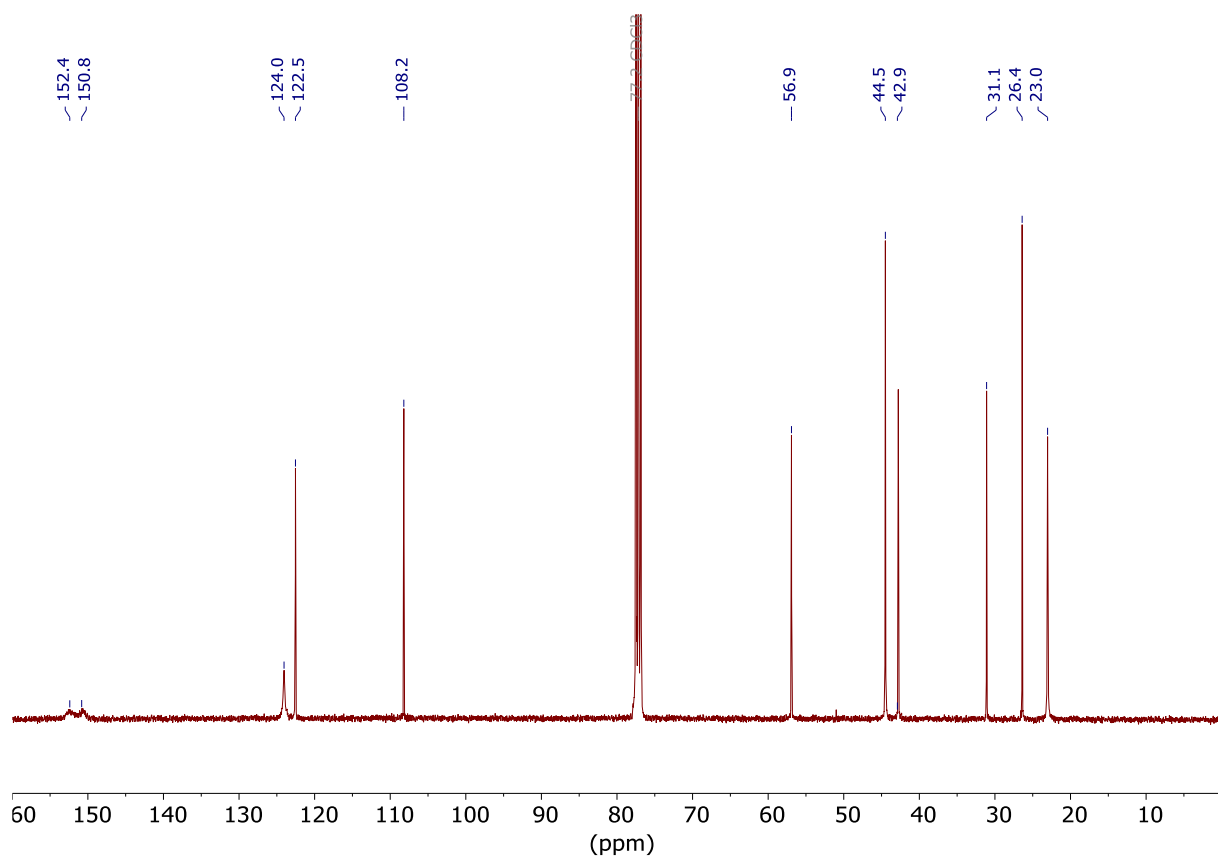
NMR Spectra of **1**



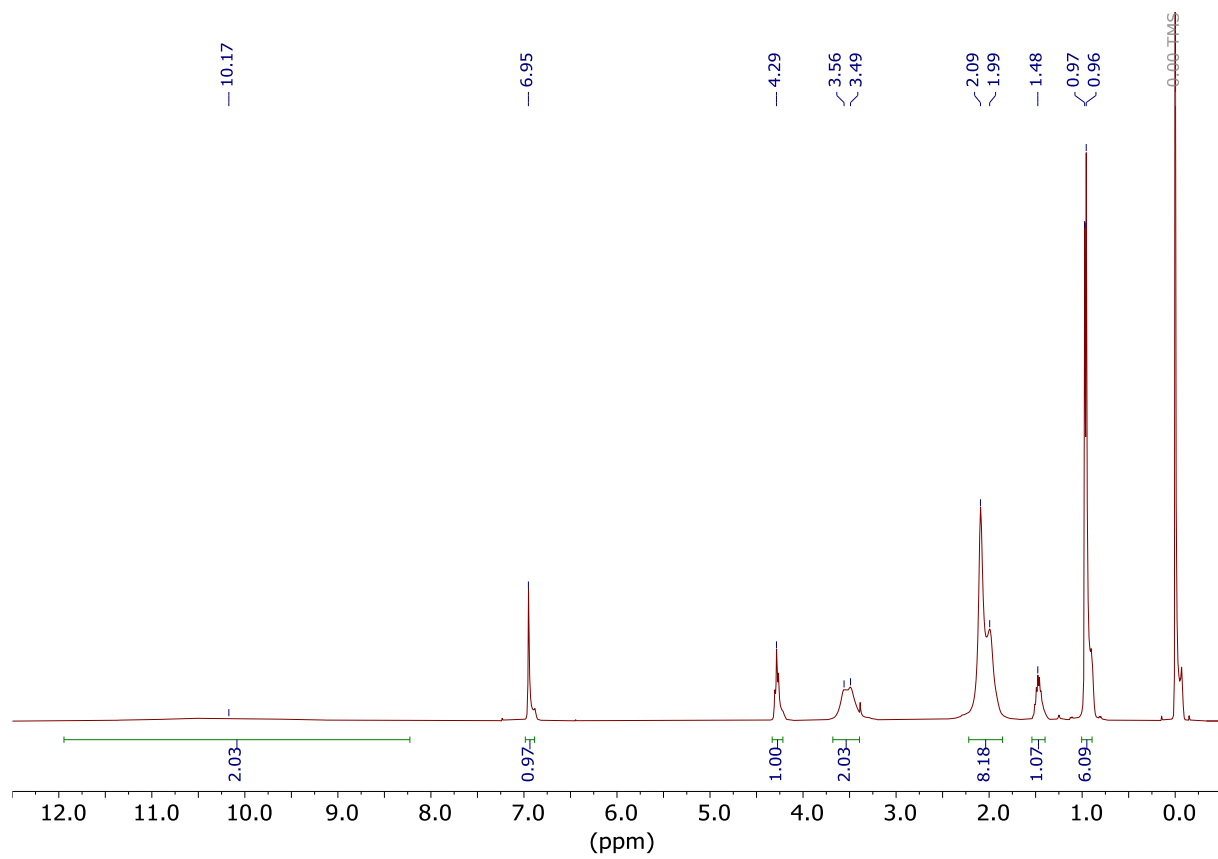
$^1\text{H}$  NMR –  $\text{CDCl}_3$



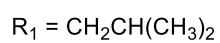
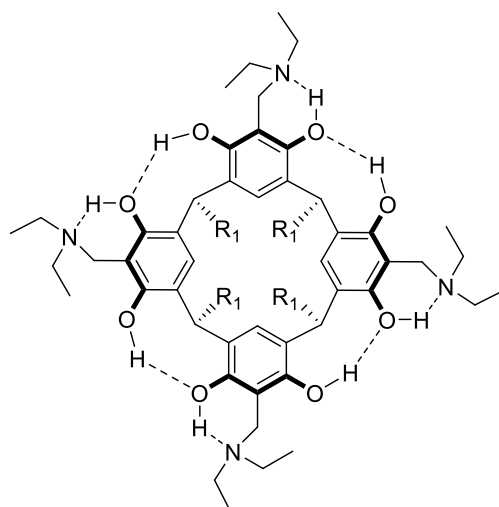
<sup>13</sup>C NMR – CDCl<sub>3</sub>



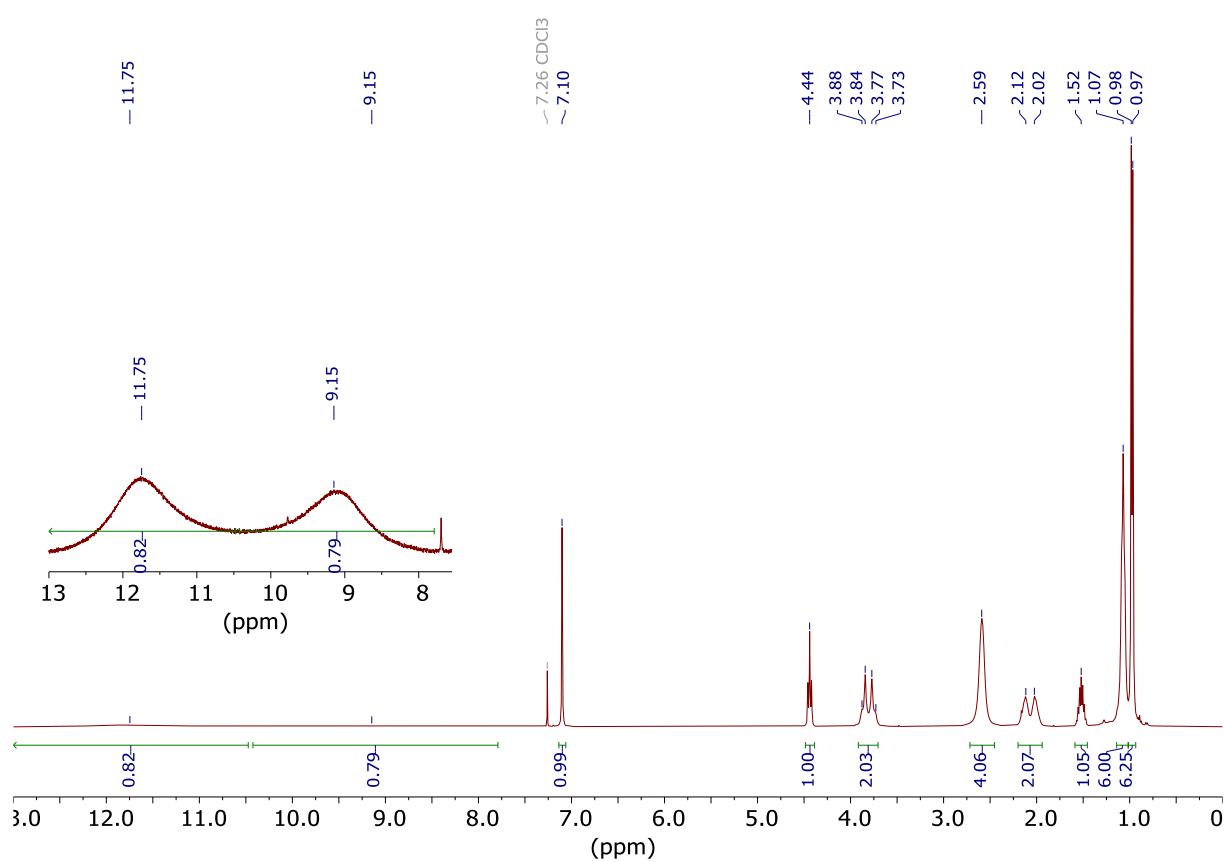
<sup>1</sup>H NMR – CCl<sub>4</sub>

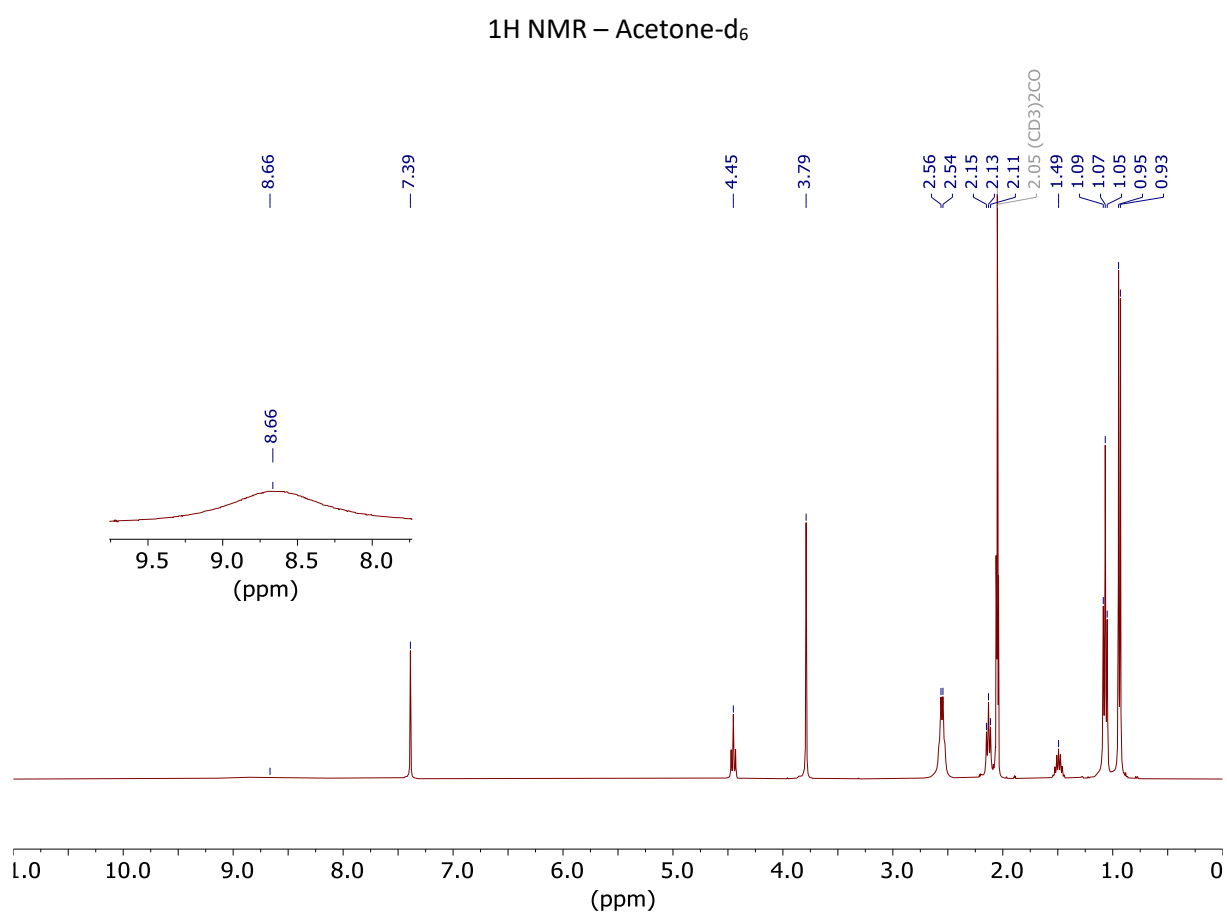
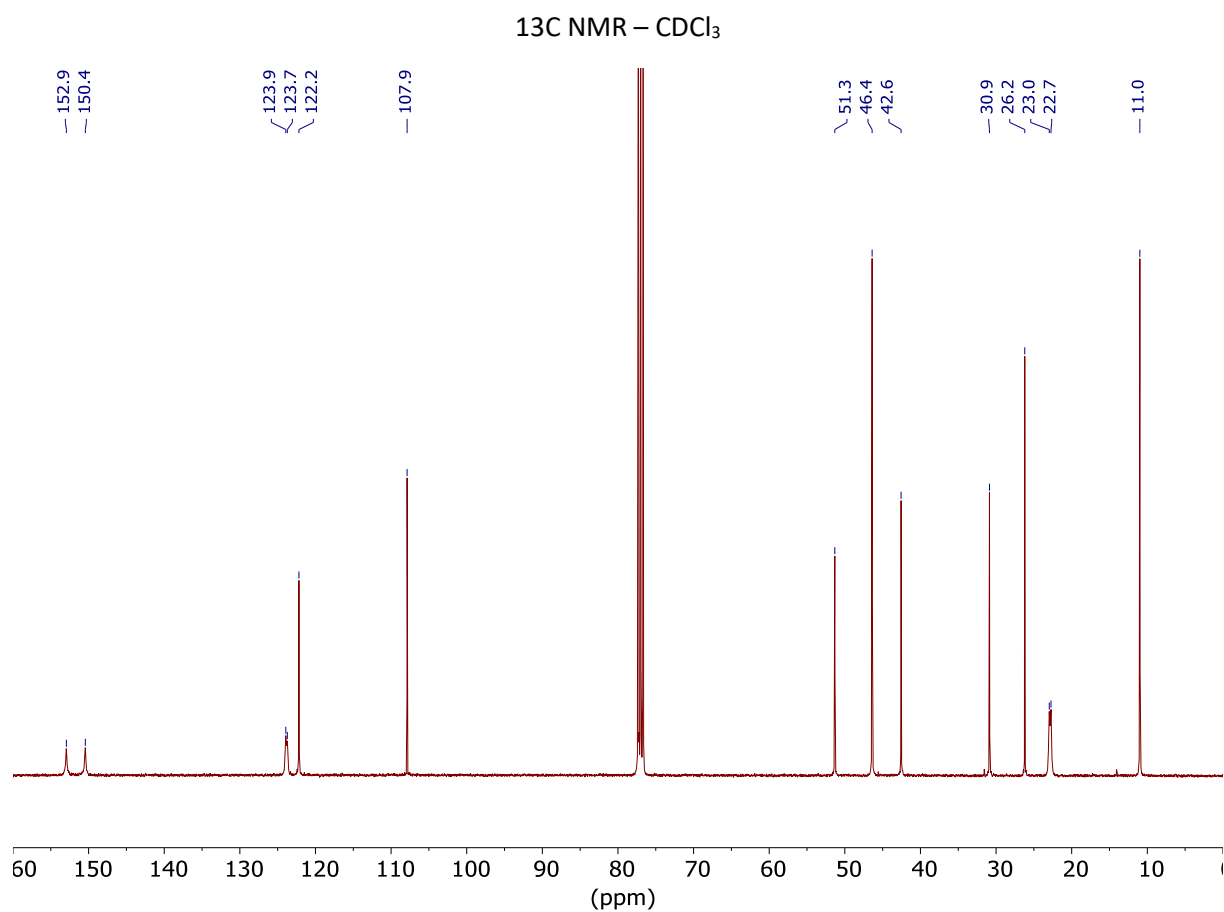


# NMR Spectra of **2**

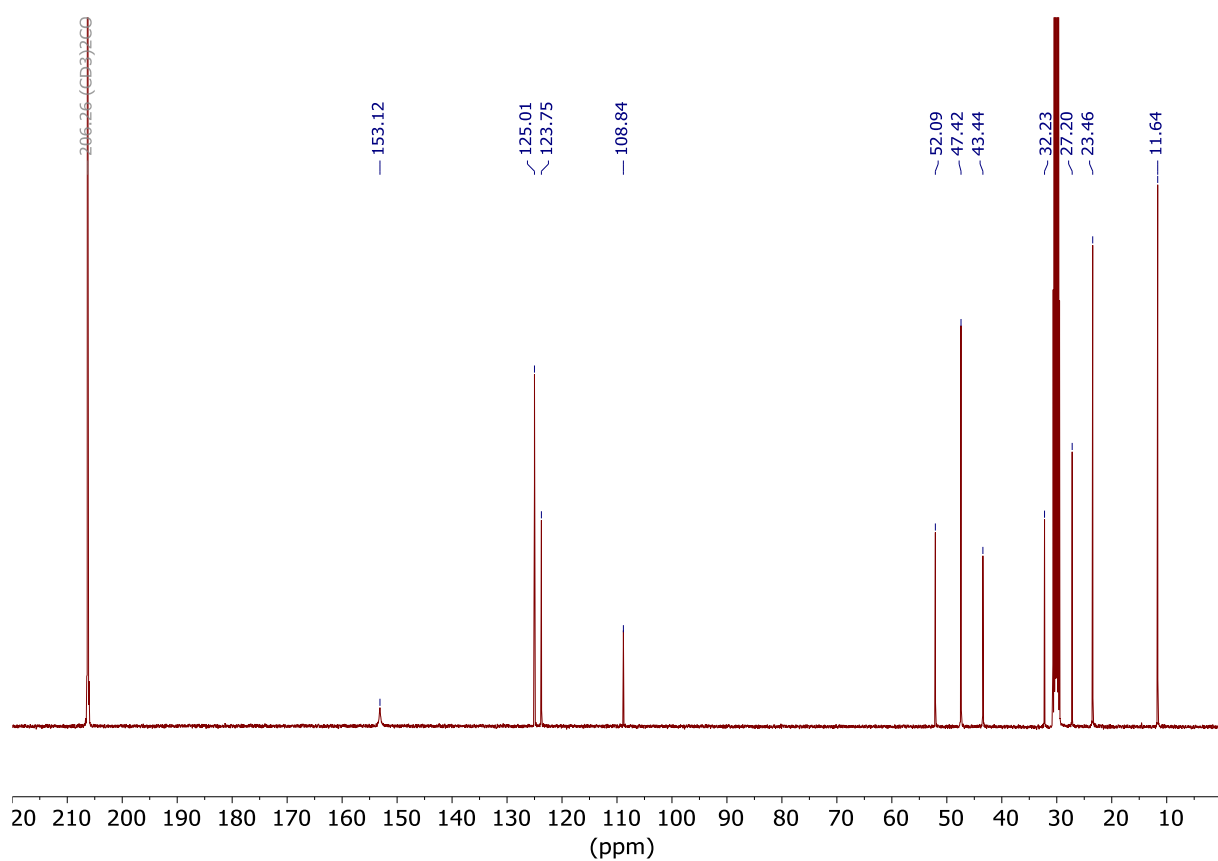


$^1\text{H}$  NMR –  $\text{CDCl}_3$

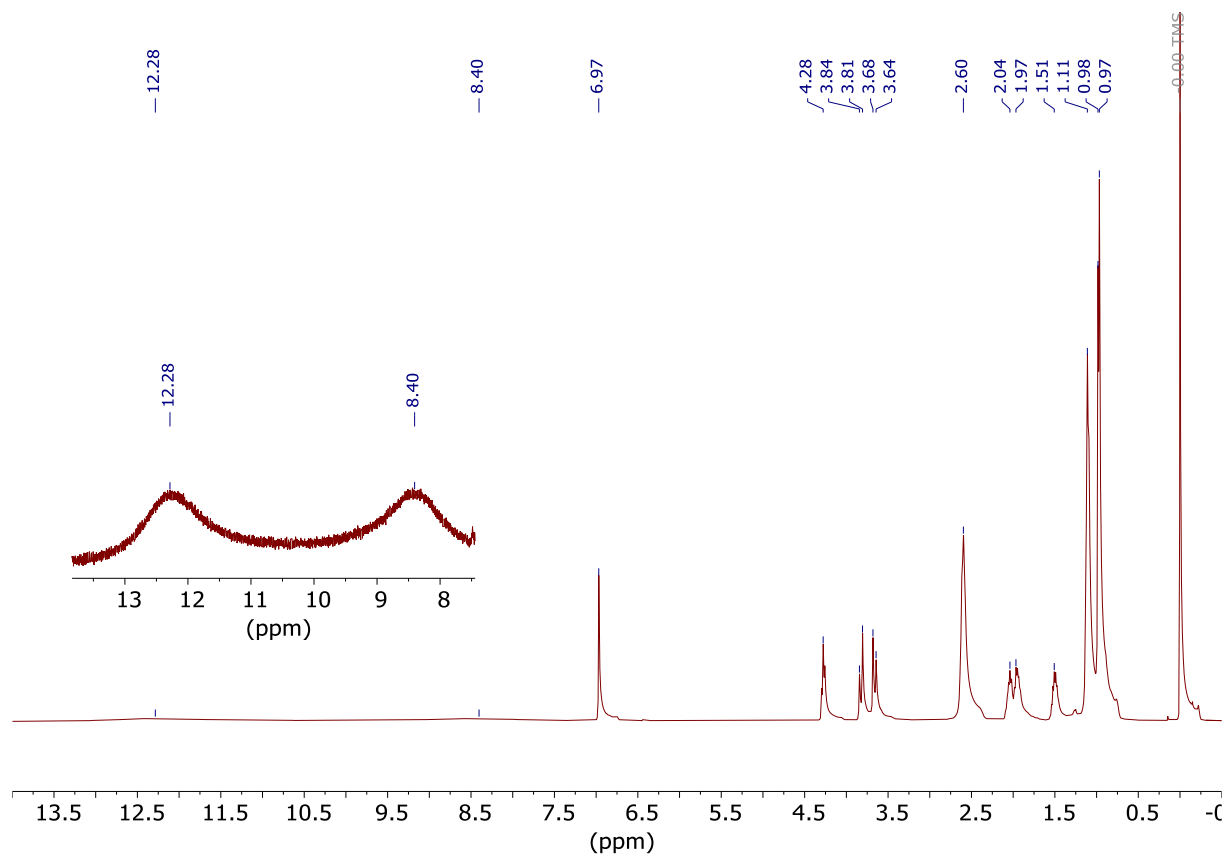




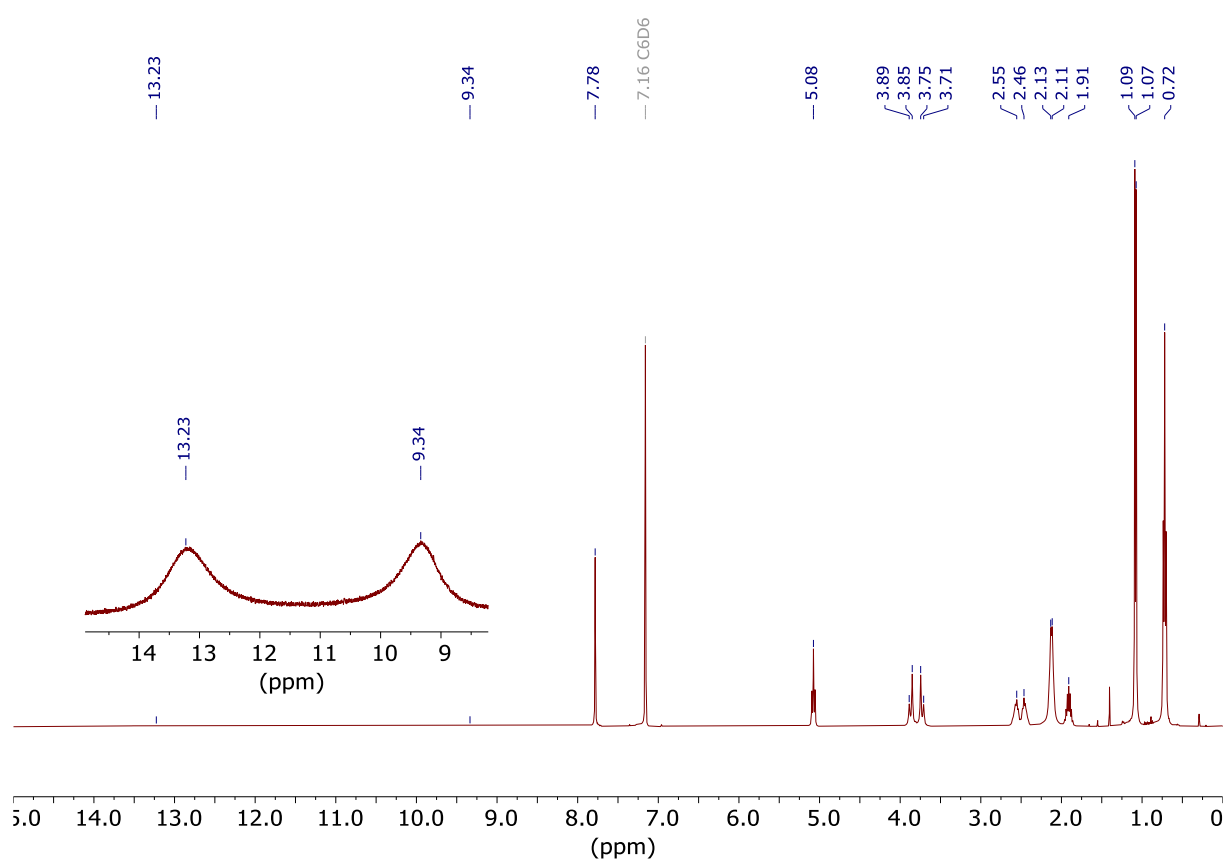
13C NMR – Acetone-d<sub>6</sub>



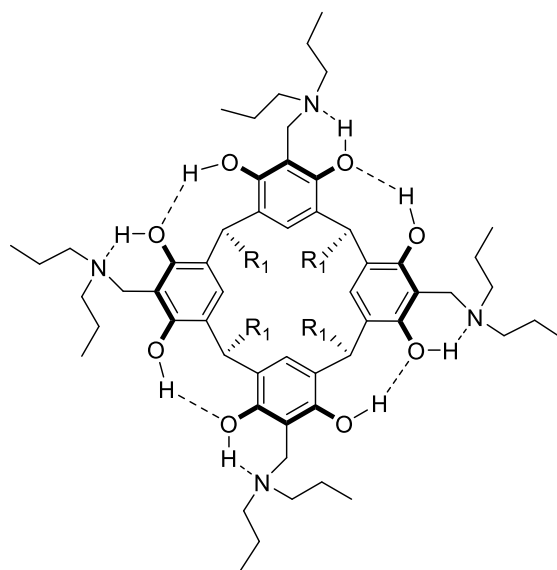
1H NMR - CCl<sub>4</sub>



# 1H NMR - Benzene-d<sub>6</sub>

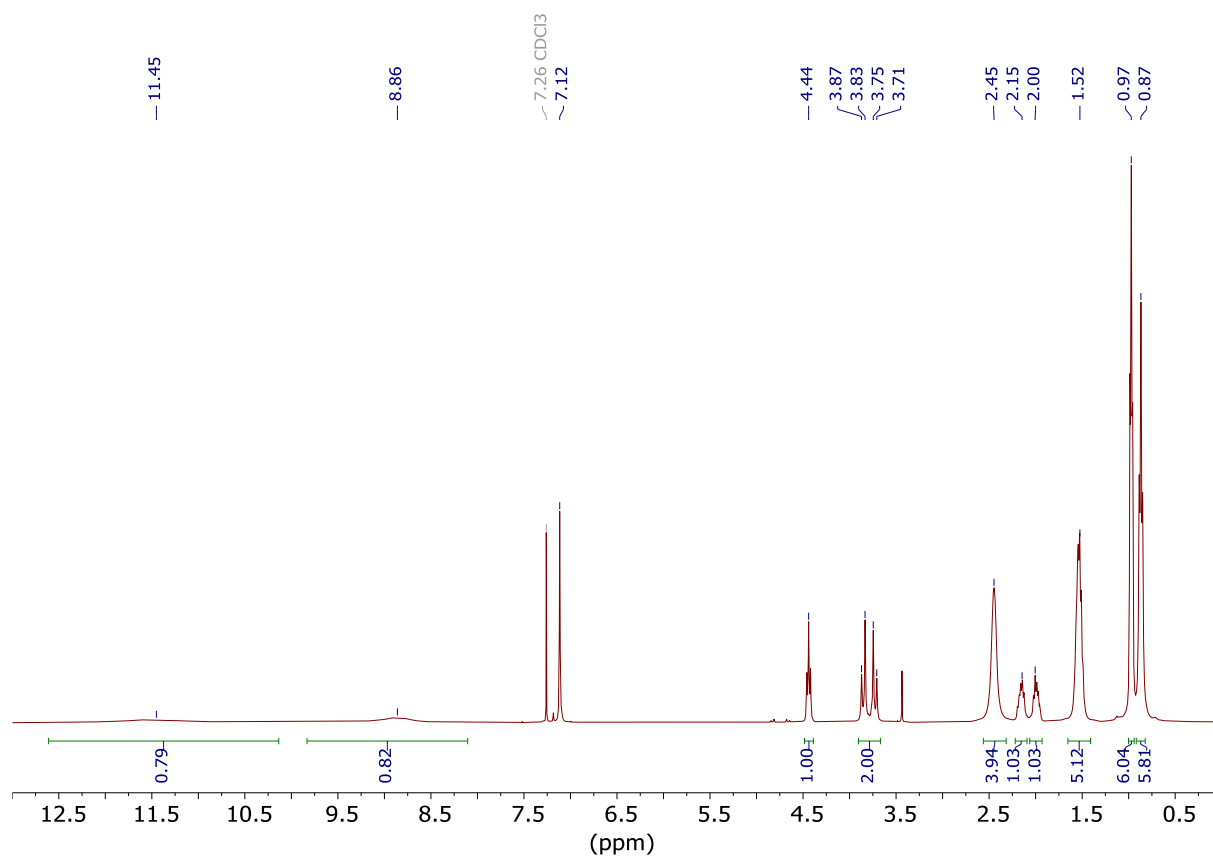


# NMR Spectra of **3**



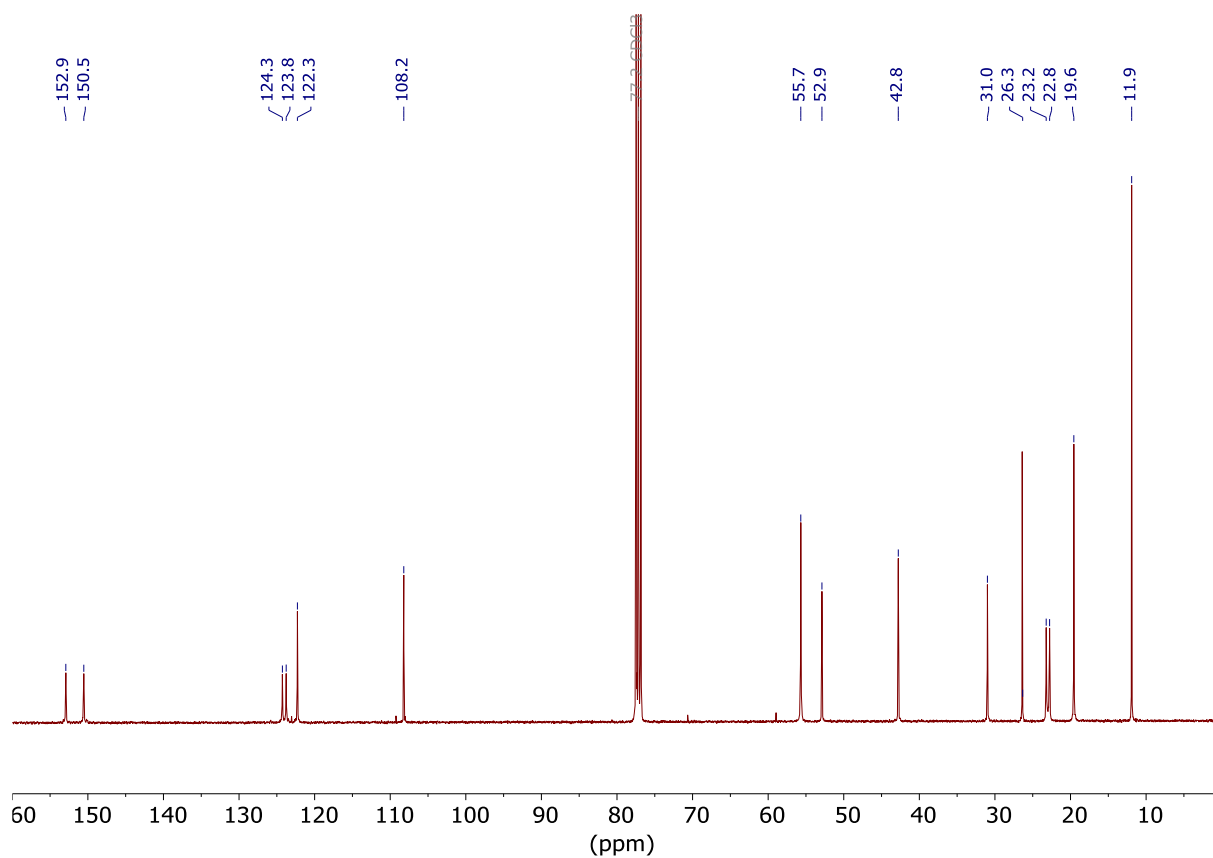
$R_1 = \text{CH}_2\text{CH}(\text{CH}_3)_2$

$^1\text{H}$  NMR –  $\text{CDCl}_3$

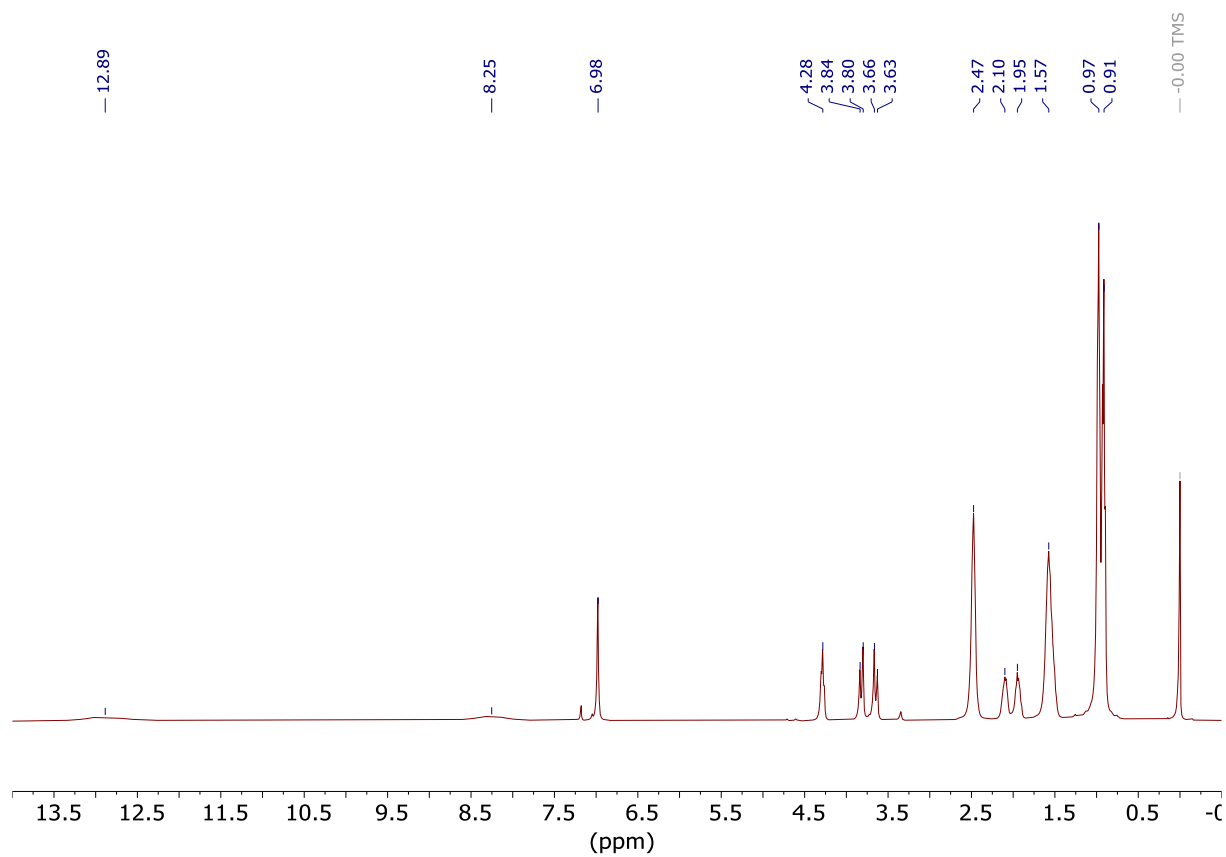




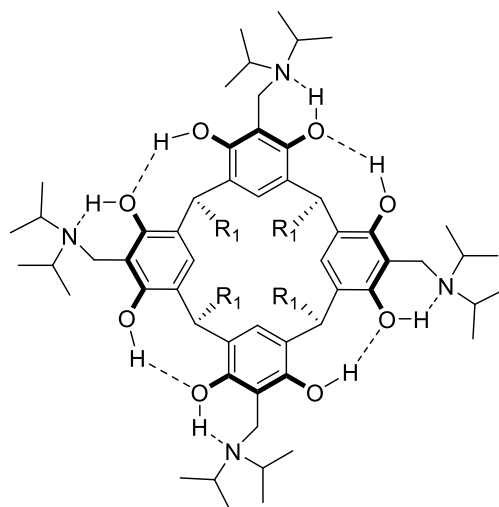
**$^{13}\text{C}$  NMR –  $\text{CDCl}_3$**



**$^1\text{H}$  NMR –  $\text{CCl}_4$**

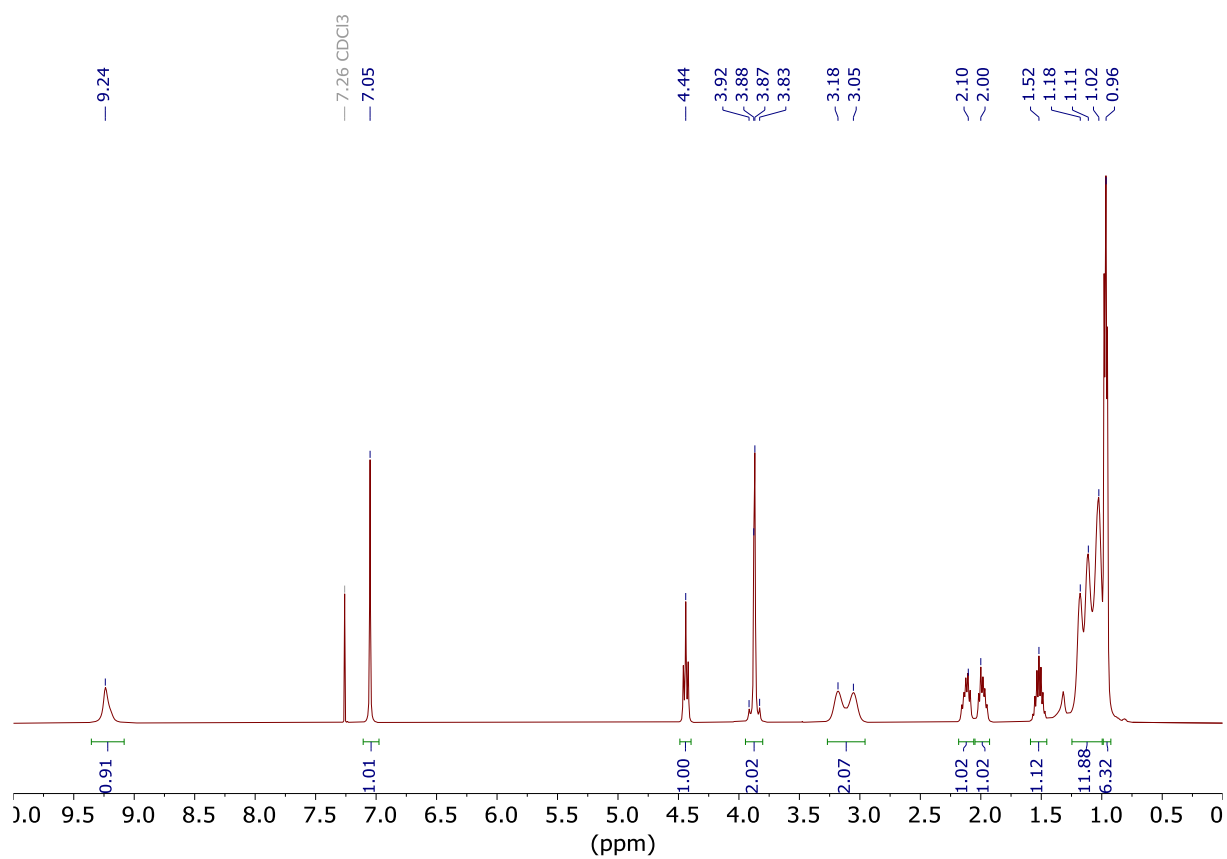


# NMR Spectra of **4**

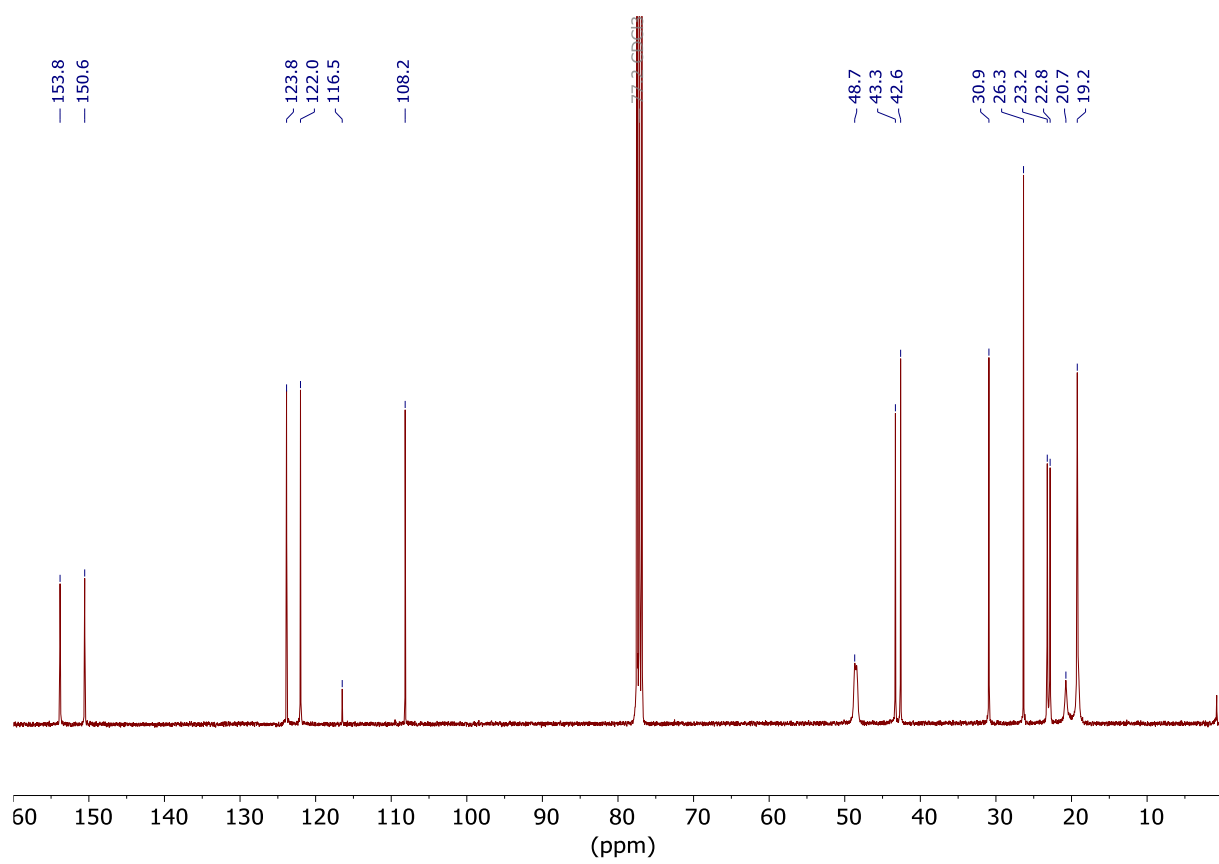


$R_1 = \text{CH}_2\text{CH}(\text{CH}_3)_2$

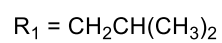
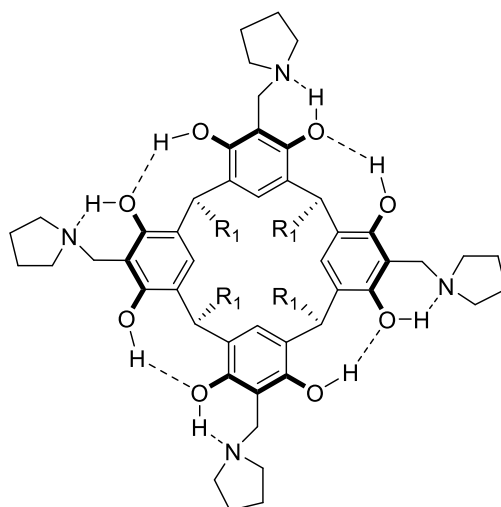
$^1\text{H}$  NMR –  $\text{CDCl}_3$



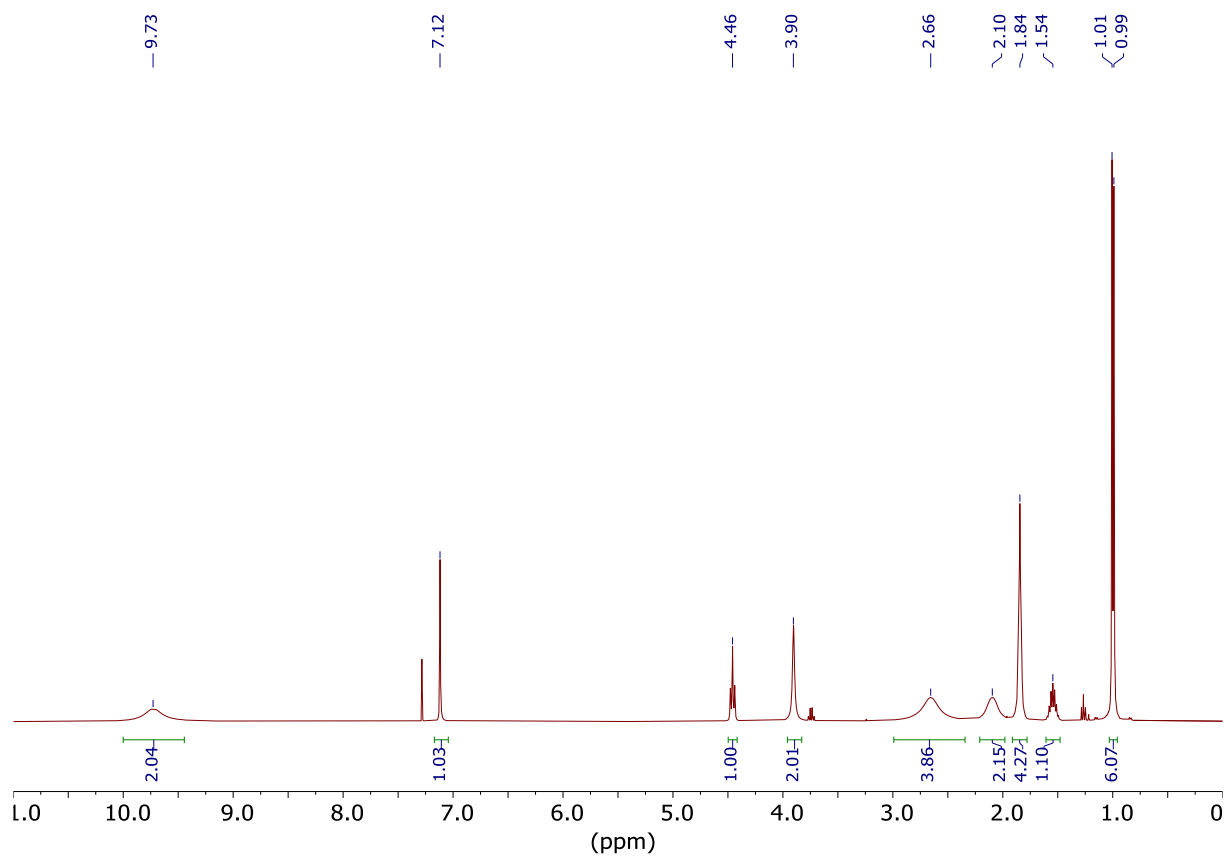
$^{13}\text{C}$  NMR –  $\text{CDCl}_3$



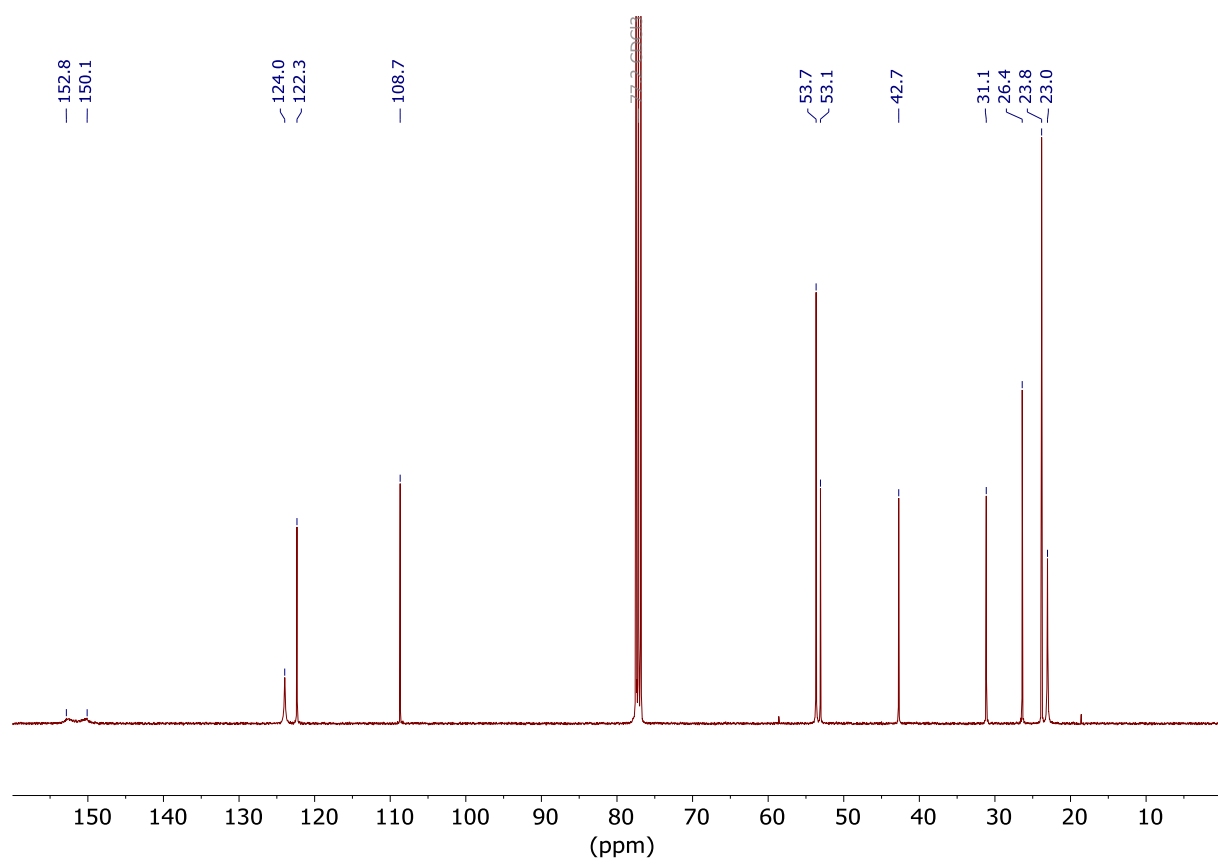
# NMR Spectra of **5**



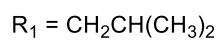
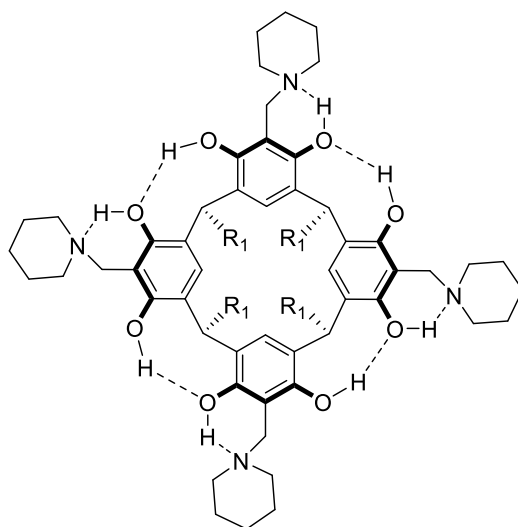
$^1\text{H}$ NMR –  $\text{CDCl}_3$



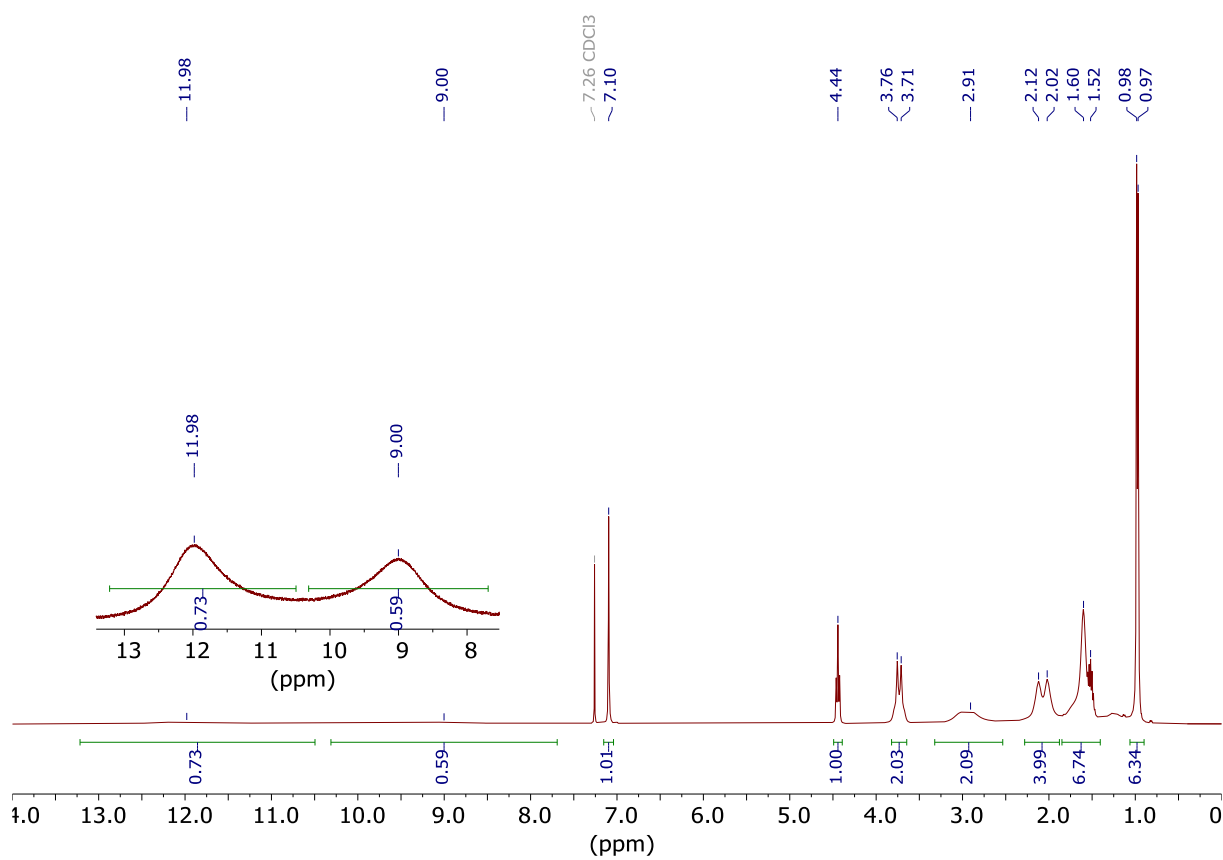
$^{13}\text{C}$  NMR –  $\text{CDCl}_3$



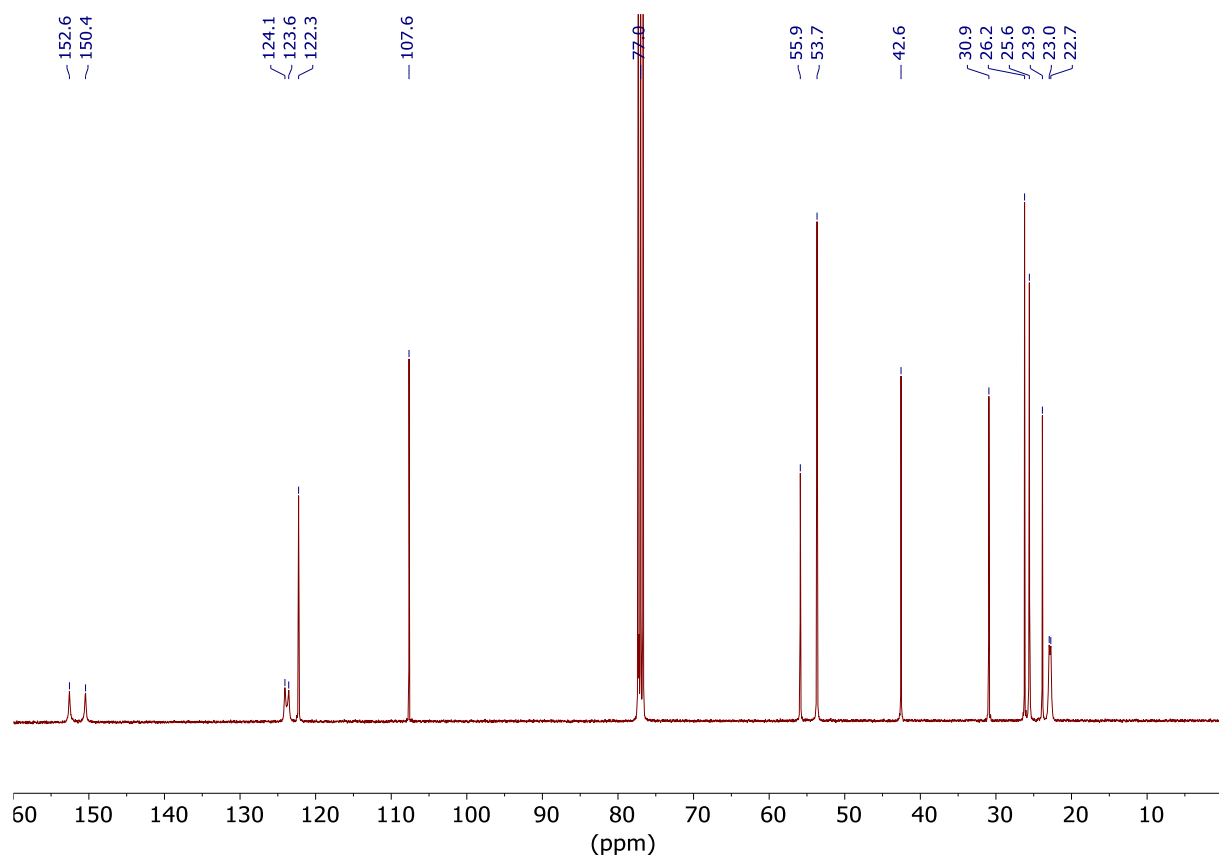
# NMR Spectra of **6**



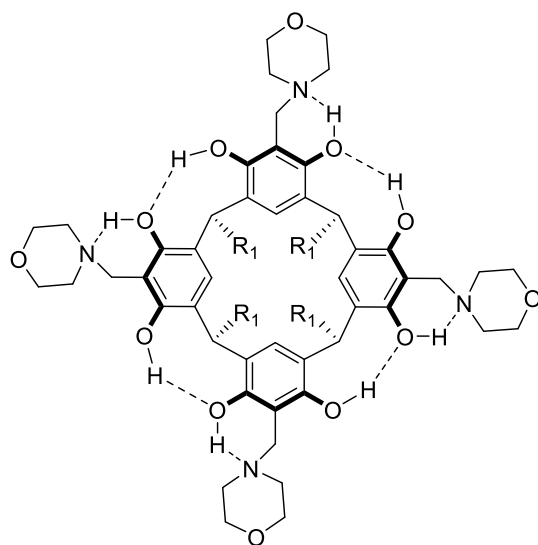
$^1\text{H}$  NMR –  $\text{CDCl}_3$



$^{13}\text{C}$  NMR –  $\text{CDCl}_3$

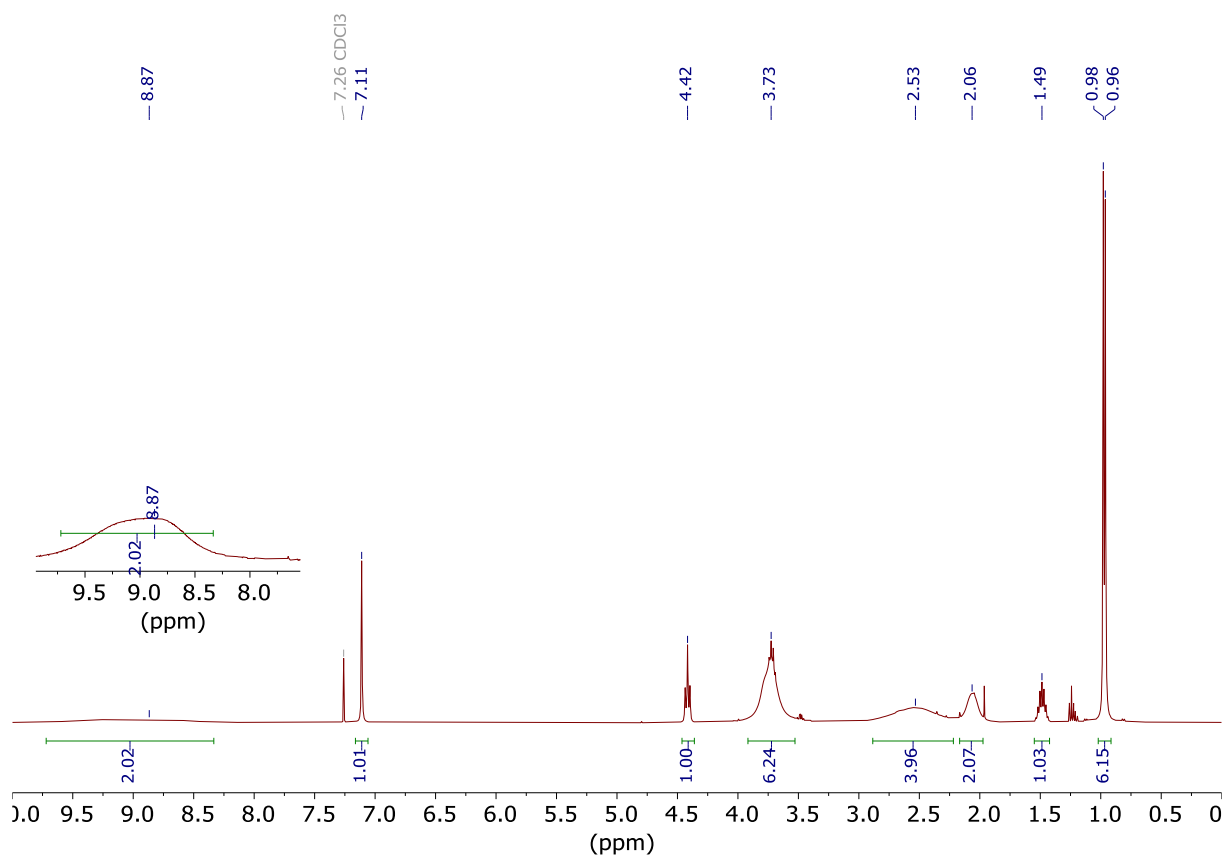


# NMR Spectra of **7**



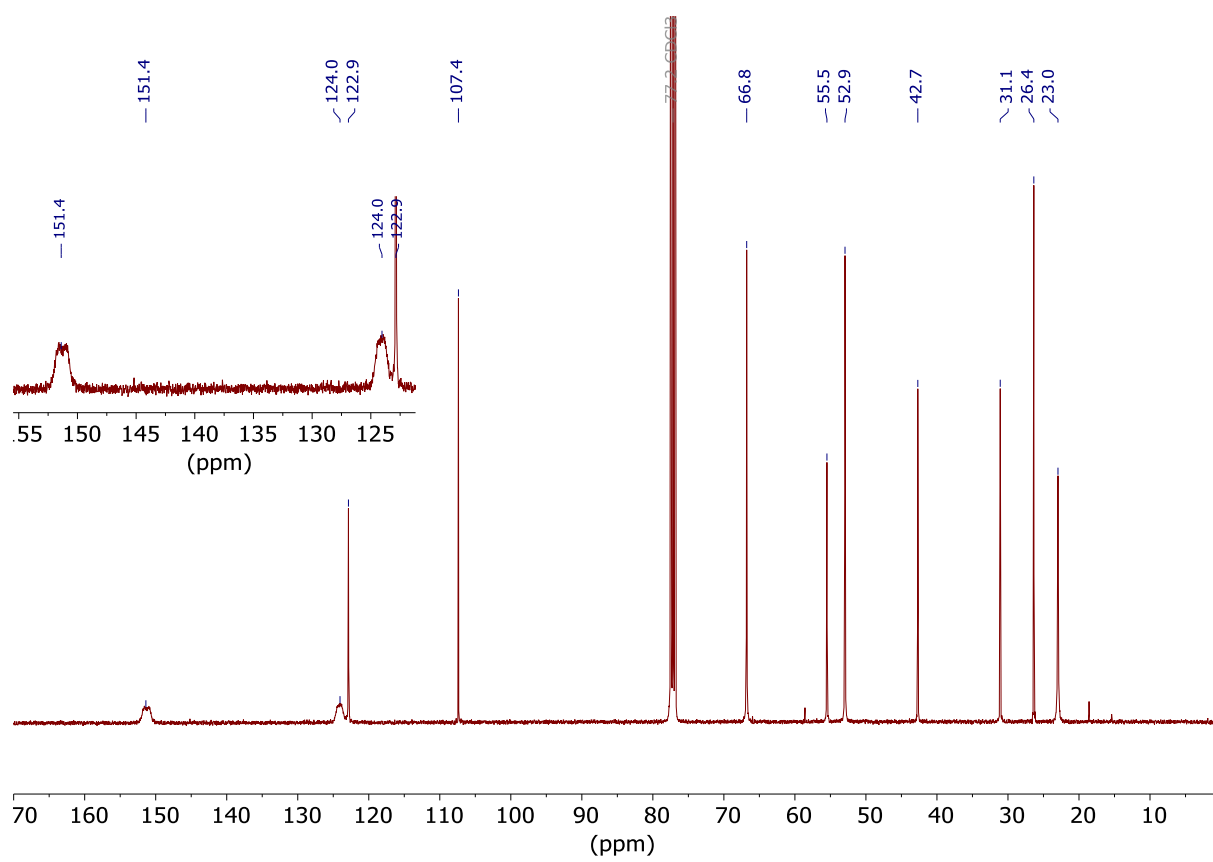
$R_1 = \text{CH}_2\text{CH}(\text{CH}_3)_2$

$^1\text{H}$  NMR –  $\text{CDCl}_3$

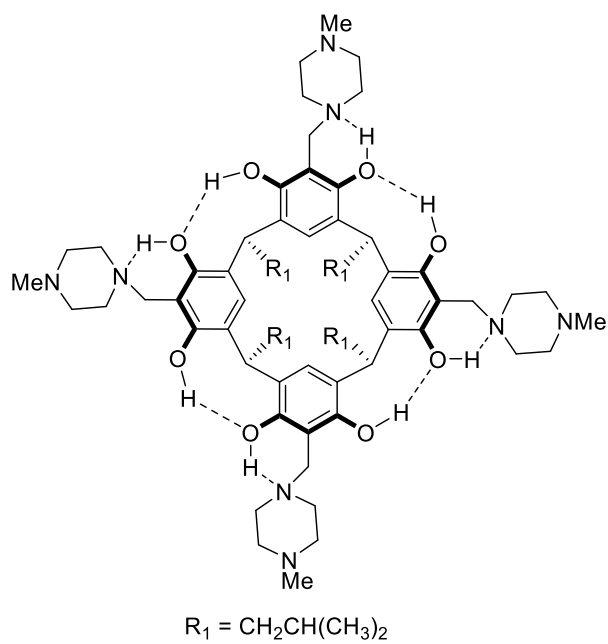




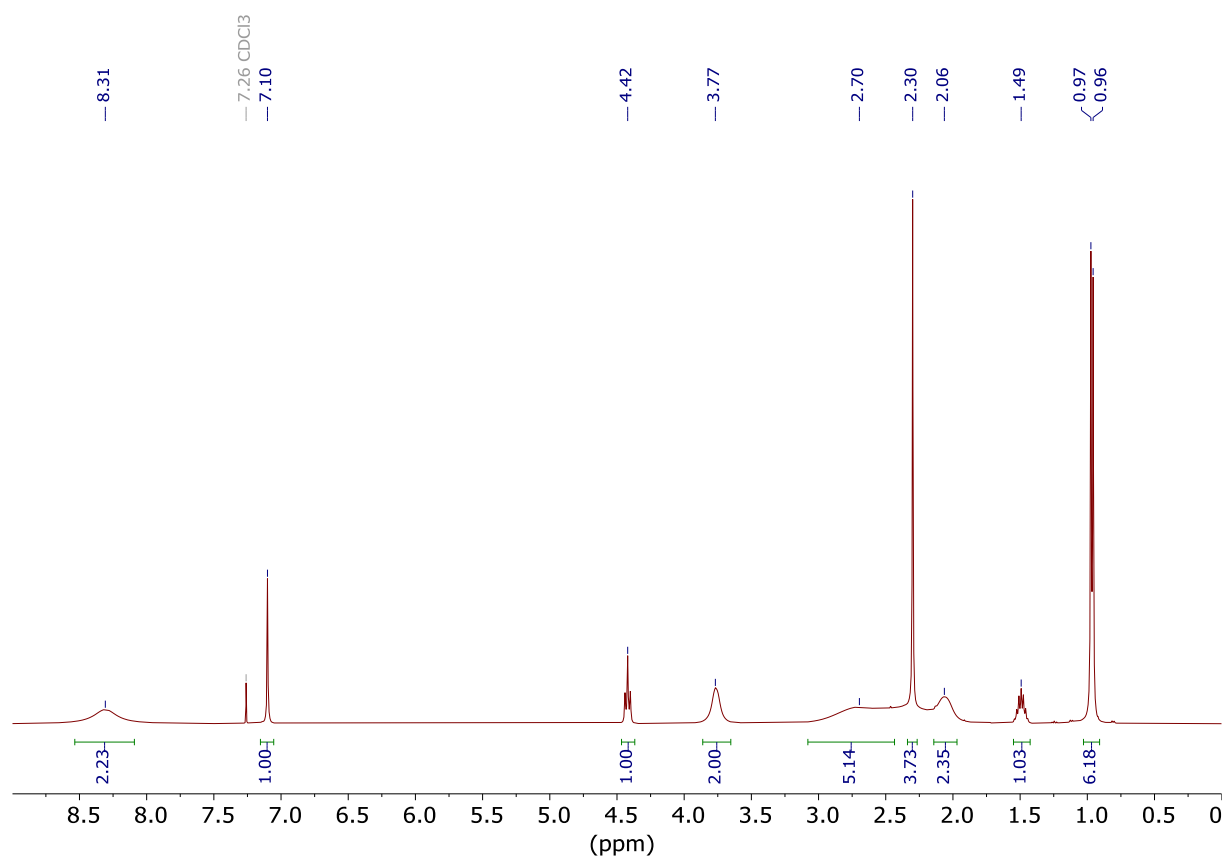
$^{13}\text{C}$  NMR –  $\text{CDCl}_3$



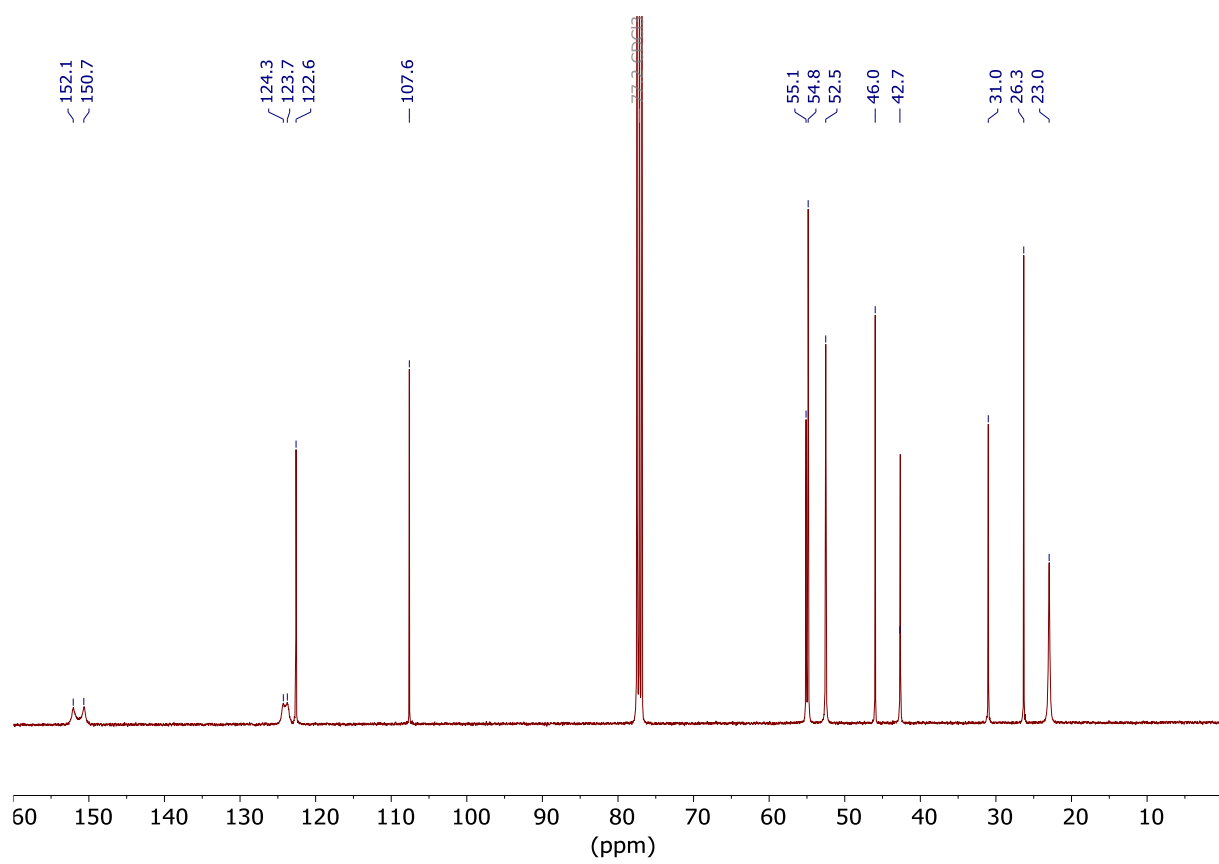
# NMR Spectra of **8**



$^1\text{H}$  NMR –  $\text{CDCl}_3$



$^{13}\text{C}$  NMR –  $\text{CDCl}_3$



## 2. The xyz coordinates of the optimized structures in CHCl<sub>3</sub>

Substrate (S)			Transition state (TS)			Intermediate state (IS)					
			1								
C	-0.76121095295846	-2.12604270645567	-2.47339497835997	C	-0.687309000	-2.390332000	-2.350802000	C	0.06314321156344	-2.2296851334007	-2.17162040347232
C	0.28542846956428	-2.0602759326219	-3.35565007719029	C	0.316923000	-2.642008000	-2.358021000	C	1.23166455134260	-2.4811867330350	-2.90807489566449
C	0.79252595207197	-1.42292115135870	-4.21942955449393	C	0.808097000	-1.739564000	-4.000837000	C	1.73869482607263	-1.53509705915084	-3.80673040725766
C	0.221159686143487	-0.14584754520107	-4.20528266873154	C	0.260761000	-0.487898000	-4.227967000	C	1.07932801010400	-0.30573679981354	-3.942300852704789
C	-0.85113667701354	0.15314176630795	-3.35465421833207	C	-0.774500000	-0.078883000	-3.364463000	C	-0.08084138404623	-0.0257860187373	-3.22176649725356
C	-1.28735286148905	-0.845921060187	-2.49049282769327	C	-1.199399000	-1.015216000	-2.430970000	C	-0.5445379758164	-0.99595962429444	-2.34196090573154
O	0.8338900816375	-3.65399448743728	-3.3577720746174	O	0.805518000	-3.931075000	-3.173521000	O	0.91375861798578	-3.66096187453379	-2.8110875375665
O	0.57760856272843	0.77478666038136	-5.06235704580386	O	0.784048000	0.411074000	-5.150288000	O	1.6373525199282	0.58589973727774	-4.81459792749729
H	-2.0953540803203	-0.61004123595903	1.81250532950008	H	-1.988179000	-0.733691000	-1.749243000	H	-1.44582697673997	-0.7876809604561	-1.78579007638458
C	-1.52447422155408	1.51252452879985	-3.36944597796770	C	-1.450808000	-1.276803000	-3.465966000	C	-0.83979259784546	1.2762146205796	-3.40458080707277
C	-0.93874009980605	2.42694110778136	-2.314793487962249	C	-0.862224000	-2.270249000	-2.484453000	C	-0.34101290913596	2.398532053798319	-2.44798302083849
C	0.1815878077836	3.25515031948748	-2.63536370129647	C	0.182717000	-3.137375000	-2.863093000	C	0.58630523344472	-2.38539080129228	-2.88337652118101
C	0.3237906746058	4.0881089674638	-1.6808227567163	C	0.779426000	-0.419746000	-1.981948000	C	1.0754078991041	-2.28731021735809	-2.03804122836456
C	0.22371306677321	4.09714692617342	-0.37823749926177	C	0.276909000	-0.479813000	-0.671369000	C	0.59256670276663	4.32692539070183	-0.72323589847507
C	-0.88049361979753	3.3044286376036	-0.03082254358999	C	-0.800185000	-3.282456000	-0.259835000	C	-0.32708760680490	3.39128659470860	-0.39128659470860
C	-1.40818263081743	2.47070051668681	-1.01000506514910	C	-1.320269000	-2.382405000	-1.1802709000	C	-0.75550998465216	2.40770733388490	-1.12517001360602
O	0.627313505044780	3.24100372497516	-5.91299251181360	O	0.613197000	-3.008476000	-5.173292000	O	1.07292226842463	3.22617665029173	-4.17345369693325
H	-2.3586085754506	1.81048019085033	0.42725015351033	H	-2.134580000	-1.04579000	-0.860373000	H	-1.44489280053611	1.66253123152661	-0.76308132152661
C	-1.46417869813426	3.34775895889502	1.36875219499172	C	-1.381350000	-3.412180000	-1.135784000	C	-0.81979328763933	3.45330156489274	1.1890825091530
C	-0.80431793840445	3.23561837470013	2.26889329711618	C	-0.716288000	-2.460045000	-2.108720000	C	-0.07170961201320	2.48491090852714	2.08682871386831
C	0.2562523982131	2.69138389934962	3.09734842215202	C	0.311103000	-2.886459000	-2.949540000	C	1.07370270409832	2.88173983081355	2.78905157093666
C	0.89249545329203	1.7613226473740	3.9279636210760	C	0.89249545329203	1.7613226473740	3.9279636210760	C	0.89249545329203	1.7613226473740	3.9279636210760
C	0.34960840285329	0.43926614379733	3.9357691278810	C	0.494617000	-0.691970000	-3.920450000	C	1.24551945099853	0.7060211341255	3.80920754034414
C	-0.05028234229279	0.04970268356672	3.14183883803713	C	-0.560386000	-0.242501000	-3.121560000	C	0.09863916302059	0.2762857145222	3.12731670789590
C	-1.21473351462524	1.00220282762828	1.215355361540803	C	-1.114763000	-1.137665000	-2.217840000	C	-0.55779109193806	1.18793853809397	2.26971537118477
O	0.6896189013397	3.98938213895828	3.0793304143300	O	0.6896189013397	3.98938213895828	3.0793304143300	O	0.6896189013397	3.98938213895828	3.0793304143300
O	1.09613278357308	-0.43159829210864	4.75879984814598	O	1.138064000	-0.110630000	4.809173000	O	1.92804403259938	-0.11273380460244	4.6651570608785
H	-2.0405990234573	0.7088655858632	1.67537319342255	H	-1.9247278000	0.977423000	1.588793000	H	-1.40275120417570	0.87607769939787	1.607910091609346
C	-0.21196862648171	-1.36315743031539	3.19197946099318	C	-1.109988000	-1.165101000	-3.295920000	C	-0.47006651917362	-1.1124027419652	3.34874066768644
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C	0.55420443374273	-2.96886551086604	2.36080314198661	C	0.55420443374273	-2.96886551086604	2.36080314198661	C	1.13899165118902	-0.9076029204355	2.72439362870592
C	1.16136524770707	-3.75455204591524	1.38107543727115	C	1.16136524770707	-3.75455204591524	1.38107543727115	C	1.679296036241859	-3.90357502813991	1.83596030706125
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C	-1.12607353487059	-2.3043694002038	0.8256070819867	C	-1.12607353487059	-2.3043694002038	0.8256070819867	C	-0.40030750170569	-2.2522946827122	1.07137011861594
C	-1.10386308121212	-2.92096605808012	3.6192130155483	C	-1.10386308121212	-2.92096605808012	3.6192130155483	C	0.162417812246752	-2.61933687030564	-0.23121292080451
O	1.21870630595781	-4.59105091394061	-0.8158487968567	O	1.21870630595781	-4.59105091394061	-0.8158487968567	O	1.61179334230694	-4.88460456230695	-0.3461095050887
H	-2.01956200016515	-1.7393389117569	0.60145242673176	H	-2.01956200016515	-1.7393389117569	0.60145242673176	H	-1.20047460089260	-1.58480815506014	0.77077941672877
C	-1.2618067586976	-3.20195740058528	3.0793304143300	C	-1.2618067586976	-3.20195740058528	3.0793304143300	C	-0.5180423115124	-2.2718851547896	1.6627871260734
C	-3.05125528266261	1.4211012747665	-3.2966271496417	C	-2.977570000	1.185140000	-3.367614000	C	-2.3630454872694	1.123802450989	-3.3534500549866
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C	-2.7329915256628	-1.4093923284616	2.04882751419861	C	-2.7329915256628	-1.4093923284616	2.04882751419861	C	-2.0011264025486	-1.1506552748562	1.6802786654093
H	-0.88495500869475	-1.79936238699475	4.1357737188607	H	-0.809909000	-1.534579000	-2.326711000	H	-1.5777702608716	-1.43545140863894	4.33809174606206
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C	-3.70365069494698	3.598393740056724	4.50392350831683	C	-3.70365069494698	3.598393740056724	4.50392350831683	C	-6.25957423384293	3.51271153984293	1.6402786654093
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H	-3.38446971805702	4.02831910593784	0.72065673981828	H	-3.38446971805702	4.02831910593784	0.72065673981828	H	-2.77843546049532	4.05930684626276	0.60250537920218
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2

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H	4.32840742927623	-6.1232748800996	2.73744603590997	H	2.33893239283052	-5.58932628270726	4.13287599639918	H	1.60186018043461	-7.1591706363200	3.2743540489631
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H	-0.19187588102092	6.08769048457491	-3.00371737238579	H	3.3700674345856	6.2805428240832	-1.52145952523652	H	-0.19847167902082	5.90313769838568	-3.44005801439327
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3

C	-0.76957974992748	-2.08301393626082	-2.55753835740033	C	-0.509534000	-2.347401000	-2.337371000	C	-0.246761000	-2.210986000	-2.084317000
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C	-1.28226575796272	-0.79508708504333	-2.53241156023940	C	-0.979532000	-1.046882000	-4.217223000	C	-0.818827000	-0.958452000	-2.234208000
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H	-3.34761266587443	-6.50578848110885	-0.51595698581343	H	-3.107729000	-6.489777000	0.105747000	H	-3.079990000	-6.46449000	-0.029003000
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C	3.70087291744578	3.36085587791746	6.42979662077328	C	2.090233000	3.004606000	7.435205000	C	3.430486000	2.635793000	6.938123000
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C	-1.2132296663371	-1.40157159479	2.06735079191249	C	-1.0625752495193	1.0625752495193	2.06735079191249	C	-0.8626680717004	1.5886569078450	1.47479221700759
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C	-3.63642052778929	-8.55442012971240	-1.783660248740817	C	-1.08472675877841	-4.5945959990311	-2.36798124259978	C	2.98026209699413	6.31136375816225	-4.4064863472703
C	-0.607162430394	1.7833949647031	6.67471011778662	C	-2.5648626139494	-2.5648626139494	-2.5648626139494	H	-2.347423996536201	-0.8846987992407	-3.88469917474739
C	-1.22017670049228	8.0879122859757	2.49482125716895	C	-2.24842489066841	8.902539066032	0.88133213706192	C	1.80348112189392	2.45927194693158	6.7329877352288
N	-2.46891923908325	2.748891973413043	2.86444802765217	N	-1.63777307777192	2.86444802765217	2.03174603074403	C	3.68206567892926	3.6918197539609	