Electronic Supplementary Information

Self-assembly of Thioether Functionalized Fullerenes on Gold and Their Activity in Electropolymerization of Styrene

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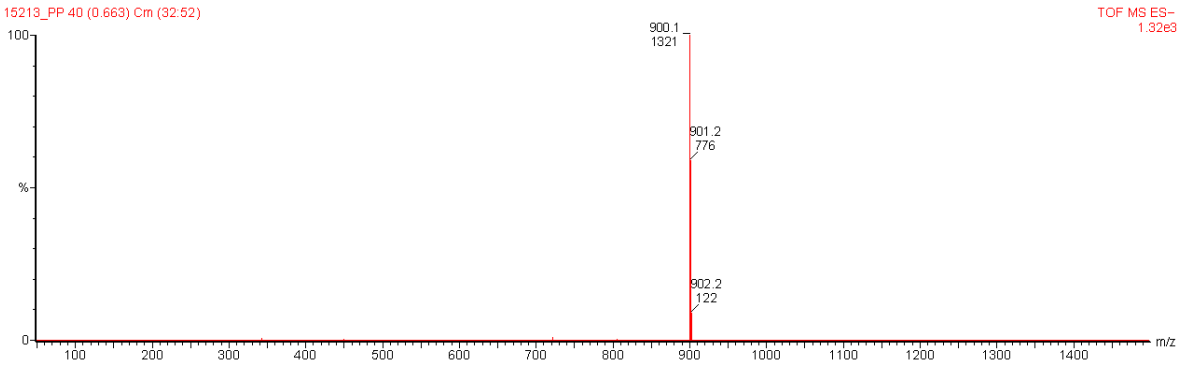

Figure S1. ESI-MS spectrum of fullerene sulphide **I** as a $[M]^-$ anion.

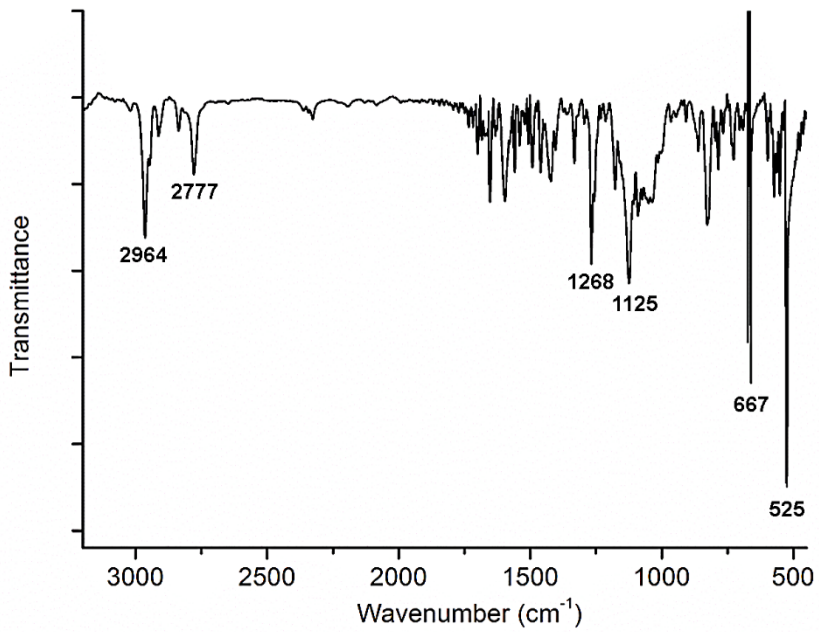

Figure S2. IR spectrum of fullerene sulphide **I** in KBr disk.

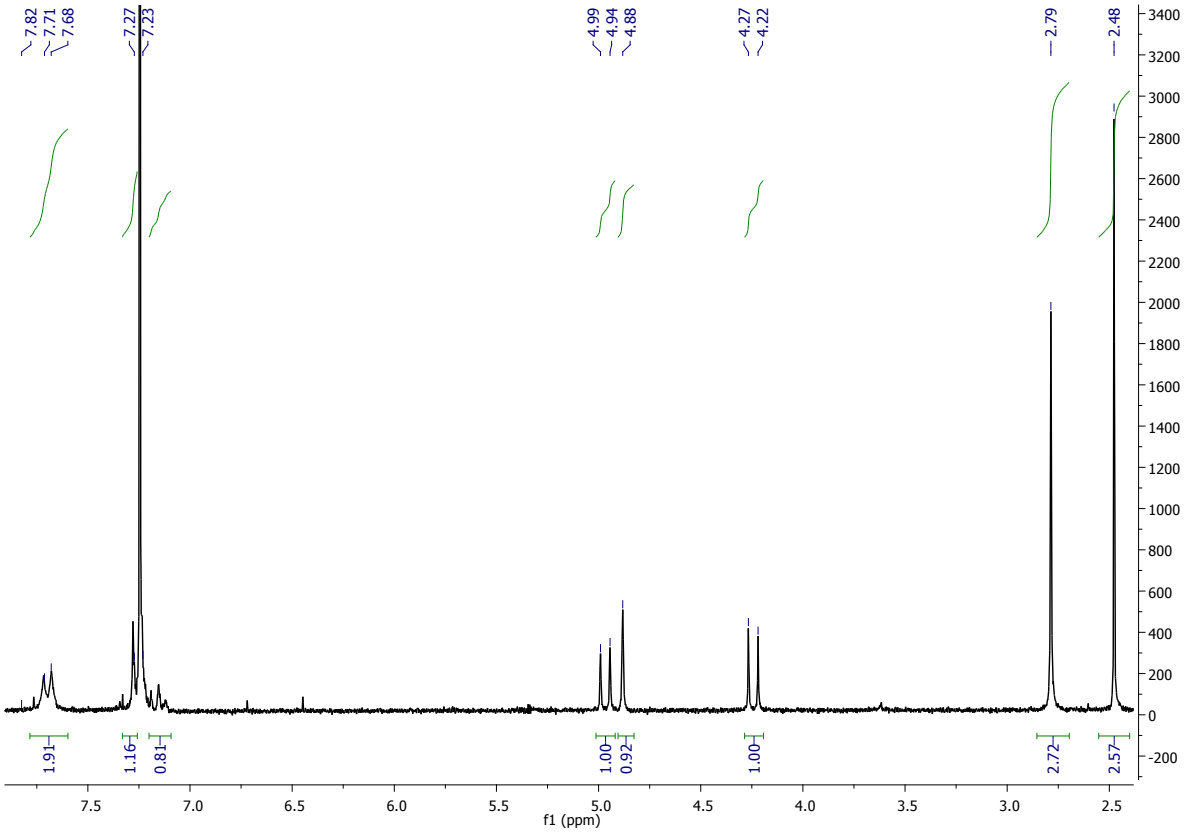

Figure S3. ^{1}H NMR spectrum of fullerene sulphide **I** in $CDCl_3$.

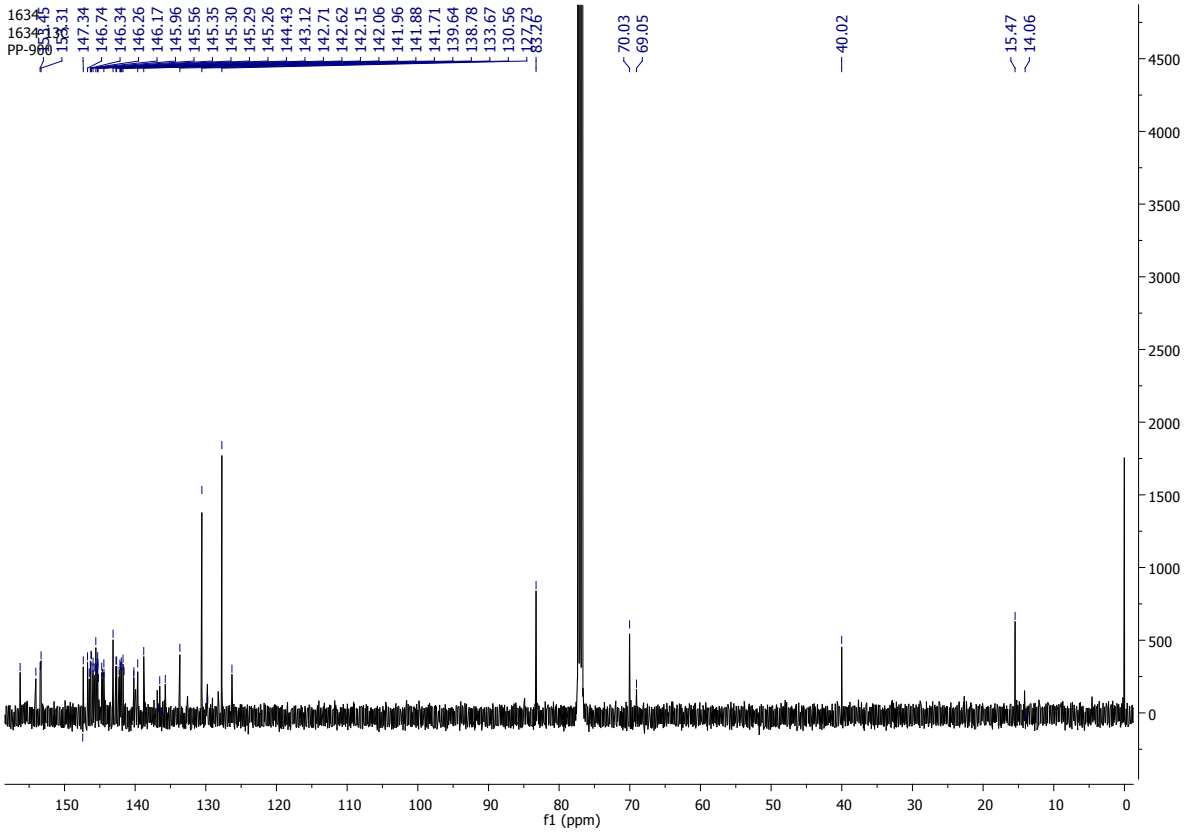

Figure S4. ^{13}C NMR spectrum of fullerene sulphide **I** in $CDCl_3$.

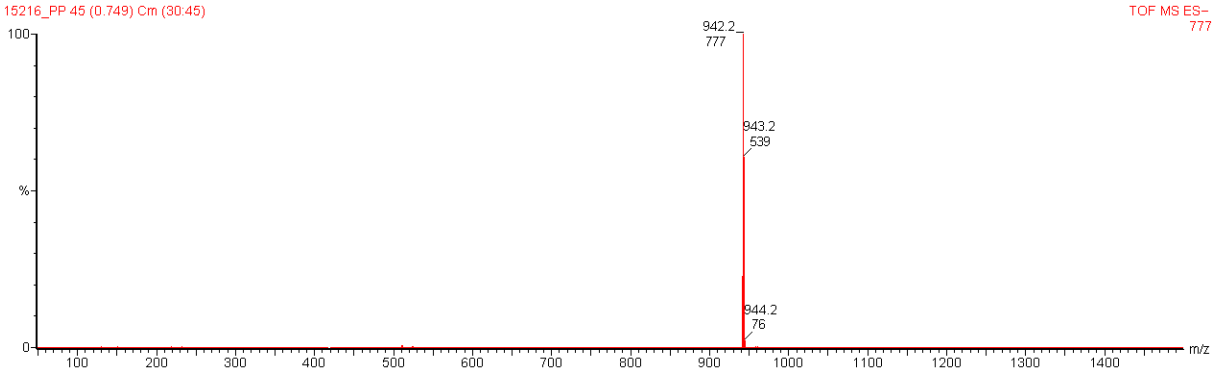

Figure S5. ESI-MS spectrum of fullerene sulphide **II** as a $[M]^-$ anion.

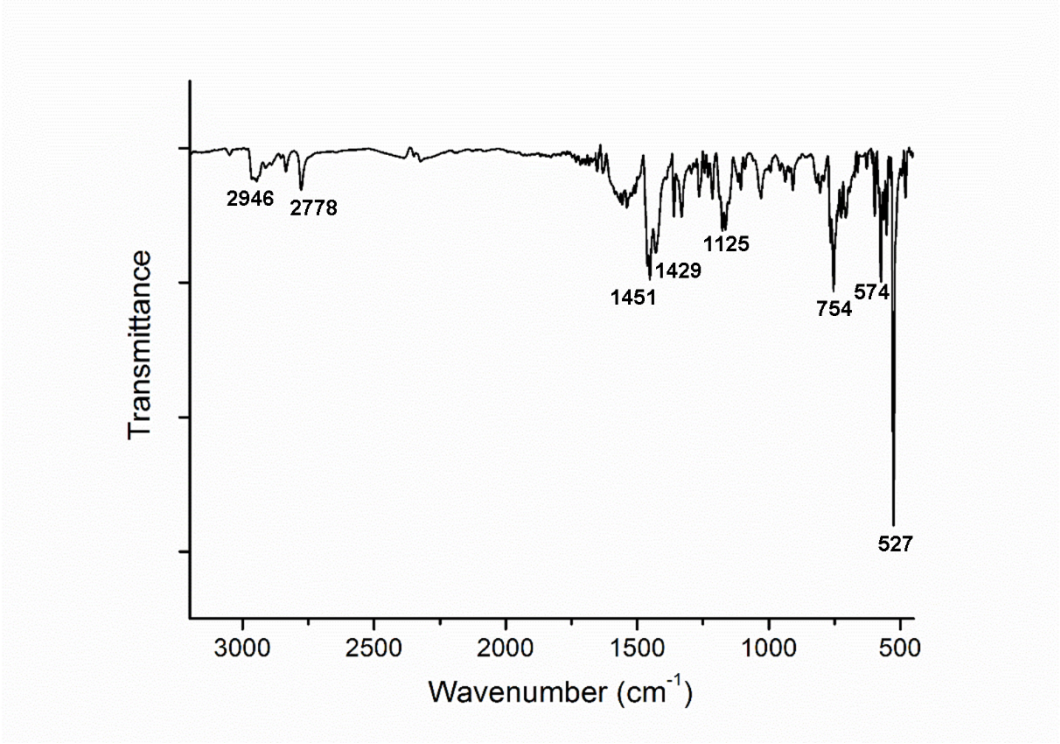

Figure S6. IR spectrum of fullerene sulphide **II** in KBr disk.

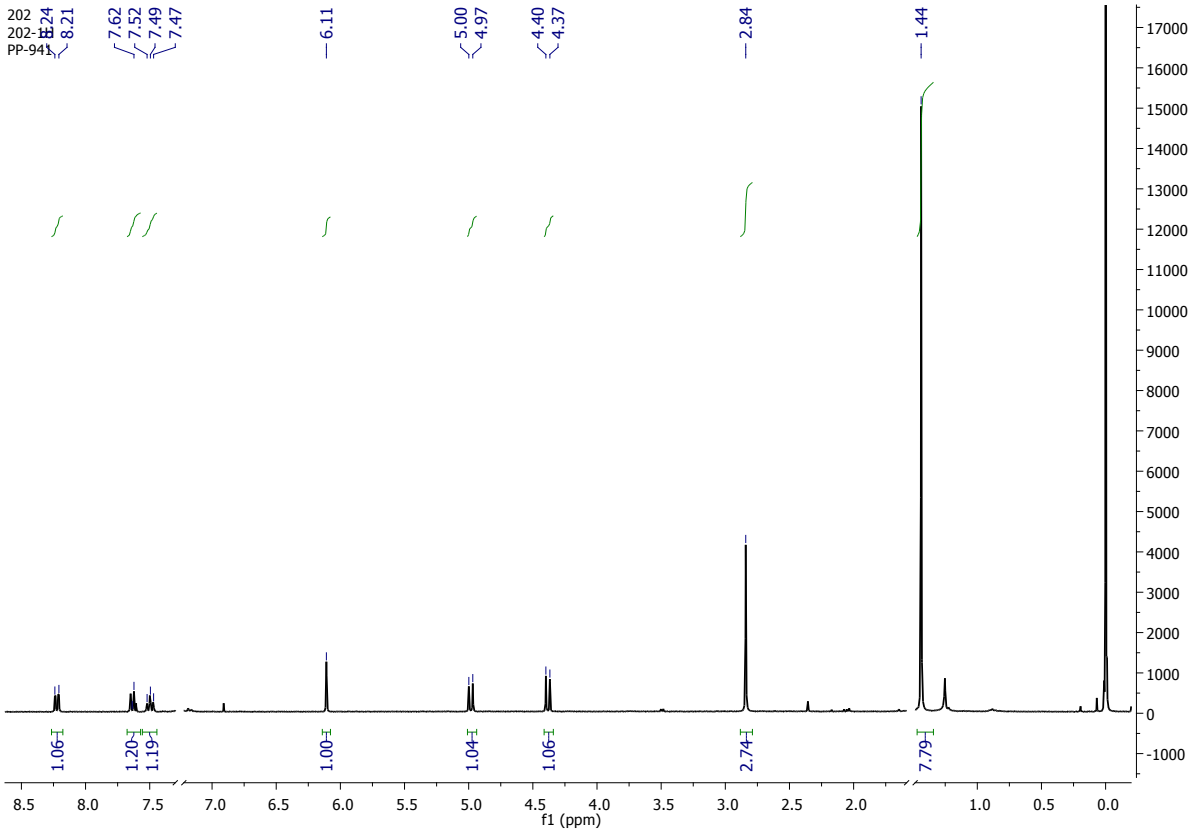

Figure S7. ^{1}H NMR spectrum of fullerene sulphide **II** in $CDCl_3$.

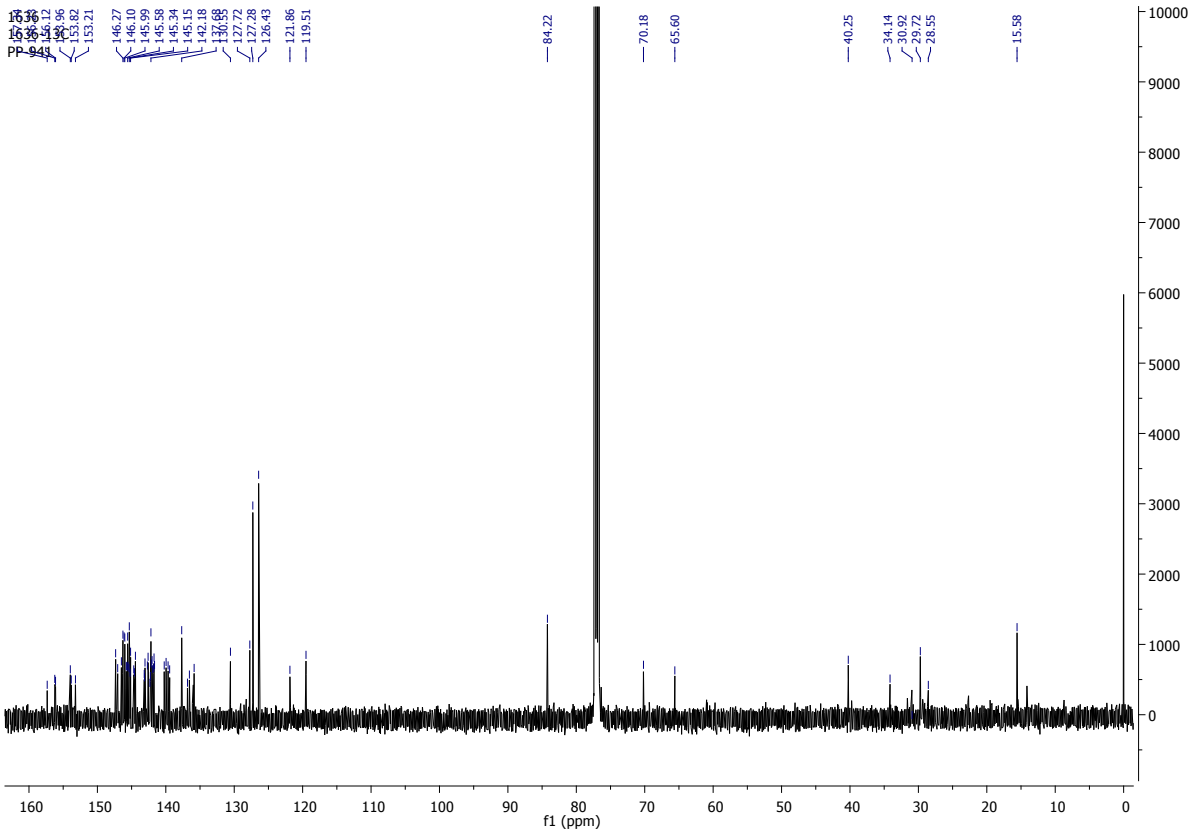

Figure S8. ^{13}C NMR spectrum of fullerene sulphide **II** in $CDCl_3$.

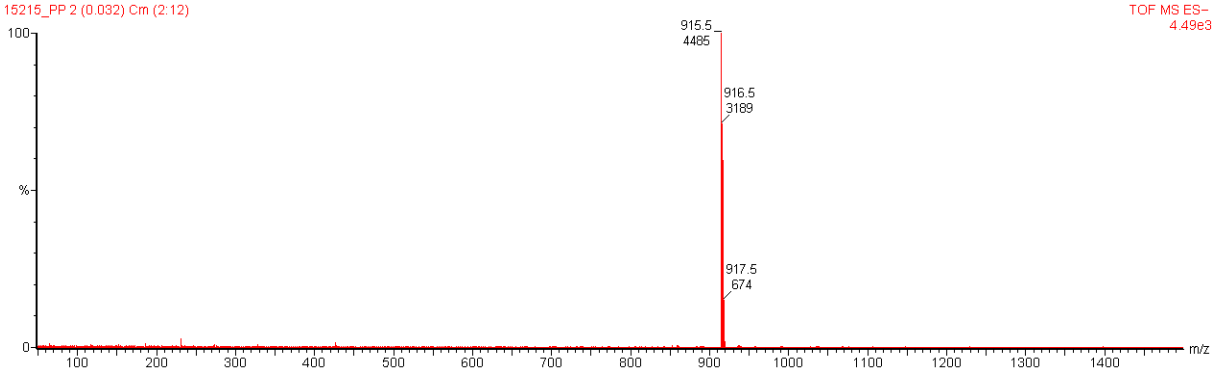

Figure S9. ESI-MS spectrum of fullerene sulphide **III** as a $[M]^-$ anion.

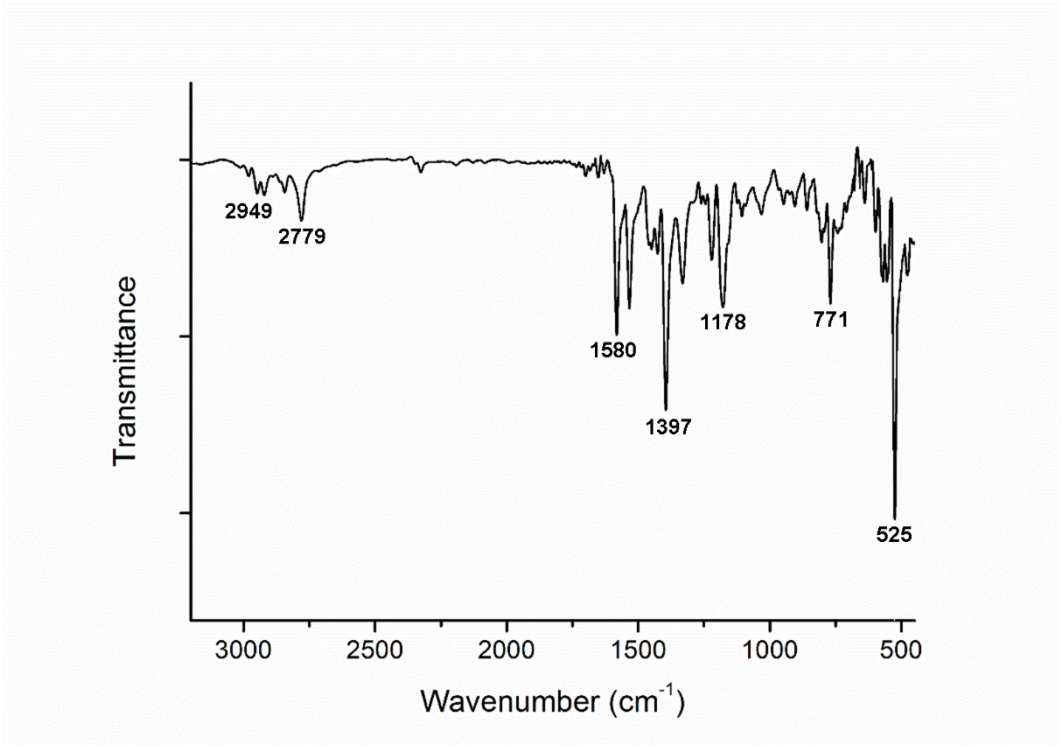

Figure S10. IR spectrum of fullerene sulphide **III** in KBr disk.

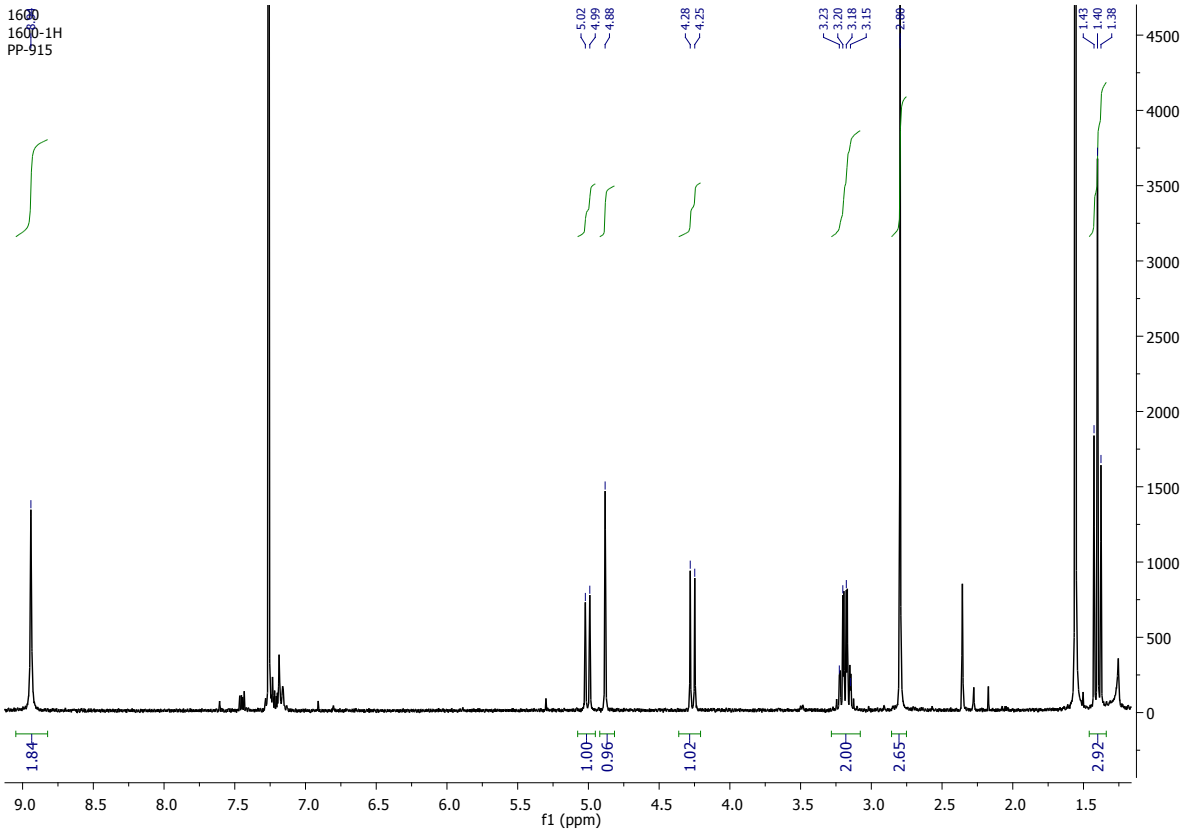

Figure S11. ^{1}H NMR spectrum of fullerene sulphide **III** in $CDCl_3$.

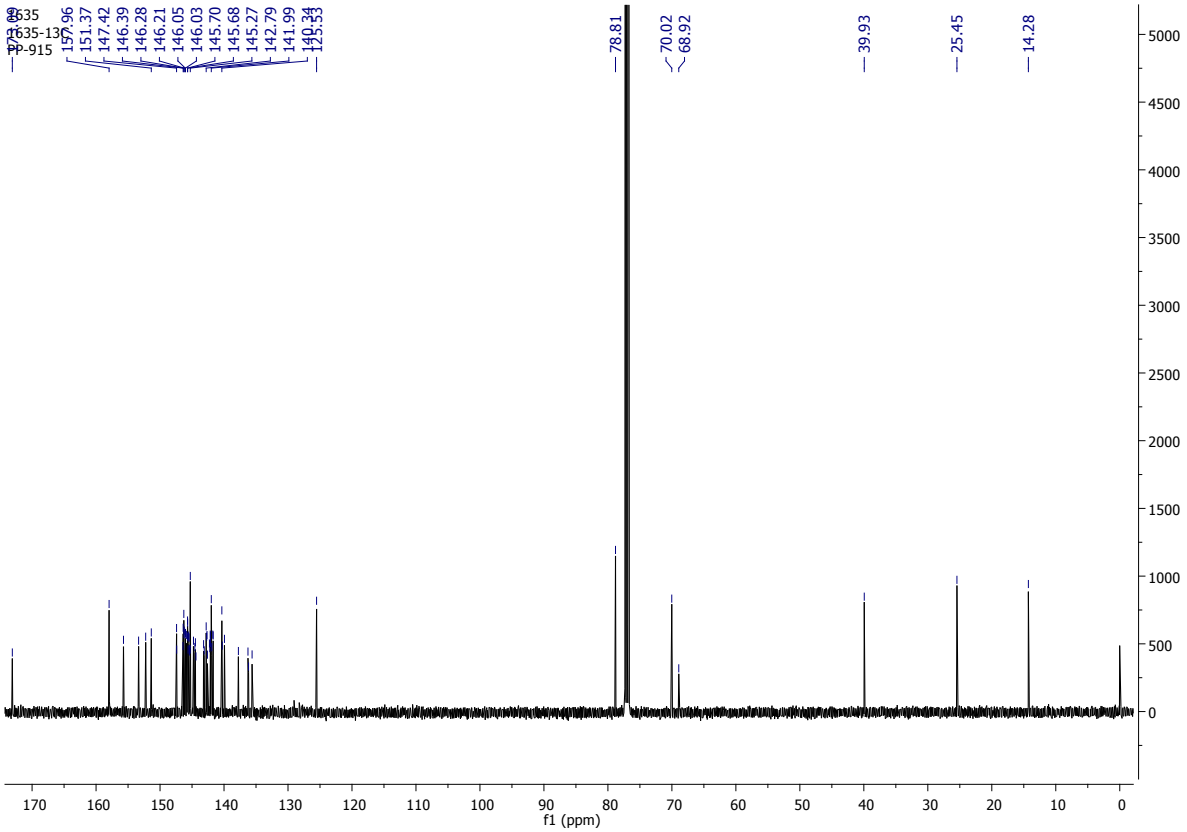

Figure S12. ^{13}C NMR spectrum of fullerene sulphide **III** in $CDCl_3$.

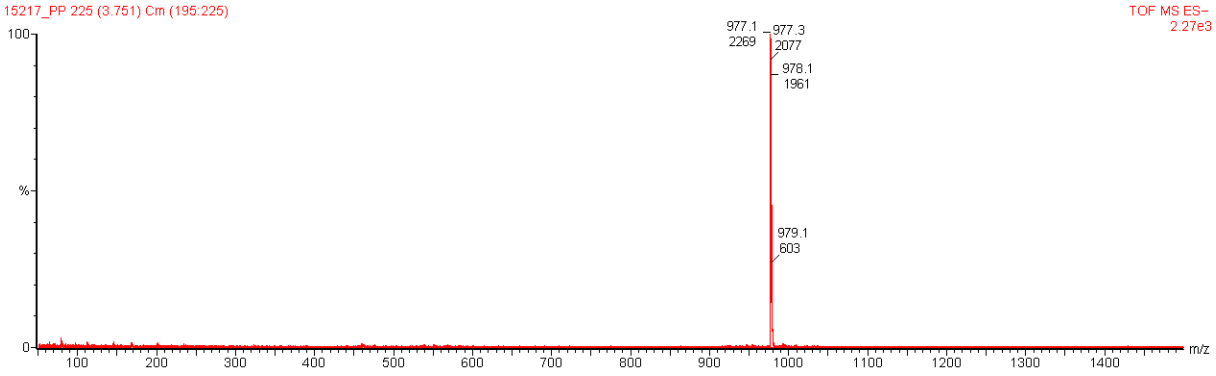

Figure S13. ESI-MS spectrum of fullerene sulphide **IV** as a $[M]^-$ anion.

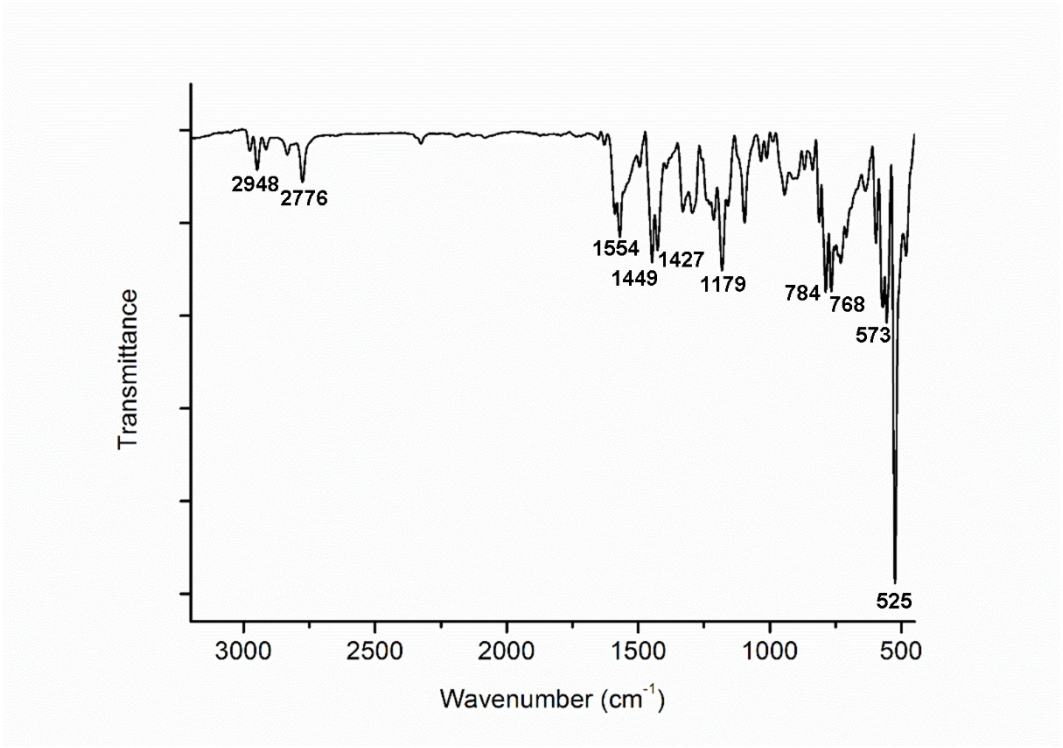

Figure S14. IR spectrum of fullerene sulphide **IV** in KBr disk.

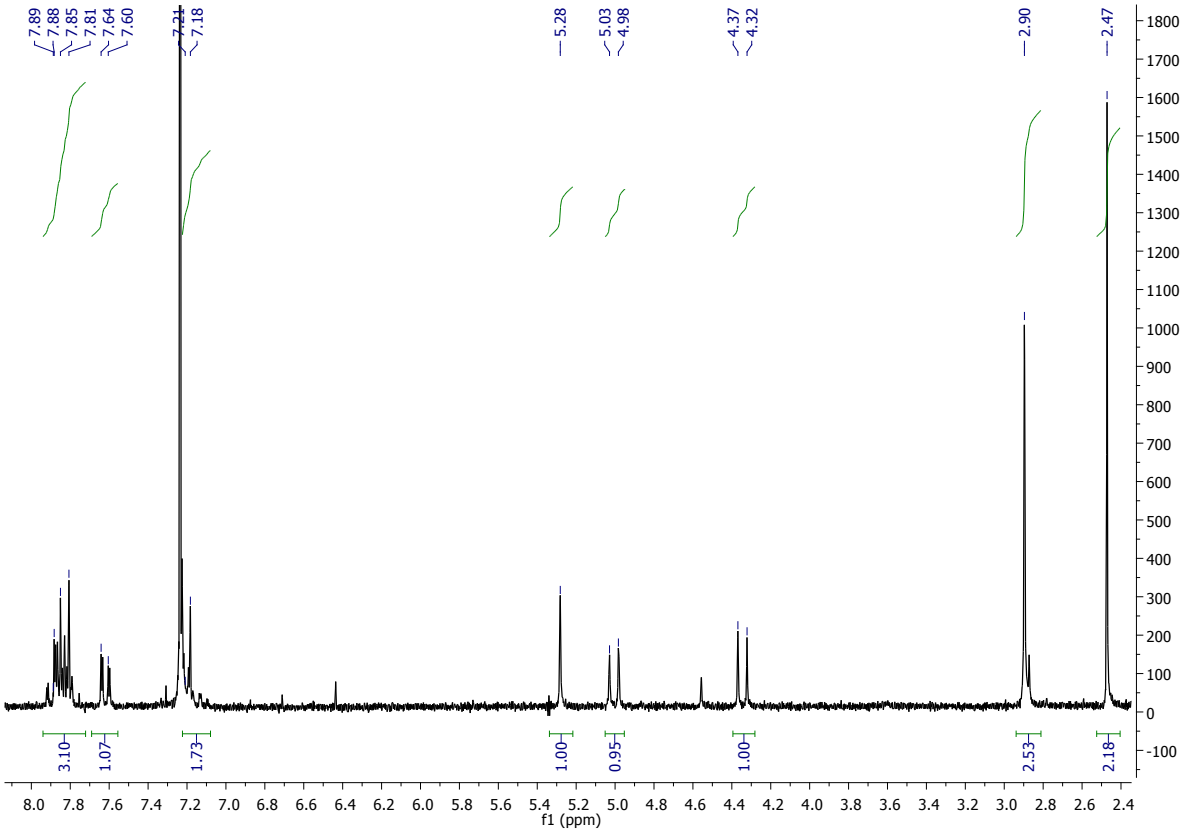

Figure S15. ^{1}H NMR spectrum of fullerene sulphide **IV** in $CDCl_3$.

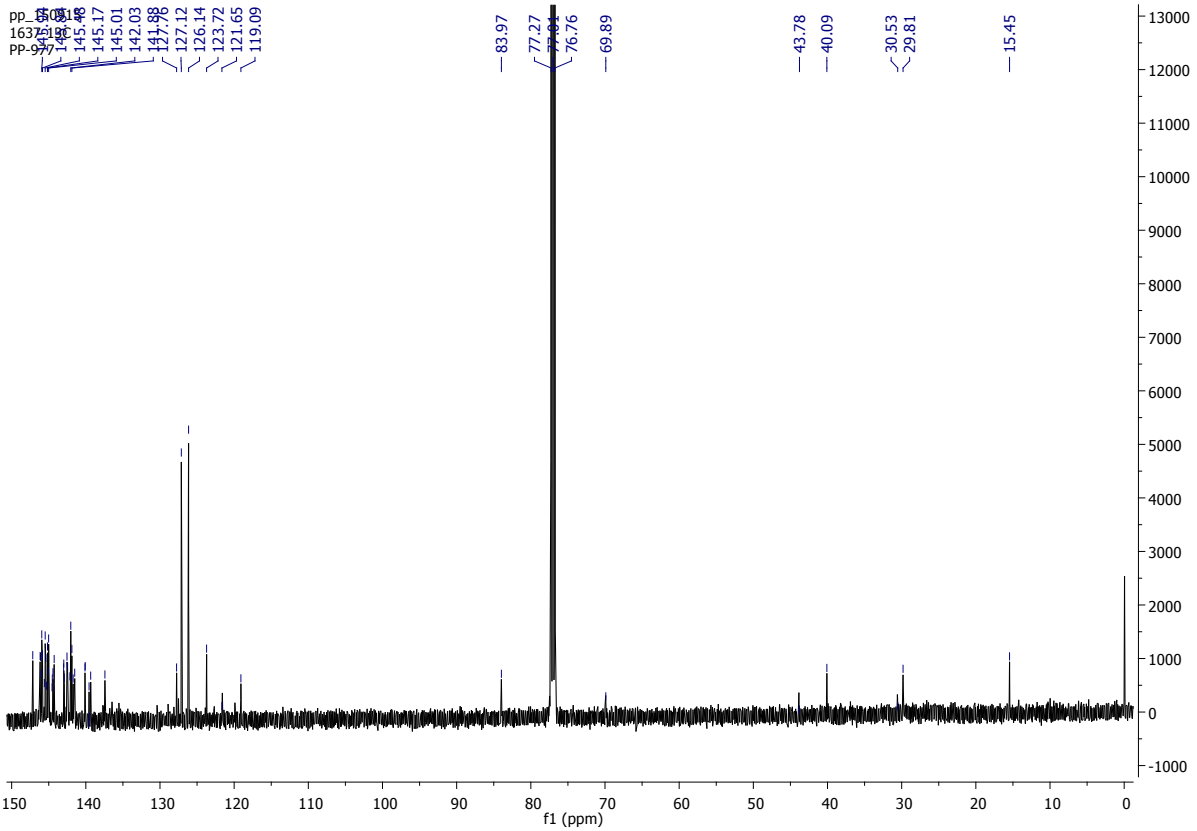

Figure S16. ^{13}C NMR spectrum of fullerene sulphide **IV** in $CDCl_3$

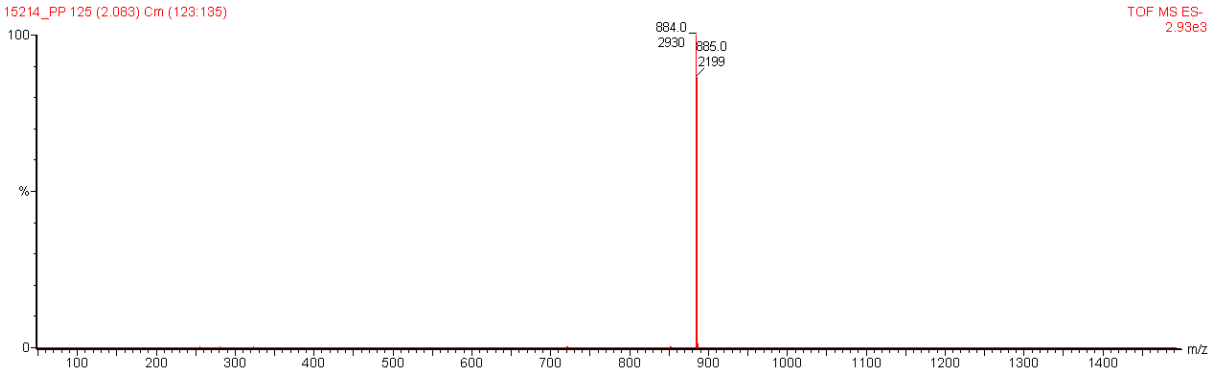

Figure S17. ESI-MS spectrum of **I-O** (methoxy analogue of fullerene sulphide **I)** as a $[M]^-$ anion.

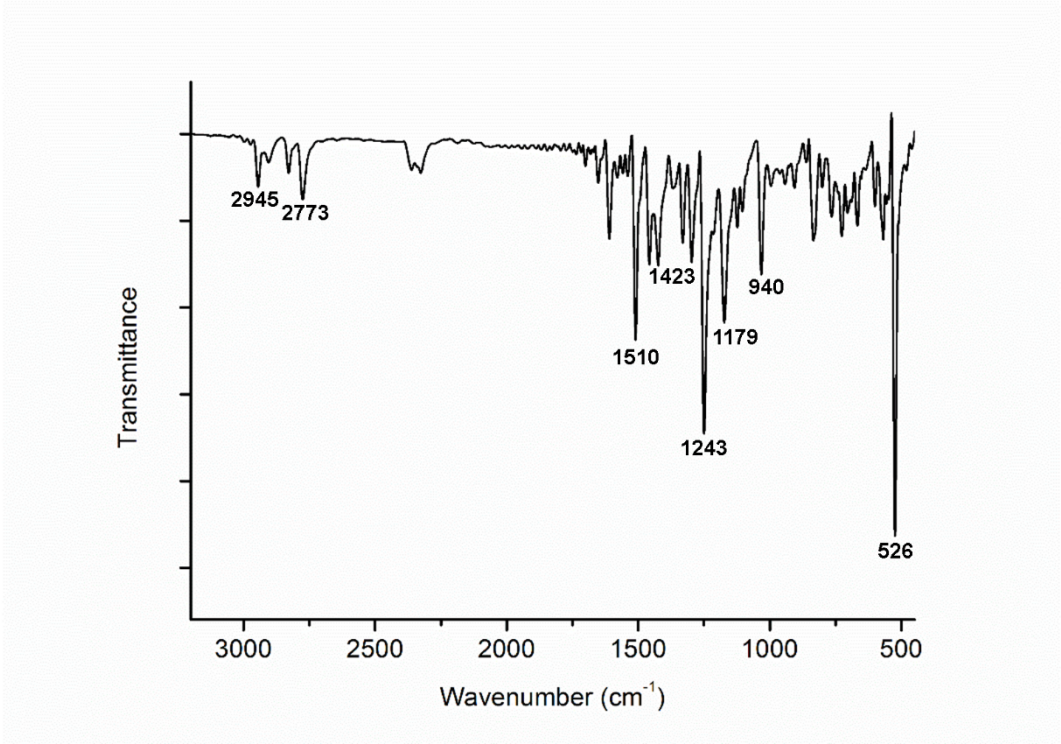

Figure S18. IR spectrum of **I-O** (methoxy analogue of fullerene sulphide **I)** in KBr disk.

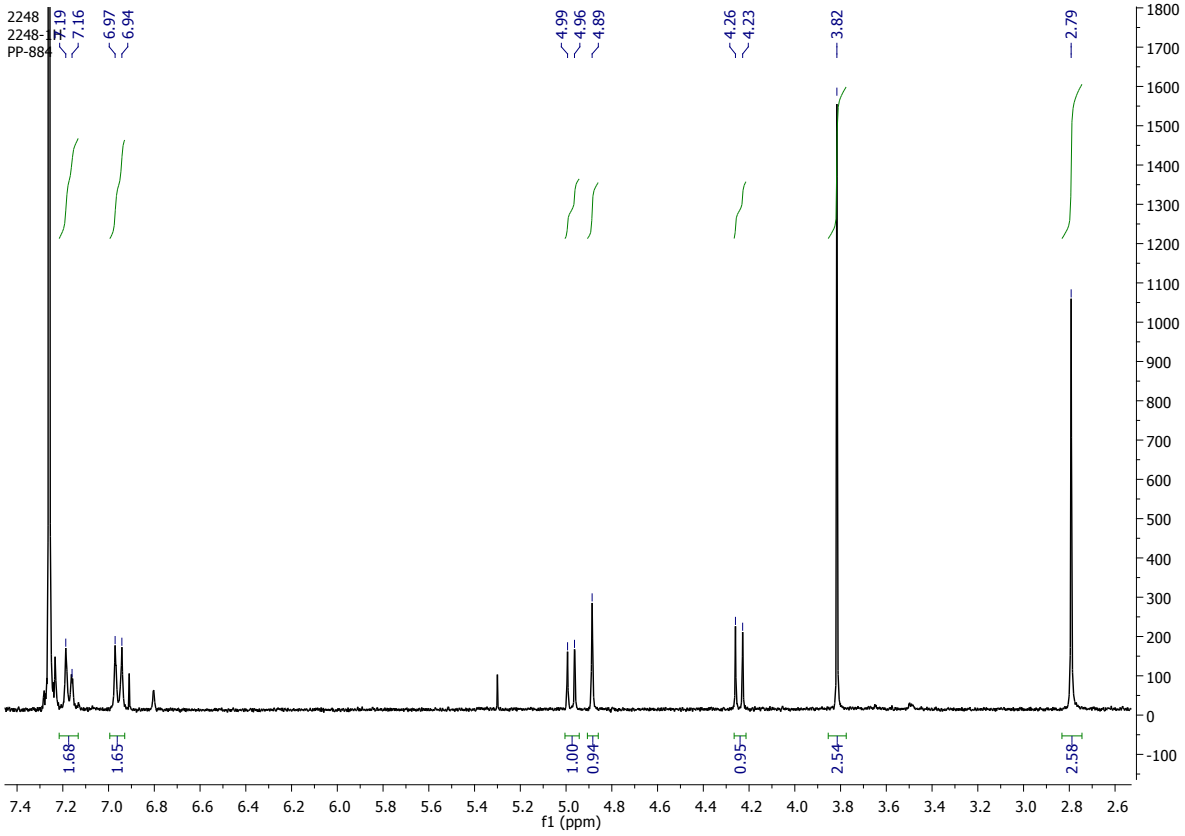

Figure S19. ^{1}H NMR spectrum of **I-O** (methoxy analogue of fullerene sulphide **I)** in $CDCl_3$.

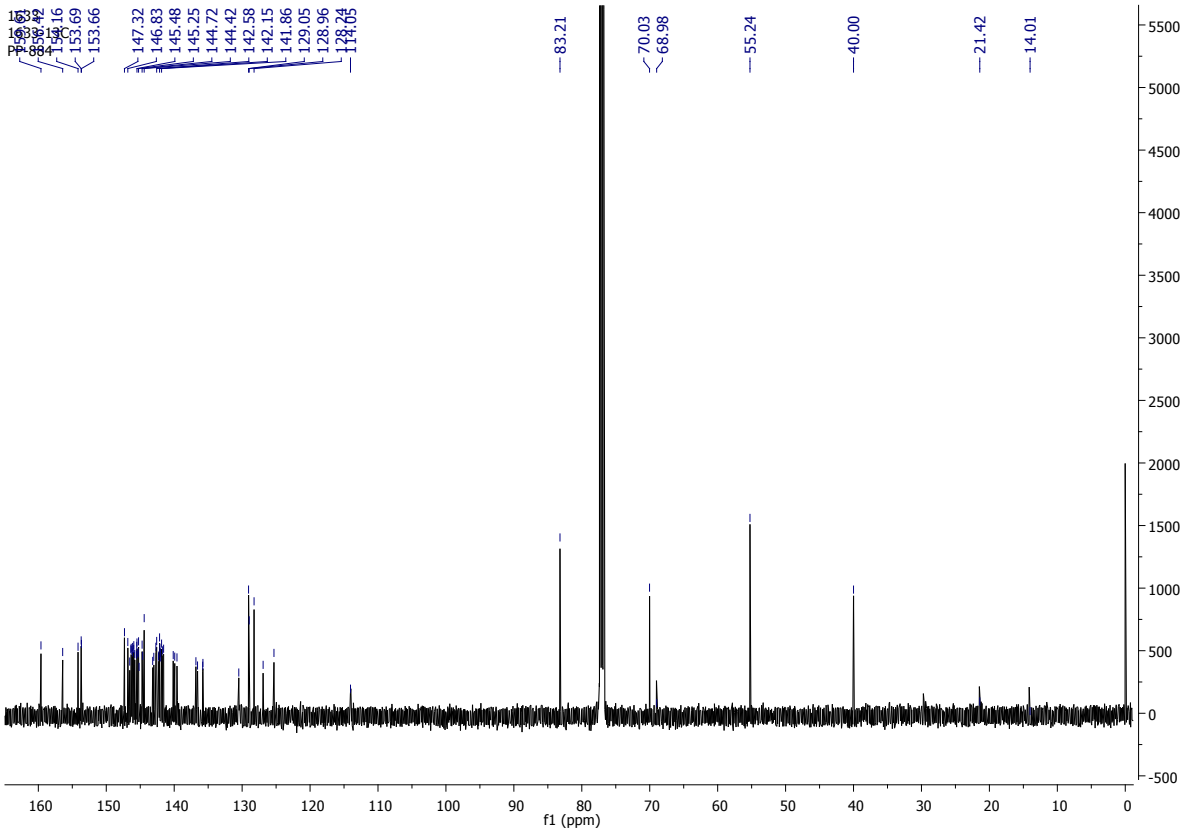

Figure S20. ^{13}C NMR spectrum of **I-O** (methoxy analogue of fullerene sulphide **I)** in $CDCl_3$

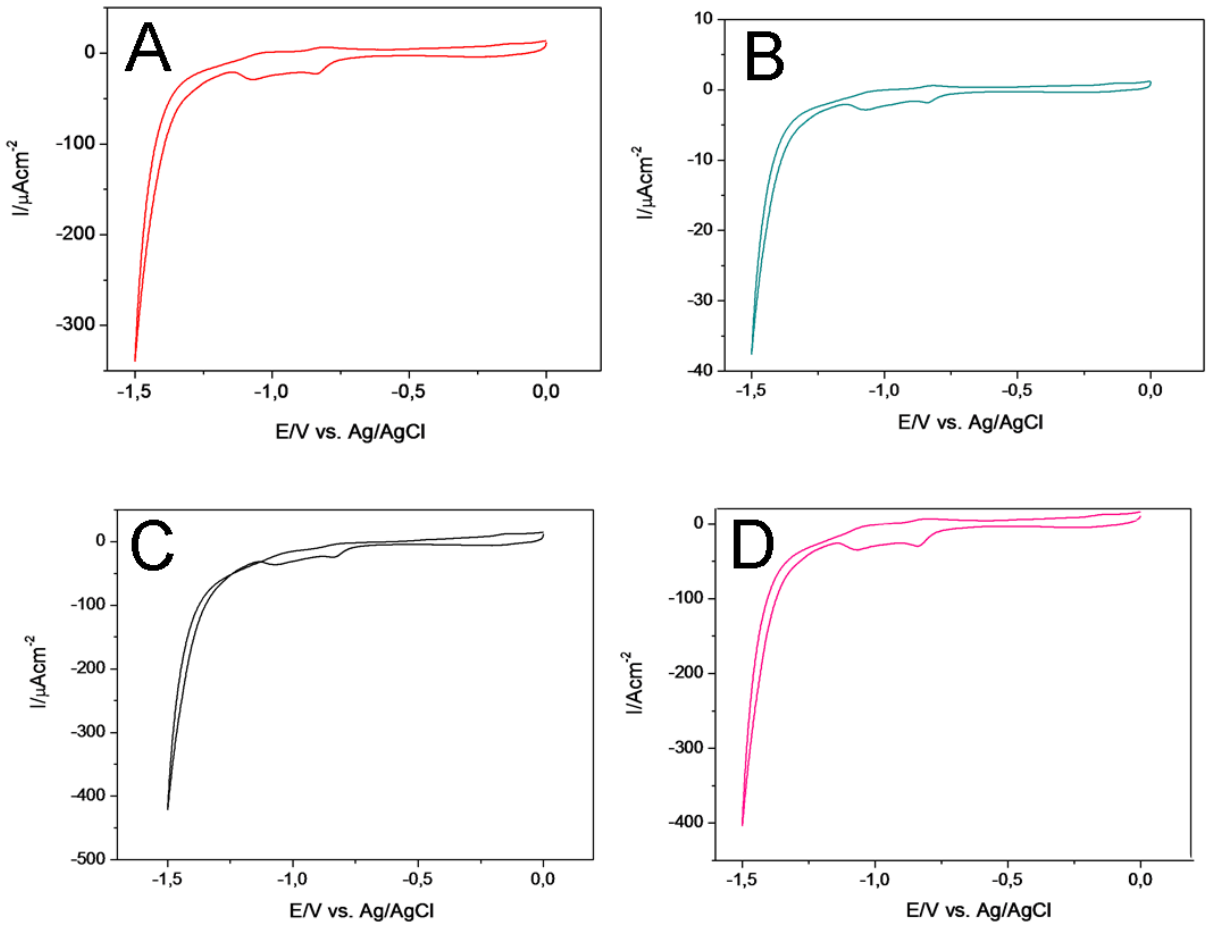

Figure S21. Desorption curves obtained for fullerene sulphides: **I** - A, **II** - B, **III** - C and **IV**- D, in 0.5M KOH, v=100mV/s.

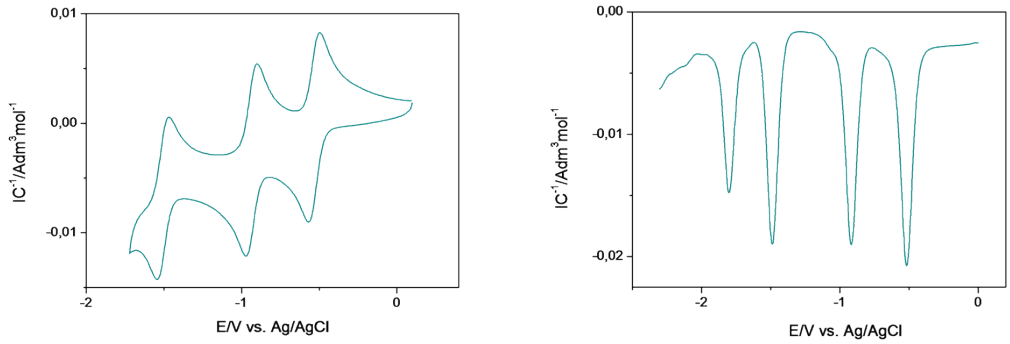

Figure S22. Voltammograms of compound **II** in 0.1M TBAHFP solution in toluene/acetonitrile (4:1), (left) CV, v = 100 mV/s; (right) DPV, tp= 3 ms, ΔE = 50 mV.

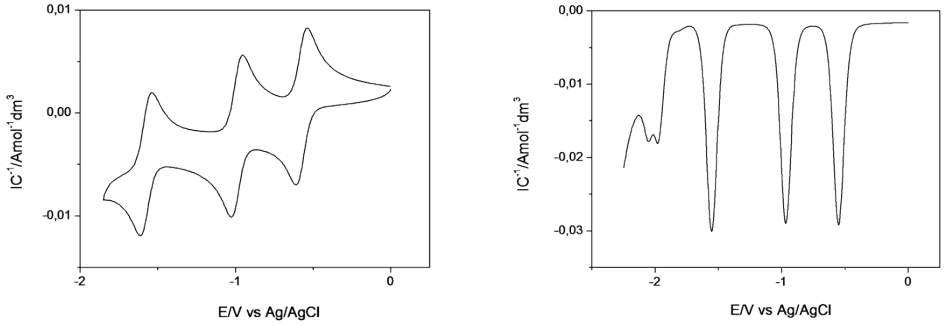

Figure S23. Voltammograms of compound **III** in 0.1M TBAHFP solution in toluene/acetonitrile (4:1), (left) CV, v = 100 mV/s; (right) DPV, tp= 3 ms, ΔE = 50 mV.

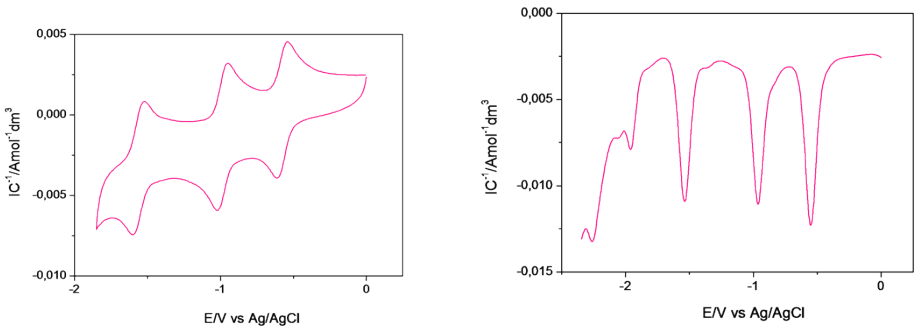

Figure S24. Voltammograms of compound **IV** in 0.1M TBAHFP solution in toluene/acetonitrile (4:1), (left) CV, v = 100 mV/s; (right) DPV, tp= 3 ms, ΔE = 50 mV.

Table S1 Comparison of electrochemical properties of C_{60} and fullerene thioethers **I-IV** obtained from CV measurements.

Compound	C_{60}	I	II	III	IV
E_{pc1} [V]	-0.467	-0.593	-0.564	-0.605	-0.542
E_{pa1} [V]	-0.396	-0.530	-0.496	-0.518	-0.610
$E_1^{0'}$ [V]	-0.432	-0.562	-0.530	-0.571	-0.576
E_{pc2} [V]	-0.874	-1.004	-0.969	-1.025	-0.947
E_{pa2} [V]	-0.807	-0.935	-0.906	-0.952	-1.021
$E_2^{0'}$ [V]	-0.841	-0.970	-0.938	-0.989	-0.984
E_{pc3} [V]	-1.40	-1.507	-1.546	-1.611	-1.597
E_{pa3} [V]	-1.324	-1.590	-1.472	-1.543	-1.528
$E_3^{0'}$ [V]	-1.362	-1.549	-1.509	-1.577	-1.563
E_{pc4} [V]	-1.895	-a)	-1.851	a)	a)
E_{pa4} [V]	-1.828	-a)	-1.747	a)	a)
$E_4^{0'}$ [V]	-1.862	-a)	-1.799	a)	a)
E_{pc5} [V]	-2.417	-a)	a)	a)	a)
E_{pa5} [V]	-2.274	-a)	a)	a)	a)
$E_5^{0'}$ [V]	-2.346	-a)	a)	a)	a)

[a)] Peak corresponding to step 5 could not be resolved due to rising of the final current

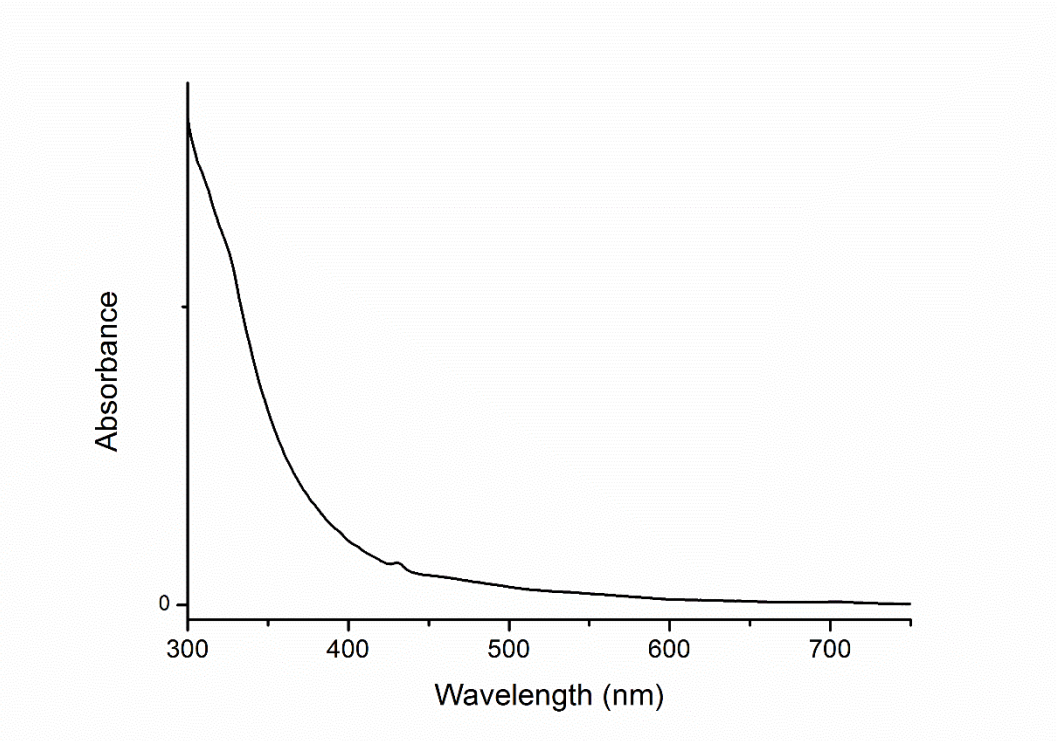

Figure S25. UV-Vis spectrum of polystyrene **F-PS** in CH_2Cl_2.

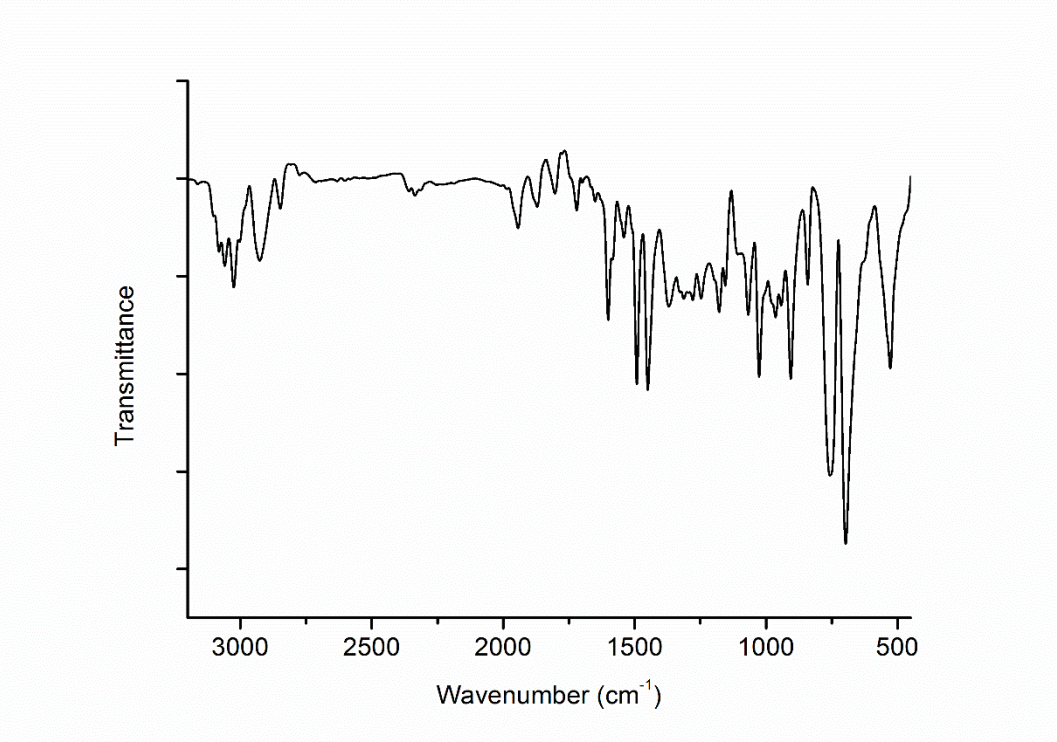

Figure S26. IR spectrum of polystyrene **F-PS** in KBr disk.