Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

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

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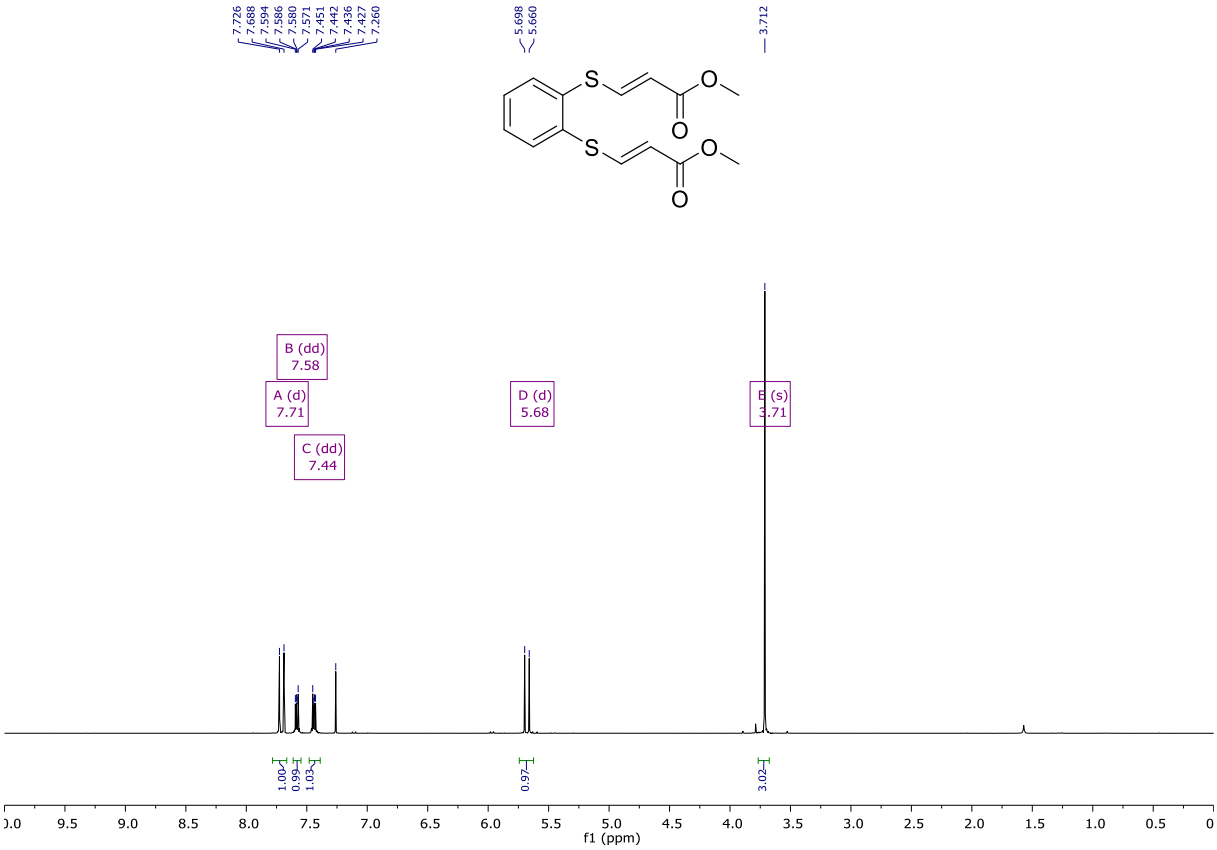
1. General information

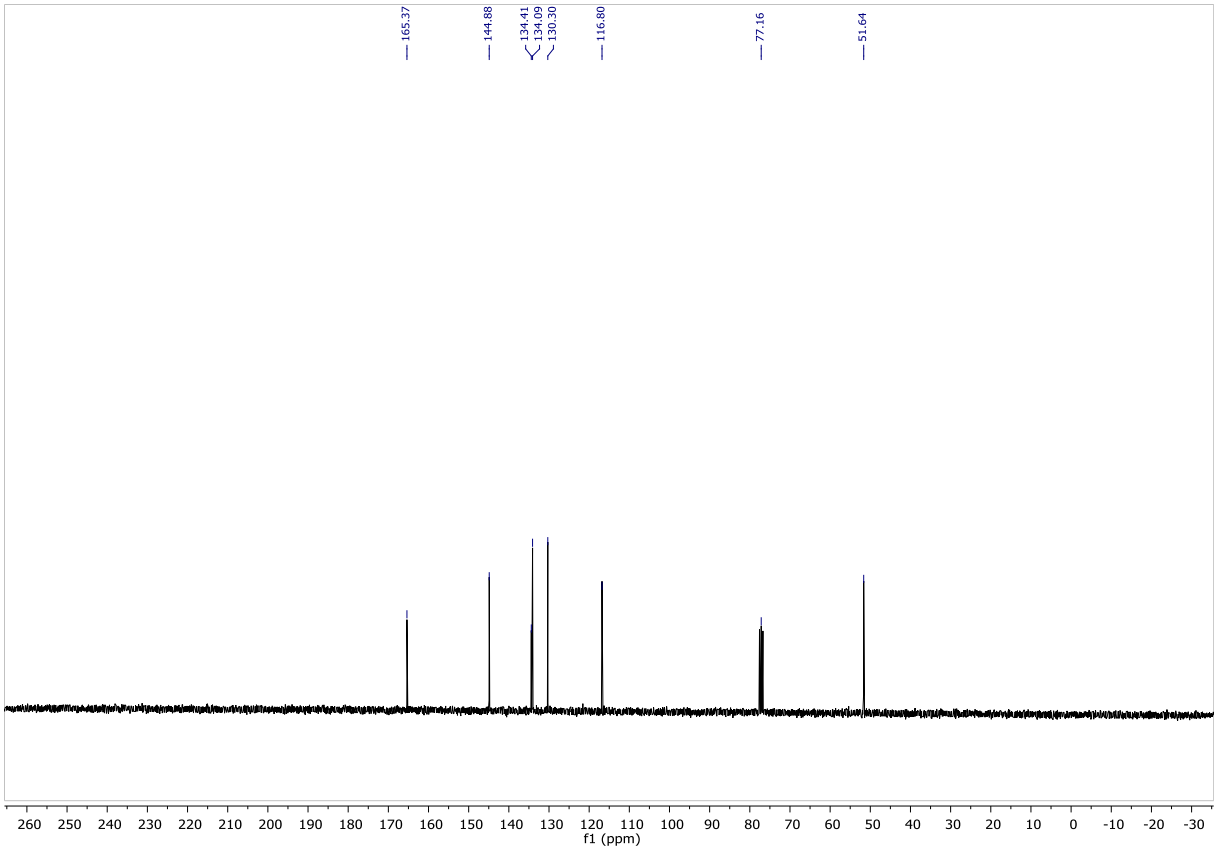
Unless otherwise noted, reactions were carried out under argon atmosphere. Methanol was dried overnight over freshly activated molecular sieves (4 Å), THF and diethyl ether were distillated from sodium/benzophenone. Other reagents and chemicals were purchased from commercial sources and used as received. 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 (δ) are reported in ppm and coupling constants (*J*) are given in Hertz (Hz). ^{1}H and ^{13}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 (λ = 254 nm) and $KMnO_4$ or *p*-anisaldehyde staining. Flash column chromatography was performed on silica Geduran® Si 60 Å (40 – 63 μm).

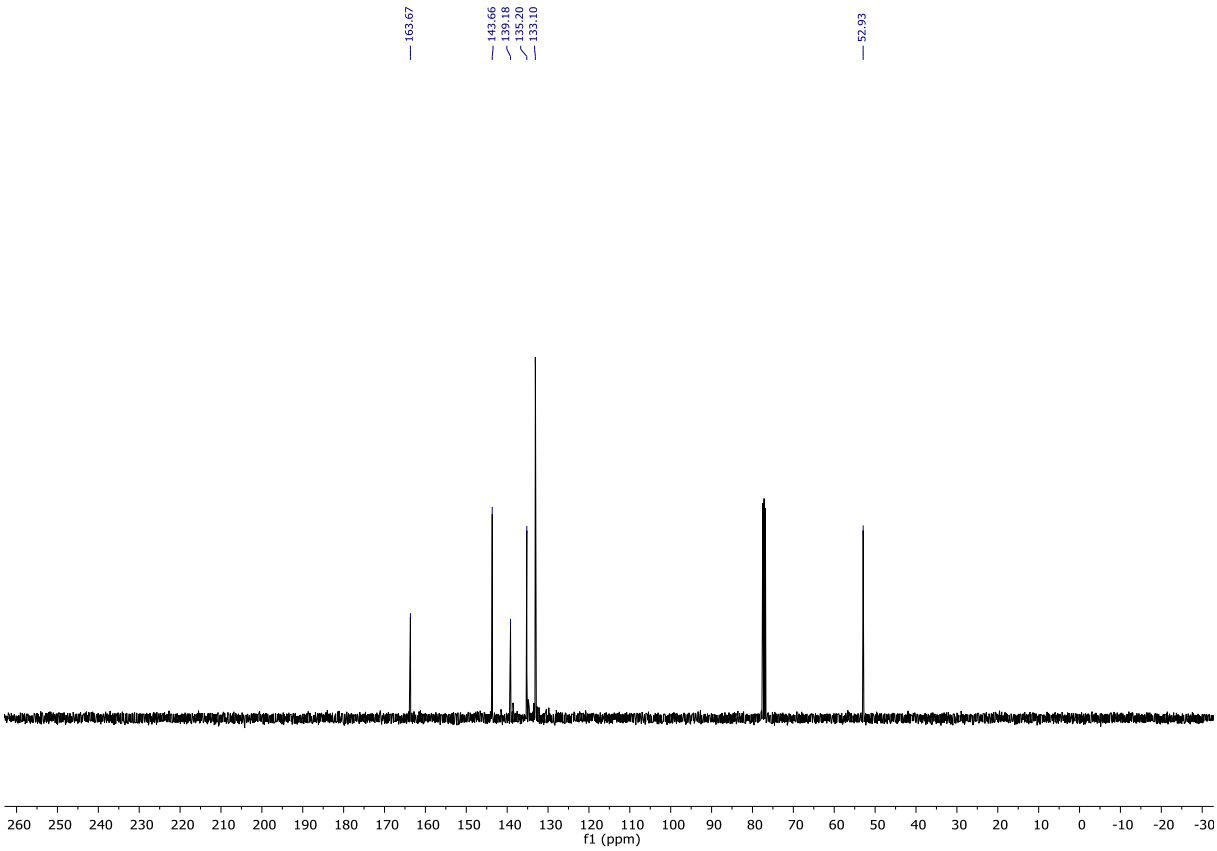
2. Spectral data

^{1}H-NMR (400 MHz) : Compound **2**

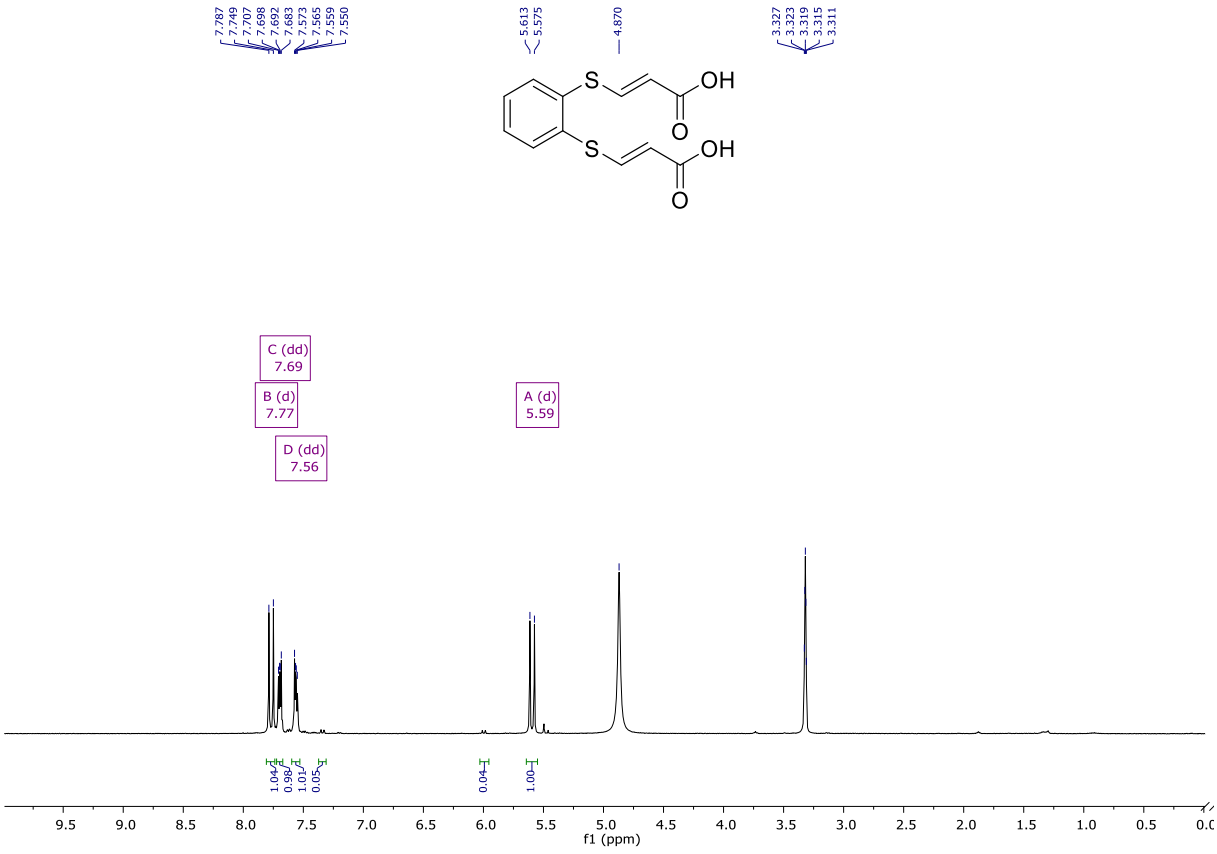


^{13}C-NMR (100 MHz) : Compound **2**

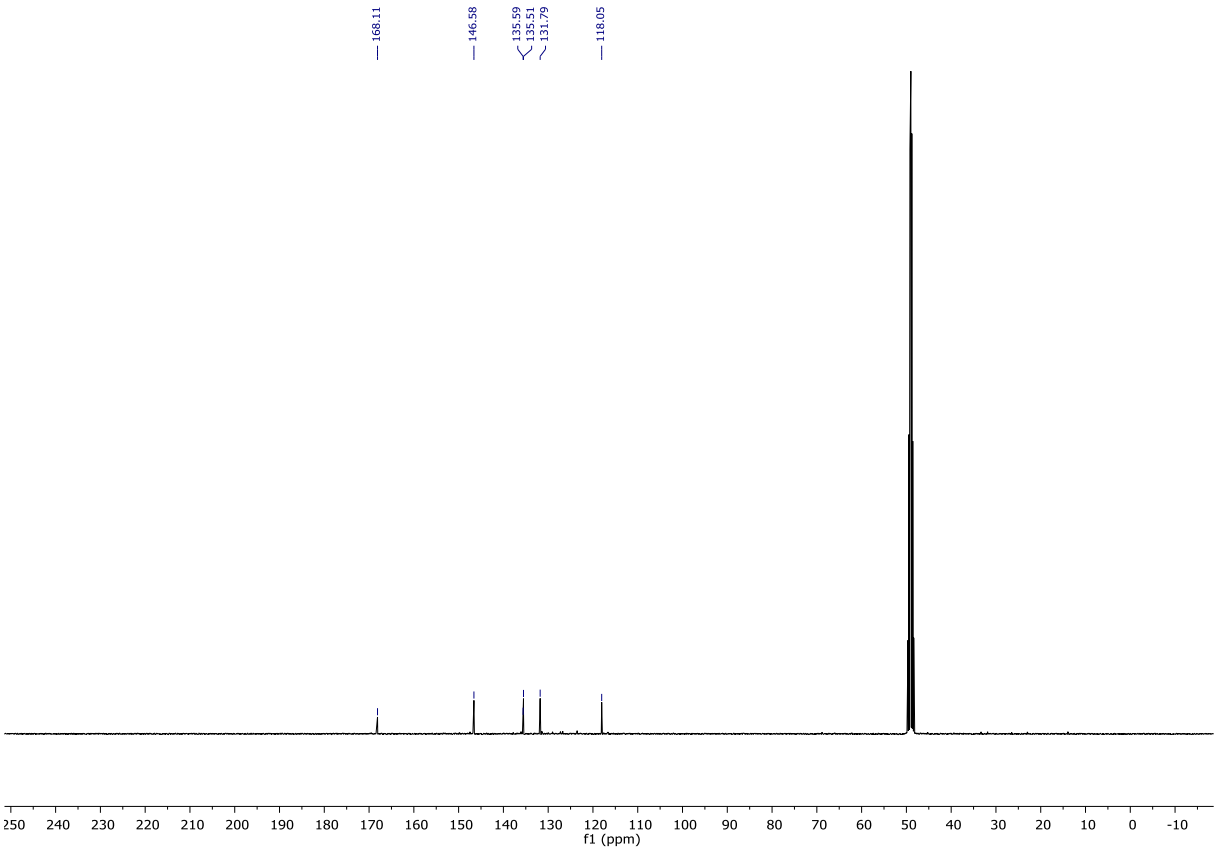




^{1}H-NMR (400 MHz) : Compound **2-OH**



^{13}C-NMR (100 MHz) : Compound **2-OH**



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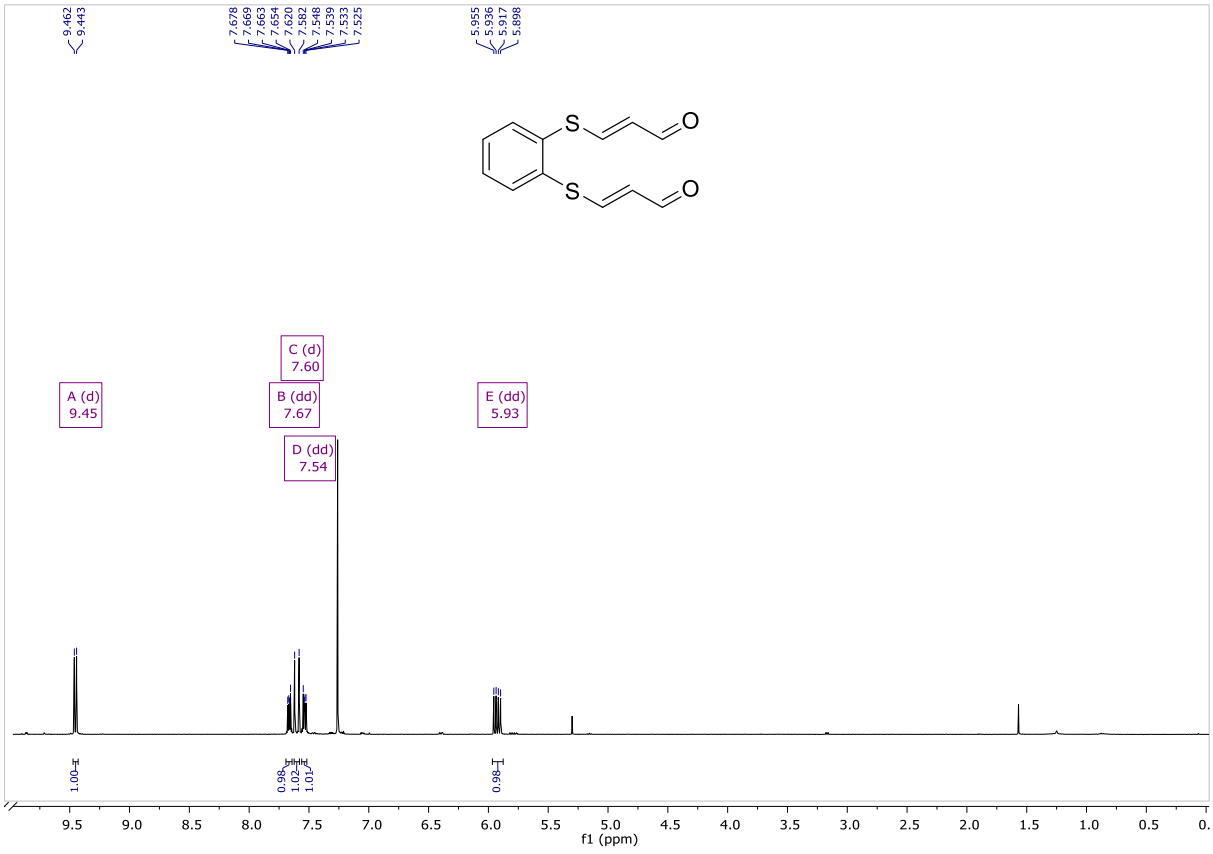
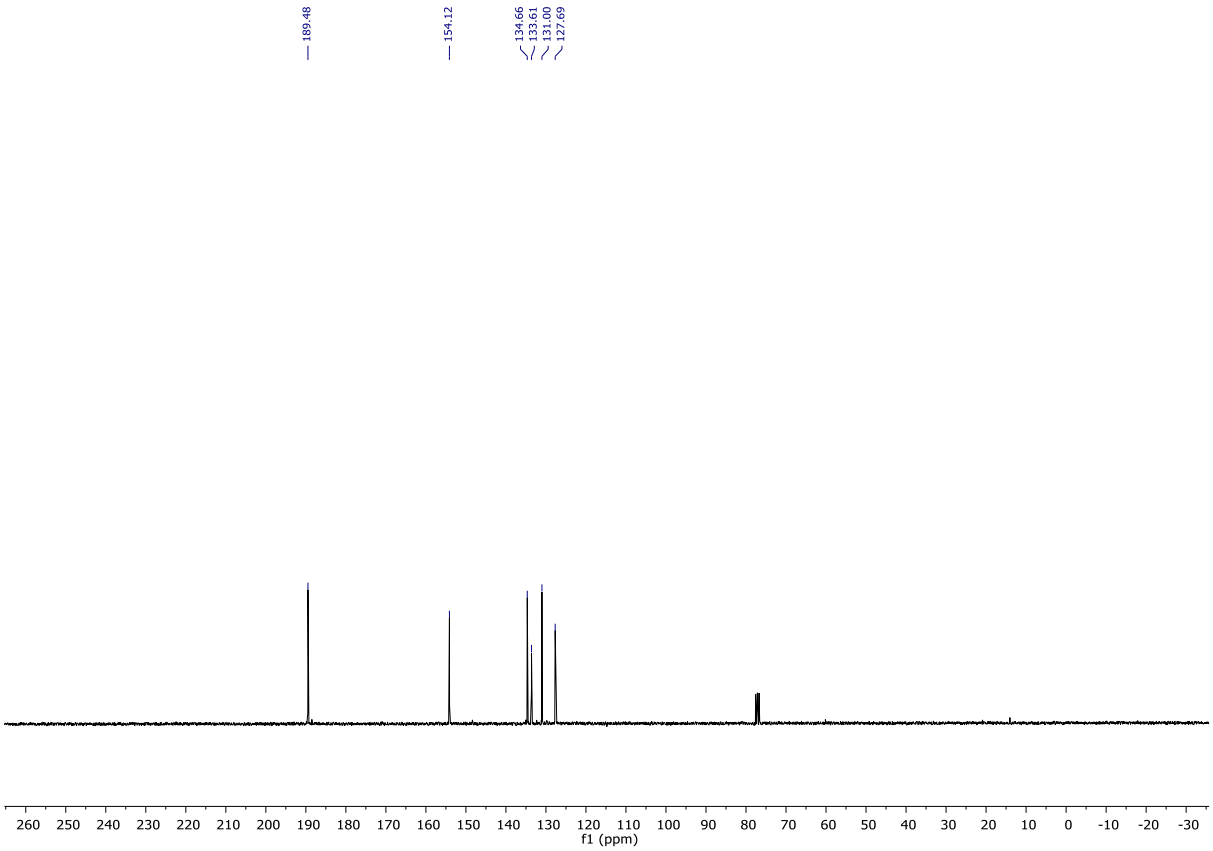
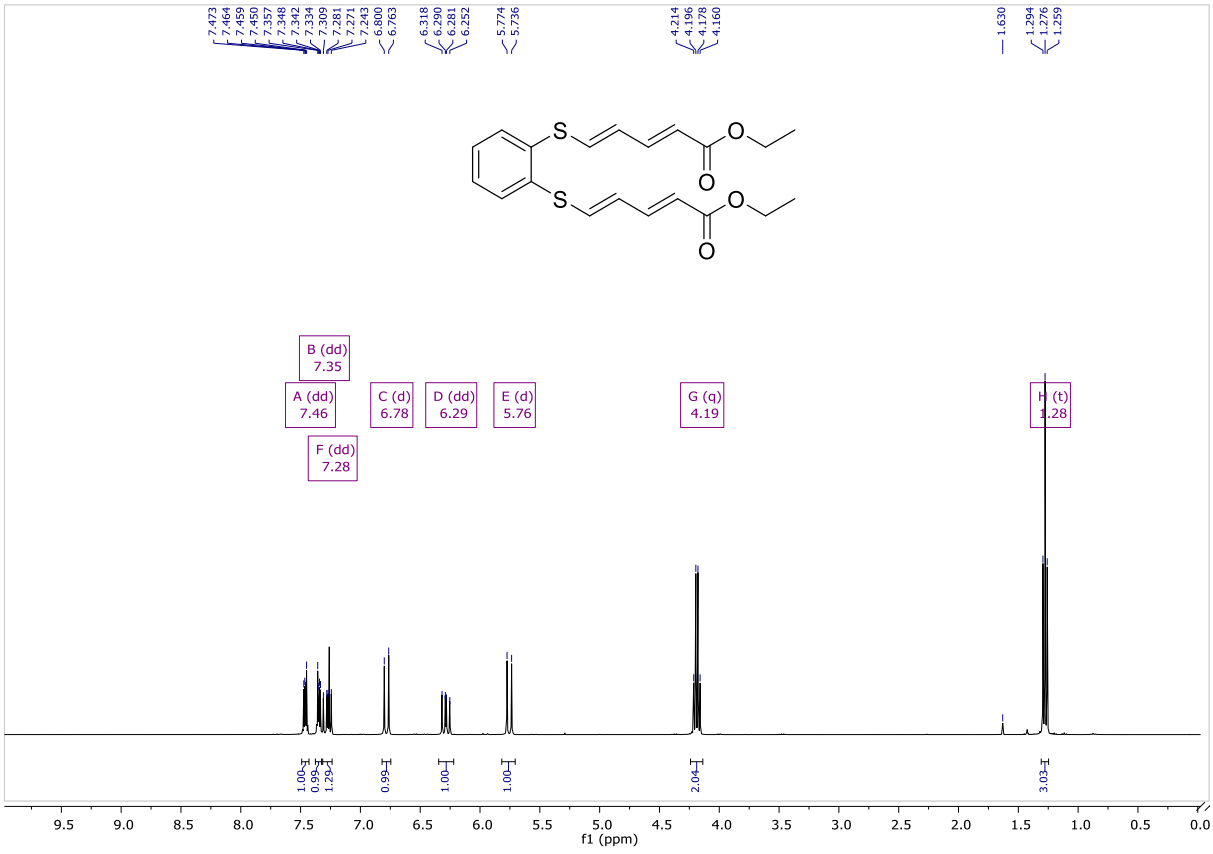


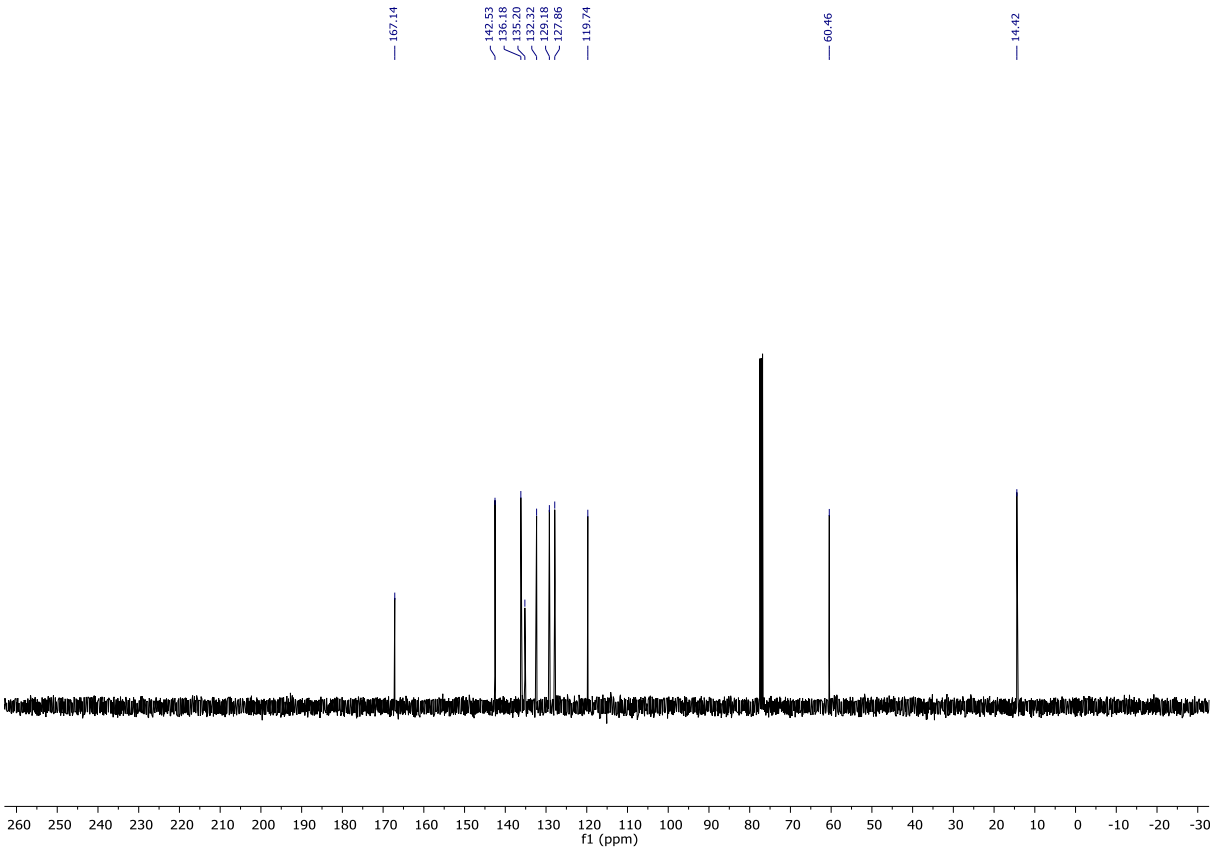
^{13}C-NMR (100 MHz) : Compound **3**



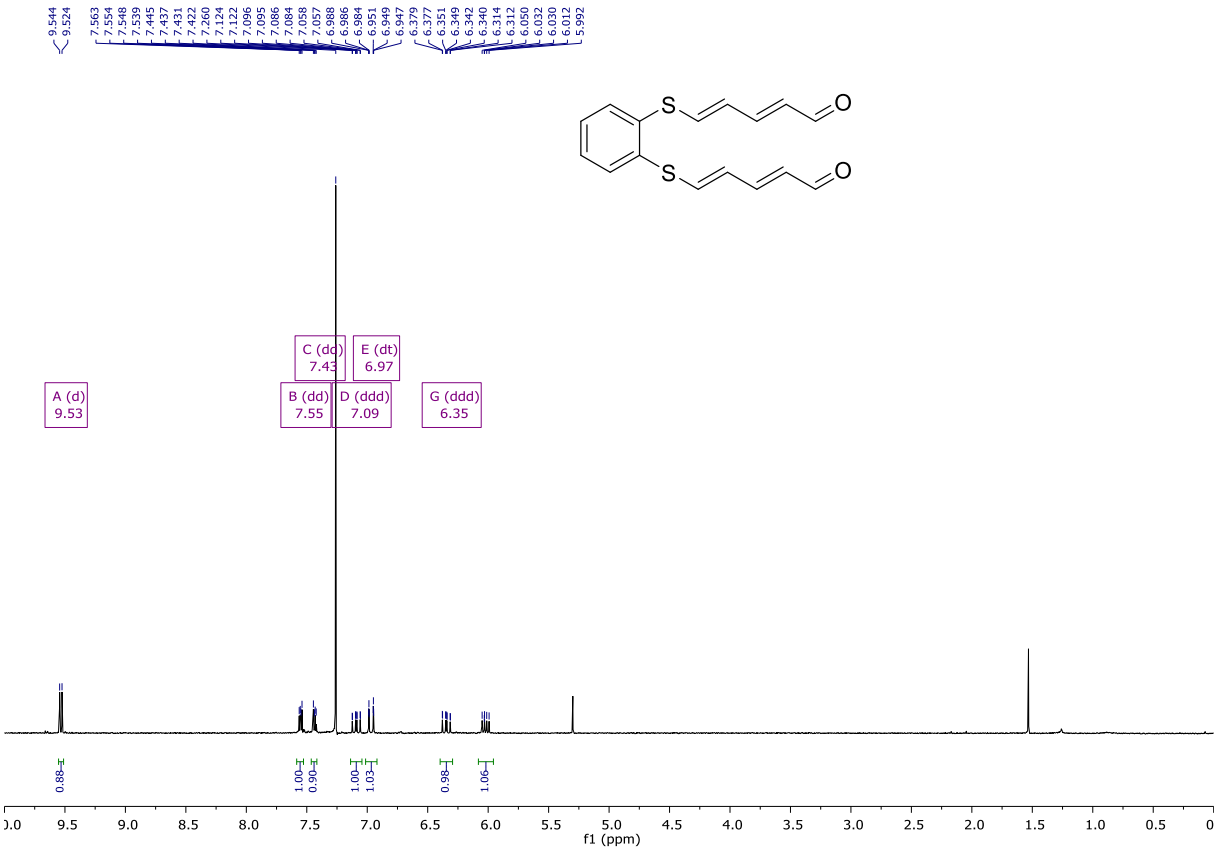
^{1}H-NMR (400 MHz) : Compound **4**



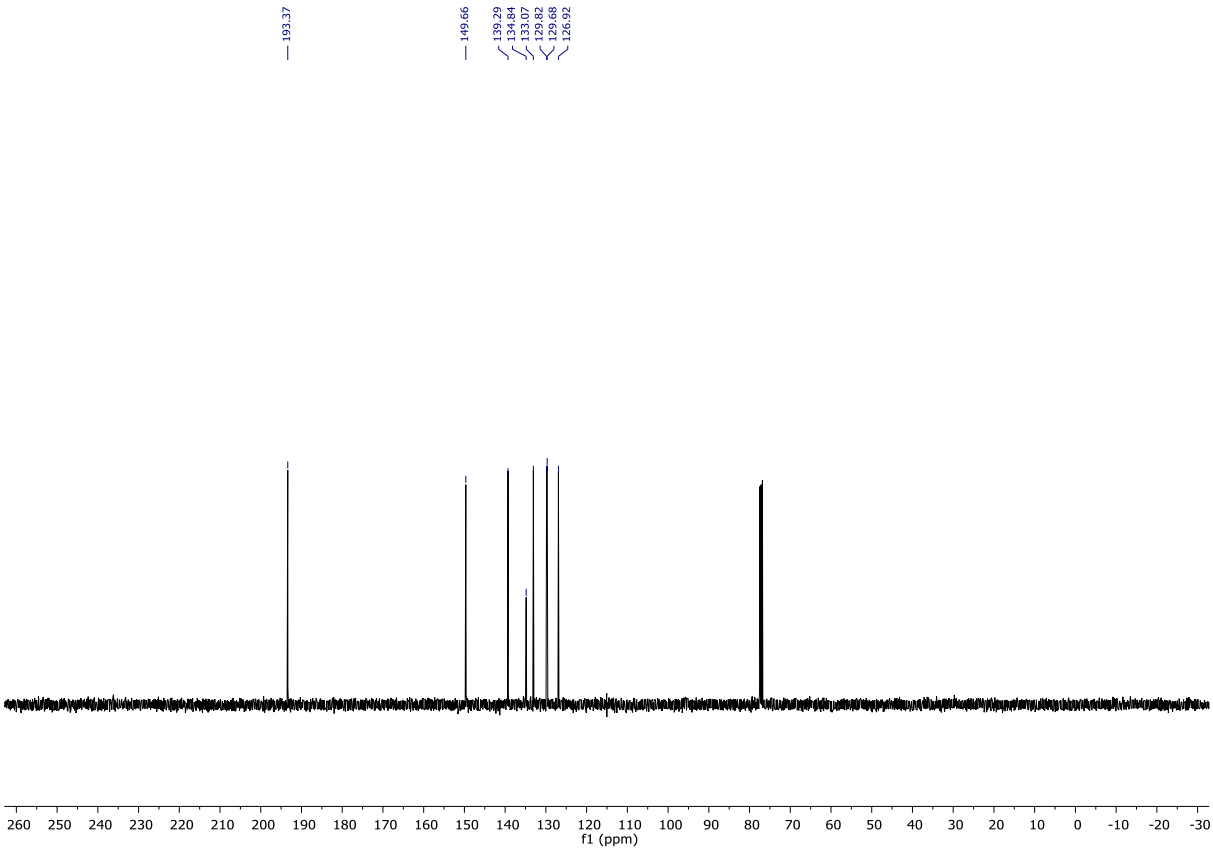
^{13}C-NMR (100 MHz) : Compound **4**



^{1}H-NMR (400 MHz) : Compound **5**



^{13}C-NMR (100 MHz) : Compound **5**



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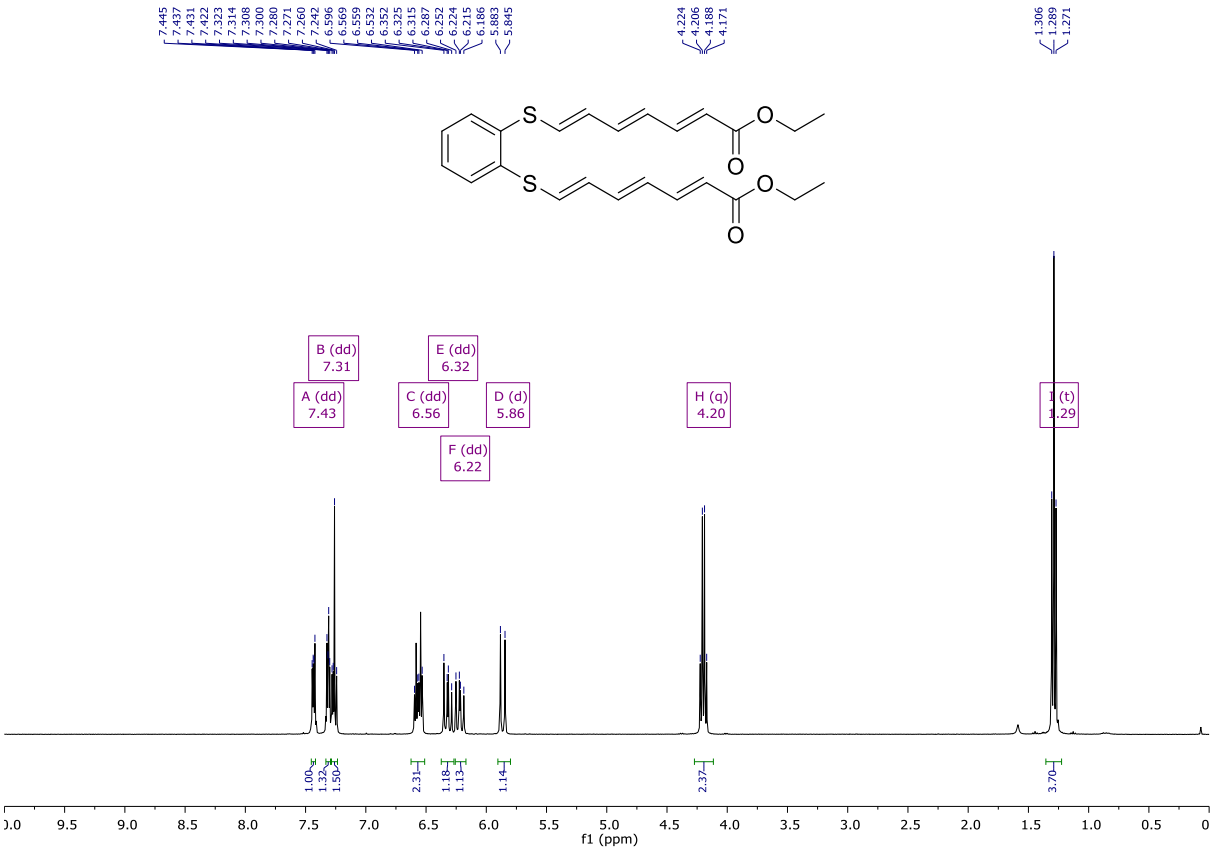
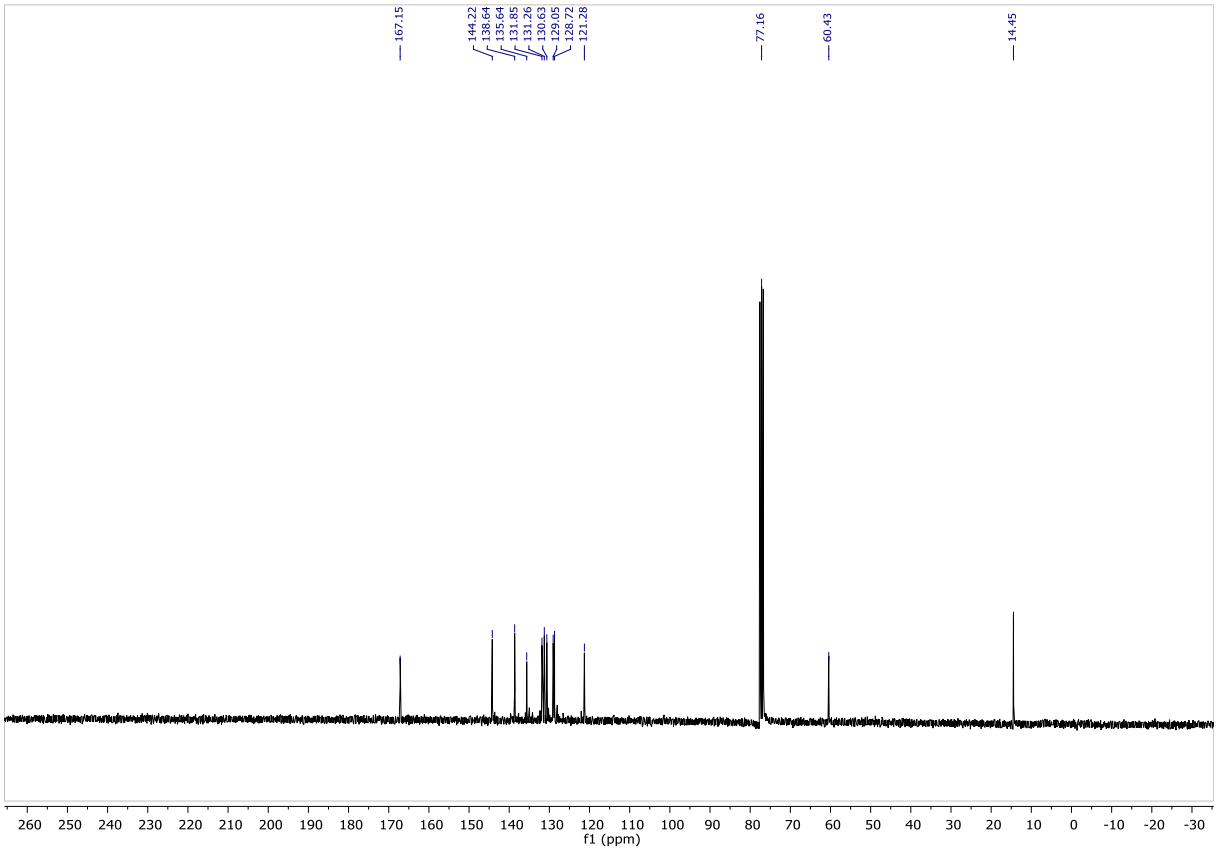
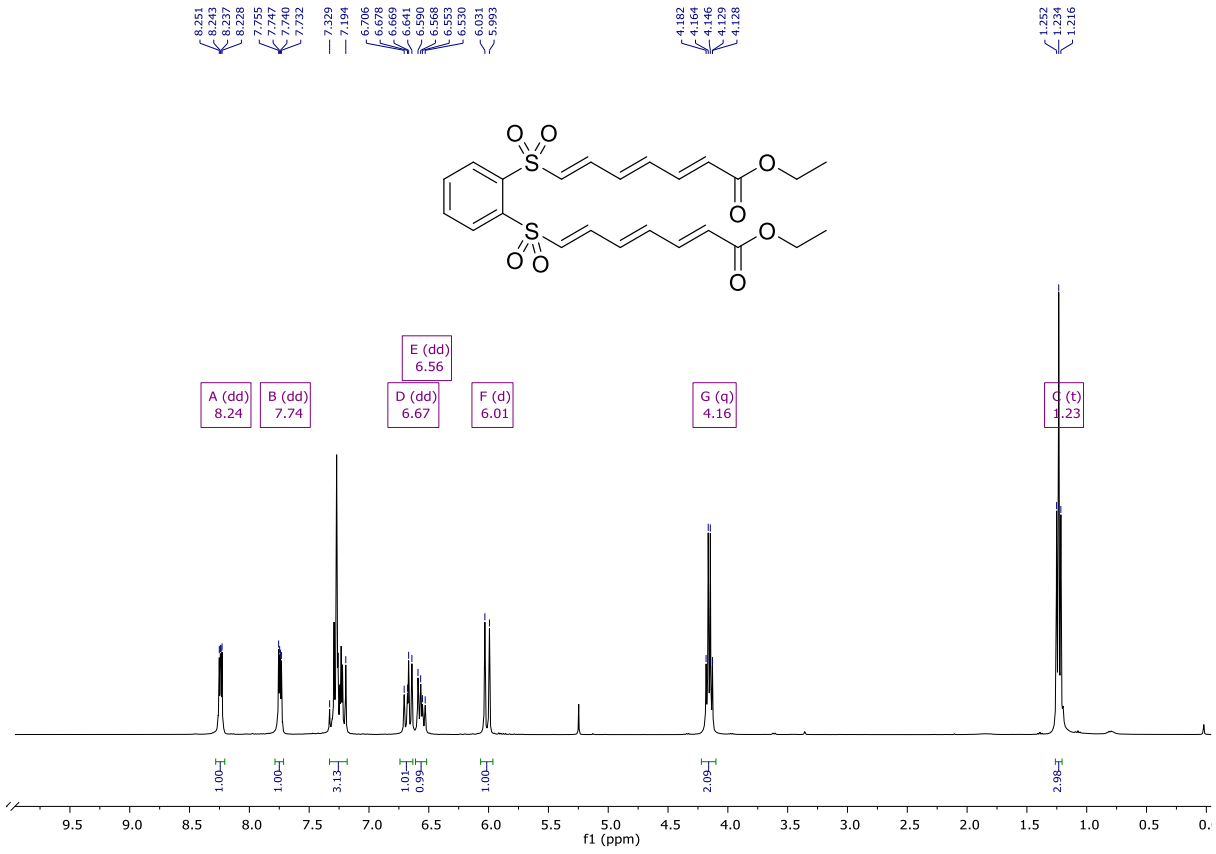


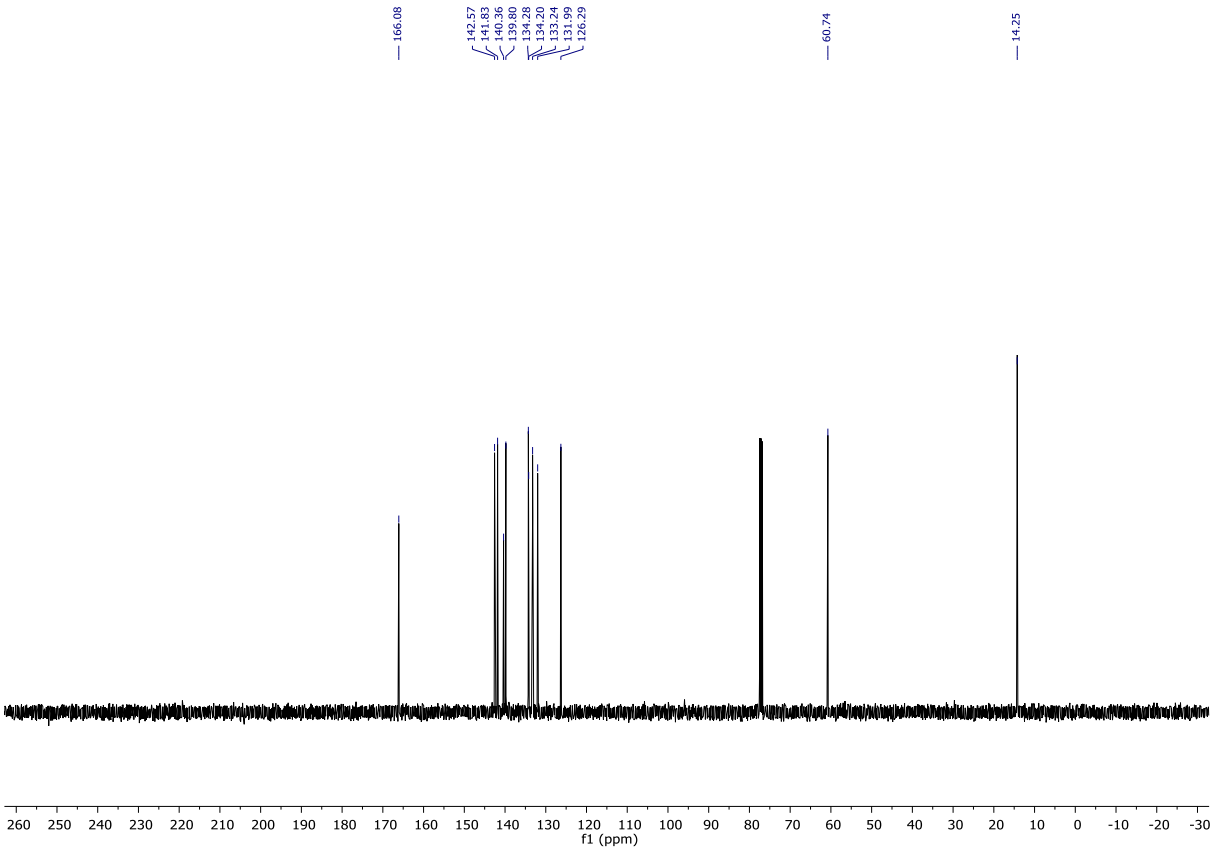
^{13}C-NMR (100 MHz) : Compound **6**



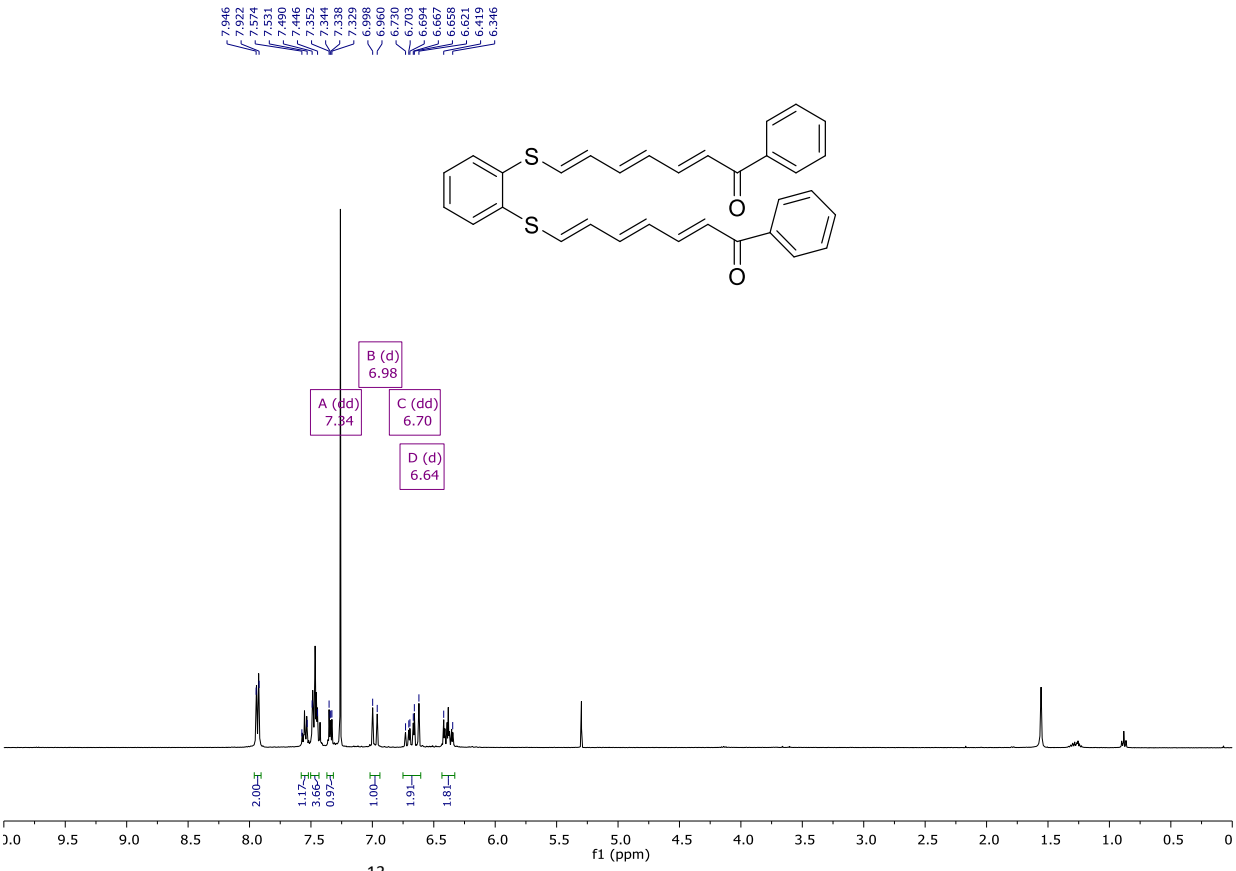
^{1}H-NMR (400 MHz) : Compound **6-O**



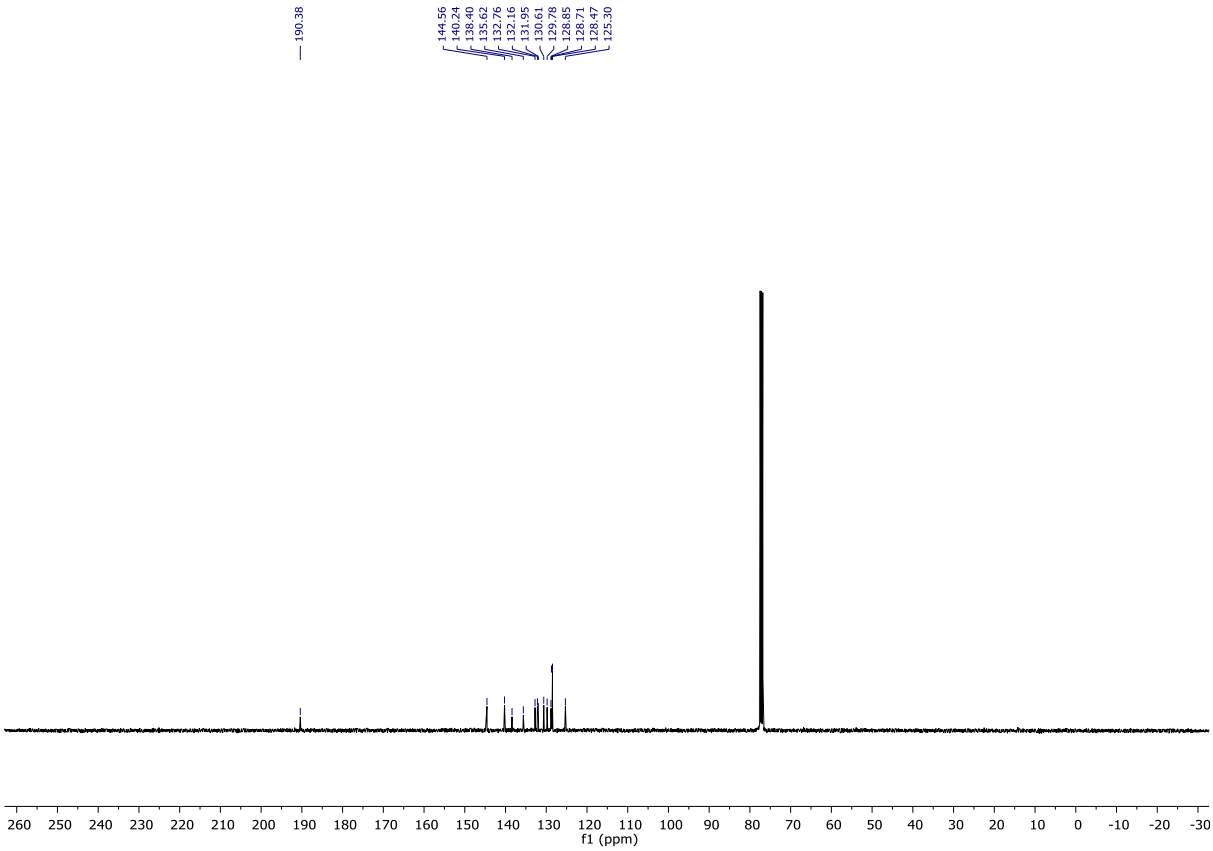
^{13}C-NMR (100 MHz) : Compound **6-O**



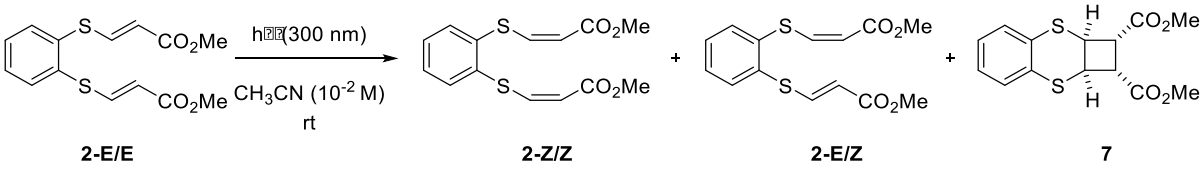
^{1}H-NMR (400 MHz) : Compound **6-COPh**



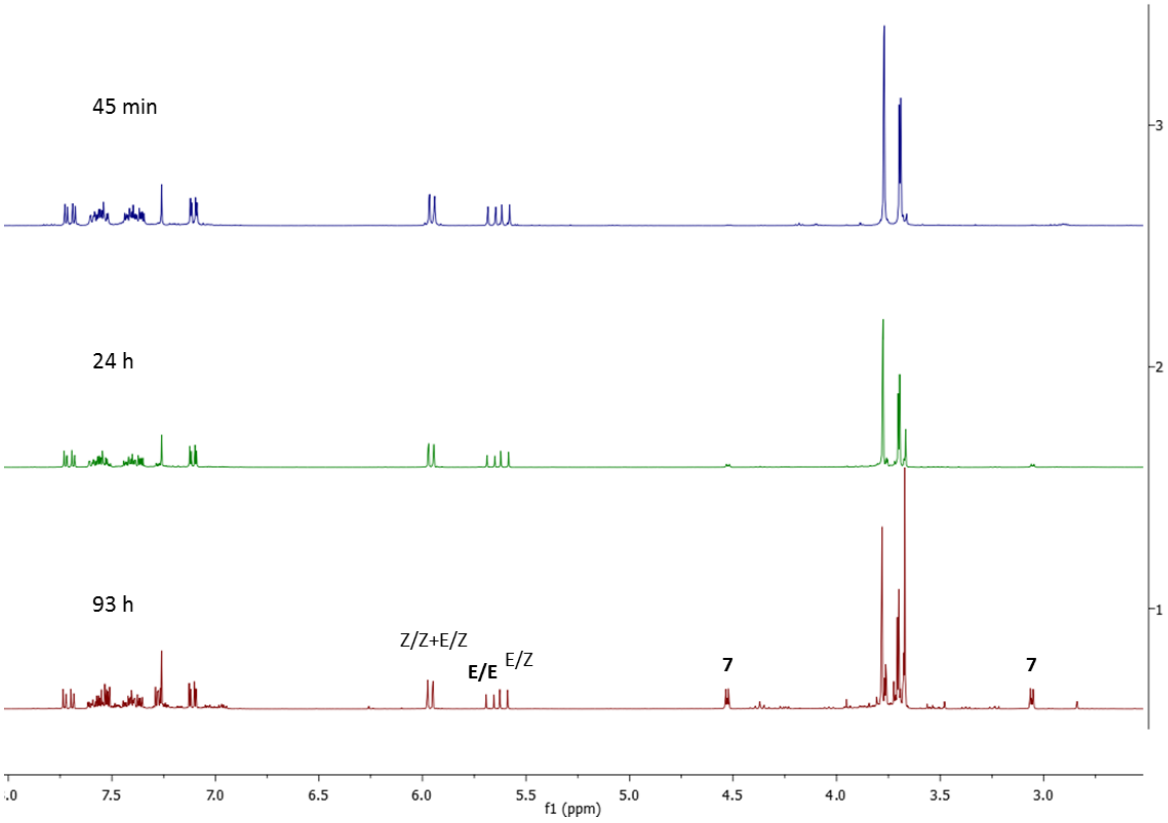
^{13}C-NMR (100 MHz) : Compound **6-COPh**



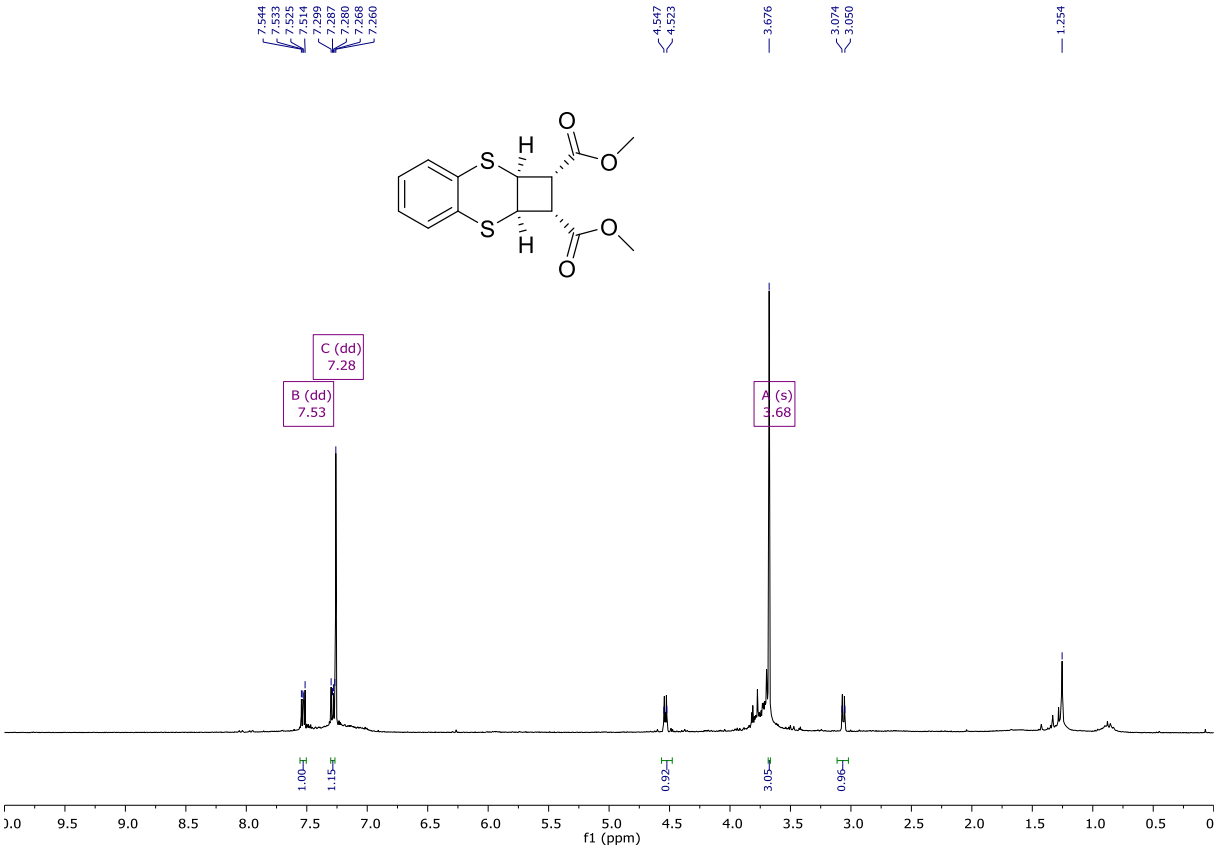
^{1}H-NMR (400 MHz) : **2-mix** + **7**



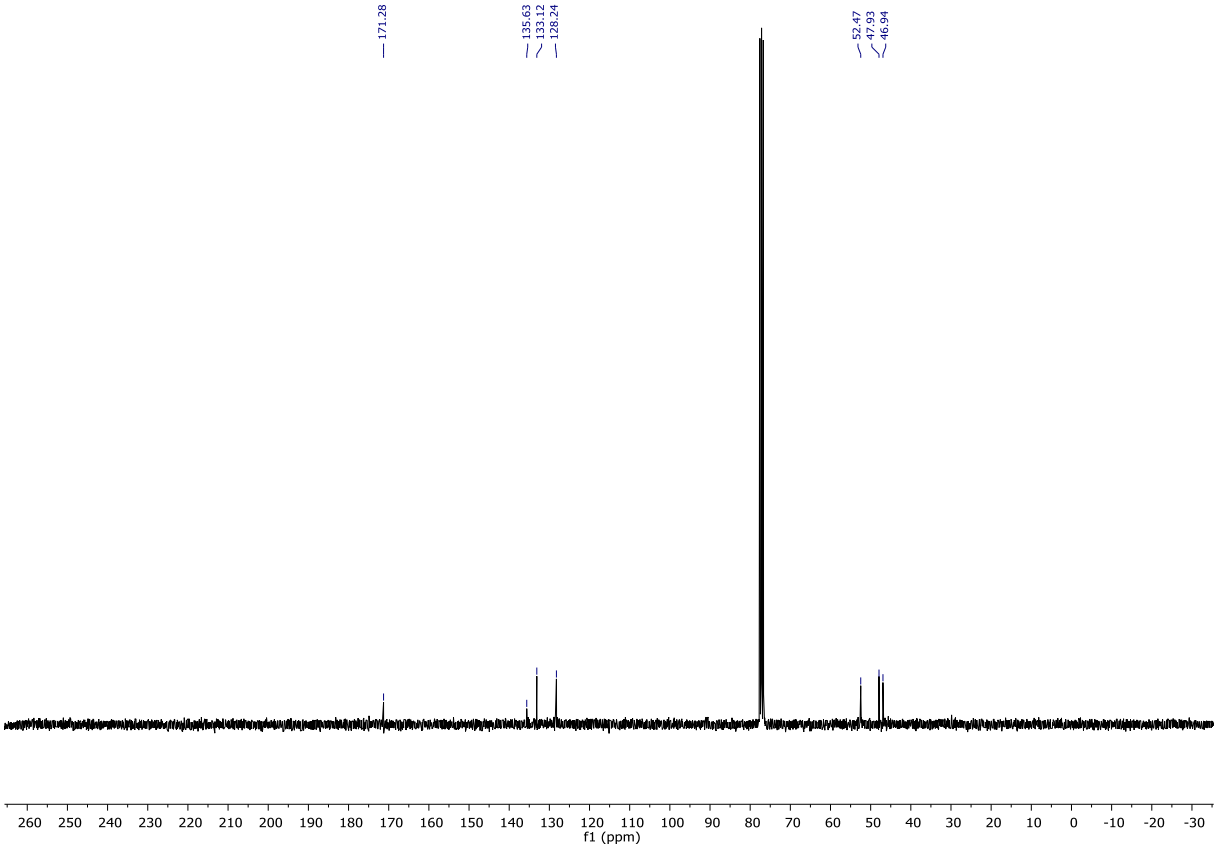
2-E/E **2-Z/Z** **2-E/Z** **7**


45 min
24 h
93 h
Z/Z+E/Z
E/E
E/Z
7
7
3
2
1
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
f1 (ppm)

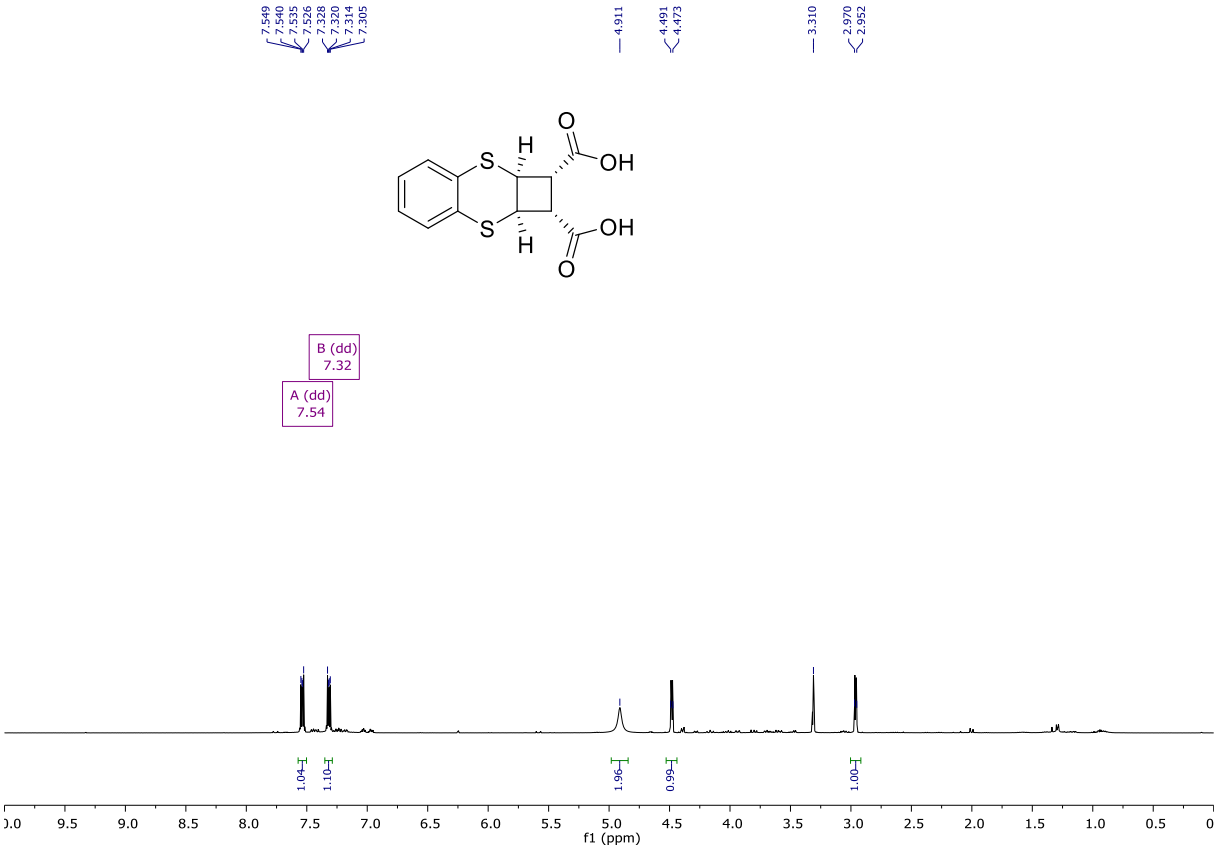
^{1}H-NMR (400 MHz) : Compound **7**



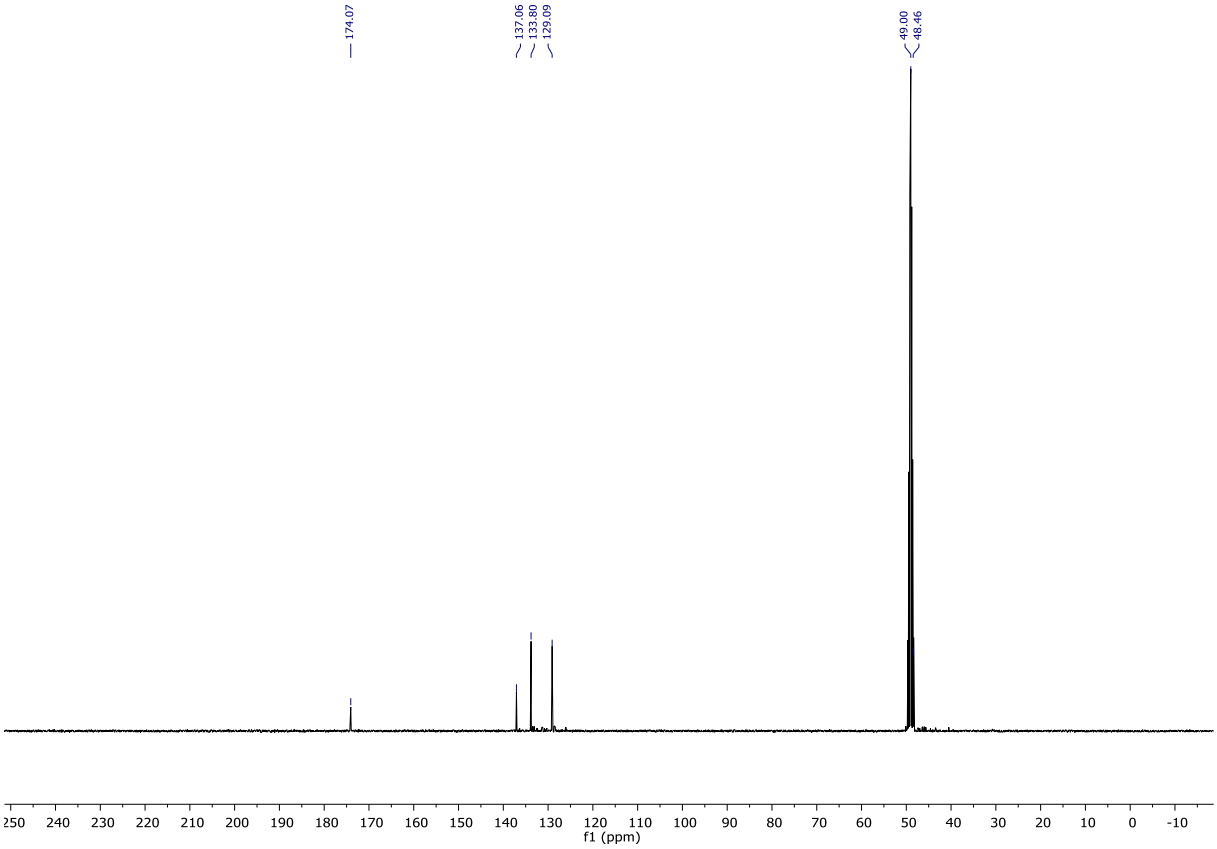
^{13}C-NMR (100 MHz) : Compound **7**



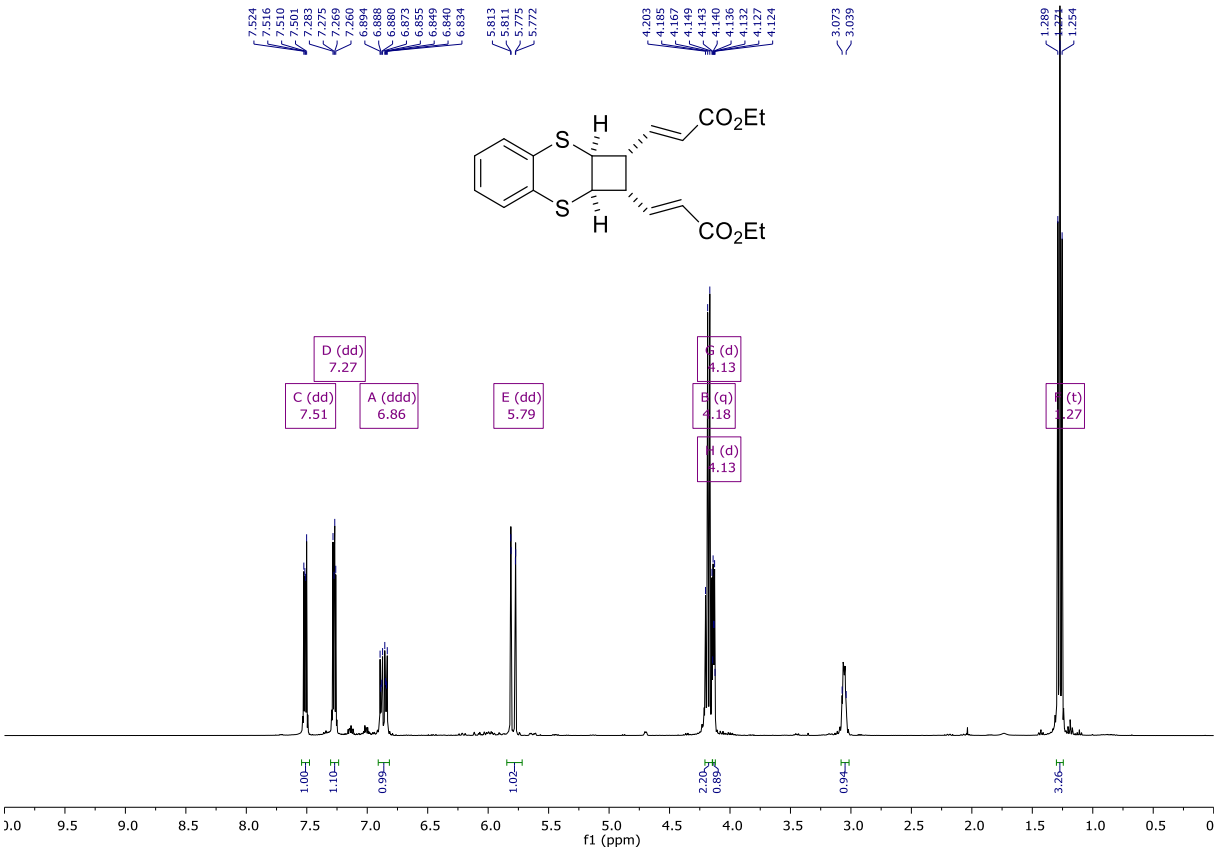
^{1}H-NMR (400 MHz) : Compound **7-OH**



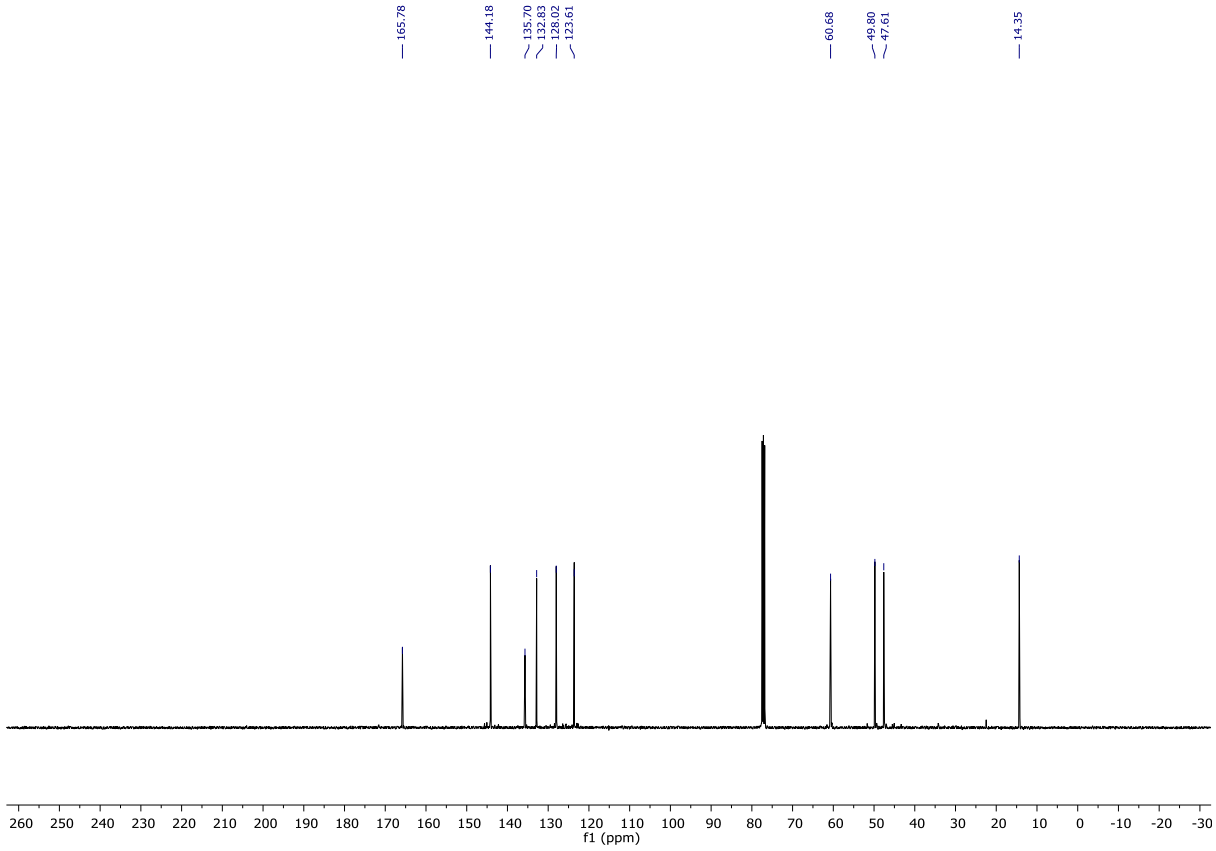
^{13}C-NMR (100 MHz) : Compound **7-OH**



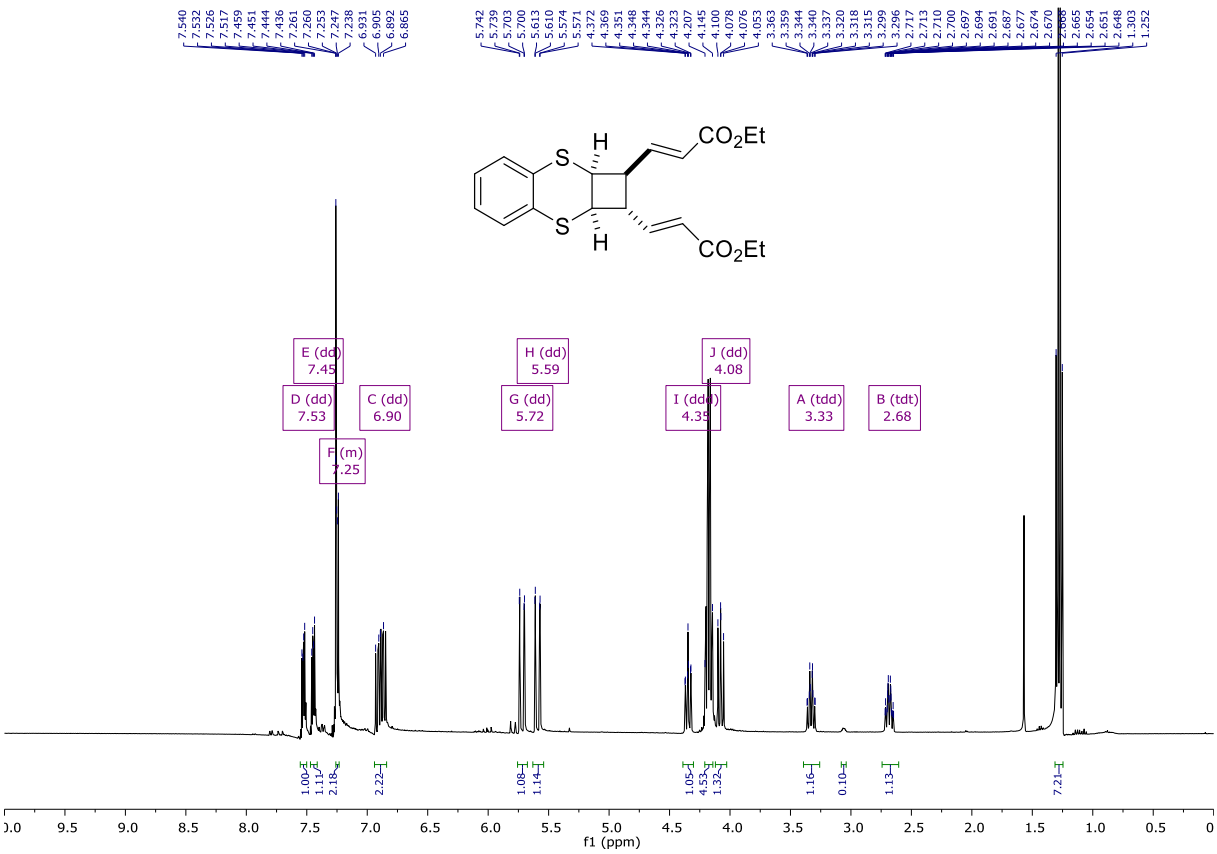
^{1}H-NMR (400 MHz) : Compound **8-sym**



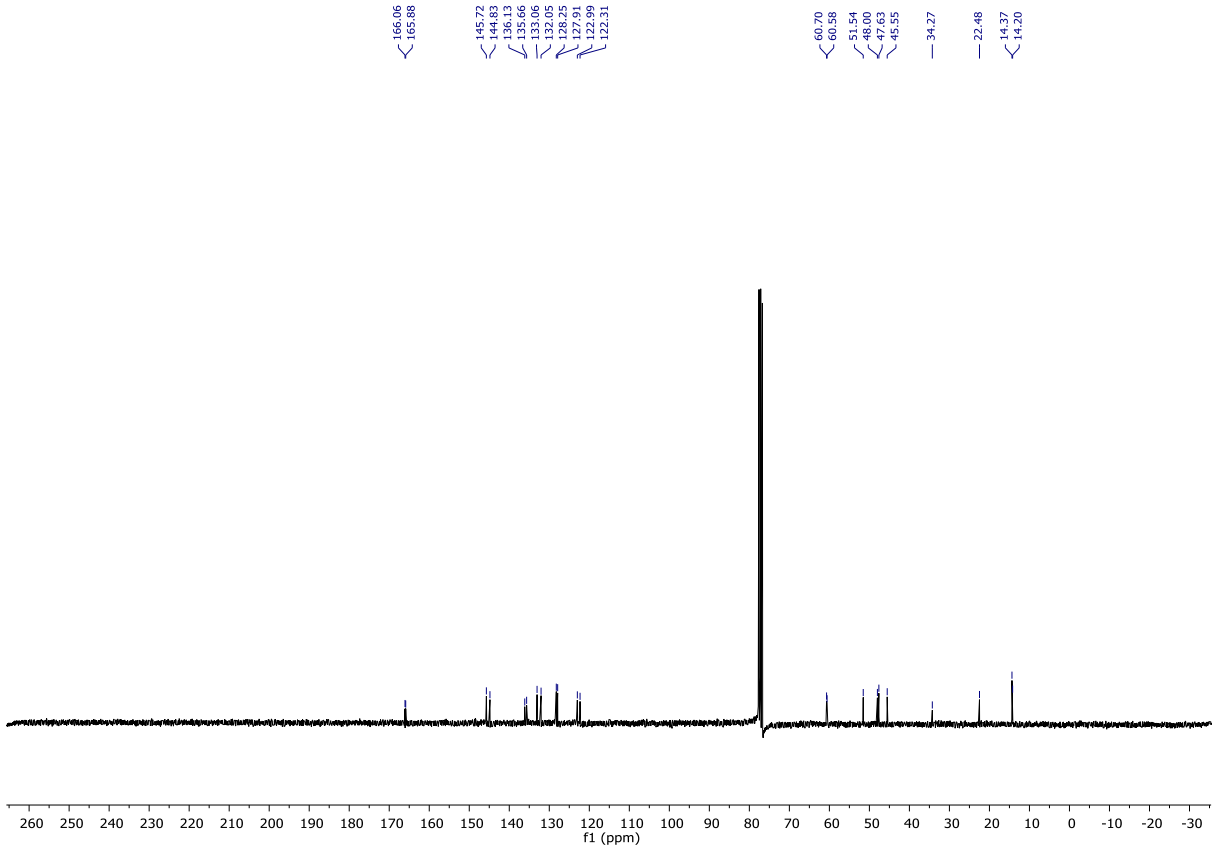
^{13}C-NMR (100 MHz) : Compound **8-sym**



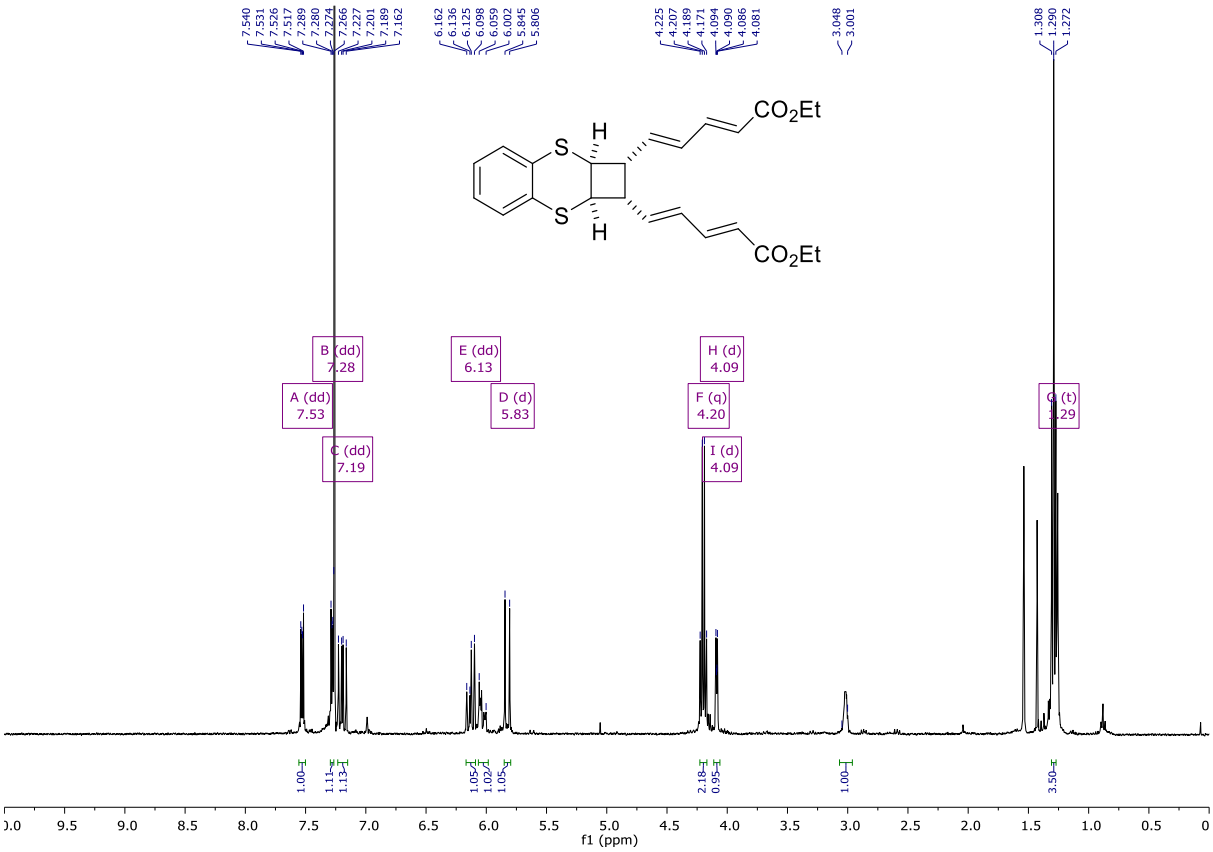
^{1}H-NMR (400 MHz) : Compound **8-dis**



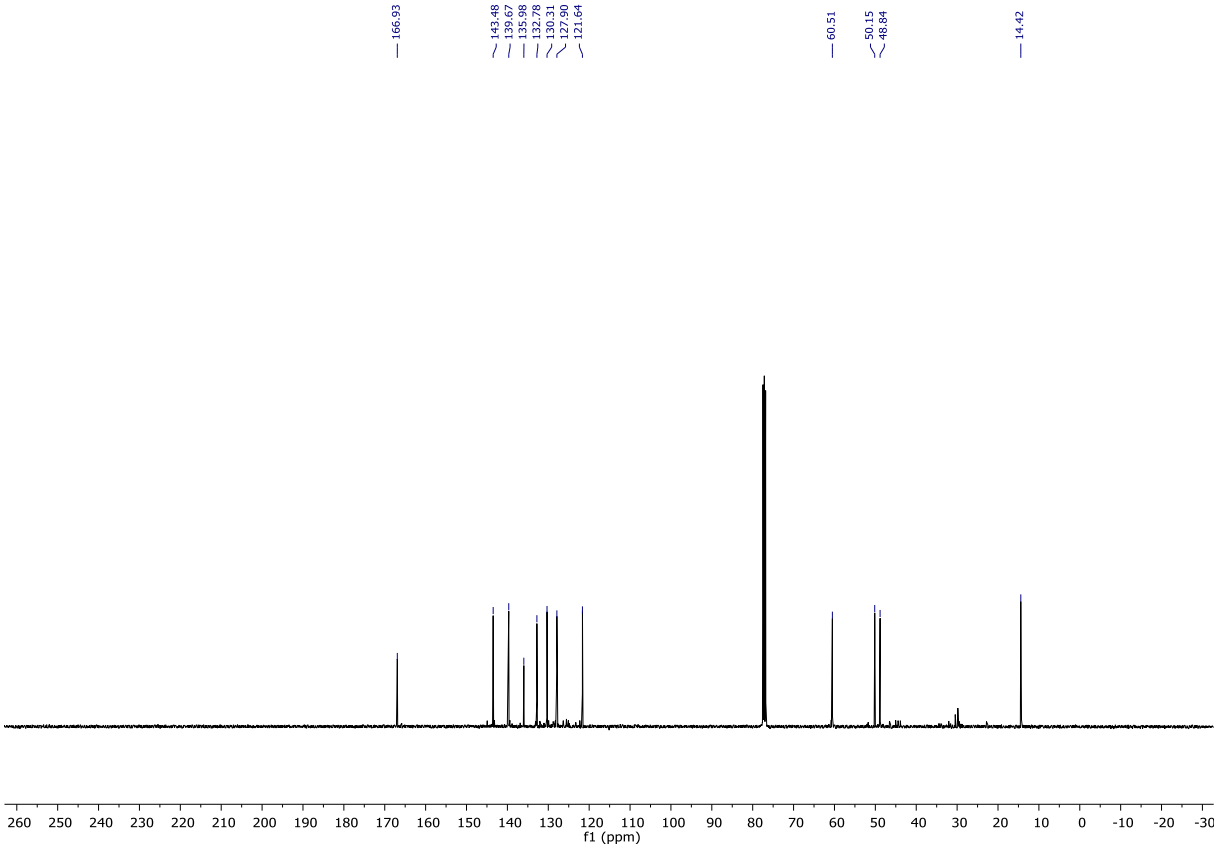
^{13}C-NMR (100 MHz) : Compound **8-dis**



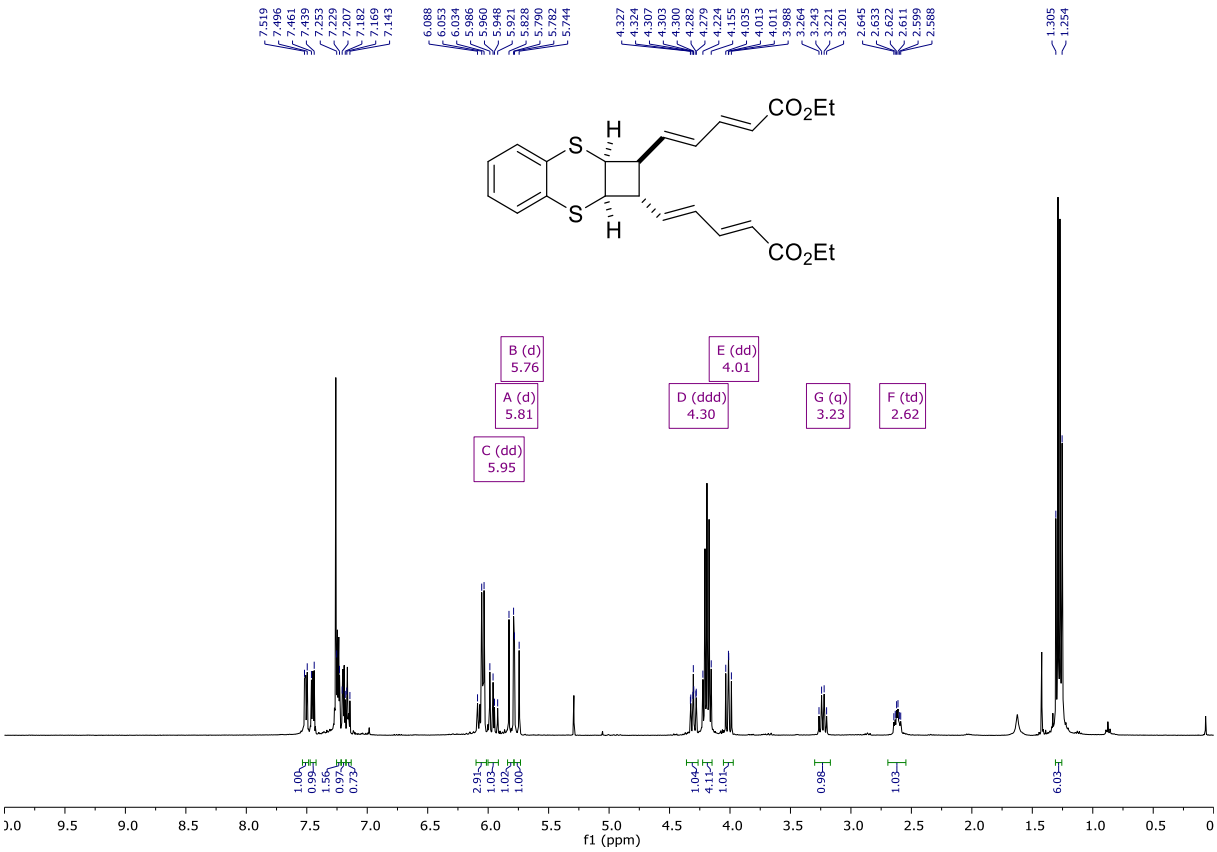
^{1}H-NMR (400 MHz) : Compound **9-sym**



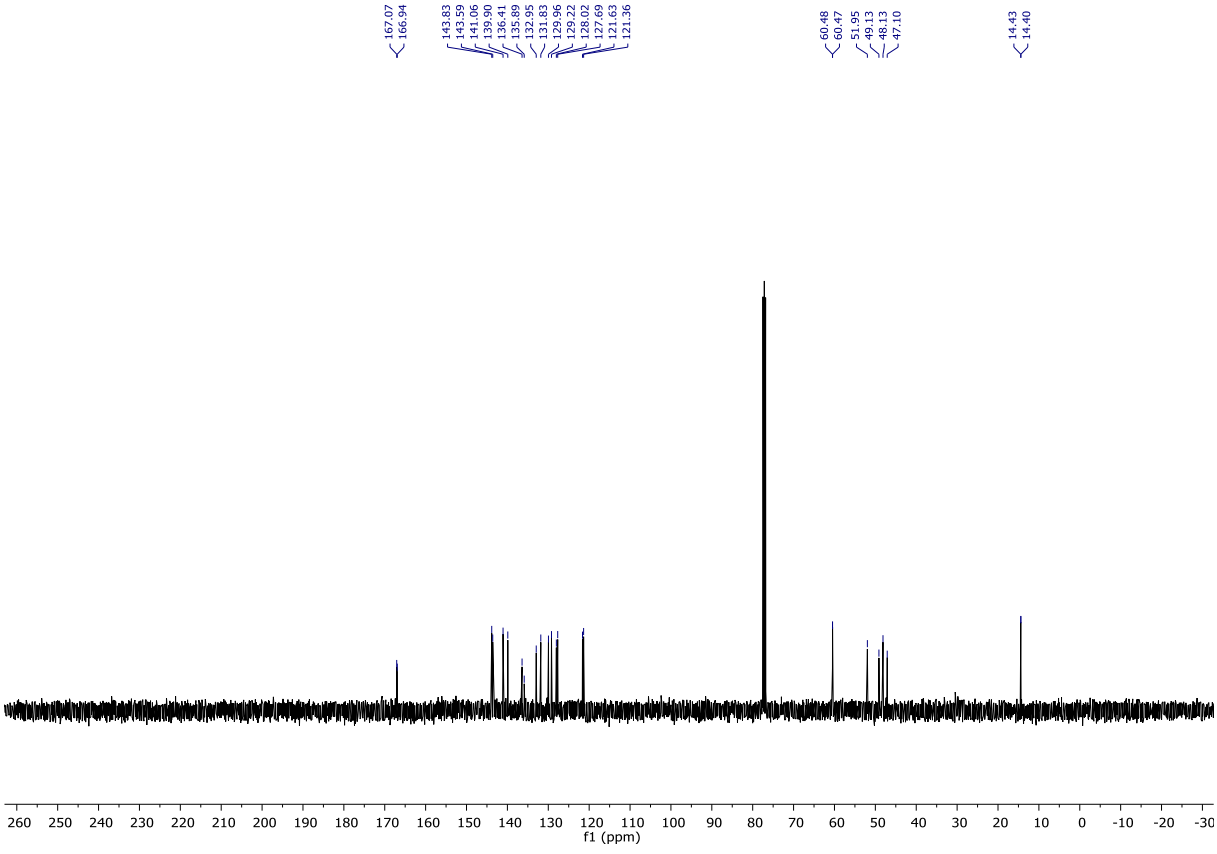
^{13}C-NMR (100 MHz) : Compound **9-sym**



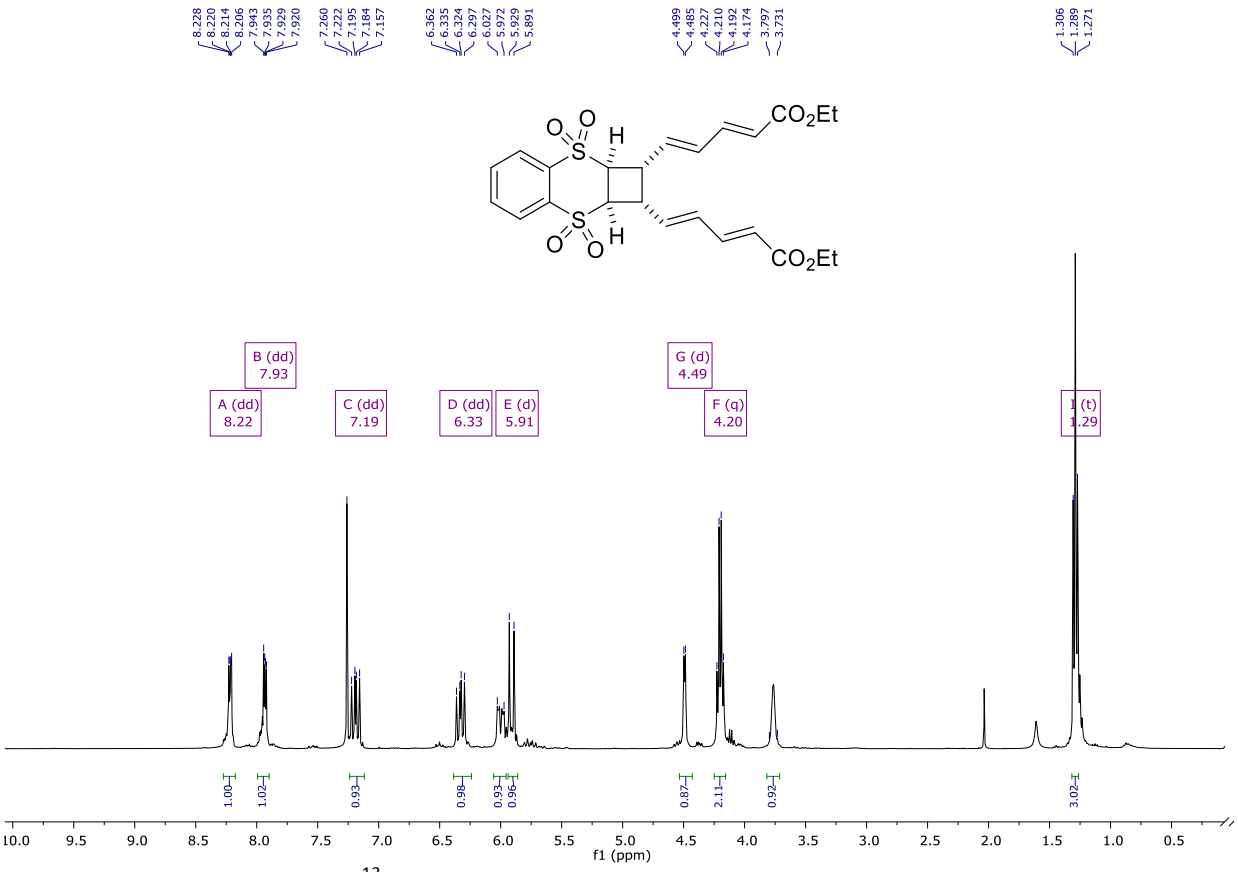
^{1}H-NMR (600 MHz) : Compound **9-dis**



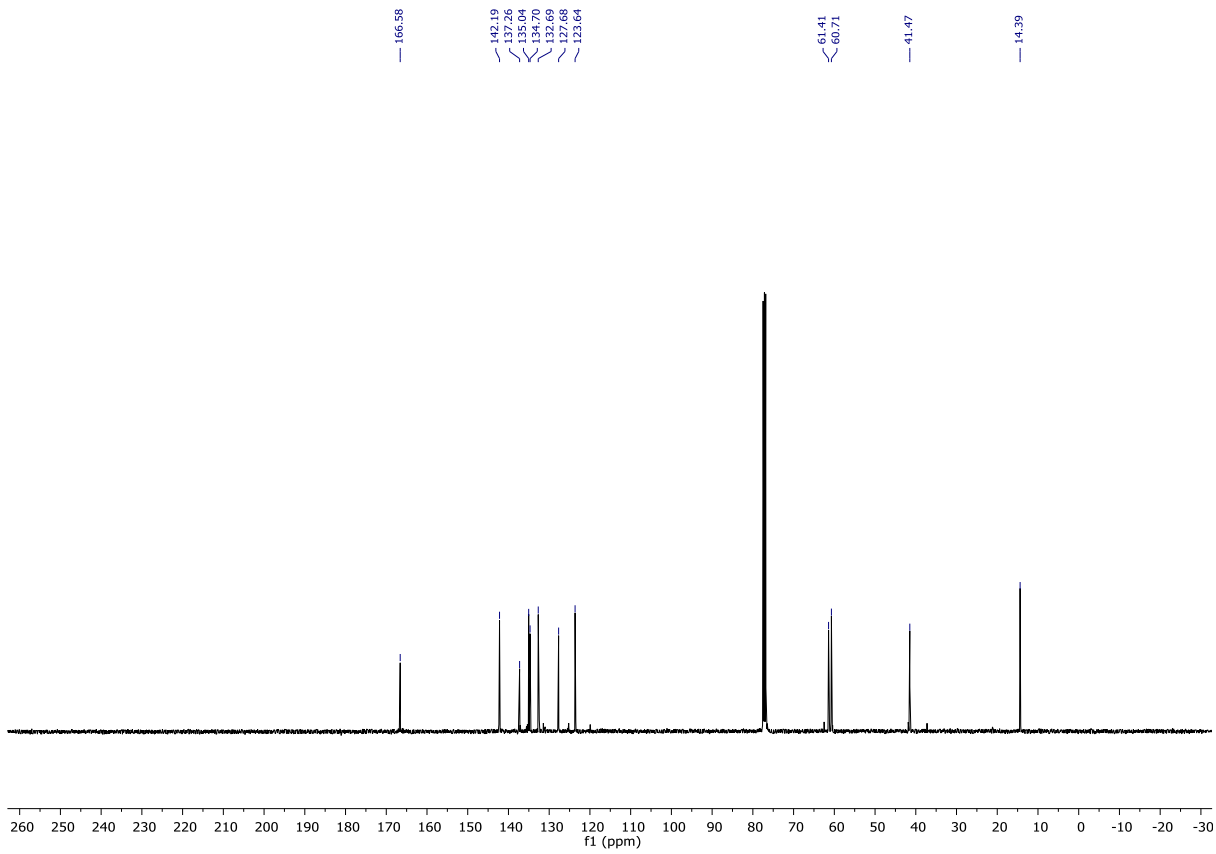
^{13}C-NMR (151 MHz) : Compound **9-dis**



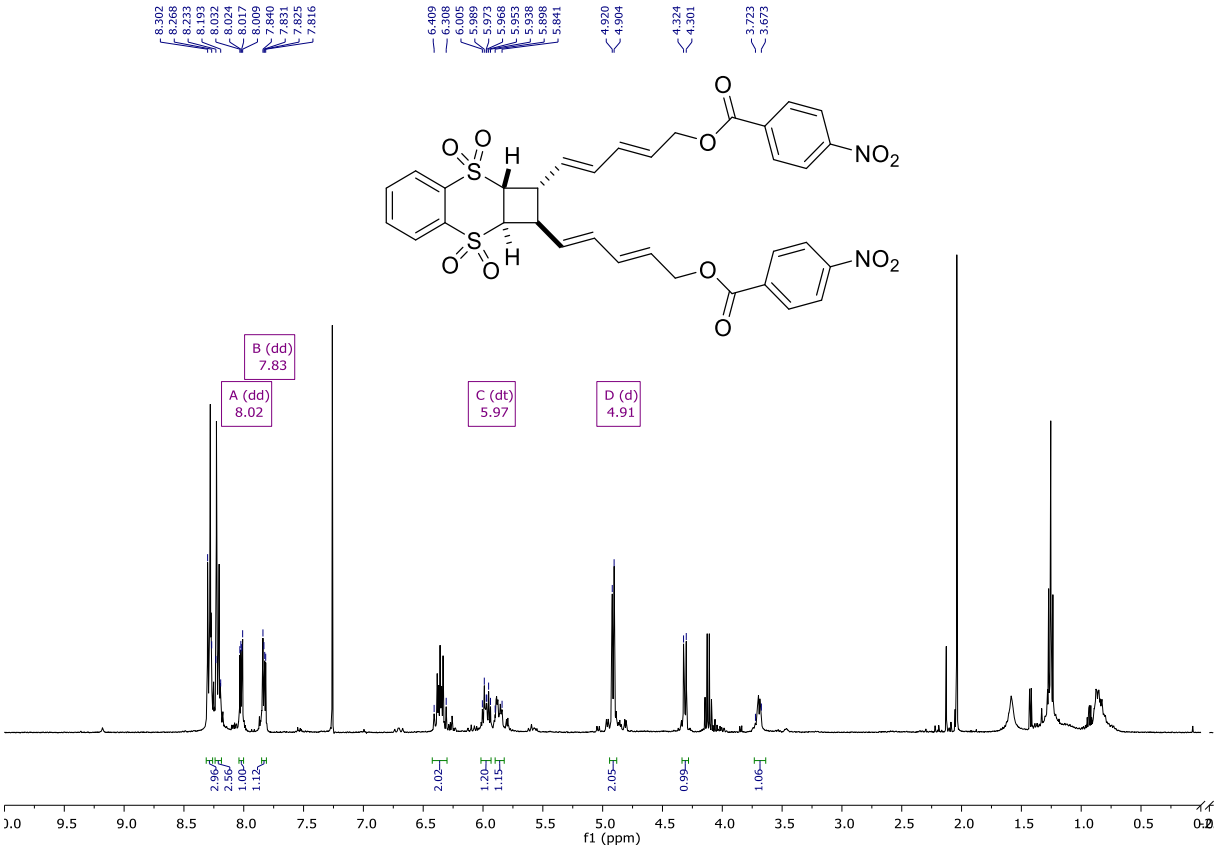
^{1}H-NMR (400 MHz) : Compound **9-O-sym**



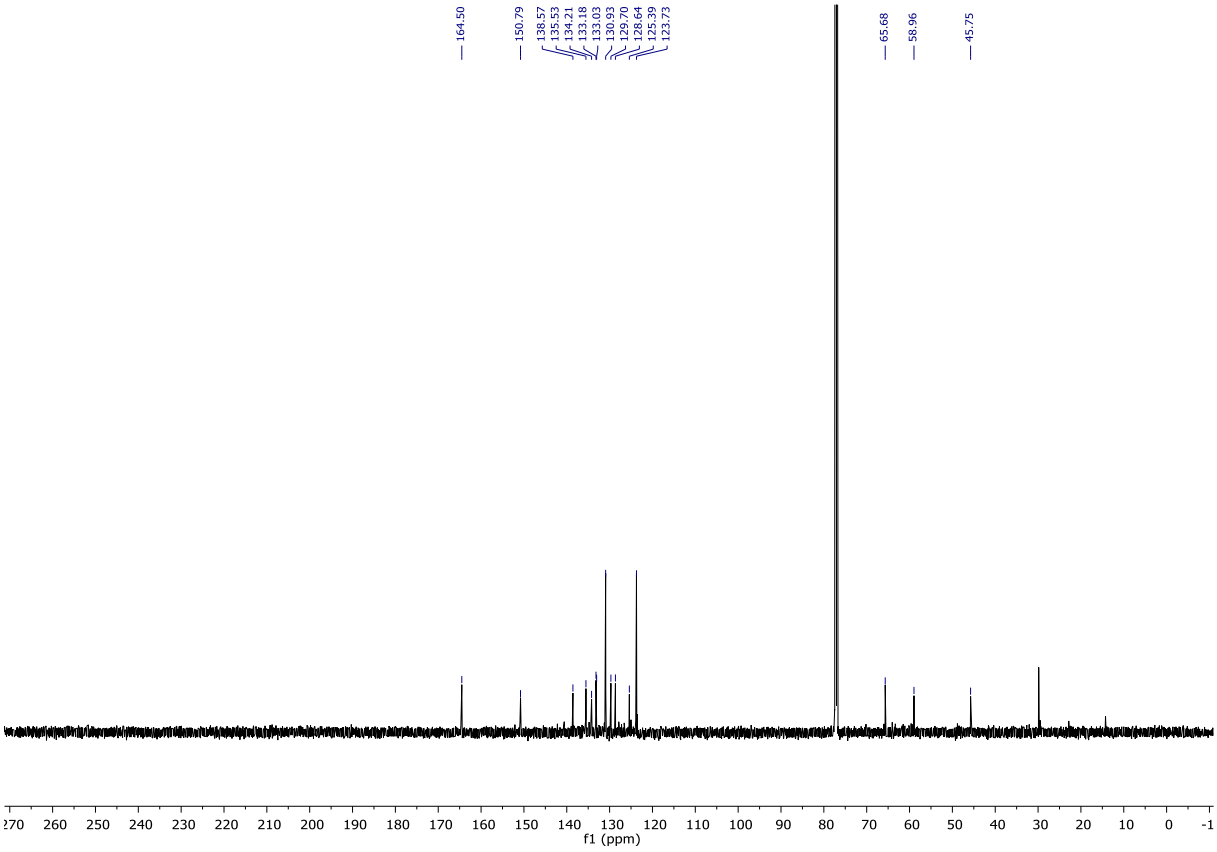
^{13}C-NMR (100 MHz) : Compound **9-O-sym**



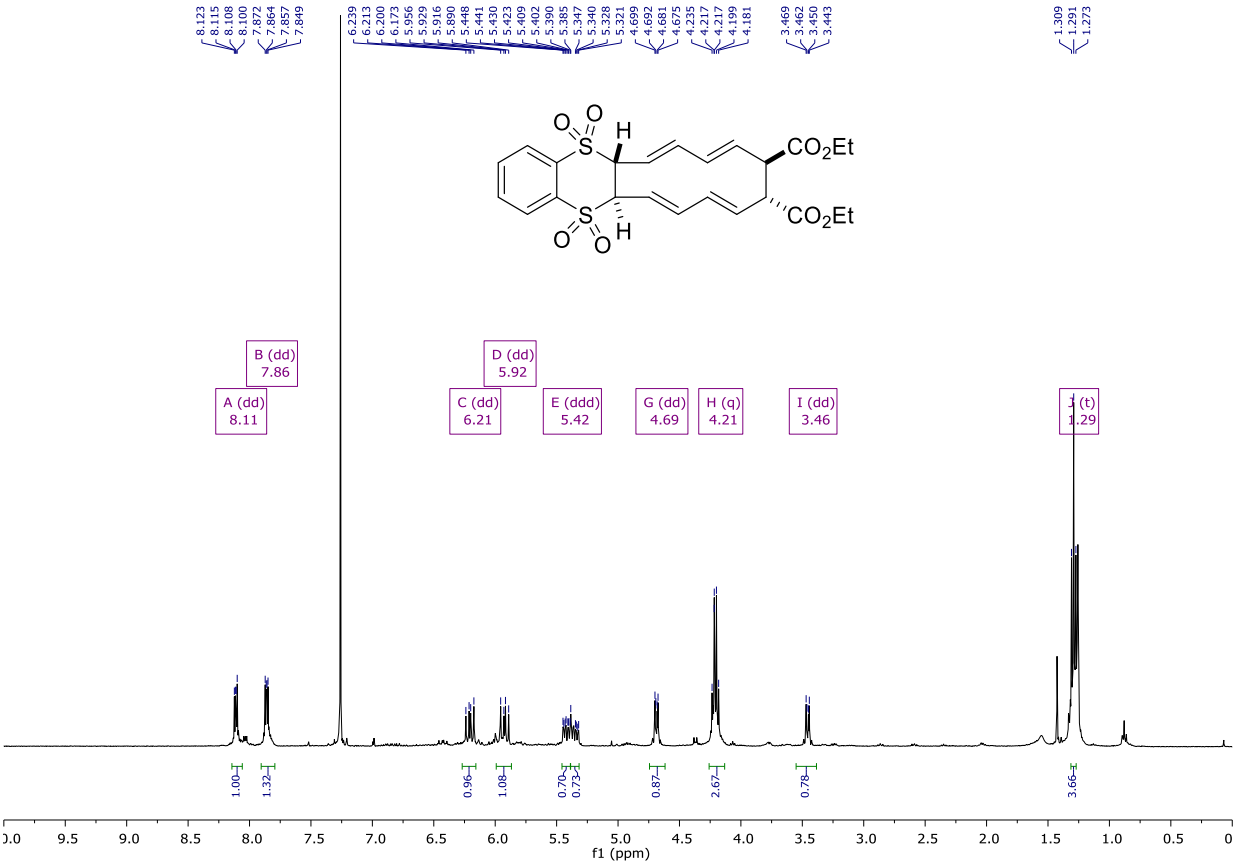
^{1}H-NMR (400 MHz) : Compound **9-O-sym'-nitroester**



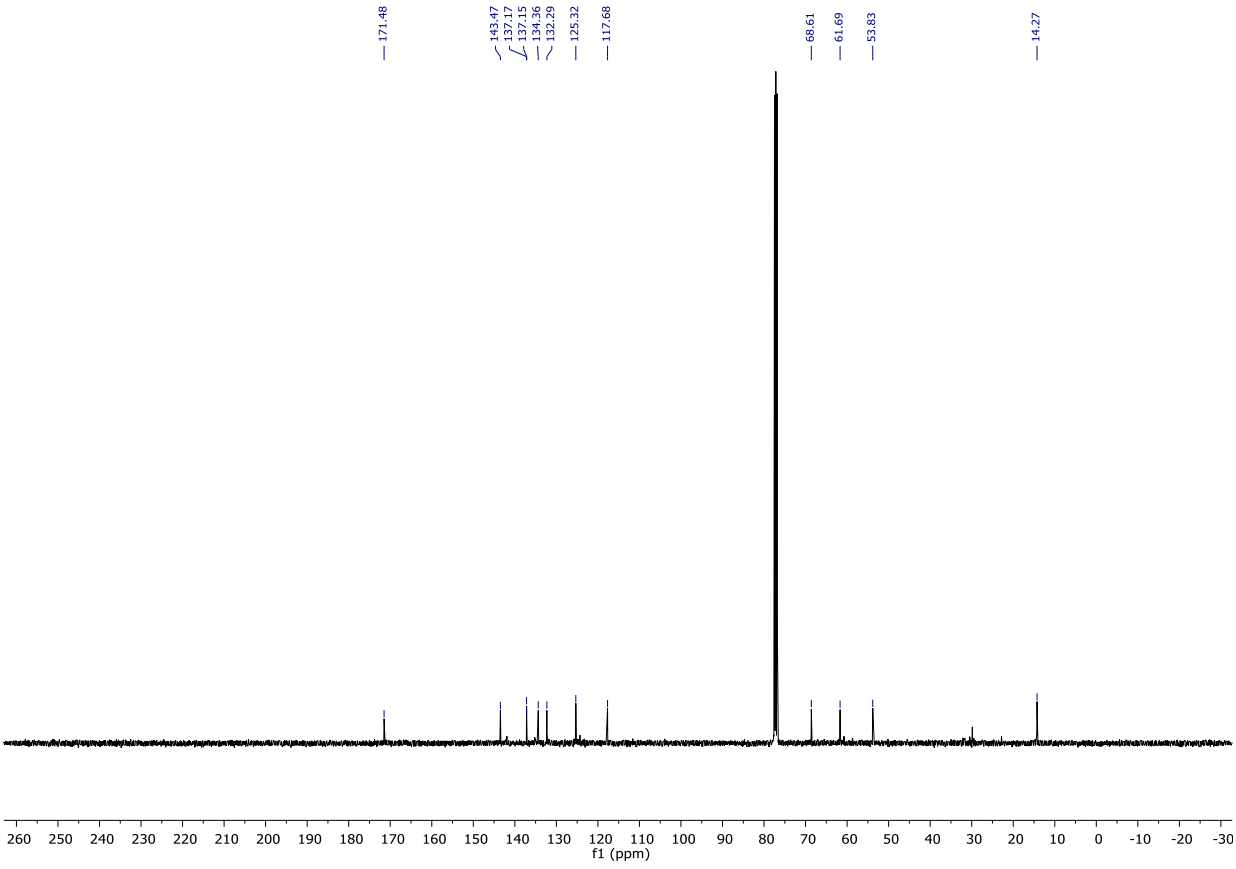
^{13}C-NMR (100 MHz) : Compound **9-O-sym'-nitroester**



^{1}H-NMR (400 MHz) : Compound **10**



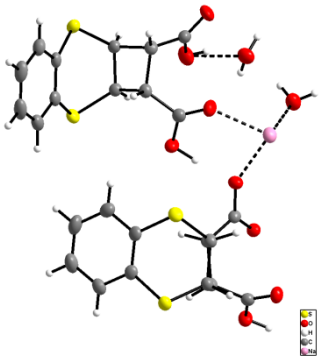
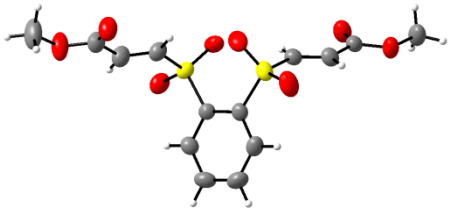
^{1}H-NMR (151 MHz) : Compound **10**



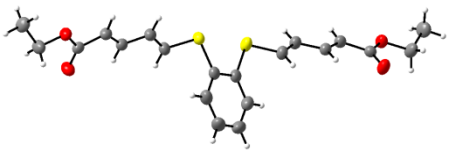
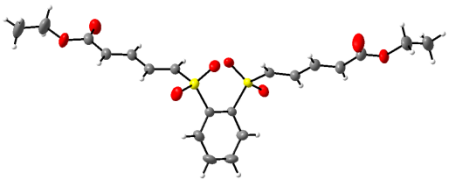
3. Crystal data: X-Ray crystal structure determination

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-Kα radiation (λ = 0.71073 Å) or a copper microfocus source (λ = 1.54178 Å). 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[1], the structure were solved with either SUPERFLIP[2], SHELXS[3] or SHELXT[4] programs and refined by full-matrix least-squares methods using SHELXL-14[5]. Specific details for each crystal structure refinements can be found in the cif files.

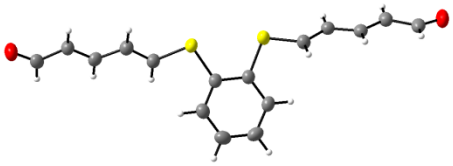
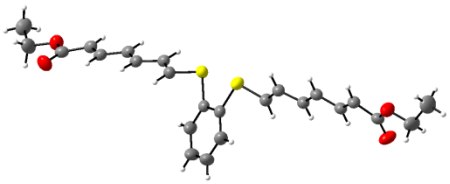
CCDC: 1535548 - 1535555

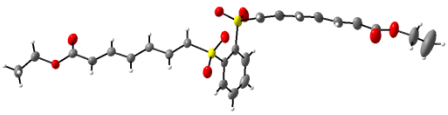
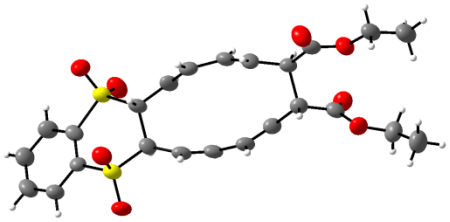
	7-OH	**2-O**
		
Chemical formula	$C_{24}H_{23}NaO_{10}S_4$	$C_{14}H_{14}O_8S_2$
M_r	622.65	374.37
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$
Temperature (K)	200	200
a, *b*, *c* (Å)	6.2958 (1), 40.1116 (9), 10.5256 (2)	8.1214 (3), 9.7223 (3), 11.2597 (3)
α,β,γ (°) ou β seul	97.680 (2)	81.884 (2), 85.392 (2), 71.440 (2)
V (Å^3)	2634.23 (9)	833.78 (5)
Z	4	2
Radiation type	Cu *K*α	Cu *K*α
μ (mm^{-1})	3.98	3.27

[1] L. J. Farrugia, *Journal of Applied Crystallography* **1999**, *32*, 837–838.
[2] L. Palatinus, G. Chapuis, *Journal of Applied Crystallography* **2007**, *40*, 786–790.
[3] G. M. Sheldrick, *Acta Cryst. A*, **2008**, 64, 112-122.
[4] G. M. Sheldrick, *Acta Crystallographica Section A*, **2015**, 71, 3-8.
[5] 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_{int}	0.103	0.040
$(\sin \theta/\lambda)_{max}$ (Å^{-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
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.36, -0.25	0.40, -0.32
	4	**4-O**
		
Chemical formula	$C_{20}H_{22}O_4S_2$	$C_{20}H_{22}O_8S_2$
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 (Å)	5.9549 (2), 15.3259 (4), 21.7847 (6)	14.7042 (3), 19.2230 (5), 8.1062 (2)
α,β,γ (°) ou β seul	93.458 (2)	95.2651 (11)
V (Å^3)	1984.54 (10)	2281.62 (9)
Z	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (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_{int}	0.024	0.023

$(\sin\theta/\lambda)_{max}$ (Å^{-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
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.23, -0.21	0.33, -0.31

	5	**6**
		
Chemical formula	$C_{16}H_{14}O_2S_2$	$C_{24}H_{26}O_4S_2$
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 (Å)	13.8437 (4), 12.6589 (4), 8.7099 (2)	6.0710 (3), 15.0757 (9), 25.2963 (14)
α,β,γ (°) ou β seul	100.811 (2)	92.595 (3)
V (Å^3)	1499.28 (7)	2312.9 (2)
Z	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	3.20	2.31
Crystal size (mm)	0.42 × 0.04 × 0.04	0.66 × 0.4 × 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_{int}	0.028	0.030
$(\sin\theta/\lambda)_{max}$ (Å^{-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
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.22, -0.19	0.22, -0.19

	6-O	**10**
		
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)
α,β,γ (°) ou β seul	100.650 (1), 92.438 (1), 101.714 (1)	93.607 (18)
V (Å^3)	2850.50 (13)	4886.8 (19)
Z	4	8
Radiation type	Mo $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	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^{-1})	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
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	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

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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

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H,0,-3.8366971916,0.6087854116,3.5237385932

H,0,-0.0781911182,4.1432018015,3.2733975237

H,0,-0.2486249959,4.0132025296,6.337559099

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4) Mono3

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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

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5) Tric

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C,0,0.1349639397,-0.0736863624,1.5310235959

C,0,1.6446673638,0.115477968,-0.0672954976

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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

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H,0,1.8838572394,1.9841215019,2.390553257

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H,0,5.7799936613,1.9779124957,-1.8923237489

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6) Pent

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H,0,6.3711070715,1.9165759175,2.0407886398

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SULFONE

1) Acyc

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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

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O,0,-2.2943596642,-3.1205543863,-1.1773595792

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C,0,-0.1274401912,-2.3902446167,0.1205350696

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C,0,2.3085065049,-2.6705075858,0.4107732806

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2) Mono1

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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

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O,0,-1.6666620152,-2.0691487473,2.2388729093

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H,0,3.1223731817,-2.5749706051,-1.196536605

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H,0,5.3597674416,-3.6905678795,-1.4242567505

H,0,-2.7551010373,-2.9857961875,-1.1264631973

H,0,-4.5149670154,-1.978585946,-2.5801277289

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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

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C,0,1.2426282245,-0.8582570931,-0.302475284

C,0,-0.0540484947,-0.4343189232,-0.5698825755

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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

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C,0,0.653576986,-2.0542804266,5.0726838826

C,0,-0.5020994833,-2.6002269905,5.8555588968

C,0,-0.6091320048,-4.1580526866,5.9469208492

C,0,-1.1362959694,-4.6468631014,7.2615915942

C,0,-0.5905654759,-5.6296928393,7.9780384053

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H,0,1.8662483936,-1.2606782744,-1.094635809

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H,0,-1.3141454958,-1.9864526814,2.9422749618

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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

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4) Mono3

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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

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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

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5) Tric1

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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

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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

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H,0,-5.1488673674,-1.2243290118,-0.694611791

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H,0,3.05455909,-2.484779143,1.4177441574

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6) Tric2

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C,0,2.720492979,1.2147693839,1.8459829248

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S,0,1.7642511909,1.9774968623,-0.5686882123

O,0,2.7631330849,2.0857689736,-1.6329145342

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C,0,-0.7210329768,-1.2371965195,-0.2043970682

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C,0,-0.9024995641,1.5116952959,-0.5464818

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7) Pent

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H,0,4.1830894921,-0.6053881459,-0.6561418015

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S,0,6.5472492841,-4.1967062439,2.4568557133

C,0,6.0252617493,-5.6467218584,0.0936864459

C,0,6.0297153509,-5.6375689875,1.4952052348

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C,0,5.6350931905,-6.7715703321,2.2041035591

C,0,5.2627446417,-7.9334252714,0.1141148097

C,0,5.2671794358,-7.9243119527,1.5094958498

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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

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SULFUR

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S,0,-2.3543678971,-2.1278425449,3.4860624699

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C,0,-9.0640531429,-3.1851720658,-0.0817671305

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2) Mono1

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3) Mono2

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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