

Benzothiazole Derivatives as Multifunctional Antioxidant Agents for Skin Damage: Structure–Activity Relationship of a Scaffold Bearing a Five-Membered Ring System

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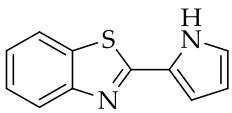
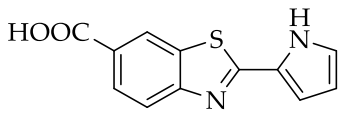
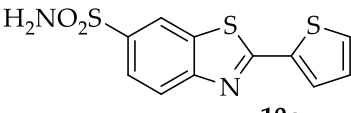
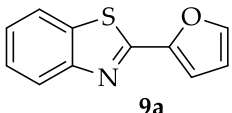
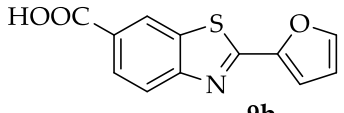
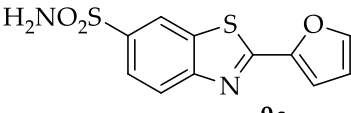
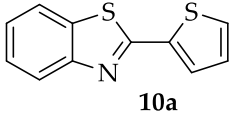
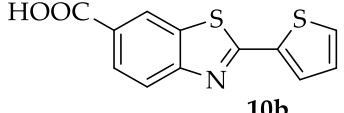
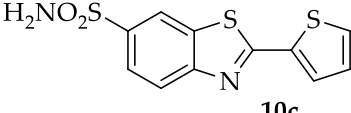
Table S1. Parameter values obtained from the UV spectra of the synthesized compounds solubilized in DMSO and MeOH.

	Solvent	λ_{max} (nm)	A	ϵ
PBSA	DMSO	310.50	1.130	23839.66
	MeOH	304.50	1.460	30801.69
8a	DMSO	333.40	2.360	29500.00
	MeOH	329.40	1.540	23692.31
8b	DMSO	348.87	0.370	5308.47
	MeOH	341.63	0.190	3089.43
8c	DMSO	344.37	0.700	13944.22
	MeOH	341.40	0.760	13263.53
9a	DMSO	322.10	1.620	21715.82
	MeOH	316.40	2.750	32505.91
9b	DMSO	331.90	1.36	23901.58
	MeOH	327.57	1.02	19318.18
9c	DMSO	329.00	0.59	10332.75
	MeOH	325.30	0.740	13805.97
10a	DMSO	321.80	0.880	12735.17
	MeOH	319.50	0.760	9706.26
10b	DMSO	340.00	1.160	17818.74
	MeOH	334.57	1.140	21268.66
10c	DMSO	336.50	0.890	20273.35
	MeOH	333.17	0.430	9704.99

Table S2. Parameter values obtained from the UV spectra of the selected compounds solubilized in different combination of solvents.

	Solvent	λ_{max} (nm)	A	ϵ
8a	HE	332.80	0.79	12153.846
	DMSO-H ₂ O 6:4	334.20	1.51	23239.769
	DMSO-H ₂ O 4:6	333.70	2.35	31333.333
9a	HE	320.70	1.18	15817.594
	DMSO-H ₂ O 6:4	323.00	1.95	301391.04
	DMSO-H ₂ O 4:6	322.77	2.43	34863.702
10a	HE	320.30	1.32	14316.703
	DMSO-H ₂ O 6:4	323.00	1.29	21535.893
	DMSO-H ₂ O 4:6	322.67	0.75	12520.868

Table S3. List of synthesized compounds.

 8a	 8b	 10c
 9a	 9b	 9c
 10a	 10b	 10c

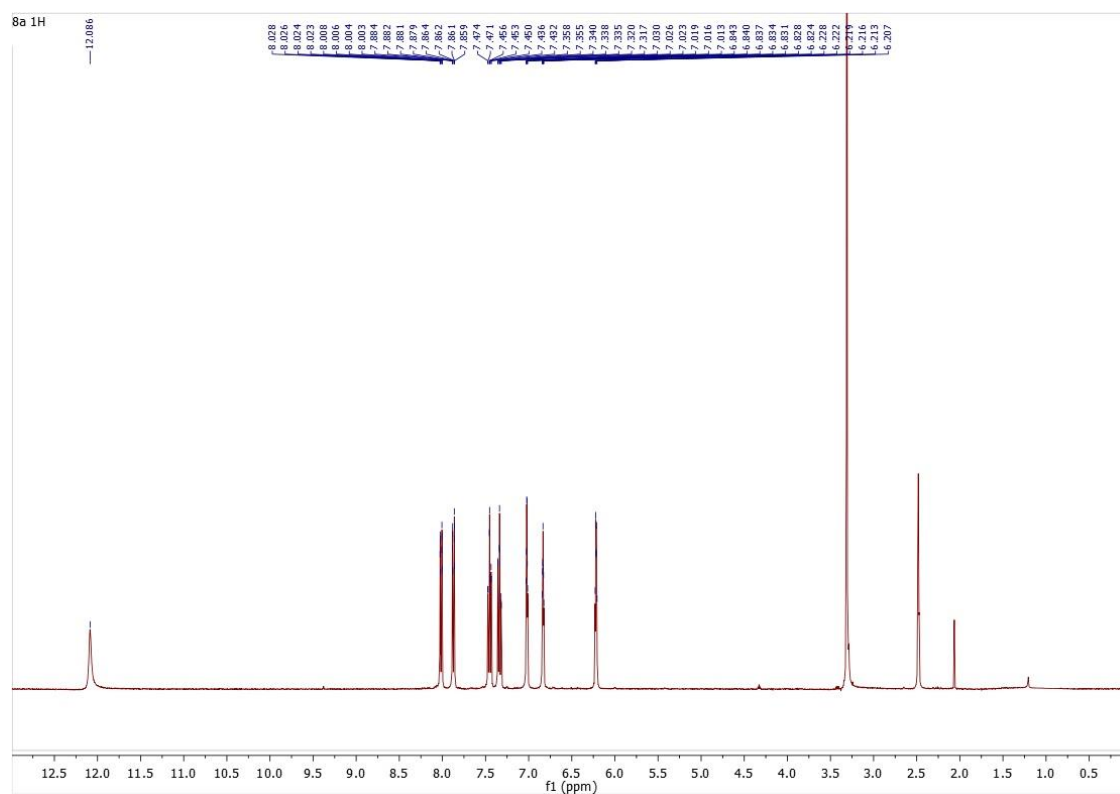


Figure S1. ^1H -NMR spectrum of compound **8a**.

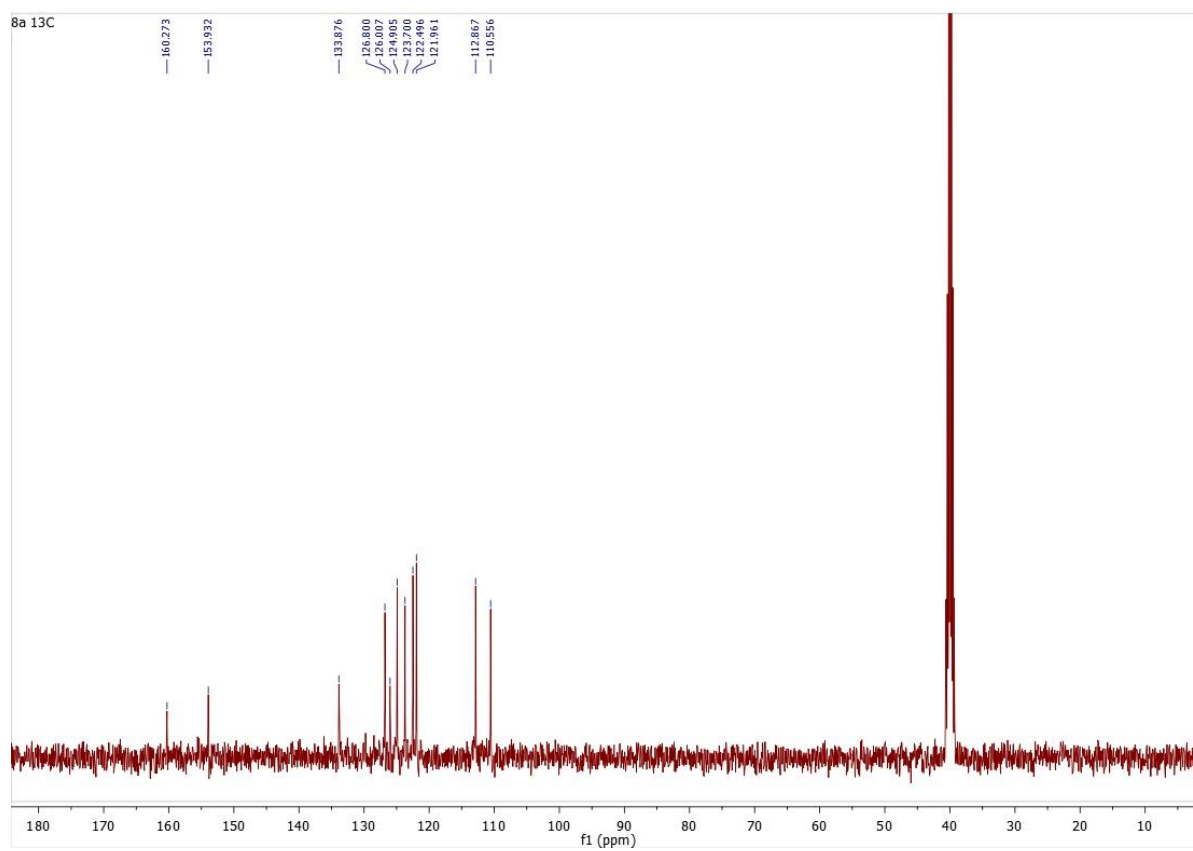


Figure S2. ^{13}C -NMR spectrum of compound **8a**.

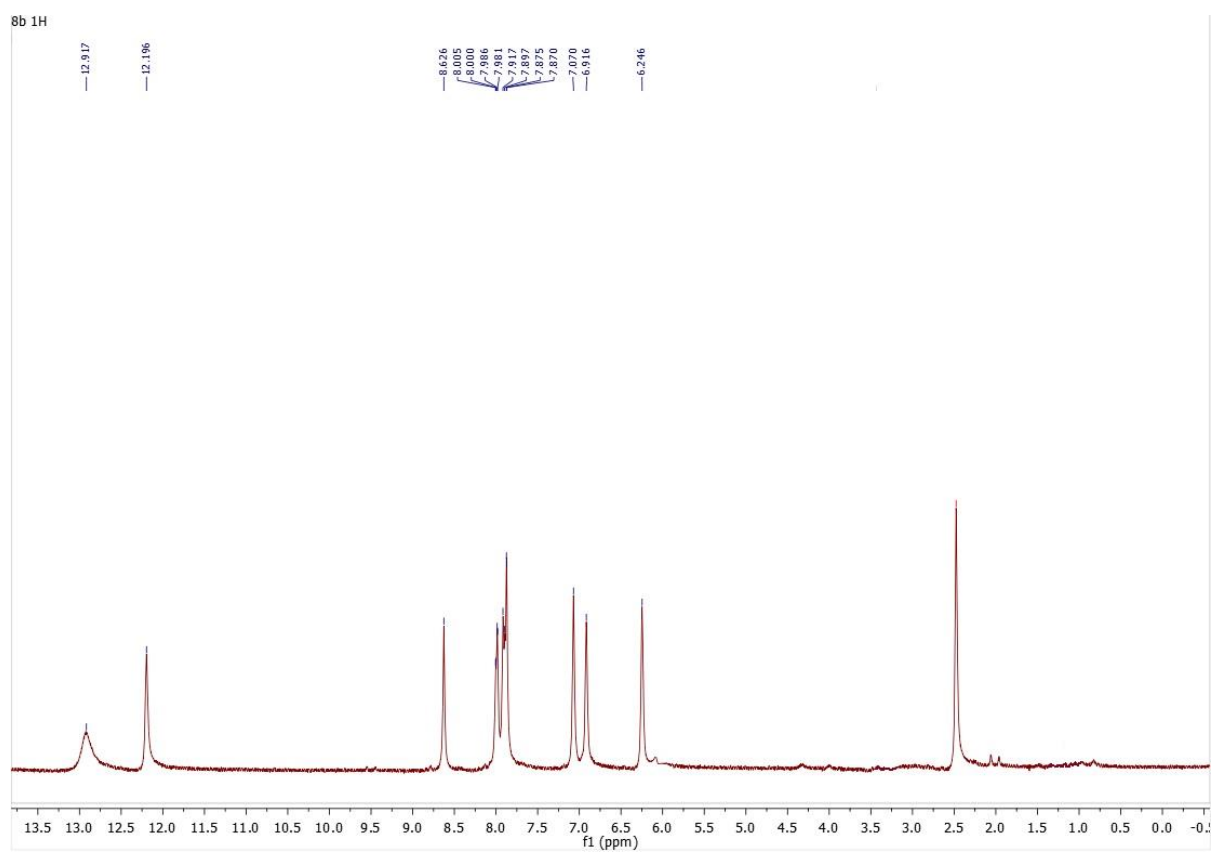


Figure S3. ^1H -NMR spectrum of compound **8b**.

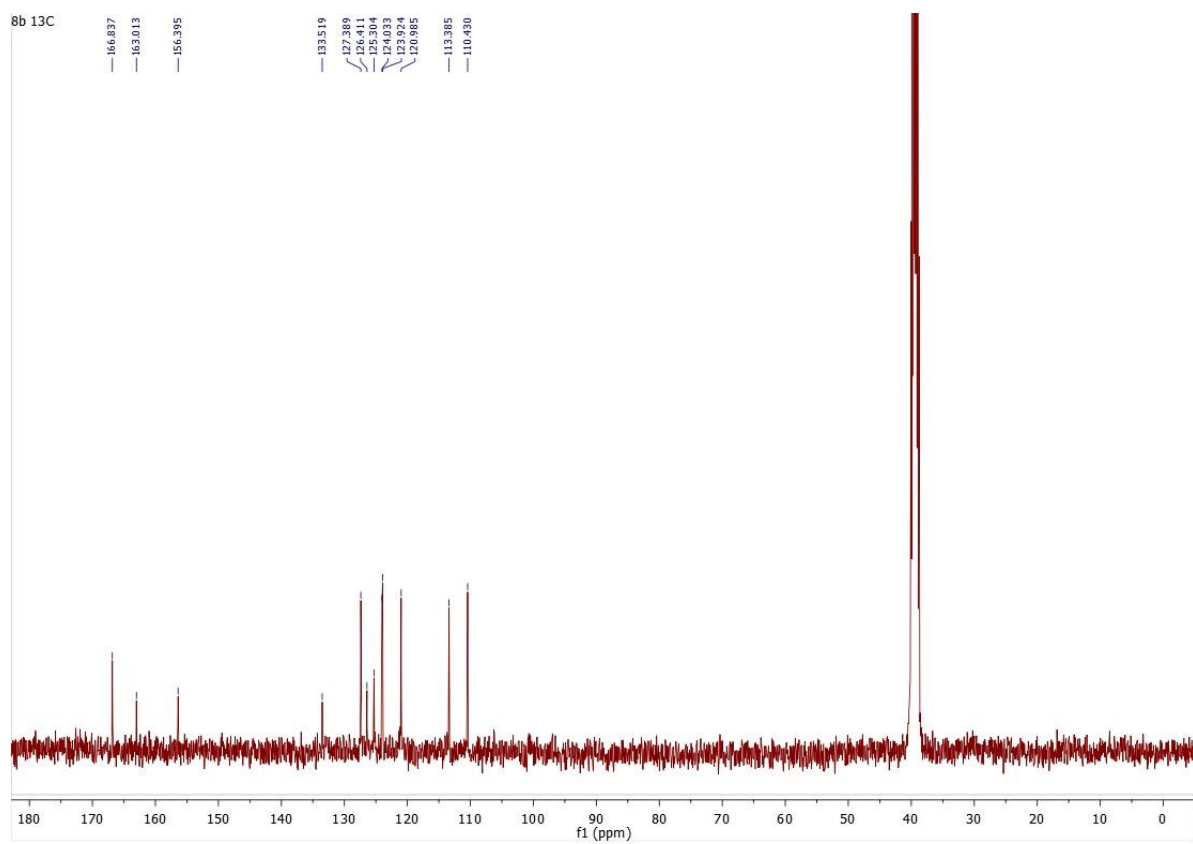


Figure S4. ^{13}C -NMR spectrum of compound **8b**.

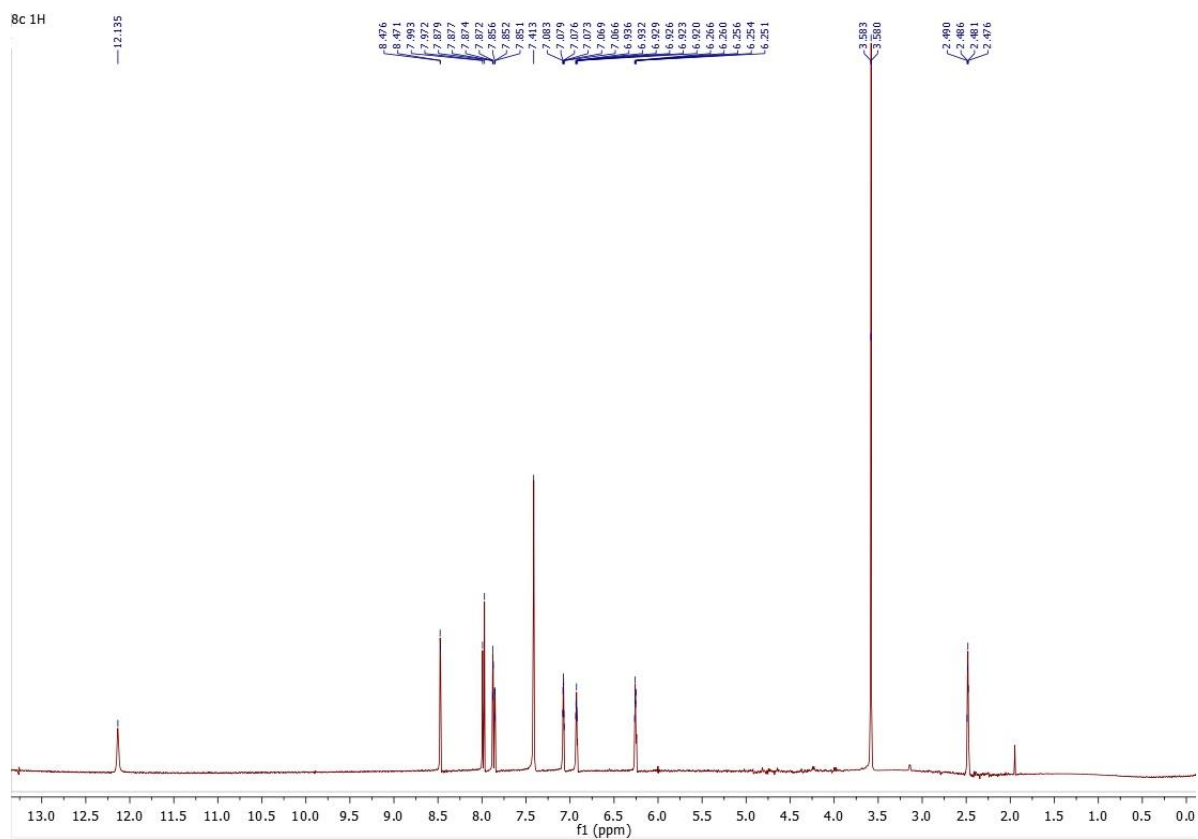


Figure S5. ^1H -NMR spectrum of compound 8c.

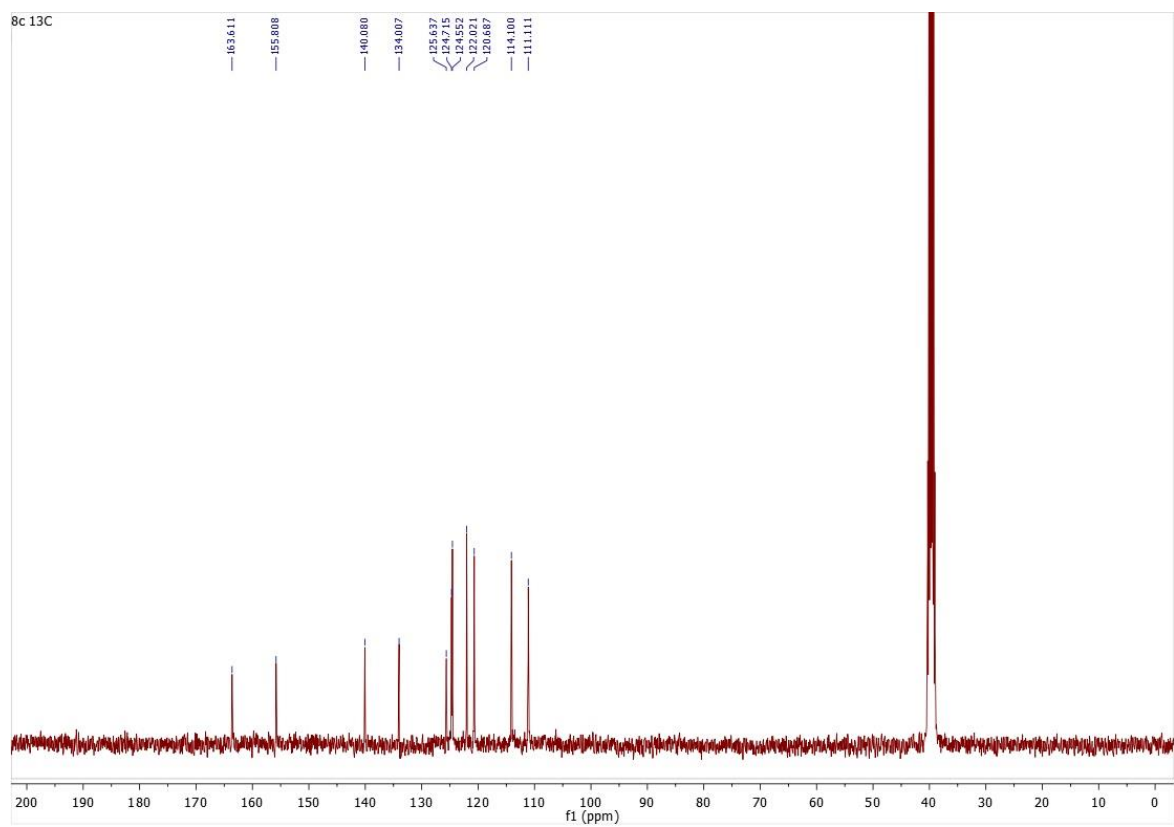


Figure S6. ^{13}C -NMR spectrum of compound 8c.

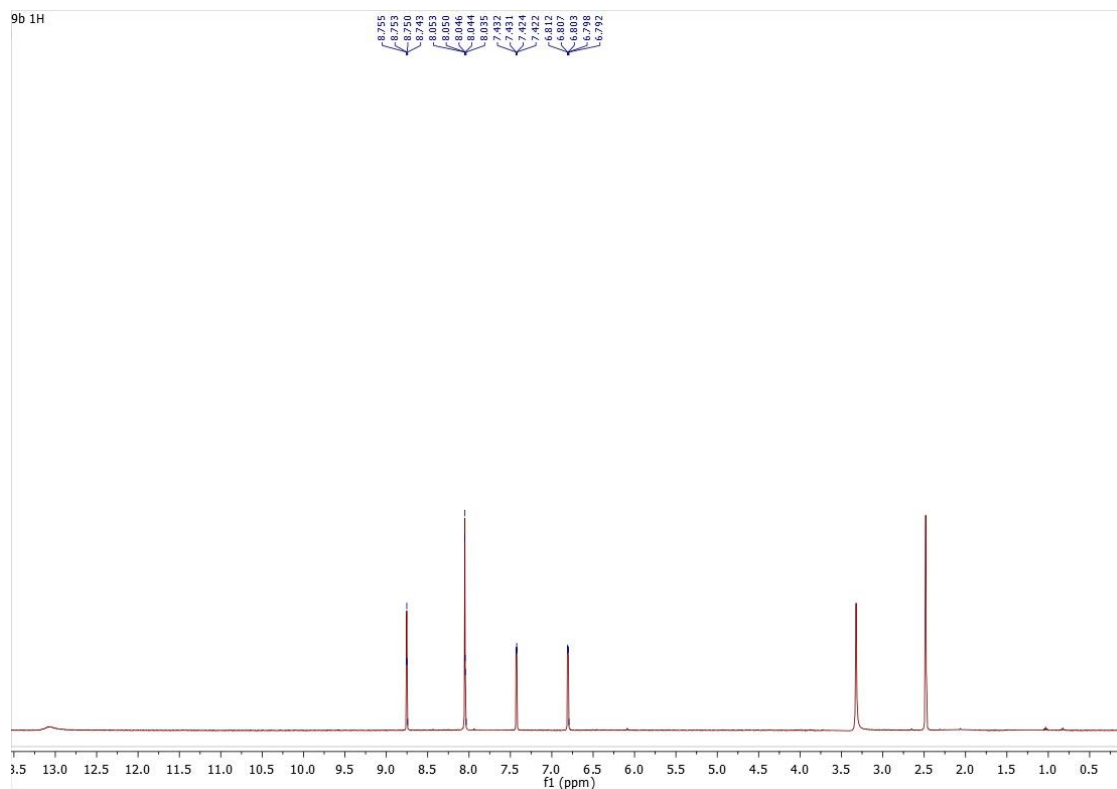


Figure S9. ^1H -NMR spectrum of compound **9b**.

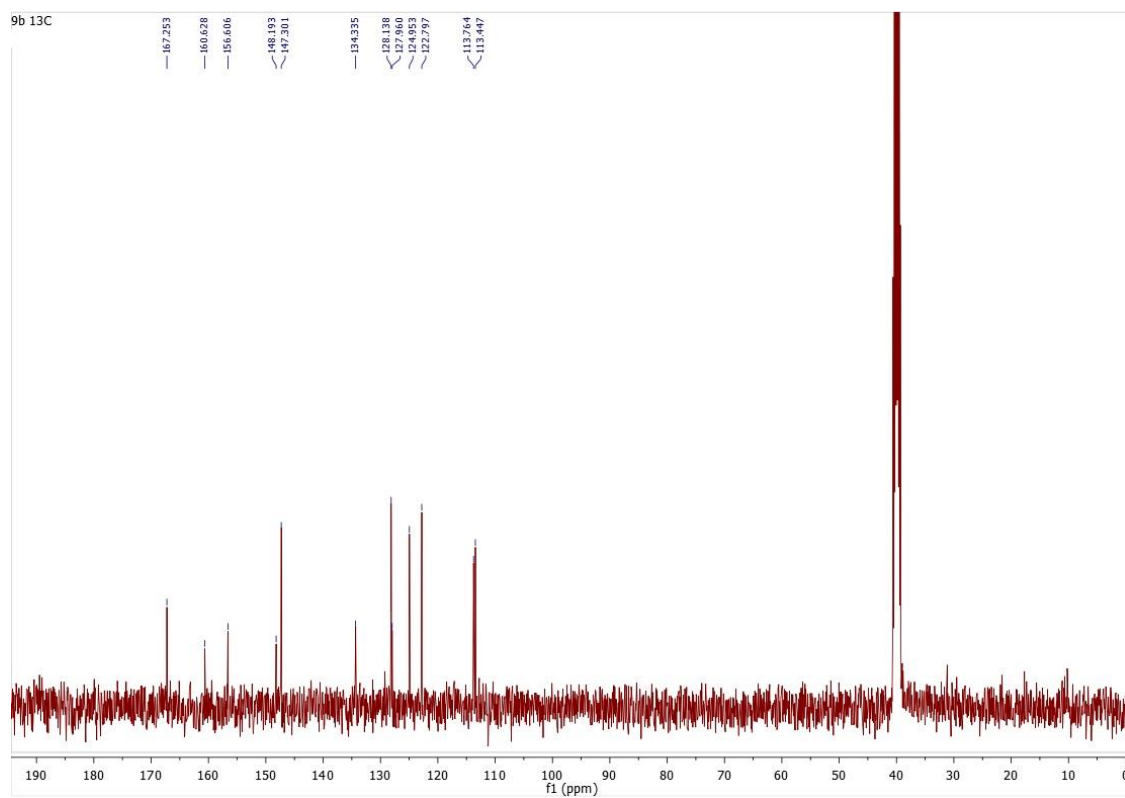


Figure S10. ^{13}C -NMR spectrum of compound **9b**.

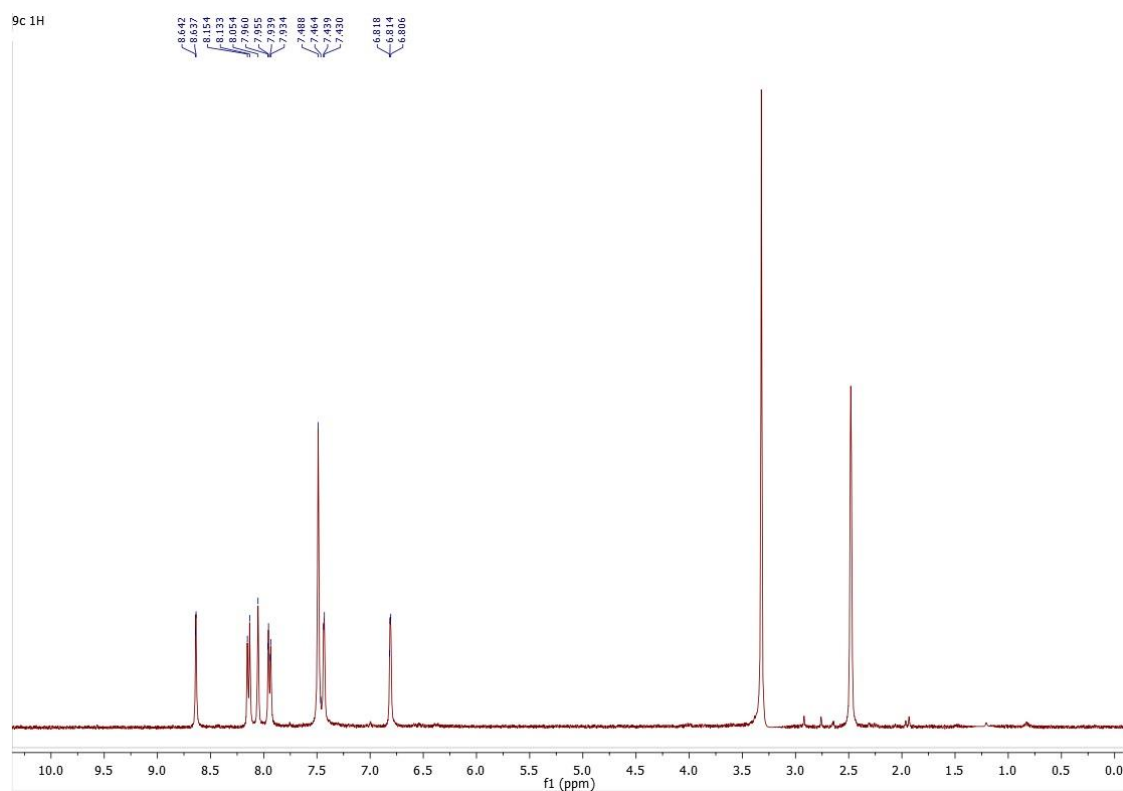


Figure S11. ^1H -NMR spectrum of compound 9c.

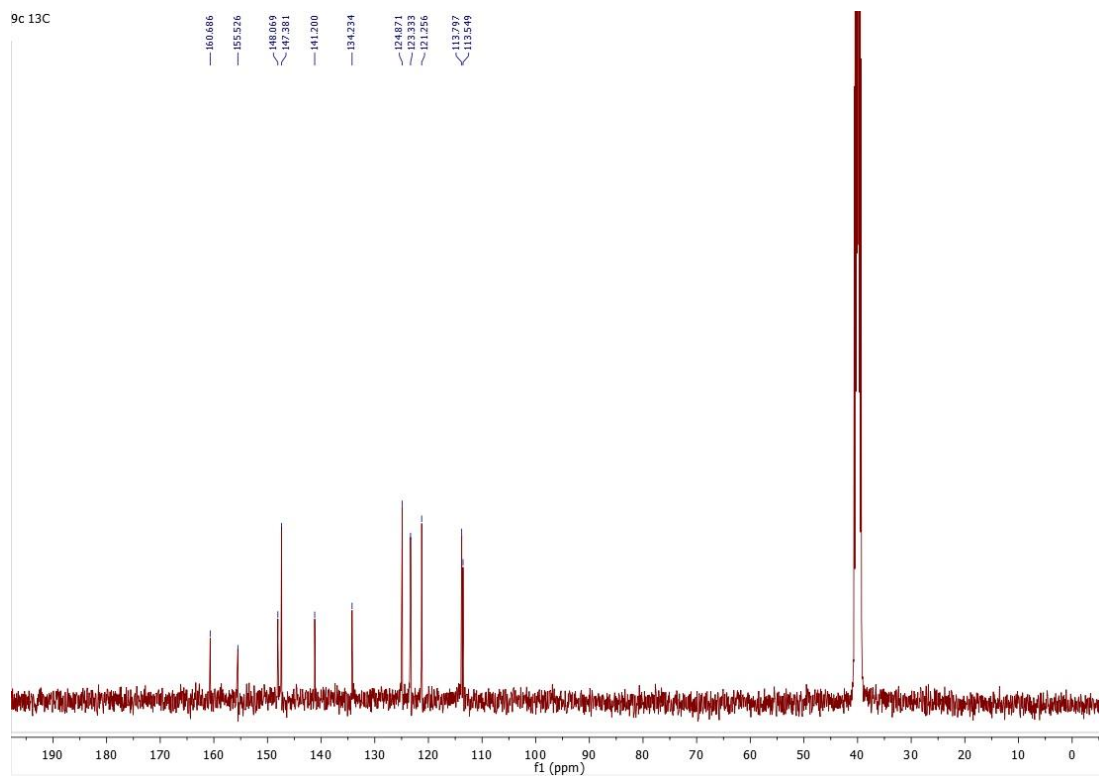


Figure S12. ^{13}C -NMR spectrum of compound 9c.

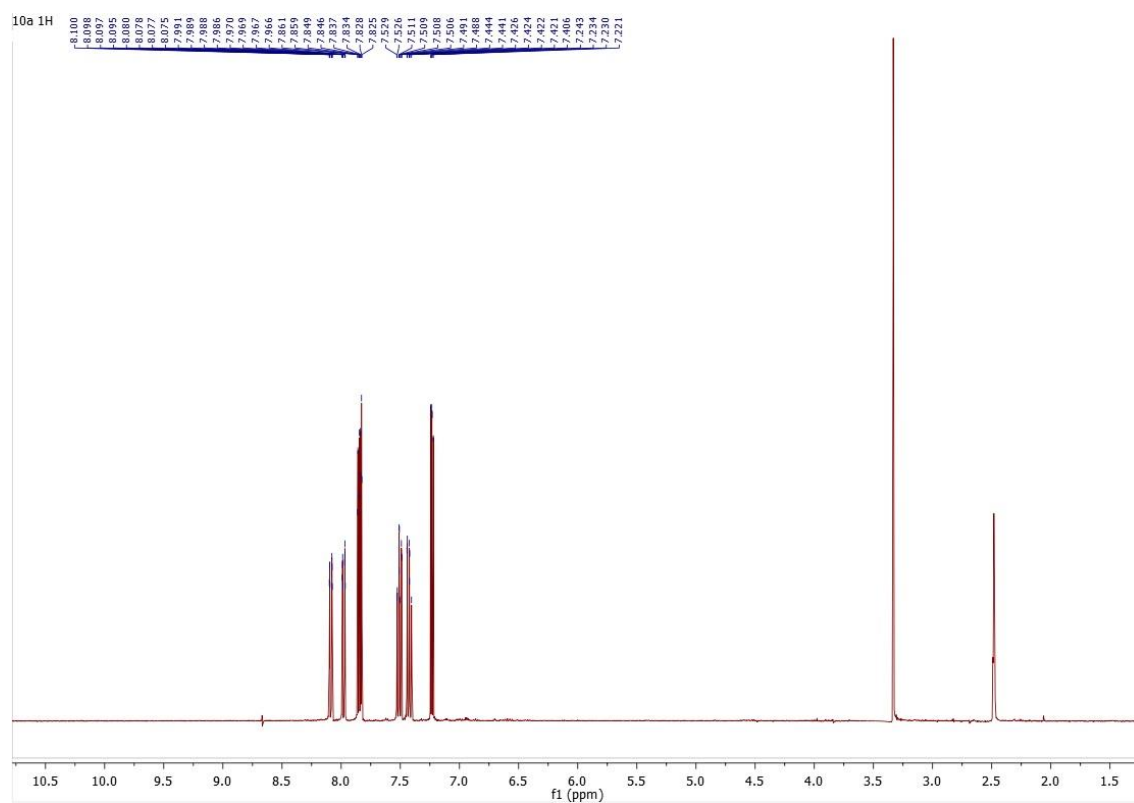


Figure S13. ^1H -NMR spectrum of compound 10a.

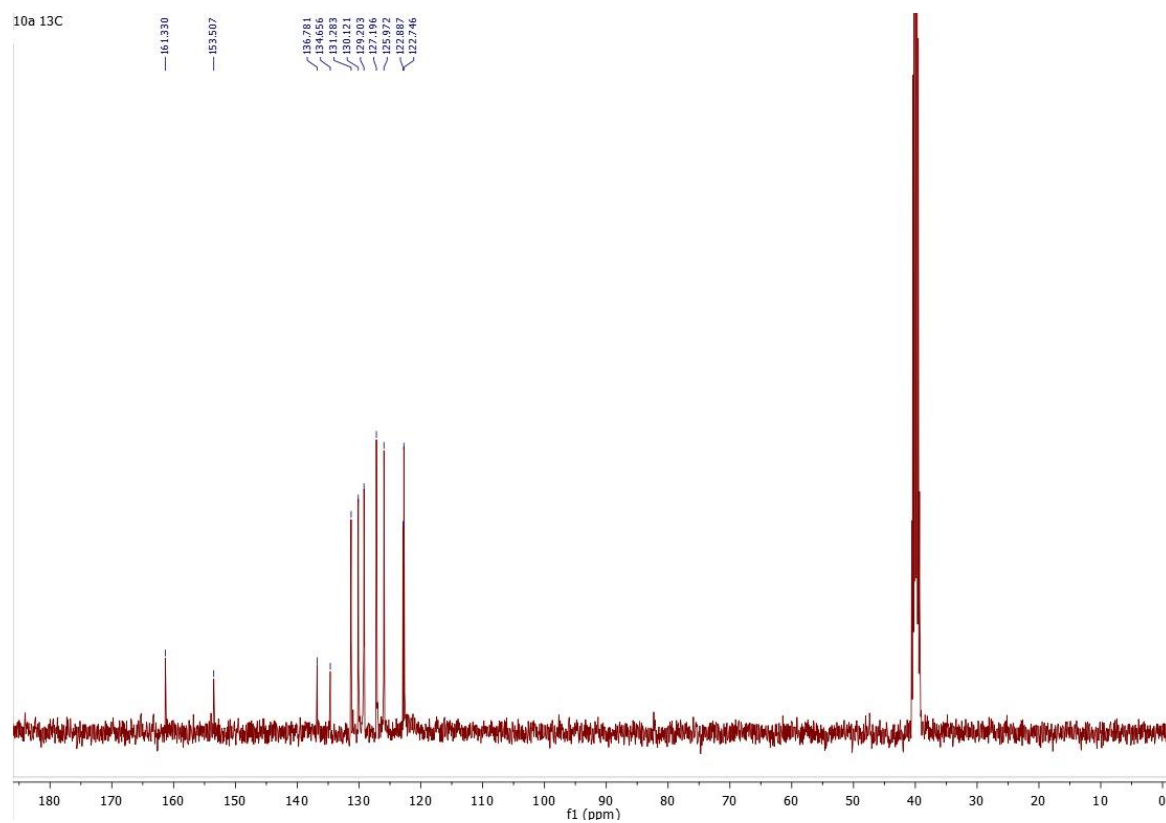


Figure S14. ^{13}C -NMR spectrum of compound 10a.

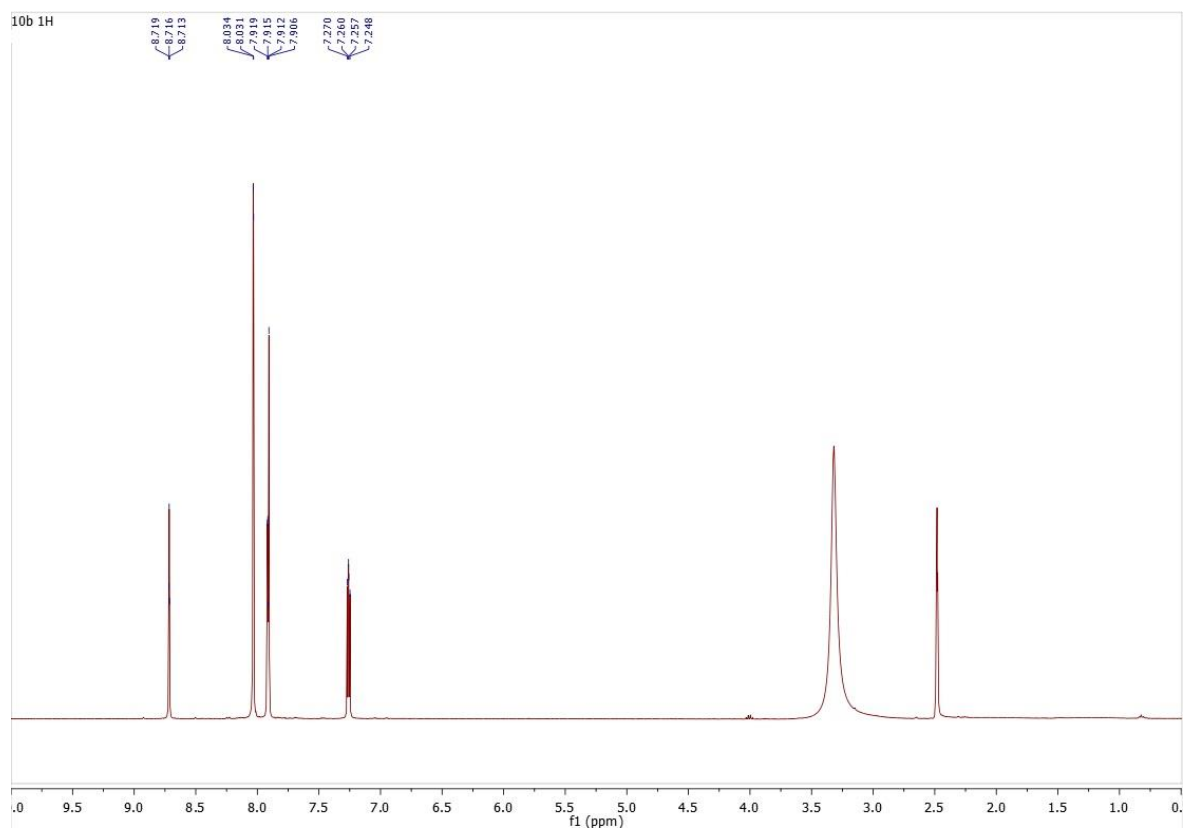


Figure S15. ^1H -NMR spectrum of compound 10b.

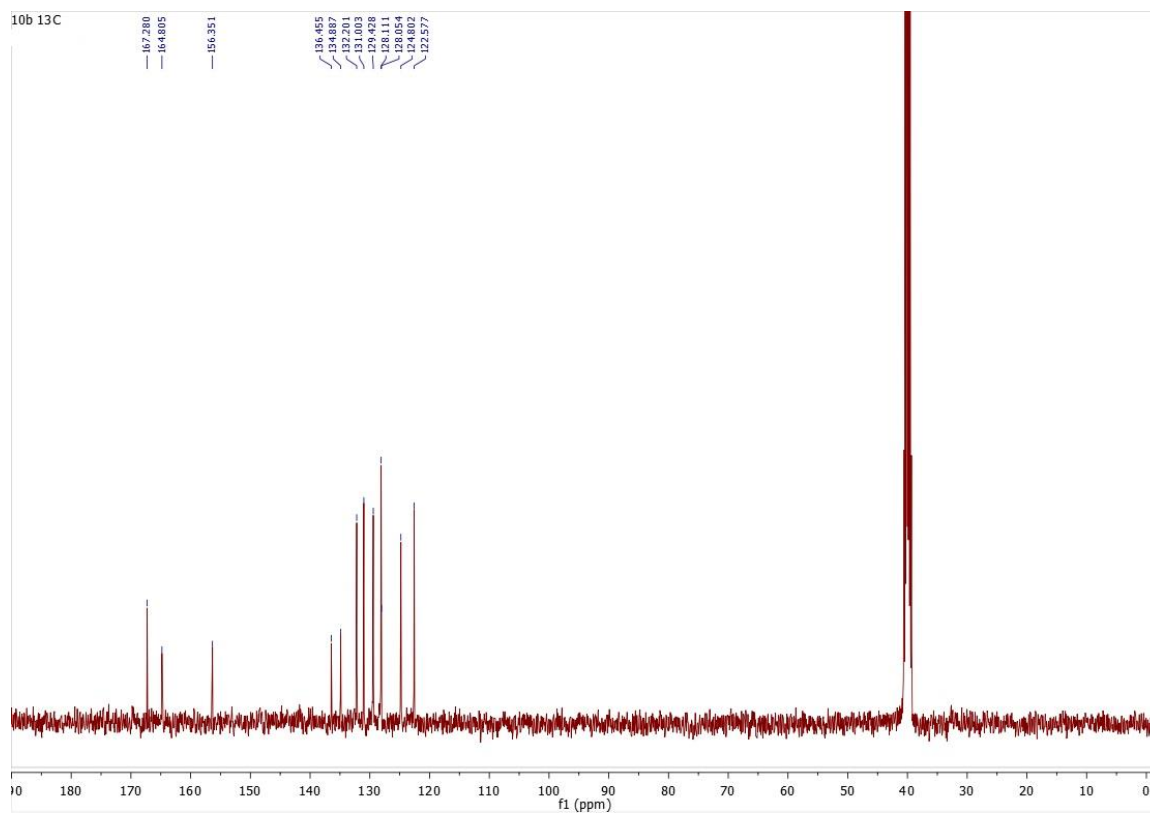


Figure S16. ^{13}C -NMR spectrum of compound 10b.

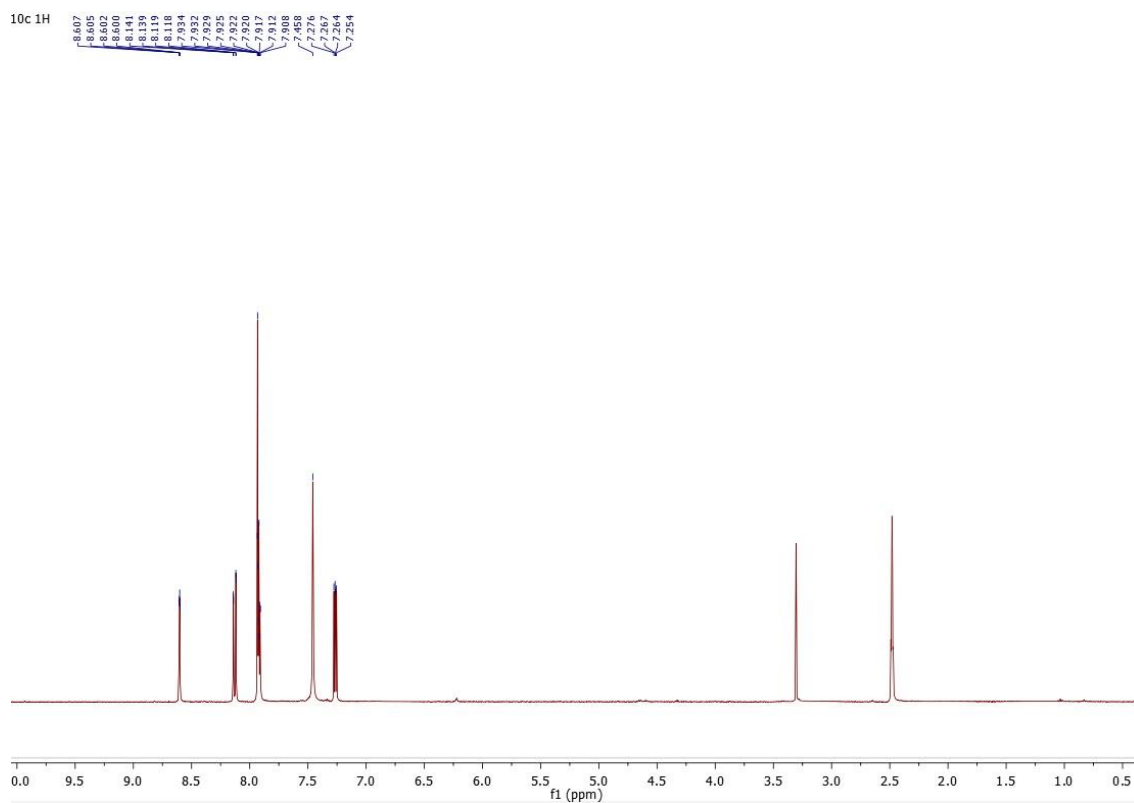


Figure S17. ^1H -NMR spectrum of compound **10c**.

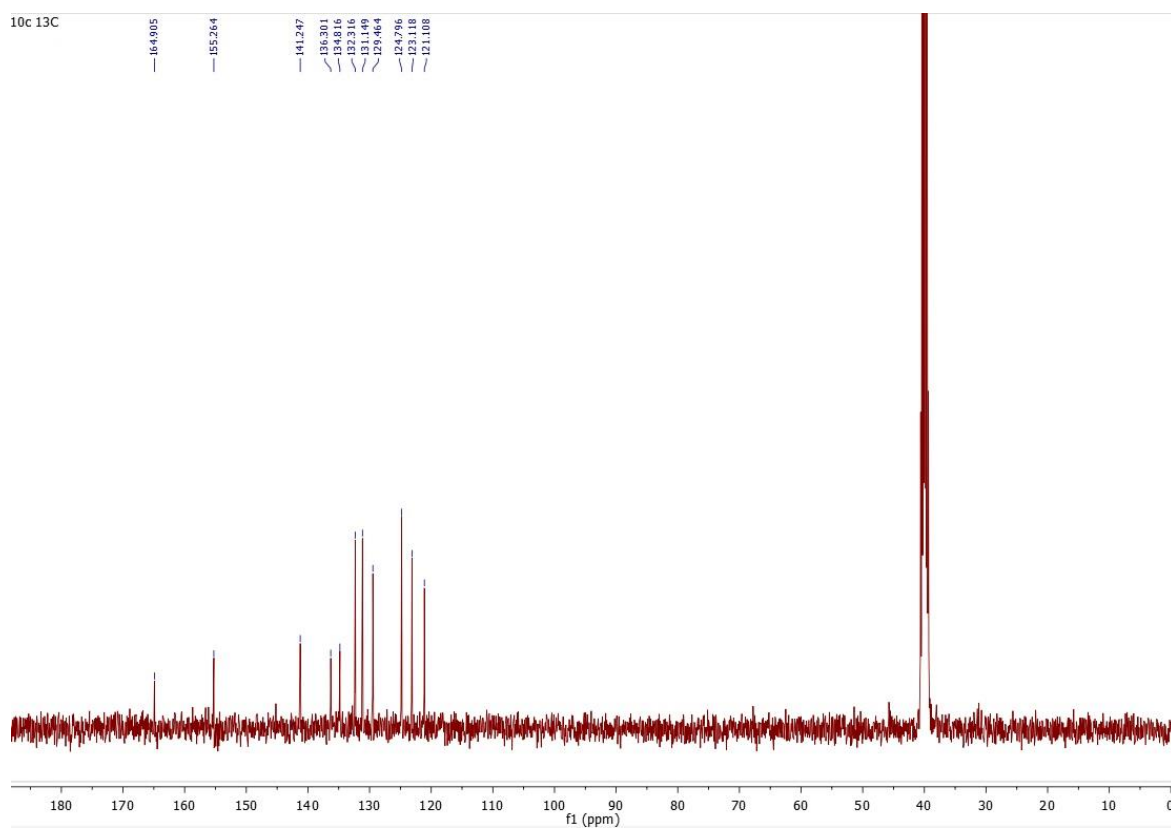


Figure S18. ^{13}C -NMR spectrum of compound **10c**.