Electronic Supporting Information for:

A comparison of optical, electrochemical and self-assembling properties of two structural isomers based on 1,6- and 1,8-pyrenedione chromophores

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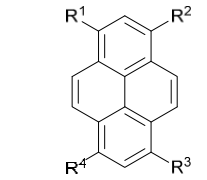
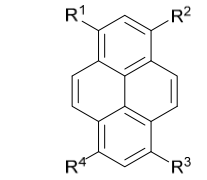
Figure 1. ^{1}H and ^{13}C NMR of 3

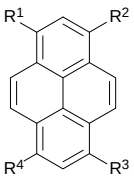


3 $R^{1,3}$ = OTIPS; $R^{2,4}$ = H

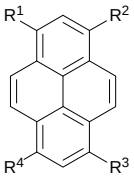


3 $R^{1,3}$ = OTIPS; $R^{2,4}$ = H

Figure 2. ^{1}H and ^{13}C NMR of 4

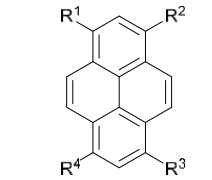


4 $R^{1,4}$ = OTIPS; $R^{2,3}$ = H

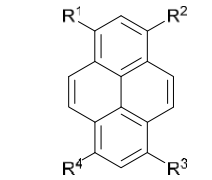


4 $R^{1,4}$ = OTIPS; $R^{2,3}$ = H

Figure 3. ^{1}H and ^{13}C NMR of 5



5 $R^{1,3}$ = OTIPS; $R^{2,4}$ = Br



5 $R^{1,3}$ = OTIPS; $R^{2,4}$ = Br

Figure 4. ^{1}H and ^{13}C NMR of 6

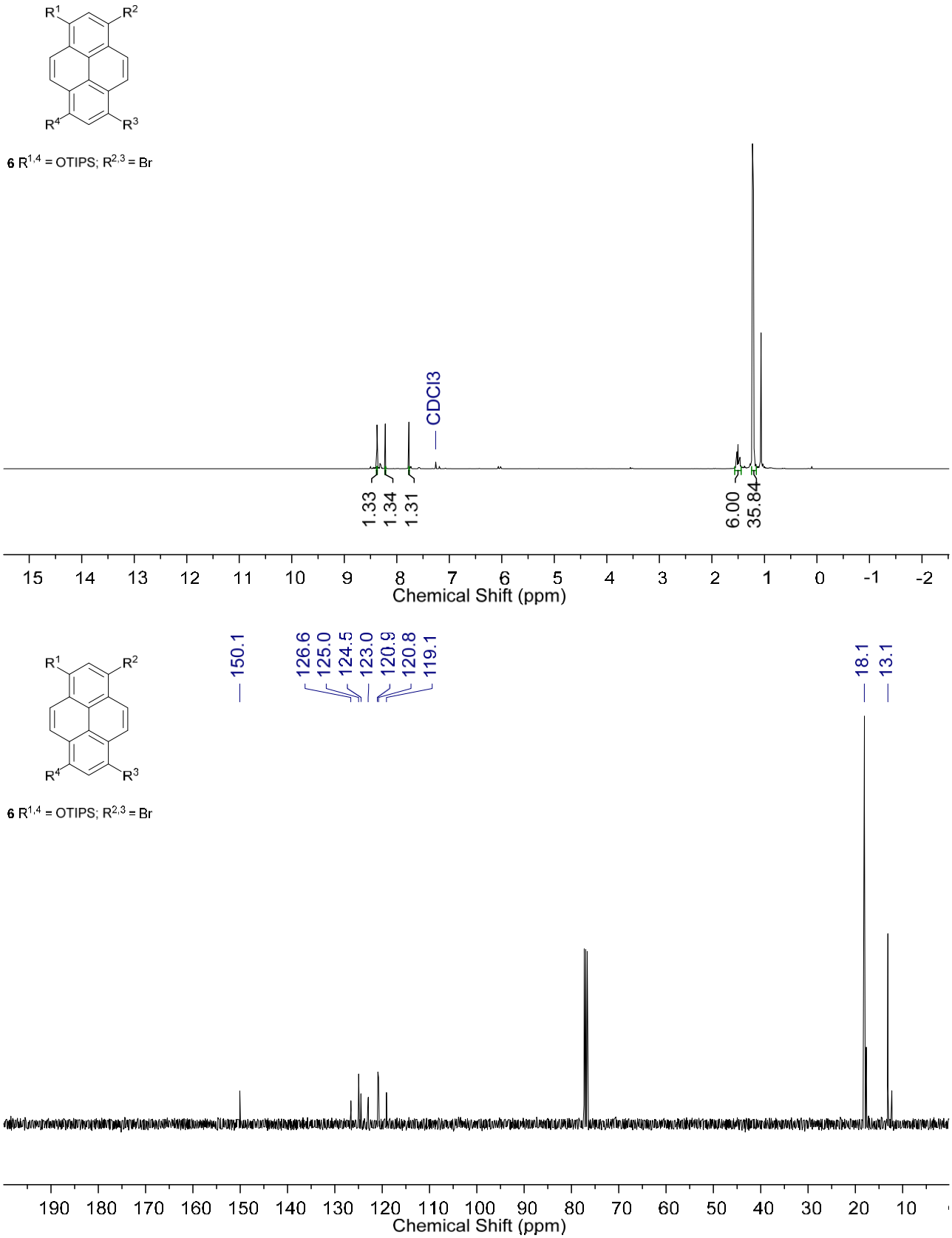
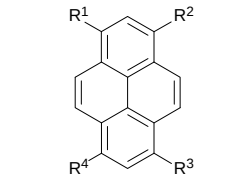
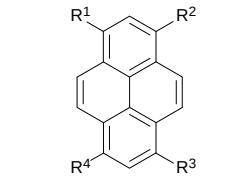


Figure 5 ^{1}H and ^{13}C NMR of 7



7 $R^{1,3}$ = OTIPS; $R^{2,4}$ = donor



7 $R^{1,3}$ = OTIPS; $R^{2,4}$ = donor

Figure 6. ^{1}H and ^{13}C NMR of 8

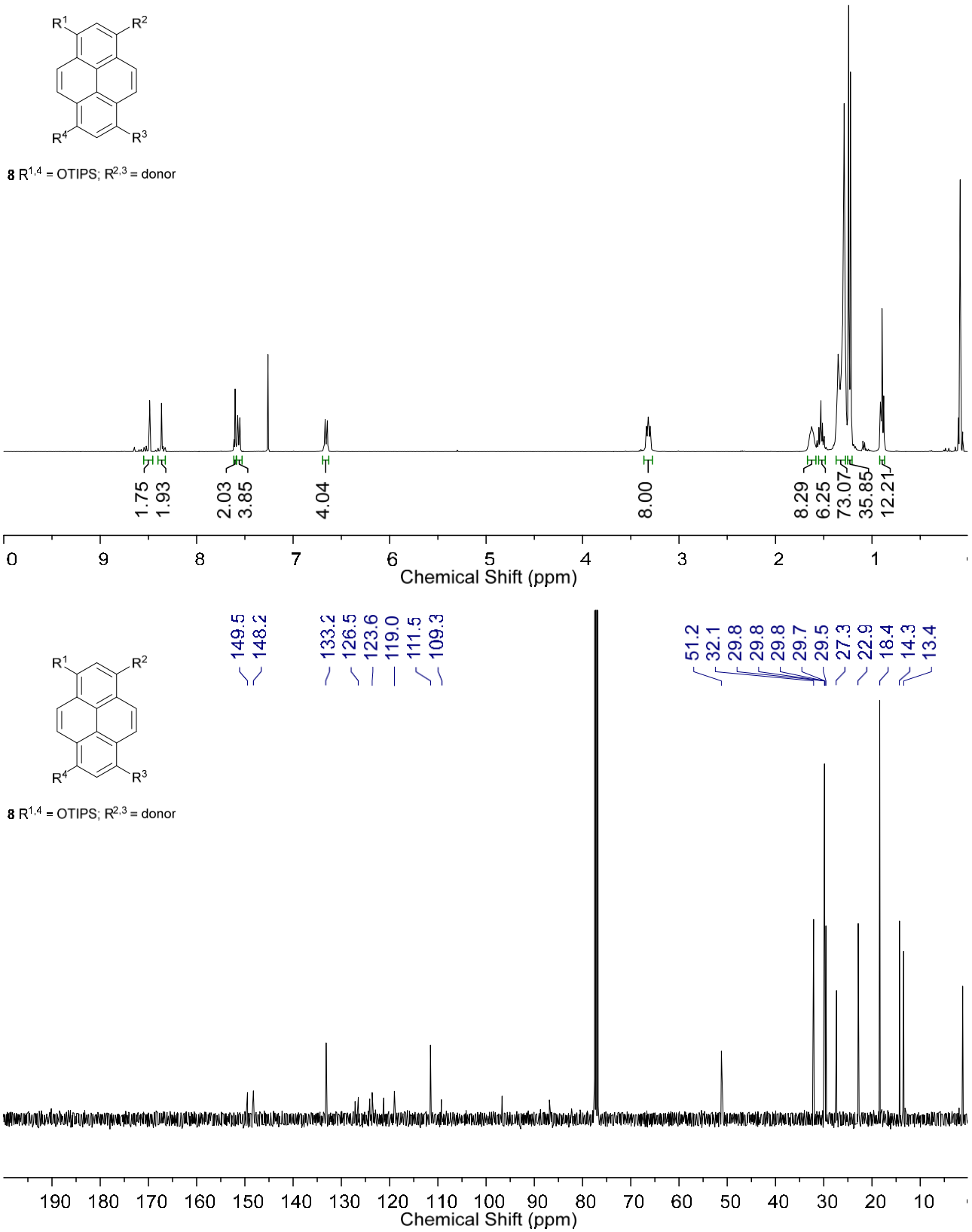


Figure 7. ^{1}H and ^{13}C NMR of 16ketPyr

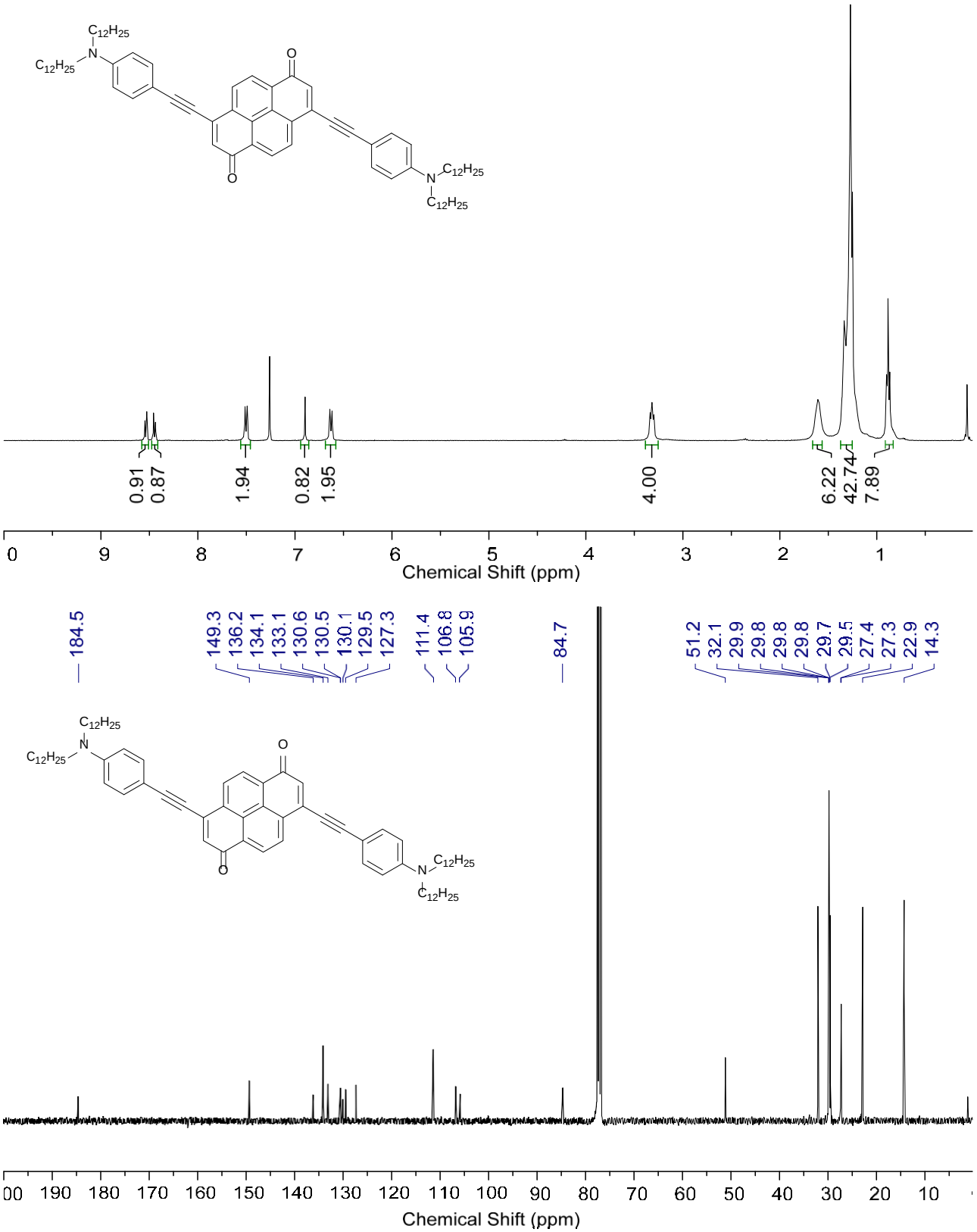
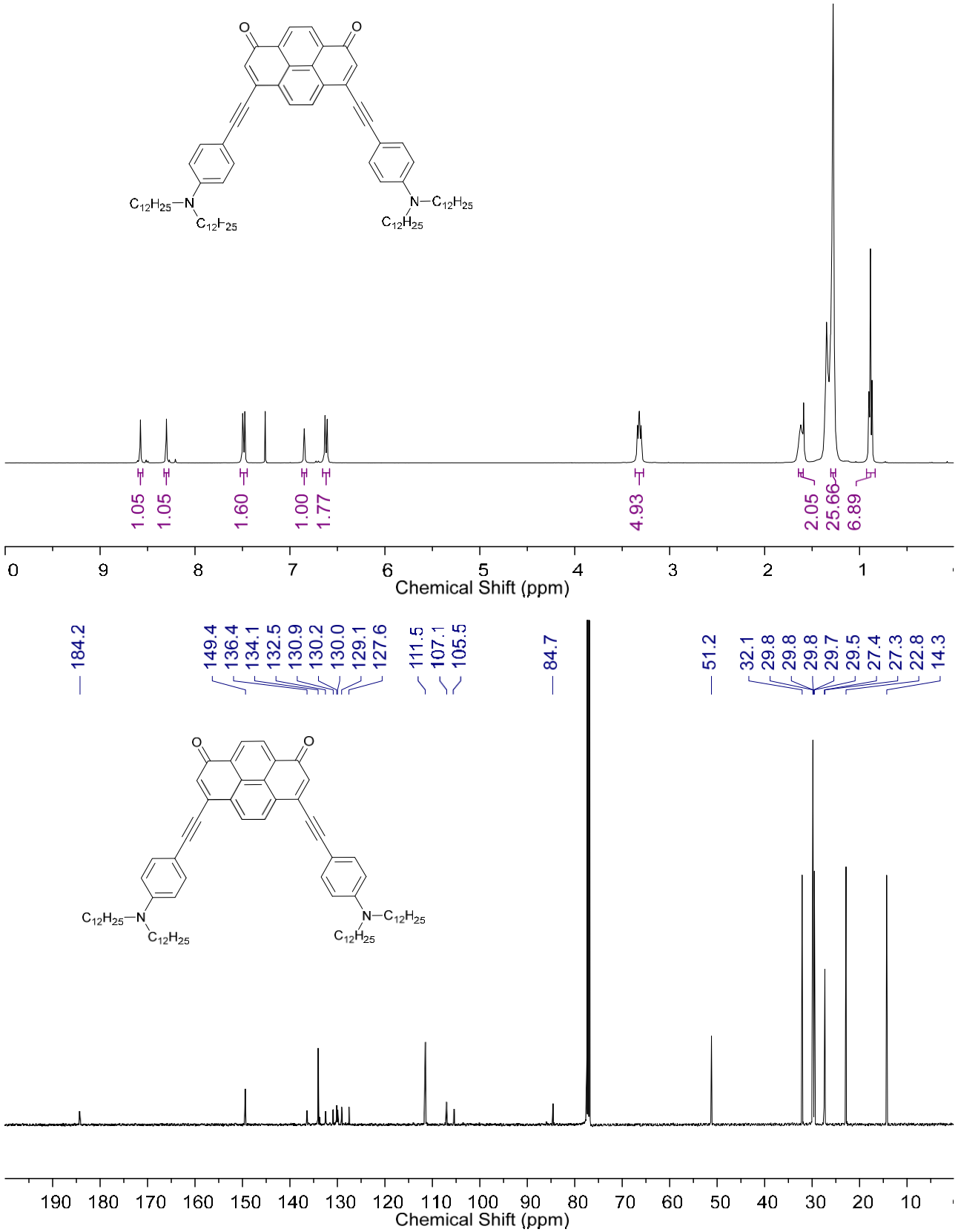


Figure 8. ^{1}H and ^{13}C NMR of 18ketPyr



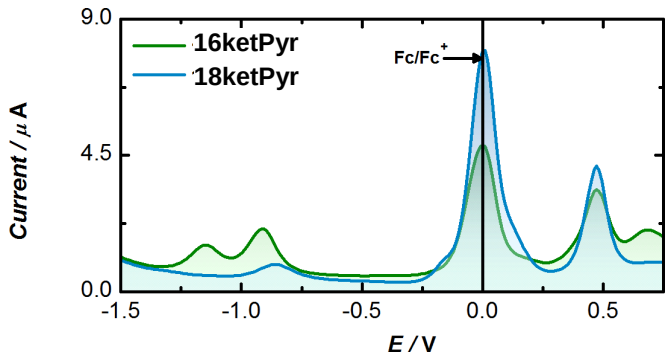


Figure 9. DPVs of **16ketPyr** and **18ketPyr** in CH_2Cl_2 solution with 0.05 M NBu_4PF_6 electrolyte. Measurements were taken with a Pt button working electrode, Ag wire reference electrode, and Pt wire counter electrode.

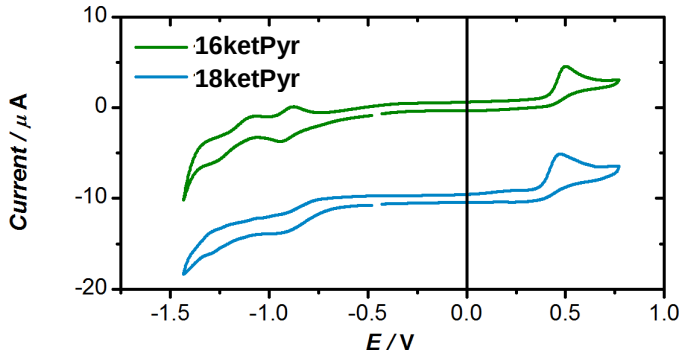


Figure 10. CVs of **16ketPyr** and **18ketPyr** in CH_2Cl_2 solution with 0.05 M *N*Bu_4PF_6 electrolyte. Measurements were taken with a scan rate of 20 mV s^{-1} using a glassy carbon working electrode, Ag wire reference electrode, and Pt wire counter electrode.

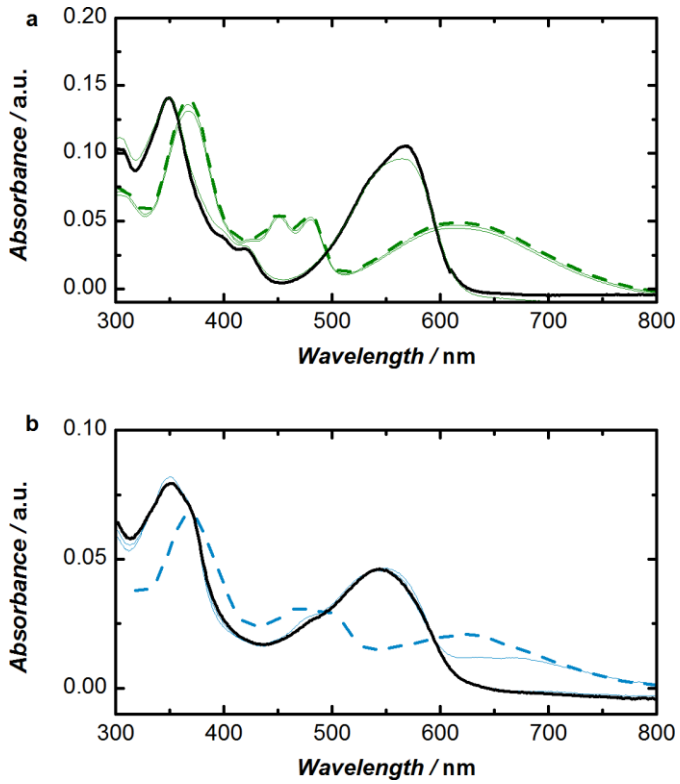


Figure 11. Spectroelectrochemical studies of (a) **16ketPyr** and (b) **18ketPyr** in $CHCl_3$ as a function of applied potential. Initial spectra (0 V applied) are dotted lines, and final spectra are solid black lines. Application of -700 mV vs Ag wire quasi reference.

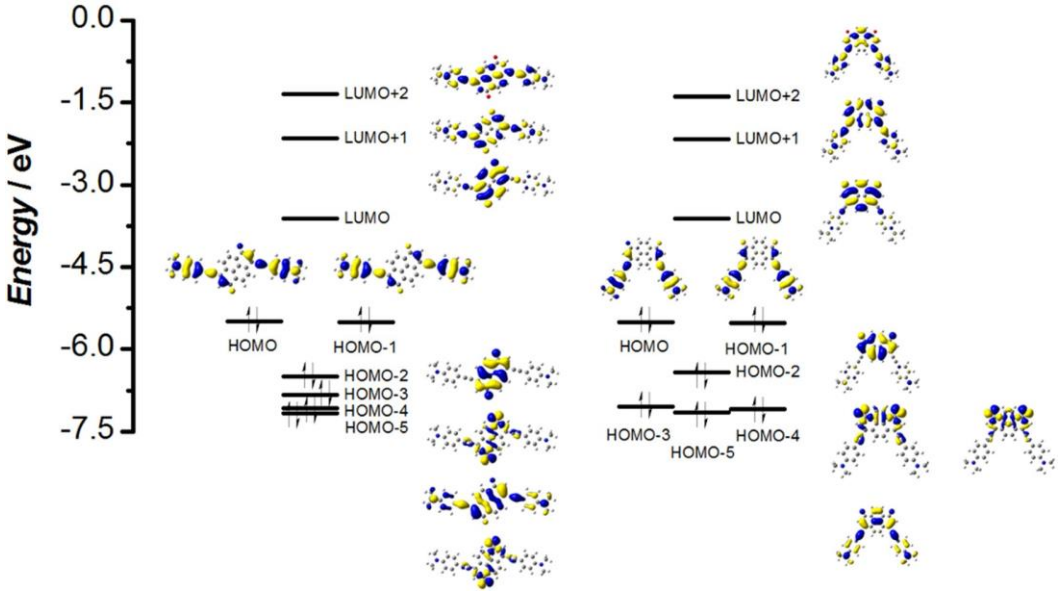


Figure 12. Molecular orbital energy levels and surfaces calculated for compounds **16ketPyr** (left) and **18ketPyr** (right). Surfaces calculated at the B3LYP/6-31+g(d) level of theory and basis set, and energy levels obtained by single point TD-DFT calculations at the same level of theory and basis set, including the PCM solvent model in chloroform.

Table 1. Allowed transitions calculated with TD-DFT for compounds **16ketPyr** and **18ketPyr**.

Compound	Major Transition	Wavelength (nm)	Energy (eV)	Oscillator Strength
16ketPyr	HOMO – LUMO (100%)	788	1.57	0.6615
	HOMO-2 – LUMO (91%) HOMO-1 – LUMO+1 (7%)	481	2.57	0.5941
	HOMO-5 – LUMO (37%) HOMO-1 – LUMO+1 (51%) HOMO-9 – LUMO (8%) HOMO-2 – LUMO (3%)	411	3.02	0.4796
	HOMO-5 – LUMO (54%) HOMO-1 – LUMO+1 (39%) HOMO-2 – LUMO (4%)	391	3.17	0.2891
18ketPyr	HOMO – LUMO (100%)	789	1.57	0.2106
	HOMO-1 – LUMO (100%)	748	1.66	0.3135
	HOMO-2 – LUMO (93%) HOMO-1 – LUMO+1 (2%)	504	2.45	0.4615
	HOMO-4 – LUMO (56%) HOMO-1 – LUMO+1 (42%)	420	2.95	0.2860
	HOMO-9 – LUMO (8%) HOMO-3 – LUMO (81%) HOMO – LUMO+1 (9%)	418	2.96	0.0527
	HOMO-3 – LUMO (10%) HOMO – LUMO+1 (89%)	406	3.05	0.7381
	HOMO-4 – LUMO (39%) HOMO-2 – LUMO (4%) HOMO-1 – LUMO+1 (55%)	396	3.13	0.0022