Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Strengthening the Acceptor Properties of Thiadiazoloquinoxalines via Planarization

Shoufa Zhou, Cunbin An, Timea Stelzig, Sreenivasa Reddy Puniredd, Xin Guo, Wojciech Pisula,* and Martin Baumgarten*

Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Corresponding authors:
martin.baumgarten@mpip-mainz.mpg.de, pisula@mpip-mainz.mpg.de

Thermal properties

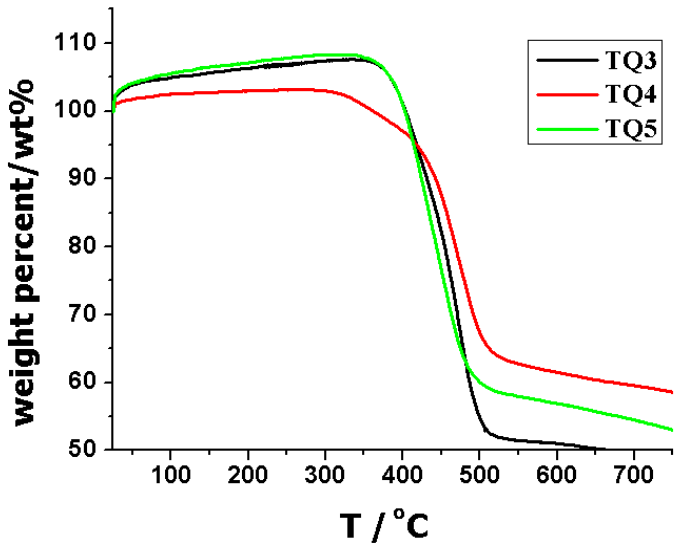


Figure S1. TGA analysis of compounds **TQ3-5**.

Differential scanning calorimetry (DSC) measurement

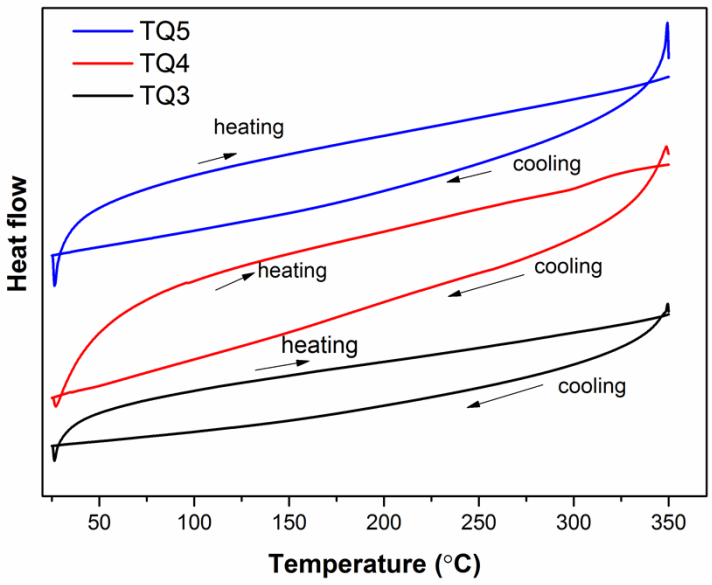


Figure S2. DSC analysis of compounds **TQ3-5**.

Photophysical spectra

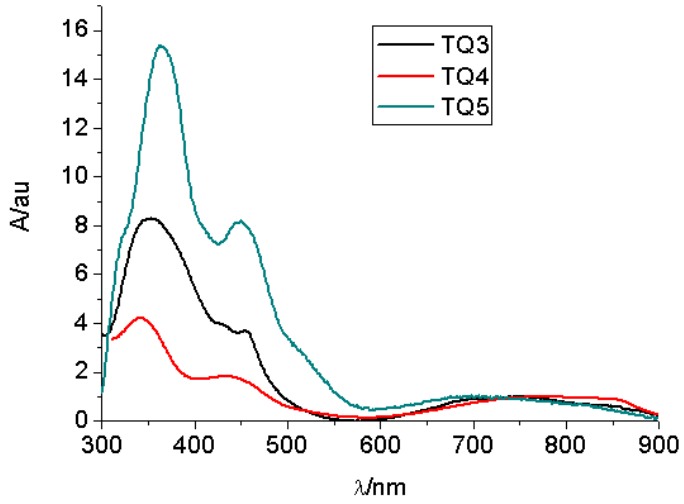


Figure S3. UV-Vis absorption spectra of compounds **TQ3-TQ5** as film.

Quantum mechanical calculations

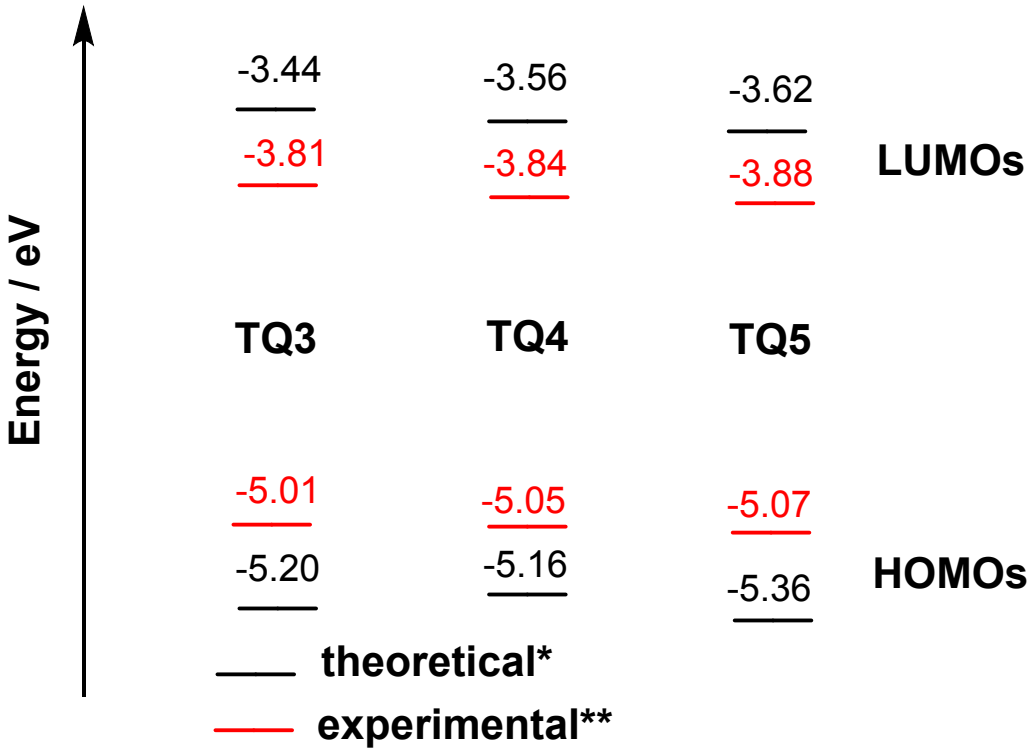
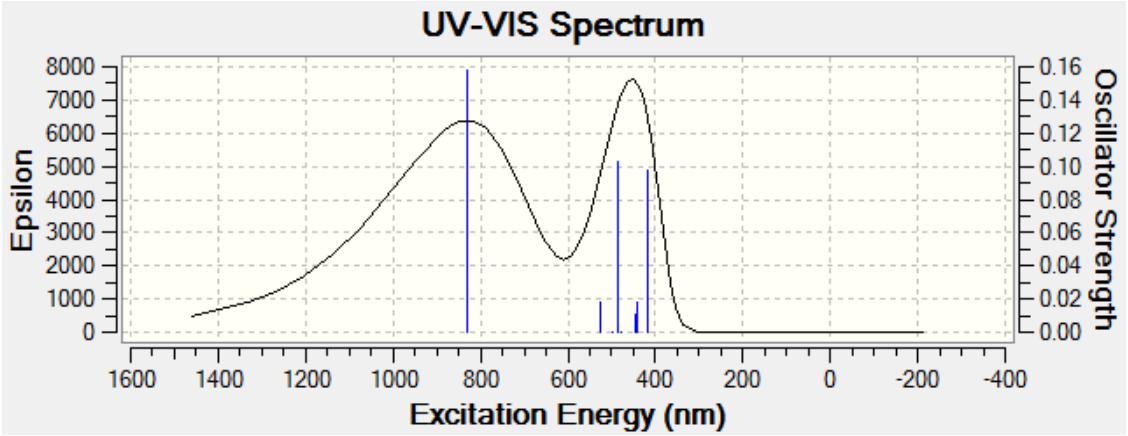


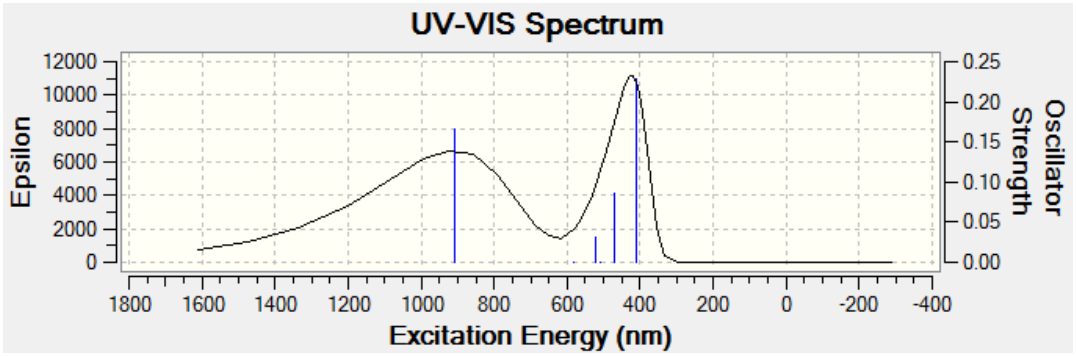
Figure S4a. Theoretical* (black) and experimental** (red, cyclic voltammetry and UV-vis) energy levels for compounds **TQ3-5**.

TQ3



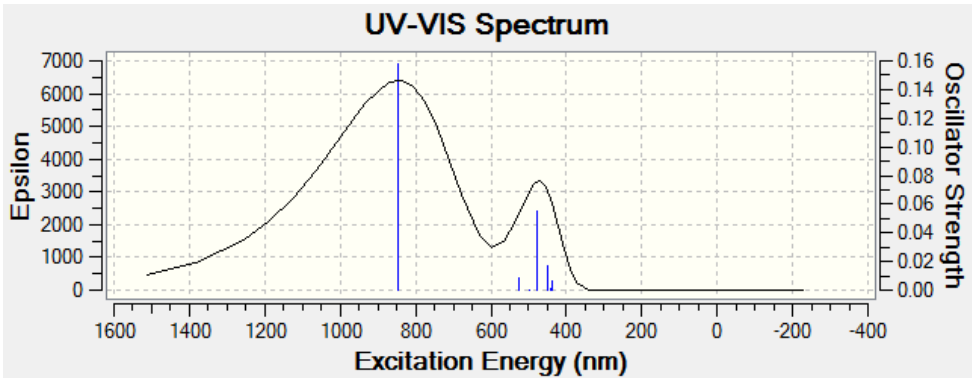
λ_{max}= 831 nm, OS= 0.16

TQ4



λ_{max}= 908 nm, OS= 0.17

TQ5



λ_{max}= 846 nm, OS= 0.16

Figure S4b. Theoretically derived (TD-DFT SCF 6-311g(d)) absorption patterns (

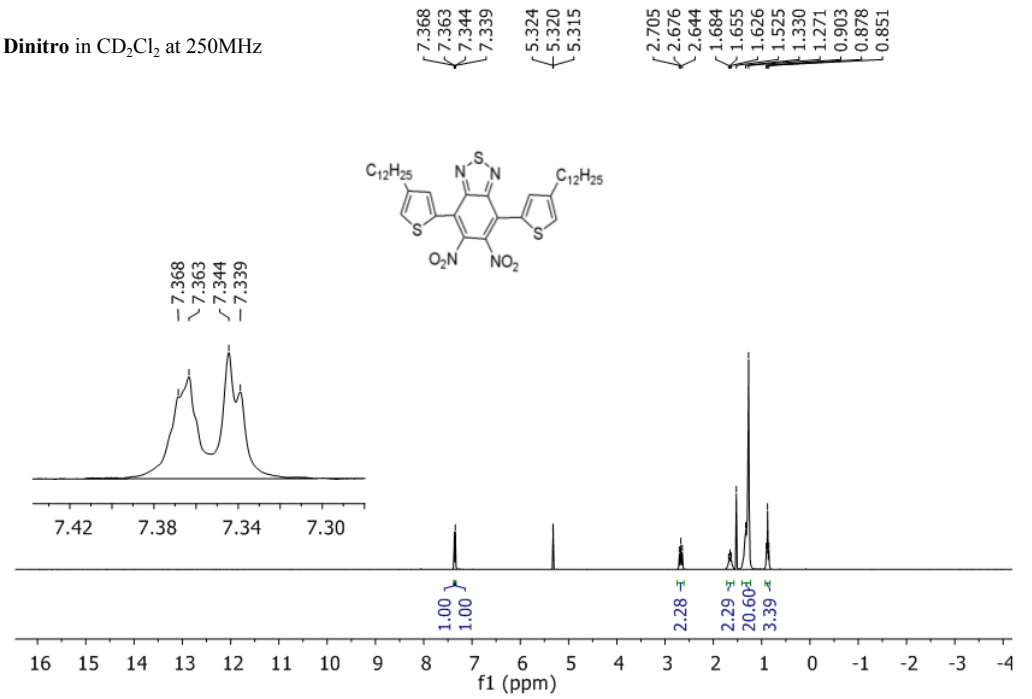
TQ3: HOMO 137 -> LUMO 138, Singlet-A, 1.4915 eV, 831.26 nm, f=0.1576;

TQ4: HOMO 139 -> LUMO 140, Singlet-A, 1.3649 eV, 908.39 nm, f=0.1654;

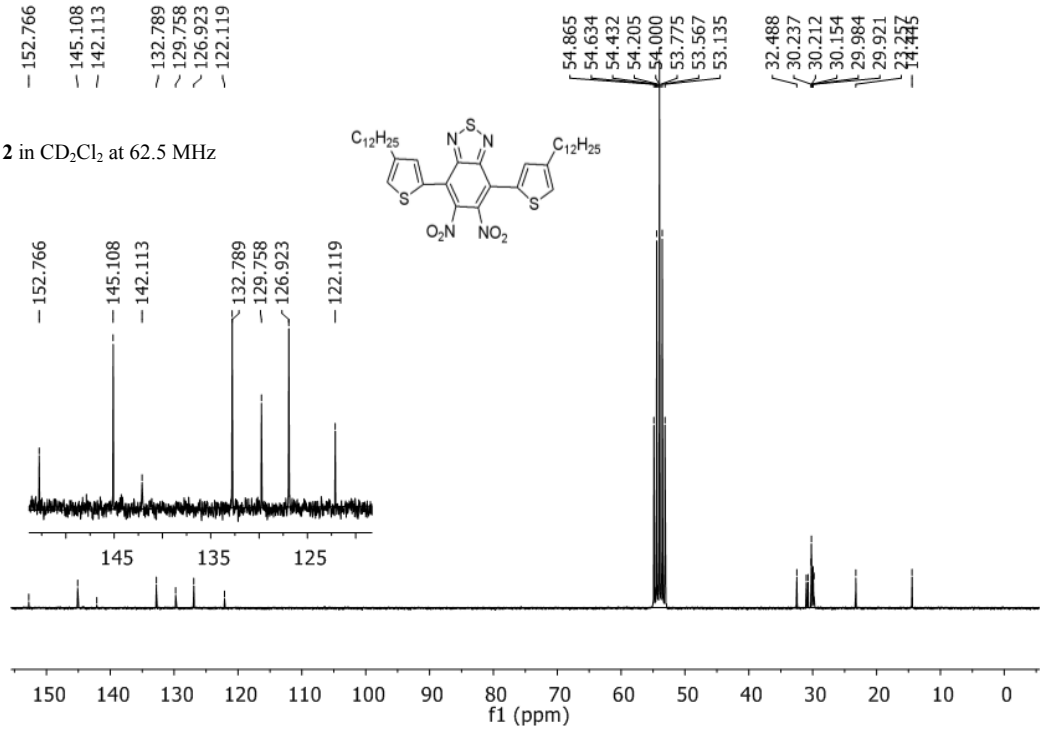
TQ5: HOMO 137 -> LUMO 138, Singlet-A, 1.4653 eV, 846.13 nm f=0.1583).

NMR Analysis of the products

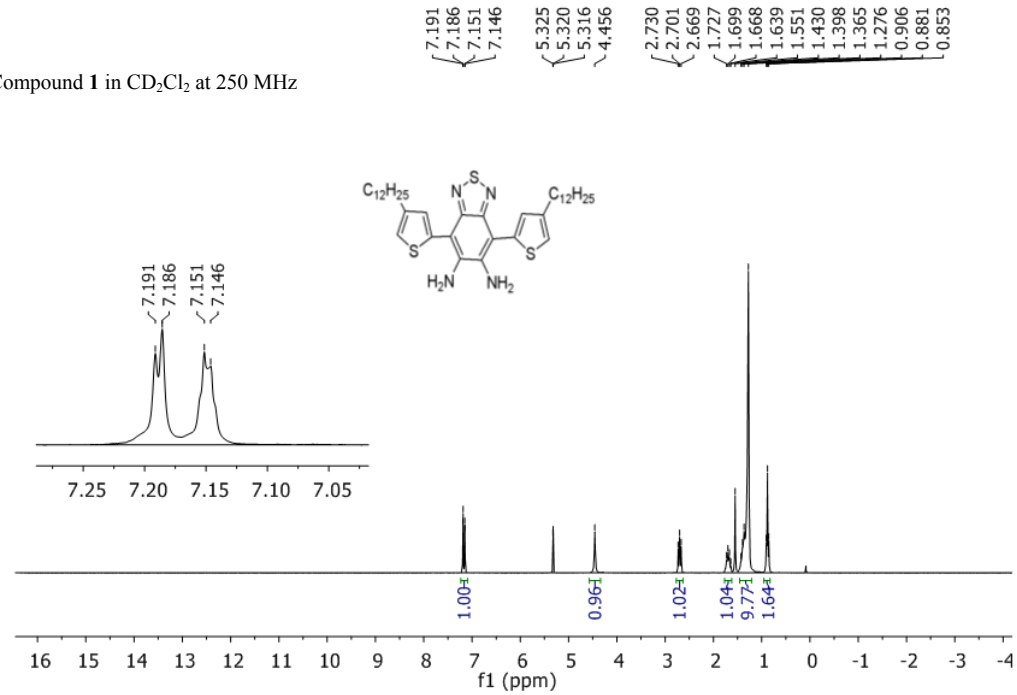
Dinitro in CD_2Cl_2 at 250MHz



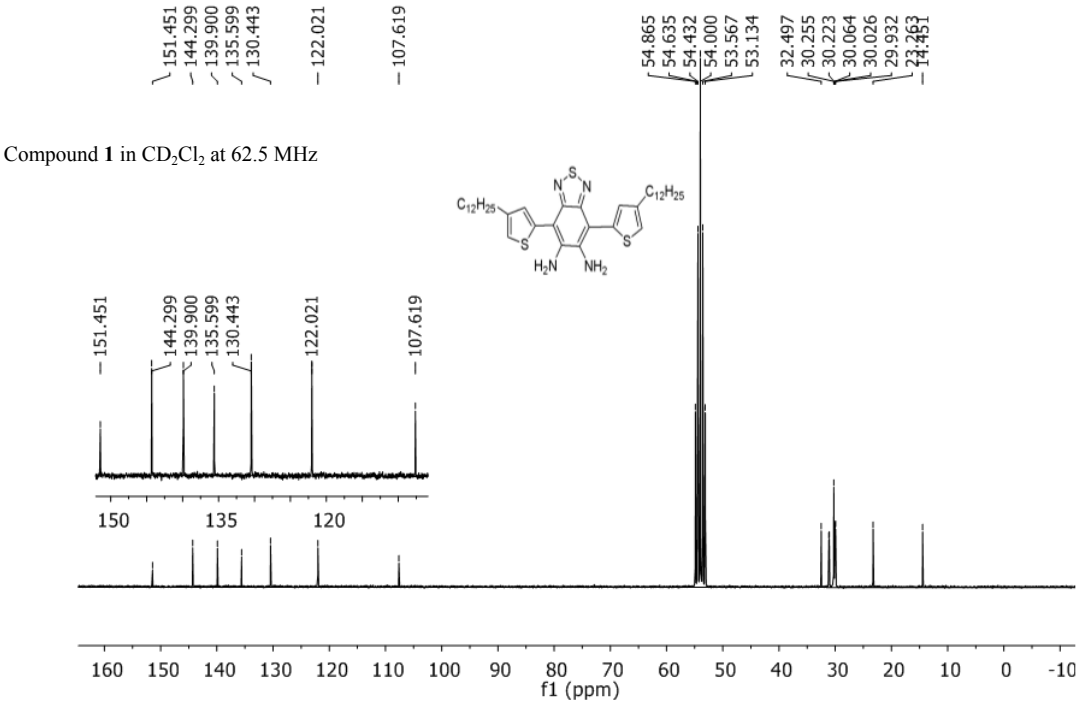
Compound **2** in CD_2Cl_2 at 62.5 MHz



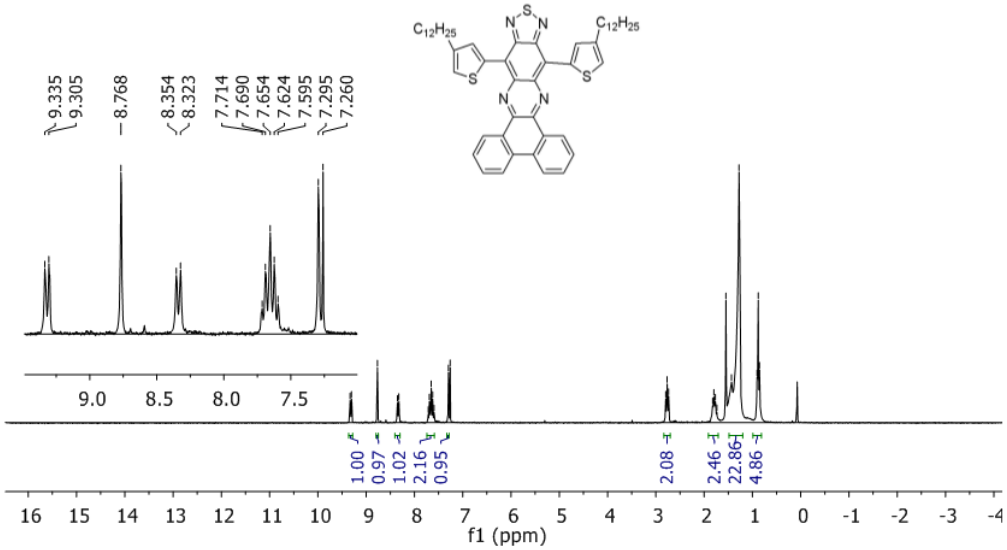
Compound **1** in CD_2Cl_2 at 250 MHz



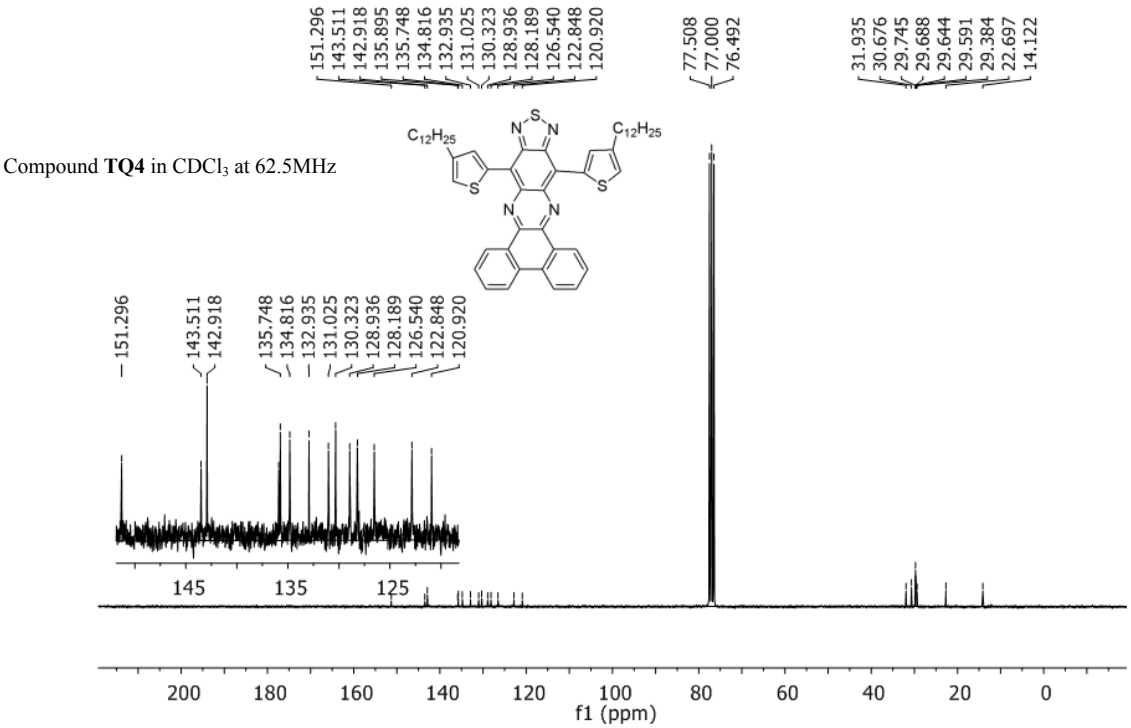
Compound **1** in CD_2Cl_2 at 62.5 MHz



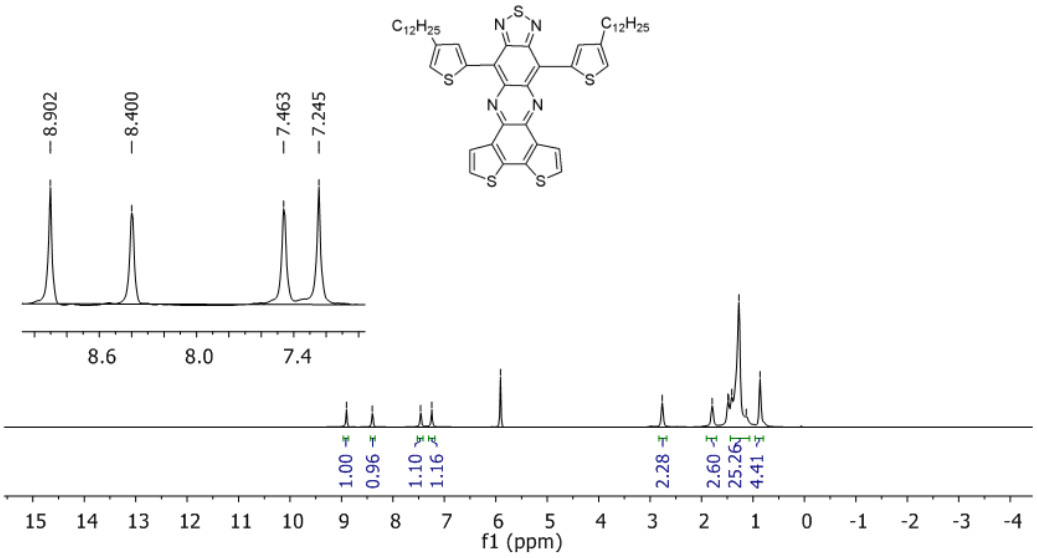
Compound **TQ3** in $CDCl_3$ at 250 MHz

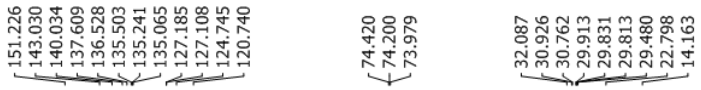


Compound **TQ4** in $CDCl_3$ at 62.5MHz

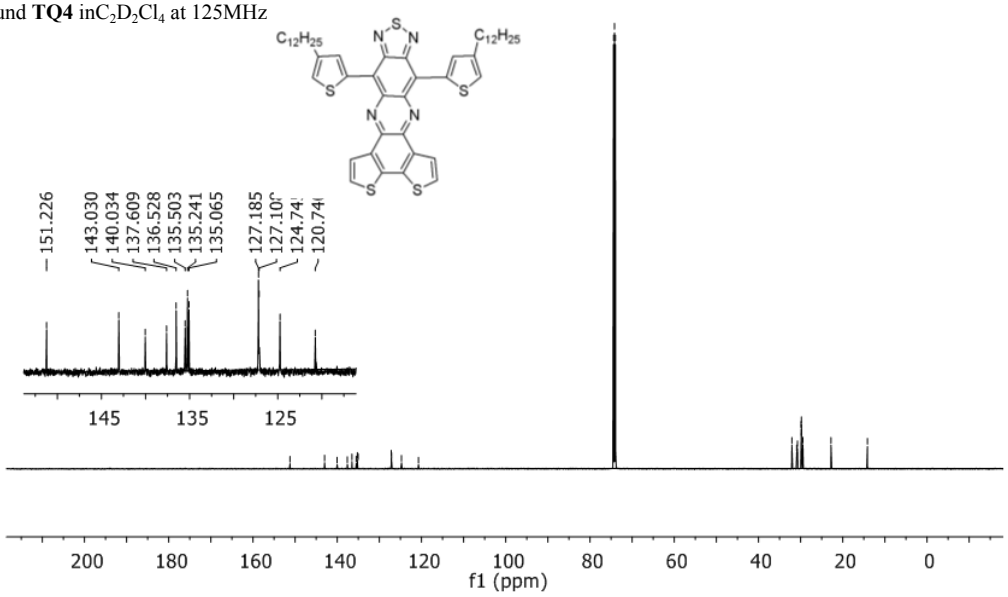


Compound **TQ4** in $C_2D_2Cl_4$ at 500 MHz

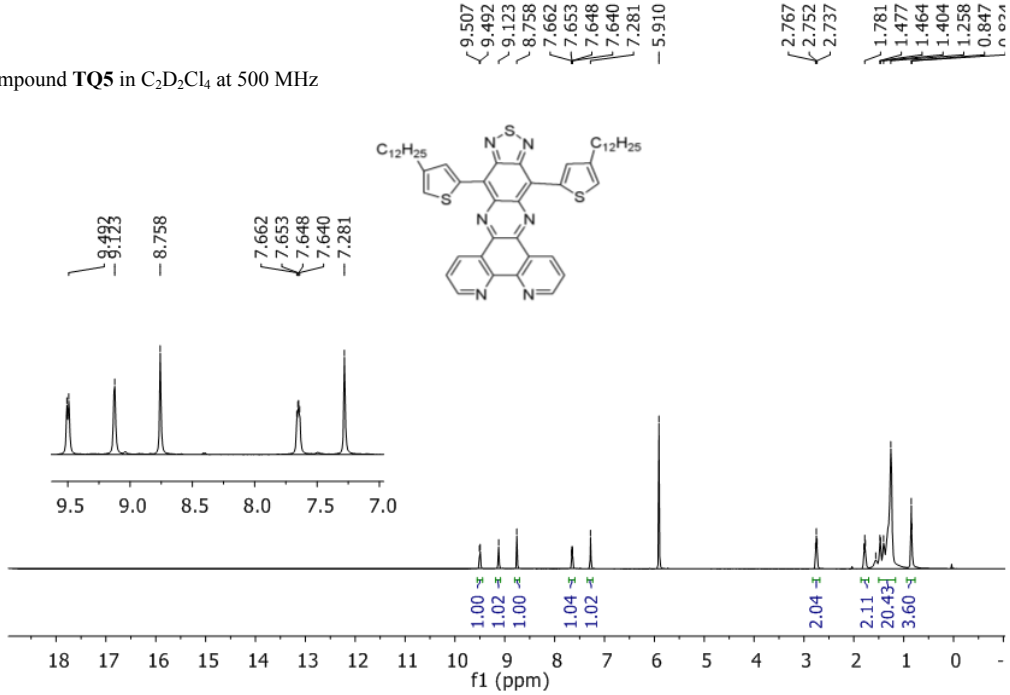




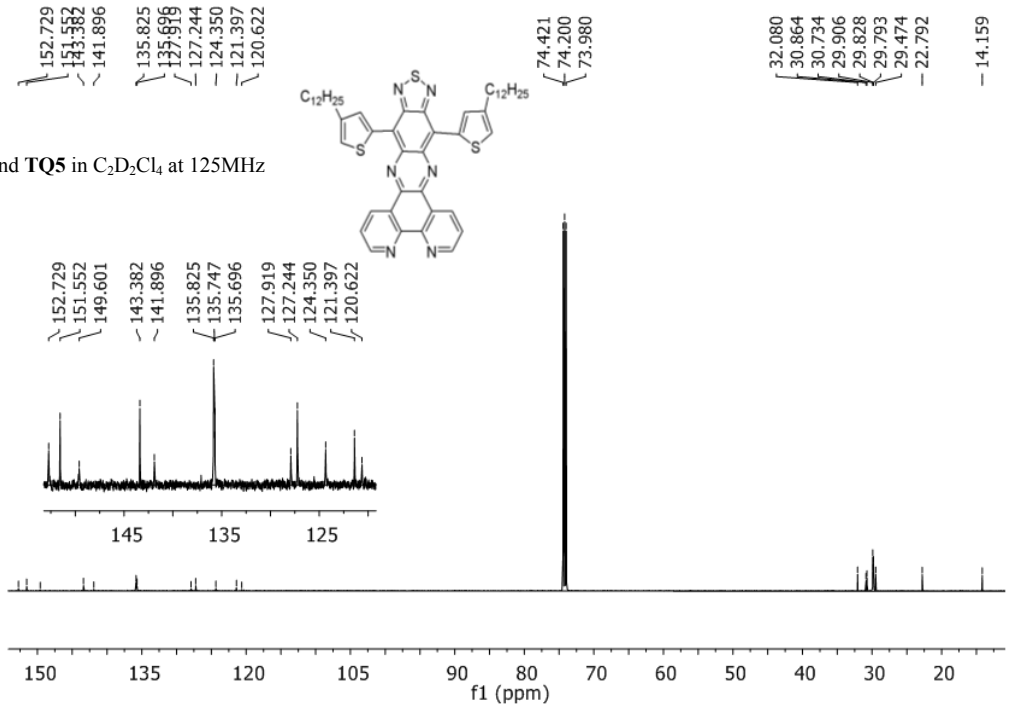
Compound **TQ4** in$C_2D_2Cl_4$ at 125MHz



Compound **TQ5** in $C_2D_2Cl_4$ at 500 MHz



Compound **TQ5** in $C_2D_2Cl_4$ at 125MHz



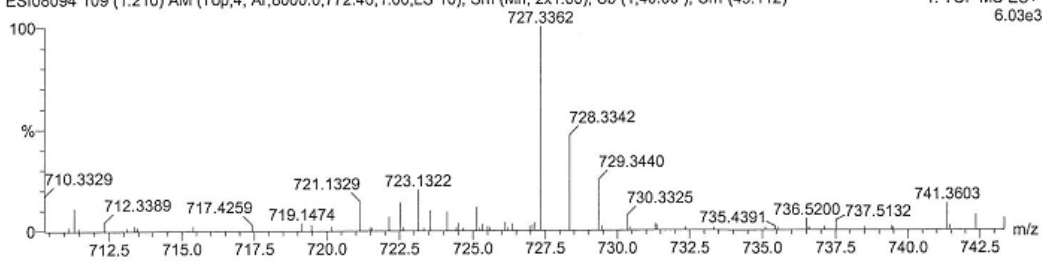
TOF MS ES+

Elemental Composition Report Page 1

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Zhou, SZTBN, Muellen
ESI08094 109 (1.210) AM (Top,4, Ar,8000.0,772.46,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (49:112) 1: TOF MS ES+ 6.03e3



Minimum:				-1.5		
Maximum:		200.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
727.3362	727.3385	-2.3	-3.2	13.5	1	C38 H55 N4 O4 S3

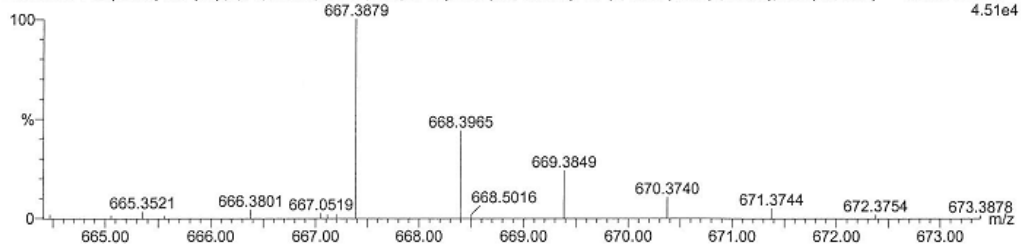
Figure S5. TOF MS ES+ spectrum of compound dinitro derivative precursor.

Elemental Composition Report Page 1

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Zhou, SZTBA, Muellen
ESI08095 116 (1.280) AM (Top,4, Ar,8000.0,622.57,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Sb (1,40.00); Cm (107:192) 1: TOF MS ES+ 4.51e4



Minimum:				-1.5		
Maximum:		200.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
667.3879	667.3902	-2.3	-3.4	11.5	1	C38 H59 N4 S3

Figure S6. TOF MS ES+ spectrum of compound **1**.

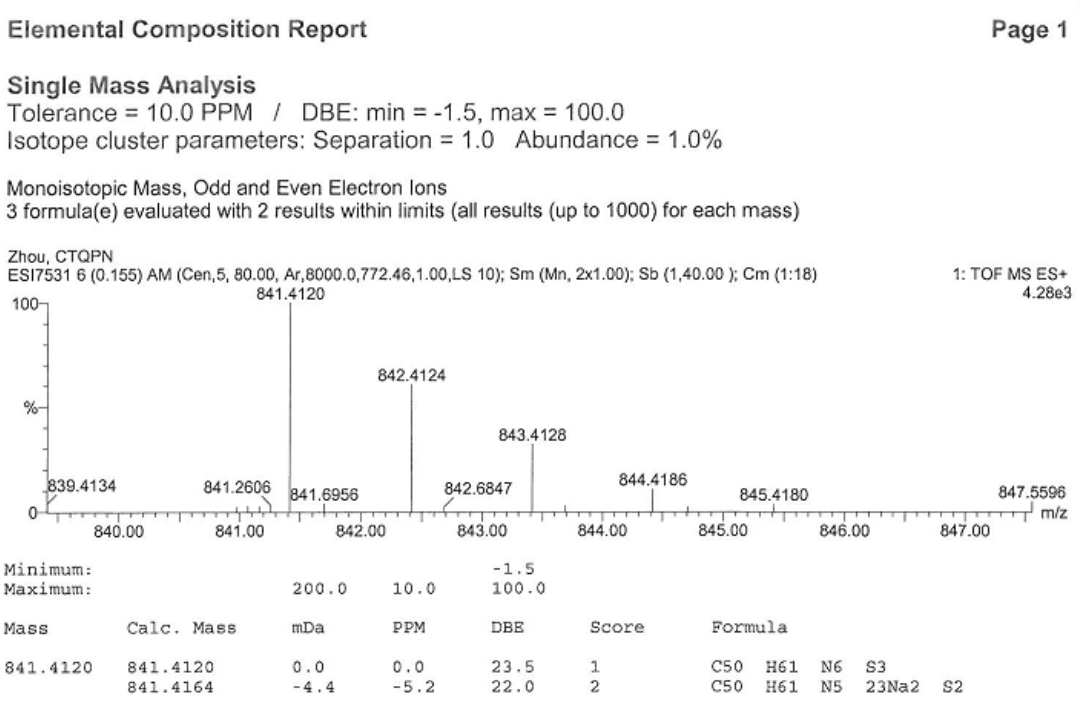


Figure S7. TOF MS ES+ spectrum of compound **TQ5**.

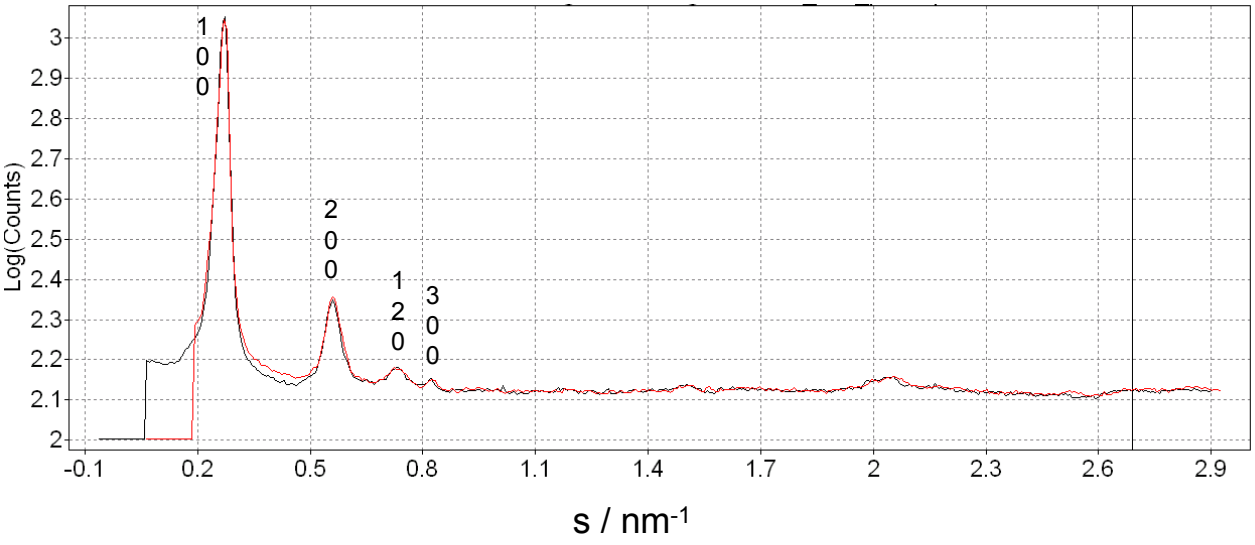


Figure S8. Equatorial integration of the 2DWAXS pattern in Figure 6c of **TQ5** and the assignment of the reflections by Miller indices. The intensity distributions are plotted as a function of the scattering vector s (defined as $s = 2\sin\theta/\lambda$, where 2θ is the scattering angle).

1. Wang, E.; Hou, L.; Wang, Z.; Hellström, S.; Mammo, W.; Zhang, F.; Inganäs, O.; Andersson, M. R. Org. Lett. 2010, 12, 4470.
2.Stokes, K. K.; Heuzé, K.; McCullough, R.D. Macromolecules 2003, 36, 7114.
3. Meyer, A.; Sigmund, E.; Luppertz, F.; Schnakenburg, G.; Gadaczek, I.; Bredow, T.; Jester, S-S.; Höger, S.; Beilstein. J. Org. Chem, 2010, 6, 1180.