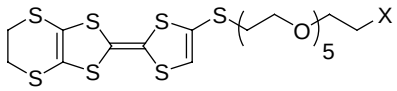
Supporting Information for the following manuscript:

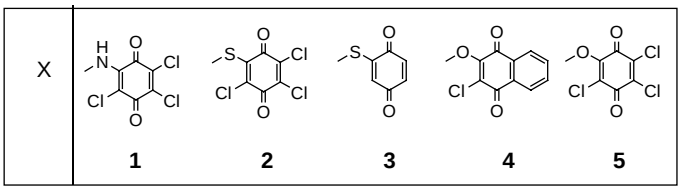
New substituted tetrathiafulvalene-quinone dyads: the influences of electron accepting abilities of quinone units on the metal ion-promoted electron-transfer processes

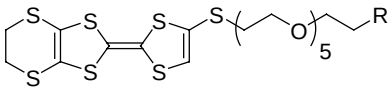
Hui Wu, Deqing Zhang,* Guanxin Zhang, Daoben Zhu*

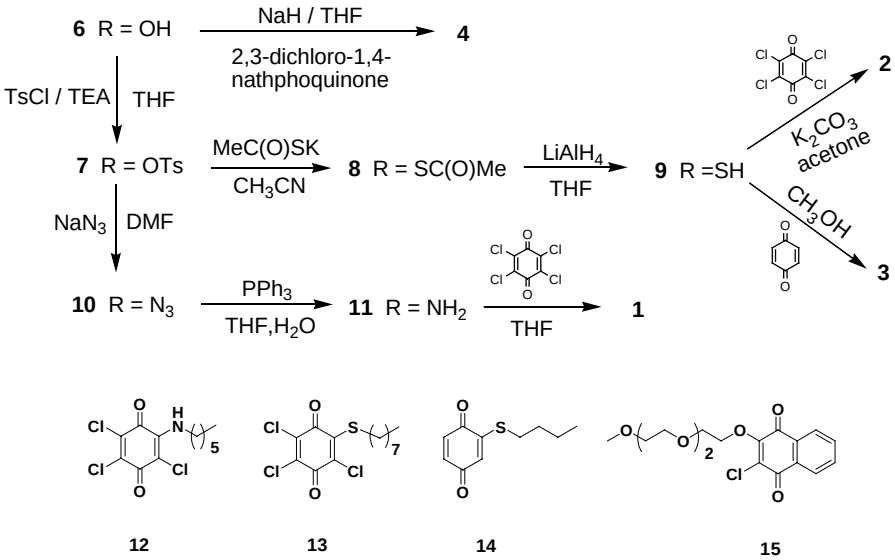
Contents

1. Synthesis of dyads 1, 2, 3, and 4 and compound 12 and 15.









General methods. ^{1}H-NMR, ^{13}C-NMR, MS (including HRMS), absorption, and ESR spectra were recorded with conventional spectrometers. Cyclic voltammetric measurements were performed in a standard three-electrode cell, with Pt as the working and counter electrodes, and Ag/AgCl electrode (saturated KCl) as the reference electrode. The scan rate was 100 mV/s, and n-Bu_4NPF_6 (0.1 M) was used as supporting electrolyte.

All solvents were purified and dried following standard procedures unless otherwise stated. Compound **13**[a] and **14**[b] was synthesized according to the literature :

(a) Grennberg, H.; Gogoll, A.; Backvall, J-E. *J. Org. Chem.* **1991**, *56*, 5808-5811.

(b) Wu, H.; Zhang, D.; Zhu, D. *Tetrahedron Lett*. **2007**, *48*, 8951-8955.

Compound 7 To a magnetically stirred solution of **6** (0.59 g, 1.0 mmol) and p-toluenesulfonyl chloride (0.29 g, 1.5 mmol) in 50 mL dry CH_2Cl_2 at ambient temperature under N_2 atmosphere was added dropwise the solution of triethylamine (1 mL, 7.2 mmol) in 10 mL CH_2Cl_2. The reaction mixture was then slowly warmed to reflux. After being refluxed for 8 h the mixture was cooled to ambient temperature and the solvents were removed under reduced pressure to give a yellow oil. After column chromatography on silica gel with CH_2Cl_2/EtOAc (5 : 1, v/v) as eluant, **7** (0.63 g) was obtained as a yellow oil in 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (2H, d, J = 7.9 Hz), 7.34 (2H, d, J = 7.9 Hz), 6.43 (1H, s), 4.16 (2H, t, J = 4.7 Hz), 3.70-3.58 (20H, m), 3.29 (4H, s), 2.93 (2H, t, J = 6.4 Hz), 2.45 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.8, 133.0, 129.8, 128.0, 126.5, 122.9, 117.8, 113.9, 113.8, 106.5, 70.7, 70.6, 70.55, 70.52, 70.46, 69.6, 69.3, 68.6, 35.3, 30.2, 21.6; HR-MS (MALDI-TOF) calcd. for $C_{27}H_{36}O_8S_8$: 744.0176; found: 744.0170.

Compound 8 Potassium thioacetate (91 mg, 0.8 mmol) was added to a solution of **7** (0.29 g, 0.4 mmol) in dry CH_3CN (25 mL). The reaction mixture was heated at 60 ^oC for 4 h before 50 mL of H_2O was added. The aqueous solution was extracted with CH_2Cl_2 (2 × 50 mL). The combined organic phases were washed with water (50 mL) and brine (50 mL), dried over Na_2SO_4, and concentrated in vacuo. After column chromatography on

silica gel with CH_2Cl_2/EtOAc (6: 1, v/v) as eluant, **8** was obtained as a yellow oil (0.24 g) in 92 % yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.43 (1H, s), 3.67-3.63 (20H, m), 3.29 (4H, s), 3.09 (2H, t, J = 6.4 Hz), 2.93 (2H, t, J = 6.4 Hz), 2.34 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.4, 126.5, 122.9, 117.8, 113.9, 113.8, 106.6, 70.59, 70.56, 70.47, 70.3, 69.7, 69.6, 35.2 30.6, 30.2, 28.8; HR-MS (MALDI-TOF) calcd. for $C_{22}H_{32}O_6S_8$: 647.9965; found: 647.9958.

Compound 10 A solution of **7** (0.74 g, 1.0 mmol) in dry DMF (30 mL) was treated with NaN_3 (0.28 g, 5.0 mmol) at 25°C under N_2. The resulting reaction mixture was warmed at 80°C for 12 h before 30 mL of H_2O was added. The aqueous solution was extracted with dichloromethane (3×50 mL), and the combined extracts were washed with H_2O (2×50 mL) and saturated aqueous NaCl (20 mL), dried ($MgSO_4$) and concentrated in vacuo. After column chromatography on silica gel with CH_2Cl_2/ EtOAc (6:1, v/v) as eluant, **10** was obtained as an orange oil (0.55 g) in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.60-6.20 (1H, br), 3.66-3.63 (20H, m), 3.39 (2H, t, J = 4.7 Hz), 3.29 (4H, s), 2.93 (2H, t, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 126.4, 122.8, 117.8, 113.81, 113.76, 106.5, 70.54, 70.47, 70.39, 69.9, 69.5, 50.6, 35.2, 30.1; HR-MS (MALDI-TOF) calcd. for $C_{20}H_{29}N_3O_5S_7$: 615.0152; found: 615.0160 .

Dyad 2 A solution of **8** (130 mg, 0.2 mmol) in dry THF (15 mL) was treated with $LiAlH_4$ (30 mg, 0.8 mmol) at 0 °C under N_2. After being stirred for 30 min, the reaction mixture was quenched with water (25 mL), and the resulting mixture was extracted with CH_2Cl_2 (2 × 25 mL). The combined organic layers were washed with water, dried (Na_2SO_4), and concentrated to give crude **9** as a yellow oil that was used directly without further purification.

To a solution of previously obtained crude oil product **9** in dry acetone was added KCO_3 (69 mg, 0.5 mmol) under N_2 atmosphere at room temperature. The mixture was stirred for 10 min whereupon tetrachloro-1,4-benzoquinone (124 mg, 0.5 mmol) was added. After being stirred for 30 min the reaction mixture was filtered. The filtrate was concentrated in vacuo. After column chromatography on silica gel with CH_2Cl_2/EtOAc (5: 1, v/v) as eluant, **2** was obtained as a red oil (67 mg) in 41 % yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.60-6.20 (1H, br), 3.74 (2H, t, J = 5.5 Hz) 3.65-3.61 (10H, m), 3.57-3.54 (8H, m), 3.47 (2H, t, J = 5.5 Hz) 3.28 (4H, s), 2.92 (2H, t, J = 6.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.7, 169.0, 147.8, 141.3, 140.2, 136.2, 126.6, 123.1, 114.09, 114.07, 71.4, 70.74, 70.68, 70.66, 70.60, 69.7, 35.3, 33.9, 30.3；MS (MALDI-TOF) m/z 814.3 (M^+); HR-MS (MALDI-TOF) calcd. for $C_{26}H_{29}Cl_3O_7S_8$: 813.8745; found: 813.8715.

Dyad 3 A solution of crude product **9** (126 mg) in CH_2Cl_2 (5mL) was added to a suspension of 1,4-benzoquinone (108 mg, 1.0 mmol) in methanol (25 mL). The mixture was stirred for 10 min. Water (25 mL) was added, and the resulting mixture was extracted with CH_2Cl_2 (2 × 25 mL). The combined organic layers were washed with water, dried (Na_2SO_4), and concentrated After column chromatography on silica gel with CH_2Cl_2/EtOAc (5: 1, v/v) as eluant, **3** was obtained as a yellow oil (74 mg) in 52 % yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.79 (1H, d, J = 10 Hz), 6.71 (1H, dd, J = 10, 2 Hz), 6.45 (1H, d, J = 2 Hz), 6.42 (1H, s), 3.76 (2H, t, J = 6.3 Hz), 3.66-3.61 (18H, m), 3.27 (4H, s), 2.99 (2H, t, J = 6.3 Hz), 2.91 (2H, t, J = 6.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 183.9, 183.7, 152.5, 137.3, 136.0, 126.5, 124.9, 122.9, 117.8, 113.9, 113.8, 106.5, 70.7, 70.6, 70.5, 70.4, 69.5, 68.0, 35.2, 30.3, 30.1; HR-MS(EI): calcd. for $C_{26}H_{32}O_7S_8$: 711.9914; found: 711.9921.

Dyad 1 A solution of **10** (0.5 g, 0.81 mmol) in THF (60 mL) was treated with PPh_3 (0.43 g, 1.62 mmol) and H_2O (0.2 mL, 11.1 mmol) at 25°C under N_2. The resulting reaction mixture was warmed at 45°C for 10 h. The reaction mixture was diluted with water and extracted with CH_2Cl_2. The organic phase was dried over $MgSO_4$ and concentrated in vacuo to give crude **11** as a yellow oil that was used directly without further purification.. The crude product of **11** was dissolved in dry THF and the solution was cooled to 0 °C. tetrachloro-1,4-benzoquinone (0.37 g, 1.5 mmol) was added. After being stirred for 30 min at this temperature the reaction mixture was concentrated in vacuo. Column chromatography of the residue on silica gel with CH_2Cl_2/ EtOAc (6:1, v/v) as eluant afforded dyad **1** as a purple oil (0.20 g) in 31% yield: ^{1}H-NMR (400 MHz, $CDCl_3$): δ 6.42 (1H, s), 4.00 (2H, m), 3.71 (2H, t, J = 5.1 Hz), 3.66-3.62 (18H, m), 3.29 (4H, s), 2.93 (2H, t, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.3, 170.0, 143.6, 142.8, 135.9, 126.8, 123.1, 114.1, 106.9, 70.9, 70.8, 70.77, 70.74, 70.67, 69.8, 69.7, 44.9, 35.5, 30.4; HR-MS (MALDI-TOF) calcd. for $C_{26}H_{30}Cl_3NO_7S_7$:796.9133; found: 796.9092.

Dyad 4 To a solution of **6** (0.59 g, 1.0 mmol) in dry THF was added petroleum ether rinsed NaH (52%, 0.23 g, 5.0 mmol) in N_2 atmosphere at room temperature. The mixture was stirred for 20 min whereupon 2,3-dichloro-1,4-nathphoquinone (0.45 g, 2.0 mmol) was added. After being heated to reflux for 6 h the reaction mixture was cooled to room temperature and filtered. The filtrate was concentrated in vacuo. After column chromatography (CH_2Cl_2/EtOAc, 5: 1) on silica gel, **4** was obtained as a yellow oil (0.38 g) in 48 % yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (1H, m), 8.07 (1H, m), 7.73 (2H, m), 6.42 (1H, s), 4.75 (2H, t, J = 4.4 Hz), 3.82 (2H, t, J = 4.4 Hz), 3.67-3.61 (12H, m), 3.55-3.49 (6H, m), 3.28 (4H, s), 2.92 (2H, t, J = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ

179.5, 178.5, 157.0, 134.1, 133.8, 131.0, 130.8, 128.8, 126.8, 126.7, 126.5, 122.8, 117.6, 113.8, 113.7, 106.5, 73.2, 70.8, 70.7, 70.54, 70.47, 70.41, 69.5, 35.2, 30.1. HR-MS(EI): calcd. for $C_{30}H_{33}ClO_8S_7$: 779.9909; found: 779.9921.

Compound 12 This was prepared in a similar manner as for dyad **1** from 1-Hexylamine as a purple solid in 46 % yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.93 (1H, s), 3.80 (2H, m), 1.66 (2H, m), 1.40-1.26 (6H, m), 0.90 (3H, t, J = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.5, 170.1, 154.2, 144.0, 142.4, 135.7, 45.4, 31.4, 30.9, 26.3, 22.6, 14.2; MS(EI): *m/z* 309 (M^+); HR-MS(EI): calcd. for $C_{12}H_{14}NO_2Cl_3$: 309.0090, 311.0061; found: 309.0086, 309.0056.

Compound 15 This was prepared in a similar manner as for dyad **4** from triethylene glycol monomethyl ether as a pale yellow oil in 53 % yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (1H, m), 8.08 (1H, m), 7.75 (2H, m), 4.76 (2H, t, J = 4.5 Hz), 3.83 (2H, t, J = 4.5 Hz), 3.64 (2H, t, J = 4.8 Hz), 3.50 (4H, m), 3.47 (2H, m), 3.34 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 179.2, 178.1, 156.8, 133.9, 133.6, 130.7, 130.6, 126.5, 73.0, 71.5, 70.6, 70.5, 70.2, 70.1, 58.6; HR-MS(EI): calcd. for $C_{17}H_{19}ClO_6$: 354.0870; found: 354.0875.

2. Absorption spectra of dyads 1, 2, 3, and 4 in the presence of metal ions

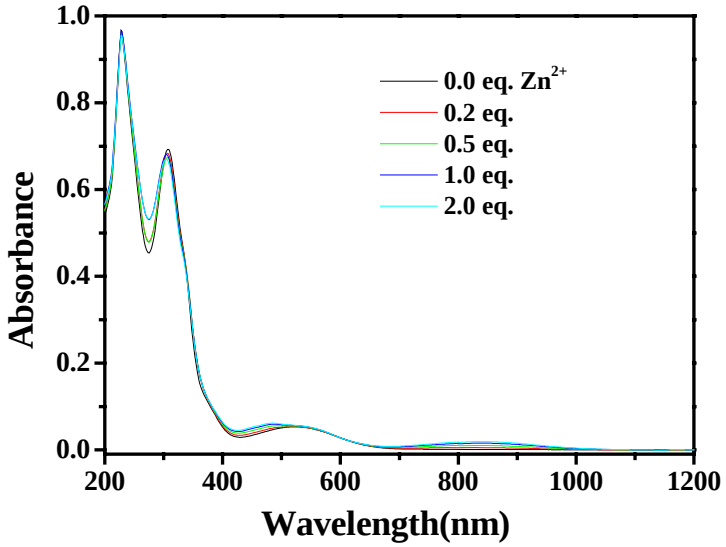


Figure S1. Absorption spectra of dyad **1** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Zn^{2+} **[**$Zn(ClO_4)_2$**]**.

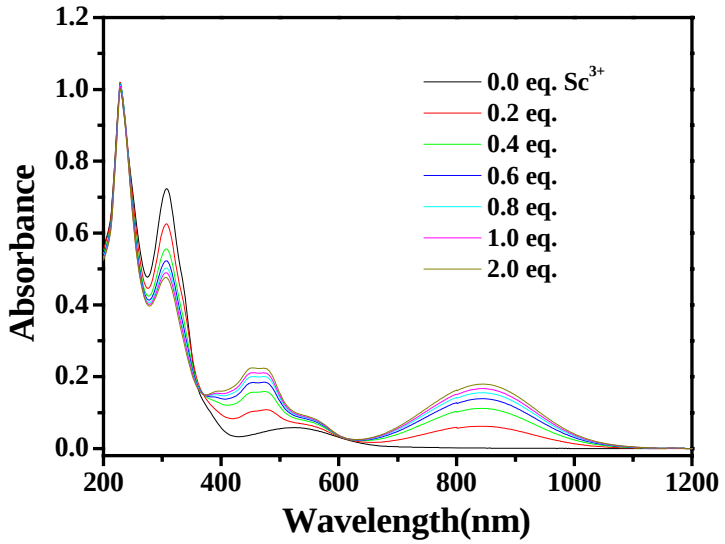


Figure S2. Absorption spectra of dyad **1** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Sc^{3+} [$Sc(SO_3CF_3)_3$].

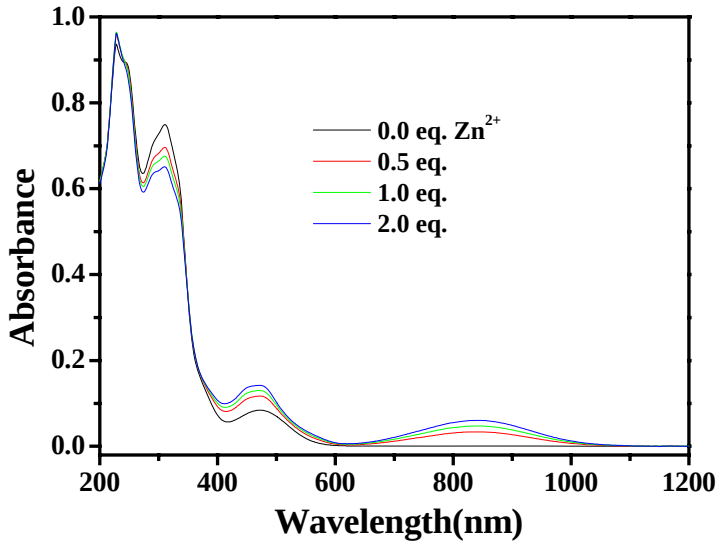


Figure S3. Absorption spectra of dyad **2** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5}M) in the presence of increasing amount of Zn^{2+} [$Zn(ClO_4)_2$].

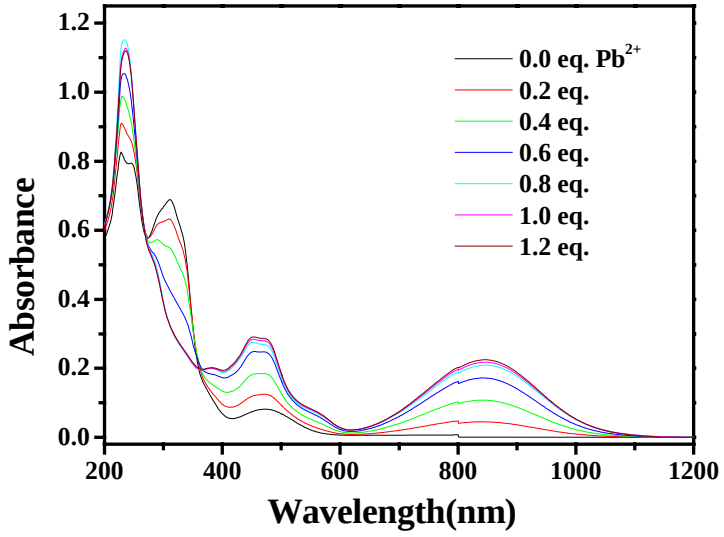


Figure S4. Absorption spectra of dyad **2** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Pb^{2+} [$Pb(ClO_4)_2$].

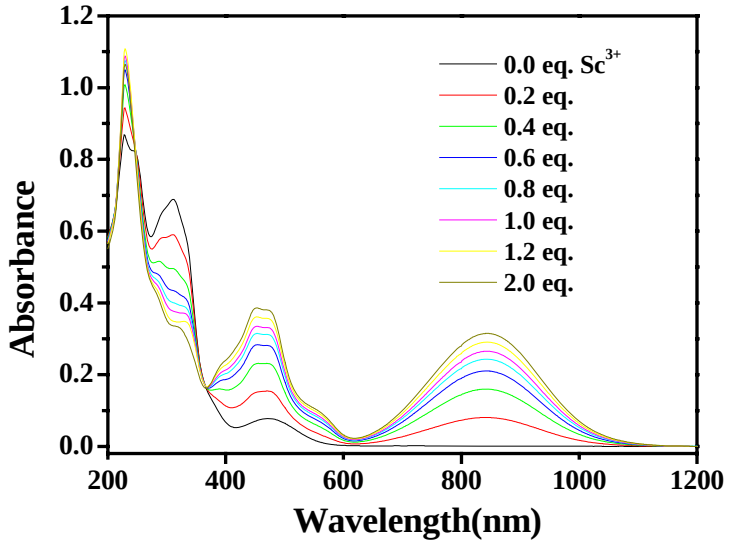


Figure S5. Absorption spectra of dyad **2** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Sc^{3+} [$Sc(SO_3CF_3)_3$].

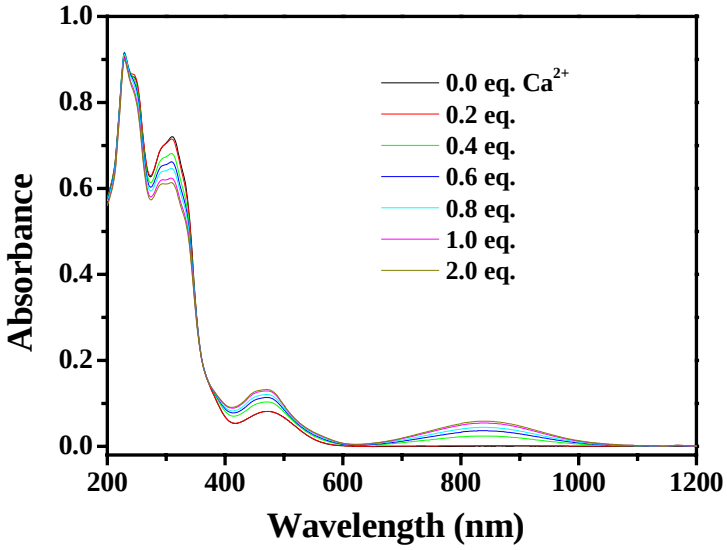


Figure S6. Absorption spectra of dyad **2** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Ca^{2+} **[**$Ca(ClO_4)_2$**]**.

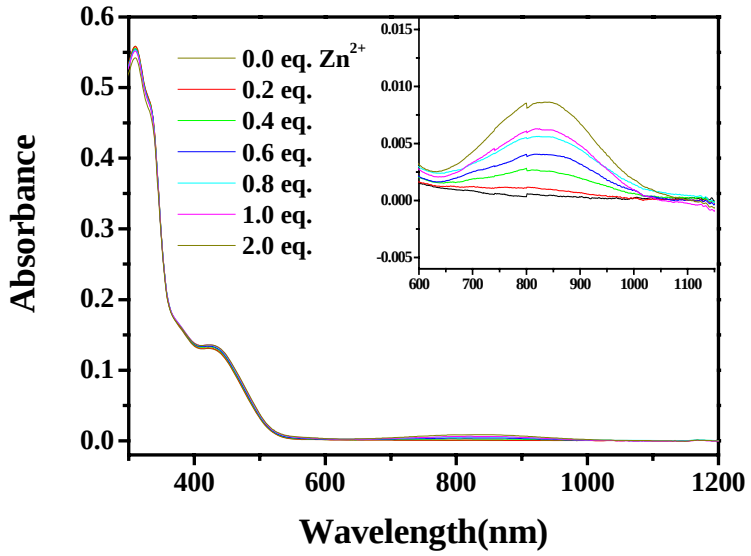


Figure S7. Absorption spectra of dyad **3** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Zn^{2+} **[**$Zn(ClO_4)_2$**]**, inset is the enlargement of the 600-1150 nm region.

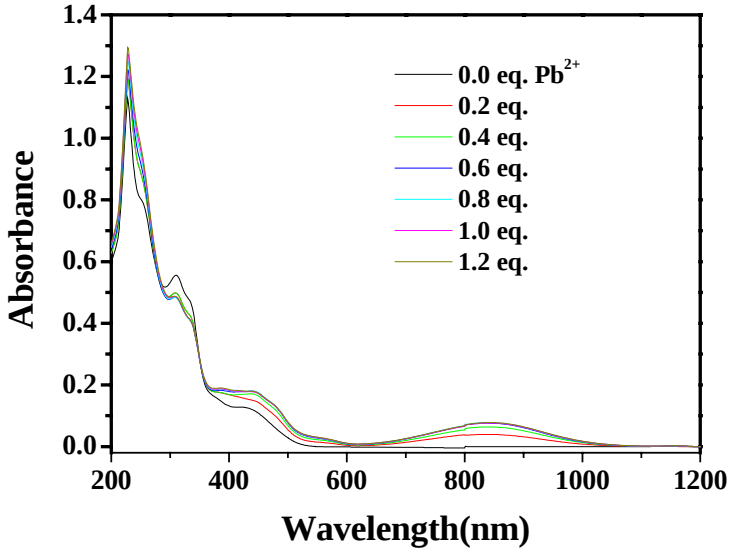


Figure S8. Absorption spectra of dyad **3** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Pb^{2+} [$Pb(ClO_4)_2$].

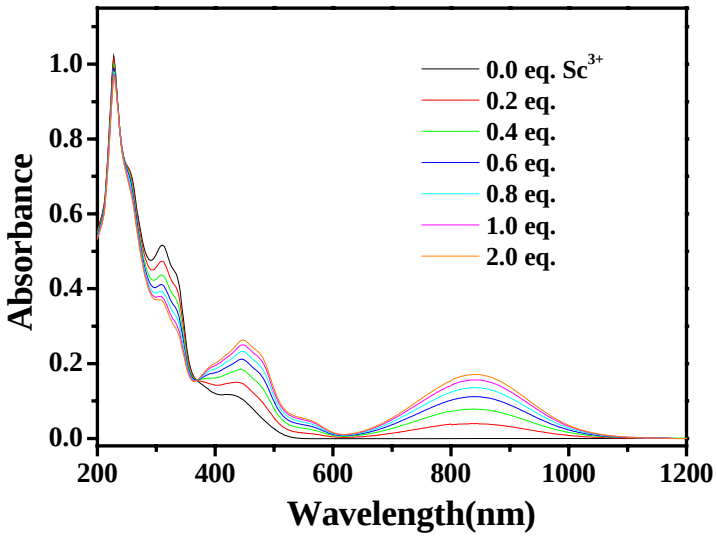


Figure S9. Absorption spectra of dyad **3** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Sc^{3+} [$Sc(SO_3CF_3)_3$].

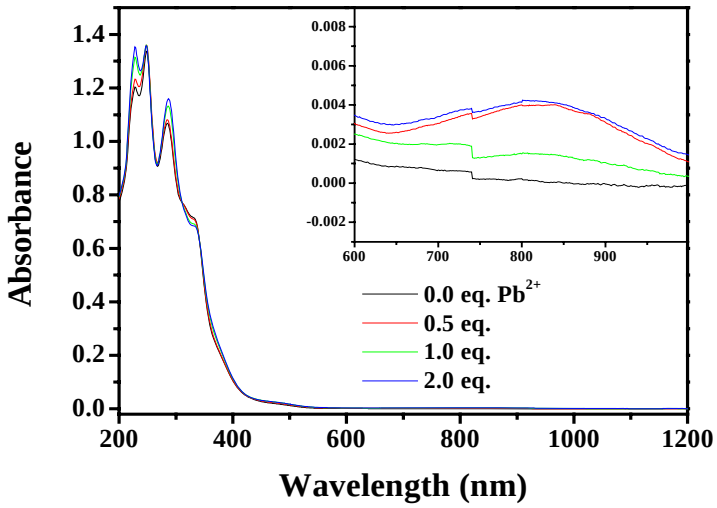


Figure S10. Absorption spectra of dyad **4** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Pb^{2+} [$Pb(ClO_4)_2$], inset is the enlargement of the 600-1000 nm region.

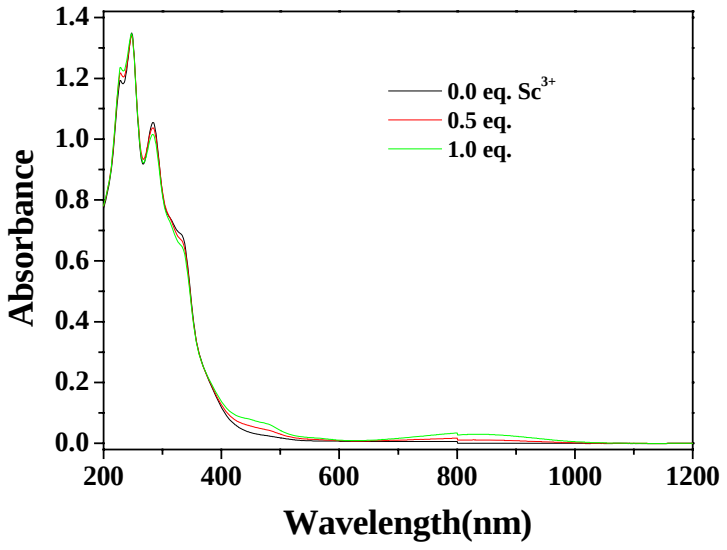


Figure S11. Absorption spectra of dyad **4** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0 × 10^{-5} M) in the presence of increasing amount of Sc^{3+} [$Sc(SO_3CF_3)_3$].

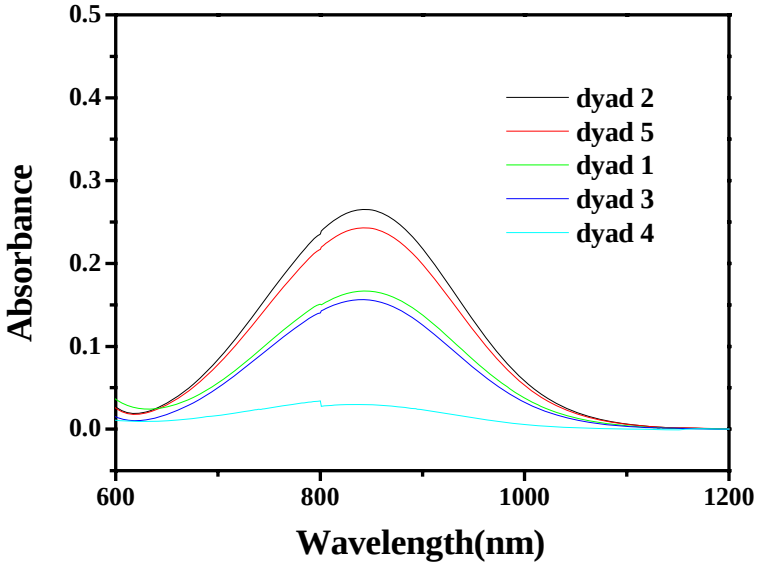


Figure S12. Absorption spectra of the 600-1200 nm region of dyads **1**, **2**, **3**, **4**, and **5** in the presence of 1.0 eq. of Sc^{3+} [$Sc(SO_3CF_3)_3$].

3. Absorption spectra of 6 after chemical and electrochemical oxidations as well as those of 6, 12 and the mixture of 6 and 12

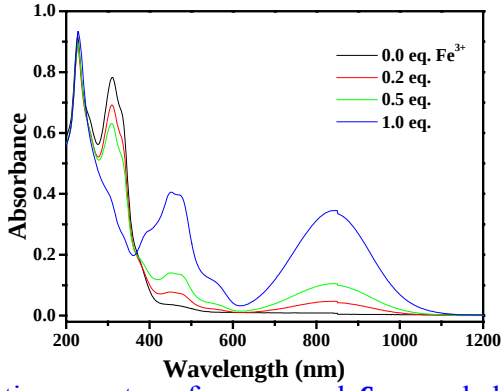


Figure S13. Absorption spectra of compound **6** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) in the presence of increasing amount of Fe^{3+} [$Fe(ClO_4)_3$].

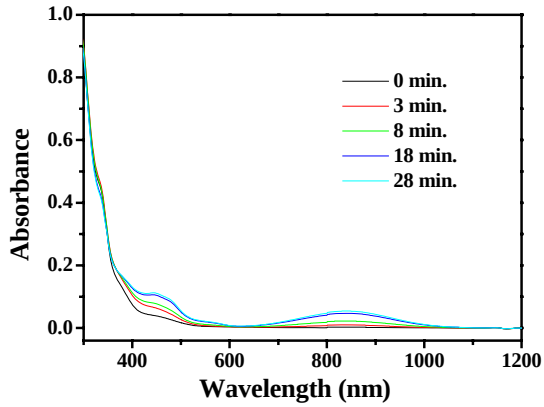


Figure S14. Absorption spectra of compound **6** recorded in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-5} M) containing *n*-Bu_4NPF_6 (27.8 mM) after applying an oxidation potential of 0.65 V (vs. Ag/AgCl).

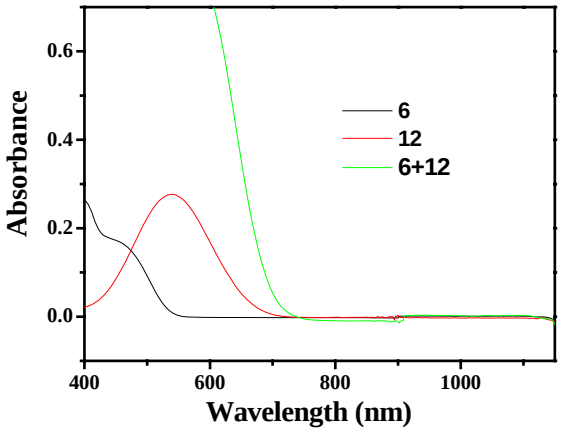


Figure S15. Absorption spectra of compound **6** (1.5×10^{-3} M), **12** (2.5×10^{-3} M) and the mixture of **6** (1.5×10^{-2} M) and **12** (2.5×10^{-2} M) recorded in CH_2Cl_2/CH_3CN (1:1, v/v).

4. ESR spectra of dyads 2, 3, 4, and 5 in the presence of metal ions.

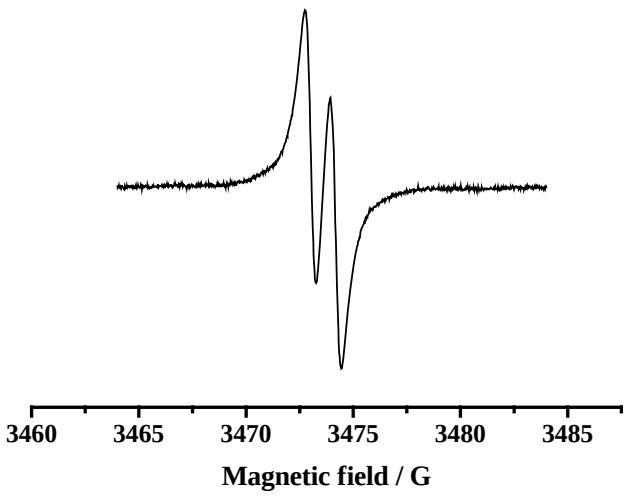


Figure S16. ESR spectrum of dyad **2** (1.0×10^{-4} M) in CH_2Cl_2/CH_3CN (1:1, v/v) in the presence of 1.0 equiv of Pb^{2+} [$Pb(ClO_4)_2$] recorded at room temperature; the solution was degassed before measurement.

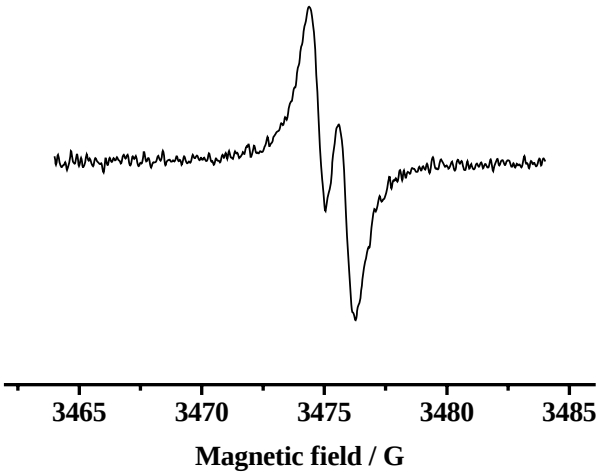


Figure S17. ESR spectrum of dyad **3** (1.0×10^{-4} M) in CH_2Cl_2/CH_3CN (1:1, v/v) in the presence of 1.0 equiv of Pb^{2+} [$Pb(ClO_4)_2$] recorded at room temperature; the solution was degassed before measurement.

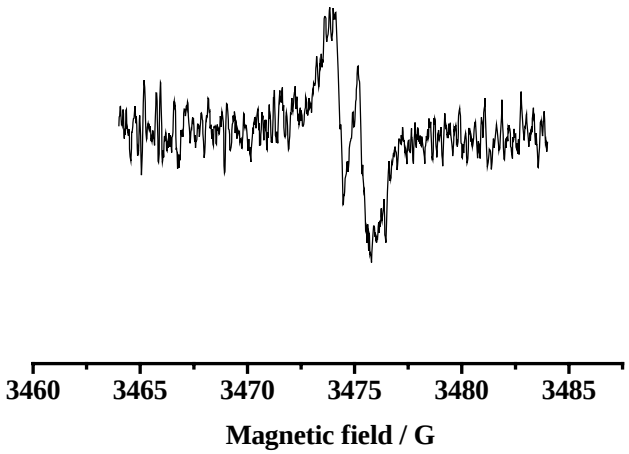


Figure S18. ESR spectrum of dyad **4** (1.0×10^{-4} M) in CH_2Cl_2/CH_3CN (1:1, v/v) in the presence of 1.0 equiv of Pb^{2+} [$Pb(ClO_4)_2$] recorded at room temperature; the solution was degassed before measurement.

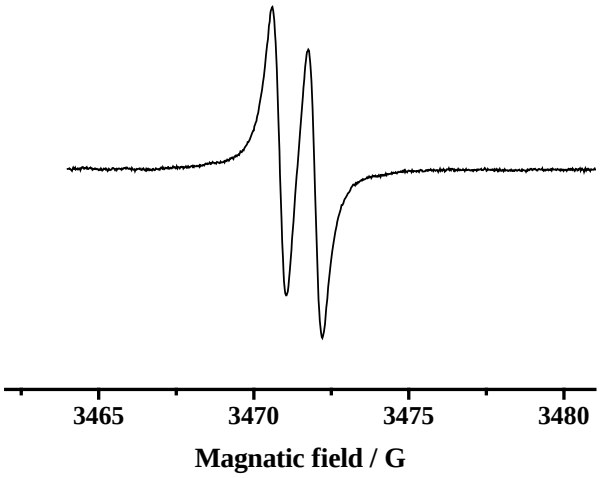


Figure S19. ESR spectrum of dyad **5** (1.0×10^{-4} M) in CH_2Cl_2/CH_3CN (1:1, v/v) in the presence of 1.0 equiv of Pb^{2+} [$Pb(ClO_4)_2$] recorded at room temperature; the solution was degassed before measurement.

5. Cyclic voltammograms of 1, 2, 3, and 4, and compounds 12-15 and those in the presence of metal ions.

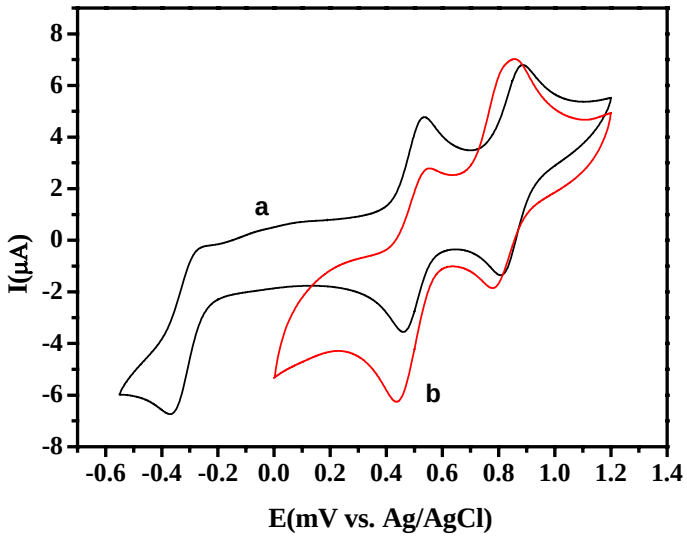


Figure S20. Cyclic voltammograms of dyad **1** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 1.2 equiv of Sc^{3+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

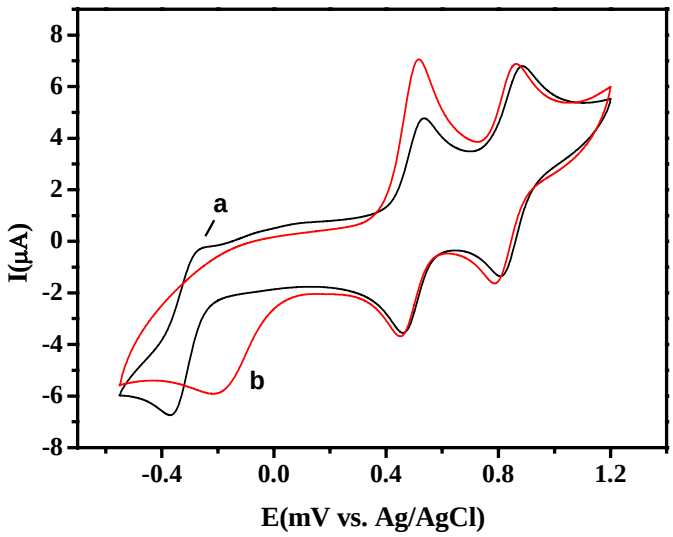


Figure S21. Cyclic voltammograms of dyad **1** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 2 equiv of Zn^{2+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

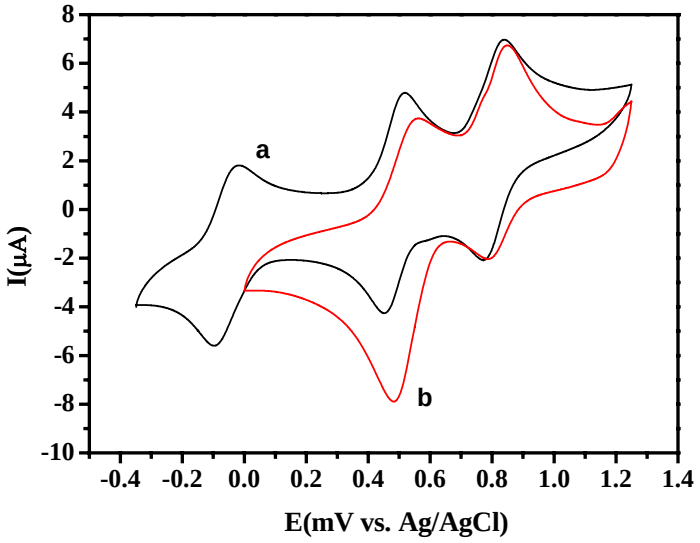


Figure S22. Cyclic voltammograms of dyad **2** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 2 equiv of Pb^{2+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

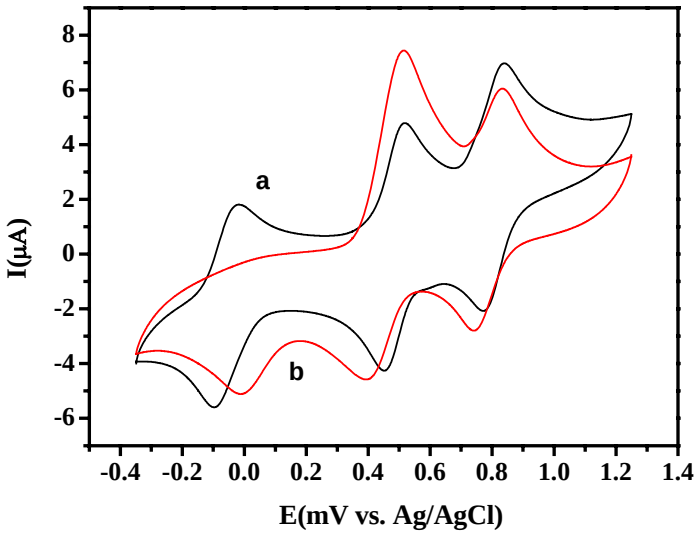


Figure S23. Cyclic voltammograms of dyad **2** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 4 equiv of Zn^{2+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

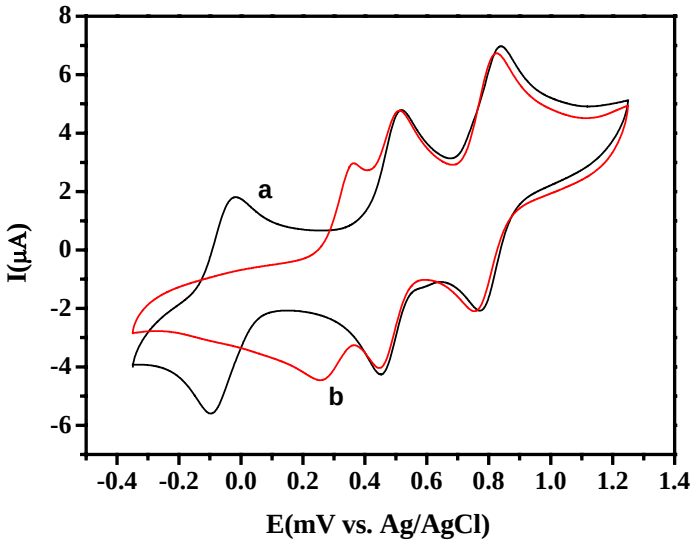


Figure S24. Cyclic voltammograms of dyad **2** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 4 equiv of Ca^{2+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

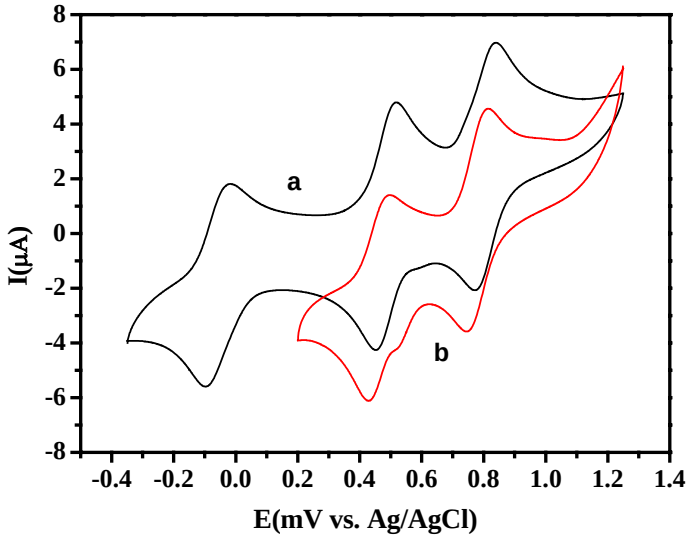


Figure S25. Cyclic voltammograms of dyad **2** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 2 equiv of Sc^{3+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

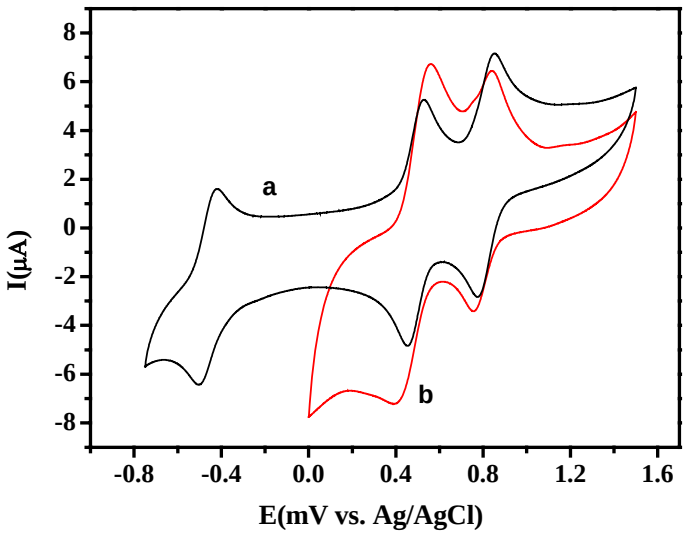


Figure S26. Cyclic voltammograms of dyad **3** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 2 equiv of Pb^{2+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

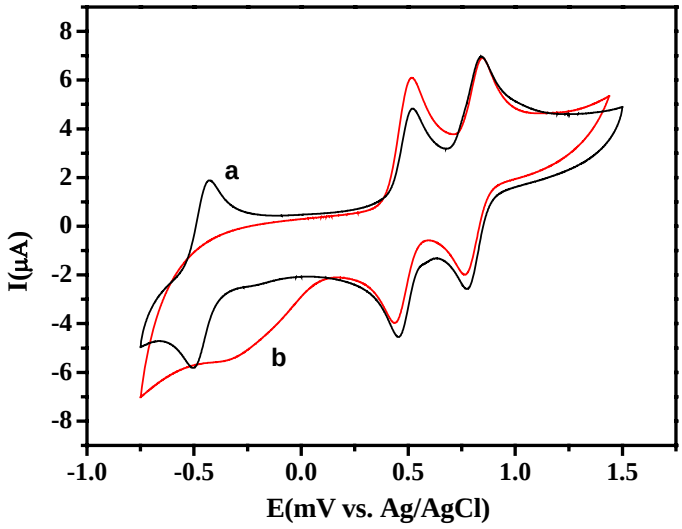


Figure S27. Cyclic voltammograms of dyad **3** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 2 equiv of Zn^{2+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

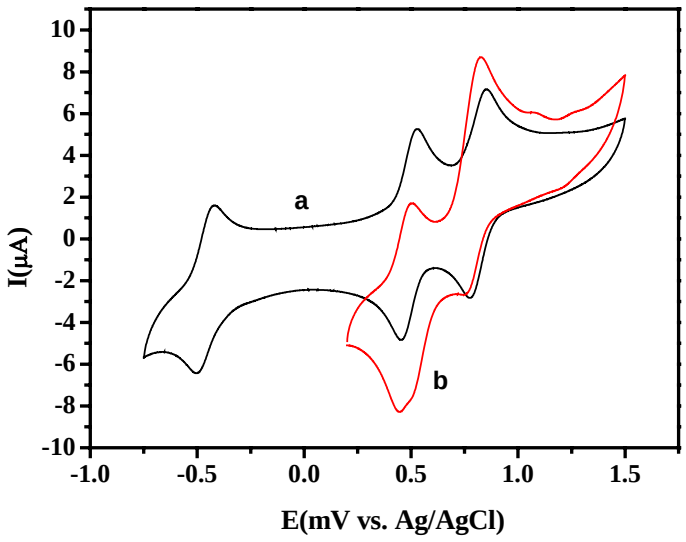


Figure S28. Cyclic voltammograms of dyad **3** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 2 equiv of Sc^{3+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

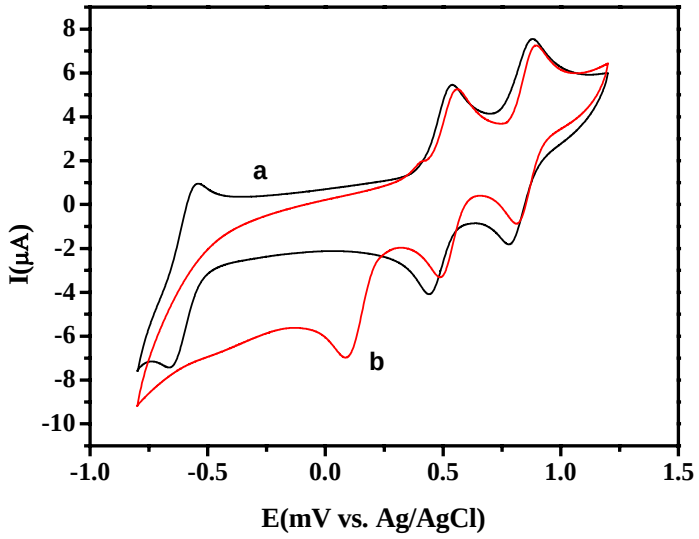


Figure S29. Cyclic voltammograms of dyad **4** (5.0×10^{-4} M) (a, black) before and (b, red) after addition of 1.2 equiv of Pb^{2+} in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

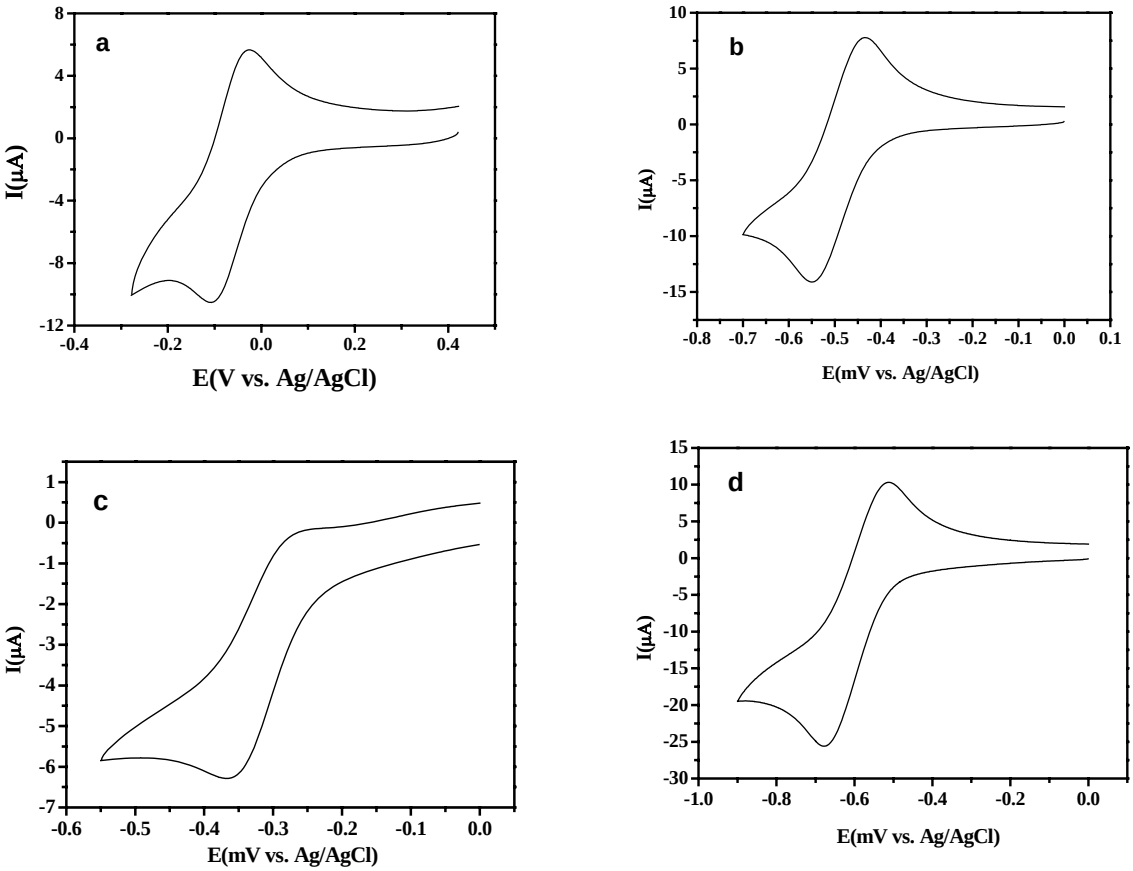


Figure S30. Cyclic voltammograms of compounds **13** (5.0×10^{-4} M) (a), **14** (5.0×10^{-4} M) (b) **12** (5.0×10^{-4} M) (c), and **15** (1.0×10^{-3} M) (d) in a mixture of CH_2Cl_2 and CH_3CN at a scan rate of 100 mV S^{-1}.

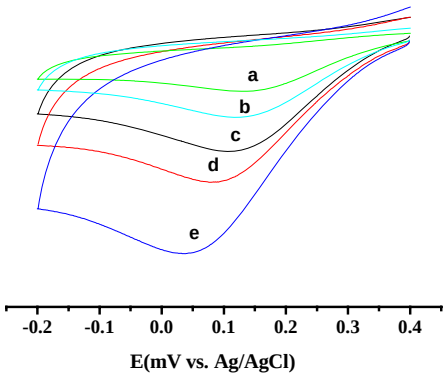


Figure S31. Cathodic waves of compound **12** in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-4} M) in the presence of 4.0 equiv of $Pb(ClO_4)_2$ at various sweep rates: (a) 10, (b) 50, (c) 100, (d) 200, (e) 300 mV s^{-1}

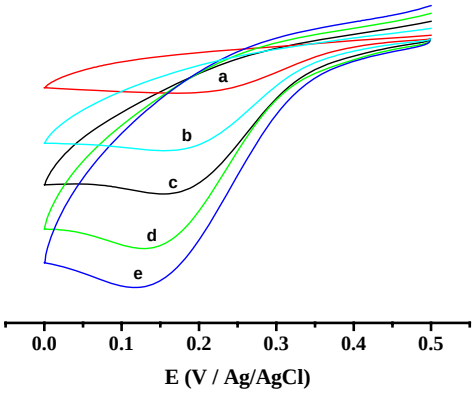


Figure S32. Cathodic waves of compound **13** in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-4} M) in the presence of 4.0 equiv of $Pb(ClO_4)_2$ at various sweep rates: (a) 10, (b) 50, (c) 100, (d) 200, (e) 300 mV s^{-1}

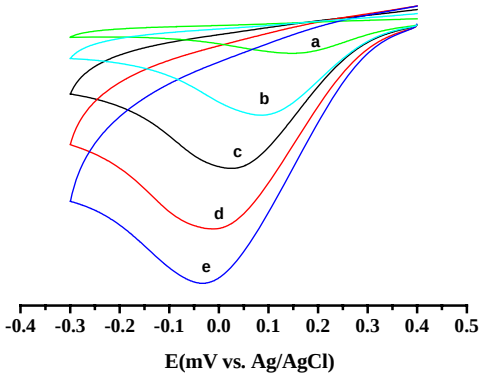


Figure S33. Cathodic waves of compound **14** in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-4} M) in the presence of 2.0 equiv of $Pb(ClO_4)_2$ at various sweep rates: (a) 10, (b) 50, (c) 100, (d) 200, (e) 300 mV s^{-1}

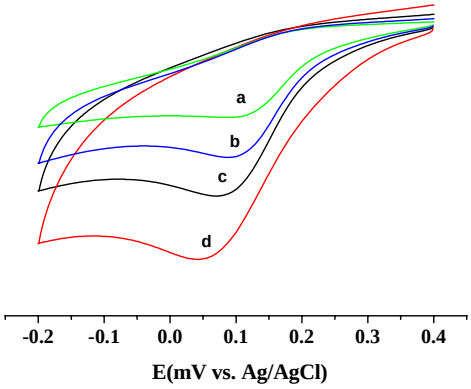


Figure S34. Cathodic waves of compound **15** in a mixture of CH_2Cl_2 and CH_3CN (1:1, v/v; 5.0×10^{-4} M) in the presence of 4.0 equiv of $Pb(ClO_4)_2$ at various sweep rates: (a) 10, (b) 50, (c) 100, (d) 200 mV s^{-1}

According to previous report (*J. Chem.. Soc. Perkin Trans. II*, **1985**, 371-378 and *Bull. Chem. Soc. Jpn.* **1983**, *56*, 2220-2227), the width of the cathodic wave ($E_{red}^{p/2} - E_{red}^{p}$) in such an irreversible system is known to depend on the transfer coefficient β according to equation (1), where *F* is the faraday constant and the other notations are conventional.

$E_{red}^{p/2} - E_{red}^{p} = 1.857\ RT/\beta F$ ……(1)

According to equation (2), the reduction potential E_{red}^{0} can be evaluated from the intercept of the linear correlation between E_{red}^{p} and $4(1 - 2\beta)$. β value is obtained from the cyclic voltammogram by using equation (1).

$E_{red}^{p} = E_{red}^{0} - 4(1 - 2\beta)\ \Delta G_0^{\ddagger}/F$…… .(2)

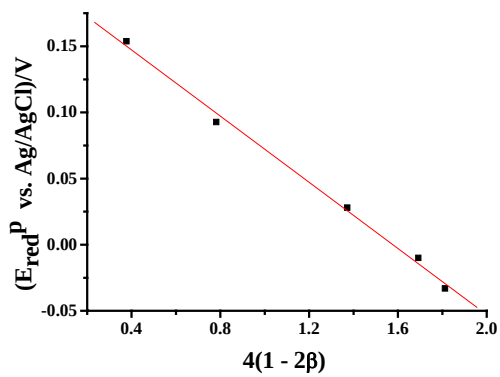


Figure S35. The plot of the cathodic-peak potentials E_{red}^{p} (vs. Ag/AgCl) of compound **12** (5.0×10^{-3} M) in the presence of 2.0 equiv of $Pb(ClO_4)_2$ vs. 4(1-2β); the reduction potential of compound **14** in the presence of Pb^{2+} was estimated to be 0.22 V.

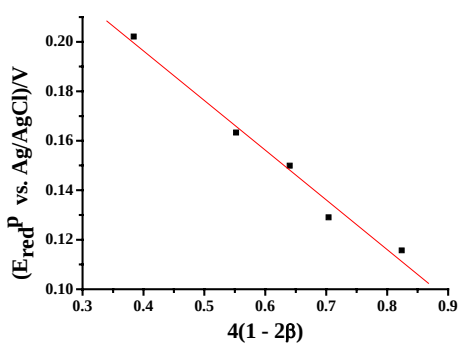


Figure S36. The plot of the cathodic-peak potentials E_{red}^{p} (vs. Ag/AgCl) of compound **13** (5.0×10^{-3} M) in the presence of 4.0 equiv of $Pb(ClO_4)_2$ vs. 4(1-2β); the reduction potential of compound **13** in the presence of Pb^{2+} was estimated to be 0.28 V.

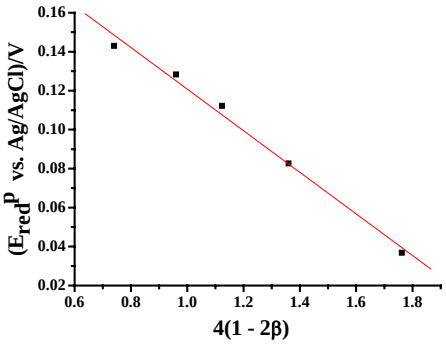


Figure S37. The plot of the cathodic-peak potentials E_{red}^{p} (vs. Ag/AgCl) of compound **14** (5.0×10^{-3} M) in the presence of 2.0 equiv of $Pb(ClO_4)_2$ vs. 4(1-2β); the reduction potential of compound **13** in the presence of Pb^{2+} was estimated to be 0.19 V.

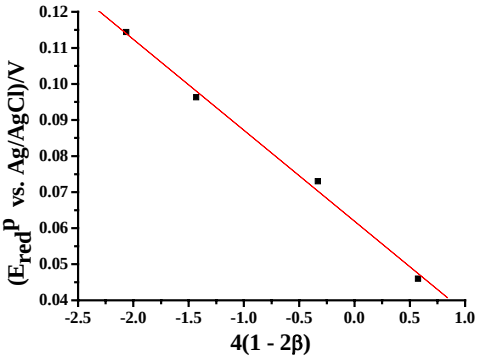
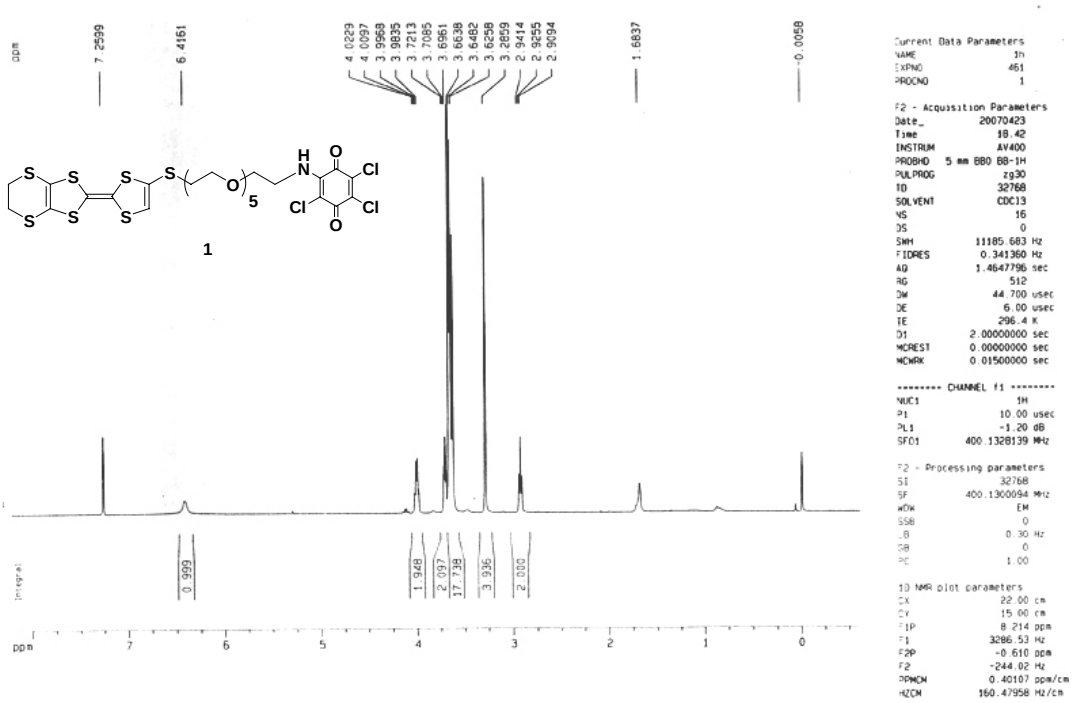
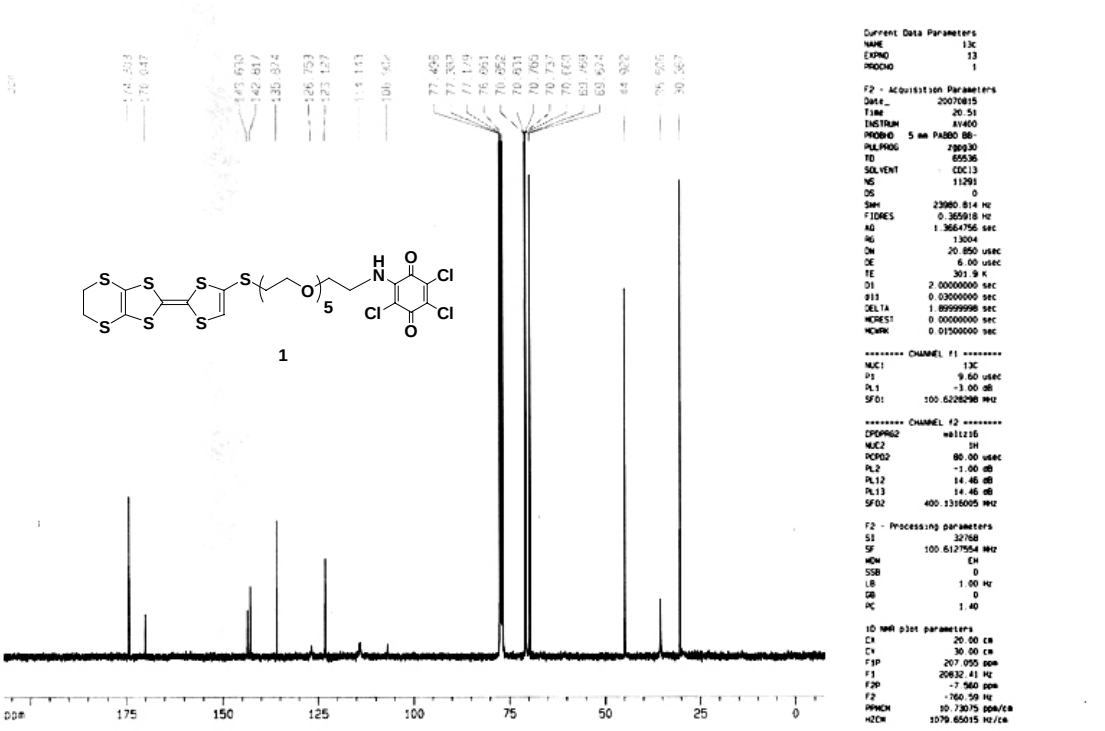
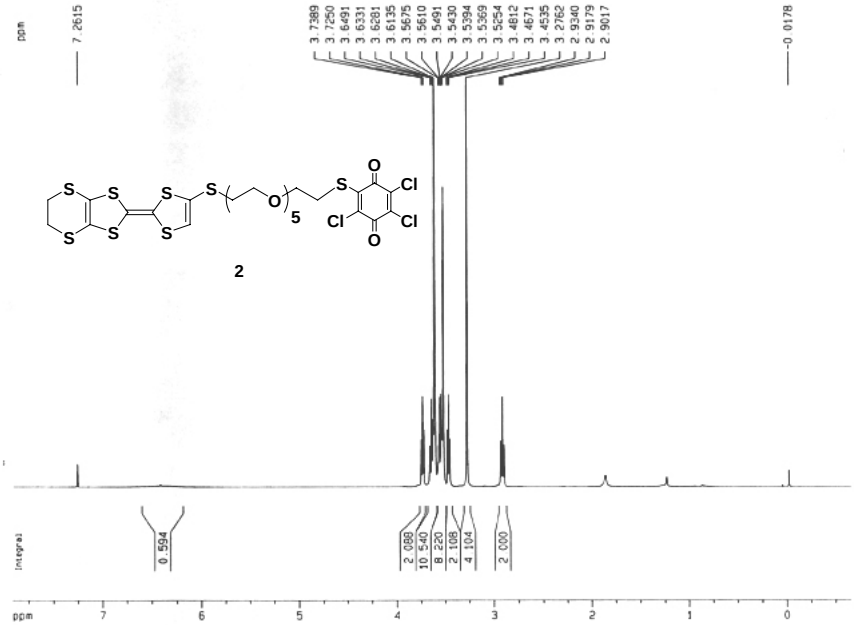


Figure S38. The plot of the cathodic-peak potentials E_{red}^{p} (vs. Ag/AgCl) of compound **15** (5.0×10^{-3} M) in the presence of 2.0 equiv of $Pb(ClO_4)_2$ vs. 4(1-2β); the reduction potential of compound **15** in the presence of Pb^{2+} was estimated to be 0.06 V.

6. The ^{1}H NMR and ^{13}C NMR of dyads 1, 2, 3, and 4, and compounds 7, 8, 10, 12, and 15.







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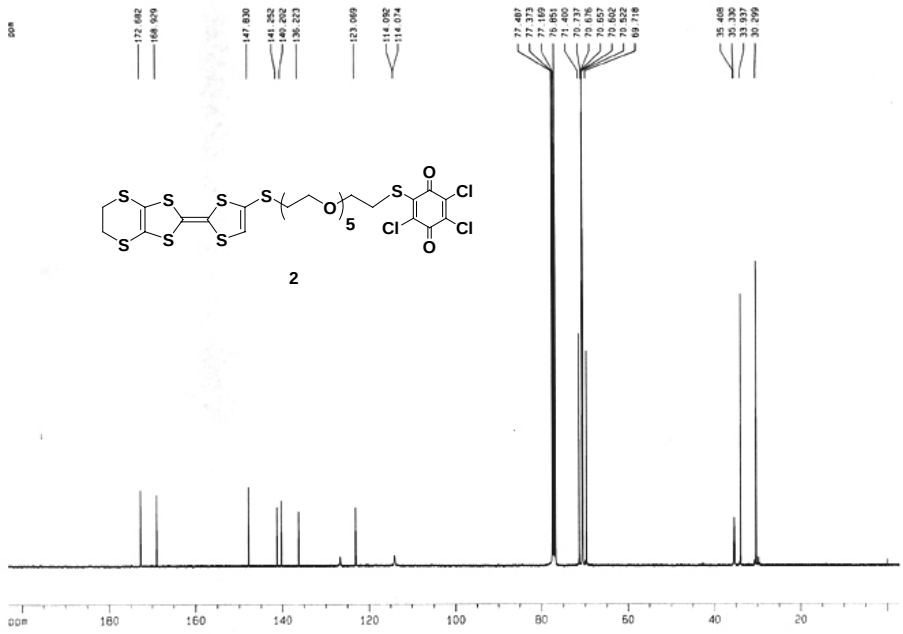

2

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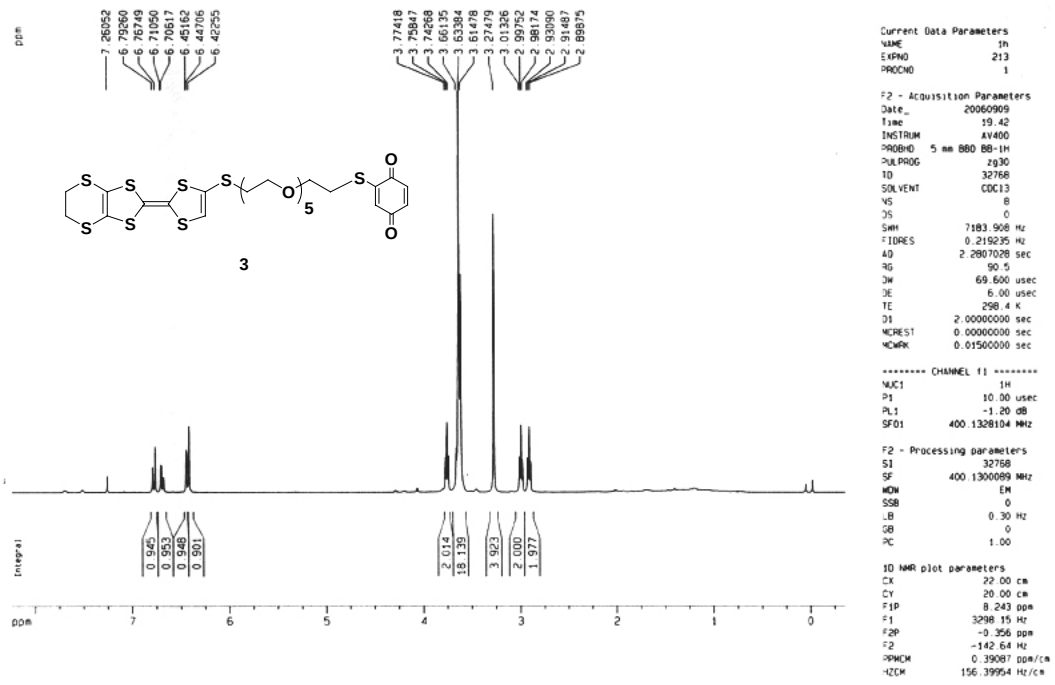
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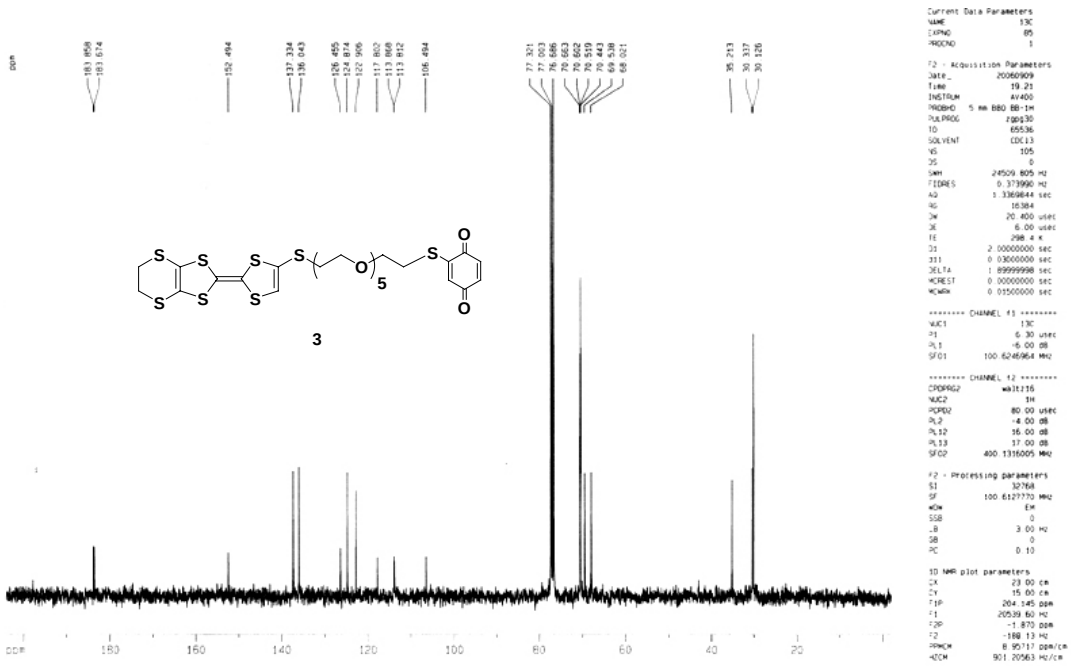
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PCPD2 80.00 usec
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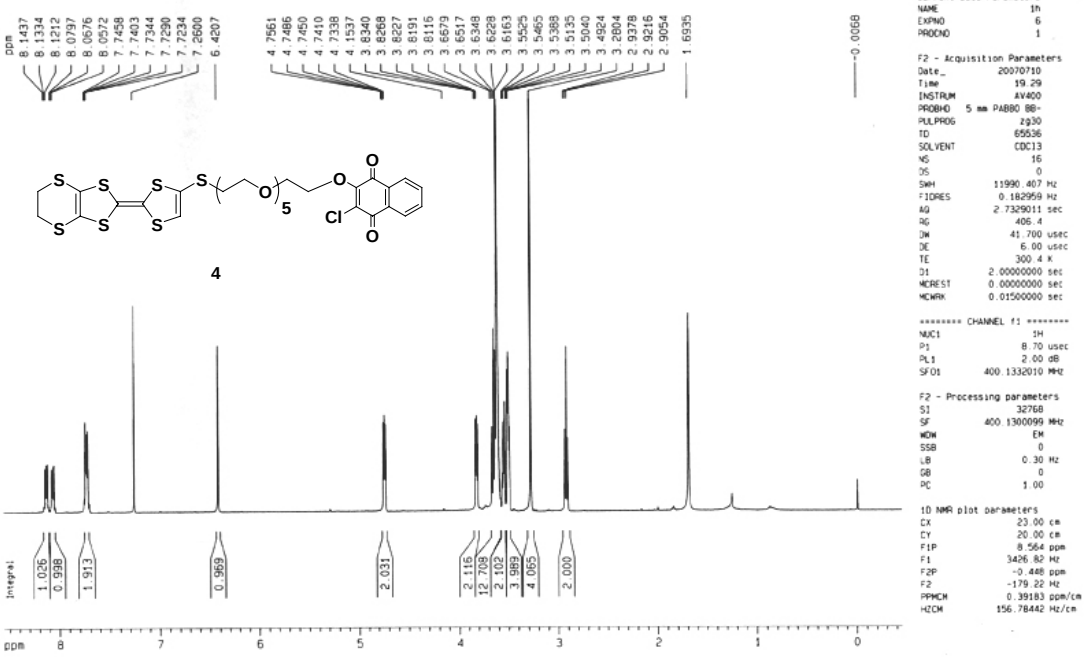
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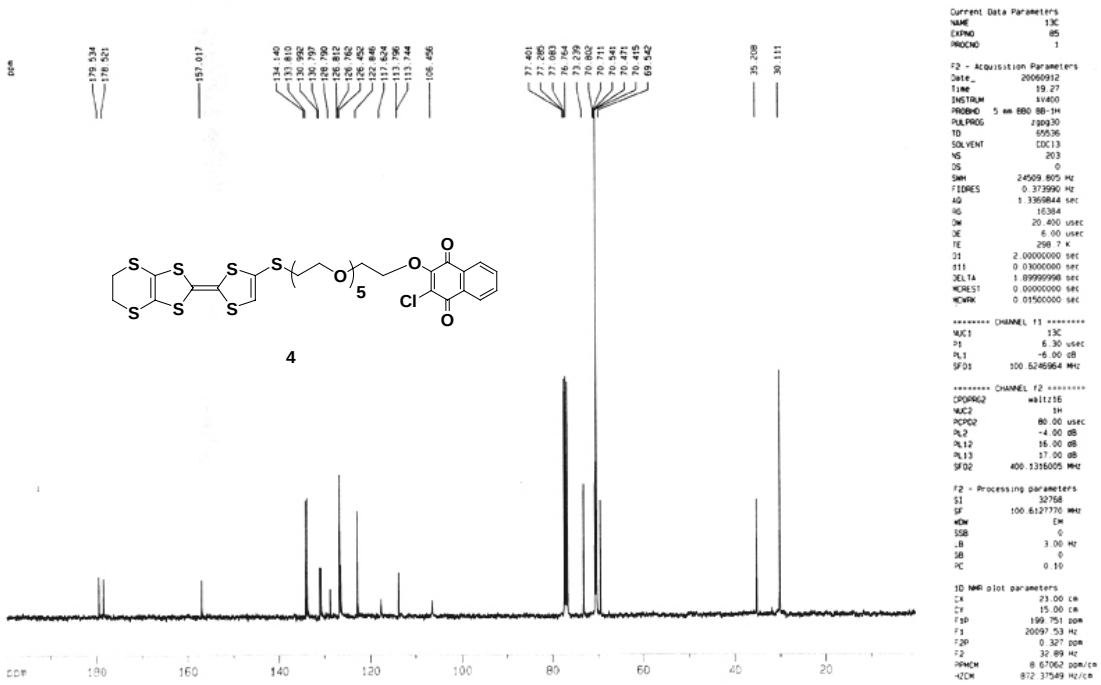
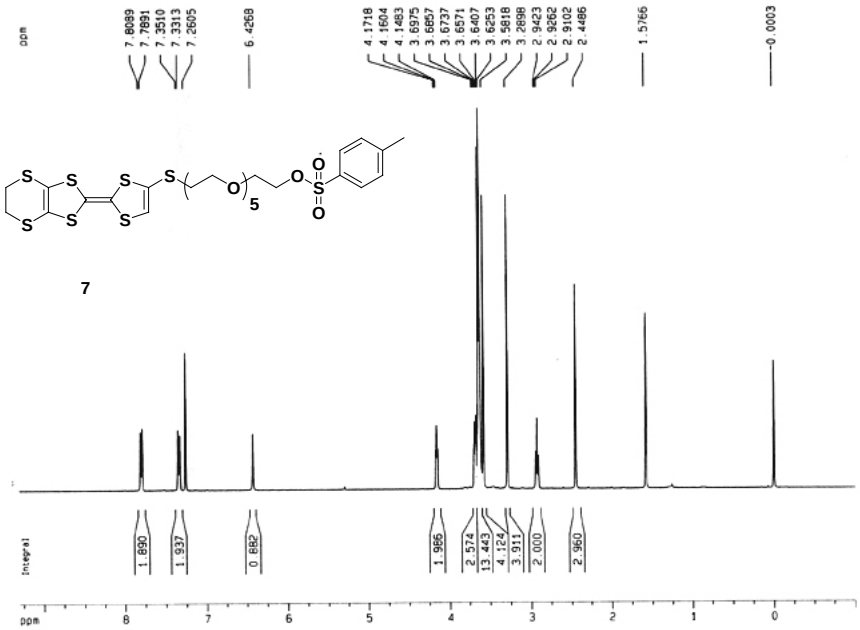
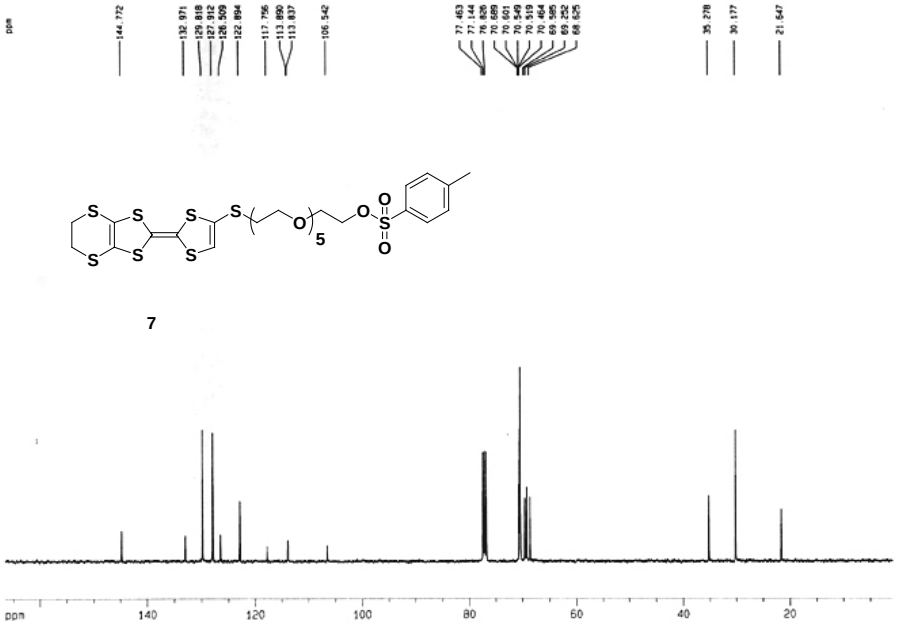
4
3
2
1
0
Current Data Parameters
NAME 1h
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070710
Time 19.29
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 406.4
DW 41.700 usec
DE 6.00 usec
TE 300.4 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.70 usec
PL1 2.00 dB
SFO1 400.1332010 MHz
F2 - Processing parameters
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.00 cm
CY 20.00 cm
F1P 8.564 ppm
F1 3426.82 Hz
F2P -0.448 ppm
F2 -179.22 Hz
PPMCM 0.39183 ppm/cm
HZCM 156.78442 Hz/cm


ppm
179.534
178.521
157.017
134.140
133.810
130.992
130.797
128.790
126.812
126.762
126.452
122.846
117.624
113.796
113.744
106.496
77.401
77.189
76.977
76.764
73.239
70.802
70.711
70.541
70.471
70.415
69.542
35.208
30.111
S
S
S
S
S
S
S
S
O
O
5
O
Cl
O
4
ppm
180
160
140
120
100
80
60
40
20
Current Data Parameters
NAME 13C
EXPNO 85
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060912
Time 19.27
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 0
SWH 24509.805 Hz
FIDRES 0.373990 Hz
AQ 1.3369844 sec
RG 16384
DW 20.400 usec
DE 6.00 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 100.6246964 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 16.00 dB
PL13 17.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127770 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.10
1D NMR plot parameters
CX 23.00 cm
CY 15.00 cm
F1P 199.751 ppm
F1 20097.53 Hz
F2P 0.327 ppm
F2 32.89 Hz
PPMCM 8.67062 ppm/cm
HZCM 872.37549 Hz/cm



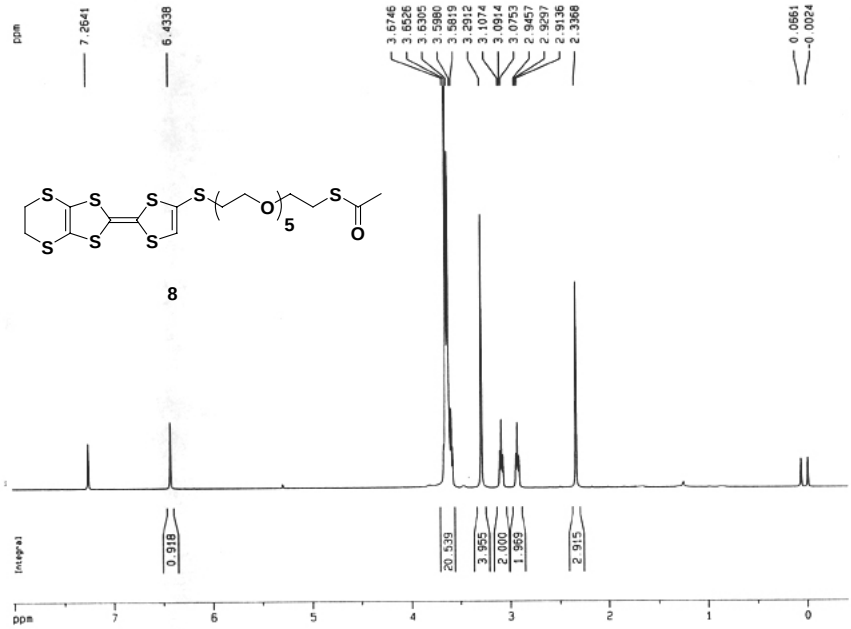
7

```
Current Data Parameters
NAME                 1h
EXPNO               441
PROCNO                1

F2 - Acquisition Parameters
Date_           20070412
Time               18.59
INSTRUM            AV400
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           11185.683 Hz
FIDRES         0.341360 Hz
AQ            1.4647796 sec
RG               1149.4
DW               44.700 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1               -1.20 dB
SFO1        400.1328139 MHz

F2 - Processing parameters
SI                32768
SF          400.1300086 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.00 cm
CY                10.00 cm
F1P               9.308 ppm
F1              3724.36 Hz
F2P              -1.000 ppm
F2              -400.22 Hz
PPMCM          0.46855 ppm/cm
HZCM          187.48091 Hz/cm
```

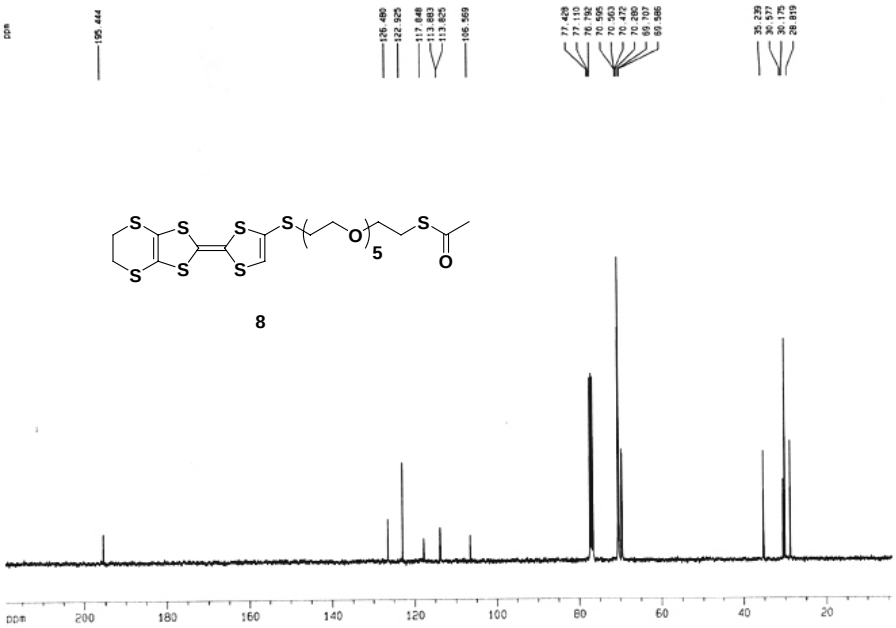


7

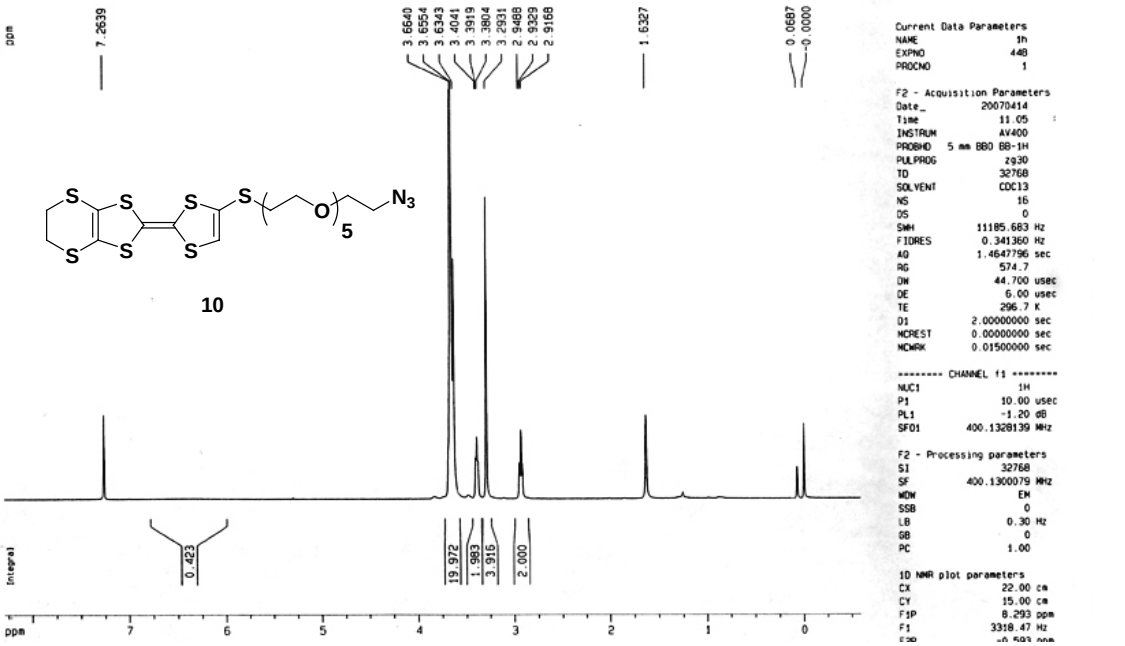
```
Current Data Parameters
NAME                 13C
EXPNO                123
PROCNO                1

F2 - Acquisition Parameters
Date_           20070412
Time               19.43
INSTRUM            AV400
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   132
DS                    0
SWH           24509.805 Hz
FIDRES         0.373990 Hz
AQ            1.3369844 sec
RG               16384
DW               20.400 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
DELTA         1.89999998 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                6.30 usec
PL1               -6.00 dB
SFO1        100.6246964 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            80.00 usec
PL2               -4.00 dB
PL12              16.00 dB
PL13              17.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127725 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 0.10

1D NMR plot parameters
CX                23.00 cm
CY                 5.00 cm
F1P             166.599 ppm
F1            16762.02 Hz
F2P               0.860 ppm
F2               86.53 Hz
PPMCM          7.20606 ppm/cm
HZCM          725.02209 Hz/cm
```

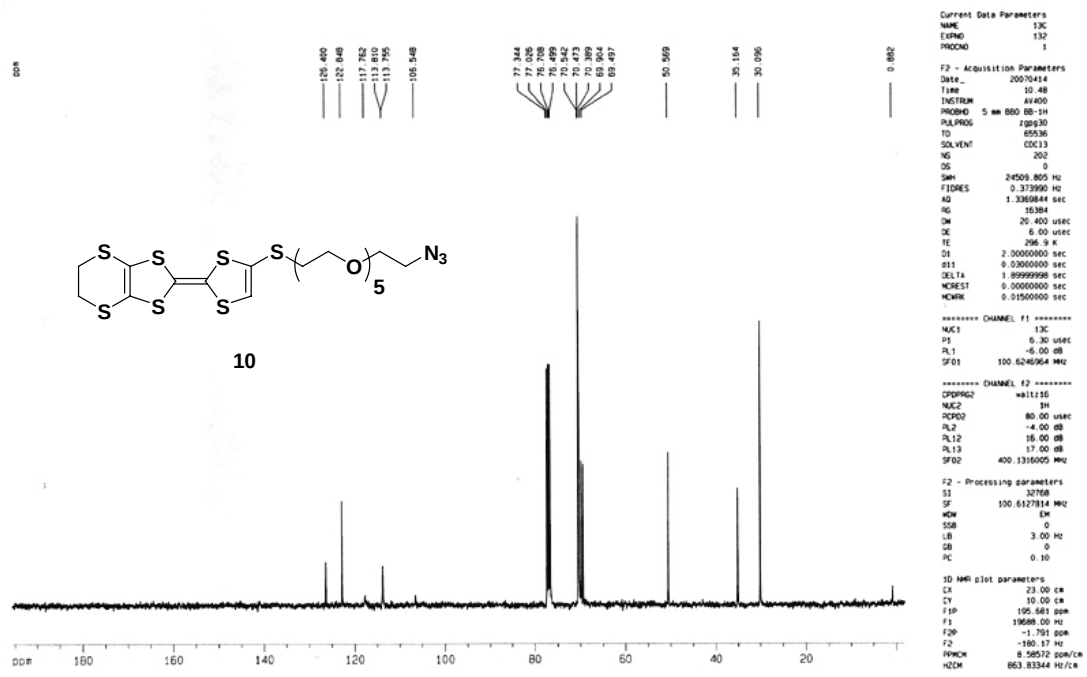


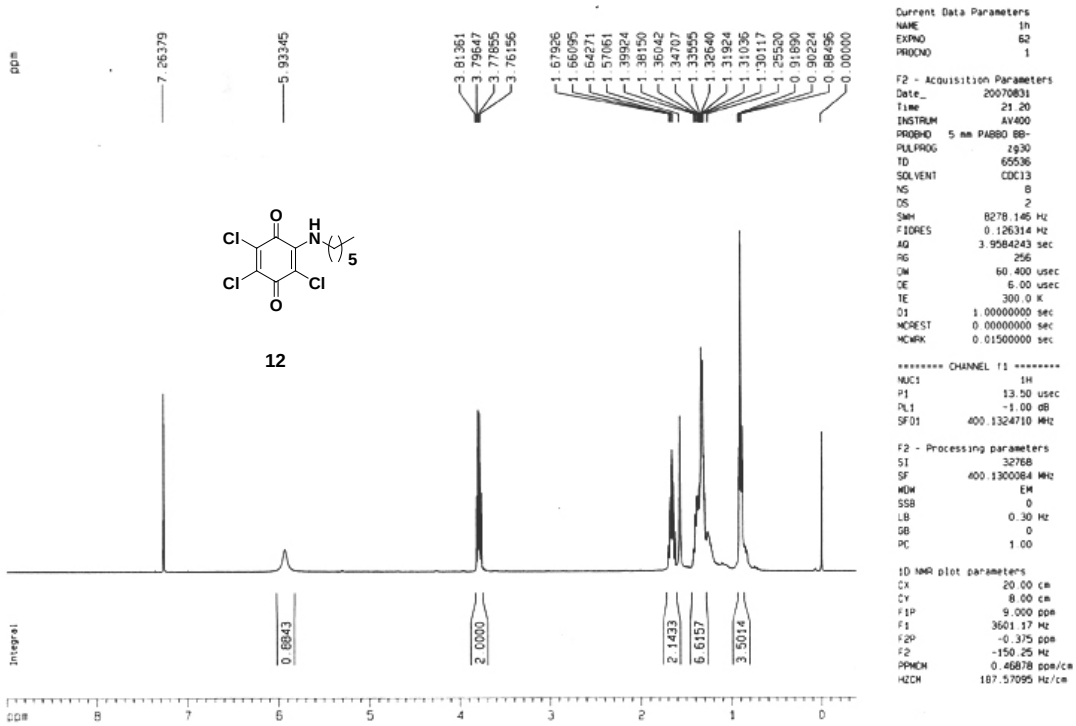

```
Current Data Parameters
NAME                 1h
EXPNO               452
PROCNO                1

F2 - Acquisition Parameters
Date_           20070416
Time              18.49
INSTRUM           AV400
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           11185.683 Hz
FIDRES         0.341360 Hz
AQ            1.4647796 sec
RG                  362
DW               44.700 usec
DE                6.00 usec
TE                296.3 K
D1            2.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 1H
P1                10.00 usec
PL1                -1.20 dB
SFO1        400.1328139 MHz

F2 - Processing parameters
SI                32768
SF          400.1300076 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.00 cm
CY                15.00 cm
F1P                8.022 ppm
F1              3209.78 Hz
F2P               -0.410 ppm
F2              -163.86 Hz
PPMCM          0.38324 ppm/cm
HZCM          153.34715 Hz/cm
```

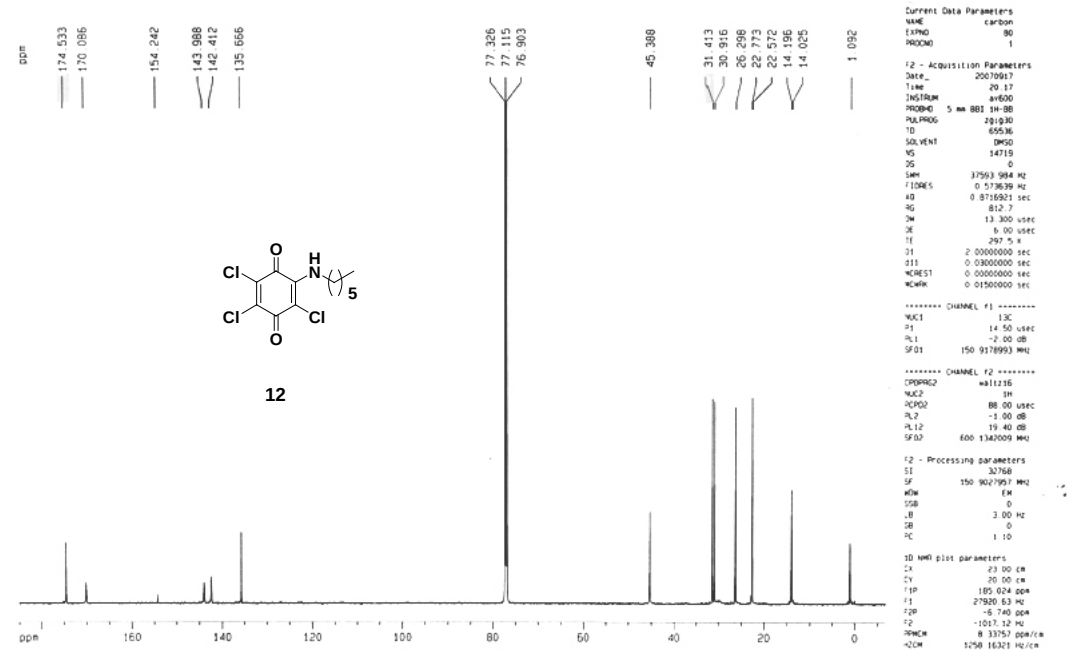


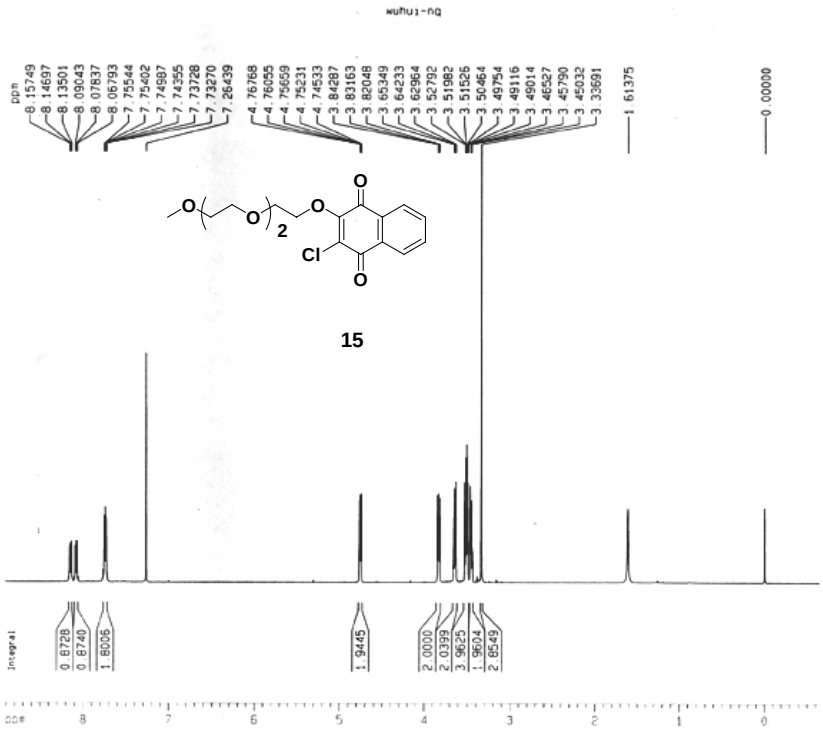

```
Current Data Parameters
NAME                 13C
EXPNO                133
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070416
Time              19.04
INSTRUM           AV400
PROBHD   5 mm BBO BB-1H
PULPROG            zgpg30
TD                65536
SOLVENT           CDCl3
NS                   197
DS                     0
SWH           24509.805 Hz
FIDRES         0.373990 Hz
AQ            1.3369844 sec
RG                  8192
DW               20.400 usec
DE                6.00 usec
TE                296.5 K
D1            2.00000000 sec
D11           0.03000000 sec
DELTA         1.89999998 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                 6.30 usec
PL1                -6.00 dB
SFO1        100.6246964 MHz

-------- CHANNEL f2 --------
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                -4.00 dB
PL12               16.00 dB
PL13               17.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127729 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 0.10

1D NMR plot parameters
CX                23.00 cm
CY                 8.00 cm
F1P              219.075 ppm
F1             22041.77 Hz
F2P                4.273 ppm
F2               429.92 Hz
PPMCM          9.33923 ppm/cm
HZCM         939.64569 Hz/cm
```


ppm
7.2639
3.6640
3.6554
3.6343
3.4041
3.3919
3.3804
3.2931
2.9488
2.9329
2.9168
1.6327
0.0687
-0.0000
10
Integral
0.423
19.972
1.983
3.916
2.000
Current Data Parameters
NAME 1h
EXPNO 448
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070414
Time 11.05
INSTRUM AV400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 11185.683 Hz
FIDRES 0.341360 Hz
AQ 1.4647796 sec
RG 574.7
DW 44.700 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
NCREST 0.00000000 sec
NCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -1.20 dB
SF01 400.1328139 MHz
F2 - Processing parameters
SI 32768
SF 400.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 15.00 cm
F1P 8.293 ppm
F1 3318.47 Hz


ppm
126.400
122.848
117.762
113.810
113.755
106.548
77.344
77.026
76.708
76.499
70.542
70.473
70.369
69.904
69.497
50.569
35.184
30.096
0.882
10
Current Data Parameters
NAME 13C
EXPNO 132
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070414
Time 10.48
INSTRUM AV400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 202
DS 0
SWH 24509.805 Hz
FIDRES 0.373990 Hz
AQ 1.3369844 sec
RG 16384
DW 20.400 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
NCREST 0.00000000 sec
NCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SF01 100.6246964 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 16.00 dB
PL13 17.00 dB
SF02 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127814 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.10
1D NMR plot parameters
CX 23.00 cm
CY 10.00 cm
F1P 195.681 ppm
F1 19688.00 Hz
F2P -1.791 ppm
F2 -180.17 Hz
PPMCM 8.58572 ppm/cm
HZCM 863.83344 Hz/cm


ppm
7.26379
5.93345
3.81361
3.79647
3.77855
3.76156
1.67926
1.66095
1.64271
1.57061
1.39924
1.38150
1.36042
1.34707
1.33595
1.32640
1.31924
1.31036
1.30117
1.25520
0.91890
0.90224
0.88496
0.00000
Cl
Cl
Cl
Cl
O
O
H
N
5
12
Integral
0.8843
2.0000
2.1433
6.6157
3.5014
ppm
8
7
6
5
4
3
2
1
0
Current Data Parameters
NAME 1h
EXPNO 62
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070831
Time 21.20
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.375 ppm
F2 -150.25 Hz
PPMCM 0.46878 ppm/cm
HZCM 187.57095 Hz/cm


ppm
174.533
170.086
154.242
143.988
142.412
135.666
77.326
77.115
76.903
45.388
31.413
30.916
26.298
22.773
22.572
14.196
14.025
1.092
Cl
Cl
Cl
Cl
O
O
H
N
5
12
ppm
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME carbon
EXPNO 80
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070917
Time 20.17
INSTRUM av600
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 14719
DS 0
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8716921 sec
RG 812.7
DW 13.300 usec
DE 6.00 usec
TE 297.5 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.50 usec
PL1 -2.00 dB
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00 usec
PL2 -1.00 dB
PL12 19.40 dB
SFO2 600.1342009 MHz
F2 - Processing parameters
SI 32768
SF 150.9027957 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.10
1D NMR plot parameters
CX 23.00 cm
CY 20.00 cm
F1P 185.024 ppm
F1 27920.63 Hz
F2P -6.740 ppm
F2 -1017.12 Hz
PPMCM 8.33757 ppm/cm
HZCM 1258.16321 Hz/cm



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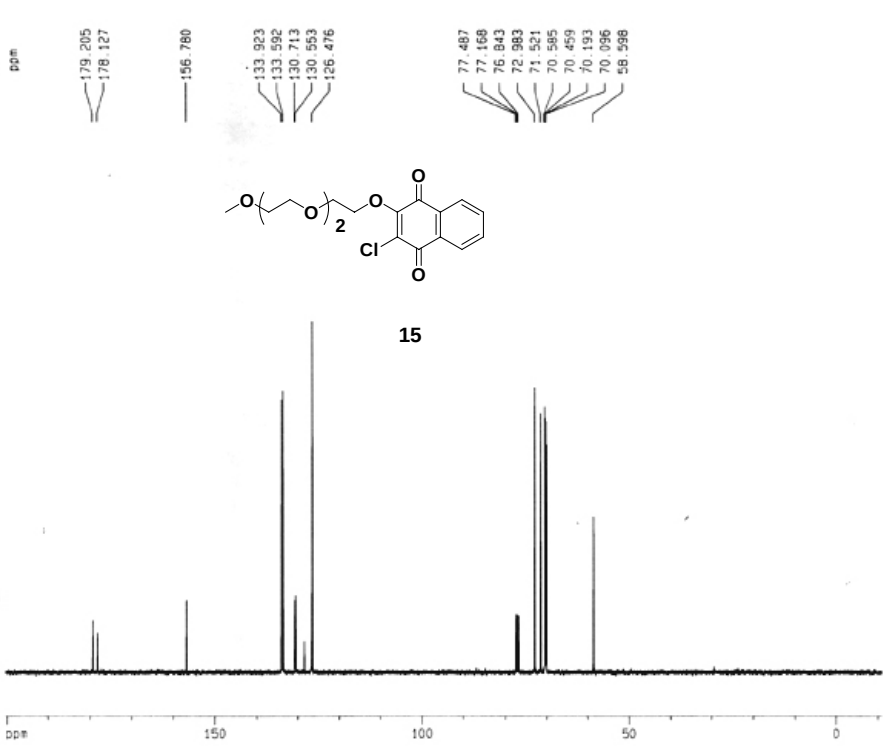
```
Current Data Parameters
NAME                 1h
EXPNO                102
PROCNO               1

F2 - Acquisition Parameters
Date_            20070929
Time               16.33
INSTRUM            AV400
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                 65536
SOLVENT            CDCl3
NS                 8
DS                 2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                 456.1
DW                 60.400 usec
DE                 6.00 usec
TE                 298.7 K
D1               1.00000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1               1H
P1                 13.50 usec
PL1                -1.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF             400.1300081 MHz
WDW                EM
SSB                0
LB                 0.30 Hz
GB                 0
PC                 1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 15.00 cm
F1P                8.912 ppm
F1                 3566.06 Hz
F2P                -0.644 ppm
F2                 -257.62 Hz
PPMCM              0.47783 ppm/cm
HZCM               191.19363 Hz/cm
```



15

```
Current Data Parameters
NAME                 13c
EXPNO                20
PROCNO               1

F2 - Acquisition Parameters
Date_            20070831
Time               21.03
INSTRUM            AV400
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 102
DS                 0
SWH              23980.814 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                 9195.2
DW                 20.850 usec
DE                 6.00 usec
TE                 300.7 K
D1               1.50000000 sec
d11              0.03000000 sec
DELTA            1.39999998 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1               13C
P1                 9.60 usec
PL1                -3.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2               1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.46 dB
PL13               14.46 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF             100.6127868 MHz
WDW                EM
SSB                0
LB                 1.00 Hz
GB                 0
PC                 1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 8.00 cm
F1P                200.363 ppm
F1                 20159.11 Hz
F2P                -10.997 ppm
F2                 -1106.44 Hz
PPMCM              10.56802 ppm/cm
HZCM               1063.27759 Hz/cm
```