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ORGANIC & BIOMOLECULAR CHEMISTRY

ELECTRONIC SUPPLEMENTARY INFORMATION FOR

Push-pull systems bearing a quinoid/aromatic thieno[3,2-b]thiophene moiety: synthesis, ground state polarization and second-order nonlinear properties

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1. General Experimental Methods

Infrared measurements were carried out in KBr using a Perkin-Elmer Fourier Transform Infrared 1600 spectrometer. Melting points were obtained on a Gallenkamp apparatus in open capillaries and are uncorrected. ^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker ARX300 or a Bruker AV400 at 300 or 400 MHz and 75 or 100 MHz respectively; δ values are given in ppm (relative to TMS) and *J* values in Hz. The apparent resonance multiplicity is described as a s (singlet), br s (broad singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). ^{1}H-^{1}H COSY and ^{1}H-^{13}C-HSQC experiments were recorded on a Bruker ARX300 or a Bruker AV400 at 300 or 400 MHz in order to establish peaks assignment and spatial relationships. Electrospray mass spectra were recorded on a Bruker Q-ToF spectrometer; accurate mass measurements were achieved using sodium formate as external reference. UV-Visible spectra were recorded with an UV-Vis UNICAM UV4 spectrophotometer. Cyclic voltammetry measurements were performed with a μ-Autolab ECO-Chemie potentiostat using a glassy carbon working electrode, Pt counter electrode, and Ag/AgCl reference electrode. The experiments were carried out under argon in CH_2Cl_2, with Bu_4NPF_6 as supporting electrolyte (0.1 mol L^{-1}). Scan rate was 100 mV s^{-1}. Elemental analyses were carried out with a Perkin-Elmer CHN2400 microanalyzer. 1064 nm FT–Raman spectra were obtained in an FT–Raman accessory kit (FRA/106–S) of a Bruker Equinox 55 FT–IR interferometer. A continuous–wave Nd–YAG laser working at 1064 nm was employed for excitation. A germanium detector operating at liquid nitrogen temperature was used. Raman scattering radiation was collected in a back–scattering configuration with a standard spectral resolution of 4 cm^{-1}. 2000 scans were averaged for each spectrum.

X-Ray data collection were carried out on a diffractometer equipped with a graphite monochromator utilizing Mo Kα radiation (λ = 0.71073 Å). The diffraction frames were integrated and corrected for absorption using the CrysAlis RED package.[1] The structures were solved by direct methods.[2] All refinements were carried out using SHELXL-97[3] against the F^2 data using full-matrix least squares methods. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed at idealized positions

(1) CrysAlisPro, Oxford Diffraction Ltd.,Version 1.171.35.15 (release 03-08-2011 CrysAlis171. NET) (compiled Aug 3 2011, 13:03:54).
(2) A. Altomare, G. Cascarano, C. Giacovazzo and A. Guagliardi, *J. Appl. Crystallogr.*, 1993, **26**, 343–350.
(3) G. M. Sheldrick, *Acta Crystallogr., Sect. A*, 2008, **64**, 112–122.

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and refined as riders with isotropic displacement parameters assigned as 1.2 times the U_{eq} value of the corresponding bonding partner (1.5 times for methyl hydrogen atoms).

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2. NMR spectra for new compounds

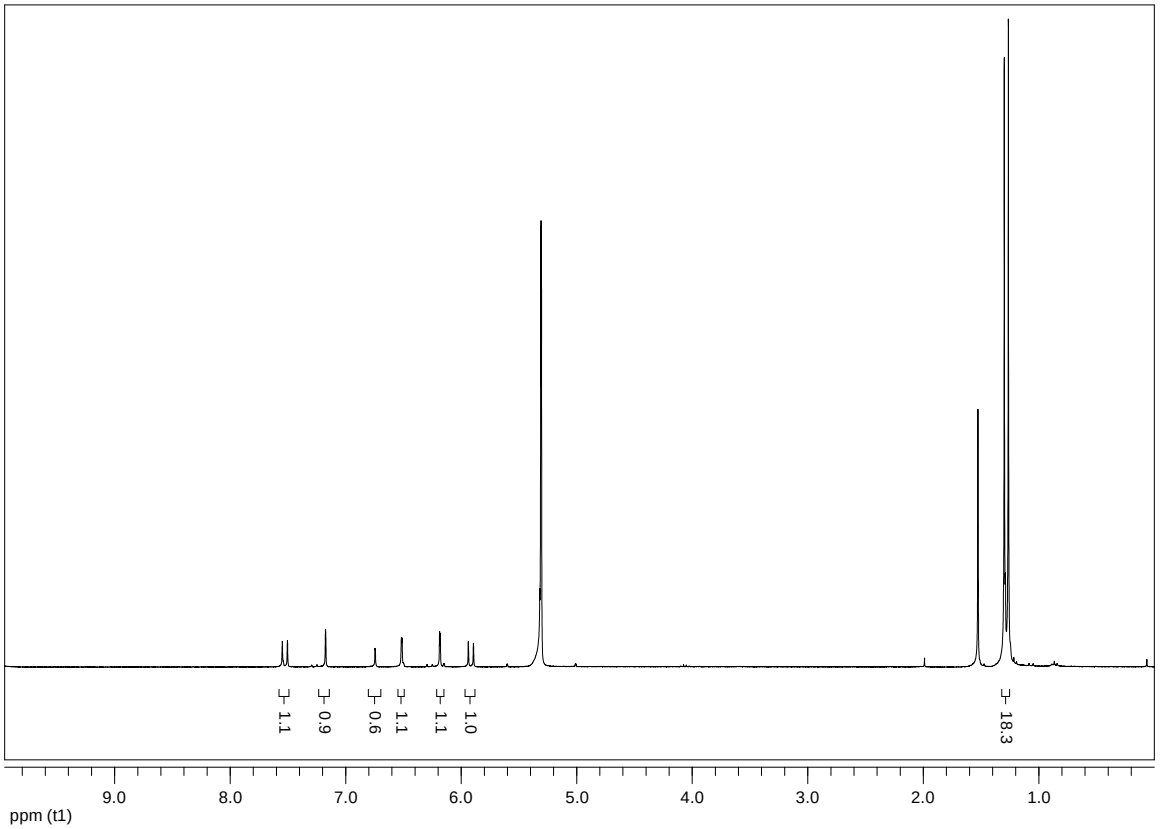
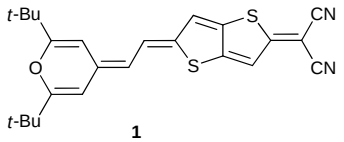


Figure S-1: ^{1}H-NMR spectrum of compound **1** (300 MHz, CD_2Cl_2).



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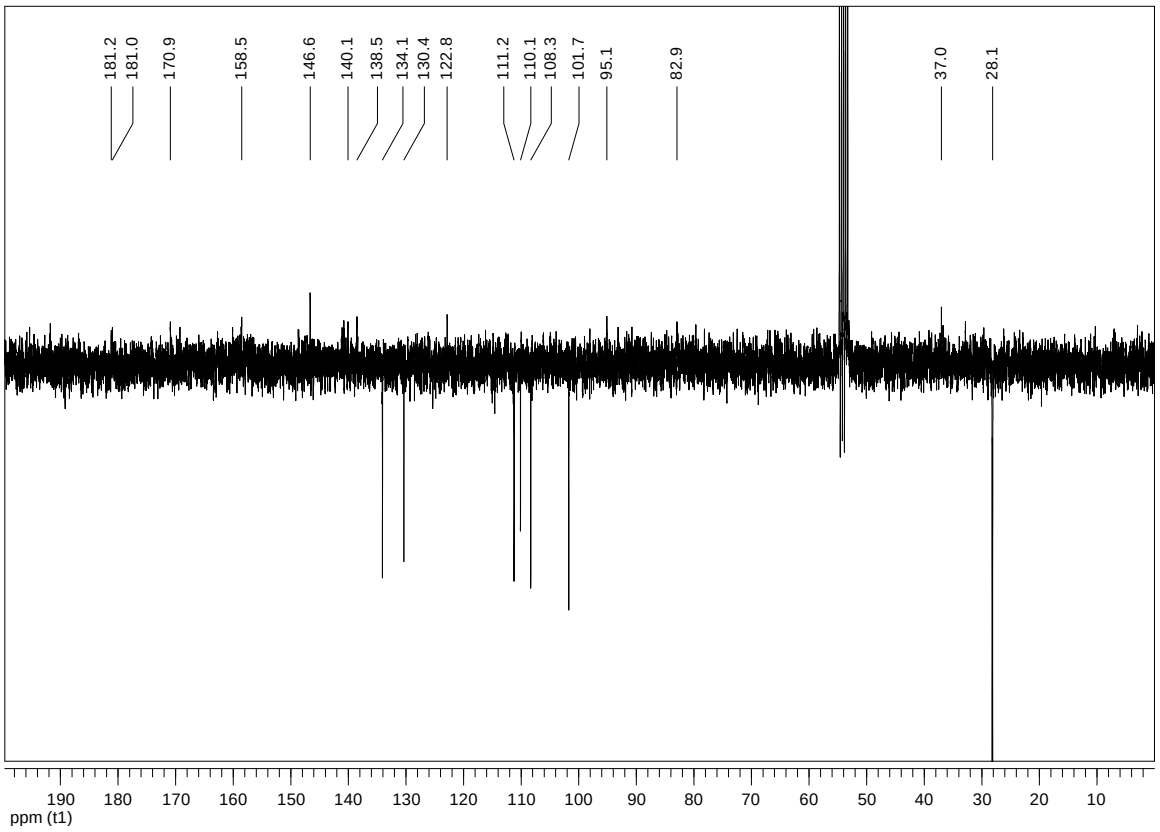
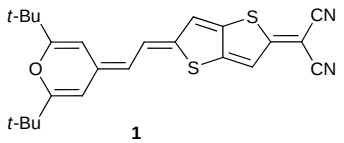


Figure S-2: ^{13}C-NMR (APT) spectrum of compound **1** (75 MHz, CD_2Cl_2).



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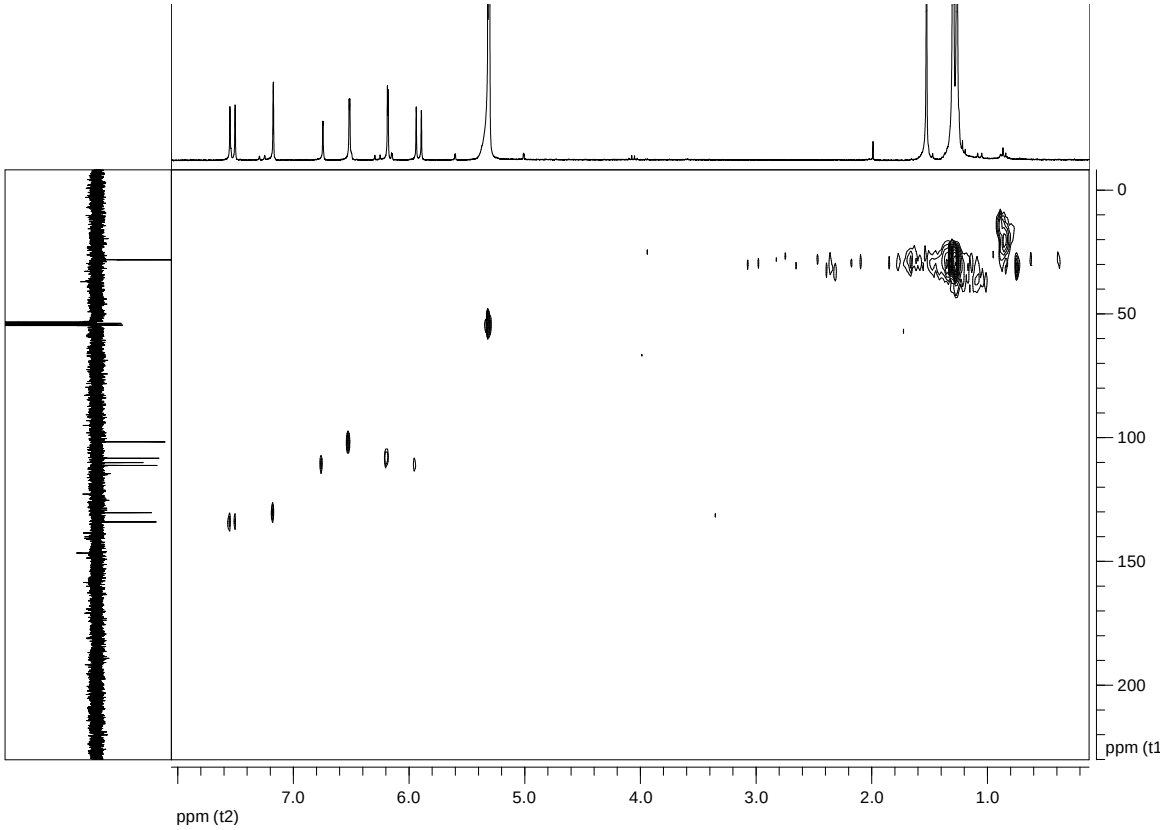
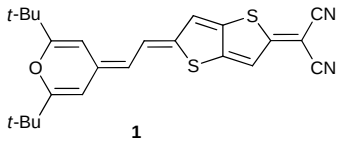


Figure S-3: ^{1}H-^{13}C-HSQC spectrum of compound **1** (300 MHz, CD_2Cl_2).



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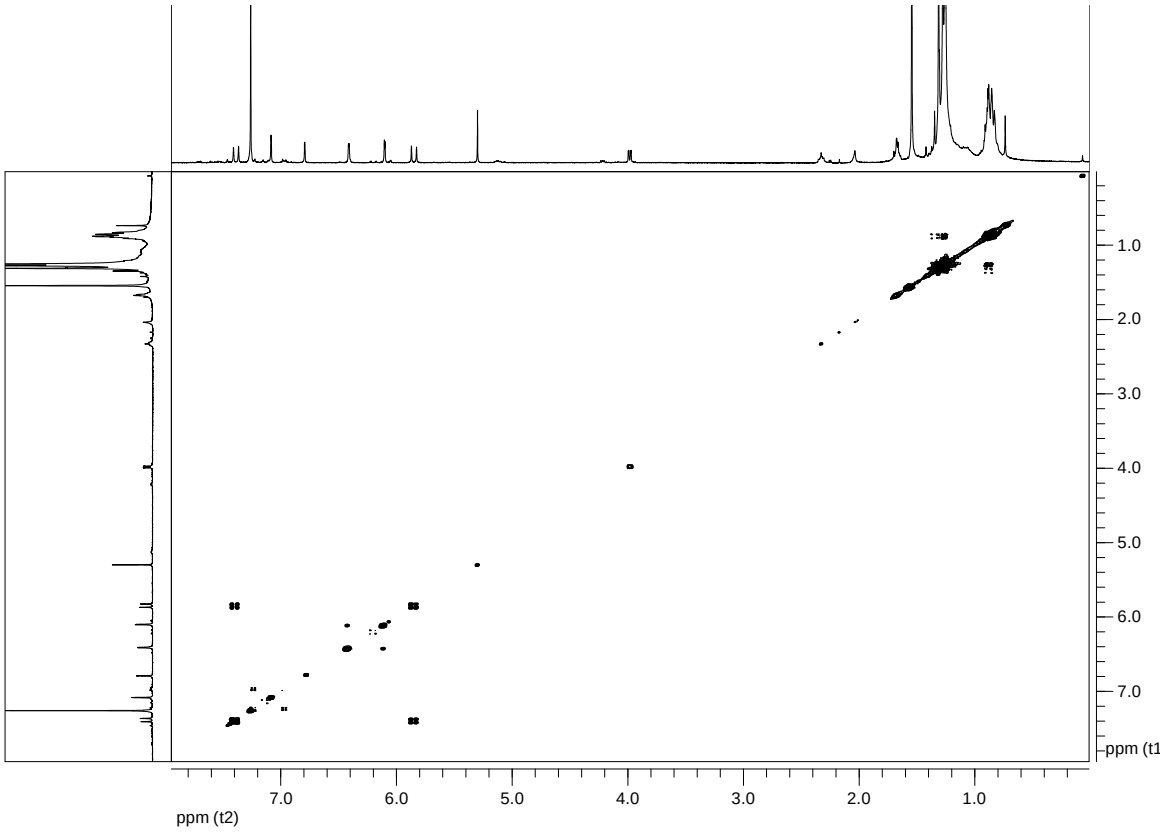
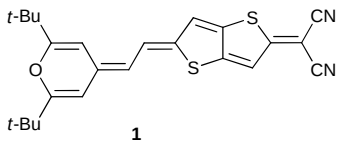


Figure S-4: ^{1}H-^{1}H-COSY spectrum of compound **1** (300 MHz, $CDCl_3$).



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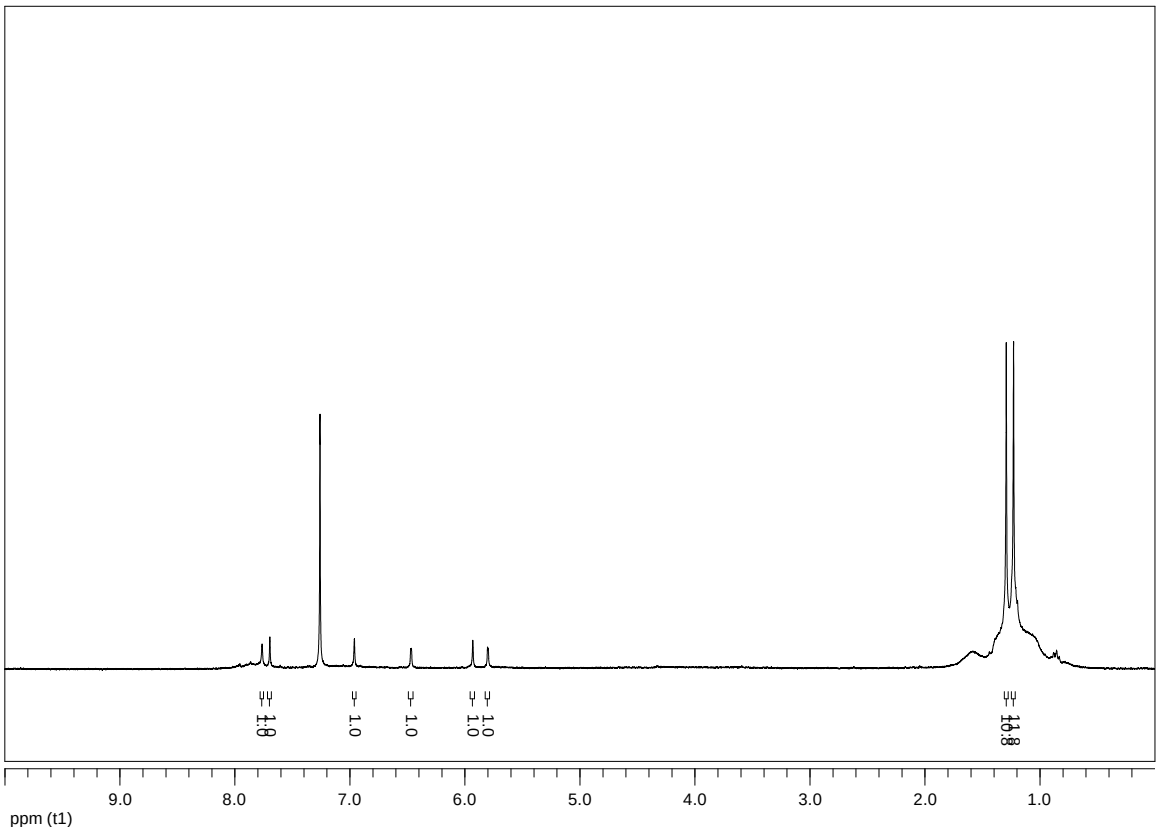
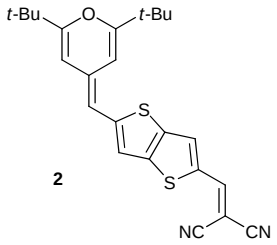


Figure S-5: ^{1}H-NMR spectrum of compound **2** (300 MHz, $CDCl_3$).



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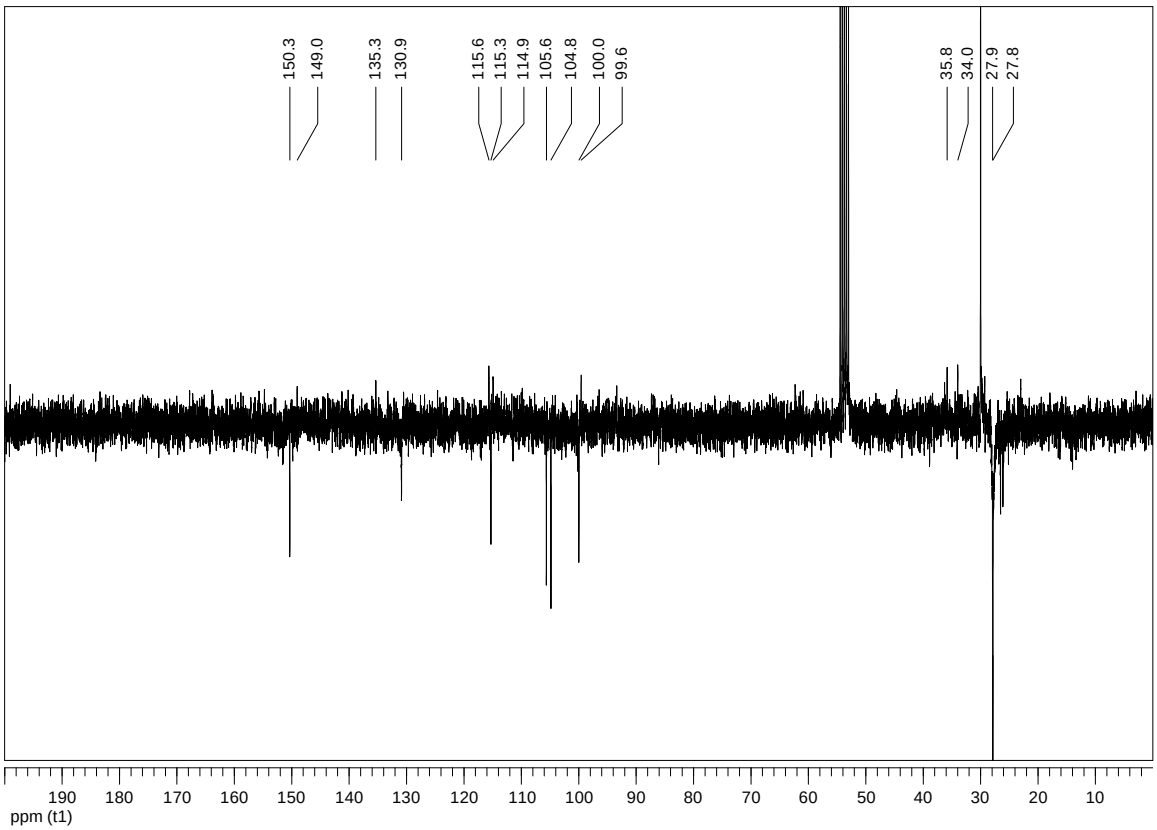
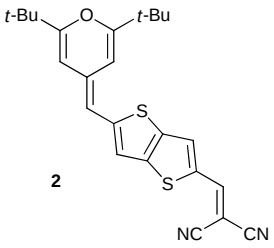


Figure S-6: ^{13}C-NMR (APT) spectrum of compound **2** (75 MHz, CD_2Cl_2).



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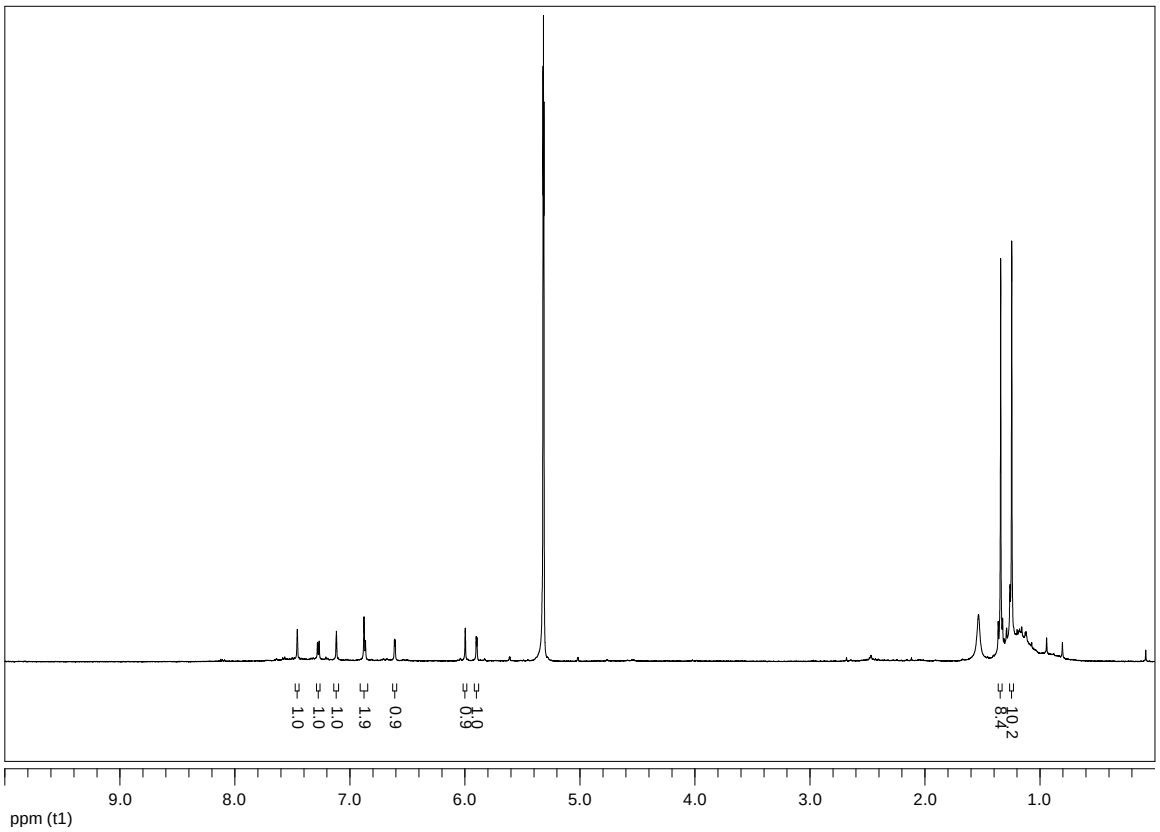
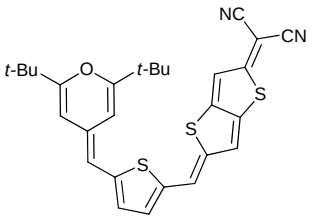


Figure S-7: ^{1}H-NMR spectrum of compound **3** (300 MHz, CD_2Cl_2).



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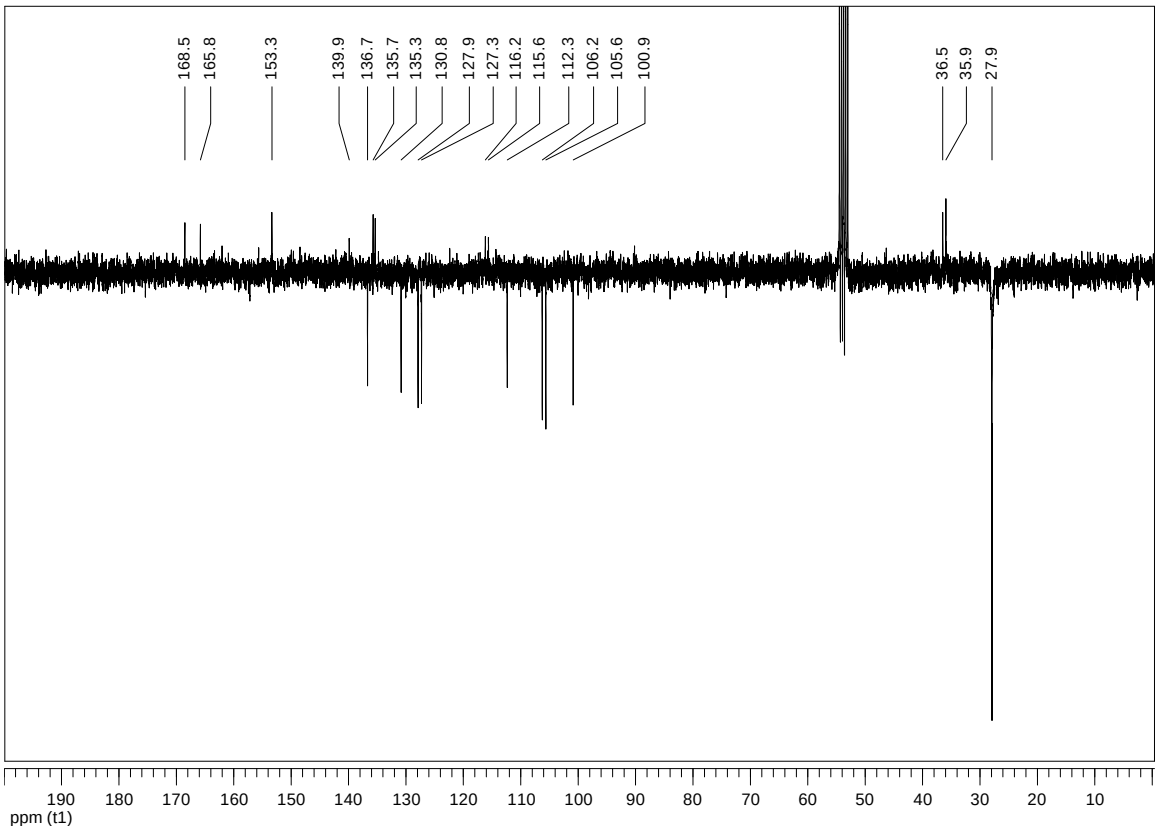
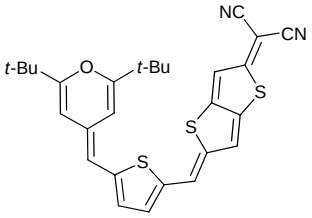


Figure S-8: ^{13}C-NMR (APT) spectrum of compound **3** (75 MHz, CD_2Cl_2).



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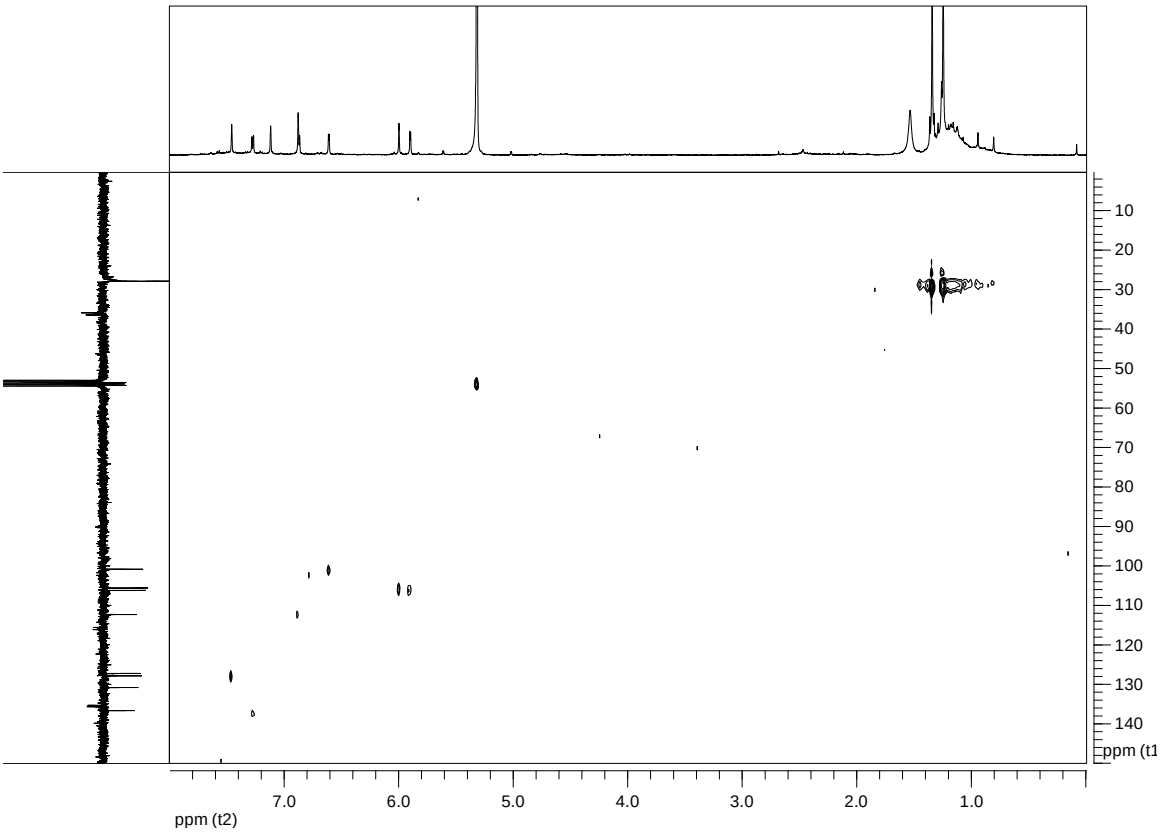
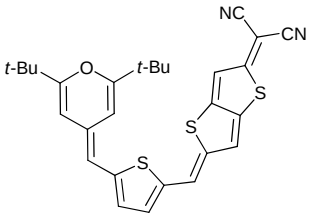


Figure S-9: ^{1}H-^{13}C-HSQC spectrum of compound **3** (400 MHz, CD_2Cl_2).



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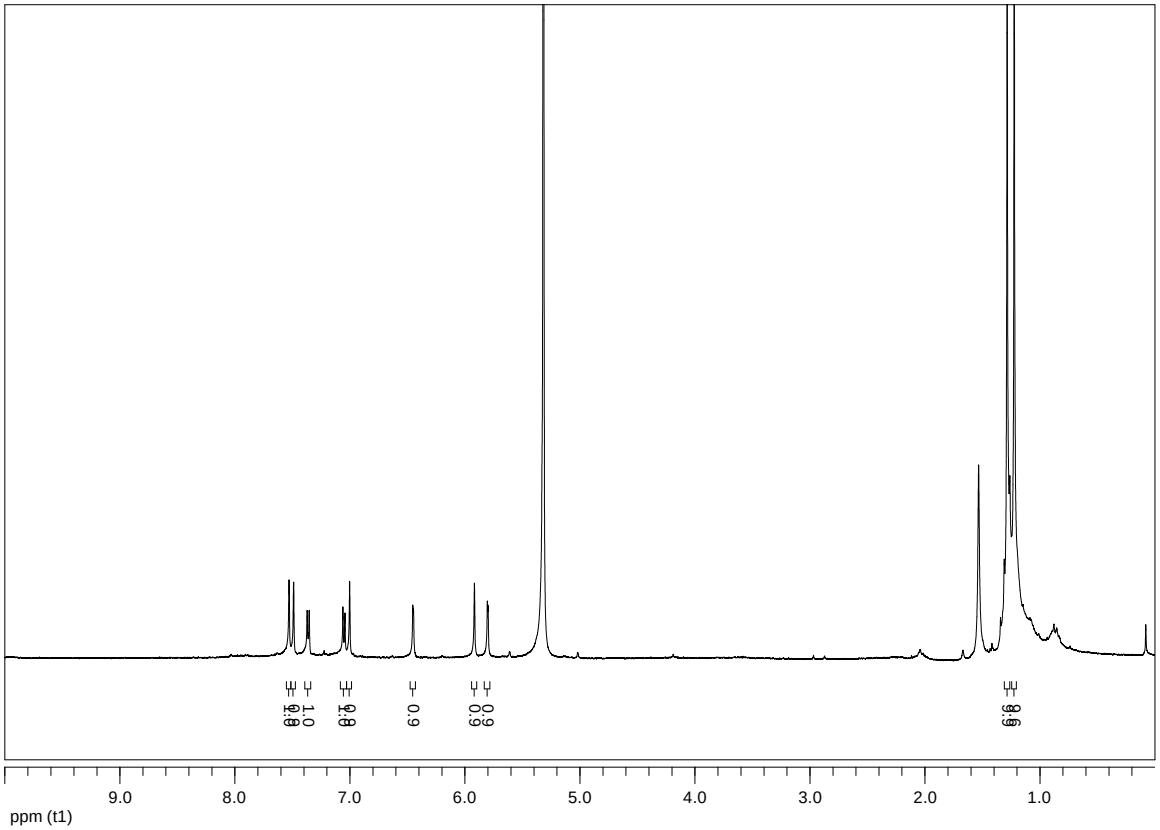
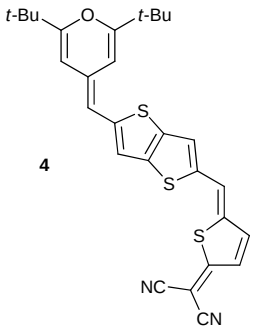


Figure S-10: ^{1}H-NMR spectrum of compound **4** (300 MHz, CD_2Cl_2).



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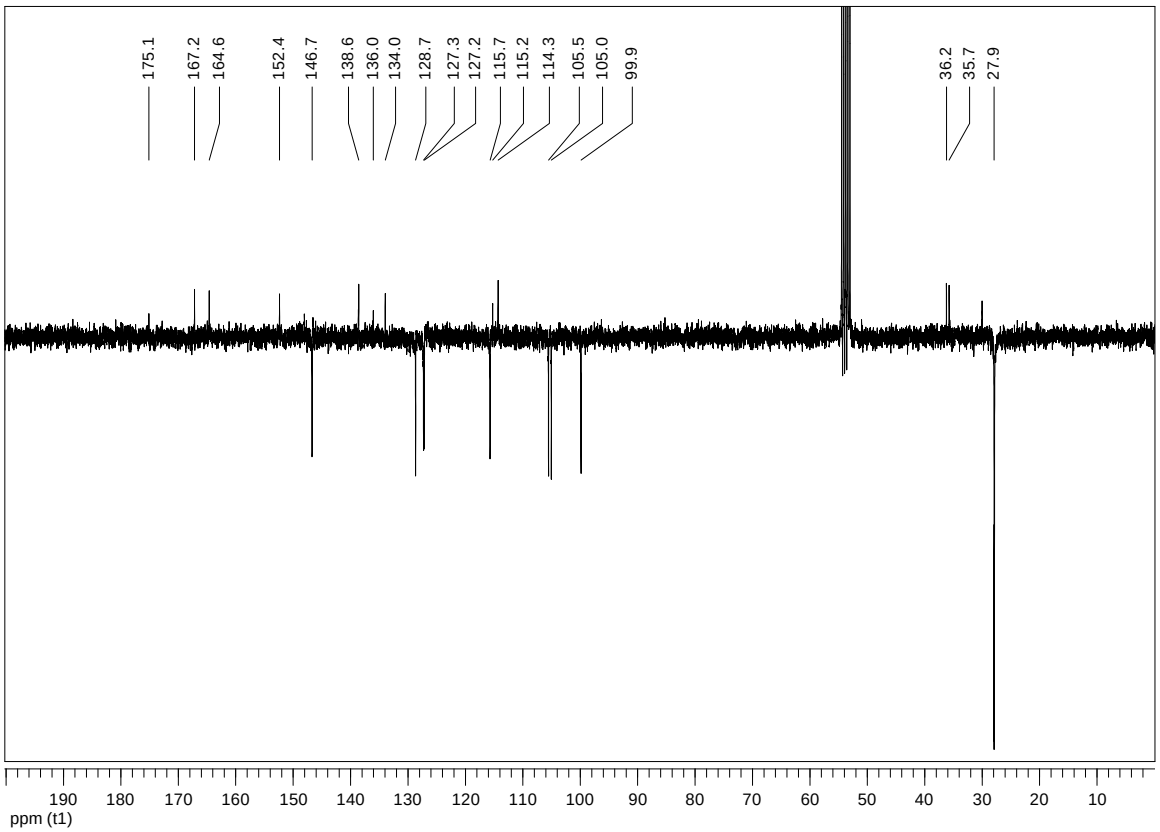
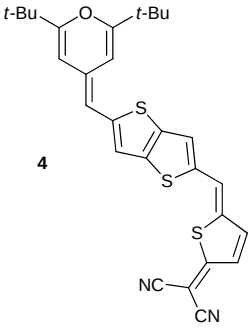


Figure S-11: ^{13}C-NMR (APT) spectrum of compound **4** (75 MHz, CD_2Cl_2).



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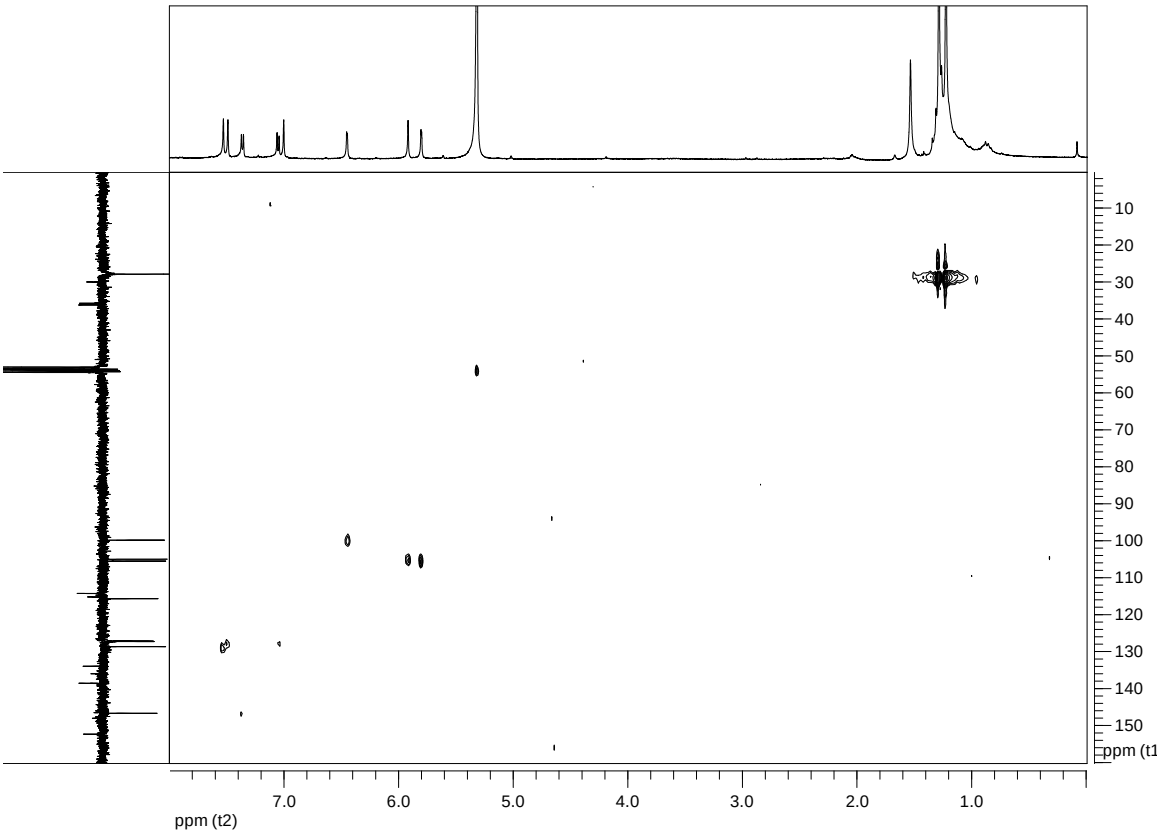
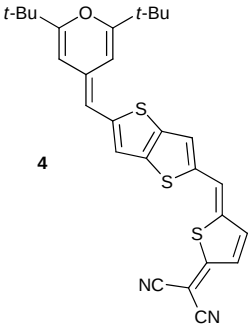


Figure S-12: ^{1}H-^{13}C-HSQC spectrum of compound **4** (400 MHz, CD_2Cl_2).



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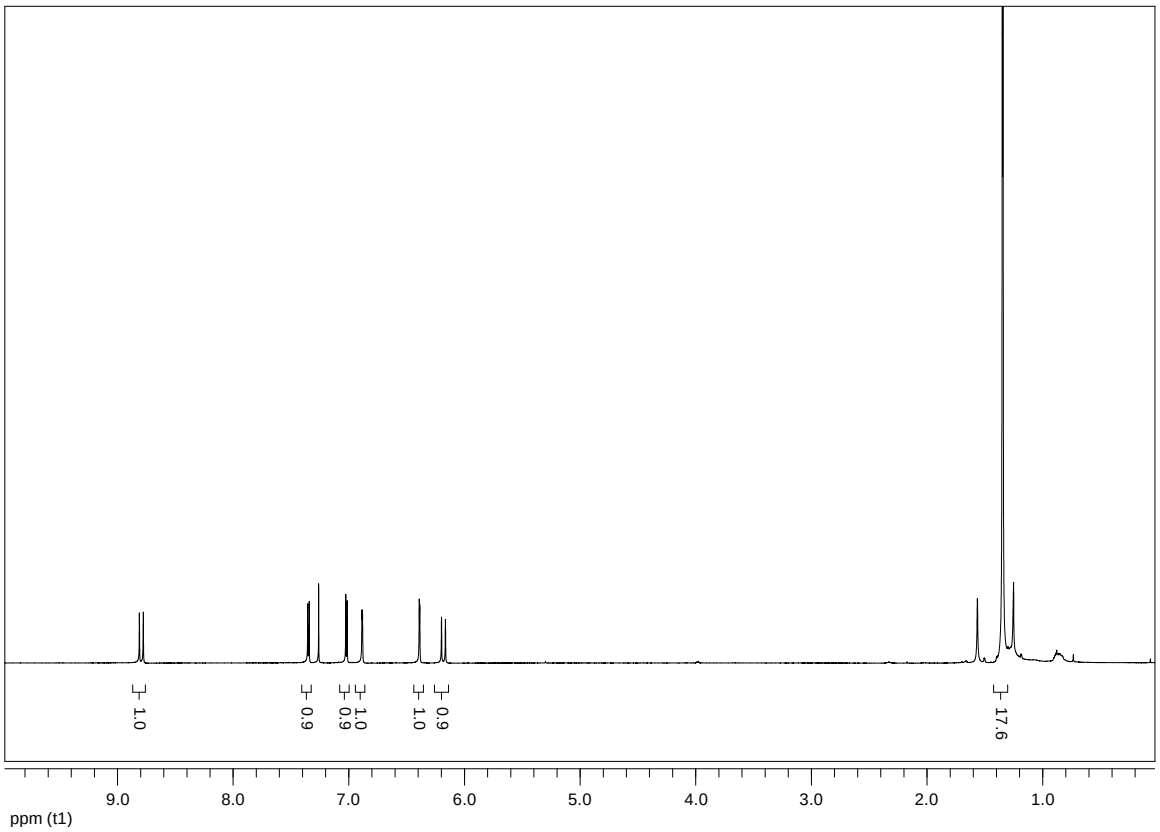
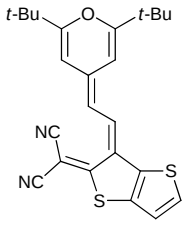


Figure S-13: ^{1}H-NMR spectrum of compound **8** (400 MHz, $CDCl_3$).



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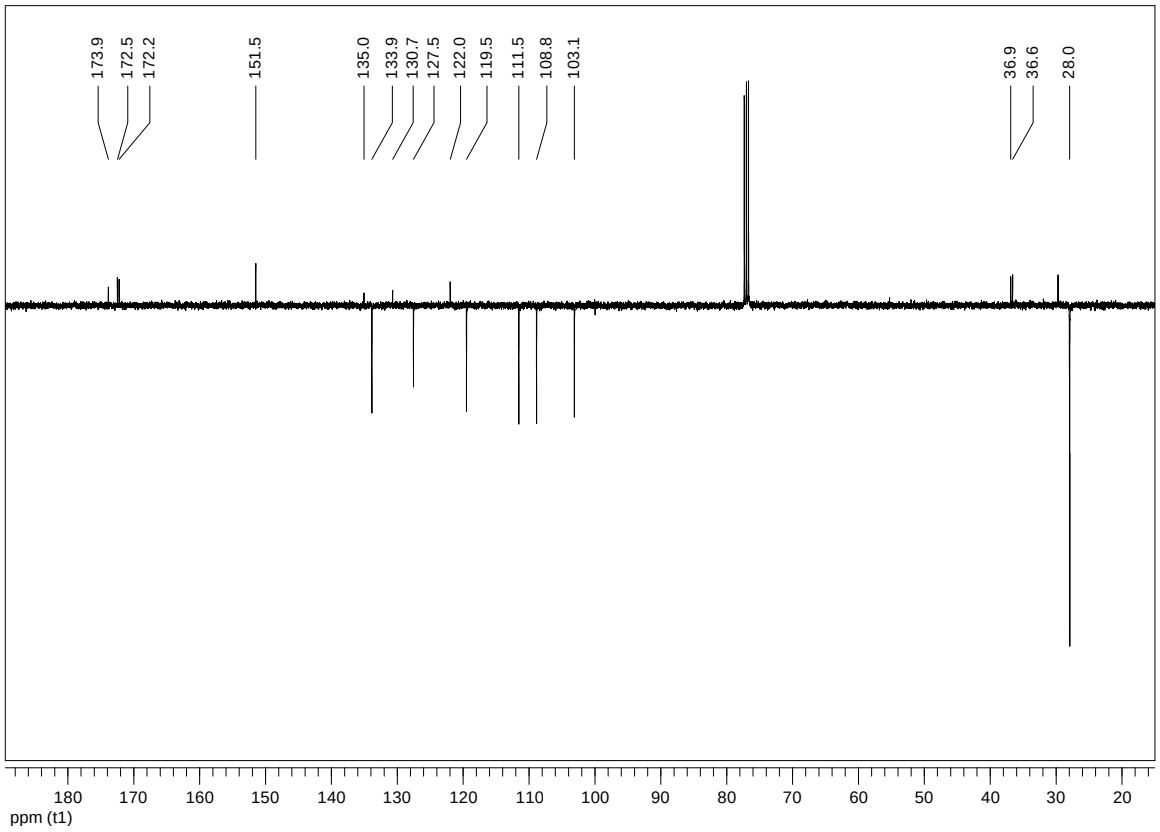
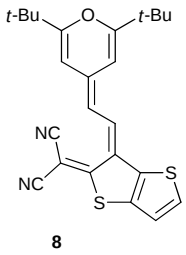


Figure S-14: ^{13}C-NMR (APT) spectrum of compound **8** (100 MHz, $CDCl_3$).



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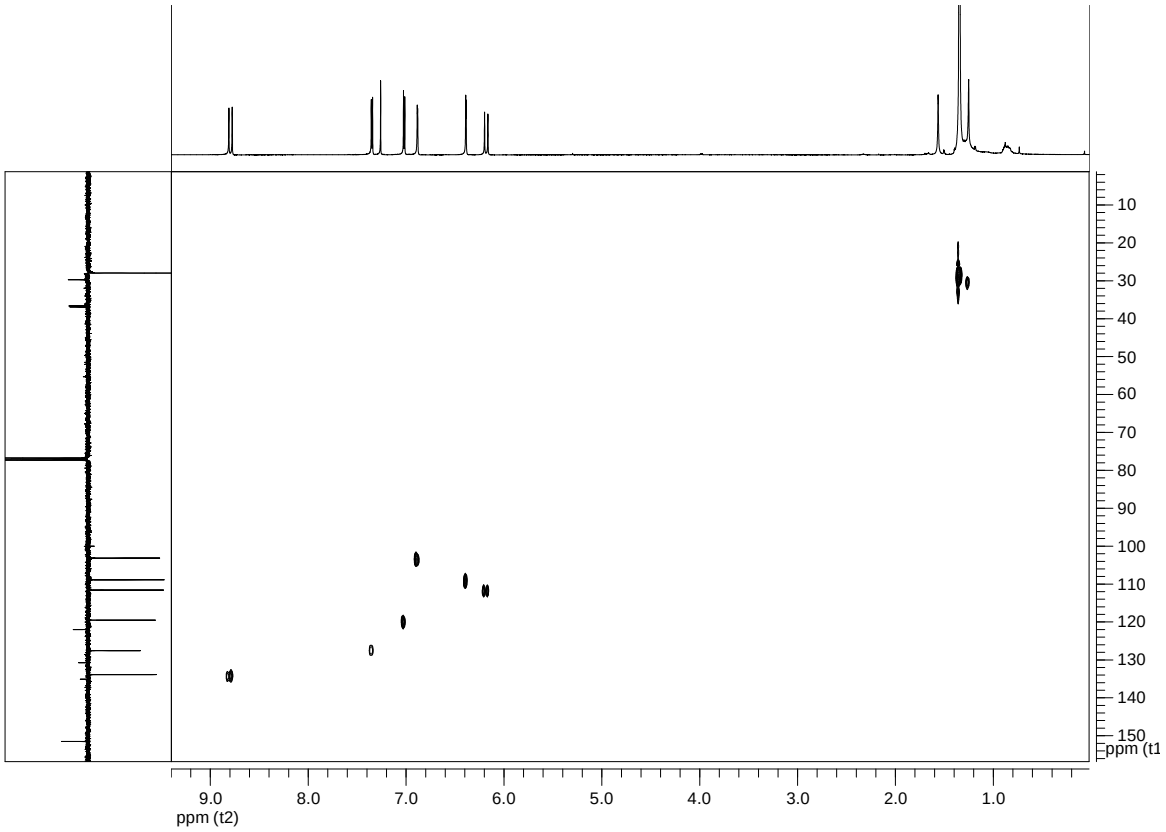
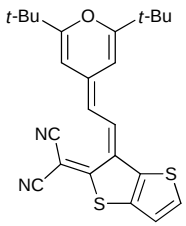


Figure S-15: ^{1}H-^{13}C-HSQC spectrum of compound **8** (400 MHz, $CDCl_3$).



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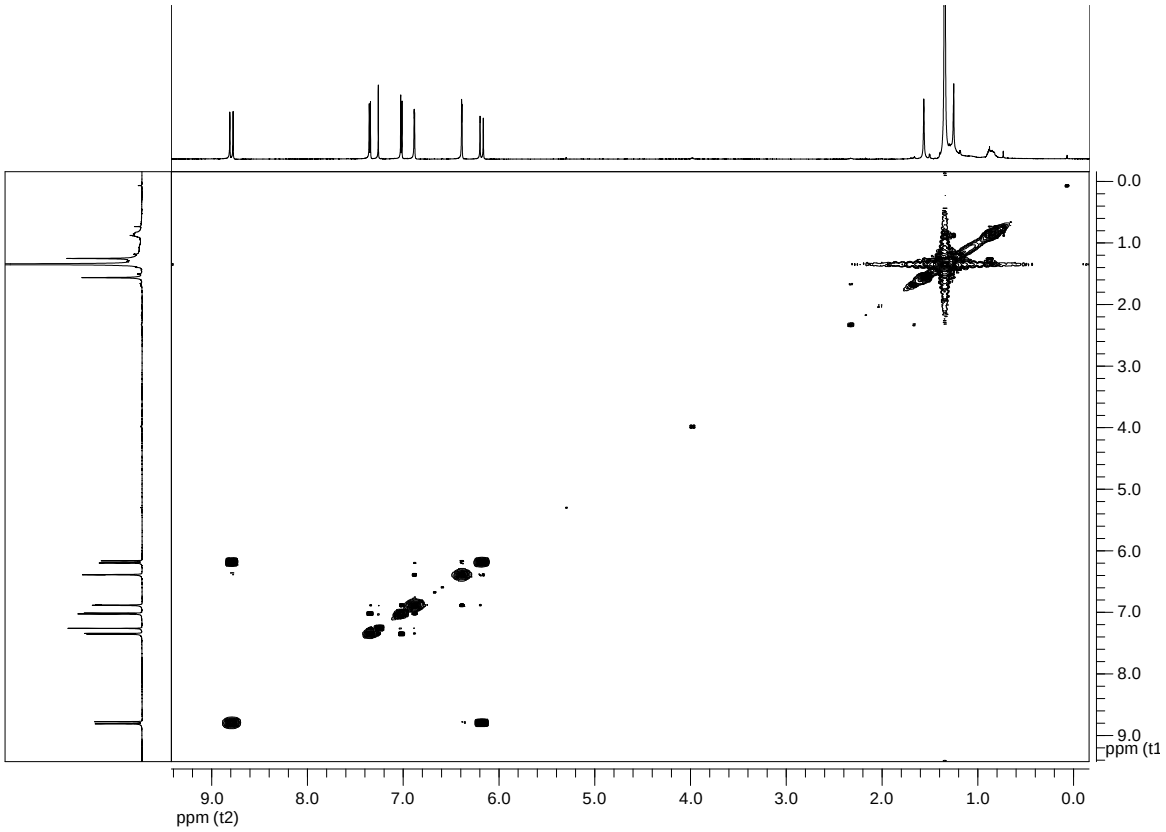
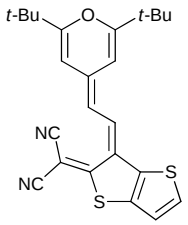


Figure S-16: ^{1}H-^{1}H-COSY spectrum of compound **8** (400 MHz, $CDCl_3$).



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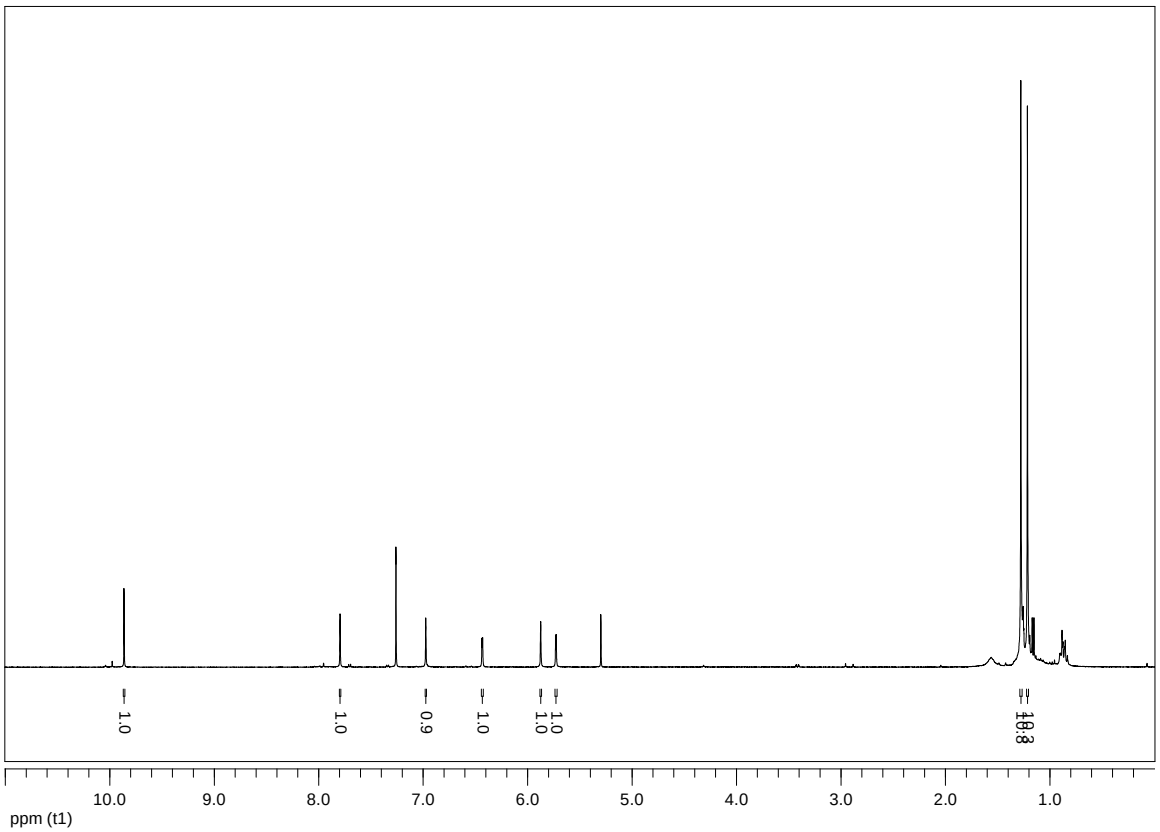
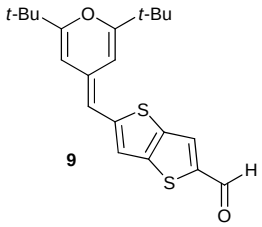


Figure S-17: ^{1}H-NMR spectrum of compound **9** (300 MHz, $CDCl_3$).



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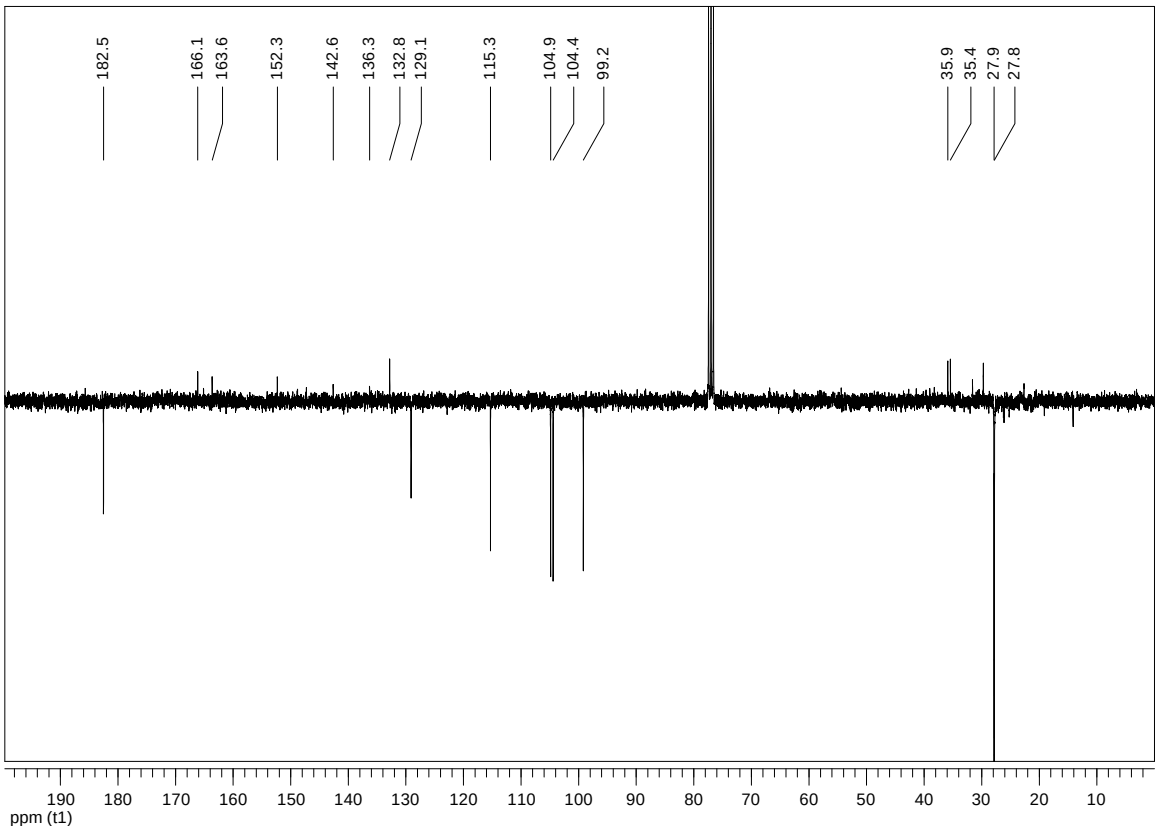
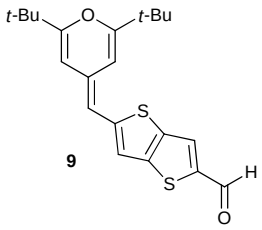


Figure S-18: ^{13}C-NMR (APT) spectrum of compound **9** (75 MHz, $CDCl_3$).



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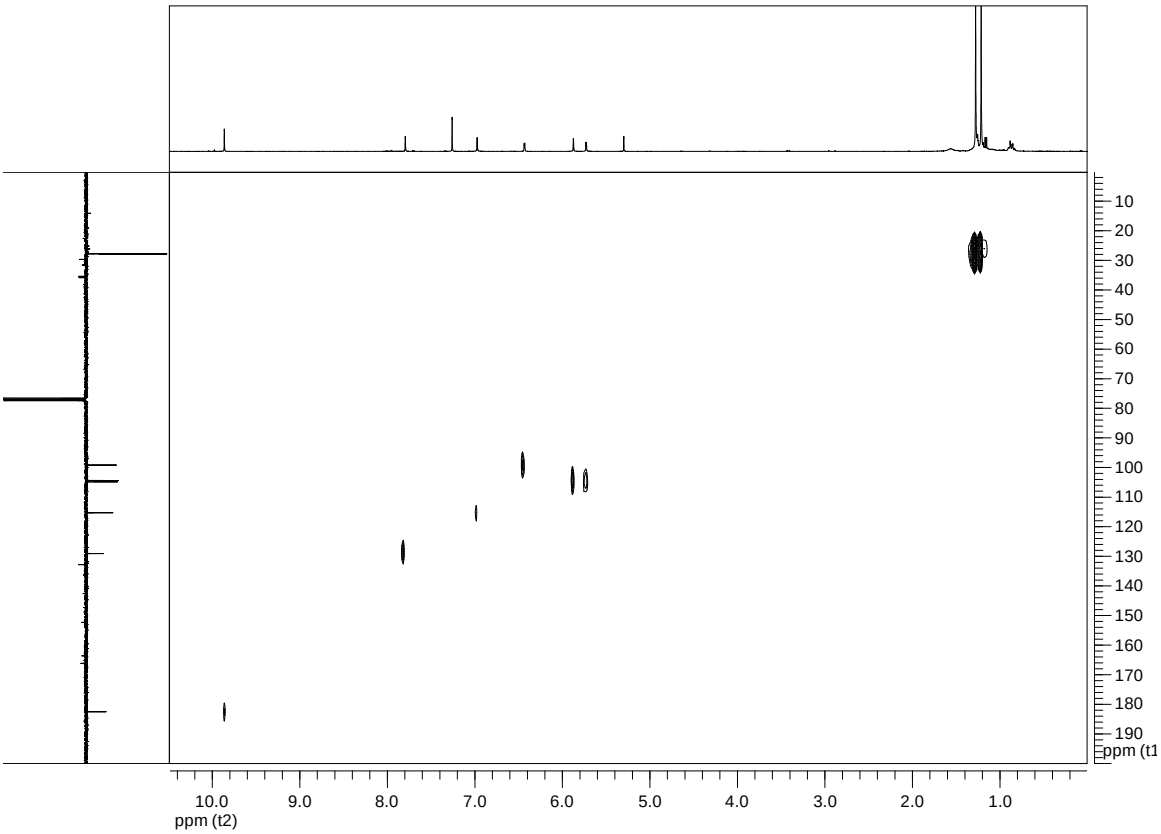
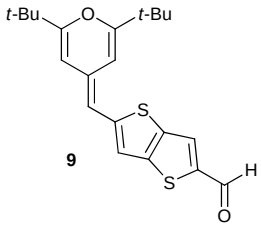


Figure S-19: ^{1}H-^{13}C-HSQC spectrum of compound **9** (300 MHz, $CDCl_3$).



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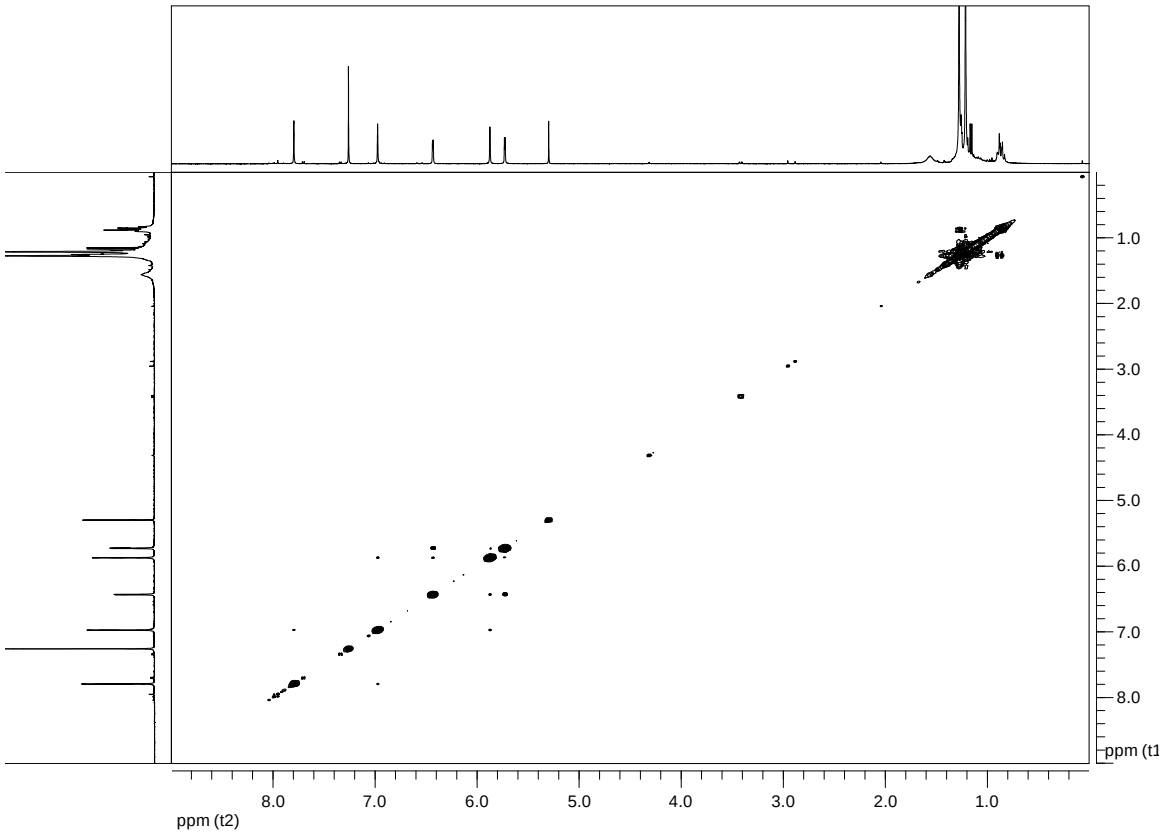
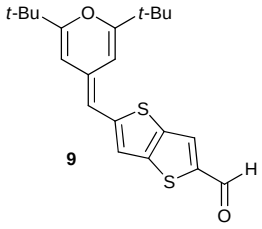


Figure S-20: ^{1}H-^{1}H-COSY spectrum of compound **9** (300 MHz, $CDCl_3$).



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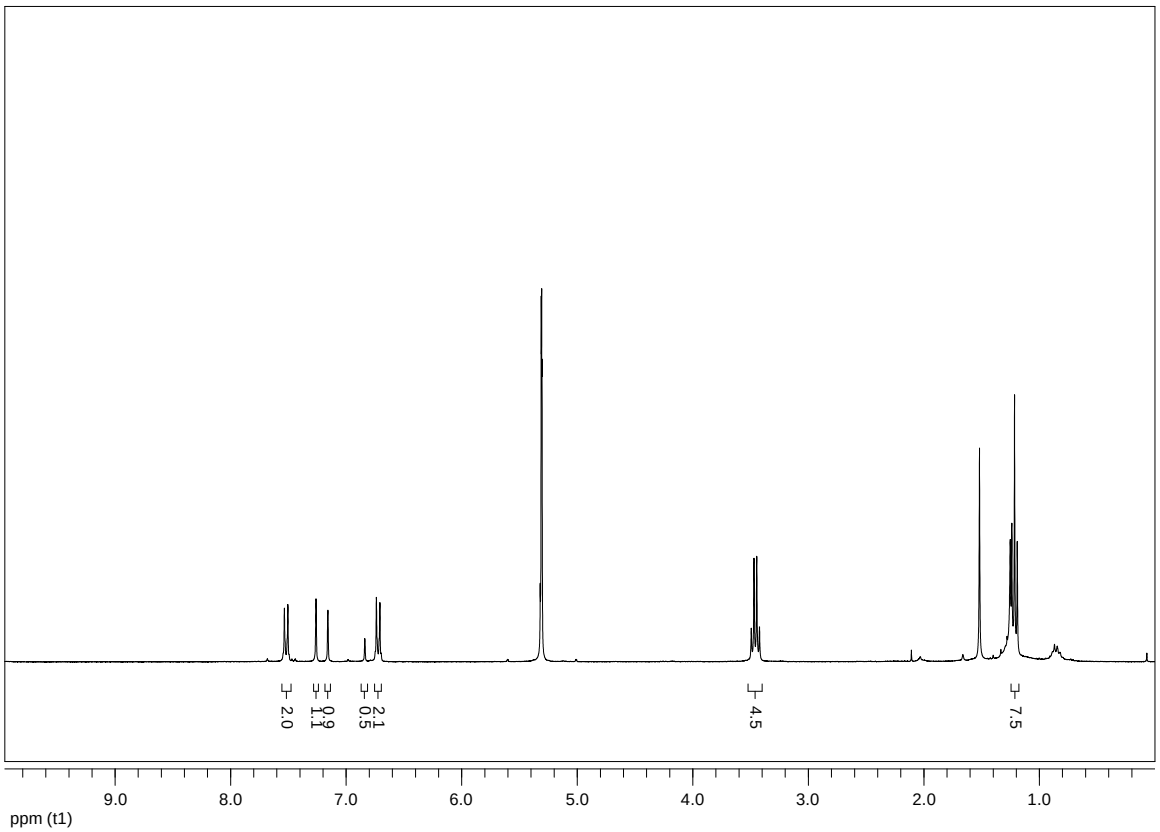
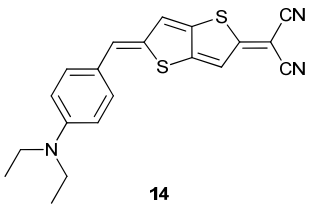


Figure S-21: ^{1}H-NMR spectrum of compound **14** (300 MHz, CD_2Cl_2).



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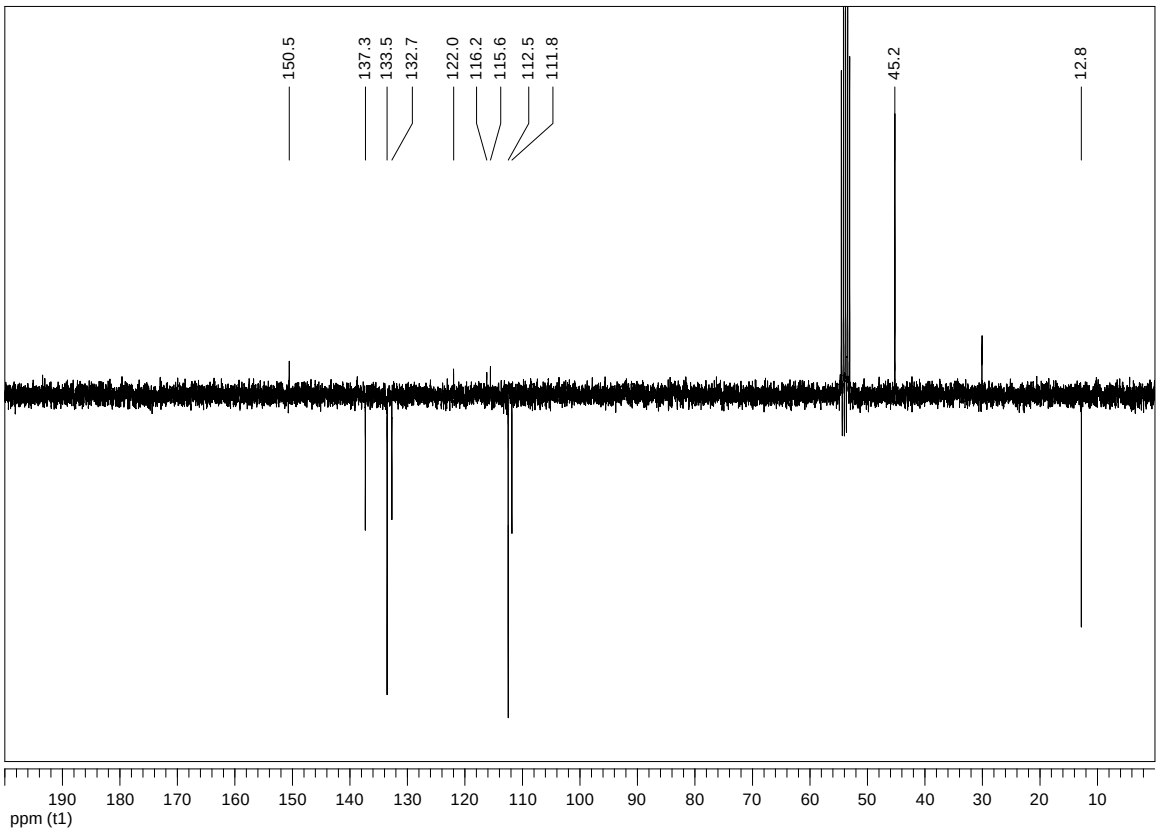
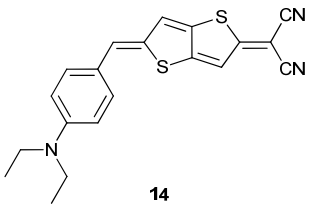


Figure S-22: ^{13}C-NMR (APT) spectrum of compound **14** (75 MHz, CD_2Cl_2).



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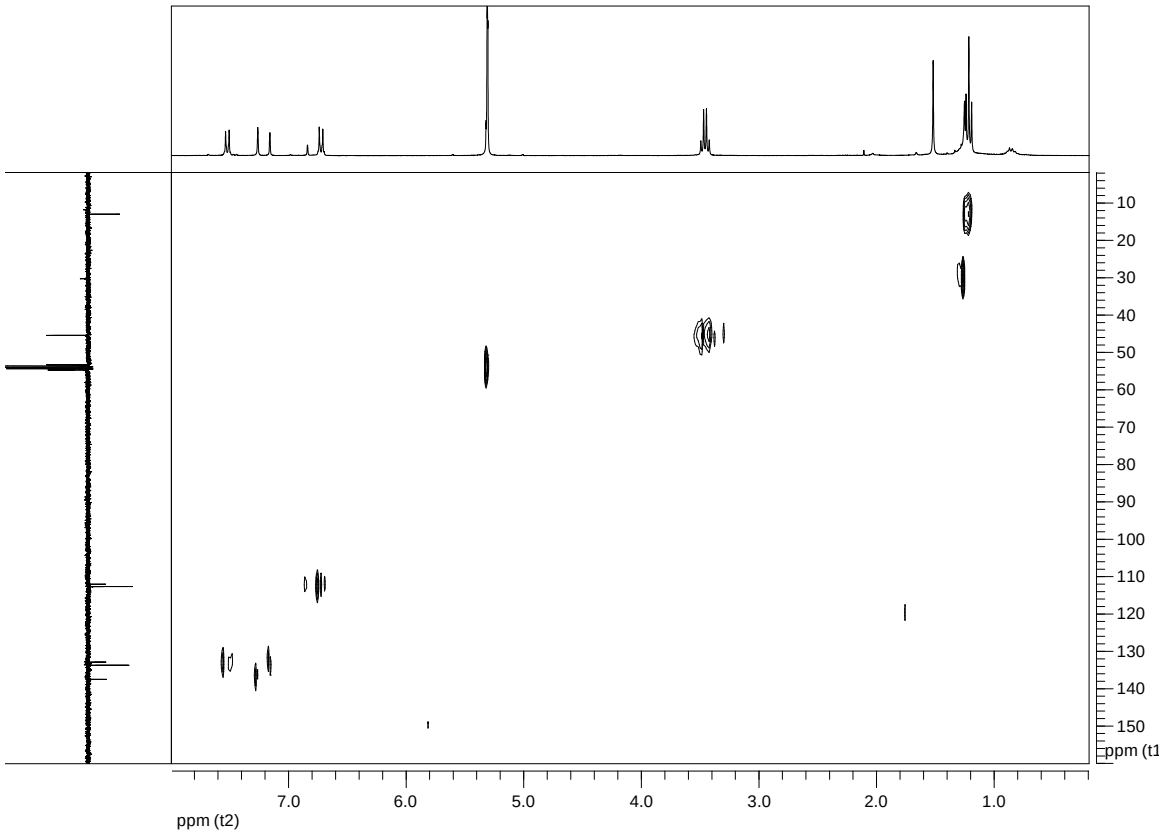
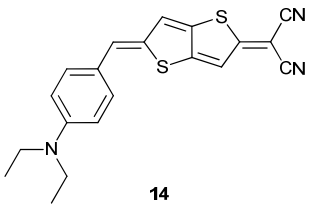


Figure S-23: ^{1}H-^{13}C-HSQC spectrum of compound **14** (300 MHz, CD_2Cl_2).



14

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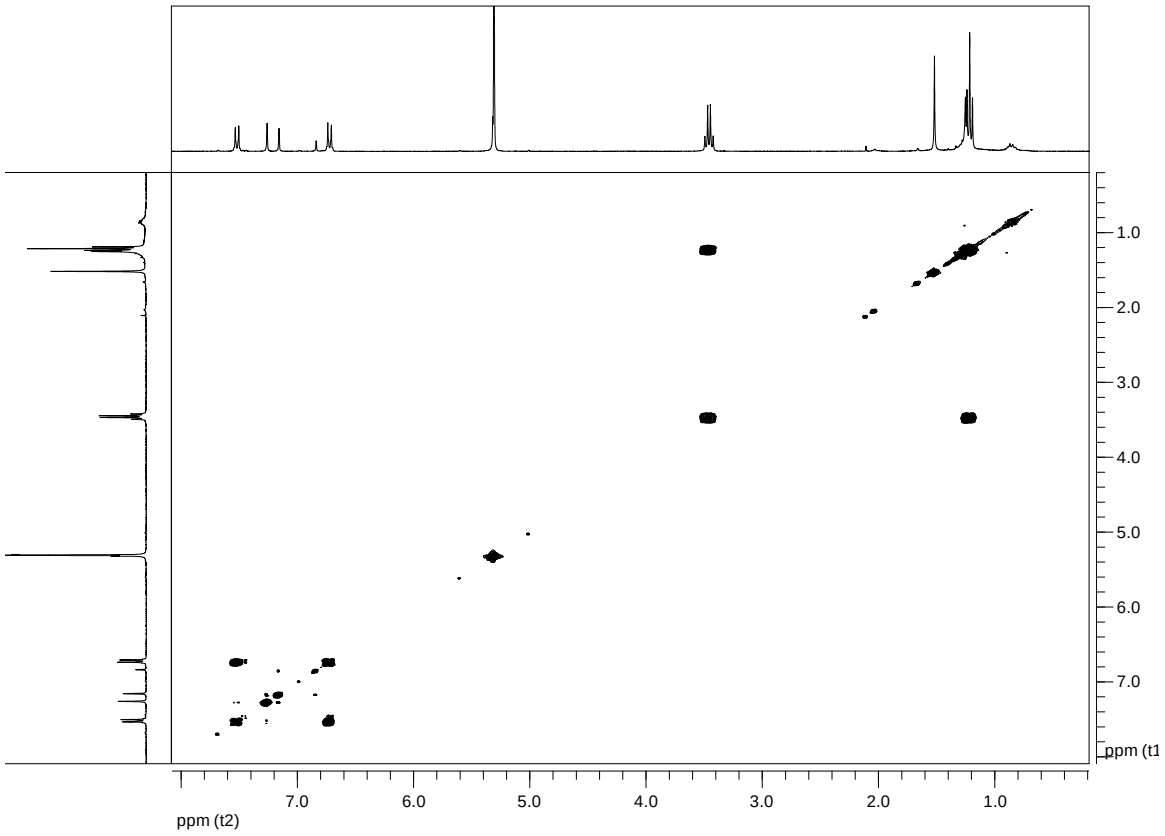
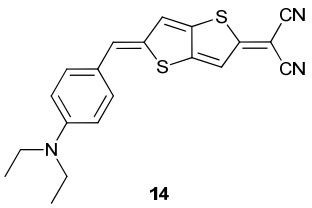


Figure S-24: ^{1}H-^{1}H-COSY spectrum of compound **14** (300 MHz, CD_2Cl_2).



14

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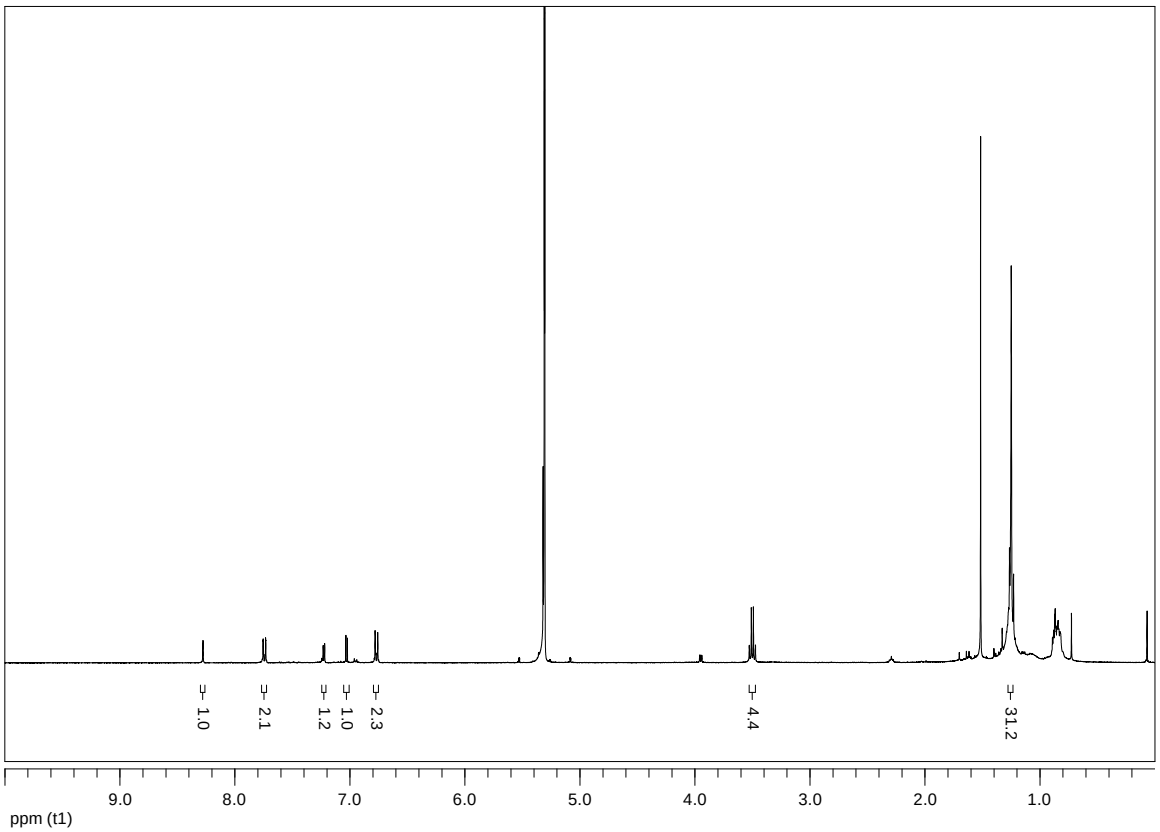
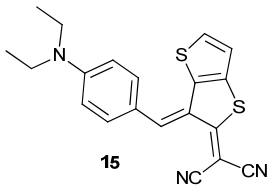


Figure S-25: ^{1}H-NMR spectrum of compound **15** (400 MHz, CD_2Cl_2).



15

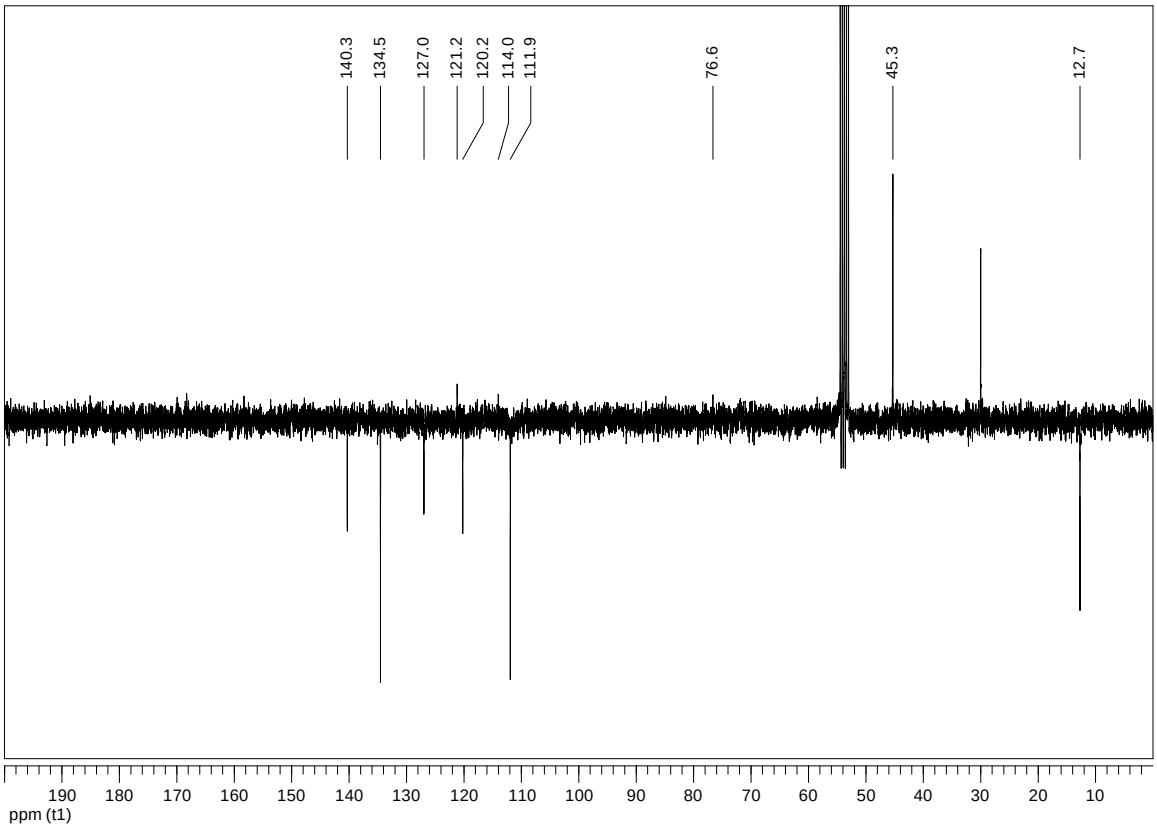
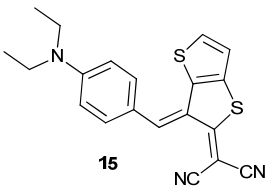


Figure S-26: ^{13}C-NMR (APT) spectrum of compound **15** (75 MHz, CD_2Cl_2).



15

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3. Normalized UV-Vis spectra

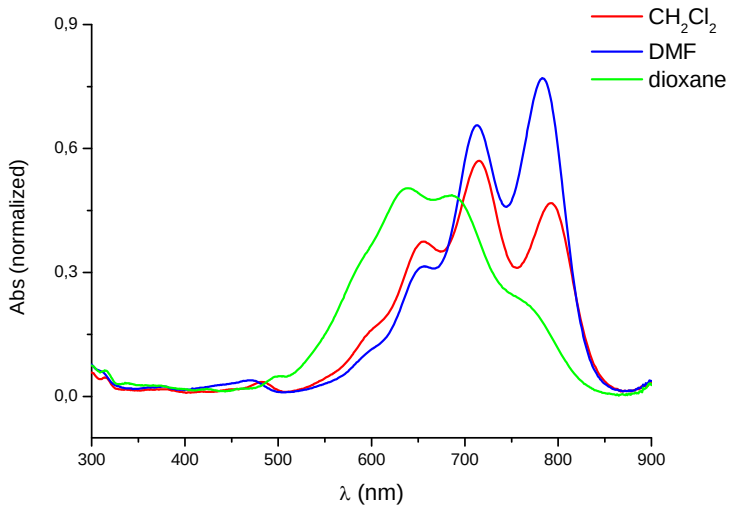

Figure S-27: Normalized UV-vis absorption spectra of compound **1** (10^{-5} M).

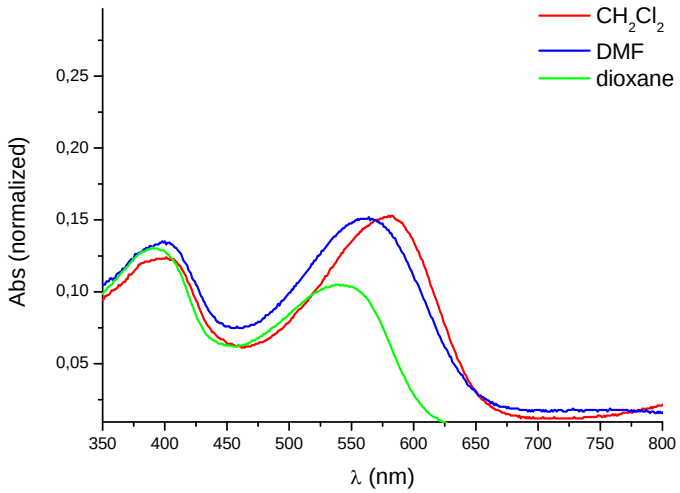

Figure S-28: Normalized UV-vis absorption spectra of compound **2** (10^{-5} M).

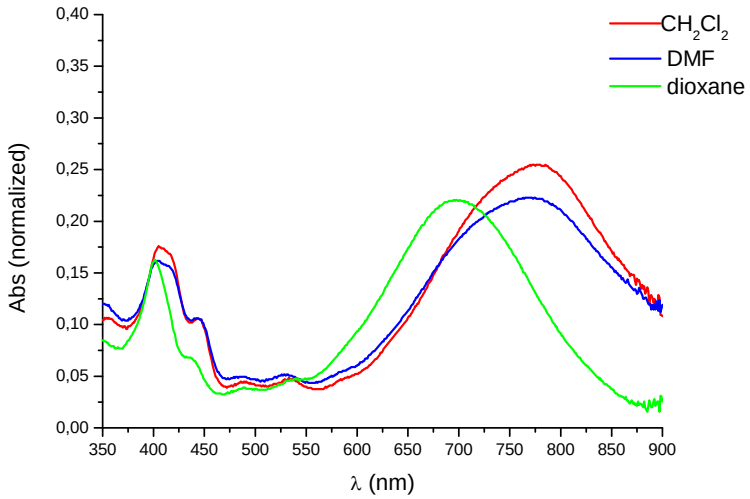

Figure S-29: Normalized UV-vis absorption spectra of compound **3** (10^{-5} M).

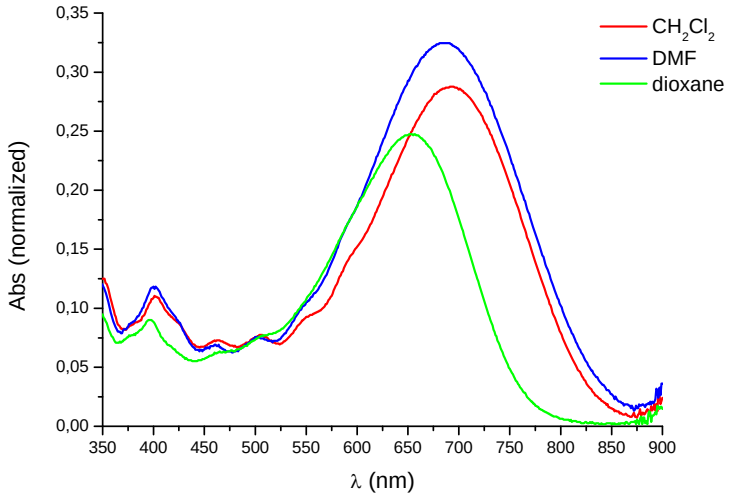

Figure S-30: Normalized UV-vis absorption spectra of compound **4** (10^{-5} M).

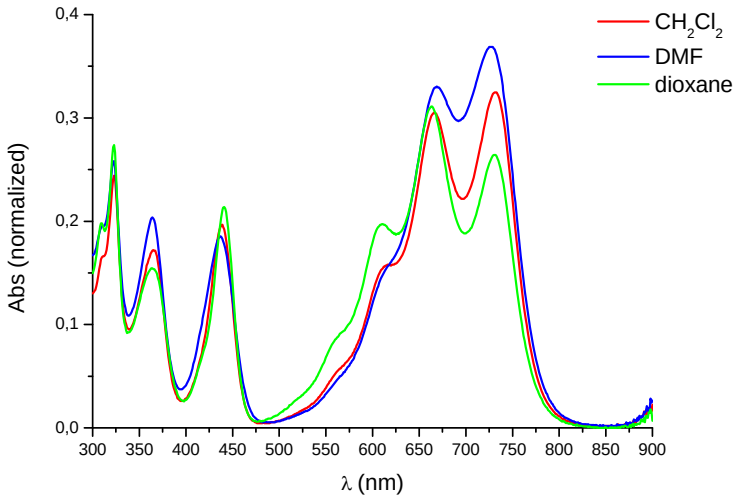

Figure S-31: Normalized UV-vis absorption spectra of compound **8** (10^{-5} M).

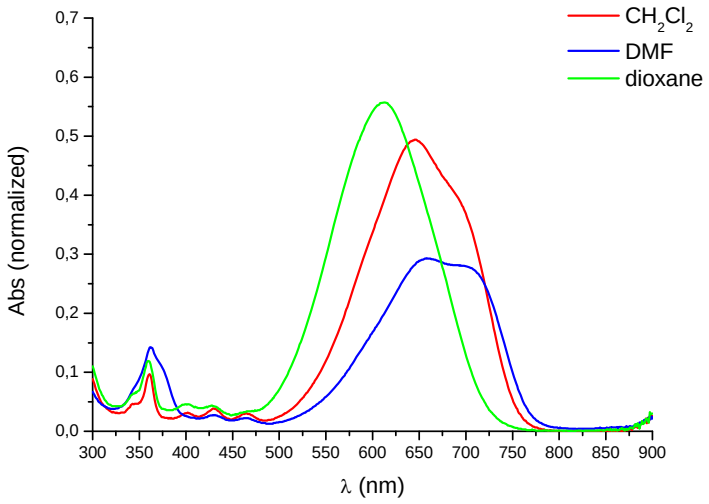

Figure S-32: Normalized UV-vis absorption spectra of compound **14** (10^{-5} M).

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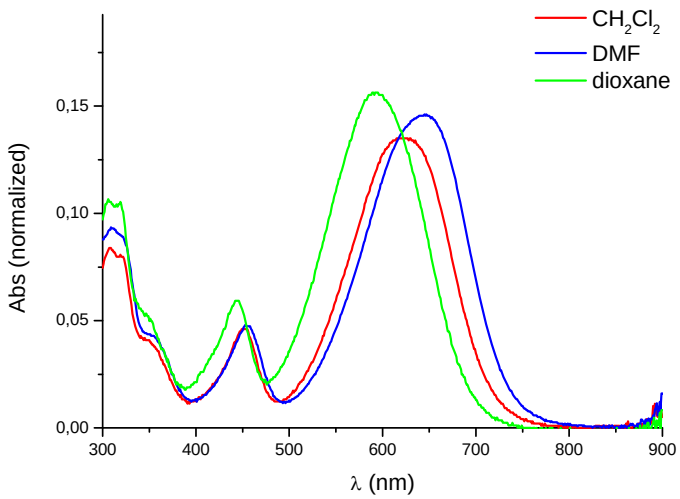

Figure S-33: Normalized UV-vis absorption spectra of compound **15** (10^{-5} M).

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4. X-Ray Diffraction

Compound 8

Single crystals were obtained by slow evaporation of a concentrated solution of the chromophore in CH_2Cl_2 at room: $C_{24}H_{24}N_2OS_2$, M_r = 420.57, crystal dimensions 0.44 × 0.11 × 0.05 mm, monoclinic space group P21/m, ρ_{calcd} = 1.179 g cm^{-3}, Z = 2, a = 11.0980(5) Å, b = 6.7887(4) Å, c = 15.8764(10) Å, α = 90 deg, β = 98.064(5) deg, γ = 90 deg, V = 1184.32(12) Å^3 at 296(1) K. Number of measured and unique reflections 7220 and 2275, respectively (R_{int}=0.0414). Final R(F)=0.0552, wR(F^2)=0.1259 for 169 parameters and 1556 reflections with I› 4σ(I) (corresponding R-values based on all 2275 reflections 0.0892 and 0.1458).

Crystal data and structure refinement for 8.

Identification code	8
Empirical formula	C24 H24 N2 O S2
Formula weight	420.57
Temperature	296(1) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/m
Unit cell dimensions	a = 11.0980(5) A alpha = 90 deg. b = 6.7887(4) A beta = 98.064(5) deg. c = 15.8764(10) A gamma = 90 deg.
Volume	1184.32(12) A^3
Z, Calculated density	2, 1.179 Mg/m^3
Absorption coefficient	0.241 mm^-1
F(000)	444
Crystal size	0.44 x 0.11 x 0.05 mm
Theta range for data collection	2.97 to 25.00 deg.
Limiting indices	-13<=h<=13, -8<=k<=8, -15<=l<=18
Reflections collected / unique	7220 / 2275 [R(int) = 0.0414]
Completeness to theta = 25.00	99.8 %

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9881 and 0.9014
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2275 / 0 / 169
Goodness-of-fit on F^2	1.011
Final R indices [I>2sigma(I)]	R1 = 0.0552, wR2 = 0.1259
R indices (all data)	R1 = 0.0892, wR2 = 0.1458
Largest diff. peak and hole	0.292 and -0.207 e.A^-3

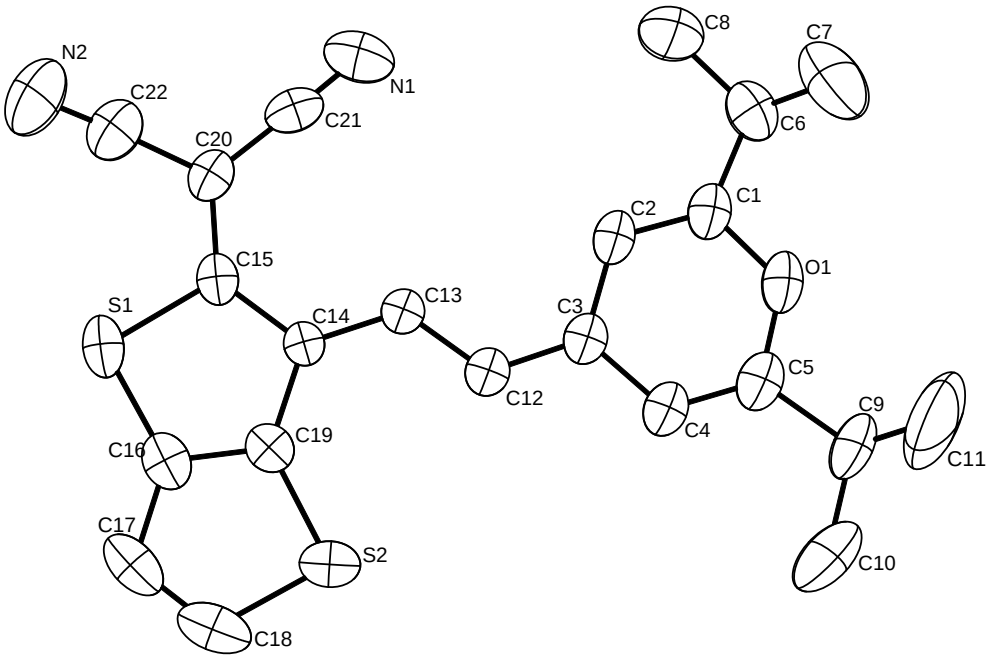

Figure S-34: ORTEP view of **8**

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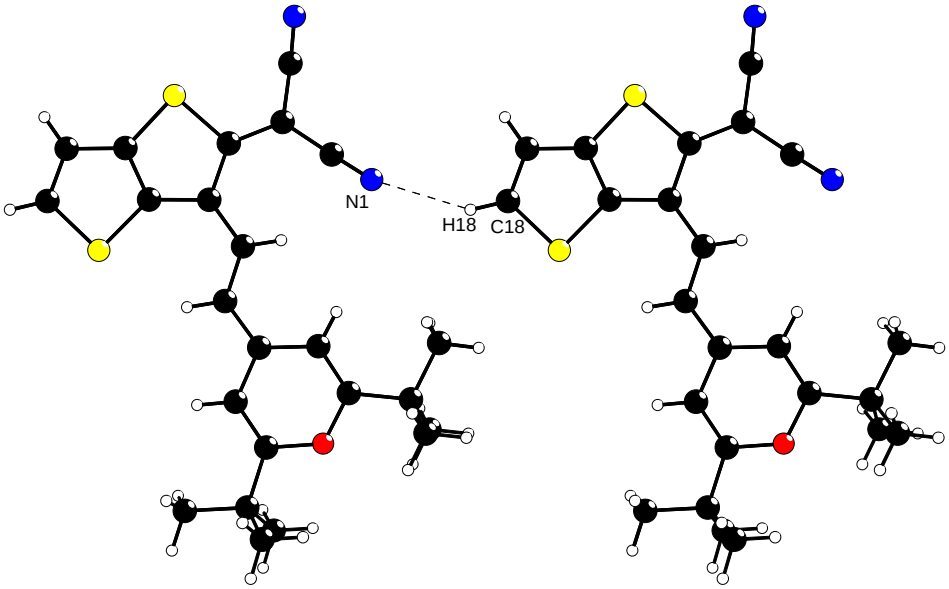

Figure S-35: Nonclassical C18-H18···N1 interaction in **8**

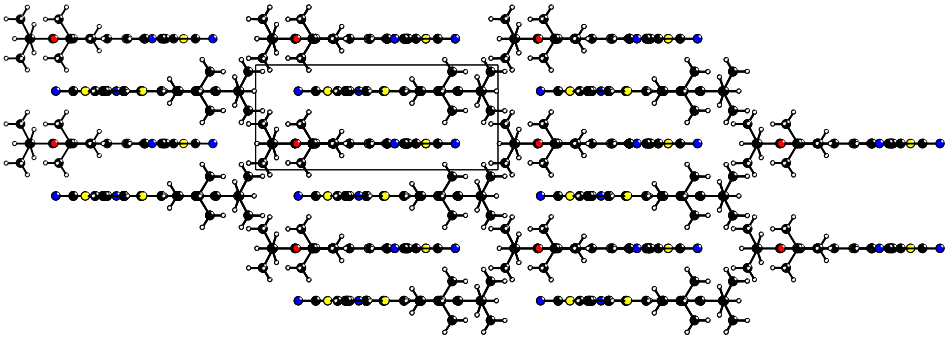

Figure S-36: Crystal packing of **8** viewed along the [100] direction.

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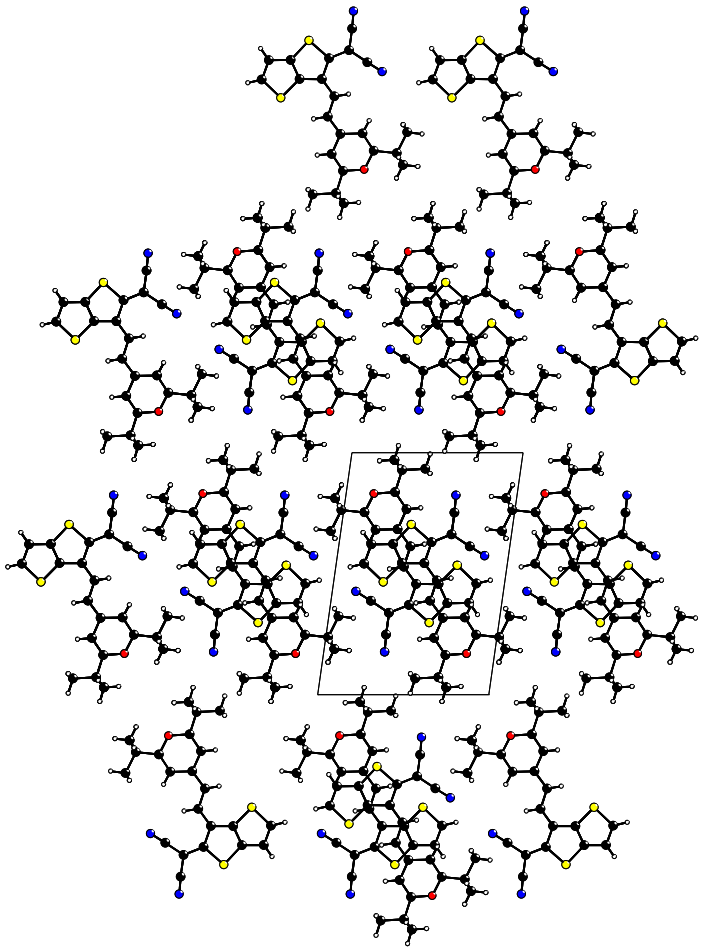

Figure S-37: Crystal packing of **8** viewed along the [010] direction.

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Compound 14

Single crystals were obtained by slow diffusion of hexane into a solution of the chromophore in CH_2Cl_2 at room temperature: $C_{20}H_{17}N_3S_2$, M_r = 363.49, crystal dimensions 0.47 × 0.14 × 0.03 mm, monoclinic space group P21/c, ρ_{calcd} = 1.334 g cm^{-3}, Z = 8, a = 8.3982(4) Å, b = 25.3341(19) Å, c = 17.1667(11) Å, α = 90 deg, β = 97.599(5) deg, γ = 90 deg, V = 3620.3(4) Å^3 at 150(1) K. Number of measured and unique reflections 24610 and 6357, respectively (R_{int}=0.0972). Final R(F)=0.0654, wR(F^2)=0.1214 for 451 parameters and 3793 reflections with I› 4σ(I) (corresponding R-values based on all 6357 reflections: 0.1243 and 0.1487).

Crystal data and structure refinement for 14.

Identification code	14
Empirical formula	C20 H17 N3 S2
Formula weight	363.49
Temperature	150(1) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 8.3982(4) A alpha = 90 deg. b = 25.3341(19) A beta = 97.599(5) deg. c = 17.1667(11) A gamma = 90 deg.
Volume	3620.3(4) A^3
Z, Calculated density	8, 1.334 Mg/m^3
Absorption coefficient	0.301 mm^-1
F(000)	1520
Crystal size	0.47 x 0.14 x 0.03 mm
Theta range for data collection	2.88 to 25.00 deg.
Limiting indices	-9<=h<=9, -30<=k<=29, -19<=l<=20
Reflections collected / unique	24610 / 6357 [R(int) = 0.0972]
Completeness to theta = 25.00	99.9 %

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Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9910 and 0.8714
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6357 / 0 / 451
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R1 = 0.0654, wR2 = 0.1214
R indices (all data)	R1 = 0.1243, wR2 = 0.1487
Largest diff. peak and hole	0.327 and -0.273 e.A^-3

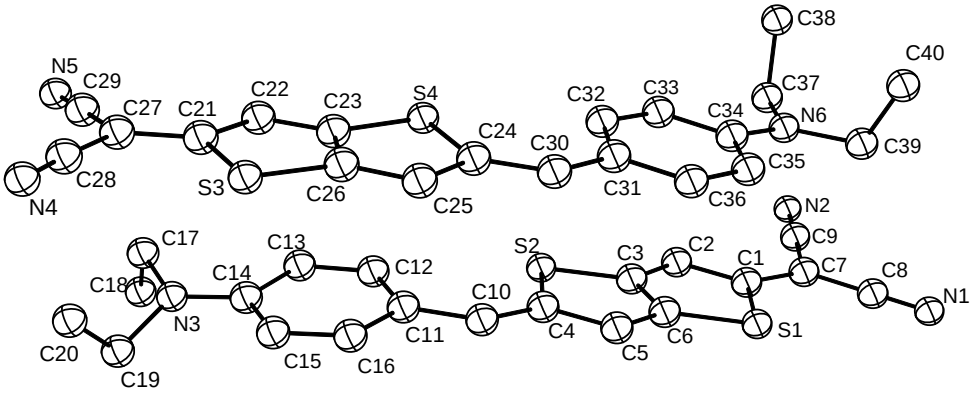

Figure S-38: ORTEP view of **14**

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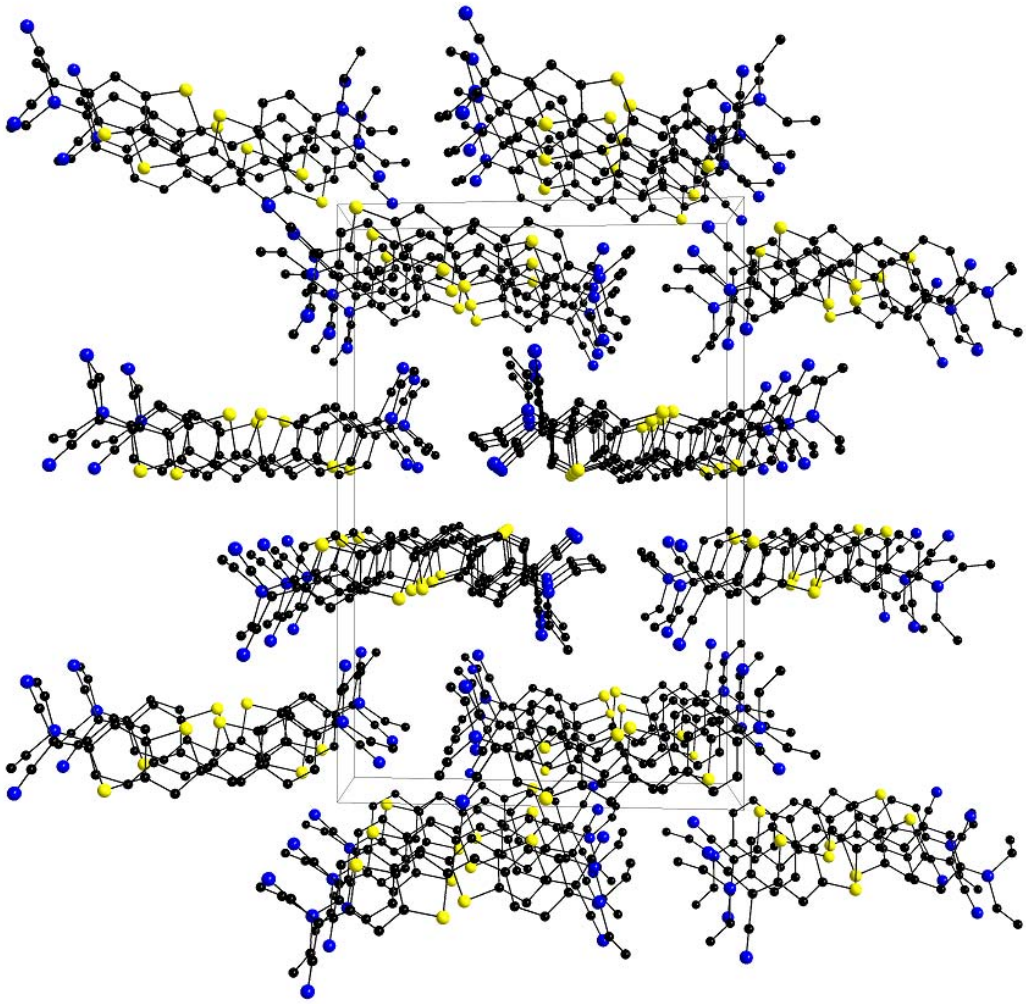

Figure S-39: Crystal packing of **14** viewed along the [100] direction.

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5. NLO measurements

Electric field induced second harmonic generation (EFISH) measurements have been performed using as the fundamental radiation the 1.9 μm output of a H2 Raman shifter pumped by a Q-switched Nd:YAG laser. This laser operates at 1064 nm, with a repetition rate of 10 Hz and pulse width of 8 ns. A computer controlled NLO spectrometer completes the SHG experimental set-up. The 1.9 μm incident light is split in two beams. The less intense one is directed to a *N*-(4-nitrophenyl)-(L)-prolinol (NPP) powder sample whose SH signal is used as a reference in order to reduce the effects of laser fluctuations. The other beam is passed through a linear polarizer and focused into the EFISH wedge shaped liquid cell.

Voltage pulses of 5 kV and 3μs are applied across the cell (2 mm gap between the electrodes) synchronously with the laser pulses. The harmonic signals from both the EFISH cell and the NPP reference are measured with two photomultipliers. Interference filters are used to remove the residual excitation light beyond the sample and the reference.

The molecular $\mu\beta$ values have been determined in dichloromethane for all compounds. Besides, **1** and **14** were measured in DMF and dioxane as well. For measurements in dioxane, experimental uncertainty is less than ±15%; concerning DMF, is not a common solvent in our EFISH experiments, so the $\mu\beta$ values in this solvent are affected by a somewhat higher uncertainty. The effect of absorption at harmonic wavelength (953 nm) of compound **3** has been corrected following reference 4. Static -zero frequency- $\mu\beta_0$ values were extrapolated using a two-level dispersion model.[5]

As a general rule, three solutions of concentration in the range (2×10^{-3}M - 4×10^{-4}M) were measured. Under the same experimental conditions, $\mu\beta_0$ deduced for the benchmark NLO chromophore DR1 in CH_2Cl_2 was 500×10^{-48} esu, quite close to the values reported in the literature.[6] On the other hand the $\mu\beta_0$ values obtained for DR1 in DMF and dioxane have been $\approx450\times10^{-48}$ esu and $\approx590\times10^{-48}$ esu, respectively.

(4) J. L. Oudar, *J. Chem. Phys*., 1977, **67**, 446–457.
(5) J. L. Oudar and D. S. Chemla, *J. Chem. Phys*., 1977, **66**, 2664–2668.
(6) (*a*) C. W. Dirk, H. E. Katz, M. L. Schilling and L. A. King, *Chem. Mater*., 1990, **2**, 700–705; (*b*) J.-M. Raimundo, P. Blanchard, N. Gallego-Planas, N. Mercier, I. Ledoux-Rak, R. Hierle and J. Roncali *J. Org. Chem.,* 2002, **67**, 205–218.

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6.- Computational Methods

Quantum-Chemistry calculations were performed using the Gaussian 09[7] package. Molecular geometries were optimized using the M06-2x[8] functional, the 6-31G*[9] basis set and the Polarizable Continuum Model (PCM).[10] Electronic spectra were calculated using the Time-Dependent Density Functional Theory (TD-DFT)[11] approach, the PCM solvent model, the M06-2x functional and the 6-311+G(2d,p) basis set. Hyperpolarizabilities were calculated using the Coupled Perturbed Hartree-Fock (CPHF) method. The Default Gaussian 09 parameters were used in every case.

Optimized geometries and calculated energies (PCM(CH_2Cl_2)-M06-2x/6-31G*)

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.001632	0.068547	0.000107
2	6	0	-5.253037	-1.125605	0.000327
3	6	0	-3.892163	-0.871062	0.000163
4	6	0	-3.541245	0.510713	-0.000198
5	6	0	-1.423560	-0.430093	-0.000186
6	6	0	-2.192079	0.760339	-0.000408
7	1	0	-5.718192	-2.103058	0.000606
8	1	0	-1.743772	1.747101	-0.000688
9	16	0	-4.978964	1.505955	-0.000269
10	16	0	-2.477000	-1.860185	0.000289
11	6	0	-7.397866	0.195619	0.000175
12	6	0	-8.212560	-0.964501	0.000335
13	7	0	-8.857757	-1.931462	0.000461
14	6	0	-8.018417	1.468411	-0.000003
15	7	0	-8.492257	2.530573	-0.000150
16	6	0	-0.043719	-0.576785	-0.000293
17	6	0	0.888769	0.462505	-0.000603
18	1	0	0.530388	1.488159	-0.000688
19	1	0	0.327330	-1.599900	0.000038
20	6	0	2.272681	0.283215	-0.000681
21	6	0	3.141870	1.427869	-0.000602

(7) Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.
(8) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc*. 2008, **120**, 215–241.
(9) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta* 1973, **28**, 213–222.
(10) J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* 2005, **105**, 2999–3093.
(11) (*a*) M. E. Casida, C. Jamorsky and K. C. Casida, *J. Chem. Phys*. 1998, **108**, 4439–4449; (*b*) R. E. Stratmann, G. E. Scuseria and N. J. Frisch, *J. Chem. Phys*. 1998, **109**, 8218–8224.

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22	6	0	2.942154	-0.984594	-0.000790
23	6	0	4.487592	1.290018	-0.000101
24	1	0	2.711178	2.421519	-0.000866
25	6	0	4.296113	-1.060134	-0.000307
26	1	0	2.384512	-1.912948	-0.001284
27	8	0	5.052130	0.056300	0.000239
28	6	0	5.537237	2.374956	0.000336
29	6	0	6.410406	2.210874	-1.256024
30	6	0	4.888984	3.759937	-0.000880
31	6	0	6.408175	2.211906	1.258351
32	1	0	6.905215	1.235569	-1.268324
33	1	0	5.810018	2.310850	-2.165942
34	1	0	7.180837	2.988148	-1.264424
35	1	0	4.270002	3.914696	0.888762
36	1	0	5.675126	4.520562	-0.000706
37	1	0	4.271314	3.913628	-0.891612
38	1	0	7.178816	2.988967	1.267329
39	1	0	5.806221	2.312913	2.167117
40	1	0	6.902694	1.236472	1.272455
41	6	0	5.102131	-2.347679	-0.000054
42	6	0	4.740905	-3.157124	1.257562
43	6	0	4.740530	-3.157992	-1.256986
44	6	0	6.606962	-2.056965	-0.000396
45	1	0	4.978182	-2.595754	2.166414
46	1	0	3.678184	-3.416033	1.278486
47	1	0	5.317264	-4.087626	1.266174
48	1	0	4.977771	-2.597364	-2.166305
49	1	0	5.316699	-4.088616	-1.264983
50	1	0	3.677770	-3.416750	-1.277581
51	1	0	7.147479	-3.007906	-0.000364
52	1	0	6.906860	-1.491819	-0.887623
53	1	0	6.907215	-1.491562	0.886547

E(RM062X) = -1909.51440963 A.U.

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.614374	1.123757	0.000131
2	6	0	2.361833	0.623073	0.000149
3	6	0	2.119708	-0.806268	-0.000025
4	6	0	3.333143	-1.603748	-0.000105
5	6	0	4.556035	-1.041651	-0.000094
6	1	0	1.547425	1.330506	0.000365
7	1	0	3.247659	-2.683652	-0.000204
8	8	0	4.706398	0.315407	-0.000014
9	6	0	0.903221	-1.436202	-0.000098
10	1	0	0.926079	-2.523846	-0.000147
11	6	0	-0.430250	-0.910602	-0.000084
12	6	0	-1.566039	-1.709210	0.000148
13	6	0	-2.545698	0.433138	-0.000305
14	6	0	-2.750699	-0.950886	0.000021
15	1	0	-1.514761	-2.790828	0.000385
16	6	0	-3.725551	1.180556	-0.000424
17	6	0	-4.857346	0.369976	-0.000157
18	1	0	-3.786038	2.263013	-0.000659
19	16	0	-0.848622	0.803123	-0.000429
20	16	0	-4.433809	-1.343988	0.000191
21	6	0	-6.171636	0.898183	-0.000198
22	1	0	-6.216920	1.985278	-0.000452
23	6	0	-7.381146	0.253372	0.000019
24	6	0	-8.592723	1.014377	-0.000097
25	7	0	-9.570493	1.636432	-0.000198
26	6	0	-7.522729	-1.168810	0.000383
27	7	0	-7.640117	-2.322166	0.000681
28	6	0	4.014084	2.582231	0.000253

29	6	0	4.856633	2.859404	-1.256937
30	6	0	2.784141	3.491802	0.000389
31	6	0	4.856819	2.859219	1.257335
32	1	0	5.755499	2.237108	-1.274639
33	1	0	4.278107	2.661589	-2.165141
34	1	0	5.164441	3.909905	-1.266046
35	1	0	2.166695	3.331254	0.890361
36	1	0	3.111146	4.535684	0.000319
37	1	0	2.166471	3.331193	-0.889415
38	1	0	5.164534	3.909747	1.266604
39	1	0	4.278486	2.661164	2.165609
40	1	0	5.755751	2.237004	1.274750
41	6	0	5.897780	-1.737184	-0.000106
42	6	0	6.674779	-1.308392	-1.256685
43	6	0	6.674556	-1.308699	1.256728
44	6	0	5.725386	-3.256571	-0.000307
45	1	0	6.137494	-1.599965	-2.164906
46	1	0	6.828567	-0.225862	-1.275486
47	1	0	7.655218	-1.795436	-1.264273
48	1	0	6.137099	-1.600498	2.164774
49	1	0	7.654998	-1.795736	1.264381
50	1	0	6.828328	-0.226171	1.275813
51	1	0	6.711622	-3.730317	-0.000365
52	1	0	5.186010	-3.597922	0.889163
53	1	0	5.186007	-3.597688	-0.889864

E(RM062X) = -1909.52523265 A.U.

3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.590426	-1.297246	0.000549
2	6	0	3.001296	-0.082154	0.000700
3	6	0	3.785189	1.133456	0.000202
4	6	0	5.216803	0.910144	-0.000159
5	6	0	5.743845	-0.329691	-0.000271
6	1	0	1.922959	-0.056917	0.001321
7	1	0	5.880312	1.766114	-0.000390
8	8	0	4.940332	-1.432302	-0.000005
9	6	0	3.301420	2.419835	0.000054
10	1	0	4.044157	3.214730	-0.000221
11	6	0	-2.816589	2.270833	0.000035
12	6	0	-4.239704	2.421671	0.000178
13	6	0	-4.039359	0.078991	-0.000307
14	6	0	-4.895677	1.228140	0.000033
15	1	0	-4.703758	3.401558	0.000451
16	6	0	-4.689438	-1.130372	-0.000480
17	6	0	-6.099918	-0.960217	-0.000252
18	1	0	-4.224483	-2.108038	-0.000760
19	16	0	-2.368741	0.546805	-0.000415
20	16	0	-6.575969	0.737627	0.000151
21	6	0	-7.058913	-1.968887	-0.000301
22	6	0	-6.657887	-3.332005	-0.000552
23	7	0	-6.306356	-4.438736	-0.000736
24	6	0	-8.445563	-1.664421	-0.000092
25	7	0	-9.570835	-1.376220	0.000063
26	6	0	-1.938038	3.324385	0.000225
27	6	0	-0.525591	3.348895	0.000189
28	6	0	0.251601	4.505864	0.000131
29	6	0	1.623878	4.265004	0.000119
30	1	0	-0.194663	5.494678	0.000119
31	6	0	1.961602	2.908126	0.000134
32	1	0	2.381874	5.039727	0.000090
33	1	0	-2.401926	4.310226	0.000448
34	16	0	0.511763	1.939998	0.000183
35	6	0	7.204004	-0.718679	-0.000682

36	6	0	7.488266	-1.558887	-1.257855
37	6	0	8.100891	0.520215	-0.001079
38	6	0	7.489059	-1.558615	1.256490
39	1	0	6.873238	-2.462813	-1.275909
40	1	0	7.286029	-0.981881	-2.166015
41	1	0	8.541135	-1.858487	-1.266642
42	1	0	7.933215	1.135790	0.888553
43	1	0	9.148122	0.204107	-0.001251
44	1	0	7.932812	1.135519	-0.890824
45	1	0	8.541850	-1.858520	1.264510
46	1	0	7.287754	-0.981276	2.164651
47	1	0	6.873798	-2.462367	1.275345
48	6	0	2.900965	-2.642636	0.000870
49	6	0	3.335756	-3.415834	1.257891
50	6	0	1.379601	-2.479848	0.001392
51	6	0	3.334846	-3.415842	-1.256494
52	1	0	4.418977	-3.564559	1.274795
53	1	0	3.042639	-2.879623	2.166185
54	1	0	2.853084	-4.398240	1.266262
55	1	0	1.032907	-1.943636	-0.888443
56	1	0	0.913394	-3.469510	0.001759
57	1	0	1.033535	-1.943276	0.891249
58	1	0	2.851960	-4.398144	-1.264613
59	1	0	3.041259	-2.879498	-2.164555
60	1	0	4.418028	-3.564769	-1.274075

E(RM062X) = -2461.23627659 A.U.

4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.417386	-0.945160	0.000029
2	6	0	4.114445	-0.598425	-0.000280
3	6	0	3.702850	0.792724	-0.000345
4	6	0	4.813855	1.729418	-0.000344
5	6	0	6.094155	1.318266	-0.000006
6	1	0	3.390273	-1.398667	-0.000550
7	1	0	4.601079	2.791622	-0.000616
8	8	0	6.406679	-0.012298	0.000329
9	6	0	2.421723	1.273284	-0.000394
10	1	0	2.316185	2.356221	-0.000470
11	6	0	1.156193	0.596280	-0.000267
12	6	0	-0.061808	1.258459	-0.000018
13	6	0	-0.794265	-0.981431	-0.000195
14	6	0	-1.152024	0.368034	0.000007
15	1	0	-0.135966	2.338843	0.000148
16	6	0	-1.883702	-1.862726	-0.000155
17	6	0	-3.098366	-1.189616	0.000039
18	1	0	-1.818045	-2.944731	-0.000285
19	16	0	0.934234	-1.154053	-0.000448
20	16	0	-2.870844	0.558767	0.000234
21	6	0	-4.362549	-1.840698	0.000076
22	1	0	-4.304128	-2.928328	0.000072
23	6	0	-5.627348	-1.329702	0.000061
24	6	0	-6.818455	-2.130052	0.000049
25	6	0	-7.979679	-1.426084	0.000063
26	1	0	-6.758600	-3.213242	0.000034
27	6	0	-7.772493	-0.005800	0.000061
28	1	0	-8.974488	-1.854751	0.000068
29	16	0	-6.071797	0.385796	0.000050
30	6	0	-8.754402	0.967076	0.000054
31	6	0	-10.129826	0.596803	0.000056
32	7	0	-11.244525	0.275368	0.000035
33	6	0	-8.422612	2.350922	0.000043
34	7	0	-8.115116	3.469816	0.000025
35	6	0	5.990064	-2.344634	0.000149

36	6	0	6.859911	-2.518820	1.256844
37	6	0	4.878608	-3.395188	-0.000200
38	6	0	6.860542	-2.518702	-1.256178
39	1	0	7.675732	-1.790785	1.276267
40	1	0	6.261565	-2.395585	2.165503
41	1	0	7.294357	-3.523674	1.264111
42	1	0	4.246054	-3.310507	-0.890086
43	1	0	5.328316	-4.392641	-0.000007
44	1	0	4.245475	-3.310481	0.889281
45	1	0	7.294624	-3.523711	-1.263540
46	1	0	6.262697	-2.394958	-2.165096
47	1	0	7.676616	-1.790939	-1.274894
48	6	0	7.344952	2.166524	0.000105
49	6	0	8.166709	1.830631	-1.256381
50	6	0	6.998622	3.656290	-0.000230
51	6	0	8.166173	1.831072	1.257057
52	1	0	8.442806	0.772659	-1.275607
53	1	0	7.599863	2.059480	-2.164596
54	1	0	9.084785	2.426854	-1.263520
55	1	0	6.423717	3.934439	0.888962
56	1	0	7.924173	4.239556	-0.000145
57	1	0	6.424078	3.934138	-0.889749
58	1	0	9.084229	2.427324	1.264385
59	1	0	7.598934	2.060210	2.164951
60	1	0	8.442294	0.773114	1.276751

E(RM062X) = -2461.23932817 A.U.

8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.563064	0.871333	-0.000082
2	6	0	-2.583794	-0.183300	-0.000022
3	6	0	-3.251953	-1.468309	0.000080
4	6	0	-4.622196	-1.412685	0.000071
5	6	0	-4.355497	-3.689007	0.000310
6	6	0	-5.271038	-2.678517	0.000208
7	1	0	-6.342838	-2.830880	0.000226
8	16	0	-5.204518	0.239615	-0.000082
9	16	0	-2.718238	-3.114650	0.000255
10	6	0	-3.408174	2.266195	-0.000133
11	6	0	-2.158193	2.934434	-0.000174
12	7	0	-1.130359	3.479601	-0.000203
13	6	0	-4.559121	3.099758	-0.000210
14	7	0	-5.518130	3.755859	-0.000267
15	6	0	-1.209875	0.051472	-0.000096
16	6	0	-0.180134	-0.882046	-0.000165
17	1	0	-0.391840	-1.946694	-0.000255
18	1	0	-0.909826	1.089413	-0.000110
19	6	0	1.171532	-0.508222	-0.000136
20	6	0	2.195633	-1.510140	-0.000246
21	6	0	1.636604	0.849105	0.000026
22	6	0	3.508013	-1.171573	-0.000204
23	1	0	1.915756	-2.556275	-0.000357
24	6	0	2.963408	1.124293	0.000056
25	1	0	0.946644	1.683687	0.000142
26	8	0	3.878912	0.128767	-0.000090
27	6	0	4.704863	-2.091813	-0.000192
28	6	0	5.541651	-1.801938	1.258468
29	6	0	4.267204	-3.557368	-0.000765
30	6	0	5.542360	-1.801192	-1.258210
31	1	0	5.882234	-0.762983	1.276329
32	1	0	4.962304	-1.996012	2.166665
33	1	0	6.421459	-2.452600	1.265245
34	1	0	3.678624	-3.801170	-0.890942
35	1	0	5.156597	-4.193819	-0.000917

36	1	0	3.678493	-3.801818	0.889146
37	1	0	6.422303	-2.451673	-1.264732
38	1	0	4.963608	-1.994989	-2.166843
39	1	0	5.882752	-0.762167	-1.275398
40	6	0	3.619054	2.484473	0.000268
41	6	0	4.497821	2.602092	-1.257479
42	6	0	2.567992	3.595860	0.000508
43	6	0	4.497904	2.601559	1.258001
44	1	0	5.271135	1.828809	-1.273969
45	1	0	3.894309	2.513960	-2.166451
46	1	0	4.988711	3.580171	-1.263699
47	1	0	1.928491	3.549400	0.887588
48	1	0	3.076634	4.564366	0.000615
49	1	0	1.928380	3.549650	-0.886501
50	1	0	4.988290	3.579886	1.264981
51	1	0	3.894558	2.512382	2.166989
52	1	0	5.271608	1.828652	1.273775
53	1	0	-4.542160	-4.753872	0.000427

E(RM062X) = -1909.52449160 A.U.

14

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.974749	0.269188	-0.018635
2	6	0	3.799948	1.069511	-0.113857
3	6	0	2.666850	0.304056	-0.043263
4	6	0	2.896747	-1.106784	0.108836
5	6	0	0.564875	-1.071598	0.076574
6	6	0	1.767720	-1.856497	0.173827
7	1	0	1.726339	-2.934259	0.284557
8	16	0	4.613407	-1.445982	0.161423
9	16	0	0.969863	0.656749	-0.101267
10	6	0	6.287670	0.720022	-0.056031
11	6	0	6.560878	2.107661	-0.201745
12	7	0	6.756960	3.245450	-0.321829
13	6	0	7.377085	-0.185947	0.048610
14	7	0	8.239011	-0.958894	0.137752
15	6	0	-0.683145	-1.622443	0.104112
16	1	0	-0.674689	-2.708157	0.199793
17	6	0	-1.997607	-1.048334	0.018593
18	6	0	-3.097903	-1.929819	0.002700
19	6	0	-2.297101	0.329844	-0.041473
20	6	0	-4.400608	-1.489662	-0.089405
21	1	0	-2.913305	-2.999314	0.066561
22	6	0	-3.592372	0.789066	-0.131515
23	1	0	-1.509266	1.073798	0.002369
24	6	0	-4.698116	-0.104429	-0.181742
25	1	0	-5.192896	-2.225707	-0.086736
26	1	0	-3.749498	1.859380	-0.153145
27	7	0	-5.983165	0.341038	-0.316865
28	6	0	-7.071631	-0.635589	-0.182410
29	6	0	-8.468968	-0.074595	-0.400865
30	1	0	-7.019231	-1.108694	0.809064
31	1	0	-6.906723	-1.426685	-0.921627
32	1	0	-9.180724	-0.899606	-0.316861
33	1	0	-8.741115	0.675827	0.346145
34	1	0	-8.578213	0.362221	-1.397118
35	6	0	-6.276853	1.767240	-0.206781
36	6	0	-6.287525	2.265419	1.237128
37	1	0	-7.242881	1.951805	-0.675653
38	1	0	-5.551186	2.320051	-0.807723
39	1	0	-6.505269	3.336673	1.270698
40	1	0	-7.052751	1.740624	1.817911
41	1	0	-5.320379	2.093650	1.719238

42	1	0	3.841676	2.145089	-0.229313

E(RM062X) = -1732.48629544 A.U.

15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.273996	-0.522653	-0.015435
2	6	0	-1.869910	-0.114846	-0.025955
3	6	0	-1.802422	1.343486	0.007085
4	6	0	-3.020172	1.968166	-0.088298
5	6	0	-1.672344	3.801080	-0.311256
6	6	0	-2.967032	3.377018	-0.265299
7	1	0	-3.827779	4.028226	-0.348163
8	16	0	-4.367900	0.845051	-0.105102
9	16	0	-0.529987	2.511438	-0.145054
10	6	0	-3.809872	-1.792862	0.124411
11	6	0	-3.054743	-2.968378	0.399173
12	7	0	-2.473396	-3.944368	0.636480
13	6	0	-5.224514	-1.966216	0.062611
14	7	0	-6.378679	-2.071293	0.009761
15	6	0	-0.862930	-1.025403	-0.235626
16	1	0	-1.164060	-2.011604	-0.577952
17	1	0	-1.309900	4.814950	-0.412547
18	6	0	0.554757	-0.844420	-0.108249
19	6	0	1.428026	-1.664626	-0.851717
20	6	0	1.146243	0.061896	0.795725
21	6	0	2.797253	-1.542506	-0.763596
22	1	0	1.008857	-2.397967	-1.535802
23	6	0	2.512277	0.183306	0.914602
24	1	0	0.514609	0.646430	1.457764
25	6	0	3.394421	-0.609713	0.128674
26	1	0	3.411315	-2.179367	-1.385237
27	1	0	2.901184	0.891960	1.633756
28	7	0	4.751188	-0.506452	0.241885
29	6	0	5.585472	-1.255244	-0.707832
30	6	0	7.085706	-1.111997	-0.500396
31	1	0	5.330207	-0.952535	-1.733535
32	1	0	5.330700	-2.316712	-0.616509
33	1	0	7.588505	-1.737200	-1.242511
34	1	0	7.432077	-0.084800	-0.642263
35	1	0	7.393283	-1.456163	0.490597
36	6	0	5.335584	0.585001	1.017355
37	6	0	5.290586	1.924571	0.285314
38	1	0	6.364918	0.319766	1.254836
39	1	0	4.821025	0.645732	1.979276
40	1	0	5.726779	2.713761	0.904190
41	1	0	5.855491	1.868687	-0.650637
42	1	0	4.260850	2.203843	0.042620

E(RM062X) = -1732.48292693 A.U.