

Innovative Triazine-Core Octupolar Chromophores: Unlocking New Frontiers in Nonlinear Optics

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UV-Vis

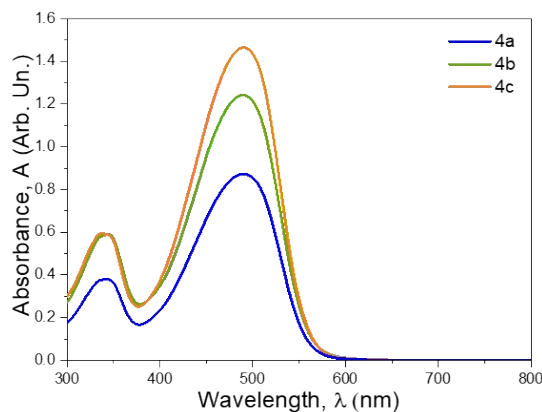


Figure S1. UV-vis absorption spectra of 4a-c solutions in THF at a concentration of 0.5mM.

NMR (¹H and ¹³C-NMR APT)

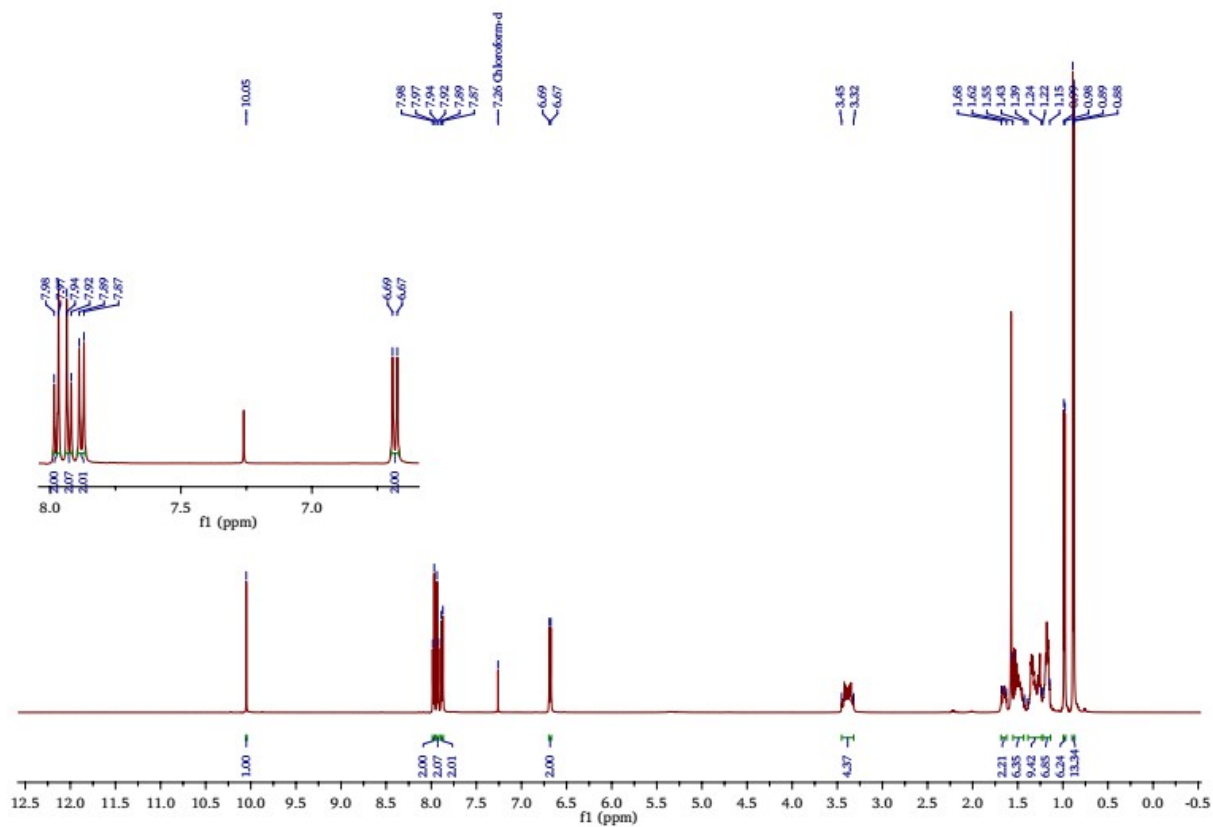


Figure S2 $^1\text{H-NMR}$ (CDCl_3) spectrum of compound 3a

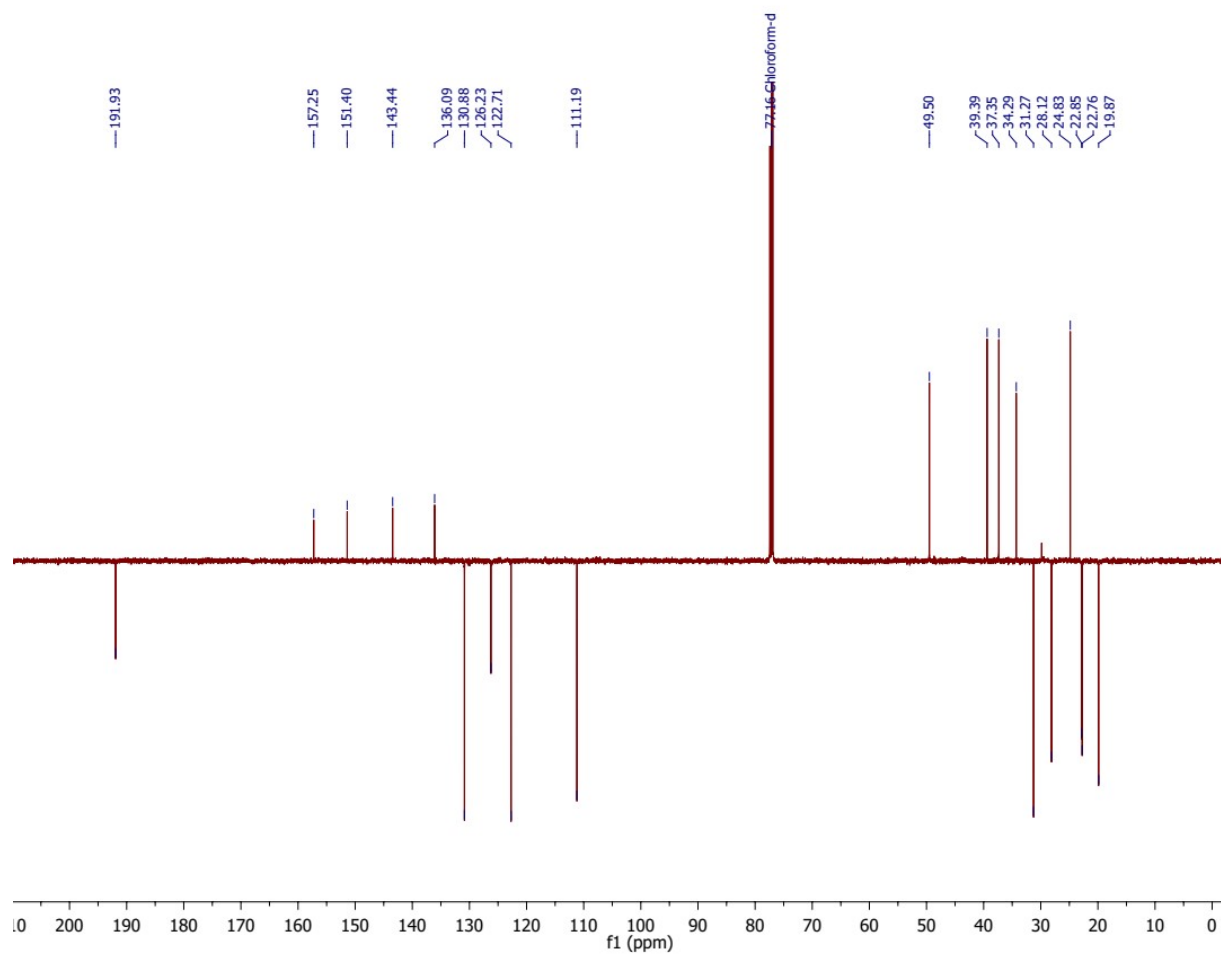


Figure S3 ¹³C-NMR (CDCl₃) spectrum of compound 3a

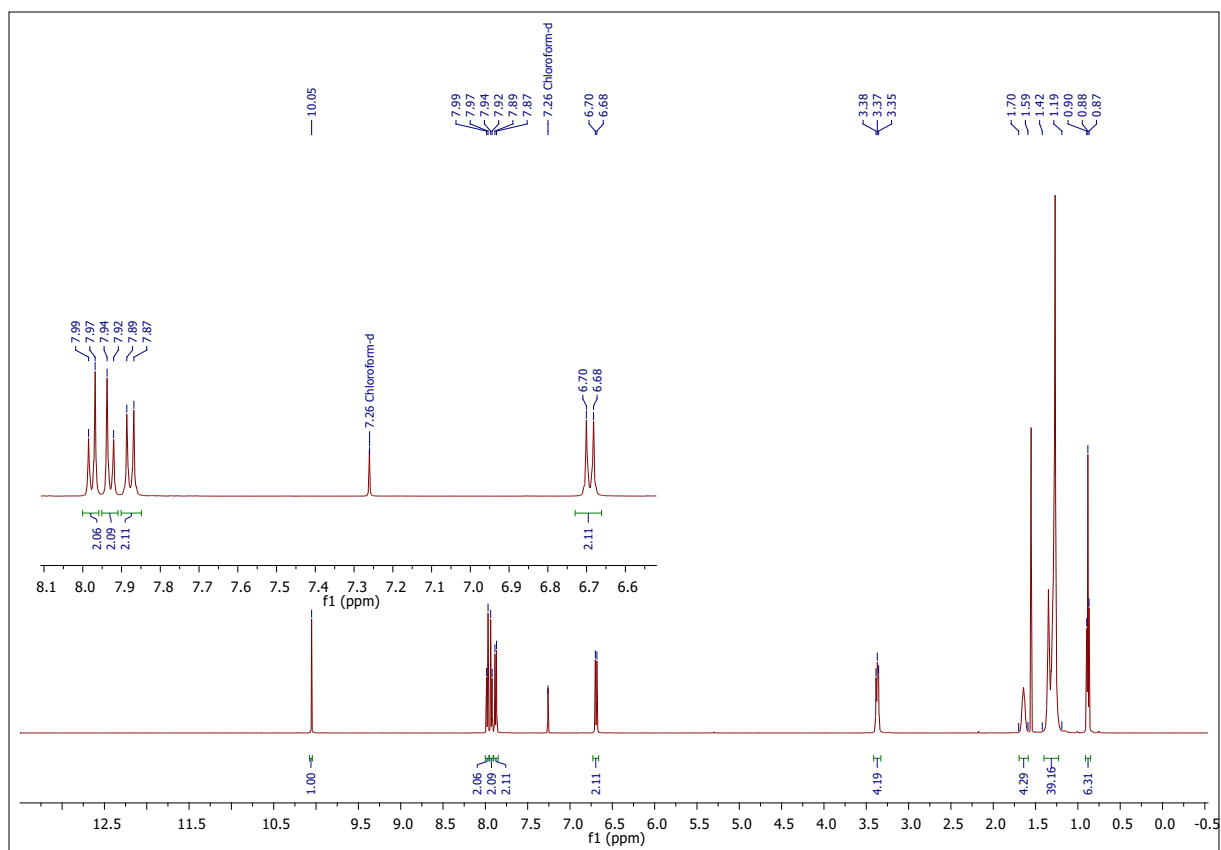


Figure S4 $^1\text{H-NMR}$ (CDCl_3) spectrum of compound 3b

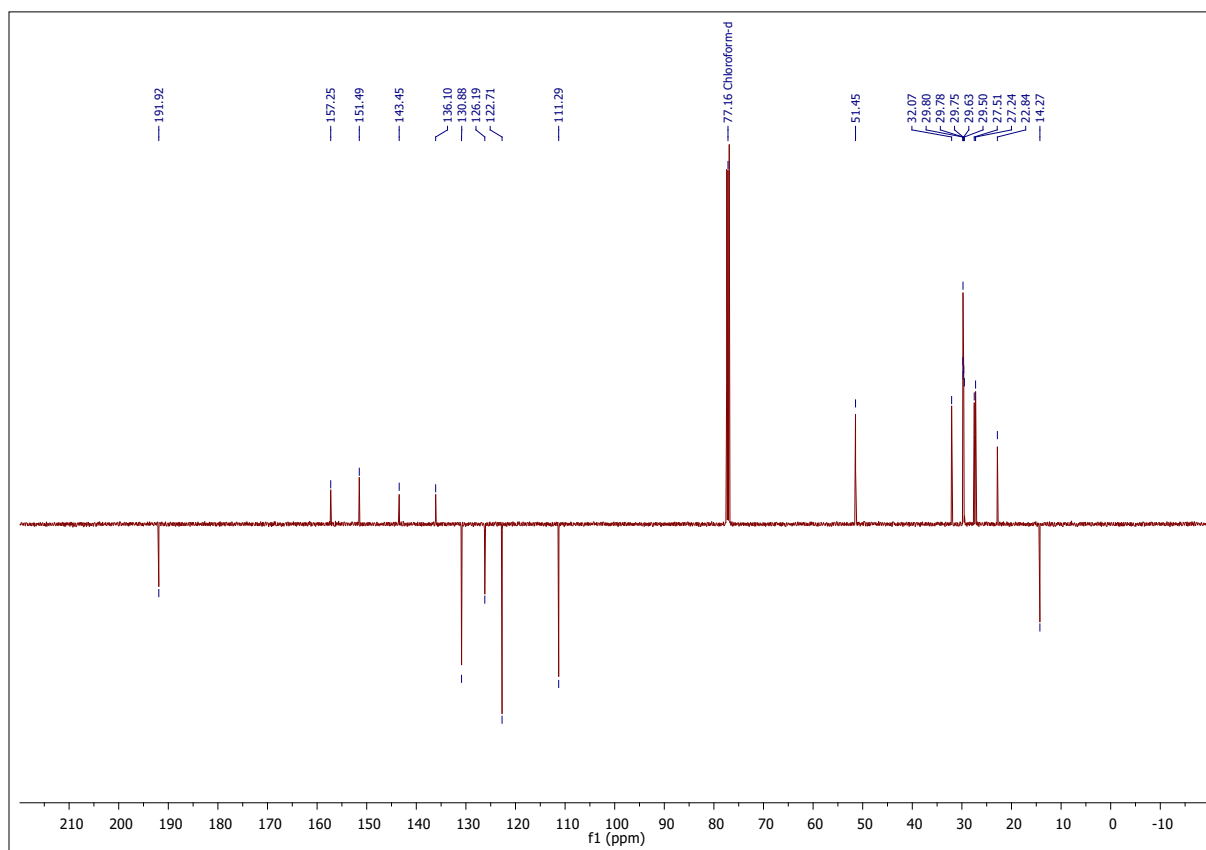


Figure S5 $^{13}\text{C-NMR}$ (CDCl_3) spectrum of compound 3b

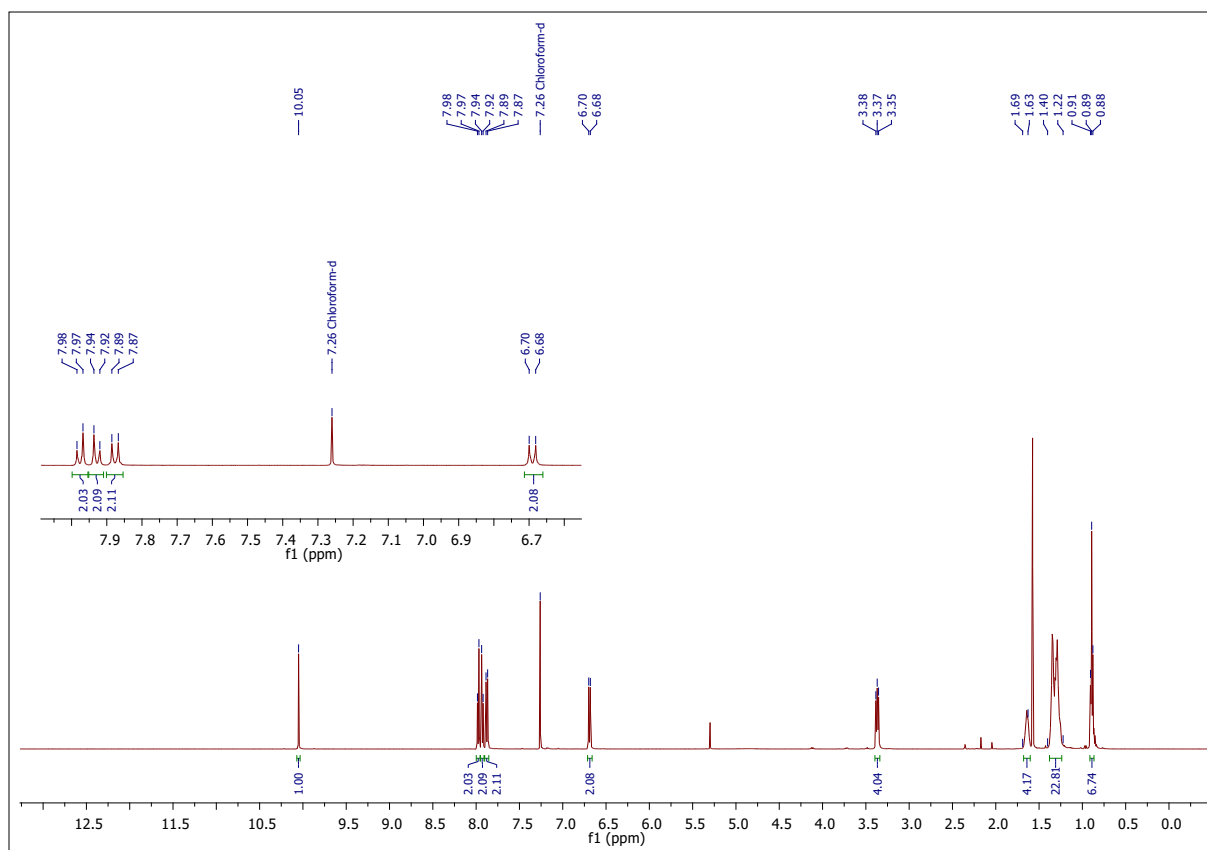


Figure S6 $^1\text{H-NMR}$ (CDCl_3) spectrum of compound 3c

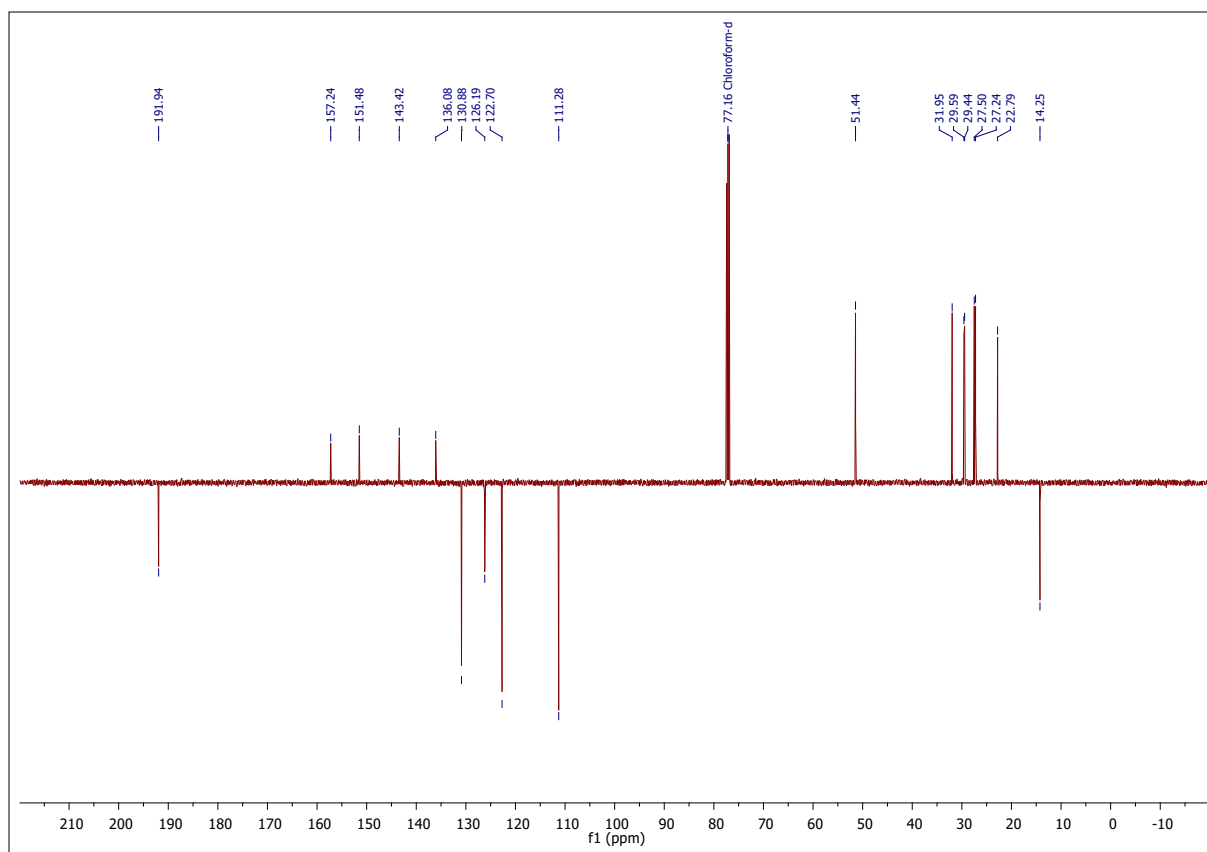


Figure S7 ^{13}C -NMR (CDCl_3) spectrum of compound 3c

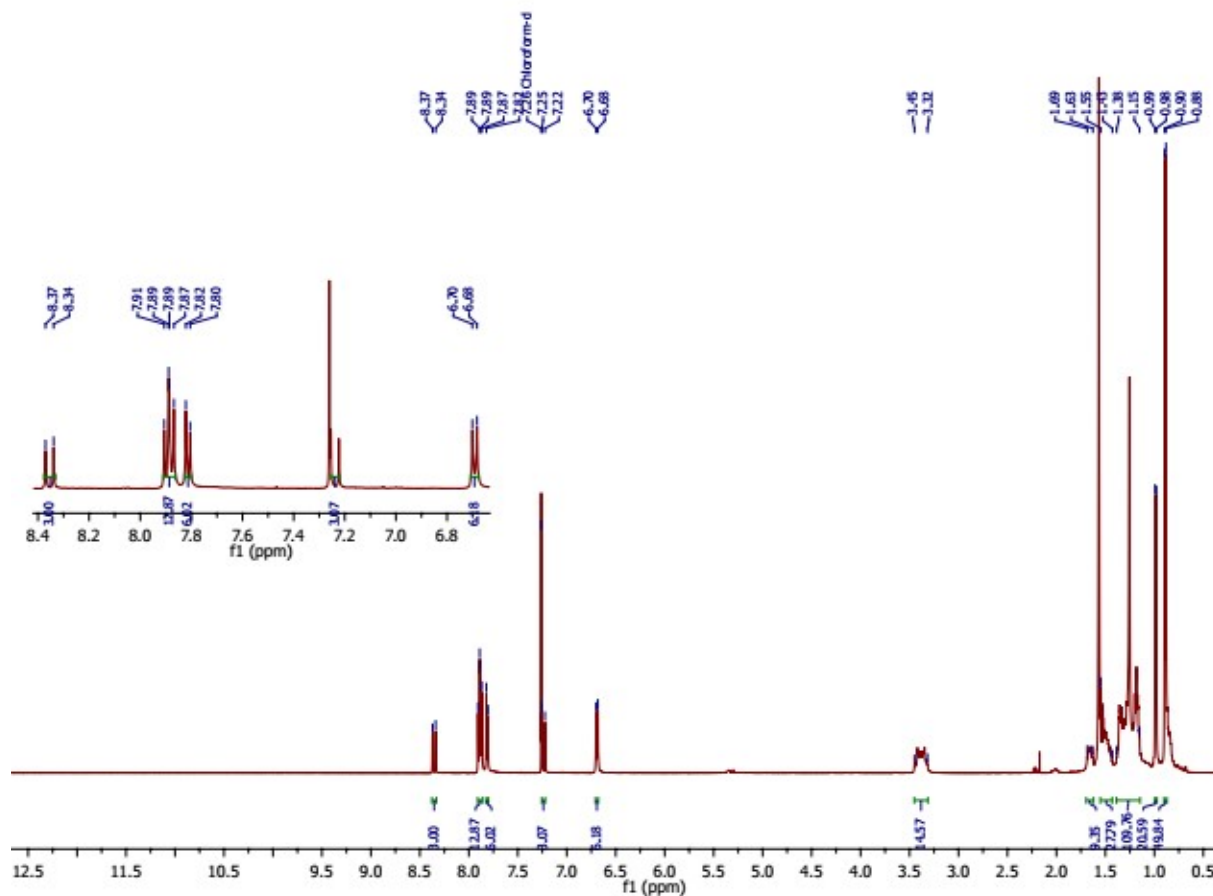


Figure S8 $^1\text{H-NMR}$ (CDCl_3) spectrum of compound 4a

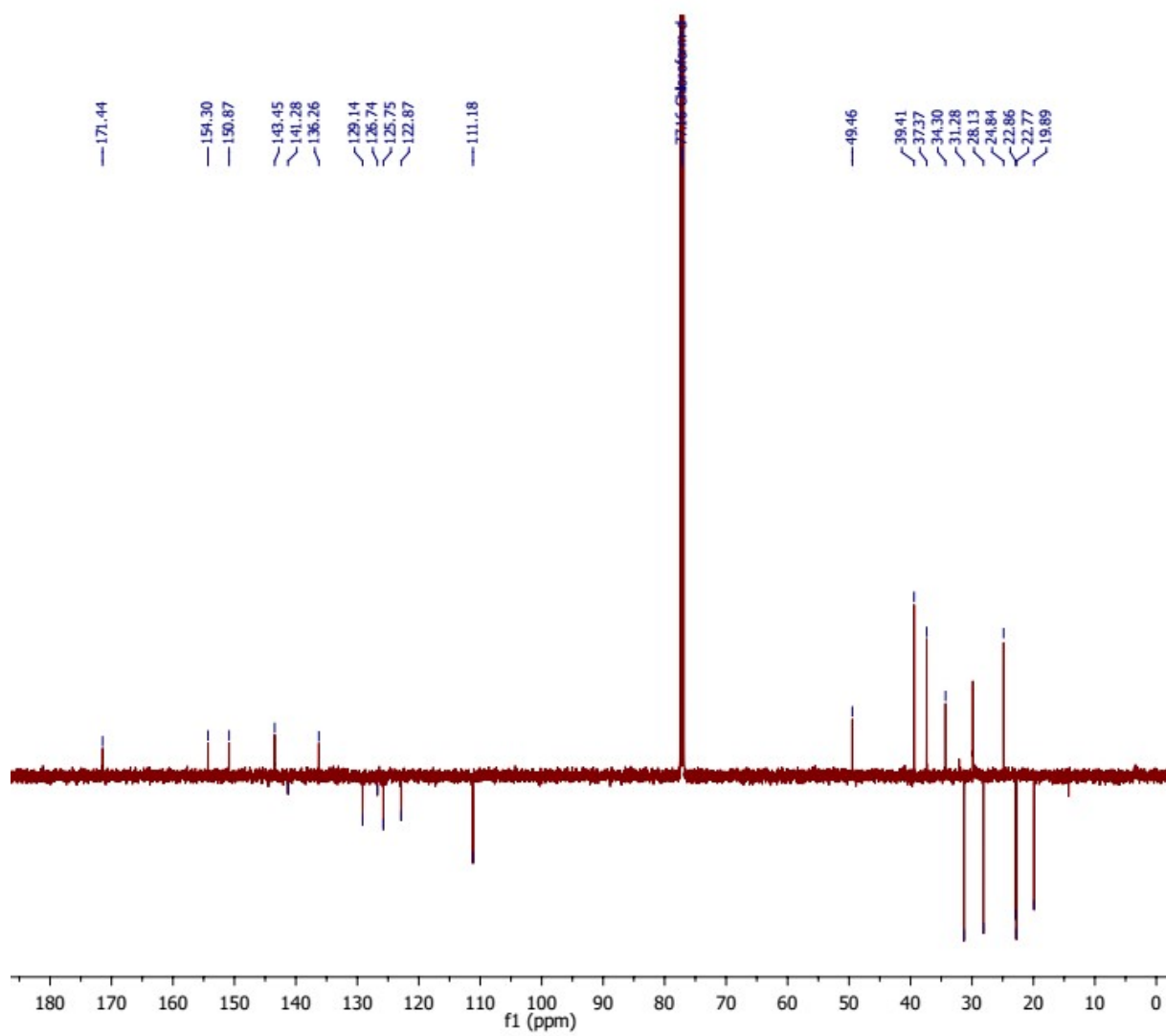


Figure S9 ¹³C-NMR (CDCl₃) spectrum of compound 4a

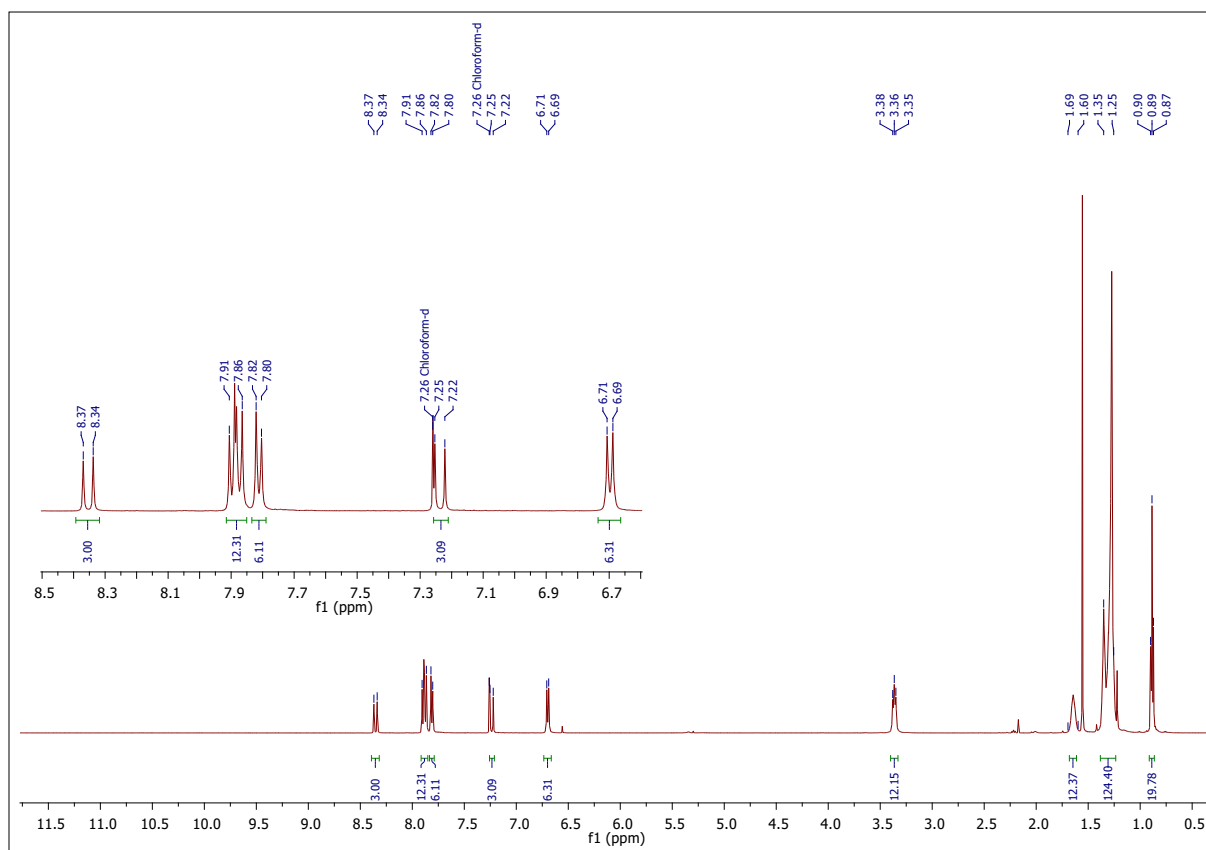


Figure S10 $^1\text{H-NMR}$ (CDCl_3) spectrum of compound 4b

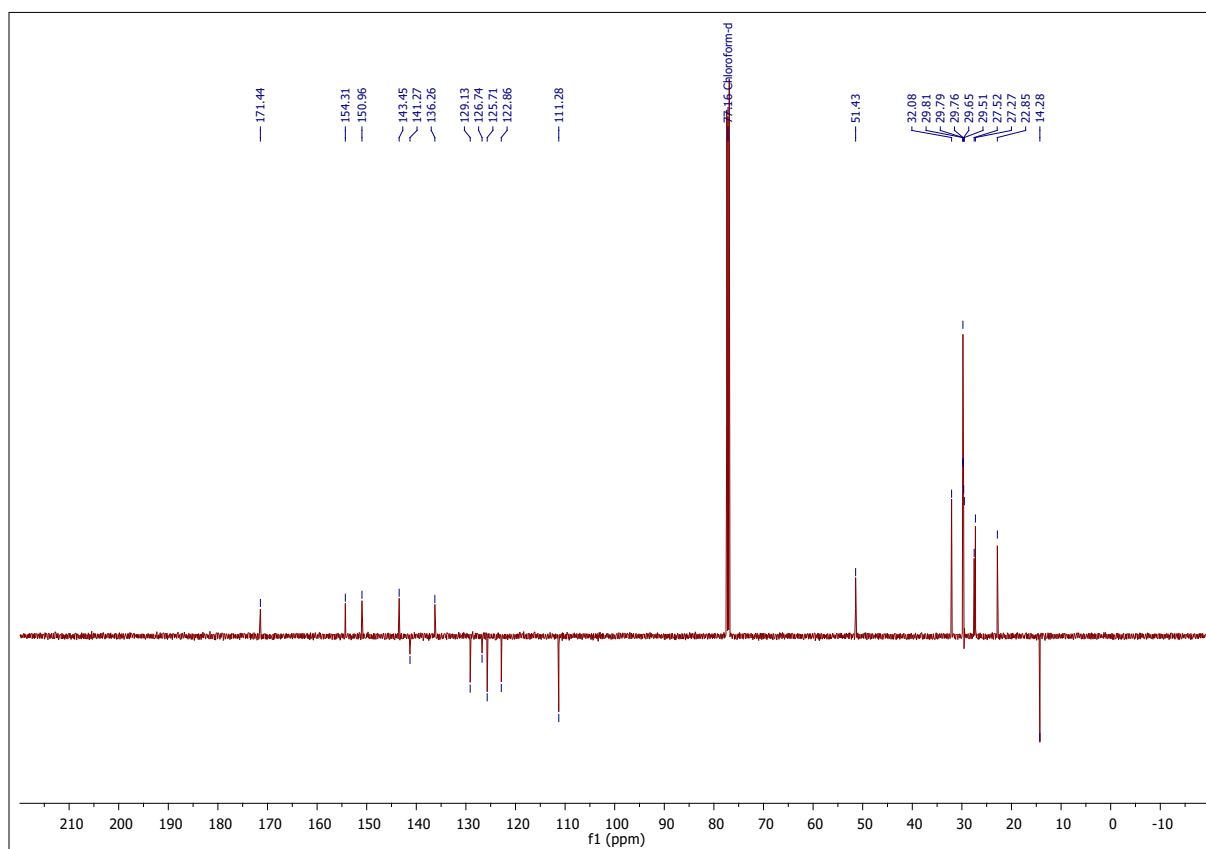


Figure S11 $^{13}\text{C-NMR}$ (CDCl_3) spectrum of compound 4b

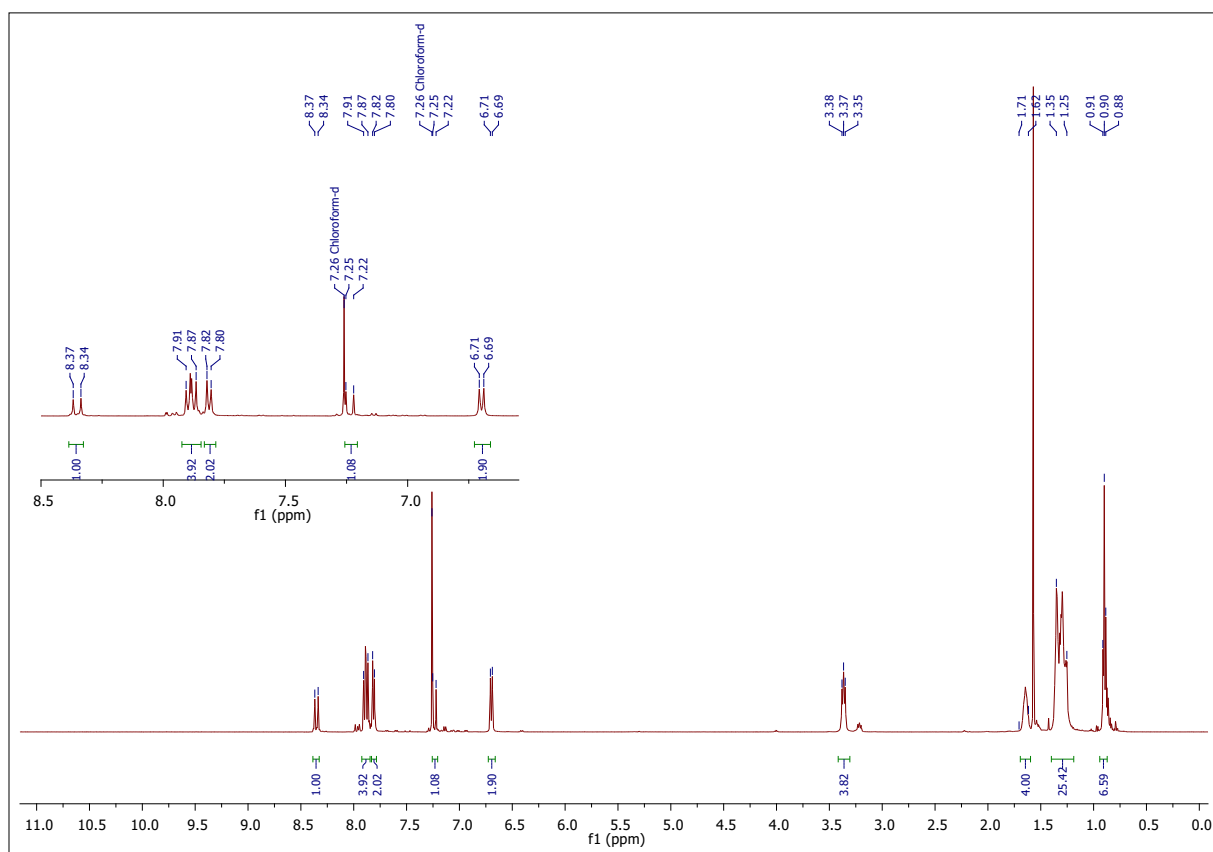


Figure S12 $^1\text{H-NMR}$ (CDCl_3) spectrum of compound 4c

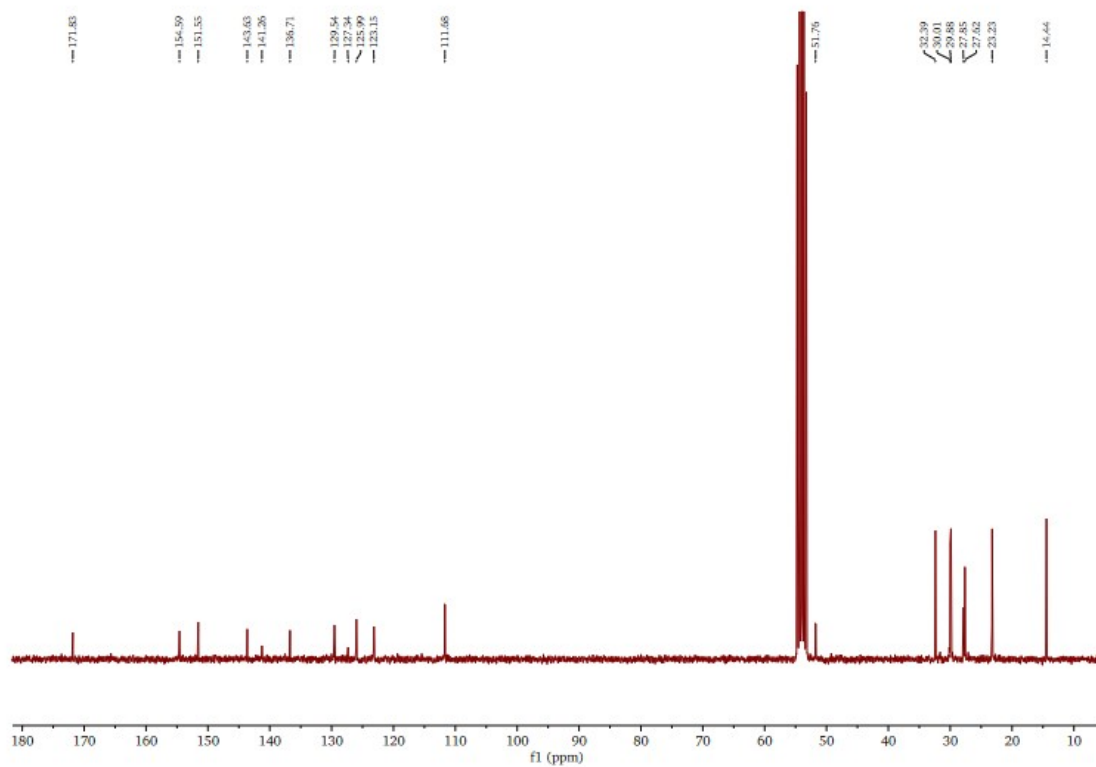
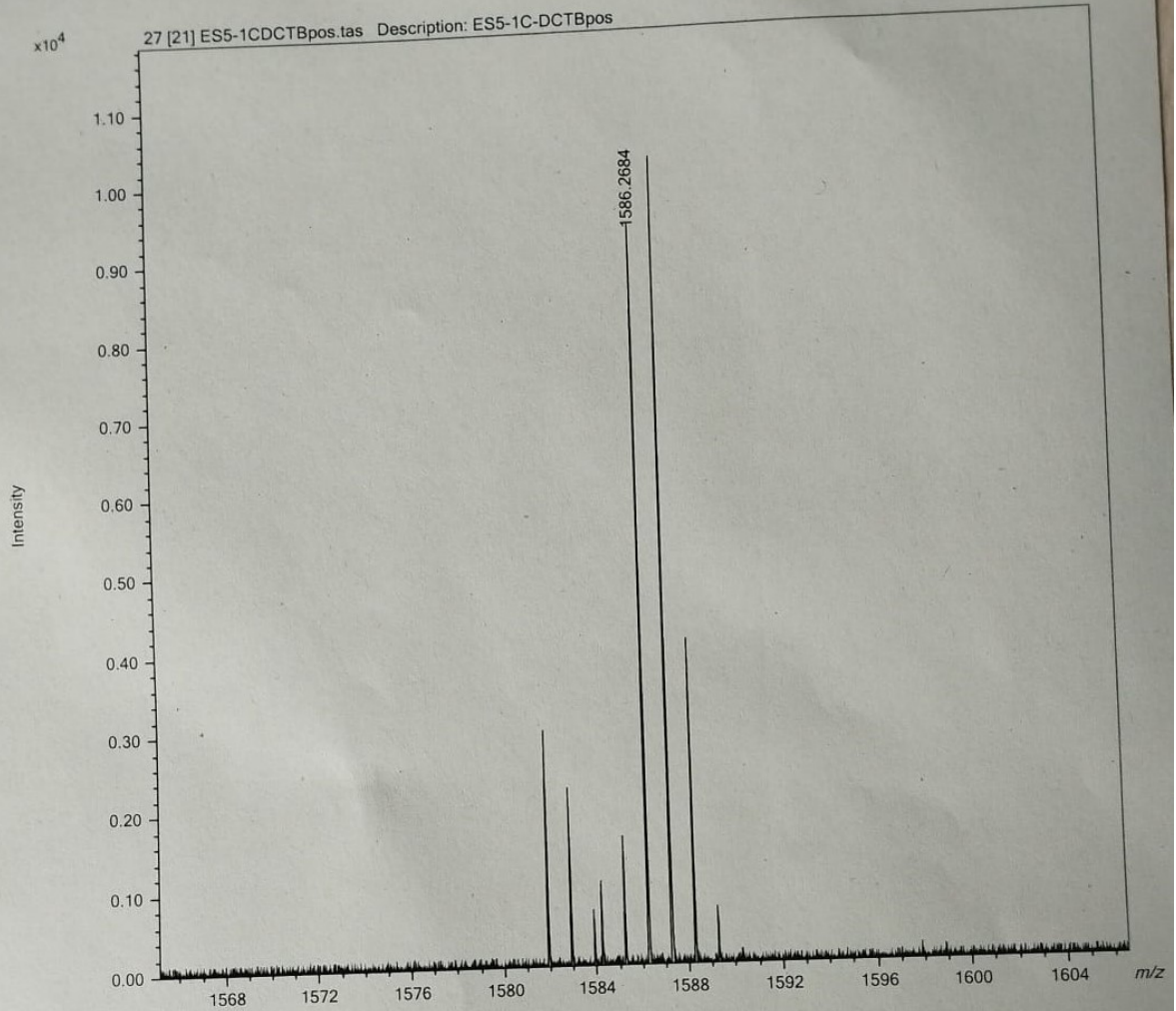


Figure S13 $^{13}\text{C-NMR}$ (CDCl_3) spectrum of compound 4c



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
1586.26844 ± 0.00476	3.0 ppm	Even	+1	-0.5 - 100.0	100

Elements

C	H	N	O	Na	Si
0 - 110	0 - 200	0 - 15	0 - 0	0 - 0	0 - 0

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C ₁₀₅ H ₁₅₇ N ₁₂	1586.26487	33.5	0.00357	0.00357	2.25

Figure S14 HMRS spectrum of compound 4a

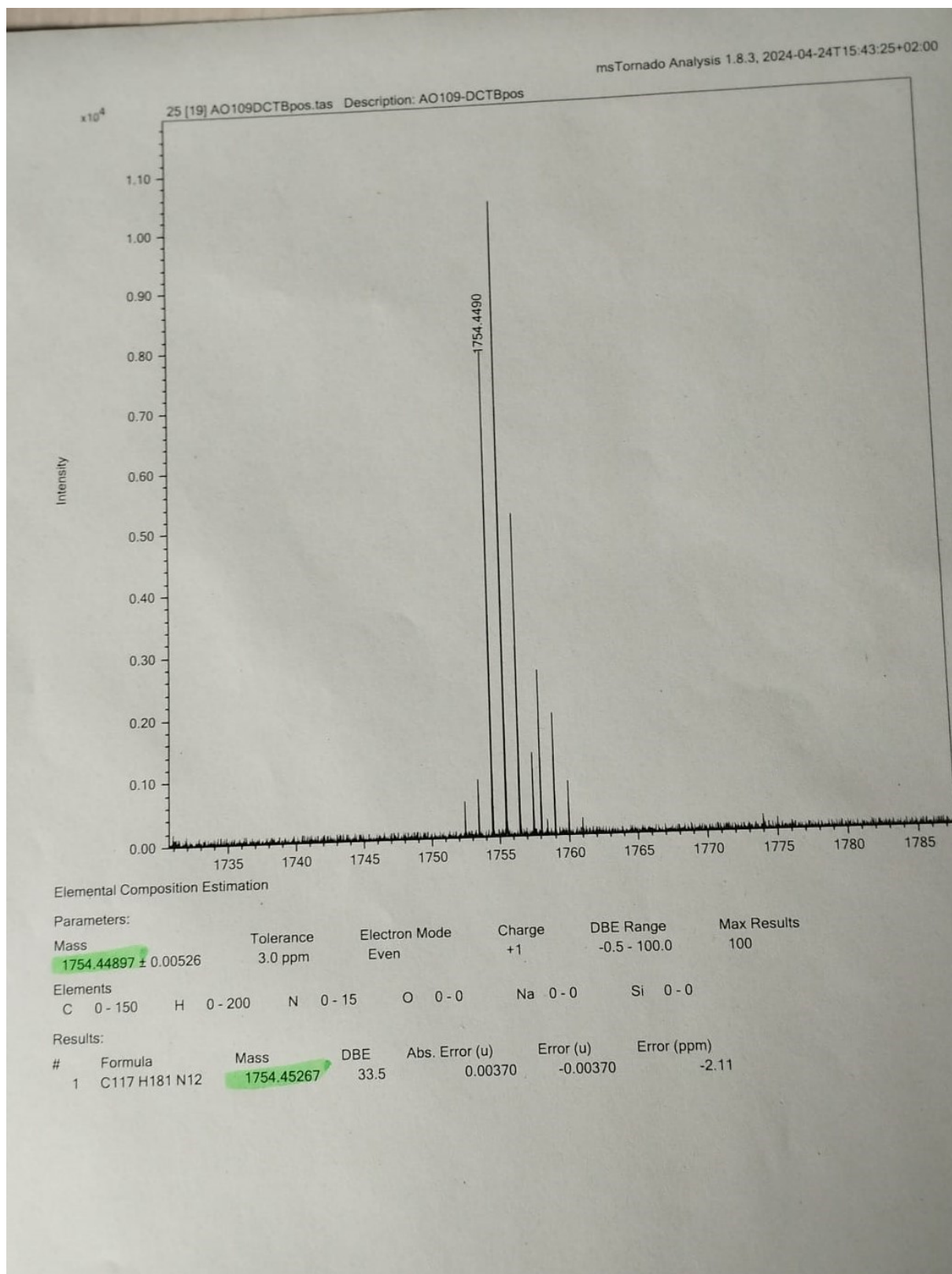
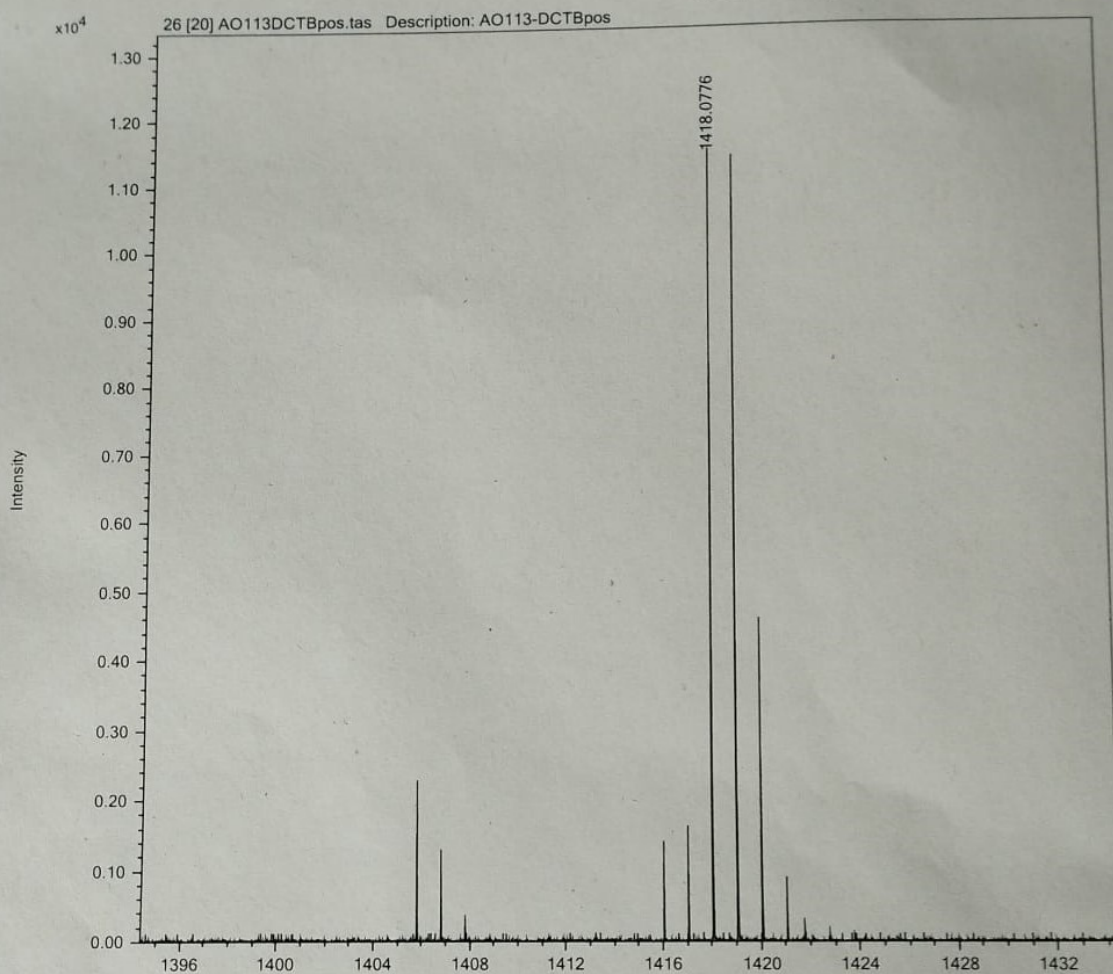


Figure S15 HMRS spectrum of compound 4b



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
1418.07757 \pm 0.00425	3.0 ppm	Even	+1	-0.5 - 100.0	100

Elements

C	0 - 150	H	0 - 200	N	0 - 15	O	0 - 0	Na	0 - 0	Si	0 - 0
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Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C ₉₃ H ₁₃₃ N ₁₂	1418.07707	33.5	0.00050	0.00050	0.35

Figure S16 HMRS spectrum of compound 4c

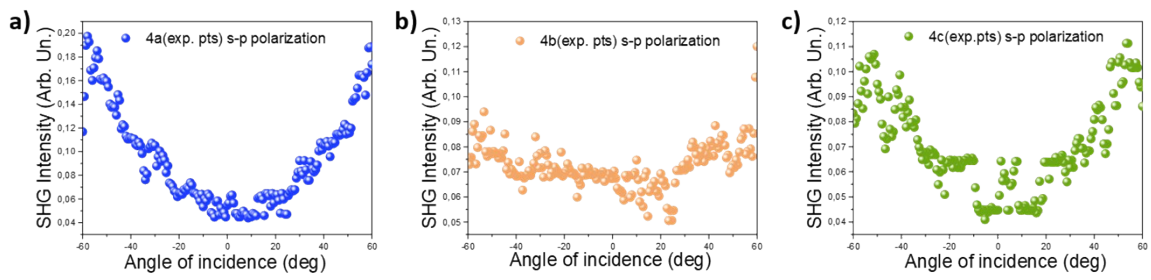


Figure S17 Maker fringes signals for all the materials measured in the s-p configuration: a) 4a, b) 4b and c) 4c