

Electronic Supplementary Information for

Pyrazole-, Isoxazole- and Pyrrole-ring Fused Derivatives of C₆₀: Synthesis and electrochemical properties as well as morphological characterization

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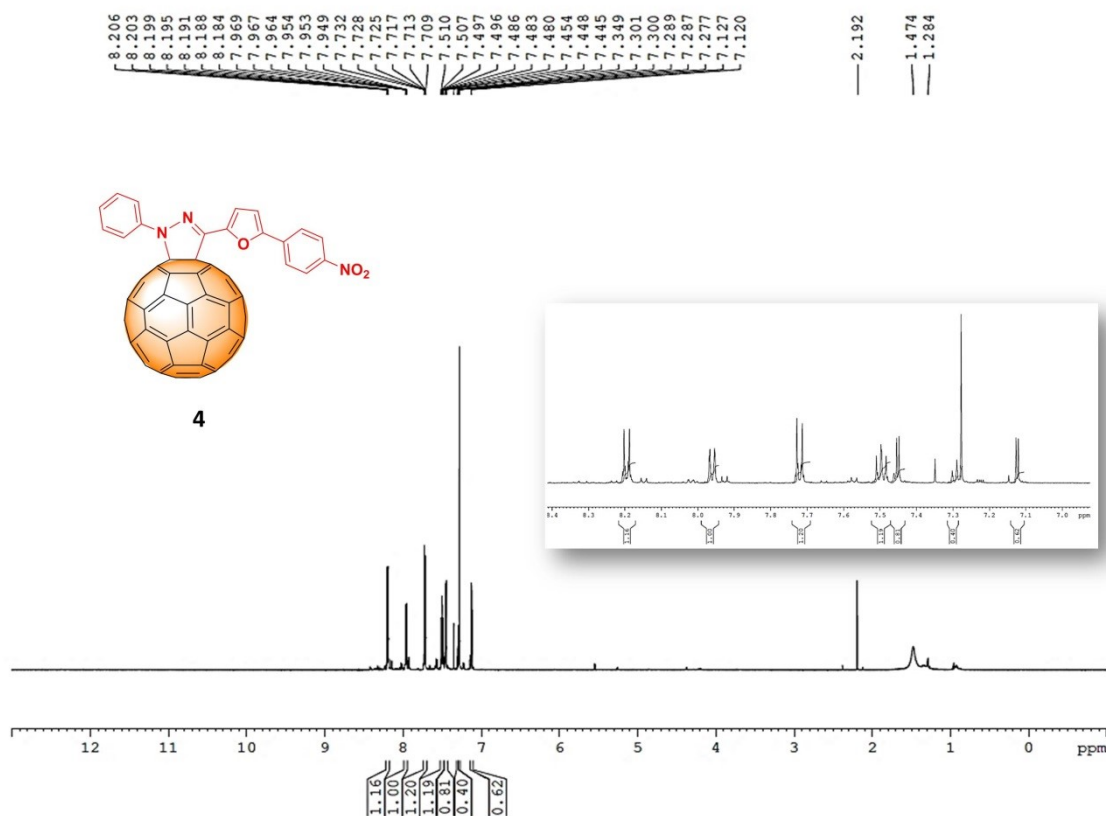
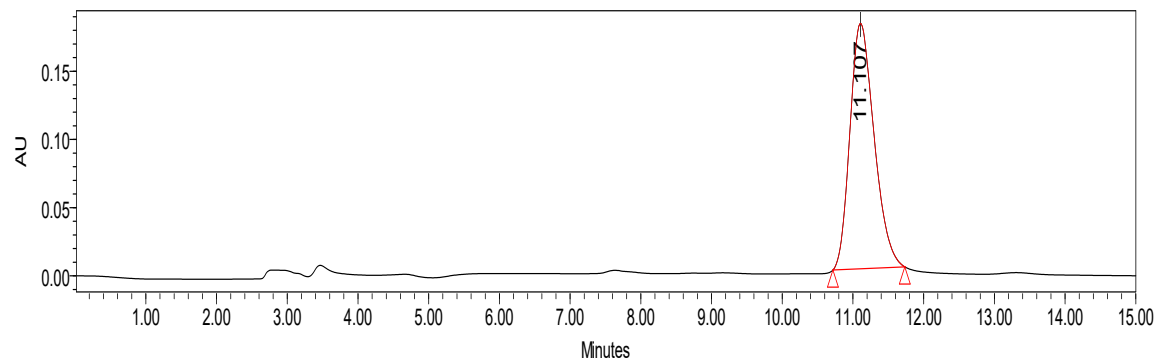


Figure S1. The ¹H NMR spectrum of compound 4 (600.13 MHz, solvent CDCl₃)



	Retention Time	Area	% Area	Height	% Height
1	11.107	4275772	100.00	180203	100.00

Figure S2. HPLC chromatogram of compound **4**

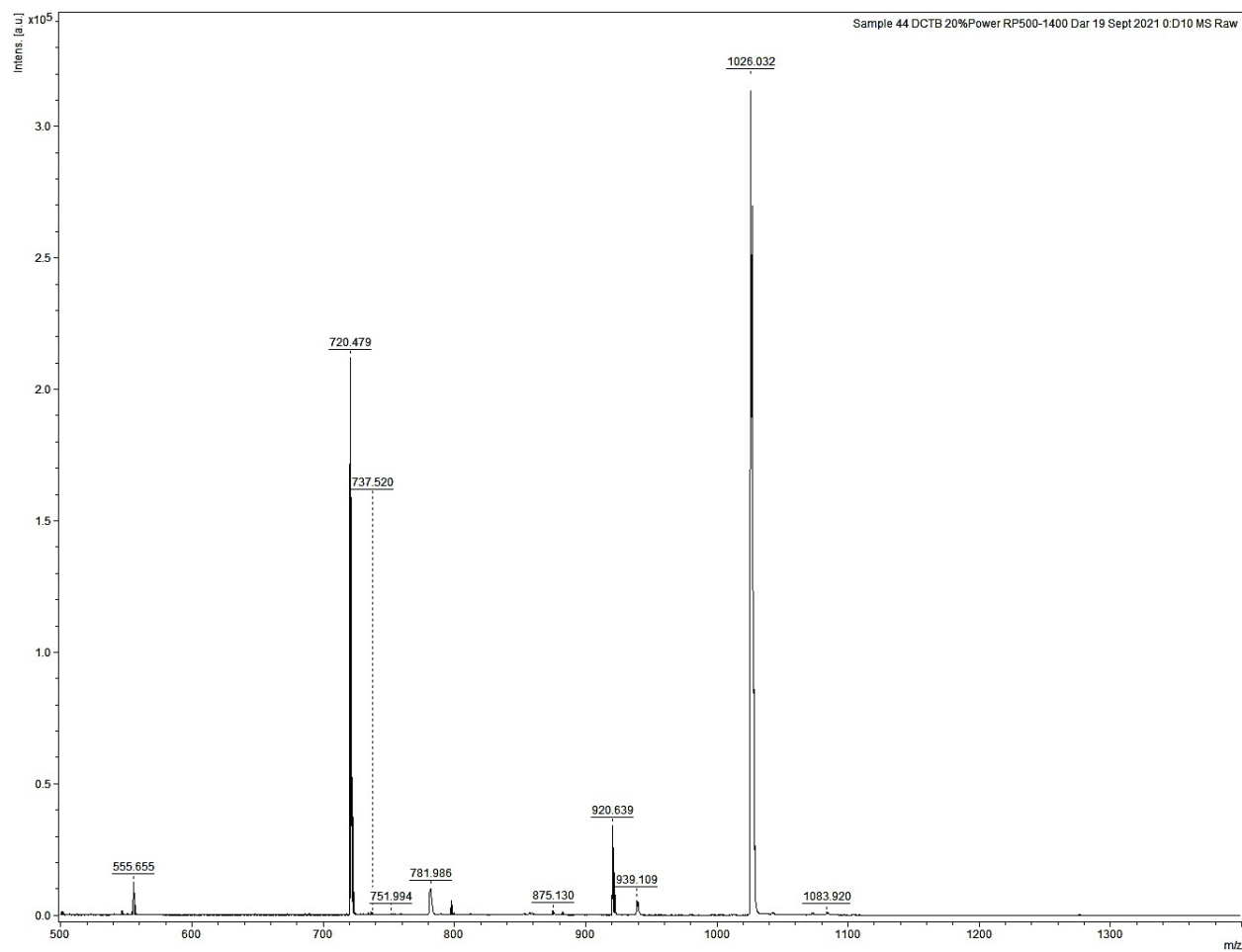


Figure S3. HRMS (ESI-TOF) of compound **4**

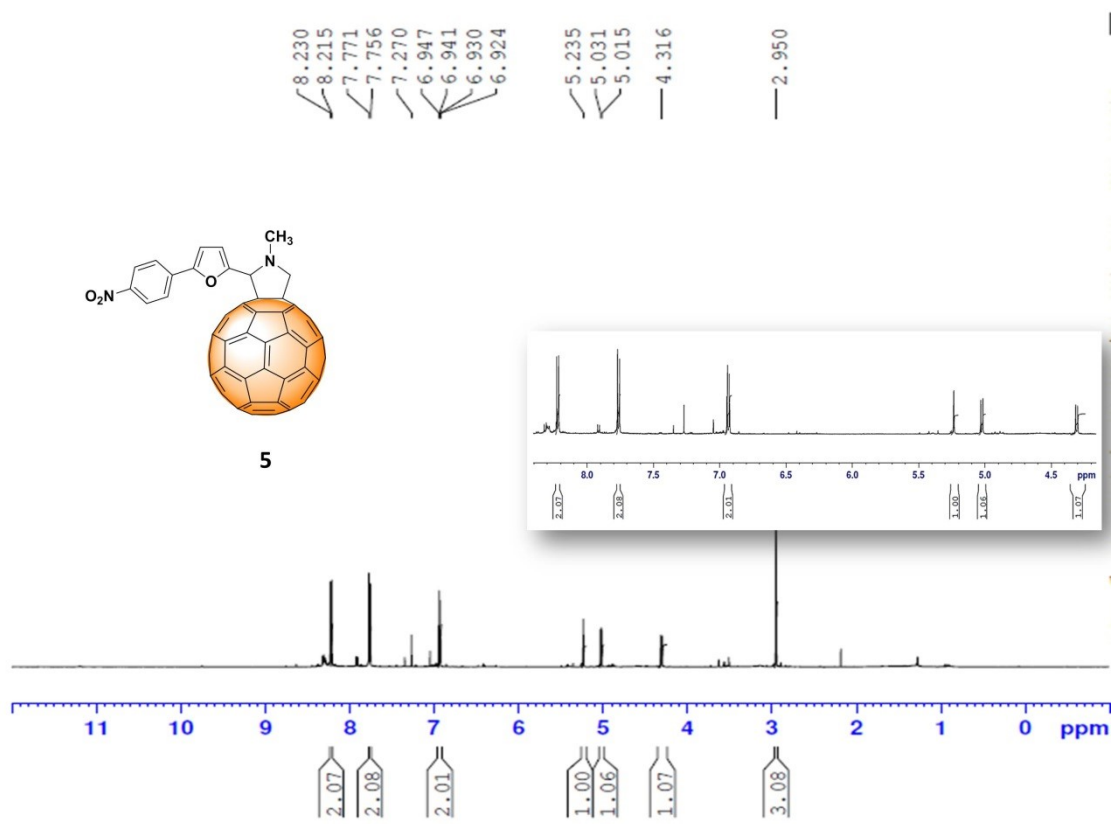


Figure S4. The ¹H NMR spectrum of compound **5** (600.13 MHz, solvent CDCl₃)

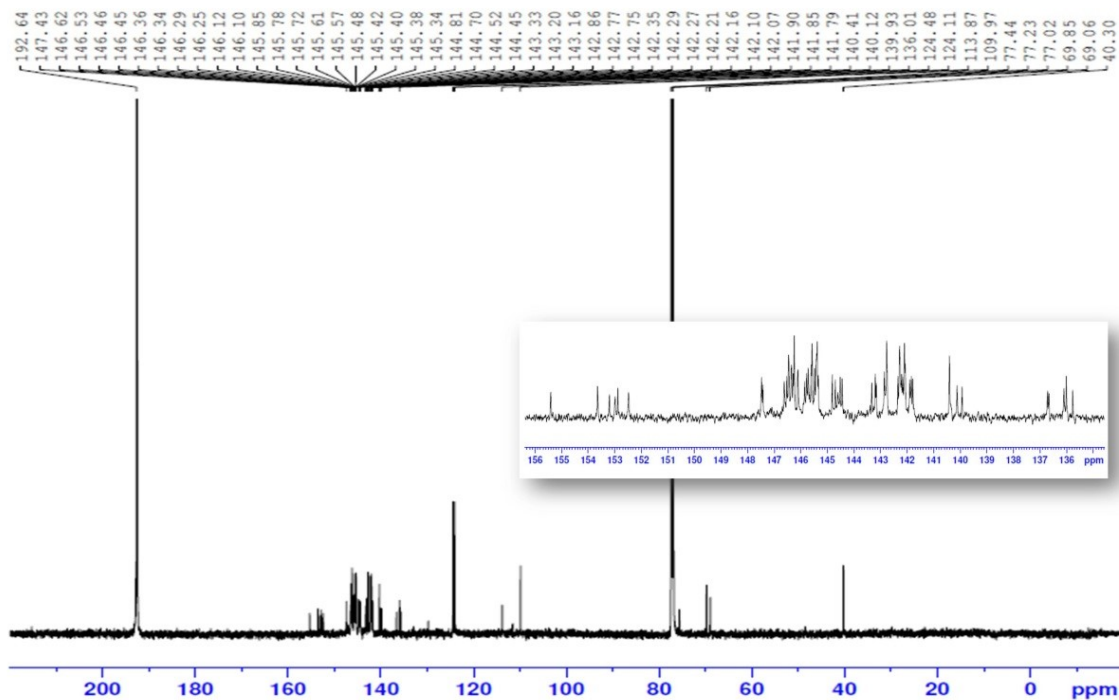


Figure S5. The ¹³C NMR spectrum of compound **5** (150 MHz, solvent CS₂ : CDCl₃ = 3:1)

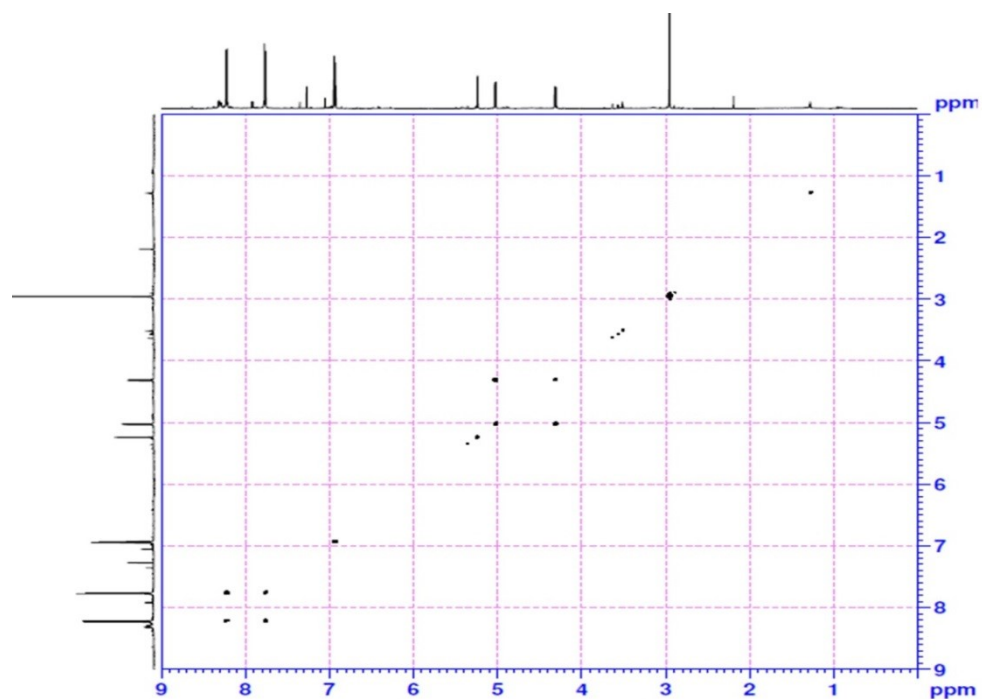


Figure S6. H-H COSY NMR spectrum of compound **5** (600.13 MHz, solvent CDCl_3)

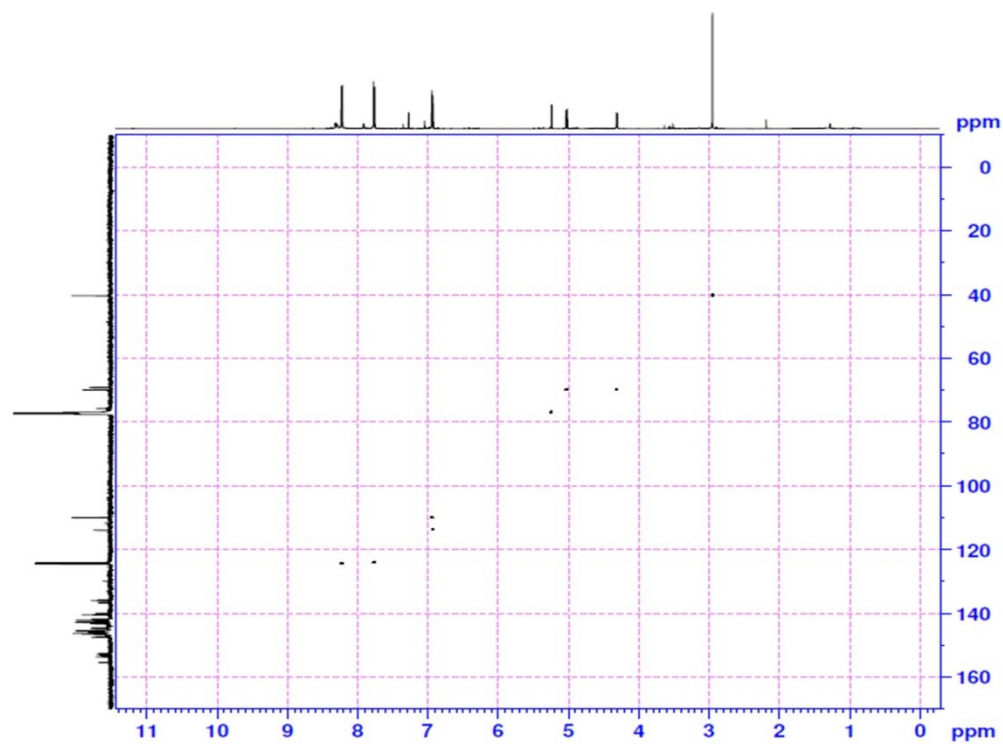


Figure S7. The HSQC spectrum of compound **5** (600.13 MHz for ^1H and ^{13}C , solvent $\text{CS}_2 : \text{CDCl}_3 = 3:1$)

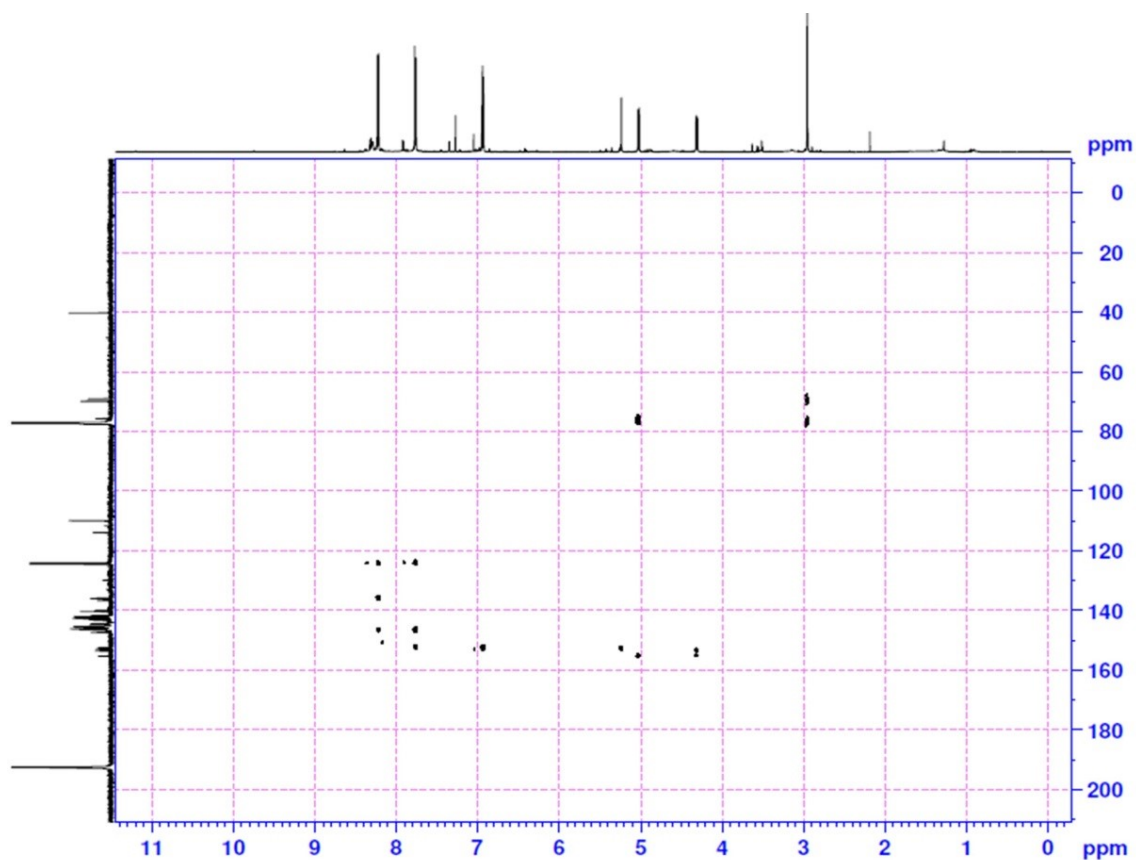
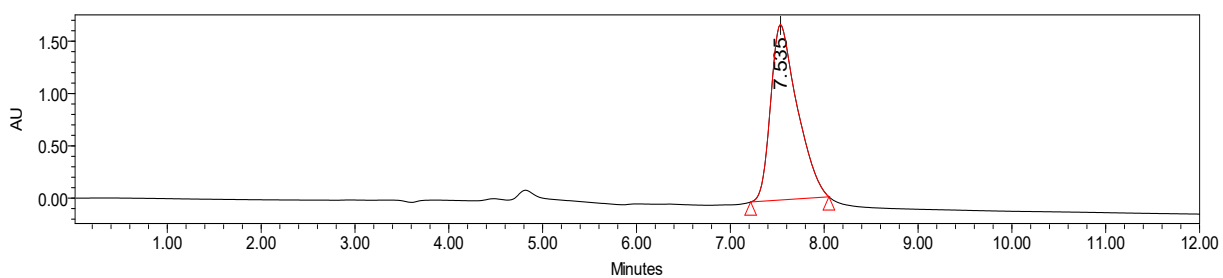


Figure S8. The HMBC spectrum of compound **5** (600.13 MHz for ^1H and ^{13}C , solvent CS_2 : $\text{CDCl}_3 = 3:1$)



	Retention Time	Area	% Area	Height	% Height
1	7.535	32994205	100.00	1677954	100.00

Figure S9. HPLC chromatogram of compound **5**

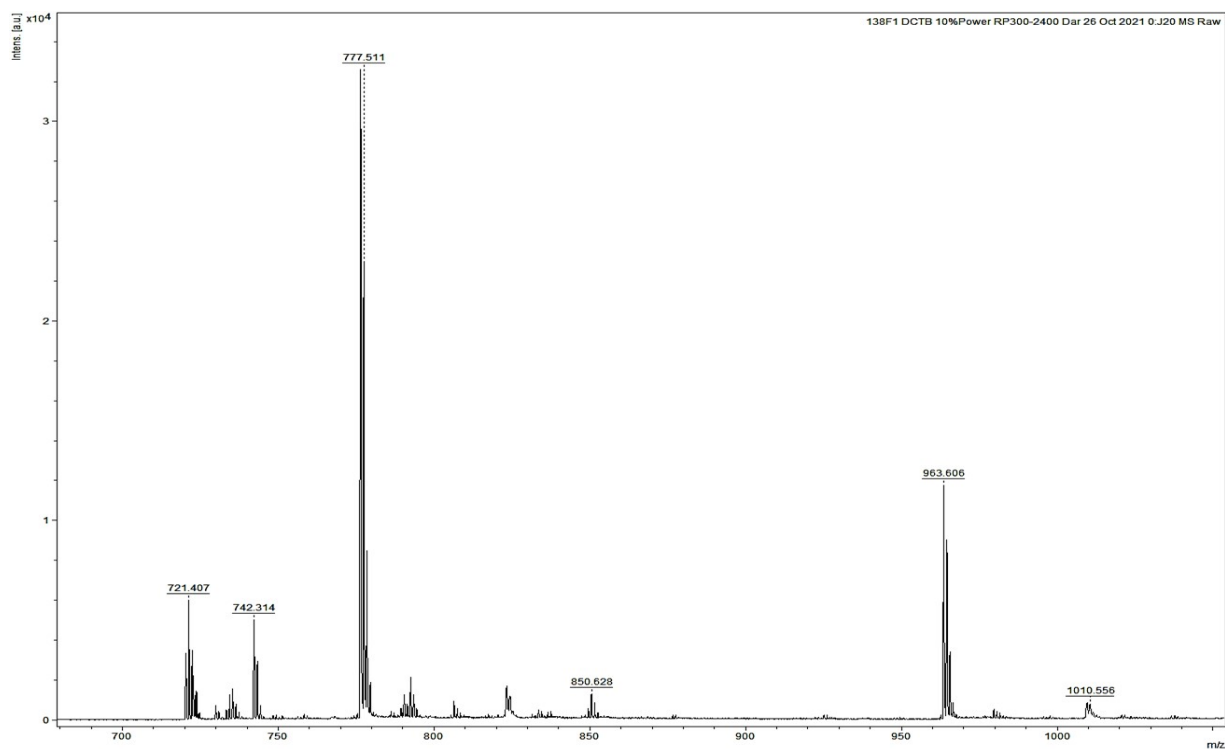


Figure S10. MALDI-TOF spectrum of compound **5**

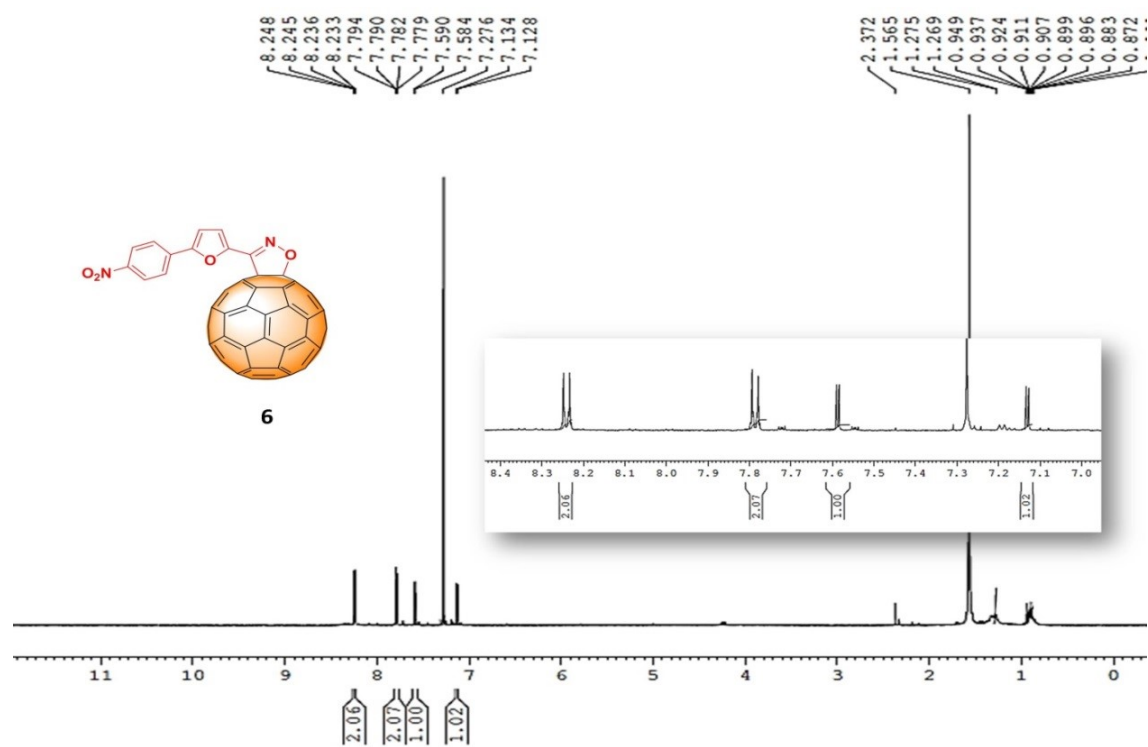


Figure S11. The ¹H NMR spectrum of compound **6** (600.13 MHz, solvent CDCl₃)

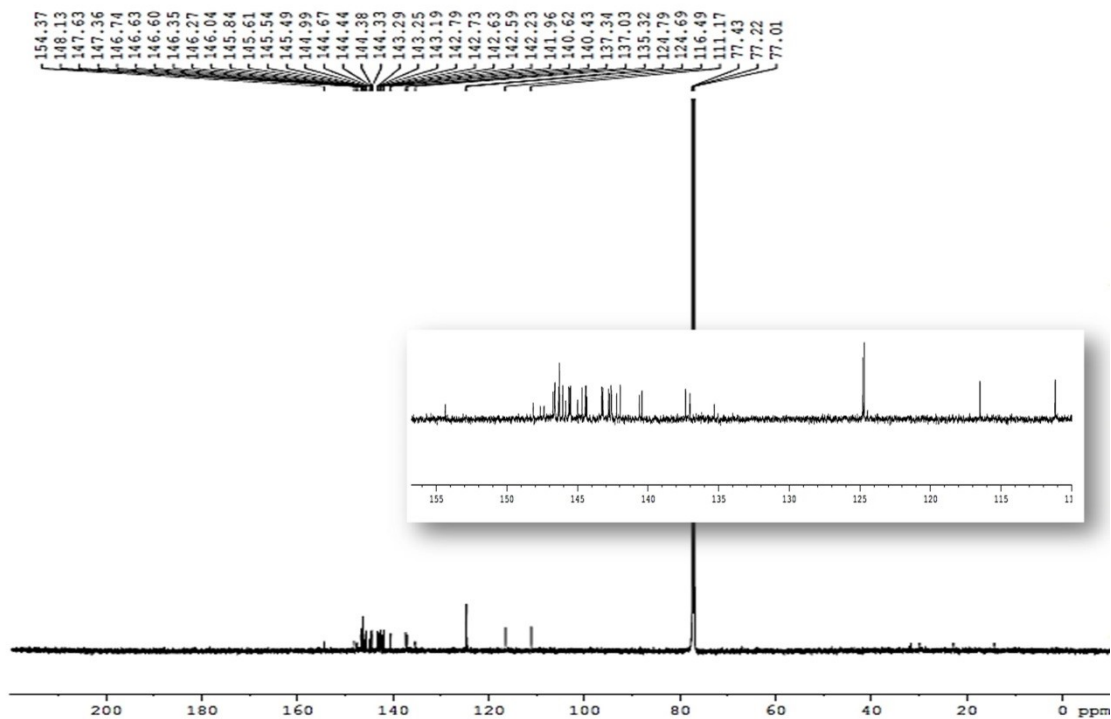


Figure S12. The ^{13}C NMR spectrum of compound **6** (150 MHz, solvent $\text{CS}_2 : \text{CDCl}_3 = 3:1$)

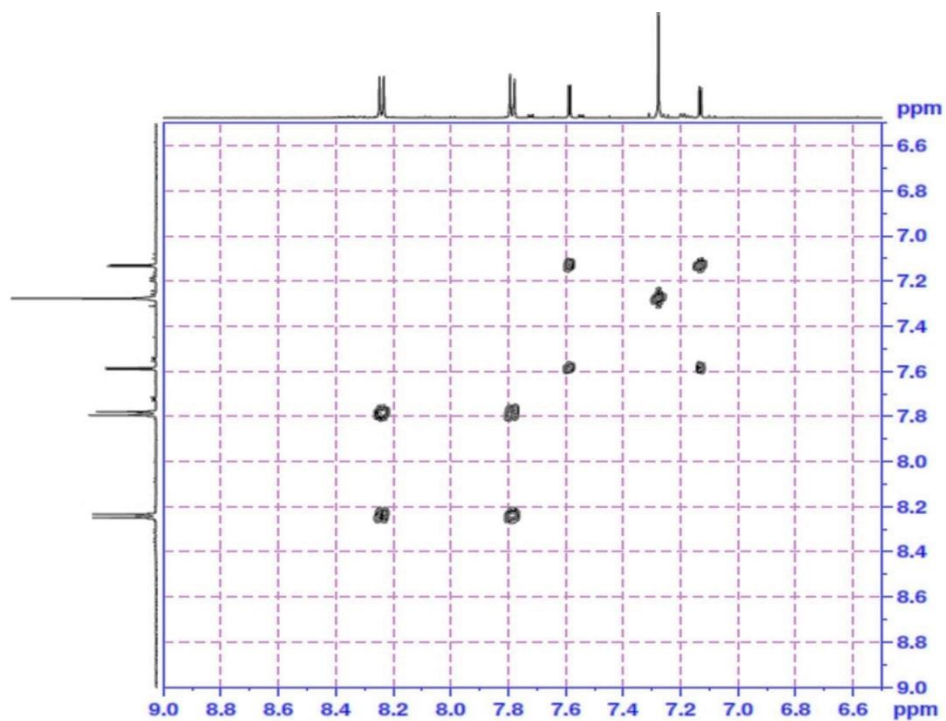


Figure S13. H-H COSY NMR spectrum of compound **6** (600.13 MHz, solvent CDCl_3)

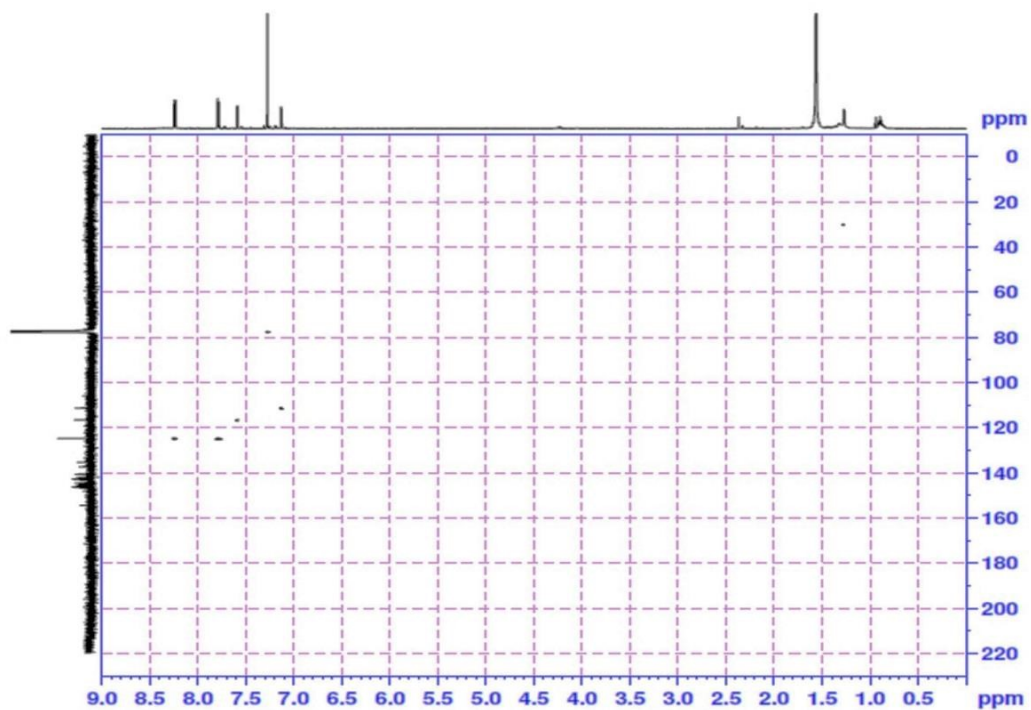


Figure S14. The HSQC spectrum of compound **6** (600.13 MHz for ^1H and ^{13}C , solvent CS_2 : $\text{CDCl}_3 = 3:1$)

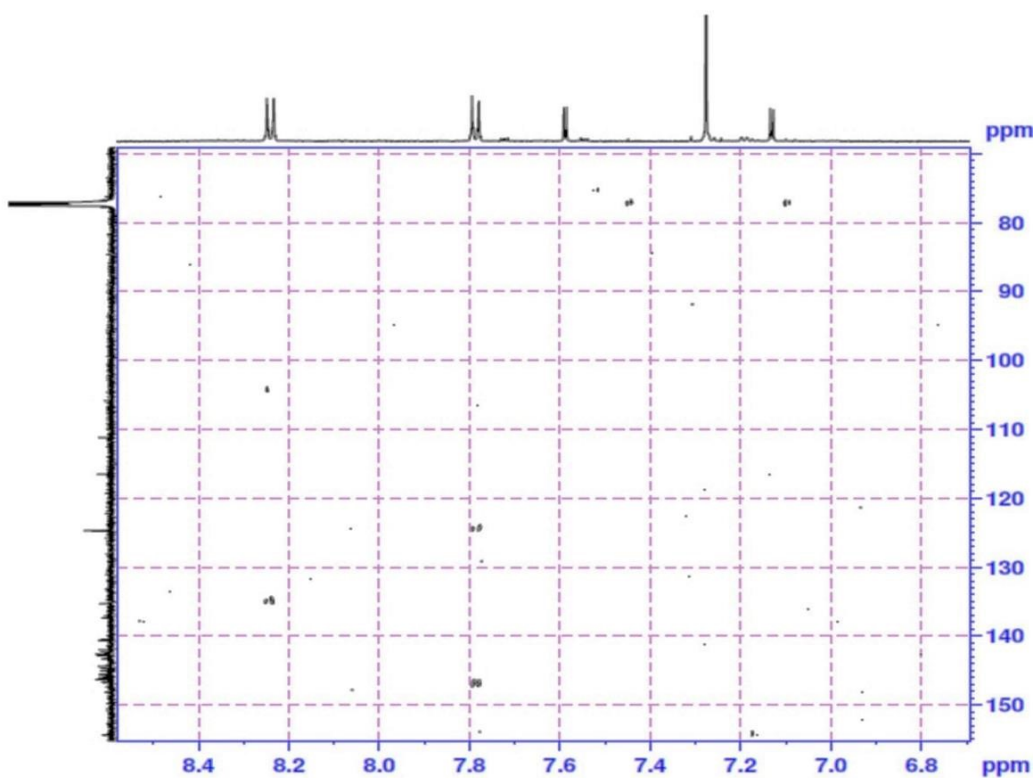
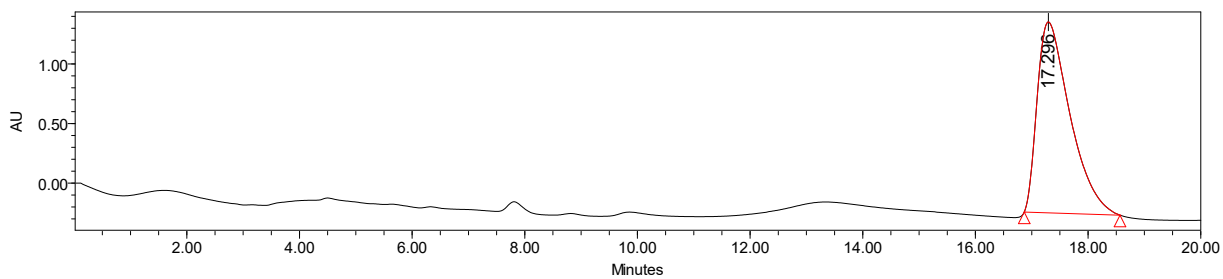


Figure S15. The HMBC spectrum of compound **6** (600.13 MHz for ^1H and ^{13}C , solvent CS_2 : $\text{CDCl}_3 = 3:1$)



	Retention Time	Area	% Area	Height	% Height
1	17.296	64839343	100.00	1603222	100.00

Figure S16. HPLC chromatogram of compound **6**

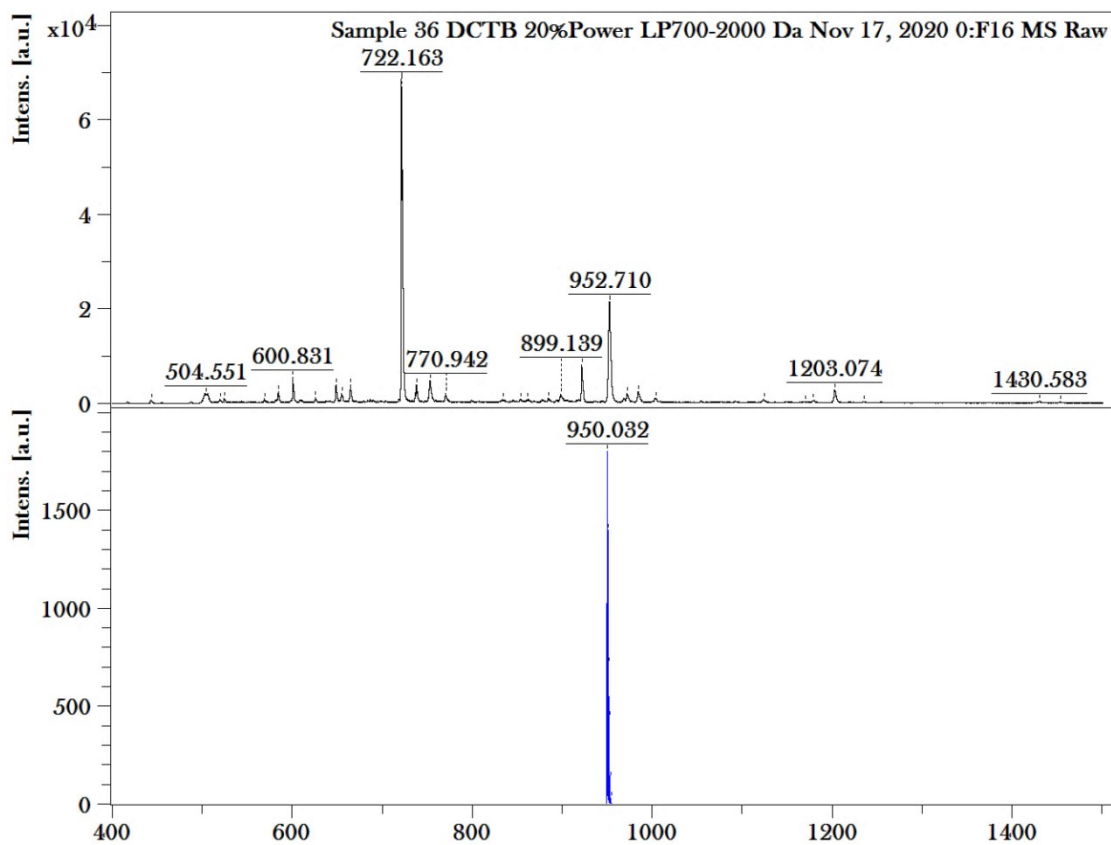


Figure S17. MALDI-TOF spectrum of compound **6**

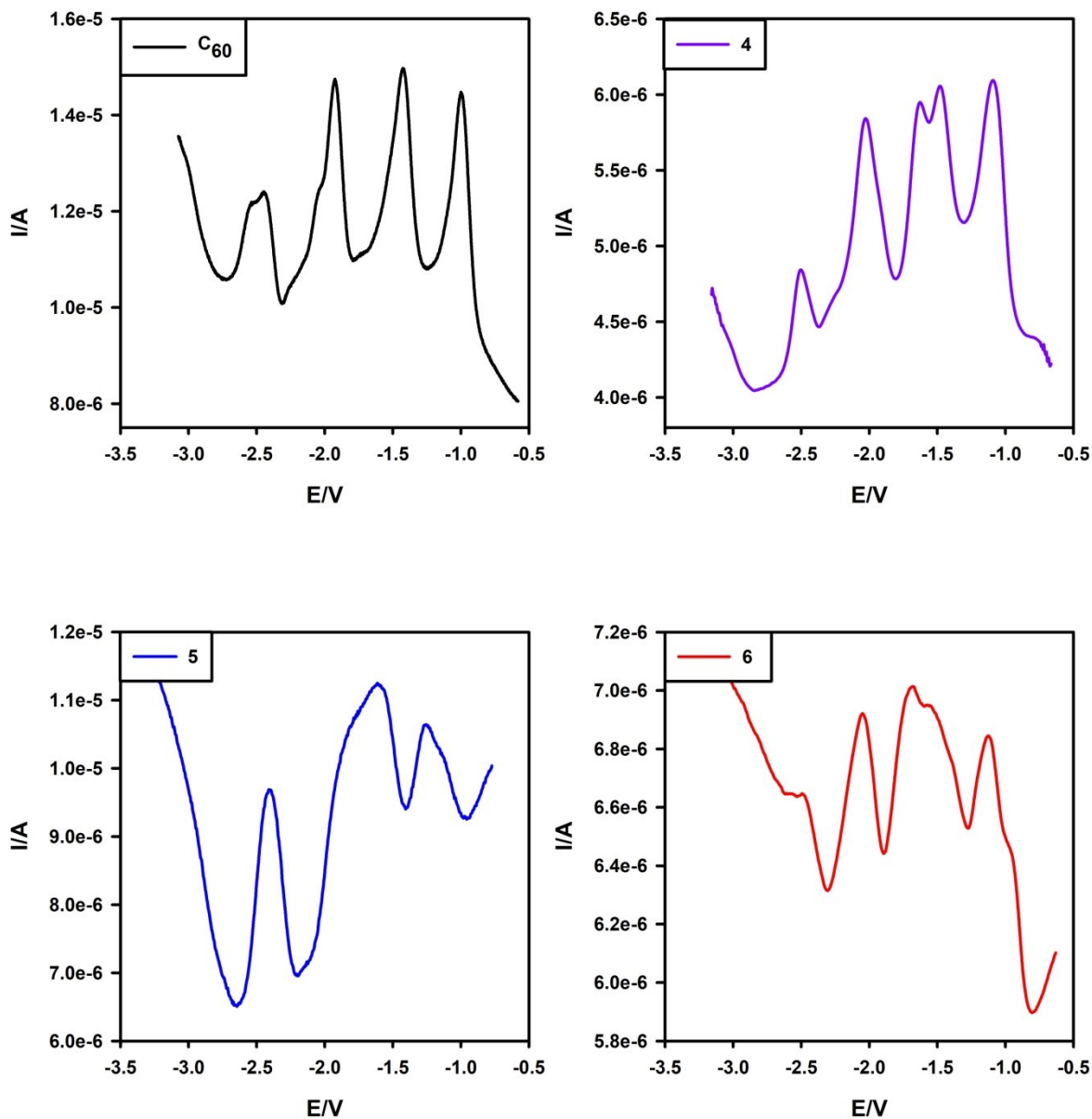


Figure S18. Square wave voltammograms of C_{60} , $FPzC_{60}$ (4), $FPyC_{60}$ (5), and $FOxC_{60}$ (6) in toluene/ CH_3CN (4:1) solutions with 0.1 M TBAP; V vs. Fc/Fc^+ ; scan rate was 100 mVs^{-1} .

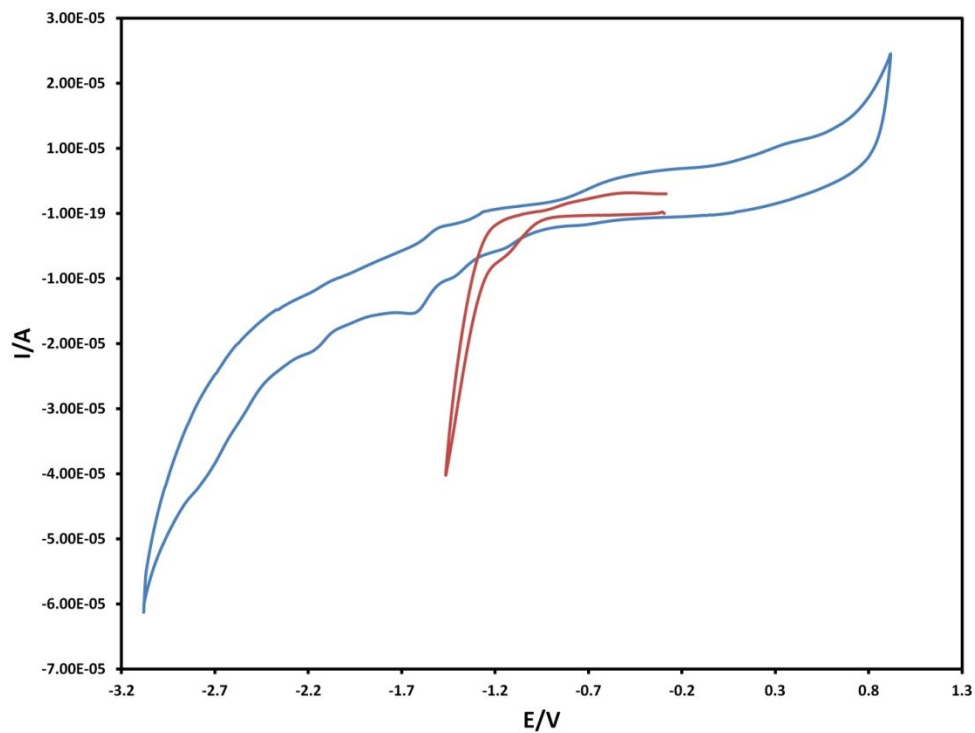


Figure S19. Cyclic voltammogram of compound **5** with the first reduction peak.

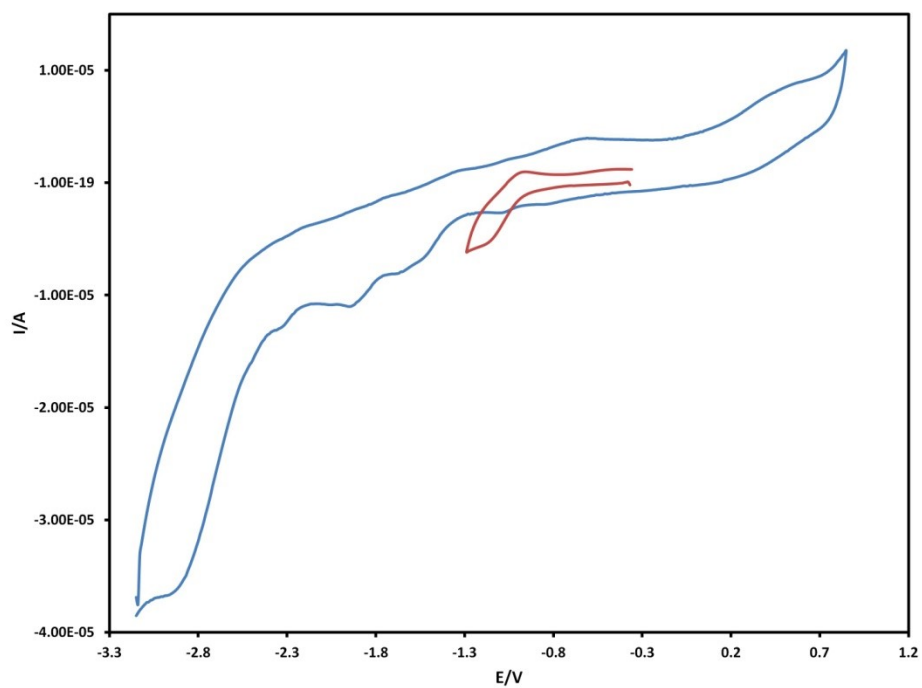


Figure S20. Cyclic voltammogram of compound **6** with the first reduction peak.