

Electronic Supplementary Information:

Anthraquinone Derivatives as Electron-Acceptors with Liquid Crystalline Properties

*Amy E. Murschell, Wang Hay Kan, Venkataraman Thangadurai and Todd C. Sutherland**

Department of Chemistry, University of Calgary, 2500 University Drive NW, Calgary, Alberta, Canada

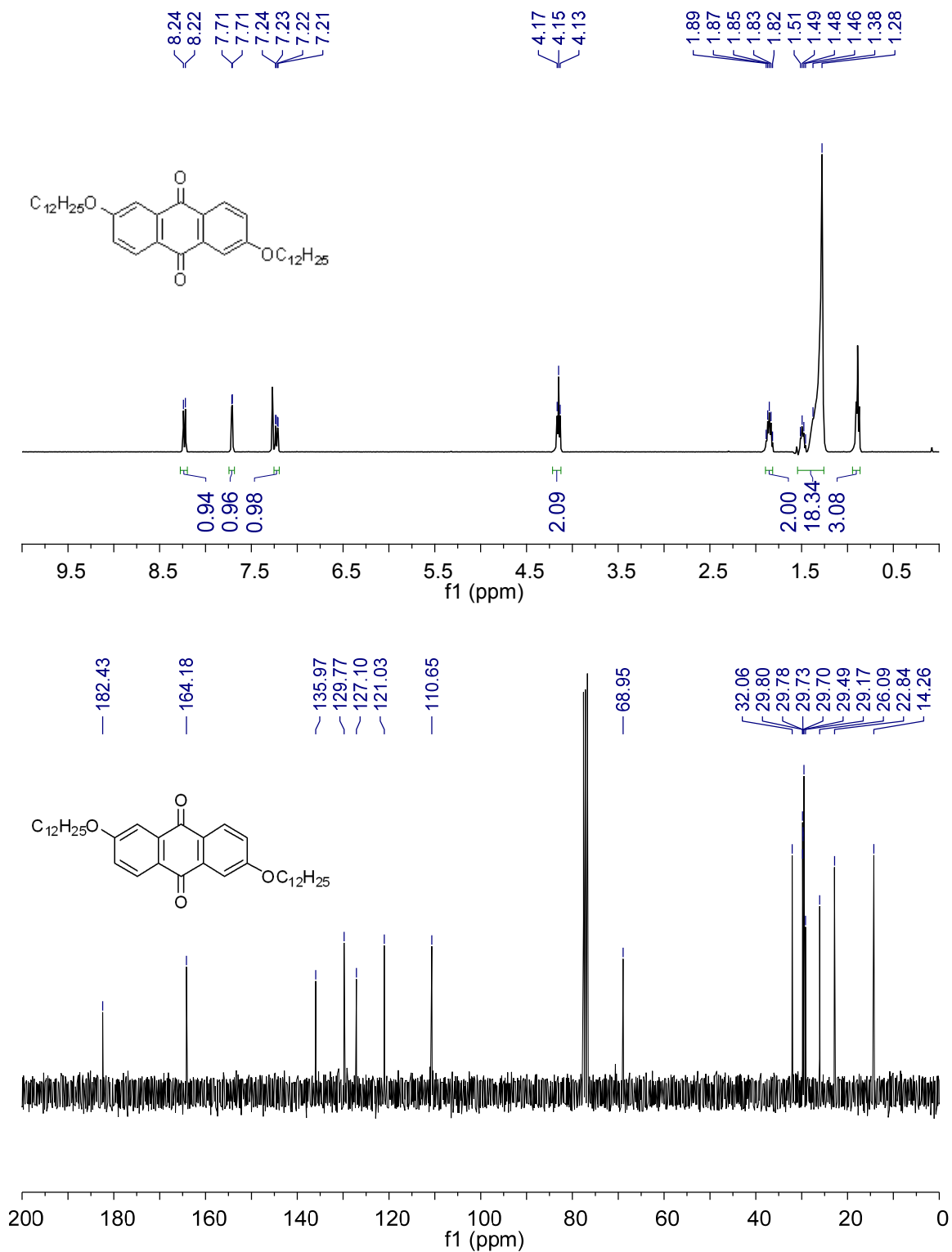
T2N 1N4

sutherlt@ucalgary.ca

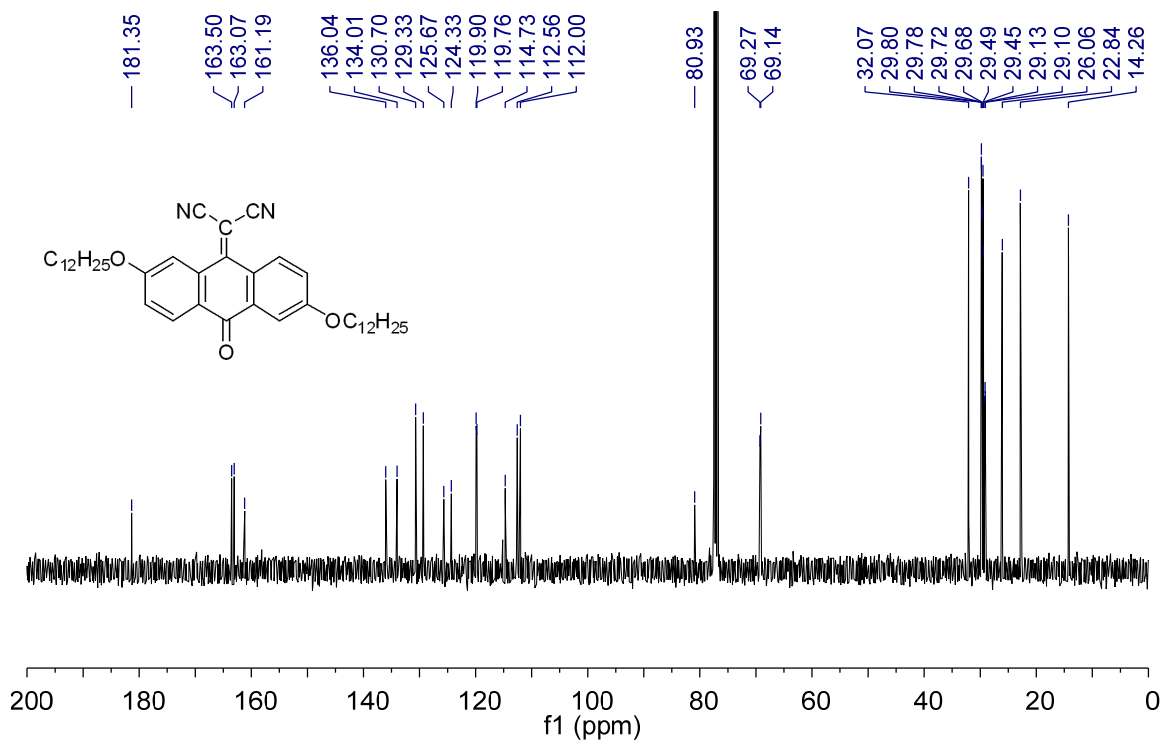
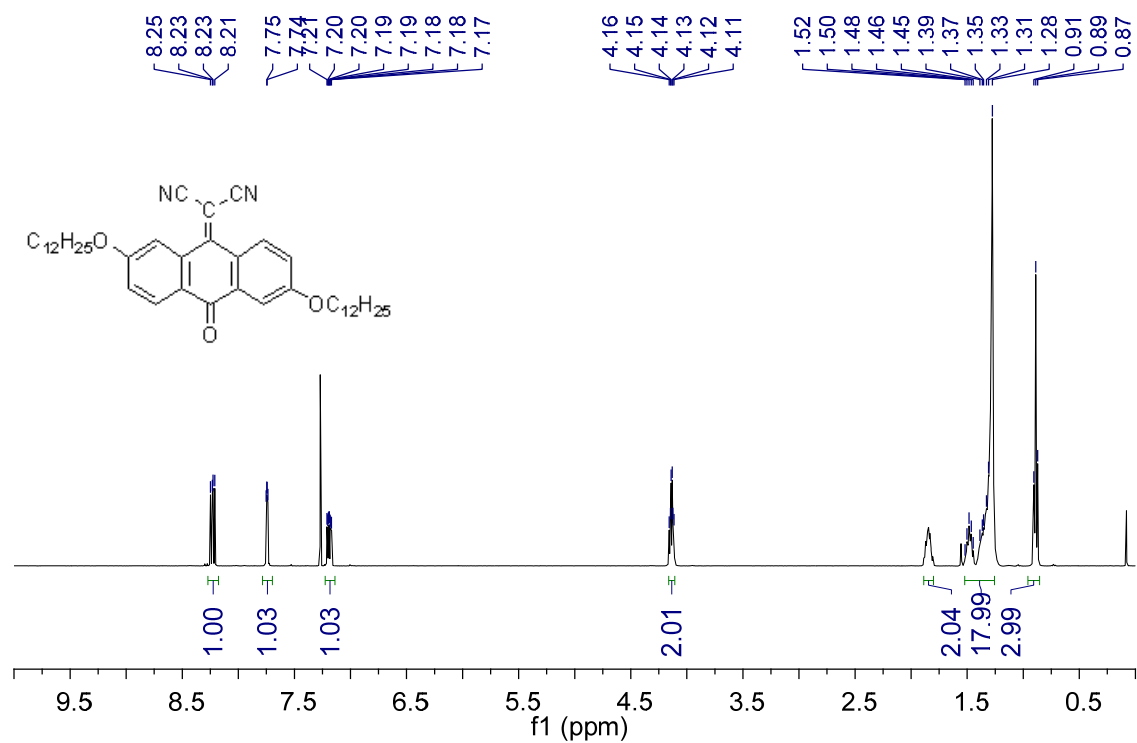
Table of Contents

NMR spectra of quinones 1 – 3	2-4
IR spectra of 1 - 3	5
Normalized absorption spectra of 1 and 2	5
Fluorescence spectra of 1 - 3	5
Cyclic voltammograms of 1 - 3	6-7
FMOs of quinones 1 – 3 and their radical anions.	7
Spin density maps of radical anions 1^{•-} , 2^{•-} and 3^{•-} .	8
DSC thermograms of quinones 1 – 3	8
P-XRD peak data table	9

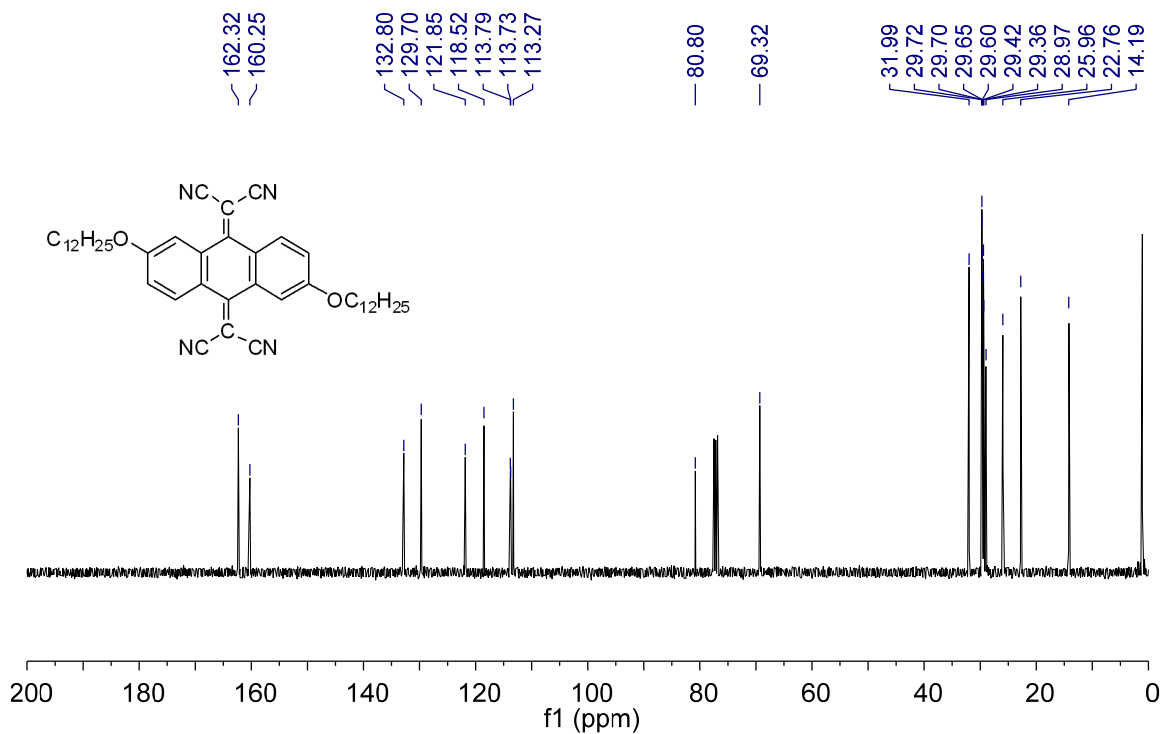
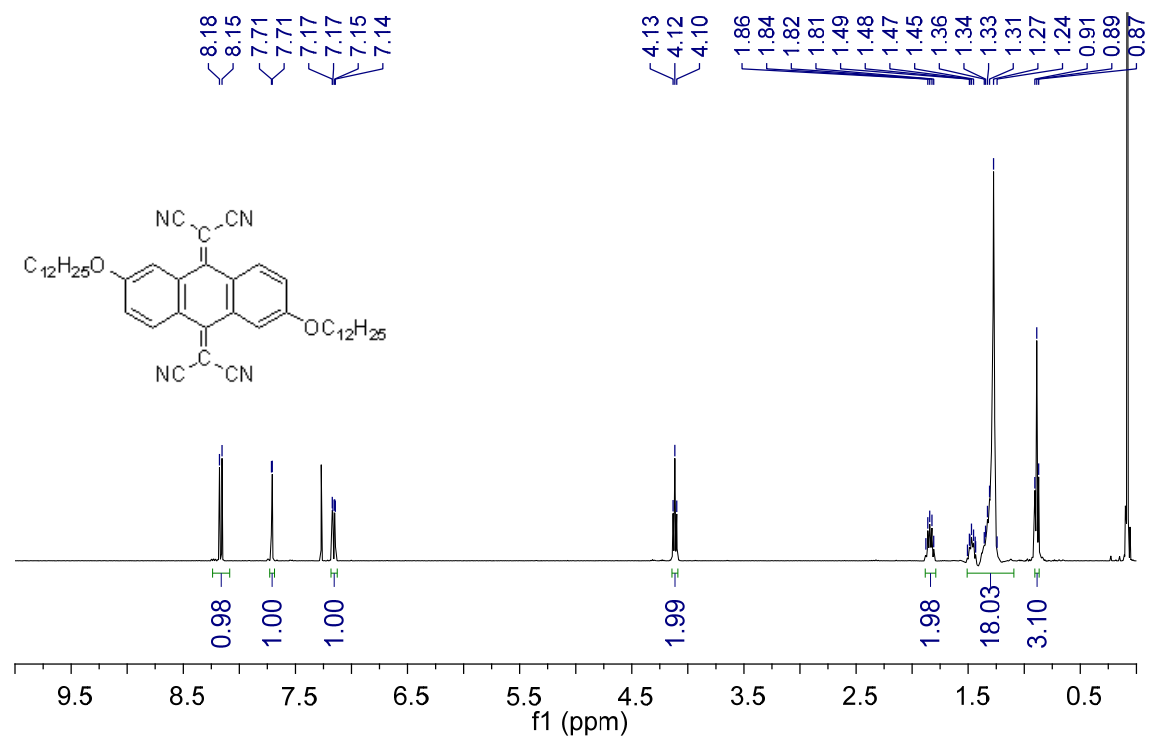
1



2



3



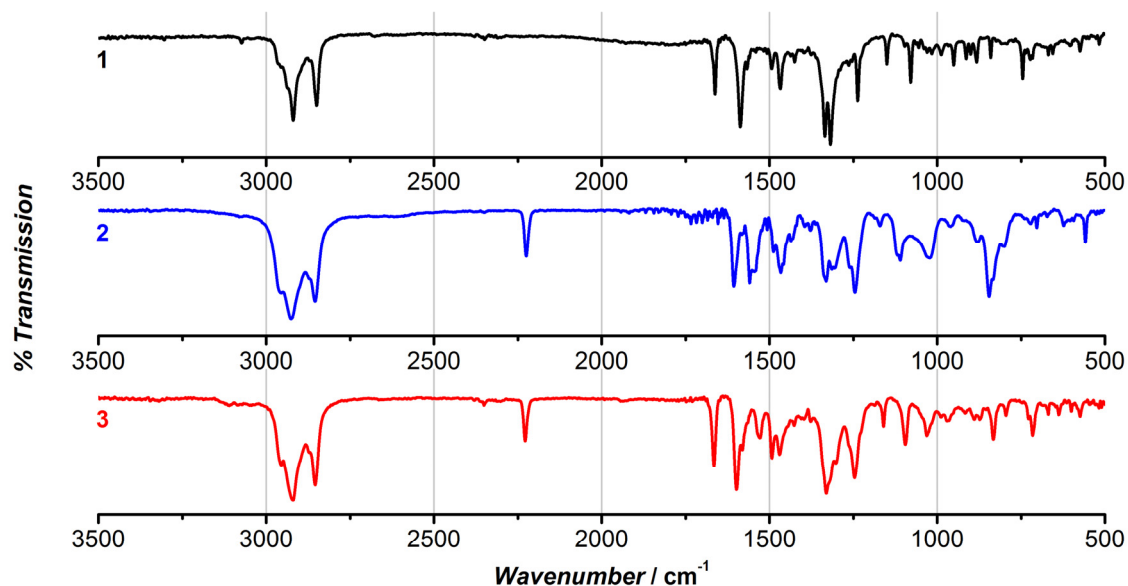


Figure 1. IR spectra of **1**, **2**, and **3** on NaCl plates.

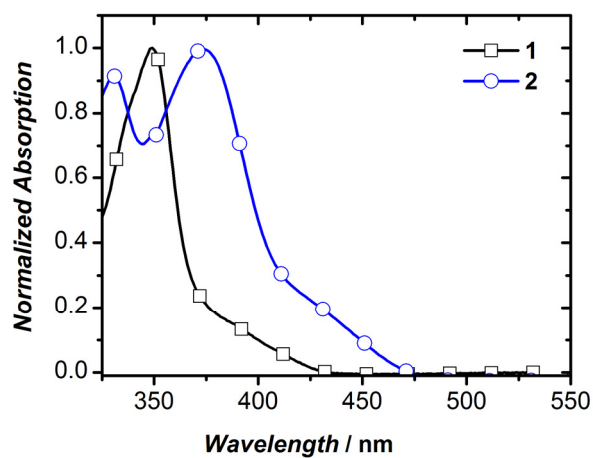


Figure 2. Normalized absorption spectra of **1** and **2** in CH_2Cl_2 highlighting the weak n- π^* transitions.

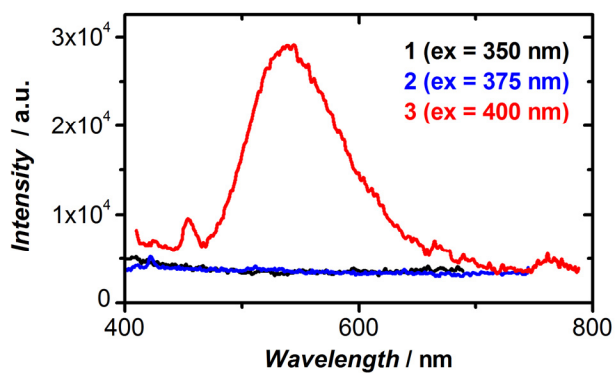


Figure 3. Fluorescence spectra of 10^{-4} M (CH_2Cl_2) quinones **1**, **2**, and **3**.

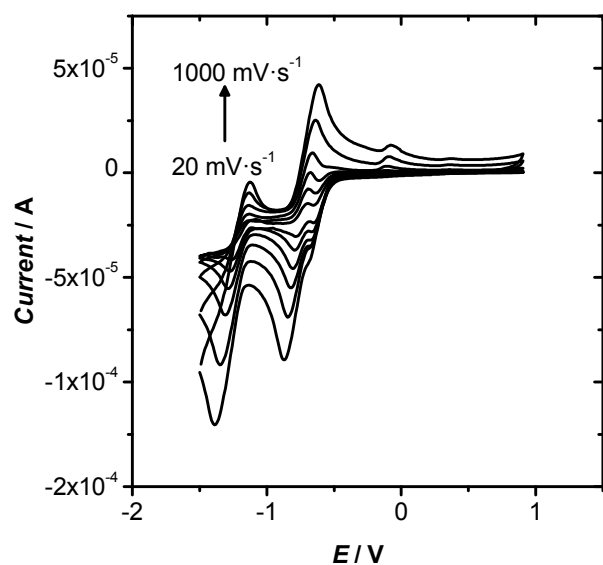


Figure 4. Cyclic voltammograms of 1.4 mM **1** in CH₂Cl₂ at 20, 50 100, 200, 500 and 1000 mV·s⁻¹.

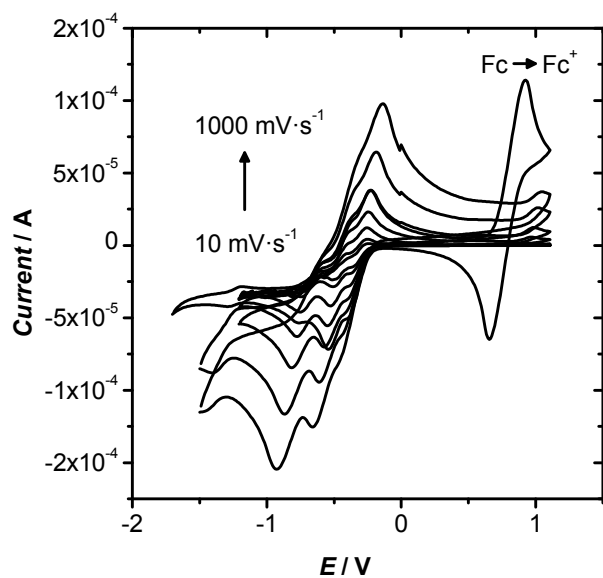


Figure 5. Cyclic voltammograms of 1.9 mM **2** in CH₂Cl₂ at 10, 20, 50 100, 200, 500 and 1000 mV·s⁻¹.

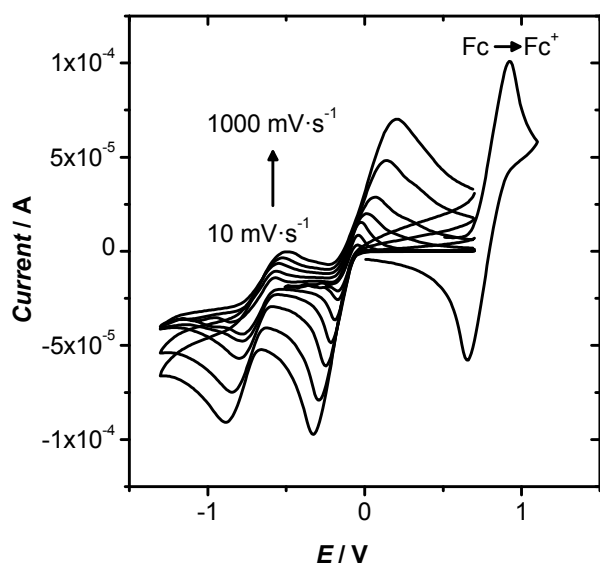


Figure 6. Cyclic voltammograms of 1.7 mM **3** in CH_2Cl_2 at 10, 20, 50 100, 200, 500 and 1000 $\text{mV}\cdot\text{s}^{-1}$.

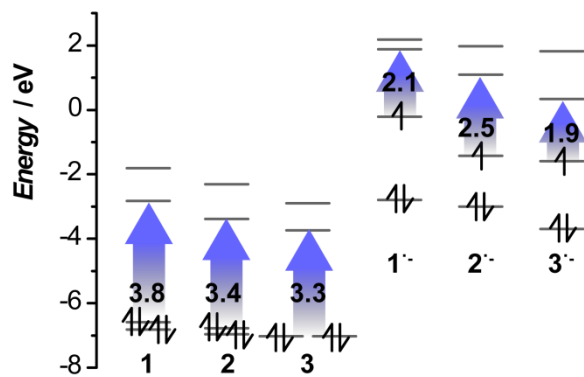


Figure 7. FMOs of quinones **1** – **3** and their radical anions.

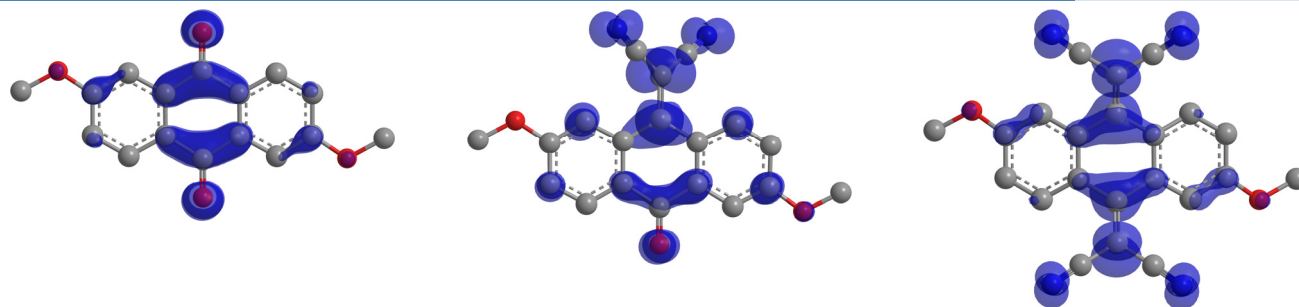


Figure 8. Spin density maps of radical anions $1^{\bullet-}$, $2^{\bullet-}$ and $3^{\bullet-}$.

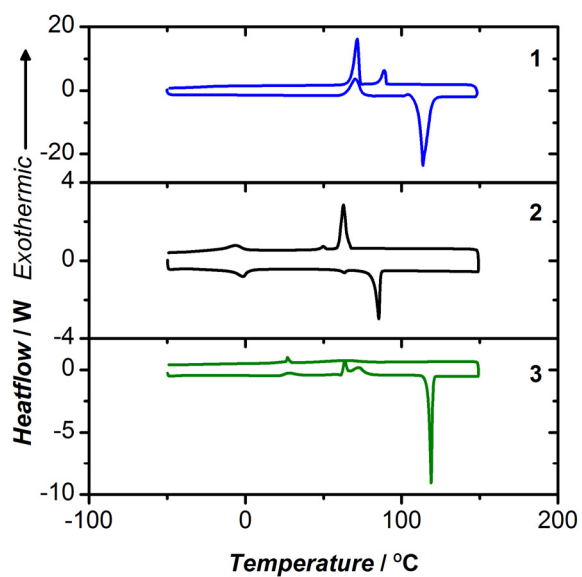


Figure 9. DSC thermograms of quinones **1** – **3** under N_2 atmosphere during heating (bottom traces) and cooling (top traces) at $5\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$ between $-50\text{ }^{\circ}\text{C}$ and $150\text{ }^{\circ}\text{C}$.

Table 1. Summary of P-XRD peaks with Miller indices.

Compound	Temperature	Measured spacing (<i>d</i>) Å	Miller index
1	85 °C	27.2	(100)
1	30 °C	19.6	(100)
		10.3	(200)
		7.3	(300)
		5.2	(400)
2	55 °C	26.9	(100)
		14.3	(200)
		9.8	(300)
		3.4	(001)
2	30 °C	26.6	(100)
		14.2	(200)
		9.7	(300)
		3.3	(001)