Star shaped ferrocenyl truxenes: synthesis, structure and properties

Rajneesh Misra,* Rekha Sharma and Shaikh M. Mobin

Supporting Information

Department of Chemistry,
Indian Institute of Technology Indore,
Indore- 452017, India.

rajneeshmisra@iiti.ac.in

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Table 1. Crystal data and structure refinement parameter for truxene **4a**.

Compound	**4a**
Empirical formula	C_{99} H_{114} Fe_3
Formula weight	1471.45
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	
a (Å)	16.3107(3)
b (Å)	b =18.4332(3)
β (°)	90.4590(10)
c (Å)	27.2131(4)
Volume	8181.6(2) A^3
Z, Calculated density	4, 1.195 Mg/m^3
Absorption coefficient	0.571 mm^{-1}
F(000)	3144
Crystal size	0.23 x 0.16 x 0.13 mm
Theta range for data collection	3.11 to 25.00 deg.
Limiting indices	-19<=h<=13, -21<=k<=21, -32<=l<=32
Reflections collected / unique	59275 / 14385 [R(int) = 0.0570]
Completeness to theta= 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9295 and 0.8799
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14385 / 0 / 925
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.1455
R indices (all data)	R1 = 0.0721, wR2 = 0.1614
Largest diff. peak and hole	0.940 and -0.511 $e.A^{-3}$

Electrochemical Data for 4b, 4c and 5a.

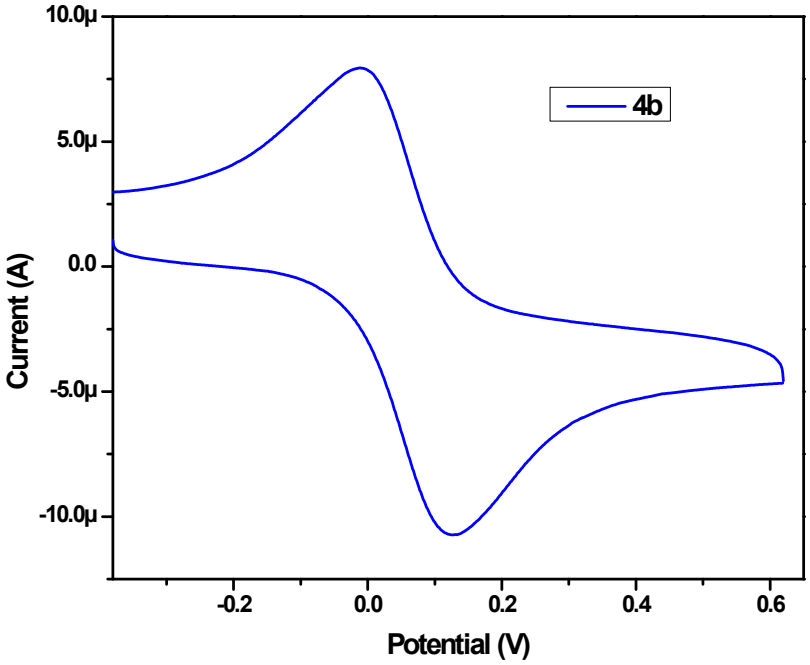


Figure S1. Cyclic voltammogram of truxene **4b.**

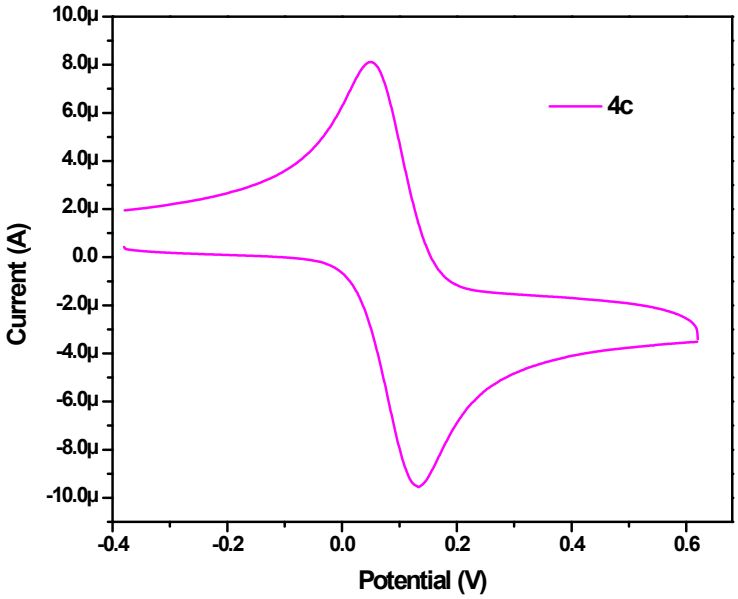


Figure S2. Cyclic voltammogram of truxene **4c.**

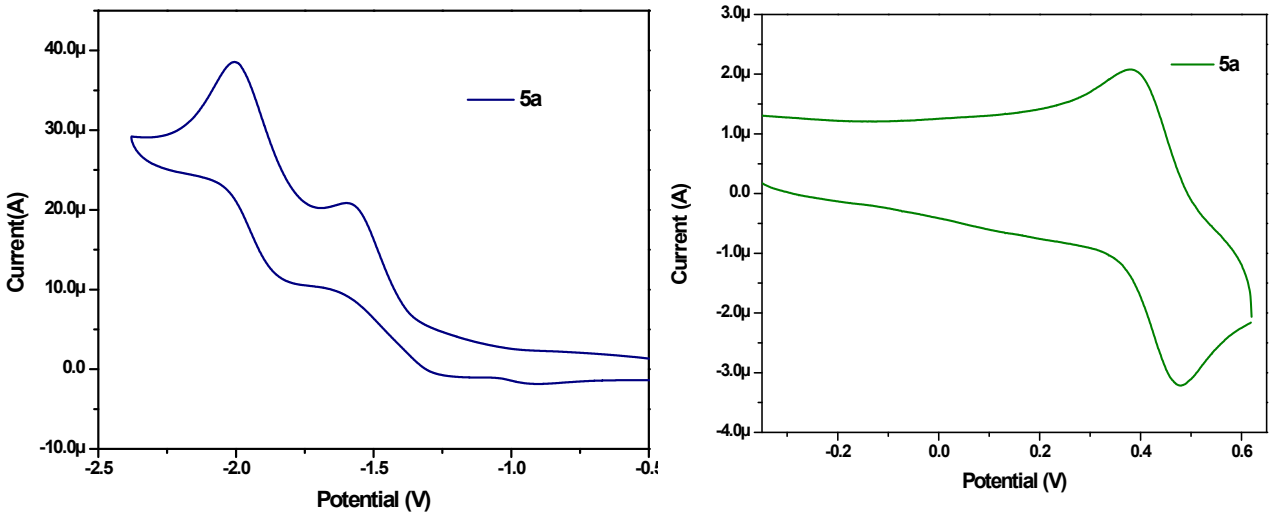
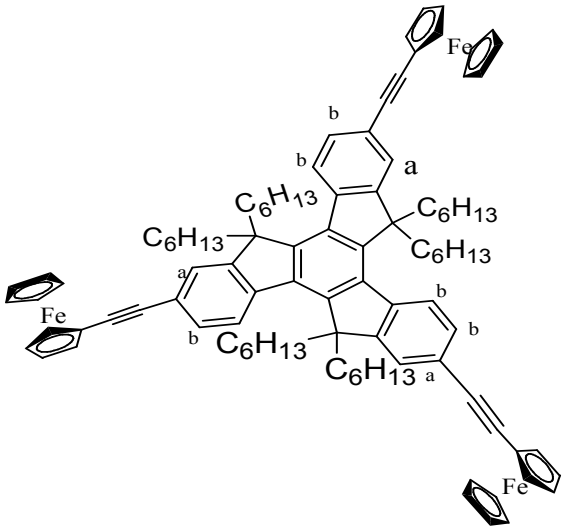


Figure S3. Cyclic voltammograms of truxene **5a.**

Copies of ^{1}H NMR, ^{13}C NMR and HRMS Spectra of the Compounds 4a-4c and 5a.



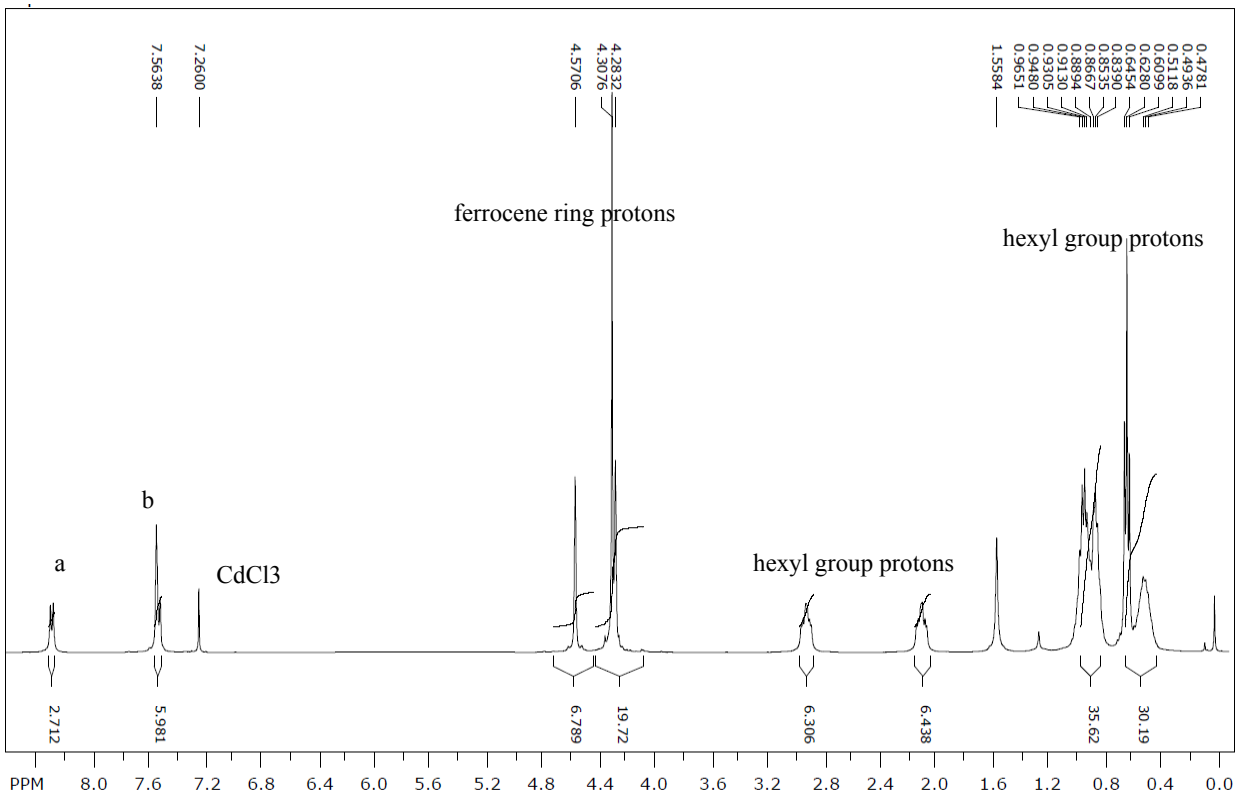


Figure S4. [1]H NMR Spectra of **4a.**

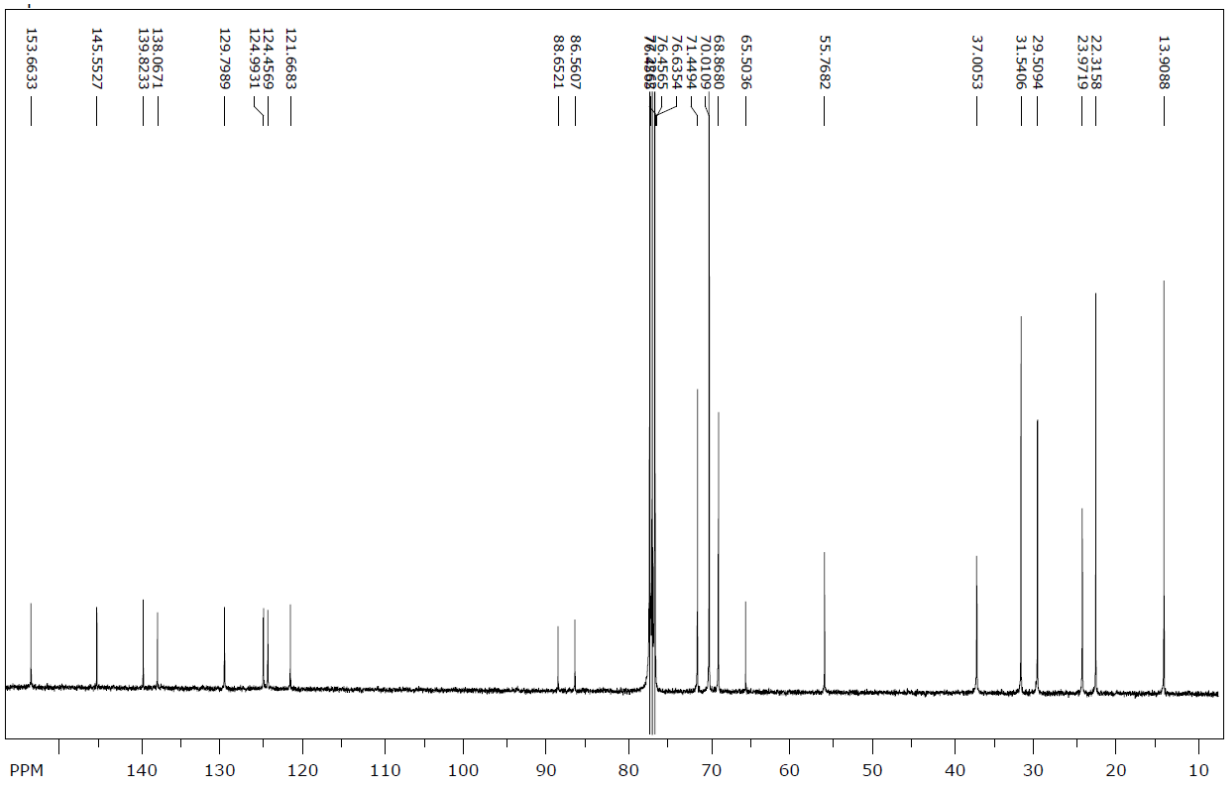


Figure S5. [13]C NMR Spectra of **4a.**

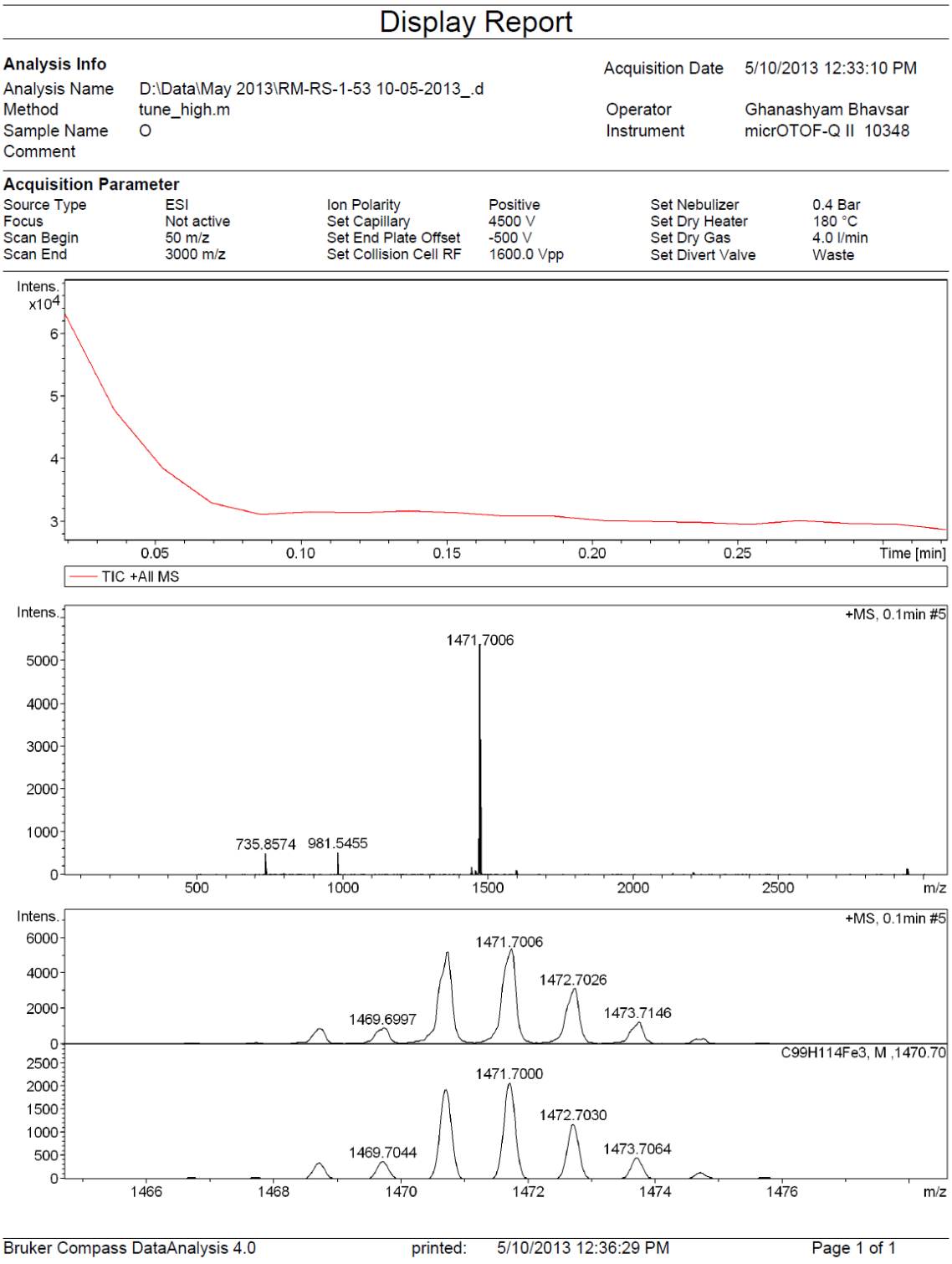
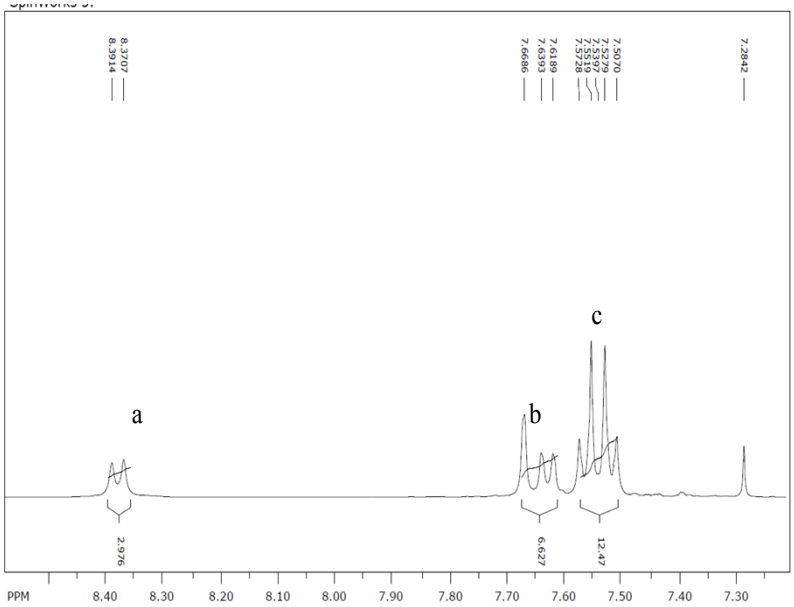
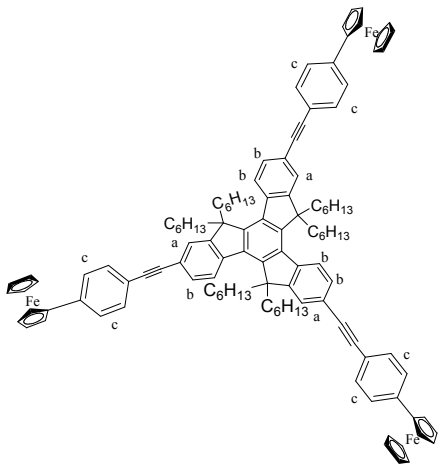


Figure S6. HRMS Spectra of **4a.**





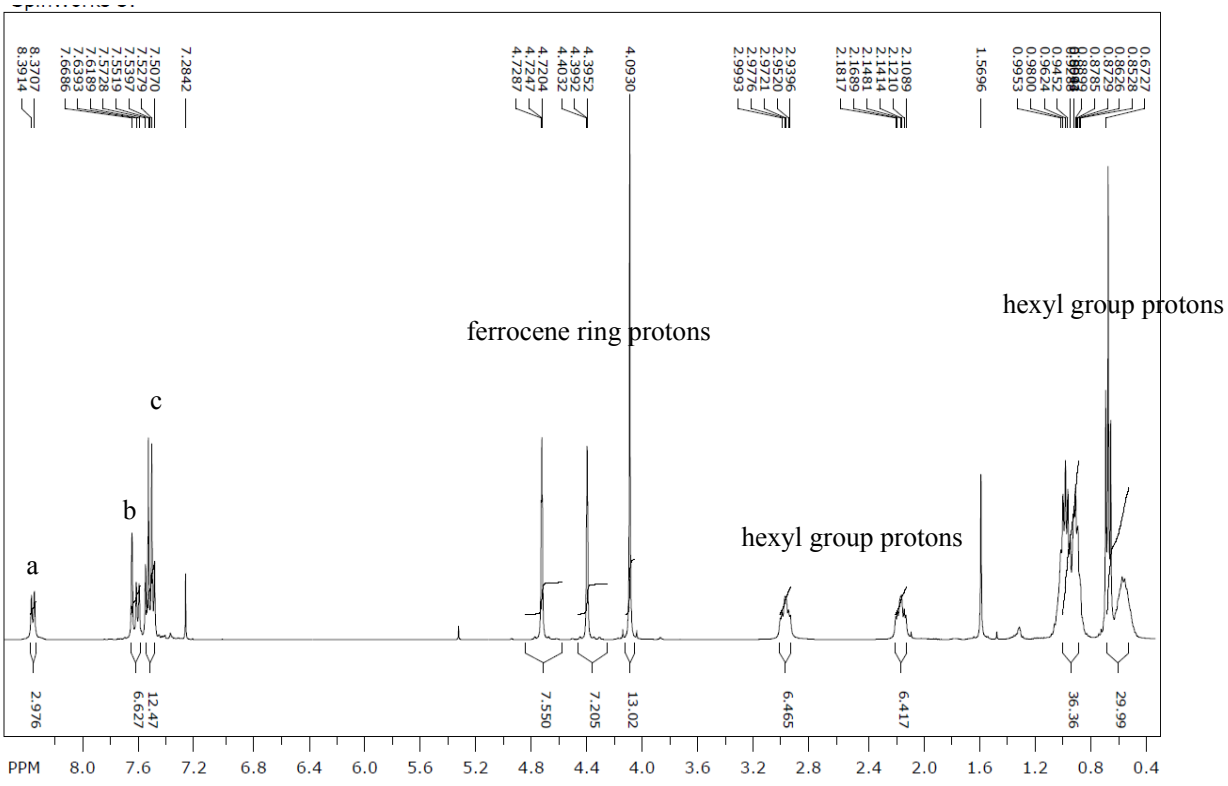


Figure S7. ^{1}H NMR Spectra of **4b.**

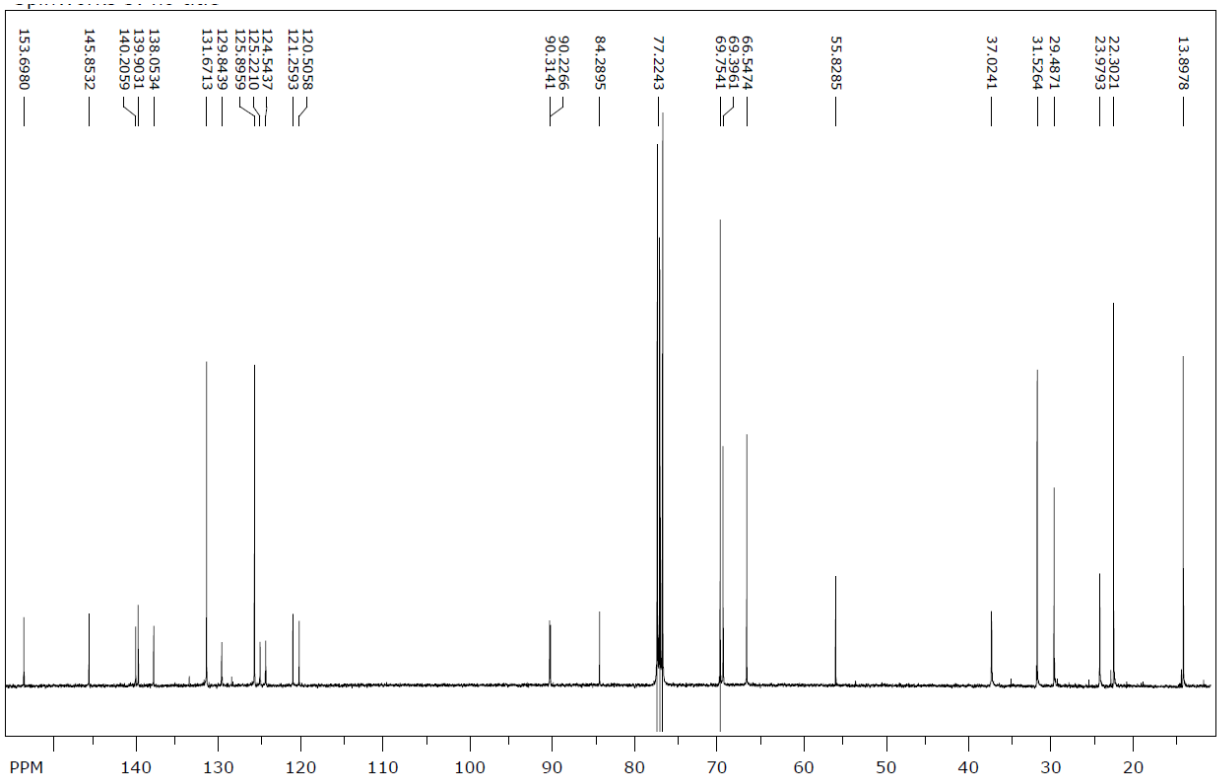


Figure S8. ^{13}C NMR Spectra of **4b.**

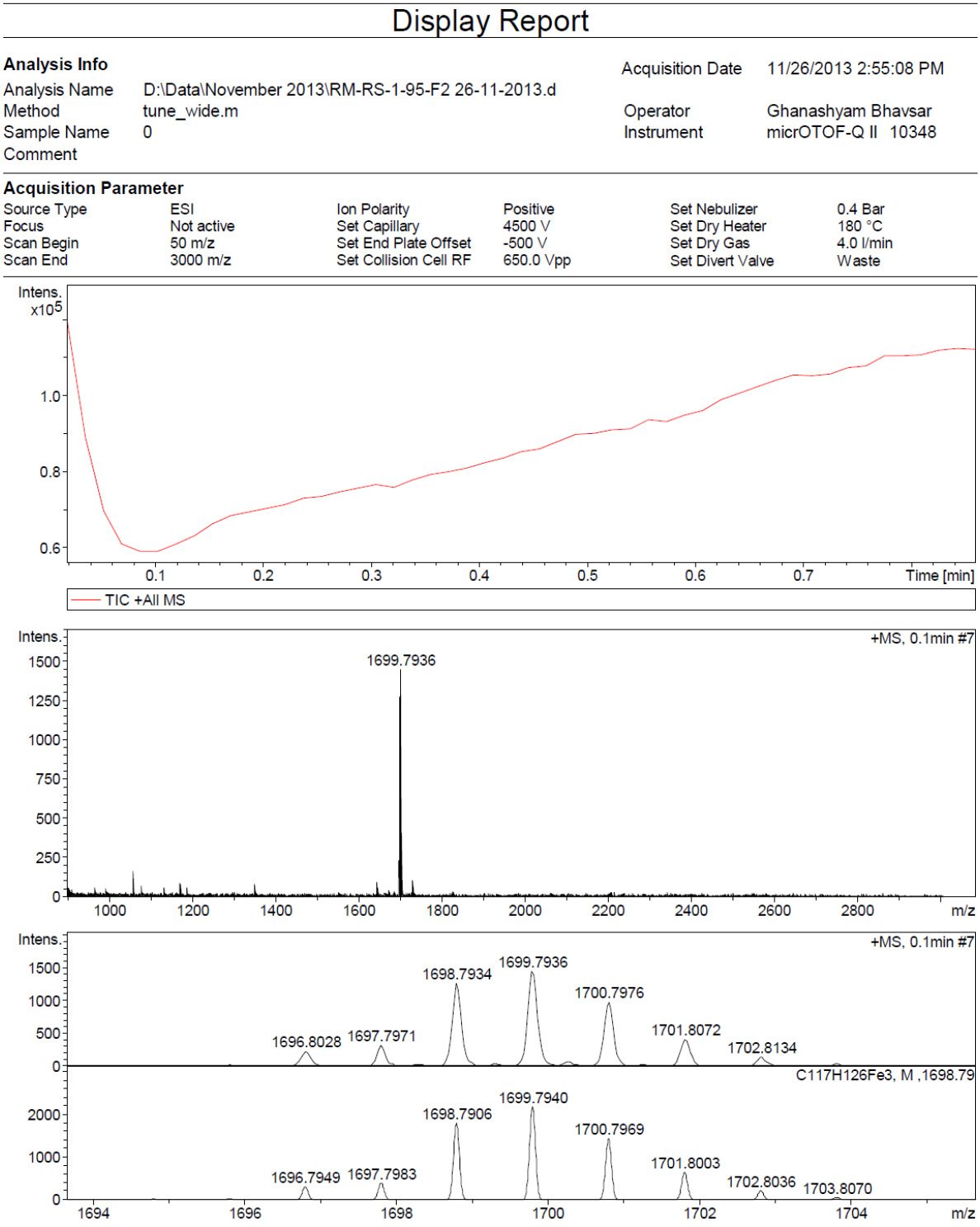
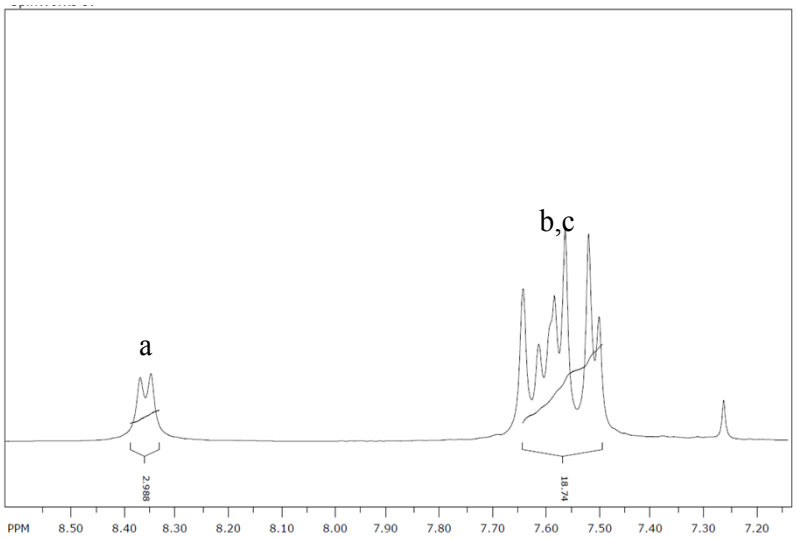
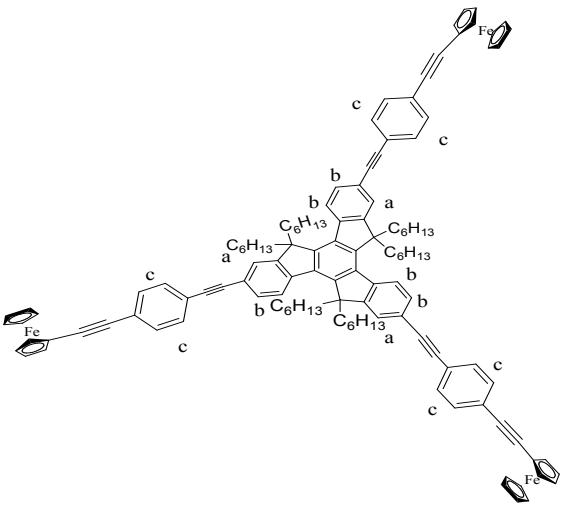


Figure S9. HRMS Spectra of **4b.**





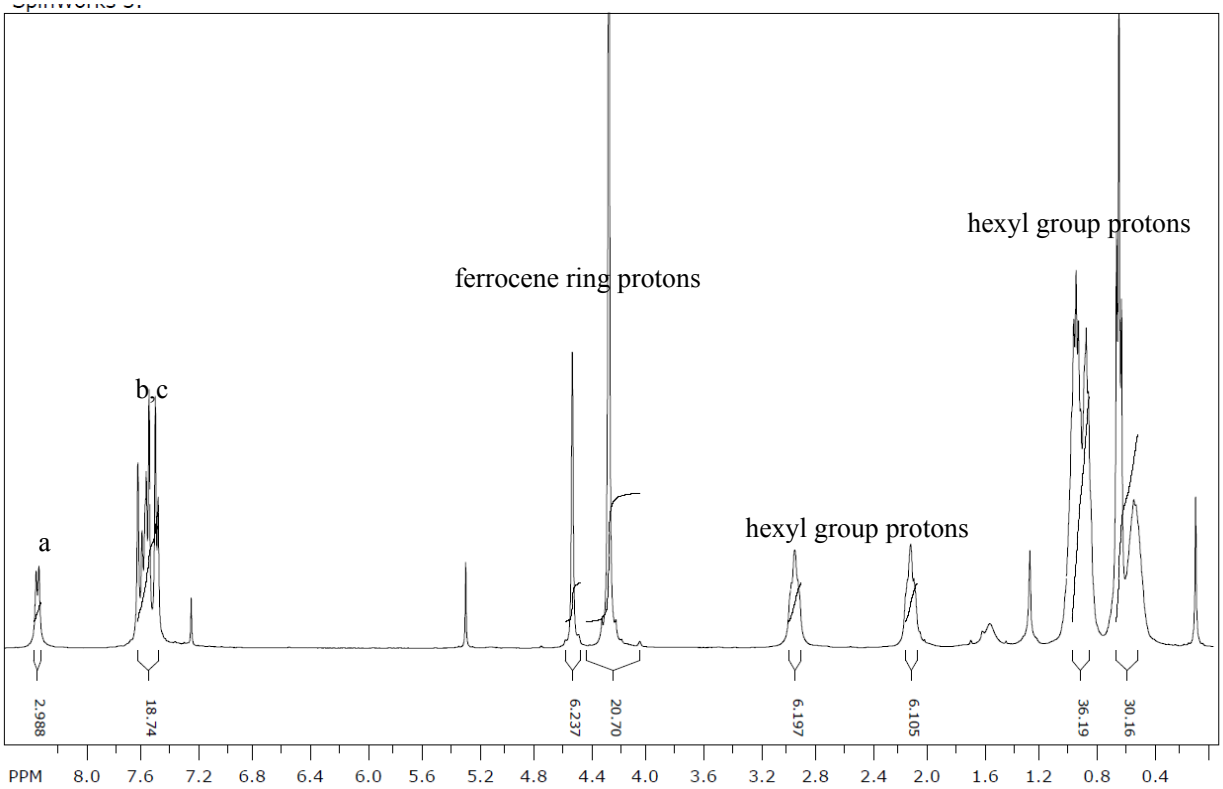


Figure S10. ^{1}H NMR Spectra of **4c.**

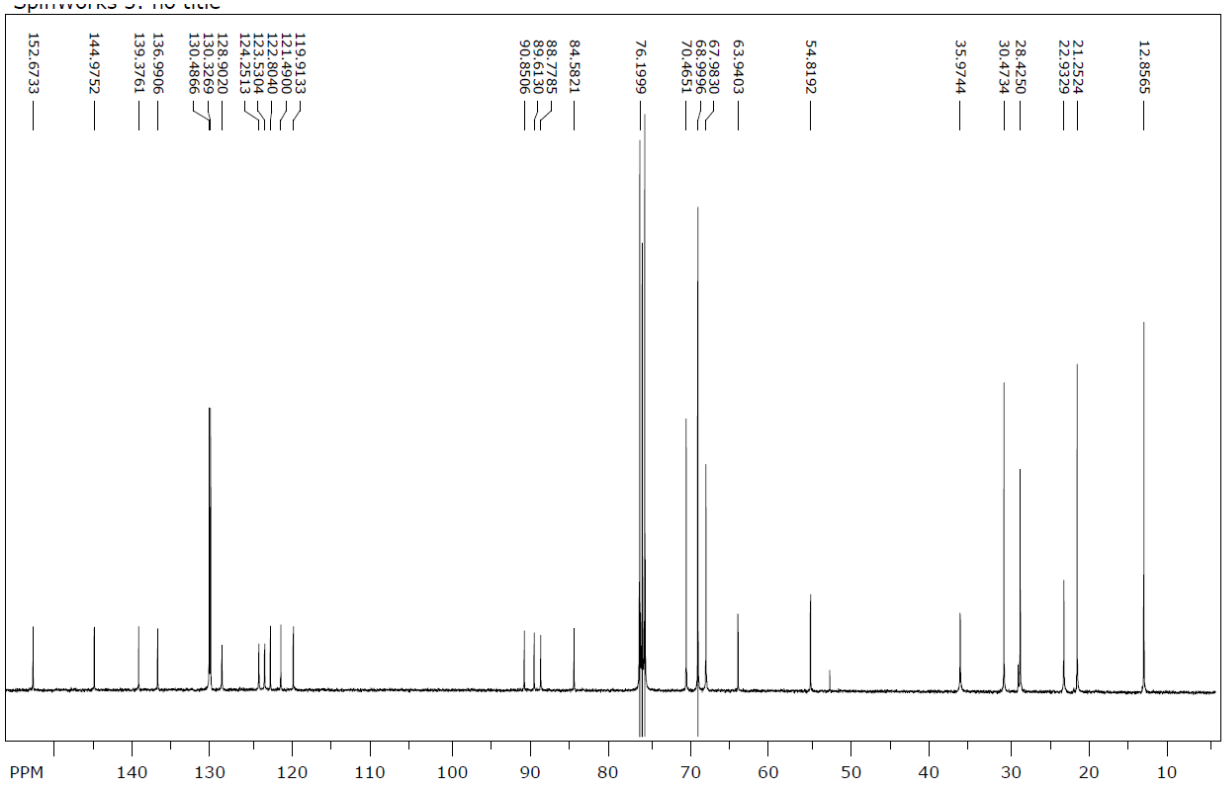


Figure S11. ^{13}C NMR Spectra of **4c.**

Display Report

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Sample Name	0	Instrument	micrOTOF-Q II 10348
Comment			

Acquisition Parameter

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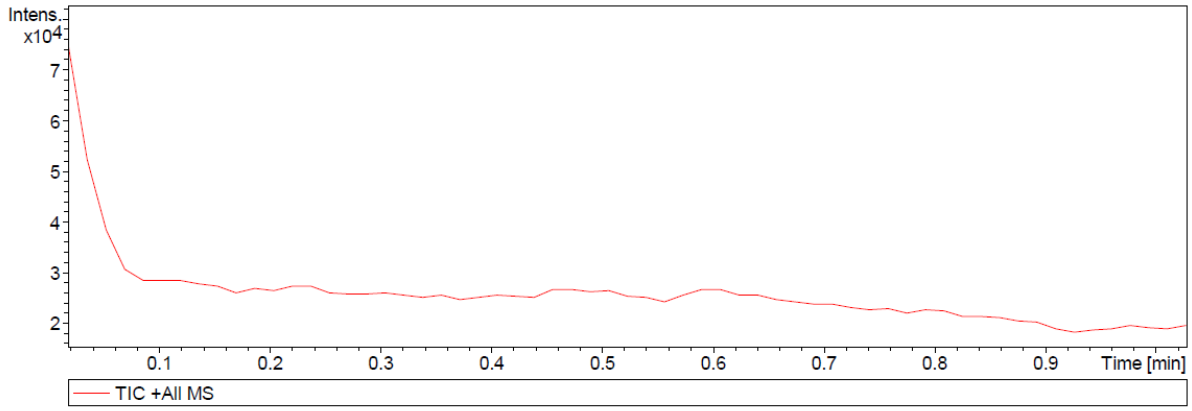
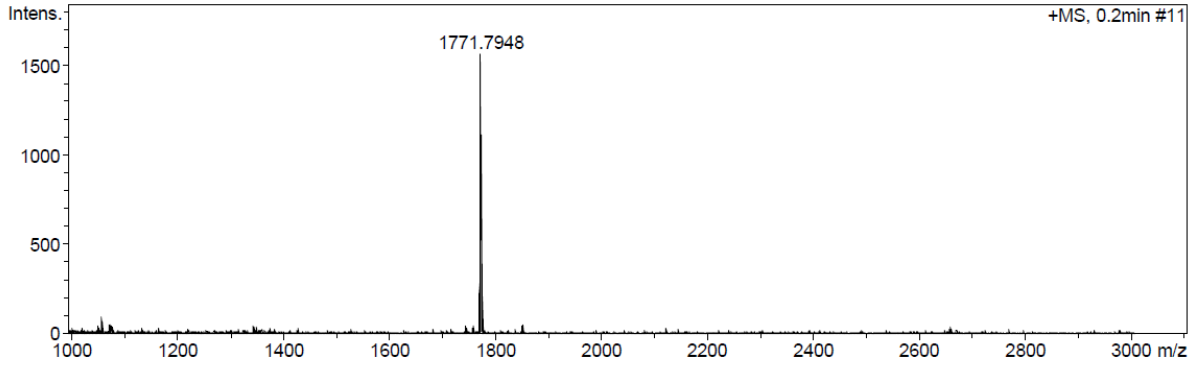
Scan End	3000 m/z	Set Collision Cell RF	1600.0 Vpp	Set Divert Valve	Waste





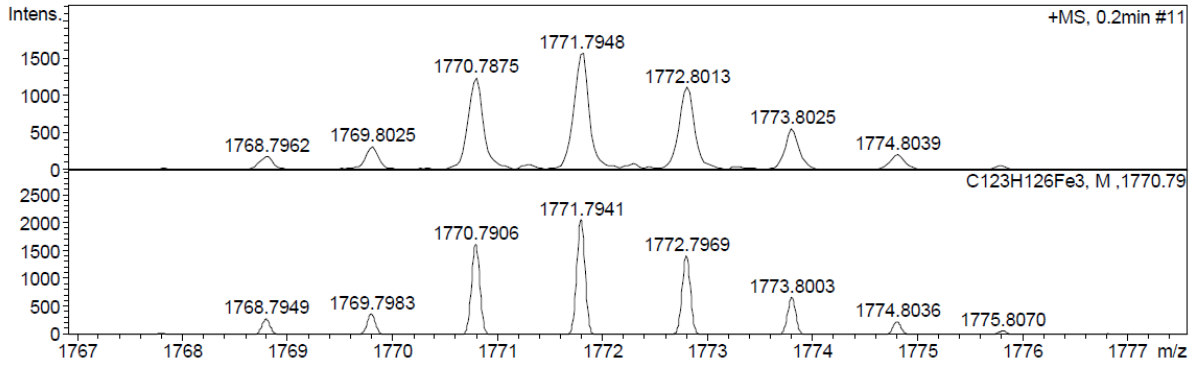


Figure S12. HRMS Spectra of **4c.**

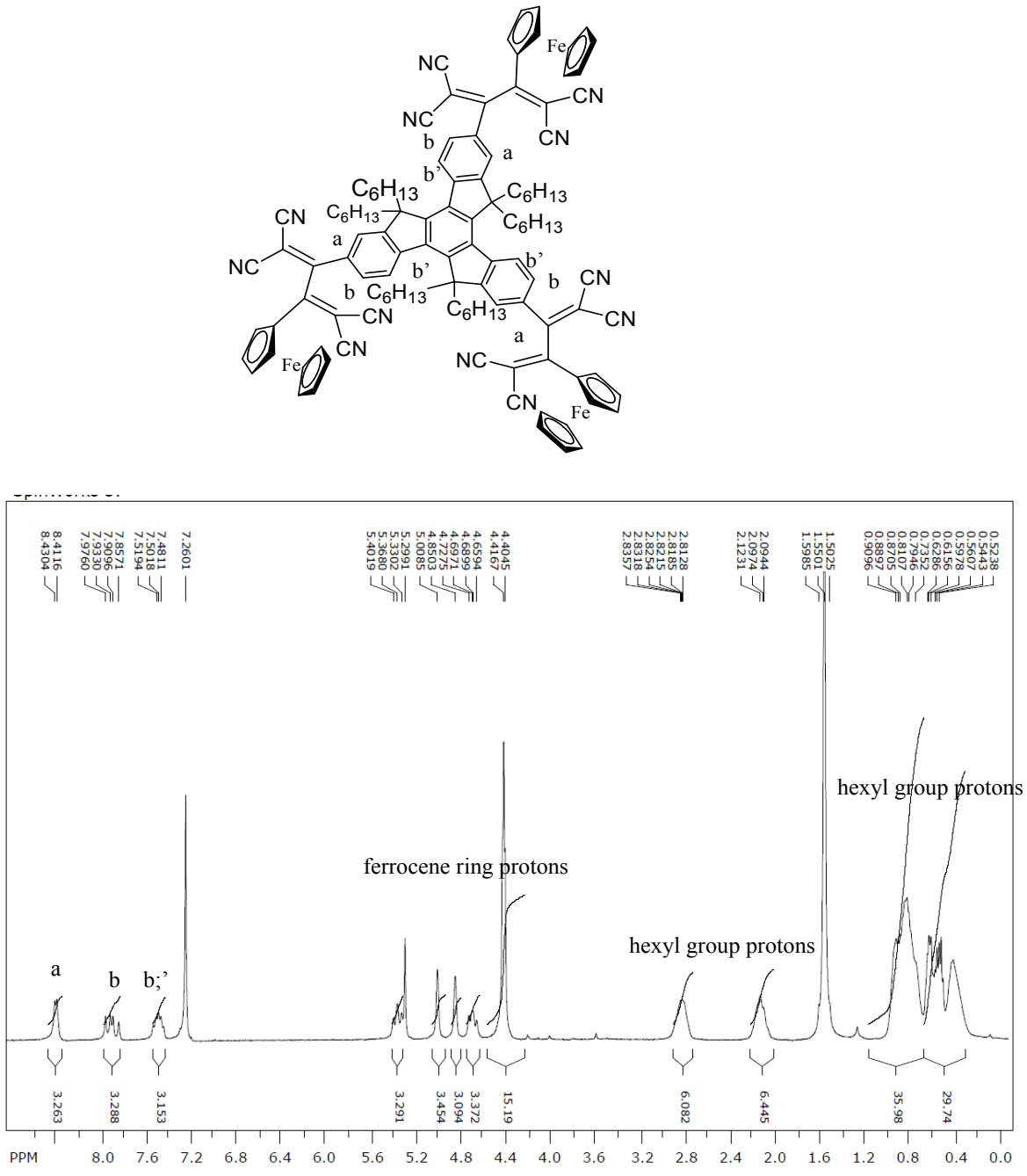


Figure S13. ^{1}H NMR Spectra of **5a.**

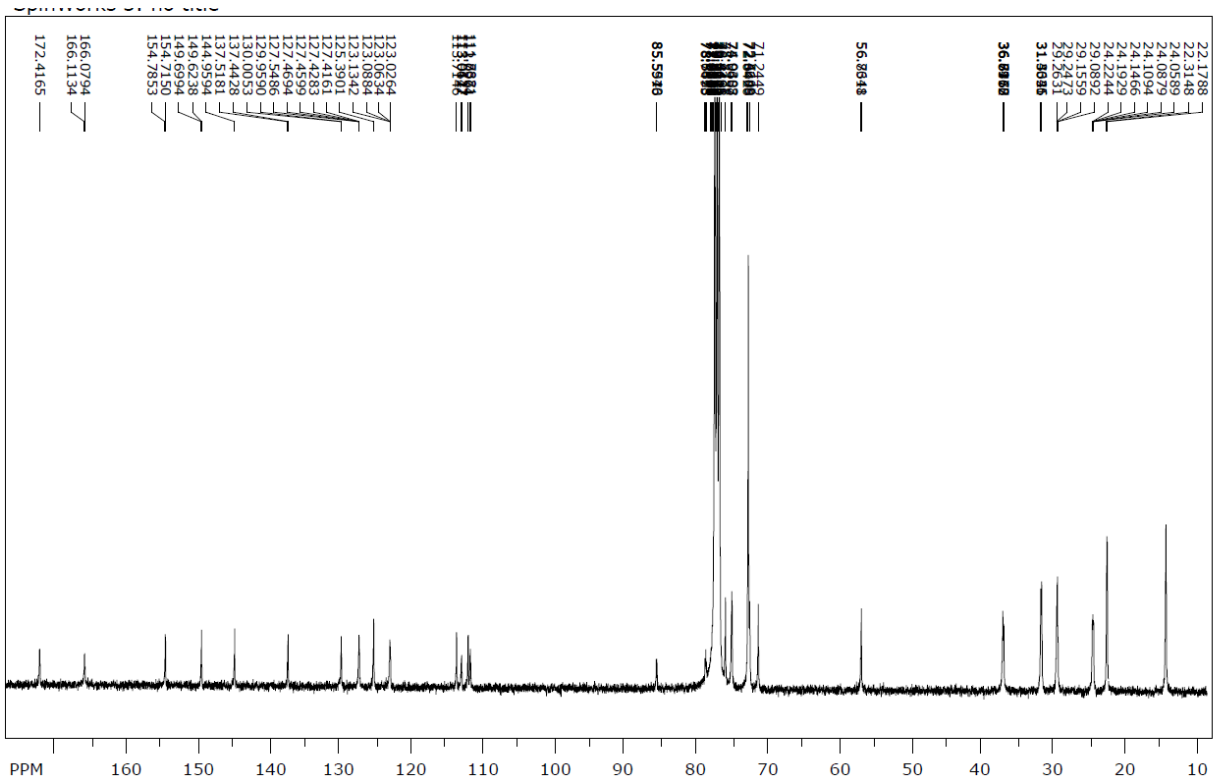


Figure S14. ^{13}C NMR Spectra of **5a.**

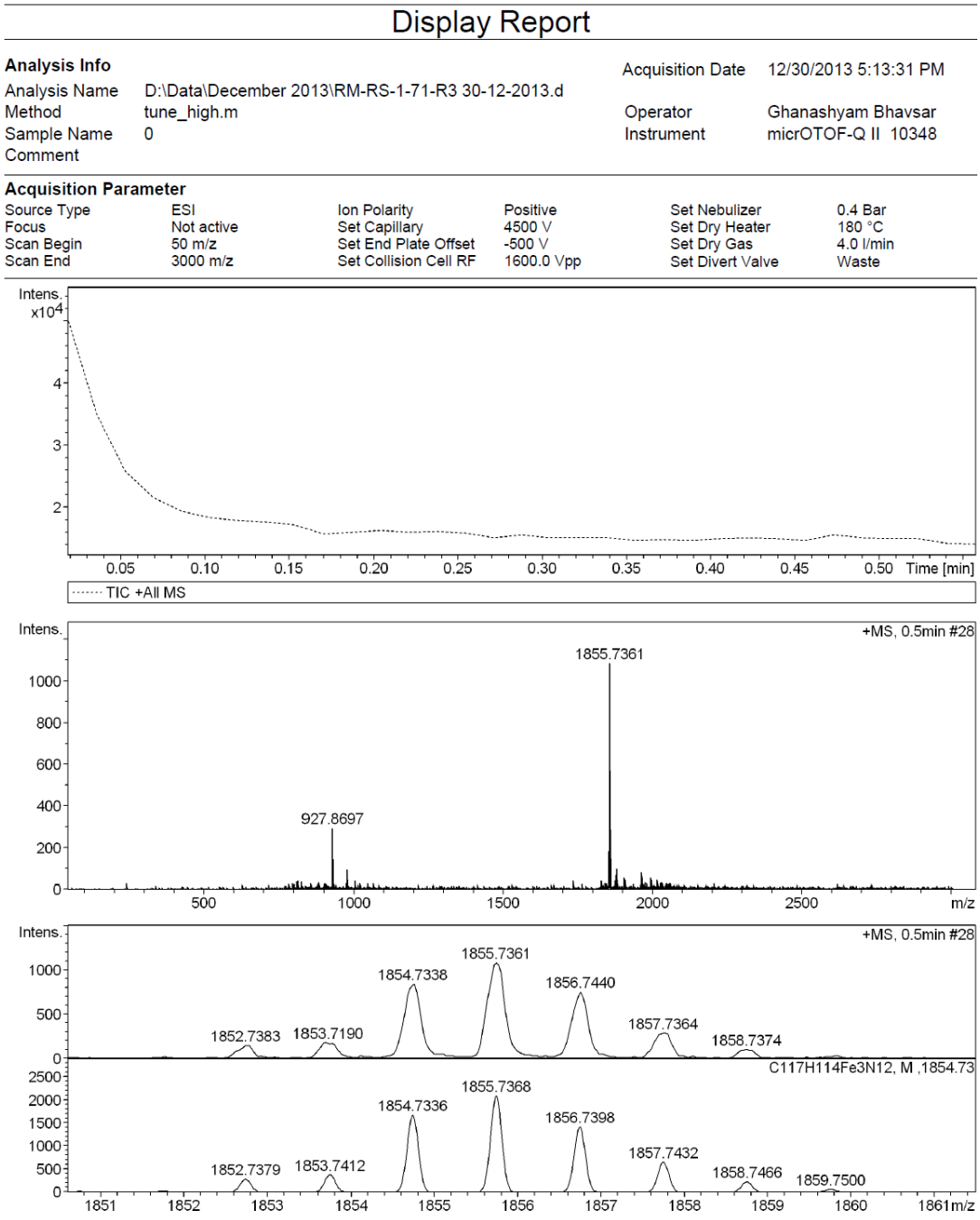


Figure S15. HRMS Spectra of **5a.**