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SUPPORTING INFORMATION

Manuscript title: **Synthesis and conformations of [2.*n*]metacyclophan-1-ene epoxides and their conversion to [*n*.1]metacyclophanes †**

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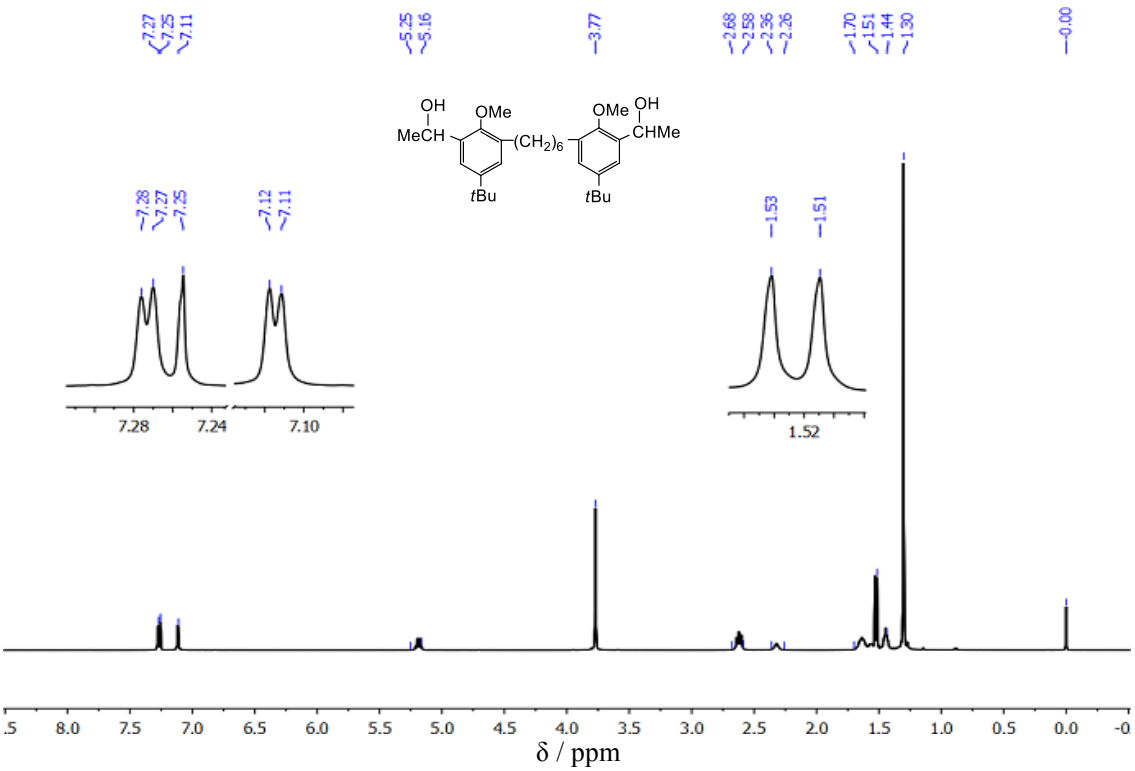


Figure S1. ^{1}H–NMR spectrum of compound **2a** (300 MHz, $CDCl_3$, 293 K).

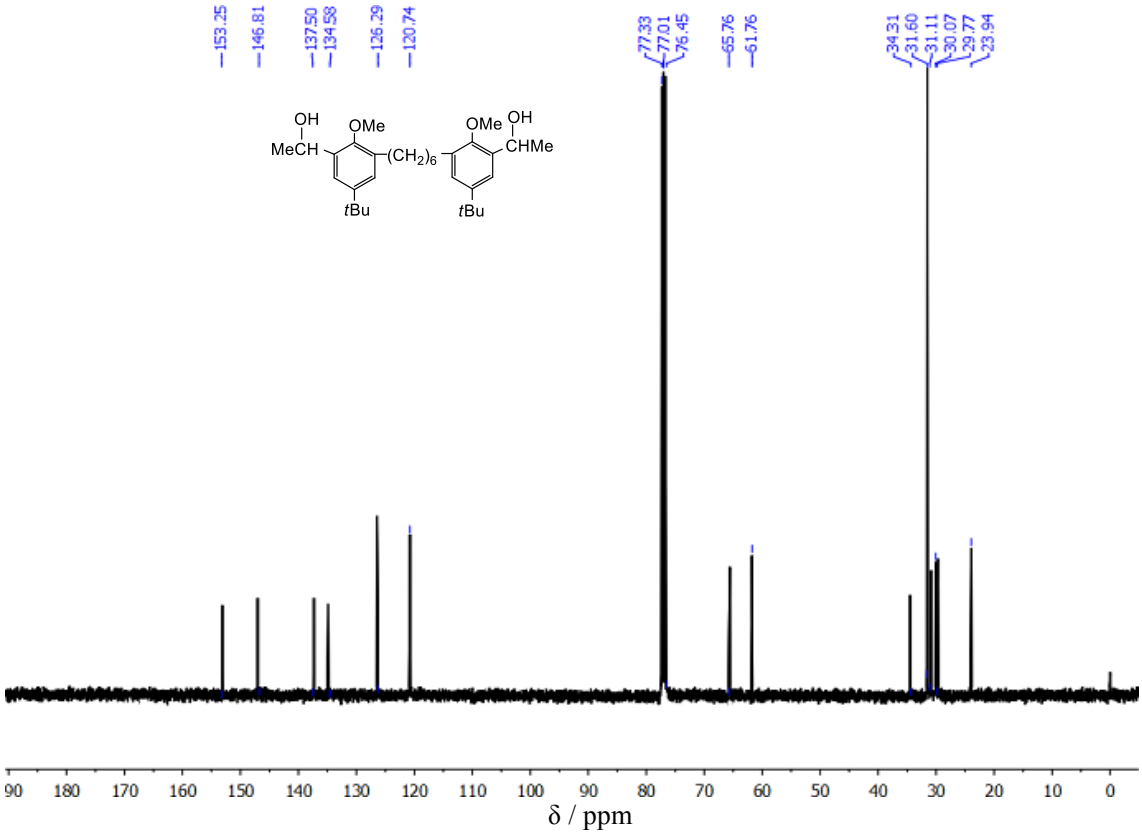


Figure S2. ^{13}C–NMR spectrum of compound **2a** (100 MHz, $CDCl_3$, 293 K).

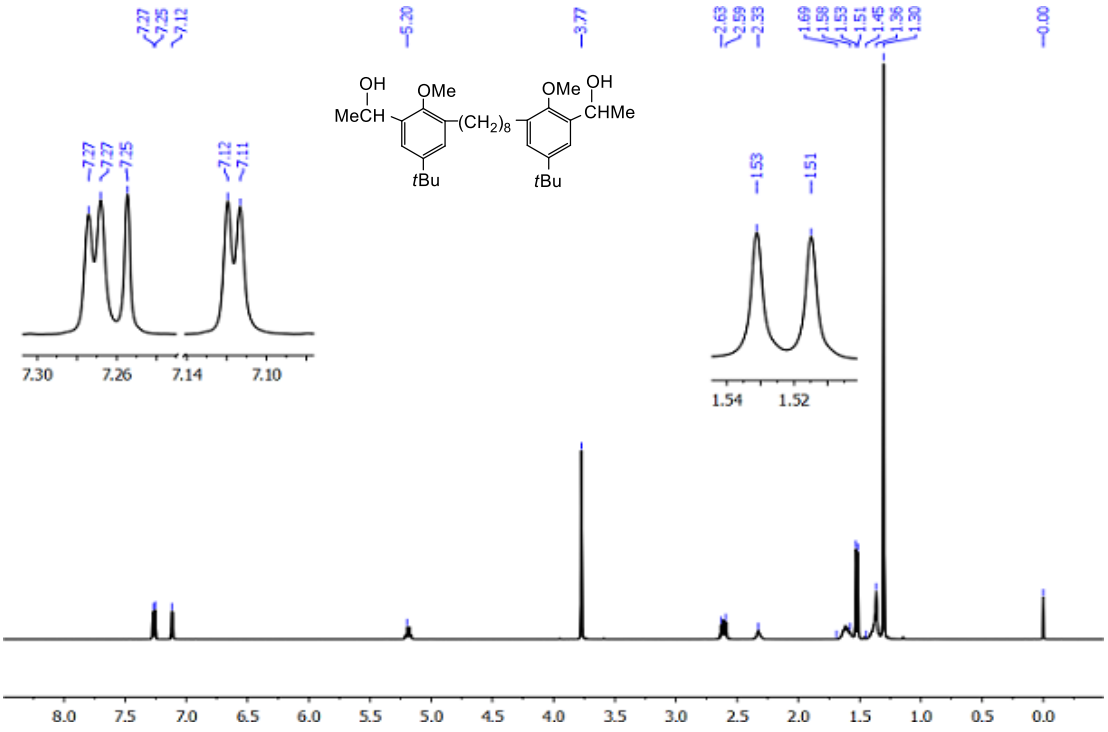


Figure S3. ^{1}H–NMR spectrum of compound **2b** (300 MHz, $CDCl_3$, 293 K).

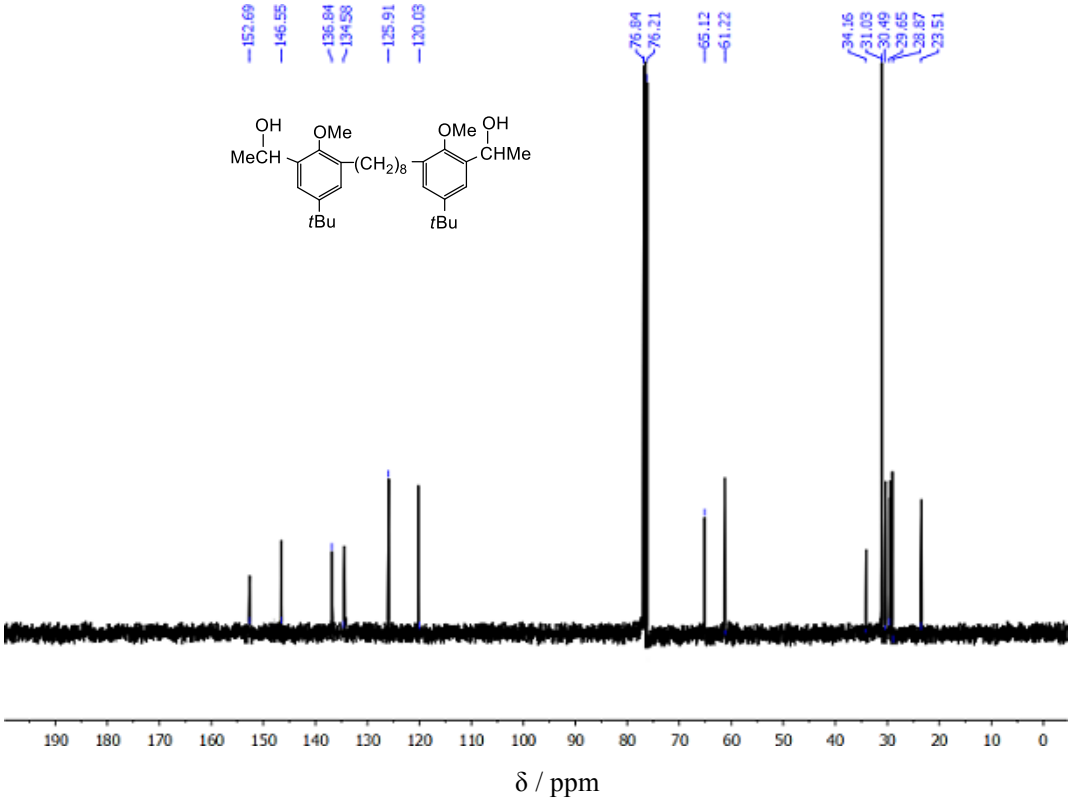


Figure S4. ^{13}C–NMR spectrum of compound **2b** (100 MHz, $CDCl_3$, 293 K).

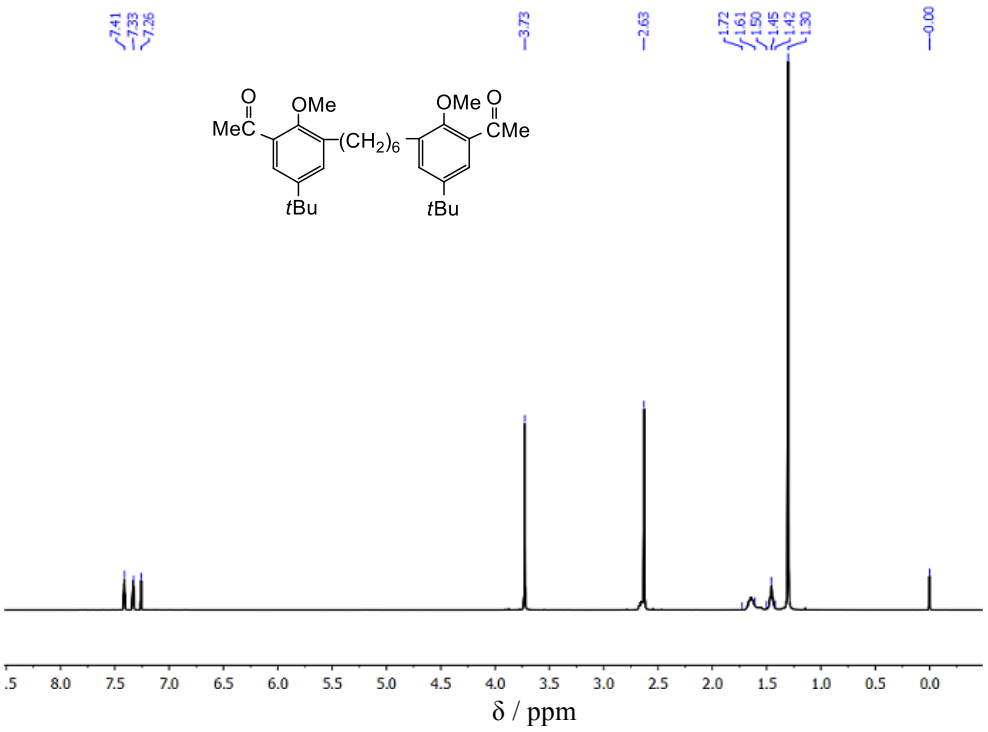


Figure S5. ^{1}H–NMR spectrum of compound **3a** (300 MHz, $CDCl_3$, 293 K).

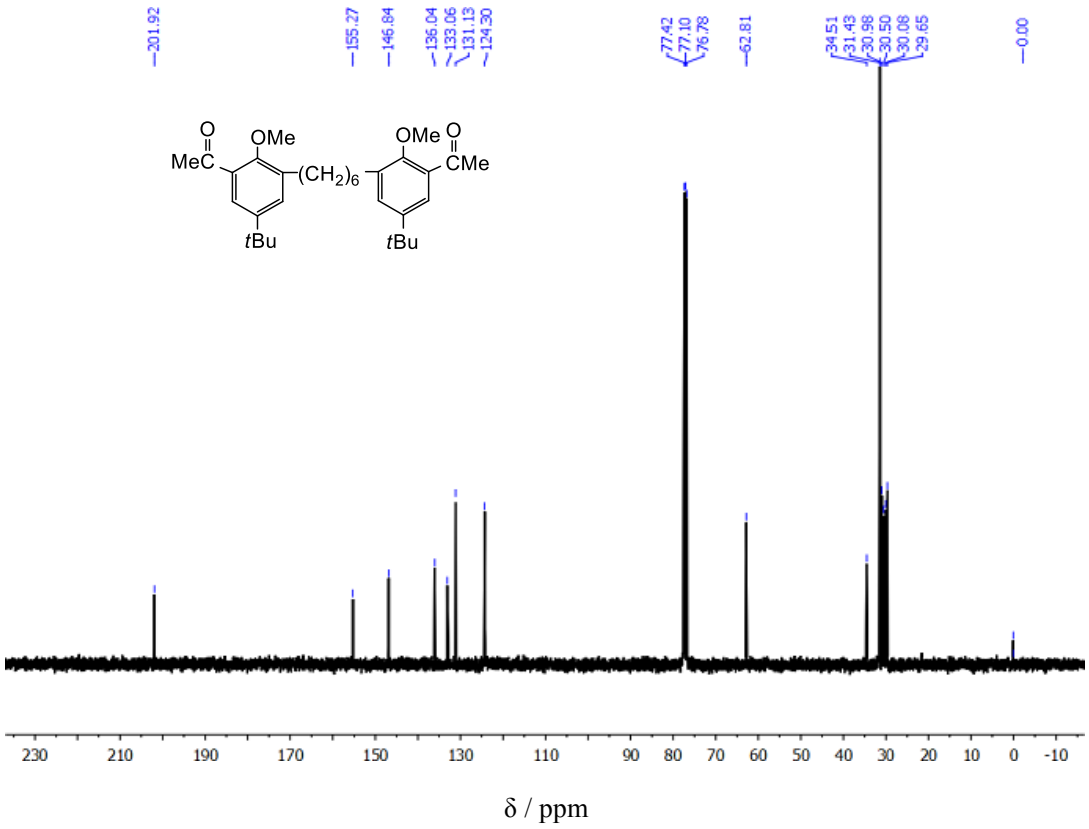


Figure S6. ^{13}C–NMR spectrum of compound **3a** (100 MHz, $CDCl_3$, 293 K).

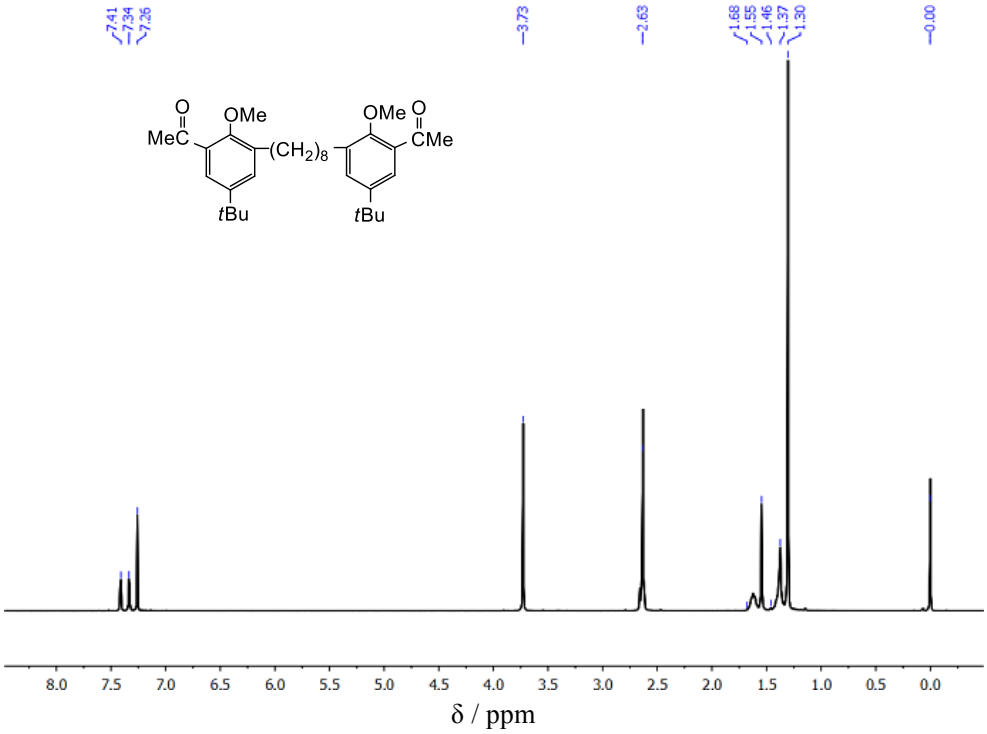


Figure S7. ^{1}H–NMR spectrum of compound **3b** (300 MHz, $CDCl_3$, 293 K).

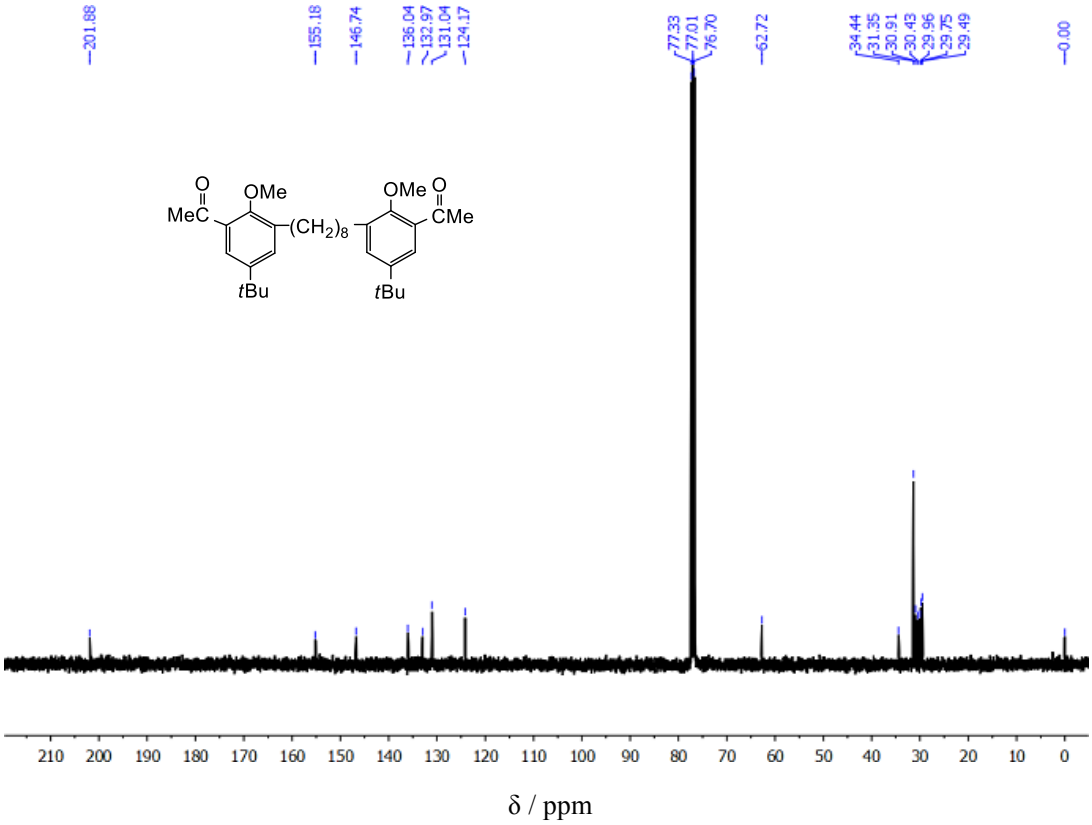


Figure S8. ^{13}C–NMR spectrum of compound **3b** (100 MHz, $CDCl_3$, 293 K).

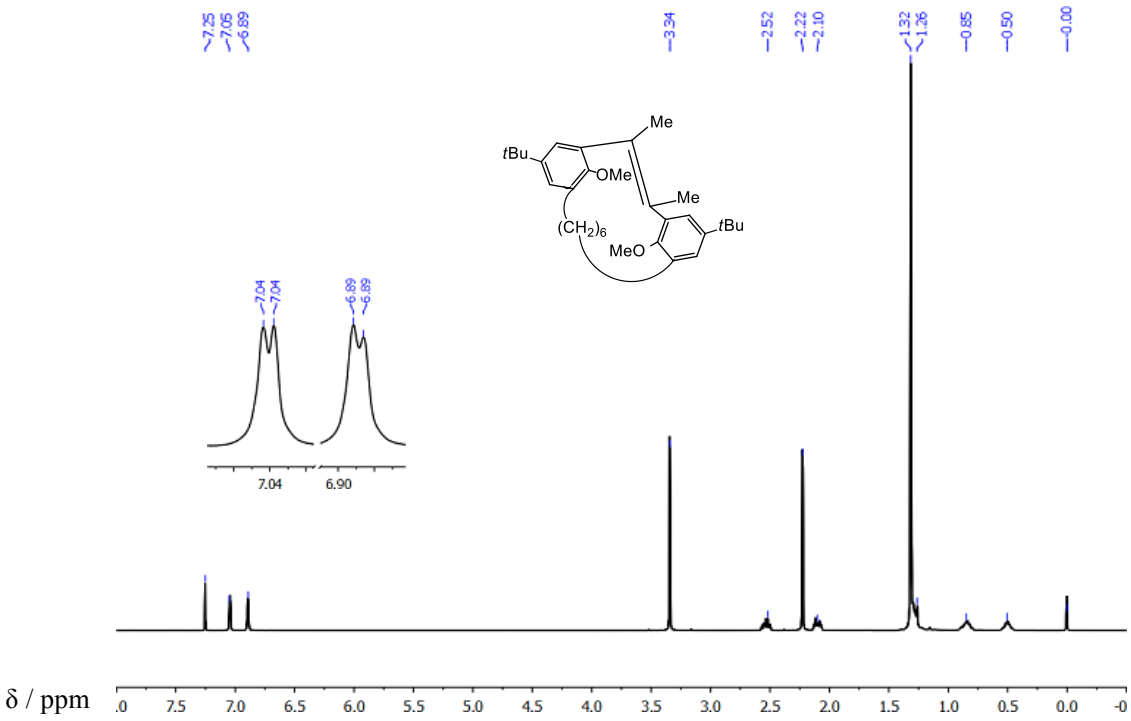


Figure S9. ^{1}H–NMR spectrum of compound *anti*-**4a** (300 MHz, $CDCl_3$, 293 K).

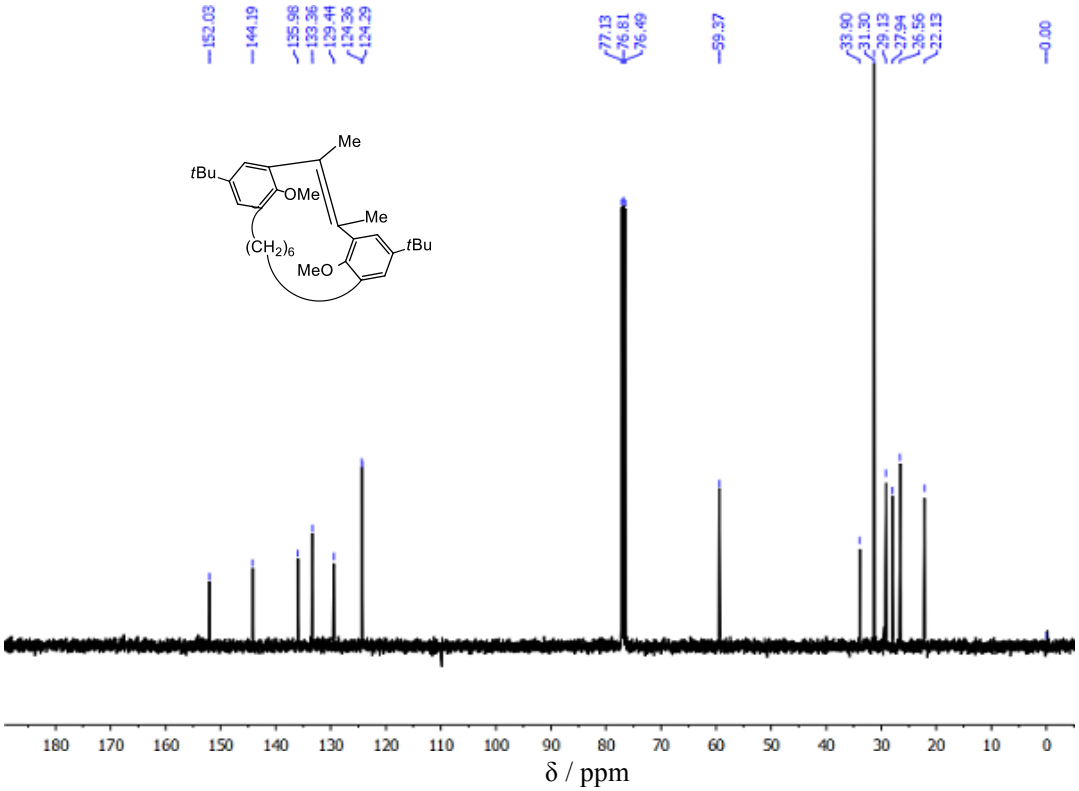


Figure S10. ^{13}C–NMR spectrum of compound *anti*-**4a** (100 MHz, $CDCl_3$, 293 K).

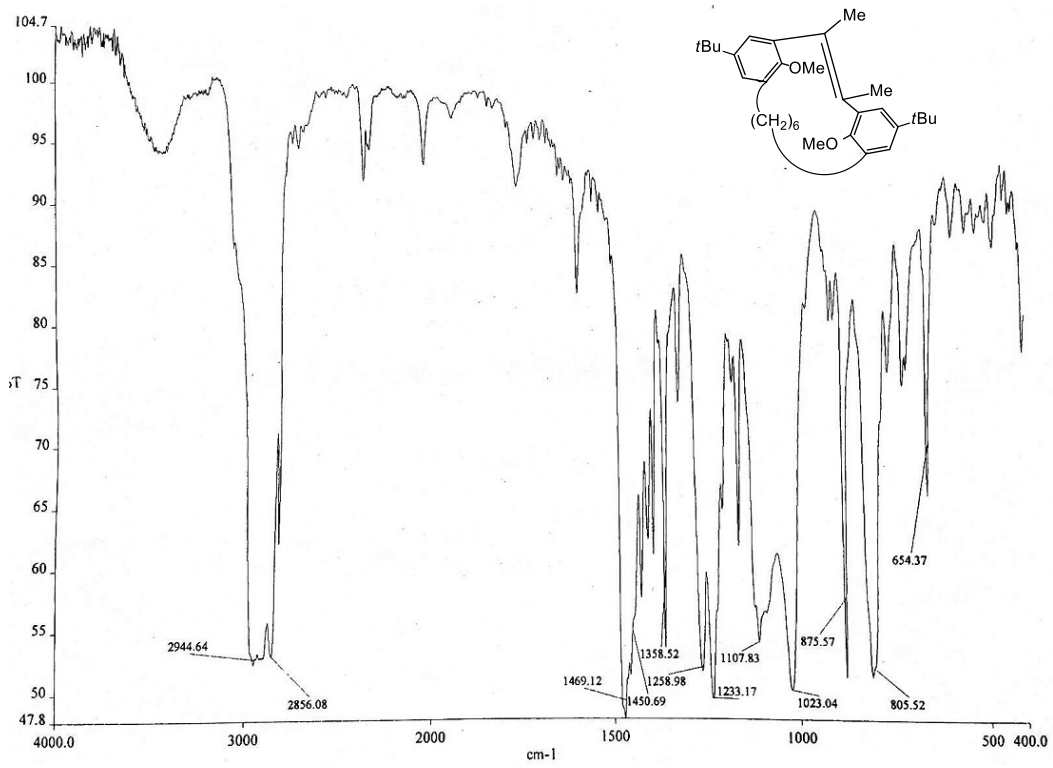


Figure S11. IR spectrum of compound *anti*-**4a**.

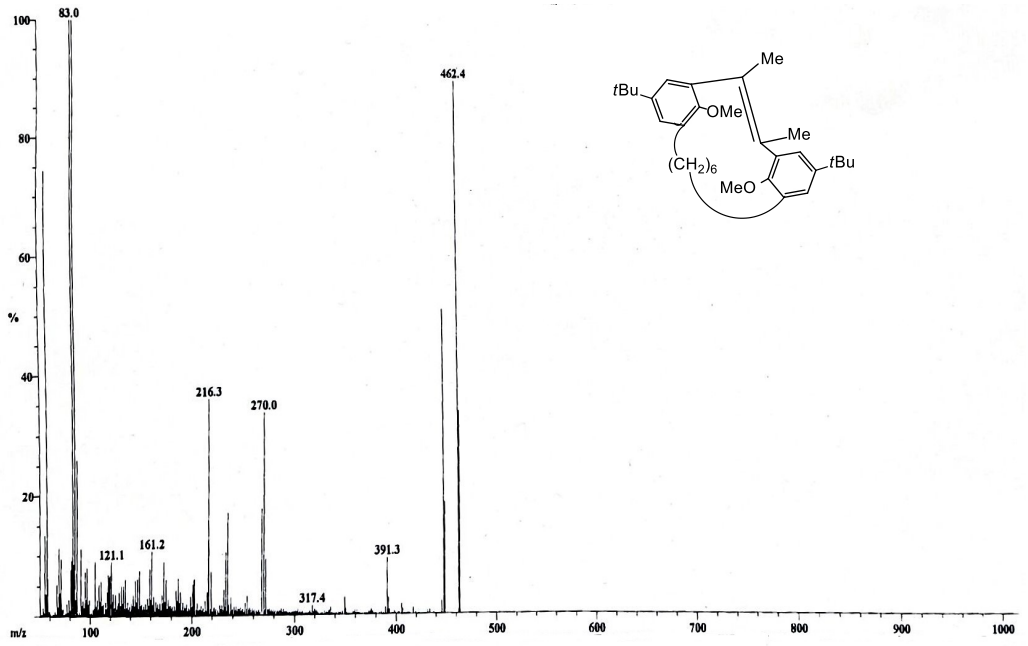


Figure S12. Mass spectrum of compound *anti*-**4a**.

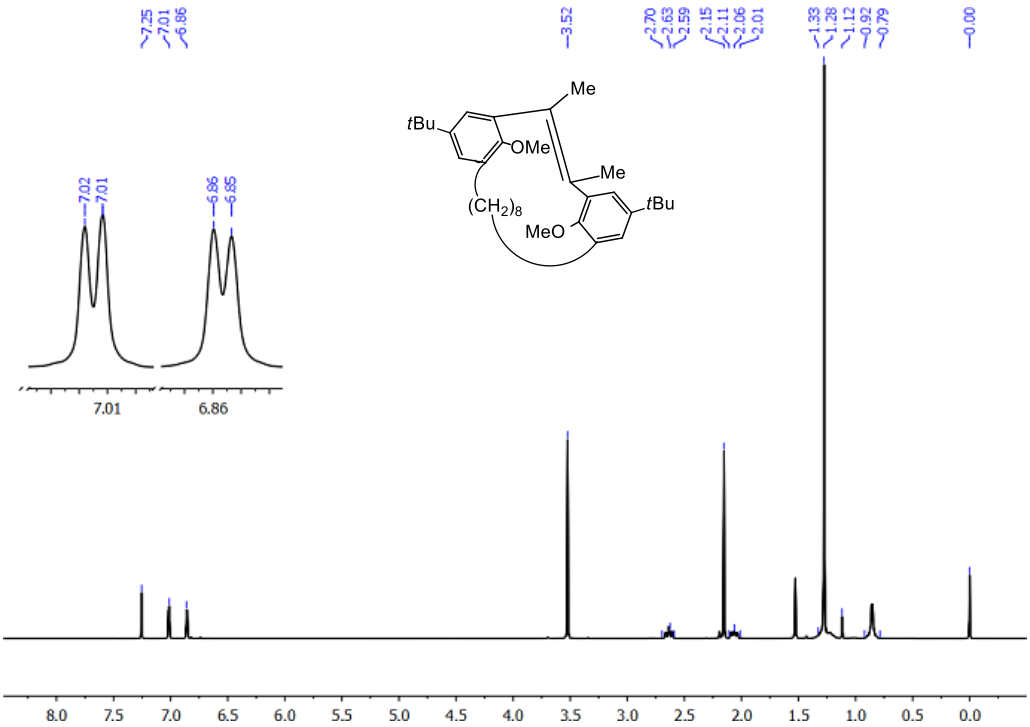


Figure S13. ^{1}H–NMR spectrum of compound *anti*-**4b** (300 MHz, $CDCl_3$, 293 K).

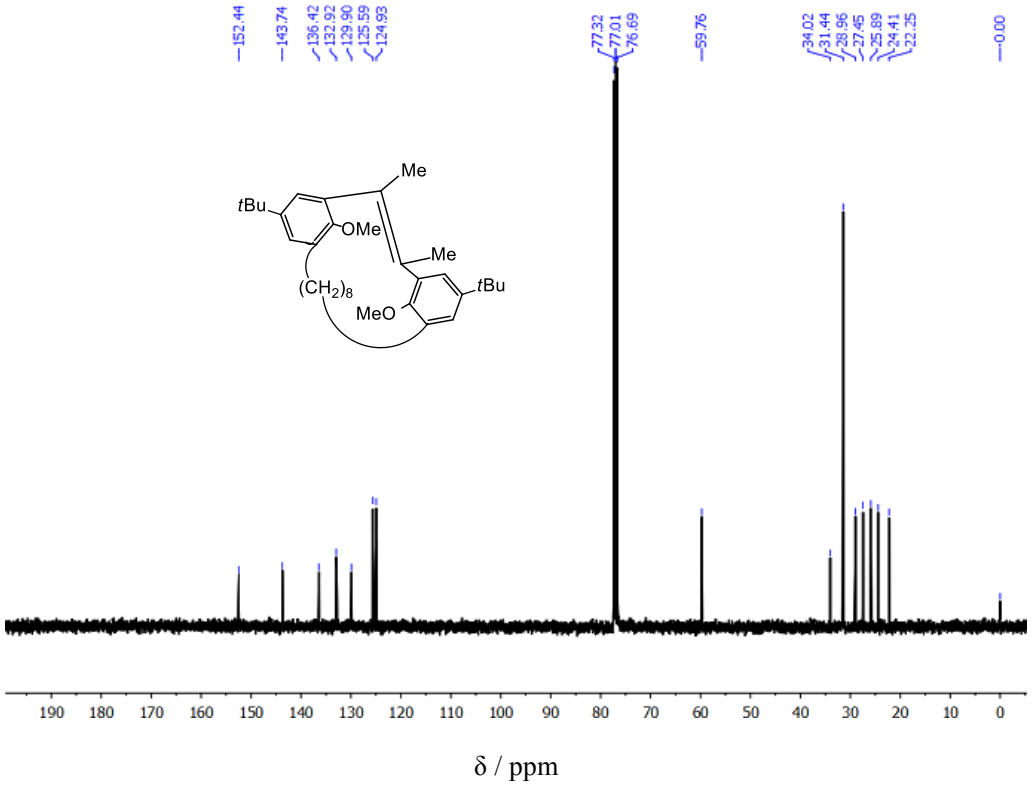


Figure S14. ^{13}C–NMR spectrum of compound *anti*-**4b** (100 MHz, $CDCl_3$, 293 K).

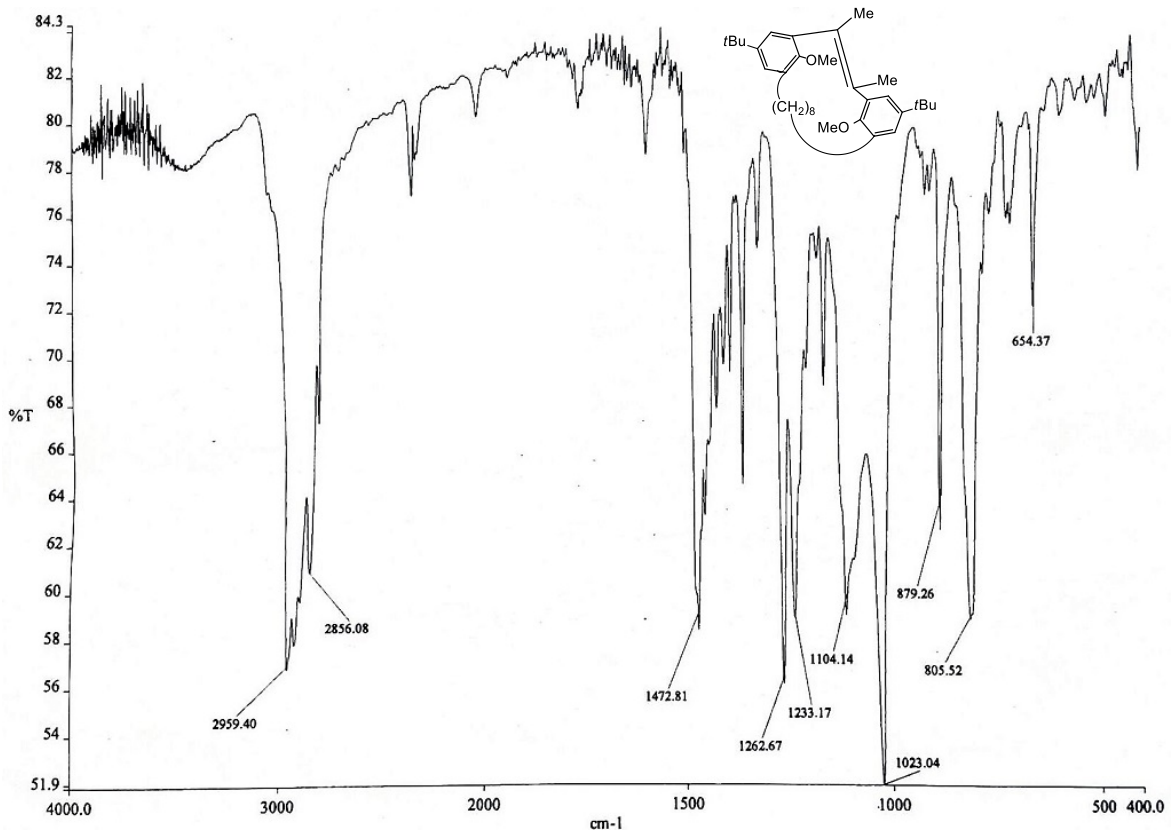


Figure S15. IR spectrum of compound *anti*-**4b**.

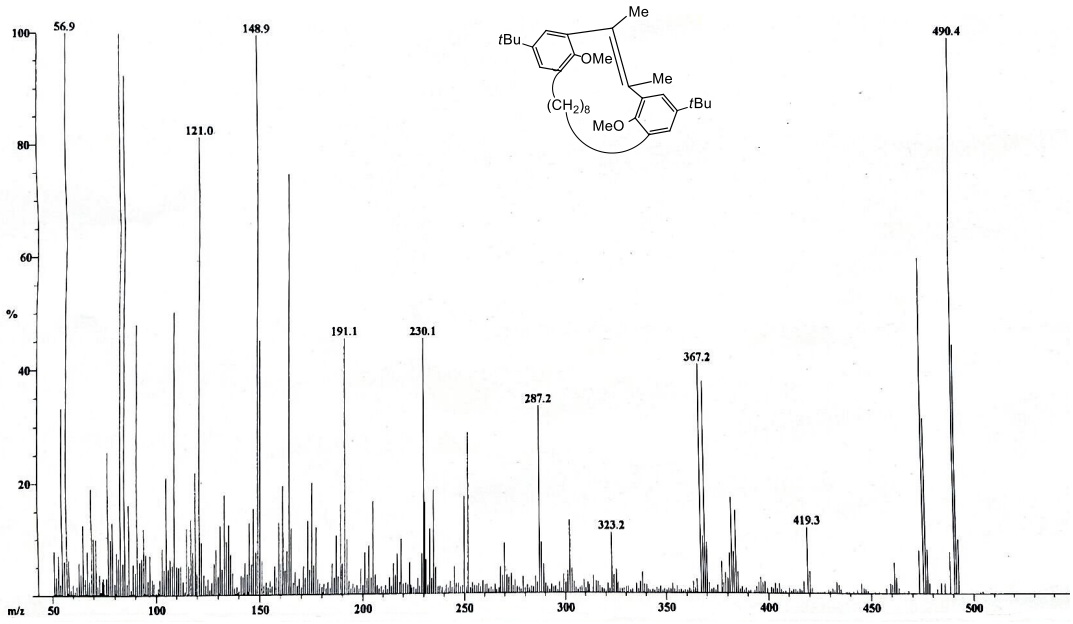


Figure S16. Mass spectrum of compound *anti*-**4b**.

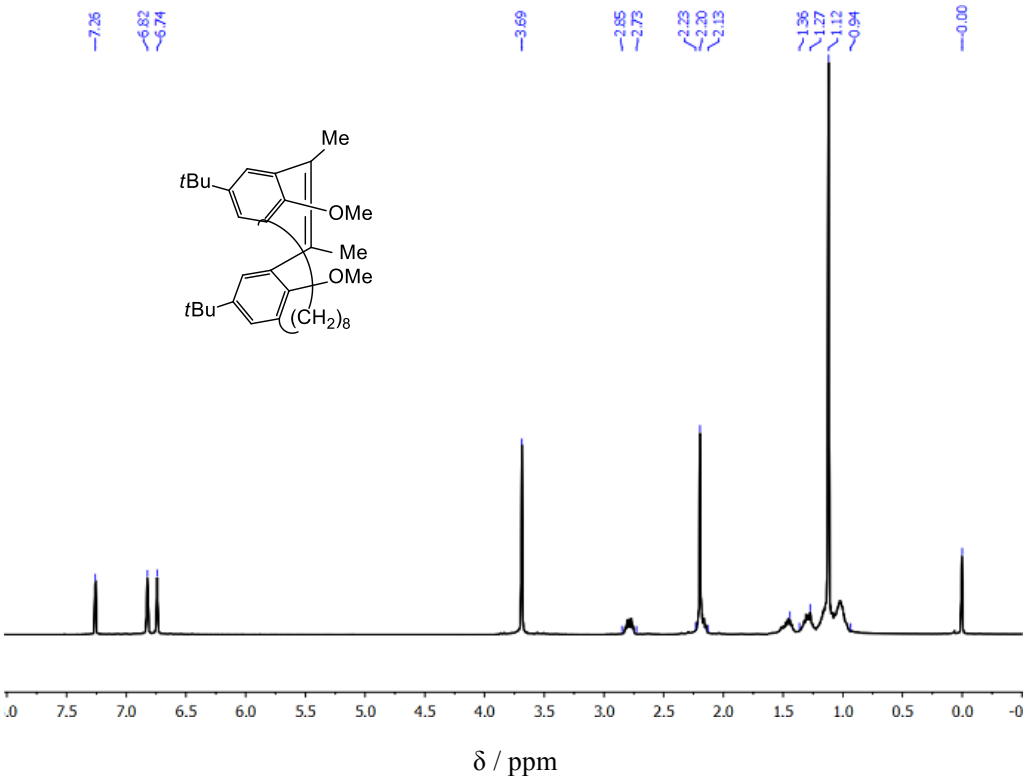


Figure S17. ^{1}H–NMR spectrum of compound *syn*-**4b** (300 MHz, $CDCl_3$, 293 K).

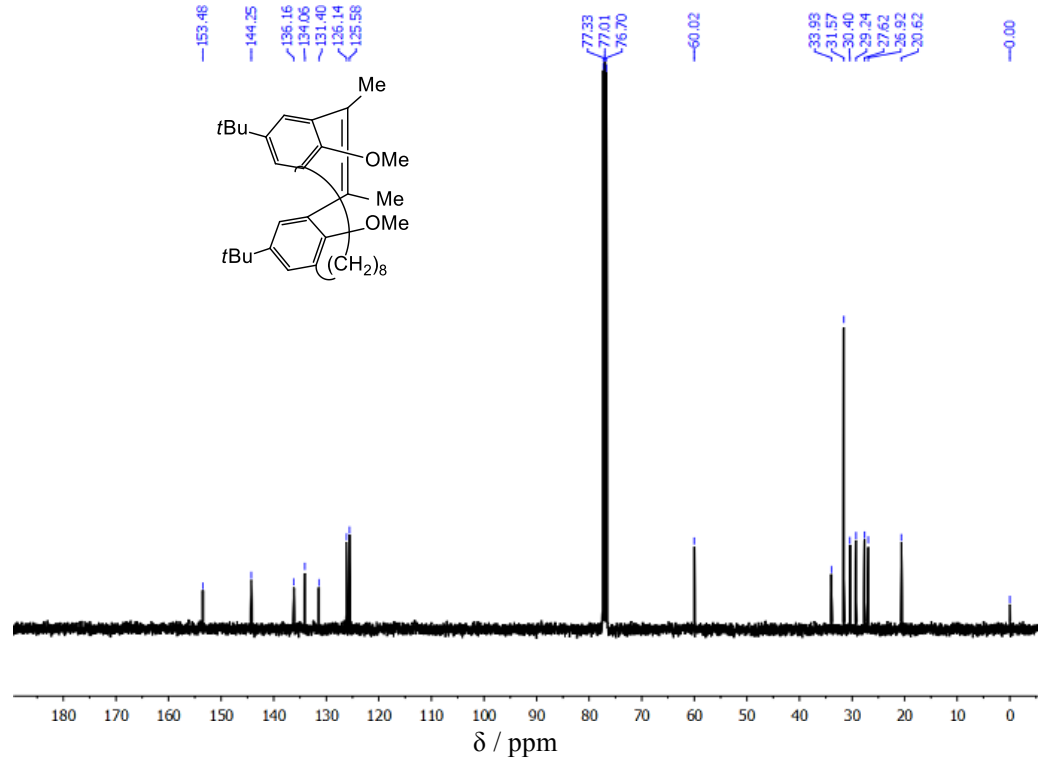


Figure S18. ^{13}C–NMR spectrum of compound *syn*-**4b** (100 MHz, $CDCl_3$, 293 K).

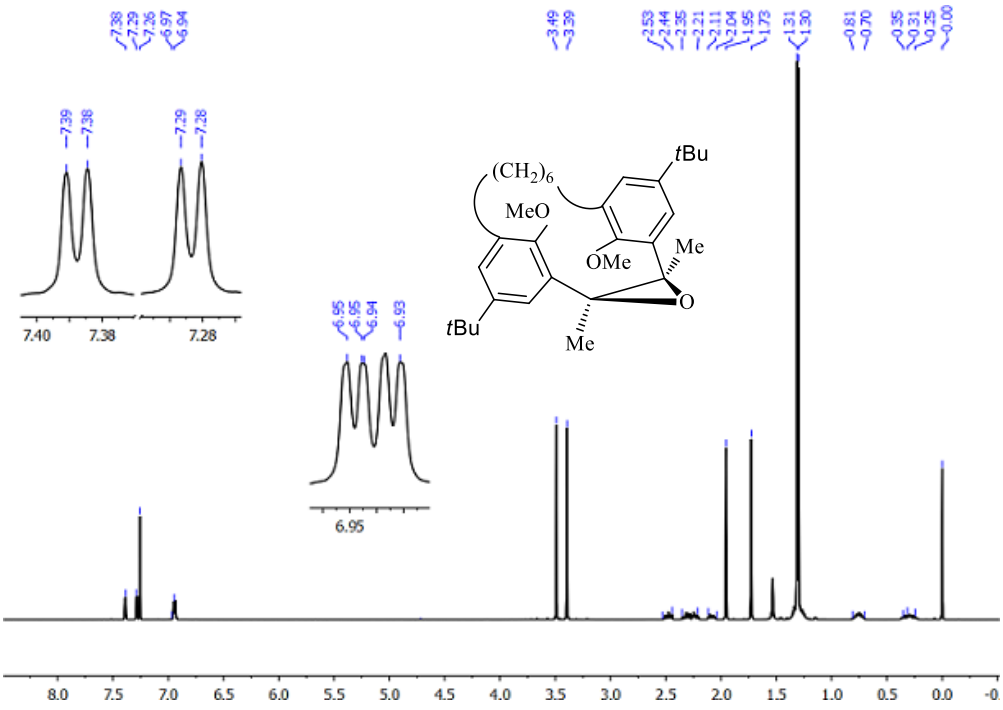


Figure S19. ^{1}H–NMR spectrum of compound *anti*-**5a** (300 MHz, $CDCl_3$, 293 K).

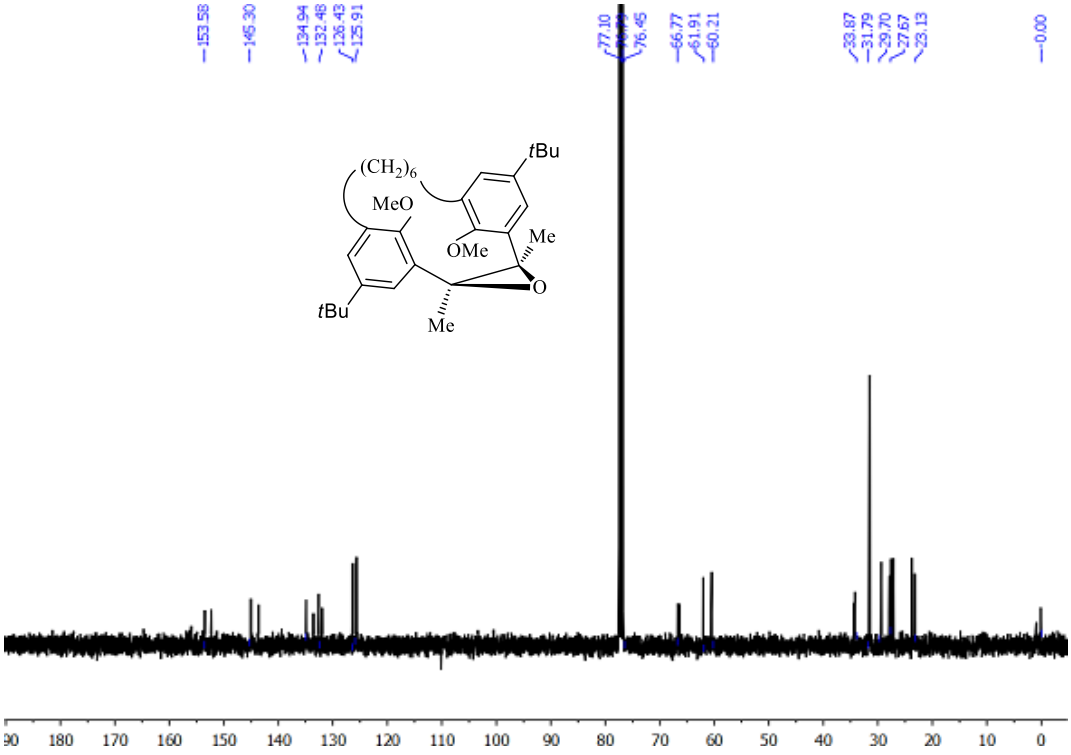


Figure S20. ^{13}C–NMR spectrum of compound *anti*-**5a** (100 MHz, $CDCl_3$, 293 K).

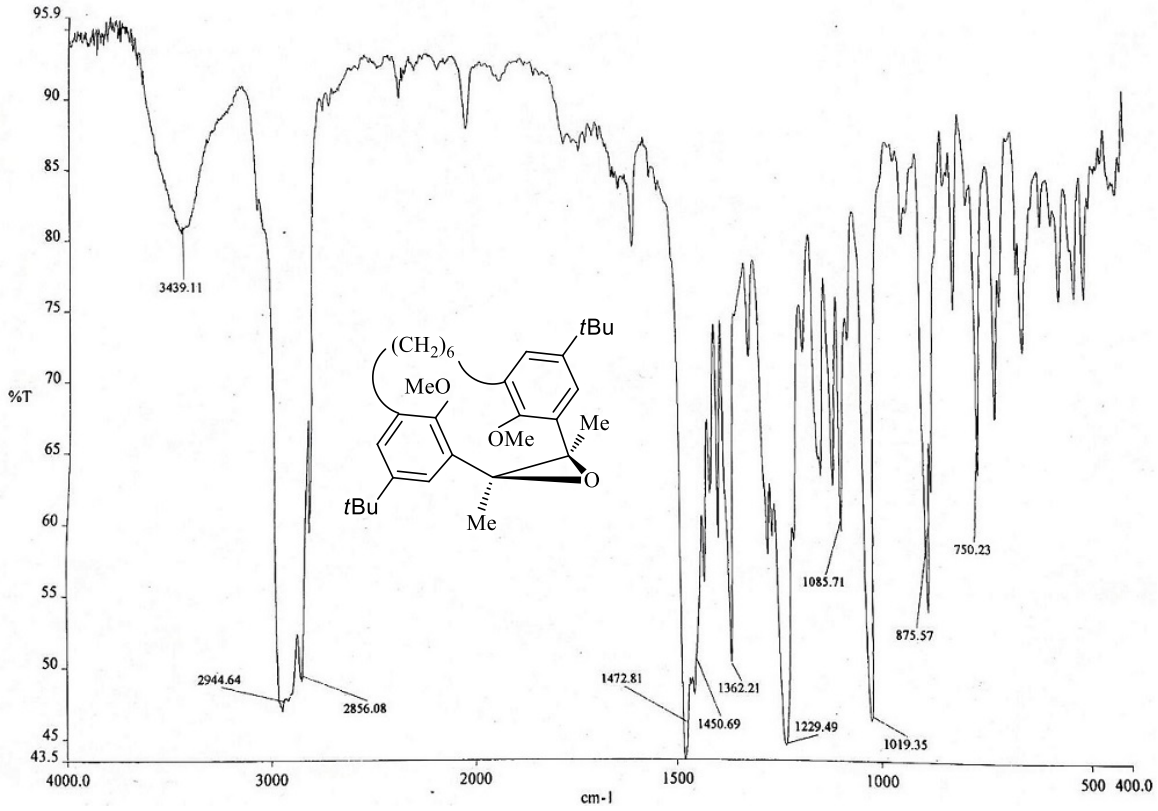


Figure S21. IR spectrum of compound *anti*-**5a**.

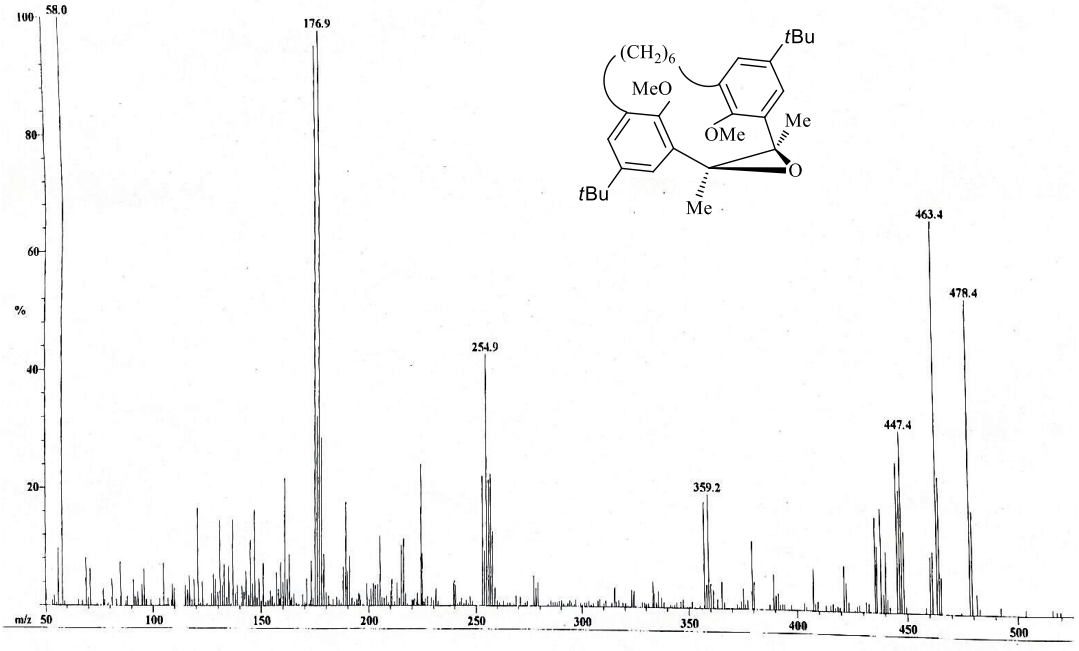


Figure S22. Mass spectrum of compound *anti*-**5a**.

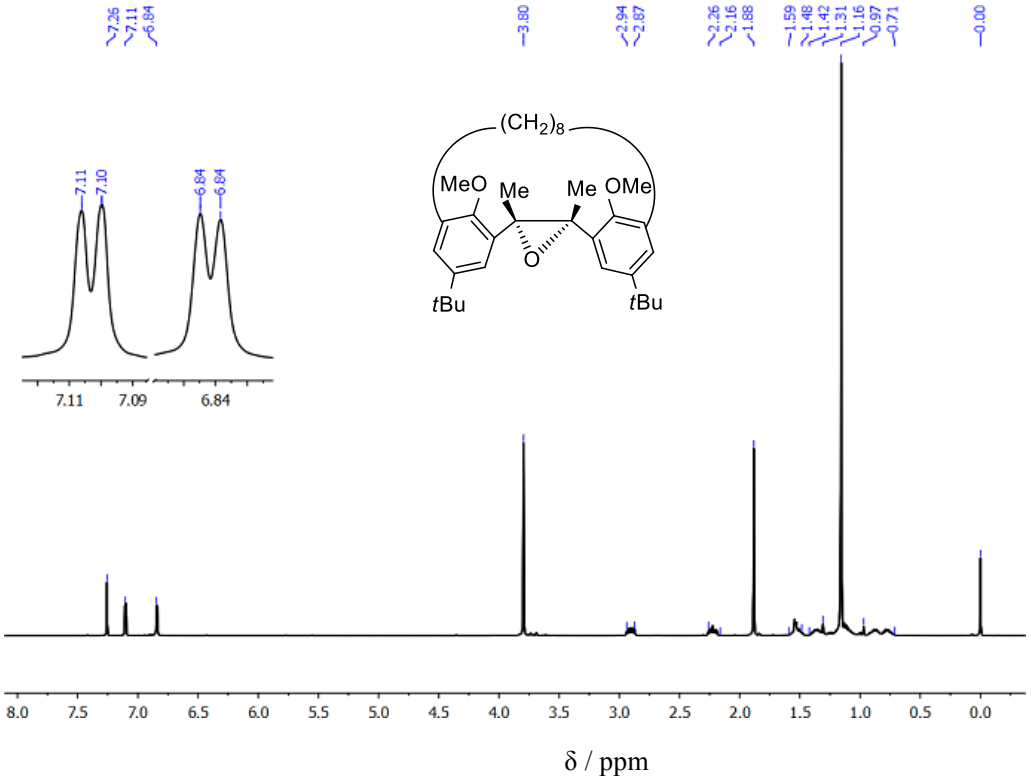


Figure S23. ^{1}H–NMR spectrum of compound *syn*-**5b** (300 MHz, $CDCl_3$, 293 K).

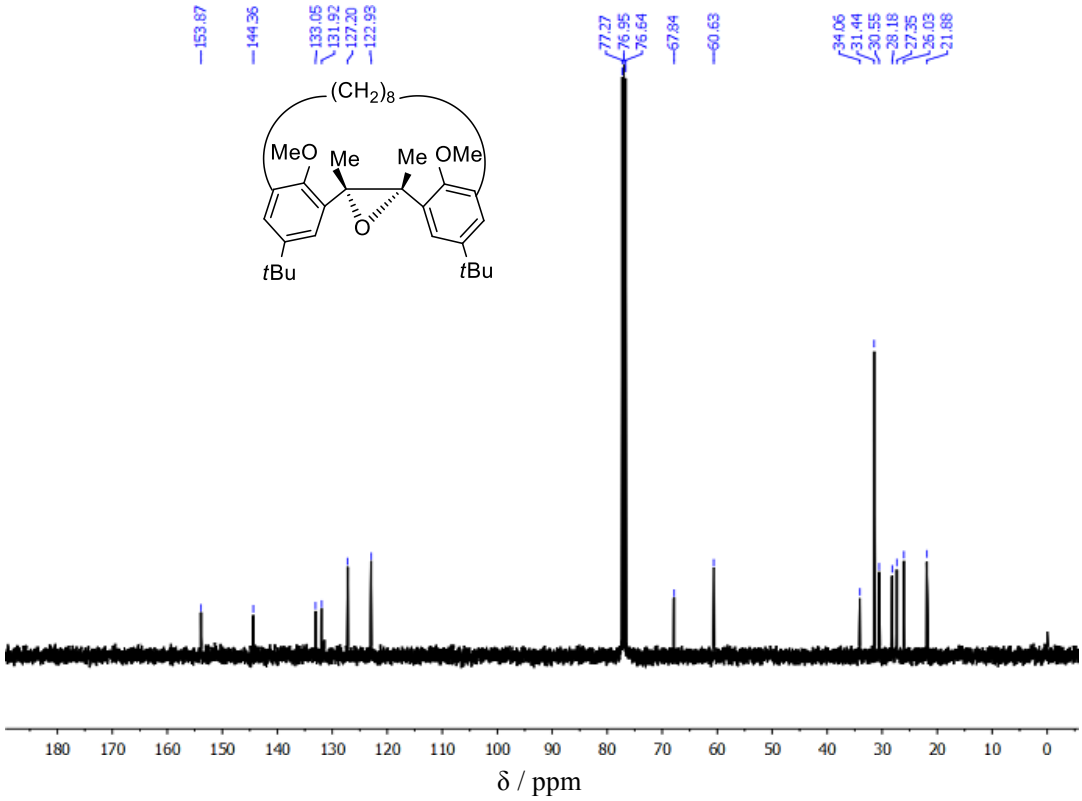


Figure S24. ^{13}C–NMR spectrum of compound *syn*-**5b** (100 MHz, $CDCl_3$, 293 K).

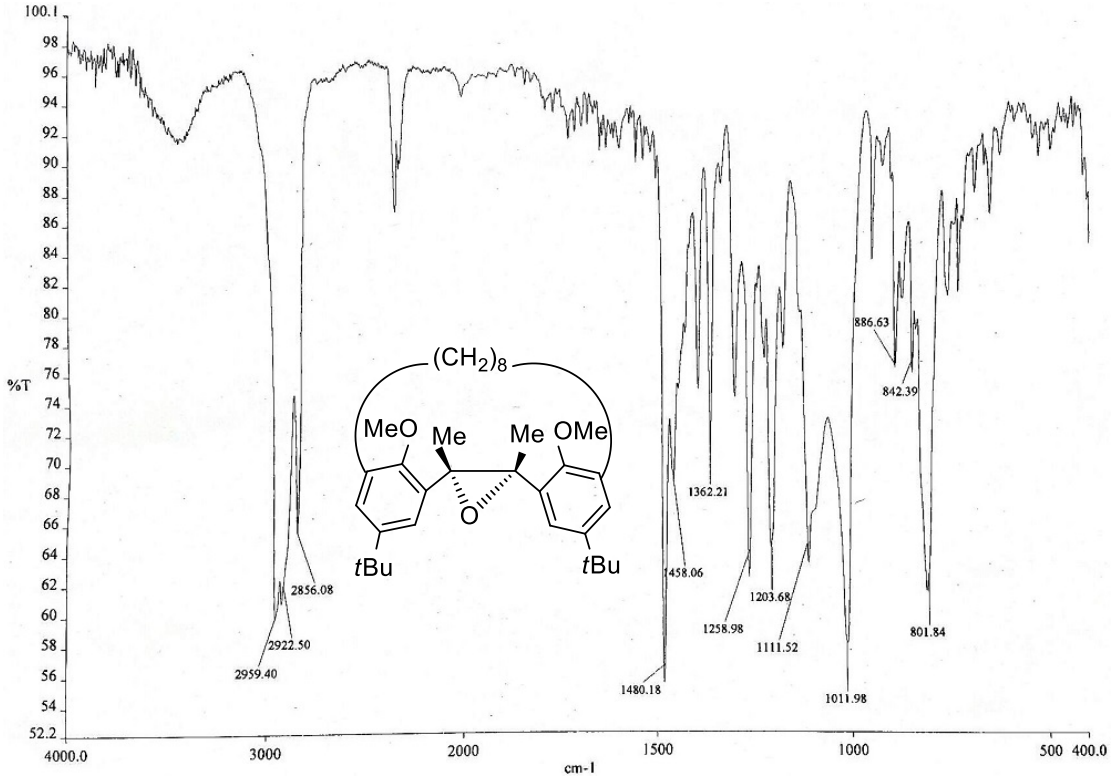


Figure S25. IR spectrum of compound *syn*-**5b**.

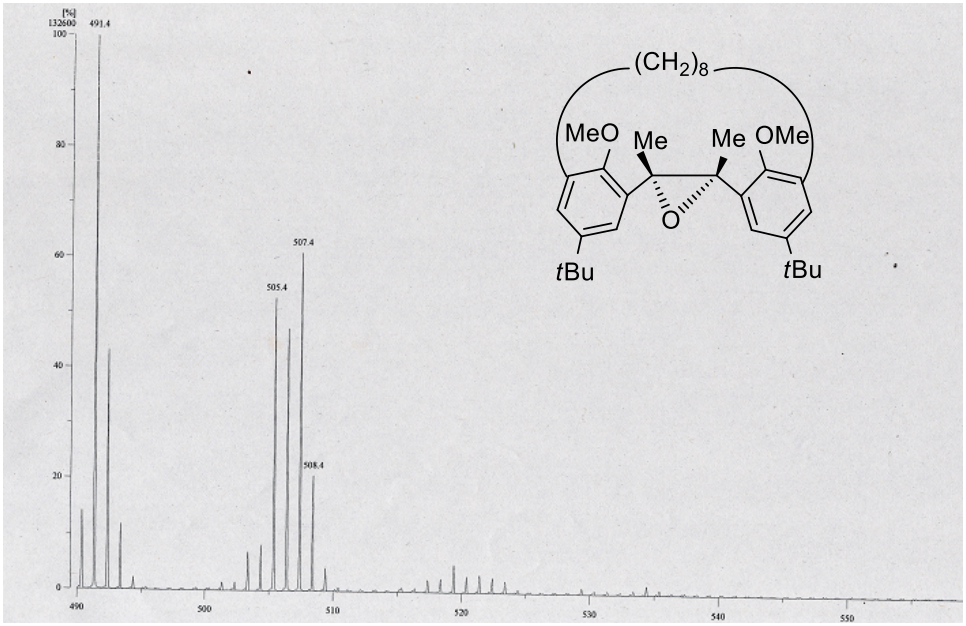


Figure S26. Mass spectrum of compound *syn*-**5b**.

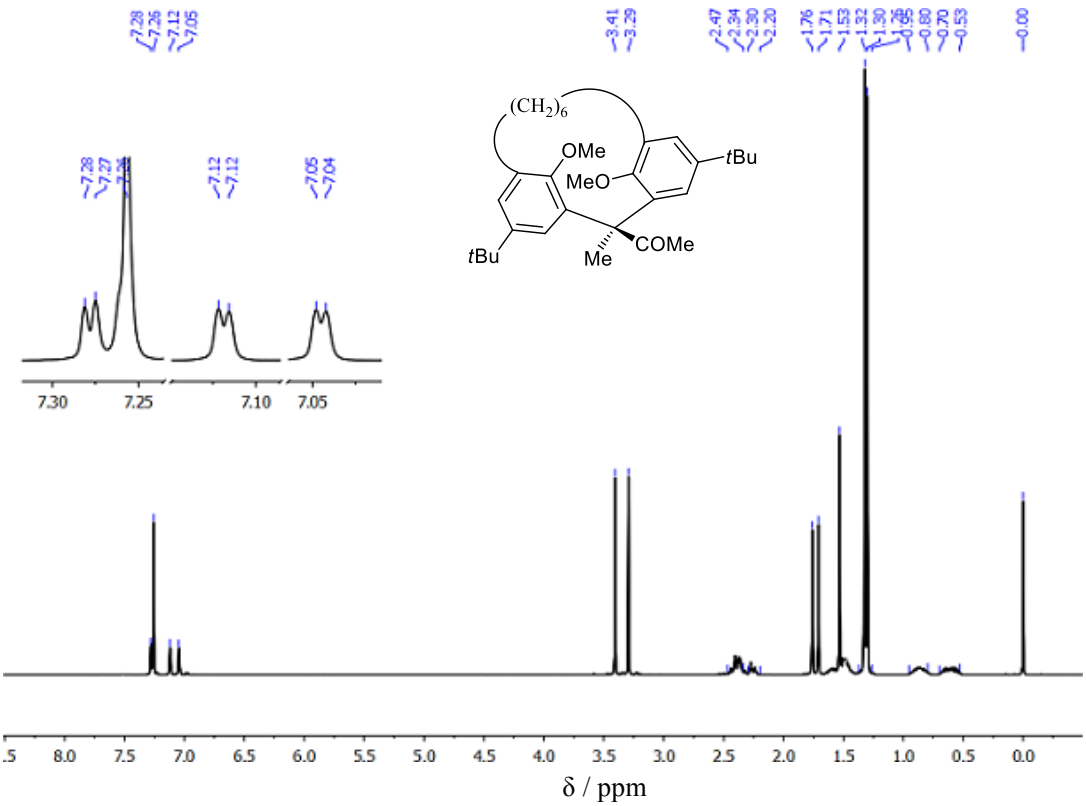


Figure S27. ^{1}H–NMR spectrum of compound *anti*-**6a** (300 MHz, $CDCl_3$, 293 K).

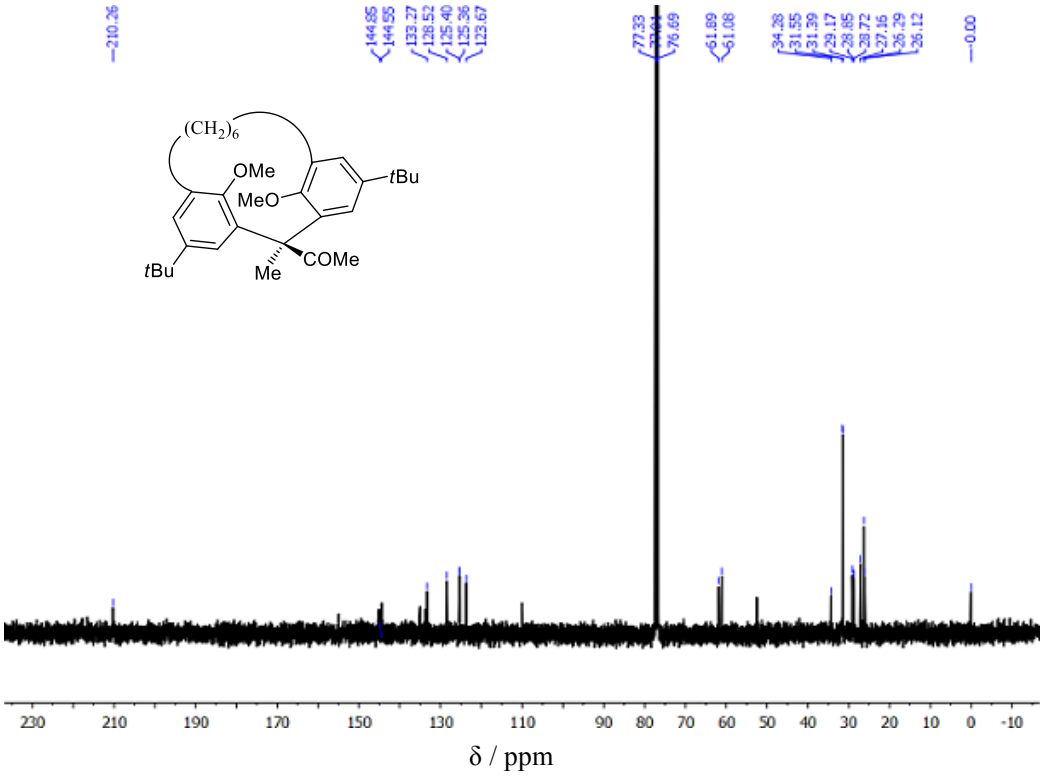


Figure S28. ^{13}C–NMR spectrum of compound *anti*-**6a** (100 MHz, $CDCl_3$, 293 K).

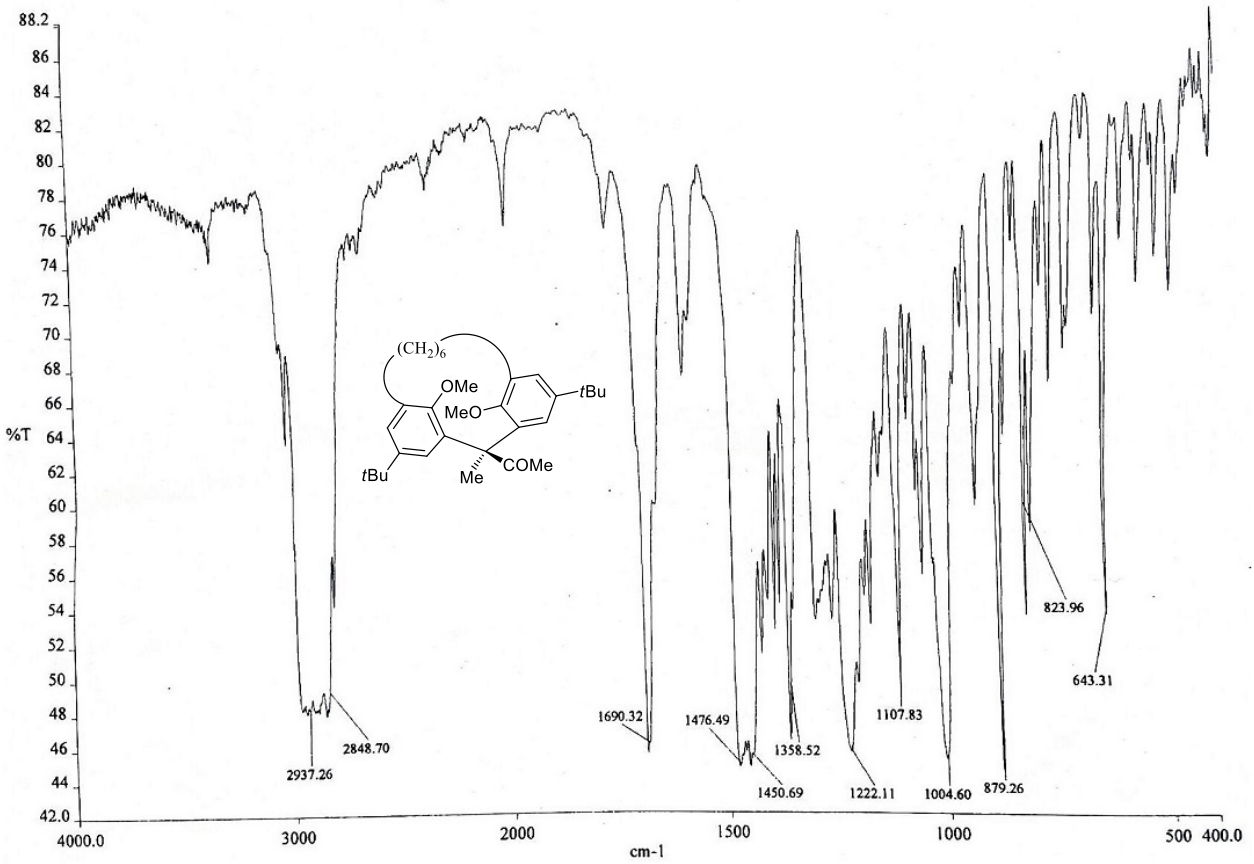


Figure S29. IR spectrum of compound *anti*-**6a**.

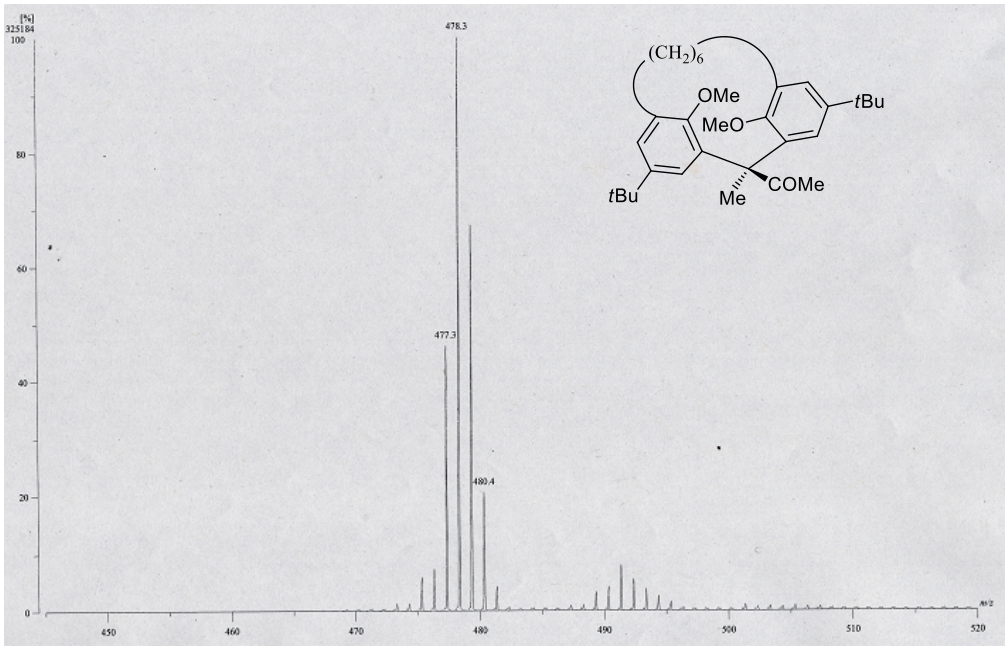


Figure S30. Mass spectrum of compound *anti*-**6a**.

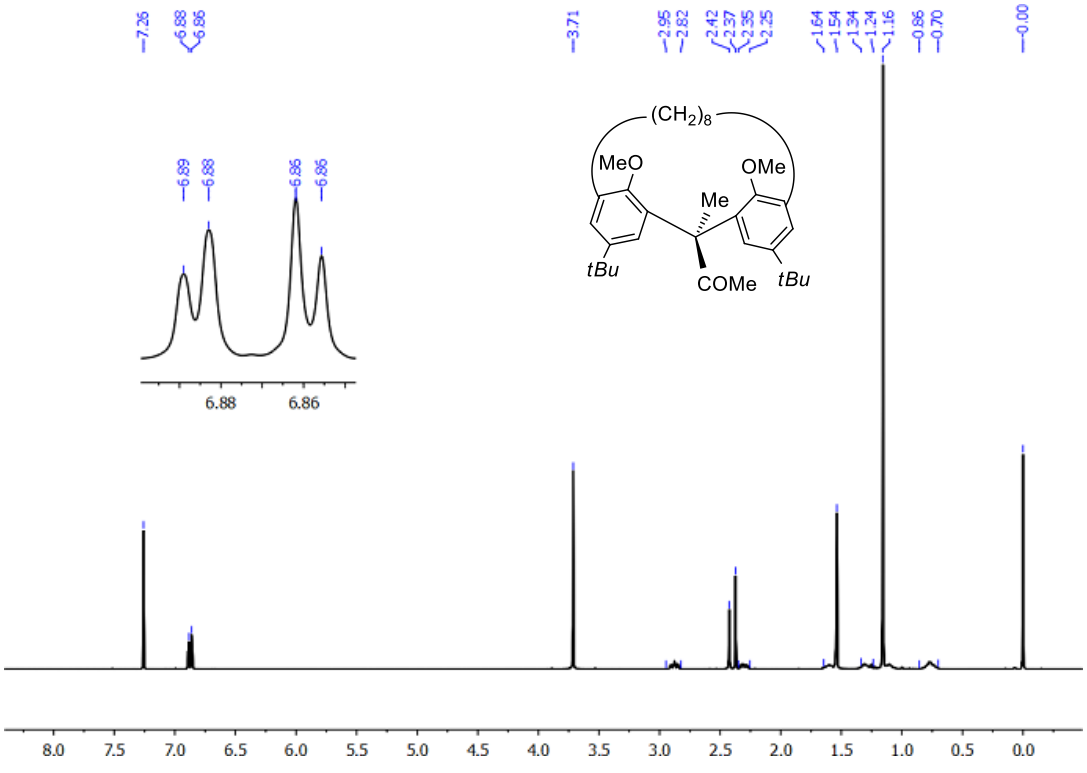


Figure S31. ^{1}H–NMR spectrum of compound *syn*-**6b** (300 MHz, $CDCl_3$, 293 K).

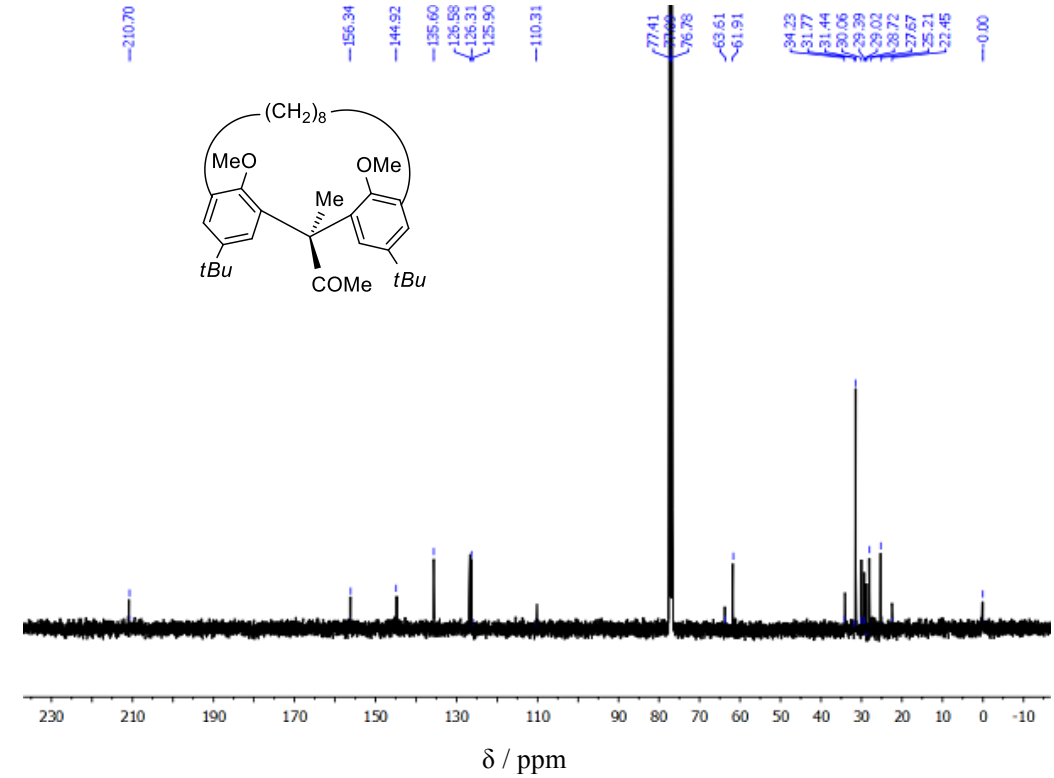


Figure S32. ^{13}C–NMR spectrum of compound *syn*-**6b** (100 MHz, $CDCl_3$, 293 K).

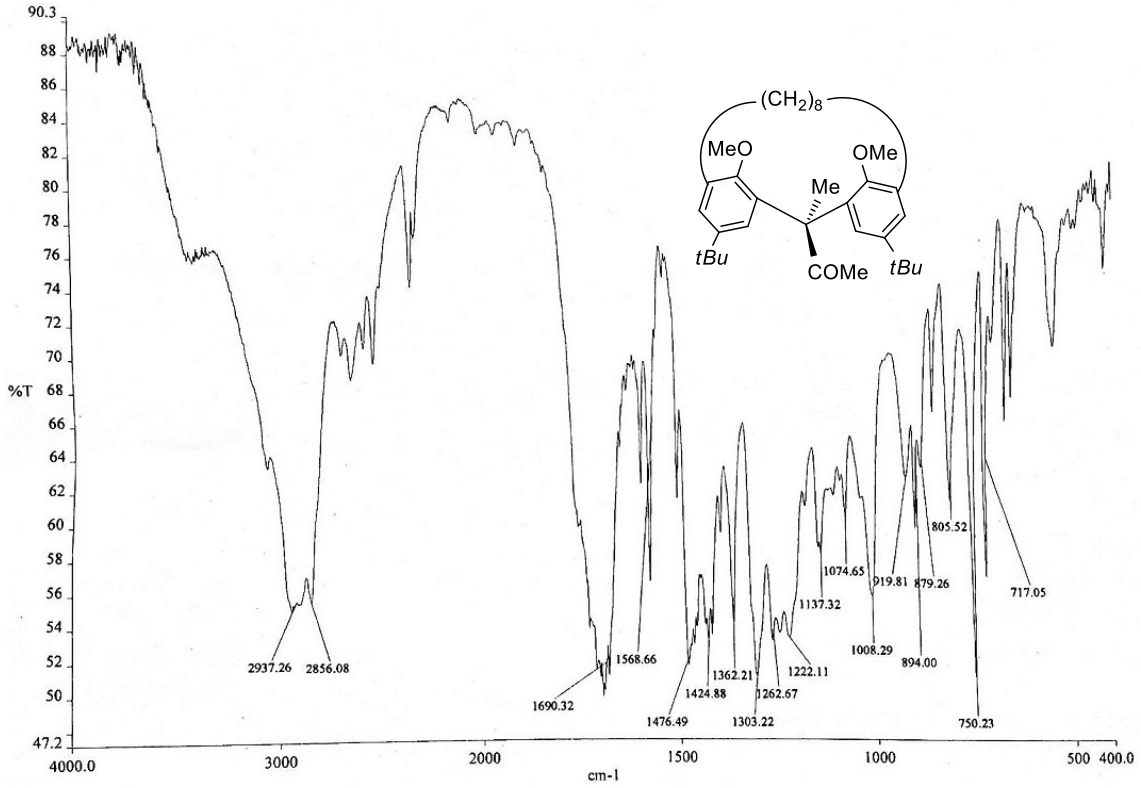


Figure S33. IR spectrum of compound *syn*-**6b**.

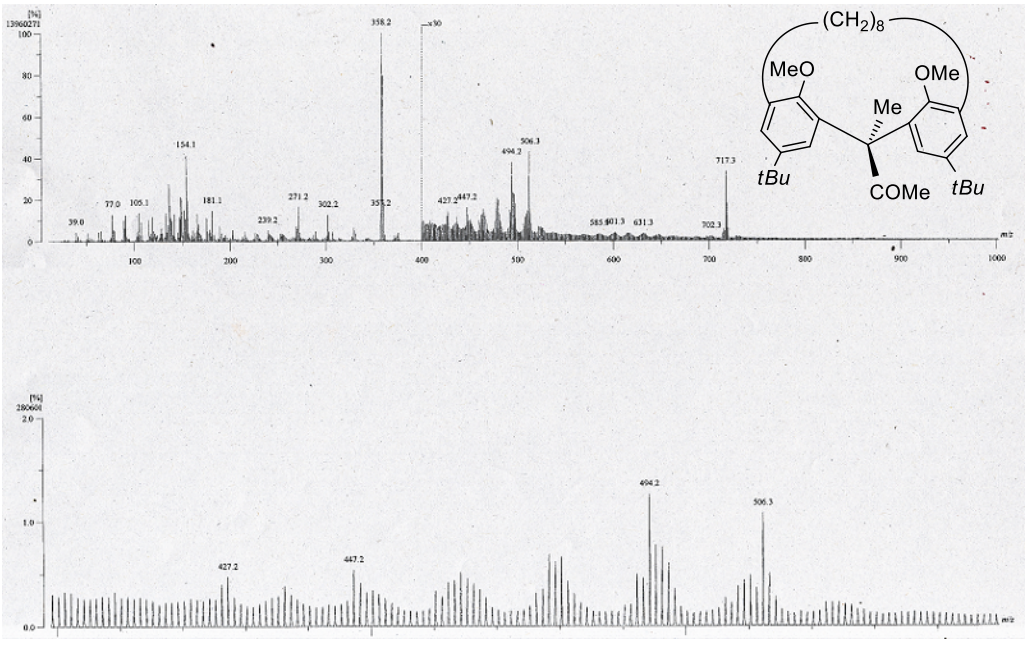
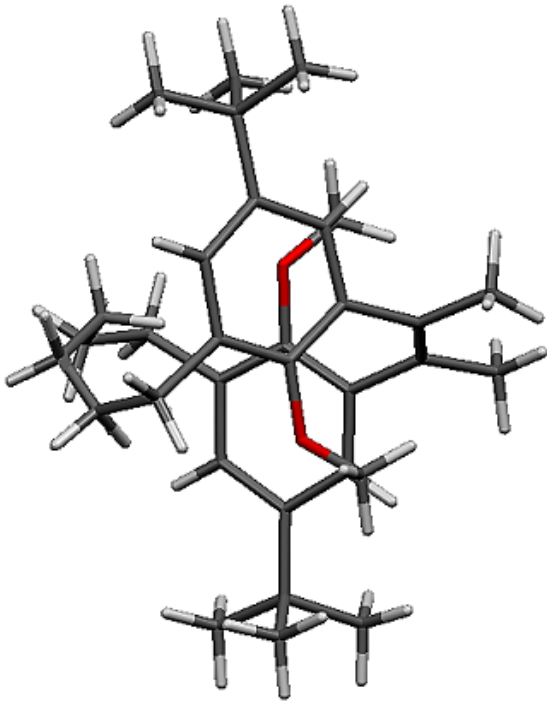
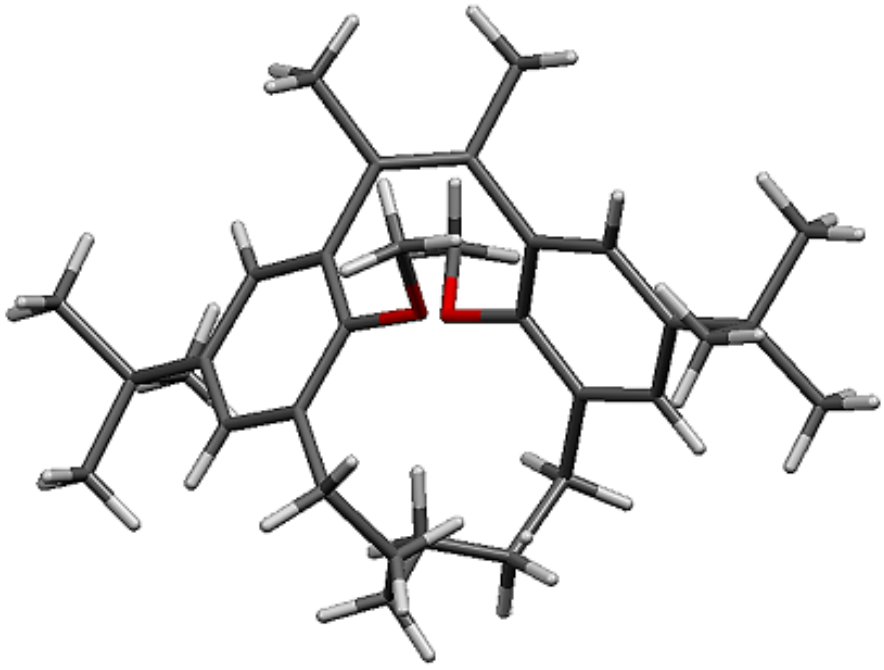


Figure S34. Mass spectrum of compound *syn*-**6b**.

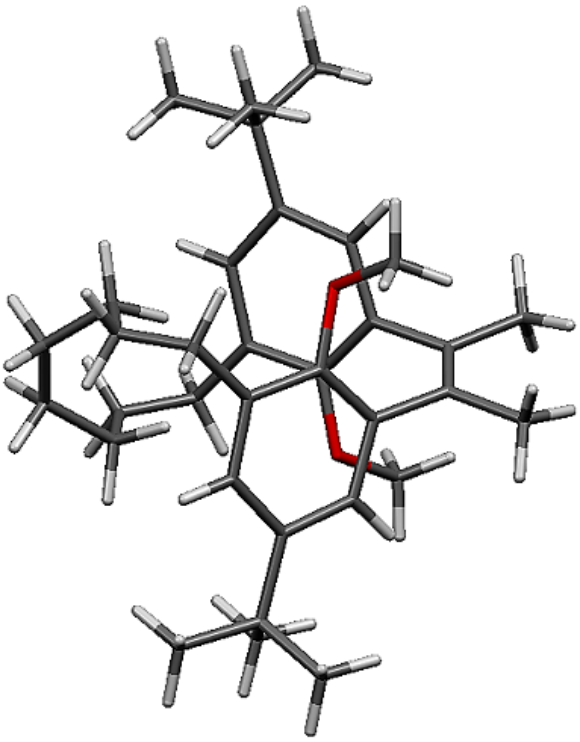


Top view

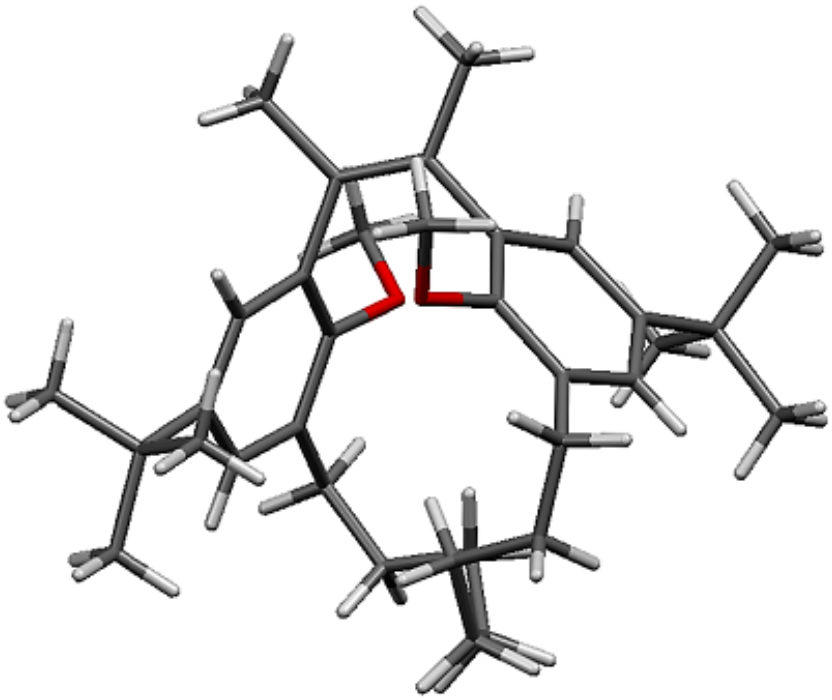


Side view

Figure S35. X-ray Crystallography of *anti*-**4a**.

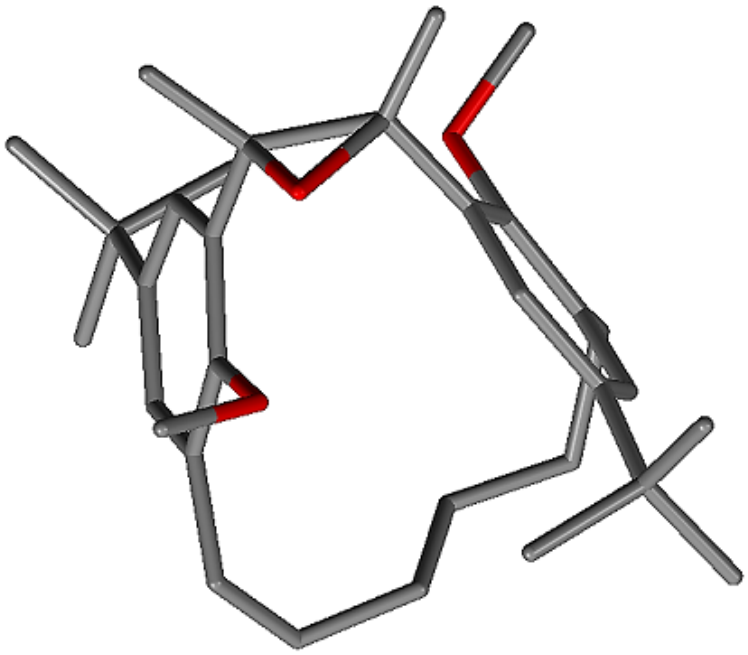


Top view

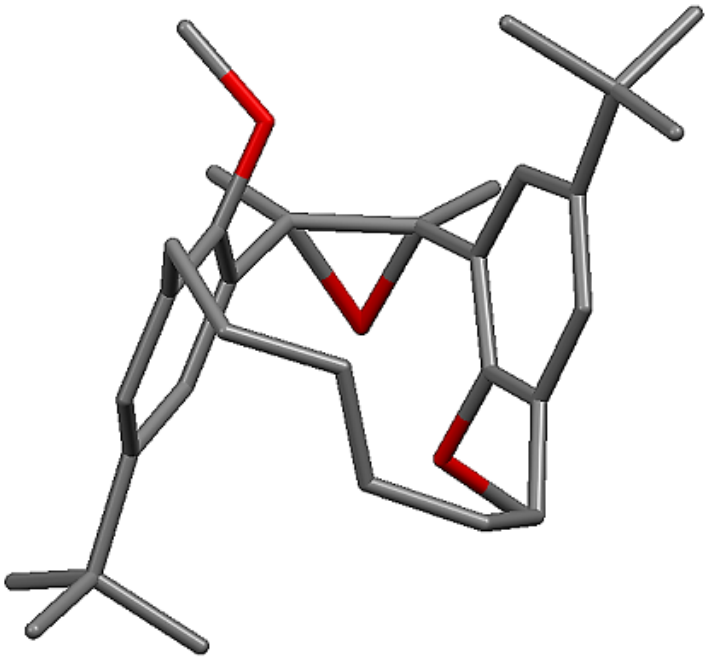


Side view

Figure S36. X-ray Crystallography of *anti*-**4b**.

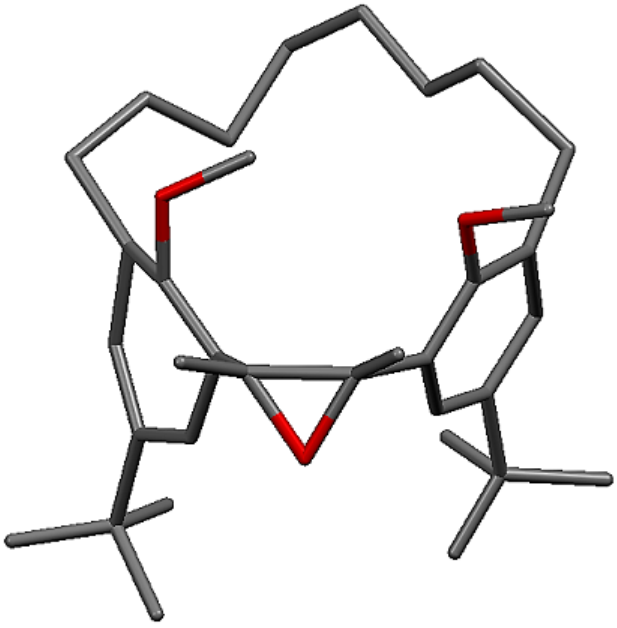


Top view

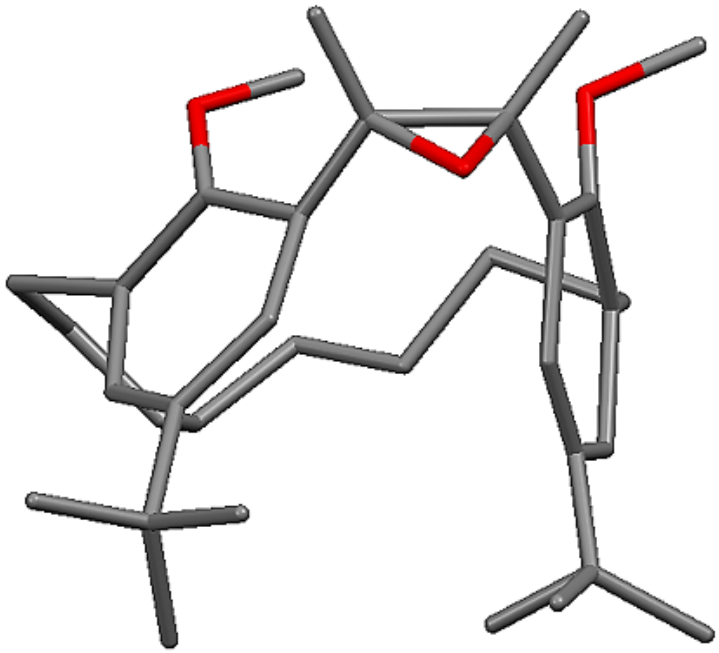


Side view

Figure S37. X-ray Crystallography of *anti*-**5a**.



Top view



Side view

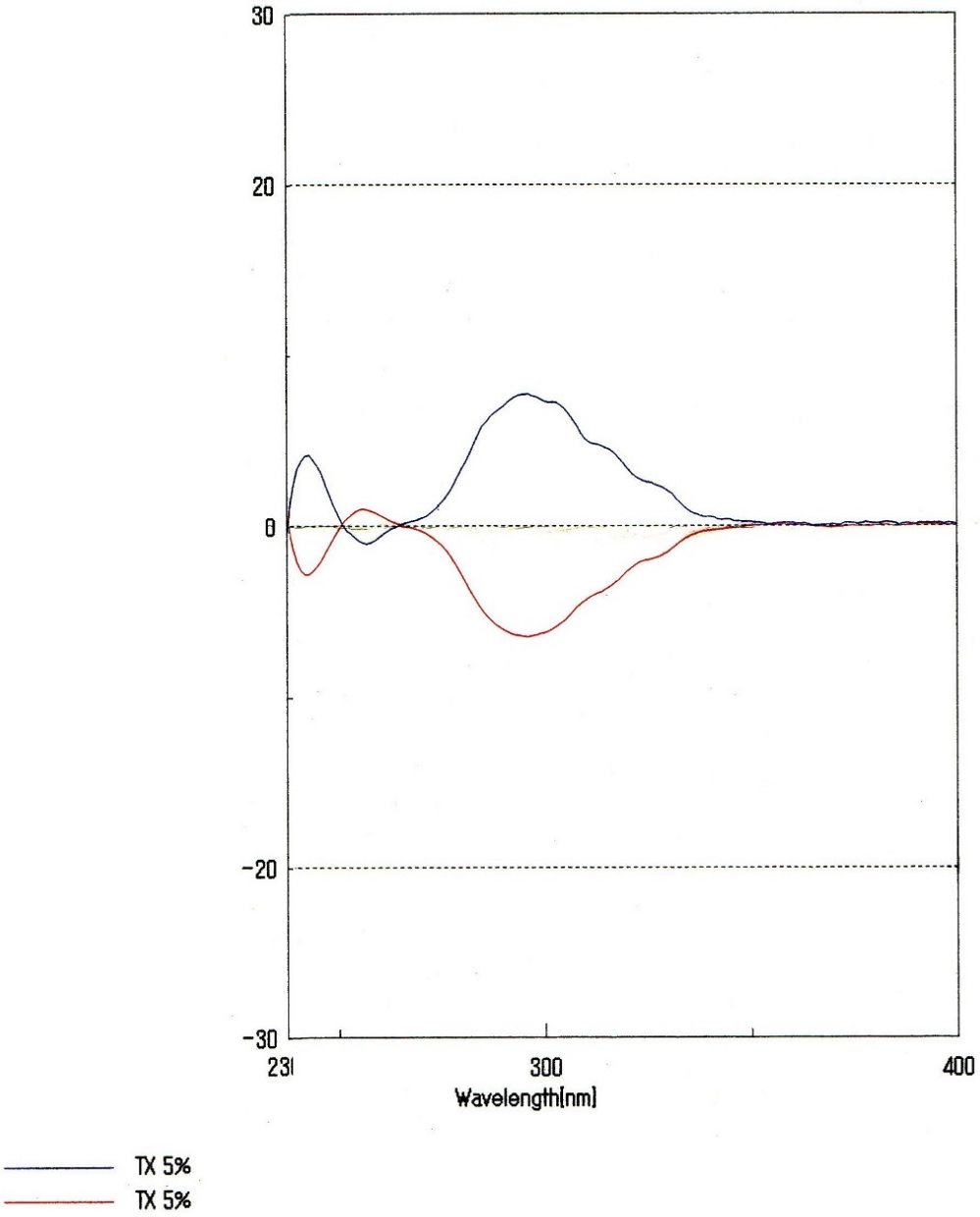
Figure S38. X-ray Crystallography of *syn*-**5b**.

Table S1. X-ray crystal structure of compounds *anti*-**4a**, *anti*-**4b**, *anti*-**5a** and *syn*-**5b**.

Parameter	*anti*-**4a**	*anti*-**4b**	*anti*-**5a**	*syn*-**5b**
Empirical formula	$C_{32}H_{46}O_2$	$C_{34}H_{50}O_2$	$C_{32}H_{46}O_3$	$C_{34}H_{50}O_3$
Formula weight	462.71	490.77	478.71	506.76
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	*P* $2_1/n$	*C 2/c*	*C 2/c*	*P* $2_1/n$
a[Å]	10.8892(5)	18.5100(18)	18.0647(12)	9.879(3)
b[Å]	14.5980(6)	11.9741(12)	10.9779(8)	36.171(5)
c[Å]	17.6382(8)	14.7028(15)	15.0137(10)	17.228(4)
α[°]	90.0000	90.0000	90.0000	90.0000
β[°]	91.421(6)	113.069(8)	109.868(8)	89.9800(2)
γ[°]	90.0000	90.0000	90.0000	90.0000
Volume[$Å^3$]	2802.9(2)	2998.1(6)	2800.2(4)	6156(2)
Z	4	4	4	10
Dcalcd[Mg/m^3]	1.096	1.087	1.135	1.367
Temperature [K]	100	100	100	123
Unique reflns	5100	2748	2566	5711
Obsd reflns	2895	1242	1445	5711
Parameters	335	192	168	385
R(int)	0.1036	0.1471	0.1450	0.0300
$R[I > 2\sigma(I)]$[a]	0.0655	0.0757	0.0649	0.0427
*wR*2[all data][b]	0.2843	0.3461	0.4263	0.5100
GOF on F^2	1.033	1.371	1.417	1.519
CCDC Number	1526807	1526816	1526819	1526822

[a] Conventional R on F_{hkl}: $\Sigma||F_o| - |F_c||/\sigma|F_o|$.

[b] Weighted R on $|F_{hkl}|^2$: $\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$



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Sample :	TPPS at pH3
Cell Length :	1 cm
Concentration :	0.0002 M
Solvent :	100 mM acetate buffer pH3
Temperature :	Room Temp.
Operator :	Nattakarn
Organization :	Saga University
Comment :	TX 5%

Figure S39. HPLC chromatogram of *anti*-**6a**.

General description for the DFT computational study

Density functional theory (DFT) computational studies were carried out to determine the geometry-optimized energies of compounds **5-6**. The starting structures were generated with the initial geometries based upon the X-ray structures. The DFT level of theory using the popular B3LYP (Becke, three-parameter, Lee-Yang-Parr)[1] exchange-correlation functional with the 6-31G(d) basis set. The individual geometry-optimized structures of these molecules were first conducted in the gas phase and then in solvent (chloroform) with the B3LYP/6-31G(D) basis set using Gaussian-*09*.[2]

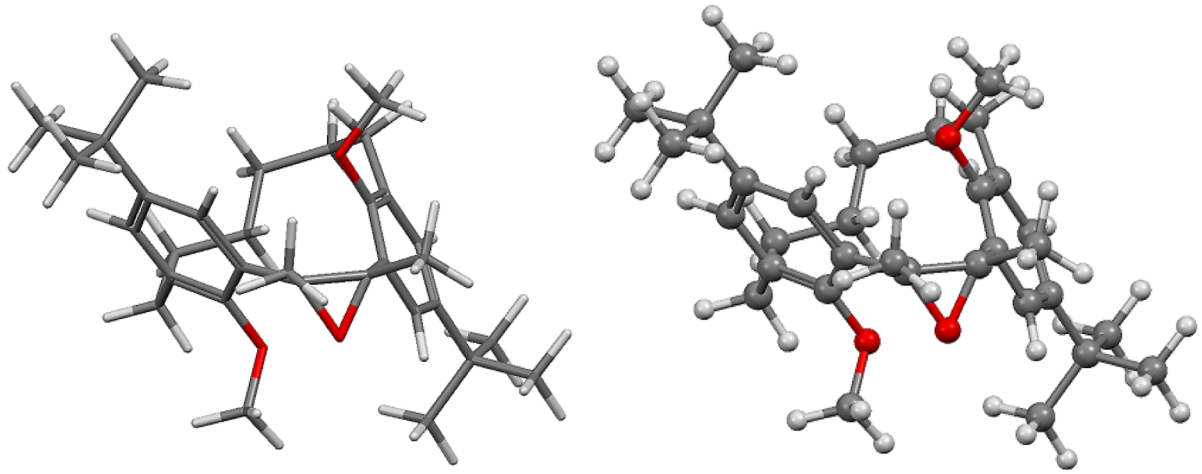

Figure S40. Geometry-optimized structure of *anti*-conformation of **5a** (in gas phase) of: *Left*: Ellipsoid *anti*-conformation of **5a** and *Right*: Ball-and-stick *anti*-conformation of **5a** in gas phase. Colour code: hydrogen = white, carbon = dark grey and oxygen atom = red.

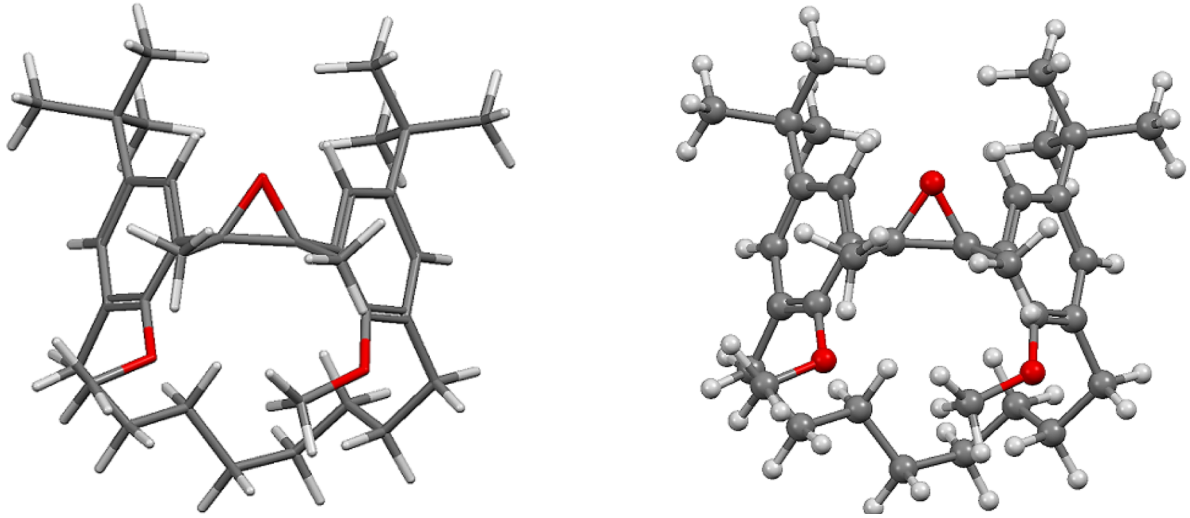

Figure S41. Geometry Geometry-optimized structure of *syn*-conformation of **5b** (in gas phase) of: *Left*: Ellipsoid *syn*-conformation of **5b** and *Right*: Ball-and-stick *syn*-conformation of **5b** in gas phase. Colour code: hydrogen = white, carbon = dark grey and oxygen atom = red.

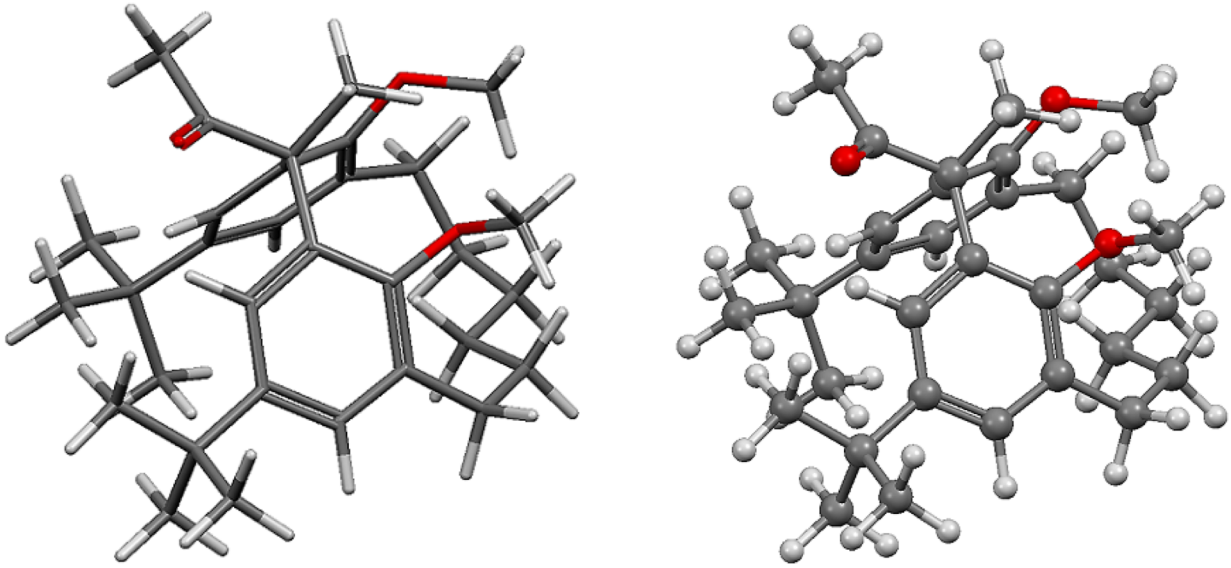

Figure S42. Geometry Geometry-optimized structure of *anti*-conformation of **6a** (in gas phase) of: *Left*: Ellipsoid *anti*-conformation of **6a** and *Right*: Ball-and-stick *anti*-conformation of **6a** in gas phase. Colour code: hydrogen = white, carbon = dark grey and oxygen atom = red.

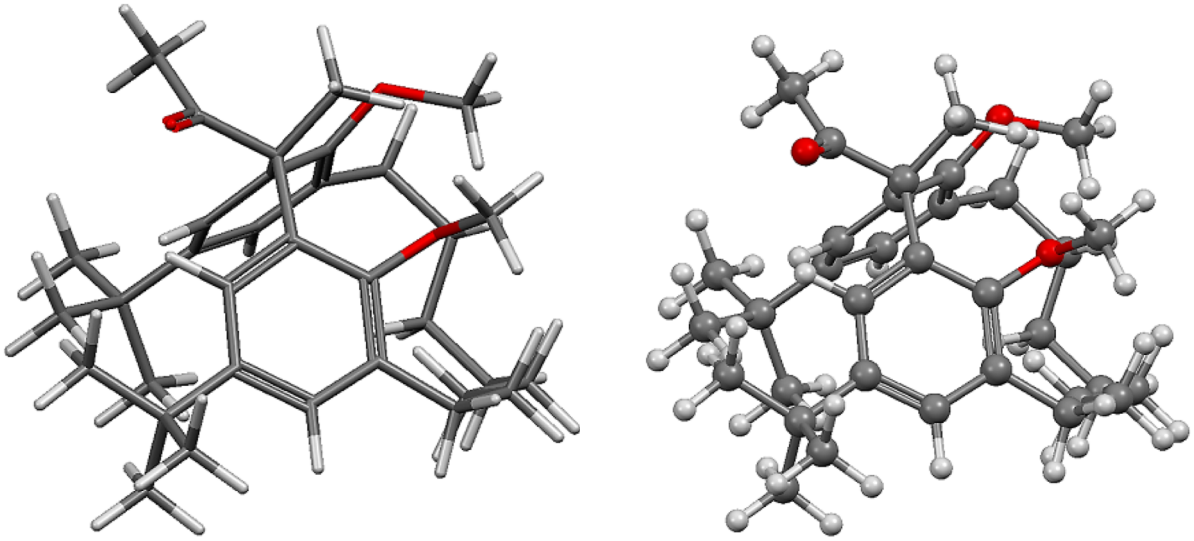

Figure S43. Geometry Geometry-optimized structure of *syn*-conformation of **6b** (in gas phase) of: *Left*: Ellipsoid *syn*-conformation of **6b** and *Right*: Ball-and-stick *syn*-conformation of **6b** in gas phase. Colour code: hydrogen = white, carbon = dark grey and oxygen atom = red.

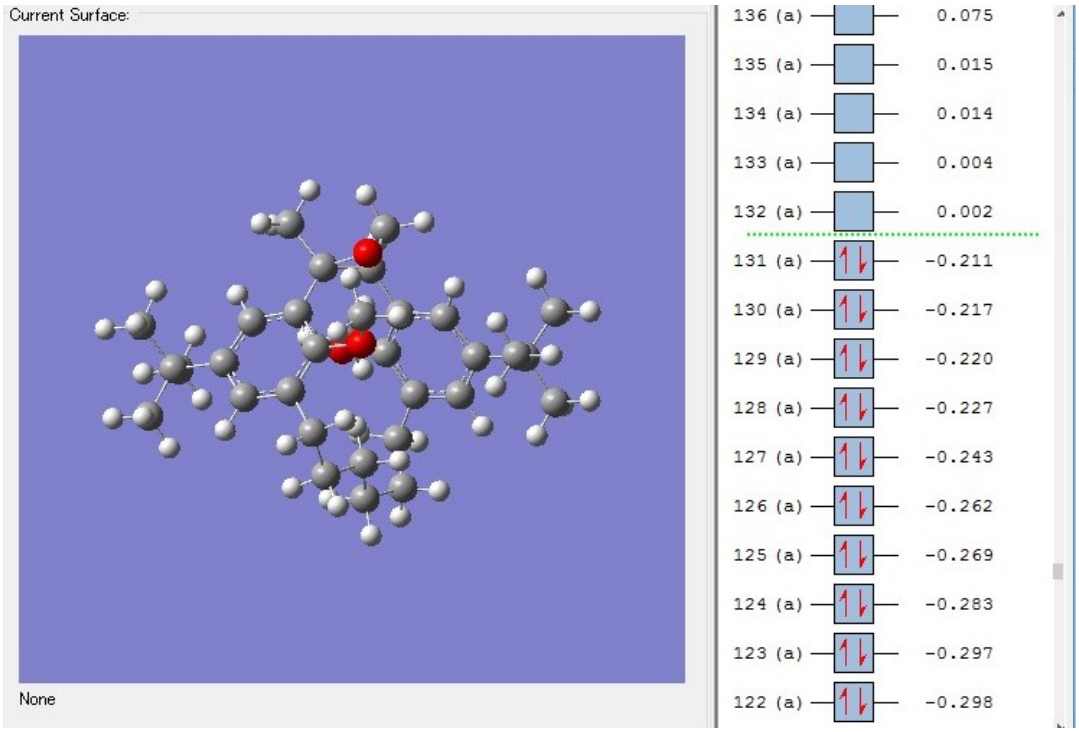

Figure S44. Computed molecular orbital plots (B3LYP/6–31G*) of *anti*-**5a**: the HOMO levels and the LUMO levels.

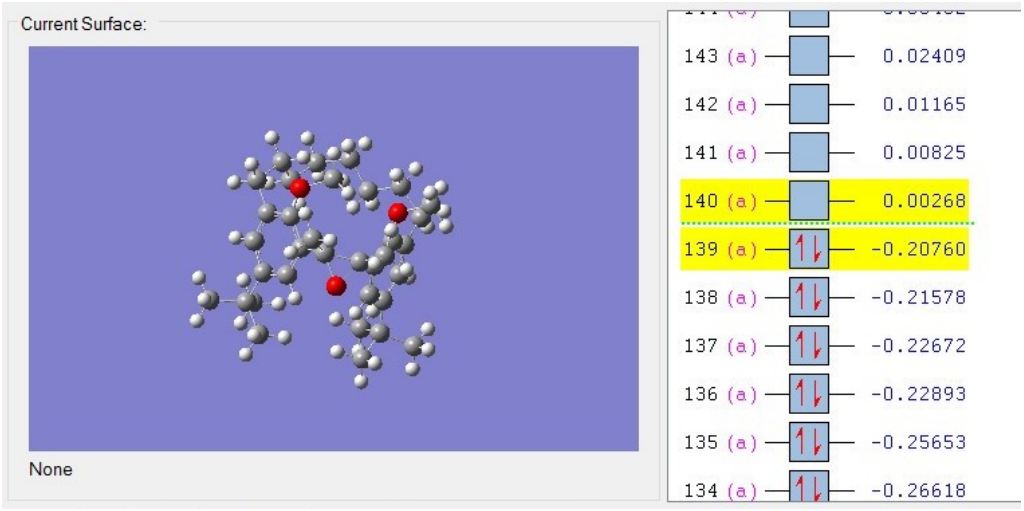

Figure S45. Computed molecular orbital plots (B3LYP/6–31G*) of *syn*-**5b**: the HOMO levels and the LUMO levels.

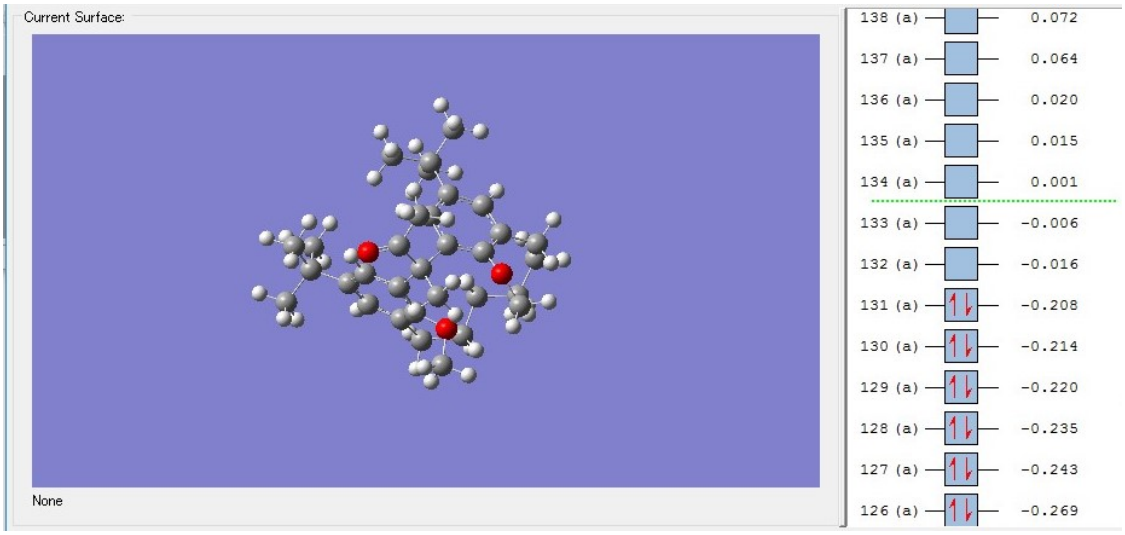

Figure S46. Computed molecular orbital plots (B3LYP/6–31G*) of *anti*-**6a**: the HOMO levels and the LUMO levels.

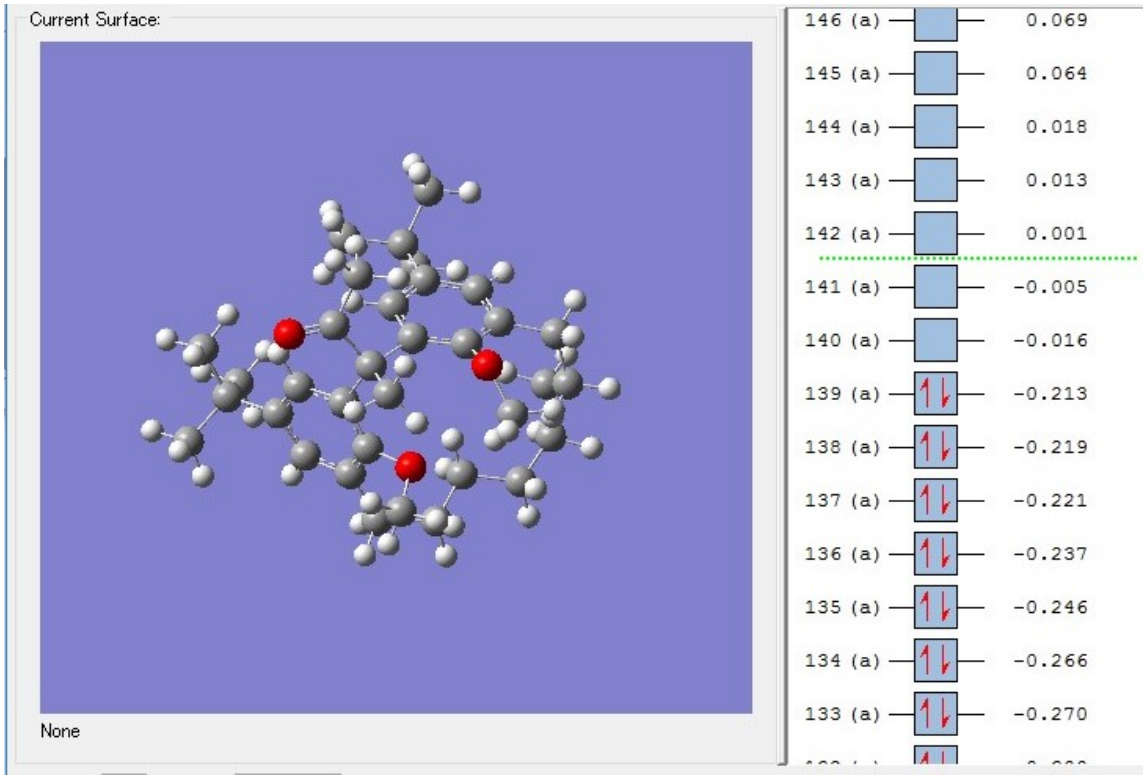

Figure S47. Computed molecular orbital plots (B3LYP/6–31G*) of *syn*-**6b**: the HOMO levels and the LUMO levels.

Table S2. The xyz file for the structure shown in **Figure S40** is given below.

81
3D

C	-0.787600	2.541100	0.206300
C	-1.723800	3.730100	-0.023100
H	-2.513900	3.741500	0.734000
H	-2.200500	3.705400	-1.009100
H	-1.163400	4.661900	0.064000
C	-1.495400	1.273000	0.642100
C	-0.979100	0.300400	1.526800
O	0.262800	0.439200	2.112900
C	0.270800	1.195200	3.321100
H	-0.392300	0.746100	4.074200
H	-0.024700	2.234000	3.141400
H	1.300400	1.175000	3.687300
C	-1.697300	-0.880400	1.786400
C	-2.965000	-1.048500	1.217100
H	-3.504100	-1.961900	1.448100
C	-3.529200	-0.098200	0.365500
C	-2.760900	1.038300	0.086600
H	-3.160200	1.772300	-0.603600
C	-4.919200	-0.262100	-0.276900
C	-5.613100	-1.567300	0.157500
H	-6.599700	-1.636600	-0.314800
H	-5.762300	-1.607300	1.242600
H	-5.041100	-2.452900	-0.141500
C	-4.778000	-0.282600	-1.817400
H	-4.331700	0.642600	-2.196900
H	-5.760800	-0.398600	-2.291500
H	-4.142100	-1.114800	-2.139800
C	-5.824800	0.921900	0.137900
H	-5.407600	1.884100	-0.177700
H	-5.951800	0.954600	1.226000
H	-6.818000	0.823800	-0.317900
C	-1.087500	-2.025300	2.574100
H	-1.799100	-2.371700	3.335500
H	-0.190100	-1.684300	3.096900
C	-0.727300	-3.215400	1.651100
H	-0.383800	-4.058700	2.266600
H	-1.644900	-3.556200	1.150700
C	0.328000	-2.865000	0.590400
H	1.319600	-2.806200	1.060400
H	0.121400	-1.862400	0.207300
C	0.358300	-3.846100	-0.588900
C	1.410800	-3.552500	-1.674200
C	1.264500	-2.198600	-2.413000
C	1.741100	-0.969400	-1.651900
C	0.946300	0.186400	-1.543100
O	-0.274300	0.276800	-2.198000
C	-0.191100	0.530400	-3.597600
H	0.306700	-0.285800	-4.136200
H	0.346200	1.465000	-3.806200

H	-1.220300	0.618400	-3.955100
C	1.334000	1.239600	-0.701800
C	0.527200	2.505100	-0.513100
C	0.917300	3.594900	-1.503200
H	0.708100	3.271700	-2.528700
H	1.994500	3.783500	-1.430600
H	0.392900	4.534500	-1.322800
O	0.438400	2.933900	0.860600
C	2.563600	1.164300	-0.045800
C	3.430700	0.077500	-0.204600
C	2.986100	-0.976800	-1.008700
H	3.610800	-1.854600	-1.130200
C	4.790100	0.066700	0.519000
C	5.617600	-1.192200	0.198100
H	6.579600	-1.145100	0.721200
H	5.827900	-1.279600	-0.874200
H	5.111000	-2.108100	0.523000
C	4.557700	0.114300	2.047800
H	4.013200	1.016000	2.346700
H	5.516400	0.108300	2.581500
H	3.974600	-0.751600	2.380800
C	5.614500	1.303300	0.088900
H	5.099100	2.239100	0.328700
H	5.803000	1.292300	-0.991000
H	6.583700	1.315100	0.602800
H	2.829700	1.984400	0.614000
H	1.820100	-2.271500	-3.359900
H	0.211800	-2.063600	-2.682800
H	1.344700	-4.347000	-2.430000
H	2.416000	-3.637700	-1.242100
H	0.527000	-4.867400	-0.215900
H	-0.636800	-3.858300	-1.059000

Table S3. The xyz file for the structure shown in **Figure S41** is given below.

87
3D

C	-0.345300	-0.234600	2.813300
O	0.302200	-1.517800	2.921900
C	1.141600	-0.396300	2.590900
C	2.140600	-0.042900	3.687000
H	2.351100	1.029100	3.709500
H	3.083400	-0.571900	3.508500
H	1.766700	-0.354000	4.663800
C	1.731300	-0.465000	1.193800
C	2.359500	0.632200	0.582000
O	2.419000	1.823800	1.293700
C	3.716000	2.304200	1.647900
H	4.400100	1.477500	1.870300
H	3.587800	2.917000	2.544800
H	4.148400	2.928700	0.858100
C	2.852500	0.537900	-0.735500

C	3.389200	1.727600	-1.515500
C	2.409900	2.907800	-1.698000
C	1.090800	2.540200	-2.391000
C	0.193700	3.763600	-2.634700
C	-1.176700	3.449200	-3.264200
C	-2.134100	2.603900	-2.403100
C	-2.579700	3.282300	-1.100200
C	-3.508300	2.419400	-0.214700
C	-2.895500	1.113100	0.249900
C	-1.925500	1.089700	1.272100
O	-1.704500	2.293400	1.919000
C	-0.395400	2.858200	1.884200
H	0.015800	2.848200	0.870400
H	0.300200	2.333000	2.542300
H	-0.506200	3.891600	2.224700
C	-1.326700	-0.123600	1.661400
C	-1.760000	-1.308600	1.045400
C	-2.751400	-1.329200	0.061600
C	-3.289600	-0.094500	-0.326100
H	-4.054500	-0.058900	-1.098300
C	-3.273800	-2.627400	-0.581400
C	-2.602000	-3.883200	0.003300
H	-3.008300	-4.779800	-0.478900
H	-2.779500	-3.975600	1.080600
H	-1.519500	-3.880600	-0.163600
C	-3.004800	-2.595800	-2.104200
H	-3.377800	-3.511500	-2.579600
H	-1.931000	-2.518200	-2.310500
H	-3.497400	-1.744900	-2.586500
C	-4.797500	-2.747200	-0.337100
H	-5.186600	-3.665700	-0.793800
H	-5.347900	-1.903300	-0.765900
H	-5.020000	-2.780100	0.735600
H	-1.308100	-2.229000	1.390400
H	-3.804100	3.015600	0.655400
H	-4.425000	2.194400	-0.775400
H	-3.105300	4.217800	-1.341200
H	-1.704300	3.570200	-0.508500
H	-3.025200	2.369900	-3.003900
H	-1.670400	1.637400	-2.171000
H	-1.013600	2.930400	-4.219800
H	-1.670800	4.398700	-3.516400
H	0.725300	4.465100	-3.293700
H	0.051500	4.300700	-1.686400
H	0.561300	1.798800	-1.780300
H	1.302500	2.047700	-3.352300
H	2.188000	3.353800	-0.721100
H	2.925000	3.682400	-2.284200
H	3.685700	1.365500	-2.508100

H	4.312100	2.107000	-1.057400
C	2.810300	-0.712400	-1.358300
C	2.284100	-1.857600	-0.745800
C	1.718500	-1.695000	0.521100
H	1.261500	-2.529400	1.036100
C	2.344000	-3.213300	-1.474000
C	1.529700	-3.136000	-2.786800
H	0.478100	-2.904700	-2.582400
H	1.570400	-4.094000	-3.319600
H	1.915600	-2.363400	-3.460300
C	3.816600	-3.551800	-1.809500
H	3.876400	-4.515600	-2.330100
H	4.420600	-3.620500	-0.897400
H	4.273500	-2.795900	-2.456700
C	1.778800	-4.362000	-0.618400
H	2.330200	-4.477900	0.321400
H	1.857200	-5.306200	-1.169300
H	0.721900	-4.210300	-0.374800
H	3.208800	-0.780900	-2.367400
C	-0.916200	0.271000	4.132100
H	-0.174900	0.288300	4.932700
H	-1.725200	-0.404200	4.434500
H	-1.344100	1.268900	4.013900

Table S4. The xyz file for the structure shown in **Figure S42** is given below.

81
3D

C	-0.172800	-0.301000	2.156100
C	0.437400	-1.315600	3.167300
H	1.102200	-2.019100	2.683000
H	-0.387800	-1.862100	3.636600
H	1.004000	-0.803800	3.950200
C	-1.009600	-0.981200	1.029300
C	-0.407900	-1.918900	0.162600
O	0.778700	-2.541300	0.533300
C	0.605600	-3.903600	0.922800
H	0.201100	-4.511400	0.104800
H	-0.062200	-3.984300	1.789500
H	1.596600	-4.279400	1.191600
C	-0.915300	-2.171200	-1.124200
C	-0.159900	-2.963000	-2.189600
C	1.375800	-2.785500	-2.307200
H	1.868800	-3.347300	-1.507700
H	1.682100	-3.267400	-3.247200
C	1.905100	-1.342700	-2.276000
H	1.514100	-0.836000	-1.392000
H	1.525900	-0.781100	-3.142400
C	3.446500	-1.293300	-2.271400
C	4.100100	0.086800	-2.038900

C	4.152700	0.631300	-0.582500
C	2.796400	1.006900	-0.005900
C	2.155300	0.331300	1.060800
O	2.834800	-0.491800	1.933300
C	3.515000	-1.676100	1.530000
H	3.201400	-2.010800	0.541500
H	3.265900	-2.455300	2.259600
H	4.600600	-1.522200	1.551800
C	0.798500	0.599700	1.337900
C	0.185300	1.676500	0.673500
C	0.832200	2.461900	-0.277900
C	2.129100	2.067400	-0.622800
H	2.658900	2.601900	-1.408100
C	0.174900	3.669700	-0.968200
C	-1.254100	3.931400	-0.456100
H	-1.673700	4.808500	-0.961800
H	-1.270800	4.132500	0.621400
H	-1.920800	3.084700	-0.656300
C	0.100300	3.420700	-2.493500
H	-0.366100	4.275400	-2.999000
H	-0.494600	2.527200	-2.714600
H	1.093600	3.277300	-2.931700
C	1.021300	4.936300	-0.697500
H	0.578300	5.807600	-1.195600
H	2.046800	4.826800	-1.065900
H	1.074100	5.149300	0.376400
H	-0.859100	1.869700	0.890800
H	4.679500	-0.082600	0.052100
H	4.782400	1.531200	-0.600100
H	3.608400	0.830900	-2.679900
H	5.140100	0.030400	-2.388700
H	3.807800	-1.678000	-3.236200
H	3.829600	-1.998800	-1.519800
H	-0.613900	-2.693900	-3.151800
H	-0.359100	-4.039300	-2.072500
C	-2.158500	-1.623700	-1.450800
C	-2.887500	-0.831100	-0.556100
C	-2.271900	-0.491900	0.653600
H	-2.777100	0.176600	1.332800
C	-4.293300	-0.331400	-0.940500
C	-4.216400	0.515900	-2.232400
H	-3.575200	1.393300	-2.087300
H	-5.215100	0.869200	-2.517600
H	-3.813500	-0.055500	-3.075300
C	-5.214100	-1.551100	-1.185100
H	-6.221200	-1.220600	-1.468400
H	-5.299800	-2.163300	-0.280000
H	-4.834800	-2.193300	-1.987300
C	-4.933200	0.533500	0.162200
H	-5.023100	-0.011300	1.108200
H	-5.940700	0.835900	-0.145800
H	-4.359300	1.447900	0.351100
H	-2.560100	-1.830500	-2.440200

C	-1.000800	0.570500	3.143000
C	-0.268800	1.698500	3.863300
H	0.811900	1.544500	3.912800
H	-0.436700	2.639400	3.327200
H	-0.690500	1.800500	4.866500
O	-2.153900	0.313800	3.434700

Table S5. The xyz file for the structure shown in **Figure S43** is given below.

87
3D

C	-0.653800	0.308900	2.171600
C	-0.196900	-0.418900	3.470600
H	0.545500	-1.180800	3.272900
H	-1.079400	-0.883000	3.923300
H	0.230300	0.285200	4.190000
C	-1.357800	-0.641700	1.155800
C	-0.742000	-1.823800	0.689200
O	0.382300	-2.322800	1.339200
C	0.123200	-3.473100	2.145600
H	-0.646500	-3.262900	2.897600
H	1.063200	-3.718800	2.647100
H	-0.193700	-4.330700	1.541400
C	-1.191400	-2.486500	-0.470300
C	-0.497600	-3.695600	-1.093500
C	1.043100	-3.725300	-1.208100
C	1.708400	-2.511900	-1.873200
C	3.234300	-2.693300	-1.962800
C	4.021600	-1.530100	-2.597900
C	3.906900	-0.168500	-1.886700
C	4.462600	-0.147400	-0.453700
C	4.156300	1.145700	0.352900
C	2.674600	1.452200	0.442500
C	1.830500	0.884800	1.429100
O	2.369200	0.317100	2.569000
C	3.027900	-0.948400	2.529200
H	2.571400	-1.610800	1.790000
H	2.908400	-1.385400	3.526100
H	4.099100	-0.837900	2.328700
C	0.434100	1.033300	1.328400
C	-0.066500	1.865700	0.308000
C	0.737700	2.527500	-0.614500
C	2.113000	2.273800	-0.533900
H	2.786200	2.725300	-1.258300
C	0.181400	3.460700	-1.704400
C	-1.345600	3.635800	-1.602800
H	-1.693600	4.313700	-2.390400
H	-1.643400	4.067700	-0.640100
H	-1.874500	2.684100	-1.728600

C	0.506200	2.874400	-3.099200
H	0.122600	3.531200	-3.889900
H	0.047600	1.886800	-3.224500
H	1.584800	2.763100	-3.252800
C	0.835000	4.856700	-1.572700
H	0.456100	5.530800	-2.350600
H	1.924100	4.808700	-1.675900
H	0.611500	5.303600	-0.597200
H	-1.141900	1.975100	0.237000
H	4.595100	1.060000	1.353100
H	4.660000	1.990000	-0.134600
H	5.553000	-0.286200	-0.482000
H	4.061100	-1.004300	0.094700
H	4.431000	0.587900	-2.489100
H	2.854900	0.135200	-1.873700
H	3.686400	-1.403600	-3.637300
H	5.080500	-1.821800	-2.656100
H	3.446500	-3.602700	-2.543600
H	3.623700	-2.894600	-0.954700
H	1.466800	-1.610000	-1.298600
H	1.293800	-2.359000	-2.881000
H	1.490000	-3.861900	-0.218700
H	1.296700	-4.628200	-1.782900
H	-0.914200	-3.805700	-2.103000
H	-0.805800	-4.608300	-0.560900
C	-2.354100	-2.014800	-1.083200
C	-3.072700	-0.918900	-0.593200
C	-2.538100	-0.240600	0.504800
H	-3.053700	0.628400	0.880500
C	-4.384200	-0.490100	-1.279300
C	-4.110000	-0.147100	-2.762800
H	-3.395100	0.679700	-2.848400
H	-5.038400	0.154700	-3.263300
H	-3.699600	-1.001000	-3.312200
C	-5.400000	-1.655500	-1.205800
H	-6.341200	-1.374900	-1.694800
H	-5.622200	-1.914800	-0.164400
H	-5.021900	-2.556200	-1.701200
C	-5.023600	0.742500	-0.612600
H	-5.252900	0.563700	0.443500
H	-5.962700	0.989400	-1.120800
H	-4.375100	1.624000	-0.675300
H	-2.705100	-2.534300	-1.971600
C	-1.609200	1.364100	2.811400
C	-0.992300	2.672300	3.292000
H	-1.040500	3.415000	2.487800
H	-1.577300	3.041700	4.137600
H	0.060800	2.568000	3.566200
O	-2.781300	1.126100	3.033500