Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Chiral chromane[4]arenes by cycloaddition reactions of *o*-quinomethine resorcin[4]arenes

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1. Crystallographic data for 3c

CCDC 1405465 contains the supplementary crystallographic data for this paper. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Crystal data for **3c**	
Moiety formula	$C_{84}H_{96}O_8 \times 1.53\ (C_7H_8) \times 0.46\ (C_3H_8O)$
Empirical formula	$C_{96.15}H_{112}O_{8.46}$
Formula weight	1403.02
Temperature (K)	100.00
Wavelength (Å)	1.54184
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions a/b/c (Å) α/β/γ (°)	14.8920(3) 16.9372(4) 17.8109(4) 63.890(2) 80.685(2) 89.895(2)
Unit cell volume (Å^3)	3968.55(15)
Z	2
Calculated density (g/cm^3)	1.174
Absorption coefficient (mm^{-1})	0.569
F(000)	1510
θ range for data collection (°)	71.51 – 3.74
Index ranges	-18 < h < 18 -20 < k < 20 -21 < l < 21
Reflections collected	60538
Independent reflections	15266 ($R_{int.}$ = 0.0387)
Completeness to θ_{max}	0.987
Refinement statistics	
Final R indices [>2σ(I)]	0.0531
R indices [all data]	0.0579
Goodness-of-fit	1.014
Largest diff. peak and hole (e/Å^3)	0.427 / -0.460

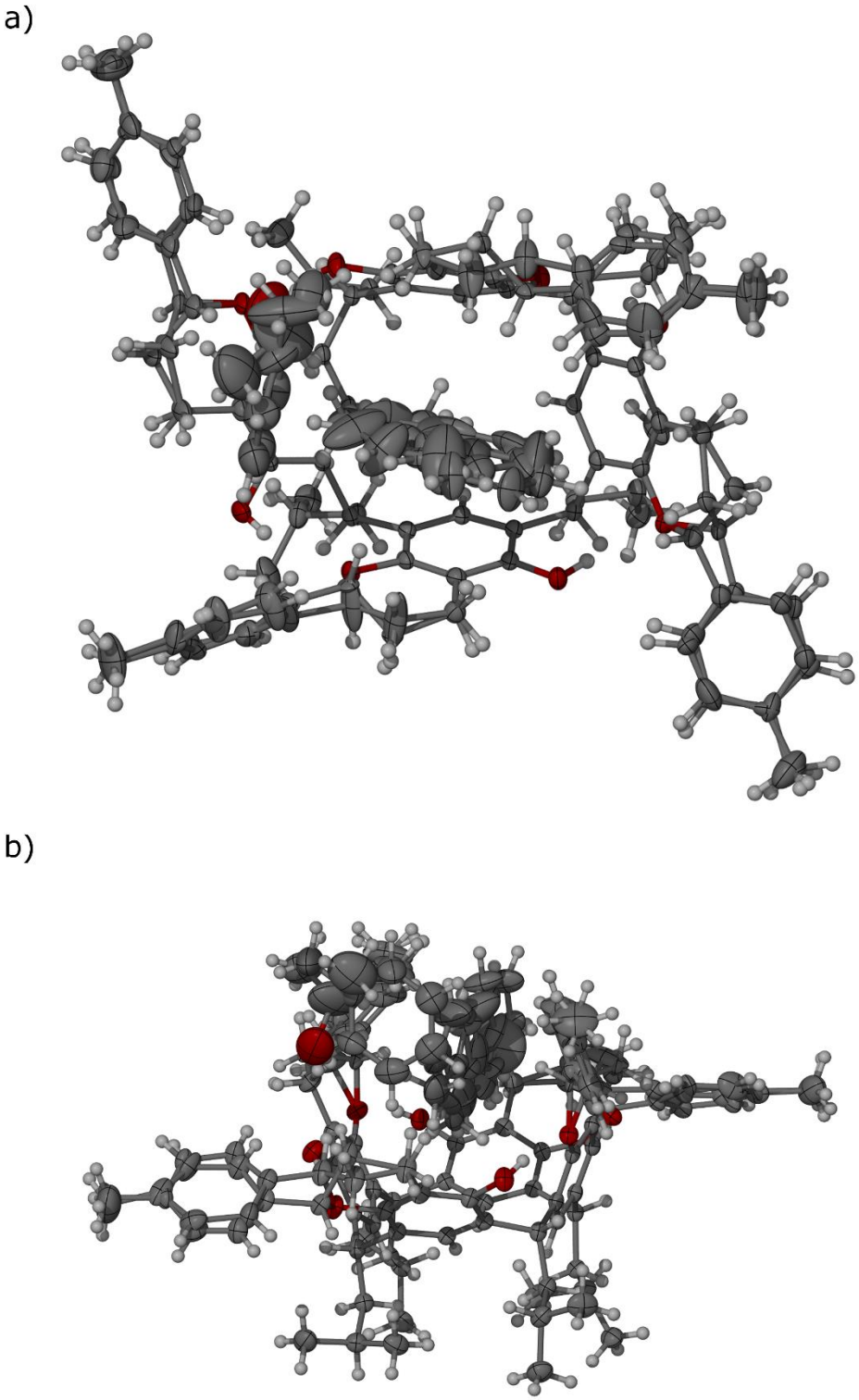
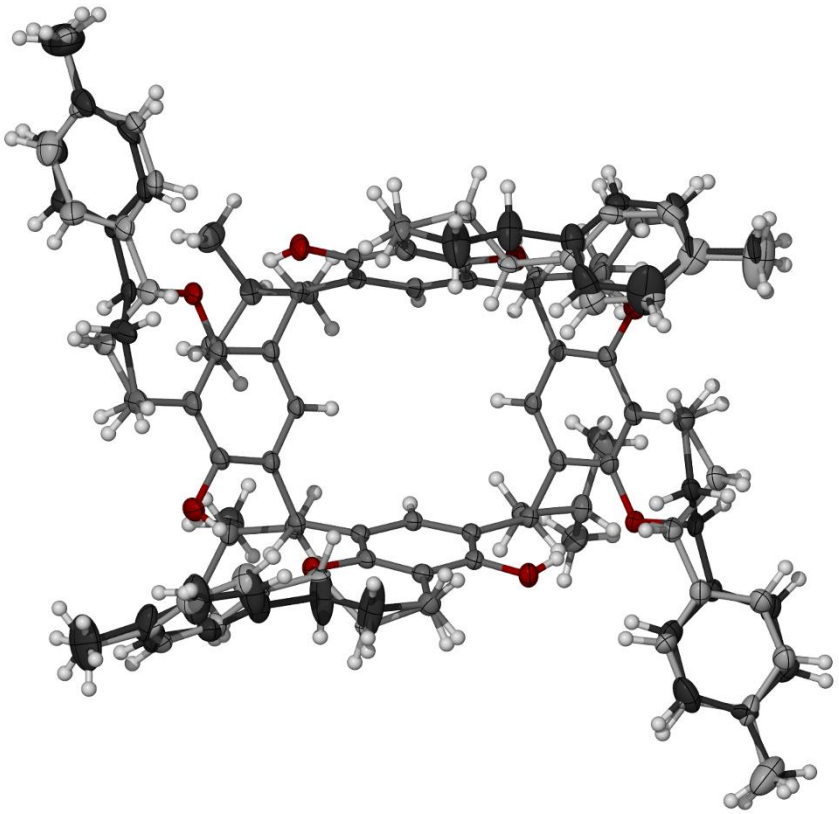


Figure S1. ORTEP representation of the asymmetric unit of the crystal structure of **3c** (whole contents of ASU is shown), thermal ellipsoids scaled at 50% probability a) top and b) side view.

a)



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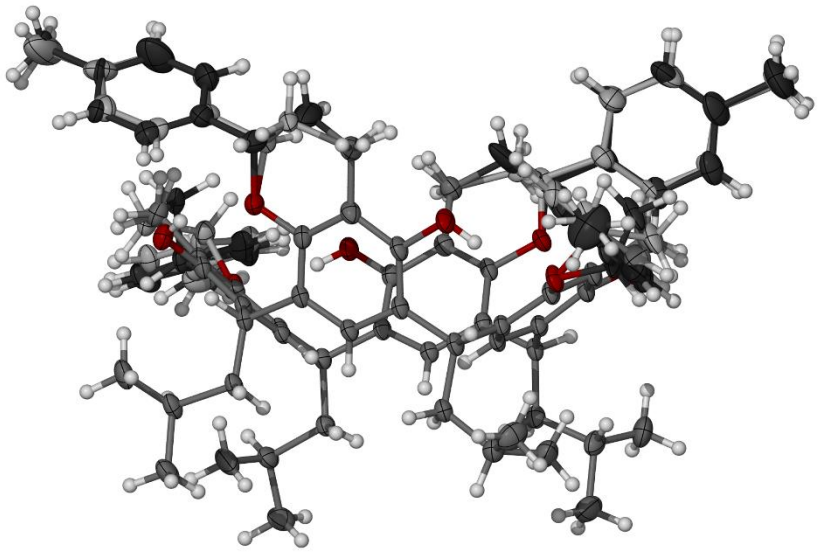

Figure S2. ORTEP representation of the asymmetric unit of the crystal structure of **3c** (solvent molecules were removed for clarity), thermal ellipsoids scaled at 50% probability a) top and b) side view (grey – common part, black - (all-*S*, all-R_M)-**3c**, occupancy 40%, light grey – (all-*R*, all-R_M)-**3c**, occupancy 60%).

2. ^{1}H and ^{13}C NMR spectra of products 3a-f.

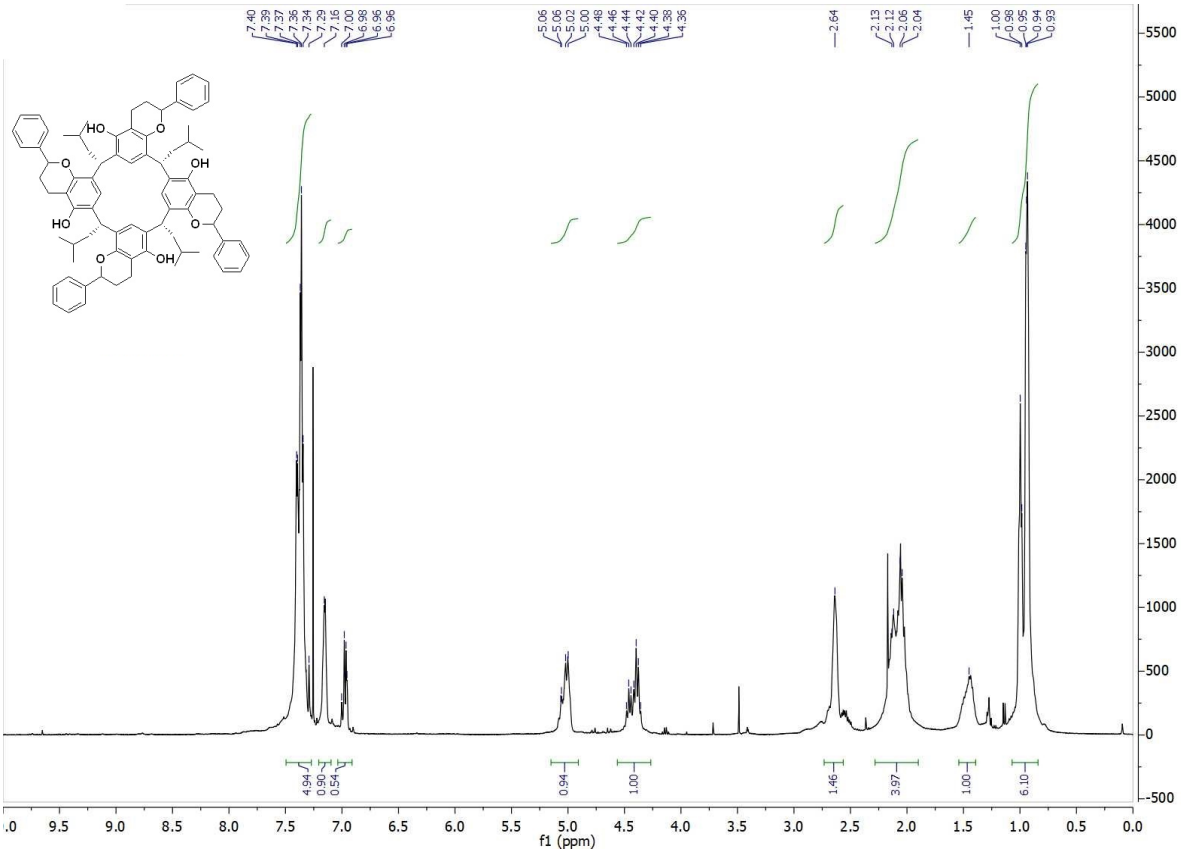

Figure S3. ^{1}H NMR spectrum of **3a** from **1a**.

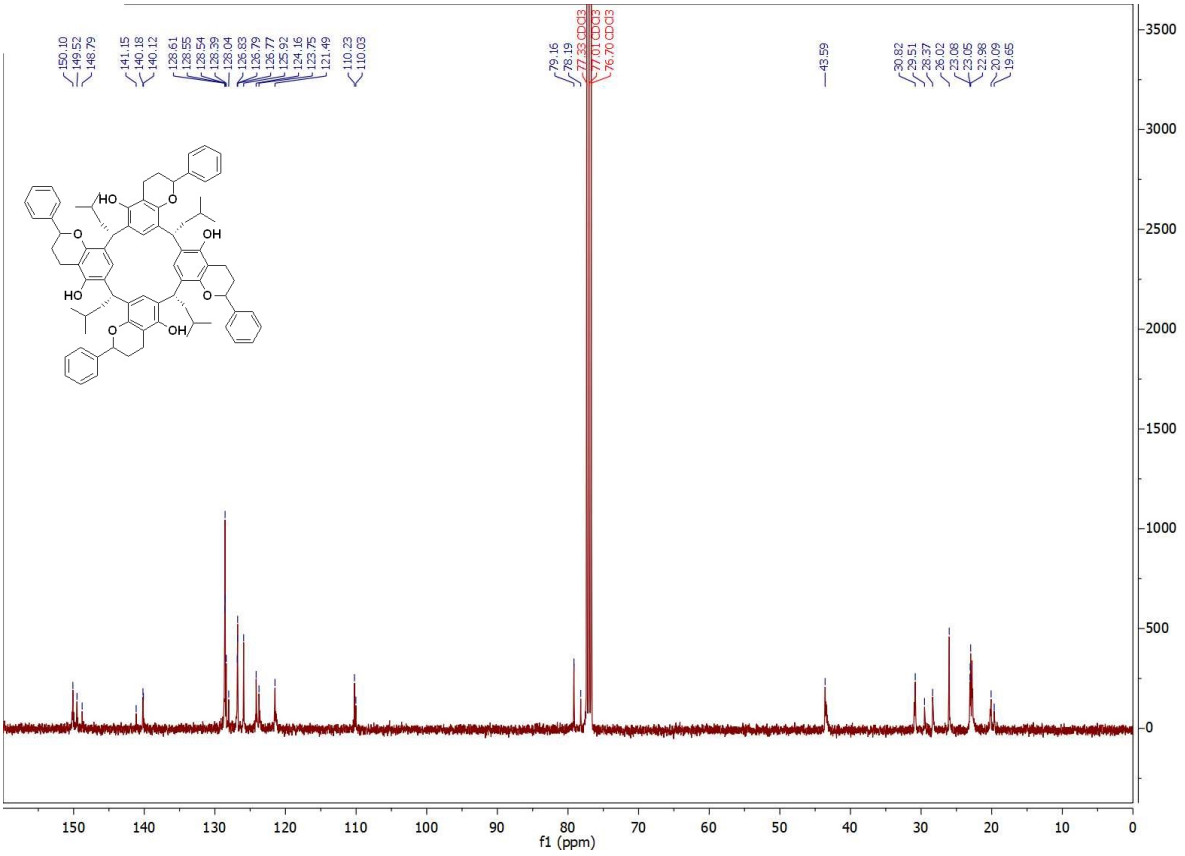

Figure S4. ^{13}C NMR spectrum of **3a** from **1a**.

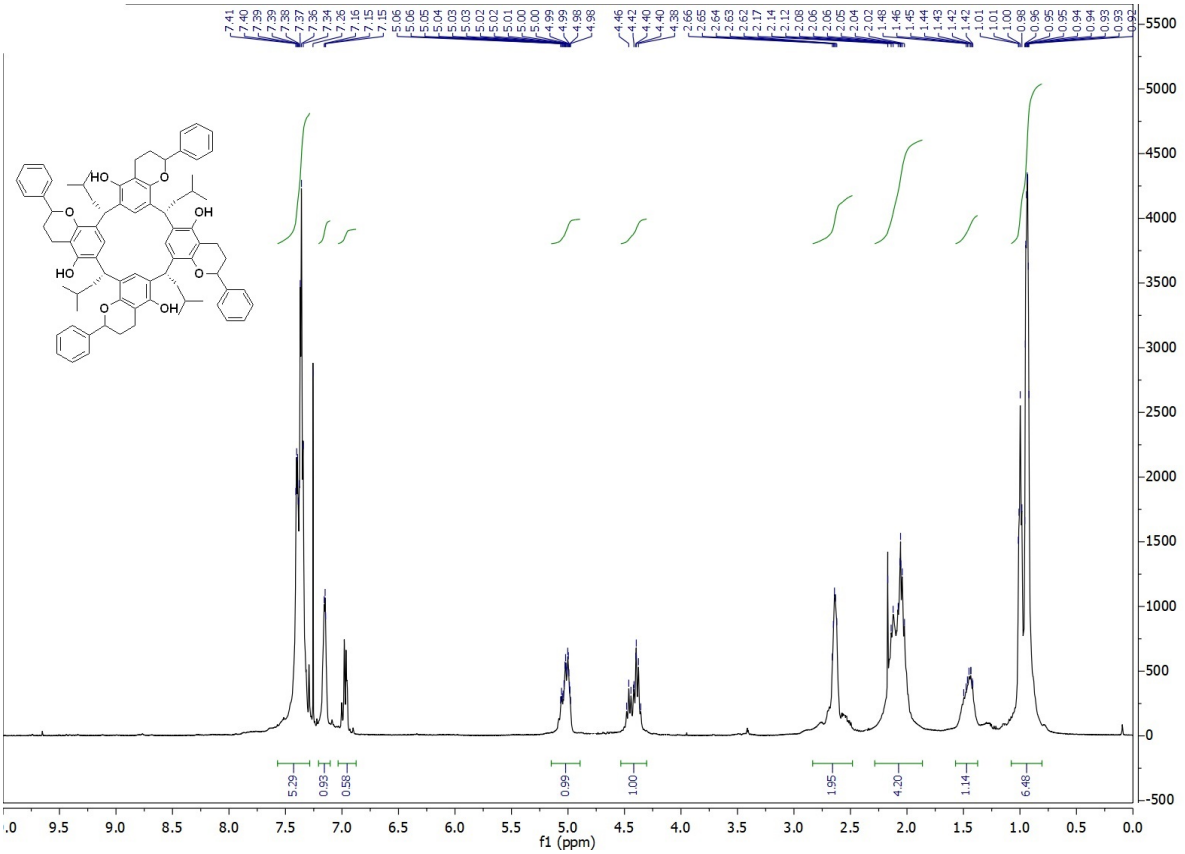

Figure S5. ^{1}H NMR spectrum of **3a** from **1b**.

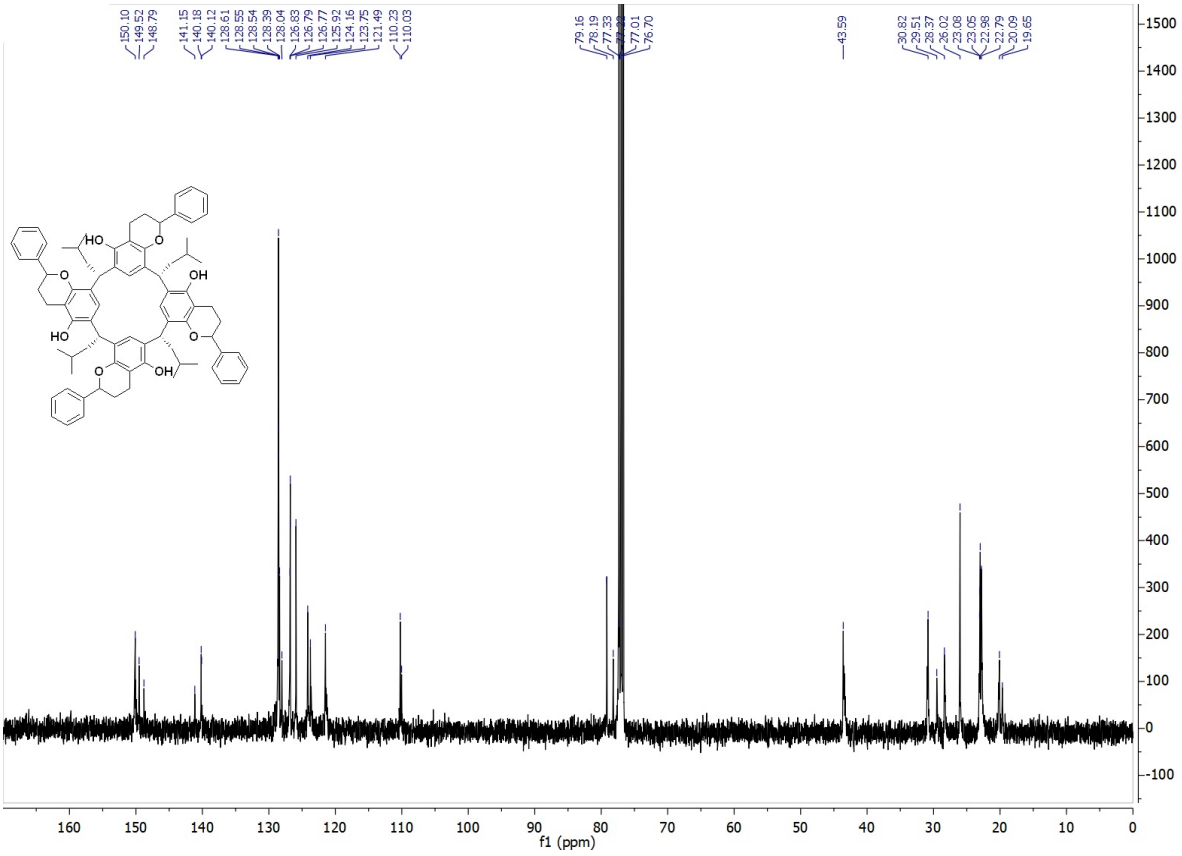

Figure S6. ^{13}C NMR spectrum of **3a** from **1b**.

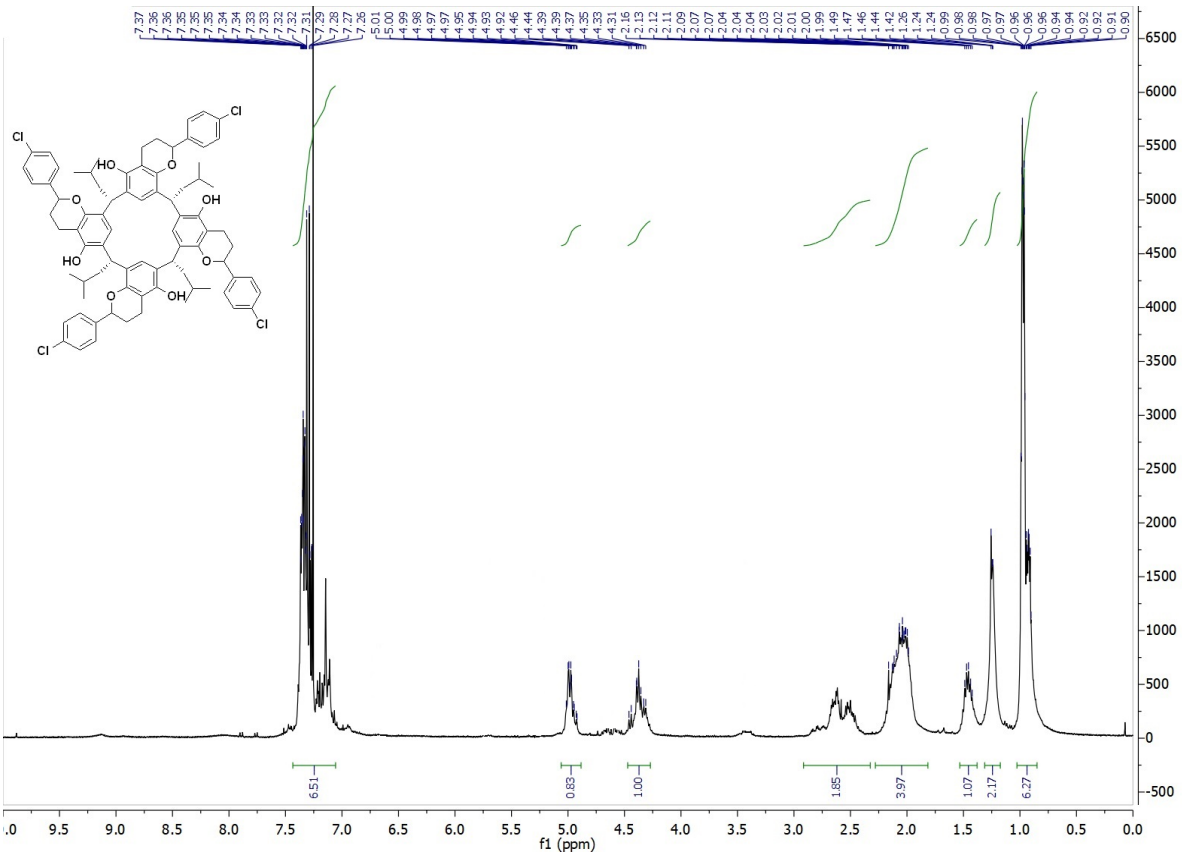

Figure S7. ^{1}H NMR spectrum of **3b** from **1a**.

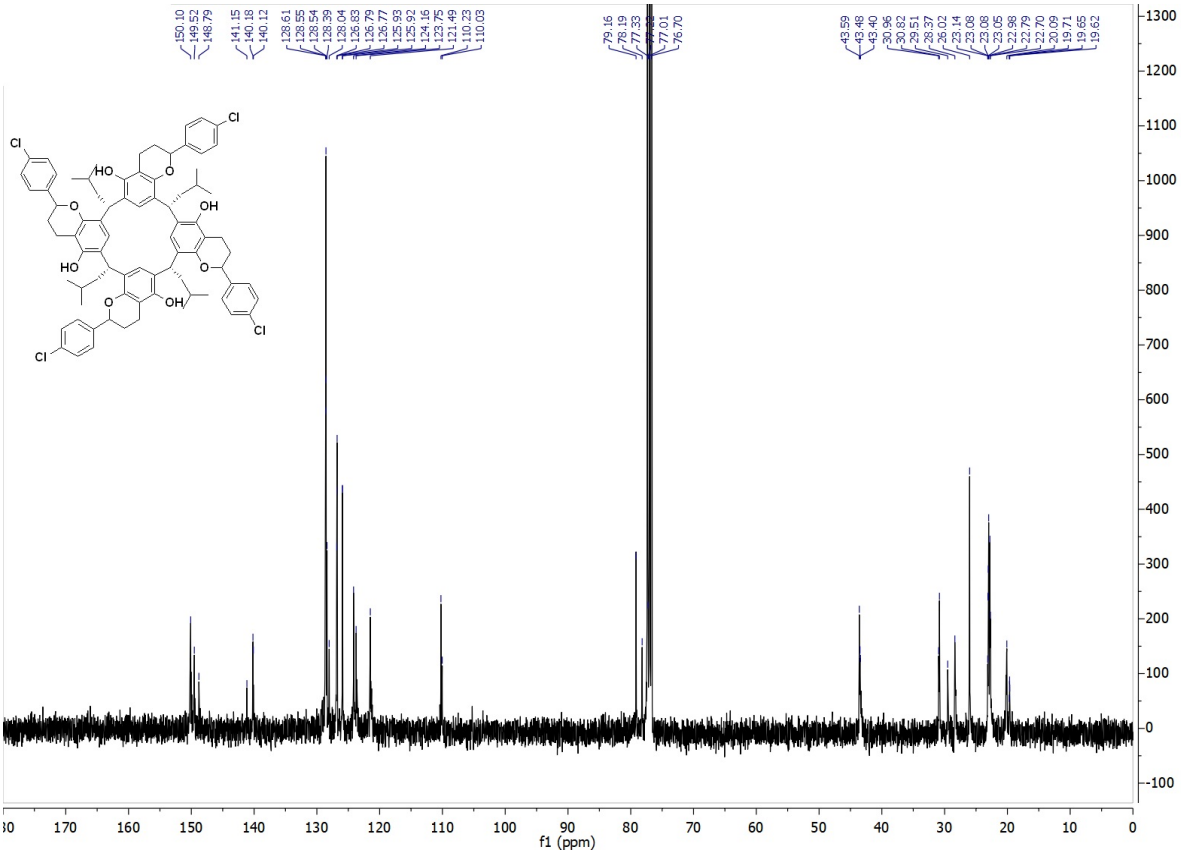

Figure S8. ^{13}C NMR spectrum of **3b** from **1a**.

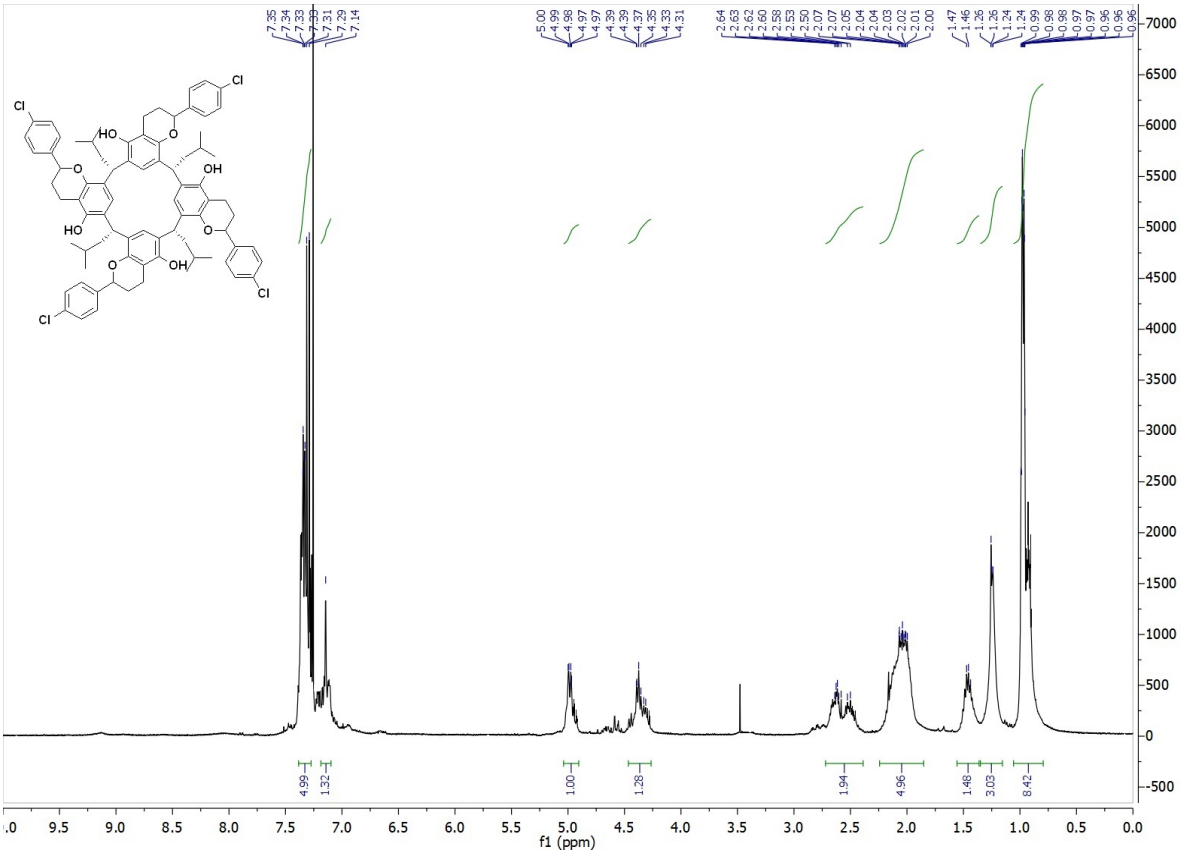

Figure S9. ^{1}H NMR spectrum of **3b** from **1b**.

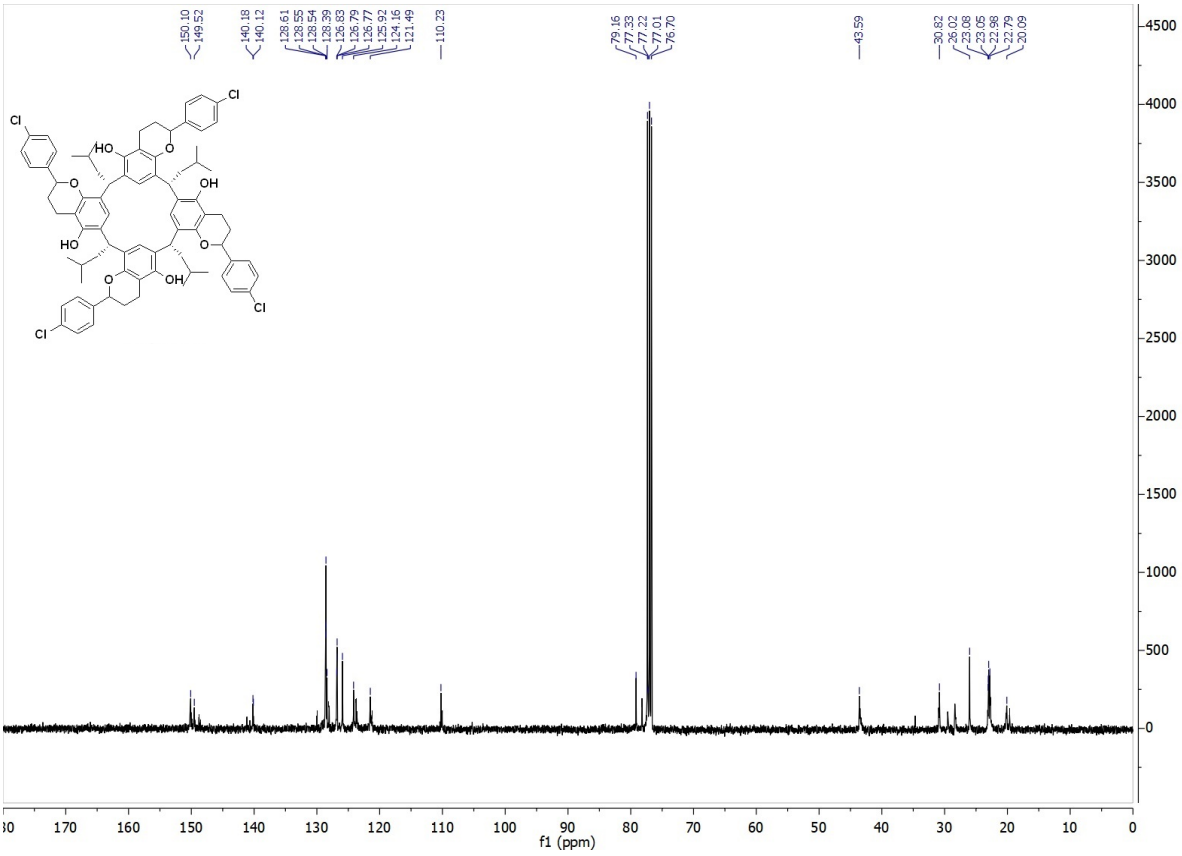

Figure S10. ^{13}C NMR spectrum of **3b** from **1b**.

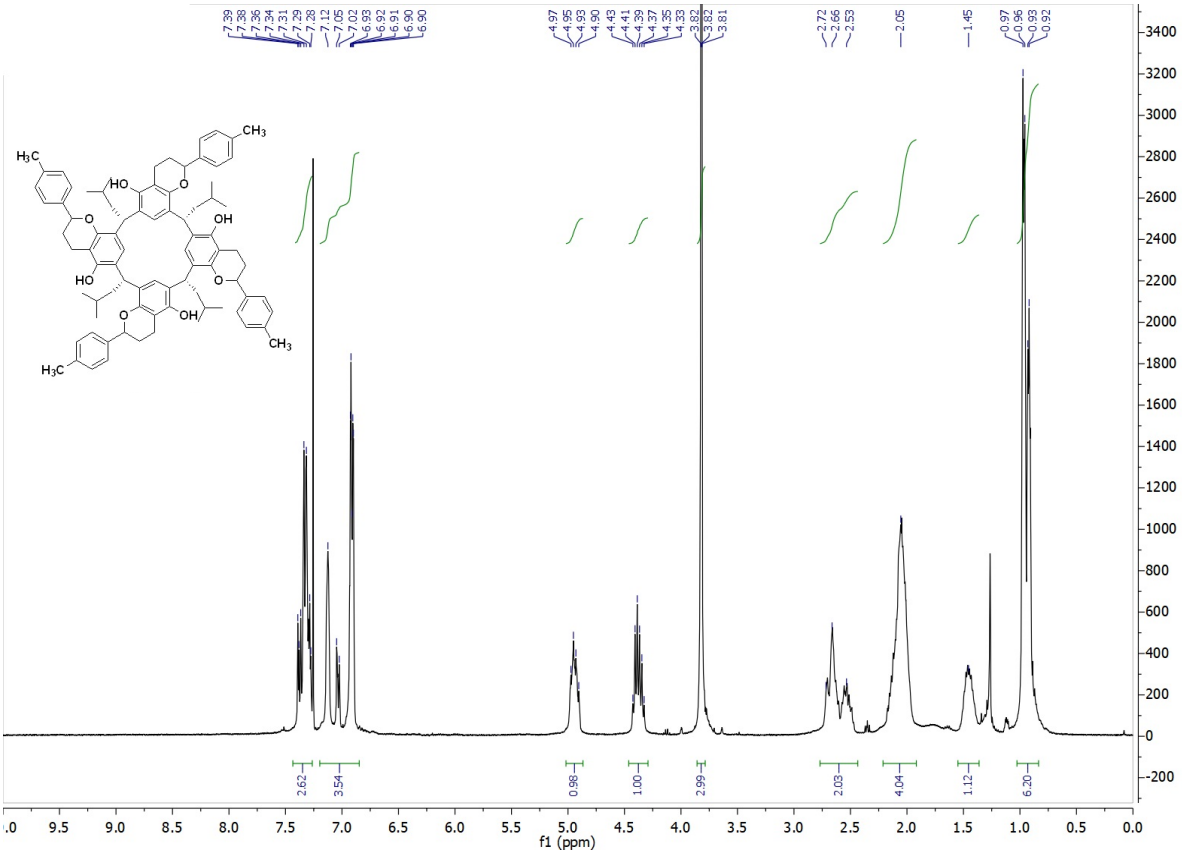

Figure S11. ^{1}H NMR spectrum of **3c** from **1a**.

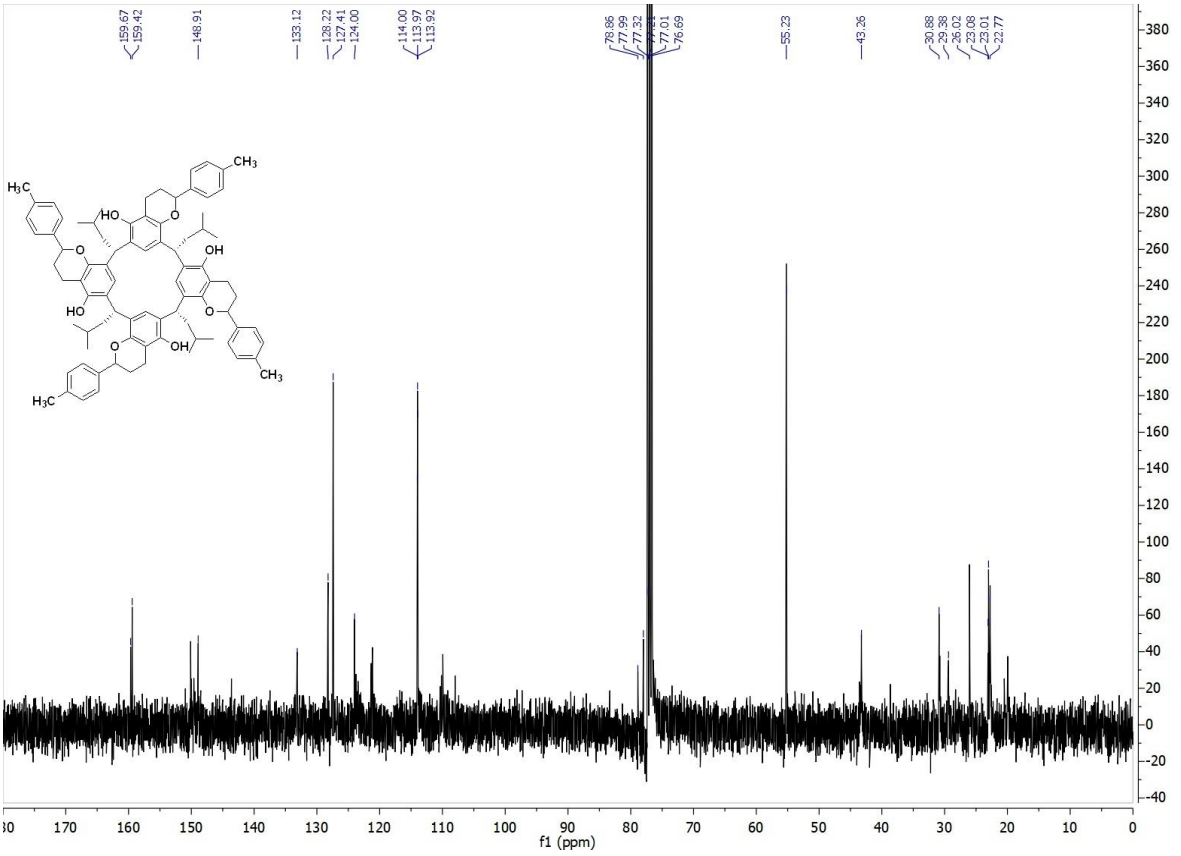

Figure S12. ^{13}C NMR spectrum of **3c** from **1a**.

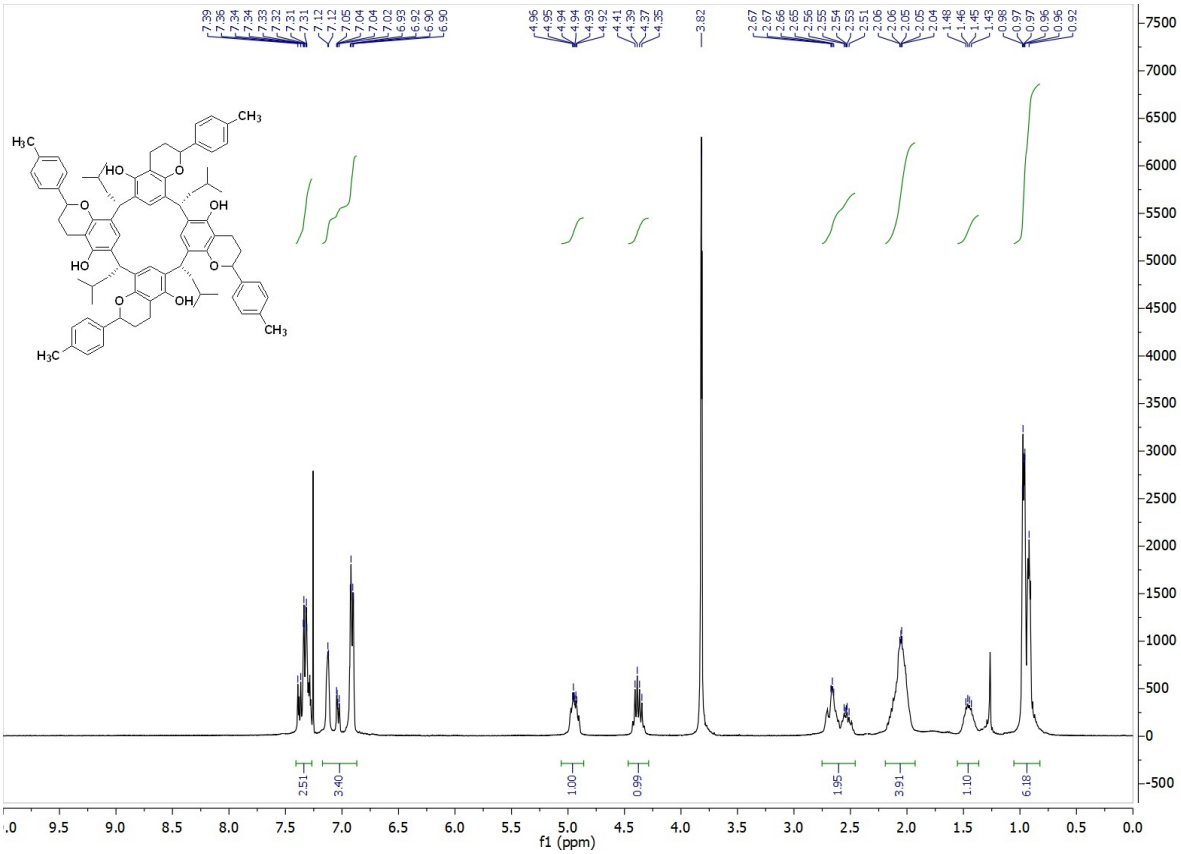

Figure S12. ^{1}H NMR spectrum of **3c** from **1b**.

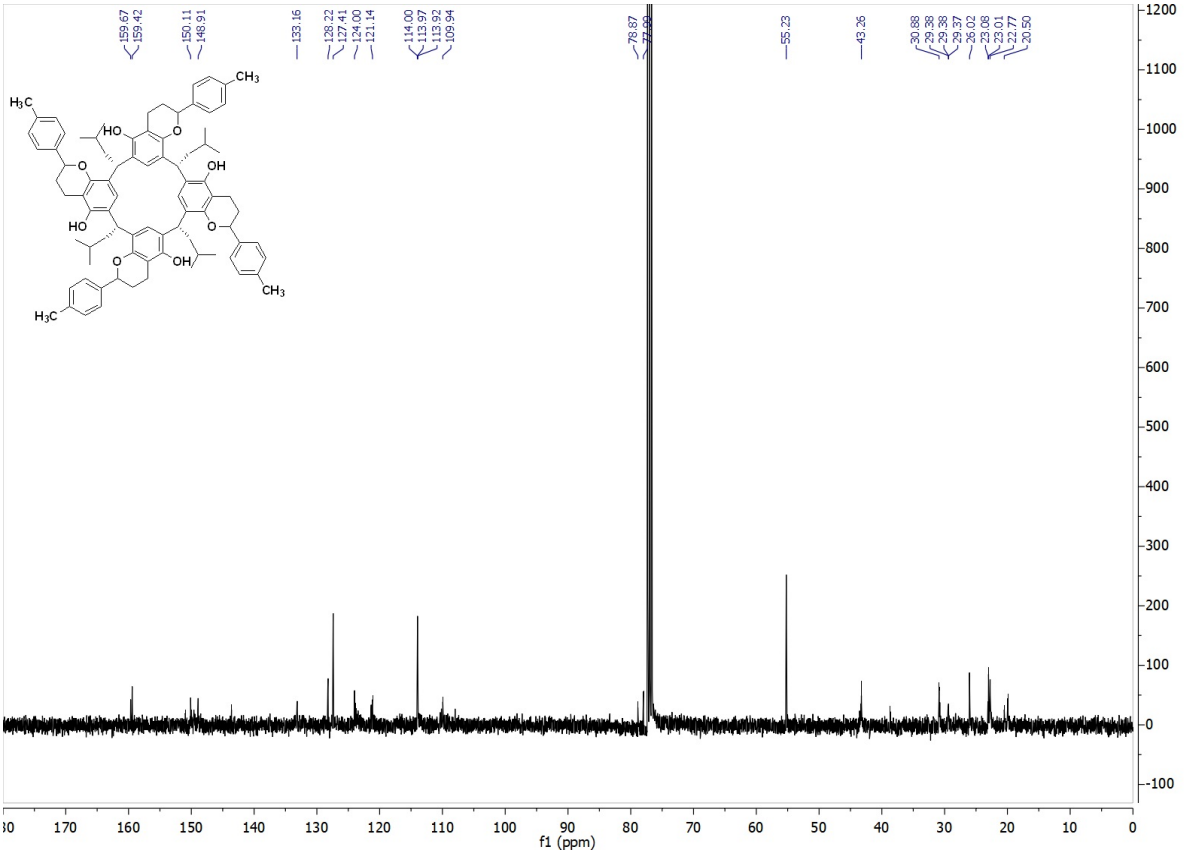

Figure S13. ^{13}C NMR spectrum of **3c** from **1b**.

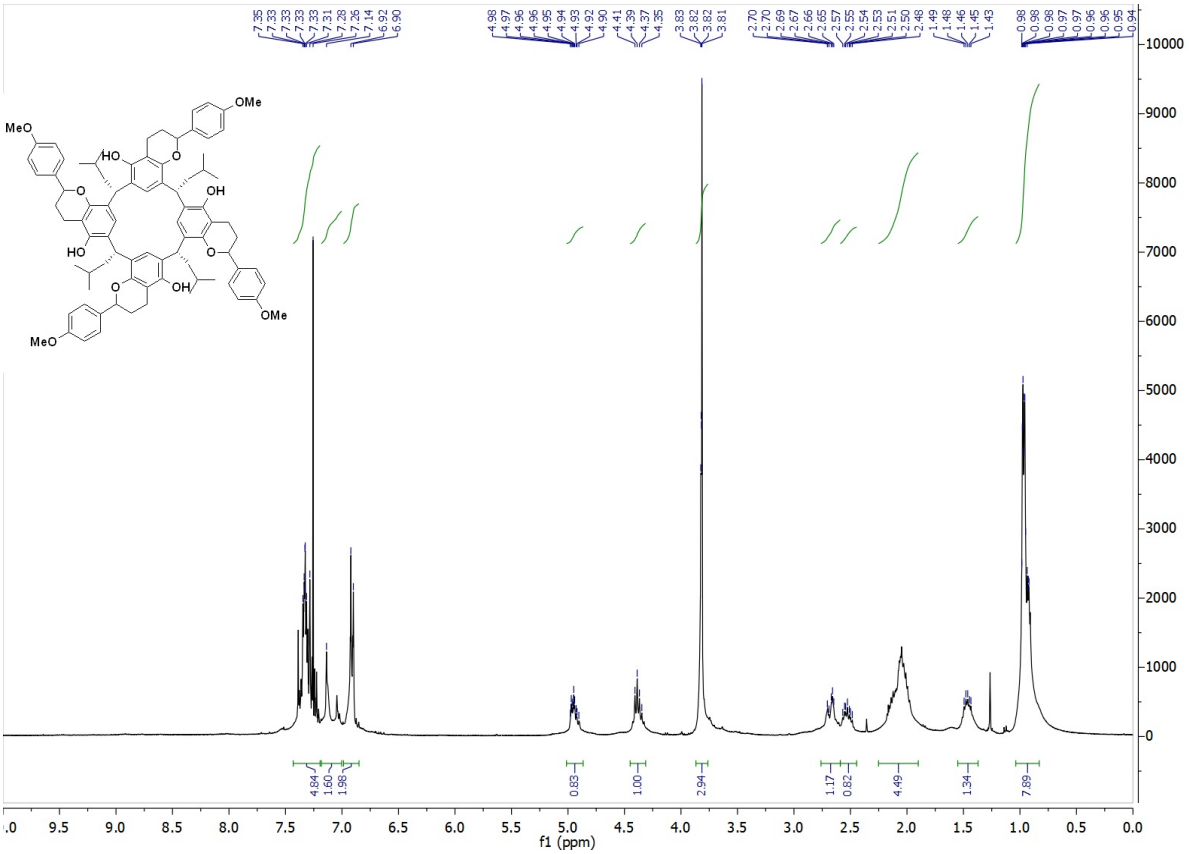

Figure S14. ^{1}H NMR spectrum of **3d** from **1a**.

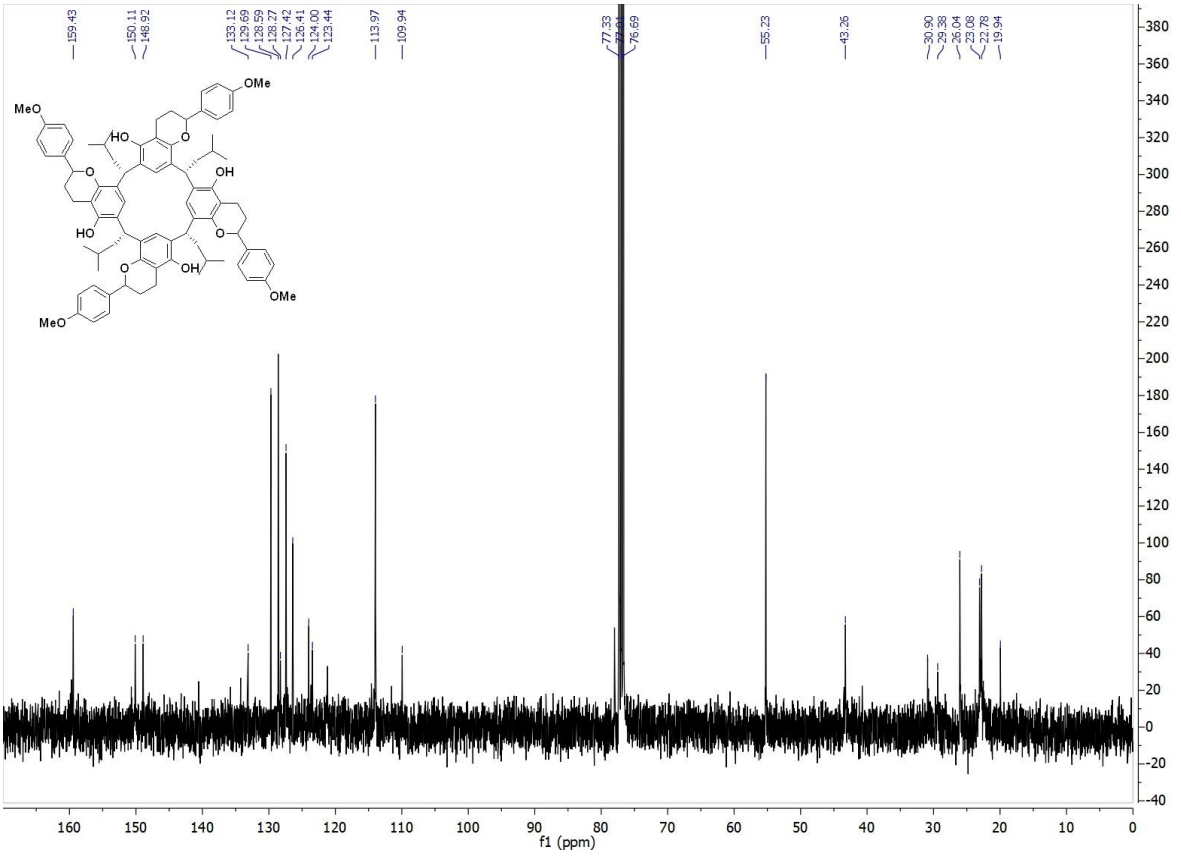

Figure S15. ^{13}C NMR spectrum of **3d** from **1a**.

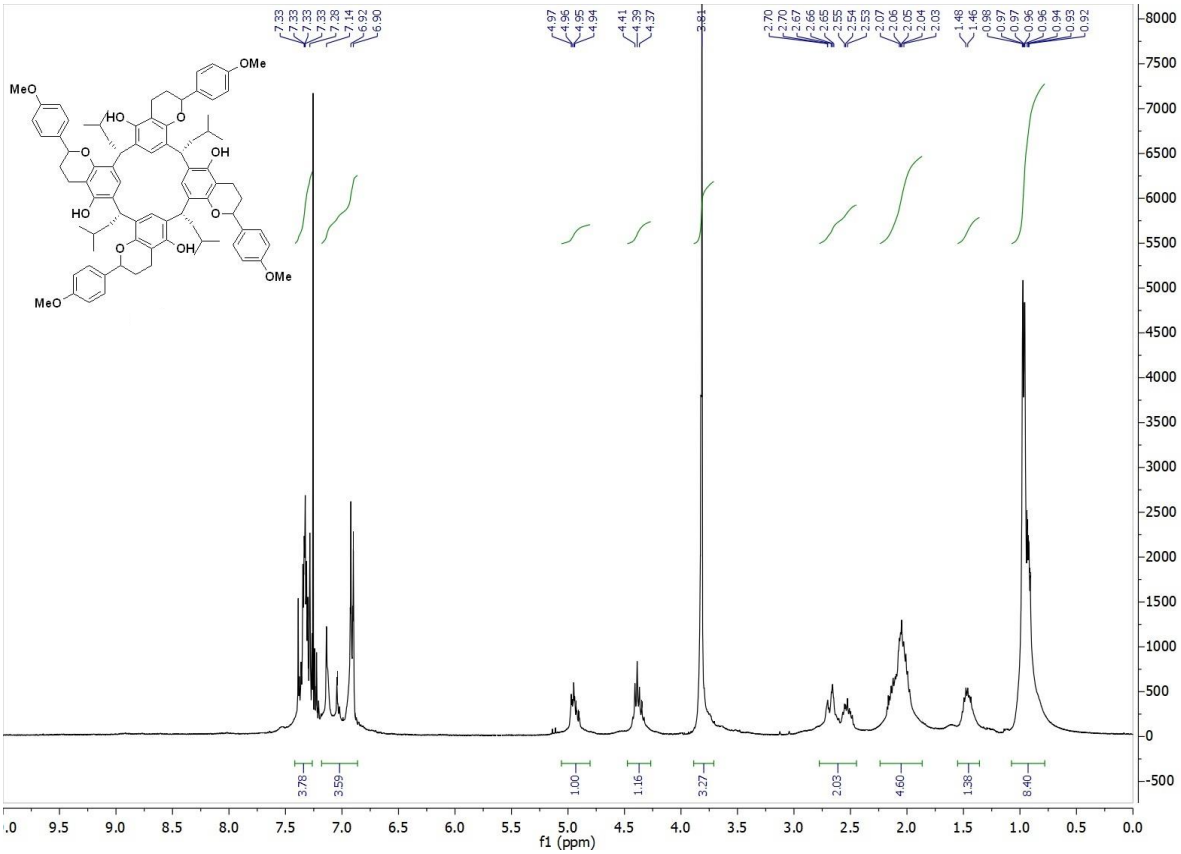

Figure S16. ^{1}H NMR spectrum of **3d** from **1b**.

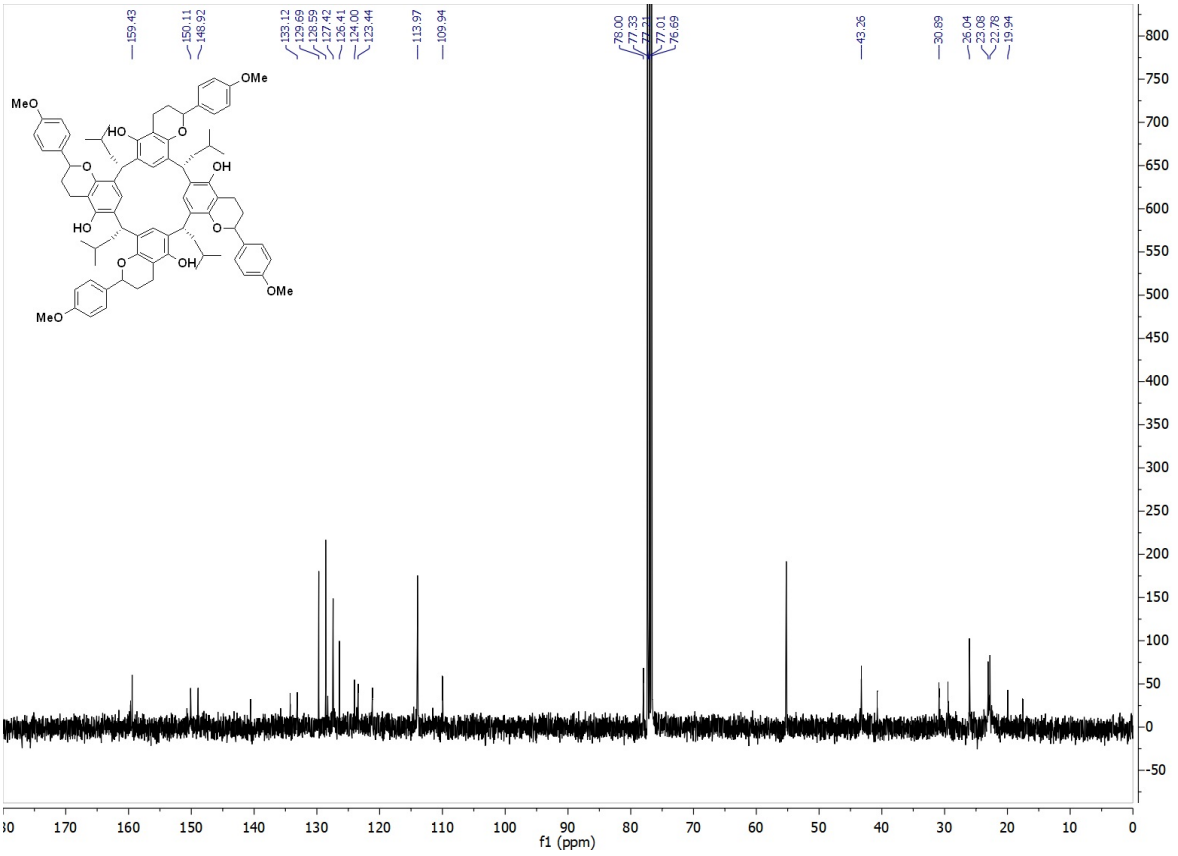

Figure S17. ^{13}C NMR spectrum of **3d** from **1b**.

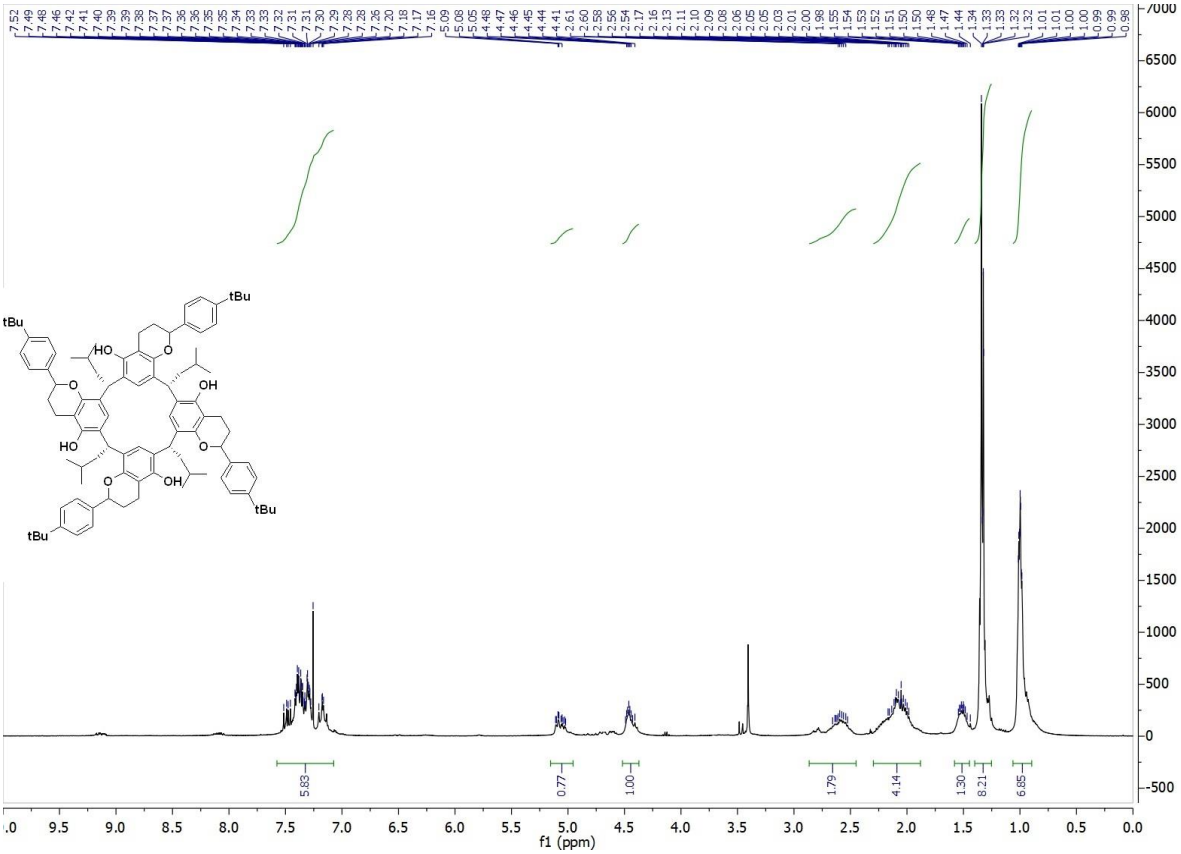

Figure S18. ^{1}H NMR spectrum of **3e** from **1a**.

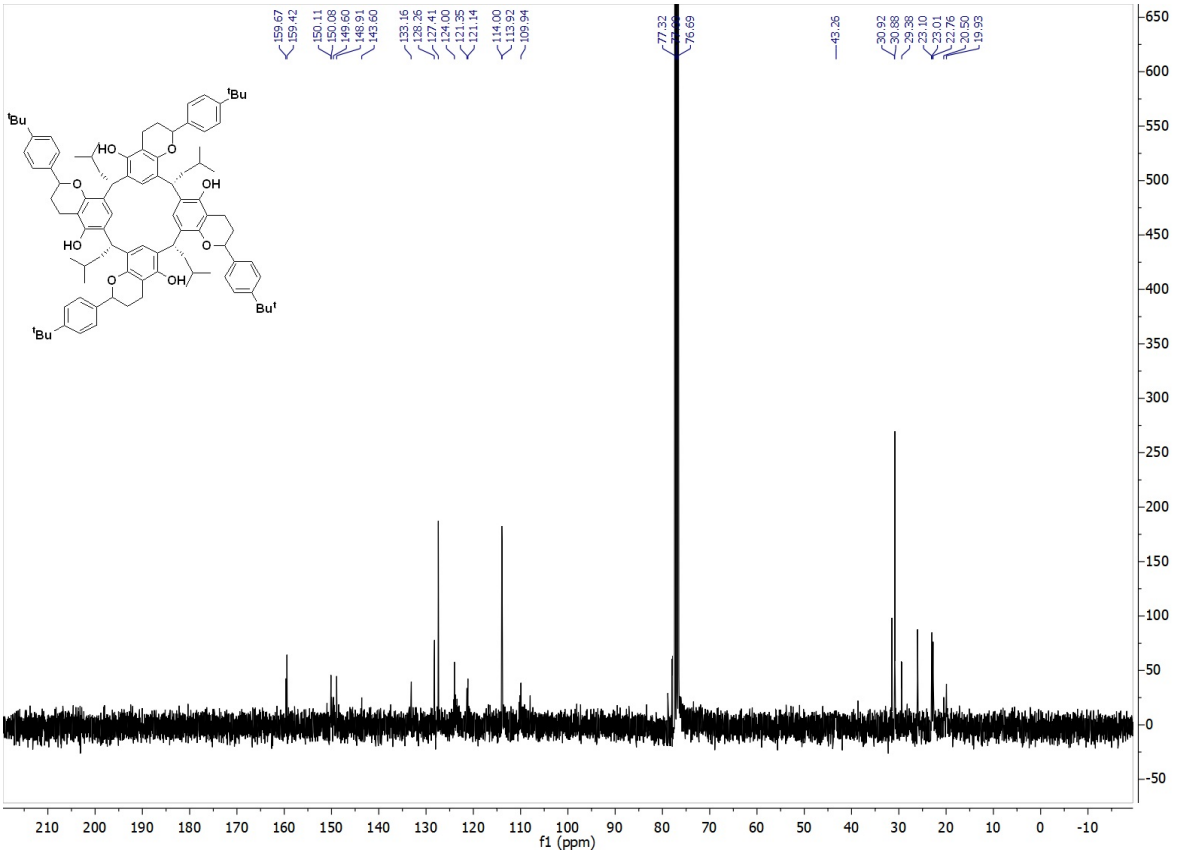

Figure S19. ^{13}C NMR spectrum of **3e** from **1a**.

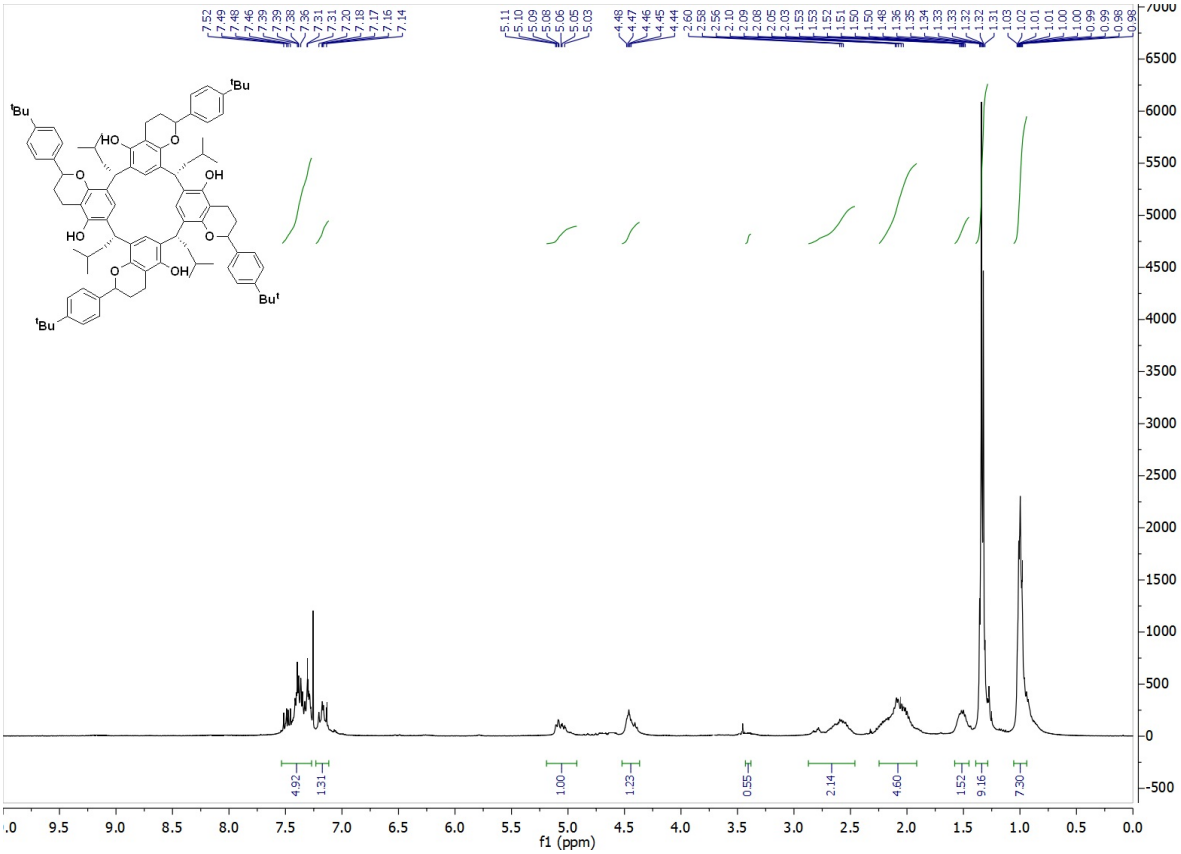

Figure S20. ^{1}H NMR spectrum of **3e** from **1b**.

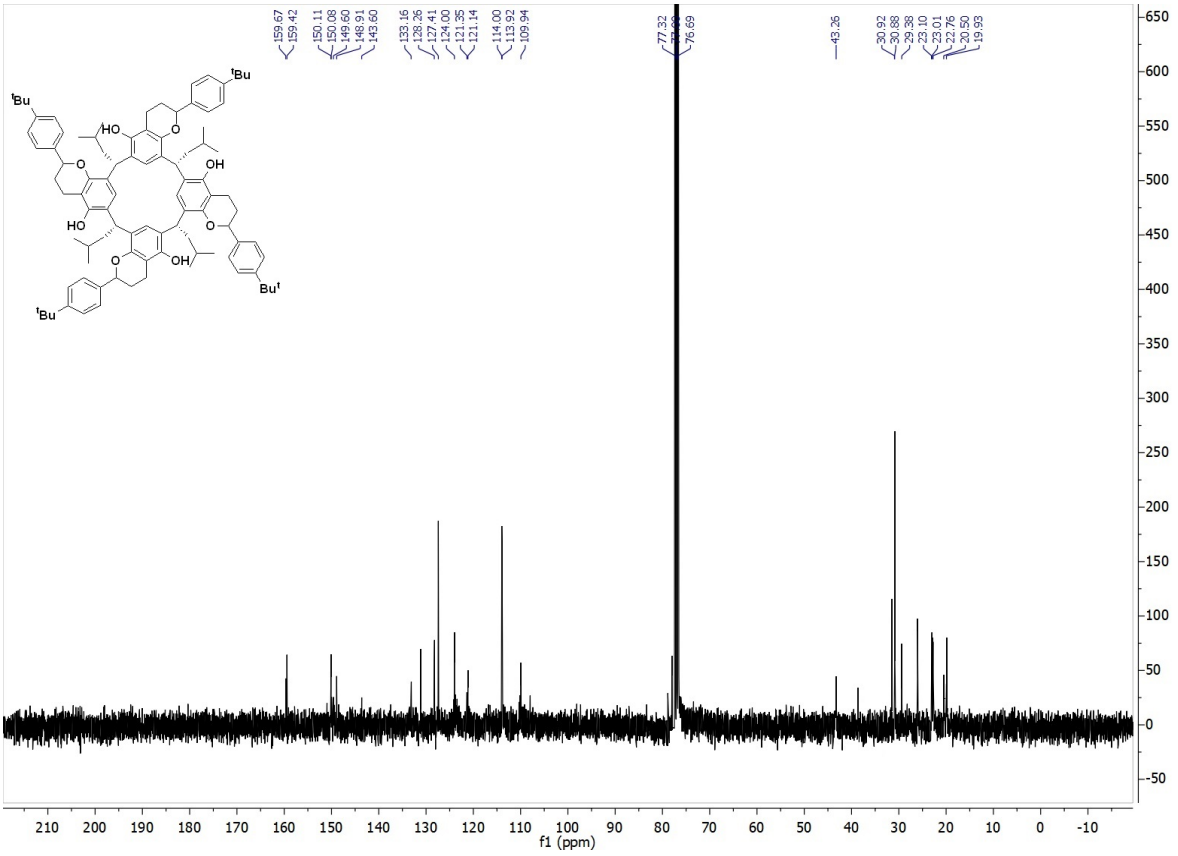

Figure S21. ^{13}C NMR spectrum of **3e** from **1b**.

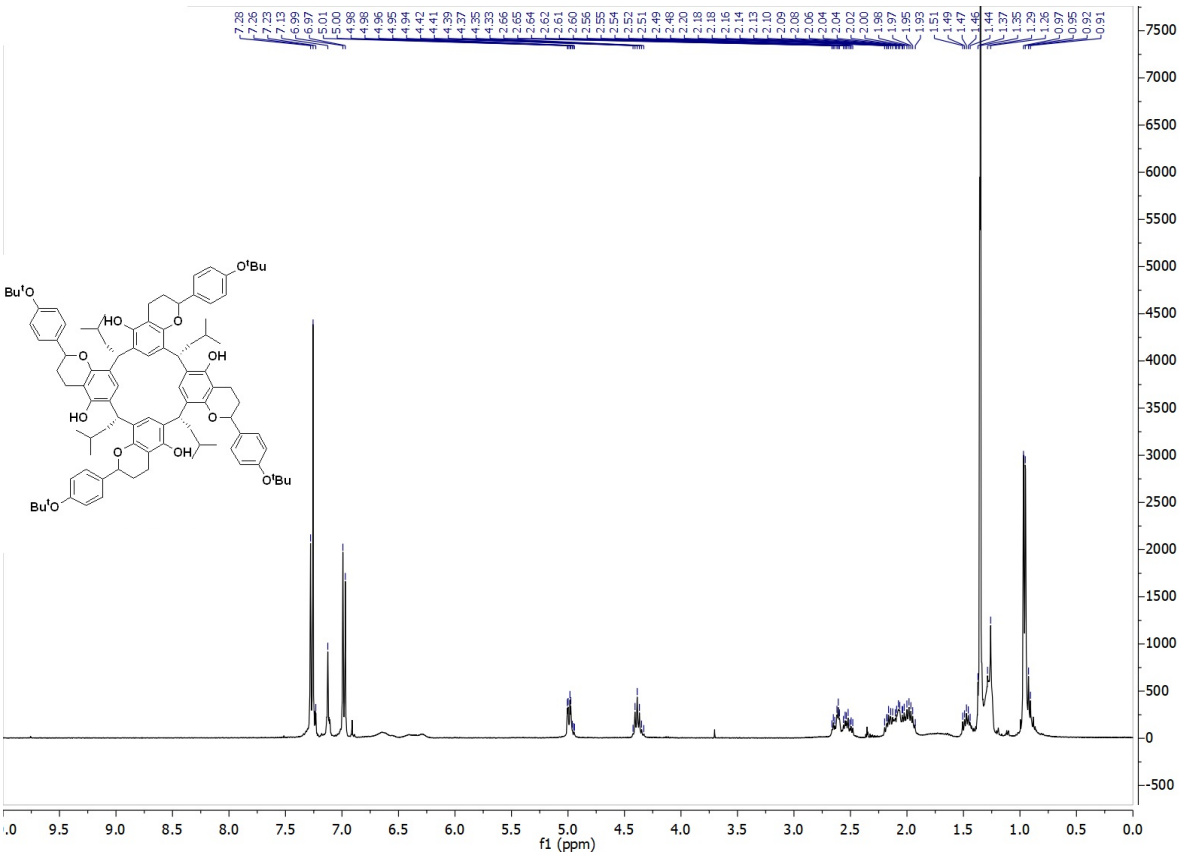

Figure S22. ^{1}H NMR spectrum of **3f** from **1a**.

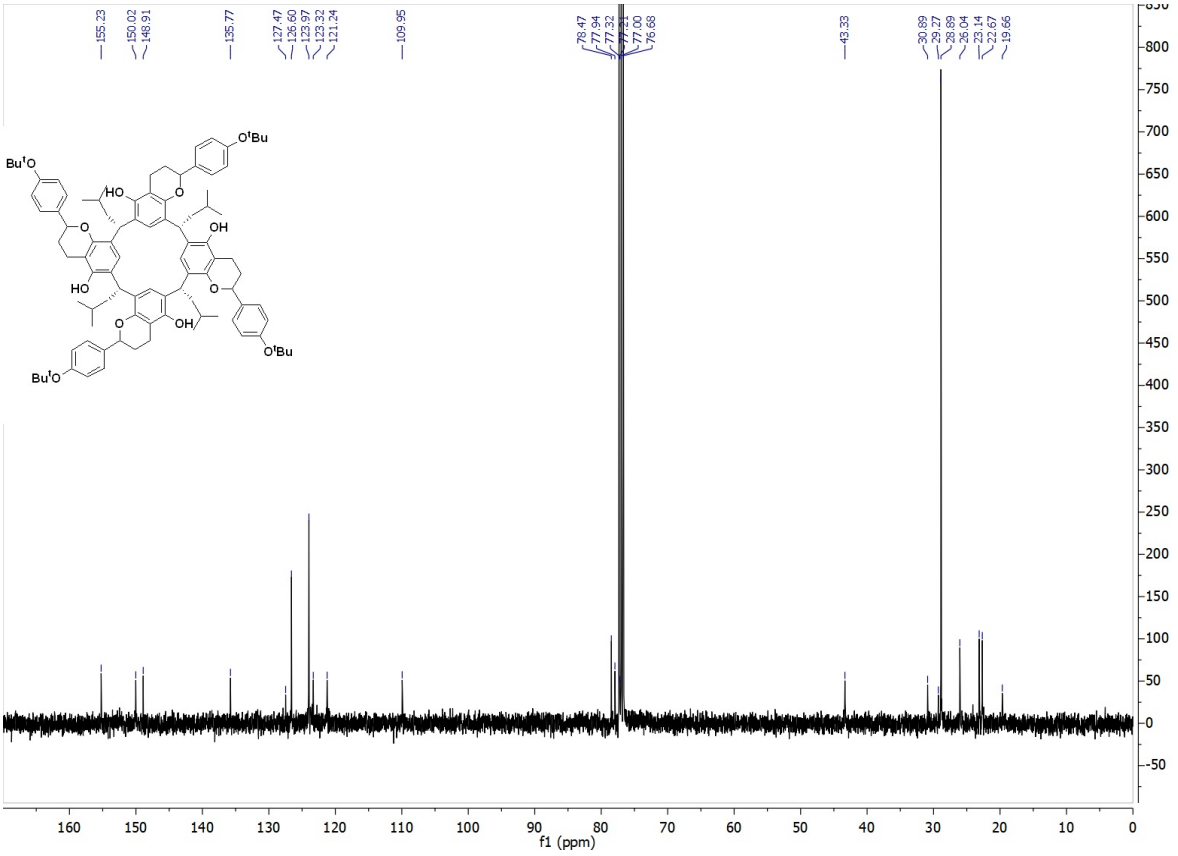

Figure S23. ^{13}C NMR spectrum of **3f** from **1a**.

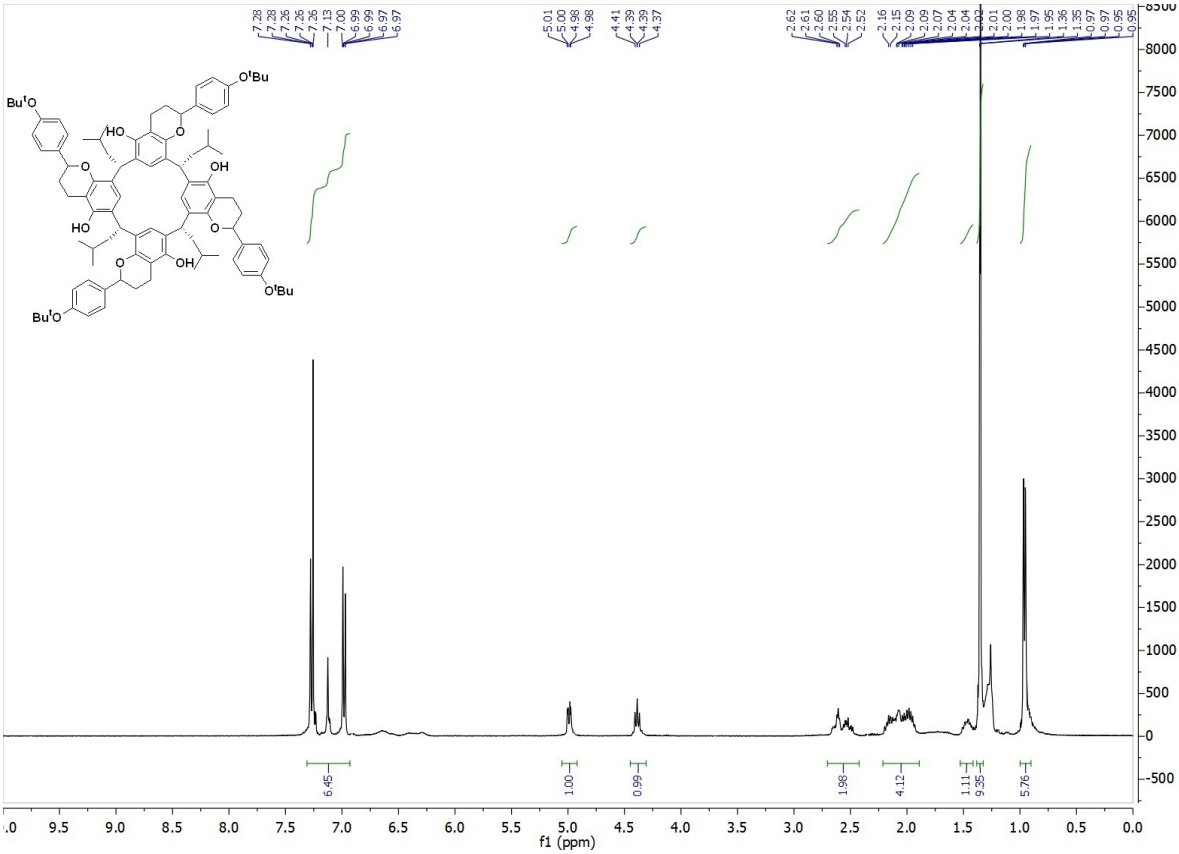

Figure S24. ^{1}H NMR spectrum of **3f** from **1b**.

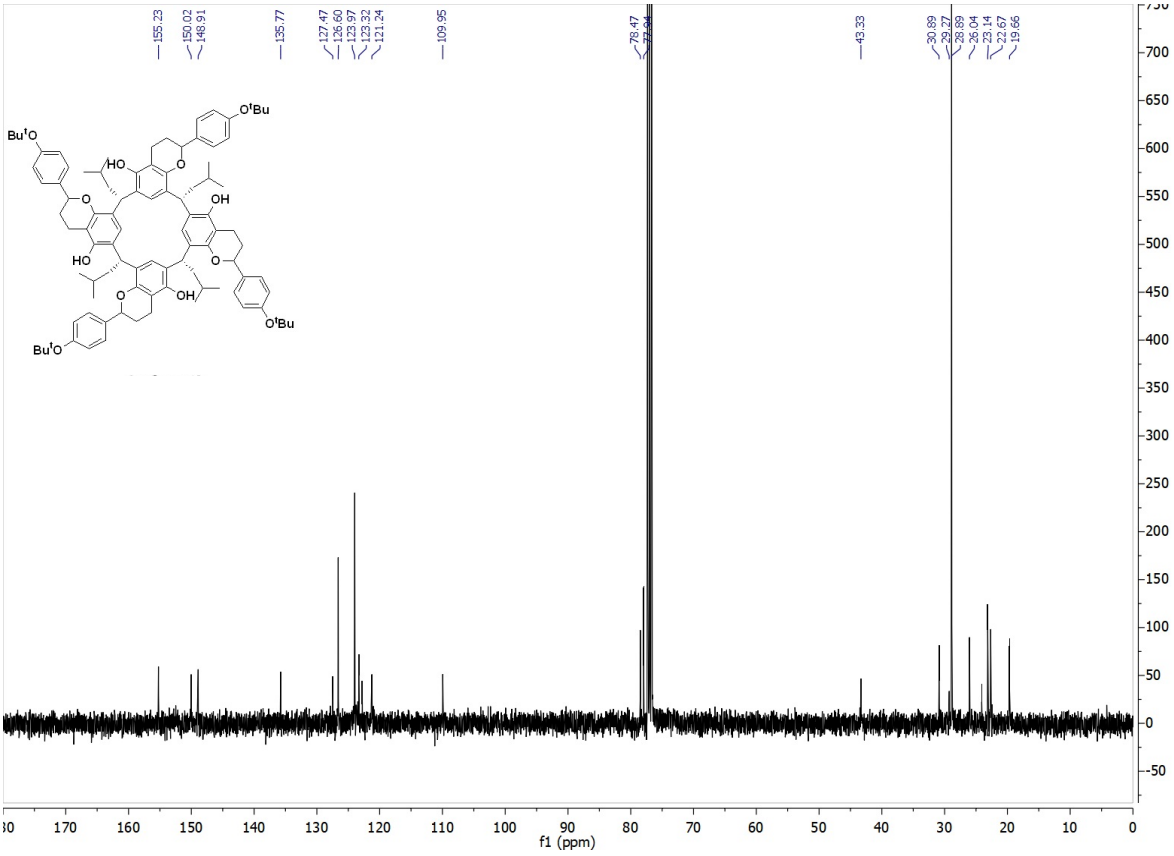

Figure S25. ^{13}C NMR spectrum of **3f** from **1b**.

3. Ab initio calculations

All theoretical calculations were performed within the density functional theory (DFT) using Gaussian 09 program suite.[1] The geometry of the initial structures was retrieved from the crystal structure of **3c** and then it was optimized by ground state method at the B3LYP/6-31G(d,p) level.
Excited electronic states were determined at the B3LYP/6-31G(d,p) level by means of the time-dependent DFT (TD DFT) approach (100 excited states). The ECD and UV spectra were simulated by overlapping Gaussian functions for each transition. Presentation of molecular orbitals was performed by using the GaussView program.

Atomic Cartesian coordinates for isomer (all-*S*, all-R_M)-3c optimized geometry:

C	0.22484900	3.27527900	1.82868500
C	0.64867600	4.07776100	0.75507800
C	1.90891000	3.92972800	0.16883900
C	2.78624900	2.96526800	0.69622700
C	2.42857000	2.17410100	1.80157000
C	1.13862500	2.34033400	2.31644500
H	0.83829900	1.72184800	3.15527300
C	3.42219600	1.18083800	2.41614700
H	4.42437600	1.52861700	2.14901900

C	3.38755500	1.18709500	3.95663500
H	2.43251000	0.84699400	4.36625300
H	3.56402300	2.19891900	4.33350200
O	4.00191100	2.88443900	0.07967200
H	4.42525300	2.02037400	0.24129200
O	-0.25439300	5.02413700	0.28213500
C	2.34033400	4.76620500	-1.01453200
H	3.14153600	5.45160300	-0.70574400
H	2.79138200	4.11775600	-1.77272700
C	1.17125900	5.56014400	-1.60397800
H	1.53033100	6.37843200	-2.23619400
H	0.53987700	4.91940100	-2.23049900
C	0.30561300	6.12677800	-0.47656300
H	0.94413600	6.70079300	0.21002100
C	-0.82285500	7.00995700	-0.95256600
C	-1.87985000	6.49946600	-1.71896600
H	-1.93377400	5.43589800	-1.92772300
C	-2.88566500	7.34063700	-2.18587900
H	-3.70333600	6.92077100	-2.76651200
C	-2.86620100	8.71739800	-1.91887800
C	-1.80952000	9.22077000	-1.15311100
H	-1.77466900	10.28215500	-0.92079200
C	-0.80526500	8.37920200	-0.67320900
H	-0.00002500	8.79402600	-0.07177300
C	-3.94919200	9.62409200	-2.45369700
H	-3.93111500	10.60143900	-1.96356600
H	-4.94344600	9.19012300	-2.30520100
H	-3.82952600	9.79321500	-3.53090700
C	3.27527900	-0.22484900	1.82868500
C	4.07776100	-0.64867600	0.75507800
C	3.92972800	-1.90891000	0.16883900
C	2.96526800	-2.78624900	0.69622700
C	2.17410100	-2.42857000	1.80157000
C	2.34033400	-1.13862500	2.31644500
H	1.72184800	-0.83829900	3.15527300
C	1.18083800	-3.42219600	2.41614700
H	1.52861700	-4.42437600	2.14901900
C	1.18709500	-3.38755500	3.95663500
H	0.84699400	-2.43251000	4.36625300
H	0.52767400	-4.16575500	4.35234000
O	2.88443900	-4.00191100	0.07967200
H	2.02037400	-4.42525300	0.24129200
O	5.02413700	0.25439300	0.28213500
C	4.76620500	-2.34033400	-1.01453200
H	4.11775600	-2.79138200	-1.77272700

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C	-1.90891000	-3.92972800	0.16883900
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C	-2.42857000	-2.17410100	1.80157000
C	-1.13862500	-2.34033400	2.31644500
H	-0.83829900	-1.72184800	3.15527300
C	-3.42219600	-1.18083800	2.41614700
H	-4.42437600	-1.52861700	2.14901900
C	-3.38755500	-1.18709500	3.95663500
H	-2.43251000	-0.84699400	4.36625300
H	-3.56402300	-2.19891900	4.33350200
O	-4.00191100	-2.88443900	0.07967200
H	-4.42525300	-2.02037400	0.24129200
O	0.25439300	-5.02413700	0.28213500
C	-2.34033400	-4.76620500	-1.01453200
H	-3.14153600	-5.45160300	-0.70574400
H	-2.79138200	-4.11775600	-1.77272700
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H	1.93377400	-5.43589800	-1.92772300
C	2.88566500	-7.34063700	-2.18587900
H	3.70333600	-6.92077100	-2.76651200
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C	3.94919200	-9.62409200	-2.45369700
H	3.93111500	-10.60143900	-1.96356600
H	4.94344600	-9.19012300	-2.30520100
H	3.82952600	-9.79321500	-3.53090700
C	-3.27527900	0.22484900	1.82868500
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C	-3.92972800	1.90891000	0.16883900
C	-2.96526800	2.78624900	0.69622700
C	-2.17410100	2.42857000	1.80157000
C	-2.34033400	1.13862500	2.31644500
H	-1.72184800	0.83829900	3.15527300
C	-1.18083800	3.42219600	2.41614700
H	-1.52861700	4.42437600	2.14901900
C	-1.18709500	3.38755500	3.95663500
H	-0.84699400	2.43251000	4.36625300
H	-0.52767400	4.16575500	4.35234000
O	-2.88443900	4.00191100	0.07967200
H	-2.02037400	4.42525300	0.24129200
O	-5.02413700	-0.25439300	0.28213500
C	-4.76620500	2.34033400	-1.01453200
H	-4.11775600	2.79138200	-1.77272700
H	-5.45160300	3.14153600	-0.70574400
C	-5.56014400	1.17125900	-1.60397800
H	-6.37843200	1.53033100	-2.23619400
H	-4.91940100	0.53987700	-2.23049900
C	-6.12677800	0.30561300	-0.47656300
H	-6.70079300	0.94413600	0.21002100
C	-7.00995700	-0.82285500	-0.95256600
C	-8.37920200	-0.80526500	-0.67320900
H	-8.79402600	-0.00002500	-0.07177300
C	-9.22077000	-1.80952000	-1.15311100
H	-10.28215500	-1.77466900	-0.92079200
C	-8.71739800	-2.86620100	-1.91887800
C	-7.34063700	-2.88566500	-2.18587900
H	-6.92077100	-3.70333600	-2.76651200
C	-6.49946600	-1.87985000	-1.71896600
H	-5.43589800	-1.93377400	-1.92772300

C	-9.62409200	-3.94919200	-2.45369700
H	-9.79321500	-3.82952600	-3.53090700
H	-10.60143900	-3.93111500	-1.96356600
H	-9.19012300	-4.94344600	-2.30520100
H	4.16575500	0.52767400	4.35234000
H	2.19891900	-3.56402300	4.33350200
H	-2.19891900	3.56402300	4.33350200
H	-4.16575500	-0.52767400	4.35234000

Atomic Cartesian coordinates for isomer (all-*R*, all-R_M)-3c optimized geometry:

C	-1.36885100	2.98588200	1.75657801
C	-1.37851700	3.87986000	0.67139201
C	-0.20145600	4.37157000	0.10287501
C	1.03072200	3.93411900	0.62218701
C	1.09296900	3.07313000	1.73198601
C	-0.12015400	2.61208700	2.25382801
H	-0.08977800	1.93179700	3.09780401
C	2.44086200	2.67336600	2.34524501
H	3.15321000	3.46121800	2.08353301
C	2.40869200	2.65950300	3.88579201
H	1.73233900	1.90427900	4.29524901
H	2.08080700	3.63207000	4.26462501
O	2.13614600	4.43542000	0.00086201
H	2.91970400	3.88571600	0.19398801
O	-2.62942900	4.26772700	0.19937201
C	-0.22865000	5.35792300	-1.04186399
H	0.05376500	4.85324700	-1.97641899
H	0.53472400	6.12542300	-0.88204699
C	-1.61206900	5.99466000	-1.18453499
H	-1.78525200	6.73098500	-0.39073499
H	-1.70956000	6.52036600	-2.13980799
C	-2.69971200	4.92328300	-1.09074399
H	-2.51952800	4.16033800	-1.86214299
C	-4.09953700	5.47163100	-1.24629199
C	-4.77308800	5.34977200	-2.46480899
H	-4.30609300	4.81166700	-3.28618199
C	-6.03850400	5.90953500	-2.63887799
H	-6.54335500	5.80340700	-3.59583699
C	-6.67380900	6.59547600	-1.59734699
C	-5.99466000	6.71016400	-0.37636799
H	-6.46638400	7.23844400	0.44869001
C	-4.72708600	6.16063400	-0.20087999
H	-4.22181700	6.25442900	0.75528701
C	-8.06119500	7.16685700	-1.76998299
H	-8.28047100	7.37662700	-2.82093599
H	-8.18416600	8.09651300	-1.20581099
H	-8.82552000	6.46668200	-1.41034299
C	2.98588200	1.36885100	1.75657801
C	3.87986000	1.37851700	0.67139201
C	4.37157000	0.20145600	0.10287501
C	3.93411900	-1.03072200	0.62218701
C	3.07313000	-1.09296900	1.73198601
C	2.61208700	0.12015400	2.25382801
H	1.93179700	0.08977800	3.09780401

C	2.67336600	-2.44086200	2.34524501
H	3.46121800	-3.15321000	2.08353301
C	2.65950300	-2.40869200	3.88579201
H	1.90427900	-1.73233900	4.29524901
H	2.45055400	-3.40768000	4.28011301
O	4.43542000	-2.13614600	0.00086201
H	3.88571600	-2.91970400	0.19398801
O	4.26772700	2.62942900	0.19937201
C	5.35792300	0.22865000	-1.04186399
H	6.12542300	-0.53472400	-0.88204699
H	4.85324700	-0.05376500	-1.97641899
C	5.99466000	1.61206900	-1.18453499
H	6.52036600	1.70956000	-2.13980799
H	6.73098500	1.78525200	-0.39073499
C	4.92328300	2.69971200	-1.09074399
H	4.16033800	2.51952800	-1.86214299
C	5.47163100	4.09953700	-1.24629199
C	5.34977200	4.77308800	-2.46480899
H	4.81166700	4.30609300	-3.28618199
C	5.90953500	6.03850400	-2.63887799
H	5.80340700	6.54335500	-3.59583699
C	6.59547600	6.67380900	-1.59734699
C	6.71016400	5.99466000	-0.37636799
H	7.23844400	6.46638400	0.44869001
C	6.16063400	4.72708600	-0.20087999
H	6.25442900	4.22181700	0.75528701
C	7.16685700	8.06119500	-1.76998299
H	8.09651300	8.18416600	-1.20581099
H	6.46668200	8.82552000	-1.41034299
H	7.37662700	8.28047100	-2.82093599
C	1.36885100	-2.98588200	1.75657801
C	1.37851700	-3.87986000	0.67139201
C	0.20145600	-4.37157000	0.10287501
C	-1.03072200	-3.93411900	0.62218701
C	-1.09296900	-3.07313000	1.73198601
C	0.12015400	-2.61208700	2.25382801
H	0.08977800	-1.93179700	3.09780401
C	-2.44086200	-2.67336600	2.34524501
H	-3.15321000	-3.46121800	2.08353301
C	-2.40869200	-2.65950300	3.88579201
H	-2.08080700	-3.63207000	4.26462501
O	-2.13614600	-4.43542000	0.00086201
H	-2.91970400	-3.88571600	0.19398801
O	2.62942900	-4.26772700	0.19937201
C	0.22865000	-5.35792300	-1.04186399

H	-0.05376500	-4.85324700	-1.97641899
H	-0.53472400	-6.12542300	-0.88204699
C	1.61206900	-5.99466000	-1.18453499
H	1.70956000	-6.52036600	-2.13980799
H	1.78525200	-6.73098500	-0.39073499
C	2.69971200	-4.92328300	-1.09074399
H	2.51952800	-4.16033800	-1.86214299
C	4.09953700	-5.47163100	-1.24629199
C	4.77308800	-5.34977200	-2.46480899
H	4.30609300	-4.81166700	-3.28618199
C	6.03850400	-5.90953500	-2.63887799
H	6.54335500	-5.80340700	-3.59583699
C	6.67380900	-6.59547600	-1.59734699
C	5.99466000	-6.71016400	-0.37636799
H	6.46638400	-7.23844400	0.44869001
C	4.72708600	-6.16063400	-0.20087999
H	4.22181700	-6.25442900	0.75528701
C	8.06119500	-7.16685700	-1.76998299
H	8.82552000	-6.46668200	-1.41034299
H	8.28047100	-7.37662700	-2.82093599
H	8.18416600	-8.09651300	-1.20581099
C	-2.98588200	-1.36885100	1.75657801
C	-3.87986000	-1.37851700	0.67139201
C	-4.37157000	-0.20145600	0.10287501
C	-3.93411900	1.03072200	0.62218701
C	-3.07313000	1.09296900	1.73198601
C	-2.61208700	-0.12015400	2.25382801
H	-1.93179700	-0.08977800	3.09780401
C	-2.67336600	2.44086200	2.34524501
H	-3.46121800	3.15321000	2.08353301
C	-2.65950300	2.40869200	3.88579201
H	-1.90427900	1.73233900	4.29524901
H	-2.45055400	3.40768000	4.28011301
O	-4.43542000	2.13614600	0.00086201
H	-3.88571600	2.91970400	0.19398801
O	-4.26772700	-2.62942900	0.19937201
C	-5.35792300	-0.22865000	-1.04186399
H	-6.12542300	0.53472400	-0.88204699
H	-4.85324700	0.05376500	-1.97641899
C	-5.99466000	-1.61206900	-1.18453499
H	-6.52036600	-1.70956000	-2.13980799
H	-6.73098500	-1.78525200	-0.39073499
C	-4.92328300	-2.69971200	-1.09074399
H	-4.16033800	-2.51952800	-1.86214299
C	-5.47163100	-4.09953700	-1.24629199

C	-6.16063400	-4.72708600	-0.20087999
H	-6.25442900	-4.22181700	0.75528701
C	-6.71016400	-5.99466000	-0.37636799
H	-7.23844400	-6.46638400	0.44869001
C	-6.59547600	-6.67380900	-1.59734699
C	-5.90953500	-6.03850400	-2.63887799
H	-5.80340700	-6.54335500	-3.59583699
C	-5.34977200	-4.77308800	-2.46480899
H	-4.81166700	-4.30609300	-3.28618199
C	-7.16685700	-8.06119500	-1.76998299
H	-8.09651300	-8.18416600	-1.20581099
H	-6.46668200	-8.82552000	-1.41034299
H	-7.37662700	-8.28047100	-2.82093599
H	-3.40768000	-2.45055400	4.28011301
H	-1.73233900	-1.90427900	4.29524901
H	-3.63207000	2.08080700	4.26462501
H	3.40768000	2.45055400	4.28011301
H	3.63207000	-2.08080700	4.26462501

Atomic Cartesian coordinates for isomer (all-*S*, all-R_M)-3c geometry form crystal structure (not optimized):

C	12.14000000	7.55800000	0.87700000
C	13.47600000	7.21300000	1.08600000
C	14.30200000	7.93200000	1.94600000
C	13.73400000	8.98300000	2.67000000
C	12.39200000	9.33900000	2.54200000
C	11.62700000	8.61500000	1.61500000
H	10.73700000	8.85500000	1.48900000
C	11.79600000	10.43900000	3.41600000
H	12.45000000	11.16800000	3.44800000
C	10.49300000	11.02600000	2.84800000
H	9.79700000	10.35500000	2.93600000
H	10.62200000	11.18300000	1.89900000
C	9.98000000	12.33300000	3.48300000
H	9.21500000	12.61800000	2.94000000
C	9.45700000	12.18400000	4.90000000
H	10.19000000	12.00400000	5.49400000
H	8.83100000	11.45700000	4.93600000
H	9.02000000	12.99600000	5.16800000
C	10.99700000	13.46300000	3.40600000
H	10.59700000	14.27700000	3.72000000
H	11.28100000	13.57600000	2.49600000
H	11.75600000	13.24800000	3.95300000
O	14.60200000	9.63100000	3.52300000
H	14.17800000	10.12200000	4.02500000
O	13.93100000	6.10800000	0.39300000
C	15.75700000	7.56800000	2.12200000
H	16.30700000	8.17400000	1.60000000
H	16.00400000	7.66700000	3.05500000
C	16.01000000	6.18000000	1.69200000
H	16.96800000	6.04900000	1.61300000
H	15.68700000	5.57800000	2.38000000
C	15.42000000	5.84000000	0.49700000
H	15.81400000	6.46700000	-0.14500000
C	15.54500000	4.50400000	-0.18700000
C	15.76500000	3.31200000	0.49300000
H	15.83500000	3.31100000	1.42000000
C	15.87900000	2.12000000	-0.21400000
H	16.02500000	1.32200000	0.24000000
C	15.77400000	2.12200000	-1.60000000
C	15.55500000	3.31500000	-2.28000000
H	15.48400000	3.31600000	-3.20700000
C	15.44000000	4.50600000	-1.57300000
H	15.29400000	5.30400000	-2.02700000

C	16.00100000	0.87000000	-2.45000000
H	15.45300000	0.91400000	-3.23700000
H	15.76700000	0.09100000	-1.94000000
H	16.92500000	0.82000000	-2.70500000
C	11.64000000	9.91300000	4.84500000
C	12.49400000	10.34100000	5.87400000
C	12.39400000	9.85000000	7.17300000
C	11.39300000	8.92100000	7.44800000
C	10.47000000	8.51300000	6.47600000
C	10.65700000	8.99900000	5.17900000
H	10.09300000	8.69200000	4.50700000
C	9.27800000	7.62200000	6.80800000
H	9.29800000	7.47300000	7.77700000
C	7.94900000	8.34200000	6.49900000
H	7.96600000	8.64700000	5.57800000
H	7.22200000	7.70700000	6.58600000
C	7.67000000	9.54300000	7.41200000
H	8.46900000	10.11000000	7.42500000
C	7.37500000	9.10600000	8.84000000
H	7.22600000	9.88100000	9.38700000
H	8.12300000	8.61100000	9.18400000
H	6.59200000	8.55100000	8.85000000
C	6.50600000	10.37000000	6.86900000
H	5.70700000	9.83700000	6.86900000
H	6.70400000	10.65000000	5.97300000
H	6.37500000	11.14200000	7.42500000
O	11.34900000	8.44100000	8.73700000
H	11.34200000	7.62100000	8.72300000
O	13.46100000	11.26600000	5.50900000
C	13.35400000	10.29600000	8.25500000
H	13.69000000	9.52400000	8.73700000
H	12.89500000	10.87200000	8.88600000
C	14.58400000	11.09600000	7.57300000
H	15.09700000	11.56100000	8.25300000
H	15.17300000	10.47600000	7.11600000
C	13.99700000	12.10900000	6.56800000
H	13.28200000	12.63400000	6.98500000
C	15.02200000	13.01100000	5.95400000
C	16.03000000	12.55000000	5.14600000
H	16.11900000	11.63800000	4.98600000
C	16.89200000	13.42000000	4.58500000
H	17.49700000	13.05200000	3.98300000
C	16.99200000	14.68300000	4.76500000
C	15.74800000	15.10800000	5.62200000
H	15.57200000	16.01900000	5.68300000

C	15.01400000	14.38600000	6.19700000
H	14.42100000	14.73700000	6.82100000
C	17.64400000	15.82200000	4.13500000
H	17.03200000	16.24400000	3.52700000
H	18.41700000	15.52100000	3.65300000
H	17.91100000	16.45100000	4.80900000
C	9.38900000	6.25400000	6.15300000
C	10.13900000	5.24800000	6.76900000
C	10.21000000	3.95800000	6.25500000
C	9.56100000	3.70100000	5.04400000
C	8.83900000	4.67600000	4.36000000
C	8.76100000	5.94500000	4.94600000
H	8.27100000	6.60700000	4.51400000
C	8.18900000	4.33800000	3.01900000
H	7.83700000	3.42700000	3.10300000
C	6.99200000	5.23700000	2.67100000
H	7.31700000	6.13600000	2.50400000
H	6.40000000	5.27700000	3.43800000
C	6.18400000	4.76700000	1.44800000
H	6.23400000	3.79000000	1.40100000
C	6.71600000	5.34100000	0.13400000
H	6.22300000	4.96800000	-0.60100000
H	7.64500000	5.11900000	0.04100000
H	6.61300000	6.29500000	0.13600000
C	4.72600000	5.16600000	1.60000000
H	4.66000000	6.12200000	1.65800000
H	4.36800000	4.77100000	2.39900000
H	4.22900000	4.85600000	0.84000000
O	9.68500000	2.40900000	4.59300000
H	9.45000000	2.37000000	3.80900000
O	10.80900000	5.60200000	7.93600000
C	10.95300000	2.85000000	6.95500000
H	10.32100000	2.16700000	7.22800000
H	11.57800000	2.44500000	6.33400000
C	11.68400000	3.32400000	8.13200000
H	11.46200000	2.72900000	8.86500000
H	12.62900000	3.20300000	7.94900000
C	11.53400000	4.50200000	8.55100000
H	10.73300000	4.23600000	9.04800000
C	12.19000000	5.01900000	9.85000000
C	13.50200000	4.65100000	10.12200000
H	13.96400000	4.10300000	9.53000000
C	14.12400000	5.10300000	11.28000000
H	15.00300000	4.85600000	11.46300000
C	13.43400000	5.92200000	12.16600000

C	12.12200000	6.28900000	11.89400000
H	11.66000000	6.83800000	12.48600000
C	11.49900000	5.83800000	10.73600000
H	10.62100000	6.08400000	10.55300000
C	14.04300000	6.24000000	13.60700000
H	13.33000000	6.44100000	14.21800000
H	14.63400000	6.99300000	13.54500000
H	14.52900000	5.47500000	13.92400000
C	9.26200000	4.28700000	1.93600000
C	9.72100000	3.06700000	1.41900000
C	10.76600000	2.99900000	0.50300000
C	11.29600000	4.20200000	0.01600000
C	10.82900000	5.44400000	0.45700000
C	9.85400000	5.44500000	1.45000000
H	9.58600000	6.26200000	1.80600000
C	11.33500000	6.75700000	-0.13800000
H	11.95200000	6.52000000	-0.86200000
C	10.18800000	7.55800000	-0.77800000
H	9.50100000	7.70900000	-0.11100000
H	10.52700000	8.42400000	-1.05400000
C	9.55600000	6.86400000	-1.99100000
H	9.22500000	5.98800000	-1.70000000
C	10.56100000	6.63700000	-3.11600000
H	10.10500000	6.29400000	-3.88800000
H	11.22400000	6.00500000	-2.83000000
H	10.98500000	7.46900000	-3.33800000
C	8.36500000	7.67200000	-2.49700000
H	8.66800000	8.52600000	-2.81100000
H	7.73800000	7.79800000	-1.78100000
H	7.93900000	7.19900000	-3.21500000
O	12.27900000	4.07800000	-0.92900000
H	12.91100000	4.56200000	-0.73200000
O	9.09200000	1.92100000	1.89700000
C	11.36000000	1.67600000	0.08500000
H	12.32900000	1.72200000	0.12000000
H	11.09600000	1.46600000	-0.82400000
C	10.82800000	0.54000000	1.08800000
H	11.06500000	-0.34000000	0.75600000
H	11.22200000	0.65500000	1.96600000
C	9.32000000	0.68700000	1.16300000
H	8.96500000	0.78800000	0.25500000
C	8.56200000	-0.39800000	1.86200000
C	7.82100000	-1.29900000	1.10500000
H	7.83500000	-1.24800000	0.17700000
C	7.05900000	-2.27500000	1.73700000

H	6.56300000	-2.87700000	1.23100000
C	7.03800000	-2.35100000	3.12400000
C	7.77900000	-1.45000000	3.88100000
H	7.76500000	-1.50100000	4.80900000
C	8.54100000	-0.47400000	3.25000000
H	9.03700000	0.12800000	3.75600000
C	6.05600000	-3.45500000	3.53500000
H	6.54600000	-4.22200000	3.84200000
H	5.51700000	-3.70200000	2.77900000
H	5.49000000	-3.13400000	4.24000000

Atomic Cartesian coordinates for isomer (all-*R*, all-R_M)-3c geometry from crystal structure (not optimized):

C	12.14100000	7.55800000	0.87700000
C	13.47600000	7.21300000	1.08600000
C	14.30200000	7.93200000	1.94600000
C	13.73400000	8.98300000	2.67000000
C	12.39200000	9.33900000	2.54200000
C	11.62600000	8.61500000	1.61500000
H	10.73700000	8.85500000	1.49000000
C	11.79600000	10.43900000	3.41600000
H	12.45000000	11.16800000	3.44900000
C	10.49400000	11.02600000	2.84800000
H	9.79800000	10.35500000	2.93600000
H	10.62400000	11.18200000	1.89900000
C	9.98100000	12.33300000	3.48300000
H	9.21700000	12.61900000	2.94100000
C	9.45700000	12.18400000	4.90000000
H	10.19000000	12.00300000	5.49400000
H	8.83100000	11.45800000	4.93600000
H	9.02000000	12.99600000	5.16900000
C	10.99800000	13.46300000	3.40600000
H	10.59800000	14.27700000	3.72000000
H	11.28200000	13.57600000	2.49500000
H	11.75700000	13.24900000	3.95400000
O	14.60200000	9.63100000	3.52300000
H	14.17700000	10.12200000	4.02500000
O	13.93100000	6.10800000	0.39400000
C	15.75700000	7.56900000	2.12300000
H	15.89600000	7.19700000	3.00800000
H	16.30500000	8.36400000	2.03900000
C	16.18500000	6.51700000	1.03700000
H	16.28300000	6.94500000	0.17200000
H	17.03200000	6.10900000	1.27600000
C	15.06100000	5.44200000	0.98800000
H	14.84100000	5.13400000	1.89100000
C	15.38600000	4.27000000	0.09600000
C	15.55700000	3.01100000	0.63600000
H	15.52200000	2.89200000	1.55600000
C	15.77700000	1.93400000	-0.18700000
H	15.95800000	1.11000000	0.20600000
C	15.74600000	2.00400000	-1.55000000
C	15.57000000	3.29700000	-2.07100000
H	15.57600000	3.41200000	-2.99300000
C	15.39200000	4.39100000	-1.27800000
H	15.27000000	5.22700000	-1.66600000

C	15.86700000	0.80200000	-2.42100000
H	16.01200000	0.02600000	-1.87700000
H	16.60800000	0.91400000	-3.02200000
H	15.05800000	0.69200000	-2.92800000
C	11.64000000	9.91300000	4.84400000
C	12.49400000	10.34100000	5.87400000
C	12.39400000	9.85000000	7.17300000
C	11.39300000	8.92100000	7.44800000
C	10.47000000	8.51300000	6.47600000
C	10.65700000	8.99900000	5.17900000
H	10.09300000	8.69100000	4.50600000
C	9.27800000	7.62200000	6.80800000
H	9.29800000	7.47300000	7.77700000
C	7.94900000	8.34200000	6.49900000
H	7.96600000	8.64700000	5.57800000
H	7.22200000	7.70800000	6.58600000
C	7.67000000	9.54300000	7.41200000
H	8.46800000	10.11100000	7.42500000
C	7.37400000	9.10600000	8.84000000
H	7.22500000	9.88100000	9.38700000
H	8.12100000	8.61200000	9.18400000
H	6.59200000	8.55100000	8.85000000
C	6.50600000	10.37000000	6.86900000
H	5.70700000	9.83700000	6.86900000
H	6.70300000	10.65100000	5.97300000
H	6.37500000	11.14200000	7.42500000
O	11.34800000	8.44100000	8.73700000
H	11.34100000	7.62200000	8.72300000
O	13.46100000	11.26600000	5.50900000
C	13.35400000	10.29600000	8.25500000
H	12.86100000	10.45600000	9.07500000
H	13.99600000	9.58900000	8.42600000
C	14.07300000	11.52300000	7.87300000
H	14.81900000	11.66400000	8.47700000
H	13.47700000	12.28400000	7.94600000
C	14.57400000	11.41900000	6.48800000
H	15.13000000	10.61500000	6.43400000
C	15.37700000	12.56400000	5.93300000
C	16.34500000	12.31400000	4.98600000
H	16.49800000	11.43900000	4.71700000
C	17.10300000	13.34200000	4.42000000
H	17.77600000	13.15400000	3.80400000
C	16.81700000	14.72100000	4.81600000
C	15.97700000	15.00400000	5.75200000
H	15.90300000	15.87000000	6.08600000

C	15.11400000	13.87800000	6.29700000
H	14.40900000	14.07000000	6.87300000
C	17.78900000	15.73700000	4.17600000
H	18.65300000	15.65500000	4.58500000
H	17.45500000	16.62800000	4.31100000
H	17.86100000	15.56200000	3.23500000
C	9.38900000	6.25400000	6.15300000
C	10.13800000	5.24800000	6.76900000
C	10.20900000	3.95800000	6.25500000
C	9.56200000	3.70100000	5.04400000
C	8.83900000	4.67600000	4.36000000
C	8.76100000	5.94400000	4.94600000
H	8.27100000	6.60700000	4.51400000
C	8.18900000	4.33800000	3.01900000
H	7.83600000	3.42600000	3.10300000
C	6.99200000	5.23700000	2.67100000
H	7.31600000	6.13600000	2.50300000
H	6.40000000	5.27700000	3.43800000
C	6.18400000	4.76700000	1.44800000
H	6.23400000	3.79000000	1.40000000
C	6.71600000	5.34100000	0.13400000
H	6.22400000	4.96800000	-0.60100000
H	7.64600000	5.12000000	0.04100000
H	6.61400000	6.29500000	0.13500000
C	4.72600000	5.16600000	1.60000000
H	4.66100000	6.12200000	1.65800000
H	4.36900000	4.77200000	2.39900000
H	4.22900000	4.85600000	0.84000000
O	9.68500000	2.40900000	4.59300000
H	9.44900000	2.37100000	3.80900000
O	10.80800000	5.60200000	7.93600000
C	10.95200000	2.85000000	6.95500000
H	11.76800000	2.64300000	6.47300000
H	10.40300000	2.05100000	6.98400000
C	11.29200000	3.30700000	8.38800000
H	11.93300000	2.69900000	8.78600000
H	10.49000000	3.30400000	8.93400000
C	11.88700000	4.73900000	8.32500000
H	12.60800000	4.77900000	7.66200000
C	12.38200000	5.19700000	9.65300000
C	13.68000000	4.88800000	10.04300000
H	14.25700000	4.49100000	9.43300000
C	14.13300000	5.16400000	11.34300000
H	14.99200000	4.91000000	11.59000000
C	13.34000000	5.79800000	12.24700000

C	12.04400000	6.10800000	11.86300000
H	11.48100000	6.53700000	12.46800000
C	11.56200000	5.79000000	10.59800000
H	10.67800000	5.97600000	10.38400000
C	13.88500000	6.20300000	13.56600000
H	13.58100000	7.09000000	13.77800000
H	14.84400000	6.19300000	13.53400000
H	13.57800000	5.59000000	14.23900000
C	9.26200000	4.28800000	1.93600000
C	9.72100000	3.06800000	1.41900000
C	10.76600000	2.99900000	0.50300000
C	11.29600000	4.20200000	0.01600000
C	10.82900000	5.44400000	0.45700000
C	9.85400000	5.44500000	1.45000000
H	9.58600000	6.26200000	1.80600000
C	11.33600000	6.75700000	-0.13800000
H	11.95300000	6.52000000	-0.86200000
C	10.18900000	7.55800000	-0.77800000
H	9.50200000	7.70900000	-0.11000000
H	10.52700000	8.42500000	-1.05400000
C	9.55700000	6.86400000	-1.99100000
H	9.22700000	5.98700000	-1.70100000
C	10.56200000	6.63700000	-3.11600000
H	10.10600000	6.29400000	-3.88800000
H	11.22500000	6.00500000	-2.82900000
H	10.98600000	7.46900000	-3.33900000
C	8.36600000	7.67100000	-2.49700000
H	8.67000000	8.52500000	-2.81200000
H	7.73800000	7.79900000	-1.78100000
H	7.94000000	7.19800000	-3.21600000
O	12.27900000	4.07700000	-0.93000000
H	12.91000000	4.56100000	-0.73200000
O	9.09200000	1.92100000	1.89700000
C	11.36000000	1.67600000	0.08500000
H	11.55300000	1.69800000	-0.86500000
H	12.19700000	1.53900000	0.55700000
C	10.43900000	0.53900000	0.37400000
H	10.91900000	-0.30000000	0.29000000
H	9.71100000	0.53800000	-0.26700000
C	9.88200000	0.66200000	1.77000000
H	10.62500000	0.68800000	2.40900000
C	8.90900000	-0.41900000	2.18900000
C	8.26800000	-1.25300000	1.27600000
H	8.46100000	-1.16800000	0.37000000
C	7.35500000	-2.20000000	1.67700000

H	6.96700000	-2.75200000	1.03500000
C	6.99200000	-2.36000000	3.00500000
C	7.66300000	-1.51000000	3.92100000
H	7.47200000	-1.58000000	4.82900000
C	8.58600000	-0.59100000	3.50100000
H	9.00900000	-0.06000000	4.13800000
C	6.09800000	-3.38000000	3.64900000
H	6.52600000	-4.23900000	3.62800000
H	5.26800000	-3.42300000	3.17000000
H	5.93100000	-3.12800000	4.56000000

[1] *Gaussian 09, Revision D.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.