

Construction of dispirocyclohexyl-3,3'-bisoxindole and dispirocyclopentyl-3,3'-bisoxindole via cycloaddition reactions of *N*-benzylbenzimidazolium salts with 2-(2-oxoindolin-3-ylidene)acetates

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Supporting Information

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Crystallographic data **3f** (CCDC 1029433), **4a** (CCDC 1029434), **4d** (CCDC 1030434) and **4f** (CCDC 1036833) have been deposited at the Cambridge Crystallographic Database Centre.

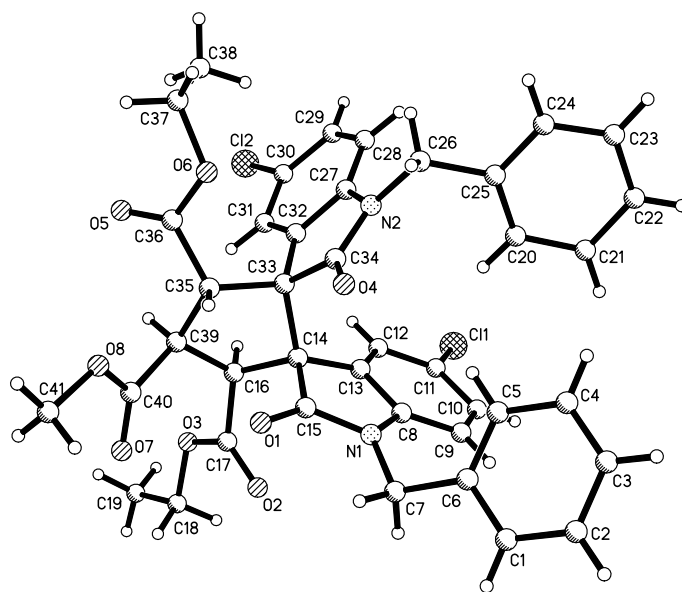


Fig. s1 Molecular structure of compound **4d**

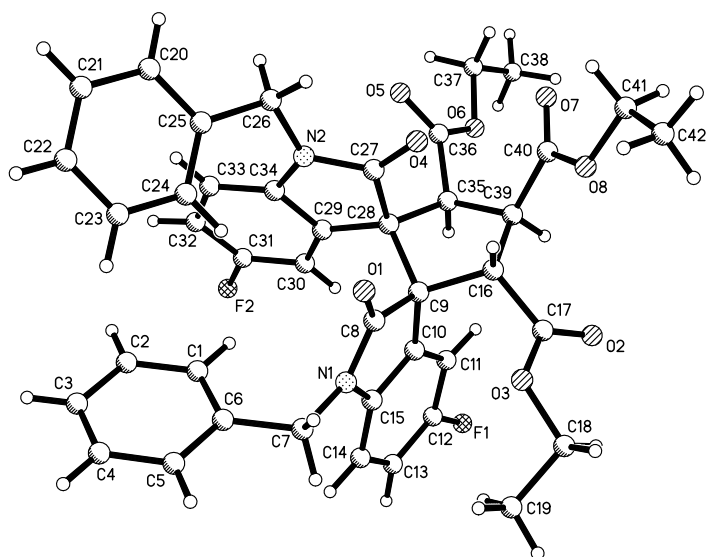


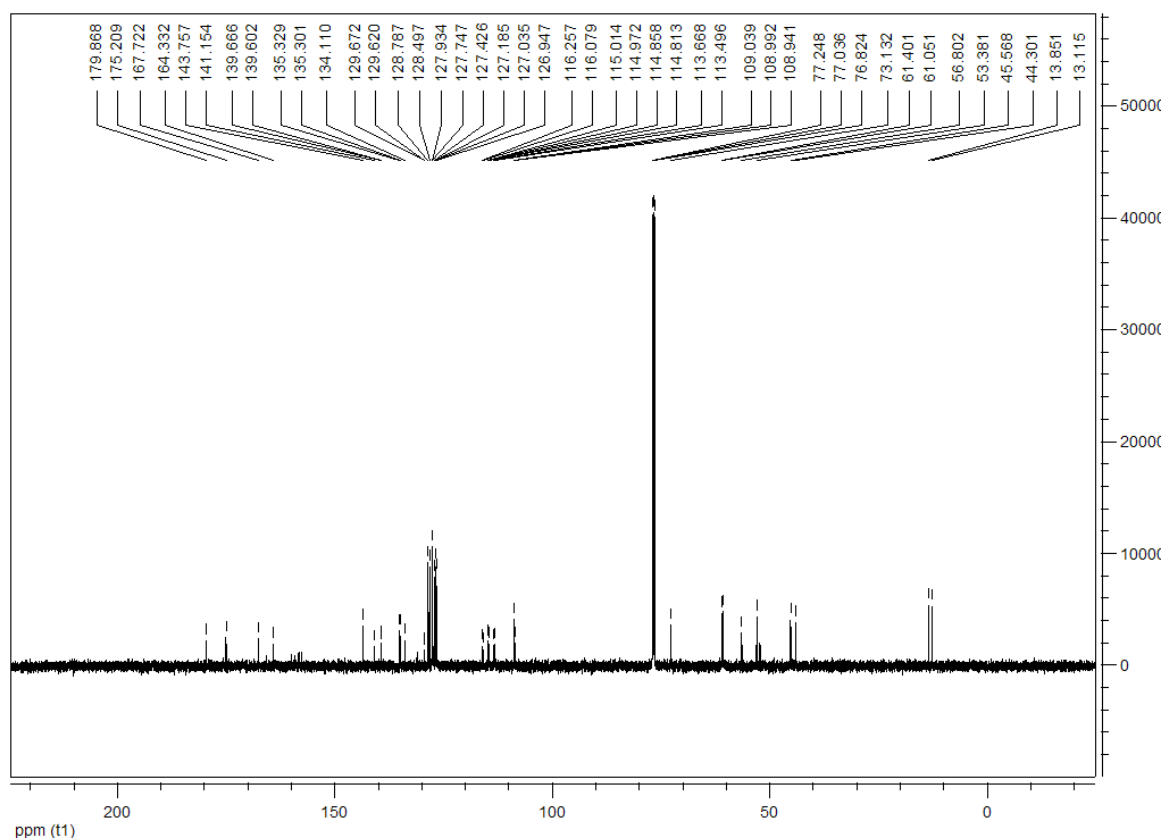
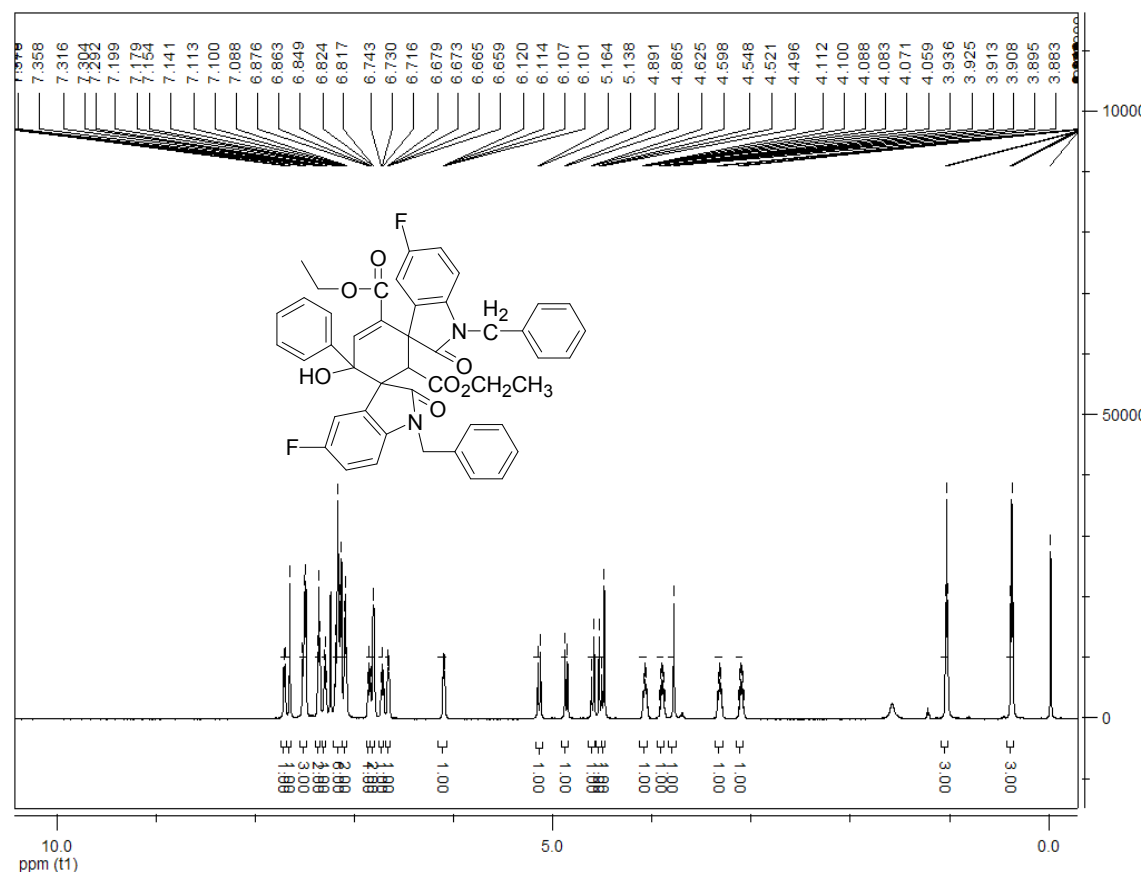
Fig. s2 Molecular structure of compound **4f**

Table s1 Crystal data of compounds 3f, 4a, 4d and 4f

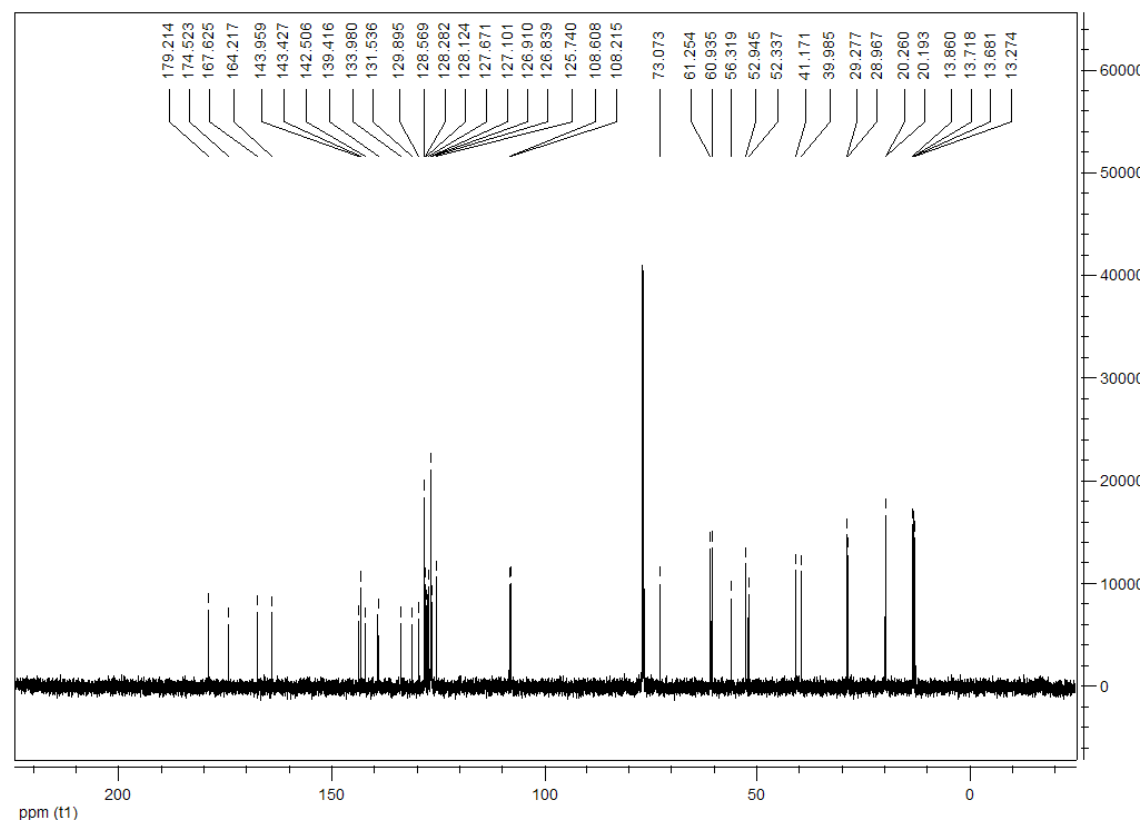
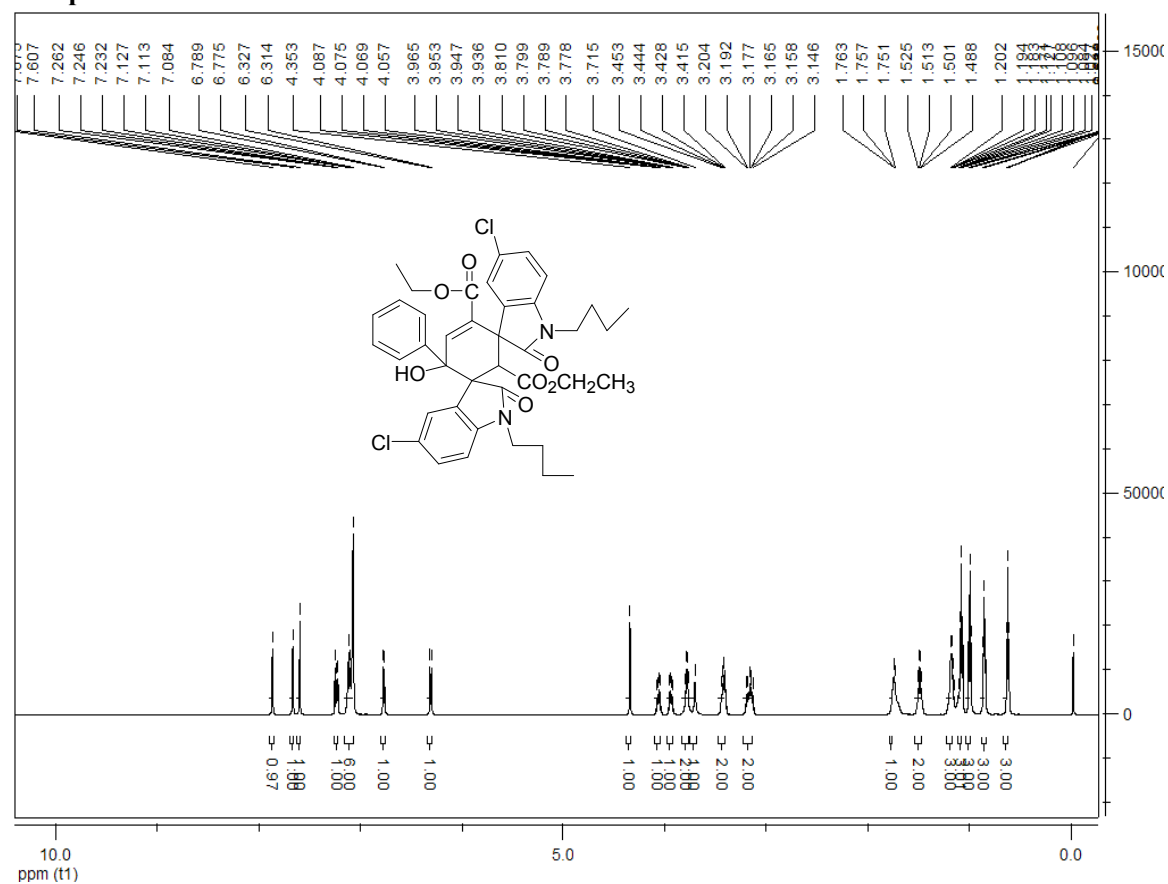
Phase	3f	4a	4d	4f
Empirical formula	C ₄₆ H ₃₇ Cl ₃ N ₂ O ₇ ·C ₃ H ₇ N O	C ₄₁ H ₃₈ N ₂ O ₈	C ₄₁ H ₃₆ Cl ₂ N ₂ O ₈	C ₄₂ H ₃₈ F ₂ N ₂ O ₈
Formula weight	909.22	686.73	755.62	736.74
Temperature(K)	296(2)	296(2)	296(2)	296(2)
Wavelength/nm	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
space group	P -1	P -1	P -1	P -1
a (Å)	11.5355(12)	10.740(3)	10.8295(16)	10.5612(11)
b (Å)	12.0272(13)	12.889(3)	12.8333(19)	12.8164(13)
c (Å)	16.4726(17)	15.381(4)	15.121(2)	15.0804(16)
α (°)	105.258(3)	68.745(3)	85.481(2)	85.716(3)
β (°)	90.346(3)	87.060(3)	76.954(2)	77.587(3)
γ (°)	91.168(3)	70.391(3)	75.004(2)	76.529(3)
Volume(Å ³)	2204.2(4)	1863.2(8)	1977.1(5)	1938.0(3)
Z	2	2	2	2
F(000)	948	724	788	772
Calc. d. (g·cm ⁻³)	1.370	1.224	1.269	1.263
Absorption coefficient (mm ⁻¹)	0.267	0.085	0.217	0.094
θ range (°)	1.28 to 27.59	1.43 to 25.00	1.38	1.63 to 27.59
Limiting indices	-14<=h<=15, -21<=l<=21	-12<=h<=12, -18<=l<=18	-13<=h<=13, -18<=l<=18	-13<=h<=13, -16<=k<=14, -19<=l<=19
Reflections collected / unique	46666/10202 [R(int)=0.0439]	12005/6557 [R(int)=0.0387]	113843/7783 [R(int)=0.0413]	25423/ 8762 [R(int)=0.0275]
Completeness to theta	99.5%	95.9%	95.2%	97.6%
Max. and min. transmission	0.923 and 0.904	0.980 and 0.972	0.958 and 0.939	0.978 and 0.969
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	10160 / 0 / 573	6287 / 0 / 463	7409 / 0 / 481	8762 / 1 / 491
Goodness-of-fit on F ²	1.031	1.030	1.184	1.098
Final R indices [I>2 sigma (I)]	R ₁ = 0.0604, wR ₂ = 0.1465	R ₁ = 0.0837, wR ₂ = 0.2365	R ₁ = 0.1064, wR ₂ = 0.2890	R ₁ = 0.0730, wR ₂ = 0.2154
R indices (all data)	R ₁ = 0.1009, wR ₂ = 0.0693	R ₁ = 0.0933, wR ₂ = 0.2499	R ₁ = 0.1257, wR ₂ = 0.3093	R ₁ = 0.1085, wR ₂ = 0.2364
Largest diff. peak	0.663 and -0.386	0.482 and -0.368	0.619 and -0.400	0.858 and -0.467

and hole($e\cdot\text{\AA}^{-3}$)

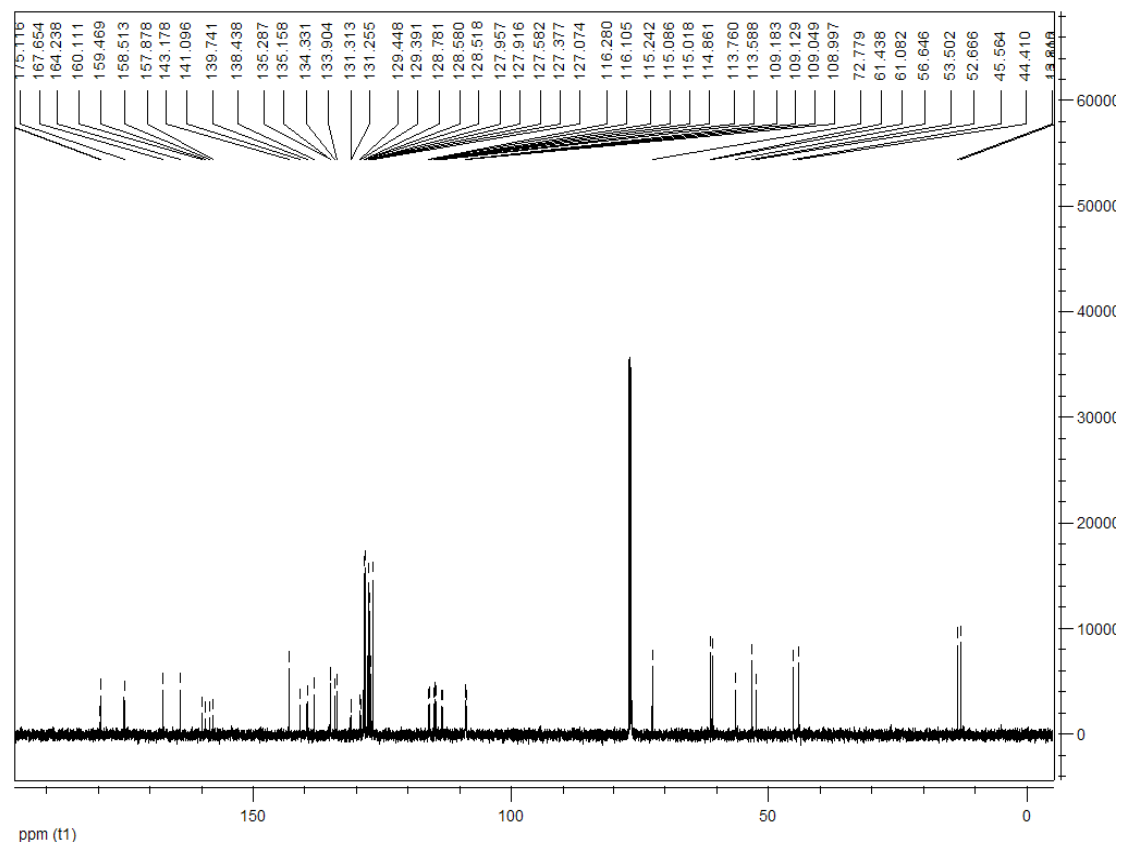
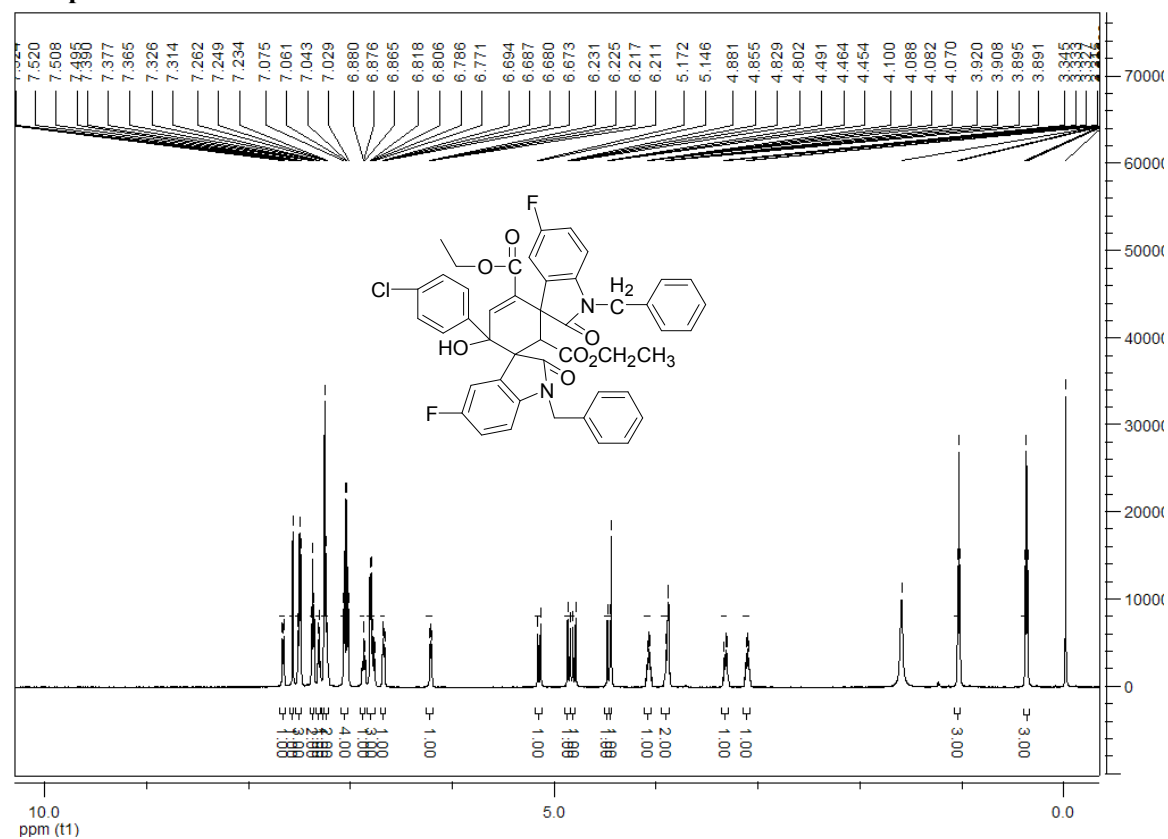
Compound 3a:



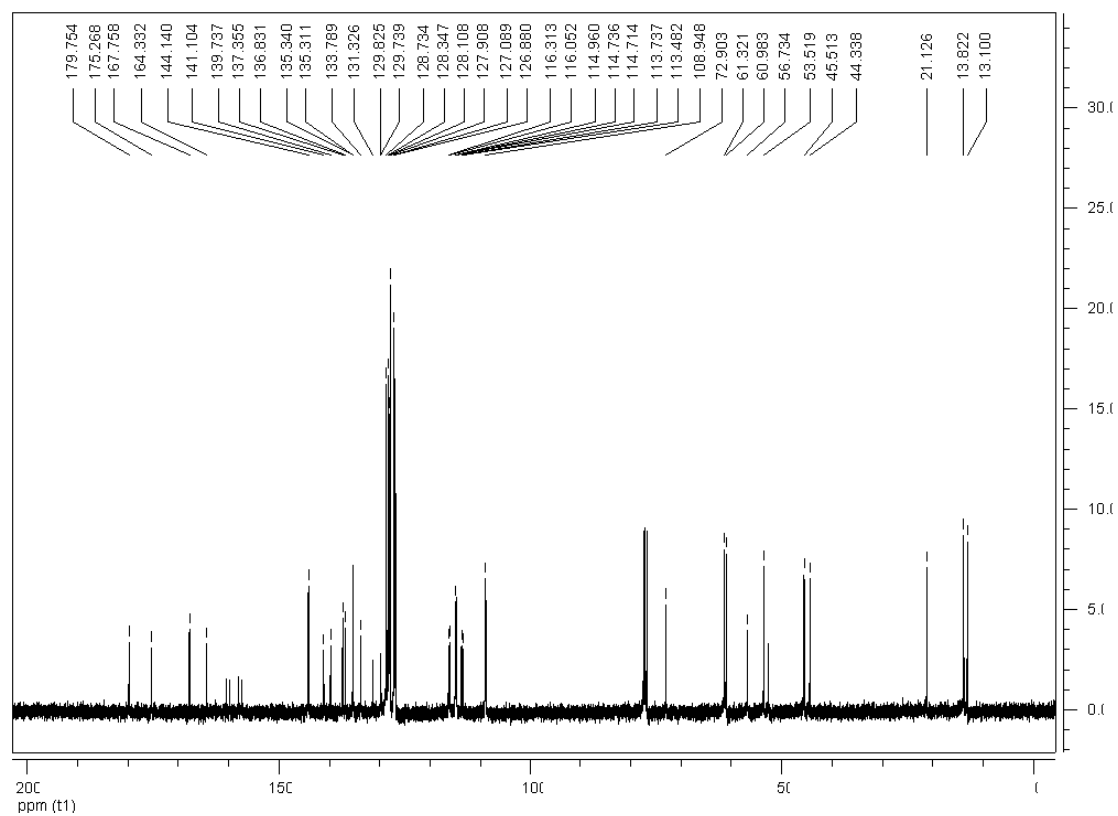
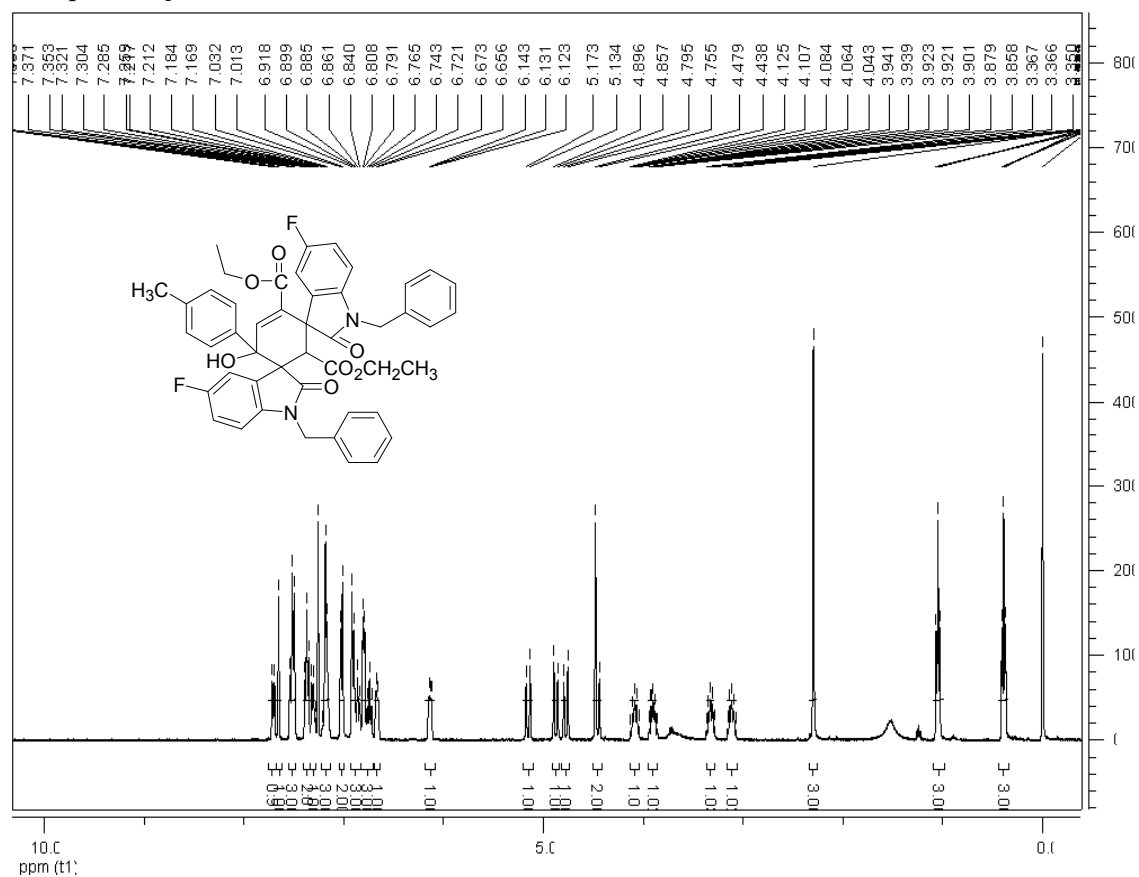
Compound 3c:



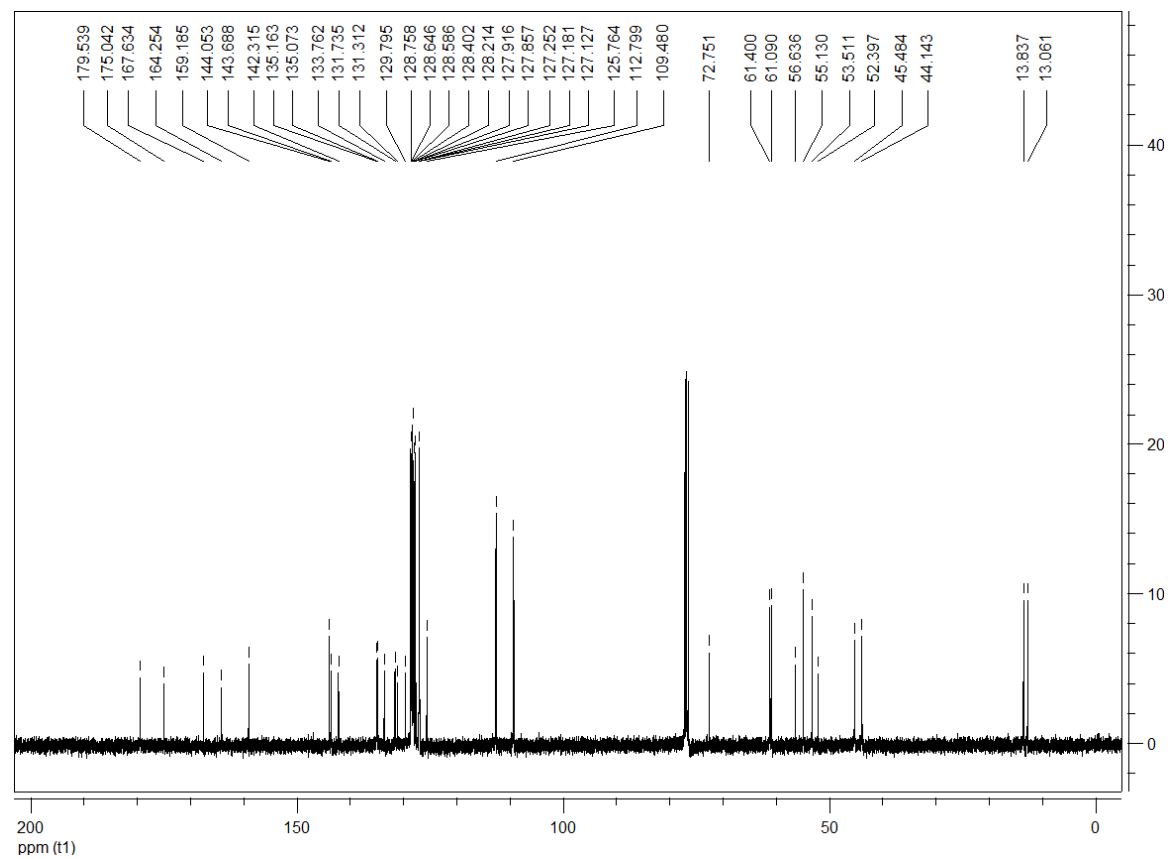
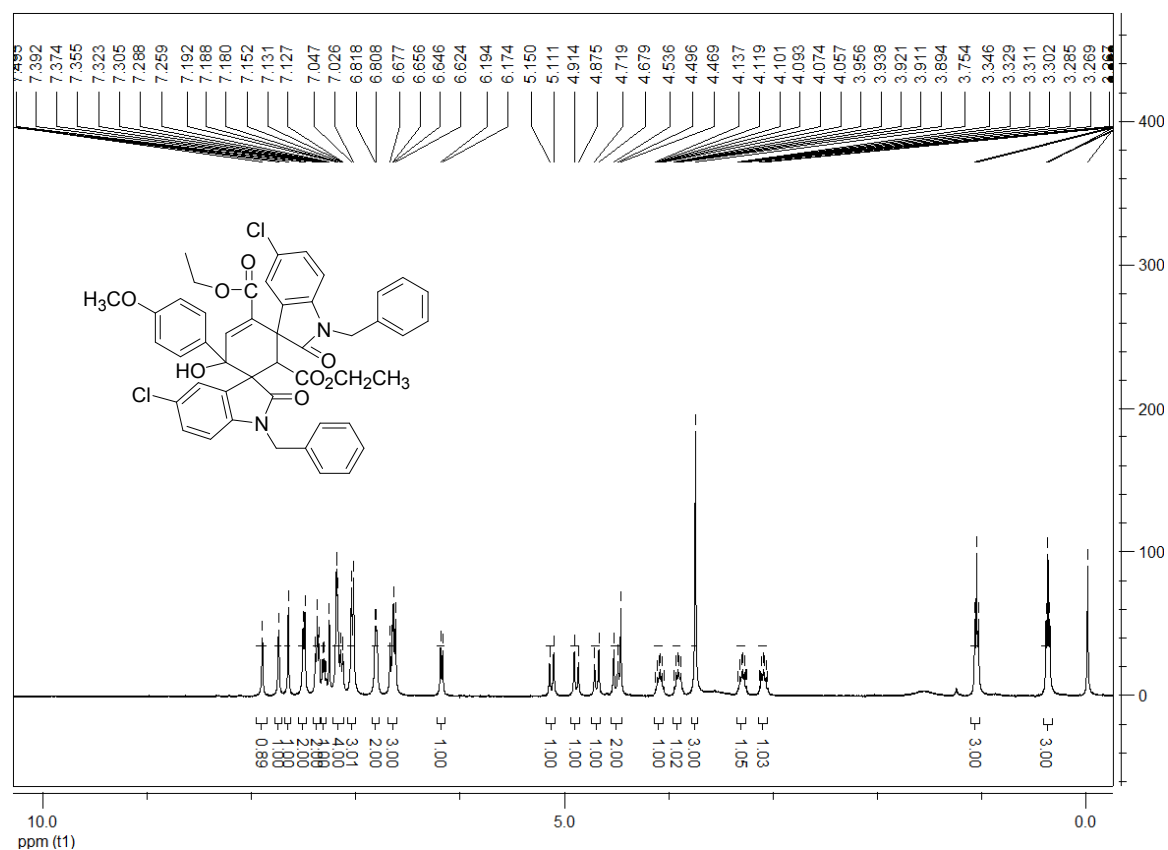
Compound 3e:



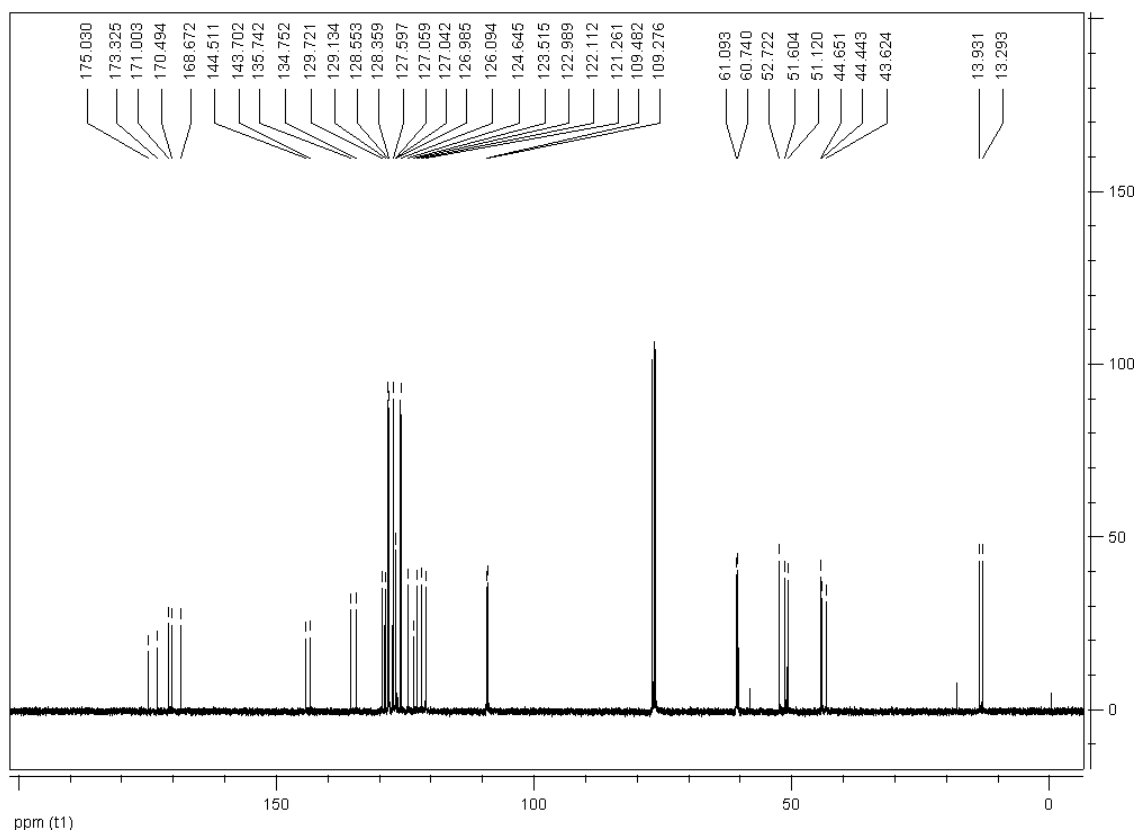
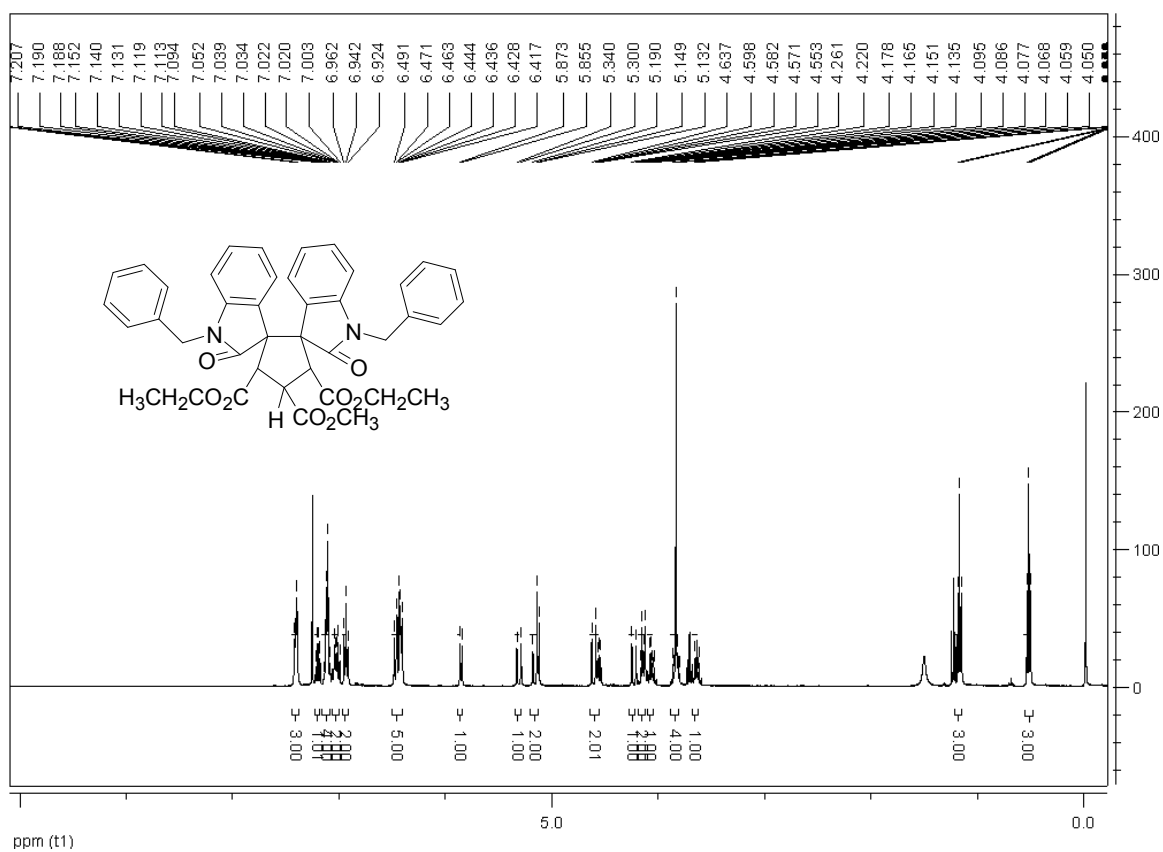
Compound 3j:



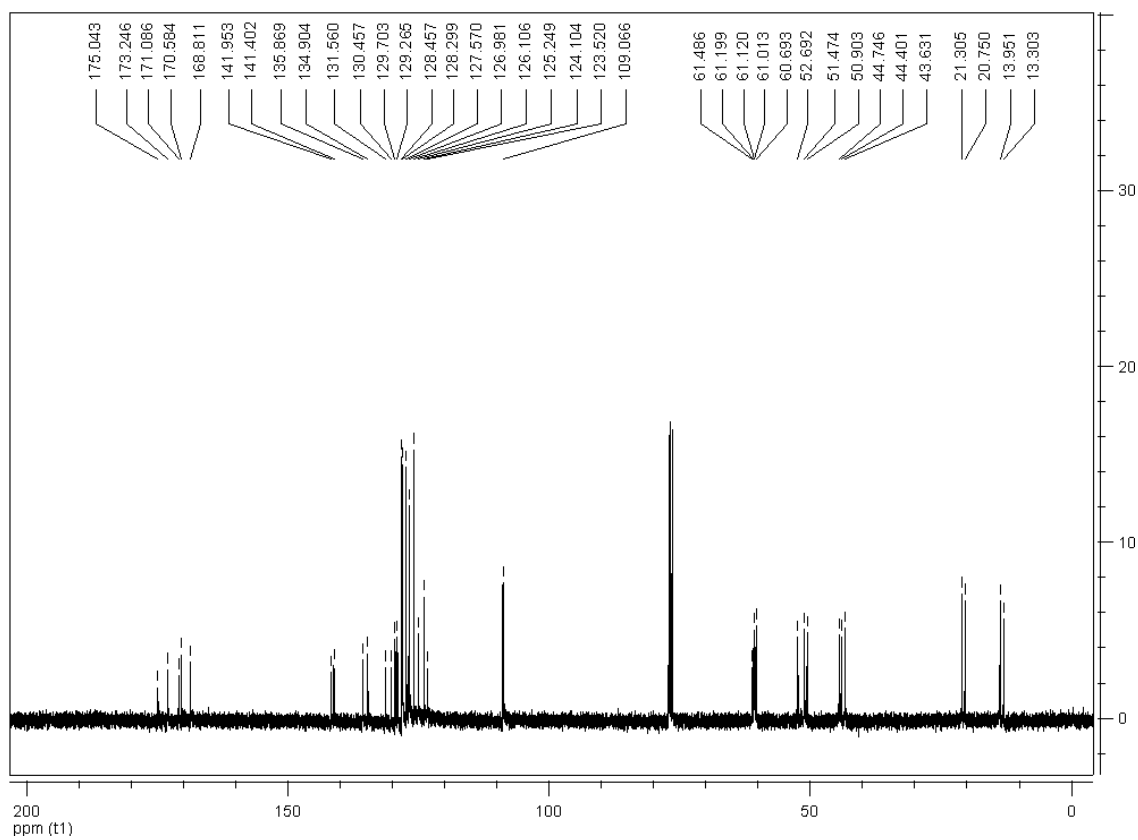
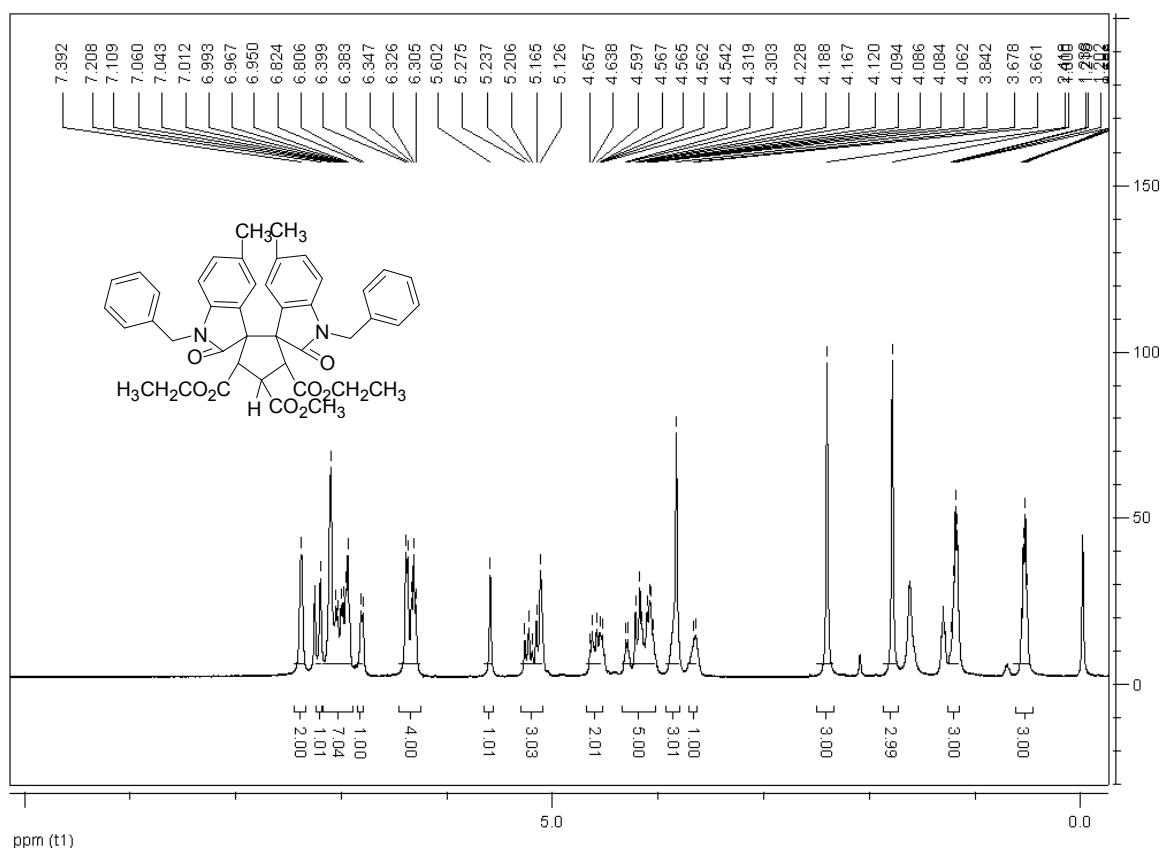
Compound 3m:



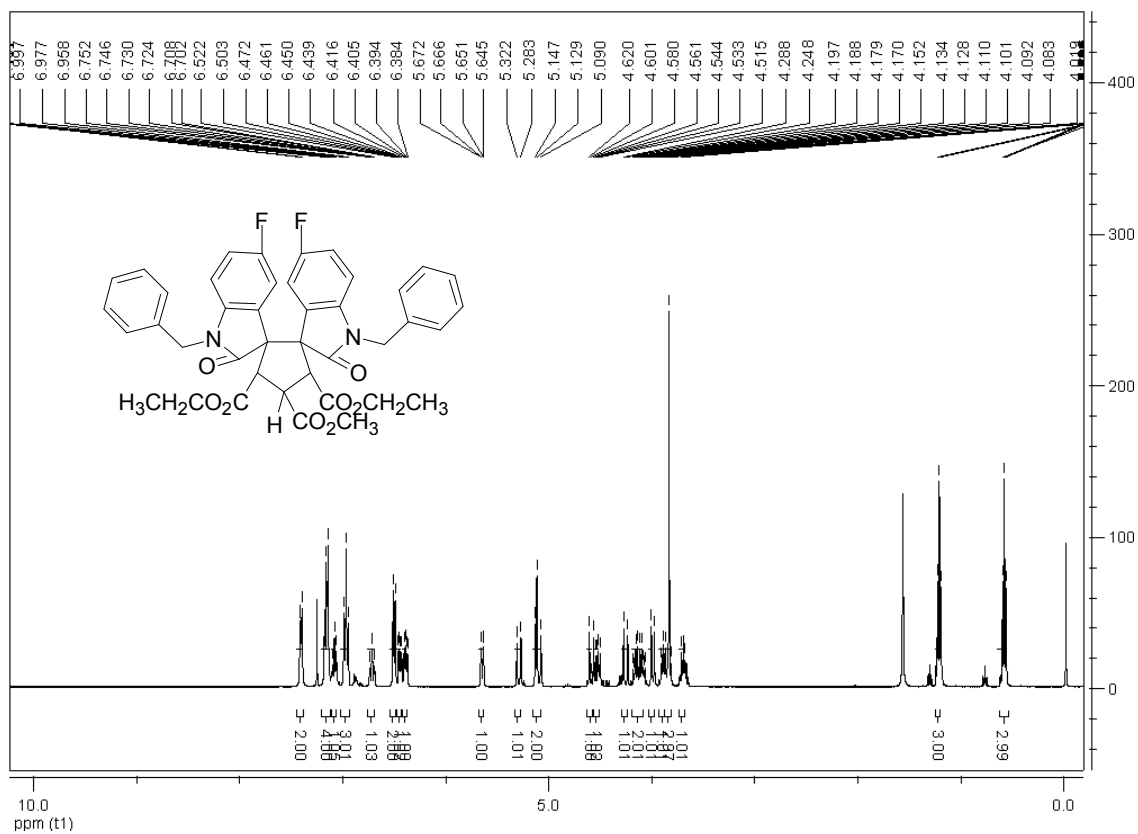
Compound 4a:



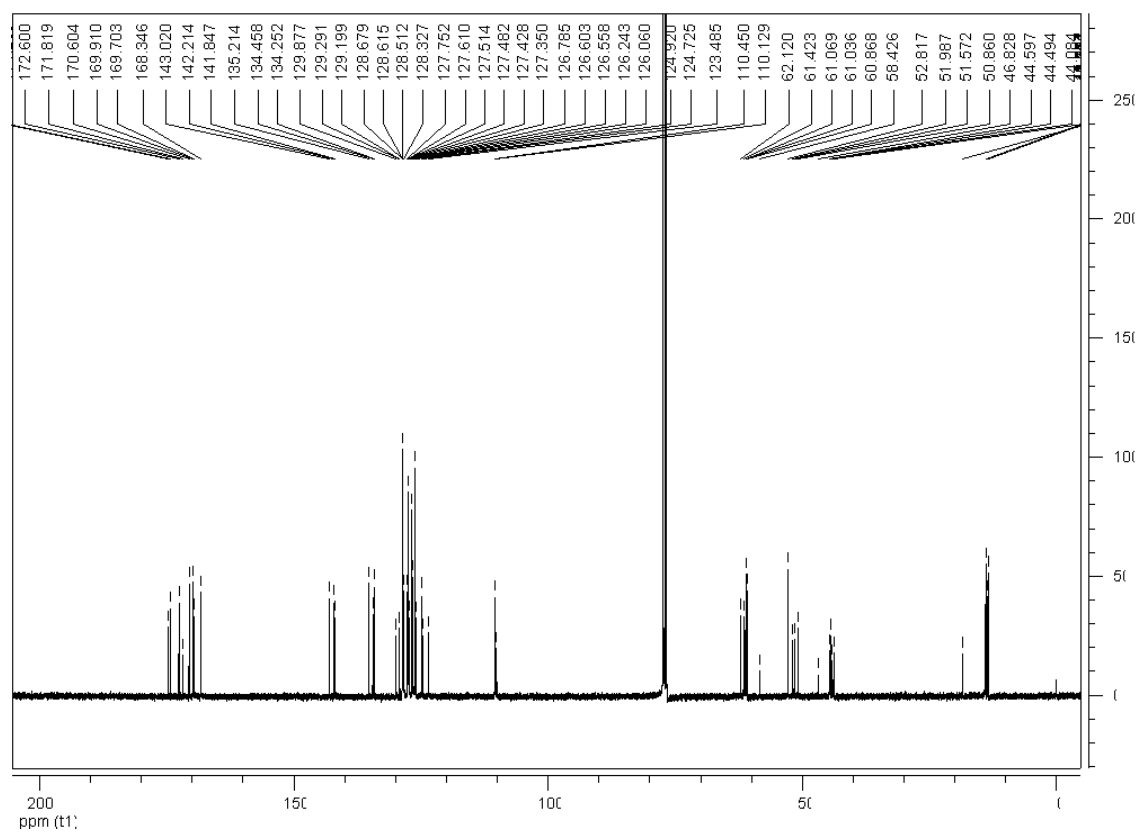
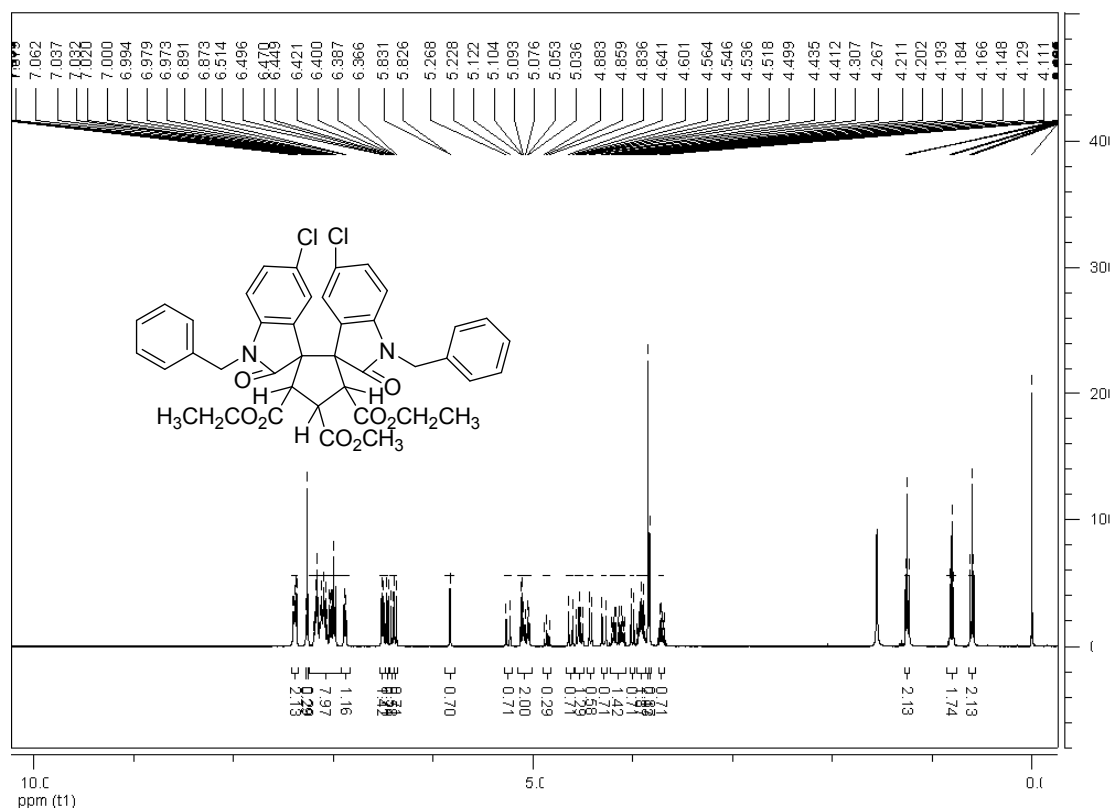
Compound 4b:



Compound 4c:



Compound 4d:



Compound: 4e:

