Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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A new entry towards diastereomeric C^1,C^2,C^3- functionalized [3]ferrocenophanes using a solid state mediated double 1,4-Michael addition type ring closing approach.

Biplob Halder[a], Tulasi Barik[a], Saurav Chatterjee *[a]
[a]*Department of Chemistry, National Institute of Technology Rourkela, Odisha-769008, India.*

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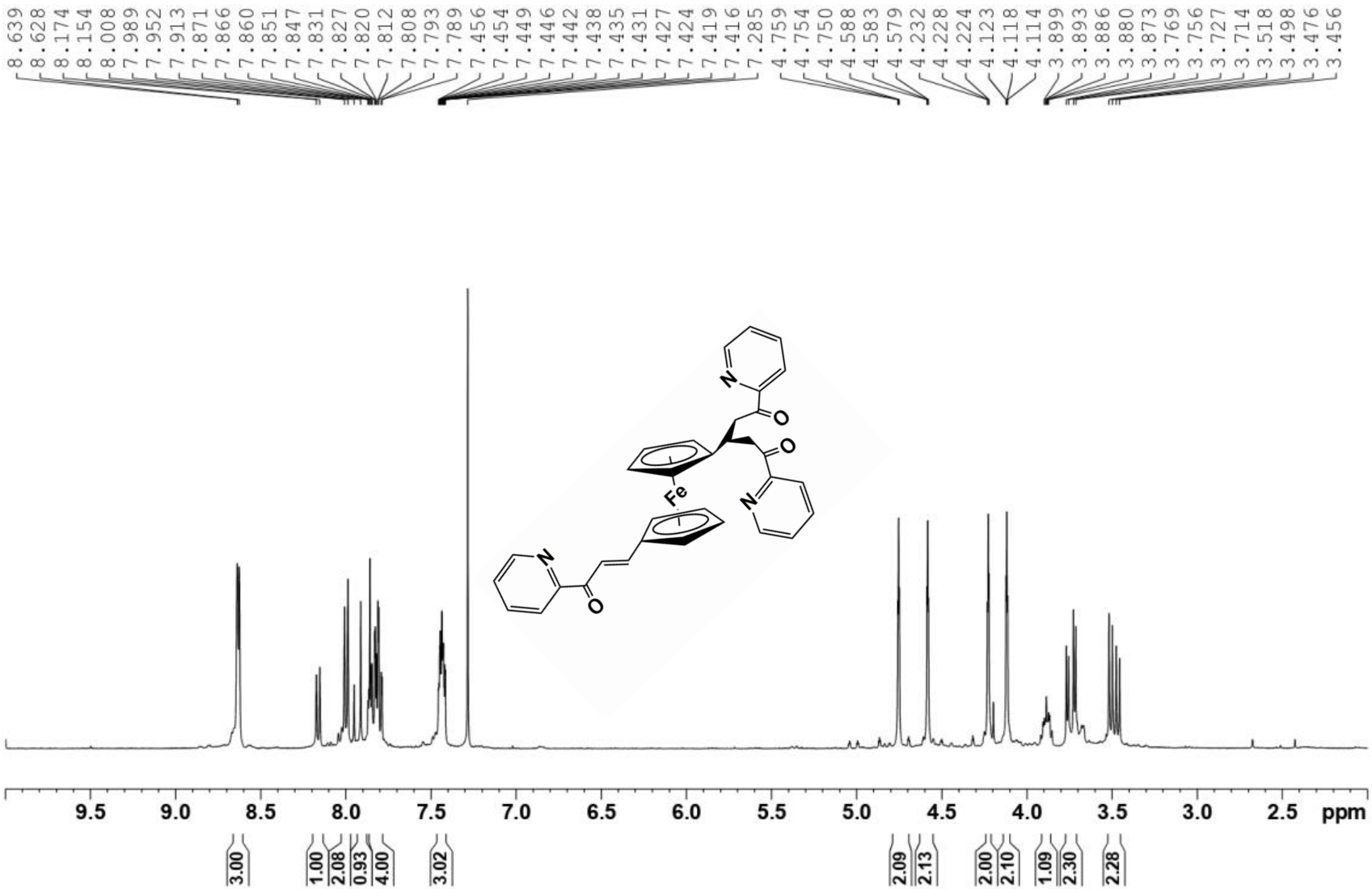


Figure S1: ^{1}H NMR of compound 4 ($CDCl_3$, 400 MHz)

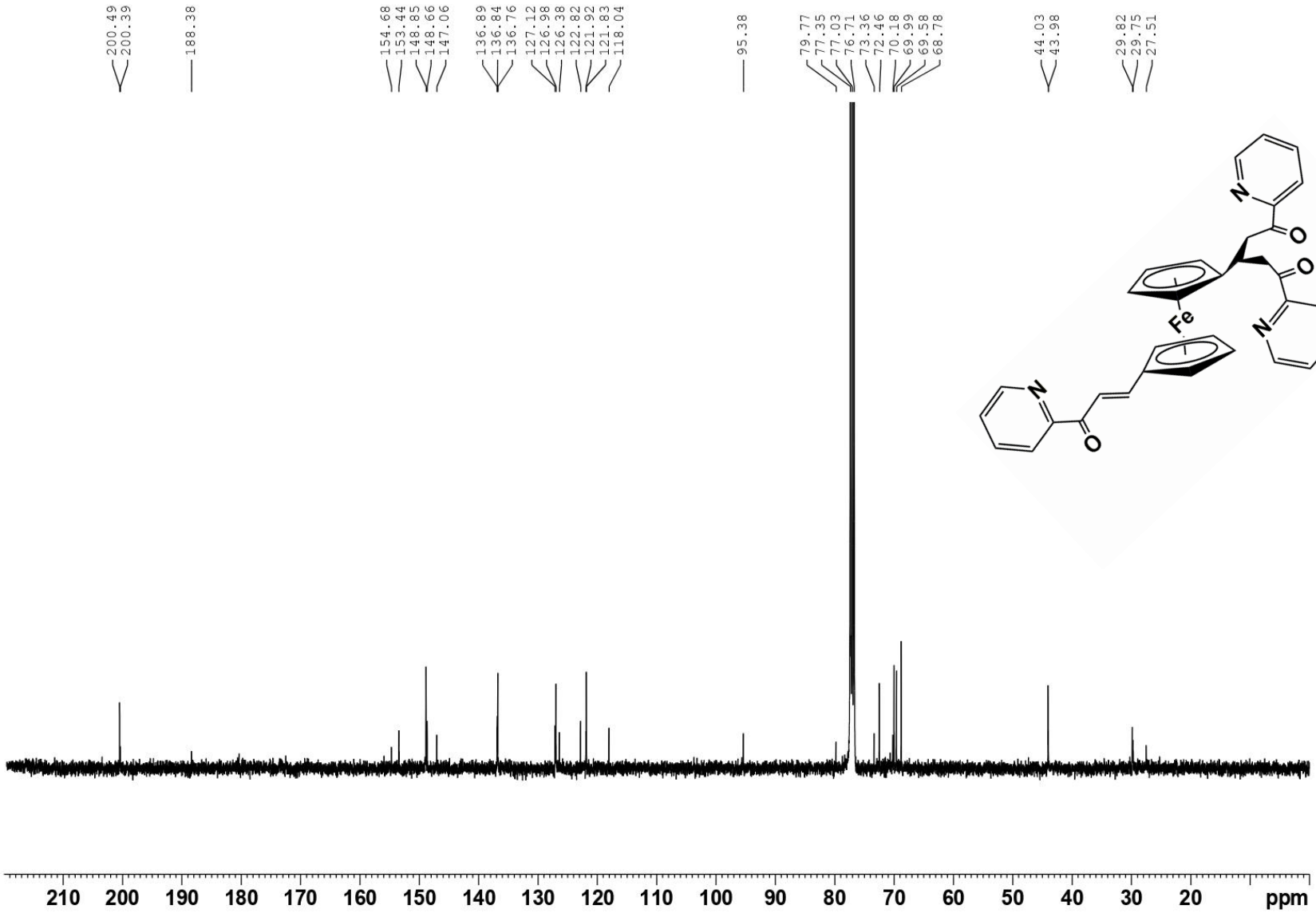


Figure S2: ^{13}C NMR of compound 4 ($CDCl_3$, 100 MHz)

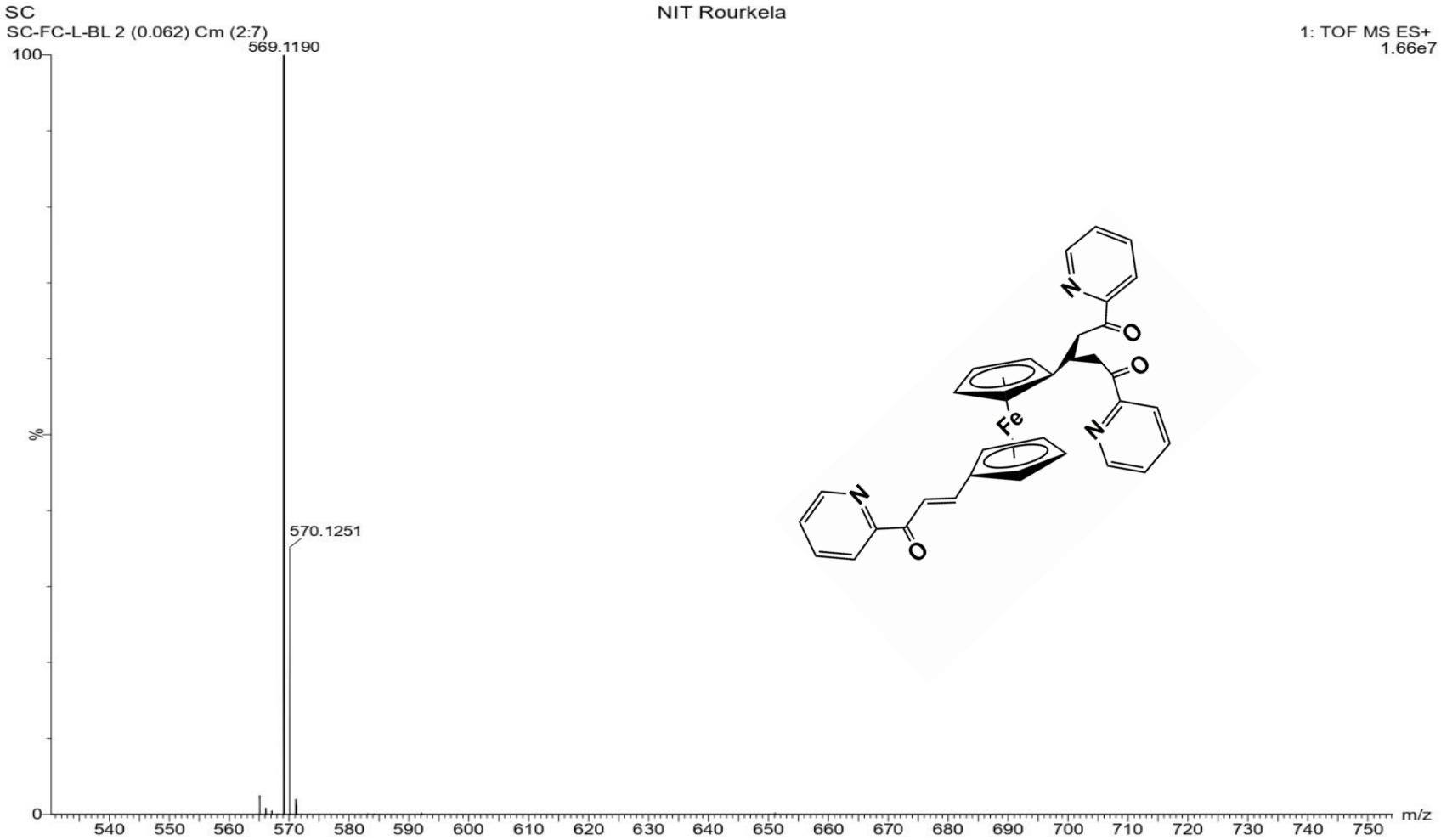


Figure S3: HRMS of compound 4. (100 pmol/µL in MeCN (positive ion mode).

Chemical formula: $C_{33}H_{27}FeN_3O_3$, Mol. Wt: 569.43 ; Observed m/z = 569.1190, $[M]^+$, 570.1251 $[M + H]^+$ **.**

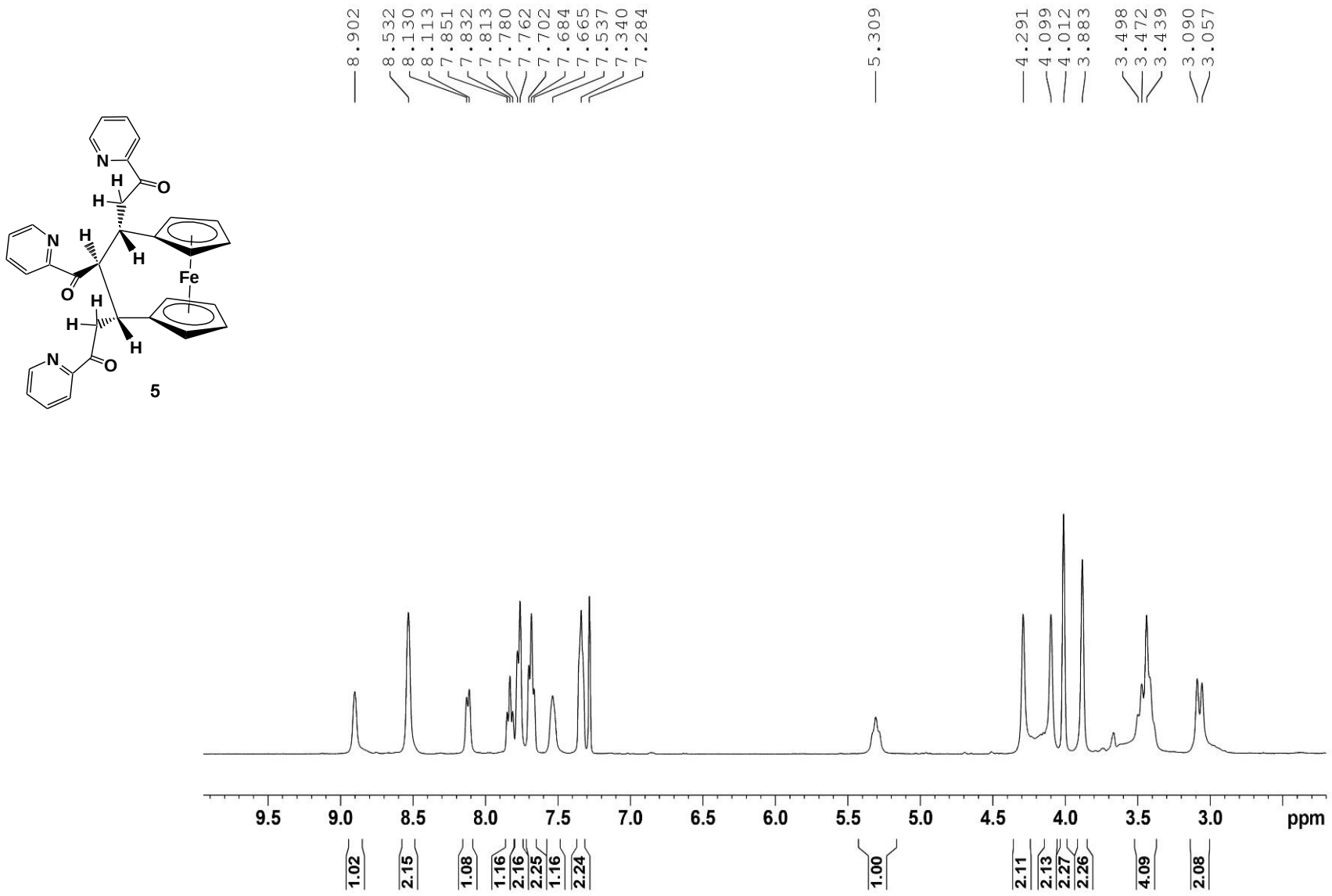


Figure S4: ^{1}H NMR of compound 5 ($CDCl_3$, 400 MHz)

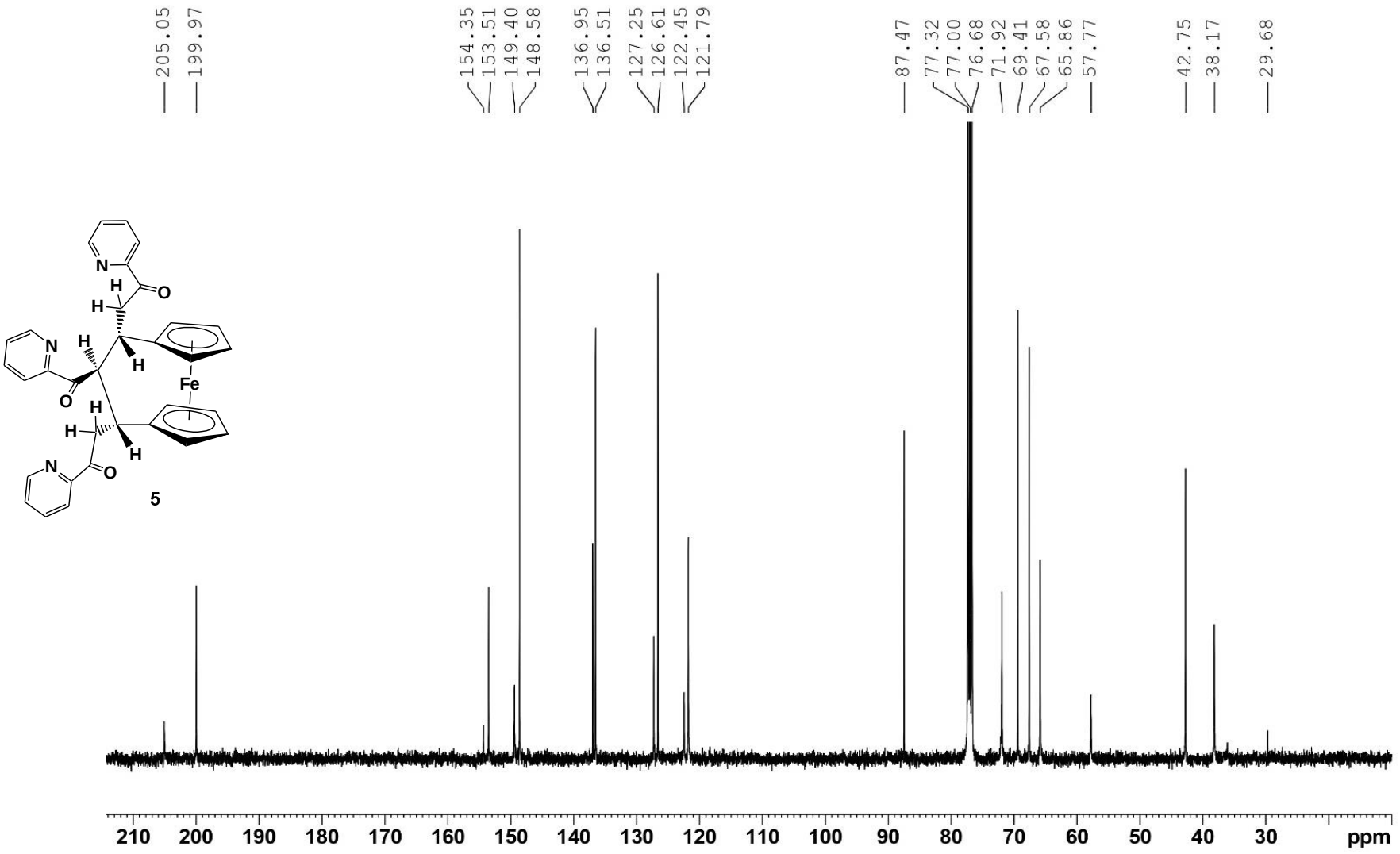


Figure S5: ^{13}C NMR of compound 5 ($CDCl_3$, 100 MHz)

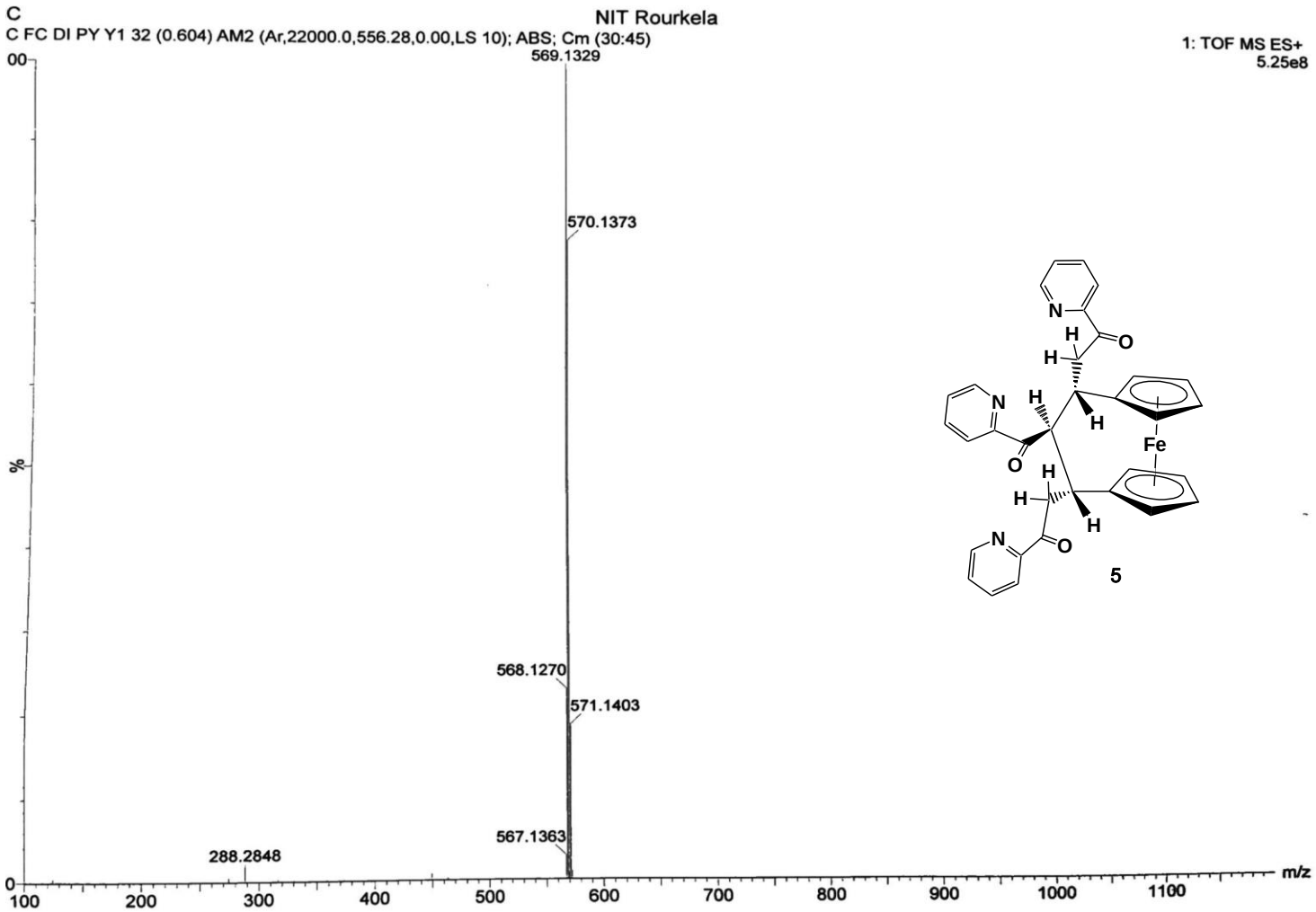


Figure S6: HRMS of compound 5. (100 pmol/µL in MeCN (positive ion mode).

Chemical formula: $C_{33}H_{27}FeN_3O_3$, Mol. Wt: 569.43 ; Observed m/z = 569.1329 $[M]^+$, 570.1373 $[M + H]^+$ **.**

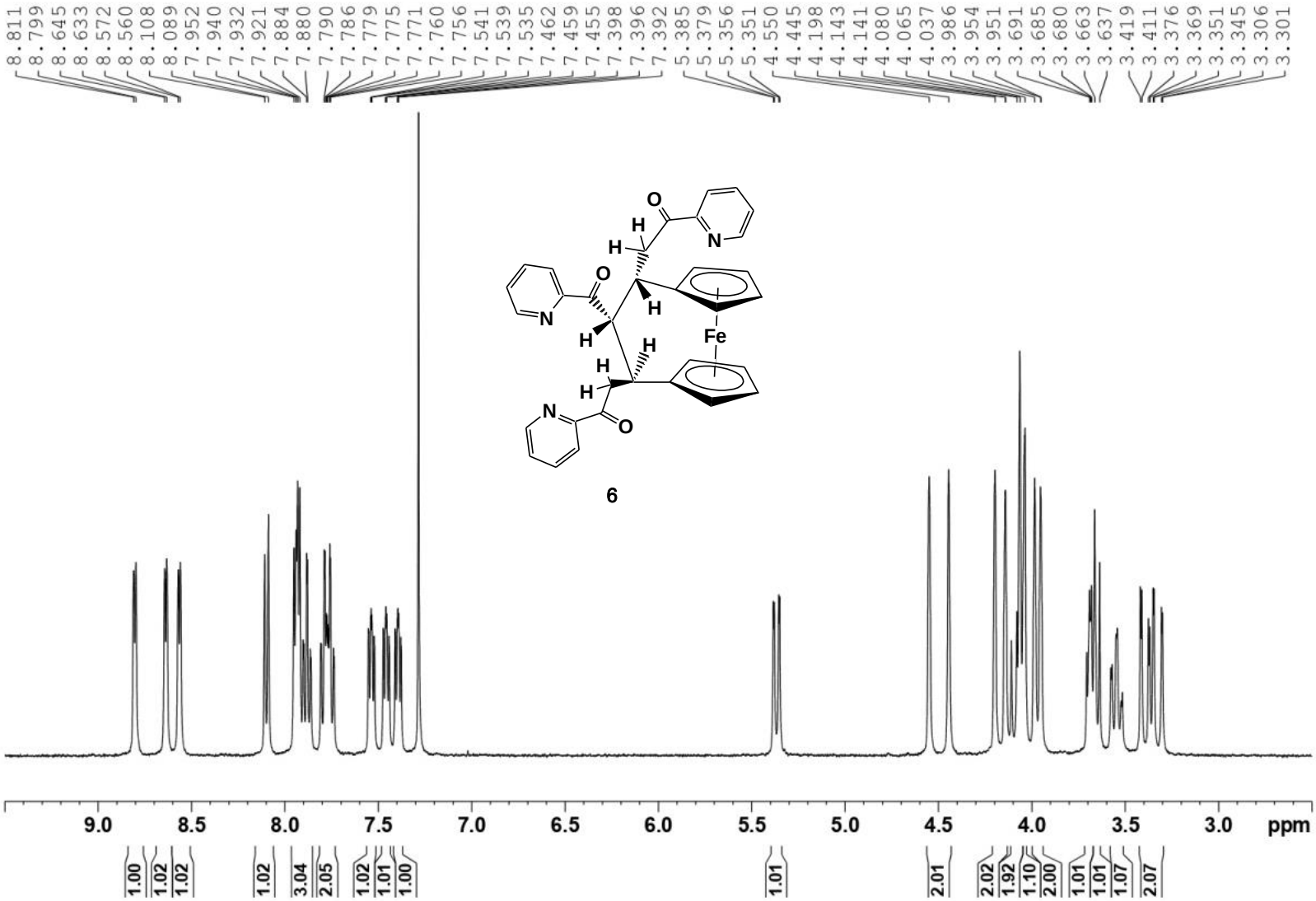
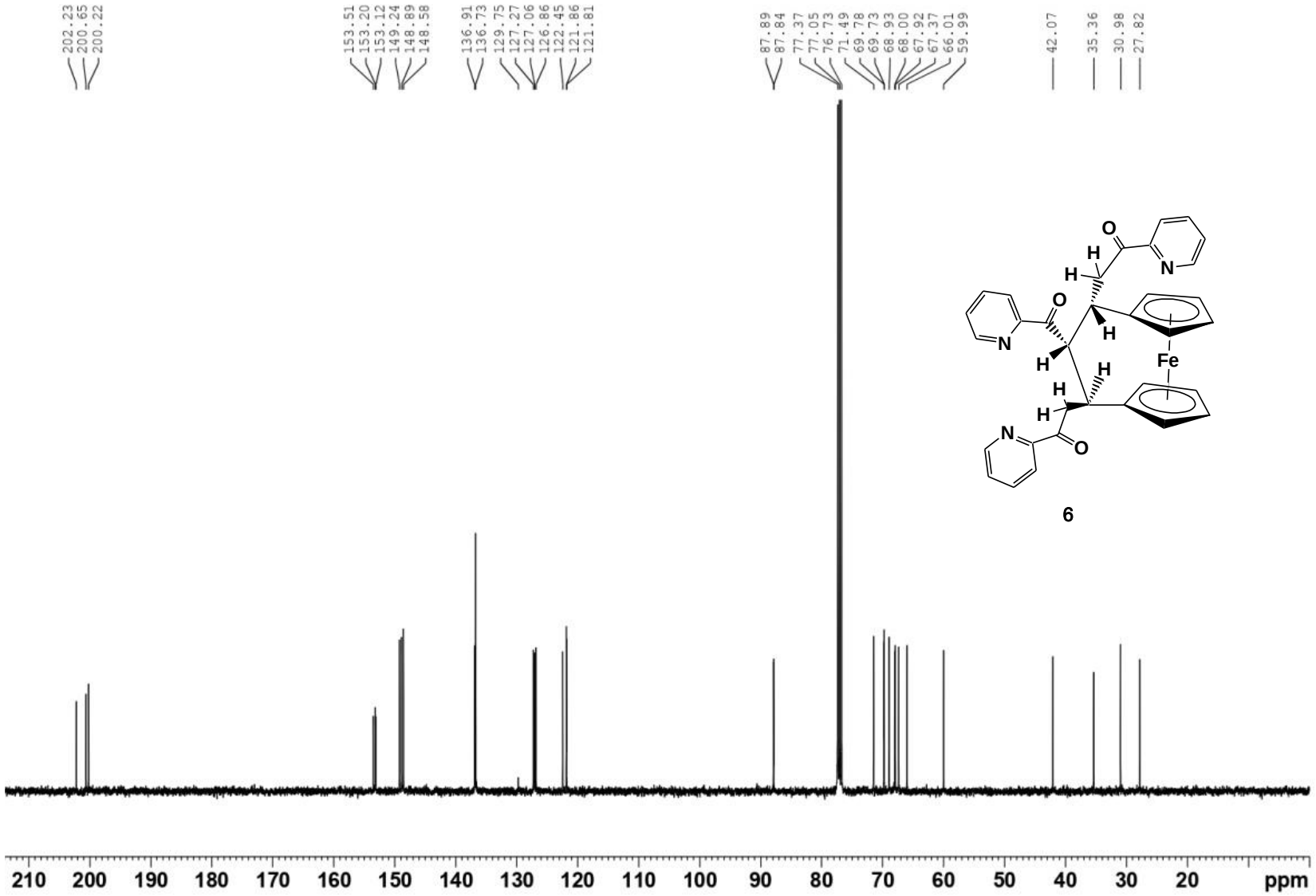


Figure S7: ^{1}H NMR of compound 6 ($CDCl_3$, 400 MHz)



6

Figure S8: ^{13}C NMR of compound 6 ($CDCl_3$, 100 MHz)

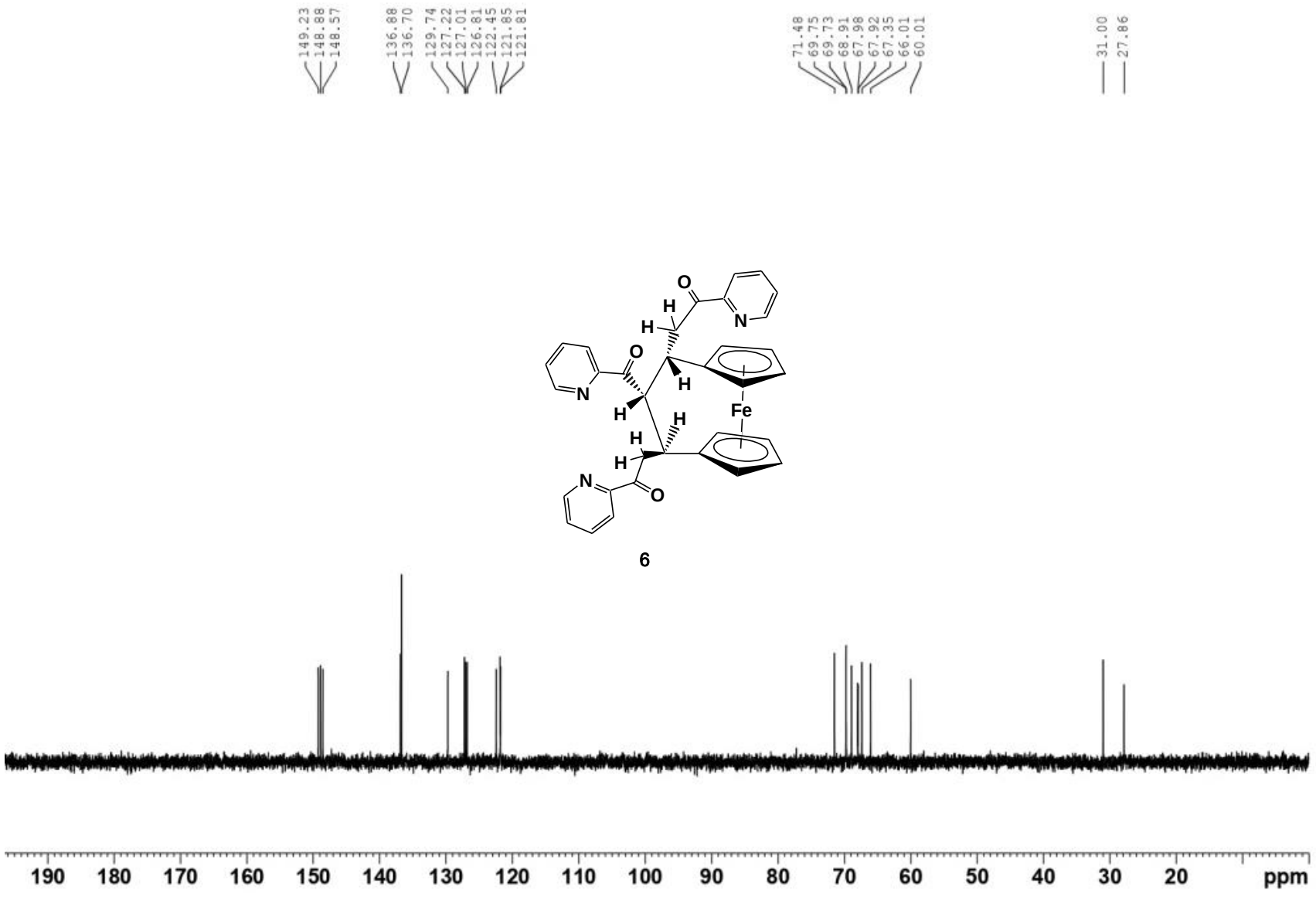


Figure S9: DEPT-90 NMR of compound 6 ($CDCl_3$, 100 MHz)

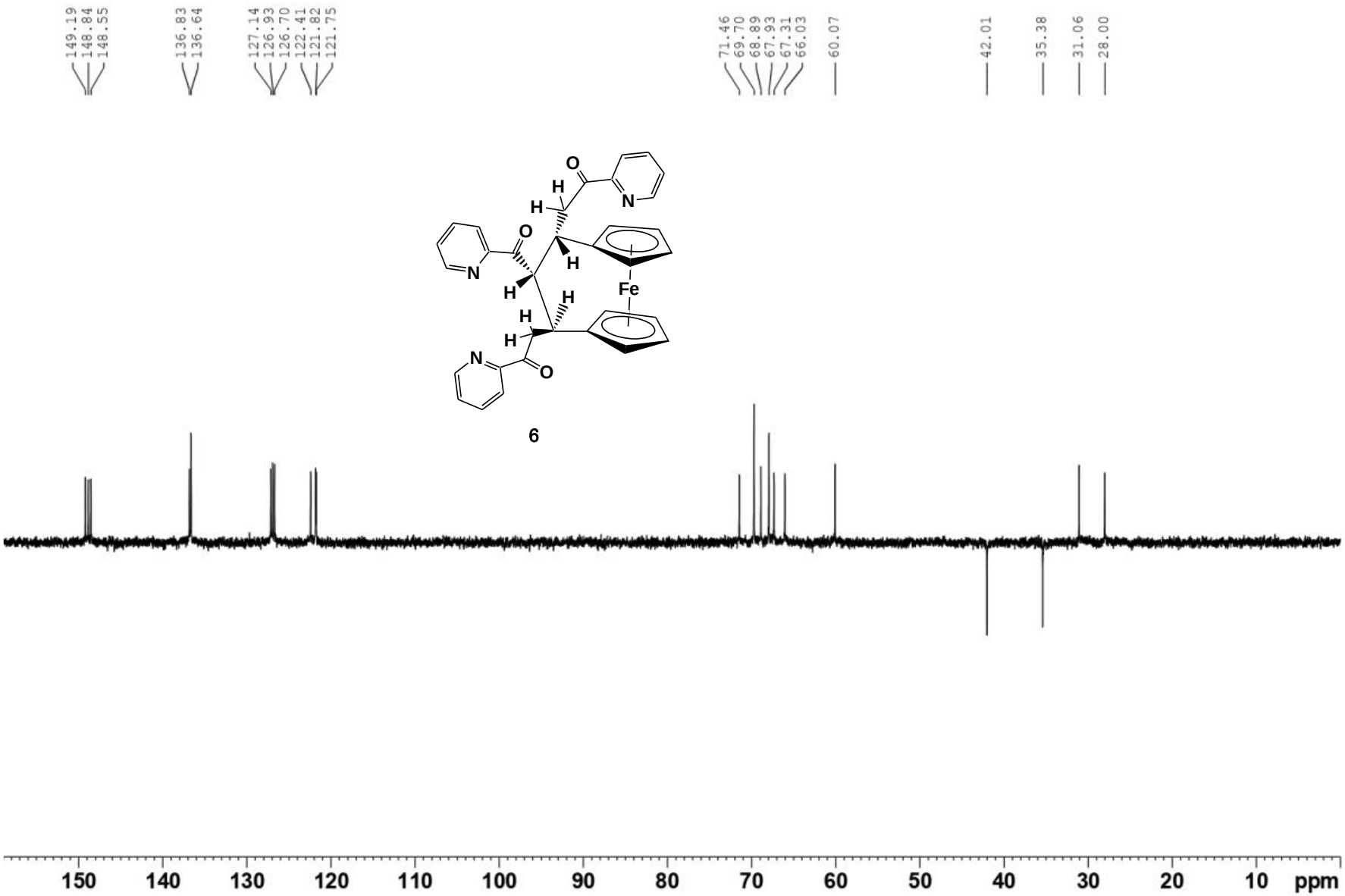


Figure S10: DEPT-135 NMR of compound 6 ($CDCl_3$, 100 MHz)

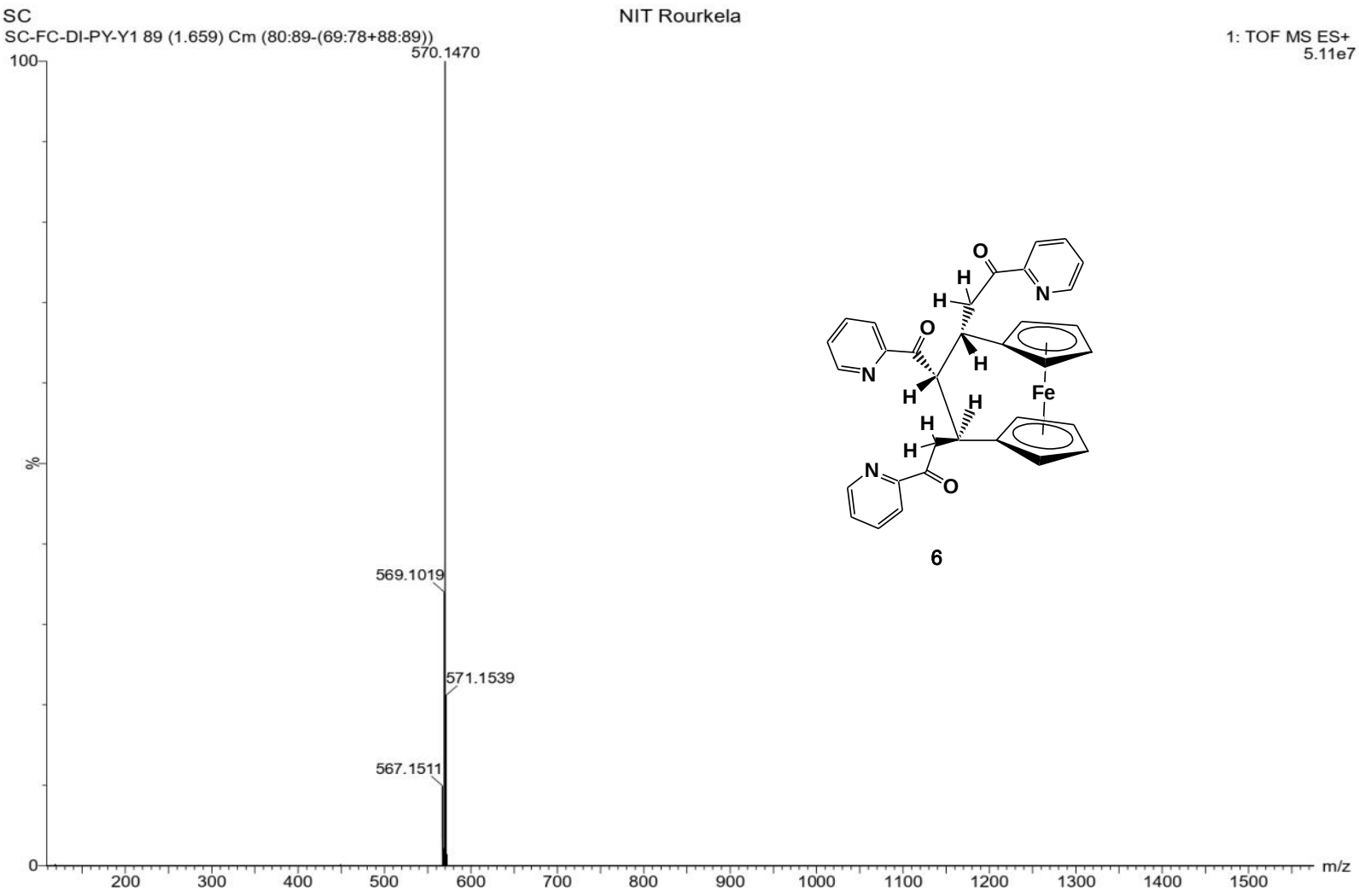


Figure S11: HRMS of compound 6. (100 pmol/µL in MeCN (positive ion mode).

Chemical formula: $C_{33}H_{27}FeN_3O_3$, Mol. Wt: 569.43 ; Observed m/z = 570.1470 $[M + H]^+$ **.**

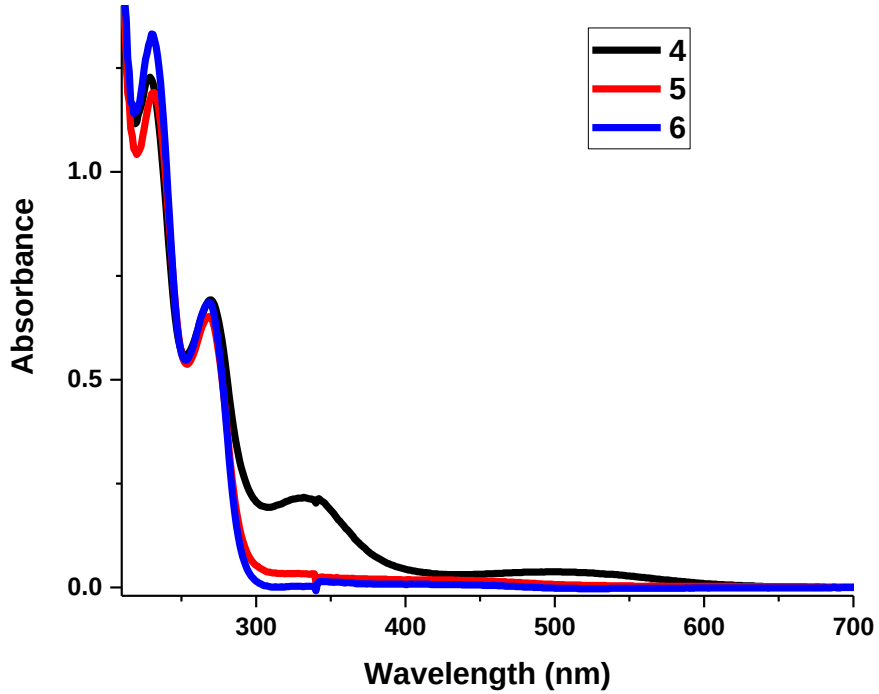
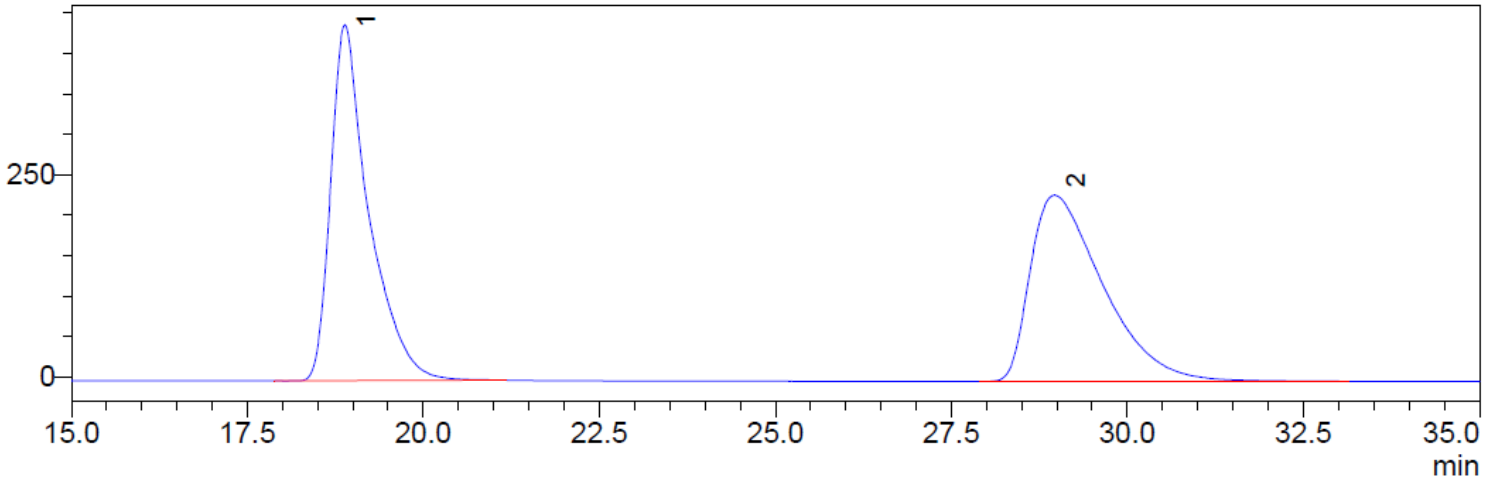


Figure S12: UV-Visible Spectra of 4-6



PDA Ch1 254nm

Peak#	Ret. Time	Area%
1	18.89	50.04
2	28.97	49.96
Total		100.00

Figure S13: Chiral HPLC of 6 showing 1R,3R and 1S,3S enantiomers

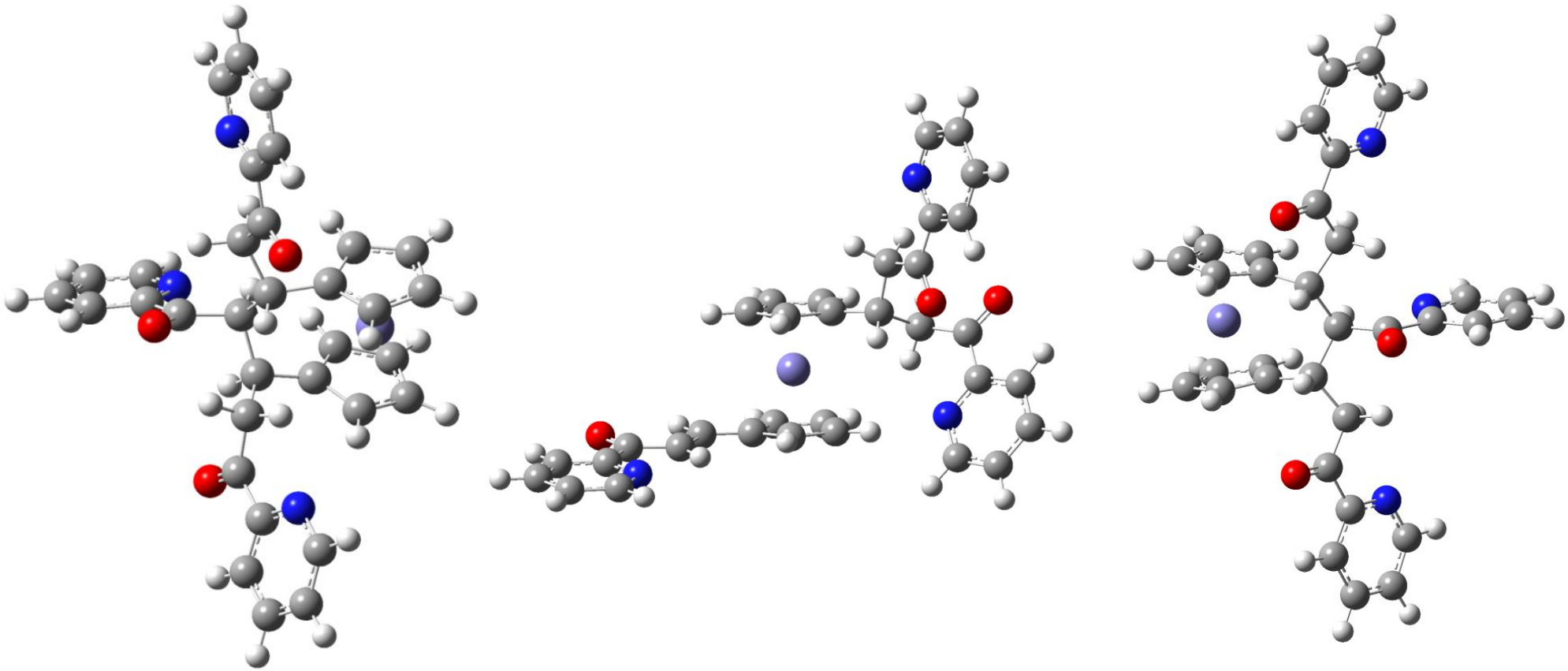


Figure S14 : Optimized geometry of 6 (- 48622.268518209 eV), 4 (- 48622.287660337 eV) and **5 (- 48622.207742644 eV)**

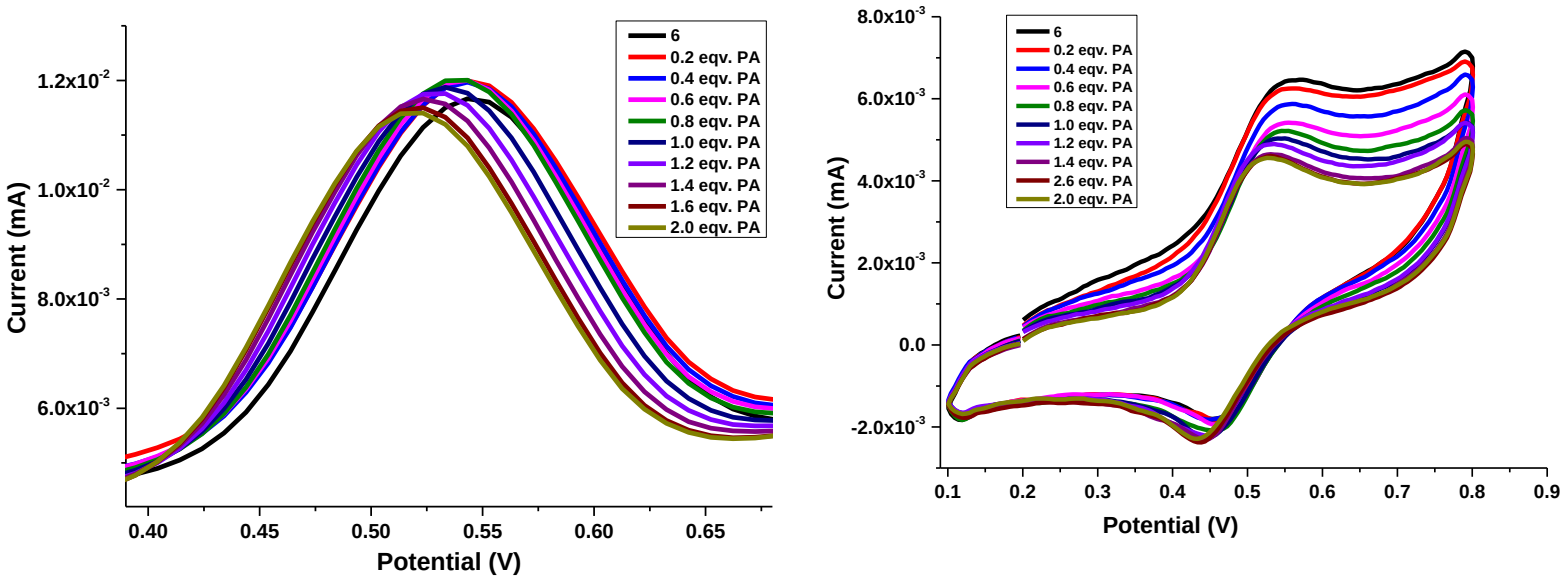


Figure S15: DPV and CV of 6 on gradual addition of Picric acid (PA)

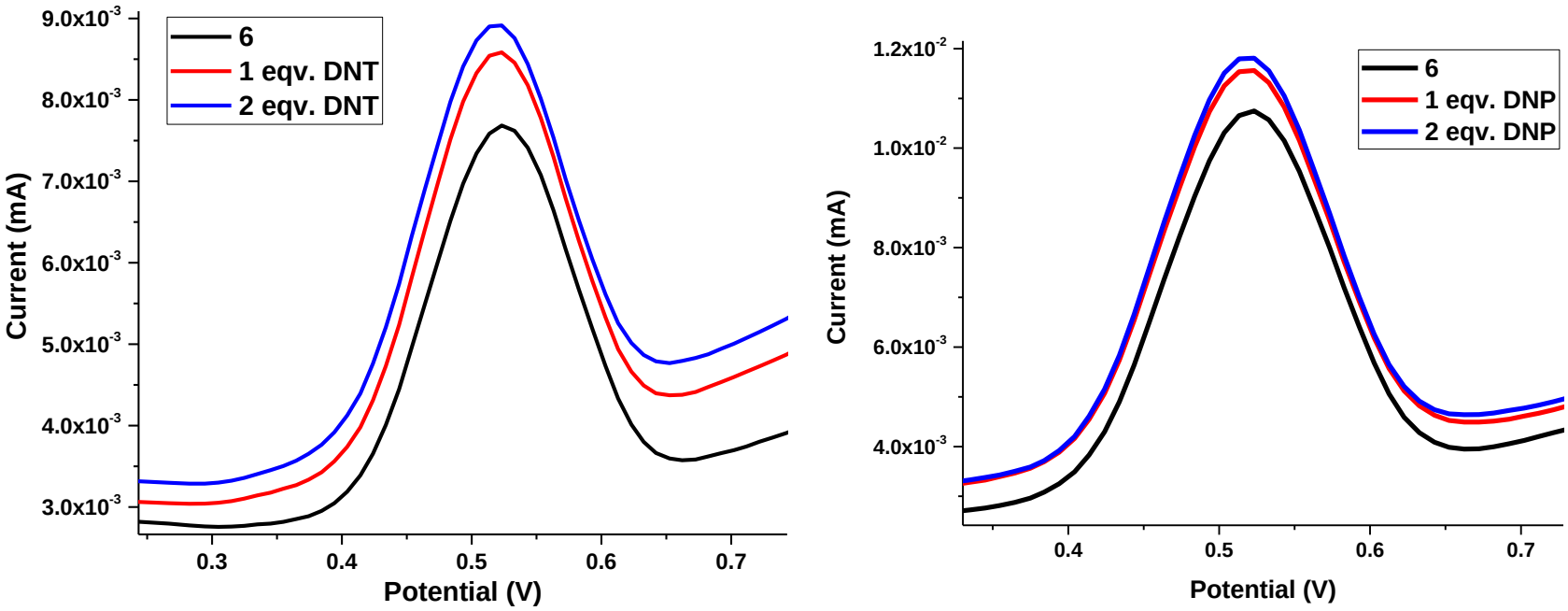
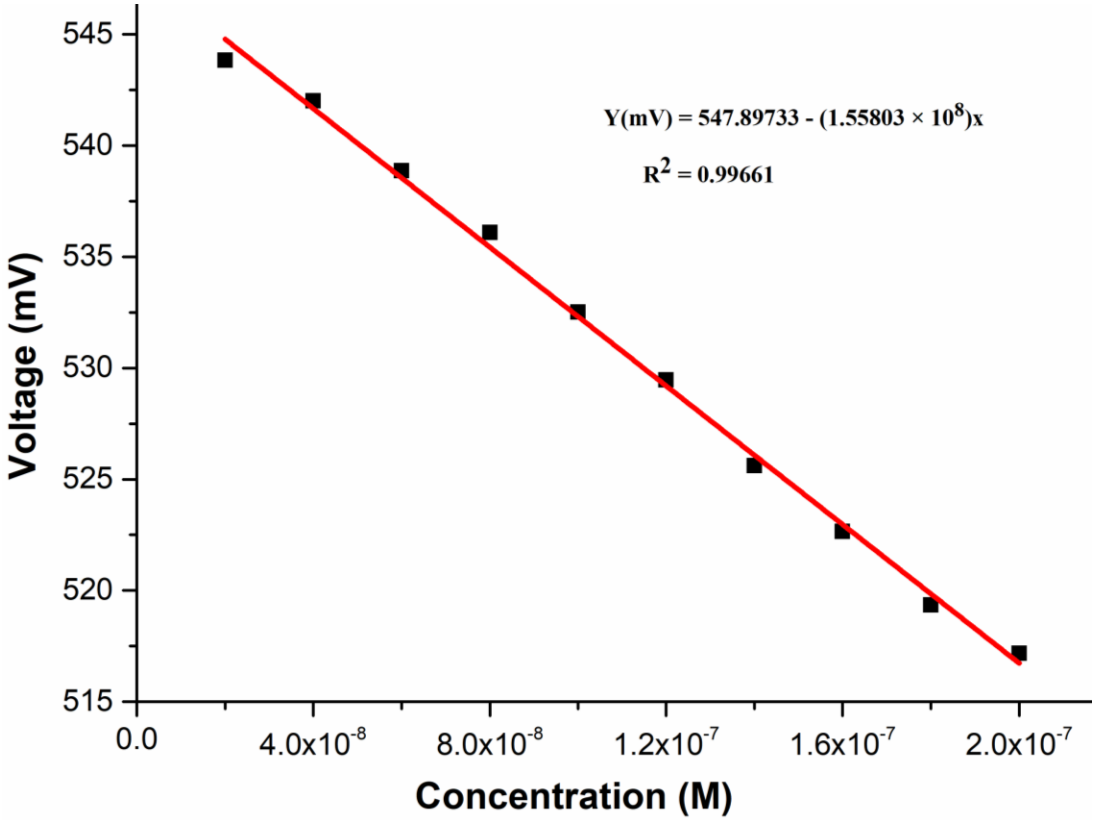


Figure S16: DPV of 6 on gradual addition of dinitrotoluene (DNT) and dinitrophenol (DNP)



$Y(mV) = 547.89733 – (1.55803 \times 10^{8})x$

$R^2 = 0.99661$

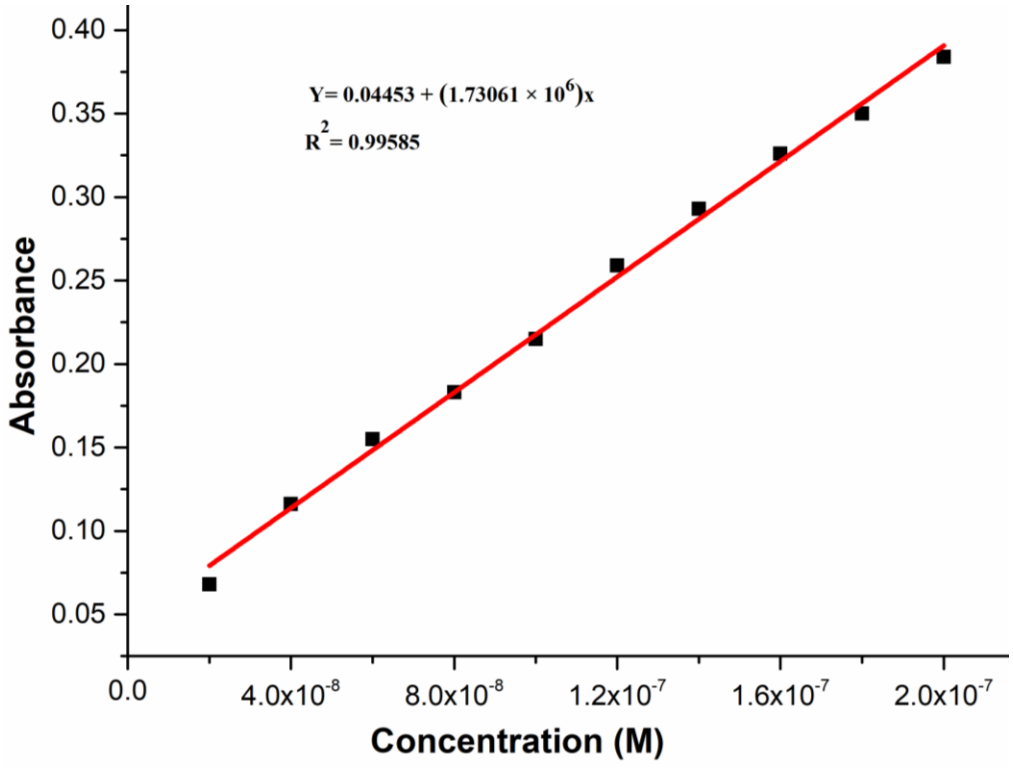
Limit of detection (LOD) = 3× SD / Slope

SD = Standard deviation of the blank

$LOD = 1.914 \times 10^{-8}$ M

LOD = 9.635 ng /mL

Figure S17: Calculation of LOD using DPV data [6.PA]



$Y = 0.04453 + (1.73061 \times 10^{6})x$

$R^2 = 0.99585$

Limit of detection (LOD) = 3× SD / Slope

SD = Standard deviation of the blank

$LOD = 1.790 \times 10^{-8}$ M

LOD = 9.011 ng /mL

Figure S18: Calculation of LOD using UV-Visible data of [6.PA]

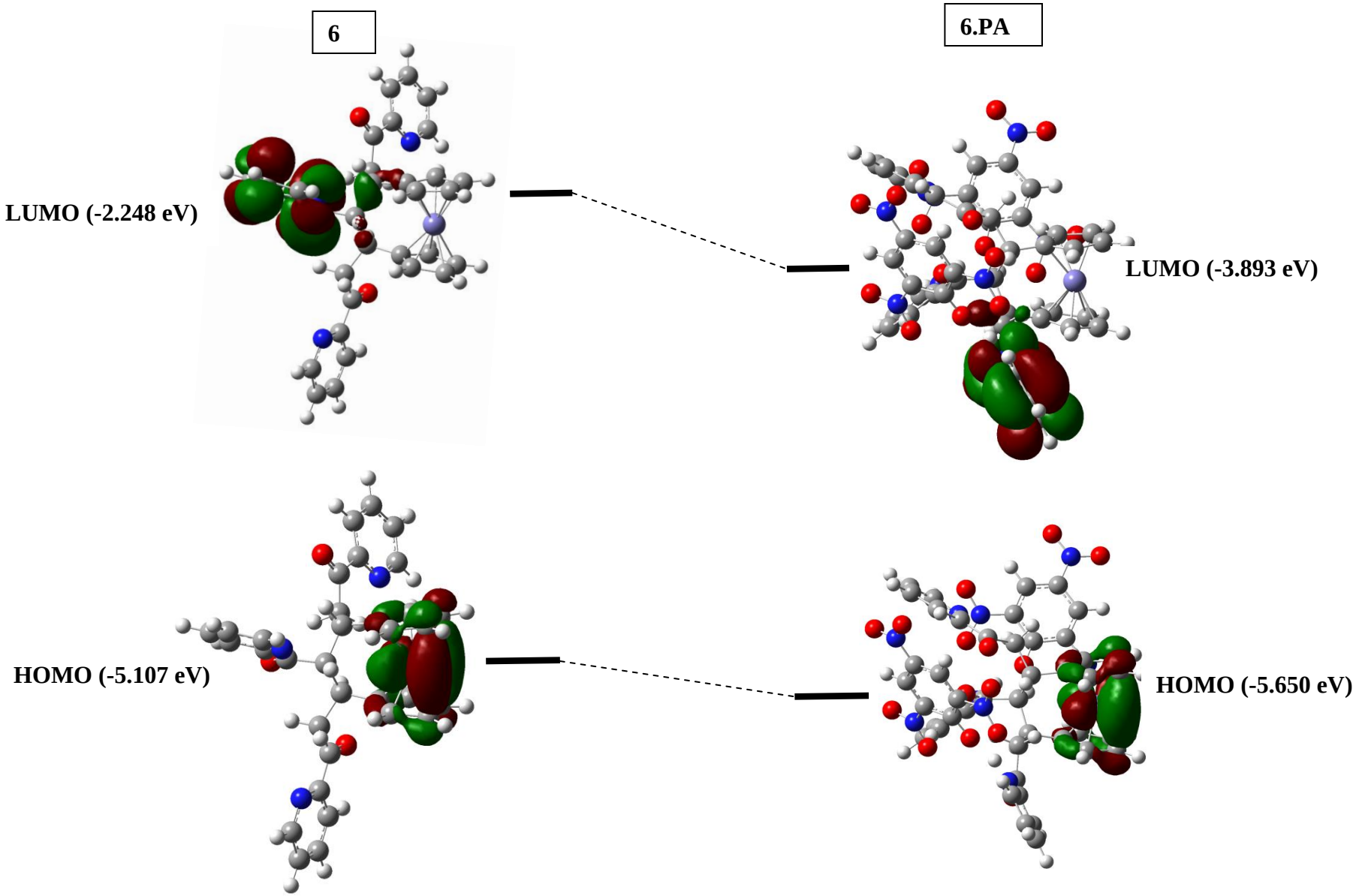
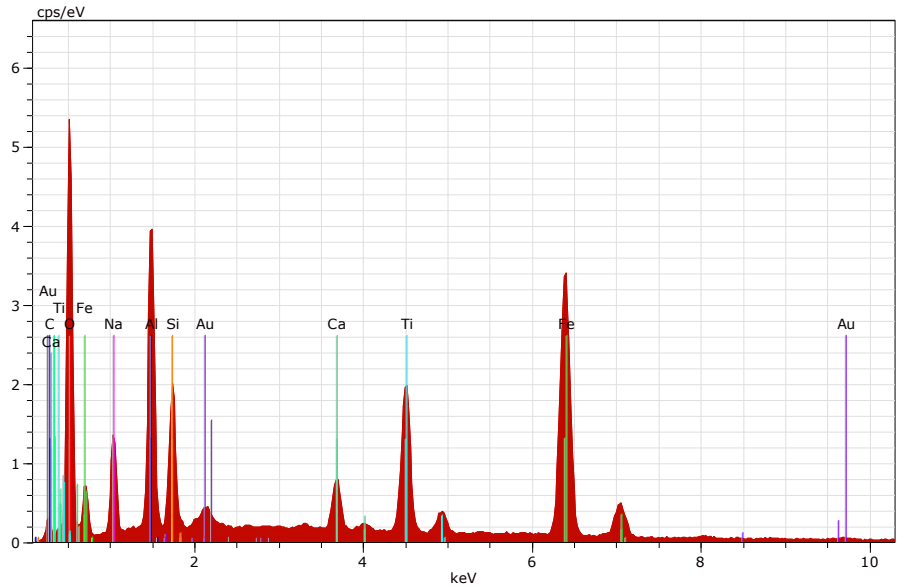
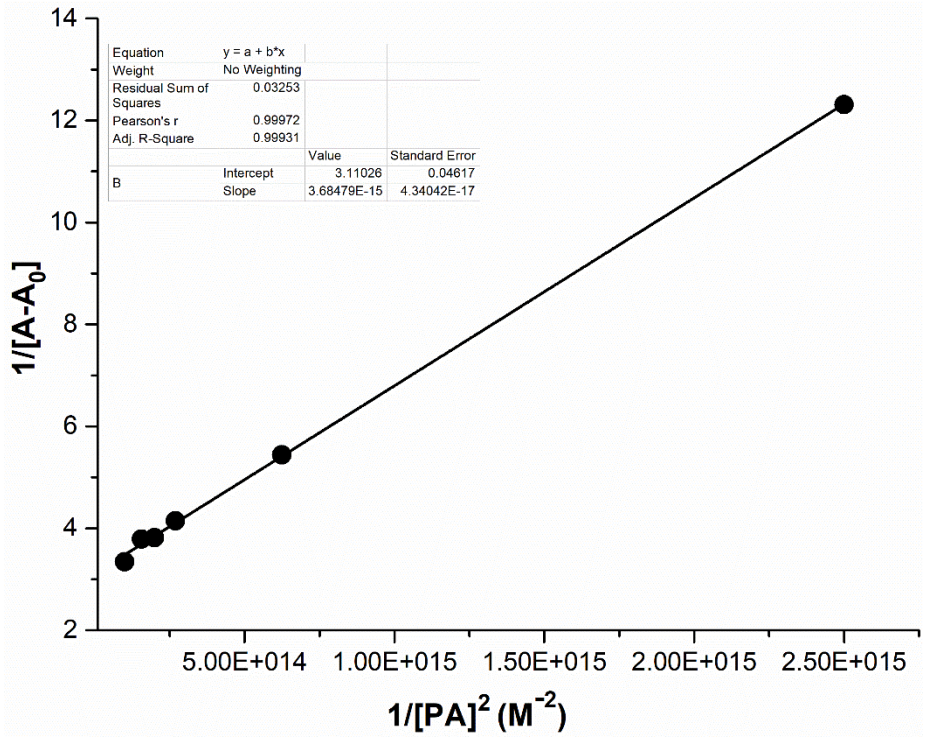


Figure S19: HOMO and LUMO for 6 and [6.PA]



El	AN	Series	unn. [wt.%]	C norm. [wt.%]	C Atom. [at.%]	C Error (1 Sigma) [wt.%]
O	8	K-series	29.30	36.44	55.39	3.69
Fe	26	K-series	21.37	26.58	11.58	0.60
Al	13	K-series	8.92	11.10	10.00	0.46
Ti	22	K-series	7.73	9.62	4.89	0.25
Na	11	K-series	5.30	6.59	6.97	0.38
Si	14	K-series	3.38	4.21	3.64	0.18
C	6	K-series	2.39	2.97	6.01	0.61
Ca	20	K-series	2.01	2.50	1.52	0.09
Au	79	L-series	0.00	0.00	0.00	0.00
		Total:	80.40	100.00	100.00	

Figure S20 : EDS of Redmud used



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