Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Electronic Supporting Information

ESI

Oxadiazole based bipolar host materials employing planarized triarylamine donors for RGB PHOLEDs with low efficiency roll-off†

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Content

A) NMR Spectra

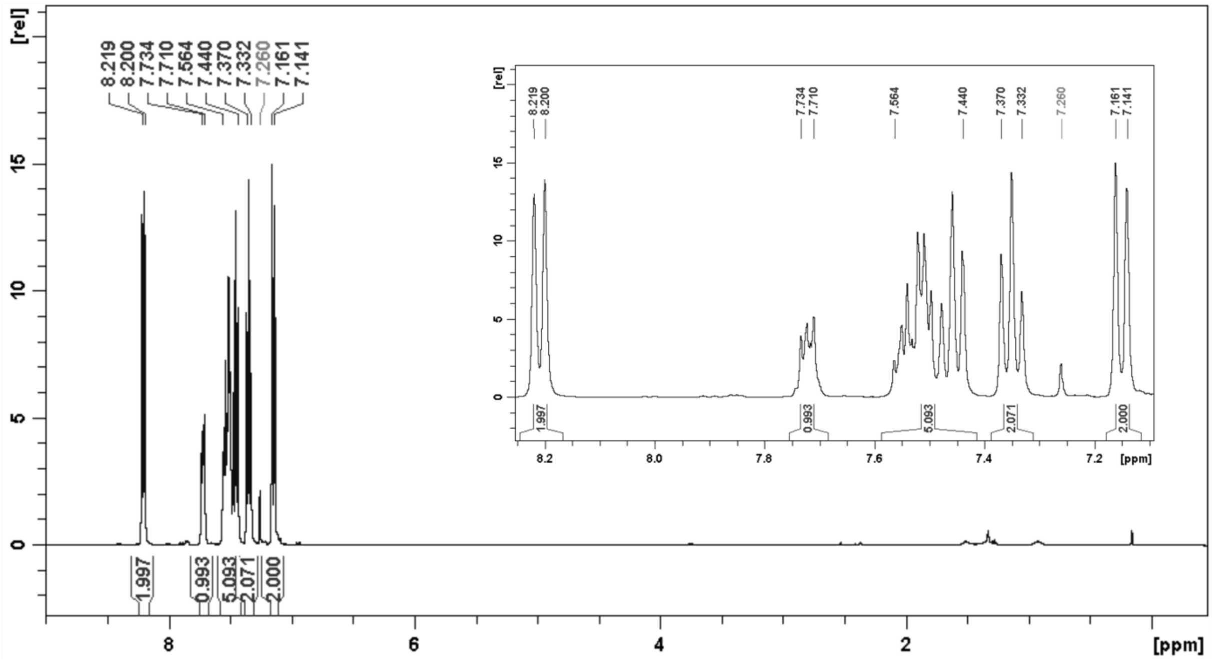


Figure S1. Proton NMR spectrum of compound **1ii**.

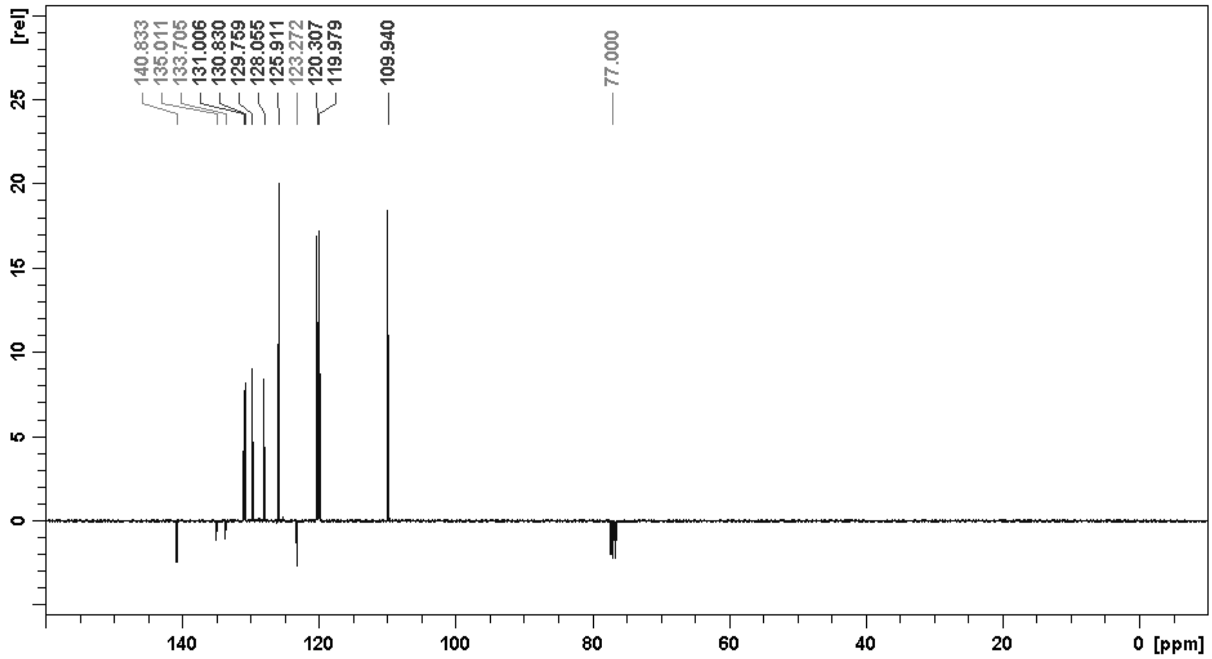


Figure S2. Carbon NMR spectrum of compound **1ii**.

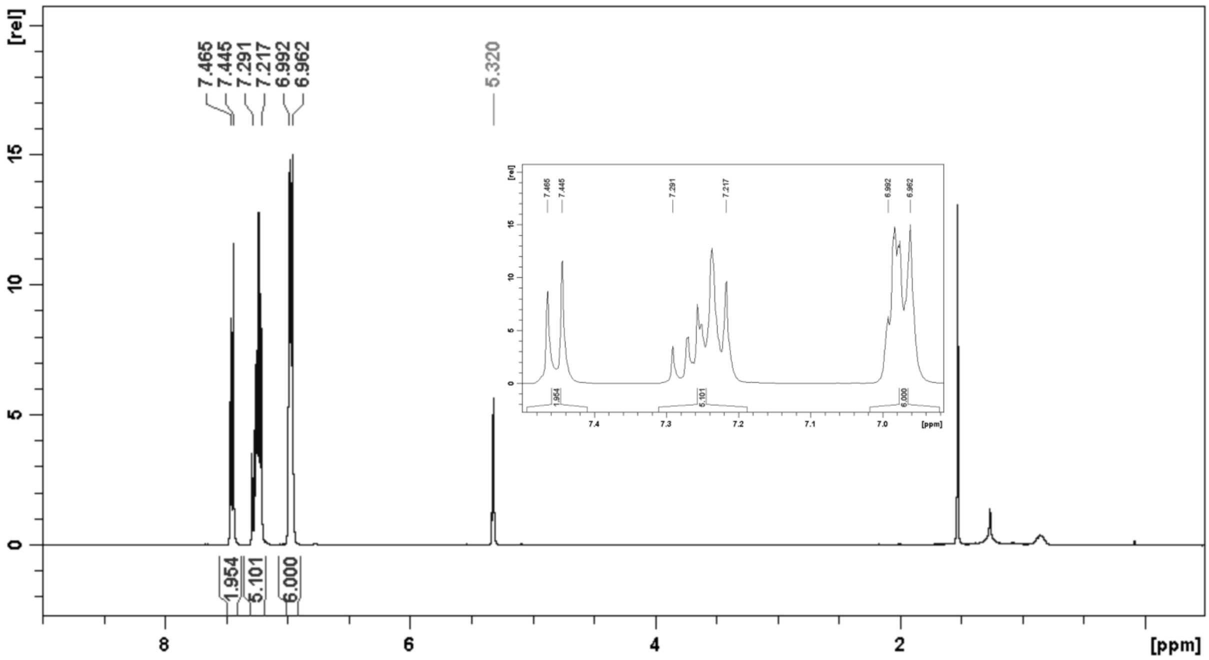


Figure S3. Proton NMR spectrum of compound **1iii**.

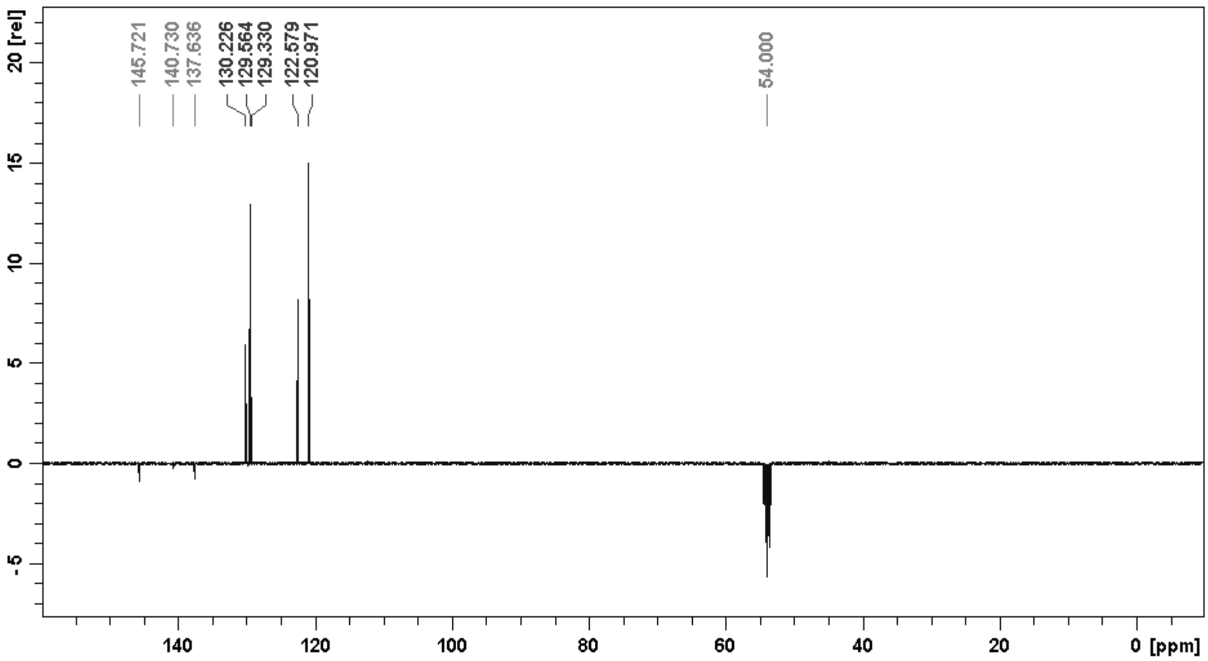


Figure S4. Carbon NMR spectrum of compound **1iii**.

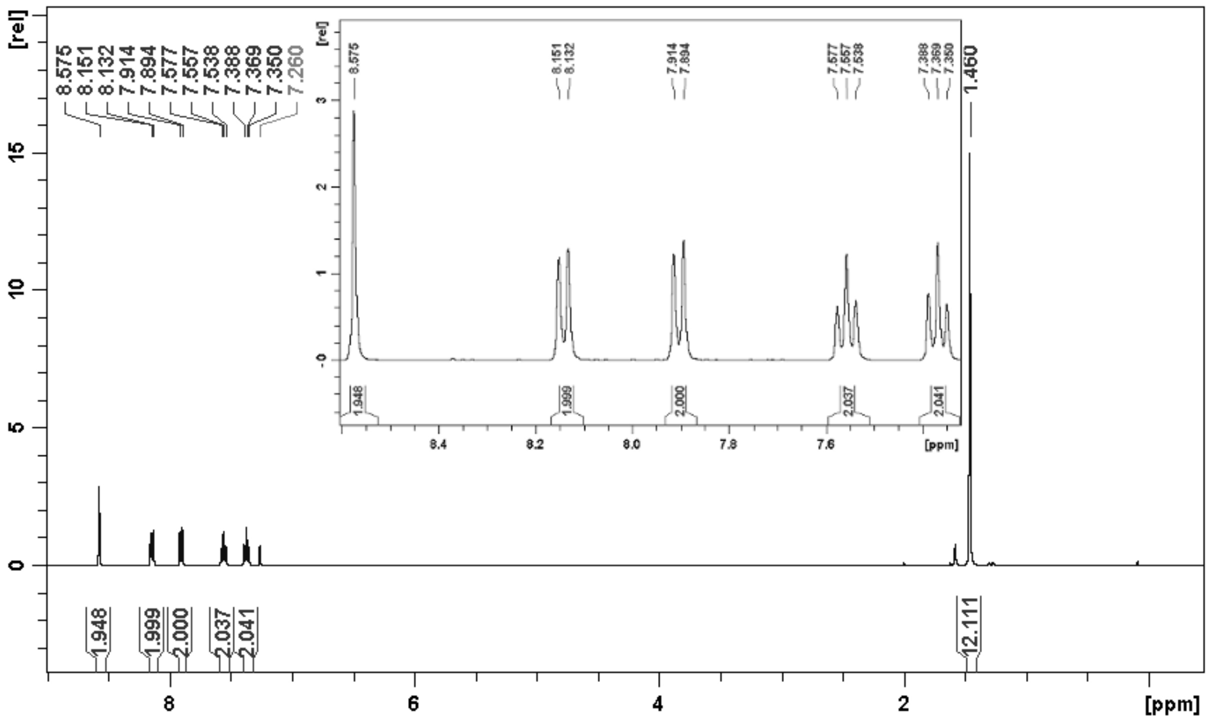


Figure S 5. Proton NMR spectrum of compound **3c**.

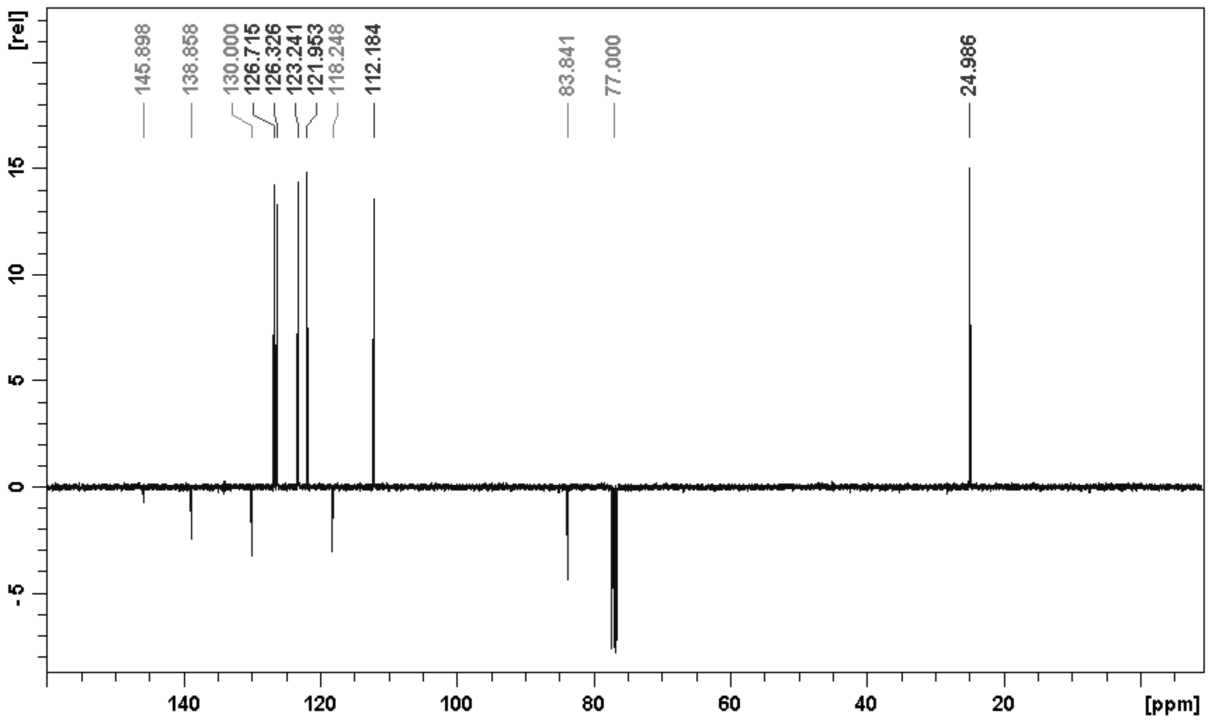


Figure S 6. Carbon NMR spectrum of compound **3c**.

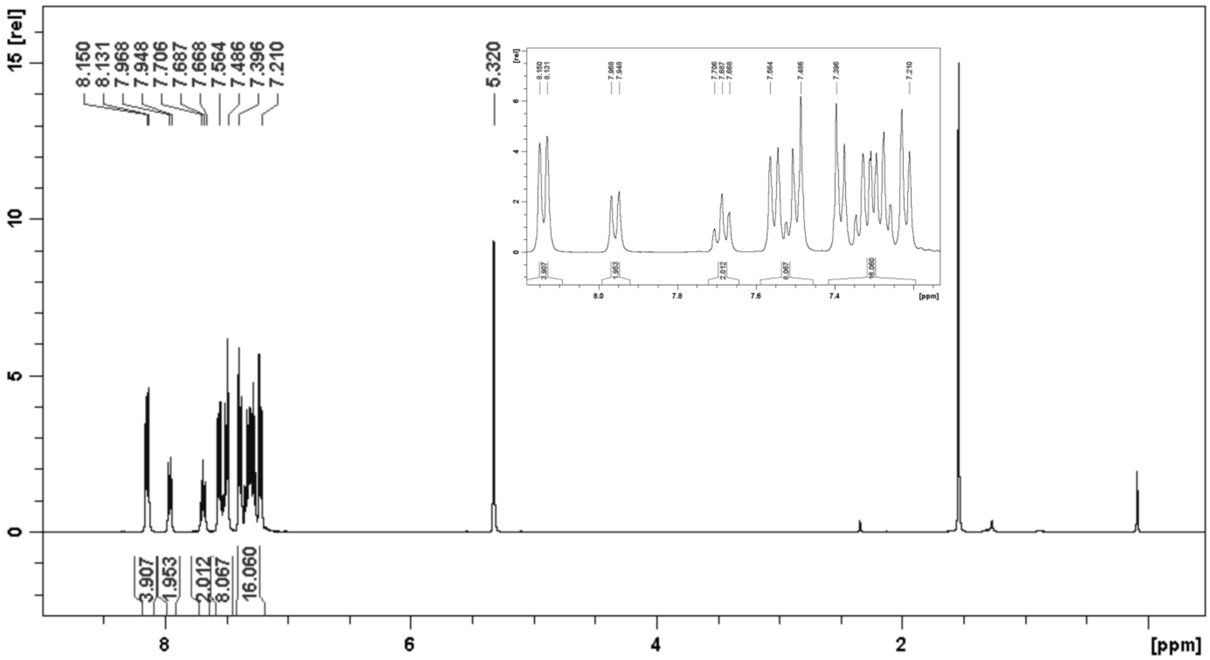


Figure S7. Proton NMR spectrum of compound o-PCzPOXD (**5b**).

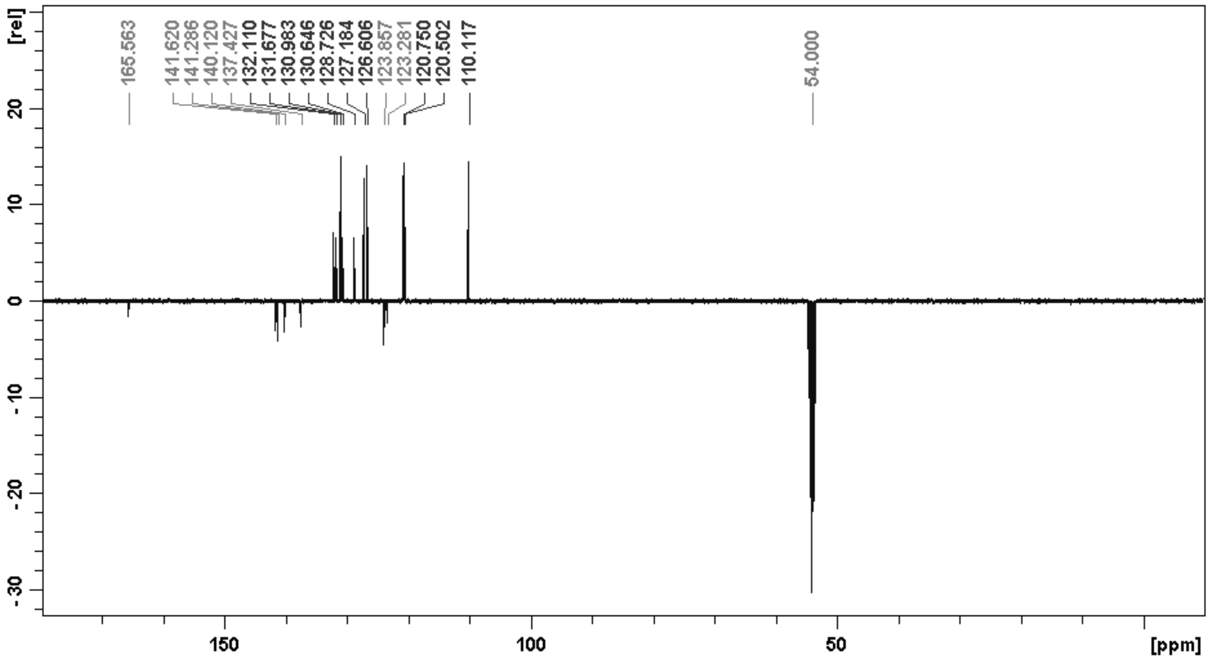


Figure S8. Carbon NMR spectrum of compound o-PCzPOXD (**5b**).

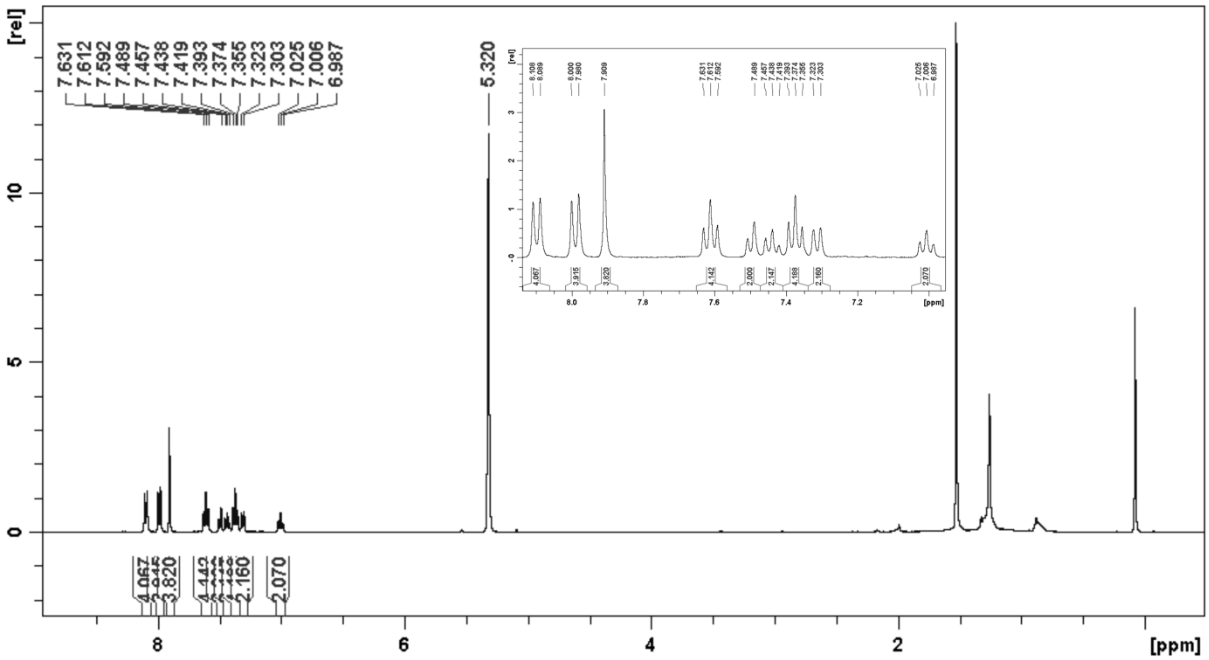


Figure S9. Proton NMR spectrum of compound o-ICzPOXD (**5c**).

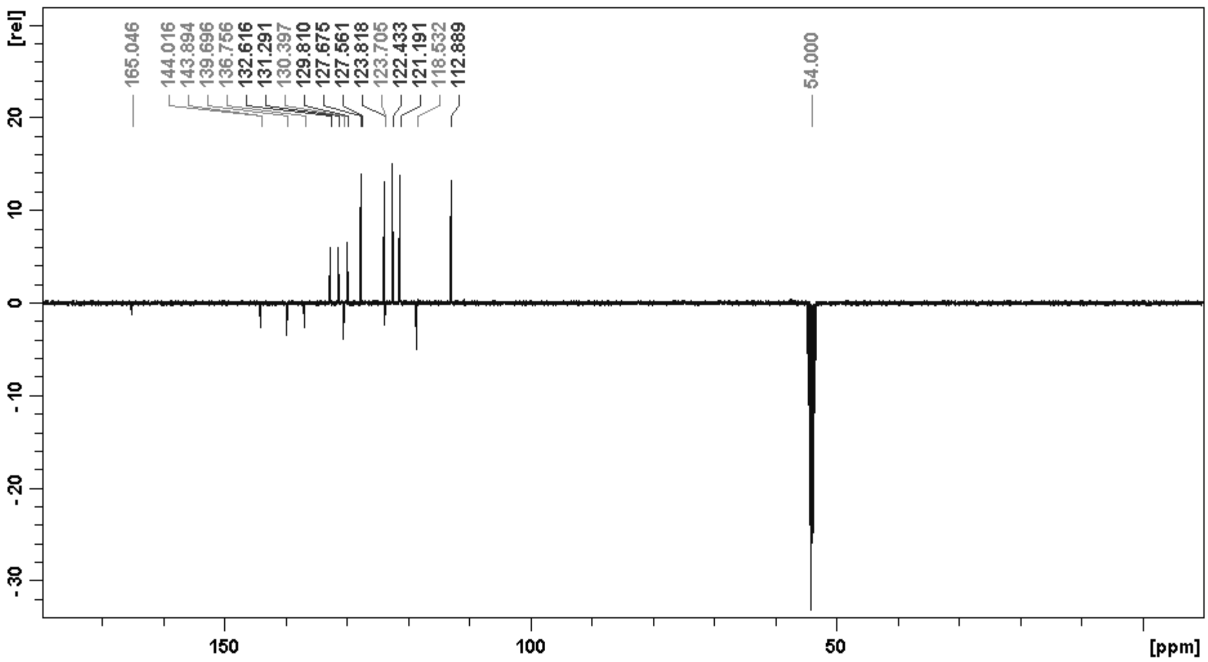


Figure S10. Carbon NMR spectrum of compound o-ICzPOXD (**5c**).

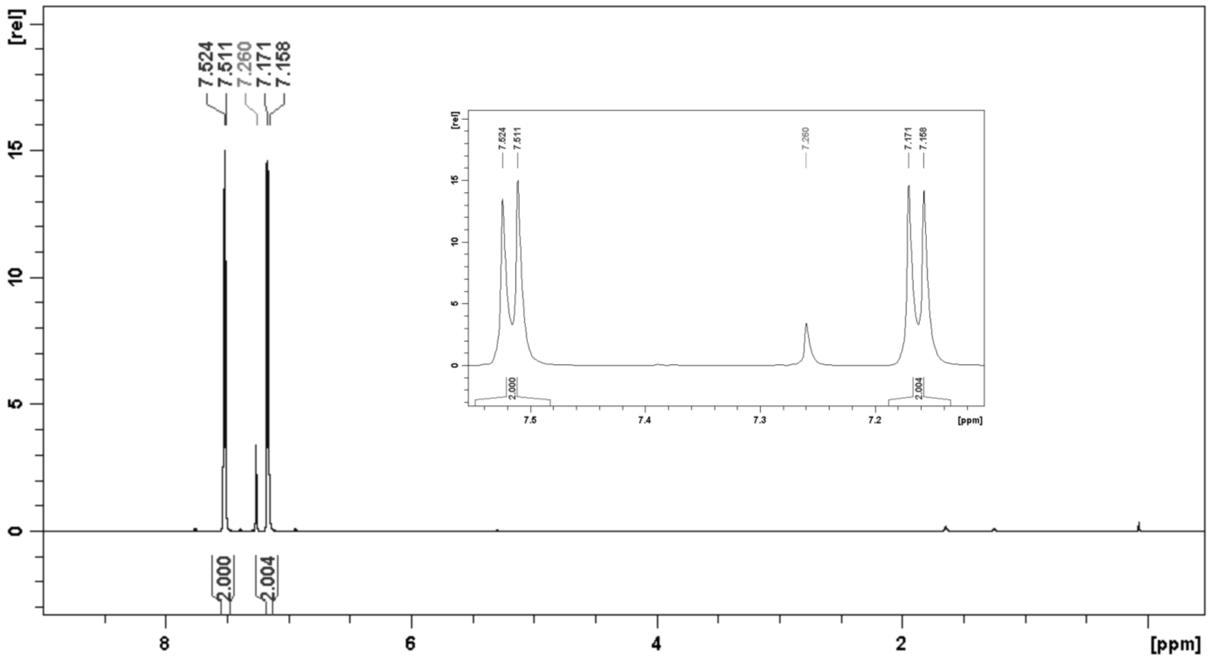
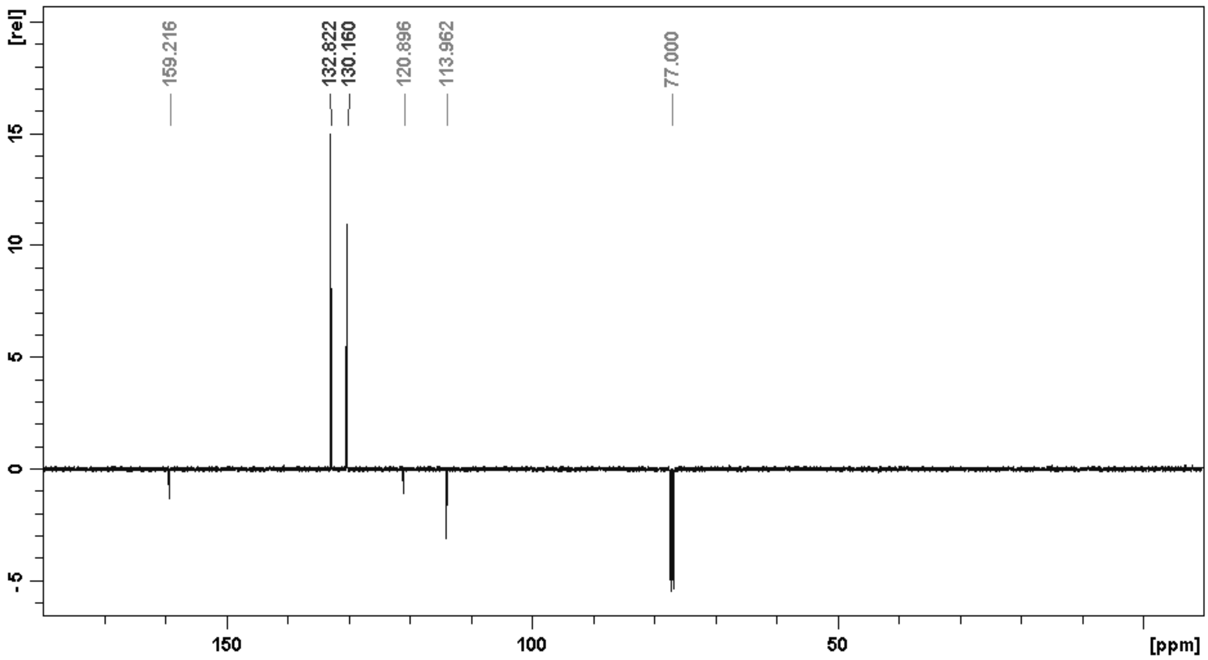


Figure S11. Proton NMR spectrum of compound **7i**.



FigureS12. Carbon NMR spectrum of compound **7i**.

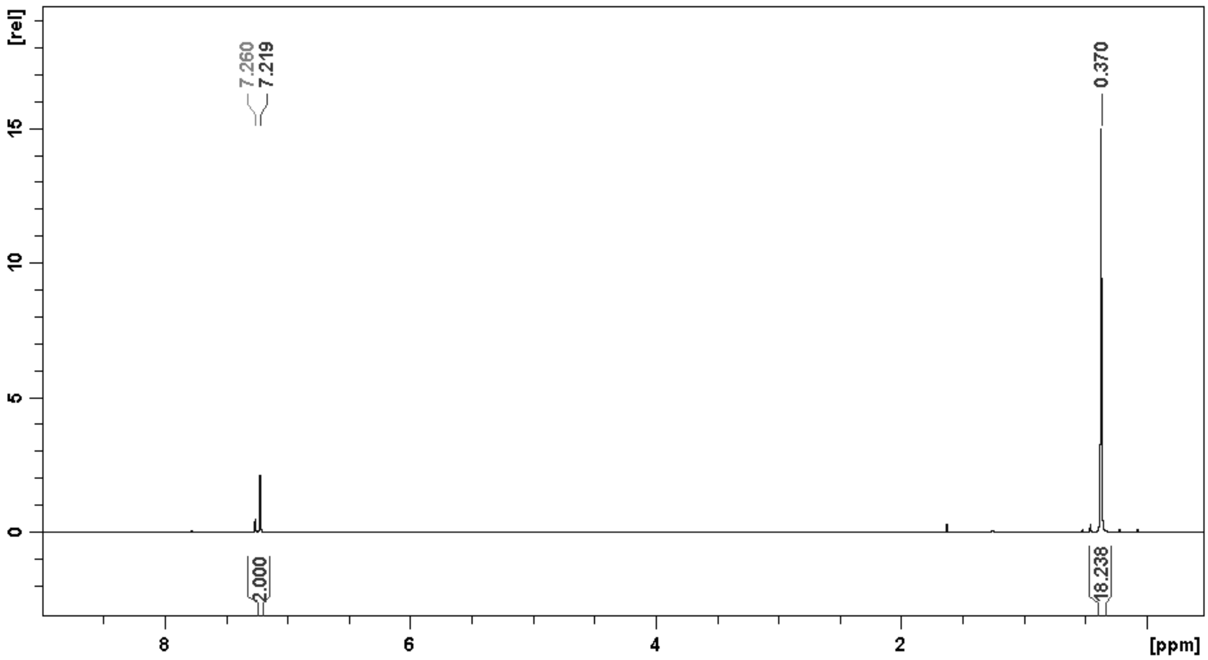


Figure S13. Proton NMR spectrum of compound **7ii**.

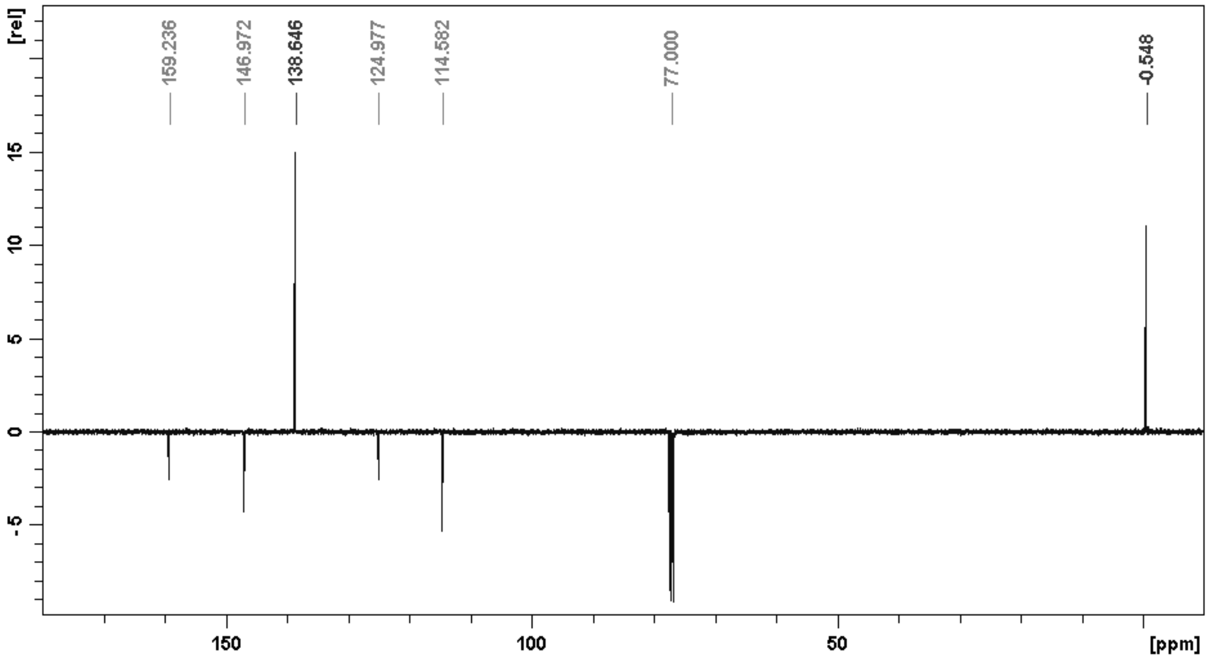


Figure S14. Carbon NMR spectrum of compound **7ii**.

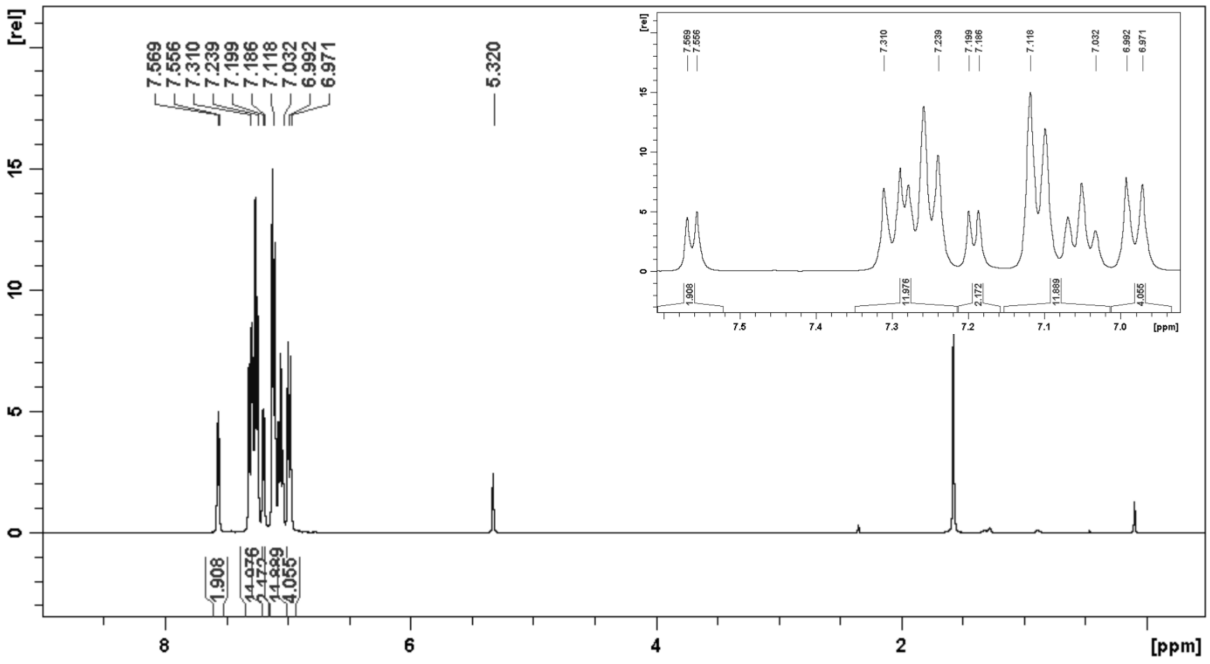


Figure S15. Proton NMR spectrum of compound o-TPATOXD (**8a**).

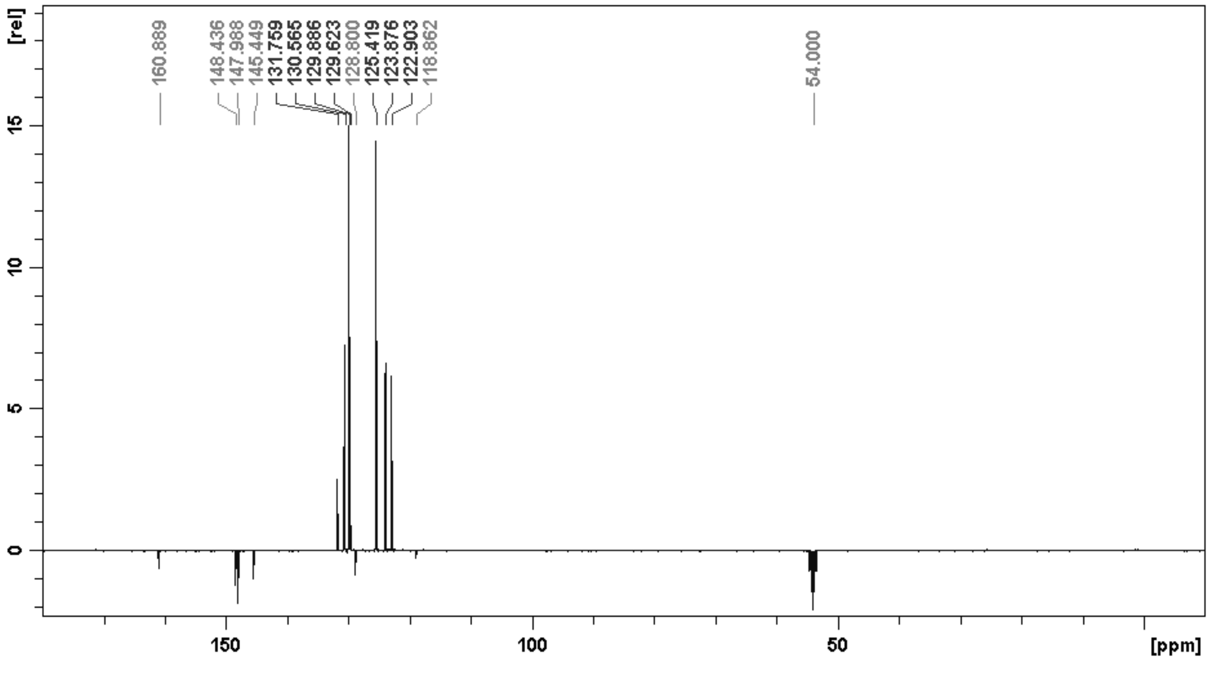


Figure S16. Carbon NMR spectrum of compound o-TPATOXD (**8a**).

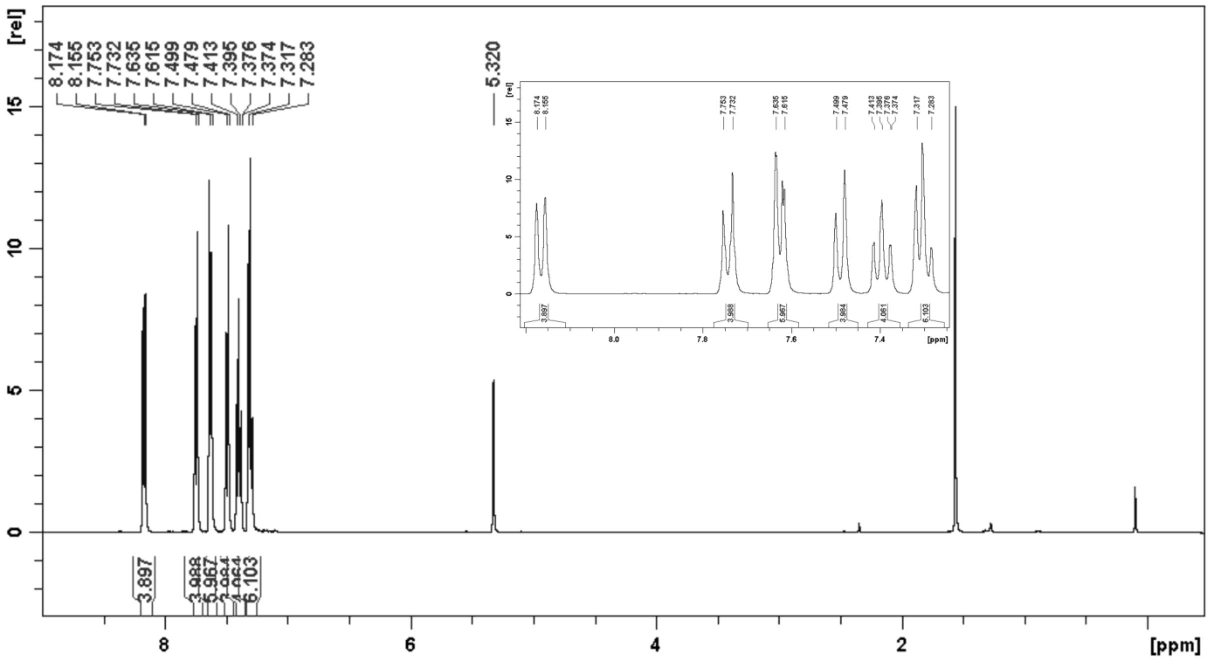


Figure S17. Proton NMR spectrum of compound o-PCzTOXD (**8b**).

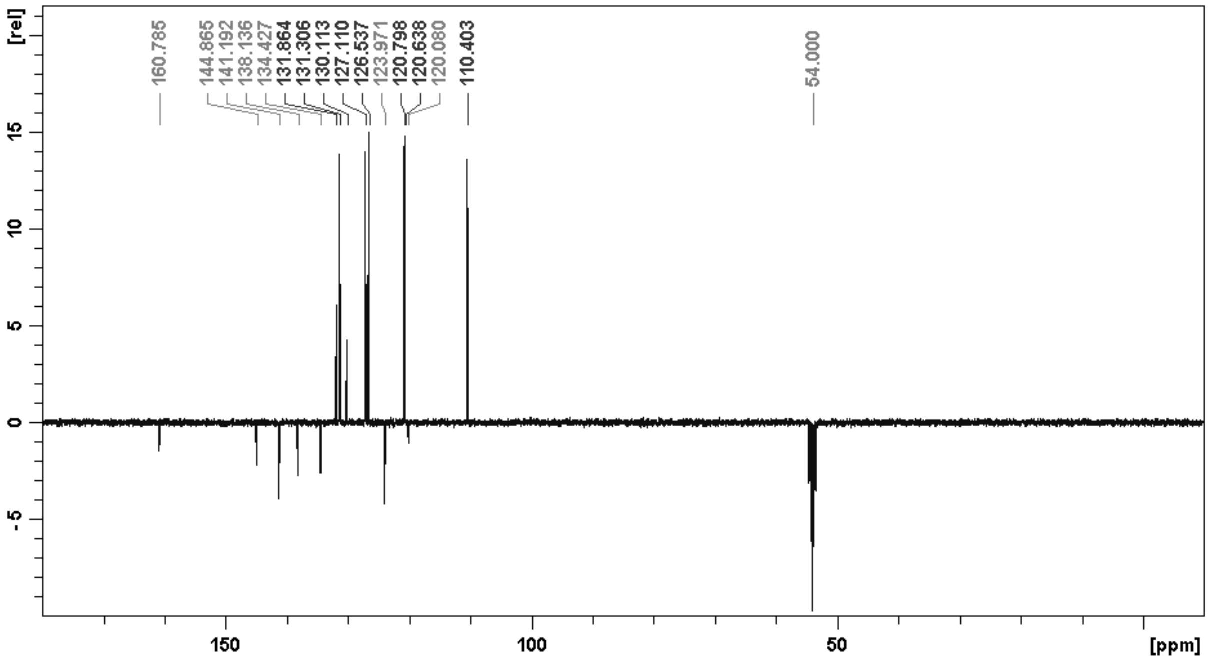


Figure S18. Carbon NMR spectrum of compound o-PCzTOXD (**8b**).

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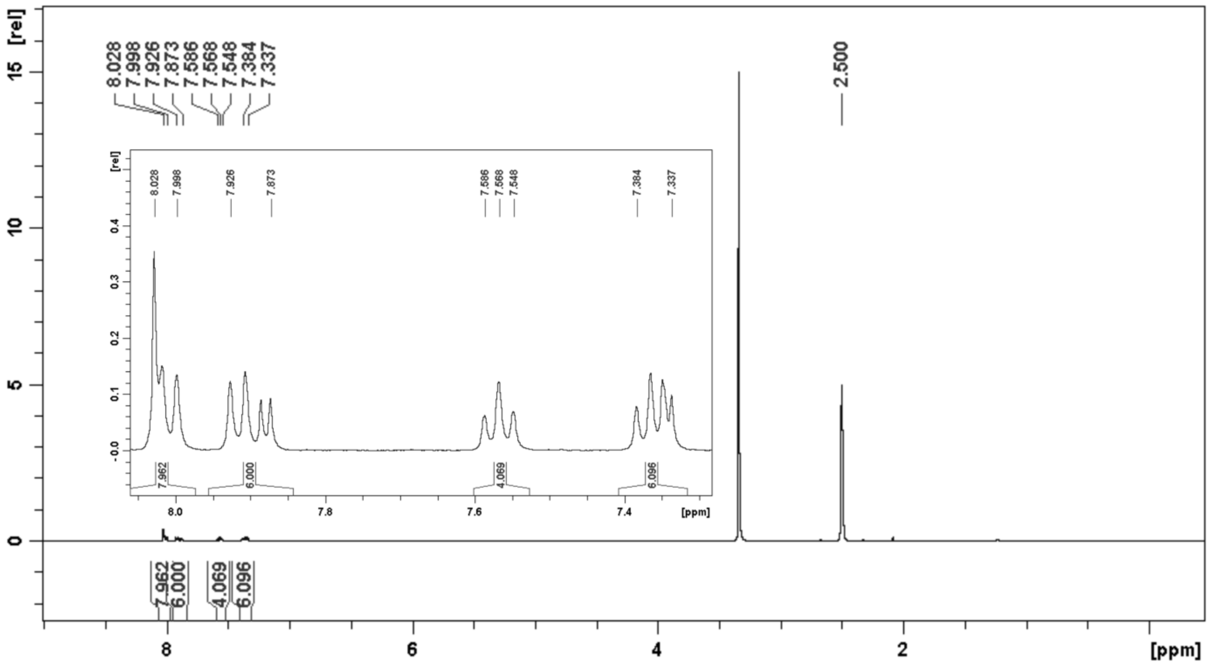

Figure S 19. Proton NMR spectrum of compound o-ICzTOXD (**8c**).

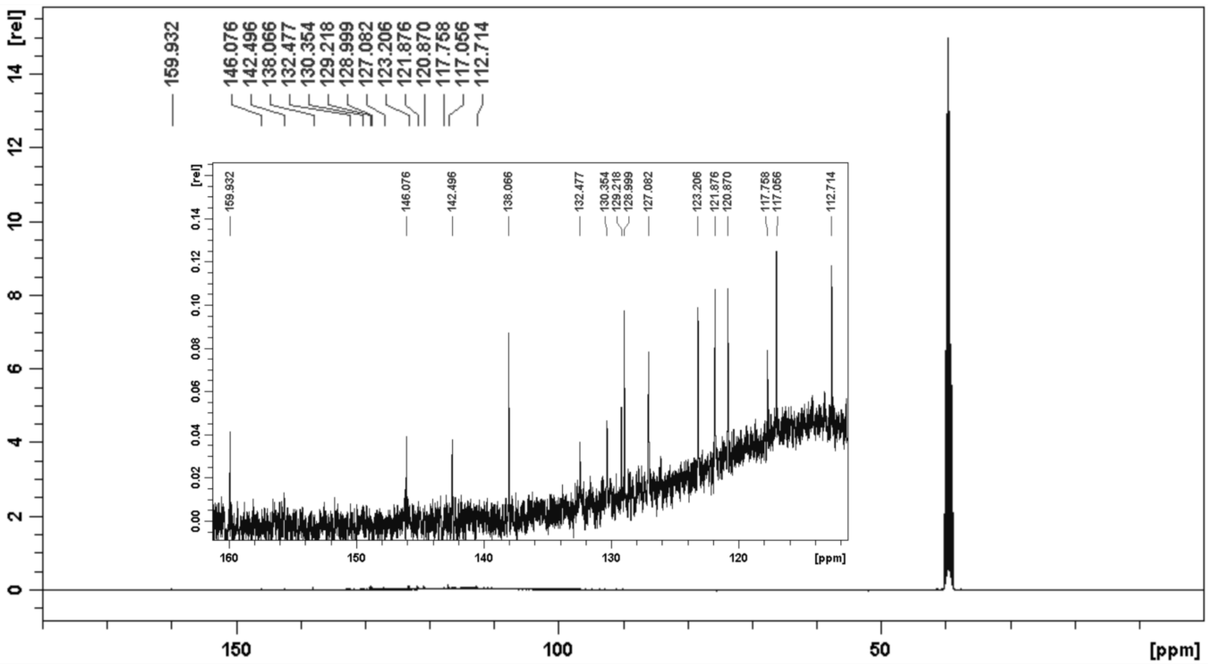

Figure S 20. Carbon NMR spectrum of compound o-ICzTOXD (**8c**).

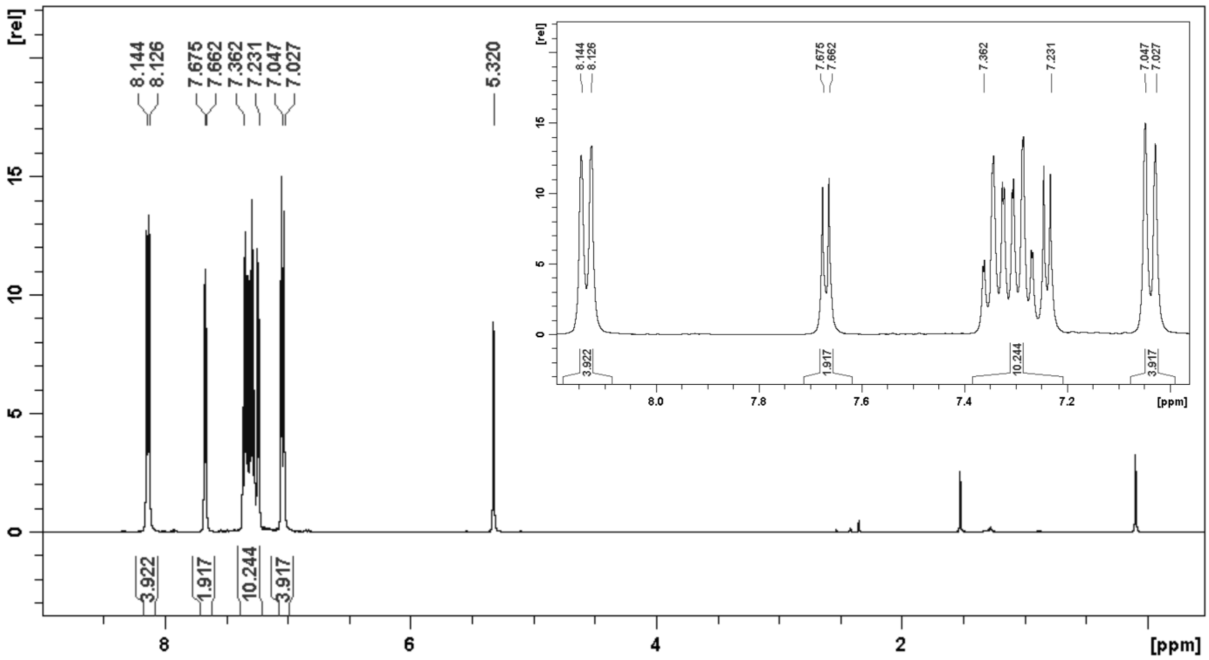

Figure S21. Proton NMR spectrum of compound o-CzTOXD (**8d**).

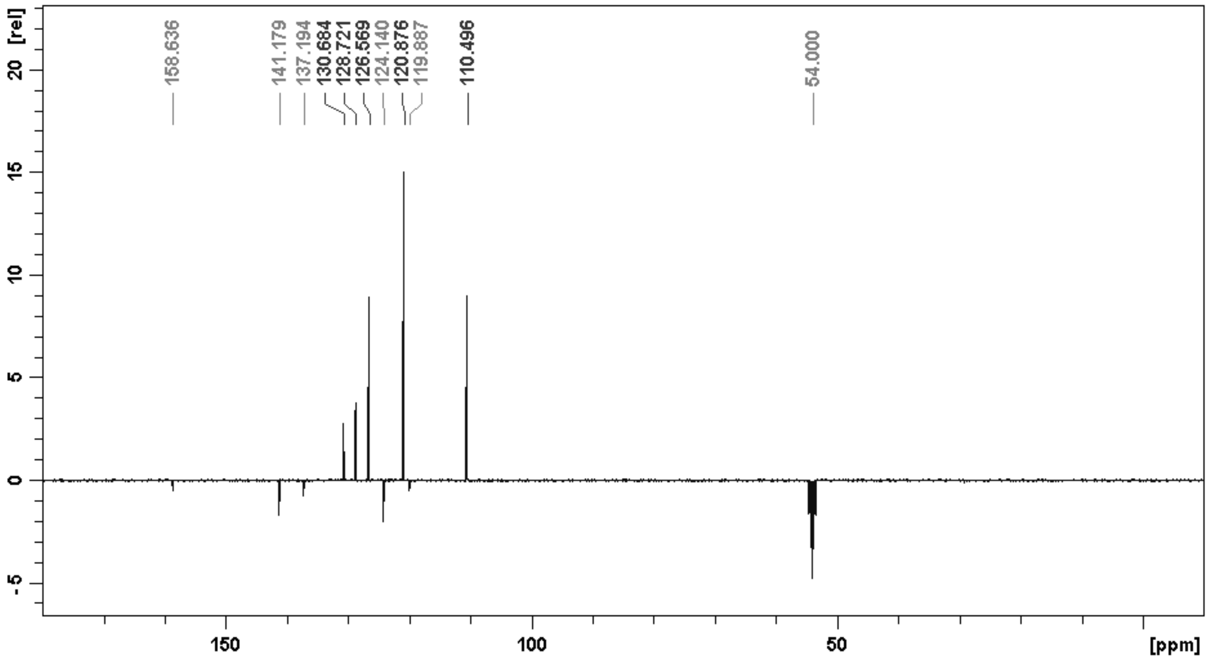

Figure S22. Carbon NMR spectrum of compound o-CzTOXD (**8d**).

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B)TGA/DSC

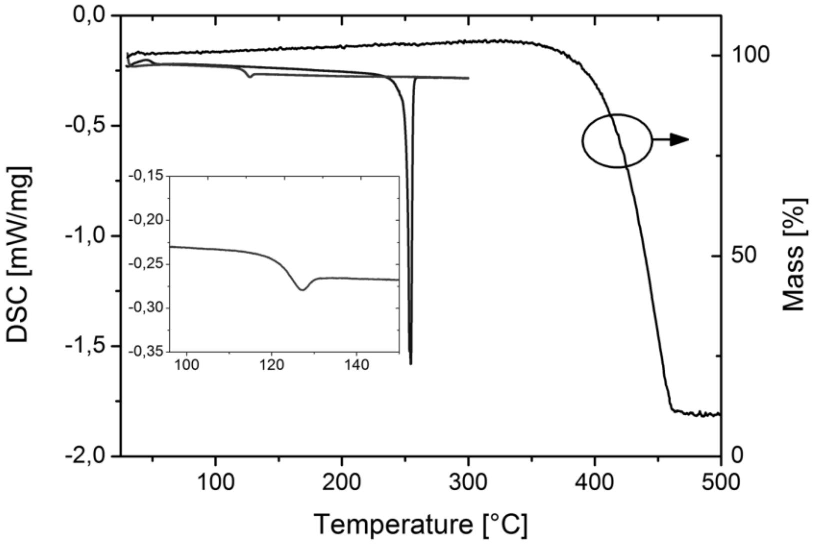

Figure S23. DSC and TG trace of o-PCzPOXD (**5b**) recorded at a heating rate of 5 °C min^{-1}.

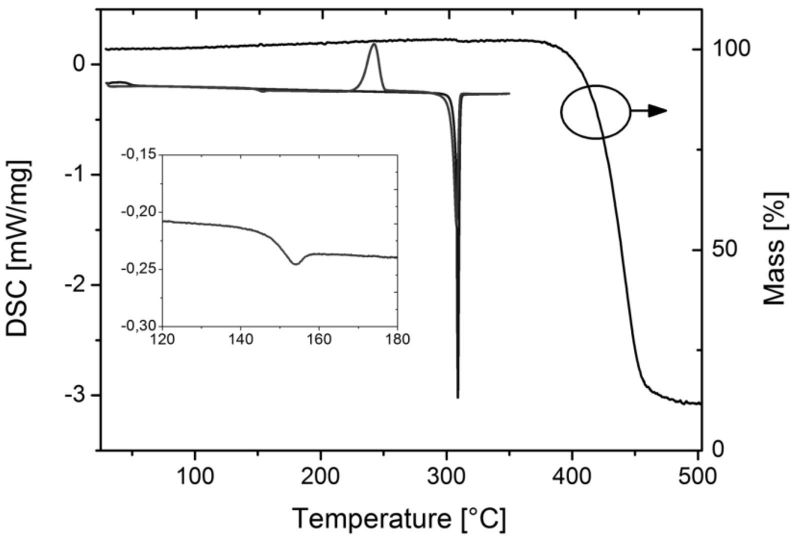

Figure S24. DSC and TG trace of o-ICzPOXD (**5c**) recorded at a heating rate of 5 °C min^{-1}.

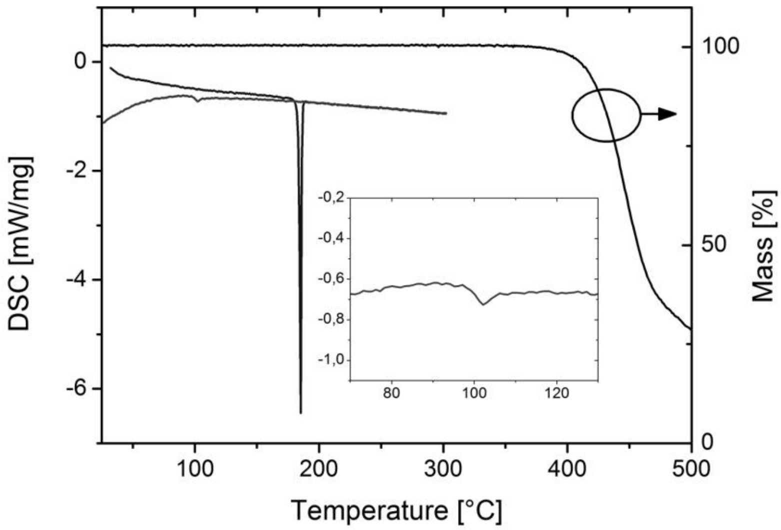

Figure S25. DSC and TG trace of o-TPATOXD (**8a**) recorded at a heating rate of 5 °C min^{-1}.

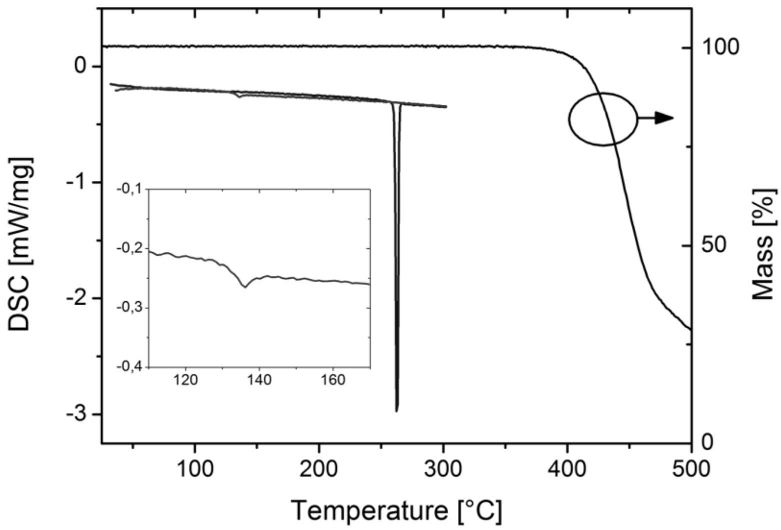

Figure S26. DSC and TG trace of o-PCzTOXD (**8b**) recorded at a heating rate of 5 °C min^{-1}.

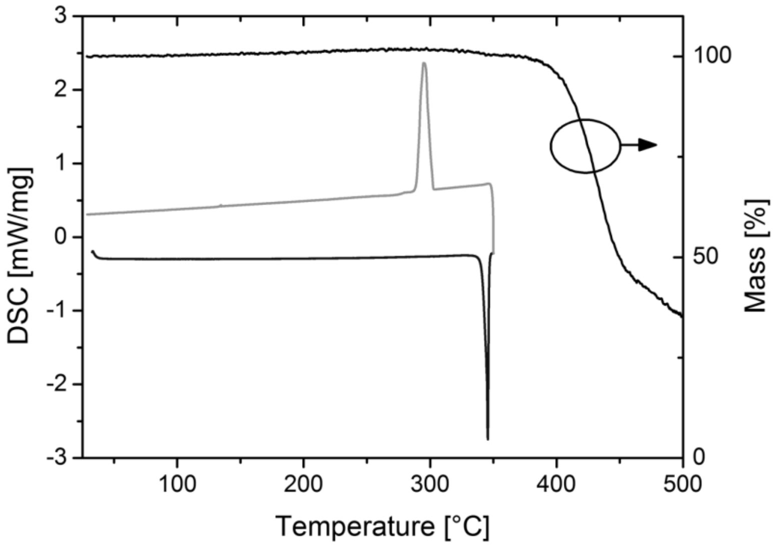

Figure S27. DSC and TG trace of o-ICzTOXD (**8c**) recorded at a heating rate of 5 °C min^{-1}.

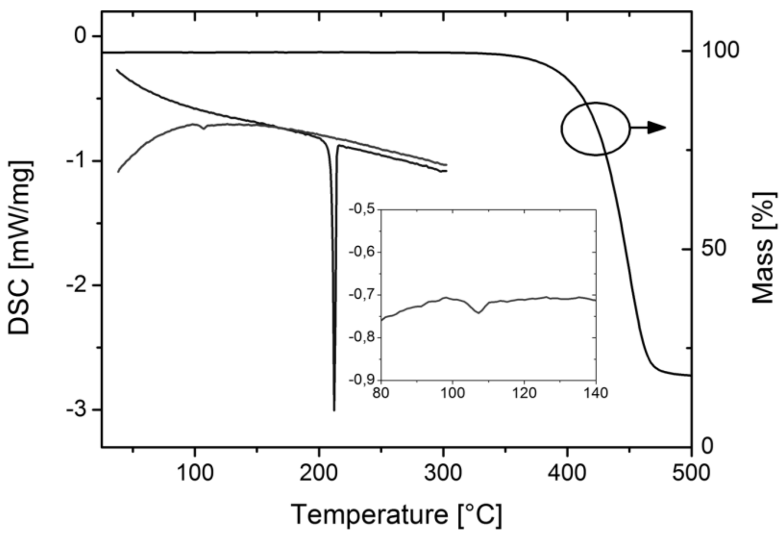

Figure S28. DSC and TG trace of o-CzTOXD (**8d**) recorded at a heating rate of 5 °C min^{-1}.

C) Cyclic Voltammetry

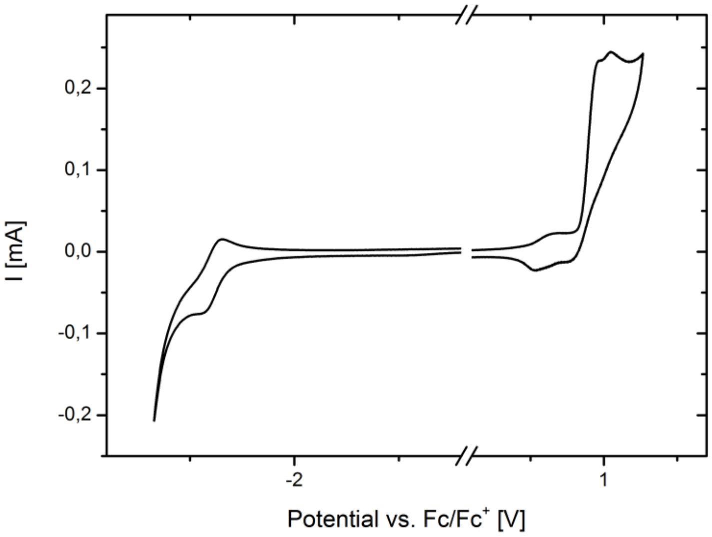

Figure S29. Cyclic voltammogram of o-PCzPOXD (**5b**).

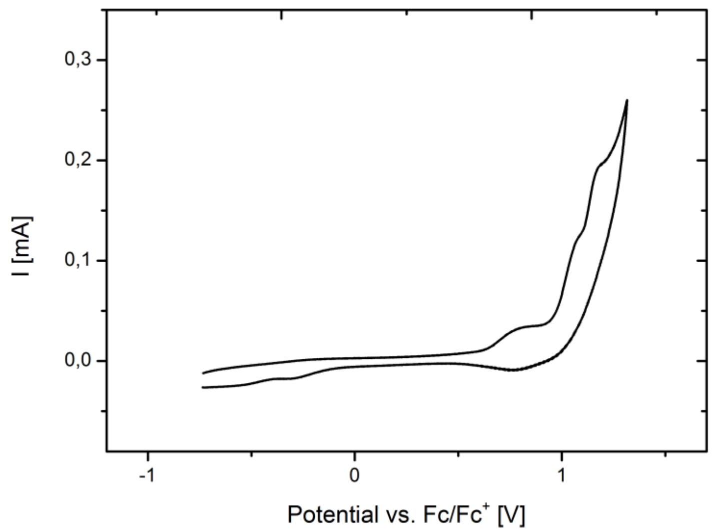

Figure S30. Cyclic voltammogram of o-ICzPOXD (**5c**).

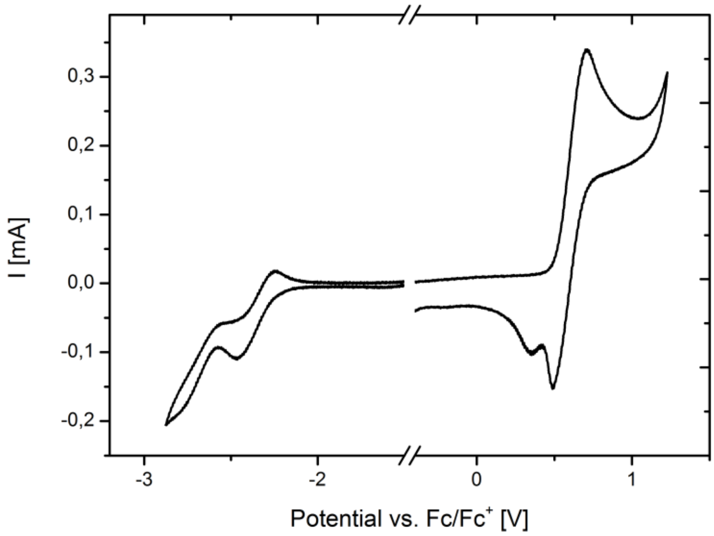

Figure S31. Cyclic voltammogram of o-TPATOXD (**8a**).

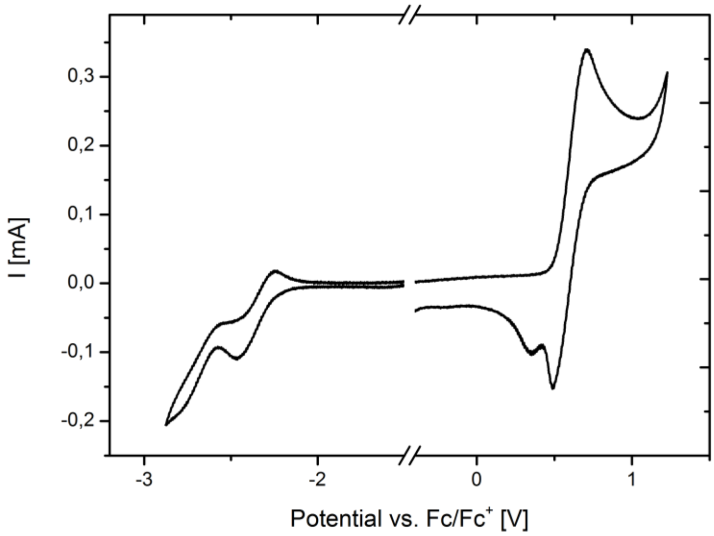

Figure S32. Cyclic voltammogram of o-PCzTOXD (**8b**).

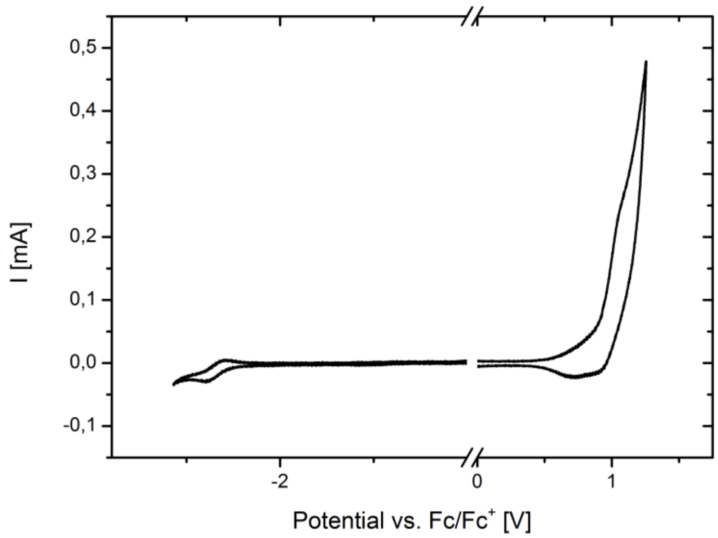

Figure S33. Cyclic voltammogram of o-ICzTOXD (**8c**).

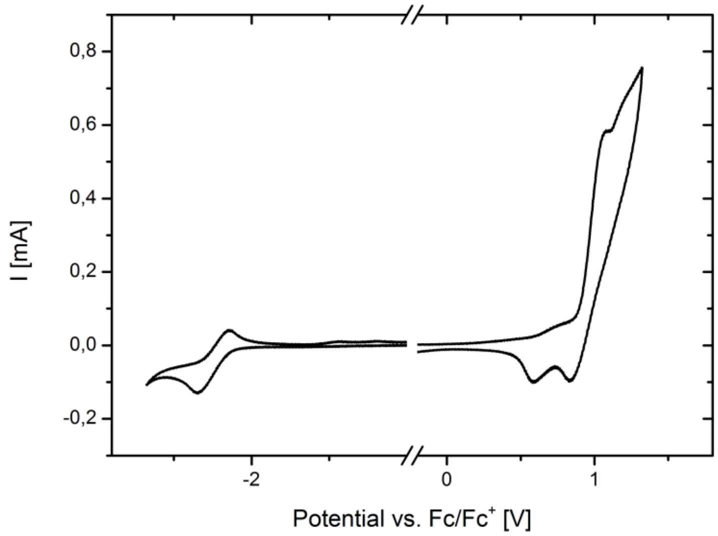

Figure S34. Cyclic voltammogram of o-CzTOXD (**8d**).

D)Phosphorescence Measurements

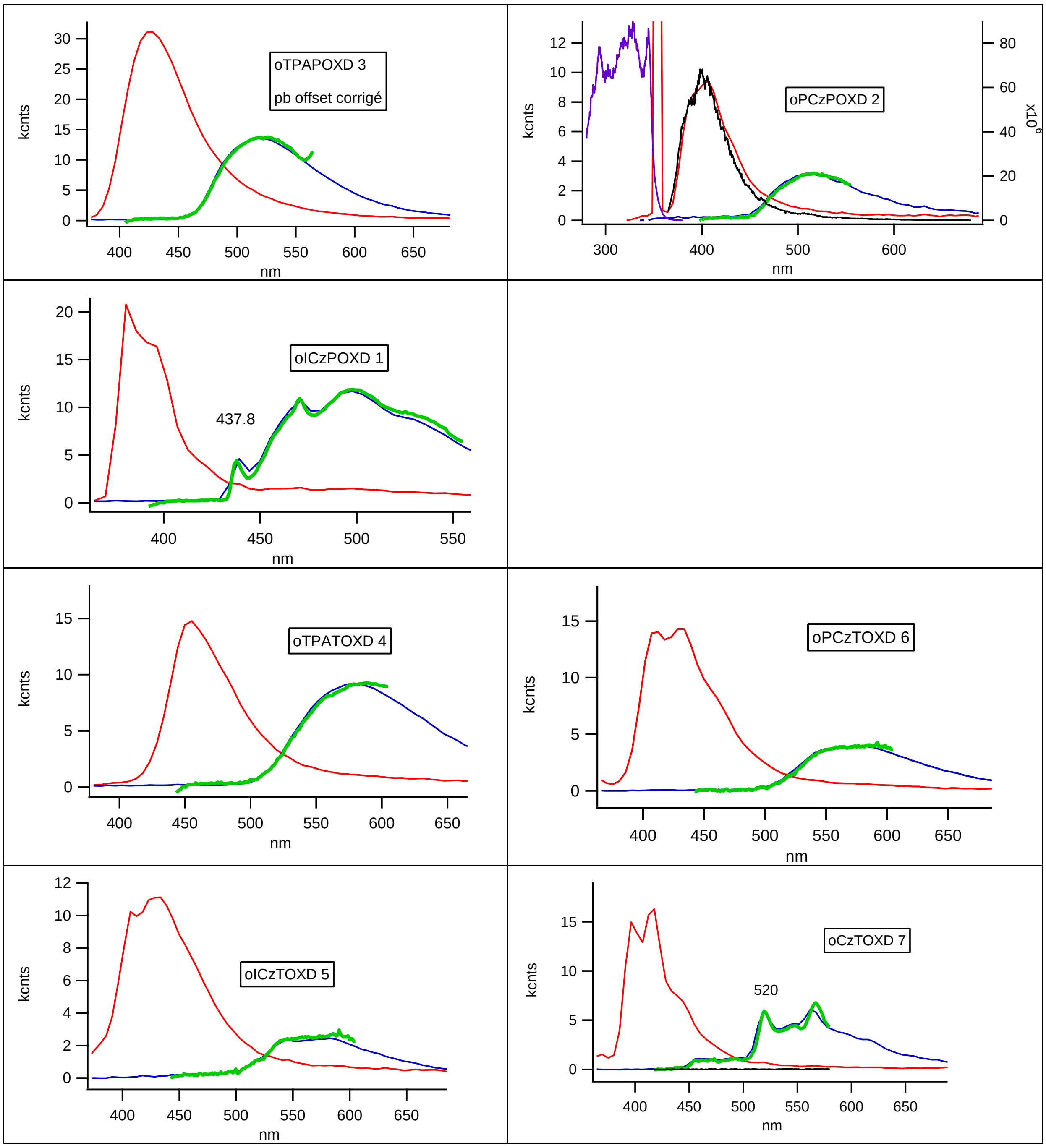

Figure S35. Singlet (red) and triplet (blue) emission spectra at 77 K with two different gratings to obtain higher resolution for the triplet emission (green).

Lifetime Measurements

The singlet and triplet lifetimes of target materials are summarized in Table S2. Some samples present single exponential decay, others a more complex behavior; results are derived from single and double exponential fits of the data. Note that the errors for the double exponential fits are significant.

Table S2. Singlet and triplet lifetimes measured in toluene solutions at ambient temperature.

Sample	**Singlet Lifetime**		**Triplet Lifetime**
	τ_1 [ns]	**τ_2 [ns]**	**τ [ms]**
o-TPAPOXD	3.25(0.003)		~790
o-PCzPOXD	0.90(0.04)	2.0(45)	335(6)
o-ICzPOXD	0.66(0.017)	64.7(12)	349(2)
o-TPATOXD	1.57(0.002)		12.3
o-PCzTOXD	0.84(0.004)		8.3
o-ICzTOXD	0.53(0.009)		8.2
o-CzTOXD	1.28(0.004)	2.02(0.17)	11.0

Experimental Parameter

The determination of the emission lifetime at room temperature was done with Dr. François-Alexandre Mianney using a picosecond 375 nm laser source in conjunction with a detection set-up as described in (Muller, P. A., Högemann, C., Allonas, X., Jacques, P., Vauthey, E., Chem. Phys. Letters 326 (2000) 321.) Low temperature experiments were performed in frozen dilute toluene solutions using a Janis closed cycle cryostat (at 5 K) and a liquid nitrogen dewar fitted with quartz windows for measurements at ~80 K.

Time resolved experiments were obtained using a Quantel Brilliant tripled Nd-YAG laser (355 nm, 20 Hz repetition rate, pulse width ~5ns). Spectra were measured using a SPEX 270 monochromator equipped with both photomultiplier and CCD. This set-up is controlled using a home-built Labview-based program which allows using different instruments such as photon counting, oscilloscope, and additional mechanical shutters.

Additional absorption measurements were performed with a Cary 5000 instrument at room temperature, as well as emission and excitation spectra at room temperature and liquid nitrogen temperature using a Fluorolog FL3-22 instrument.

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E) DFT Calculations

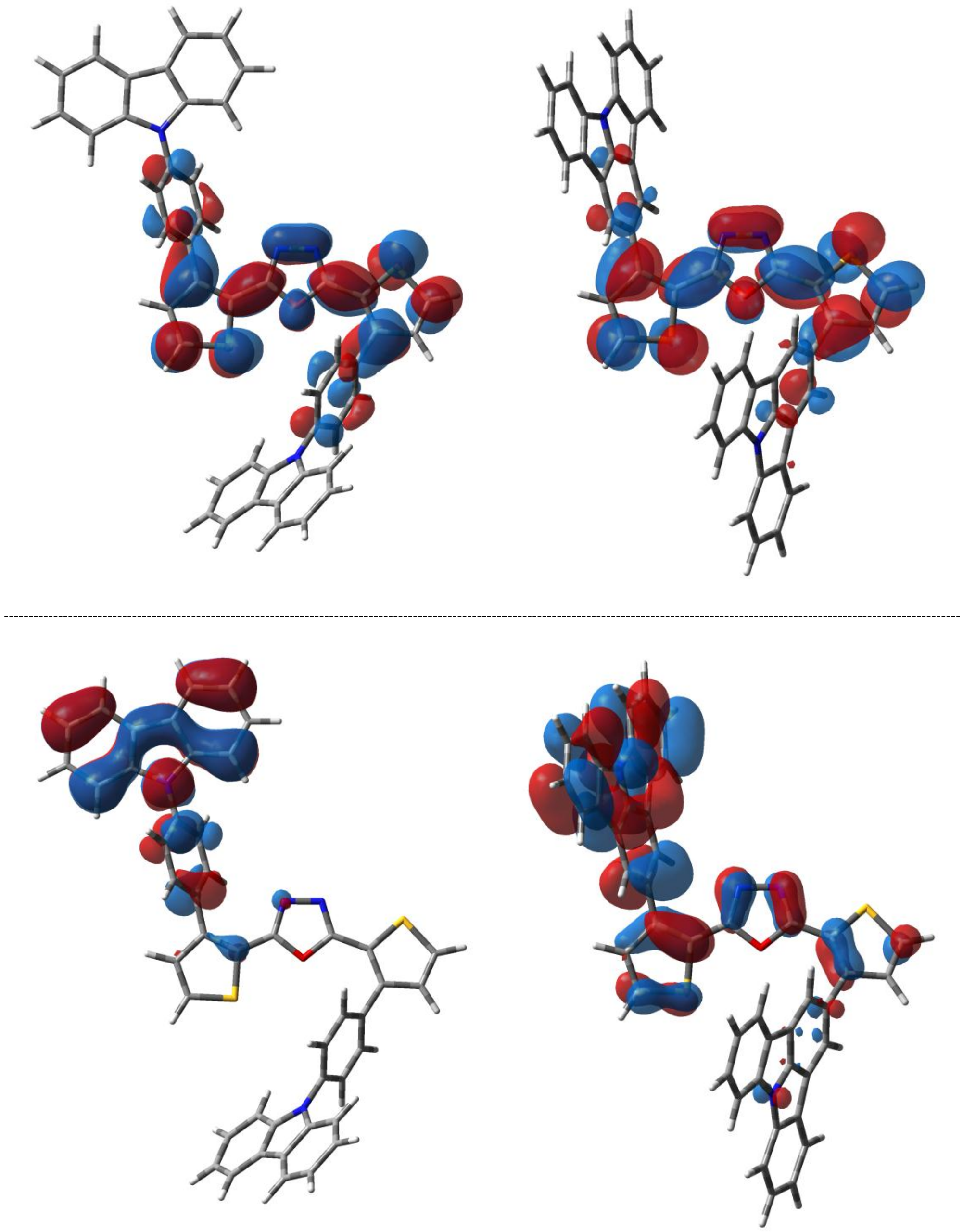


Figure S36. HOMO (bottom) and LUMO (top)
of **o-PCzTOXD** (left) and **o-ICzTOXD** (right).

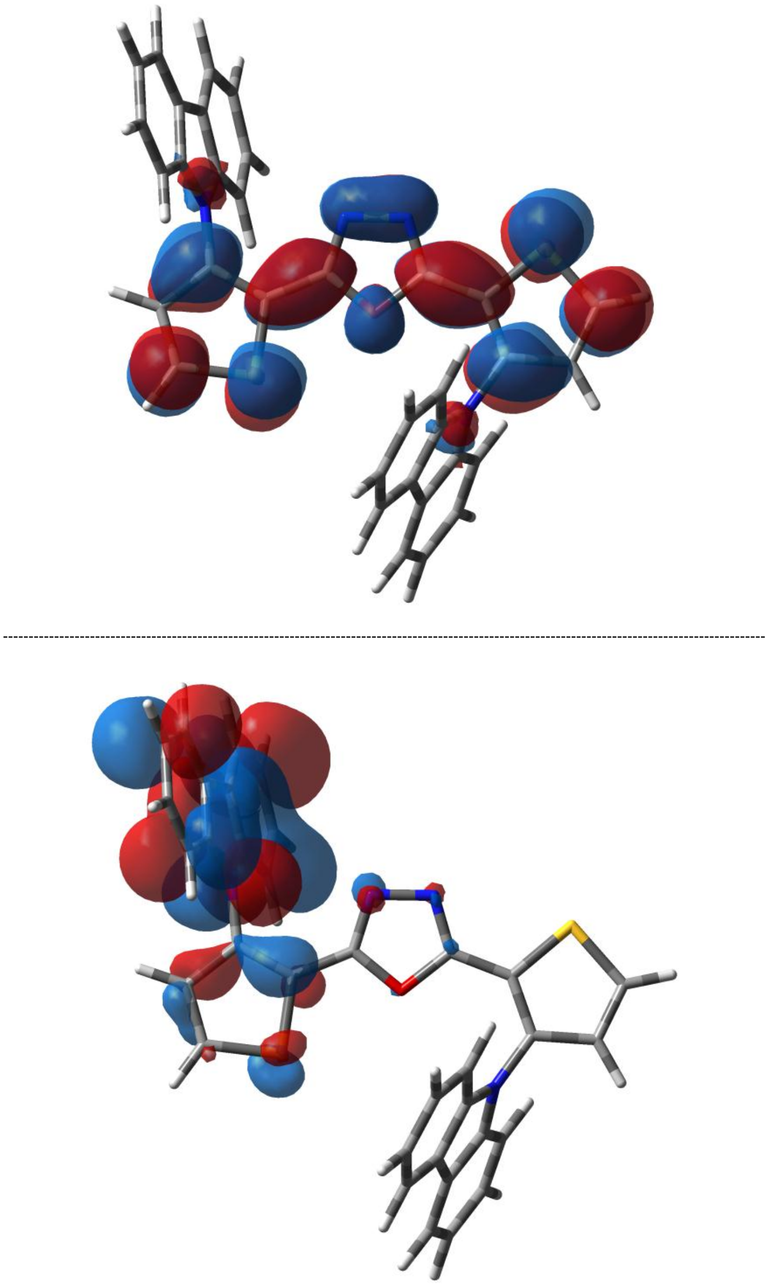
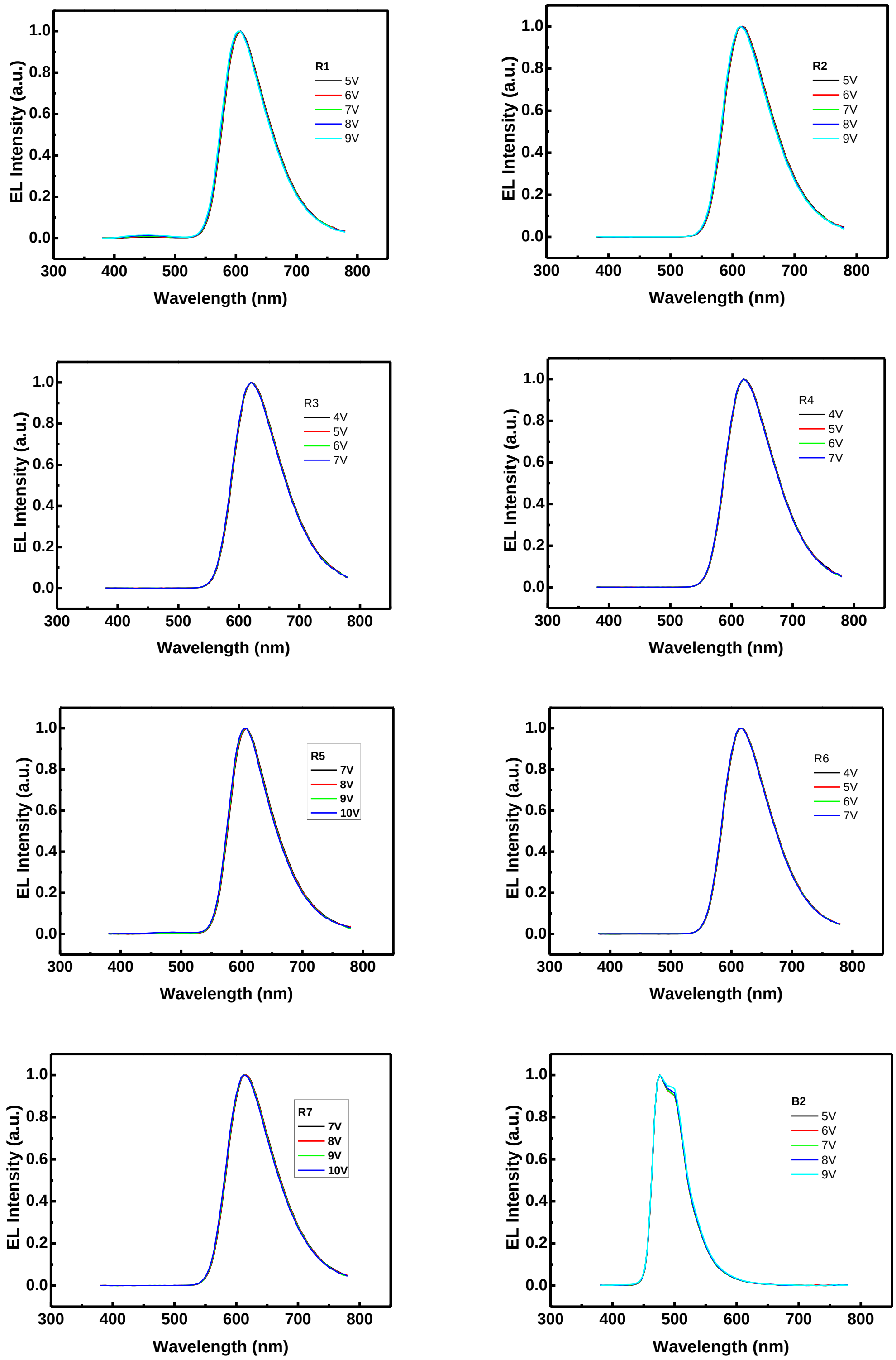


Figure S367. HOMO (bottom) and LUMO (top) of **o-CzTOXD**

F) EL Spectra


EL Intensity (a.u.)
Wavelength (nm)
R1
5V
6V
7V
8V
9V
R2
5V
6V
7V
8V
9V
R3
4V
5V
6V
7V
R4
4V
5V
6V
7V
R5
7V
8V
9V
10V
R6
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6V
7V
8V
9V

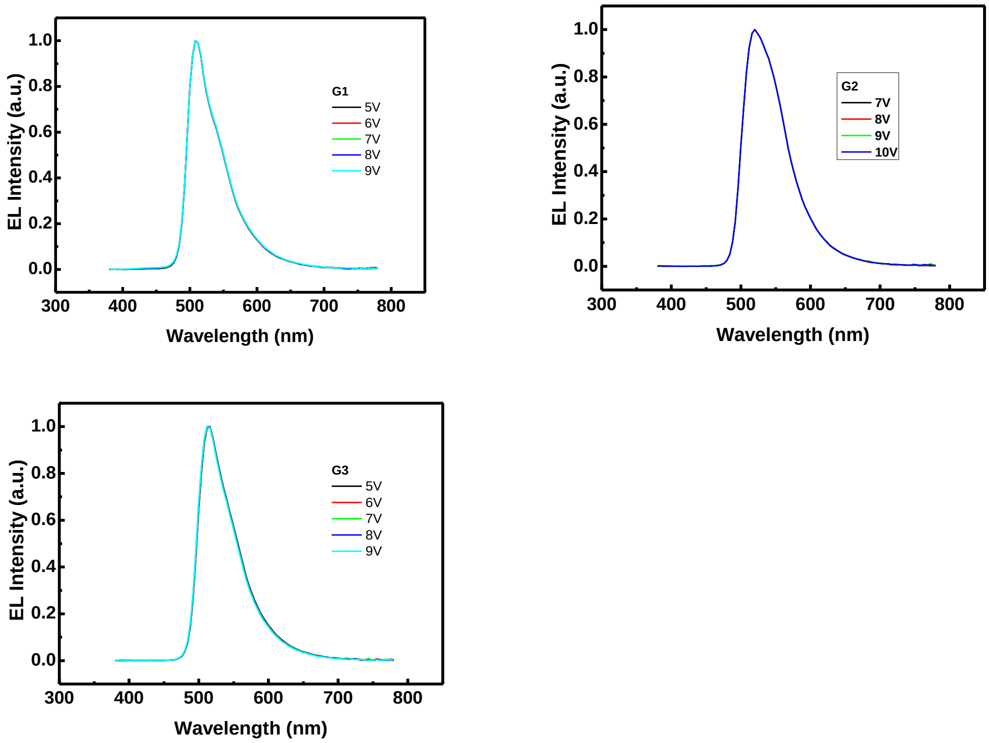

Figure S38. Electroluminescence (EL) spectra of all devices discussed in this study.

G)Crystal Structure of Compound 3c

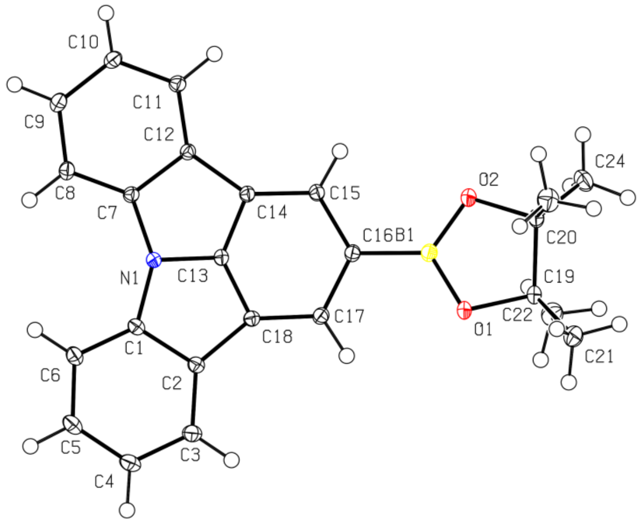

Figure S39. Molecular structure of **3c**; B, C, N, and O atoms are represented by yellow, white, blue and red ellipsoids drawn at 50% probability levels, H atoms by spheres of arbitrary radius.