

RSC ADVANCES

ELECTRONIC SUPPLEMENTARY INFORMATION FOR

Polarization, second-order nonlinear optical properties and electrochromism in 4*H*-pyranylidene chromophores with a quinoid/aromatic thiophene ring bridge.

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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. ^1H - 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). 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 type III 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.

In situ UV-Vis-NIR spectroelectrochemical studies were conducted on a Cary 5000 spectrophotometer from Varian operating in a maximal 175–3300 nm range and FT-infrared spectra were taken using a Bruker Vertex 70 FTIR interferometer. In both case, a C3 epsilon potentiostat from BASi was used for the electrolysis using a thin layer cell from a demountable omni cell from Specac. In this cell a three electrodes system was coupled to conduct in situ spectroelectrochemistry. A Pt gauze was used as the working electrode, a Pt wire was used as the counter electrode, and an Ag wire was used as the pseudo-reference electrode. The spectra were collected a constant potential electrolysis and the potentials were changed in interval of 15 mV. The electrochemical medium used was 0.1 M Bu_4NPF_6 in fresh distilled CH_2Cl_2 , at room temperature with sample concentrations of 10^{-3} M .

X-Ray data collection was carried out on a Xcalibur, Sapphire 3 diffractometer equipped with a graphite monochromator (Mo $\kappa\alpha$ radiation, $\lambda = 0.71073$ Å). The diffraction frames were integrated and corrected for absorption using the CrysAlisPro package.¹ The structures were solved using Superflip² and refined against the F^2 data using full-matrix least squares methods with SHELXL-2013 (**1c**) and SHELXL-97 (**2**).³ All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed at idealized positions 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).

¹ CrysAlisPro, Agilent Technologies, version 1.171.36.28 (release 01-02-2013 CrysAlis171.NET; compiled Feb 1 2013,16:14:44).

² L. Palatinus and G. Chapuis, *J. Appl. Cryst.*, 2007, **40**, 786–790. <http://superspace.epfl.ch/superflip>, Version: 04/17/13 12:45.

³ G. M. Sheldrick, *Acta Crystallogr. A*, 2008, **64**, 112–122.

2. NMR spectra for new compounds

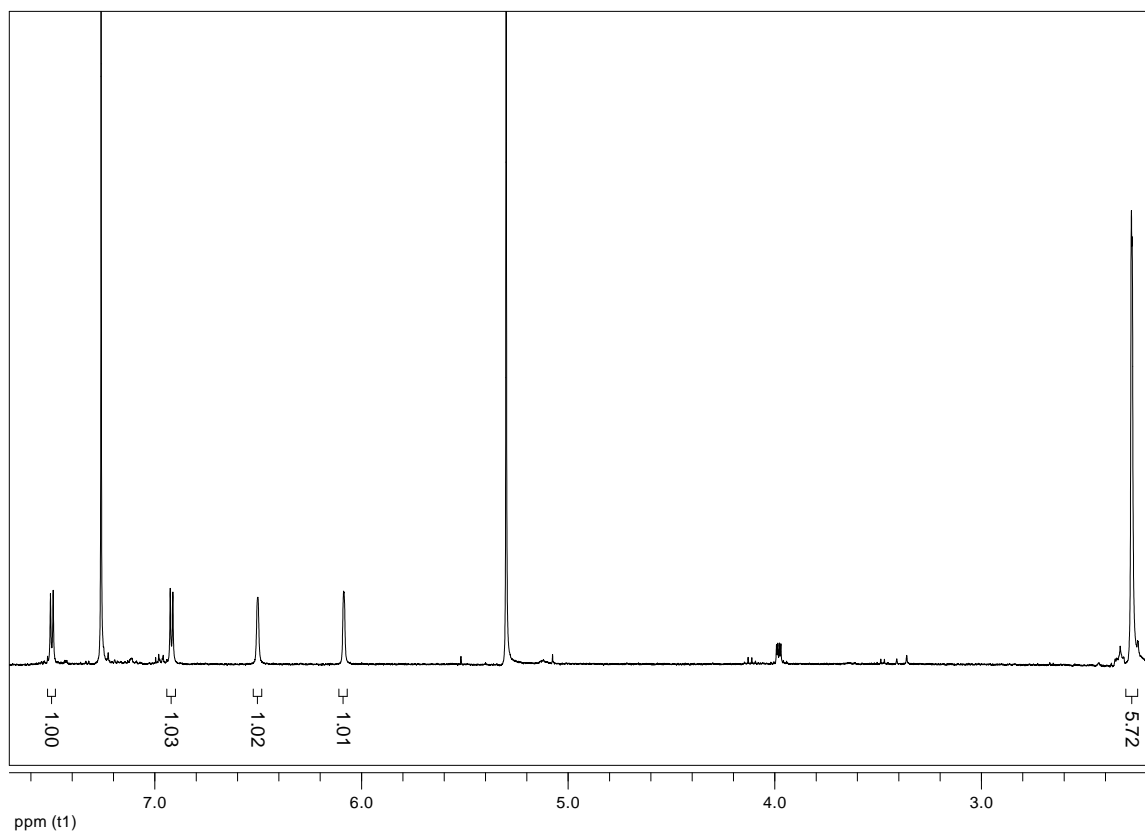
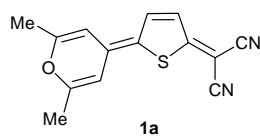


Figure S-1: ¹H-NMR spectrum of compound **1a** (400 MHz, CDCl₃).



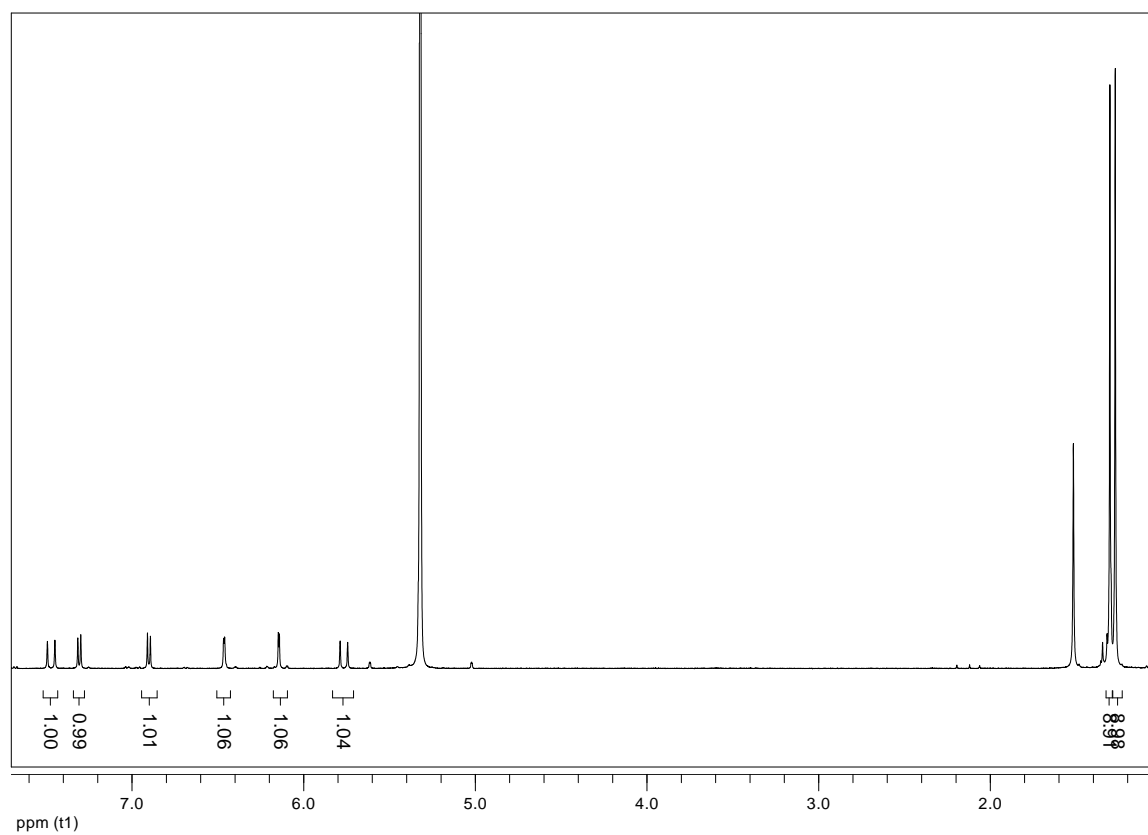
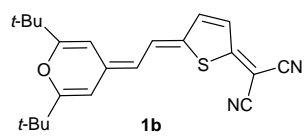


Figure S-2: ¹H-NMR spectrum of compound **1b** (300 MHz, CD₂Cl₂).



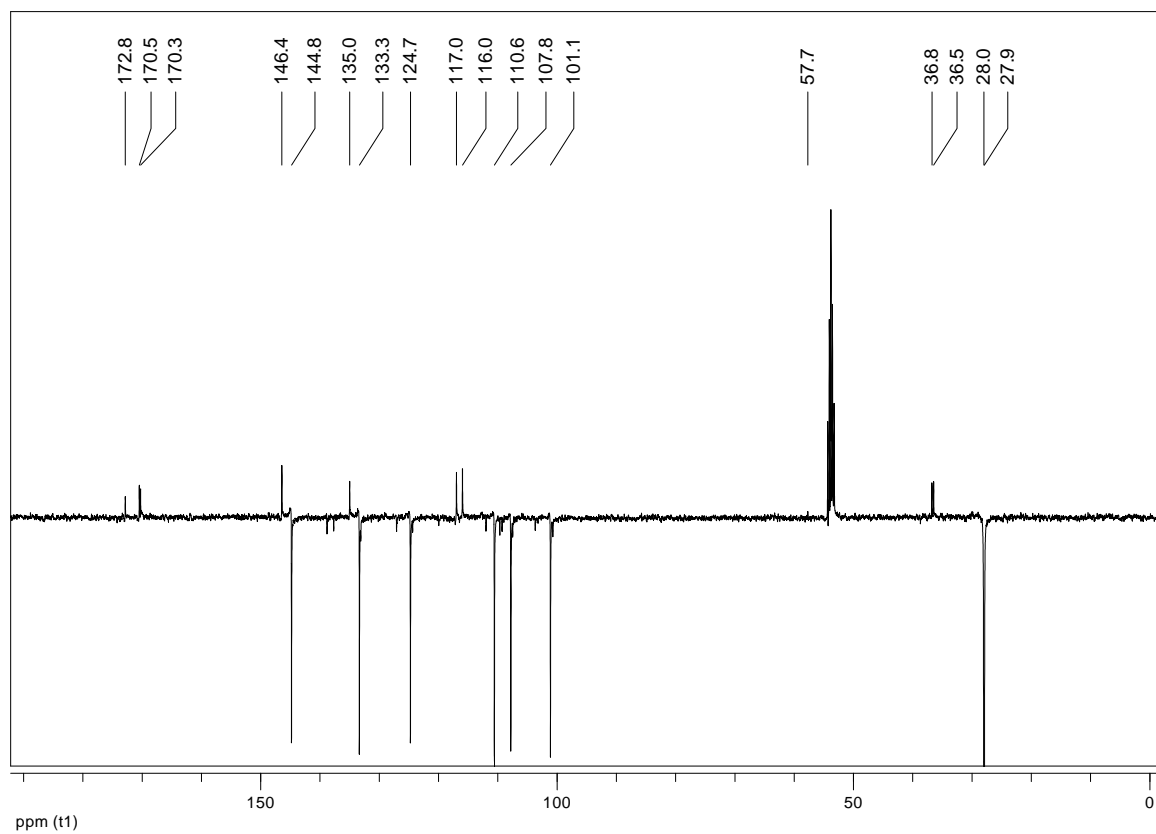
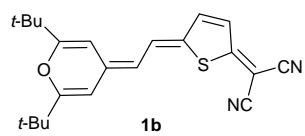


Figure S-3: ^{13}C -NMR (APT) spectrum of compound **1b** (100 MHz, CD_2Cl_2).



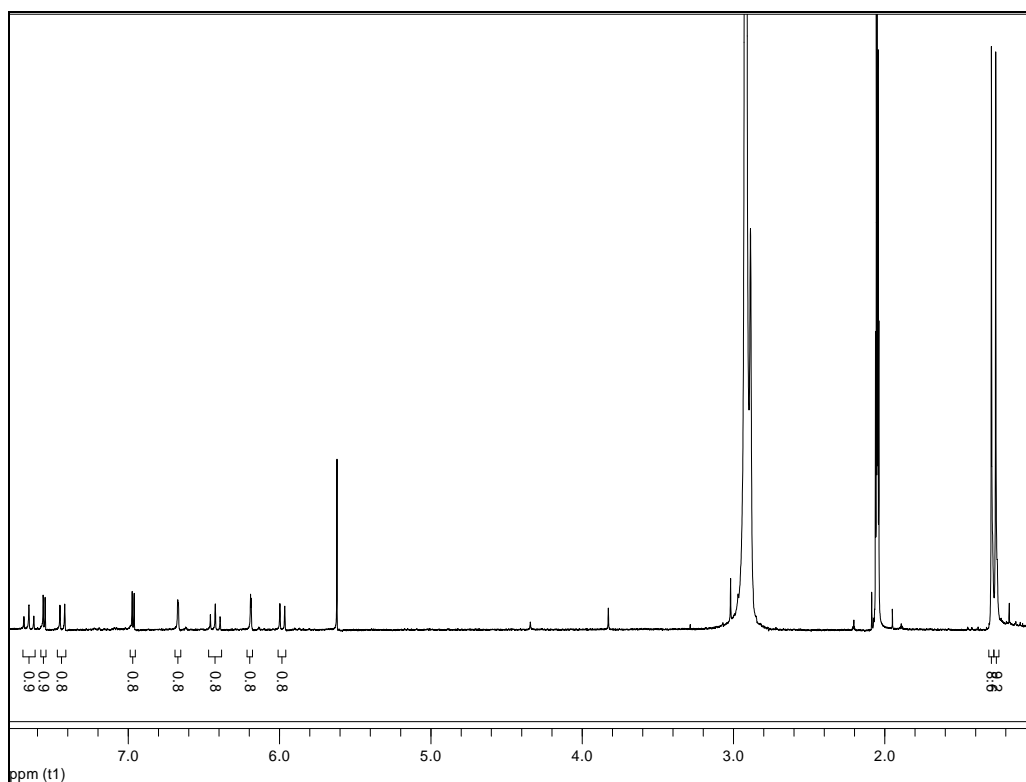
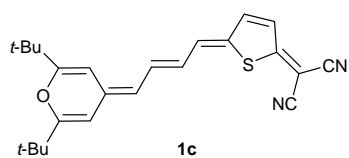


Figure S-4: ^1H -NMR spectrum of compound **1c** (400 MHz, CD_3COCD_3).



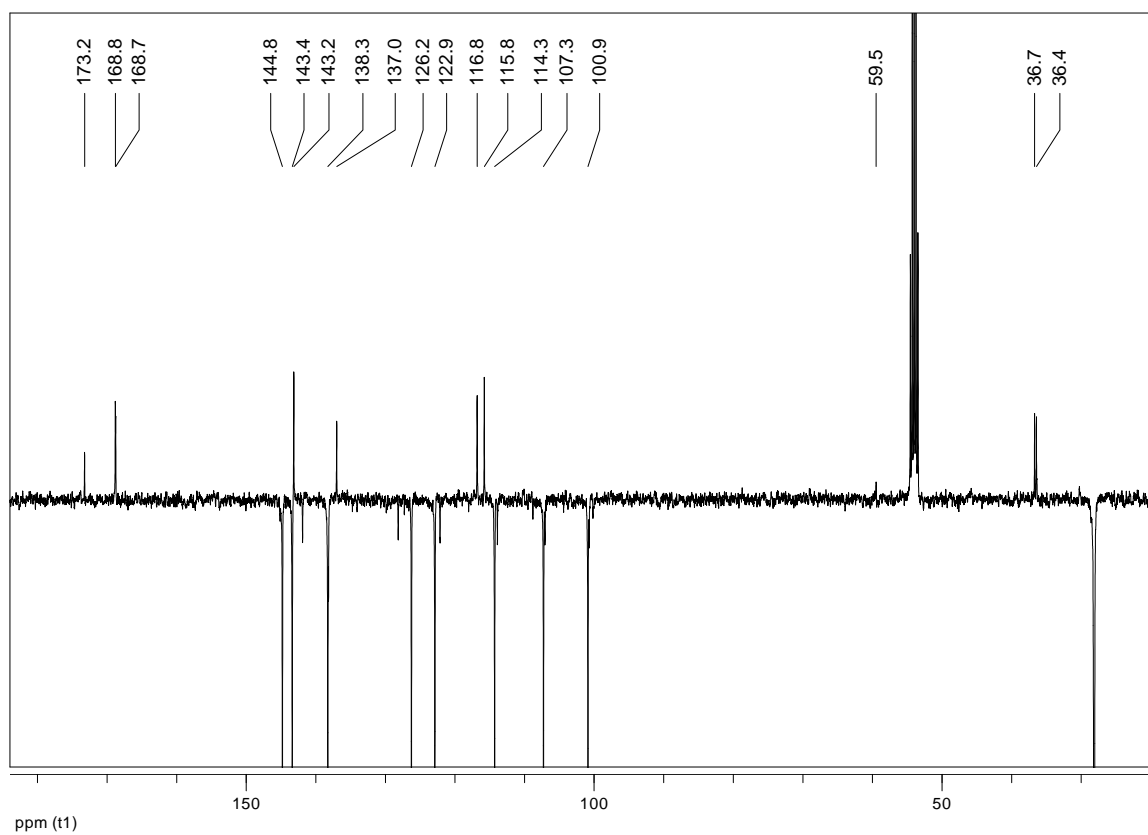
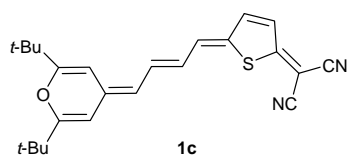


Figure S-5: ^{13}C -NMR (APT) spectrum of compound **1c** (100 MHz, CD_2Cl_2).



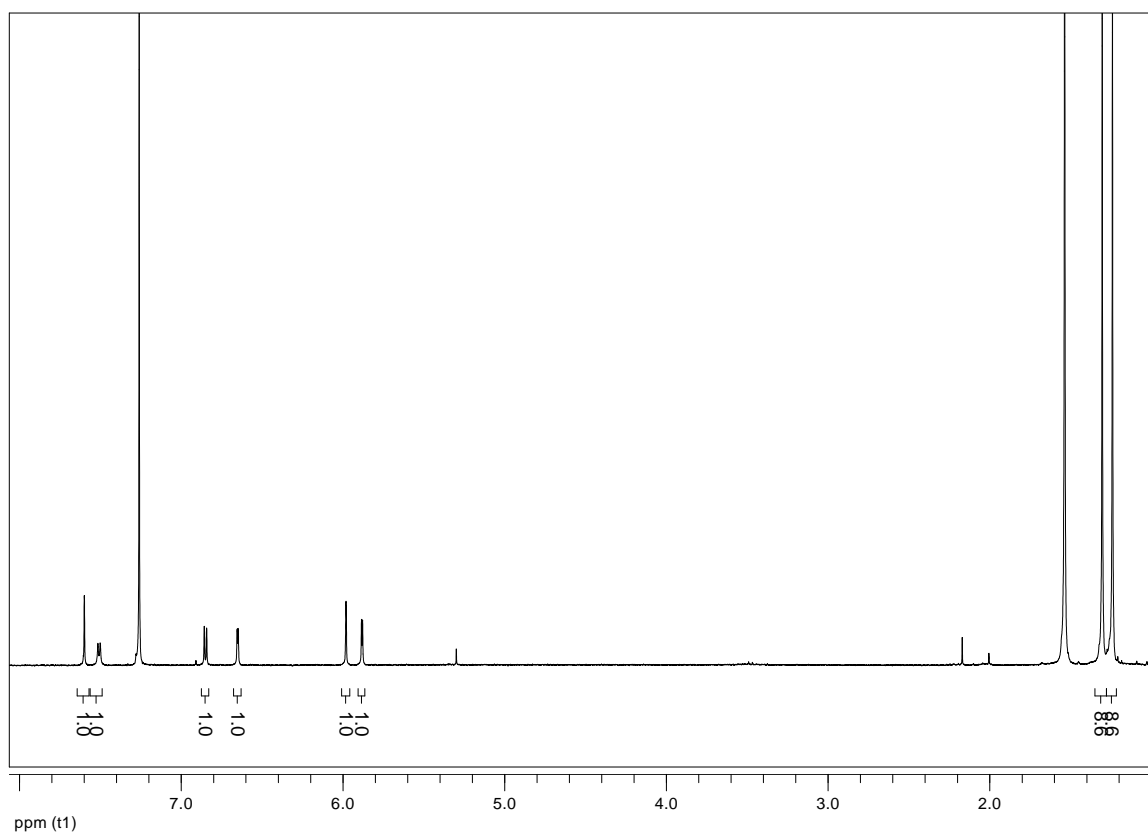
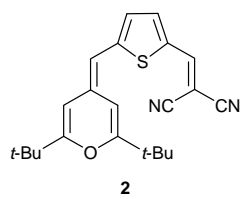


Figure S-6: ¹H-NMR spectrum of compound **2** (300 MHz, CDCl₃).



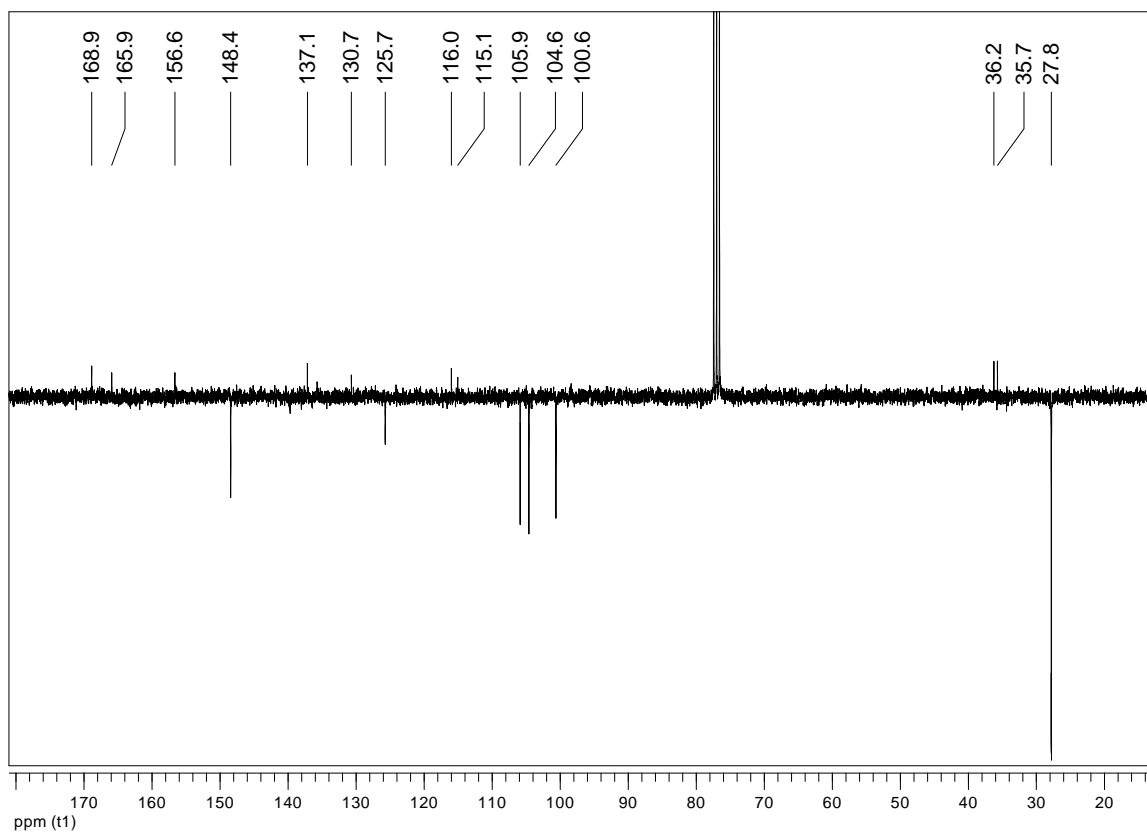
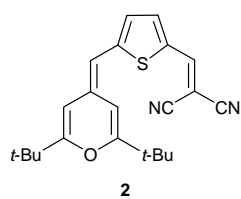


Figure S-7: ^{13}C -NMR (APT) spectrum of compound **2** (75 MHz, CDCl_3).



3. UV-Vis spectra

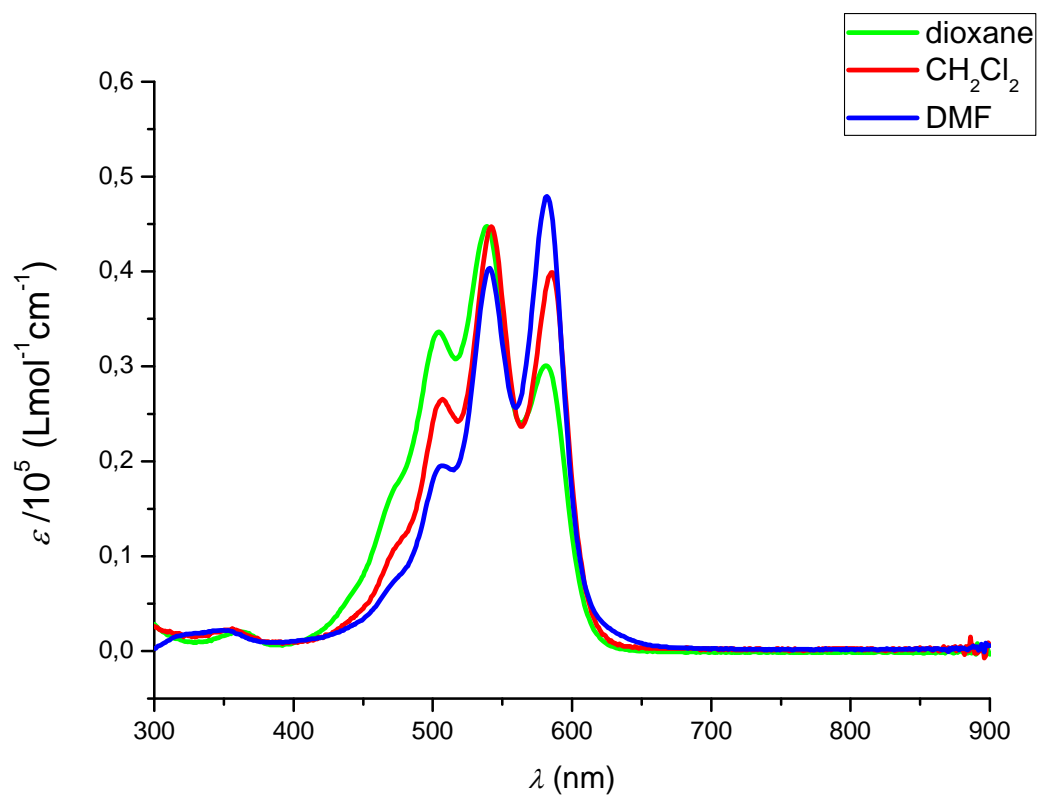
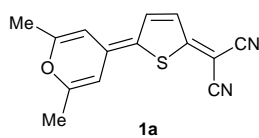


Figure S-8: UV-vis absorption spectra of compound **1a**.



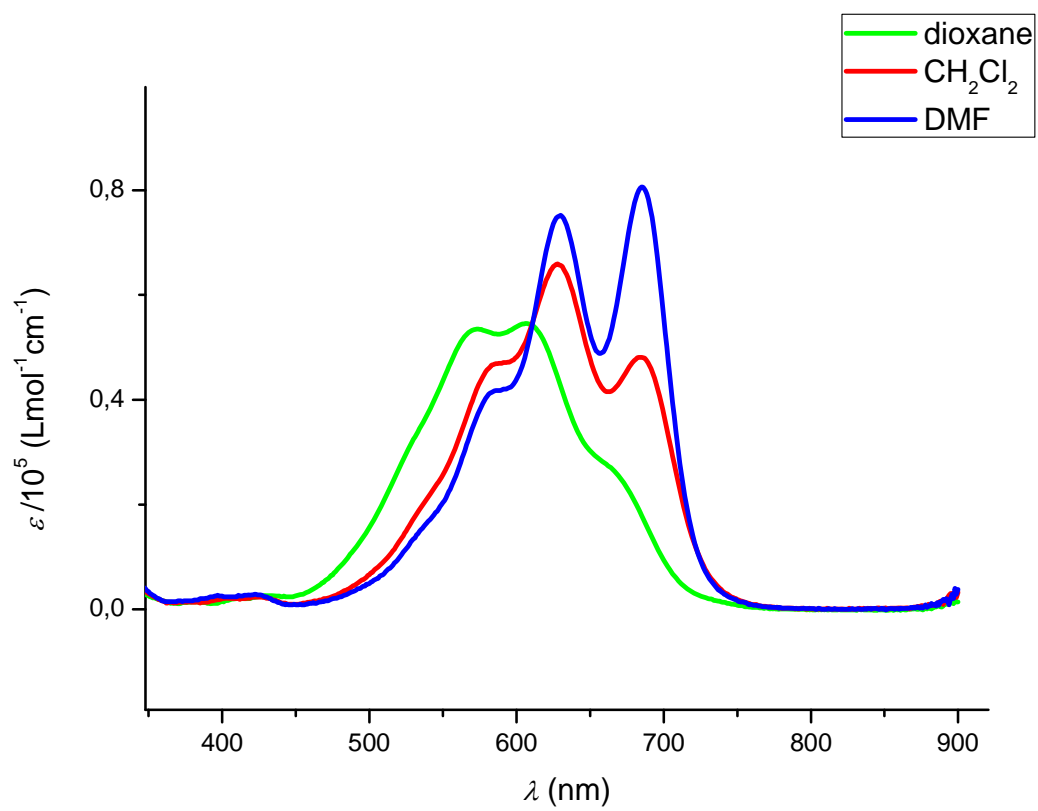
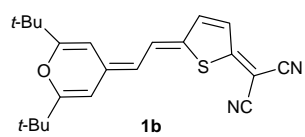


Figure S-9: UV-vis absorption spectra of compound **1b**.



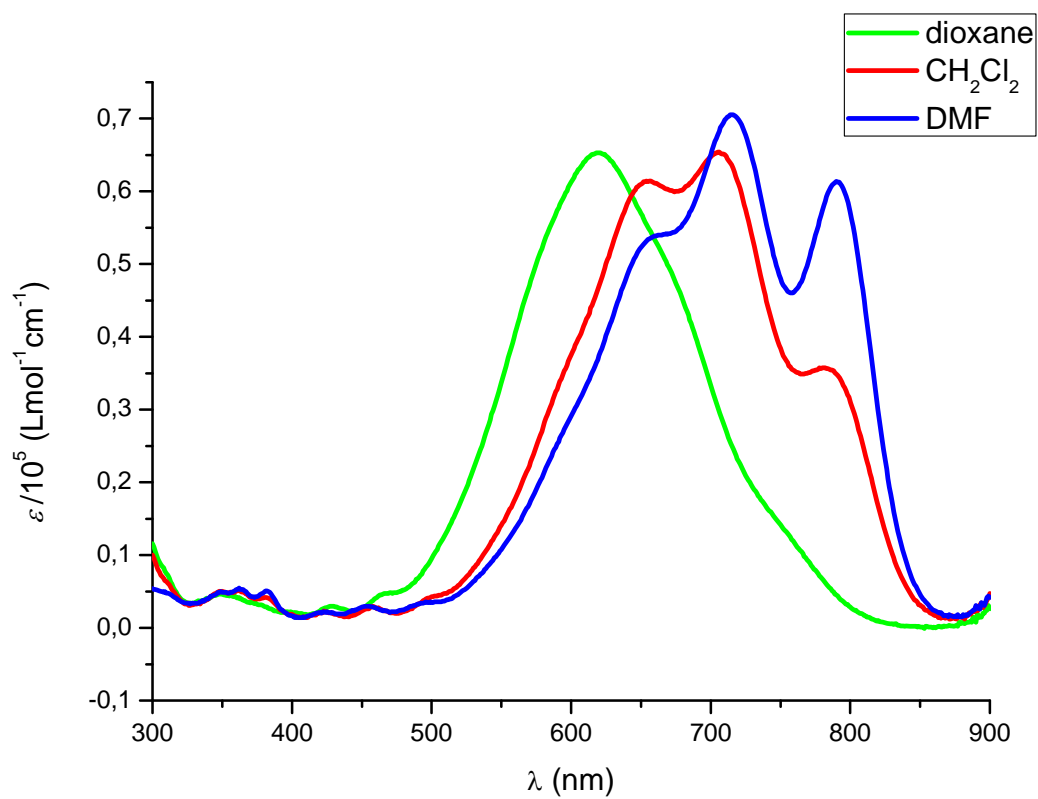
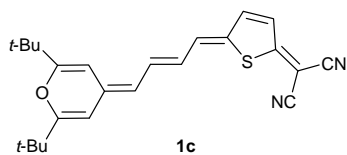


Figure S-10: UV-vis absorption spectra of compound **1c**.



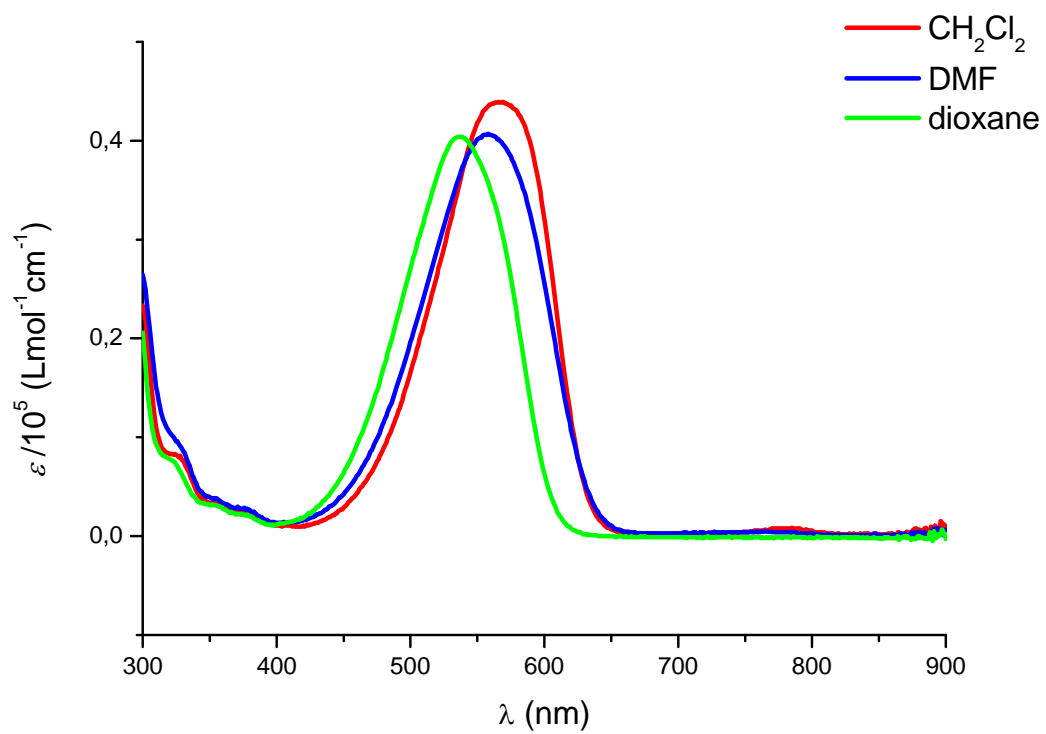
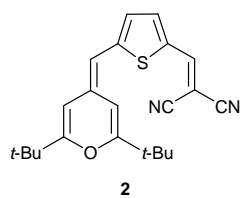


Figure S-11: UV-vis absorption spectra of compound **2**.



4. X-Ray Diffraction

X-Ray crystal structure of compound 1c: Single crystals were obtained by slow diffusion of hexane into a solution of **1c** in dichloromethane at room temperature: C₂₄H₂₆N₂OS, $M_r = 390.53$, crystal dimensions $0.45 \times 0.06 \times 0.05$ mm, orthorhombic space group *Pnma*, $\rho_{\text{calcd}} = 1.215$ g cm⁻³, $Z = 4$, $a = 16.4908(5)$, $b = 6.9106(3)$, $c = 18.7394(6)$ Å, $V = 2135.57(13)$ Å³ at 150(1) K. Number of measured and unique reflections 13243 and 2021, respectively ($R_{\text{int}}=0.0584$). Final $R(F)=0.0451$, $wR(F^2)=0.0865$ for 163 parameters and 1570 reflections with $I > 2\sigma(I)$ (corresponding R -values based on all 2021 reflections 0.0699 and 0.0955).

Crystal data and structure refinement for 1c.

Identification code	1c
Empirical formula	C ₂₄ H ₂₆ N ₂ O S
Formula weight	390.53
Temperature	150(1) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, <i>P n m a</i>
Unit cell dimensions	$a = 16.4908(5)$ Å $\alpha = 90$ deg. $b = 6.9106(3)$ Å $\beta = 90$ deg. $c = 18.7394(6)$ Å $\gamma = 90$ deg.
Volume	2135.57(13) Å ³
Z , Calculated density	4, 1.215 Mg/m ³
Absorption coefficient	0.168 mm ⁻¹
$F(000)$	832
Crystal size	0.450 x 0.060 x 0.050 mm
Theta range for data collection	3.142 to 24.998 deg.
Limiting indices	$-19 \leq h \leq 19$, $-8 \leq k \leq 7$, $-21 \leq l \leq 22$
Reflections collected / unique	13243 / 2021 [$R_{\text{int}} = 0.0584$]
Completeness to theta = 25.000	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.96493

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2021 / 0 / 163
Goodness-of-fit on F^2	1.084
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0451, wR2 = 0.0865
R indices (all data)	R1 = 0.0699, wR2 = 0.0955
Extinction coefficient	n/a
Largest diff. peak and hole	0.261 and -0.254 e. \AA^{-3}

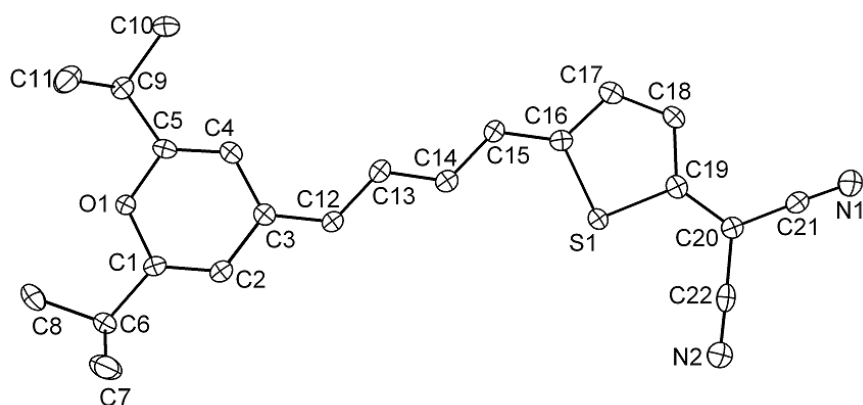


Figure S-12: ORTEP view of **1c**.

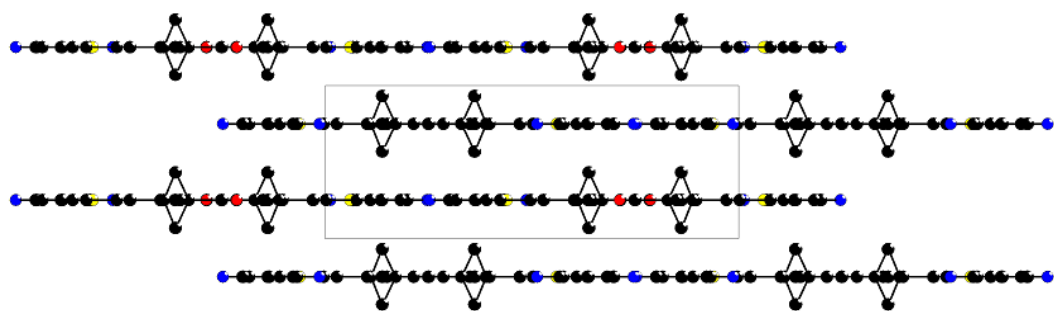


Figure S-13: Crystal packing of **1c** viewed along the $[100]$ direction.

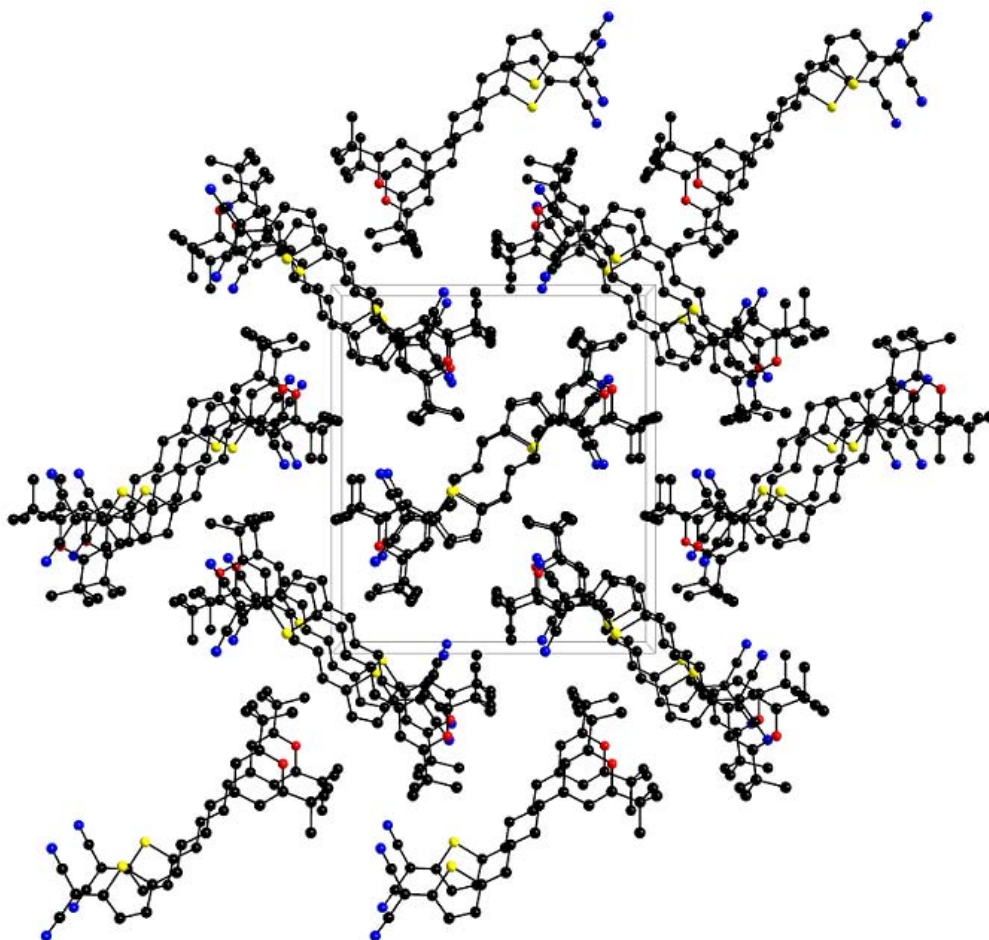


Figure S-14: Crystal packing of **1c** viewed along the [010] direction.

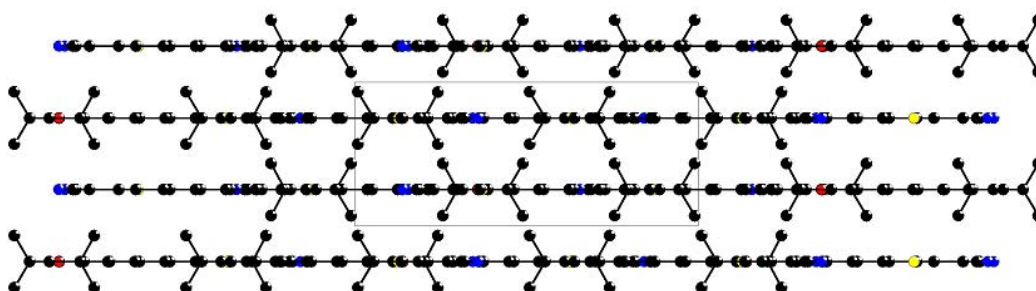


Figure S-15: Crystal packing of **1c** viewed along the [001] direction.

Compound 2

X-Ray crystal structure of compound 2: Single crystals were obtained by slow diffusion of hexane into a solution of **2** in dichloromethane at room temperature: C₂₂H₂₄N₂OS. $M_r = 364.49$, crystal dimensions $0.42 \times 0.06 \times 0.02$ mm, monoclinic space group $P21/m$, $\rho_{\text{calcd}} = 1.168 \text{ g cm}^{-3}$, $Z = 2$, $a = 9.1986(13)$, $b = 6.8265(10)$, $c = 17.101(3) \text{ \AA}$, $\beta = 105.222(16)$, $V = 1036.2(3) \text{ \AA}^3$ at $150(1) \text{ K}$. Number of measured and unique reflections 11105 and 1945, respectively ($R_{\text{int}} = 0.1603$).

Crystal data and structure refinement for 2.

Identification code	2
Empirical formula	C ₂₂ H ₂₄ N ₂ O S
Formula weight	364.49
Temperature	150(1) K
Wavelength	0.71073 \AA
Crystal system, space group	Monoclinic, $P21/m$
Unit cell dimensions	$a = 9.1986(13) \text{ \AA}$ $\alpha = 90\text{deg.}$ $b = 6.8265(10) \text{ \AA}$ $\beta = 105.222(16) \text{ deg.}$ $c = 17.101(3) \text{ \AA}$ $\gamma = 90 \text{ deg.}$
Volume	$1036.2(3) \text{ \AA}^3$
Z , Calculated density	2, 1.168 Mg/m ³
Absorption coefficient	0.168 mm^{-1}
$F(000)$	388
Crystal size	$0.42 \times 0.06 \times 0.02 \text{ mm}$
Theta range for data collection	3.23 to 24.98 deg.
Limiting indices	$-10 \leq h \leq 10$, $-8 \leq k \leq 8$, $-19 \leq l \leq 20$
Reflections collected / unique	11105 / 1945 [$R_{\text{int}} = 0.1603$]
Completeness to $\theta = 24.98$	97.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9966 and 0.9327

Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1945 / 0 / 151
Goodness-of-fit on F ²	1.042
Final R indices [I>2sigma(I)]	R1 = 0.1046, wR2 = 0.2063
R indices (all data)	R1 = 0.1895, wR2 = 0.2475
Largest diff. peak and hole	0.486 and -0.279 e.A ⁻³

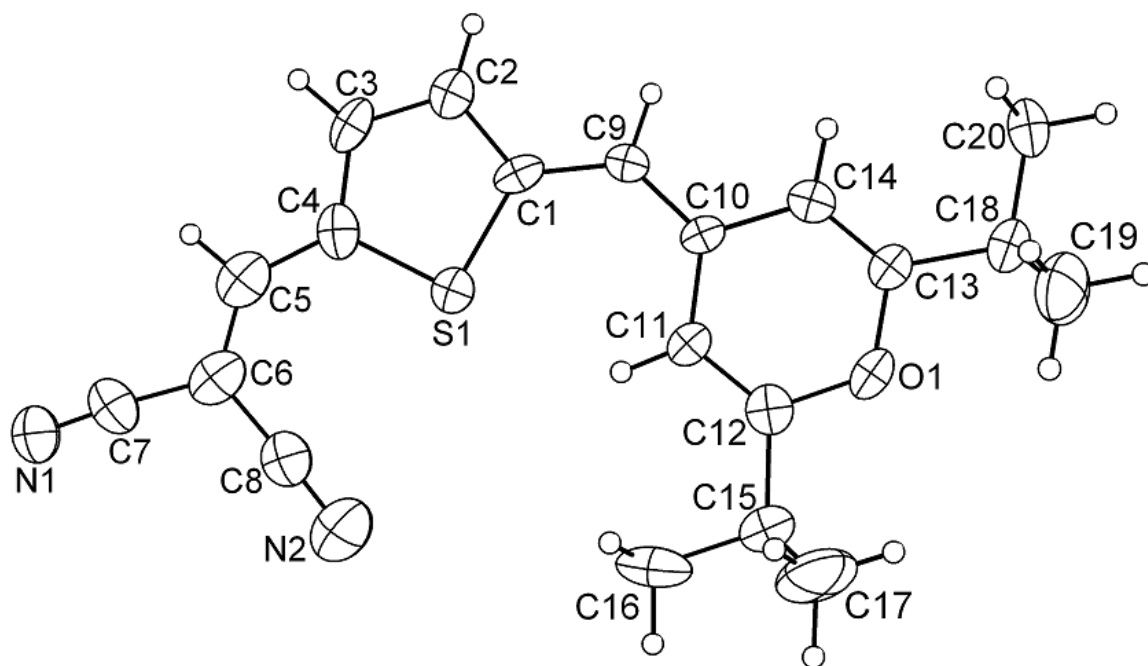


Figure S-16: ORTEP view of **2**.

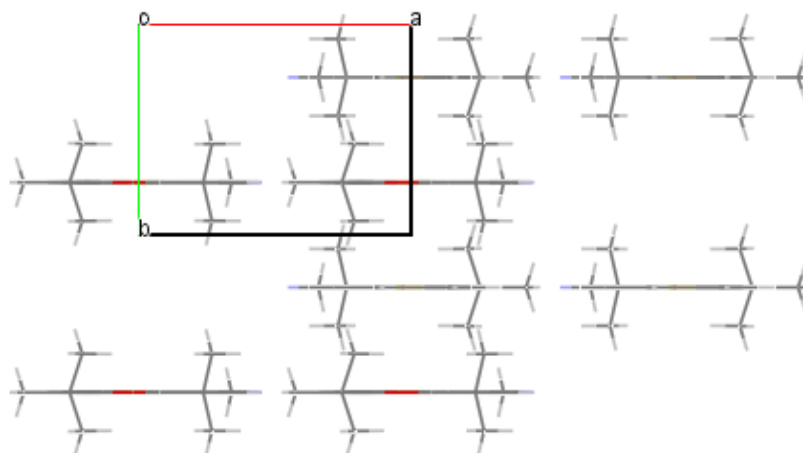


Figure S-17: Crystal packing of **2** viewed along the [001] direction.

5. Voltammograms

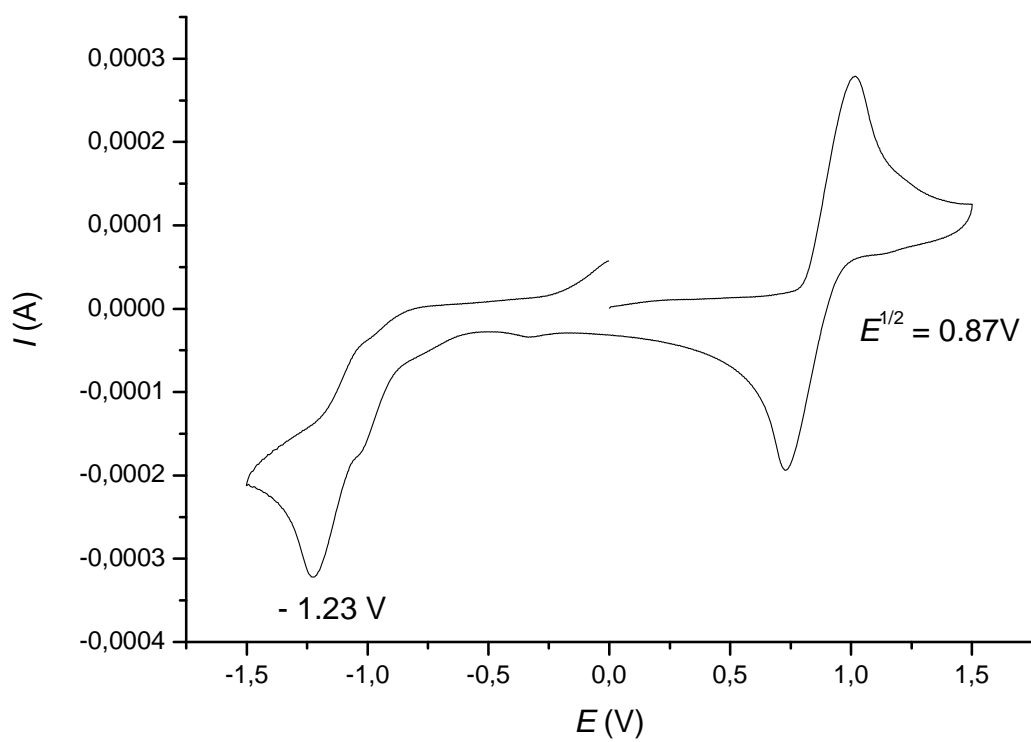
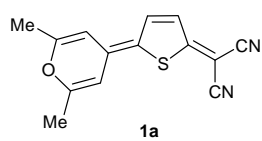


Figure S-18: Voltammogram of compound **1a**.



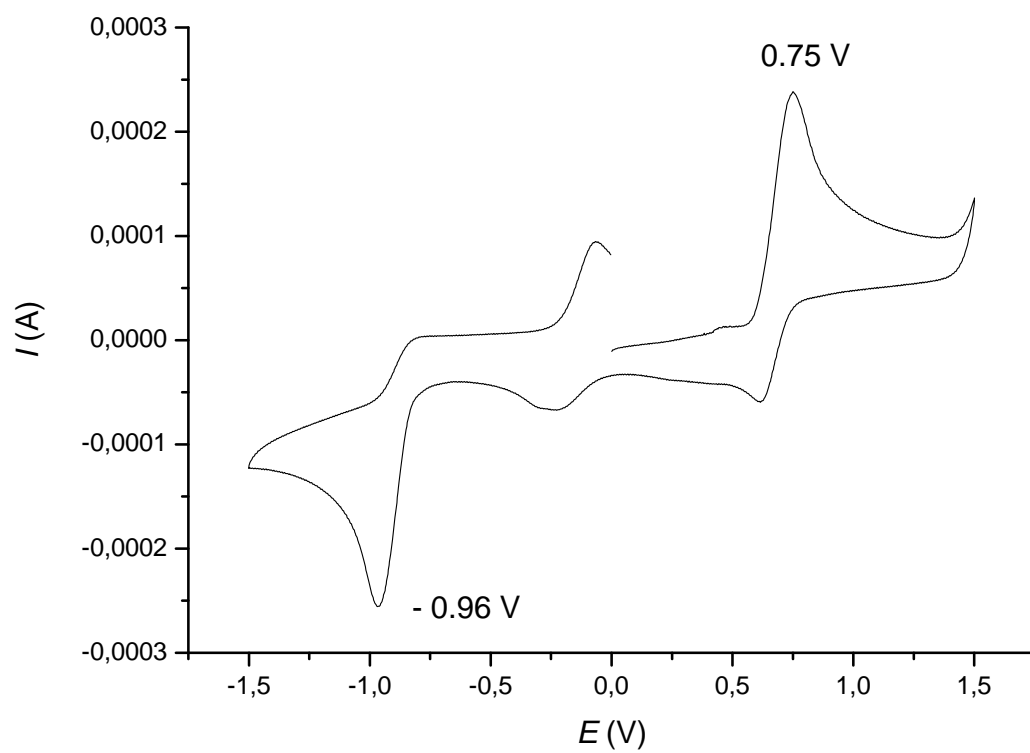
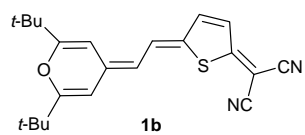


Figure S-19: Voltammogram of compound **1b**.



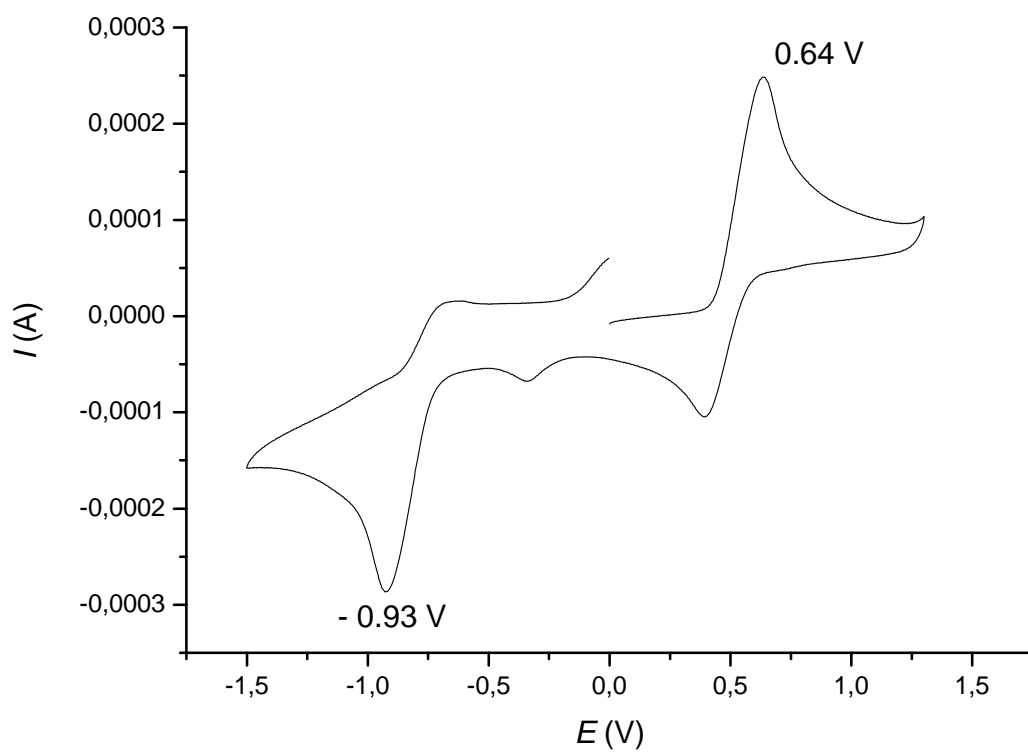
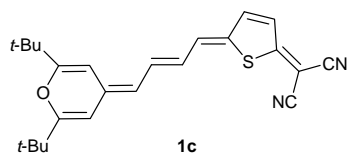


Figure S-20: Voltammogram of compound **1c**.



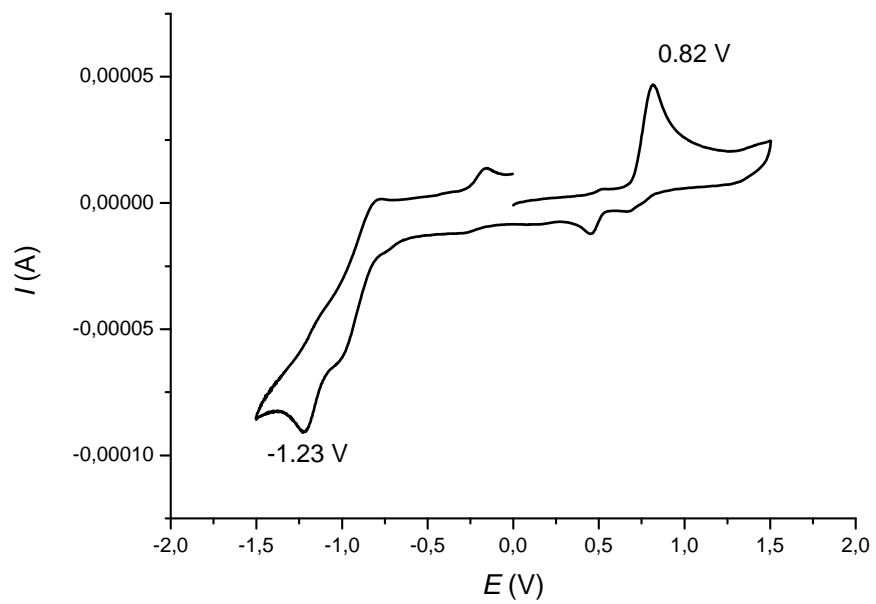
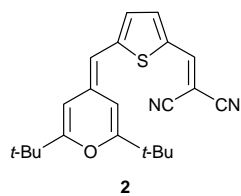


Figure S-21: Voltammogram of compound **2**.



6. HRMS spectra of new compounds

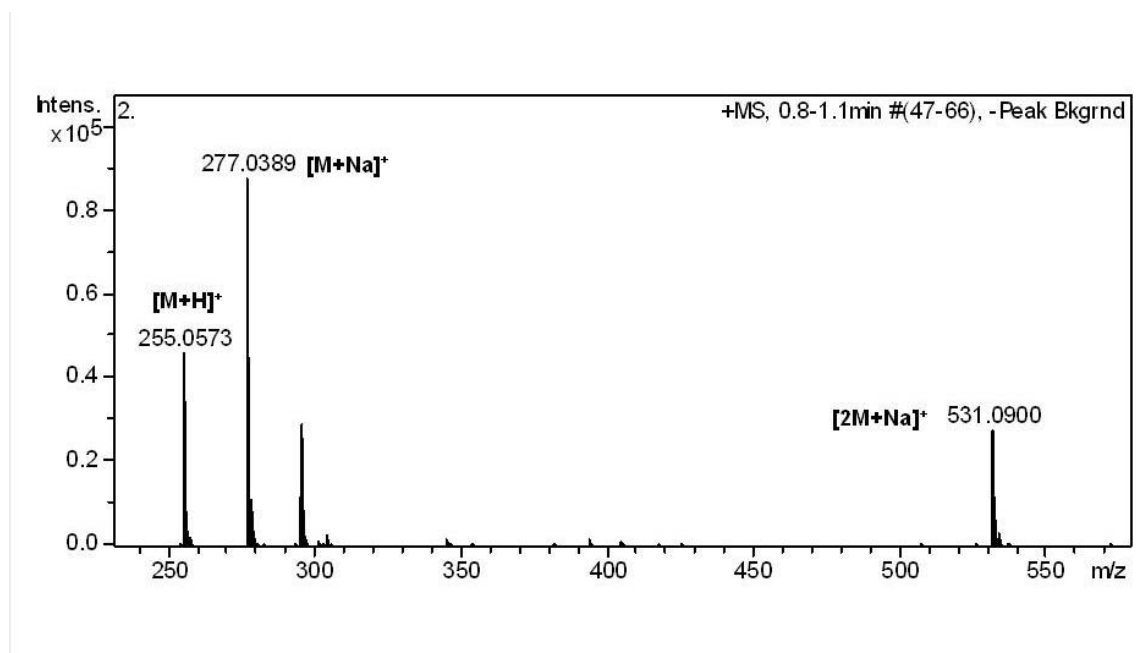
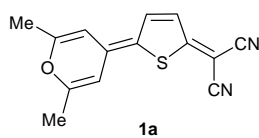


Figure S-22: HRMS spectra (ESI⁺) of compound 1a.



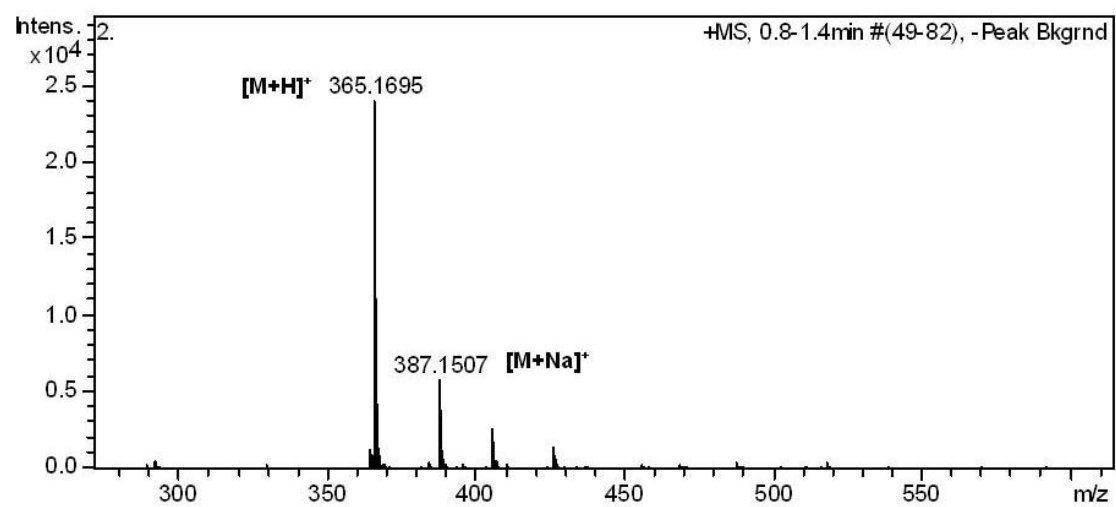
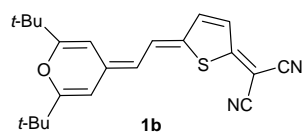


Figure S-23: HRMS spectra (ESI⁺) of compound **1b**.



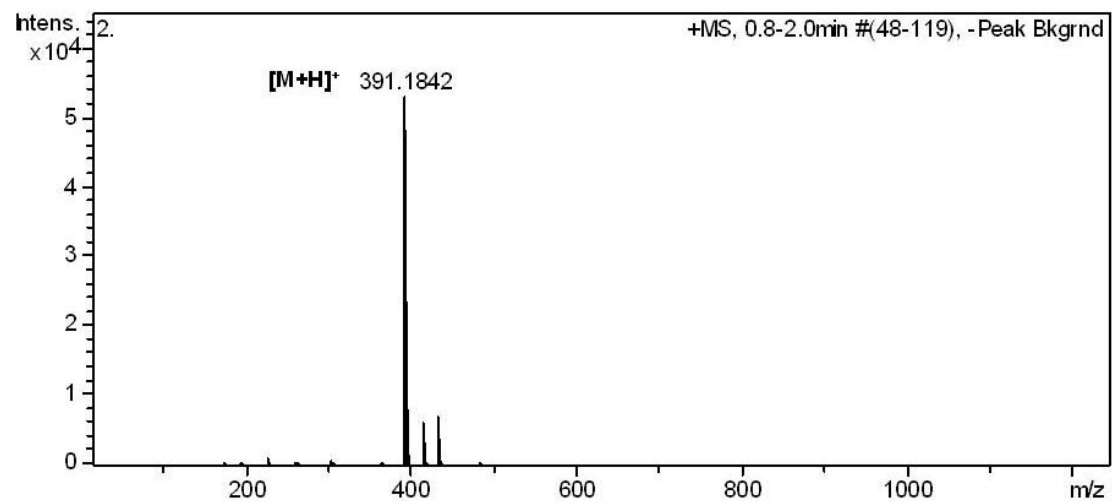
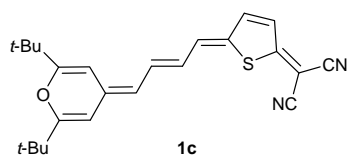


Figure S-24: HRMS spectra (ESI⁺) of compound **1c**.



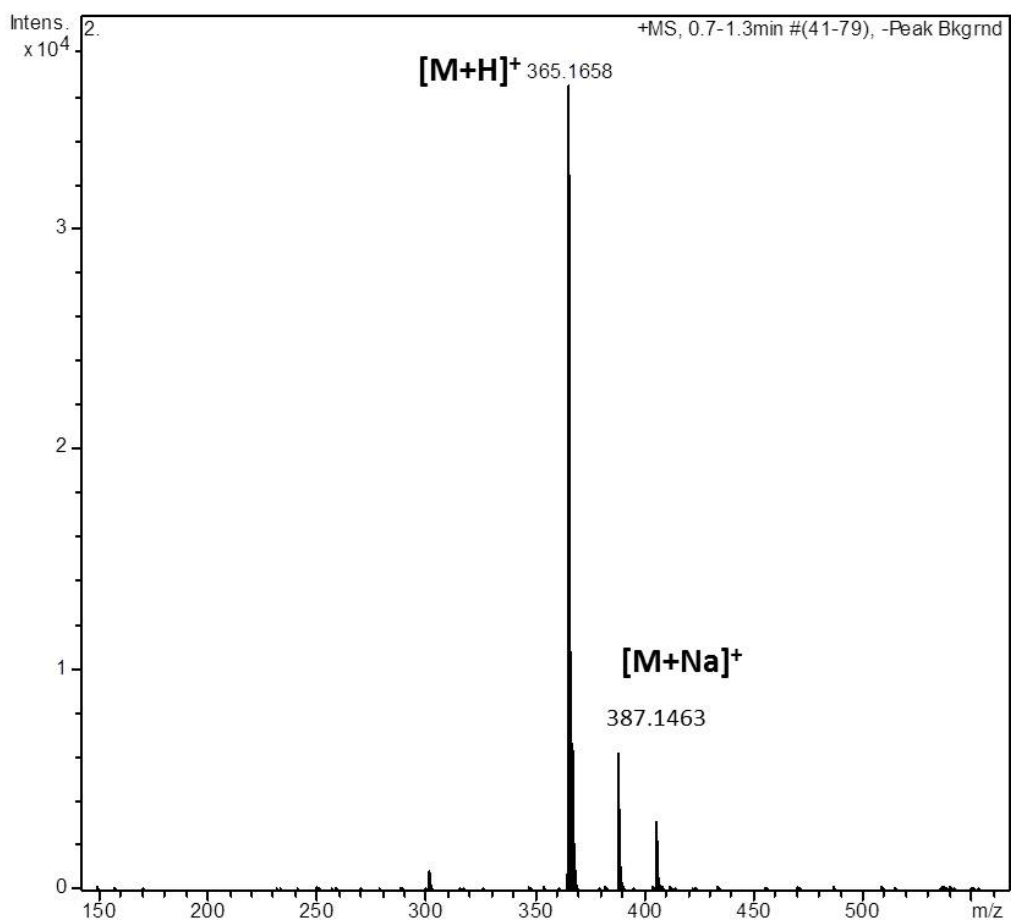
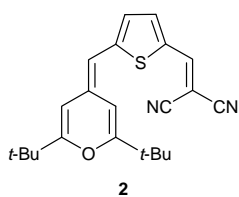


Figure S-25: HRMS spectra (ESI⁺) of compound **2**.



7. 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 H_2 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 second one is passed through a linear (vertical) polarizer and focused into the EFISH wedge shaped liquid cell. Voltage pulses of 5 kV and 3 μs 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 of the reported compounds have been determined in dichloromethane. Several solutions of concentration in the range 10^{-3} – 10^{-4} M were measured.

8.- Computational Methods

Theoretical calculations were performed using Gaussian 09,^[4] and the default parameters provided by this software package. All the calculations performed estimated solvent effects by using a Polarizable Continuum Model (PCM).^[5] Equilibrium geometries in solution were obtained using the M06-2x hybrid meta-GGA exchange-correlation functional^[6] and the medium size 6-31G* basis set.^[7] Mulliken charges and molecular orbital energies were calculated by single point calculations using the 6-311+G(2d,p) basis set. Vertical excitation energies were calculated by time-dependent single point calculations using the M06-2x/6-311+G(2d,p) model chemistry. Molecular Orbital contour plots were obtained using the Avogadro software^[8] at 0.04 isosurface value.

Calculated Equilibrium Geometries and Energies. (PCM-M06-2x/6-31G* in dichloromethane)

1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.436603	-0.305989	-0.000007
2	6	0	1.958584	-1.646923	-0.000012
3	6	0	0.590955	-1.730369	-0.000023
4	6	0	-0.078653	-0.483085	-0.000030
5	1	0	2.632899	-2.494480	-0.000004
6	16	0	1.115300	0.823578	-0.000024
7	6	0	3.768439	0.109381	0.000007
8	6	0	4.811730	-0.853234	0.000023
9	7	0	5.647525	-1.660254	0.000039
10	6	0	4.106465	1.486961	0.000009
11	7	0	4.342417	2.624819	0.000011
12	6	0	-1.444776	-0.240421	-0.000025
13	6	0	-1.996744	1.086256	-0.000022
14	6	0	-2.415474	-1.301220	-0.000022
15	6	0	-3.334869	1.283209	0.000010
16	1	0	-1.353813	1.959030	-0.000043
17	6	0	-3.739312	-1.028759	0.000010
18	1	0	-2.110529	-2.339716	-0.000041

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19	8	0	-4.201405	0.244909	0.000037
20	6	0	-4.035976	2.596778	0.000013
21	6	0	-4.847523	-2.023482	0.000021
22	1	0	0.058634	-2.675015	-0.000027
23	1	0	-3.315666	3.414759	0.000050
24	1	0	-4.674971	2.677807	-0.884282
25	1	0	-4.675027	2.677774	0.884270
26	1	0	-5.476169	-1.882622	0.884349
27	1	0	-5.476212	-1.882591	-0.884272
28	1	0	-4.448990	-3.038036	-0.000006

E(RM062X) = -1122.04903014 A.U.

1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.007702	-0.268682	-0.000182
2	6	0	4.769904	-1.673893	-0.000627
3	6	0	3.437837	-1.988797	-0.000663
4	6	0	2.563241	-0.872003	-0.000268
5	1	0	5.582612	-2.390001	-0.000899
6	16	0	3.509969	0.621798	0.000147
7	6	0	6.247831	0.366672	-0.000006
8	6	0	7.440591	-0.404786	-0.000293
9	7	0	8.401381	-1.057436	-0.000530
10	6	0	6.349596	1.781867	0.000511
11	7	0	6.394281	2.942906	0.000955
12	6	0	-1.069090	0.100048	0.000139
13	6	0	-1.865388	1.298265	0.000343
14	6	0	-1.819666	-1.128517	-0.000020
15	6	0	-3.216491	1.245053	0.000206
16	1	0	-1.370467	2.261498	0.000507
17	6	0	-3.172222	-1.116199	0.000038
18	1	0	-1.316128	-2.085280	-0.000095
19	8	0	-3.860323	0.051301	0.000043
20	1	0	3.051427	-3.002900	-0.000969
21	6	0	1.186293	-0.917155	-0.000224
22	1	0	0.767253	-1.921916	-0.000515
23	6	0	0.317748	0.183711	0.000115
24	1	0	0.750223	1.182303	0.000345
25	6	0	-4.190541	2.399153	-0.000256
26	6	0	-5.069980	2.297837	-1.258838
27	6	0	-5.073259	2.296501	1.255896
28	6	0	-3.449375	3.736837	0.001444
29	1	0	-4.461470	2.355419	-2.166898
30	1	0	-5.632583	1.360281	-1.273815
31	1	0	-5.783606	3.127524	-1.268748
32	1	0	-4.467099	2.352513	2.165624
33	1	0	-5.786434	3.126578	1.265105
34	1	0	-5.636454	1.359270	1.268081
35	1	0	-4.180870	4.550066	0.001281
36	1	0	-2.822260	3.846828	0.892026
37	1	0	-2.820437	3.848206	-0.887678
38	6	0	-4.105133	-2.304999	0.000356
39	6	0	-4.987224	-2.234031	1.259246
40	6	0	-4.990622	-2.232327	-1.256029
41	6	0	-3.319573	-3.617295	-0.001600
42	1	0	-4.376715	-2.271058	2.166994
43	1	0	-5.580851	-1.315976	1.274578
44	1	0	-5.672456	-3.087255	1.269244
45	1	0	-4.382557	-2.267643	-2.165487
46	1	0	-5.675517	-3.085823	-1.265567
47	1	0	-5.584699	-1.314521	-1.268244
48	1	0	-4.023314	-4.454520	-0.001424
49	1	0	-2.689658	-3.706584	-0.892590
50	1	0	-2.687558	-3.708041	0.887753

E(RM062X) = -1435.18246040 A.U.

1c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.311625	-0.193832	-0.000088
2	6	0	6.183395	-1.614831	-0.000206
3	6	0	4.881072	-2.032647	-0.000258
4	6	0	3.921272	-0.985342	-0.000184
5	1	0	7.049735	-2.264958	-0.000247
6	16	0	4.749233	0.577657	-0.000045
7	6	0	7.498000	0.534921	-0.000012
8	6	0	8.748106	-0.140433	-0.000047
9	7	0	9.757774	-0.714393	-0.000077
10	6	0	7.487734	1.954352	0.000101
11	7	0	7.438233	3.115028	0.000193
12	6	0	-2.125347	0.370972	-0.000014
13	6	0	-3.062621	1.465923	0.000150
14	6	0	-2.727954	-0.939507	-0.000159
15	6	0	-4.396052	1.252109	0.000189
16	1	0	-2.687848	2.481936	0.000249
17	6	0	-4.070799	-1.088197	-0.000123
18	1	0	-2.113917	-1.829305	-0.000296
19	8	0	-4.896610	-0.010883	0.000070
20	1	0	4.573644	-3.073215	-0.000348
21	6	0	2.553904	-1.131667	-0.000210
22	6	0	1.595122	-0.100904	-0.000124
23	1	0	2.188927	-2.158883	-0.000299
24	1	0	1.927537	0.936256	-0.000009
25	6	0	0.243607	-0.367835	-0.000141
26	6	0	-0.762115	0.617065	-0.000019
27	1	0	-0.049486	-1.417169	-0.000248
28	1	0	-0.443925	1.657372	0.000093
29	6	0	-5.501075	2.281939	0.000358
30	6	0	-6.363747	2.075464	-1.257068
31	6	0	-6.363788	2.075013	1.257681
32	6	0	-4.926267	3.699496	0.000620
33	1	0	-5.768058	2.209534	-2.165530
34	1	0	-6.804790	1.075005	-1.273471
35	1	0	-7.175344	2.809641	-1.265320
36	1	0	-5.768125	2.208742	2.166210
37	1	0	-7.175376	2.809195	1.266177
38	1	0	-6.804842	1.074552	1.273702
39	1	0	-5.750031	4.419060	0.000731
40	1	0	-4.315942	3.884766	0.890249
41	1	0	-4.315907	3.885080	-0.888920
42	6	0	-4.857012	-2.379140	-0.000174
43	6	0	-5.743324	-2.412316	1.257313
44	6	0	-5.743326	-2.412253	-1.257659
45	6	0	-3.923629	-3.591008	-0.000206
46	1	0	-5.133426	-2.380821	2.165721
47	1	0	-6.437453	-1.567651	1.273559
48	1	0	-6.327179	-3.337943	1.265897
49	1	0	-5.133436	-2.380639	-2.166069
50	1	0	-6.327119	-3.337918	-1.266322
51	1	0	-6.437512	-1.567637	-1.273831
52	1	0	-4.525135	-4.504509	-0.000279
53	1	0	-3.286248	-3.607166	-0.890116
54	1	0	-3.286321	-3.607273	0.889753

E(RM062X) = -1512.55019014 A.U.

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.881843	1.070360	-0.023891
2	6	0	0.847085	0.202909	-0.036986
3	6	0	1.064110	-1.226780	-0.018695
4	6	0	2.460811	-1.610077	0.000242
5	6	0	3.449216	-0.694163	0.014310
6	1	0	-0.146051	0.622024	-0.069796
7	1	0	2.715625	-2.662855	0.006554
8	8	0	3.167616	0.640068	0.007907
9	6	0	0.094321	-2.201218	-0.021302
10	1	0	0.443940	-3.231093	-0.018639
11	6	0	-1.327734	-2.089491	-0.026159
12	6	0	-2.195072	-3.188614	-0.049687
13	16	0	-2.239305	-0.607457	0.005529
14	6	0	-3.541197	-2.838169	-0.046404
15	1	0	-1.825877	-4.206989	-0.069920
16	6	0	-3.766308	-1.462160	-0.017634
17	1	0	-4.359021	-3.550930	-0.064771
18	6	0	4.940022	-0.937946	0.037326
19	6	0	5.249197	-2.435956	0.044339
20	6	0	5.562799	-0.290330	-1.211586
21	6	0	5.525983	-0.286178	1.301674
22	1	0	4.829551	-2.928089	0.927721
23	1	0	4.858999	-2.930240	-0.851250
24	1	0	6.333752	-2.577656	0.062616
25	1	0	5.375372	0.786839	-1.232241
26	1	0	6.645426	-0.451809	-1.204546
27	1	0	5.153841	-0.732828	-2.125583
28	1	0	6.608873	-0.444349	1.324665
29	1	0	5.334768	0.790436	1.315199
30	1	0	5.093485	-0.728495	2.204870
31	6	0	1.804333	2.579843	-0.040962
32	6	0	2.554970	3.094697	-1.281287
33	6	0	0.350704	3.055816	-0.088204
34	6	0	2.480520	3.118614	1.231654
35	1	0	3.605674	2.792242	-1.260836
36	1	0	2.099548	2.711920	-2.200248
37	1	0	2.511880	4.188147	-1.305017
38	1	0	-0.213526	2.720223	0.788159
39	1	0	0.333228	4.149498	-0.100285
40	1	0	-0.160947	2.701096	-0.989026
41	1	0	2.445596	4.212616	1.226735
42	1	0	1.964218	2.761318	2.128404
43	1	0	3.527587	2.807595	1.284295
44	6	0	-5.046614	-0.871101	-0.009085
45	6	0	-5.405224	0.456001	0.025218
46	1	0	-5.870242	-1.582044	-0.032661
47	6	0	-4.462839	1.528510	0.064818
48	7	0	-3.694997	2.397466	0.098640
49	6	0	-6.786829	0.822208	0.025270
50	7	0	-7.908196	1.117040	0.025083

E(RM062X) = -1435.18520382 A.U.