

Supporting Information for —

**Efficient Multigram Procedure for the Synthesis of Large
Hydrazone-linked Molecular Cages**

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I. General Methods and Materials

^1H NMR spectra were recorded at 298 K on a Varian Unity Inova 500 (500 MHz) spectrometer, a Bruker ARX 500 (500 MHz) spectrometer or a Bruker Avance-III-800 (800 MHz) spectrometer. ^{13}C (^1H) NMR spectra were recorded at 298 K on a Bruker ARX 500 (125 MHz) spectrometer or a Bruker Avance-III-800 (200 MHz) spectrometer with a QCI cryoprobe. Samples for NMR spectroscopy were dissolved in CDCl_3 , CD_2Cl_2 or DMSO-d_6 . The spectra were referenced to the residual solvent peak (CDCl_3 : 7.26 ppm for ^1H and 77.16 ppm for ^{13}C (^1H) NMR), or to tetramethylsilane (TMS, 0.00 ppm for ^1H and ^{13}C (^1H) NMR) as the internal standard. Chemical shift values are reported in parts per million (ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad peak), coupling constants (Hz), and number of protons. The raw ^1H NMR and ^{13}C (^1H) NMR spectral data were processed and analyzed with the MestReNova software suite (version 14.0.1).

II. DOSY NMR Spectroscopy

The NMR samples for ^1H DOSY NMR spectroscopy were prepared in CD_2Cl_2 (0.3 mL) at room temperature and recorded with chloroform-d-matched Shigemi NMR tubes. The ^1H DOSY NMR spectra were acquired on a Bruker Avance-III-800 (800 MHz) spectrometer, equipped with a 5mm QCI Z-gradient cryoprobe, and a Z-axis field gradient module. The DOSY pulse program used was a standard double-stimulated-echo experiment with bipolar gradient pulses and convection compensation. All experiments were acquired at 298 K and DOSY spectra were processed/analyzed using Bruker's TopSpin (version 4.1.1) software. The hydrodynamic radii were estimated using the Stokes-Einstein equation. This equation was solved for r using values for η from the literature.

$$r = \frac{k_B \cdot T}{6 \cdot \pi \cdot \eta \cdot D}$$

D is the measured diffusion coefficient (m^2/s)

k_B is Boltzmann constant ($1.3806485 \cdot 10^{-23} \text{ kg m}^2/\text{s}^2 \text{ K}$)

T is the temperature (K)

r is the solvodynamic radius of the analyte (m)

η is the viscosity of the solvent (0.00041 kg/m s)

Table S1. Diffusion coefficients measured by ^1H DOSY NMR spectroscopy in CD_2Cl_2 for the molecular cages **10**, **11**, **12**, and **13**. The corresponding solvodynamic radii r were determined with the Stokes-Einstein Equation. See Figures SX–SX for the ^1H DOSY NMR spectra.

Compound	T [K]	Log D [$\log(\text{m}^2/\text{s})$]	$D \cdot 10^{-10}$ [m^2/s]	r (nm)
10	298	−9.56	2.75	1.9
11	298	−9.67	2.14	2.5
12	298	−9.70	2.00	2.7
13	298	−9.85	1.41	3.8

III. Computational Details

Quantum Mechanical Calculations. All structures were optimized with the Jaguar software package^{1,2} at the B3LYP/LACVP* level^{3,4,5,6} of theory. The structures of the molecular cages **10**, **11**, **12**, and **13** were optimized for model compounds with the peripheral $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups. Due to their very large structures (the model of cage **13**, for example, contains over 600 atoms), we had to optimize the structures of the molecular cages in cartesian coordinates, with loose (Jaguar keyword: `iaccg = 3`) convergence criteria in order to be able to get the geometry optimizations to converge.

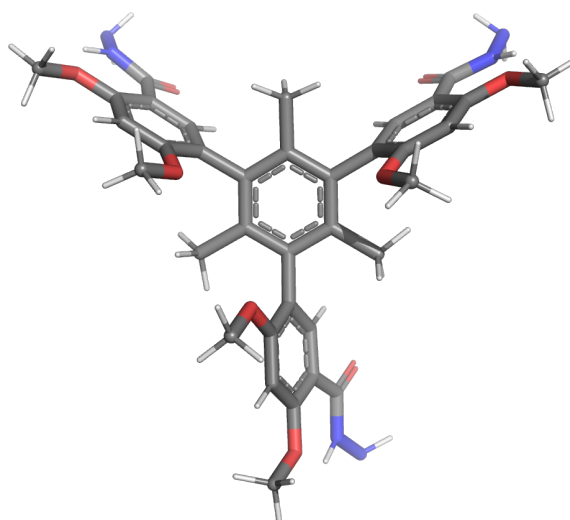
To calculate the rotational barrier for conversion of *syn-9* to *anti-9*, we first performed a minimum energy dihedral scan at the B3LYP/LACVP* level, which performed a rotation around one of the rotationally restricted phenyl-phenyl single in *syn-9*. This initial dihedral scan revealed structures close to the *syn-9* to *anti-9* transition state and the two structures closest to the transition state (one to either side of the transition state) were then used as the input for an LST transition state search (with an initial LST guess of 0.5) in Jaguar. The transition state search (which was also performed at the B3LYP/LACVP* level) then yielded the geometry of the transition state for the *syn-9* to *anti-9* atropoisomer conversion. The nature of the transition state was verified by a frequency calculation at the B3LYP/LACVP* level, which showed one imaginary frequency at 32 cm^{-1} .

Finally, to ensure that we found the correct transition state for the *syn-9* to *anti-9* conversion, we performed an intrinsic reaction coordinate scan (Figure 2a) at the B3LYP/LACVP* level, which proceeded energetically downhill in both directions from the transition state to afford *anti-9* in the forward direction, and *syn-9* in the reverse direction. To calculate the rotational barrier, we then performed single point calculations at the B3LYP/aug-cc-pVDZ level on the

optimized structures of *syn-9*, *anti-9*, and the *syn-9* to *anti-9* transition state, which provided an overall activation energy of 28.5 kcal/mol for the *syn-9* to *anti-9* interconversion.

IV. DFT-optimized Cartesian Coordinates (in Å)

Model of *syn-9* (with the $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups)

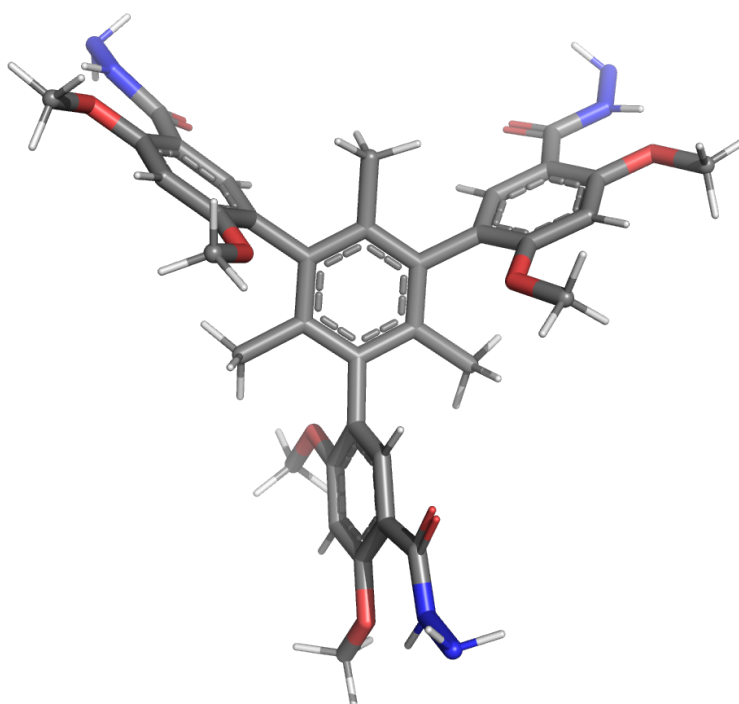


C	3.75030	17.27560	6.42920
C	4.92550	17.11730	5.66850
C	6.18920	17.10980	6.28980
C	6.27410	17.26230	7.68970
C	5.10560	17.43230	8.45960
C	3.84660	17.43420	7.82430
C	4.65330	16.69080	1.36670
C	4.55870	17.95650	1.95630
C	4.64490	18.09530	3.34580
C	4.82930	16.97070	4.17720
C	4.91640	15.73040	3.55250
C	4.83450	15.54210	2.16300
H	4.41640	18.82980	1.33620
H	5.04790	14.83610	4.15250
C	0.31030	17.99920	10.26180
C	0.97390	16.75460	10.28570
C	2.10810	16.61760	9.46980
C	2.61120	17.62790	8.65440
C	1.92270	18.85910	8.66260
C	0.78340	19.04030	9.45480
H	2.60430	15.65320	9.49560
H	0.26890	19.99030	9.44570

C	10.10290	17.29860	9.71320
C	9.44560	18.50050	9.42480
C	8.21600	18.48850	8.75820
C	7.61580	17.27350	8.36440
C	8.30830	16.10180	8.65340
C	9.54250	16.06510	9.32380
H	9.88860	19.44140	9.71870
H	7.88630	15.14390	8.36860
C	2.40420	17.30250	5.73910
H	2.20160	18.30260	5.33550
H	2.36950	16.59920	4.90270
H	1.59580	17.05380	6.42960
C	5.18230	17.64810	9.95790
H	4.59010	16.90720	10.50340
H	6.20720	17.58630	10.32310
H	4.78240	18.63310	10.22870
C	7.44160	16.95810	5.44960
H	8.32070	17.33980	5.97180
H	7.63870	15.90520	5.20780
H	7.34630	17.49010	4.49830
O	-0.80220	18.15520	11.05110
C	-1.50090	19.39190	11.04320
H	-2.33720	19.26620	11.73310
H	-0.86440	20.21480	11.39170
H	-1.88800	19.62660	10.04390
O	11.30660	17.28330	10.37340
O	4.56660	16.52670	0.00630
C	4.38230	17.66100	-0.82780
H	3.44020	18.17630	-0.60200
H	5.21740	18.36660	-0.73470
H	4.34710	17.27620	-1.84880
C	11.86570	18.50240	10.84070
H	12.10630	19.17830	10.01040
H	11.19070	19.00880	11.54210
H	12.78610	18.22760	11.35910
O	2.43180	19.83810	7.86390
O	4.55870	19.30040	3.97620
O	7.52260	19.62160	8.45780
C	4.40670	20.47550	3.20020
H	3.47030	20.46600	2.62560
H	5.25050	20.61920	2.51180
H	4.38160	21.30200	3.91330
C	1.78400	21.09670	7.81510
H	2.36450	21.70290	7.11690
H	0.75300	21.00980	7.44610
H	1.77500	21.58850	8.79750
C	8.05450	20.87850	8.83670
H	7.33090	21.62230	8.49720
H	9.02300	21.07140	8.35520
H	8.17070	20.95860	9.92590

C	10.11100	14.68950	9.55310
O	9.56010	13.68410	9.10060
N	11.25440	14.58230	10.29240
H	11.77340	15.39840	10.57720
N	11.88470	13.33770	10.48660
C	4.93710	14.11310	1.69910
O	5.00830	13.18170	2.50330
N	4.92620	12.55580	-0.14730
H	4.74870	14.60590	-0.30660
N	4.95960	13.87320	0.35370
C	0.61990	15.54430	11.10920
O	1.32490	14.53320	11.09900
N	-0.51300	15.59510	11.87060
H	-1.03170	16.45360	11.97840
N	-0.85600	14.54290	12.74170
H	-1.09500	13.73750	12.16010
H	0.00400	14.26350	13.21860
H	11.25330	12.76860	11.05390
H	11.89690	12.86970	9.57780
H	5.83700	12.13710	0.05070
H	4.27540	12.03530	0.44500

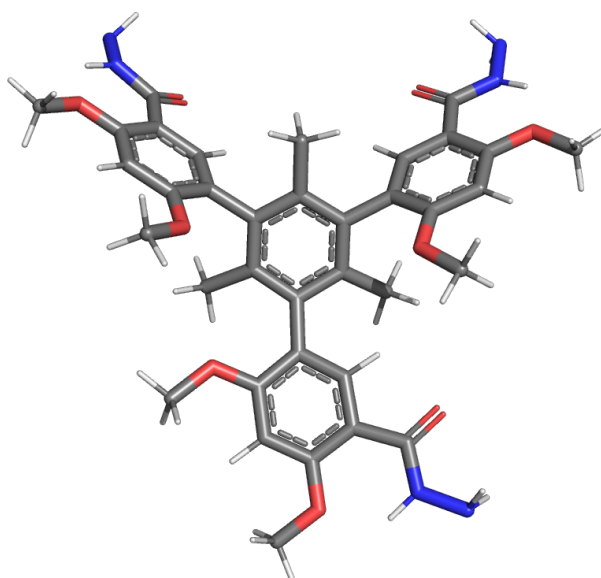
Model of *anti*-9 (with the $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups)



C	3.81490	17.60990	6.39620
C	5.02070	17.41900	5.69640
C	6.20280	17.07080	6.38340
C	6.16390	16.88850	7.77980
C	4.95800	17.06880	8.48980
C	3.79420	17.44720	7.79540
C	5.23990	17.93400	1.40340
C	5.14600	19.05120	2.24130
C	5.06530	18.88770	3.62880
C	5.06970	17.60100	4.20770
C	5.15430	16.51670	3.34000
C	5.24500	16.63190	1.94360
H	5.13930	20.04450	1.81650
H	5.15430	15.50860	3.74100
C	0.15660	18.17780	10.02990
C	1.07240	19.23260	9.83680
C	2.23250	18.94690	9.09720
C	2.52400	17.69910	8.55700
C	1.58340	16.66900	8.77090
C	0.41140	16.90710	9.49820
H	2.92830	19.76700	8.95600
H	-0.29690	16.10580	9.65180
C	9.76260	15.80050	9.93170
C	9.24580	17.09750	10.03170
C	8.08510	17.45190	9.33480
C	7.41280	16.51300	8.52240
C	7.96270	15.23650	8.44360
C	9.12450	14.83630	9.12430
H	9.74660	17.83090	10.64700
H	7.48330	14.48280	7.82810
C	2.55470	18.00790	5.65810
H	2.43800	19.09920	5.64240
H	2.57760	17.66560	4.62010
H	1.66420	17.59280	6.13550
C	4.91880	16.86880	9.99050
H	3.93240	16.54140	10.32500
H	5.65300	16.12460	10.31050
H	5.14870	17.80370	10.51770
C	7.50340	16.92330	5.61770
H	8.36620	17.03170	6.27660
H	7.58340	15.93960	5.13750
H	7.57920	17.67090	4.82270
O	-0.98500	18.43790	10.74640
C	-1.92640	17.39720	10.96880
H	-2.73150	17.84590	11.55390
H	-2.33360	17.01560	10.02380
H	-1.48130	16.57030	11.53700
O	10.89910	15.42920	10.60600

O	5.32320	18.06670	0.03960
C	5.31380	19.36270	-0.54140
H	4.38200	19.89620	-0.31540
H	6.16940	19.96010	-0.20210
H	5.38760	19.20570	-1.61910
C	11.55010	16.36460	11.45340
H	11.91450	17.23210	10.88870
H	10.88680	16.70370	12.25900
H	12.39980	15.83250	11.88500
O	1.89470	15.45970	8.23270
O	4.98320	19.93330	4.49600
O	7.54010	18.69760	9.38850
C	4.98710	21.25690	3.98960
H	4.12760	21.44150	3.33150
H	5.91440	21.47800	3.44450
H	4.91780	21.90850	4.86250
C	1.00570	14.36950	8.41230
H	1.46910	13.52160	7.90460
H	0.87400	14.12760	9.47540
H	0.02460	14.56960	7.96090
C	8.15930	19.69320	10.18540
H	7.54380	20.58760	10.07330
H	9.17960	19.90930	9.84130
H	8.18780	19.40420	11.24430
C	9.54820	13.40960	8.89500
O	8.92130	12.66710	8.13630
N	10.65350	12.95460	9.55600
H	11.23350	13.57790	10.09620
N	11.16800	11.66490	9.31870
C	5.34210	15.33010	1.19390
O	5.23130	14.24690	1.77190
N	5.57400	14.20530	-0.93170
H	5.51500	16.25060	-0.65640
N	5.57900	15.37970	-0.15140
C	0.95650	20.64820	10.33460
O	1.80390	21.50090	10.05700
N	-0.11650	20.96710	11.11760
H	-0.87330	20.31440	11.25640
N	-0.34210	22.29070	11.54360
H	0.40190	22.52500	12.20220
H	-0.16470	22.89230	10.73570
H	10.47690	10.99770	9.66670
H	11.16270	11.52820	8.30560
H	6.42610	13.69000	-0.70190
H	4.81880	13.61890	-0.56900

Transition State for *syn-9* to *anti-9* conversion (with the $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups)

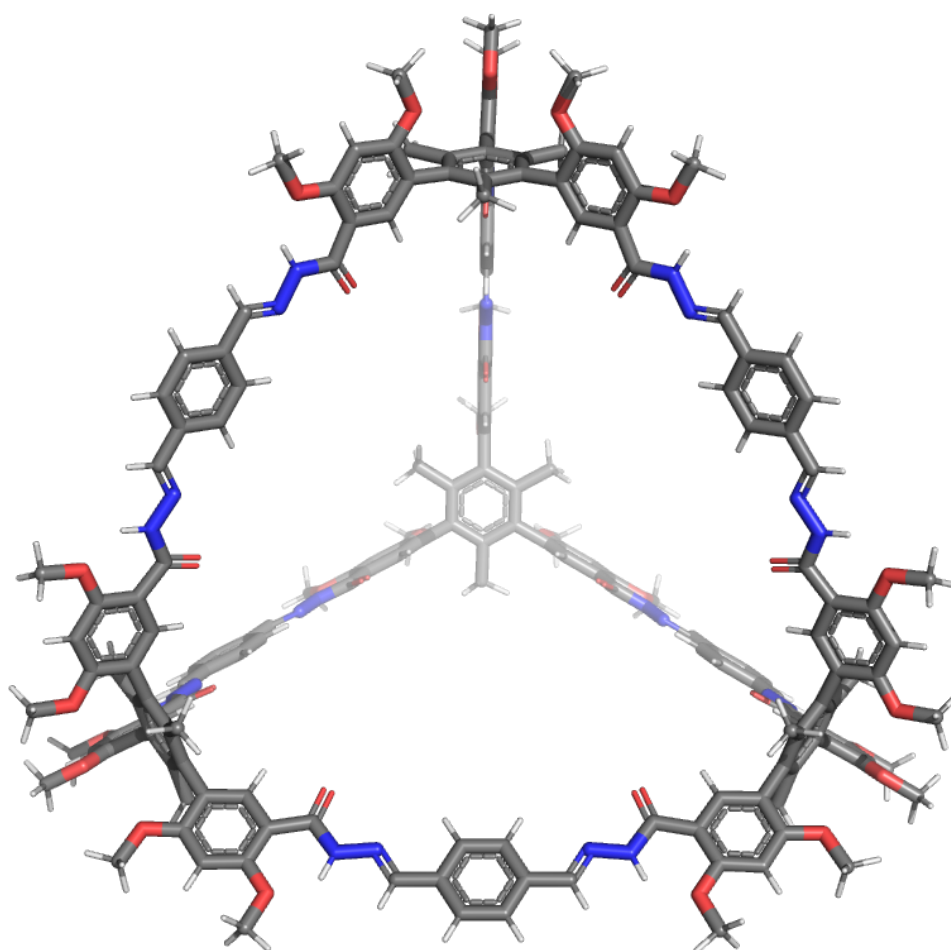


C	3.67790	17.02520	6.25430
C	4.90530	17.14470	5.56850
C	6.12250	17.27150	6.26020
C	6.10920	17.02630	7.64490
C	4.89050	16.88270	8.33850
C	3.64980	17.16110	7.67710
C	4.98360	17.11380	1.23820
C	4.50780	18.23670	1.92500
C	4.47320	18.24560	3.32380
C	4.91720	17.13160	4.06780
C	5.37940	16.03490	3.34660
C	5.42990	15.97890	1.94450
H	4.16670	19.10120	1.37390
H	5.72260	15.15180	3.87550
C	0.32830	18.42270	10.27530
C	1.62880	18.23990	10.78040
C	2.61790	17.85960	9.87050
C	2.46130	17.61250	8.49140
C	1.19020	18.06350	8.01610
C	0.13990	18.37390	8.89690
H	3.59460	17.80670	10.31350
H	-0.82760	18.61840	8.48460
C	9.72480	16.58280	9.98210
C	8.85350	17.65020	10.22600
C	7.69970	17.81220	9.45260
C	7.38780	16.90230	8.41590

C	8.29230	15.86820	8.19080
C	9.46150	15.66770	8.94210
H	9.07100	18.35490	11.01560
H	8.09540	15.14330	7.40830
C	2.49870	16.52600	5.43560
H	2.06700	17.28400	4.77660
H	2.85600	15.70850	4.79930
H	1.70510	16.12820	6.06610
C	4.96460	16.22570	9.71400
H	4.01630	15.75490	9.98120
H	5.72330	15.43740	9.67260
H	5.24950	16.89300	10.53450
C	7.40610	17.58240	5.52080
H	8.15720	17.99430	6.19840
H	7.84370	16.69150	5.05220
H	7.22660	18.30680	4.71990
O	-0.69130	18.69880	11.14910
C	-2.01180	18.86070	10.65050
H	-2.64550	19.00830	11.52680
H	-2.08890	19.73850	9.99660
H	-2.34340	17.96770	10.10660
O	10.85440	16.39610	10.73890
O	5.02510	17.07740	-0.13390
C	4.58200	18.20240	-0.87860
H	3.52280	18.41700	-0.68850
H	5.18170	19.09320	-0.65340
H	4.71330	17.93460	-1.92860
C	11.09660	17.24080	11.85520
H	11.25070	18.28190	11.54540
H	10.27310	17.19180	12.57840
H	12.00990	16.86470	12.31970
O	1.02630	18.26790	6.68550
O	4.02130	19.30840	4.04580
O	6.81740	18.82730	9.65040
C	3.58880	20.47410	3.36810
H	2.72970	20.27020	2.71390
H	4.39630	20.92050	2.77220
H	3.28780	21.17640	4.14800
C	-0.17870	18.81400	6.18310
H	-0.02210	18.92920	5.10880
H	-1.03330	18.14430	6.34790
H	-0.39500	19.79450	6.62760
C	6.98980	19.70030	10.75610
H	6.12840	20.36980	10.74020
H	7.91210	20.29020	10.66560
H	6.99650	19.14940	11.70490
C	10.28360	14.47080	8.54670
O	9.97320	13.76760	7.58290
N	11.38620	14.17530	9.29620
H	11.70710	14.79600	10.02330

N	12.24650	13.11660	8.94520
C	5.95370	14.69030	1.36870
O	6.20660	13.72260	2.08870
N	6.54020	13.41780	-0.59970
H	5.81500	15.35070	-0.59270
N	6.15780	14.62550	0.01880
C	2.10130	18.45720	12.19180
O	3.29820	18.41170	12.49310
N	1.15550	18.71100	13.14250
H	0.18790	18.84980	12.89200
N	1.50800	19.01170	14.47240
H	1.91040	18.16410	14.87680
H	2.28870	19.66960	14.42850
H	11.71650	12.25030	9.05910
H	12.40100	13.18620	7.93710
H	7.51000	13.23890	-0.33210
H	6.01030	12.67430	-0.13960

Model of the phenyl-linked molecular cage 10 (with the $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups)



C	0.74150	-3.67680	-7.87080
C	-0.42300	-2.93400	-8.10980
C	-1.69680	-3.51060	-7.91490
C	-1.79250	-4.84400	-7.49000
C	-0.62860	-5.60480	-7.24410
C	0.62990	-5.01550	-7.43480
C	-0.16460	1.07840	-9.69890
C	-0.22120	-0.02040	-10.56080
C	-0.30900	-1.31520	-10.04230
C	-0.33510	-1.53800	-8.65010
C	-0.28390	-0.42050	-7.82680
C	-0.19920	0.89940	-8.30060
H	-0.19790	0.13200	-11.63020
H	-0.30470	-0.54570	-6.74890
C	4.23620	-7.35370	-6.96610
C	3.72030	-6.66690	-5.84860
C	2.54710	-5.91810	-6.04350
C	1.88060	-5.82390	-7.25820
C	2.43310	-6.51970	-8.35290
C	3.59750	-7.27900	-8.20780
H	2.15730	-5.39630	-5.17520
H	4.00560	-7.80850	-9.05650
C	-5.69810	-6.68730	-7.25170
C	-4.96820	-6.72370	-8.44350
C	-3.70060	-6.13870	-8.50750
C	-3.13760	-5.50140	-7.38200
C	-3.88910	-5.49620	-6.21360
C	-5.16710	-6.07120	-6.10050
H	-5.38530	-7.20400	-9.31680
H	-3.49550	-5.01520	-5.32380
C	2.11550	-3.08500	-8.10910
H	2.77660	-3.25590	-7.25320
H	2.59260	-3.55270	-8.98050
H	2.06910	-2.00970	-8.28950
C	-0.76710	-7.05250	-6.82110
H	0.18930	-7.48000	-6.51560
H	-1.46720	-7.15760	-5.98590
H	-1.16110	-7.66060	-7.64640
C	-2.93320	-2.68740	-8.20850
H	-3.84020	-3.18810	-7.86920
H	-2.88450	-1.70730	-7.72290
H	-3.03100	-2.50600	-9.28630
O	5.38250	-8.09730	-6.80310
C	5.91910	-8.81560	-7.90330
H	6.80710	-9.32380	-7.52220
H	5.20800	-9.56140	-8.28010
H	6.20980	-8.14130	-8.71860
O	-6.95070	-7.25130	-7.17200

O	-0.07350	2.35950	-10.19330
C	-0.00690	2.57400	-11.59500
H	0.87340	2.08690	-12.03290
H	-0.91330	2.21630	-12.09910
H	0.07580	3.65470	-11.72650
C	-7.53970	-7.82990	-8.32670
H	-7.64830	-7.09300	-9.13240
H	-6.95680	-8.68620	-8.68830
H	-8.52840	-8.17340	-8.01560
O	1.76710	-6.40110	-9.53540
O	-0.37370	-2.42480	-10.83020
O	-2.94140	-6.13910	-9.63840
C	-0.34040	-2.27080	-12.23680
H	0.59440	-1.80040	-12.57200
H	-1.19160	-1.67960	-12.60210
H	-0.40180	-3.28030	-12.64850
C	2.25600	-7.08720	-10.67280
H	1.56450	-6.84920	-11.48380
H	3.26500	-6.75090	-10.94870
H	2.26920	-8.17470	-10.51690
C	-3.46000	-6.73260	-10.81390
H	-2.68980	-6.60350	-11.57710
H	-4.38350	-6.23780	-11.14500
H	-3.65580	-7.80510	-10.67690
C	-5.79820	-5.93260	-4.73800
O	-5.21300	-5.38970	-3.81500
N	-7.07590	-6.45250	-4.60760
H	-7.51140	-6.89850	-5.41200
N	-7.72340	-6.39060	-3.42520
C	-0.15670	1.95030	-7.22040
O	-0.19980	1.65710	-6.03620
N	-0.03210	4.27860	-6.78120
H	-0.03190	3.44110	-8.66430
N	-0.06760	3.25910	-7.66360
C	4.26190	-6.62500	-4.44230
O	3.71330	-5.97730	-3.56550
N	5.41020	-7.36480	-4.21510
H	5.82310	-7.88420	-4.98660
N	5.97330	-7.39650	-2.98950
C	7.03720	-8.10550	-2.85270
C	9.02610	-8.36110	0.92100
C	9.52680	-9.04820	-0.19360
C	8.87850	-8.96720	-1.42330
C	7.71570	-8.19740	-1.56420
C	7.21190	-7.50950	-0.44090
C	7.85440	-7.58960	0.77760
H	10.43020	-9.64740	-0.09600
H	9.27730	-9.50350	-2.28240
H	6.31110	-6.91560	-0.55670
H	7.47210	-7.06000	1.64420

C	-8.90340	-6.89970	-3.37360
C	-11.13940	-6.87350	0.26930
C	-11.67930	-7.44550	-0.89120
C	-10.95350	-7.45220	-2.07950
C	-9.67210	-6.88580	-2.13280
C	-9.13300	-6.30650	-0.96520
C	-9.85200	-6.30060	0.21250
H	-12.67250	-7.89000	-0.86070
H	-11.38180	-7.90220	-2.97340
H	-8.14160	-5.86800	-1.01360
H	-9.44050	-5.85730	1.11350
C	0.05500	5.46780	-7.26230
C	0.17290	8.88740	-4.69560
C	0.24020	9.03820	-6.08820
C	0.20150	7.92500	-6.92350
C	0.09590	6.63450	-6.38560
C	0.02920	6.48480	-4.98470
C	0.06650	7.58880	-4.15630
H	0.32260	10.03450	-6.51910
H	0.25390	8.05680	-8.00270
H	-0.05260	5.48430	-4.57230
H	0.01470	7.47630	-3.07810
H	0.10120	5.65190	-8.34640
H	7.47330	-8.66390	-3.69480
H	-9.37230	-7.36600	-4.25320
C	-1.18990	13.47440	4.56890
C	0.05830	13.42070	3.92770
C	1.24970	13.32580	4.67600
C	1.18430	13.27070	6.07940
C	-0.06340	13.30970	6.73480
C	-1.23920	13.41730	5.97480
C	0.32620	13.69310	-0.37710
C	0.38450	14.84950	0.40680
C	0.30040	14.75840	1.79890
C	0.14940	13.50960	2.43390
C	0.10280	12.38320	1.62160
C	0.18590	12.42320	0.22000
H	0.49510	15.81540	-0.06430
H	-0.00790	11.40150	2.07140
C	-5.00570	13.77700	8.06930
C	-4.55660	12.49590	7.68630
C	-3.33550	12.42730	6.99420
C	-2.55730	13.53390	6.67920
C	-3.04100	14.79650	7.07700
C	-4.25360	14.91640	7.76330
H	-2.99750	11.43540	6.71100
H	-4.60940	15.89230	8.06070
C	4.83510	13.16760	8.39570
C	4.24830	14.39060	8.05640
C	3.06550	14.42140	7.31070

C	2.44840	13.22610	6.88730
C	3.06020	12.03120	7.24720
C	4.24610	11.94990	7.99670
H	4.71070	15.31460	8.37200
H	2.61540	11.08880	6.94370
C	-2.47670	13.63040	3.78490
H	-2.91740	14.62080	3.96070
H	-2.31550	13.52020	2.71110
H	-3.22350	12.89110	4.09270
C	-0.14970	13.28060	8.24650
H	-0.95920	12.62990	8.58890
H	0.77940	12.92970	8.69670
H	-0.35420	14.28460	8.64090
C	2.57850	13.31970	3.94910
H	3.40830	13.12670	4.62910
H	2.60040	12.55760	3.16300
H	2.75760	14.28750	3.46250
O	-6.19750	13.87750	8.75010
C	-6.65760	15.14970	9.18160
H	-7.59750	14.96390	9.70510
H	-5.94520	15.62070	9.87060
H	-6.84260	15.81810	8.33130
O	6.00040	13.12110	9.12700
O	0.40460	13.76570	-1.74940
C	0.53400	15.02960	-2.38290
H	-0.32510	15.67630	-2.16480
H	1.45990	15.53560	-2.08230
H	0.56750	14.82290	-3.45440
C	6.62990	14.32780	9.53090
H	6.92220	14.93590	8.66570
H	5.98160	14.91690	10.19150
H	7.52480	14.02680	10.07920
O	-2.25990	15.86610	6.75710
O	0.35760	15.84480	2.61920
O	2.44590	15.57920	6.95060
C	0.49220	17.13280	2.04720
H	-0.35610	17.37770	1.39320
H	1.42600	17.22960	1.47620
H	0.51140	17.83100	2.88660
C	-2.67820	17.16340	7.14010
H	-1.90060	17.84330	6.78590
H	-3.63550	17.43630	6.67490
H	-2.76920	17.25560	8.23120
C	3.02060	16.81460	7.33460
H	2.36020	17.58730	6.93570
H	4.02590	16.94470	6.91060
H	3.07570	16.91580	8.42730
C	4.72280	10.54420	8.26870
O	4.11300	9.56880	7.86040
N	5.88870	10.44160	9.00890

H	6.35150	11.29280	9.32000
N	6.40690	9.23350	9.31790
C	0.11460	11.07370	-0.45110
O	0.00050	10.04190	0.19150
N	0.14160	9.94730	-2.54590
H	0.28030	11.98790	-2.30760
N	0.18840	11.09220	-1.83340
C	-5.21070	11.16050	7.93810
O	-4.70890	10.11680	7.55200
N	-6.40560	11.20270	8.63730
H	-6.77460	12.10500	8.92970
N	-7.06740	10.06480	8.93530
C	-8.17030	10.18140	9.58720
C	7.49140	9.22840	10.00970
C	0.21260	10.05830	-3.82560
H	0.30540	11.04040	-4.31400
H	7.97150	10.16480	10.33260
C	9.37100	-4.71320	12.65790
C	10.24870	-4.10330	11.73480
C	10.64460	-4.77750	10.57170
C	10.15610	-6.08060	10.32740
C	9.28350	-6.69900	11.23450
C	8.89360	-6.00650	12.40280
C	11.86380	-0.21280	12.71240
C	12.51390	-1.37680	13.13660
C	11.99000	-2.63230	12.81540
C	10.80570	-2.74920	12.05900
C	10.18760	-1.57160	11.65820
C	10.67480	-0.28790	11.95720
H	13.42350	-1.30490	13.71500
H	9.27320	-1.61620	11.07510
C	6.40990	-8.00340	15.32830
C	5.79220	-7.22630	14.32730
C	6.63430	-6.59820	13.39360
C	8.01970	-6.70070	13.40650
C	8.59710	-7.49480	14.41870
C	7.80100	-8.13680	15.37150
H	6.14680	-5.99750	12.63210
H	8.26090	-8.73710	16.14310
C	11.60080	-8.22830	6.86100
C	12.29100	-8.29770	8.07520
C	11.81900	-7.60070	9.19120
C	10.64560	-6.82230	9.11780
C	9.99050	-6.77630	7.89330
C	10.42540	-7.45900	6.74390
H	13.19080	-8.89100	8.15070
H	9.08230	-6.19070	7.79180
C	8.99500	-3.96930	13.92240
H	8.23440	-4.50370	14.49180
H	9.87140	-3.83520	14.56990

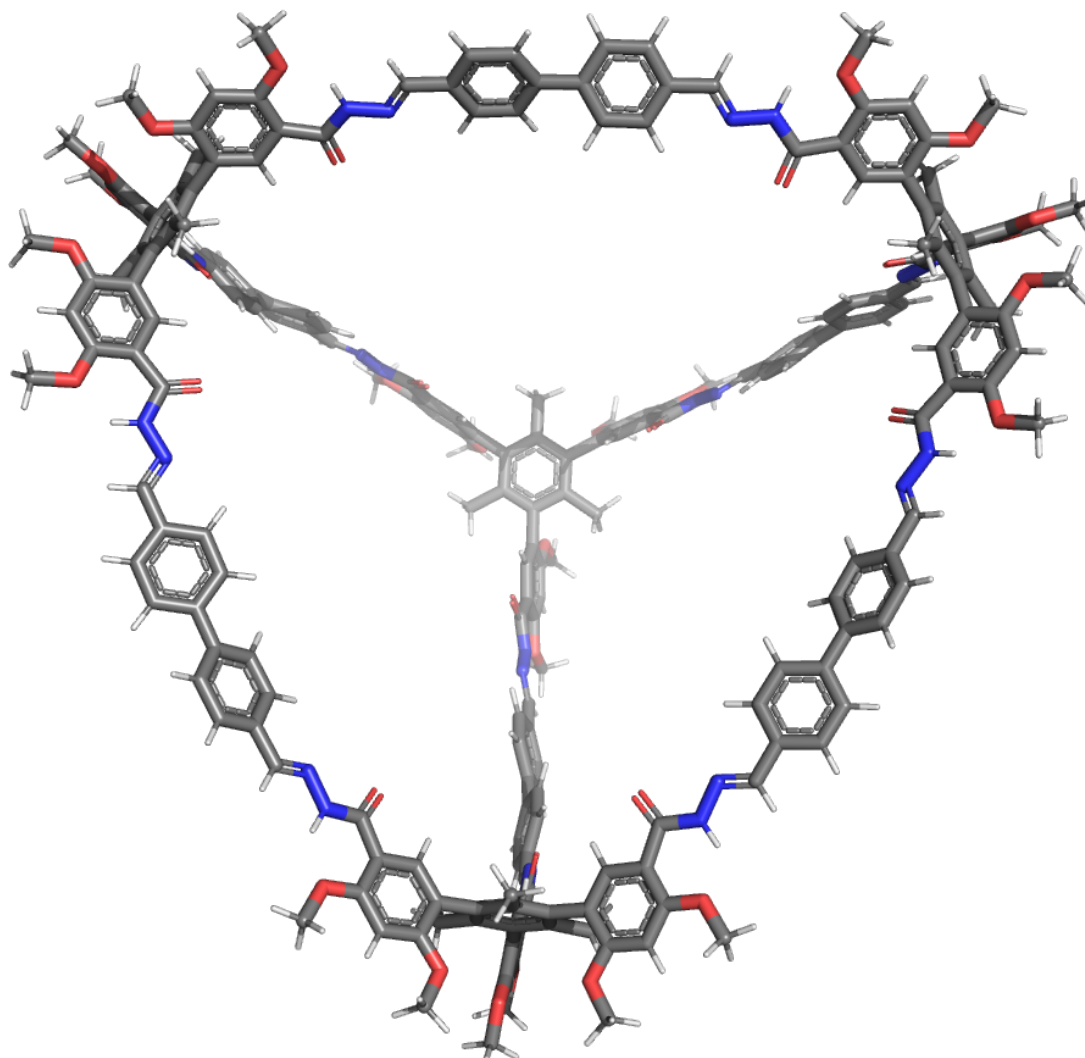
H	8.60930	-2.96920	13.69750
C	8.78080	-8.10970	11.00780
H	7.69500	-8.17040	11.13550
H	9.02350	-8.47170	10.00740
H	9.22740	-8.80100	11.73470
C	11.61610	-4.15340	9.59140
H	12.57220	-4.69310	9.59710
H	11.23190	-4.19730	8.56670
H	11.81880	-3.10820	9.83070
O	5.60930	-8.62520	16.25970
C	6.19860	-9.39570	17.29630
H	5.36790	-9.76680	17.89990
H	6.76160	-10.24680	16.89310
H	6.85810	-8.78360	17.92420
O	12.04900	-8.90840	5.75140
O	12.36760	1.02950	13.02110
C	13.56330	1.13730	13.77890
H	13.45010	0.68580	14.77250
H	14.41030	0.67240	13.25910
H	13.75040	2.20740	13.88830
C	13.21770	-9.70940	5.84020
H	14.09780	-9.10710	6.09800
H	13.09600	-10.51460	6.57550
H	13.35650	-10.14430	4.84840
O	9.95600	-7.58860	14.40480
O	12.57060	-3.80150	13.20410
O	12.44660	-7.62530	10.40000
C	13.76510	-3.75790	13.96240
H	13.61940	-3.24290	14.92190
H	14.57880	-3.26760	13.41050
H	14.03540	-4.79890	14.15110
C	10.60280	-8.34550	15.41100
H	11.67170	-8.26520	15.20300
H	10.39880	-7.94580	16.41400
H	10.30760	-9.40340	15.37880
C	13.61620	-8.40760	10.55250
H	13.92620	-8.27970	11.59160
H	14.42400	-8.06630	9.89040
H	13.42060	-9.47190	10.36220
C	9.55040	-7.26580	5.53050
O	8.54640	-6.57350	5.57000
N	9.96140	-7.91990	4.38080
H	10.80750	-8.48440	4.41200
N	9.26070	-7.80200	3.23350
C	9.83580	0.84150	11.41490
O	8.82670	0.63470	10.76000
N	9.60320	3.20030	11.28310
H	11.13440	2.22870	12.26130
N	10.28470	2.11760	11.71240
C	4.32120	-6.96770	14.11770

O	3.91860	-6.26490	13.20510
N	3.46930	-7.57890	15.02170
H	3.86730	-8.15190	15.76260
N	2.13190	-7.43070	14.91870
C	1.41270	-8.03790	15.79470
C	9.70890	-8.43620	2.20840
C	10.07780	4.35250	11.60060
C	8.14240	7.98330	10.40620
C	7.60620	6.72990	10.04310
C	8.22920	5.55710	10.42610
C	9.41560	5.58640	11.18910
C	9.95050	6.83200	11.55010
C	9.32260	8.01350	11.16420
H	6.69310	6.70590	9.45720
H	7.81490	4.59360	10.14650
H	10.86530	6.87470	12.13880
H	9.75210	8.97080	11.45460
H	10.99860	4.45420	12.19500
C	-12.77180	-3.41170	9.92940
C	-12.36950	-2.80620	11.12880
C	-11.63850	-3.53520	12.09340
C	-11.31450	-4.87780	11.84510
C	-11.71980	-5.50250	10.64340
C	-12.44430	-4.76600	9.69440
C	-13.59440	1.24210	12.04080
C	-14.39670	0.15850	12.41060
C	-13.99250	-1.14670	12.11700
C	-12.77920	-1.39600	11.44240
C	-12.00740	-0.29300	11.09720
C	-12.36980	1.03710	11.37230
H	-15.33080	0.33170	12.92500
H	-11.06650	-0.43770	10.57570
C	-13.97640	-6.58420	6.08030
C	-12.68850	-6.01110	6.06070
C	-12.22280	-5.44280	7.25880
C	-12.95370	-5.41540	8.44040
C	-14.23930	-5.99560	8.41590
C	-14.74350	-6.57750	7.24920
H	-11.23030	-5.00410	7.23090
H	-15.72940	-7.01960	7.25000
C	-9.25840	-7.16010	14.89990
C	-10.65620	-7.11480	14.86840
C	-11.31510	-6.38670	13.87300
C	-10.59160	-5.68380	12.88700
C	-9.20530	-5.76010	12.94840
C	-8.49780	-6.47830	13.92870
H	-11.22900	-7.64330	15.61660
H	-8.60410	-5.23210	12.21580
C	-13.58740	-2.65400	8.90140
H	-13.15430	-2.74840	7.90010

H	-14.60880	-3.05310	8.84650
H	-13.65520	-1.59140	9.14020
C	-11.39540	-6.96560	10.42270
H	-11.65040	-7.28970	9.41210
H	-10.33080	-7.16610	10.58410
H	-11.95010	-7.59580	11.13030
C	-11.25670	-2.85770	13.39360
H	-10.59220	-3.48020	13.99310
H	-10.75430	-1.90150	13.21330
H	-12.15030	-2.64040	13.99350
O	-14.45750	-7.14970	4.92130
C	-15.74650	-7.74470	4.90930
H	-15.89130	-8.11980	3.89430
H	-15.80750	-8.58090	5.61710
H	-16.52920	-7.01090	5.13980
O	-8.59260	-7.86600	15.87540
O	-13.98060	2.53330	12.31920
C	-15.22680	2.77720	12.95360
H	-16.06310	2.40000	12.35170
H	-15.26280	2.32800	13.95400
H	-15.30750	3.86230	13.04350
C	-9.33010	-8.52970	16.89100
H	-9.93490	-7.82300	17.47290
H	-9.97870	-9.30880	16.47110
H	-8.58730	-8.99240	17.54370
O	-14.94210	-5.94450	9.58220
O	-14.72860	-2.24270	12.45400
O	-12.67250	-6.30270	13.79300
C	-15.96920	-2.06230	13.11140
H	-16.67320	-1.48280	12.49830
H	-15.84690	-1.56620	14.08410
H	-16.37130	-3.06520	13.26870
C	-16.23760	-6.51300	9.63000
H	-16.59480	-6.35420	10.64960
H	-16.92400	-6.02200	8.92630
H	-16.21620	-7.59110	9.41850
C	-13.46230	-6.94720	14.77500
H	-14.49940	-6.72610	14.51420
H	-13.25250	-6.56110	15.78200
H	-13.31300	-8.03570	14.76840
C	-6.99660	-6.40000	13.80030
O	-6.46470	-5.76270	12.90600
N	-6.26990	-7.09120	14.75610
H	-6.76950	-7.60620	15.47800
N	-4.92020	-7.08660	14.72720
C	-11.38050	2.07050	10.89400
O	-10.35500	1.75670	10.31080
N	-10.90720	4.39610	10.77520
H	-12.58510	3.58440	11.65310
N	-11.71610	3.38710	11.16190

C	-11.72420	-5.91550	4.90480
O	-10.61820	-5.41600	5.03360
N	-12.17950	-6.42010	3.69830
H	-13.10840	-6.83390	3.65780
N	-11.40420	-6.37450	2.59410
C	-11.89660	-6.87480	1.51640
C	-4.31320	-7.75440	15.64320
C	-0.04220	-7.95270	15.76360
C	-0.81430	-8.63000	16.71820
C	-2.20460	-8.56210	16.68200
C	-2.85520	-7.81530	15.68980
C	-2.07710	-7.12980	14.73370
C	-0.69880	-7.19700	14.76980
H	-0.32170	-9.21670	17.49160
H	-2.79200	-9.09560	17.42700
H	-2.58500	-6.55210	13.96820
H	-0.09780	-6.67340	14.03330
C	-11.28650	5.59090	11.06320
C	-8.95930	9.01040	9.96220
C	-10.16610	9.16100	10.66140
C	-10.92150	8.04710	11.01930
C	-10.48870	6.75470	10.68790
C	-9.27400	6.60510	9.98670
C	-8.52520	7.70980	9.63100
H	-10.51530	10.15770	10.92540
H	-11.85650	8.18000	11.56070
H	-8.94040	5.60420	9.73210
H	-7.59070	7.59650	9.09110
H	-12.22660	5.78370	11.60240
H	-4.86560	-8.30650	16.41880
H	1.86440	-8.64690	16.59240
H	-8.56150	11.16520	9.88820
H	-12.90160	-7.32320	1.49420
H	10.62050	-9.05030	2.26120

Model of the biphenyl-linked molecular cage 11 (with the $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups)



C	0.73480	-4.50800	-10.53920
C	-0.43510	-3.77710	-10.78220
C	-1.70620	-4.36440	-10.59040
C	-1.79090	-5.69790	-10.16890
C	-0.62040	-6.45020	-9.92260
C	0.63260	-5.84910	-10.10360
C	-0.22190	0.27350	-12.27110
C	-0.43740	-0.79000	-13.15190
C	-0.50510	-2.09920	-12.66840
C	-0.35800	-2.37090	-11.29290
C	-0.14360	-1.28800	-10.44990
C	-0.06500	0.04350	-10.88820
H	-0.55180	-0.59940	-14.20920

H	-0.02340	-1.45360	-9.38390
C	4.27500	-8.06600	-9.40340
C	3.58820	-7.50750	-8.30640
C	2.40650	-6.80260	-8.58370
C	1.89000	-6.62660	-9.86140
C	2.60310	-7.20450	-10.93100
C	3.78230	-7.91980	-10.70360
H	1.88260	-6.38080	-7.73190
H	4.31510	-8.35860	-11.53480
C	-5.65250	-7.60680	-9.79910
C	-4.89070	-7.77300	-10.95930
C	-3.64010	-7.16020	-11.07120
C	-3.12700	-6.36380	-10.02670
C	-3.91270	-6.22500	-8.88920
C	-5.17450	-6.82230	-8.72960
H	-5.26970	-8.37650	-11.77140
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H	0.21550	-8.32980	-9.23690
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H	-1.18580	-8.49980	-10.30260
C	-2.94770	-3.54580	-10.87450
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H	-2.89790	-2.56620	-10.38770
H	-3.05320	-3.36570	-11.95140
O	5.43620	-8.76160	-9.15760
C	6.15160	-9.34210	-10.23790
H	7.01860	-9.83220	-9.79070
H	5.54410	-10.08960	-10.76290
H	6.49200	-8.58010	-10.95040
O	-6.88800	-8.19860	-9.67300
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H	-0.26450	2.92250	-14.21700
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H	-1.01400	-3.96720	-15.29870
C	2.73400	-7.58520	-13.29270
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C	-3.30830	-8.06190	-13.26560
H	-2.51580	-8.01740	-14.01540
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H	0.00660	2.58900	-11.17370
N	0.16270	2.37370	-10.19140
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O	3.18590	-7.18000	-5.97680
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C	6.88780	-8.51650	-5.15210
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C	-4.32210	17.96610	7.86020
H	-3.18220	14.31650	7.43990
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C	4.71200	15.14290	8.52290
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H	0.45590	13.37370	-3.85210
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H	15.00510	-10.09190	9.41330
H	11.29780	-6.84510	9.52080
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H	12.49490	-4.96850	16.28390
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C	13.95800	-5.25110	11.18390
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C	8.54420	-10.14170	19.15910
H	7.70140	-10.53600	19.73030
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H	9.09430	-9.41910	19.77490
O	13.80580	-9.69620	7.08170
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H	15.82710	-10.15820	7.31520
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O	12.36200	-8.25850	16.39390
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C	16.62790	-4.81970	14.93710
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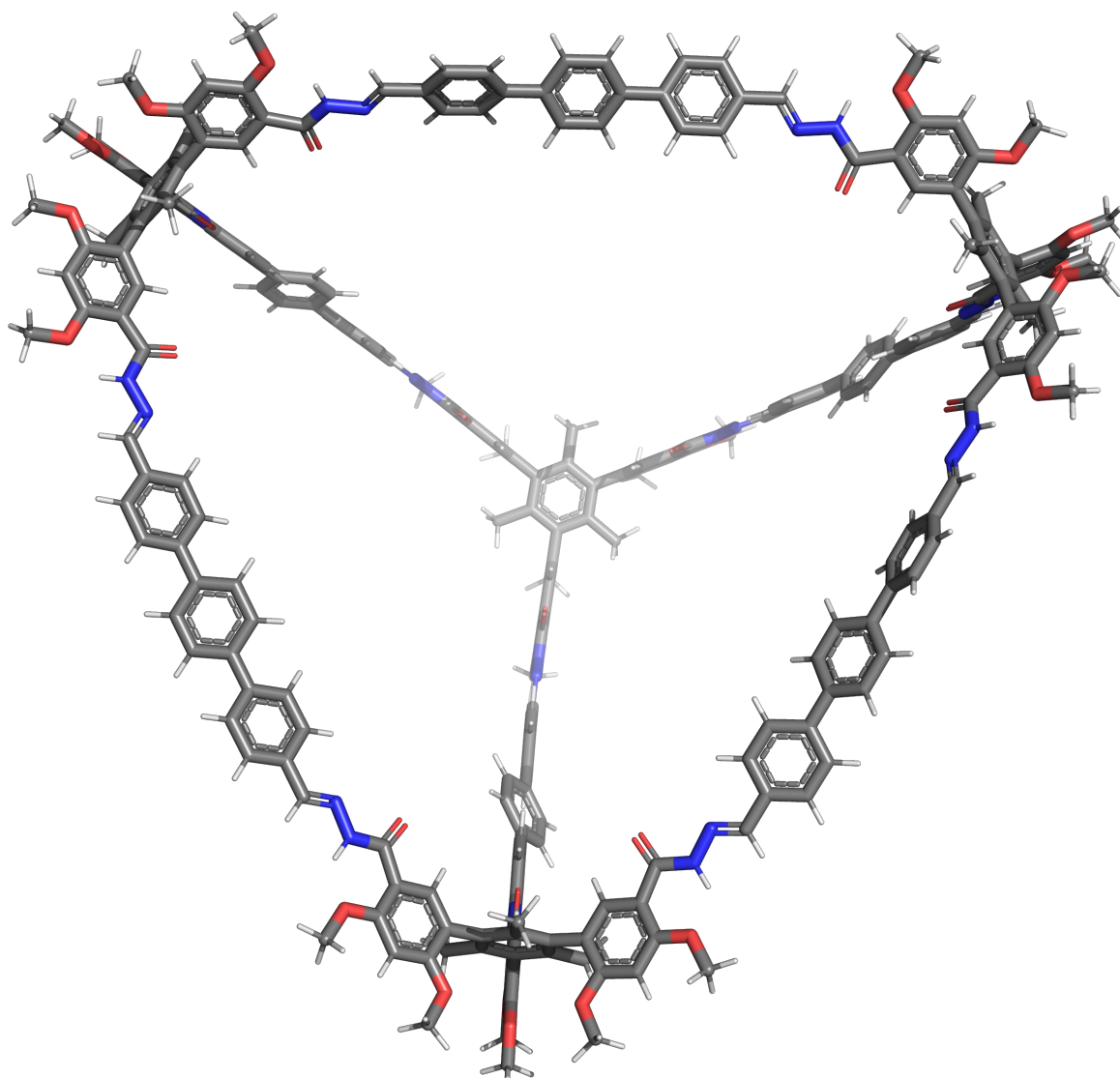
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O	-14.52500	-6.82960	14.82060
C	-17.68170	-2.55050	14.77490
H	-18.50270	-2.03990	14.25290
H	-17.44590	-2.00220	15.69720
H	-17.99420	-3.56490	15.03090
C	-18.27960	-6.64380	10.75180
H	-18.67050	-6.39710	11.74110
H	-18.89610	-6.15130	9.98740
H	-18.32610	-7.73180	10.60570
C	-15.30160	-7.62500	15.69750
H	-16.33930	-7.47930	15.39030
H	-15.18600	-7.30780	16.74310
H	-15.04720	-8.69050	15.61430
C	-8.86440	-6.48060	15.11740
O	-8.34710	-5.64230	14.39690
N	-8.13530	-7.33580	15.92270
H	-8.64010	-7.99770	16.50810
N	-6.78340	-7.30030	15.96150
C	-13.74130	1.72250	11.72420
O	-12.83870	1.44440	10.94990
N	-13.35900	4.08070	11.61510
H	-14.82080	3.17050	12.73670
N	-14.06190	3.01960	12.07610
C	-13.51840	-6.69200	6.23860
O	-12.34590	-6.41100	6.42780
N	-14.01730	-7.05520	5.00190
H	-15.00260	-7.29920	4.92890
N	-13.22680	-7.11750	3.90690
C	-13.81430	-7.44680	2.81150
C	-11.76660	-7.64480	-0.94850
C	-13.14360	-7.89840	-0.85870
C	-13.79710	-7.84520	0.36810
C	-13.09860	-7.53440	1.54470
C	-11.71580	-7.29760	1.46500
C	-11.06920	-7.35650	0.24270

H	-13.71370	-8.10430	-1.76090
H	-14.86940	-8.02690	0.41440
H	-11.16790	-7.07090	2.37420
H	-9.99620	-7.19590	0.20470
C	-6.22460	-8.16720	16.72980
C	-1.97100	-8.56140	17.10900
C	-2.84450	-9.42510	17.78690
C	-4.22270	-9.27990	17.66790
C	-4.77630	-8.27030	16.86530
C	-3.90760	-7.39030	16.19760
C	-2.53640	-7.53600	16.32320
H	-2.44190	-10.23900	18.38400
H	-4.88280	-9.97180	18.18800
H	-4.32970	-6.59830	15.58680
H	-1.88280	-6.83050	15.81940
C	-13.72030	5.22380	12.08190
C	-11.71890	8.91880	11.21360
C	-12.77050	8.85610	12.13940
C	-13.42710	7.65580	12.38980
C	-13.05330	6.47310	11.73200
C	-12.02230	6.53410	10.77930
C	-11.37840	7.73400	10.52630
H	-13.04840	9.74440	12.69900
H	-14.22410	7.62560	13.13060
H	-11.73720	5.62920	10.25150
H	-10.59880	7.76340	9.77150
H	-14.54540	5.30430	12.80620
H	-14.89340	-7.66150	2.78290
H	-6.82330	-8.88570	17.31020

Model of the terphenyl-linked molecular cage 12 (with the $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups)



C	4.81940	-7.12580	-10.77130
C	3.66230	-6.38710	-11.06560
C	2.38400	-6.95870	-10.91150
C	2.26900	-8.28490	-10.45750
C	3.42100	-9.04090	-10.16190
C	4.68690	-8.45430	-10.32540
C	3.97280	-2.38340	-12.65760
C	3.96490	-3.48570	-13.51700
C	3.86550	-4.77920	-12.99800
C	3.77300	-4.99520	-11.60830
C	3.78310	-3.87590	-10.78680
C	3.88280	-2.55760	-11.26030
H	4.03520	-3.33720	-14.58490

H	3.71860	-3.99890	-9.71030
C	8.26230	-10.77120	-9.62090
C	7.62760	-10.14200	-8.53090
C	6.46360	-9.40650	-8.80320
C	5.91720	-9.26860	-10.07170
C	6.57030	-9.92670	-11.13330
C	7.73220	-10.67060	-10.91070
H	5.98250	-8.92700	-7.95650
H	8.22260	-11.16580	-11.73620
C	-1.63530	-10.10070	-10.11320
C	-0.91360	-10.20460	-11.30640
C	0.34910	-9.61530	-11.41560
C	0.91500	-8.91410	-10.33170
C	0.16860	-8.83330	-9.16410
C	-1.10430	-9.40490	-9.00770
H	-1.33250	-10.74070	-12.14580
H	0.56880	-8.30190	-8.30670
C	6.19990	-6.53130	-10.95860
H	6.85360	-6.77160	-10.11440
H	6.67640	-6.93610	-11.86140
H	6.16280	-5.44510	-11.05940
C	3.32350	-10.48190	-9.70230
H	3.87810	-10.64200	-8.77160
H	2.28930	-10.78510	-9.53190
H	3.75670	-11.15880	-10.45020
C	1.16160	-6.13870	-11.27100
H	0.23860	-6.64650	-10.99060
H	1.17510	-5.16290	-10.77410
H	1.12740	-5.94620	-12.35130
O	9.41020	-11.48860	-9.37800
C	10.05720	-12.16390	-10.44630
H	10.92110	-12.66250	-10.00260
H	9.39860	-12.91480	-10.89990
H	10.39910	-11.46200	-11.21760
O	-2.87950	-10.67420	-9.98670
O	4.07050	-1.10360	-13.15400
C	4.17770	-0.89470	-14.55480
H	5.07840	-1.37010	-14.96270
H	3.29300	-1.26910	-15.08450
H	4.24790	0.18650	-14.68970
C	-3.44220	-11.38640	-11.07870
H	-3.58330	-10.73600	-11.95100
H	-2.82040	-12.24580	-11.35850
H	-4.41450	-11.74200	-10.73220
O	6.00240	-9.78650	-12.36380
O	3.84940	-5.89390	-13.78020
O	1.10310	-9.67660	-12.54720
C	3.95820	-5.75050	-15.18460
H	4.90470	-5.27210	-15.47160
H	3.12180	-5.17230	-15.60080

H	3.93040	-6.76400	-15.59000
C	6.58910	-10.44450	-13.47170
H	5.95770	-10.20310	-14.32920
H	7.61040	-10.08750	-13.66320
H	6.60880	-11.53410	-13.33240
C	0.59760	-10.36590	-13.67550
H	1.36780	-10.28140	-14.44500
H	-0.33320	-9.91340	-14.04460
H	0.42030	-11.42790	-13.45720
C	-1.72370	-9.17750	-7.65290
O	-1.13920	-8.56160	-6.77570
N	-2.99020	-9.70310	-7.47670
H	-3.42880	-10.20140	-8.24820
N	-3.64540	-9.54100	-6.30710
C	3.89260	-1.50680	-10.17920
O	3.83620	-1.80030	-8.99480
N	4.00570	0.82850	-9.75120
H	4.02610	-0.02550	-11.62550
N	3.97010	-0.20050	-10.62440
C	8.02080	-10.17450	-7.07880
O	7.27410	-9.76870	-6.20210
N	9.28830	-10.66120	-6.81670
H	9.85910	-10.99170	-7.59180
N	9.72790	-10.78310	-5.54600
C	10.93460	-11.19610	-5.38870
C	14.31160	-12.36060	2.44830
C	14.78650	-13.09140	1.34760
C	14.25280	-12.90760	0.07740
C	13.21900	-11.98500	-0.15100
C	12.74280	-11.25550	0.95110
C	13.27420	-11.44070	2.22020
H	15.60000	-13.79860	1.48500
H	14.63440	-13.50190	-0.74870
H	11.95710	-10.51880	0.80890
H	12.86790	-10.87250	3.05210
C	-4.83020	-10.03280	-6.23820
C	-7.21650	-9.67590	-2.69970
C	-7.72050	-10.29970	-3.85030
C	-6.93980	-10.41760	-4.99500
C	-5.63290	-9.91110	-5.02650
C	-5.12260	-9.28290	-3.87700
C	-5.90210	-9.17150	-2.73820
H	-8.72220	-10.72070	-3.83660
H	-7.34470	-10.91500	-5.87450
H	-4.11470	-8.88080	-3.90480
H	-5.50240	-8.65960	-1.86720
C	4.10690	2.00520	-10.25790
C	4.27210	5.53830	-7.83540
C	4.35780	5.61350	-9.23360
C	4.30080	4.46340	-10.01330

C	4.16020	3.19950	-9.42120
C	4.07790	3.11680	-8.02030
C	4.13240	4.26560	-7.24820
H	4.44000	6.58480	-9.71420
H	4.35670	4.54570	-11.09740
H	3.98070	2.13930	-7.55820
H	4.09440	4.18010	-6.16580
H	4.16260	2.16050	-11.34620
H	11.58680	-11.41450	-6.24770
H	-5.28810	-10.55790	-7.08980
C	3.80950	17.34950	6.42470
C	5.00280	17.24150	5.69340
C	6.24370	17.12170	6.34980
C	6.28160	17.10590	7.75450
C	5.09260	17.20290	8.50340
C	3.86740	17.33110	7.83070
C	4.91830	17.43320	1.38200
C	5.02420	18.60590	2.13610
C	5.05560	18.54100	3.53160
C	4.97650	17.30240	4.19830
C	4.87590	16.16020	3.41640
C	4.84280	16.17380	2.01340
H	5.08100	19.56410	1.64000
H	4.81130	15.18720	3.89280
C	0.24100	17.86150	10.11080
C	0.63620	16.55680	9.74730
C	1.82140	16.43170	9.00600
C	2.60900	17.50730	8.62090
C	2.18240	18.79440	9.00380
C	1.00910	18.96990	9.74170
H	2.11680	15.42370	8.73220
H	0.69570	19.96340	10.02810
C	10.08530	16.94620	9.78810
C	9.51720	18.17880	9.45260
C	8.28430	18.22690	8.79670
C	7.59860	17.04210	8.46260
C	8.19150	15.83810	8.81510
C	9.42600	15.73890	9.47510
H	10.03200	19.09560	9.70090
H	7.69170	14.90400	8.57970
C	2.47120	17.51750	5.73460
H	2.07850	18.53080	5.89240
H	2.54490	17.34970	4.65870
H	1.72670	16.82170	6.13490
C	5.11820	17.20700	10.01800
H	4.34130	16.55640	10.43110
H	6.08090	16.87380	10.40850
H	4.93100	18.21680	10.40520
C	7.51310	17.04380	5.52510
H	8.38650	16.82690	6.14190

H	7.44140	16.26670	4.75690
H	7.69490	17.99220	5.00250
O	-0.91770	18.01670	10.83740
C	-1.34270	19.31720	11.21880
H	-2.27120	19.17510	11.77520
H	-0.60360	19.80600	11.86570
H	-1.53770	19.94780	10.34250
O	11.29930	16.88190	10.43280
O	4.88360	17.47920	0.00680
C	4.94180	18.73330	-0.65760
H	4.09310	19.37160	-0.38170
H	5.88080	19.25800	-0.44150
H	4.89180	18.50740	-1.72460
C	11.99160	18.07880	10.75620
H	12.24160	18.65260	9.85510
H	11.40760	18.70650	11.44080
H	12.91250	17.76480	11.25150
O	2.97670	19.82970	8.61220
O	5.15970	19.64190	4.32650
O	7.67550	19.39150	8.44200
C	5.21460	20.92330	3.72730
H	4.31010	21.13650	3.14140
H	6.09670	21.03330	3.08160
H	5.28360	21.63460	4.55300
C	2.61010	21.15110	8.96460
H	3.38730	21.79610	8.54920
H	1.63920	21.43220	8.53400
H	2.57330	21.28600	10.05430
C	8.31460	20.61980	8.73620
H	7.64900	21.39910	8.35910
H	9.28810	20.70190	8.23350
H	8.45480	20.75660	9.81730
C	9.86500	14.32620	9.75920
O	9.17790	13.36320	9.45510
N	11.09260	14.20330	10.38100
H	11.61330	15.04580	10.61530
N	11.58640	12.98690	10.69650
C	4.72830	14.81040	1.38200
O	4.65770	13.79250	2.05360
N	4.63720	13.63730	-0.68190
H	4.78000	15.68350	-0.49890
N	4.71450	14.79900	0.00030
C	-0.05120	15.25020	10.04800
O	0.40790	14.17950	9.68050
N	-1.23040	15.35630	10.75990
H	-1.55860	16.28010	11.03300
N	-1.95130	14.25850	11.07280
C	-3.04560	14.45740	11.71650
C	-8.22210	7.96640	13.97890
C	-8.75370	9.19810	13.56410

C	-7.92360	10.25470	13.20770
C	-5.99460	8.89400	13.66730
C	-6.82390	7.83850	14.02350
H	-9.83090	9.31390	13.47810
H	-8.36400	11.18130	12.84880
H	-4.91740	8.77440	13.74520
H	-6.38200	6.90980	14.37410
C	12.72760	12.96740	11.28670
C	16.51480	5.61610	13.67970
C	16.62270	6.77230	14.46860
C	16.01870	7.96340	14.08430
C	15.28210	8.05320	12.89260
C	15.17520	6.89660	12.10260
C	15.77610	5.70470	12.48790
H	17.14910	6.72410	15.41830
H	16.08140	8.82680	14.73990
H	14.64110	6.94180	11.15740
H	15.69630	4.83780	11.83760
C	4.65770	13.72490	-1.96380
C	4.32280	6.75270	-6.99310
C	3.55760	6.84560	-5.81860
C	3.60810	7.97850	-5.01700
C	5.18960	8.97820	-6.52830
C	5.13930	7.84410	-7.33040
H	2.88940	6.03230	-5.54910
H	2.97920	8.03410	-4.13260
H	5.86420	9.78860	-6.79170
H	5.77560	7.78400	-8.20950
H	4.73460	14.69730	-2.47350
H	-3.37340	15.47030	11.99610
H	13.27080	13.89560	11.52060
C	17.42020	-8.04450	17.55440
C	18.32580	-7.68790	16.54350
C	18.60070	-8.56000	15.47290
C	17.94890	-9.80240	15.42360
C	17.03760	-10.18040	16.43240
C	16.77930	-9.29960	17.49690
C	20.39440	-3.90760	16.83060
C	20.95860	-5.06210	17.38190
C	20.28840	-6.28460	17.28420
C	19.04470	-6.37710	16.62930
C	18.51890	-5.21110	16.09080
C	19.14920	-3.95910	16.16970
H	21.91270	-5.00830	17.88610
H	17.55990	-5.23800	15.58310
C	14.10760	-10.47570	20.68530
C	13.56570	-9.95050	19.49510
C	14.47040	-9.57940	18.48750
C	15.84870	-9.70810	18.59890
C	16.35140	-10.25580	19.79710

C	15.48930	-10.63330	20.83110
H	14.04230	-9.18060	17.57340
H	15.89140	-11.04680	21.74470
C	18.80750	-12.56410	12.21300
C	19.48240	-12.67370	13.43320
C	19.20290	-11.78020	14.47120
C	18.24220	-10.76140	14.31050
C	17.60230	-10.67750	13.08110
C	17.85310	-11.54770	12.00820
H	20.22090	-13.44970	13.57440
H	16.87410	-9.89130	12.90910
O	13.23980	-10.83400	21.69030
O	19.06010	-13.43370	11.17750
O	21.03760	-2.69400	16.92000
O	17.70430	-10.38540	19.87470
O	20.77710	-7.44560	17.80330
O	19.82480	-11.82970	15.68230
C	17.08780	-11.22880	10.75120
O	16.46750	-10.18480	10.62580
N	17.11540	-12.20320	9.76960
H	17.66130	-13.04730	9.92920
N	16.52650	-11.98760	8.57330
C	18.36980	-2.83090	15.54580
O	17.28760	-3.01410	15.00960
N	18.32040	-0.48850	15.17010
H	19.85710	-1.49460	16.10490
N	18.95830	-1.58340	15.63580
C	12.11630	-9.77410	19.13080
O	11.76860	-9.51950	17.98850
N	11.21590	-9.89600	20.17420
H	11.56350	-10.11780	21.10460
N	9.88780	-9.84520	19.93710
C	9.11020	-9.93510	20.95610
C	4.84000	-9.97010	20.54250
C	5.44520	-9.94320	21.80840
C	6.83010	-9.93120	21.93710
C	7.65780	-9.93680	20.80480
C	7.05810	-9.95780	19.53340
C	5.67890	-9.97640	19.41040
H	4.82490	-9.90470	22.69980
H	7.27740	-9.90280	22.92920
H	7.69540	-9.97490	18.65480
H	5.23670	-10.02930	18.41970
C	16.56120	-12.95270	7.72590
C	14.88850	-12.52930	3.79960
C	15.37790	-13.76640	4.24670
C	15.92290	-13.90020	5.51980
C	15.98840	-12.80380	6.39140
C	15.49990	-11.56170	5.95010
C	14.96490	-11.43210	4.68010

H	15.30510	-14.63800	3.60180
H	16.28700	-14.87160	5.84970
H	15.56290	-10.70840	6.61810
H	14.62560	-10.45570	4.34640
C	18.91060	0.63990	15.34170
C	17.14120	4.34270	14.09620
C	16.50250	3.11380	13.84050
C	17.06730	1.91140	14.23350
C	18.30540	1.89250	14.89990
C	18.95050	3.11220	15.15240
C	18.37710	4.31710	14.75970
H	15.53110	3.11060	13.35410
H	16.55940	0.97040	14.04650
H	19.91430	3.11530	15.65870
H	18.90530	5.24840	14.94670
H	19.88880	0.70990	15.84130
H	9.50540	-10.01980	21.97960
H	17.02240	-13.92160	7.96960
C	-13.62700	-5.28930	14.16200
C	-13.17970	-4.76790	15.39600
C	-12.46400	-5.57030	16.29700
C	-12.19020	-6.91260	15.95670
C	-12.62730	-7.44480	14.73550
C	-13.35040	-6.62540	13.84190
C	-14.17430	-0.67980	16.38600
C	-15.04800	-1.71770	16.72450
C	-14.72600	-3.03970	16.40410
C	-13.51990	-3.35010	15.74420
C	-12.68060	-2.29180	15.42270
C	-12.96120	-0.94870	15.71870
H	-15.97490	-1.49720	17.23410
H	-11.74290	-2.48470	14.91290
C	-14.88270	-8.37690	10.20060
C	-13.59080	-7.81160	10.19480
C	-13.13380	-7.24830	11.39770
C	-13.87420	-7.22450	12.57190
C	-15.15740	-7.80700	12.53920
C	-15.65830	-8.37400	11.36410
H	-12.13980	-6.81260	11.37990
H	-16.64610	-8.81140	11.35520
C	-10.11780	-9.39910	18.82070
C	-11.51530	-9.40520	18.76510
C	-12.18350	-8.59700	17.84050
C	-11.46710	-7.77410	16.94740
C	-10.08220	-7.78060	17.04780
C	-9.36740	-8.57040	17.96260
H	-12.08000	-10.03500	19.43730
H	-9.49430	-7.14590	16.39230
C	-14.42290	-4.40390	13.22510
H	-14.57640	-4.87610	12.25330

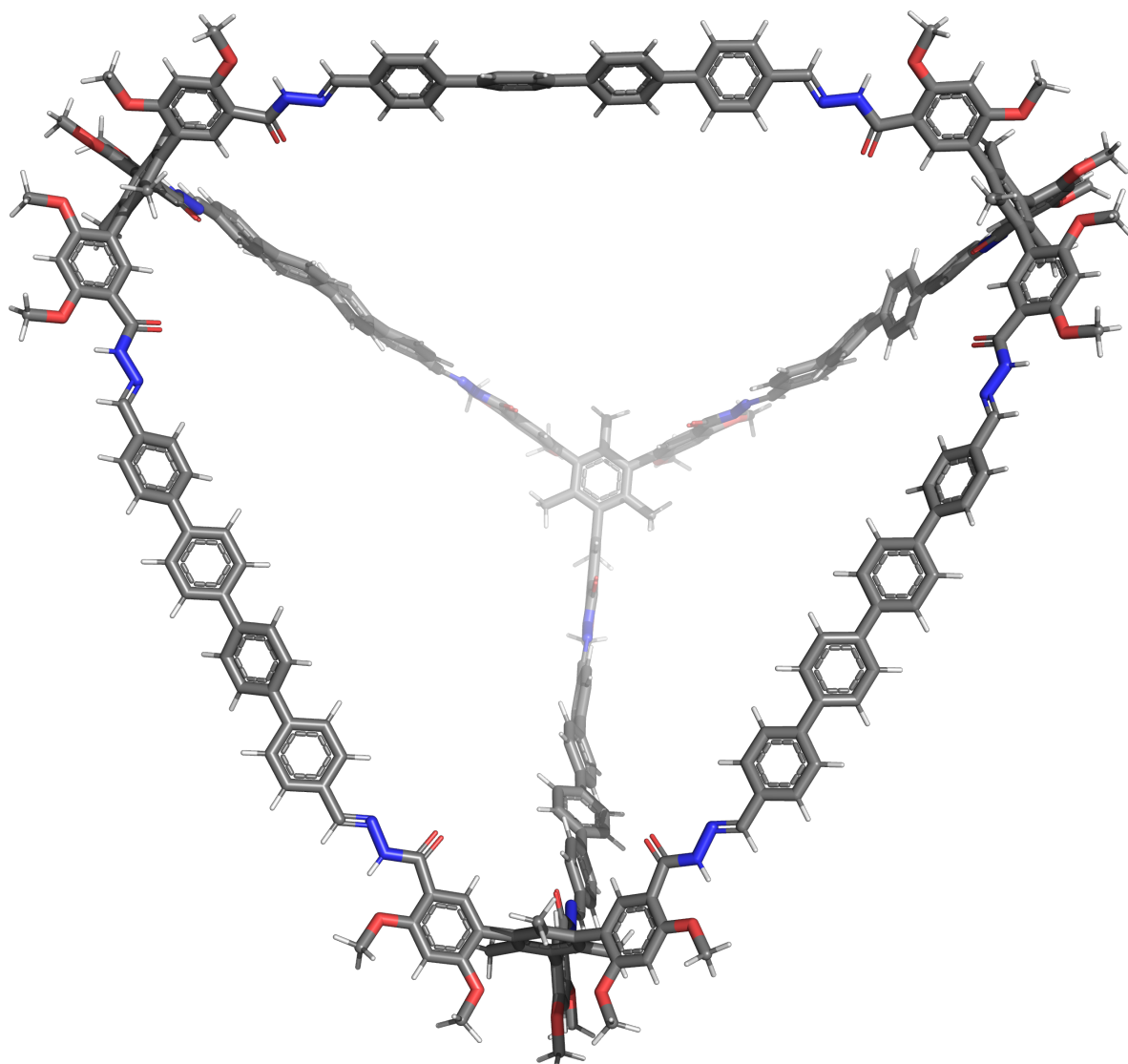
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H	-13.91980	-3.44550	13.05940
C	-12.36780	-8.89190	14.37430
H	-11.97550	-8.98640	13.35680
H	-11.65230	-9.35140	15.05710
H	-13.29710	-9.47540	14.41560
C	-12.00960	-5.03450	17.63920
H	-10.92940	-5.15480	17.77460
H	-12.24520	-3.97540	17.74770
H	-12.49480	-5.57760	18.46040
O	-15.35890	-8.93020	9.03390
C	-16.65850	-9.50250	9.00480
H	-16.80150	-9.86440	7.98470
H	-16.74100	-10.34450	9.70330
H	-17.42910	-8.75670	9.23640
O	-9.43680	-10.19220	19.71520
O	-14.47530	0.62690	16.69410
C	-15.68060	0.93090	17.38100
H	-16.56050	0.63580	16.79590
H	-15.71390	0.44550	18.36430
H	-15.68240	2.01460	17.51320
C	-10.16280	-11.02320	20.60930
H	-10.80820	-10.43070	21.26940
H	-10.76970	-11.76100	20.06930
H	-9.41250	-11.54190	21.20930
O	-15.85750	-7.77650	13.70670
O	-15.53560	-4.09380	16.70150
O	-13.54060	-8.54920	17.73840
C	-16.75210	-3.85560	17.38600
H	-17.42750	-3.21340	16.80420
H	-16.58100	-3.39970	18.37080
H	-17.21490	-4.83550	17.51960
C	-17.15990	-8.33010	13.74480
H	-17.51420	-8.18570	14.76750
H	-17.83970	-7.81680	13.05100
H	-17.15220	-9.40410	13.51340
C	-14.32640	-9.33860	18.61220
H	-15.36520	-9.12510	18.35190
H	-14.15560	-9.07240	19.66430
H	-14.13290	-10.41150	18.47570
C	-7.87300	-8.38680	17.91370
O	-7.35820	-7.48520	17.27150
N	-7.13340	-9.31940	18.61800
H	-7.62410	-10.04260	19.13950
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H	-13.01670	1.60190	16.01630
N	-12.15490	1.35260	15.53530

C	-12.60490	-7.73520	9.05730
O	-11.50890	-7.21440	9.19250
N	-13.02260	-8.29740	7.86550
H	-13.95080	-8.71190	7.81630
N	-12.21000	-8.31650	6.78650
C	-12.68280	-8.86410	5.72470
C	-8.03260	-9.54990	-1.47440
C	-9.41360	-9.30570	-1.53920
C	-10.17480	-9.18420	-0.38310
C	-8.20530	-9.54400	0.95090
C	-7.44430	-9.66450	-0.20430
H	-9.88730	-9.16780	-2.50760
H	-11.23360	-8.95260	-0.46260
H	-7.72860	-9.67430	1.91860
H	-6.38370	-9.88650	-0.12350
C	-5.17620	-10.15210	19.33170
C	3.36930	-9.99910	20.38590
C	2.54510	-10.65920	21.31150
C	1.16520	-10.69720	21.14830
C	0.54590	-10.07880	20.05040
C	1.37080	-9.41880	19.12400
C	2.74880	-9.37810	19.28890
H	2.99360	-11.16730	22.16090
H	0.55520	-11.19990	21.89400
H	0.92720	-8.94620	18.25210
H	3.35320	-8.84160	18.56300
C	-11.60050	3.52390	15.43010
C	-9.09680	6.83300	14.34890
C	-10.31490	7.03390	15.01490
C	-11.12160	5.95610	15.36460
C	-9.52120	4.43430	14.38620
C	-8.72050	5.51070	14.04180
H	-10.61820	8.04150	15.28680
H	-12.05720	6.13340	15.89200
H	-9.22780	3.41950	14.13600
H	-7.79680	5.33300	13.49810
H	-12.53460	3.77060	15.95740
H	-13.69750	-9.28930	5.69790
H	-5.71810	-11.00520	19.76710
C	-10.73890	4.64200	15.05770
C	-3.72770	-10.12780	19.50950
C	-2.96260	-9.02160	19.10080
C	-1.59000	-9.01500	19.28280
C	-0.92200	-10.10660	19.87200
C	-1.69190	-11.20760	20.27740
C	-3.07170	-11.21610	20.10310
H	-3.46900	-8.17200	18.65330
H	-1.02180	-8.13640	18.99110
H	-1.20170	-12.07720	20.70670
H	-3.64800	-12.08510	20.41570

C	13.36420	11.71650	11.68520
C	12.76460	10.47200	11.42450
C	13.38890	9.29920	11.81690
C	14.62990	9.31610	12.48350
C	15.22170	10.56170	12.74230
C	14.59990	11.74160	12.34840
H	11.80290	10.44960	10.92140
H	12.89690	8.34850	11.63160
H	16.19150	10.60350	13.23090
H	15.08230	12.69660	12.54940
C	11.50420	-11.39570	-4.05960
C	10.71860	-11.26310	-2.90140
C	11.27880	-11.45810	-1.65010
C	12.64030	-11.78740	-1.49770
C	13.41830	-11.91870	-2.65810
C	12.85870	-11.73070	-3.91740
H	9.66670	-11.01750	-3.00850
H	10.64640	-11.38350	-0.77010
H	14.47840	-12.14080	-2.57160
H	13.48410	-11.82730	-4.80310
C	4.42530	9.07010	-5.35420
C	4.59020	12.54060	-2.81300
C	4.65860	12.67390	-4.20760
C	4.60850	11.55570	-5.03280
C	4.48280	10.26830	-4.49010
C	4.41100	10.14280	-3.08910
C	4.46510	11.25310	-2.26290
H	4.74490	13.66500	-4.64960
H	4.63830	11.68200	-6.11180
H	4.34160	9.15320	-2.64600
H	4.42280	11.14750	-1.18340
C	-9.58730	-9.30280	0.88640
C	-11.89620	-8.95750	4.50010
C	-10.58320	-8.45890	4.43780
C	-9.84910	-8.57020	3.26910
C	-10.39100	-9.17780	2.12000
C	-11.70400	-9.66670	2.18660
C	-12.44450	-9.55920	3.35830
H	-10.16240	-7.98250	5.31770
H	-8.84500	-8.15730	3.22990
H	-12.13590	-10.16260	1.32150
H	-13.45680	-9.95790	3.39470
C	-6.52610	10.12560	13.25080
C	-3.91720	13.35370	12.10530
C	-3.58180	12.02040	11.81230
C	-4.42680	10.98870	12.18590
C	-5.63710	11.24090	12.86100
C	-5.96670	12.57350	13.14950
C	-5.11980	13.61270	12.77940
H	-2.65680	11.81920	11.28090

H	-4.16440	9.96670	11.92720
H	-6.88150	12.79360	13.69340
H	-5.38970	14.63880	13.02270
H	22.58720	-1.55740	17.52150
C	22.29030	-2.60620	17.58380
H	22.20620	-2.89720	18.63830
H	23.04850	-3.22720	17.09090
H	22.18850	-8.44940	18.82400
C	22.01170	-7.42270	18.49700
H	22.83780	-7.10370	17.84700
H	21.97090	-6.76500	19.37630
H	12.87430	-11.61980	23.50740
C	13.74660	-11.40960	22.88550
H	14.28070	-12.34590	22.68180
H	14.41160	-10.71590	23.41540
H	19.35300	-10.97880	20.85820
C	18.27550	-10.96140	21.03480
H	18.06630	-10.36280	21.93200
H	17.91880	-11.98810	21.19540
H	21.21770	-12.60400	16.90640
C	20.85380	-12.77950	15.89190
H	20.47980	-13.80970	15.81640
H	21.68120	-12.64300	15.18200
H	20.07960	-14.97850	10.38470
C	20.05340	-14.43700	11.33220
H	21.03910	-13.99550	11.52500
H	19.79930	-15.13320	12.14150
C	17.17120	-7.08970	18.70390
H	16.30300	-7.38700	19.29310
H	18.03850	-7.05690	19.37670
H	17.00350	-6.06900	18.34660
C	16.38060	-11.54420	16.35600
H	15.60140	-11.66560	17.10950
H	15.92870	-11.71110	15.37240
H	17.12280	-12.33880	16.50670
C	19.61530	-8.14840	14.42550
H	19.65900	-8.85730	13.59740
H	19.38280	-7.16060	14.01300
H	20.61810	-8.08110	14.86730

Model of the quarterphenyl-linked molecular cage 13 (with the $-(\text{CH}_2)_4(\text{OCH}_2\text{CH}_2)_3\text{OCH}_3$ substituents replaced by methyl groups)



C	3.15390	-6.93440	-13.32500
C	2.10270	-6.04380	-13.60020
C	0.76150	-6.44320	-13.43370
C	0.47780	-7.74690	-12.98750
C	1.52180	-8.65010	-12.70570
C	2.85210	-8.23440	-12.87750
C	2.95540	-2.08440	-15.11590
C	2.86030	-3.16920	-15.99300
C	2.57790	-4.44680	-15.50060
C	2.39280	-4.66720	-14.12020
C	2.47880	-3.56190	-13.28370
C	2.75540	-2.25960	-13.73170

H	3.00650	-3.02020	-17.05310
H	2.32910	-3.68380	-12.21560
C	6.08650	-11.01320	-12.18670
C	5.61290	-10.23420	-11.11120
C	4.55420	-9.35110	-11.37850
C	3.96620	-9.20460	-12.62800
C	4.46090	-10.00860	-13.67440
C	5.51020	-10.90510	-13.45590
H	4.19440	-8.75860	-10.54310
H	5.87830	-11.51360	-14.26940
C	-3.63280	-9.01660	-12.61160
C	-2.96410	-9.15160	-13.83230
C	-1.63160	-8.74560	-13.94930
C	-0.94520	-8.19310	-12.84920
C	-1.63720	-8.09030	-11.65060
C	-2.97330	-8.48650	-11.48420
H	-3.47770	-9.56950	-14.68610
H	-1.13680	-7.68810	-10.77570
C	4.59940	-6.53320	-13.52980
H	5.21580	-6.80760	-12.66770
H	5.02360	-7.04460	-14.40400
H	4.69840	-5.45890	-13.68860
C	1.23940	-10.06890	-12.25490
H	1.80480	-10.31980	-11.35120
H	0.18080	-10.22570	-12.04320
H	1.53970	-10.78760	-13.02870
C	-0.34770	-5.46580	-13.76770
H	-1.33110	-5.86520	-13.51580
H	-0.22090	-4.51990	-13.23030
H	-0.34370	-5.22480	-14.83880
O	7.12540	-11.88370	-11.95190
C	7.61430	-12.69860	-13.00720
H	8.41840	-13.29610	-12.57330
H	6.83290	-13.36650	-13.39010
H	8.01500	-12.09320	-13.83000
O	-4.94550	-9.40300	-12.47390
O	3.24100	-0.81990	-15.57730
C	3.43120	-0.60390	-16.96810
H	4.28320	-1.17980	-17.35100
H	2.52970	-0.85920	-17.53850
H	3.63760	0.46260	-17.07800
C	-5.63360	-9.96380	-13.58200
H	-5.69790	-9.25380	-14.41620
H	-5.15210	-10.88840	-13.92370
H	-6.63890	-10.19210	-13.22280
O	3.85760	-9.85180	-14.88600
O	2.46730	-5.54250	-16.30150
O	-0.92040	-8.85100	-15.10520
C	2.63590	-5.39440	-17.69920
H	3.64250	-5.03330	-17.95110

H	1.89020	-4.71100	-18.12800
H	2.49540	-6.39100	-18.12260
C	4.29090	-10.64130	-15.97850
H	3.66100	-10.35230	-16.82230
H	5.34270	-10.44640	-16.22930
H	4.16060	-11.71400	-15.78100
C	-1.53890	-9.41810	-16.24530
H	-0.77900	-9.41230	-17.02950
H	-2.40340	-8.82610	-16.57590
H	-1.85970	-10.45250	-16.06060
C	-3.50670	-8.30530	-10.08810
O	-2.77610	-8.01620	-9.15400
N	-4.87350	-8.45820	-9.94830
H	-5.42540	-8.71850	-10.76300
N	-5.45950	-8.33630	-8.73800
C	2.77870	-1.21570	-12.64560
O	2.44430	-1.47400	-11.50020
N	3.25570	1.05680	-12.14300
H	3.47940	0.19170	-14.00190
N	3.22010	0.03730	-13.02990
C	6.09140	-10.22180	-9.68230
O	5.49170	-9.61350	-8.81030
N	7.26370	-10.91430	-9.44150
H	7.70870	-11.40790	-10.21250
N	7.79870	-10.96520	-8.20150
C	8.91600	-11.58940	-8.08700
C	15.09660	-12.59710	3.22220
C	15.70560	-12.98220	2.01740
C	15.03520	-12.86870	0.80550
C	13.72690	-12.36250	0.74120
C	13.11700	-11.97880	1.94620
C	13.78580	-12.09520	3.15830
H	16.72600	-13.35600	2.02790
H	15.52970	-13.19250	-0.10640
H	12.11200	-11.56580	1.93260
H	13.27770	-11.80620	4.07400
C	-6.73660	-8.46850	-8.70080
C	-8.92250	-8.16790	-5.03110
C	-9.58690	-8.33340	-6.25500
C	-8.87230	-8.43600	-7.44360
C	-7.47210	-8.36660	-7.44530
C	-6.80070	-8.19620	-6.22190
C	-7.51620	-8.10270	-5.04030
H	-10.67070	-8.41170	-6.27020
H	-9.40520	-8.57750	-8.38220
H	-5.71720	-8.13170	-6.22500
H	-6.98470	-7.94810	-4.10540
C	3.70840	2.17920	-12.57430
C	3.89680	5.66090	-10.08280
C	4.39430	5.68430	-11.39400

C	4.32990	4.55070	-12.19840
C	3.77490	3.35690	-11.71470
C	3.28540	3.32490	-10.39760
C	3.34530	4.45730	-9.60320
H	4.80630	6.60610	-11.79660
H	4.70690	4.59360	-13.21880
H	2.86670	2.39860	-10.01700
H	2.98340	4.40980	-8.58000
H	4.06290	2.29940	-13.60850
H	9.41240	-12.04640	-8.95640
H	-7.32530	-8.65790	-9.61100
C	3.79010	21.21110	6.55910
C	4.96960	21.06530	5.81080
C	6.21650	20.93320	6.45120
C	6.27710	20.94750	7.85630
C	5.10450	21.10160	8.62120
C	3.87050	21.23330	7.96380
C	4.82390	21.17260	1.49510
C	4.91840	22.36090	2.22650
C	4.97010	22.32260	3.62260
C	4.92220	21.09550	4.31390
C	4.83960	19.93720	3.55310
C	4.78710	19.92360	2.15010
H	4.95140	23.31040	1.71200
H	4.80770	18.97160	4.04770
C	0.27060	21.86400	10.26290
C	0.67210	20.54440	9.96710
C	1.85260	20.38710	9.22430
C	2.62690	21.44590	8.76980
C	2.19730	22.74860	9.09210
C	1.03050	22.95560	9.83250
H	2.15400	19.36800	9.00320
H	0.71490	23.96090	10.07130
C	10.09120	20.57950	9.84410
C	9.61840	21.83910	9.46300
C	8.38230	21.95940	8.82140
C	7.59970	20.82080	8.54590
C	8.09750	19.58900	8.94790
C	9.32950	19.41830	9.59710
H	10.20870	22.72120	9.66500
H	7.51690	18.69060	8.76510
C	2.44710	21.38010	5.88030
H	2.11390	22.42430	5.93870
H	2.48880	21.10220	4.82560
H	1.67660	20.77070	6.36220
C	5.14940	21.16040	10.13500
H	4.43070	20.46580	10.58240
H	6.13920	20.91600	10.52320
H	4.88520	22.16520	10.49020
C	7.46980	20.80570	5.60950

H	8.35040	20.61910	6.22440
H	7.38430	19.98830	4.88560
H	7.64610	21.72340	5.03360
O	-0.88410	22.04890	10.98870
C	-1.30980	23.36490	11.31270
H	-2.23190	23.24700	11.88510
H	-0.56540	23.88490	11.92810
H	-1.51560	23.95390	10.41000
O	11.30670	20.44090	10.47430
O	4.76790	21.19160	0.12000
C	4.80500	22.43310	-0.56930
H	3.95320	23.06860	-0.29660
H	5.74100	22.97080	-0.37380
H	4.74600	22.18580	-1.63100
C	12.08900	21.59250	10.75590
H	12.37550	22.11760	9.83600
H	11.55720	22.28300	11.42190
H	12.98680	21.22660	11.25780
O	2.98210	23.76690	8.64080
O	5.06700	23.44020	4.39460
O	7.86080	23.15320	8.42650
C	5.11970	24.70920	3.76860
H	4.21040	24.91370	3.18700
H	5.99580	24.80270	3.11240
H	5.19900	25.43700	4.57890
C	2.61540	25.10240	8.93580
H	3.38690	25.72910	8.48360
H	1.63960	25.36140	8.50260
H	2.58920	25.28680	10.01850
C	8.58540	24.34160	8.68490
H	7.97140	25.15510	8.29280
H	9.55770	24.34440	8.17350
H	8.74350	24.49460	9.76130
C	9.65160	17.99080	9.95440
O	8.84720	17.08630	9.79130
N	10.92150	17.78360	10.45810
H	11.53830	18.58370	10.58080
N	11.32780	16.54890	10.82360
C	4.70790	18.54550	1.54310
O	4.76850	17.53510	2.22700
N	4.48400	17.33620	-0.49270
H	4.51680	19.39160	-0.34120
N	4.55100	18.51230	0.17030
C	-0.00330	19.25210	10.34680
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C	19.62540	-9.05250	16.35220
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C	4.02210	15.19810	-4.79150
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C	-5.03920	-10.72770	21.36850
C	-4.19750	-9.80760	20.72600
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C	10.96020	-11.94100	-4.33720
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C	9.01100	-11.23670	-5.61550
H	11.32580	-12.69070	-7.64430
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H	8.03330	-10.76780	-5.66640
C	18.10660	-7.91210	19.67430
H	17.23660	-8.27920	20.22110
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C	17.49290	-12.16980	16.94090
H	16.72460	-12.38850	17.68400
H	17.03830	-12.25990	15.94840
H	18.26330	-12.94870	17.01070
C	20.63740	-8.52230	15.35650
H	20.72420	-9.16710	14.48070
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H	21.62990	-8.44310	15.81910
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H	13.82670	-13.00530	23.93090
H	15.22980	-13.64040	23.02760
H	15.37330	-12.11350	23.95540
C	19.24840	-12.10270	21.59080
H	20.32720	-12.10570	21.42120
H	19.03470	-11.60820	22.54830
H	18.88610	-13.13910	21.63160
C	23.05250	-3.17240	19.04920
H	23.32180	-2.11460	19.06430
H	22.91590	-3.52700	20.07860
H	23.85580	-3.74390	18.56800
C	22.87380	-8.04370	19.64890
H	23.06650	-9.08460	19.91690
H	23.71340	-7.66320	19.05130
H	22.78410	-7.44510	20.56590
C	21.42870	-14.43620	11.74090
H	21.48550	-14.89750	10.75300
H	22.37550	-13.92660	11.95830
H	21.24830	-15.21320	12.49420
C	22.14980	-13.07790	16.40750
H	22.51310	-12.95440	17.42970
H	21.84890	-14.12350	16.25530
H	22.95610	-12.82860	15.70410

V. ^1H , ^{13}C (^1H), and ^1H DOSY NMR Spectra

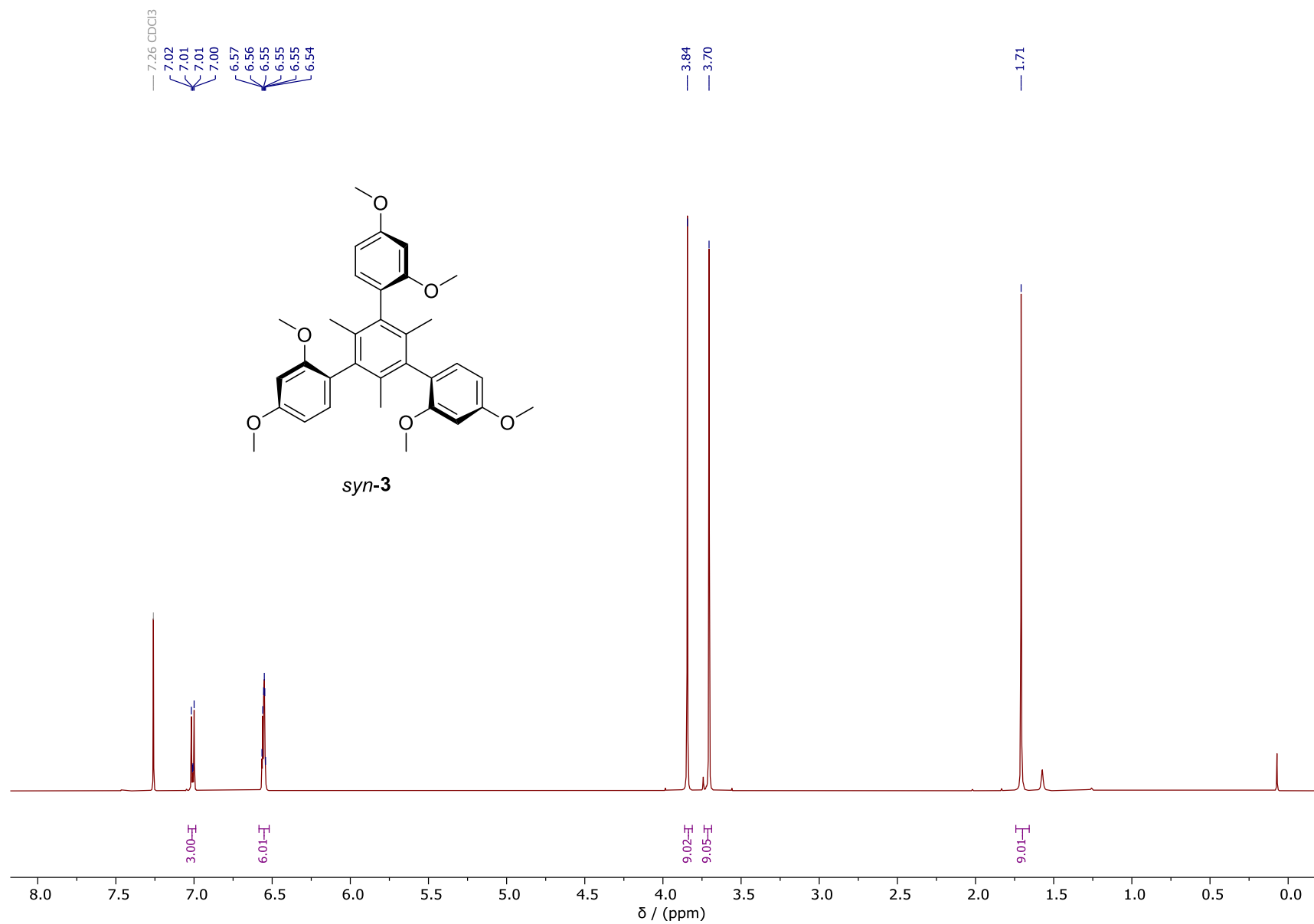


Figure S1. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *syn-3*.

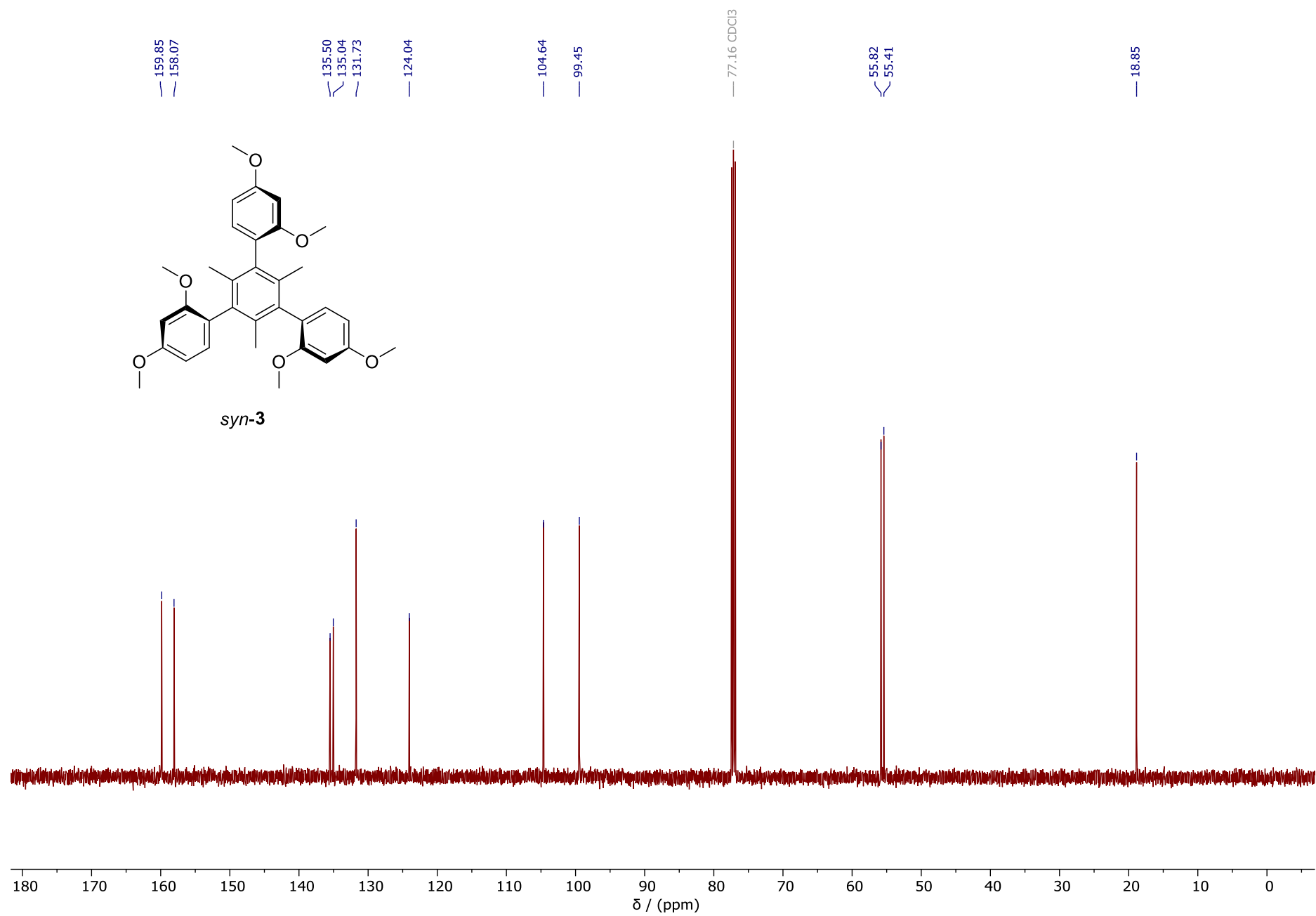


Figure S2. ^{13}C (^1H) NMR spectrum (125 MHz, CDCl_3 , 298 K) of *syn-3*.

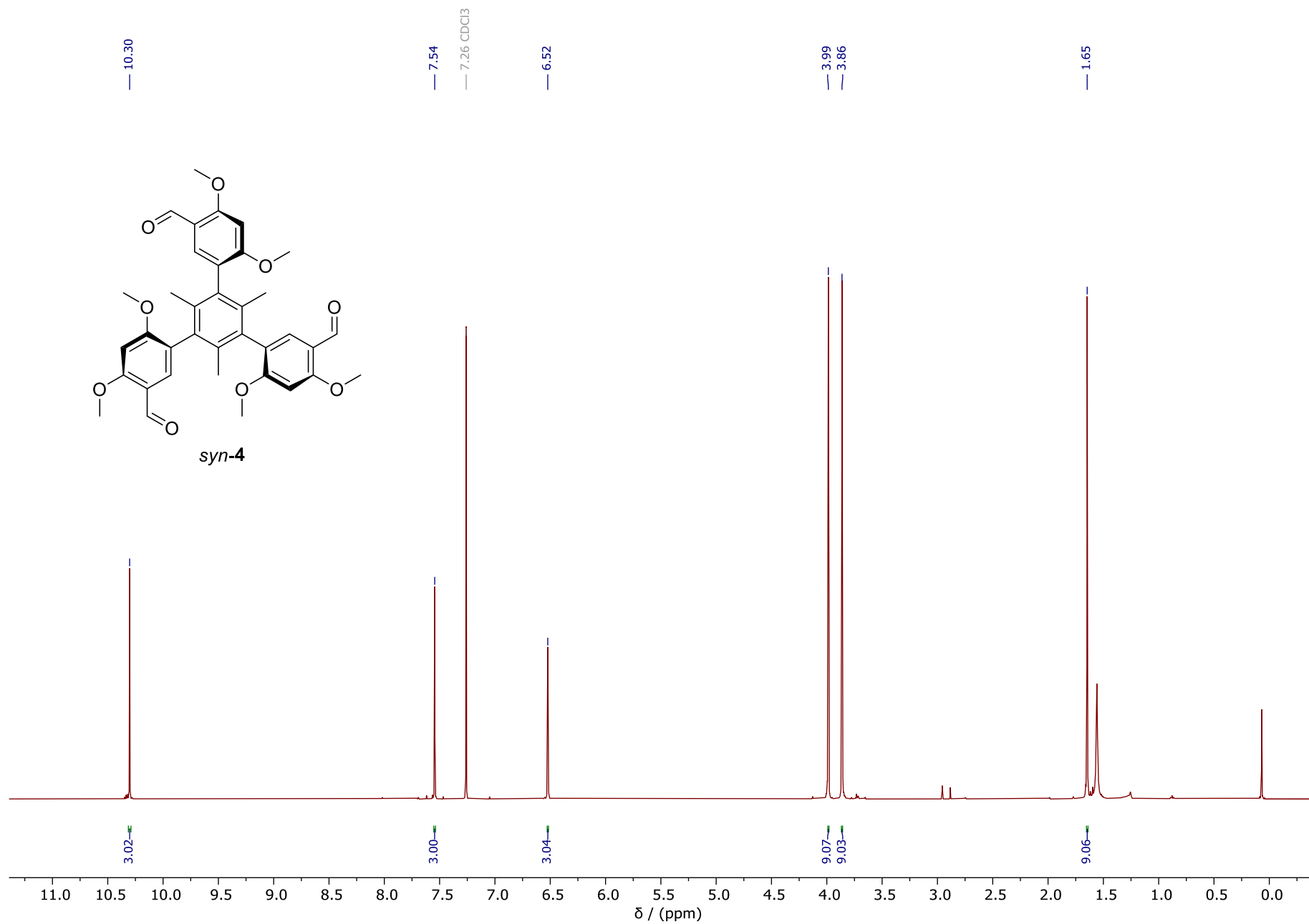


Figure S3. ¹H NMR spectrum (500 MHz, CDCl₃, 298 K) of *syn-4*.

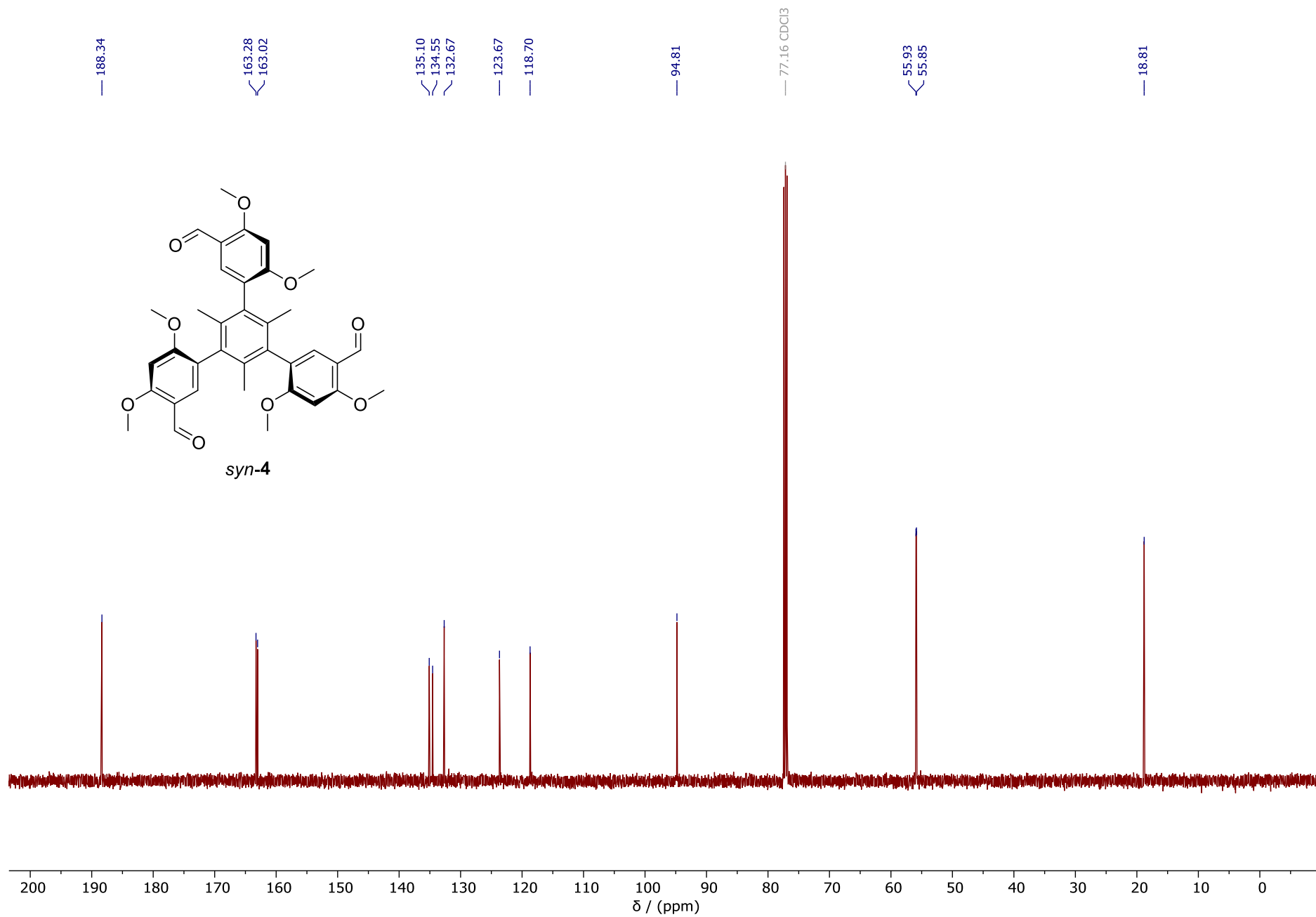


Figure S4. ^{13}C (^1H) NMR spectrum (125 MHz, CDCl_3 , 298 K) of *syn-4*.

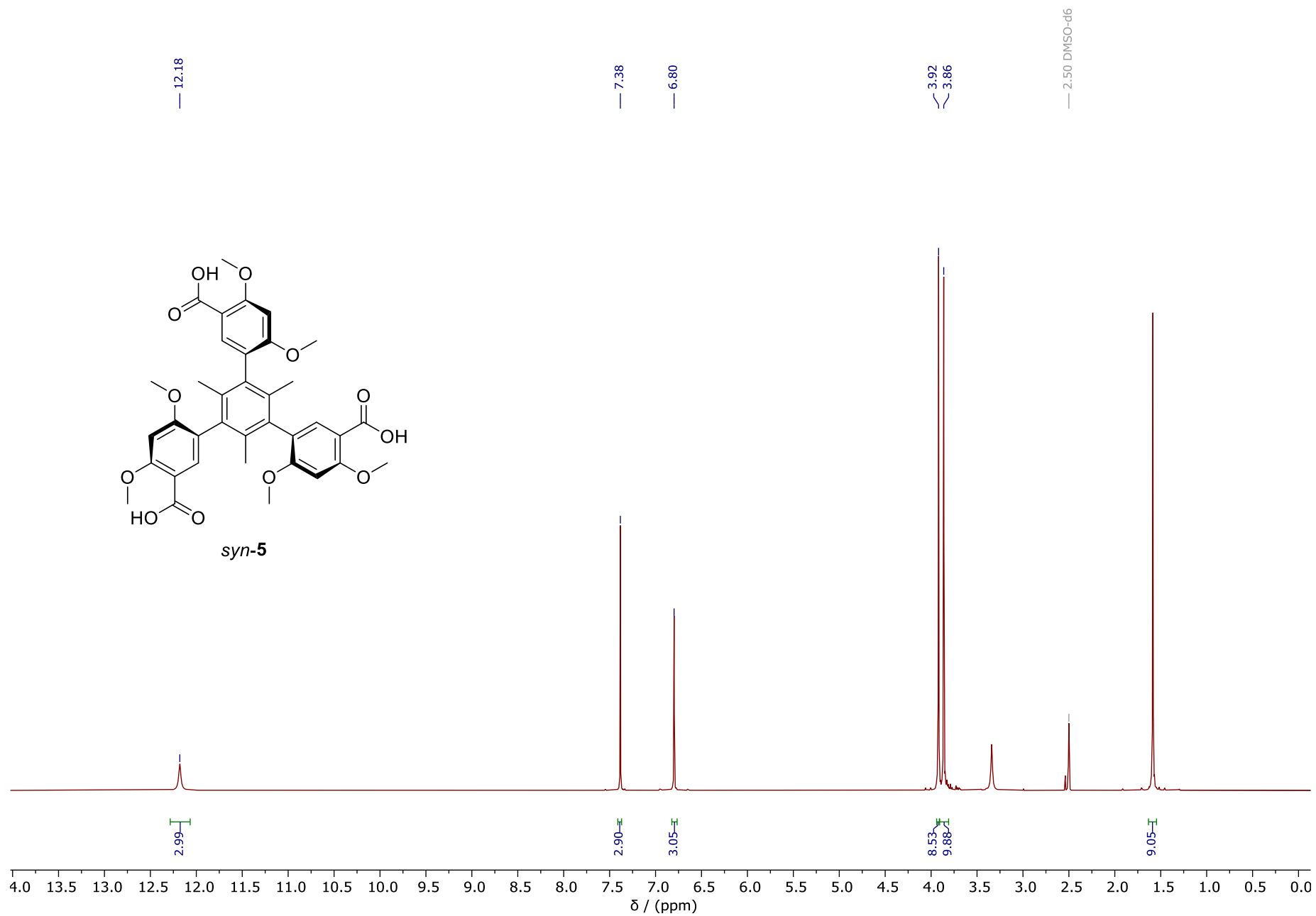


Figure S5. ¹H NMR spectrum (500 MHz, DMSO-d₆, 298 K) of *syn-5*.

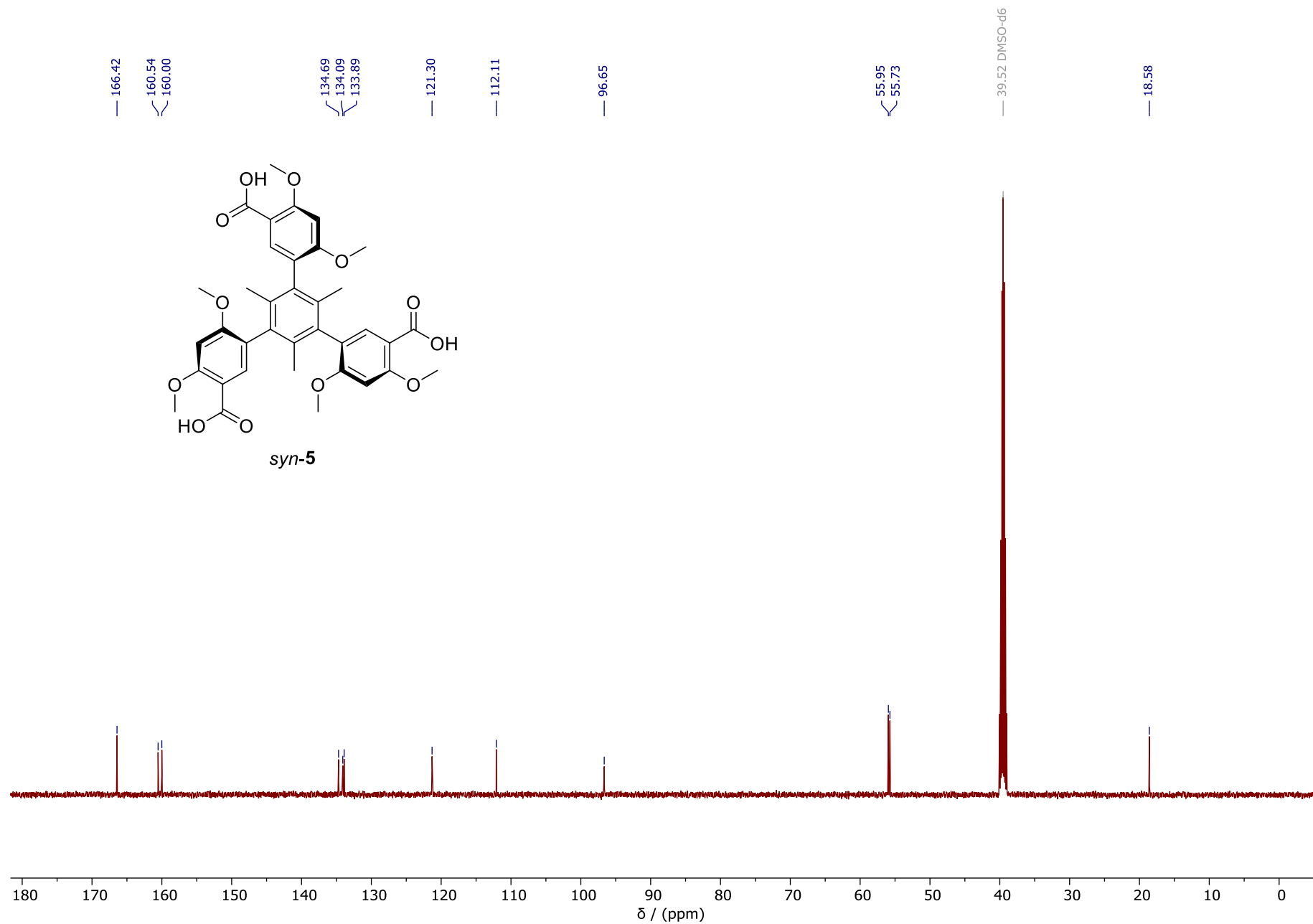


Figure S6. ^{13}C (^1H) NMR spectrum (125 MHz, DMSO-d_6 , 298 K) of *syn-5*.

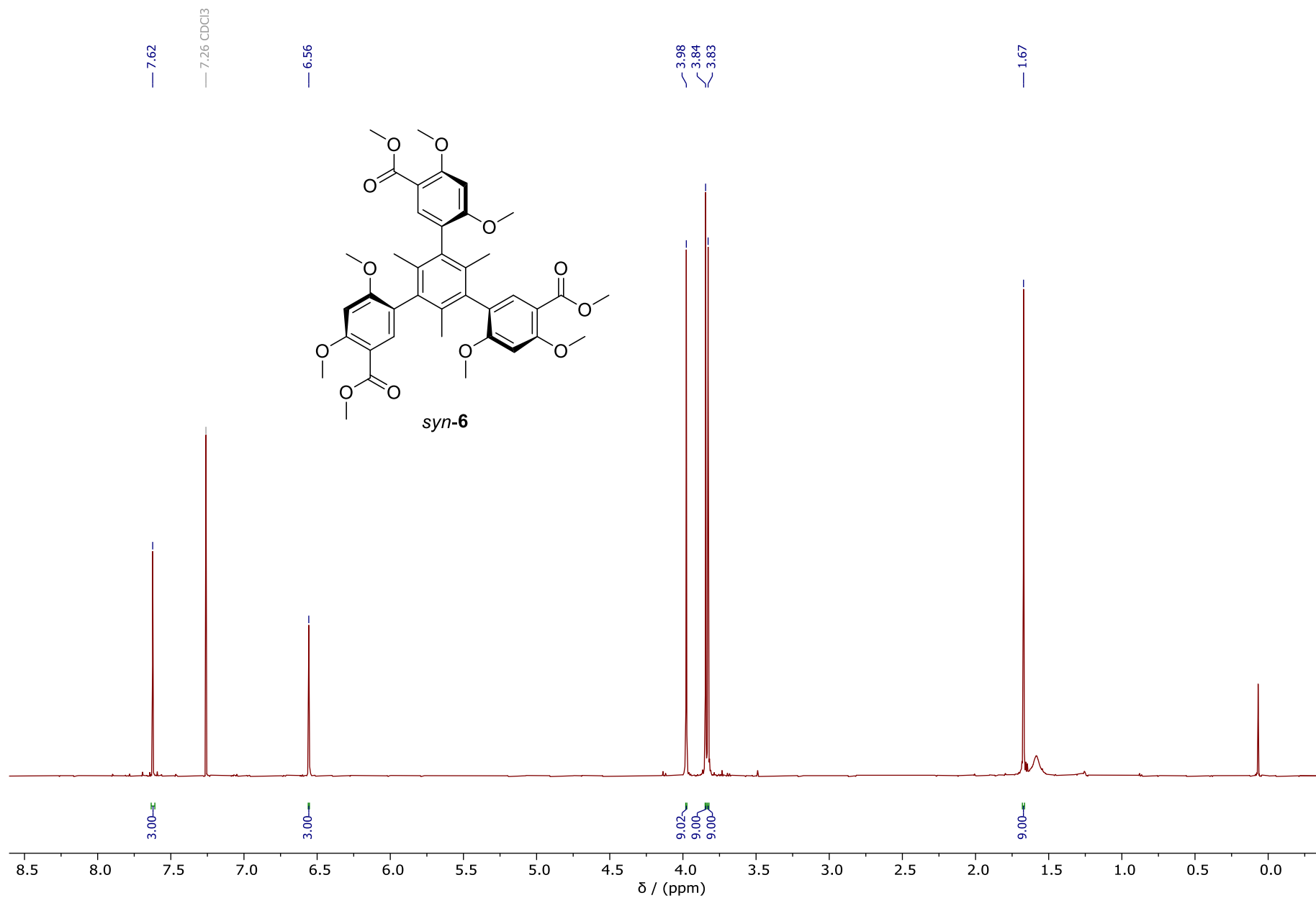


Figure S7. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *syn-6*.

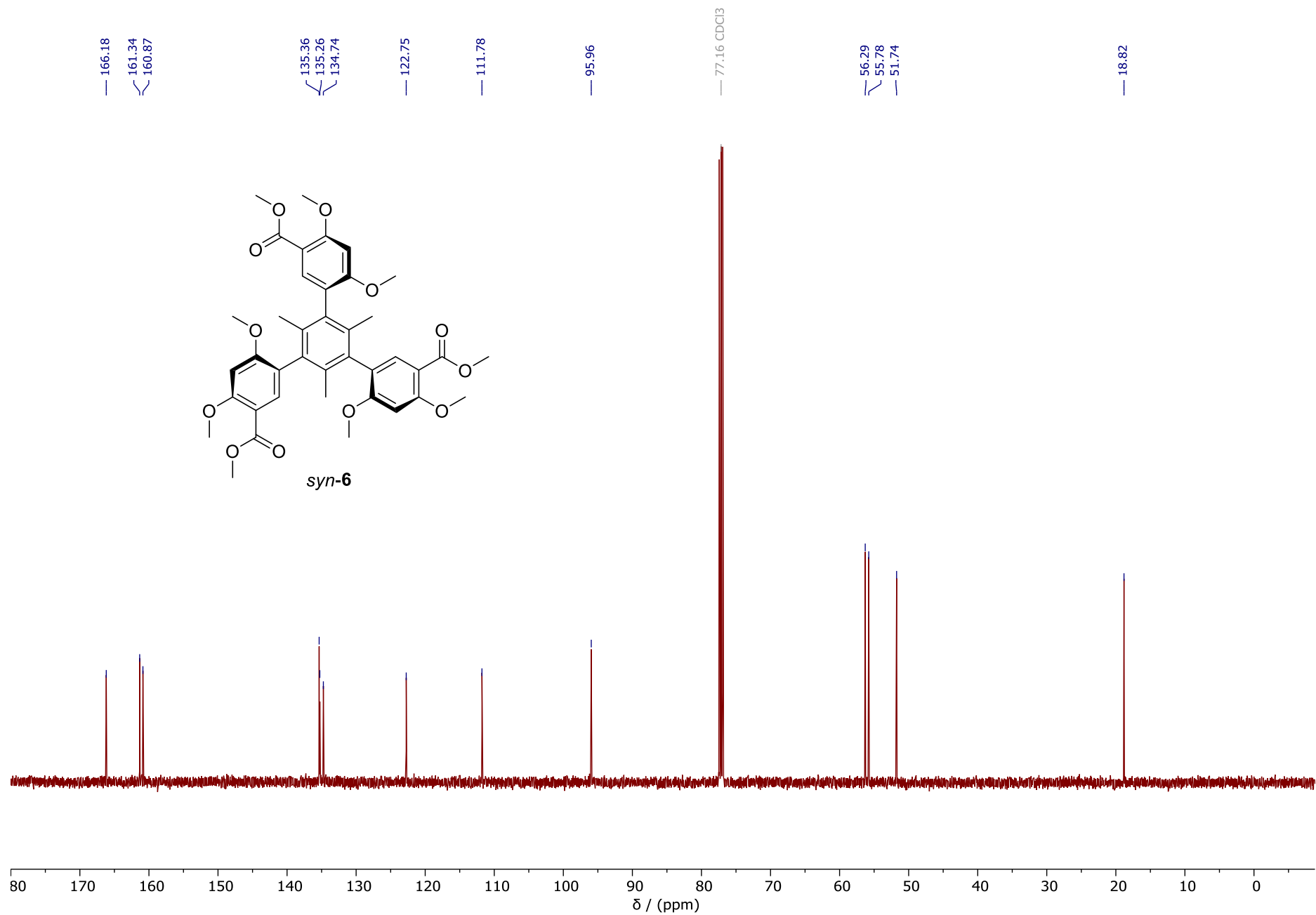


Figure S8. ^{13}C (^1H) NMR spectrum (125 MHz, CDCl_3 , 298 K) of *syn-6*.

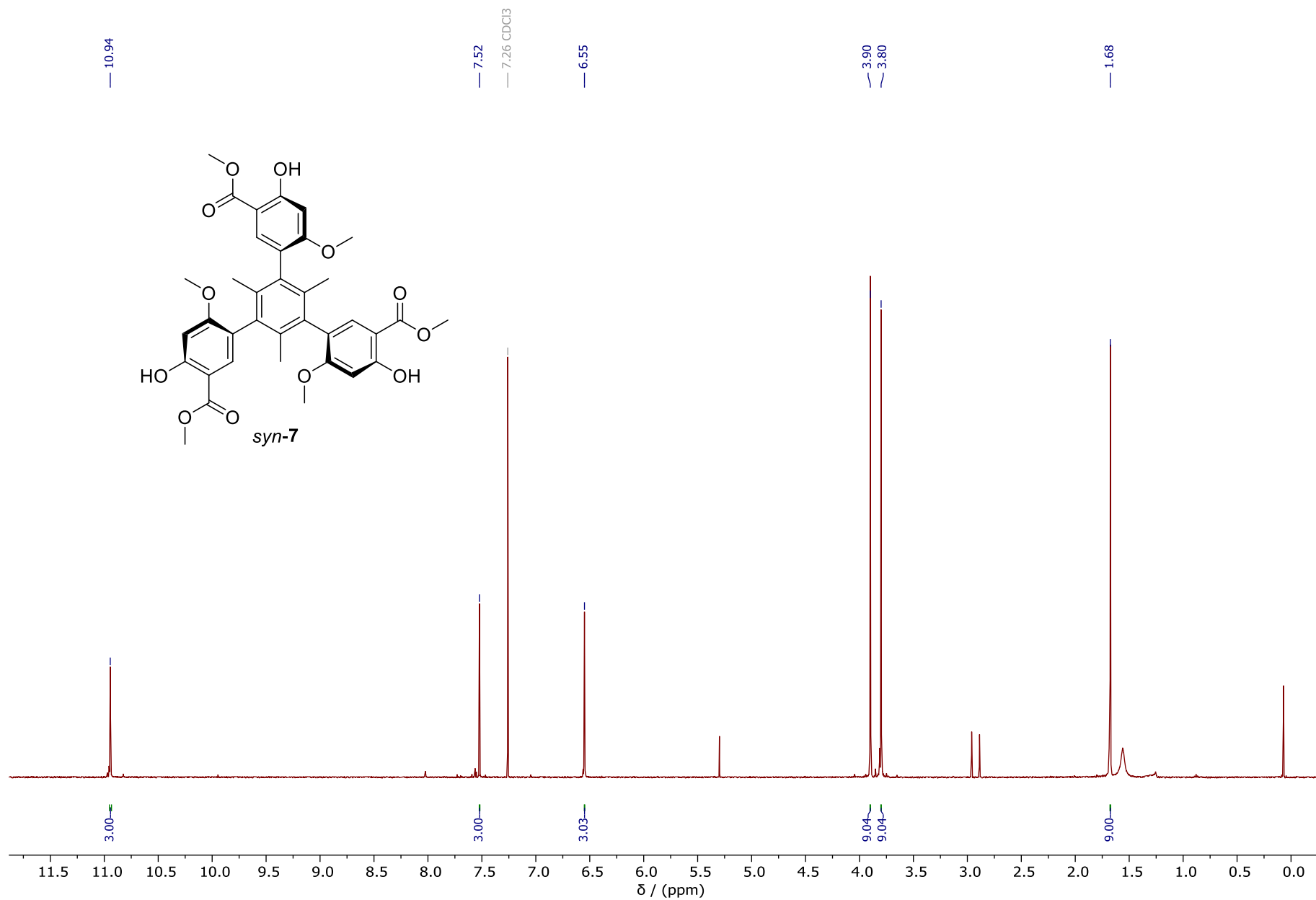


Figure S9. ¹H NMR spectrum (500 MHz, CDCl₃, 298 K) of *syn-7*.

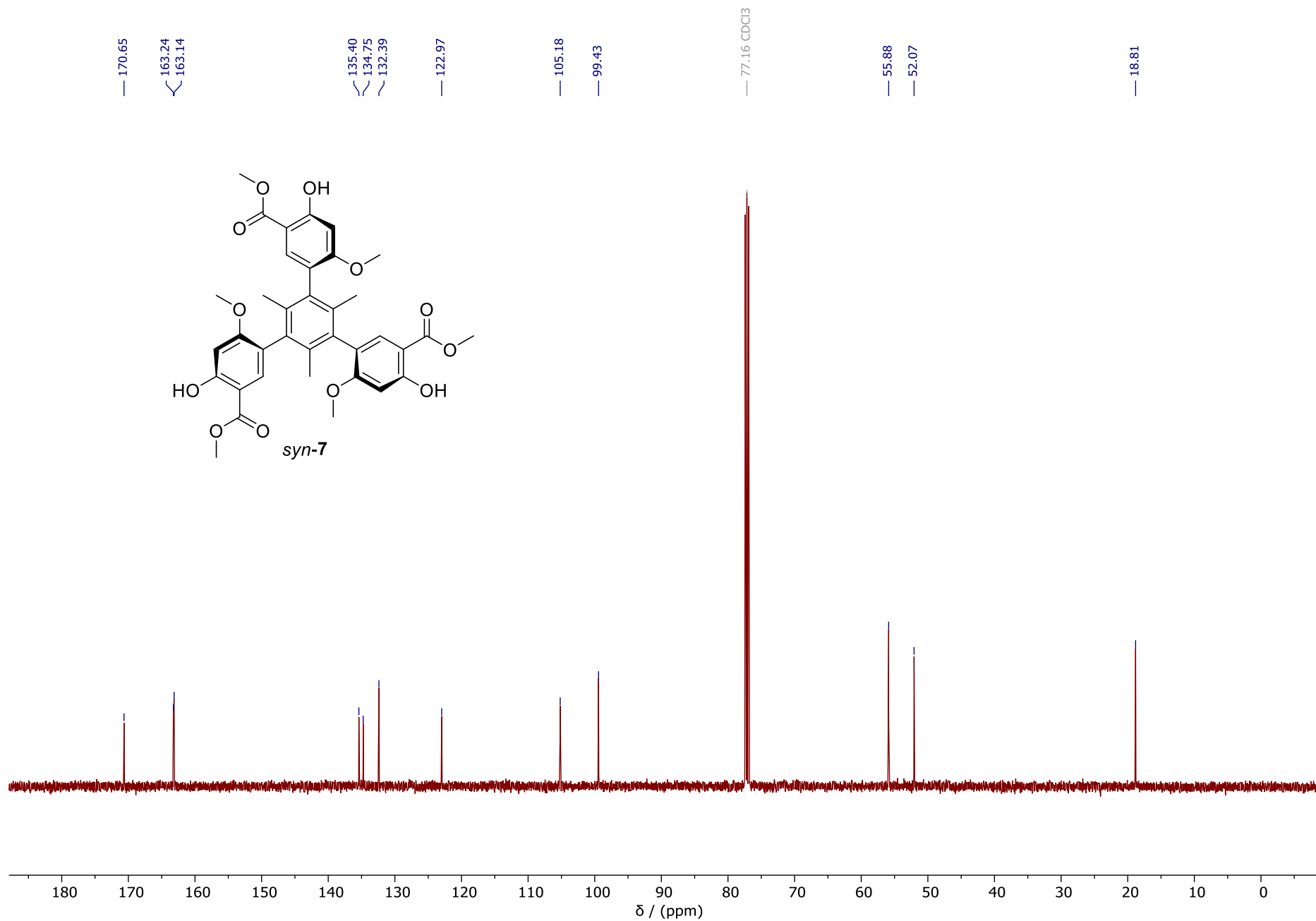


Figure S10. ^{13}C (^1H) NMR spectrum (125 MHz, CDCl_3 , 298 K) of *syn-7*.

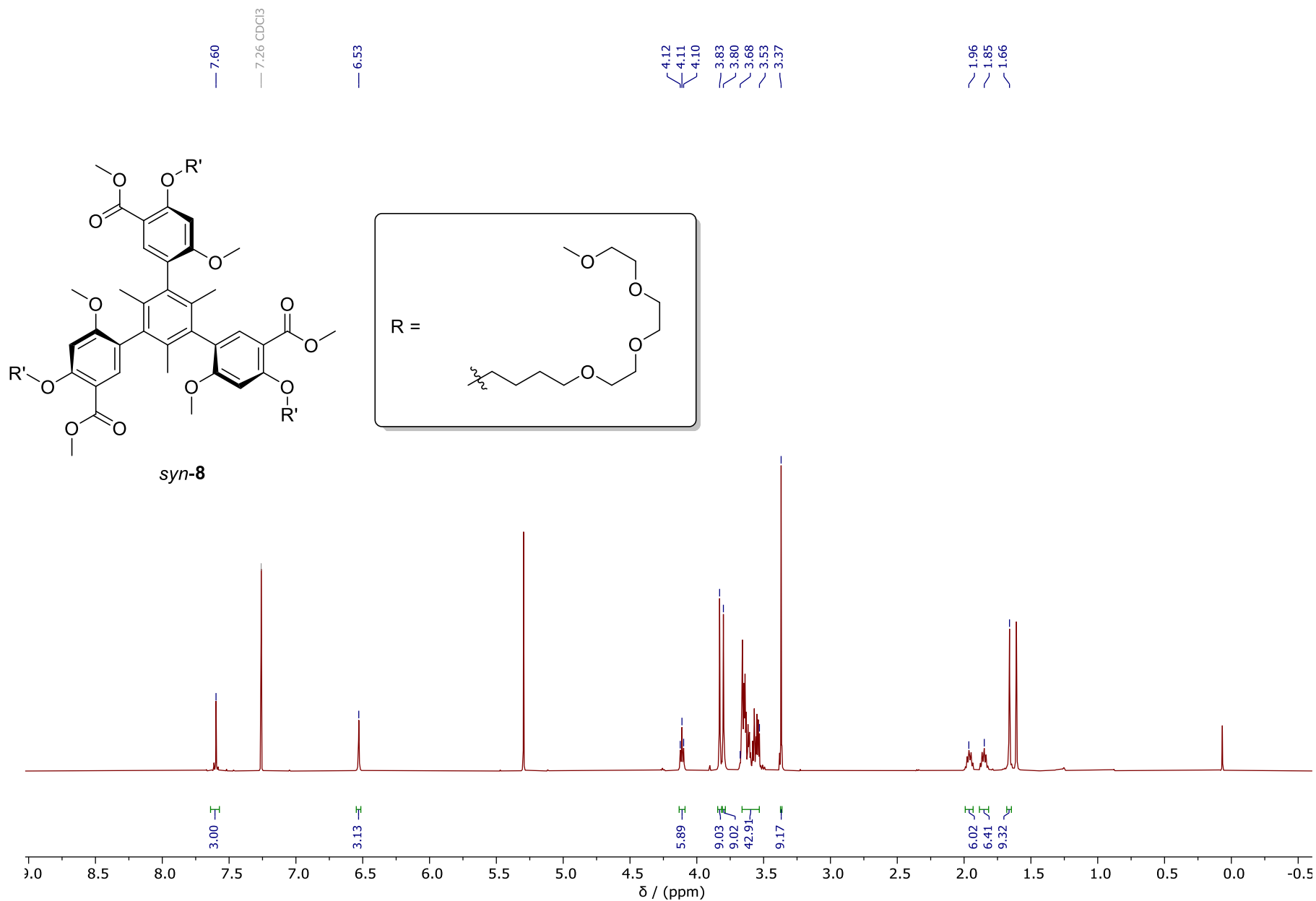


Figure S11. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of **yn-8**.

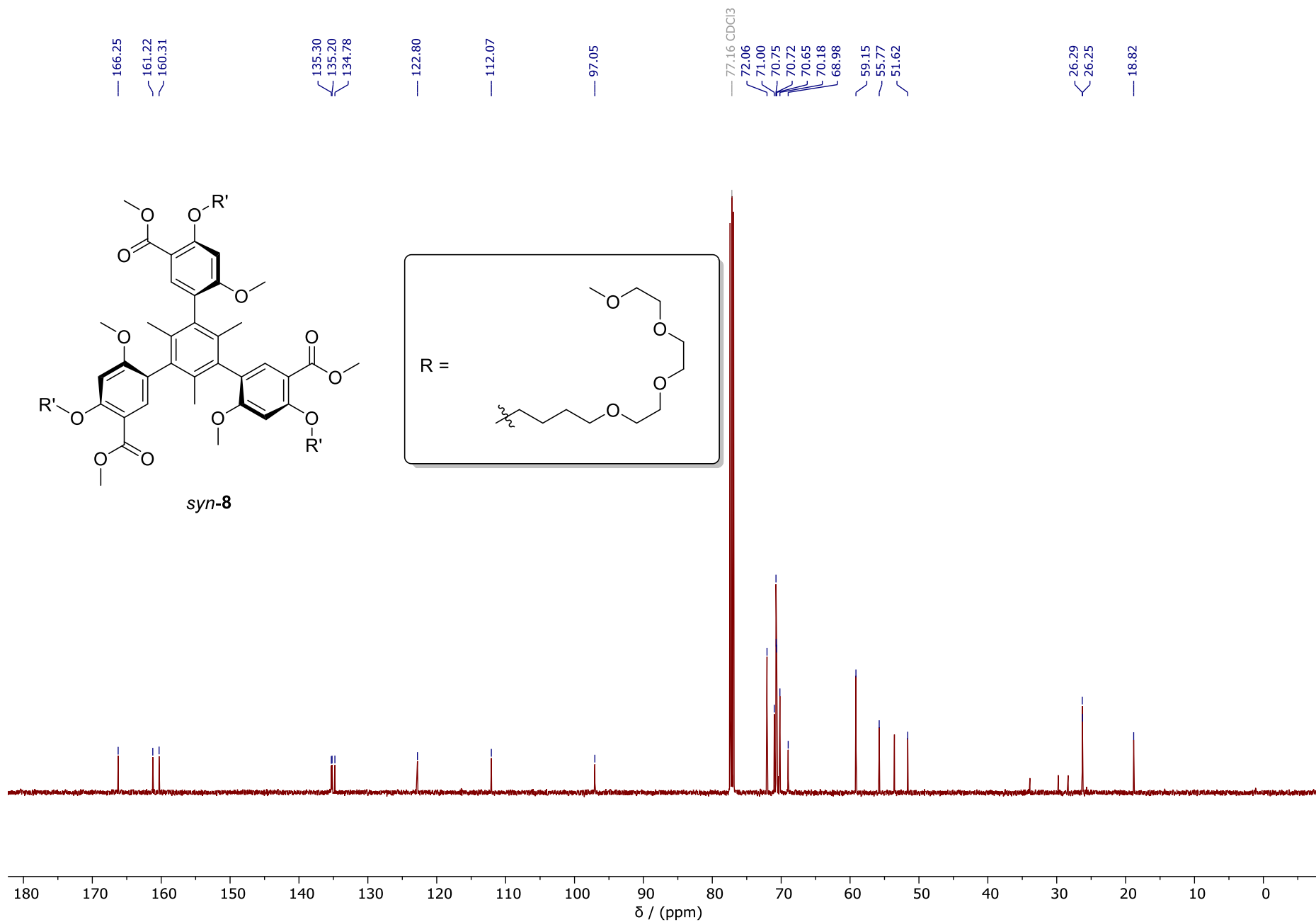


Figure S12. ^{13}C (^1H) NMR spectrum (125 MHz, CDCl_3 , 298 K) of *syn-8*.

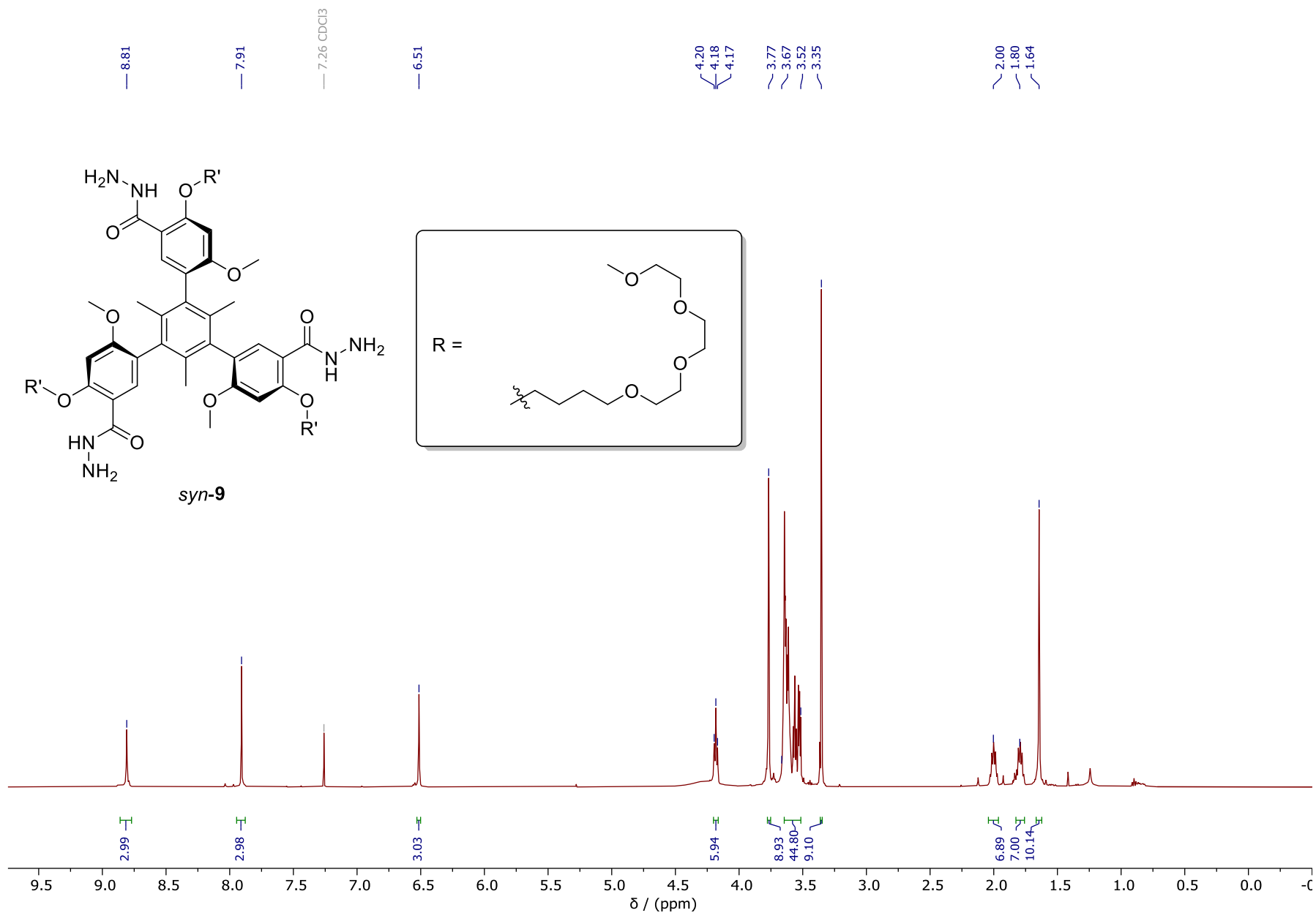


Figure S13. ^1H NMR spectrum (500 MHz, CDCl_3 , 298 K) of *syn-9*.

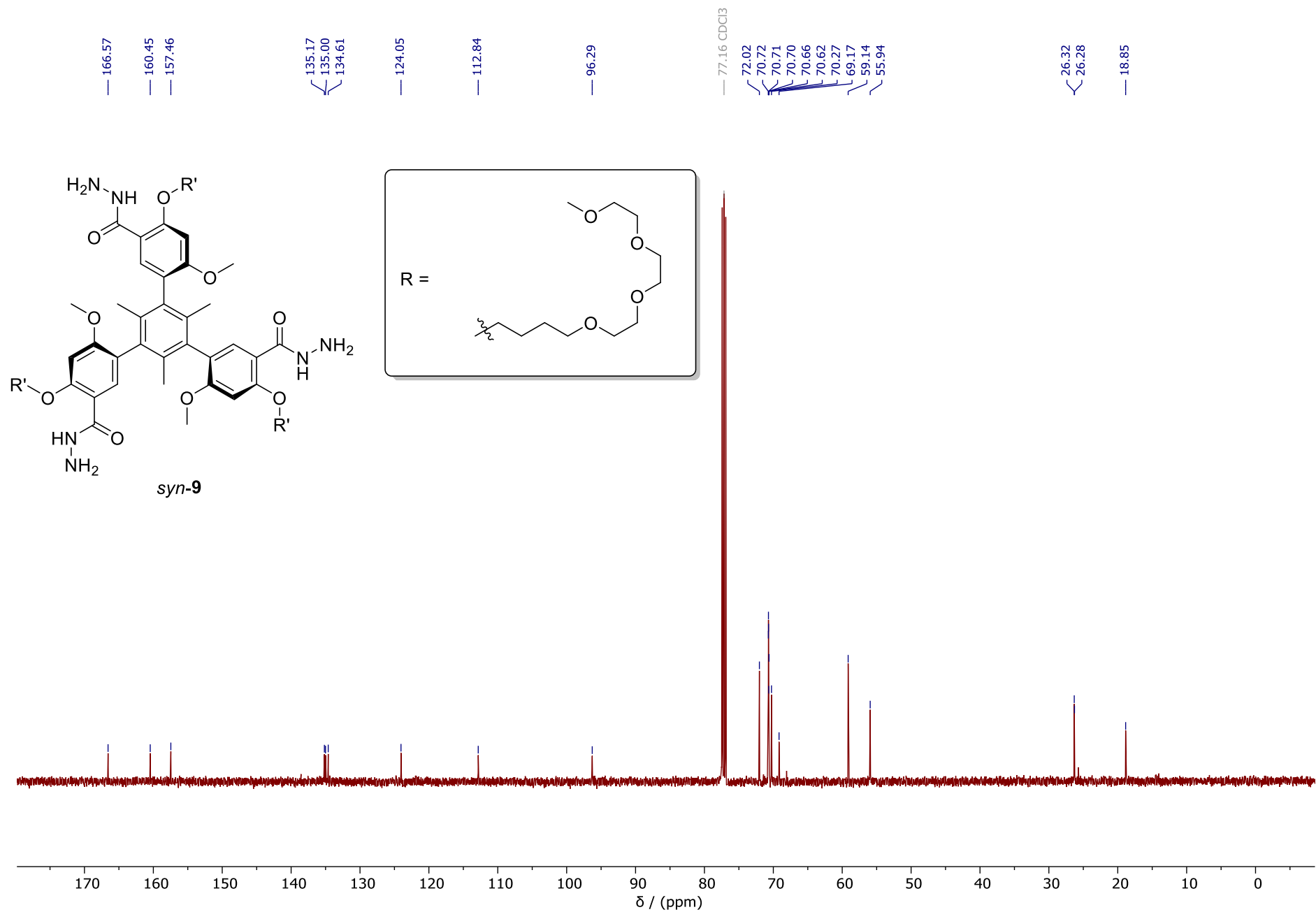


Figure S14. ^{13}C (^1H) NMR spectrum (125 MHz, CDCl_3 , 298 K) of *syn-9*.

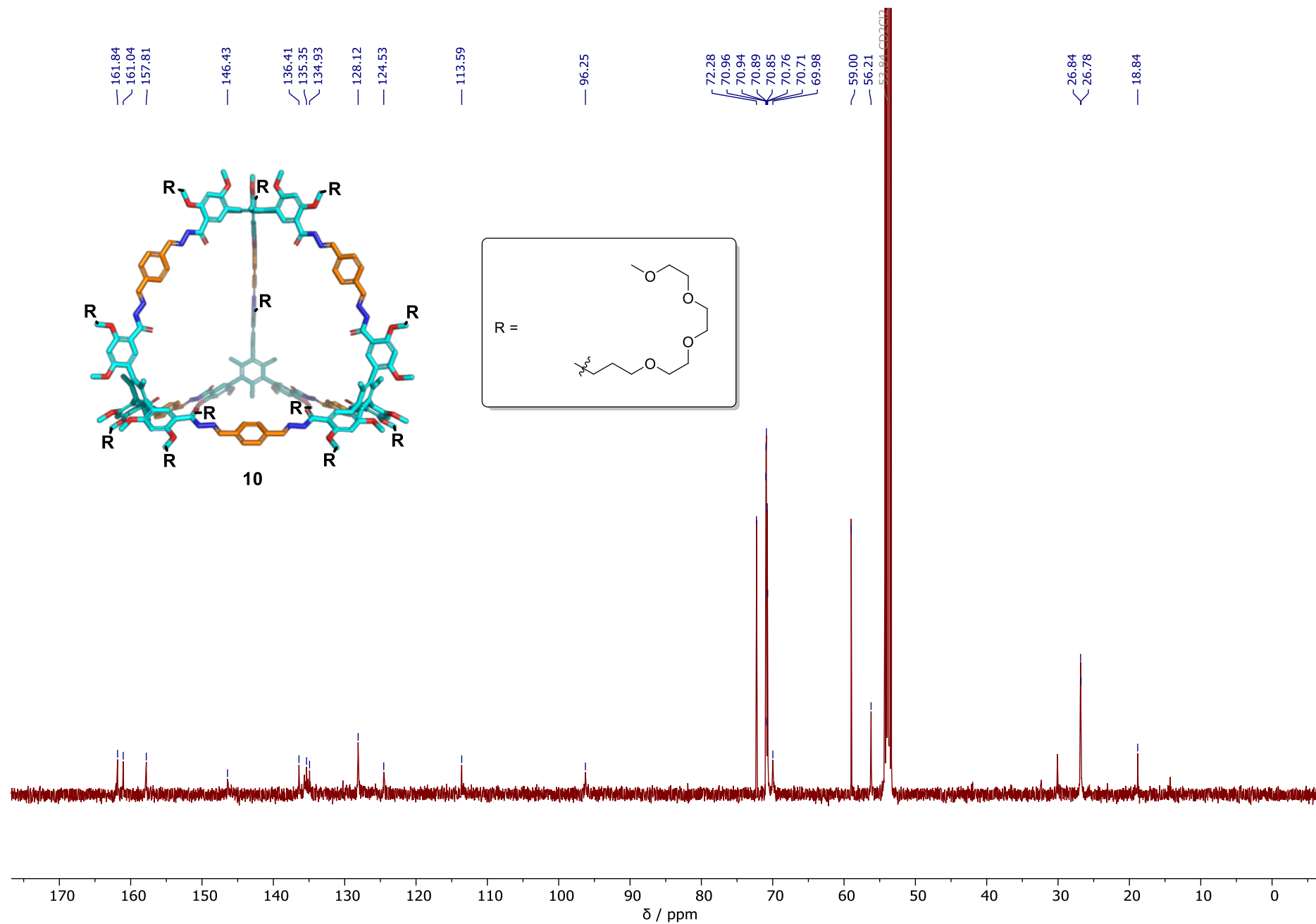


Figure S16. ^{13}C (^1H) NMR spectrum (125 MHz, CDCl_3 , 298 K) of **10**.

DOSY 74 1 C:\Bruker\TopSpin4.1.1\data

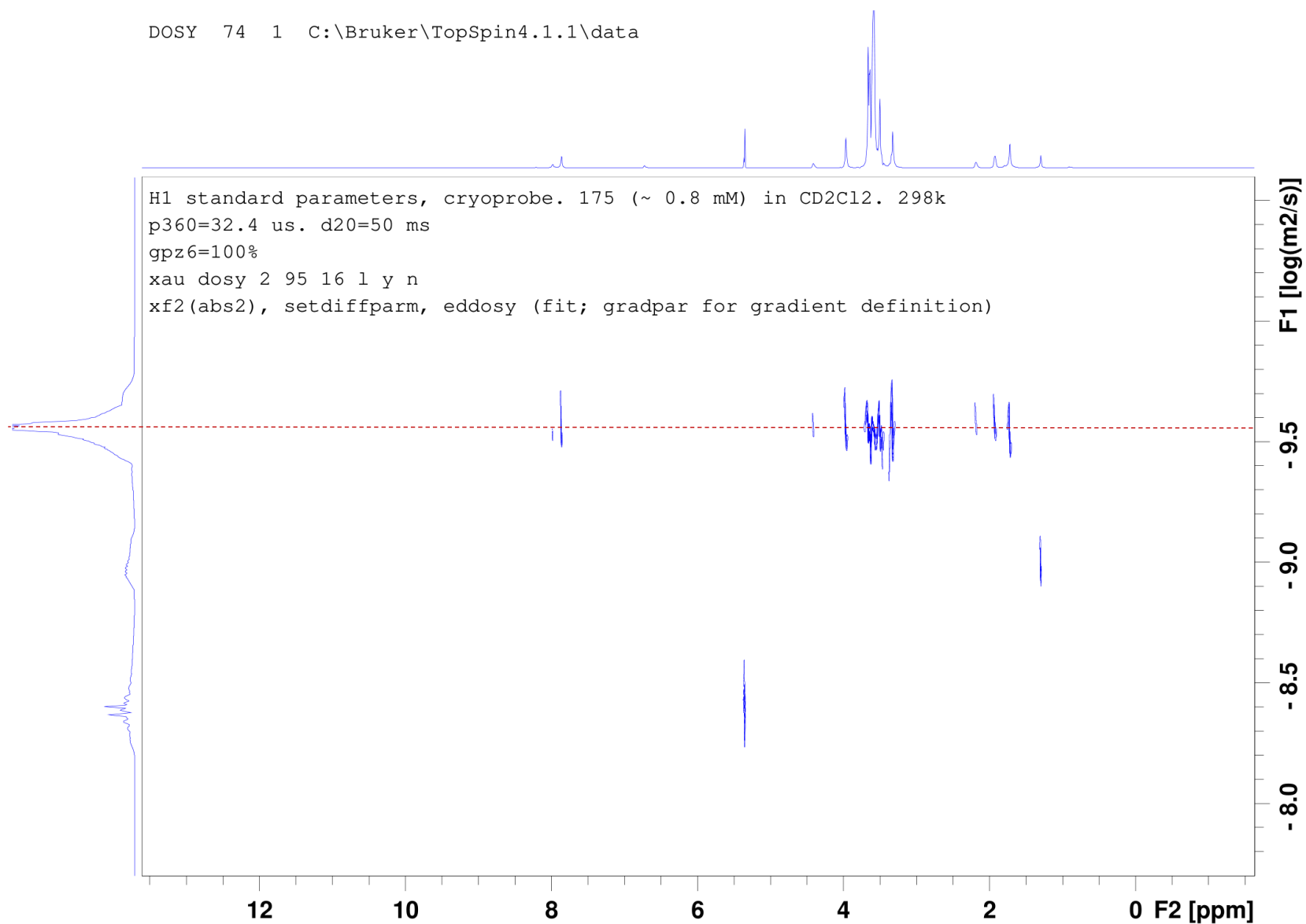


Figure S17. ¹H DOSY NMR spectrum (800 MHz, CD₂Cl₂) of **10**.

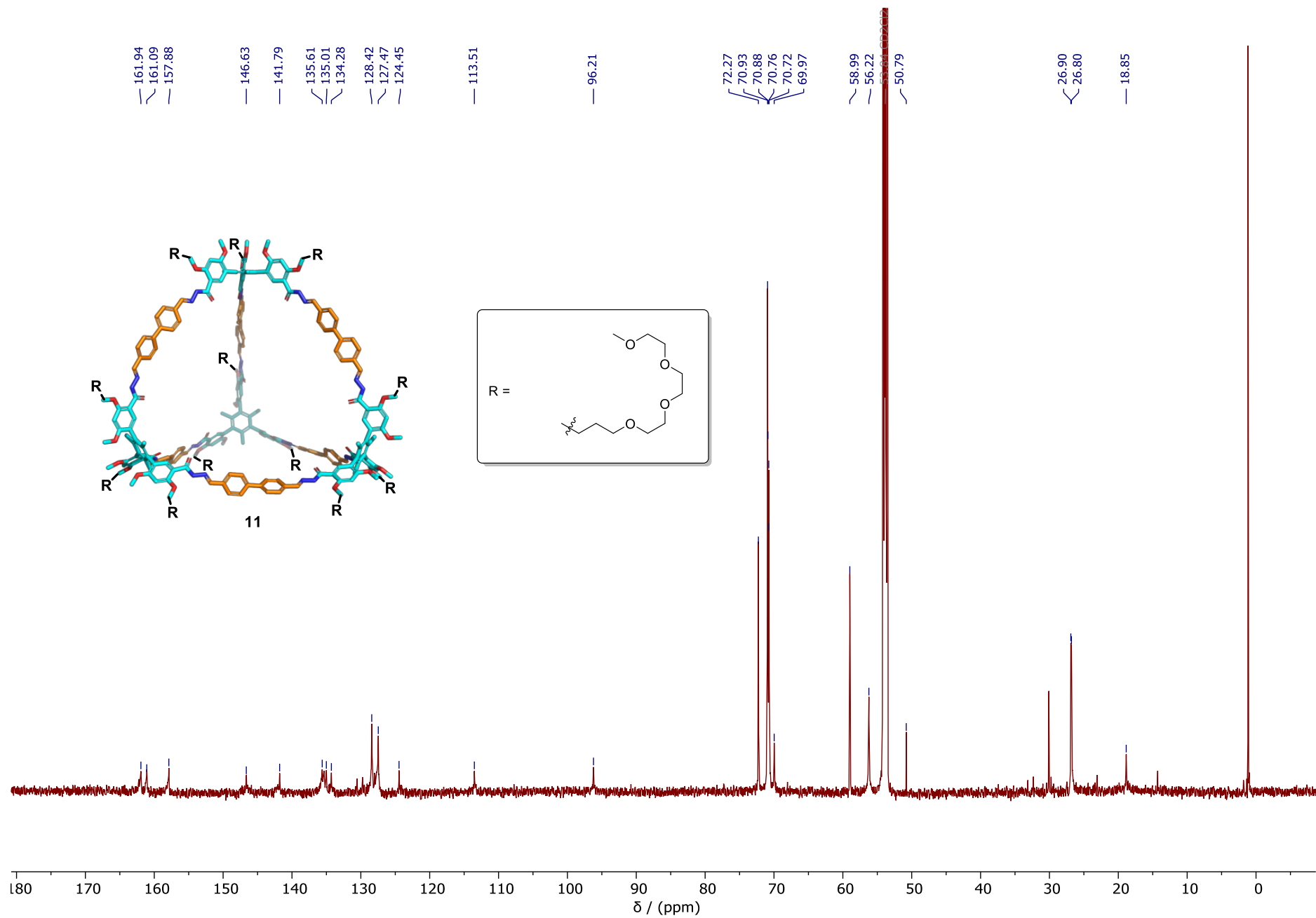


Figure S19. ^{13}C (^1H) NMR spectrum (200 MHz, CDCl_3 , 298 K) of **11**.

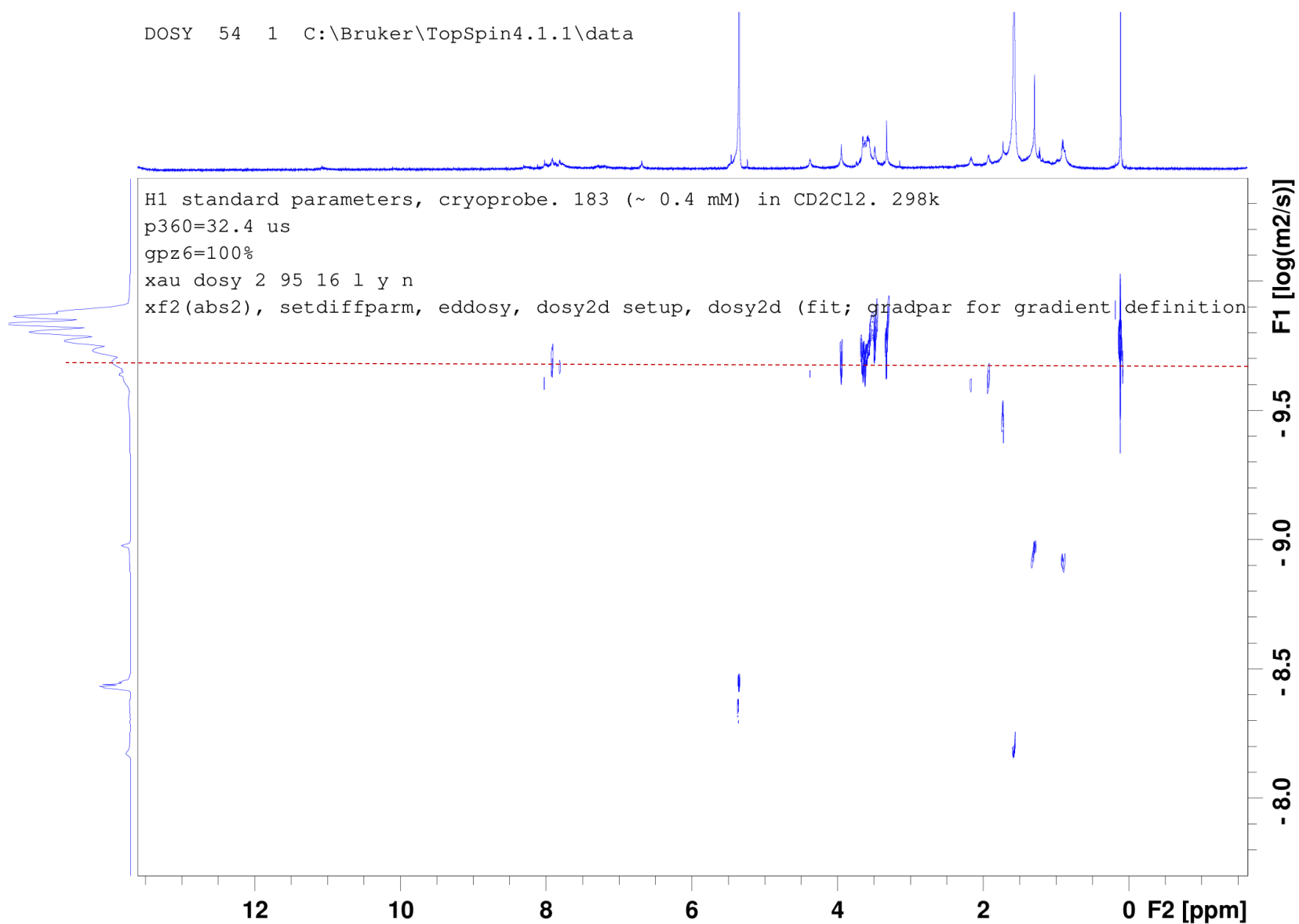


Figure S20. ¹H DOSY NMR spectrum (800 MHz, CD₂Cl₂) of **11**.

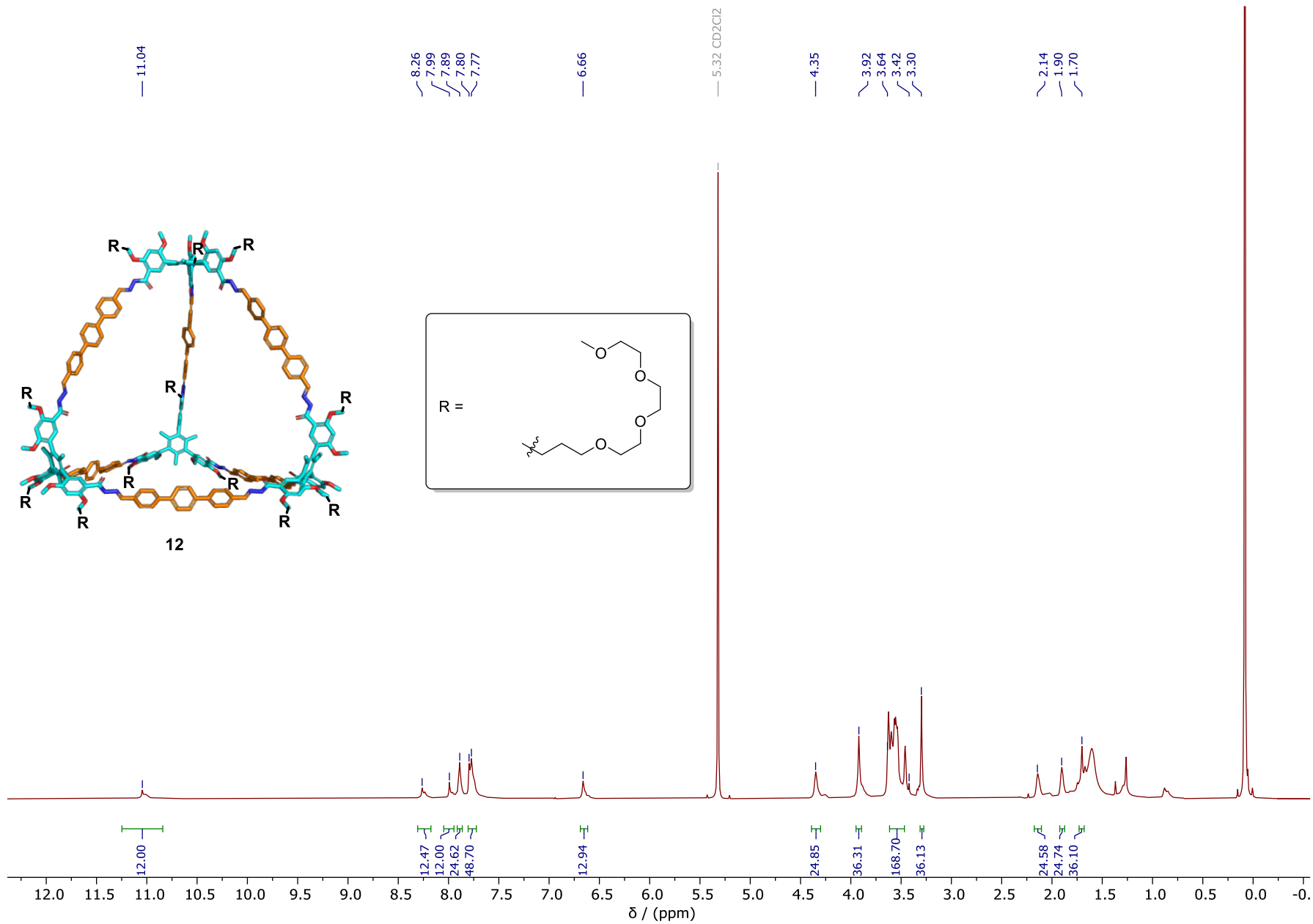


Figure S21. ^1H NMR spectrum (800 MHz, CD_2Cl_2 , 298 K) of **12**.

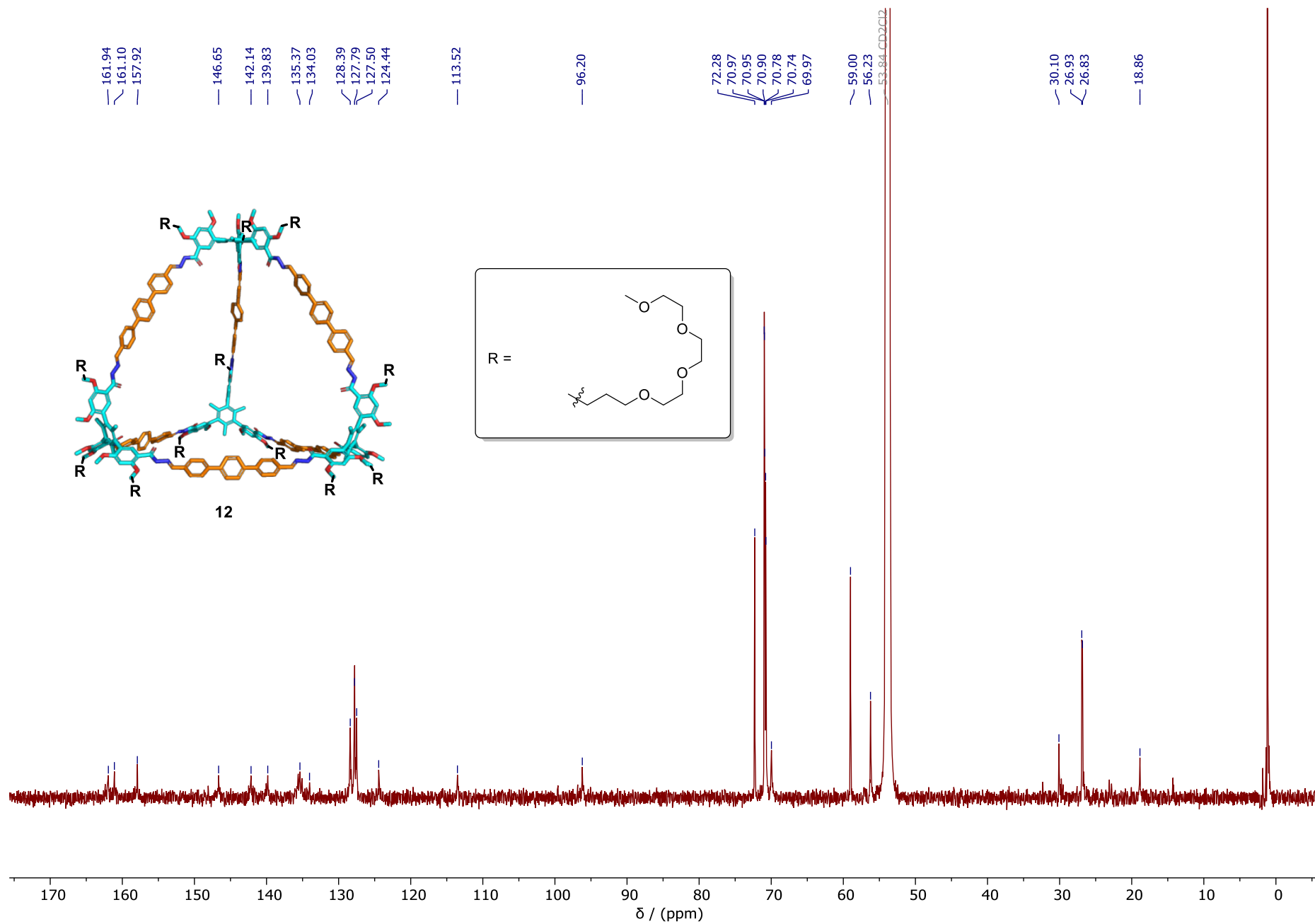


Figure S22. ^{13}C (^1H) NMR spectrum (200 MHz, CDCl_3 , 298 K) of **12**.

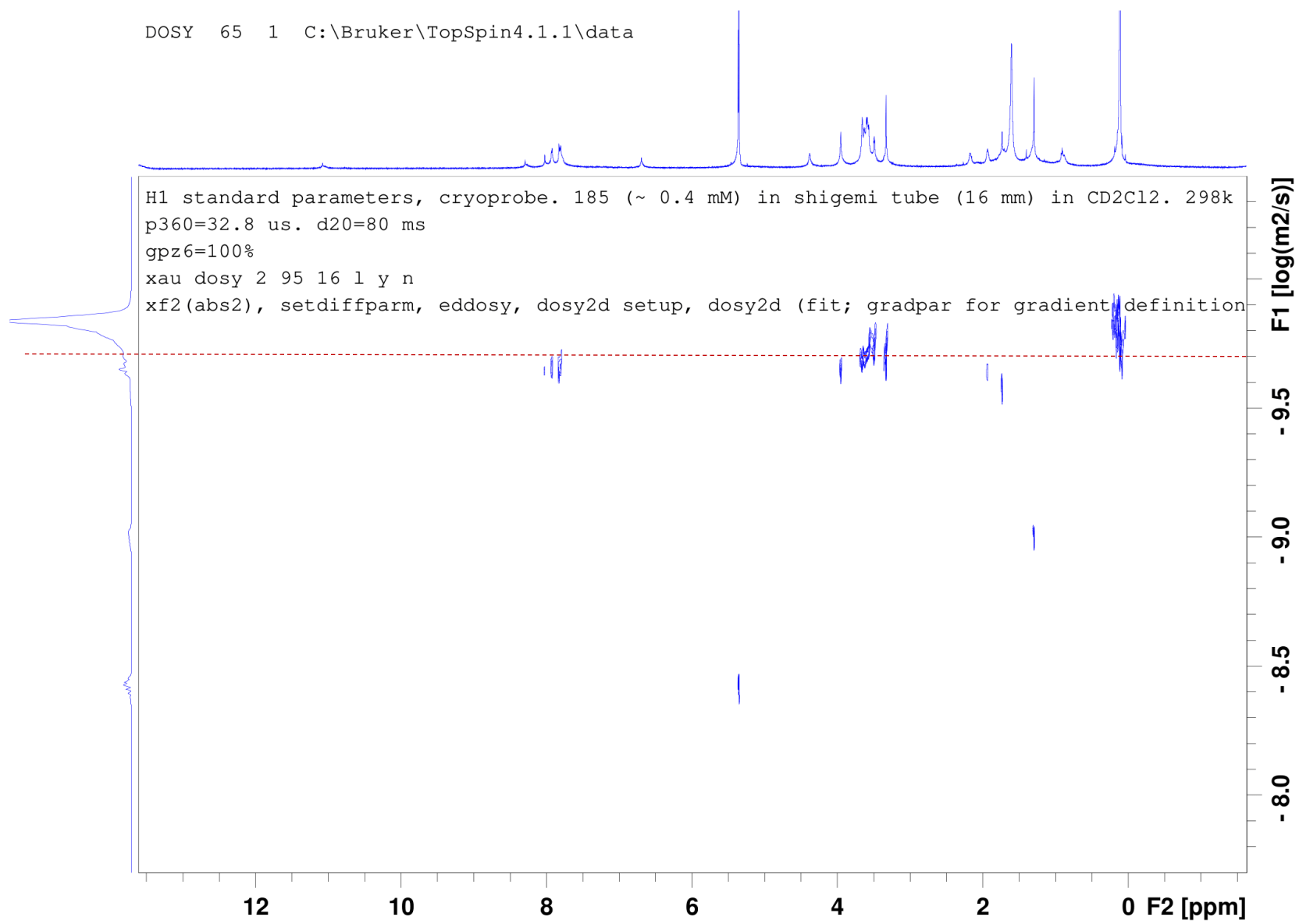


Figure S23. ^1H DOSY NMR spectrum (800 MHz, CD_2Cl_2) of **12**.

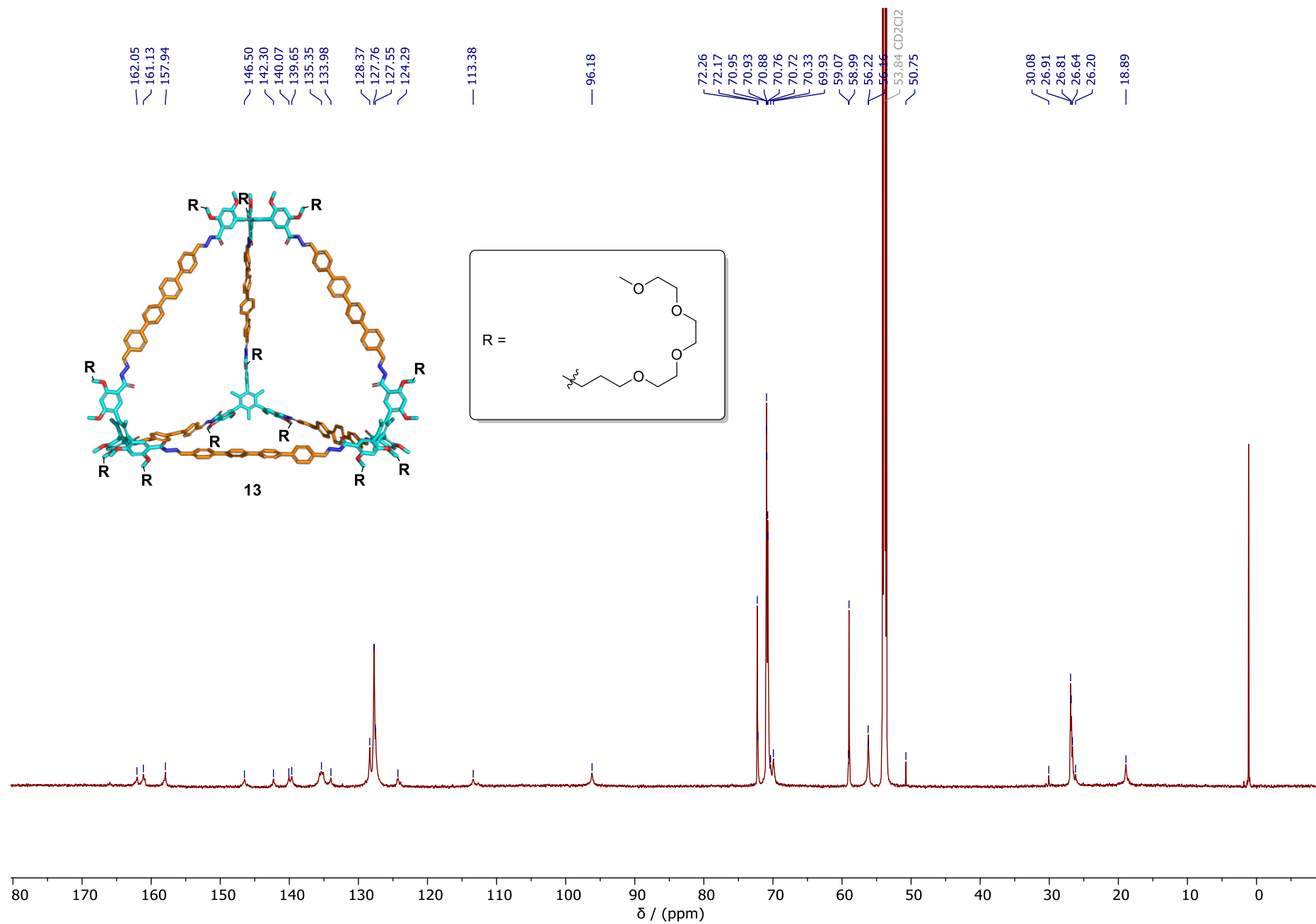


Figure S25. ^{13}C (^1H) NMR spectrum (200 MHz, CDCl_3 , 298 K) of **13**.

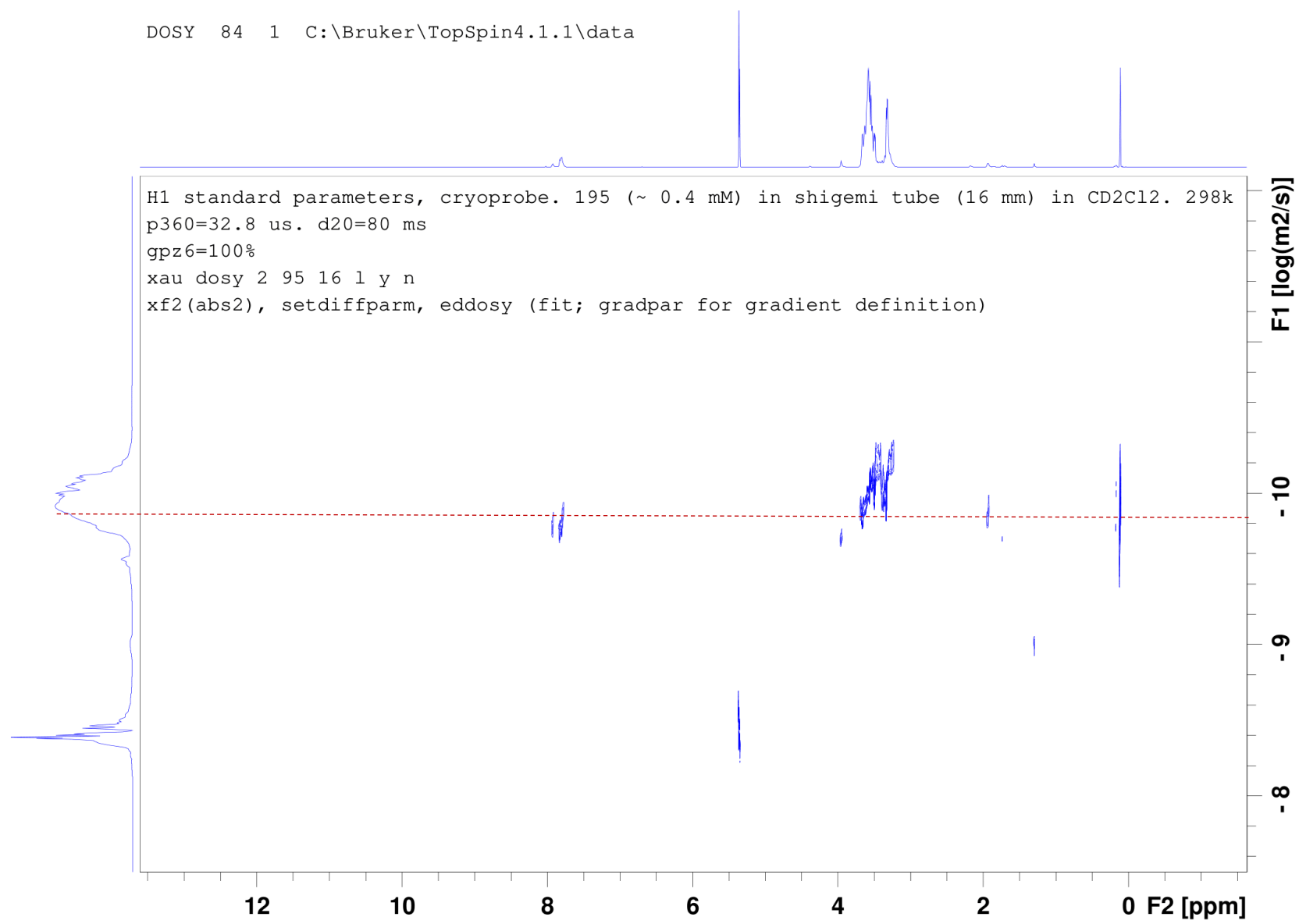


Figure S26. ¹H DOSY NMR spectrum (800 MHz, CD₂Cl₂) of **13**.

VI. Mass Spectra

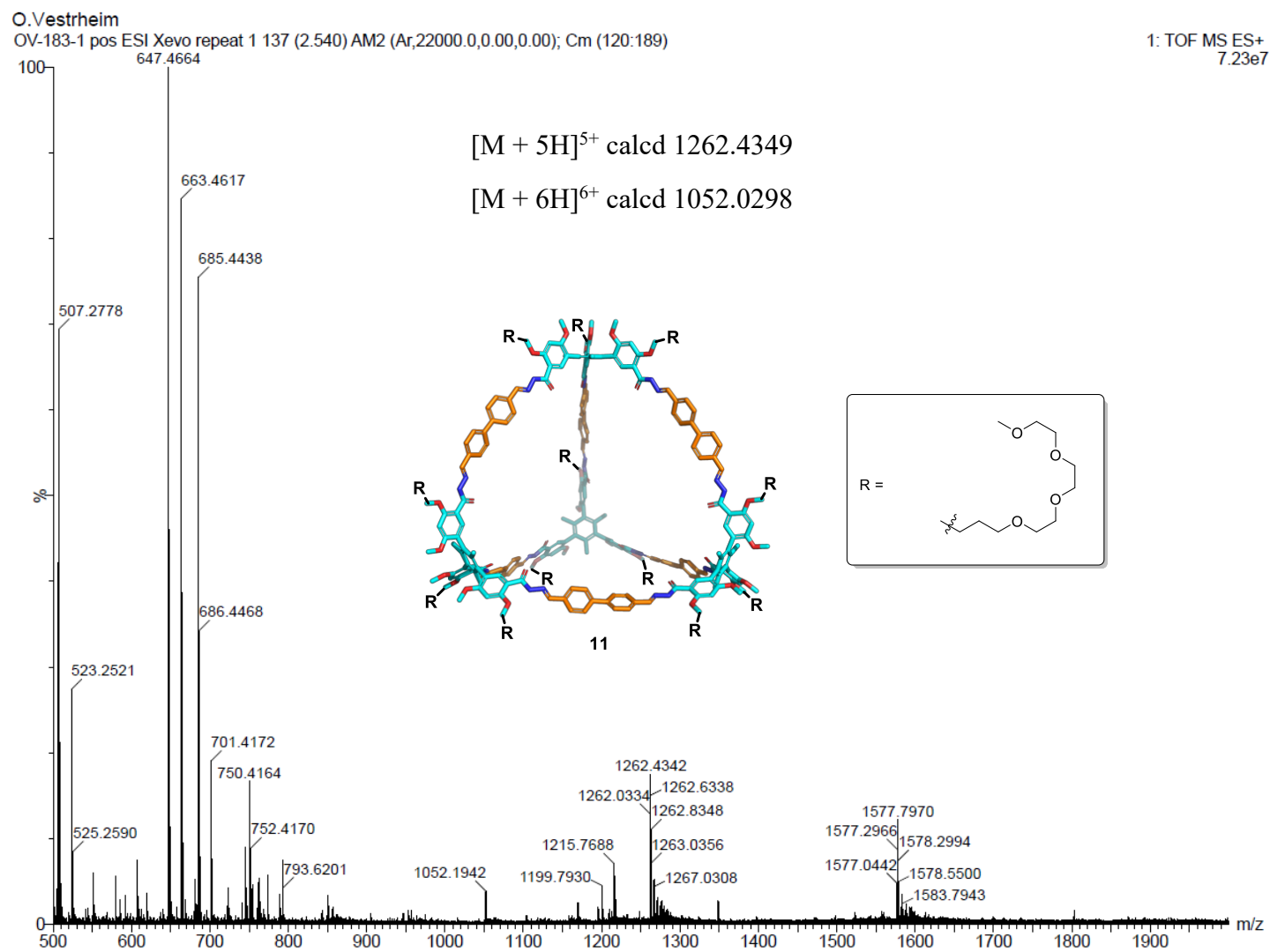


Figure S27. HRMS (ESI+) spectrum of 11.

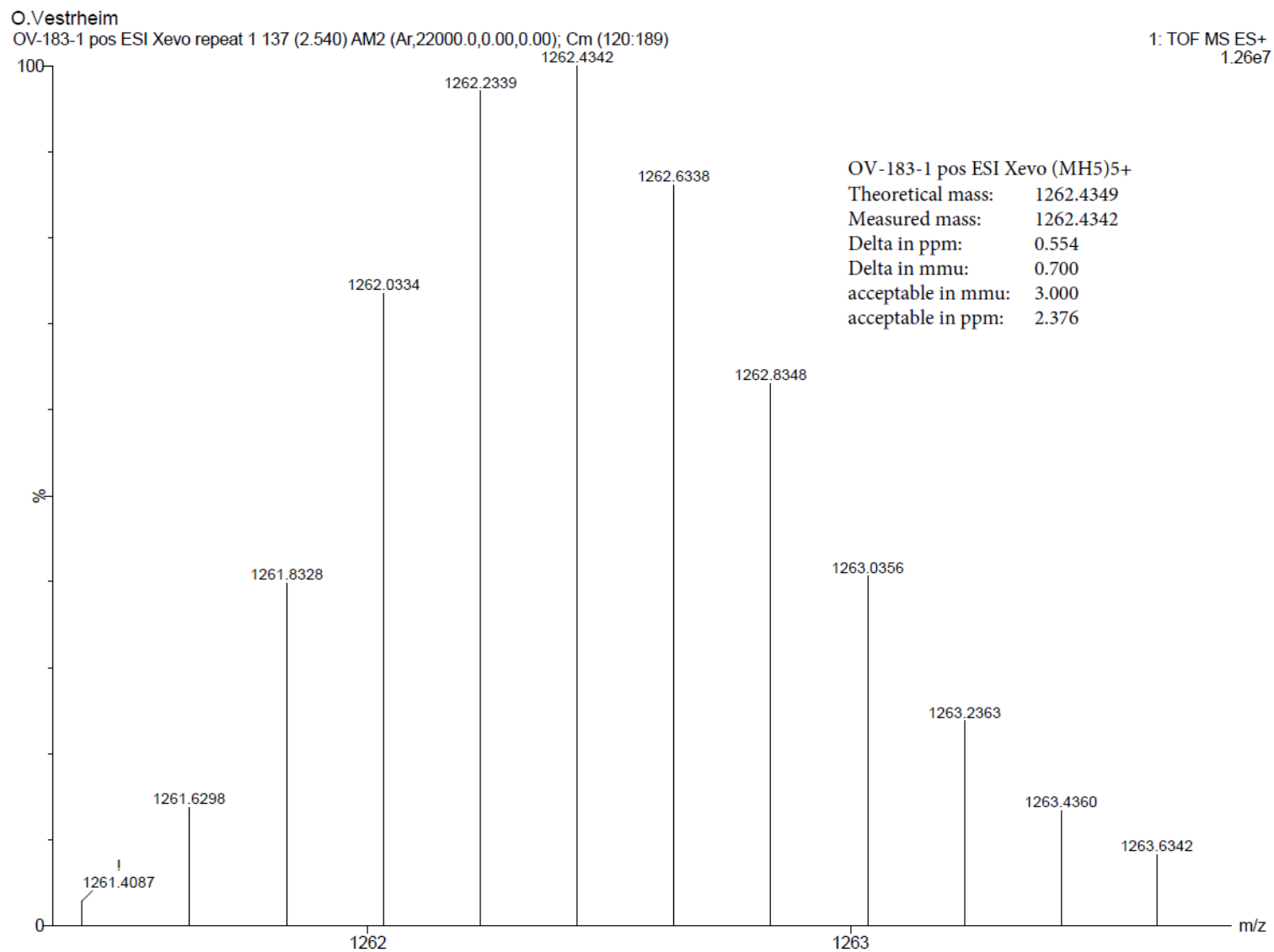


Figure S28. Isotopic distribution of the $[M + 5H]^{5+}$ peak of the HRMS (ESI+) spectrum of **11**.

O. Vestrheim

OV-183-1 pos ESI Xevo repeat 1 137 (2.540) AM2 (Ar,22000.0,0.00,0.00); Cm (120:189)

1: TOF MS ES+
2.76e6

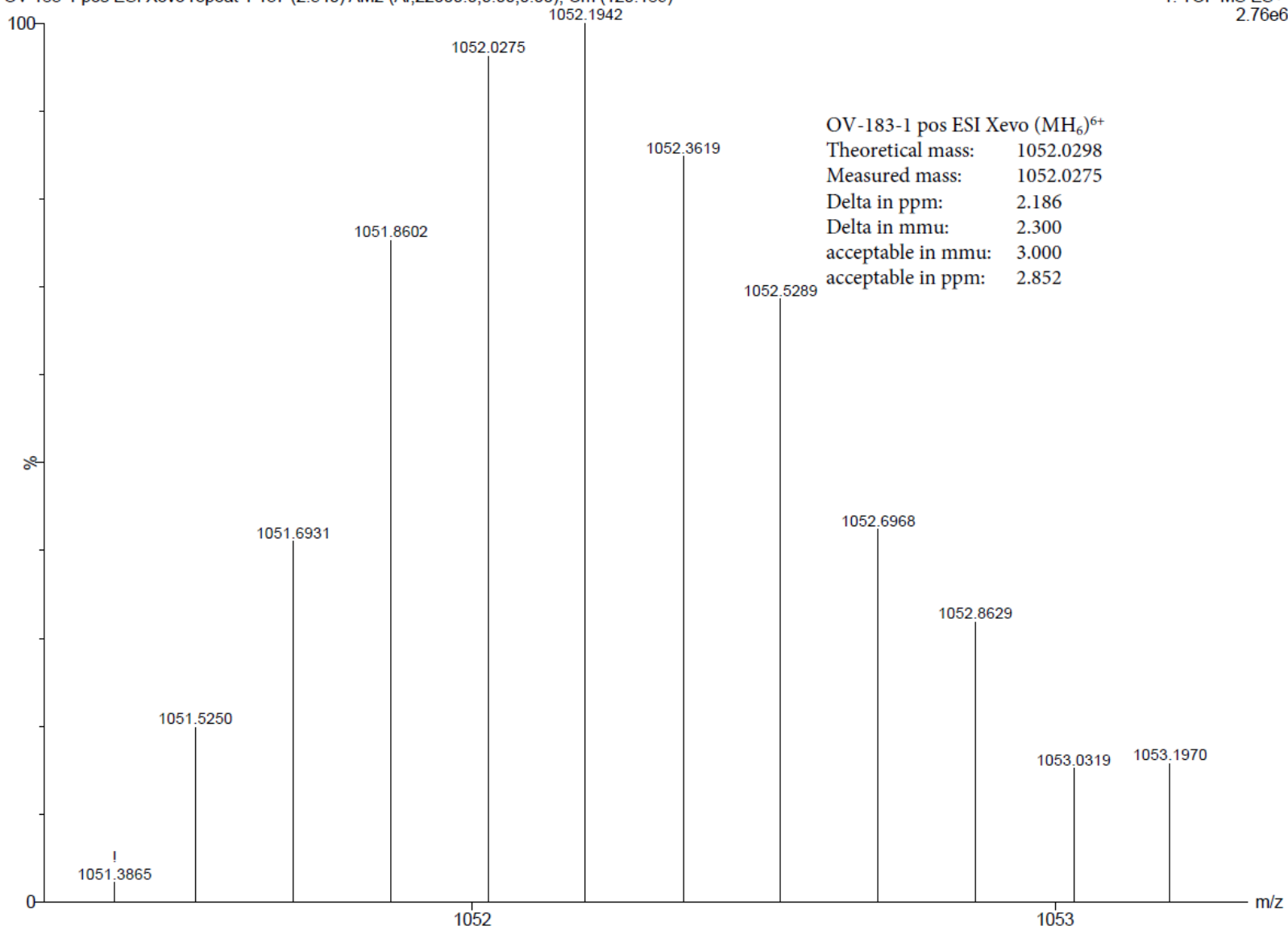
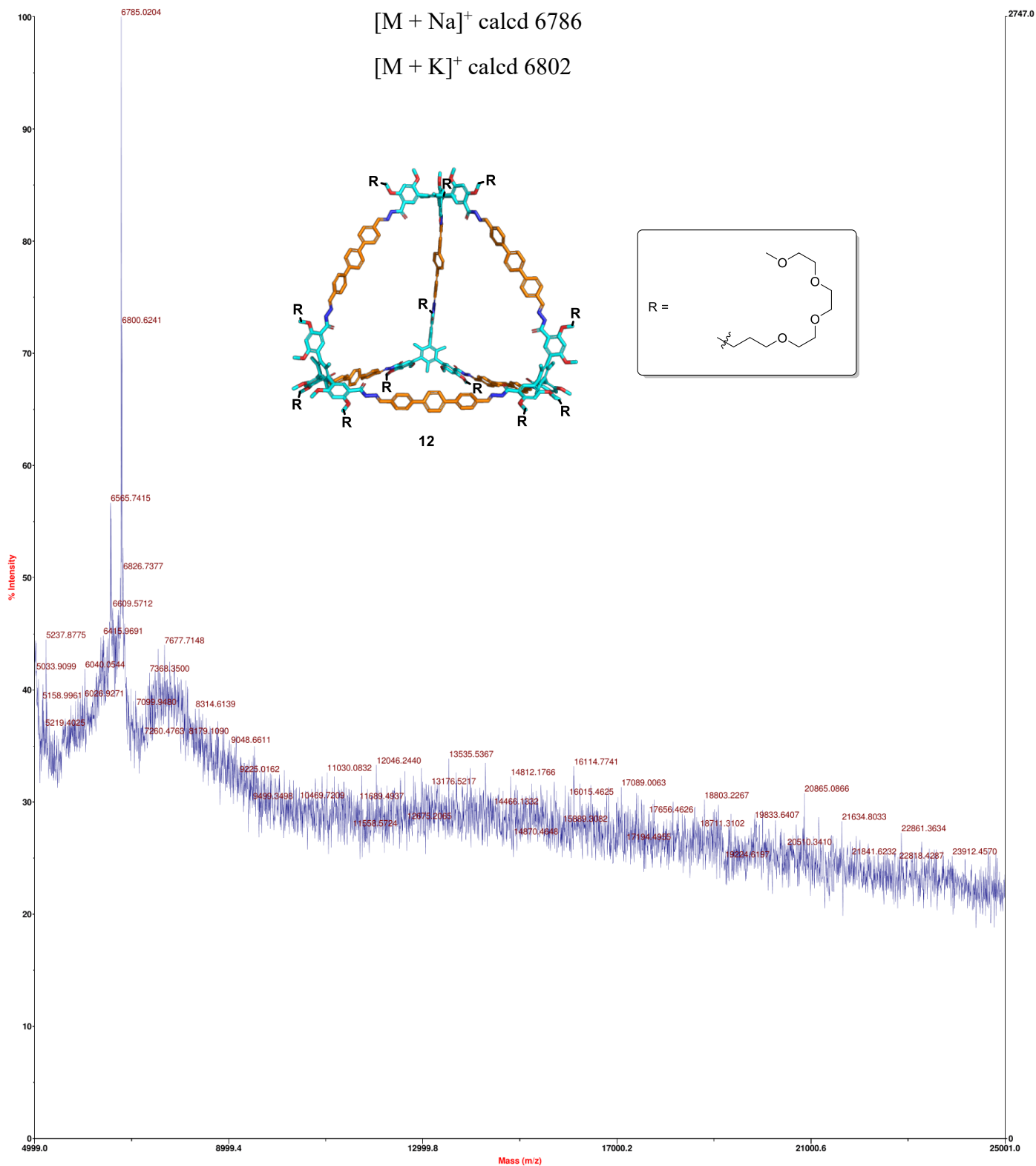
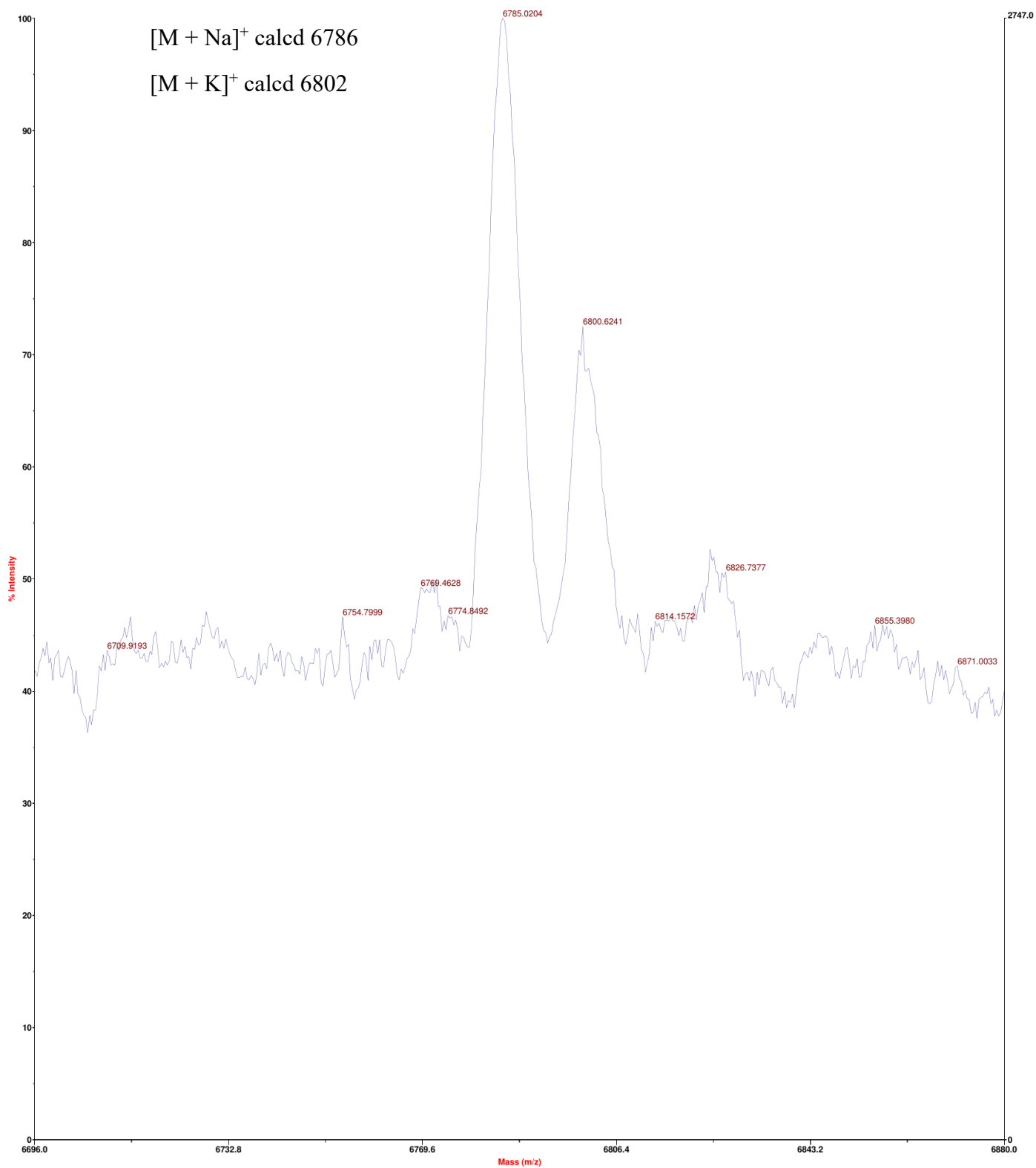


Figure S29. Isotopic distribution of the $[M + 6H]^{6+}$ peak of the HRMS (ESI+) spectrum of **11**.



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Figure S30. MALDI-TOF mass spectrum (DCTB matrix) of **12**.

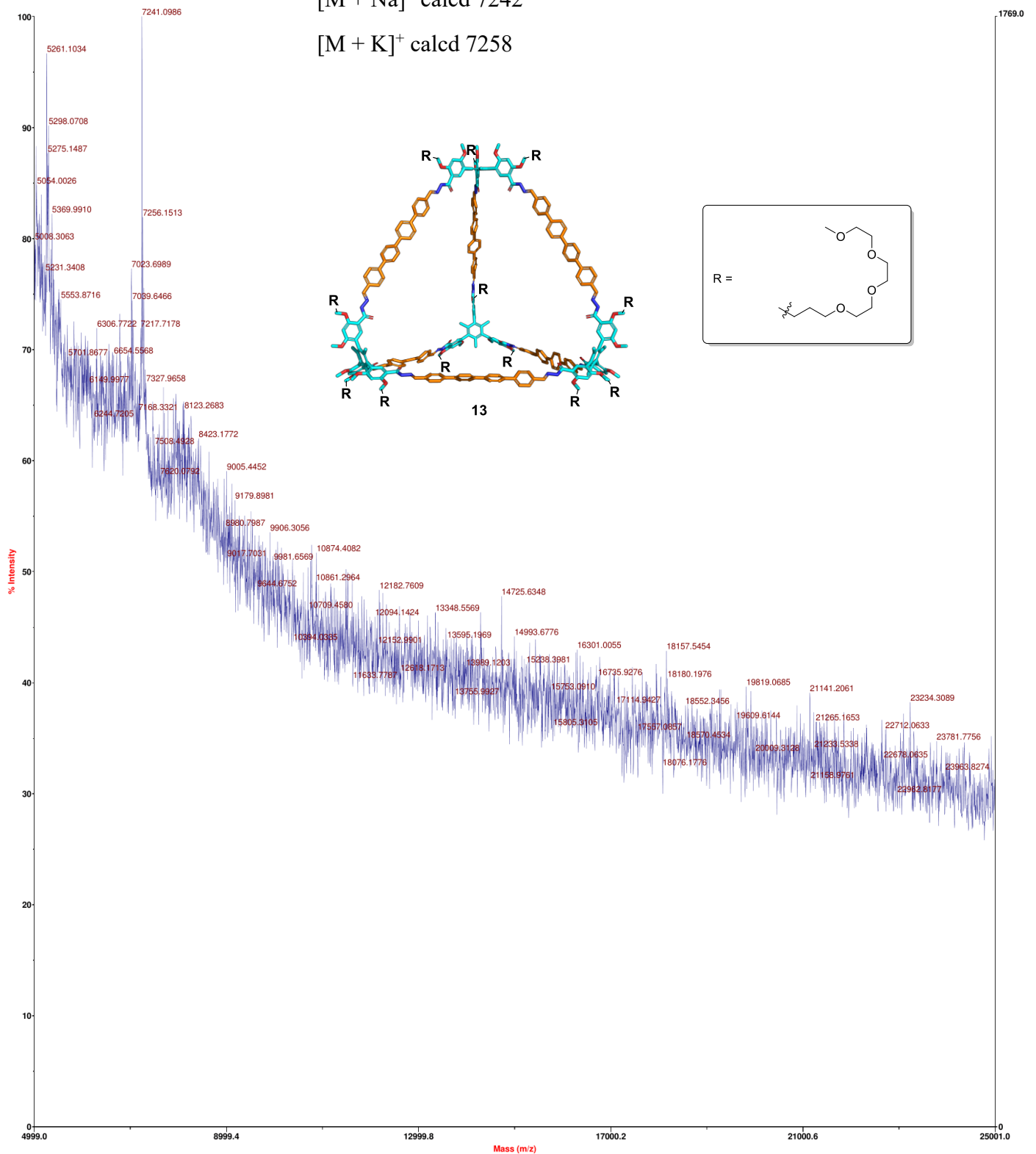


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Figure S31. Partial MALDI-TOF mass spectrum (DCTB matrix) of **12**.

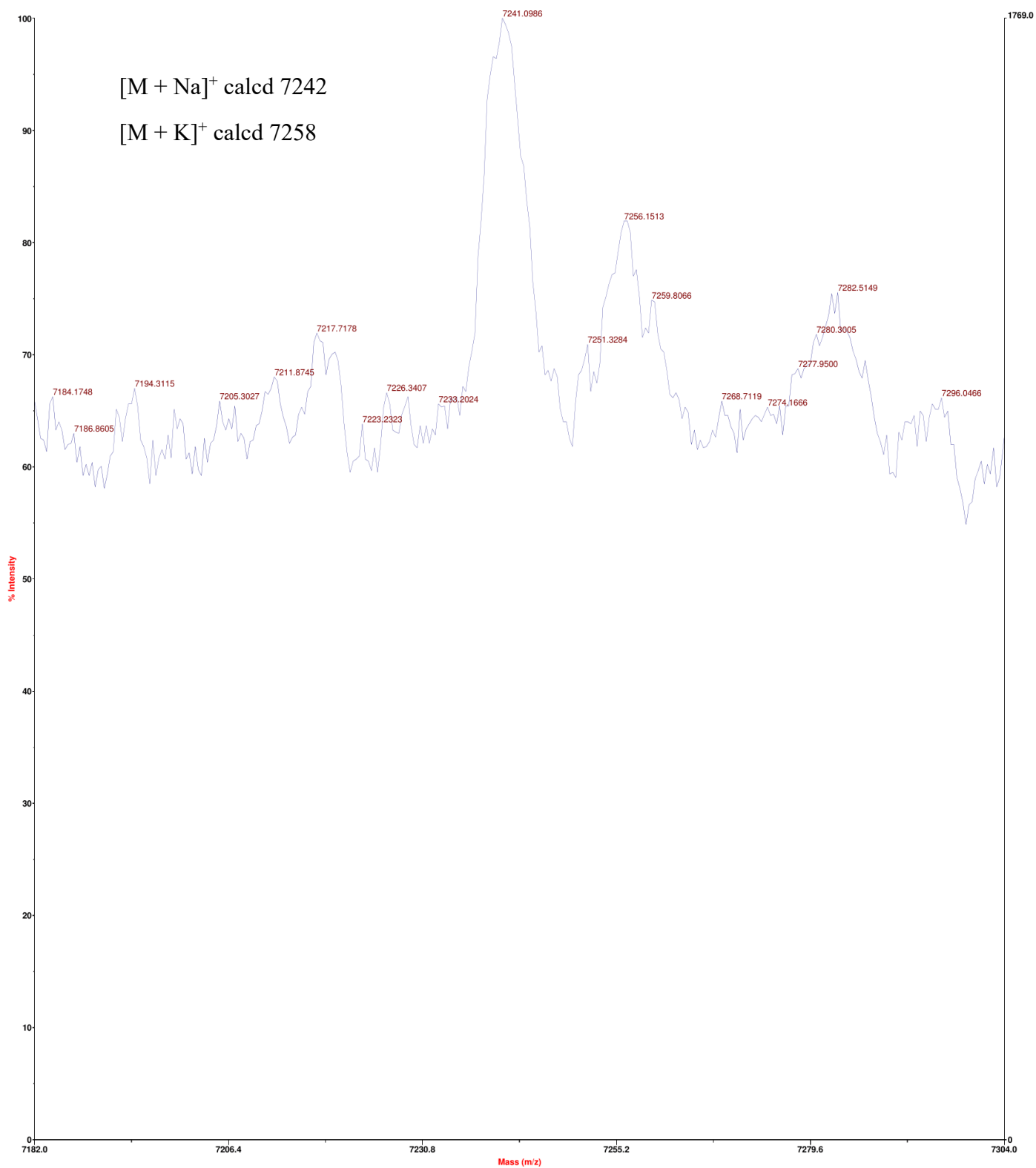
$[M + Na]^+$ calcd 7242

$[M + K]^+$ calcd 7258



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Figure S32. MALDI-TOF mass spectrum (DCTB matrix) of **13**.



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Acquired: 09:18:00, January 31, 2023

Figure S33. Partial MALDI-TOF mass spectrum (DCTB matrix) of 13.

VII. Supplemental References

- (1) Jaguar, version 11.8, Schrodinger, Inc., New York, NY, 2022.
- (2) A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang, R. A. Friesner, *Int. J. Quantum Chem.* **2013**, *113*, 2110–2142.
- (3) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648–5652.
- (4) C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B* **1988**, *37*, 785–789.
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- (6) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623–11627.