

## Photochemical Studies on Bis-Sulfide and -Sulfone Tethered Polyenic Derivatives

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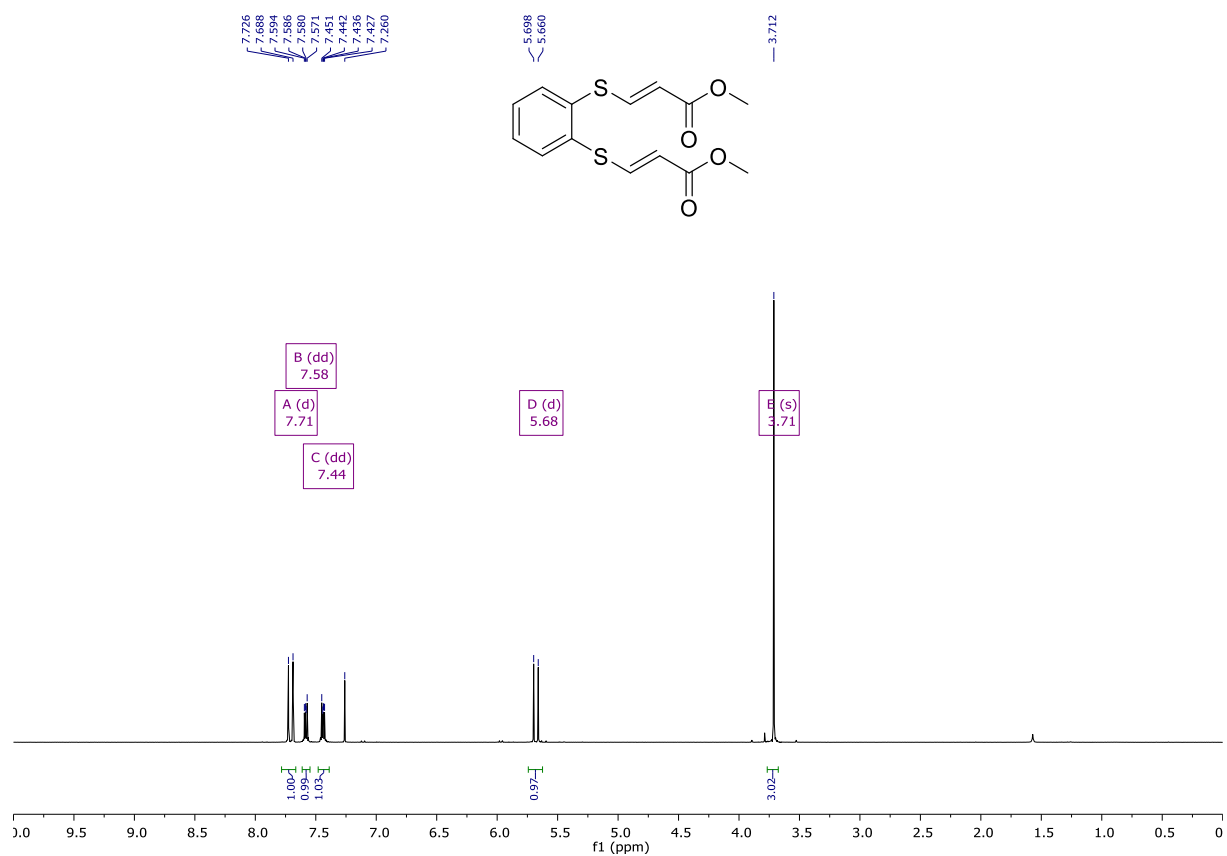
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## 1. General information

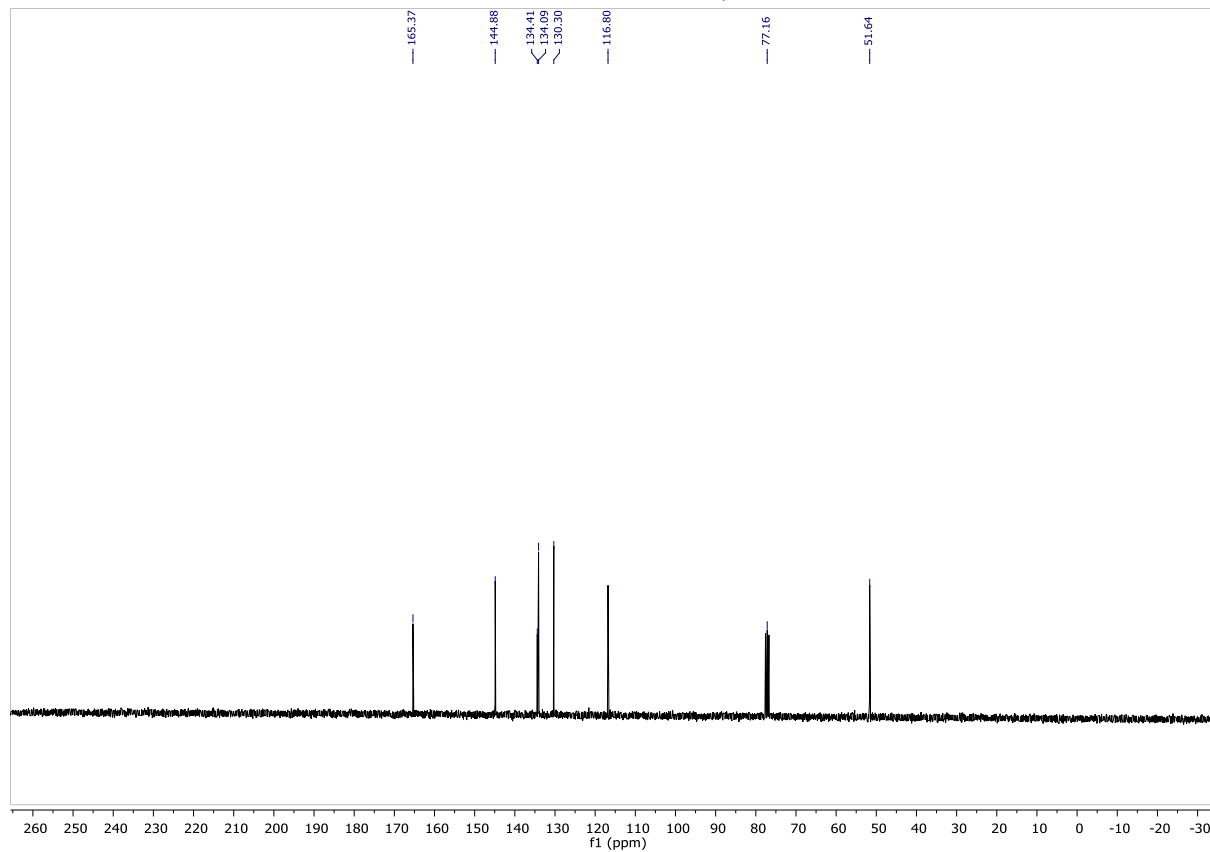
Unless otherwise noted, reactions were carried out under argon atmosphere. Methanol was dried overnight over freshly activated molecular sieves (4 Å), THF and diethyl ether were distilled from sodium/benzophenone. Other reagents and chemicals were purchased from commercial sources and used as received. Infrared (IR) spectra were recorded on a Bruker Tensor 27 (ATR diamond) spectrophotometer. Melting points were determined on a melting point apparatus SMP3 (Stuart scientific) and are uncorrected. NMR spectra were recorded at room temperature on Bruker AVANCE 600, 400 or 300 spectrometers. Chemical shifts ( $\delta$ ) are reported in ppm and coupling constants ( $J$ ) are given in Hertz (Hz).  $^1\text{H}$  and  $^{13}\text{C}$  NMR assignments were based on COSY, HSQC and HMBC experiments. Abbreviations used for peak multiplicity are: s (singlet); bs (broad singlet); d (doublet); t (triplet); q (quartet); m (multiplet) and for assignments: cp (cyclopropyl); cb (cyclobutyl); cpe (cyclopentyl); ch (cyclohexyl). High resolution mass spectrometry was performed on a microTOF (ESI). Thin layer chromatography (TLC) was performed on Merck silica gel 60 F 254 and detected with a UV lamp ( $\lambda = 254 \text{ nm}$ ) and  $\text{KMnO}_4$  or *p*-anisaldehyde staining. Flash column chromatography was performed on silica Geduran<sup>®</sup> Si 60 Å (40 – 63  $\mu\text{m}$ ).

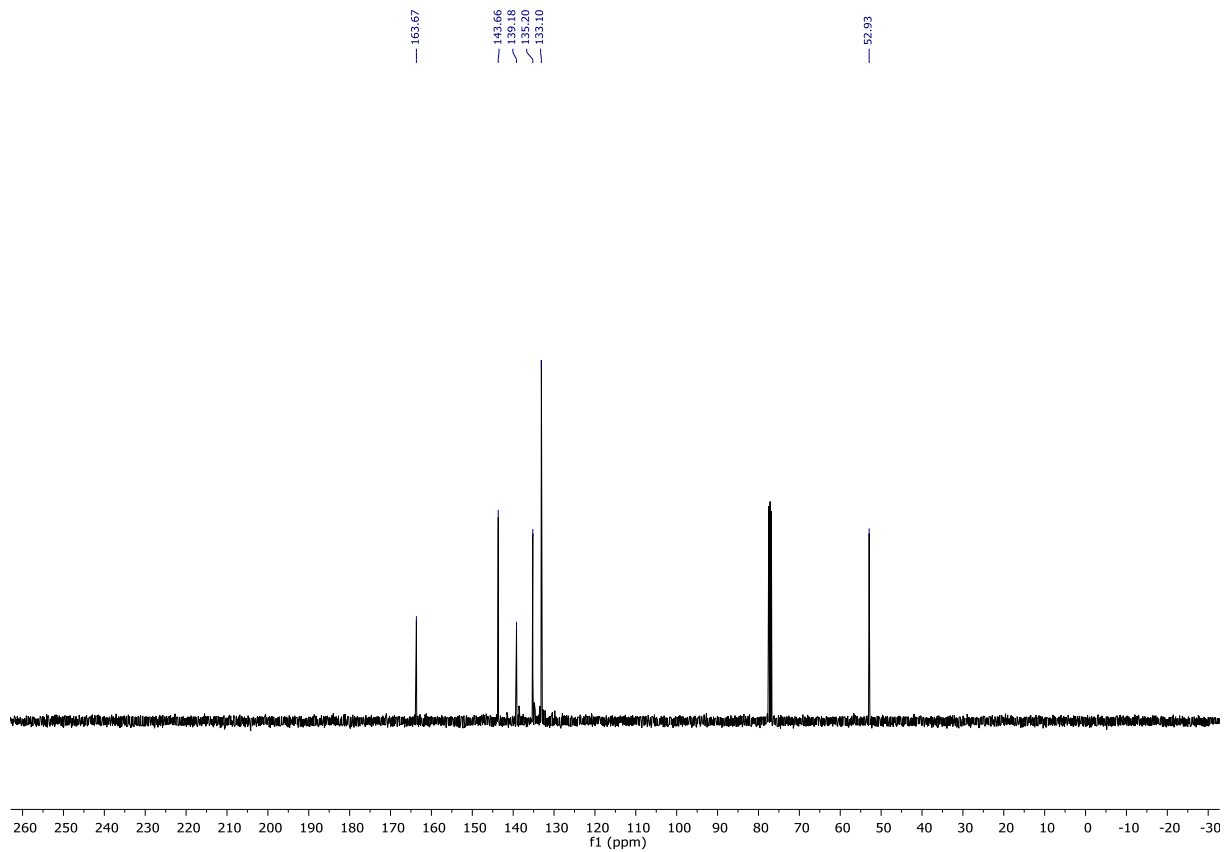
## 2. Spectral data

### <sup>1</sup>H-NMR (400 MHz) : Compound 2

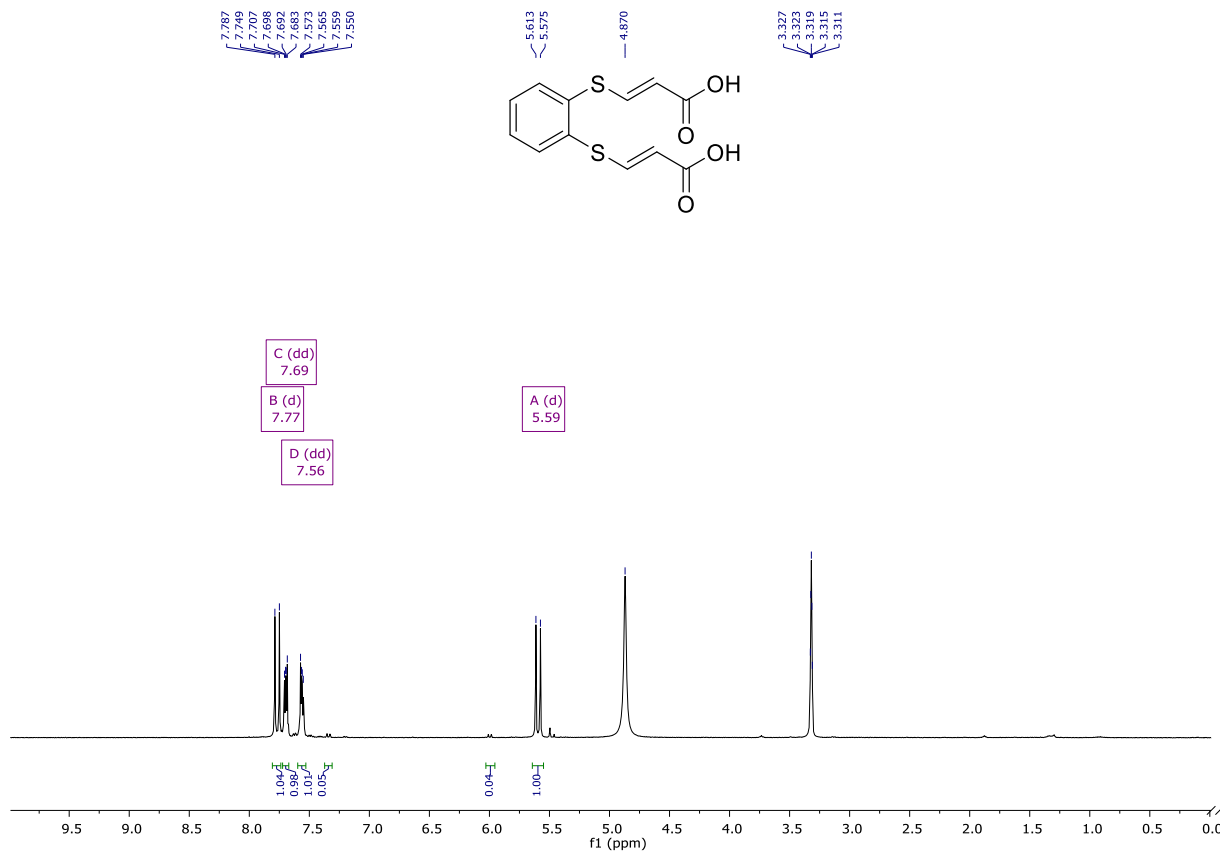


### <sup>13</sup>C-NMR (100 MHz) : Compound 2

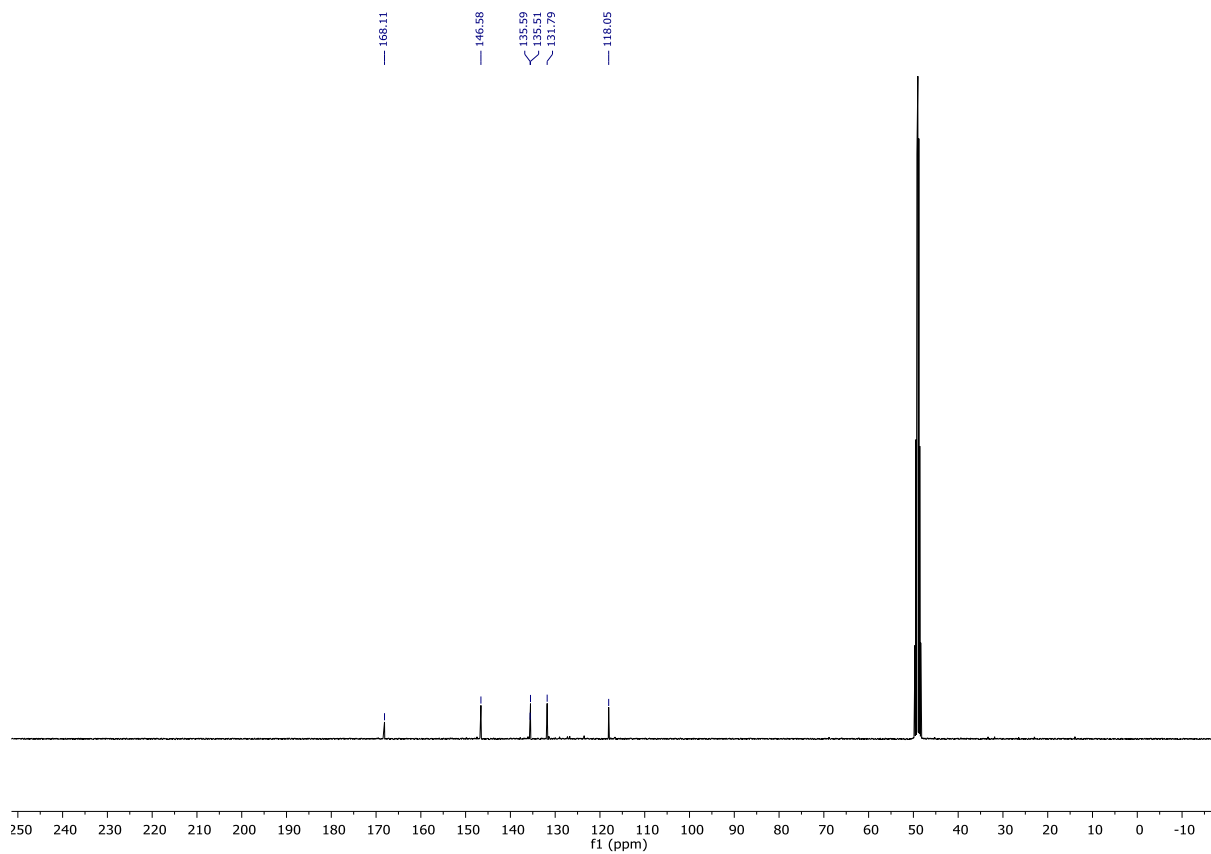




<sup>1</sup>H-NMR (400 MHz) : Compound 2-OH



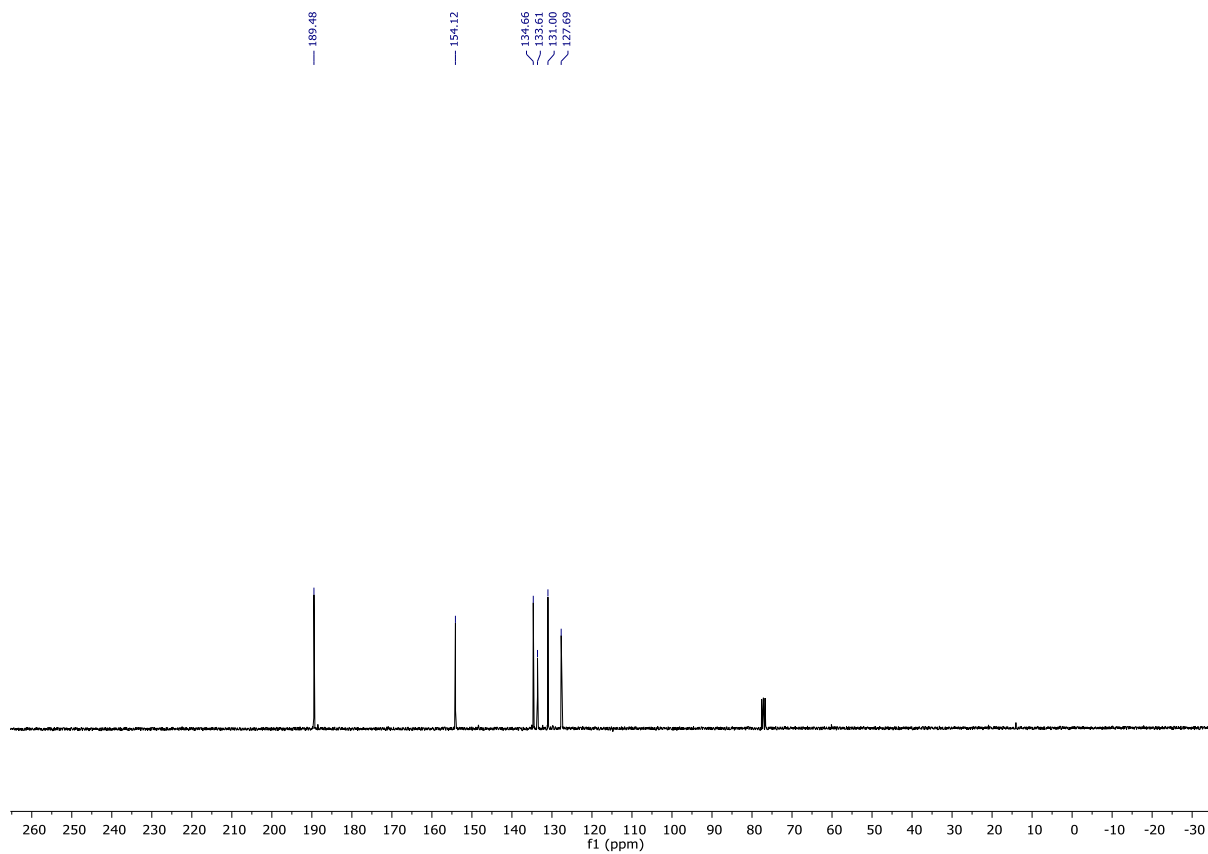
<sup>13</sup>C-NMR (100 MHz) : Compound 2-OH



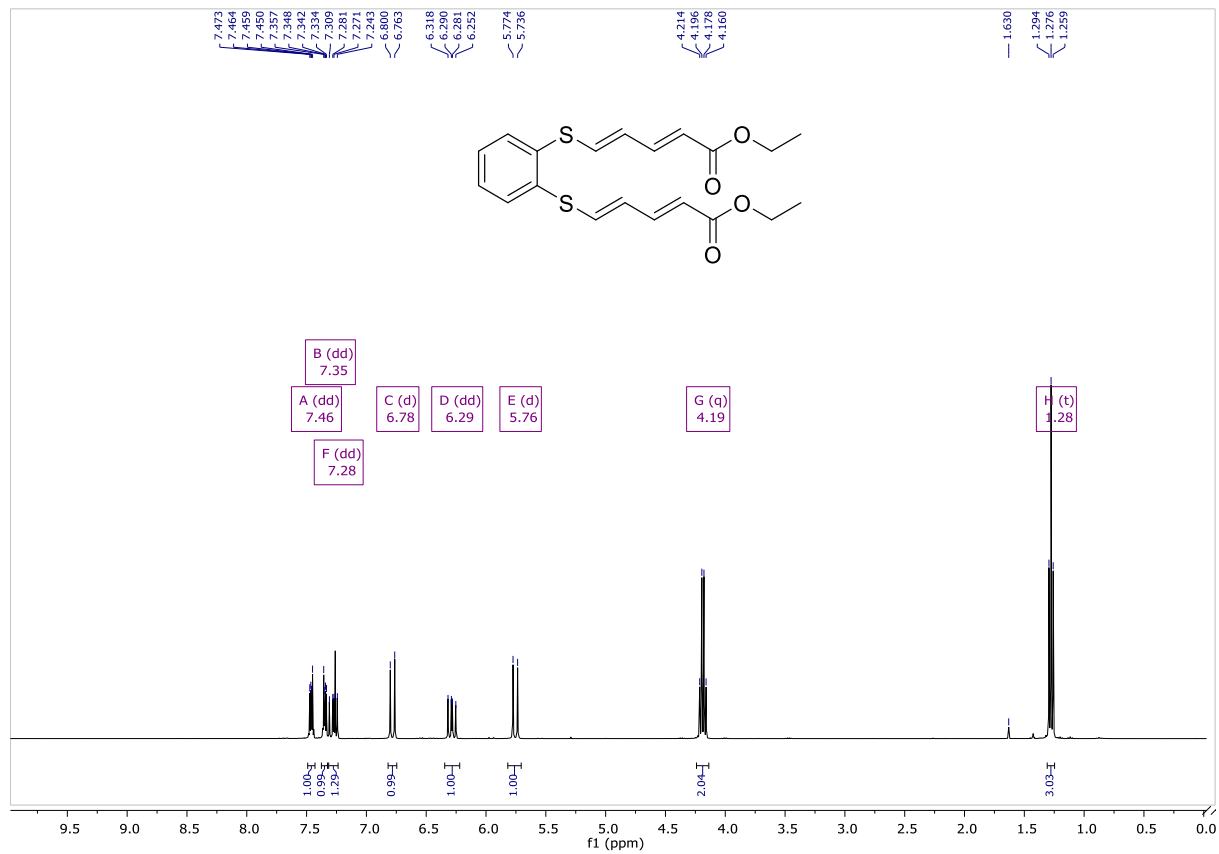
<sup>1</sup>H-NMR (400 MHz) : Compound 3



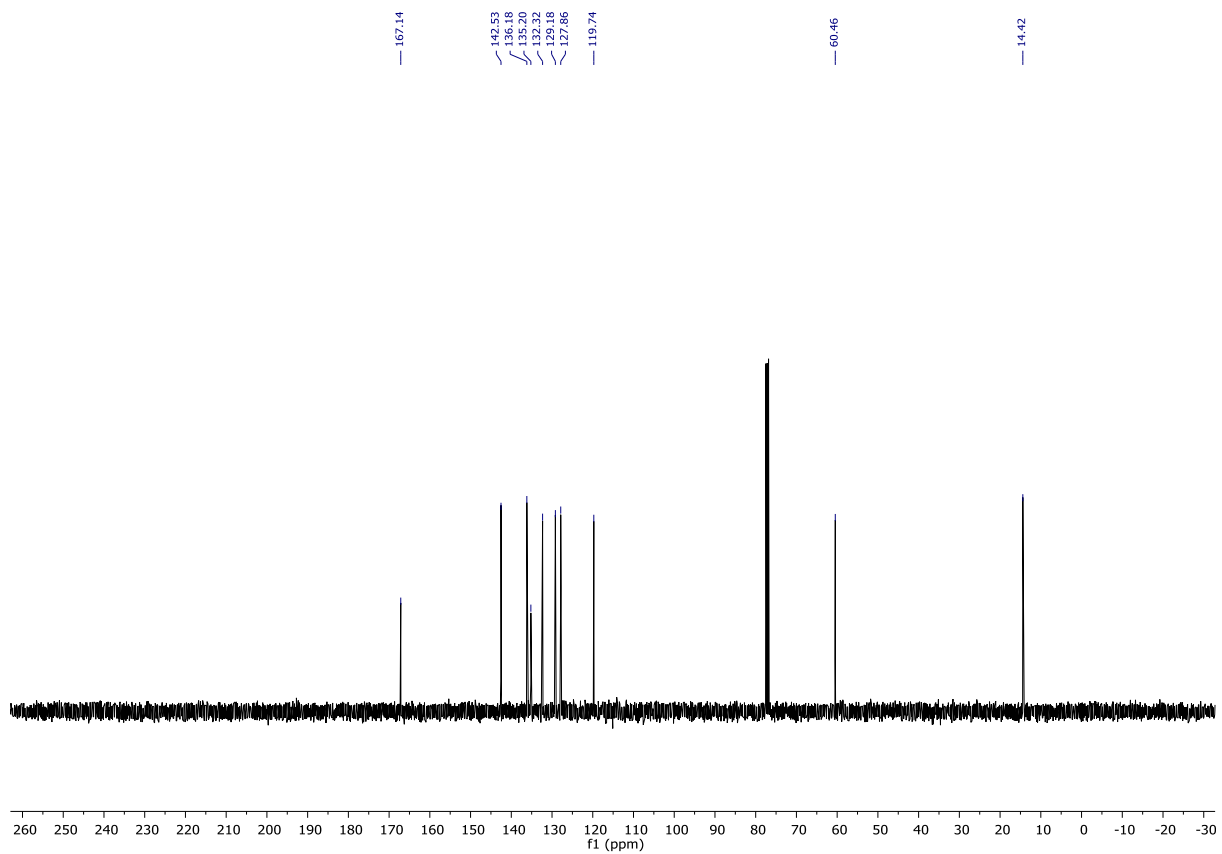
<sup>13</sup>C-NMR (100 MHz) : Compound 3



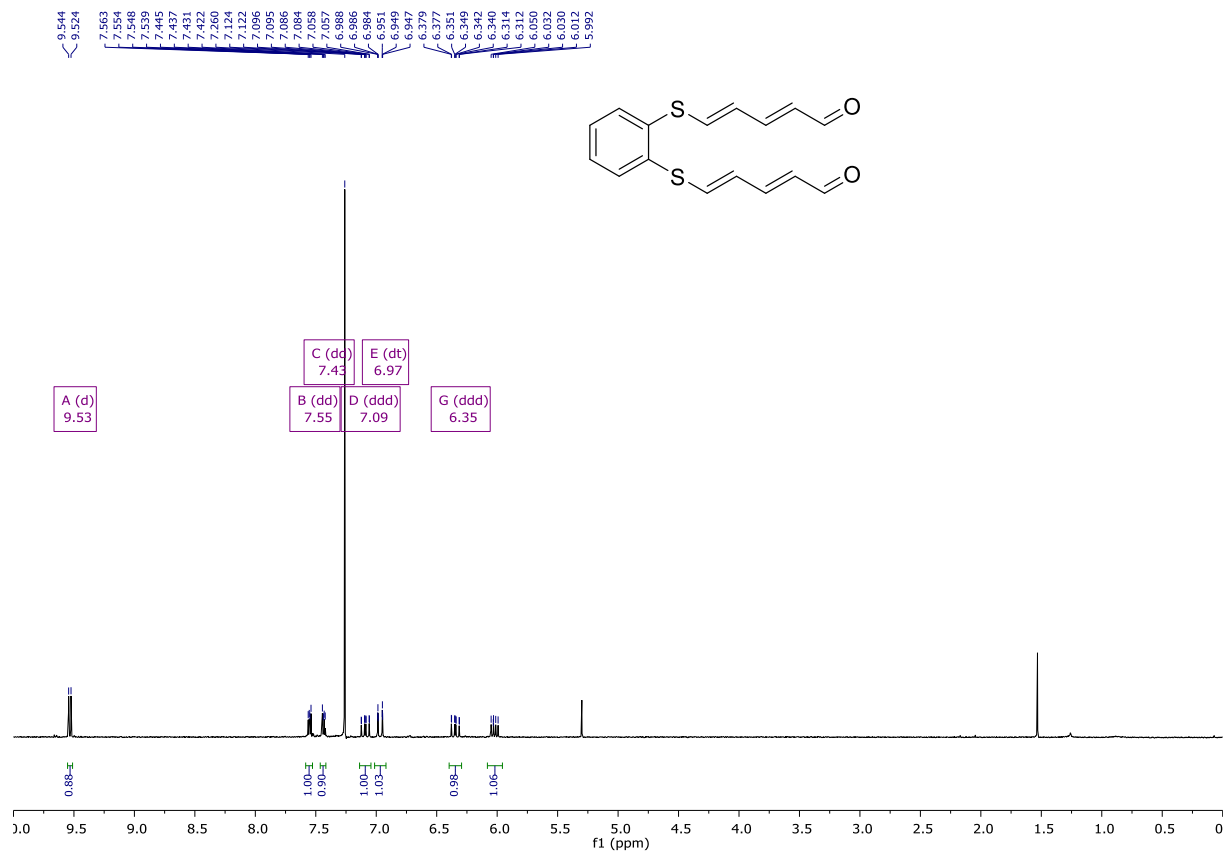
<sup>1</sup>H-NMR (400 MHz) : Compound 4



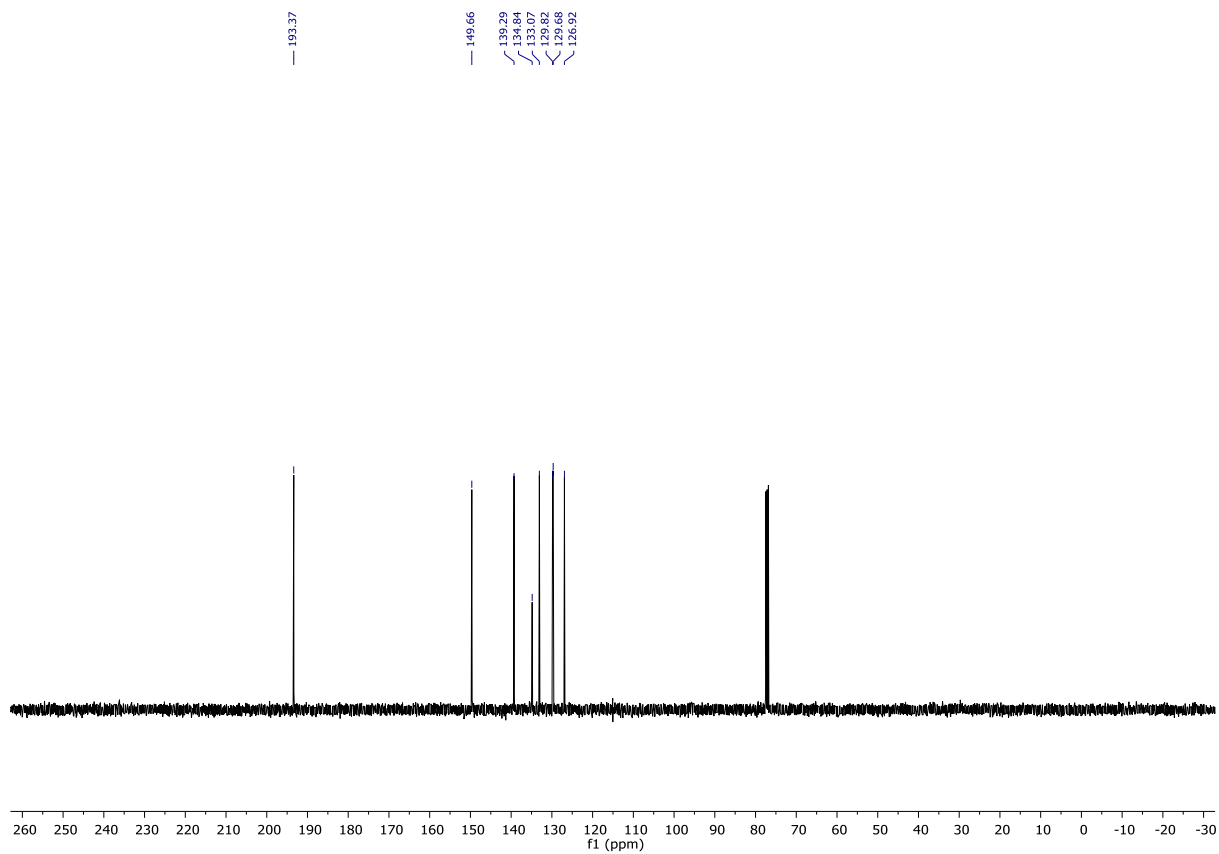
<sup>13</sup>C-NMR (100 MHz) : Compound 4



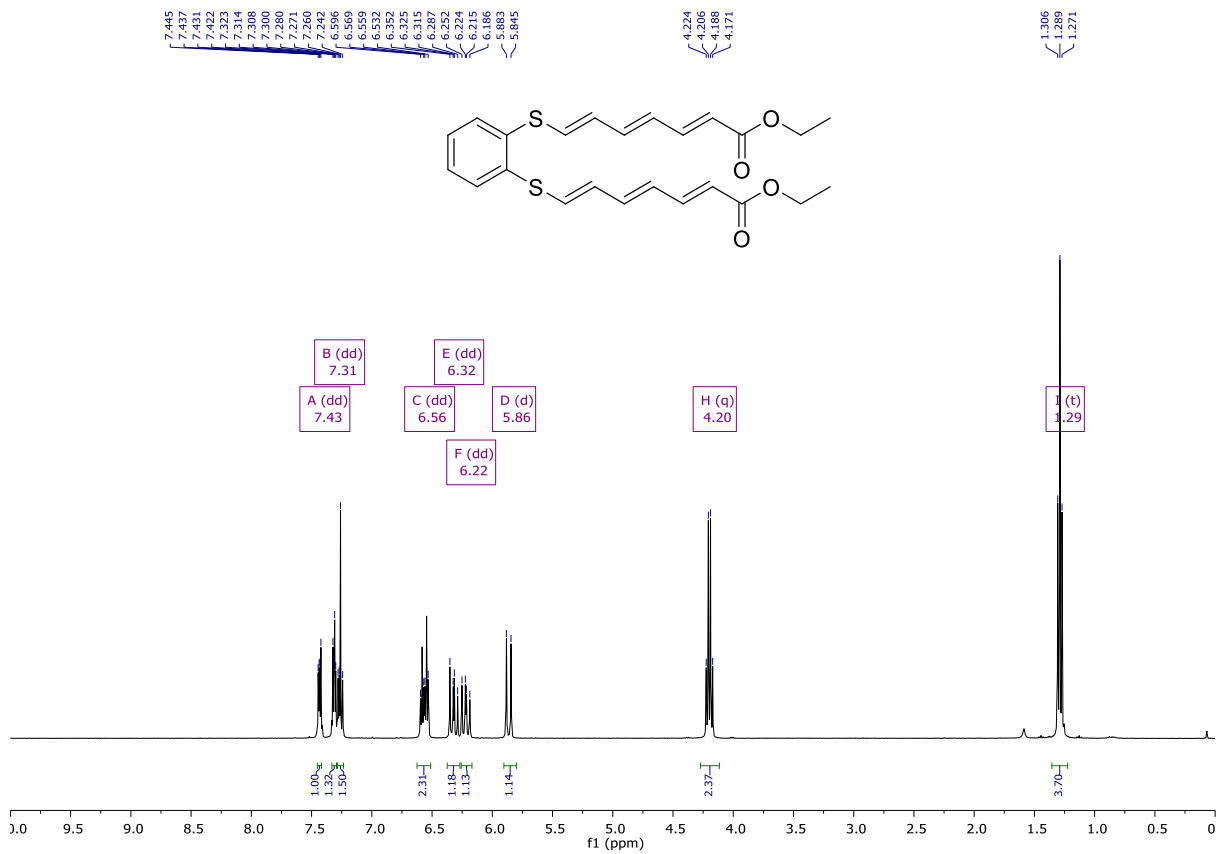
<sup>1</sup>H-NMR (400 MHz) : Compound 5



<sup>13</sup>C-NMR (100 MHz) : Compound 5

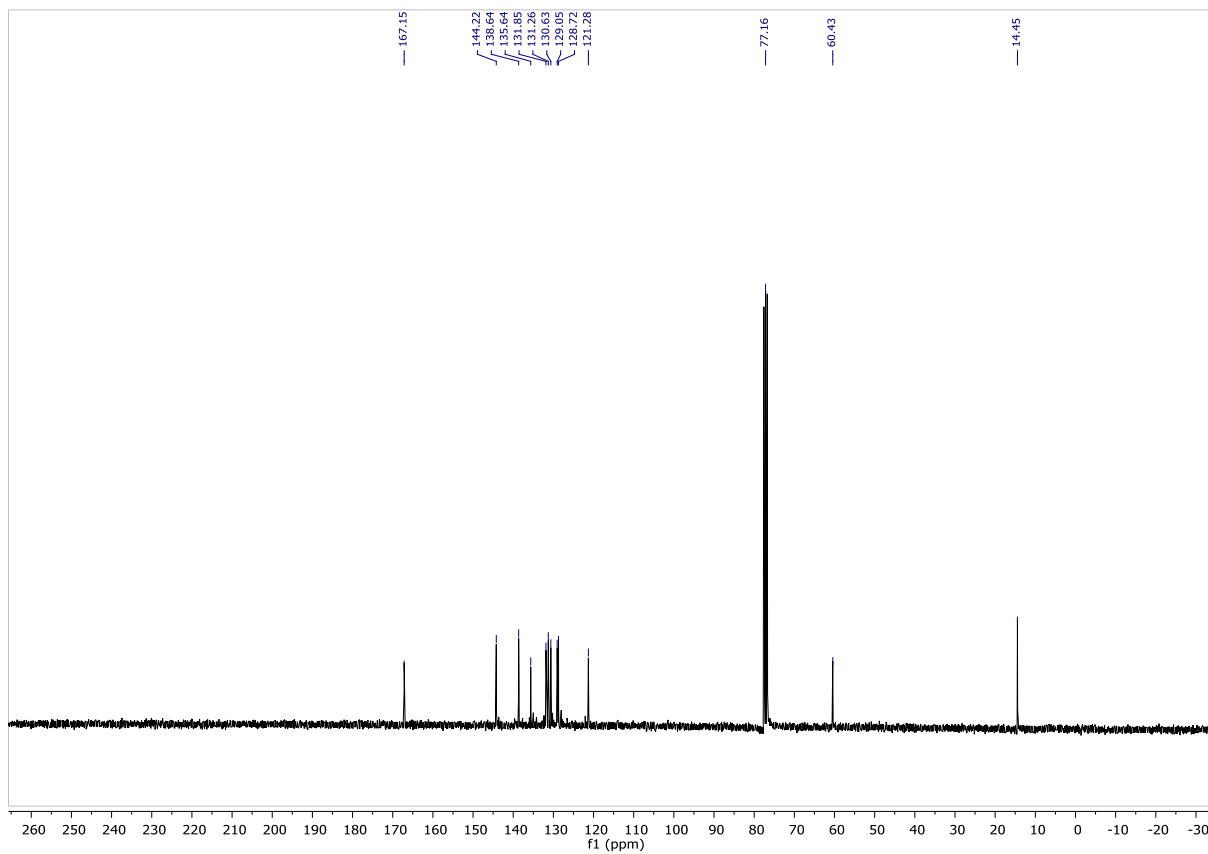


<sup>1</sup>H-NMR (400 MHz) : Compound 6

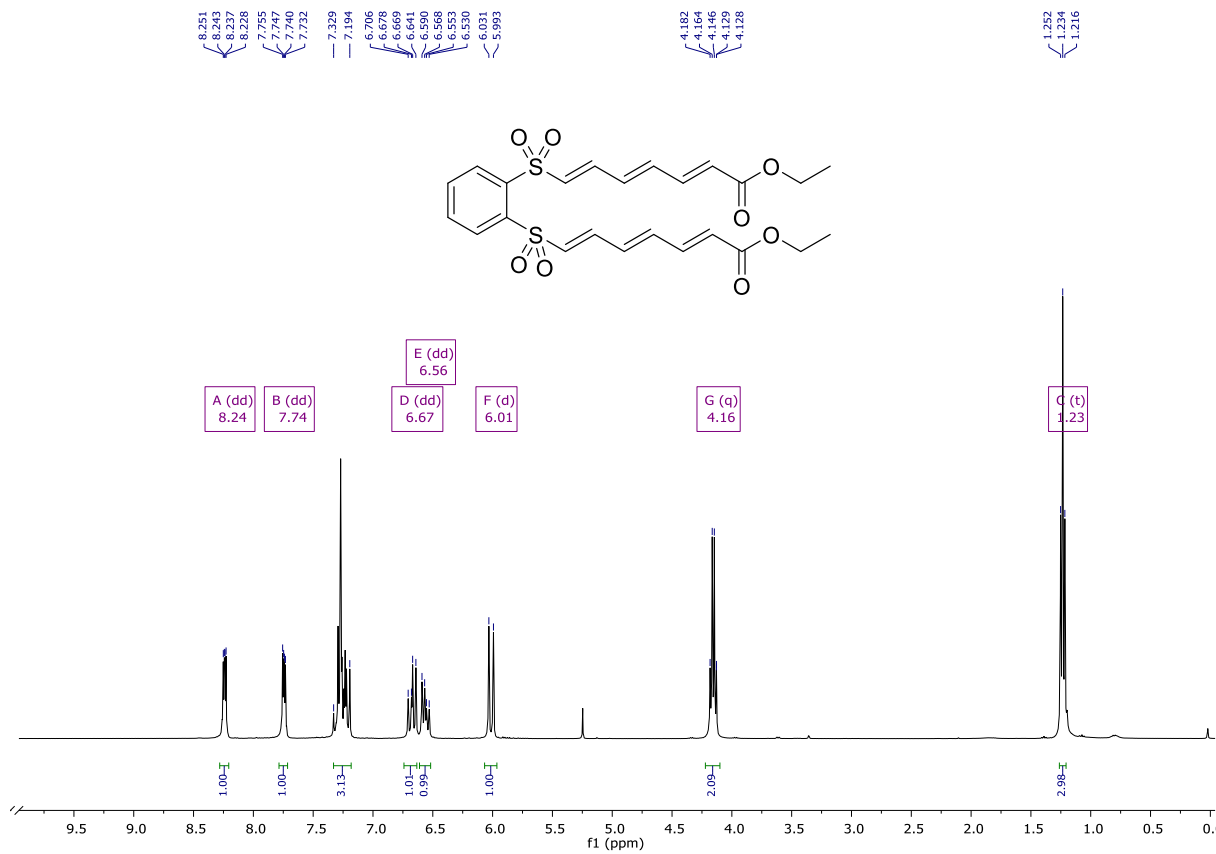


<sup>13</sup>C-NMR (100 MHz) : Compound 6

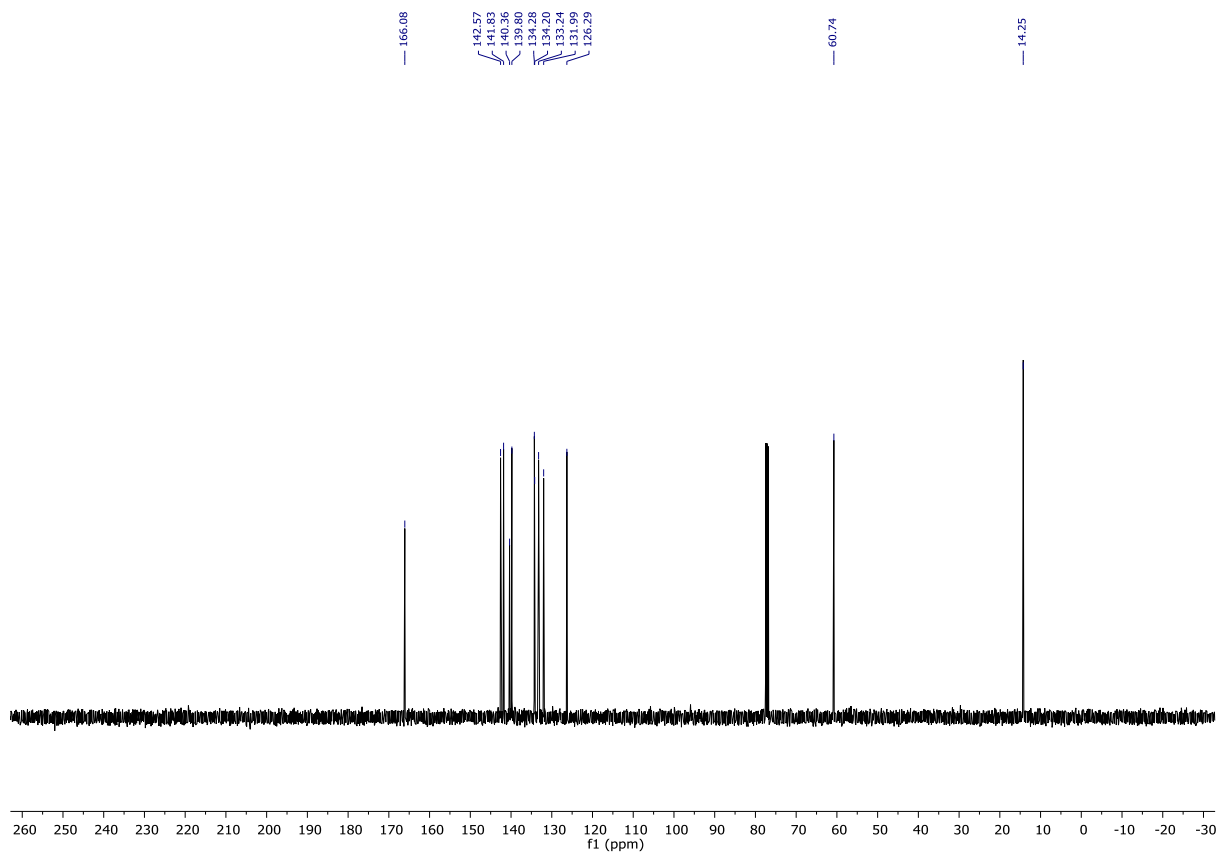




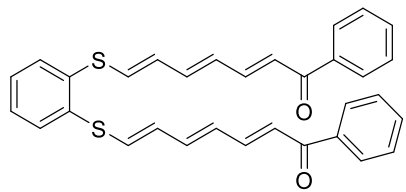
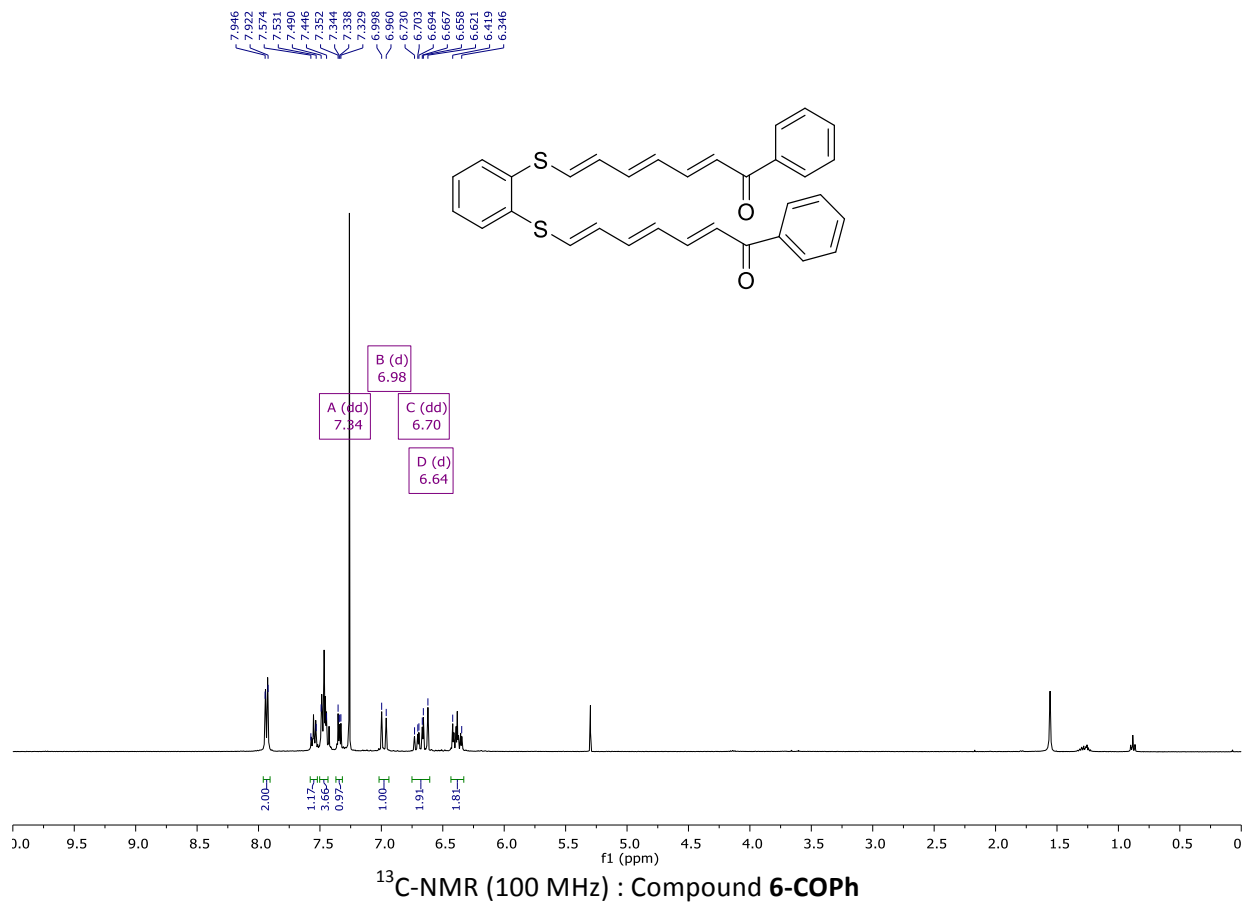
<sup>1</sup>H-NMR (400 MHz) : Compound 6-O

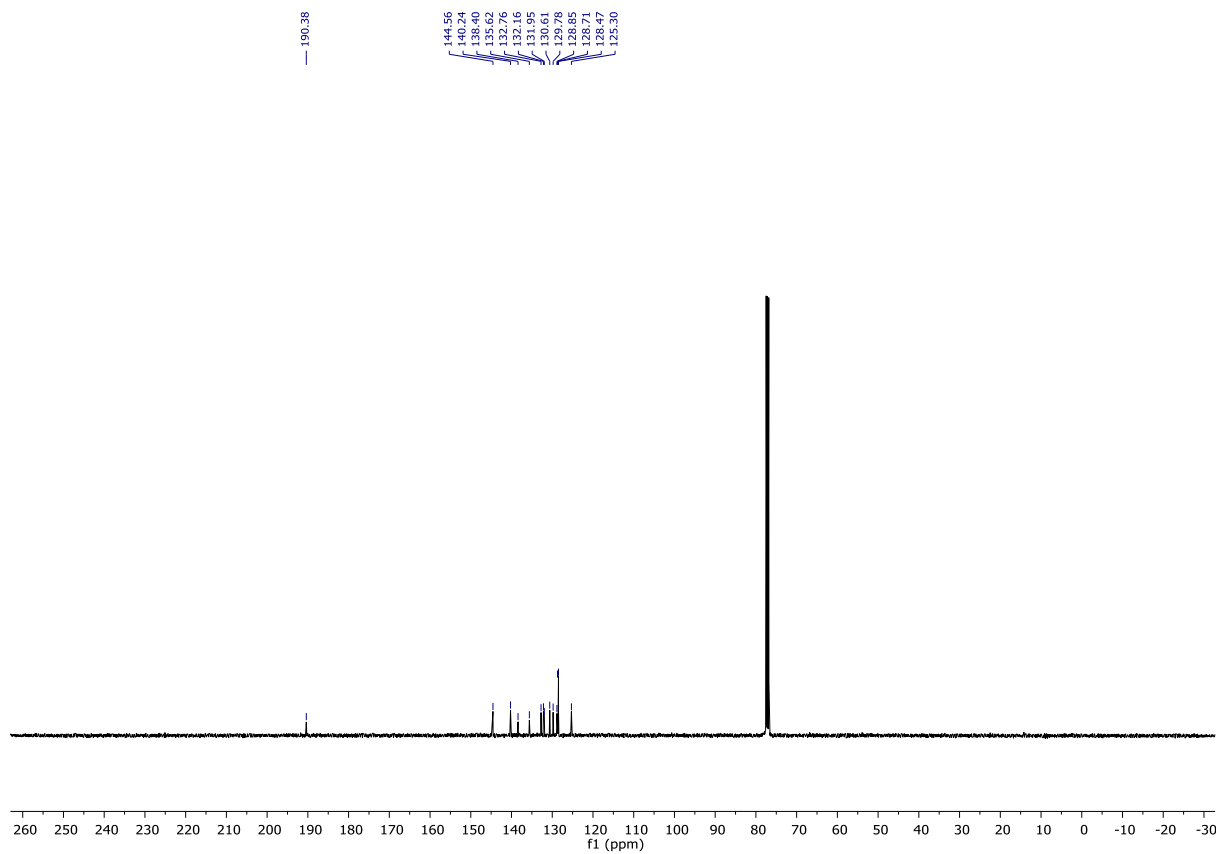


<sup>13</sup>C-NMR (100 MHz) : Compound 6-O

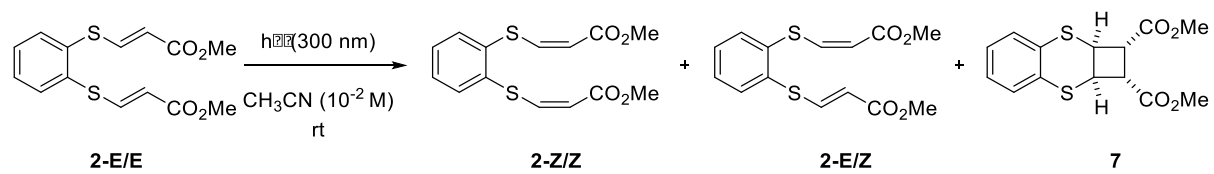


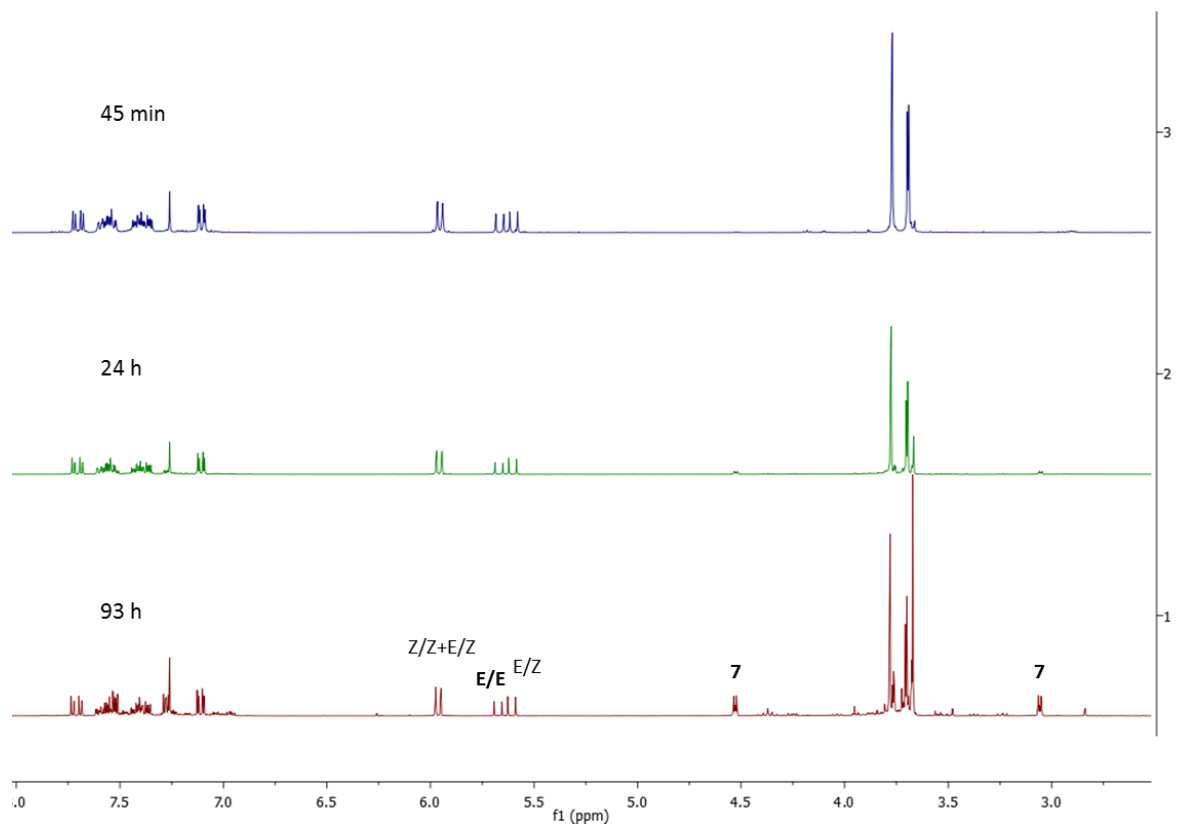
<sup>1</sup>H-NMR (400 MHz) : Compound 6-COPh



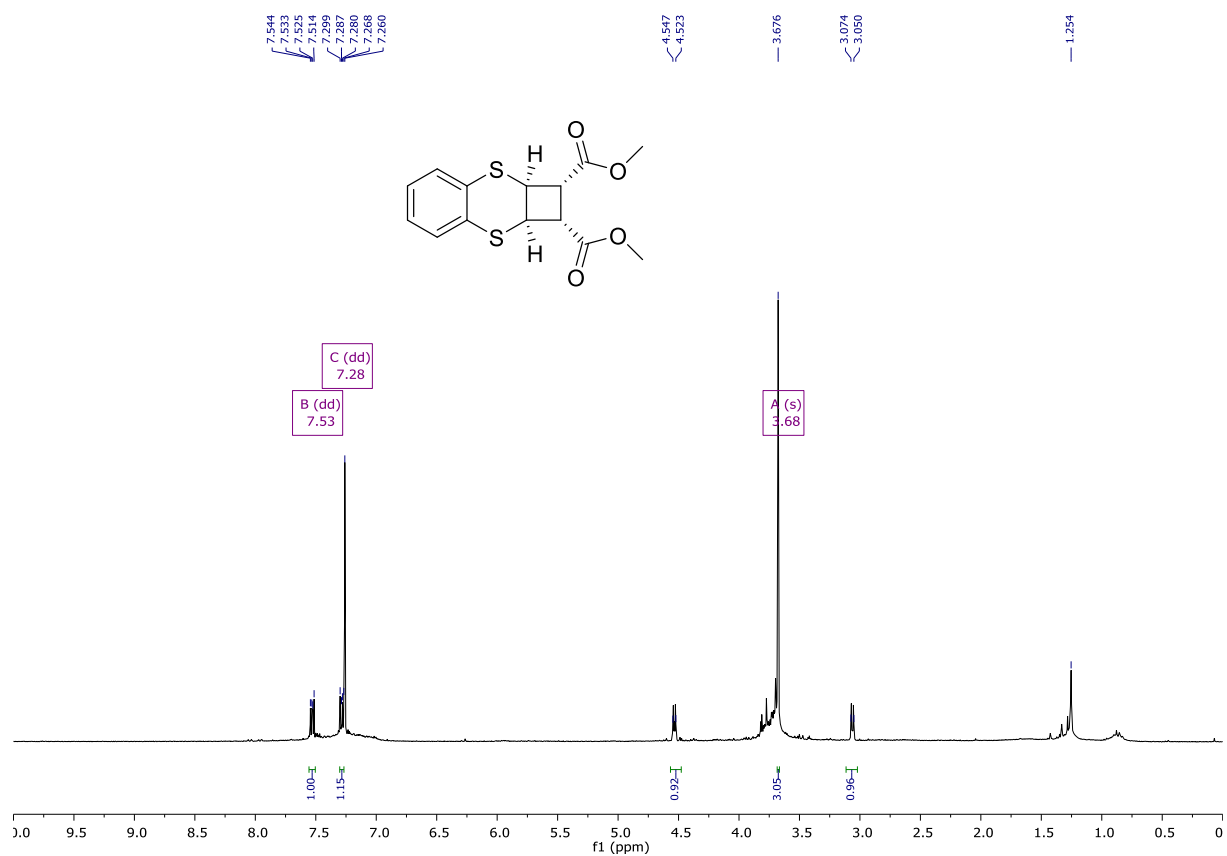


$^1\text{H-NMR}$  (400 MHz) : **2-mix** + **7**

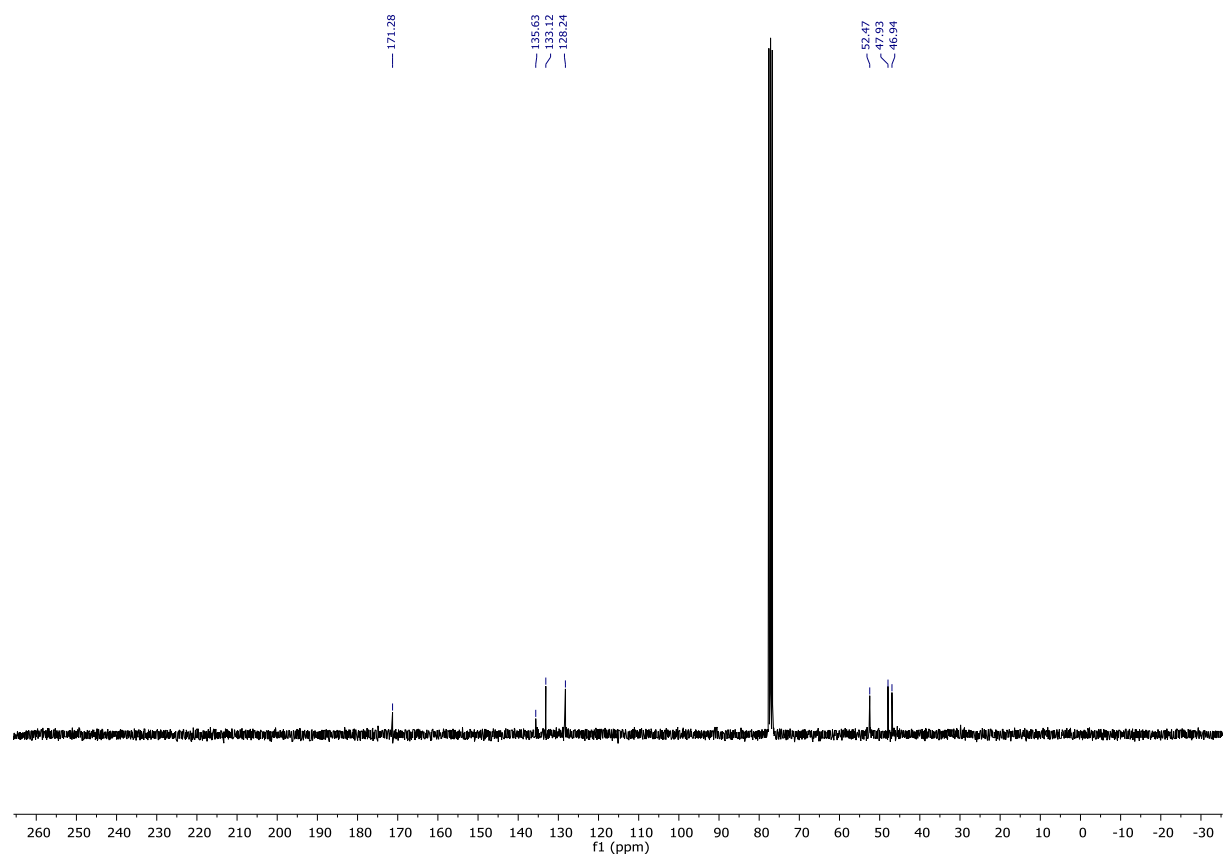




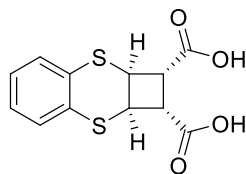
<sup>1</sup>H-NMR (400 MHz) : Compound 7



<sup>13</sup>C-NMR (100 MHz) : Compound 7

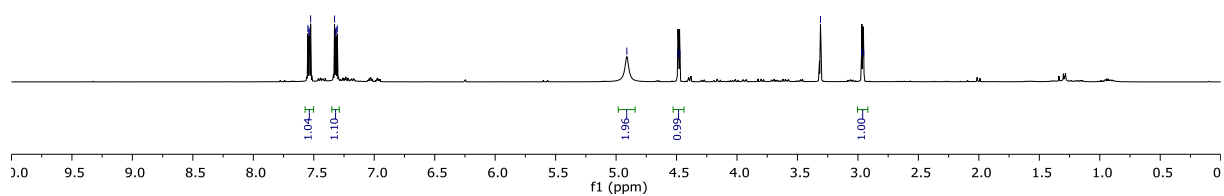


<sup>1</sup>H-NMR (400 MHz) : Compound 7-OH

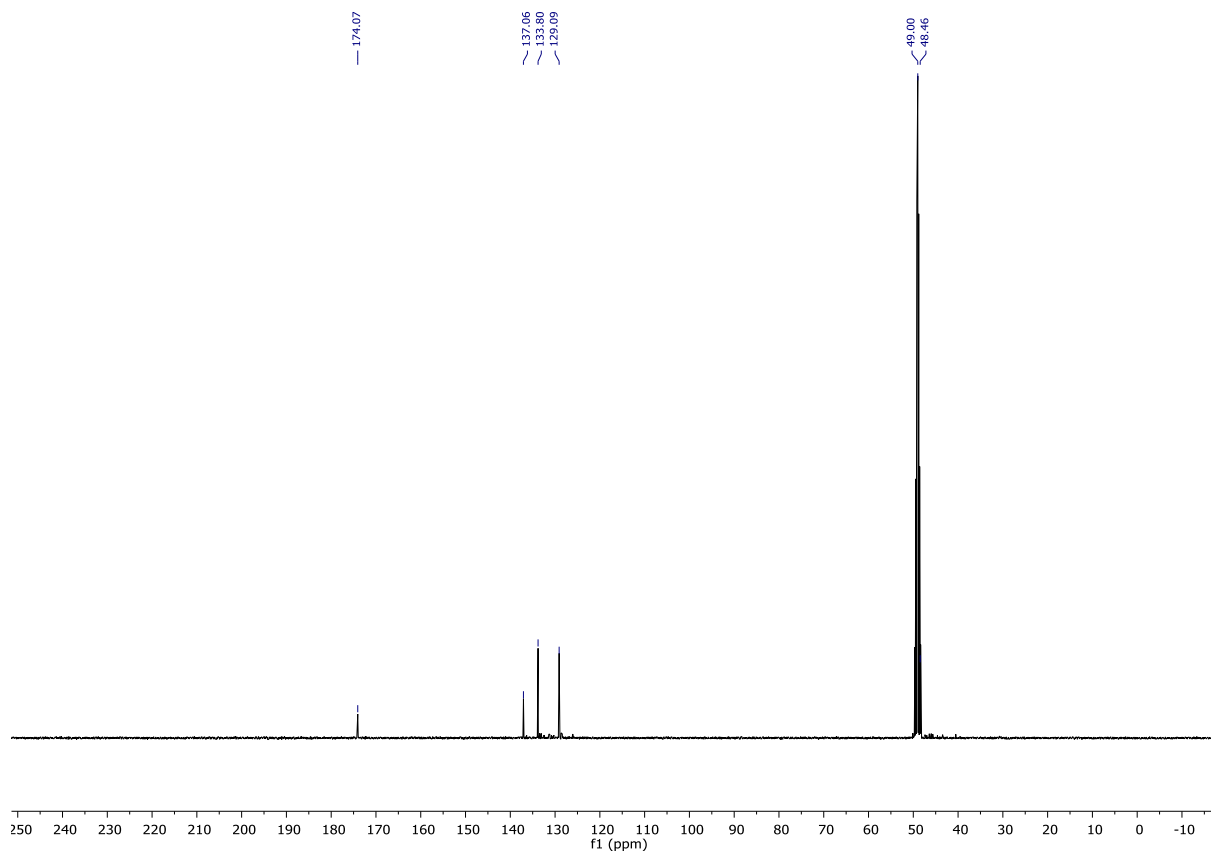


B (dd)  
7.32

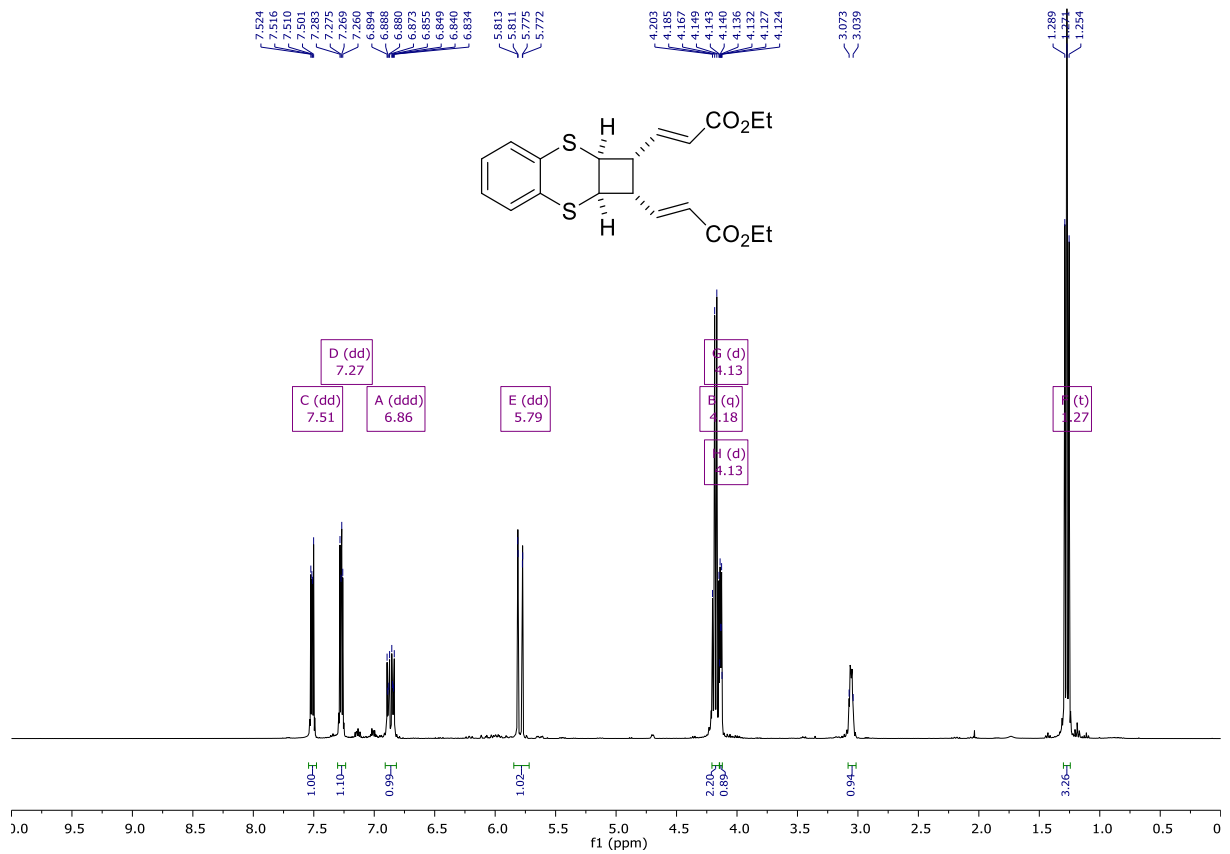
A (dd)  
7.54



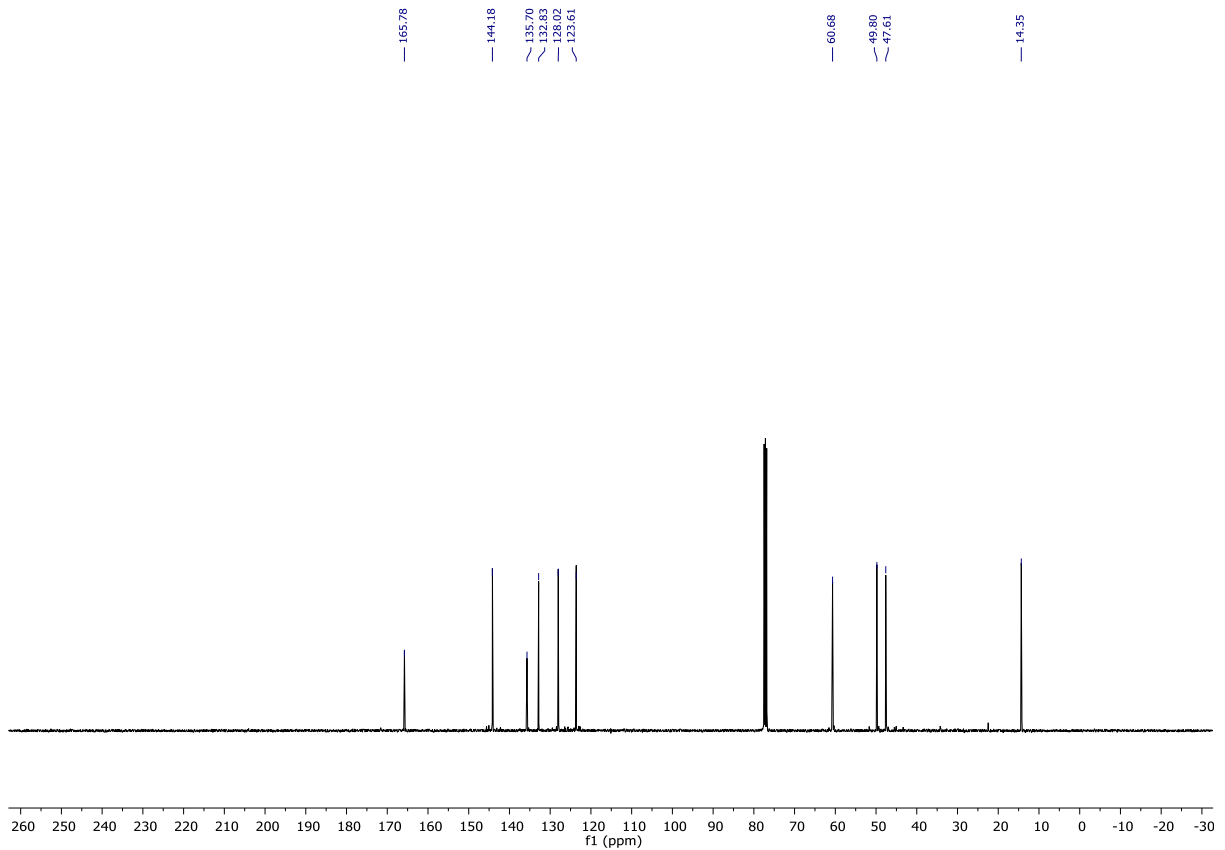
<sup>13</sup>C-NMR (100 MHz) : Compound 7-OH



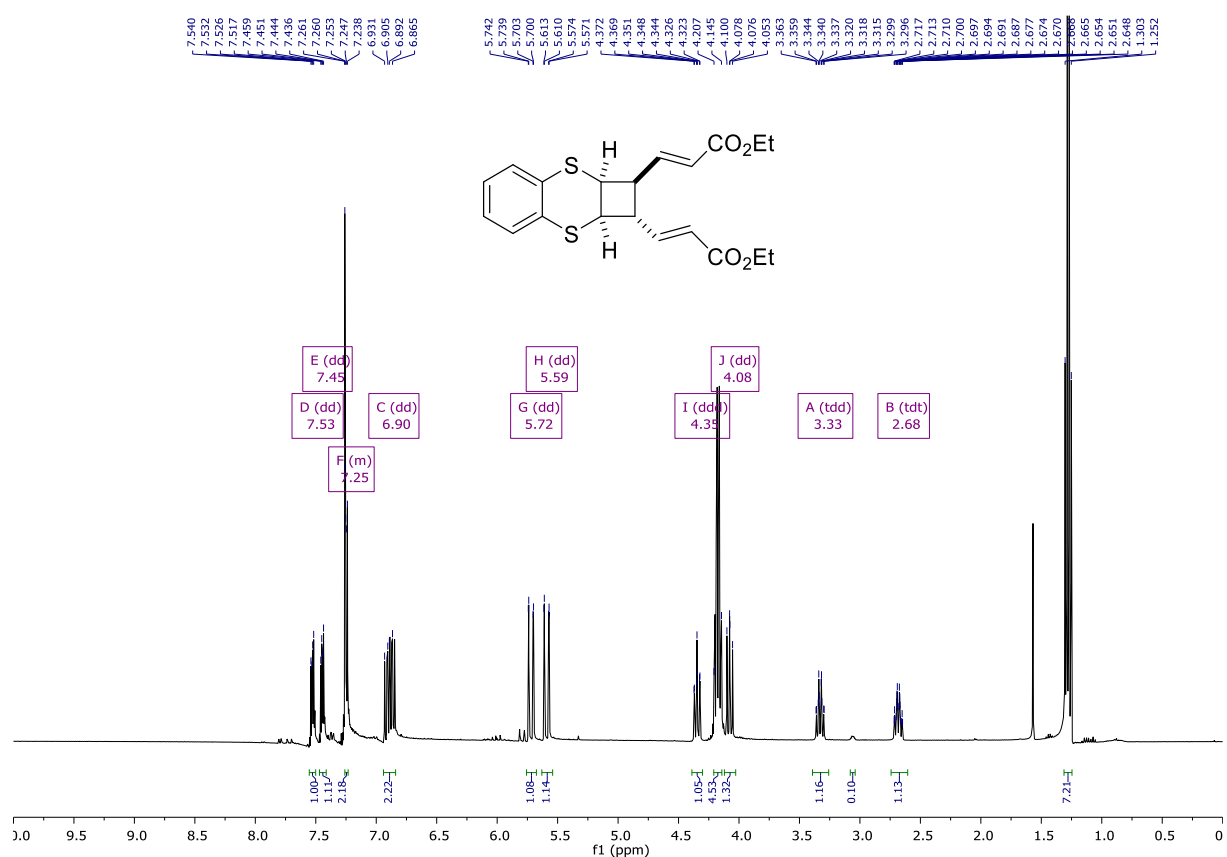
<sup>1</sup>H-NMR (400 MHz) : Compound **8-sym**



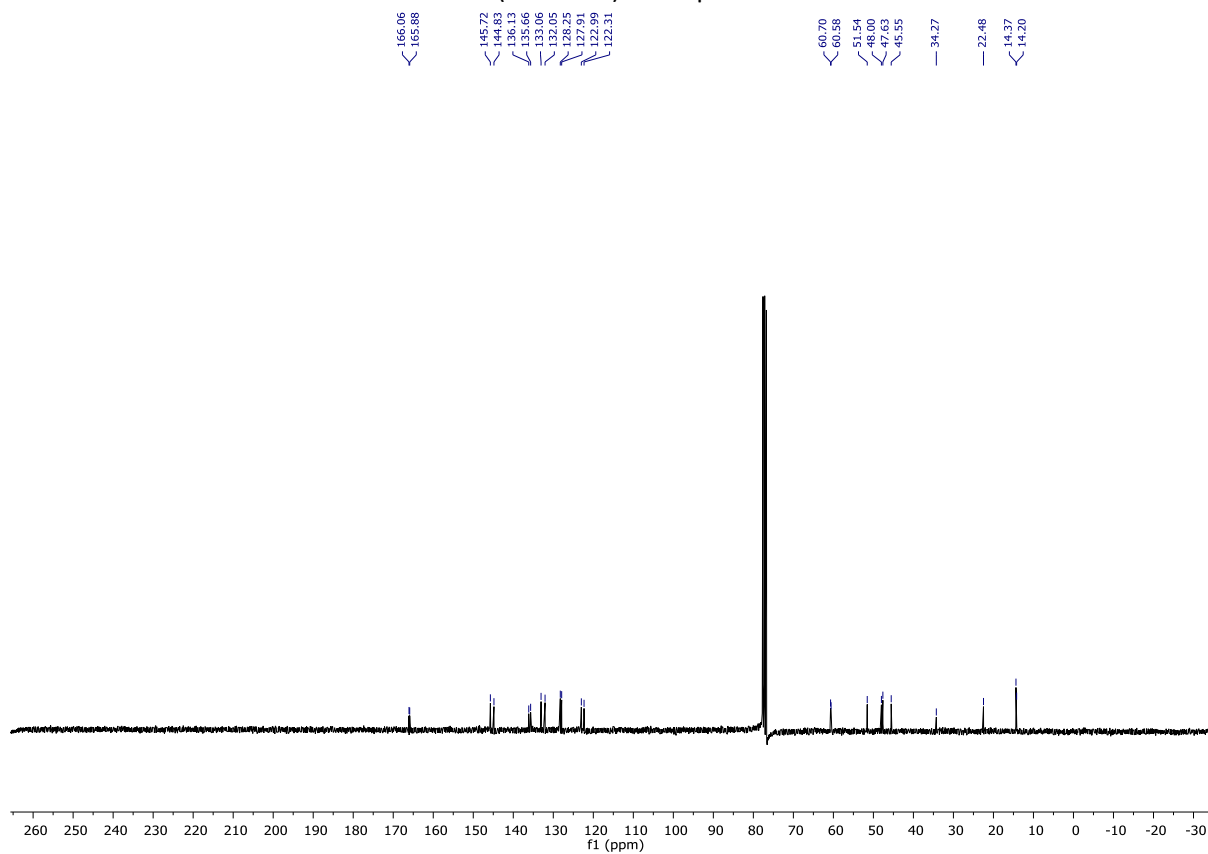
<sup>13</sup>C-NMR (100 MHz) : Compound **8-sym**



<sup>1</sup>H-NMR (400 MHz) : Compound 8-dis

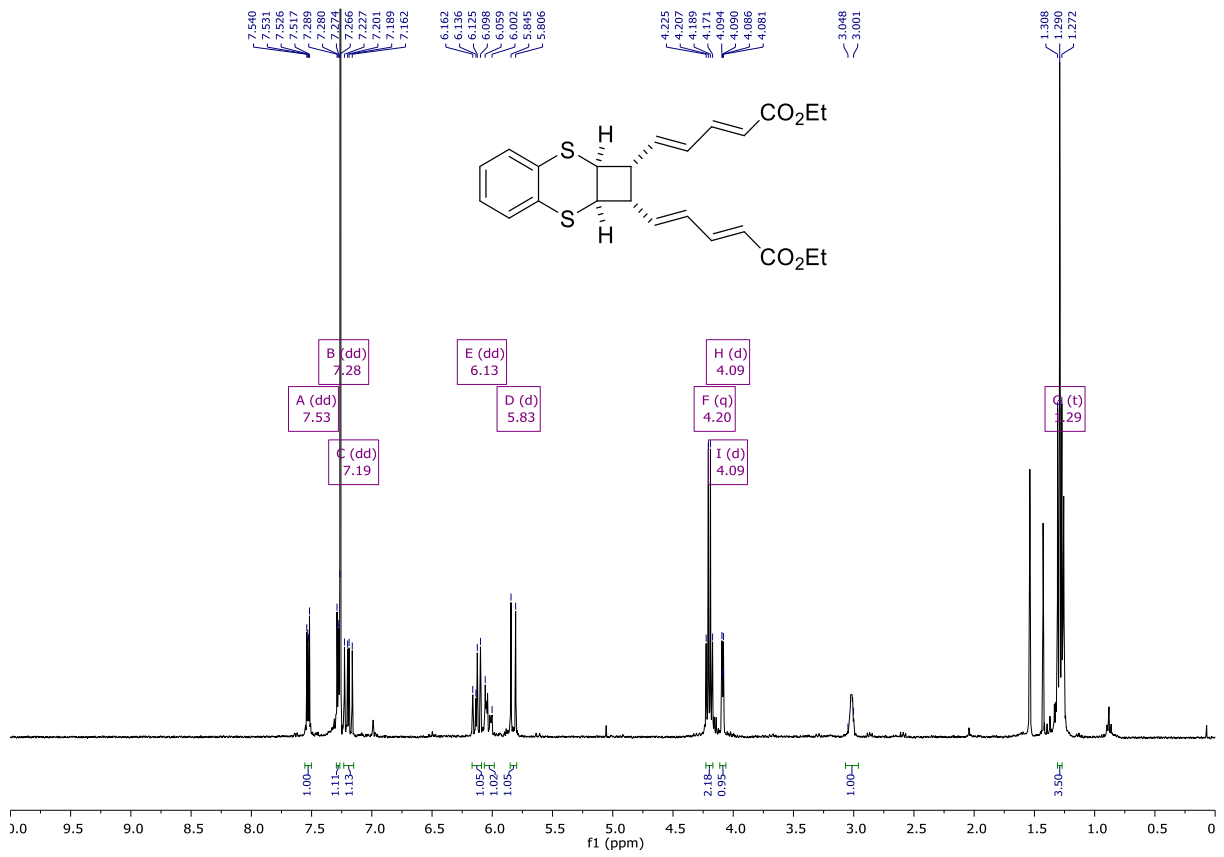


<sup>13</sup>C-NMR (100 MHz) : Compound 8-dis

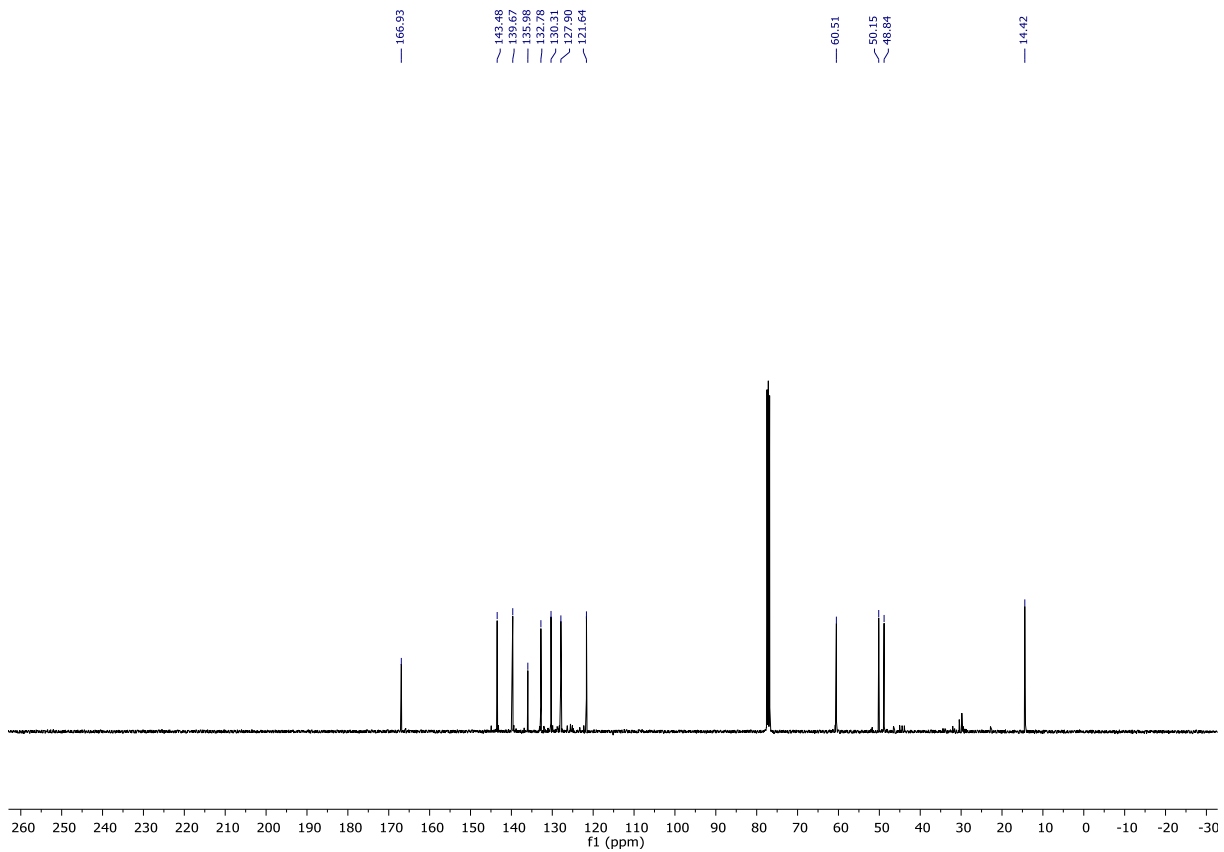




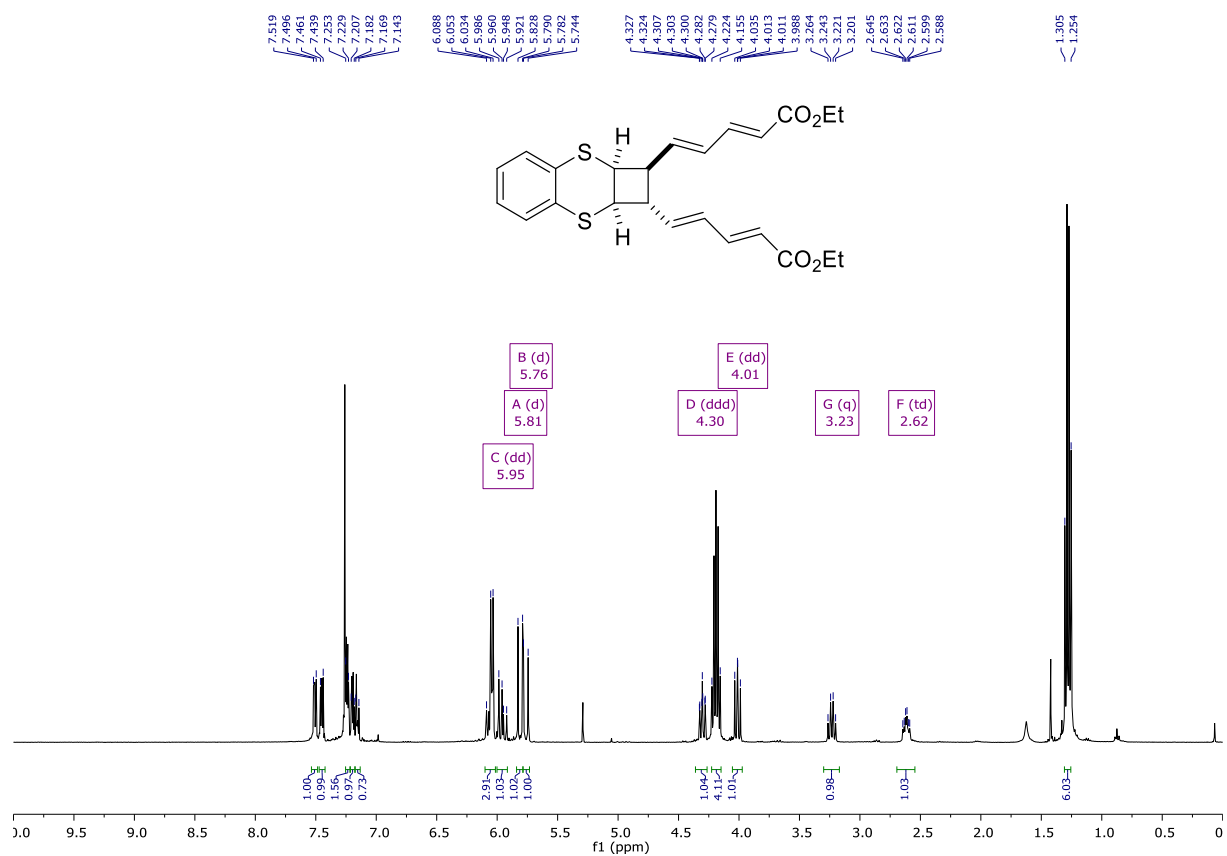
<sup>1</sup>H-NMR (400 MHz) : Compound 9-sym



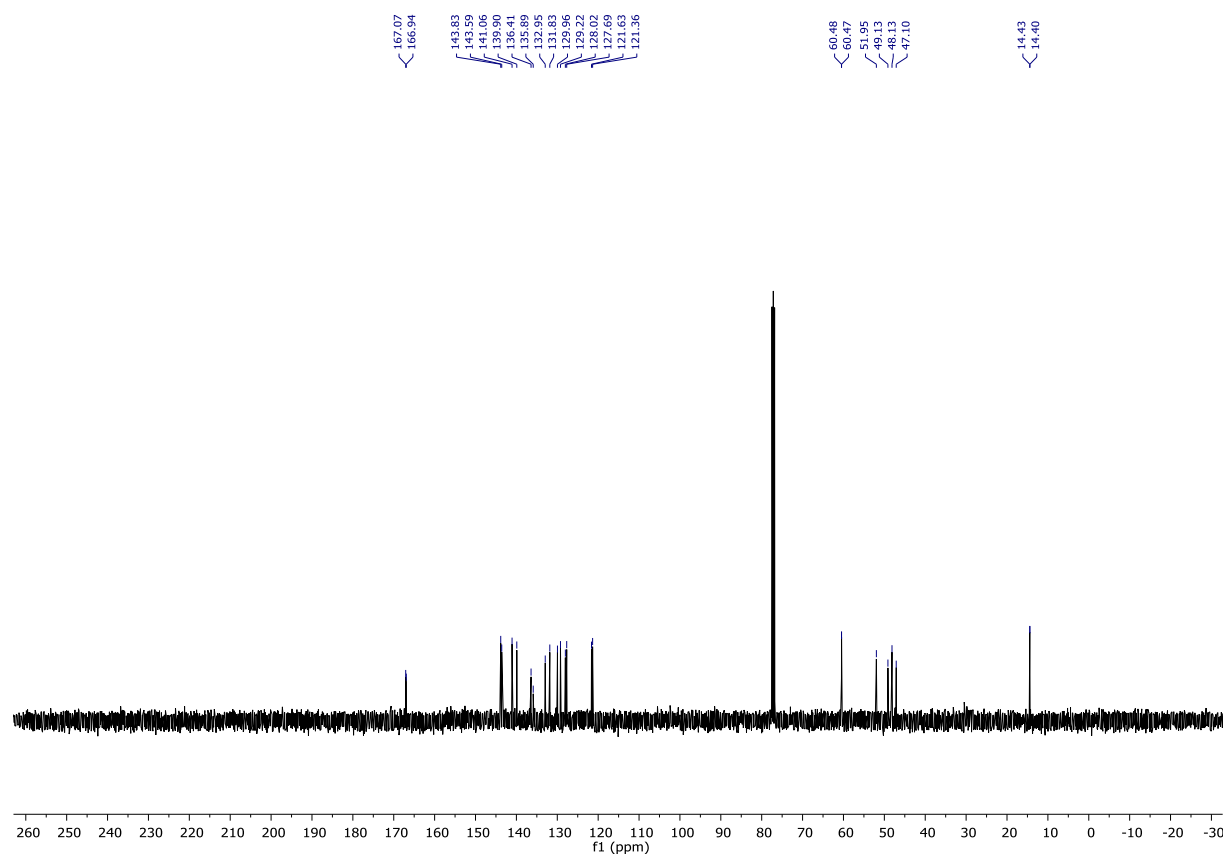
<sup>13</sup>C-NMR (100 MHz) : Compound 9-sym



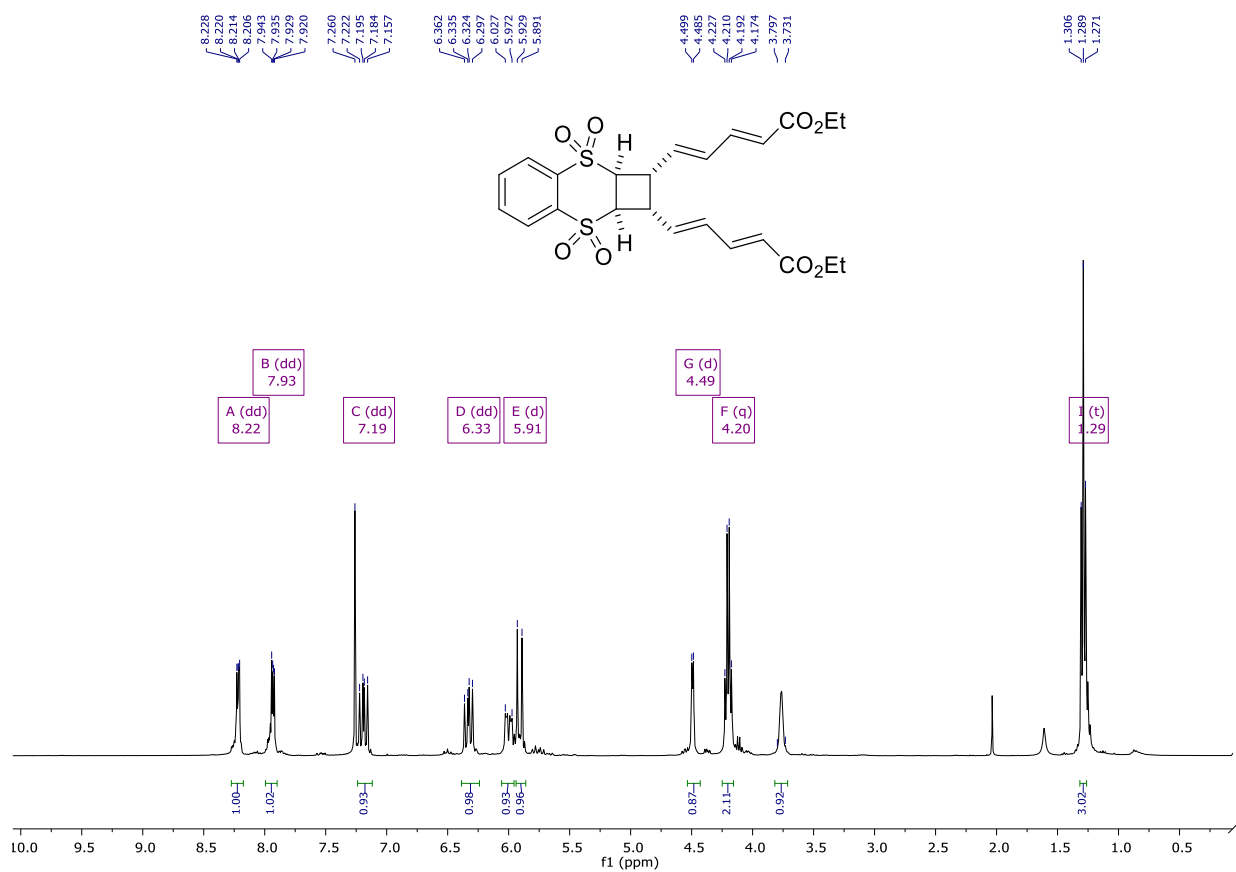
# <sup>1</sup>H-NMR (600 MHz) : Compound 9-dis



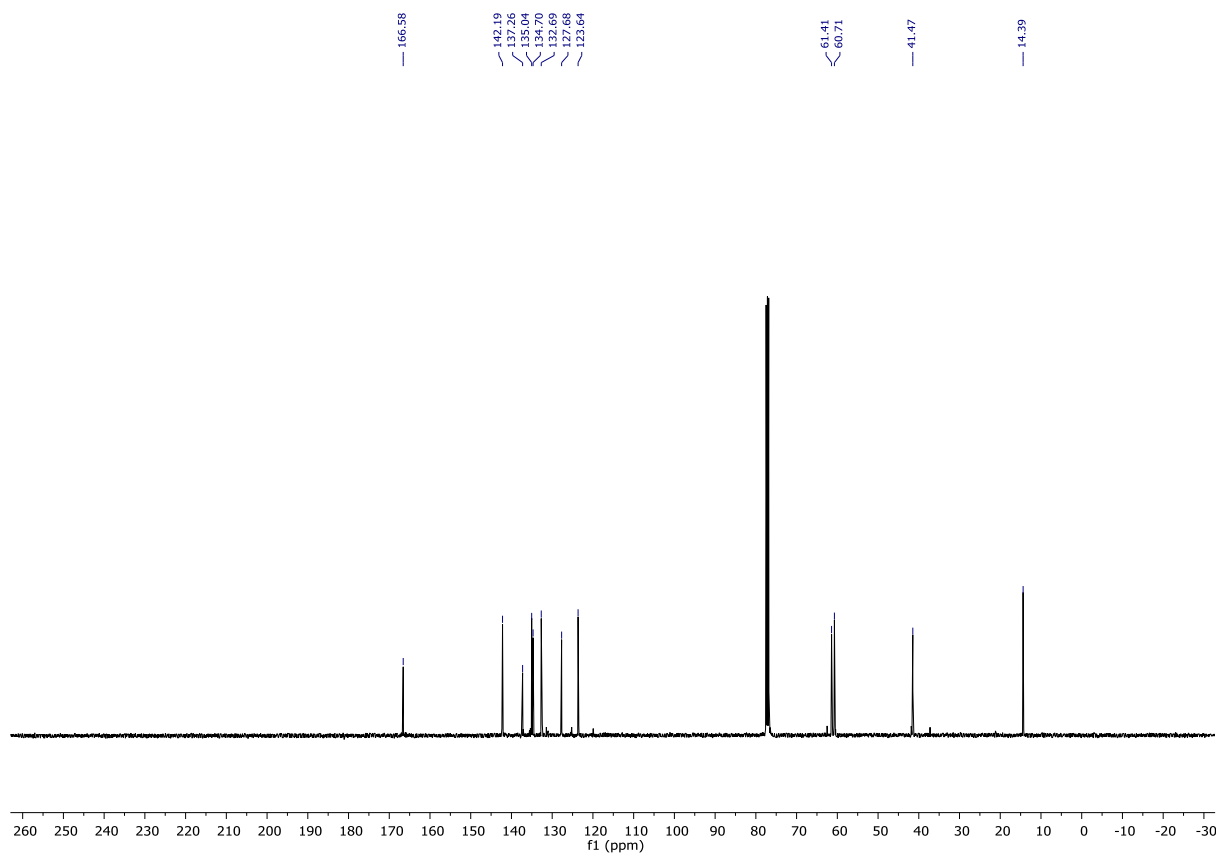
# <sup>13</sup>C-NMR (151 MHz) : Compound 9-dis



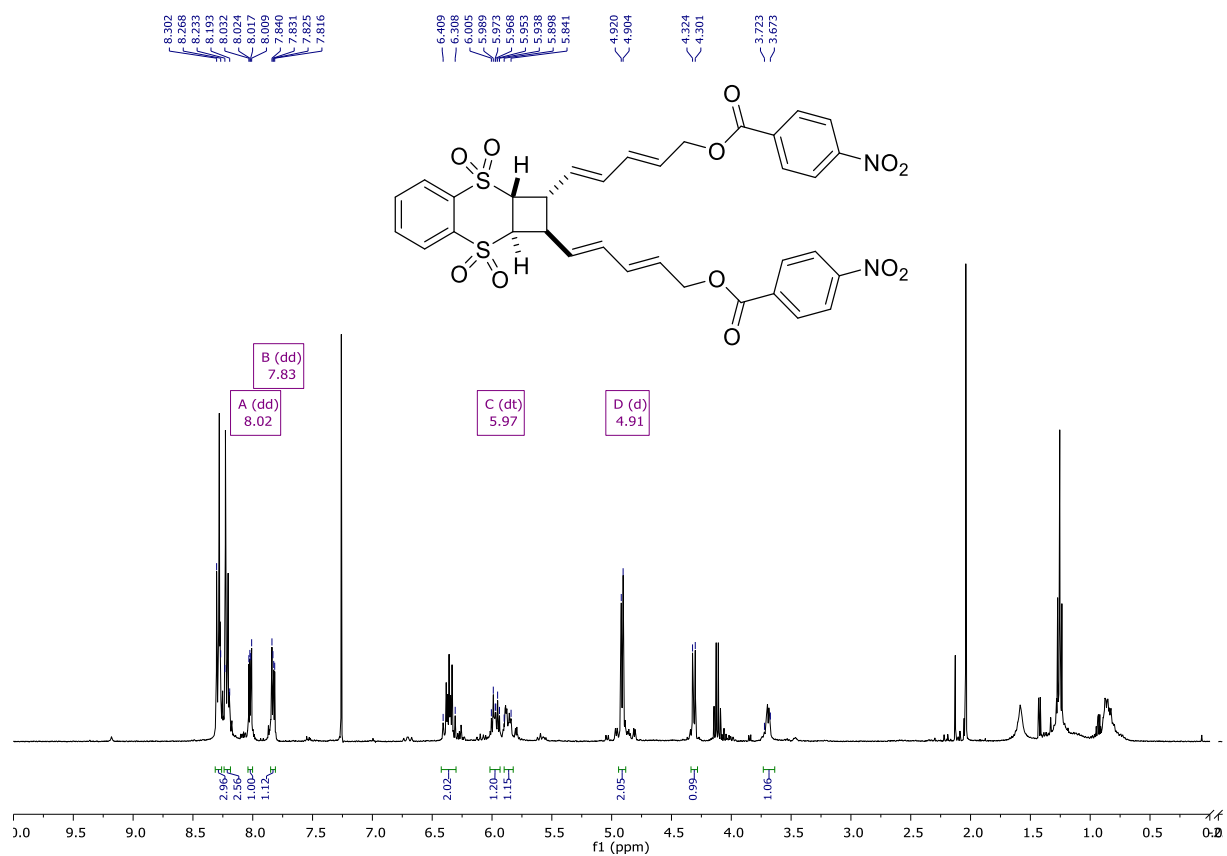
<sup>1</sup>H-NMR (400 MHz) : Compound 9-O-sym



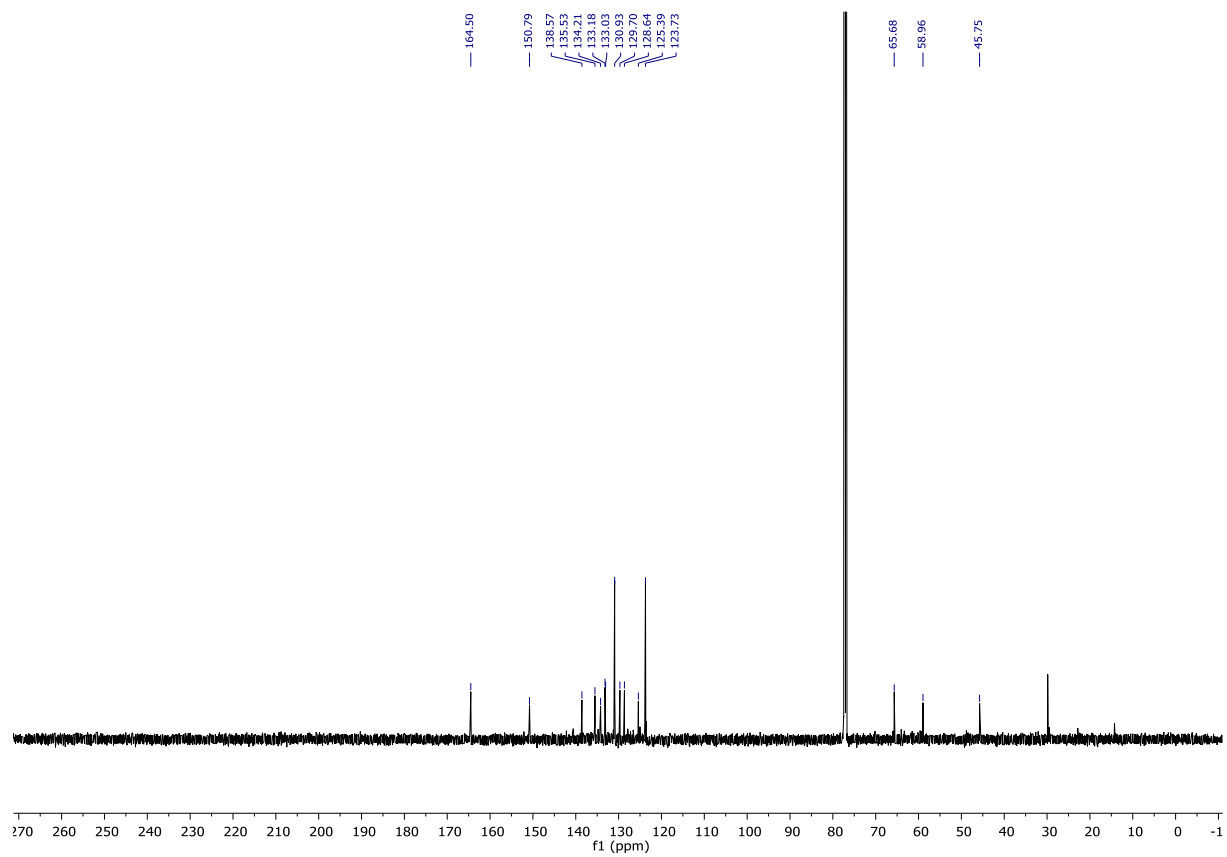
<sup>13</sup>C-NMR (100 MHz) : Compound 9-O-sym

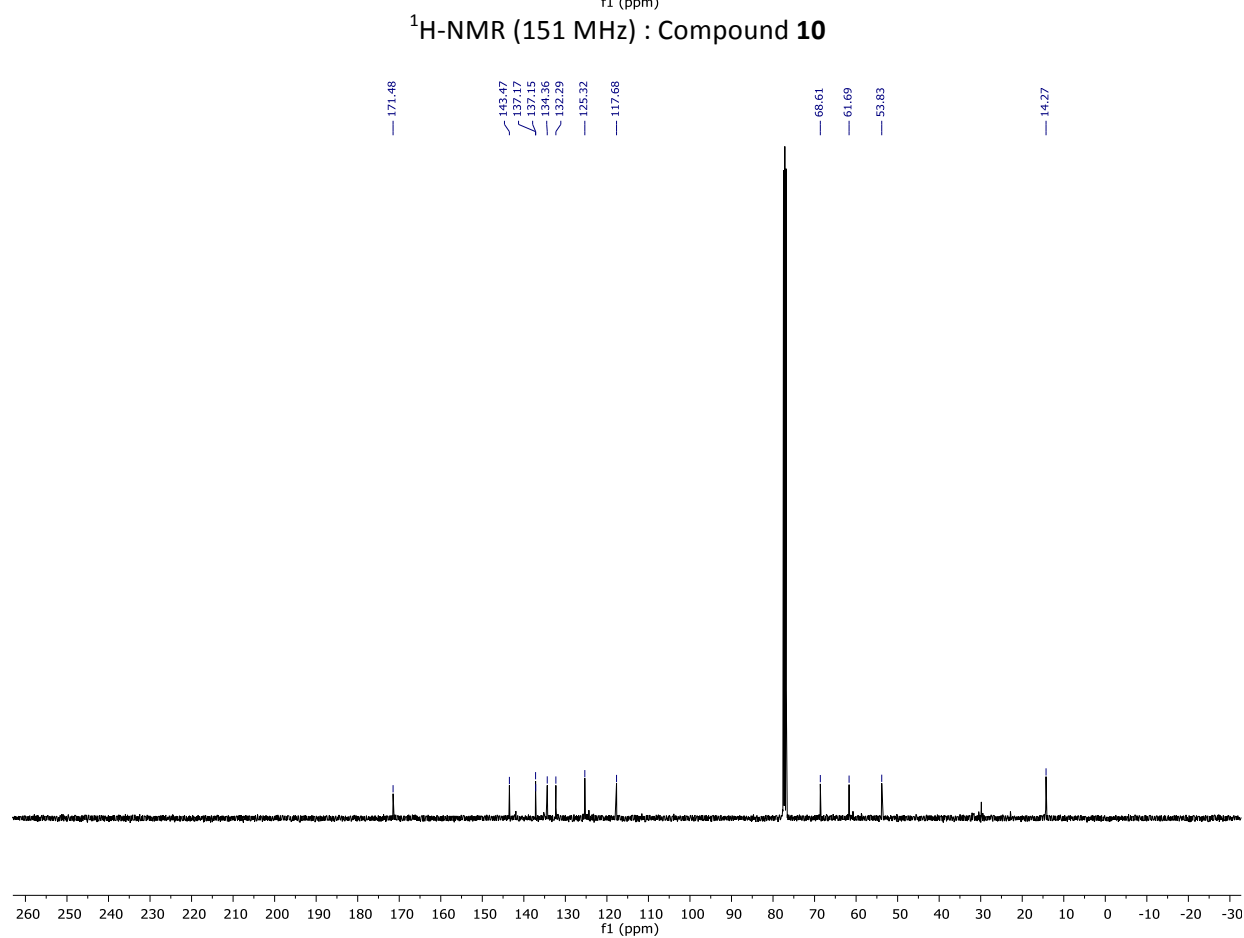
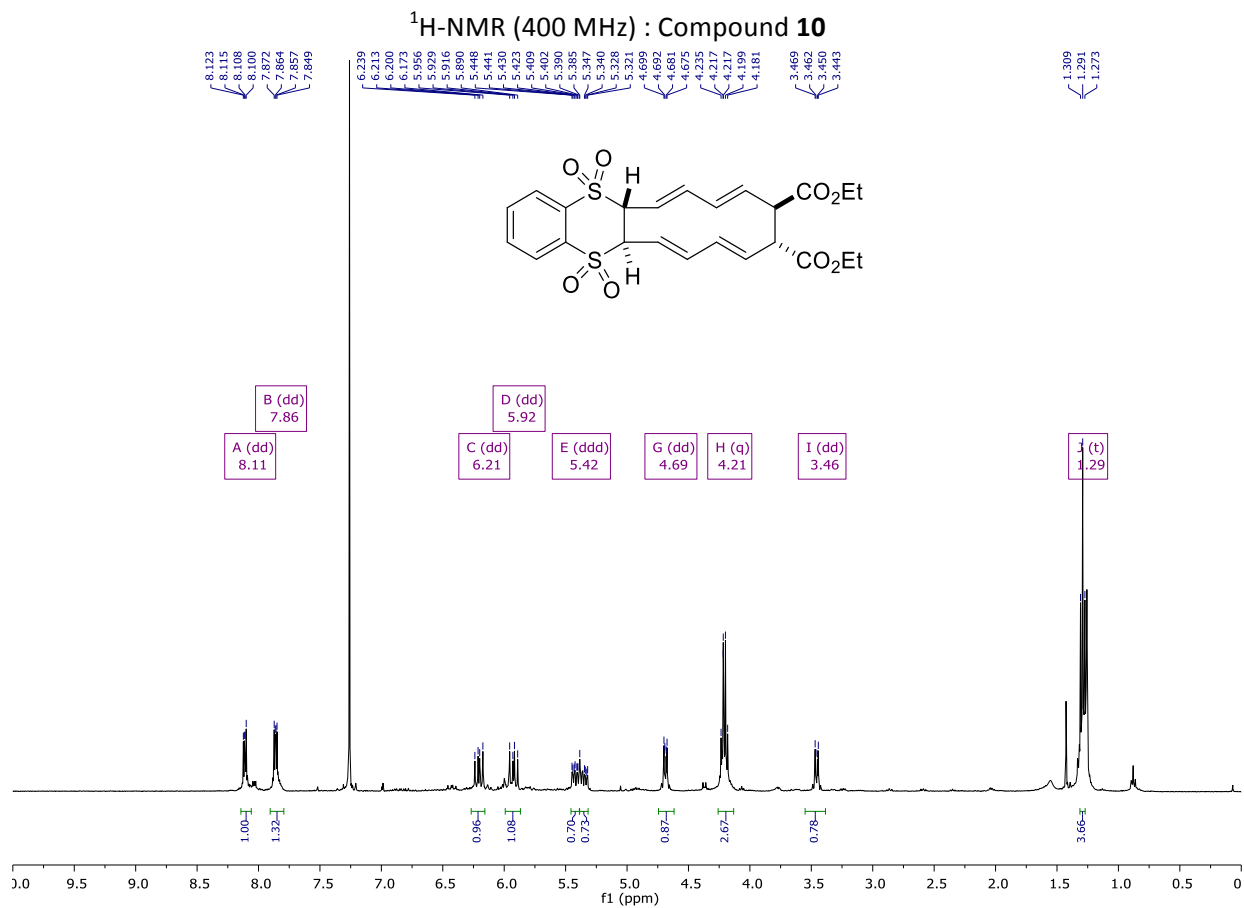


<sup>1</sup>H-NMR (400 MHz) : Compound **9-O-sym'-nitroester**



<sup>13</sup>C-NMR (100 MHz) : Compound **9-O-sym'-nitroester**





### 3. Crystal data: X-Ray crystal structure determination

A single crystal of each compound was selected, mounted onto a cryoloop, and transferred in a cold nitrogen gas stream. Intensity data were collected with a BRUKER Kappa-APEXII diffractometer with graphite-monochromated Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) or a copper microfocus source ( $\lambda = 1.54178 \text{ \AA}$ ). Data collection were performed with APEX2 suite (BRUKER). Unit-cell parameters refinement, integration and data reduction were carried out with SAINT program (BRUKER). SADABS (BRUKER) was used for scaling and multi-scan absorption corrections. In the WinGX suite of programs<sup>1</sup>, the structure were solved with either SUPERFLIP<sup>2</sup>, SHELXS<sup>3</sup> or SHELXT<sup>4</sup> programs and refined by full-matrix least-squares methods using SHELXL-14<sup>5</sup>. Specific details for each crystal structure refinements can be found in the cif files.

CCDC: 1535548 - 1535555

	7-OH	2-O
Chemical formula	C <sub>24</sub> H <sub>23</sub> NaO <sub>10</sub> S <sub>4</sub>	C <sub>14</sub> H <sub>14</sub> O <sub>8</sub> S <sub>2</sub>
$M_r$	622.65	374.37
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$
Temperature (K)	200	200
$a, b, c$ (Å)	6.2958 (1), 40.1116 (9), 10.5256 (2)	8.1214 (3), 9.7223 (3), 11.2597 (3)
$\alpha, \beta, \gamma$ (°) ou $\beta$ seul	97.680 (2)	81.884 (2), 85.392 (2), 71.440 (2)
$V$ (Å <sup>3</sup> )	2634.23 (9)	833.78 (5)
$Z$	4	2
Radiation type	Cu K $\alpha$	Cu K $\alpha$
$\mu$ (mm <sup>-1</sup> )	3.98	3.27

<sup>1</sup> L. J. Farrugia, *Journal of Applied Crystallography* **1999**, 32, 837–838.

<sup>2</sup> L. Palatinus, G. Chapuis, *Journal of Applied Crystallography* **2007**, 40, 786–790.

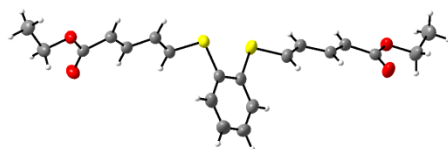
<sup>3</sup> G. M. Sheldrick, *Acta Cryst. A*, **2008**, 64, 112–122.

<sup>4</sup> G. M. Sheldrick, *Acta Crystallographica Section A*, **2015**, 71, 3–8.

<sup>5</sup> G. M. Sheldrick, *Acta Crystallographica Section C* **2015**, 71, 3–8.

Crystal size (mm)	0.12 × 0.10 × 0.08	0.15 × 0.07 × 0.02
Absorption correction	Multi-scan	Multi-scan
$T_{\min}, T_{\max}$	0.604, 0.753	0.629, 0.753
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	26845, 4834, 3506	14037, 3015, 2497
$R_{\text{int}}$	0.103	0.040
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.602	0.600
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.044, 0.106, 1.03	0.040, 0.113, 1.03
No. of reflections	4834	3015
No. of parameters	357	219
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	0.36, -0.25	0.40, -0.32

**4**



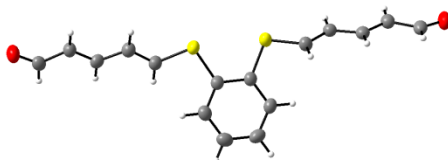
**4-O**



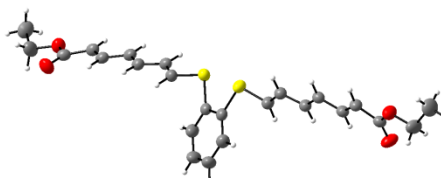
Chemical formula	$\text{C}_{20}\text{H}_{22}\text{O}_4\text{S}_2$	$\text{C}_{20}\text{H}_{22}\text{O}_8\text{S}_2$
$M_r$	390.49	454.49
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	200	200
$a, b, c$ ( $\text{\AA}$ )	5.9549 (2), 15.3259 (4), 21.7847 (6)	14.7042 (3), 19.2230 (5), 8.1062 (2)
$\alpha, \beta, \gamma$ ( $^\circ$ ) ou $\beta$ seul	93.458 (2)	95.2651 (11)
$V$ ( $\text{\AA}^3$ )	1984.54 (10)	2281.62 (9)
$Z$	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	2.61	2.49
Crystal size (mm)	0.24 × 0.17 × 0.12	0.38 × 0.09 × 0.07
Absorption correction	Multi-scan	Multi-scan
$T_{\min}, T_{\max}$	0.646, 0.753	0.426, 0.585
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	17607, 3572, 3001	15366, 4031, 3789
$R_{\text{int}}$	0.024	0.023

$(\sin \theta/\lambda)_{\max}$ ( $\text{\AA}^{-1}$ )	0.600	0.602
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.032, 0.089, 1.05	0.030, 0.079, 1.06
No. of reflections	3572	4031
No. of parameters	237	274
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ( $\text{e \AA}^{-3}$ )	0.23, -0.21	0.33, -0.31

**5**

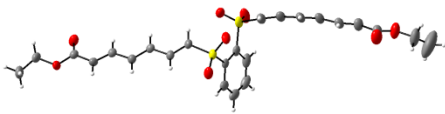
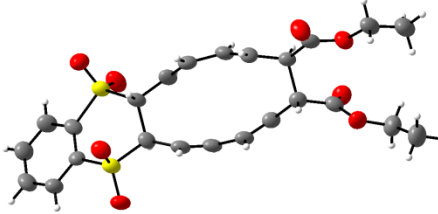


**6**



Chemical formula	$\text{C}_{16}\text{H}_{14}\text{O}_2\text{S}_2$	$\text{C}_{24}\text{H}_{26}\text{O}_4\text{S}_2$
$M_r$	302.39	442.57
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Temperature (K)	200	200
$a, b, c$ ( $\text{\AA}$ )	13.8437 (4), 12.6589 (4), 8.7099 (2)	6.0710 (3), 15.0757 (9), 25.2963 (14)
$\alpha, \beta, \gamma$ ( $^\circ$ ) ou $\beta$ seul	100.811 (2)	92.595 (3)
$V$ ( $\text{\AA}^3$ )	1499.28 (7)	2312.9 (2)
$Z$	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	3.20	2.31
Crystal size (mm)	0.42 $\times$ 0.04 $\times$ 0.04	0.66 $\times$ 0.4 $\times$ 0.04
Absorption correction	Multi-scan	Multi-scan
$T_{\min}, T_{\max}$	0.418, 0.521	0.608, 0.753
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	8954, 2649, 2126	22816, 4187, 3467
$R_{\text{int}}$	0.028	0.030
$(\sin \theta/\lambda)_{\max}$ ( $\text{\AA}^{-1}$ )	0.601	0.601
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.039, 0.101, 1.12	0.033, 0.091, 1.03
No. of reflections	2649	4187
No. of parameters	181	274
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ( $\text{e \AA}^{-3}$ )	0.22, -0.19	0.22, -0.19



	<b>6-O</b>	<b>10</b>
		
Chemical formula	$C_{24}H_{26}O_8S_2$	$C_{24}H_{26}O_8S_2$
$M_r$	506.57	506.57
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$
Temperature (K)	200	200
$a, b, c$ (Å)	7.2168 (2), 16.2188 (4), 25.3953 (6)	22.865 (6), 20.080 (4), 10.665 (2)
$\alpha, \beta, \gamma$ (°) ou $\beta$ seul	100.650 (1), 92.438 (1), 101.714 (1)	93.607 (18)
$V$ (Å <sup>3</sup> )	2850.50 (13)	4886.8 (19)
$Z$	4	8
Radiation type	Mo $K\alpha$	Cu $K\alpha$
$\mu$ (mm <sup>-1</sup> )	0.23	2.38
Crystal size (mm)	0.15 × 0.08 × 0.07	0.13 × 0.11 × 0.03
Absorption correction	Multi-scan	Multi-scan
$T_{min}, T_{max}$	0.7, 0.745	0.597, 0.75
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	48777, 13088, 8204	29958, 5475, 4050
$R_{int}$	0.034	0.079
$(\sin \theta/\lambda)_{max}$ (Å <sup>-1</sup> )	0.651	0.530
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.055, 0.153, 1.04	0.083, 0.238, 1.07
No. of reflections	13088	5475
No. of parameters	617	714
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.70, -0.54	0.77, -0.49

#### 4. Computational data

##### NON SUBSTITUTED

##### 1) Acyclic (Monomer)

C,0,-0.0093885685,-0.0022316765,0.0048922532  
C,0,0.0109530854,0.0025897579,1.3472496057  
C,0,1.2181692509,0.0032302984,2.1498860907  
C,0,1.2342238763,0.0080411274,3.5015958882  
C,0,2.4415814912,0.0089157996,4.3041443526  
C,0,2.4623254306,0.0136609223,5.6464032045  
H,0,0.9088383374,-0.0060928134,-0.5767318342  
H,0,-0.9405887529,-0.002734429,-0.5514943411  
H,0,-0.9326148766,0.0061337463,1.8928188578  
H,0,2.1658367224,-0.0004079247,1.6105068418  
H,0,0.2867058847,0.0116248606,4.0412654691  
H,0,3.3849887852,0.005138949,3.7582278414  
H,0,1.5443417343,0.0171441463,6.2284333295  
H,0,3.3937520896,0.0137436157,6.2024202261

##### 2) Mono1

C,0,0.1784611244,-0.1227046361,-0.231758383  
C,0,0.0999838559,0.0977231813,1.0884675282  
C,0,1.1924300498,-0.1092348749,2.0266922471  
C,0,1.1074491334,0.1103191999,3.3503966869  
C,0,2.2138942062,-0.1032734687,4.324565792  
C,0,2.6497338703,1.0623518486,5.3128462733  
C,0,1.581897027,2.0487830791,5.6559895407  
C,0,1.6850542992,3.3801294952,5.502777773  
C,0,0.6411044546,4.3300391636,5.8562256106

C,0,0.7383920155,5.6586610062,5.704884968  
C,0,1.9795273756,-1.0044993375,5.5755457073  
C,0,2.8607938831,-0.0393386956,6.4036984513  
H,0,2.2877265773,-2.0510178666,5.4977528123  
H,0,0.9323889807,-0.9792777672,5.8953774157  
H,0,3.9044135283,-0.3653277362,6.4440915272  
H,0,2.5336855073,0.2052482635,7.4181230939  
H,0,3.5509354615,1.5961461036,4.9943014389  
H,0,3.1096662851,-0.4460449241,3.7942475938  
H,0,0.1617762146,0.4693550238,3.7584278385  
H,0,0.6572007458,1.6471223437,6.0750609359  
H,0,2.6043434383,3.7971373638,5.0899497274  
H,0,2.1335180049,-0.4667066751,1.6063537455  
H,0,-0.8373029162,0.4585785759,1.5120705424  
H,0,-0.274682276,3.9082558139,6.2709249168  
H,0,1.6334795934,6.1194519205,5.2948613638  
H,0,-0.070542232,6.3256658972,5.9836397878  
H,0,-0.6666319498,0.0486209912,-0.8901584859  
H,0,1.0941764866,-0.4815651994,-0.694865863

### 3) Mono2

C,0,-0.1655534547,0.0527154563,0.0785366717  
C,0,-0.0915532612,0.0717094172,1.4103224698  
C,0,2.9158921345,0.0738215497,4.0299410118  
C,0,1.6049943083,0.3033259067,3.9404923086  
C,0,0.9911362969,1.5378349617,3.3578595284  
C,0,-0.1038574337,1.3080716167,2.2477123639  
C,0,-1.2040162244,1.4630501726,3.3535966237  
C,0,-0.1320364487,2.1691171774,4.2681403697

C,0,-0.1388801712,3.665787708,4.2526514156  
C,0,-2.4826963059,2.1525315789,3.0077958331  
C,0,-0.1918079428,4.438572704,5.33853154  
C,0,-3.6968968935,1.6150417189,3.1355093893  
H,0,-0.2308652867,0.9702400831,-0.5017248996  
H,0,-0.1649543227,-0.8774289981,-0.4818564933  
H,0,-0.0267171098,-0.8740232222,1.9484086029  
H,0,3.3078655603,-0.8354586013,4.4755926136  
H,0,3.6456069099,0.78976046,3.6595658989  
H,0,0.9149607863,-0.4458835032,4.3317493729  
H,0,-0.1257398575,2.1872466936,1.5928803522  
H,0,1.7841364097,2.232617231,3.0628365497  
H,0,-1.4288409757,0.4773211152,3.7778952989  
H,0,-0.1312384392,1.8171856384,5.3048461681  
H,0,-2.3929761657,3.1651628665,2.6145025763  
H,0,-3.8366971916,0.6087854116,3.5237385932  
H,0,-0.0781911182,4.1432018015,3.2733975237  
H,0,-0.2486249959,4.0132025296,6.337559099  
H,0,-4.5954534128,2.157419152,2.8568889642  
H,0,-0.1801346923,5.5221776802,5.2699990827

#### 4) Mono3

C,0,-0.0012575731,0.0227663915,-0.010866064  
C,0,-0.0088802786,0.0091205275,1.3230115238  
C,0,1.2028719636,0.0039772442,2.1933929165  
C,0,1.3410042027,-1.0958190631,3.3024738518  
C,0,2.0867196453,-2.3500618705,2.9915561072  
C,0,1.6211358772,-3.5880866378,3.1647883217  
C,0,1.3346488874,1.0827032356,3.3236692027

C,0,2.0735020942,2.3470427467,3.0382617704  
C,0,1.6033302887,3.578710879,3.2417485277  
C,0,2.01501949,-0.0134211693,4.2149004866  
C,0,1.742164735,-0.0288297937,5.6816314923  
C,0,2.6705091055,-0.0370344827,6.6395352385  
H,0,0.608219521,3.748790014,3.645758687  
H,0,2.1929793838,4.4613995862,3.0132072721  
H,0,3.0786663304,2.2235995583,2.6308673535  
H,0,0.9283542567,0.0313115111,-0.5749101654  
H,0,-0.9207505451,0.0259684137,-0.5884295391  
H,0,-0.9659586357,0.00104138,1.8478926704  
H,0,2.1106862794,0.0125876131,1.5765358512  
H,0,0.3389327027,1.309963191,3.7256752877  
H,0,3.0973291505,-0.0084020759,4.0324180753  
H,0,0.3466223225,-1.3365951253,3.6998862355  
H,0,3.7320131714,-0.0326403307,6.4037712453  
H,0,2.4061295942,-0.0484967815,7.6926405522  
H,0,0.6879191732,-0.0338590967,5.9646625314  
H,0,3.0926476951,-2.2129947643,2.5904513058  
H,0,0.6253728524,-3.7716624366,3.5612171192  
H,0,2.2153033422,-4.4627521294,2.9178414017

##### 5) Tric

C,0,0.0950217541,0.1059208748,-0.0153997843  
C,0,0.1349639397,-0.0736863624,1.5310235959  
C,0,1.6446673638,0.115477968,-0.0672954976  
C,0,1.68645667,-0.0872119289,1.5022660406  
C,0,2.2739872753,1.515190979,0.1018392726  
C,0,2.3330900625,1.3034305972,1.6601268456

C,0,3.8326302552,1.5342635381,0.0348349371  
C,0,3.8937491208,1.2917380335,1.6049505876  
C,0,4.4290954188,2.8038164213,-0.4874402633  
C,0,4.5770917176,2.3270672273,2.4419274318  
C,0,5.3653451747,2.8731236311,-1.4348374031  
C,0,5.5747385123,2.0818394819,3.2926093663  
H,0,-0.3479021362,-0.7479187362,-0.536252733  
H,0,-0.3026918643,-1.016685033,1.8708520806  
H,0,-0.3903146979,1.0150463626,-0.3864922391  
H,0,-0.3088942521,0.7351576366,2.1211773988  
H,0,2.1225079573,-0.5558951406,-0.7876362022  
H,0,2.1840775233,-0.9246309991,2.0012866952  
H,0,1.7616033716,2.3504449006,-0.3863849918  
H,0,4.316602734,0.3093285673,1.8453424928  
H,0,4.2493954494,0.690460726,-0.527429209  
H,0,1.8838572394,1.9841215019,2.390553257  
H,0,4.0428189191,3.73189541,-0.0647085207  
H,0,4.2059725323,3.3483096527,2.3513289928  
H,0,5.7799936613,1.9779124957,-1.8923237489  
H,0,5.9782224003,1.0804923344,3.4236555226  
H,0,5.753861611,3.8241927057,-1.7867040735  
H,0,6.0267026888,2.8703025101,3.8870432675

## 6) Pent

C,0,-0.003456779,0.0042192774,-0.0002958454  
C,0,-0.0038188135,0.0041926262,1.5573624901  
C,0,1.5474872641,-0.000439466,-0.0108933264  
C,0,1.5471198353,-0.0005309537,1.5686921684  
C,0,2.1815066088,1.4045684481,-0.0152133478

C,0,2.181133635,1.4044479623,1.5734884419  
C,0,3.7215488917,1.3836887646,-0.0149035973  
C,0,3.7211841809,1.3833962815,1.5738949069  
C,0,4.3553745252,2.7887937683,-0.0098960161  
C,0,4.3552585828,2.7883001778,1.5696790747  
C,0,5.9062977426,2.7846276538,0.0010921984  
C,0,5.9062510329,2.7834089707,1.5587813856  
H,0,-0.4437981593,-0.898657112,-0.4333125928  
H,0,-0.4444115424,-0.8986458672,1.9902015777  
H,0,-0.4685904885,0.8703754828,-0.4833070156  
H,0,-0.4691093433,0.8703900335,2.0401412484  
H,0,2.0363027699,-0.7636938218,-0.62457049  
H,0,2.0356040312,-0.7638856451,2.1825111848  
H,0,1.6969659437,2.164196029,-0.6398106308  
H,0,1.6963776651,2.1640274349,2.1979803923  
H,0,4.2063598457,0.6242312013,-0.6394903209  
H,0,4.2055477842,0.6236018941,2.1984259722  
H,0,3.8664950749,3.5521251141,-0.623422273  
H,0,3.8667553416,3.5515697187,2.1835844351  
H,0,6.37197333,1.9191253306,-0.4825259604  
H,0,6.3711070715,1.9165759175,2.0407886398  
H,0,6.3469431956,3.6857070688,1.9926081554  
H,0,6.3462592929,3.6881451566,-0.4309671781

## SULFONE

### 1) Acyc

C,0,-2.4972890521,0.50143948,0.3771432591  
C,0,-2.499793902,-0.9016764223,0.2398749197  
C,0,-3.2857278061,-1.6795296277,1.0990484528

C,0,-4.0495843233,-1.0899260864,2.104026209  
C,0,-4.0290975754,0.2923572242,2.2582505496  
C,0,-3.264901662,1.0767646405,1.3954941644  
S,0,-1.5007425765,-1.9121455465,-0.9060974921  
H,0,-3.306902702,-2.7538534279,0.954815237  
H,0,-4.6563160855,-1.7119747699,2.7544225203  
S,0,-1.7610345442,1.7658222655,-0.7491911352  
O,0,-2.3346120174,1.5650742462,-2.0826889649  
O,0,-1.9650268522,3.0481869672,-0.0466043136  
C,0,-0.0085280008,1.4858861917,-0.8022237309  
H,0,0.2850003023,0.6426205498,-1.4131936322  
C,0,0.822627017,2.3529546828,-0.1955758819  
H,0,0.385738522,3.1788328822,0.362448271  
C,0,2.2633343495,2.2636845563,-0.2460027386  
H,0,2.699902138,1.4383258059,-0.8062788574  
C,0,3.0773218981,3.1554165953,0.3661194136  
H,0,2.6302203752,3.9801391985,0.9210749297  
C,0,4.5240164904,3.0969208204,0.3363481259  
H,0,4.9686274605,2.2722158494,-0.2193577967  
C,0,5.3219328025,3.9891694604,0.9446096356  
H,0,6.4028764313,3.912265771,0.8979483986  
H,0,4.913647337,4.8251160945,1.5063644224  
H,0,-3.2613609072,2.1563705244,1.4862589386  
H,0,-4.6144638455,0.7691331582,3.0382471346  
O,0,-2.2943596642,-3.1205543863,-1.1773595792  
O,0,-0.9828709191,-1.0976051833,-2.0143387176  
C,0,-0.1274401912,-2.3902446167,0.1205350696  
C,0,1.1365150369,-2.2322075826,-0.3100853025  
H,0,-0.401915035,-2.8831029299,1.0479151097



C,0,2.3085065049,-2.6705075858,0.4107732806  
H,0,1.2891829167,-1.7501142759,-1.2742623582  
C,0,3.5659290245,-2.5206123876,-0.0679337553  
H,0,2.1582770722,-3.1437795164,1.3799053336  
C,0,4.762177739,-2.947716556,0.6274939588  
H,0,3.7054668911,-2.0535548481,-1.0430875661  
C,0,6.0037733663,-2.802111568,0.1375930592  
H,0,4.6218471737,-3.4121938813,1.6026364055  
H,0,6.8763462452,-3.1360979222,0.6884799553  
H,0,6.1817305671,-2.3463778438,-0.8328999318

## 2) Mono1

C,0,-3.9501965612,-1.35074938,-1.8983592353  
C,0,-2.9756982519,-1.9248813436,-1.0814051198  
C,0,-2.2592811495,-1.121725994,-0.1938445054  
C,0,-2.4973583779,0.2592906627,-0.1498159544  
C,0,-3.4485674182,0.8353261435,-0.9909106221  
C,0,-4.1873356073,0.0235391185,-1.8522201786  
S,0,-1.0824836956,-1.9633066377,0.8973550486  
O,0,-0.6376447911,-3.1694894851,0.1804273958  
S,0,-1.5893061286,1.3603522945,0.959894137  
O,0,-2.0605849697,1.1850861306,2.3383575483  
C,0,0.3460124222,-0.8229549518,1.0095920624  
C,0,1.2929736623,-0.794061344,-0.2336323996  
C,0,2.7397862008,-0.9647921676,0.1003556276  
C,0,1.8252168322,1.7346215647,-0.8407963489  
C,0,1.8247574537,2.9898139136,-0.3628713718  
C,0,2.8249546257,3.9891096386,-0.7100461368  
C,0,2.8210328892,5.2472020851,-0.2480284522

O,0,-1.6666620152,-2.0691487473,2.2388729093  
C,0,3.5374488286,-1.8934553159,-0.4536607895  
C,0,4.9443620599,-2.0659162165,-0.1250816327  
C,0,5.7362592688,-2.994565501,-0.6791836706  
C,0,0.0981018511,0.7017369242,0.8485936682  
C,0,0.8045322193,0.6830074169,-0.5311506558  
O,0,-1.591717732,2.6939469126,0.3353053008  
H,0,-3.5873139694,1.9107913211,-0.9693181505  
H,0,-4.9368835987,0.4694505042,-2.4981495096  
H,0,0.7991762777,-1.1223652956,1.9577514179  
H,0,1.0024366118,-1.5136801077,-1.0030682516  
H,0,3.1573139706,-0.2840525254,0.8431085861  
H,0,3.1223731817,-2.5749706051,-1.196536605  
H,0,5.3563587069,-1.3862559363,0.6203072301  
H,0,6.7814223761,-3.089967735,-0.4048744151  
H,0,5.3597674416,-3.6905678795,-1.4242567505  
H,0,-2.7551010373,-2.9857961875,-1.1264631973  
H,0,-4.5149670154,-1.978585946,-2.5801277289  
H,0,0.641383363,1.2773322149,1.6035155255  
H,0,0.0610150048,0.6404967257,-1.3384790472  
H,0,2.6057660307,1.4293342432,-1.5377048684  
H,0,1.0281497282,3.3106722447,0.307405974  
H,0,3.6149451955,3.6705852912,-1.3899313649  
H,0,3.5856508177,5.9617432463,-0.5339918905  
H,0,2.0476972988,5.6008227062,0.4287764214

### 3) Mono2

C,0,-0.8357421495,0.0776727069,0.4647027058  
C,0,-0.3319580437,0.1777490545,1.765527655

C,0,0.986040217,-0.2519278255,2.0421675817  
C,0,1.7514327627,-0.7711068101,0.9937313045  
C,0,1.2426282245,-0.8582570931,-0.302475284  
C,0,-0.0540484947,-0.4343189232,-0.5698825755  
S,0,-1.5084152752,0.9518729138,2.9326387972  
C,0,-2.1341754236,-0.3599555661,3.9692945604  
C,0,-1.8268626968,-1.6513538941,3.8422346743  
C,0,-1.8552505805,-2.6075724966,4.9881469605  
C,0,-1.6450388014,-4.1318467465,4.7514575346  
C,0,-2.8365341168,-5.0341548205,4.7645863249  
C,0,-3.1674358458,-5.8654799015,3.7757616216  
S,0,1.9632736362,-0.1738978494,3.6226290765  
C,0,0.8500377036,-0.7444843804,4.889959304  
C,0,0.653576986,-2.0542804266,5.0726838826  
C,0,-0.5020994833,-2.6002269905,5.855588968  
C,0,-0.6091320048,-4.1580526866,5.9469208492  
C,0,-1.1362959694,-4.6468631014,7.2615915942  
C,0,-0.5905654759,-5.6296928393,7.9780384053  
O,0,3.0009589699,-1.2075699962,3.4498182615  
O,0,2.3373262139,1.2161064317,3.8881676546  
O,0,-0.7518691584,1.812583925,3.8558068681  
O,0,-2.5989512215,1.5190802995,2.1262891225  
H,0,2.7554389845,-1.1150815937,1.2133187197  
H,0,1.8662483936,-1.2606782744,-1.094635809  
H,0,-2.6065317943,0.0642080105,4.8526771479  
H,0,-1.3141454958,-1.9864526814,2.9422749618  
H,0,-2.7020343508,-2.4119882785,5.6536624223  
H,0,-1.0928955935,-4.2747408434,3.8145255987  
H,0,-3.4668209642,-4.9893857749,5.6523017683

H,0,-4.0486138366,-6.497030988,3.8311859292  
H,0,-2.5667289658,-5.9465850366,2.8728788864  
H,0,-1.8445944081,0.4266842091,0.277254115  
H,0,-0.4624120294,-0.4960411716,-1.5734671621  
H,0,0.2947038579,0.0550410715,5.3658163001  
H,0,1.2729031354,-2.751651387,4.5094428681  
H,0,-0.6155258458,-2.0653489272,6.8030731168  
H,0,0.3175989689,-4.689047846,5.7067447802  
H,0,-2.0233553444,-4.1433878938,7.6488233425  
H,0,-1.0078884337,-5.9404899302,8.9306847652  
H,0,0.2953787498,-6.1593546485,7.6368234724

#### 4) Mono3

C,0,3.1050452225,-1.3459359947,2.6413757913  
C,0,2.7418700556,-1.7695219659,1.3643394096  
C,0,2.2831013906,-0.8572739774,0.4074480067  
C,0,2.1882732093,0.5136435984,0.7312182206  
C,0,2.5529597421,0.9189315312,2.0194334146  
C,0,3.0074139883,0.0024781991,2.9676301144  
S,0,1.8828091444,-1.6394423305,-1.1915802146  
O,0,2.6400924779,-2.8994023698,-1.2468647726  
S,0,1.7472872712,1.9585462617,-0.3500297128  
O,0,2.7869067125,2.1181574314,-1.368290618  
C,0,0.148167483,-2.0345050871,-1.1310029121  
C,0,-0.6983313393,-1.7896164291,-0.1188791138  
C,0,-2.1423232957,-1.856170895,-0.2631775301  
C,0,-2.2550685065,1.4806544724,-0.9752060248  
C,0,-3.3345032863,1.492751146,-0.1685481786  
C,0,-4.5329978184,0.6303604228,-0.3935109453

C,0,-5.7532831797,0.8534892862,0.5433959134  
O,0,2.034990308,-0.6540770735,-2.2727671634  
C,0,-2.9741663624,-1.2328024901,0.5924328839  
C,0,-4.3742753532,-0.8384610891,0.2774695676  
C,0,-5.3330346137,-0.3665460617,1.4025255621  
C,0,0.1976326593,1.5462240745,-1.1112585055  
C,0,-0.9532106483,1.9525301691,-0.5456563127  
O,0,1.4773684629,3.0493074364,0.6075994319  
H,0,2.473876934,1.9715632187,2.2640990116  
H,0,3.2864055239,0.3517773389,3.9569412132  
H,0,-0.1757337877,-2.4064267248,-2.1002197376  
H,0,-0.3162186064,-1.3925159756,0.8192764768  
H,0,-2.5315342846,-2.2716018854,-1.1922171326  
H,0,-2.5460728032,-0.8016035241,1.498366386  
H,0,-4.8496251937,-1.5671467393,-0.3871711158  
H,0,-6.1181946378,-1.0650218663,1.7037148747  
H,0,-4.7798997782,-0.0682239757,2.2995674489  
H,0,2.8289724135,-2.8124533494,1.0822794234  
H,0,3.46451089,-2.0684014243,3.3671347365  
H,0,0.2877962236,0.9199245481,-1.9900900148  
H,0,-0.9012220873,2.5698859797,0.3493512447  
H,0,-2.299027069,0.938152832,-1.9184134626  
H,0,-3.2654933208,2.0147279081,0.7873344093  
H,0,-4.756415468,0.5652510598,-1.4630043433  
H,0,-6.7004010766,0.6938213624,0.0213808529  
H,0,-5.8008675958,1.8220089522,1.0494634169

5) Tric1

C,0,0.1629117334,0.7805931552,-1.2688605099

S,0,1.7199996596,1.6729805612,-0.940045829  
C,0,2.4837709107,0.7007605894,0.3791010185  
C,0,2.4837613445,-0.7007790636,0.3792149131  
S,0,1.7199761992,-1.6732039322,-0.9397733187  
C,0,0.1629009094,-0.7808483117,-1.2687368148  
C,0,3.0967274003,1.4011954176,1.417456196  
C,0,3.7370678446,0.6978816495,2.4382469623  
C,0,3.7370581463,-0.6975826448,2.4383604618  
C,0,3.0967079899,-1.4010535142,1.4176840666  
O,0,1.3604566136,-2.9741658255,-0.3532917514  
O,0,2.5500151859,-1.6062143524,-2.1470834348  
O,0,2.5500376075,1.6057808758,-2.1473448931  
O,0,1.3604991025,2.9740438475,-0.3537778168  
C,0,-0.8673836804,-0.7886004322,-0.1126844213  
C,0,-0.867367882,0.7885432409,-0.112804436  
C,0,-2.333546849,0.78718415,-0.5988399688  
C,0,-3.3796380655,0.7952399364,0.5601517558  
C,0,-4.6693097585,1.4885603584,0.2478489522  
C,0,-5.2425257417,2.4064252458,1.0268131862  
C,0,-2.3335602708,-0.7872875973,-0.5987334829  
C,0,-3.3796705559,-0.7951746471,0.56023867  
C,0,-4.669367378,-1.4884648965,0.2479691441  
C,0,-5.2426798094,-2.4061822359,1.0270360944  
H,0,3.0545940619,2.4849216698,1.417340015  
H,0,4.2242475991,1.2429180306,3.2404674872  
H,0,-0.1640975245,-1.2338363921,-2.2098224774  
H,0,-0.6179603565,-1.4120642131,0.7484881666  
H,0,-2.5704464103,-1.4066277086,-1.468379904  
H,0,-2.9766409019,-1.2036679813,1.4937682564

H,0,-5.1488673674,-1.2243290118,-0.694611791  
H,0,-6.1743872449,-2.8895095923,0.7494884591  
H,0,-4.8001907186,-2.7070626931,1.9736439847  
H,0,3.05455909,-2.484779143,1.4177441574  
H,0,4.2242302091,-1.2424952618,3.2406697249  
H,0,-0.1640859218,1.2334354155,-2.210016626  
H,0,-0.6179265527,1.4121328017,0.7482719067  
H,0,-2.5704410476,1.4064105928,-1.4685649727  
H,0,-2.9765614672,1.2038111119,1.4936270628  
H,0,-5.1488741397,1.2243179844,-0.69466896  
H,0,-6.1742167273,2.8897713528,0.7492430059  
H,0,-4.7999702356,2.7074134631,1.9733557608

6) Tric2

C,0,3.2537289339,-0.9689183943,2.7197632181  
C,0,2.8140359396,-1.5386346232,1.5256167858  
C,0,2.3315771147,-0.7418769312,0.4823907176  
C,0,2.281958729,0.6622537662,0.6391089716  
C,0,2.720492979,1.2147693839,1.8459829248  
C,0,3.2073144618,0.4113499691,2.8775911568  
S,0,1.8994487769,-1.7035735364,-1.01343758  
O,0,2.4167731315,-3.064240887,-0.8051937435  
S,0,1.7642511909,1.9774968623,-0.5686882123  
O,0,2.7631330849,2.0857689736,-1.6329145342  
C,0,0.1186938854,-1.7405616584,-1.109613819  
C,0,-0.7210329768,-1.2371965195,-0.2043970682  
C,0,-2.1043811941,-0.8020363828,-0.5507884497  
C,0,-2.1771917563,0.7831511182,-0.8623530128  
C,0,-3.2985284551,0.9153952393,0.1983699287

C,0,-4.729940429,0.6405341595,-0.3183509835  
C,0,-5.8326191453,0.8525503194,0.7494845347  
O,0,2.3080331324,-0.9337770112,-2.1982934313  
C,0,-3.1496064126,-0.6055095166,0.5834231553  
C,0,-4.5979840082,-0.8711176489,0.1326918006  
C,0,-5.6635681424,-0.6181602682,1.2330748929  
C,0,0.2268785305,1.388279506,-1.2508169009  
C,0,-0.9024995641,1.5116952959,-0.5464818  
O,0,1.4525684086,3.139586335,0.2841231938  
H,0,2.6651952132,2.2903139132,1.9670018318  
H,0,3.5453285694,0.8732741665,3.7999822152  
H,0,-0.1844509142,-2.025406564,-2.1147866466  
H,0,-0.3366015233,-0.9368919756,0.7688244911  
H,0,-2.4857872894,-1.3869042455,-1.3940071652  
H,0,-2.8497889838,-0.9588369829,1.5752254921  
H,0,-4.7638514622,-1.7270895566,-0.5282636596  
H,0,-6.5648960822,-1.2254017354,1.1159533742  
H,0,-5.3029602927,-0.7459708874,2.2589535955  
H,0,2.8563046268,-2.6110354768,1.3744801884  
H,0,3.6302375397,-1.6060893922,3.5135683624  
H,0,0.3478293986,0.8445570719,-2.1801035936  
H,0,-0.8610509133,2.0765173546,0.3845439871  
H,0,-2.4874879132,0.9793084743,-1.8947069006  
H,0,-3.1849198434,1.7385988458,0.9109941109  
H,0,-4.9528340189,0.9622086619,-1.3400909479  
H,0,-6.8153835499,1.0469046188,0.3114943397  
H,0,-5.6299107765,1.6370361588,1.4859051799

7) Pent



C,0,0.0048642769,0.187255371,-0.0034907966  
C,0,0.00967879,0.1972437257,1.5542125876  
C,0,1.5546304041,0.1307759595,-0.0188916519  
C,0,1.5595127533,0.1409084285,1.5607569518  
C,0,2.1293494373,-1.2996269553,-0.0163724122  
C,0,2.1342690345,-1.2894277989,1.5730322126  
C,0,3.6693185054,-1.3346144155,-0.0210063132  
C,0,3.6742423233,-1.3243934394,1.5685806938  
H,0,-0.3988206393,1.1040820926,-0.4417624259  
H,0,-0.4959011407,-0.6622707995,-0.4796724144  
H,0,-0.3913283813,1.1196300073,1.9831784243  
H,0,-0.4880980029,-0.6460874083,2.0443357933  
H,0,2.0720044258,0.868355801,-0.6397734652  
H,0,2.0806827997,0.8863733939,2.168916434  
H,0,1.6165540791,-2.0427769971,-0.6367745628  
H,0,1.6253628834,-2.0245422536,2.206081275  
H,0,4.1830894921,-0.6053881459,-0.6561418015  
H,0,4.1918872955,-0.587067375,2.1910938495  
S,0,6.5366342024,-4.2185791686,-0.8899902705  
S,0,6.5472492841,-4.1967062439,2.4568557133  
C,0,6.0252617493,-5.6467218584,0.0936864459  
C,0,6.0297153509,-5.6375689875,1.4952052348  
C,0,5.6261886561,-6.7898706279,-0.5978156883  
C,0,5.6350931905,-6.7715703321,2.2041035591  
C,0,5.2627446417,-7.9334252714,0.1141148097  
C,0,5.2671794358,-7.9243119527,1.5094958498  
H,0,5.5954983109,-6.7650389167,-1.6816275706  
H,0,5.611290799,-6.7325810204,3.2876718908  
H,0,4.9630900659,-8.8269376474,-0.4241806634

H,0,4.9709894021,-8.8107044832,2.0613101268  
O,0,5.8527752996,-4.3315934258,-2.1882895165  
O,0,7.9950654179,-4.0745630717,-0.8289508425  
O,0,5.8716734079,-4.2927155979,3.7608466848  
O,0,8.0052527016,-4.0535248582,2.3846560736  
C,0,5.786198503,-2.8117375707,-0.0042230237  
C,0,5.7910890957,-2.801582768,1.5575567525  
H,0,6.3003351115,-1.9408339846,2.0020021457  
H,0,6.2927013357,-1.9569322207,-0.4630402322  
C,0,4.2385310162,-2.7690607255,-0.0055161903  
C,0,4.2434466284,-2.75891508,1.568004954  
H,0,3.7473769197,-3.5016920741,2.196235104  
H,0,3.7385201383,-3.5198123038,-0.6210127244

## SULFUR

## 1) Acyc

C,0,-0.7527088426,-1.5174833468,1.2901995078  
C,0,-0.7925372515,-1.8608580947,2.6488481428  
C,0,0.417322847,-1.9603598292,3.3705231713  
C,0,1.629717792,-1.7134500694,2.7113385044  
C,0,1.656498025,-1.4125088622,1.3518731621  
C,0,0.4613822513,-1.3141993992,0.6389755927  
S,0,-2.3543678971,-2.1278425449,3.4860624699  
C,0,-3.3591958485,-2.7750879681,2.1892448354  
C,0,-4.6714464632,-2.4812535083,2.0717456612  
C,0,-5.5522769673,-3.1146015642,1.1186902539  
C,0,-6.8711369539,-2.8317012397,0.999041063  
C,0,-7.7547880303,-3.4594863183,0.0388007346  
C,0,-9.0640531429,-3.1851720658,-0.0817671305

S,0,0.382683327,-2.3531624263,5.1187145756  
C,0,1.9106586269,-3.2075695751,5.3324430084  
C,0,2.6628959673,-3.0825798752,6.4463014897  
C,0,3.8334561901,-3.883756474,6.716844198  
C,0,4.5893973486,-3.7705317977,7.8346377911  
C,0,5.768281181,-4.5670117527,8.1045751913  
C,0,6.5193568732,-4.4612948048,9.2130307918  
H,0,2.5557526627,-1.7594042804,3.2748769411  
H,0,2.6077487385,-1.2371856996,0.8586881019  
H,0,-2.8825911202,-3.5074346512,1.5412986921  
H,0,-5.1085392206,-1.7326052148,2.7310124418  
H,0,-5.1126488286,-3.8632076704,0.4593562989  
H,0,-7.3136708475,-2.0877995535,1.6617860905  
H,0,-7.3050812222,-4.2022875333,-0.6200126113  
H,0,-9.685516669,-3.6835796562,-0.8179240563  
H,0,-9.5514709711,-2.452131304,0.5556851333  
H,0,-1.6848456103,-1.4105735633,0.7453000182  
H,0,0.4693736626,-1.0612492885,-0.4168646166  
H,0,2.1669701152,-3.9220050419,4.5531992773  
H,0,2.3800551514,-2.3465168304,7.1975440214  
H,0,4.1150948718,-4.6194676848,5.9633066944  
H,0,4.3055915002,-3.0395688371,8.5920069788  
H,0,6.0455714498,-5.2956239876,7.3428301422  
H,0,7.3948770456,-5.0821417973,9.3697725922  
H,0,6.2772481393,-3.7483893592,9.9968779939

## 2) Mono1

C,0,-0.0573697765,-0.0686332139,0.1457378689  
S,0,0.0513252725,-0.0321625632,1.9712428699

C,0,1.8213727706,-0.0178414749,2.180633501  
C,0,2.6465581743,0.8350412539,1.4184720252  
S,0,1.9760451498,1.9927504596,0.2398383183  
C,0,0.7617809878,0.9693030365,-0.6714984873  
C,0,2.3966899711,-0.8418346288,3.1572119418  
C,0,3.7670477298,-0.7971445561,3.4057811457  
C,0,4.5848388195,0.0452530017,2.6500262146  
C,0,4.0291623846,0.8412978666,1.6506097339  
C,0,1.3088175855,-0.1780082909,-1.5960592876  
C,0,0.6245371815,-1.2288427133,-0.6269686317  
C,0,-0.2089096285,-2.3160917035,-1.2275185952  
C,0,-1.4844277453,-2.6120631418,-0.9265548849  
C,0,-2.2287226602,-3.7036271354,-1.5387908384  
C,0,-3.4962137536,-4.0191809535,-1.2378959734  
C,0,0.8131768946,-0.1323369762,-3.0023183295  
C,0,1.6018685918,-0.1010071644,-4.0907686006  
C,0,1.1091581815,-0.0395097051,-5.4583136841  
C,0,1.893501049,-0.0064385458,-6.5451516482  
H,0,1.7569917088,-1.5114592416,3.7239323374  
H,0,4.1958078923,-1.4314200681,4.1756441545  
H,0,0.1469227768,1.7063356159,-1.1953759589  
H,0,2.4000436778,-0.2425413148,-1.5825580477  
H,0,-0.2692754086,-0.1170174066,-3.1382755537  
H,0,2.684682998,-0.1212153783,-3.9627704983  
H,0,0.0264034651,-0.0204591982,-5.5816060508  
H,0,1.479084942,0.0392957118,-7.5466711726  
H,0,2.9773612653,-0.0231309108,-6.4641622244  
H,0,4.6612644662,1.4853284837,1.046885487  
H,0,5.655816505,0.0723359454,2.8266167927

H,0,-1.1270035391,0.0151219984,-0.0640579375  
H,0,1.4113683476,-1.6803420849,-0.0091992715  
H,0,0.3029349564,-2.9276712305,-1.9720389381  
H,0,-2.0167722044,-2.0289442221,-0.1758662087  
H,0,-1.6966464825,-4.2886831082,-2.2888143619  
H,0,-4.0089030223,-4.8439467058,-1.7214012029  
H,0,-4.0592631235,-3.4611984755,-0.4940651962

### 3) Mono2

C,0,0.411965203,-0.3086651472,-0.1933025338  
C,0,0.1505085831,-0.2859992277,1.1774468165  
C,0,1.1717748417,-0.0842490462,2.1163174431  
C,0,2.503289744,0.0902549354,1.6536709391  
C,0,2.7474642673,0.0557976909,0.273429241  
C,0,1.7160245273,-0.136327636,-0.6466855137  
S,0,0.6538360398,0.0550552181,3.8370669954  
S,0,3.9170244137,0.5079659948,2.6922442719  
C,0,1.2026531636,-1.4768793889,4.5624152399  
C,0,1.4355289379,-2.6196779697,3.9073348434  
C,0,2.3551254785,-3.6857982608,4.4127771804  
C,0,3.9085253286,-3.3804204581,4.1350304864  
C,0,4.0676498046,-4.8340934429,3.5761681463  
C,0,4.8450688896,-5.7473966729,4.4729484524  
C,0,5.8544568973,-6.5256041749,4.0809869236  
C,0,2.4937509837,-5.0009455939,3.584142838  
C,0,1.8815935171,-6.2508652007,4.130401584  
C,0,1.0140860583,-7.0236463108,3.4751846275  
C,0,4.2325119312,-0.97793324,3.6237059959  
C,0,4.079613384,-2.2353202128,3.1904173126

H,0,3.7663023181,0.1908450717,-0.0741393809  
H,0,1.9381661393,-0.1528636744,-1.7094544224  
H,0,1.4569955755,-1.3602639169,5.6140783886  
H,0,1.1796116004,-2.6717607429,2.8498500419  
H,0,2.2043813512,-3.8824940033,5.4803812178  
H,0,2.1153334031,-4.8352676265,2.5686213721  
H,0,2.1708488363,-6.5280941645,5.1441905763  
H,0,0.5912508428,-7.917328917,3.9242127847  
H,0,0.6942419737,-6.7898748067,2.4622999875  
H,0,-0.8638331516,-0.4181441452,1.5389643653  
H,0,-0.4019283794,-0.4619249594,-0.895457109  
H,0,4.4771261631,-0.7724496412,4.663802787  
H,0,3.8208739315,-2.4075694719,2.1459213988  
H,0,4.4654413726,-3.1938517635,5.0595806594  
H,0,4.4909941294,-4.8769796477,2.5669743911  
H,0,4.5603101697,-5.7499441717,5.5263676887  
H,0,6.3921059265,-7.1594188821,4.779695897  
H,0,6.1802116191,-6.5565280434,3.044075695

#### 4) Mono3

C,0,0.1351820754,-0.1102531618,-0.1901346373  
C,0,0.0350444415,-0.2839129621,1.1884155764  
C,0,1.190520409,-0.2643041685,1.9688462512  
C,0,2.4548408016,-0.0789183427,1.3921674007  
C,0,2.5599147864,0.0816212058,-0.0098186656  
C,0,1.3869480621,0.0657085387,-0.7788540954  
S,0,3.8619014248,0.0442692614,2.5062295255  
S,0,4.0875138925,0.442096552,-0.9044673298  
C,0,4.3807978466,-1.6356414805,2.7247270093

C,0,3.7775202069,-2.7609630375,2.3004545339  
C,0,4.4457764668,-4.0482040871,2.2442692853  
C,0,4.0041236632,-5.0623089883,1.4755442294  
C,0,4.8514331245,-6.1794009864,0.9729787874  
C,0,4.191952796,-7.3940327199,0.2654271575  
C,0,5.1925742266,-7.2713714399,-0.9128566304  
C,0,5.6404720382,-5.8691782817,-0.4111102489  
C,0,5.1079289179,-4.6717057413,-1.1275052012  
C,0,5.5495875384,-3.4214010603,-0.8910424842  
C,0,4.8258154107,-2.2131387563,-1.2429854141  
C,0,5.0883175736,-1.0204650298,-0.6755711476  
H,0,1.4700084758,0.1920456013,-1.8532055314  
H,0,-0.7555176739,-0.1163786615,-0.8114913493  
H,0,5.3554954883,-1.6716978253,3.2077750591  
H,0,2.8091615701,-2.6945490451,1.8094827295  
H,0,5.4283403973,-4.1199006759,2.7130703274  
H,0,3.035060144,-4.943833589,0.9882062624  
H,0,5.5867613936,-6.4902520377,1.7231266795  
H,0,4.1843742189,-8.3383325244,0.8173111399  
H,0,3.1630903477,-7.1717795918,-0.0376672445  
H,0,1.1228002931,-0.3802939204,3.04560819  
H,0,-0.9332159684,-0.4252918838,1.6587930788  
H,0,5.9347640714,-0.8977118542,-0.0055209054  
H,0,3.9649595759,-2.3146543656,-1.9026137826  
H,0,6.4321607679,-3.2883638726,-0.2652394038  
H,0,4.2025843099,-4.8050758868,-1.7223599309  
H,0,6.7164981955,-5.7554277416,-0.243286515  
H,0,6.0020494023,-8.0049410151,-0.8618450321  
H,0,4.7681307827,-7.3046771214,-1.9209566411

## 5) Tric1

C,0,0.004567465,0.000349821,0.0174445337

C,0,0.0271640106,0.0004117075,1.5616375797

C,0,1.4568067576,-0.0002137691,2.1692314882

C,0,1.466024235,1.5612186954,2.1678678885

C,0,0.0364627433,1.5764125044,1.5602722304

C,0,0.0138384394,1.5740658076,0.0160822582

S,0,1.6910984107,-0.8508173225,3.7762722492

C,0,0.6029568659,0.083356671,4.8338445135

C,0,0.611281557,1.4924035546,4.8326134184

S,0,1.7103737785,2.4118043372,3.773419274

C,0,-0.2306921011,-0.6007392053,5.7291022387

C,0,-1.0197707594,0.1007689914,6.6382544875

C,0,-1.0115208901,1.4973201017,6.6370331008

C,0,-0.2142181097,2.1878658297,5.7266639945

C,0,-1.4309086173,0.0003671272,-0.5974470961

C,0,-1.4215535909,1.5898936701,-0.5988038665

C,0,-1.5378487023,2.2810356291,-1.921515738

C,0,-2.4513376003,3.2063215224,-2.2179435042

C,0,-1.5553126142,-0.6916091989,-1.9189844068

C,0,-2.4796339556,-1.6065713471,-2.2138735088

H,0,-0.2173400449,3.2733449062,5.7061693795

H,0,-1.6358801773,2.0490432547,7.3333116717

H,0,2.2236076745,-0.4507162223,1.5303812438

H,0,-0.7152876281,-0.6074786026,2.0842004771

H,0,0.7454145334,-0.6216832209,-0.4946418905

H,0,-2.1872505844,-0.4030358123,0.0852637226

H,0,-0.8154055645,-0.4310586727,-2.6762162324



H,0,-2.5164483471,-2.0892182532,-3.1858594697  
H,0,-3.2360340414,-1.9055002705,-1.4921041673  
H,0,-0.2466387786,-1.6861399177,5.7105062999  
H,0,-1.6505974402,-0.4423209442,7.3354903664  
H,0,2.2380782565,2.0015179699,1.5282314383  
H,0,-0.6987532376,2.1939256676,2.0817815066  
H,0,0.7619510402,2.1864391701,-0.4970827862  
H,0,-2.1730751327,2.003330888,0.0832270301  
H,0,-0.8010943976,2.0104956325,-2.6783181392  
H,0,-2.4825025419,3.6877132421,-3.1907491362  
H,0,-3.2041344099,3.5153695358,-1.4966689724

6) Tric2

C,0,0.0900864117,0.091713371,-0.0251679429  
C,0,-0.0425975846,-0.303373594,1.4753368443  
C,0,1.5002452315,-0.2763986663,1.6315822275  
C,0,2.1905155116,-1.6225282588,1.3250963008  
C,0,2.3327629677,-1.2066169284,-0.1904194459  
C,0,1.6350348559,0.1357431101,0.1096552523  
C,0,3.8790883912,-1.1712662716,-0.055561897  
C,0,3.7327966165,-1.607365156,1.4958665412  
C,0,4.6588101356,-2.1750987267,-0.8431230314  
C,0,5.9903868899,-2.1310032273,-0.963648099  
S,0,7.0588100385,-3.4937396989,-1.3815053245  
C,0,4.4038842973,-2.915998385,1.767759189  
C,0,5.6893571439,-3.0151531003,2.1238080179  
S,0,6.7238247294,-4.4557235883,1.950805155  
C,0,6.1528924507,-4.9441379373,-0.8124431088  
C,0,5.6447539697,-5.785057928,-1.8124399702

C,0,5.0182980159,-6.9930266539,-1.5028039691  
C,0,4.8826116291,-7.3760226017,-0.172095388  
C,0,5.3748239359,-6.5480083377,0.837768589  
C,0,6.014855895,-5.3352685893,0.5461227621  
H,0,5.2735866976,-6.8410190514,1.8774383114  
H,0,4.3956773134,-8.3113713205,0.0868766482  
H,0,6.5529410342,-1.2391550726,-0.6947735955  
H,0,4.1397878441,-3.0955855035,-1.1077268466  
H,0,4.3170170134,-0.1712788264,-0.1600968837  
H,0,1.939157252,-1.7949356531,-1.0260955117  
H,0,2.1370315411,1.043413212,-0.2395675374  
H,0,-0.3529745531,1.0640838625,-0.2580825001  
H,0,-0.2906736541,-0.634647516,-0.7509496078  
H,0,5.7547878962,-5.4805820812,-2.8479269348  
H,0,4.6394705322,-7.6241339143,-2.301083058  
H,0,6.2512106386,-2.1460820239,2.4600455672  
H,0,3.887416399,-3.8104837863,1.4210766041  
H,0,4.1034922127,-0.8321793326,2.1772199325  
H,0,1.67994458,-2.5295426162,1.6654954335  
H,0,1.9045793496,0.3065532668,2.4650388286  
H,0,-0.5506004997,0.4552117639,2.0775620309  
H,0,-0.5150373887,-1.2694958594,1.6826809911

#### 7) Pent

C,0,-0.0338473474,-0.0004921582,-0.0135793373  
C,0,-0.0142199797,-0.0004217755,1.5291968807  
C,0,1.4103514973,-0.0003568267,2.1161474441  
C,0,1.4138897783,-1.5888574746,2.1079481288  
C,0,-0.0106511689,-1.5890751352,1.5209366692

C,0,-0.0302183832,-1.5730470354,-0.0217696454  
C,0,1.4367615099,-0.0127282515,3.6574340462  
C,0,1.4402403192,-1.5922738046,3.6492840273  
C,0,2.8636466458,-0.0236915843,4.2650952278  
C,0,2.8670656407,-1.5812976116,4.2570876254  
C,0,-1.4591594847,-1.5677078512,-0.6303678022  
C,0,-1.462820155,-0.0061153046,-0.622122699  
S,0,-1.7042062457,0.8526761258,-2.2238554975  
C,0,-0.6099601494,-0.06619336,-3.2883335201  
C,0,-0.6065566692,-1.4752730193,-3.29577729  
S,0,-1.6963669921,-2.4106215803,-2.2411417786  
C,0,0.2165873894,0.6302057225,-4.180717613  
C,0,1.0100510302,-0.0589880312,-5.0953955863  
C,0,1.0134318338,-1.4555499113,-5.102768577  
C,0,0.2233327839,-2.1581985073,-4.195443523  
H,0,2.9152191625,-2.0194585502,5.2580522618  
H,0,3.6374101081,-2.0596993001,3.6429137727  
H,0,2.9099214327,0.4043636563,5.2705111135  
H,0,3.6318539683,0.4643734866,3.6558686458  
H,0,0.6913077377,-2.2107437043,4.1537155191  
H,0,0.6851351758,0.5971979294,4.1682219474  
H,0,2.1582743315,-2.2099532425,1.5971936164  
H,0,2.1519353084,0.6292857547,1.6118238295  
H,0,-0.7528064263,-2.2203210518,2.0229038261  
H,0,-0.7591531437,0.6222324642,2.0377365702  
H,0,0.2355312449,-3.2437233097,-4.1815612661  
H,0,0.2235342339,1.7155697697,-4.155367323  
H,0,1.641310152,-1.9977932977,-5.8033378463  
H,0,1.6352770957,0.4936572955,-5.7901847636

H,0,-2.2336991527,0.4335998285,0.0194341898

H,0,-2.2280156261,-2.0178120977,0.006394043

H,0,0.7045410517,0.614994013,-0.5330941434

H,0,0.711042123,-2.1796742487,-0.5475771073