

Supplementary Information

Tandem Diels–Alder/Oxidation–Aromatization Reactions involving 2-Styrylchromones and Arynes

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1. X-ray crystallographic data of compound **4a**

The structure of **4a** was determined by X-ray crystallographic analysis. The crystal was prepared from the solution of **4a** in mixed hexane/dichloromethane at ambient temperature. For more details, see CCDC 1832632, The Cambridge Crystallographic Data Center.

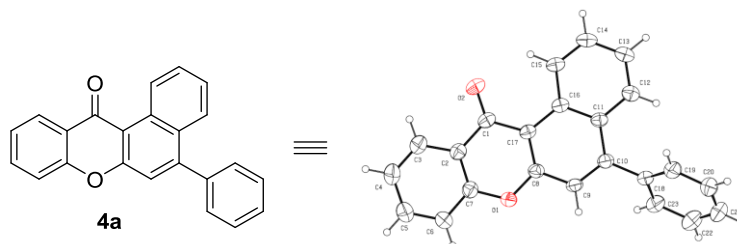


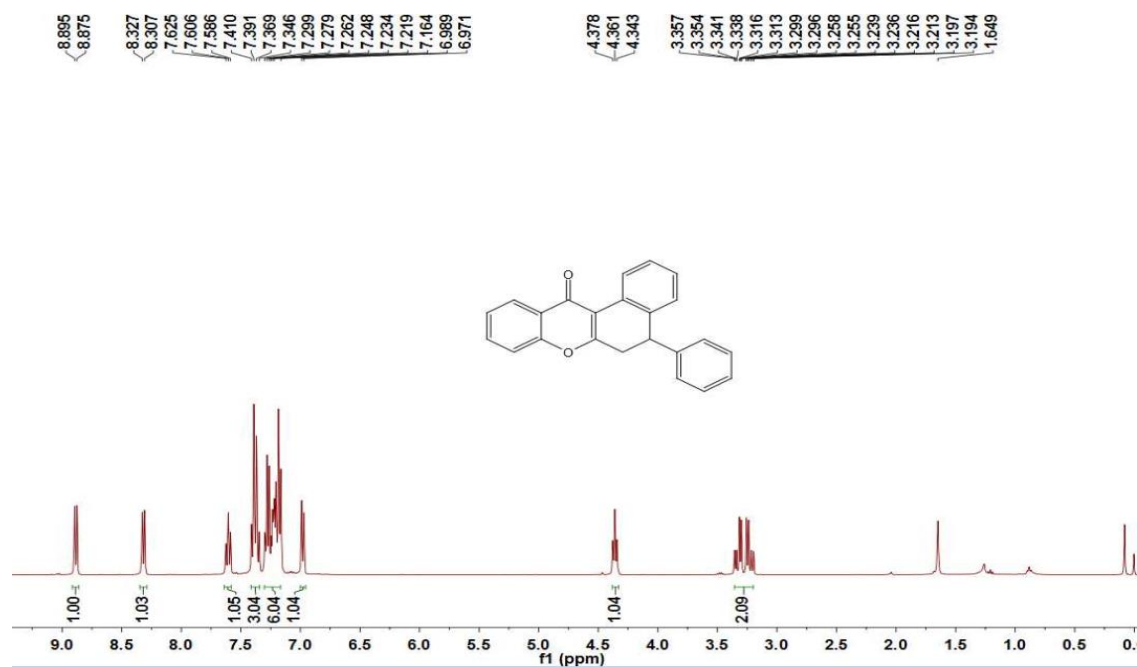
Figure S1. ORTEP diagram of **4a** (30% probability factor for the thermal ellipsoids).

Table 1 Crystal data and structure refinement for 170623_s3_wz (4a**).**

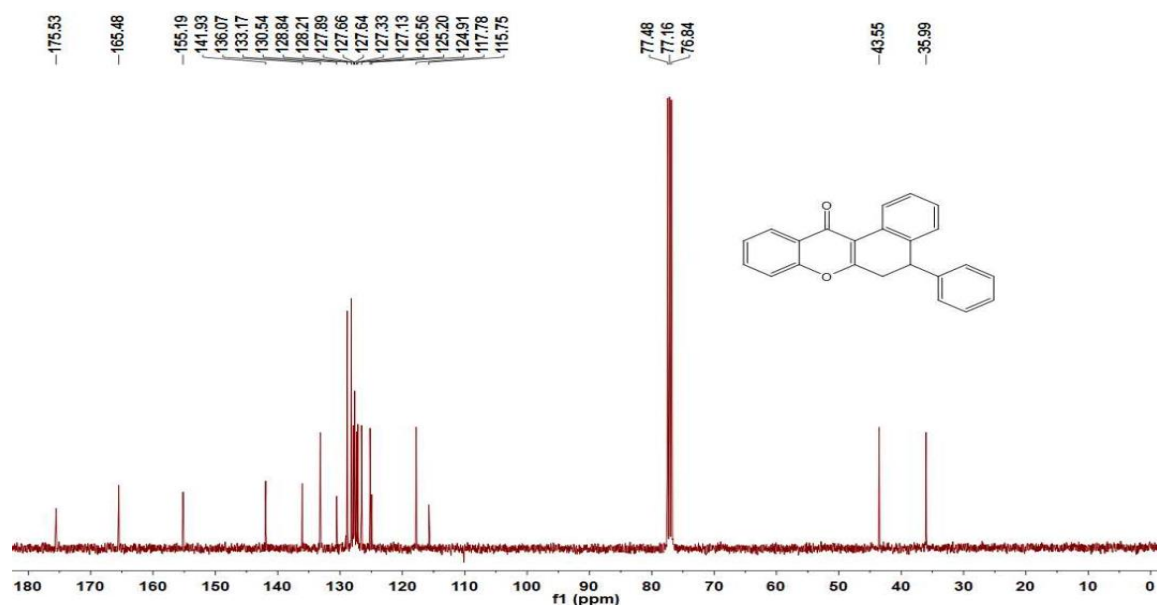
Identification code	170623_s3_wz (4a)
Empirical formula	C ₂₃ H ₁₄ O ₂
Formula weight	322.34
Temperature/K	293.15
Crystal system	orthorhombic
Space group	Pbcn
a/Å	9.1068(5)
b/Å	13.5461(9)
c/Å	26.1677(13)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	3228.1(3)
Z	8
ρ _{calc} /g/cm ³	1.327
μ/mm ⁻¹	0.084
F(000)	1344.0
Crystal size/mm ³	0.4 × 0.4 × 0.4
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.016 to 52.742
Index ranges	-10 ≤ h ≤ 11, -16 ≤ k ≤ 15, -32 ≤ l ≤ 32
Reflections collected	18344
Independent reflections	3312 [R _{int} = 0.0309, R _{sigma} = 0.0255]
Data/restraints/parameters	3312/0/226
Goodness-of-fit on F ²	1.024
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0540, wR ₂ = 0.1203
Final R indexes [all data]	R ₁ = 0.0861, wR ₂ = 0.1393
Largest diff. peak/hole / e Å ⁻³	0.14/-0.16

2. Experimental Spectra

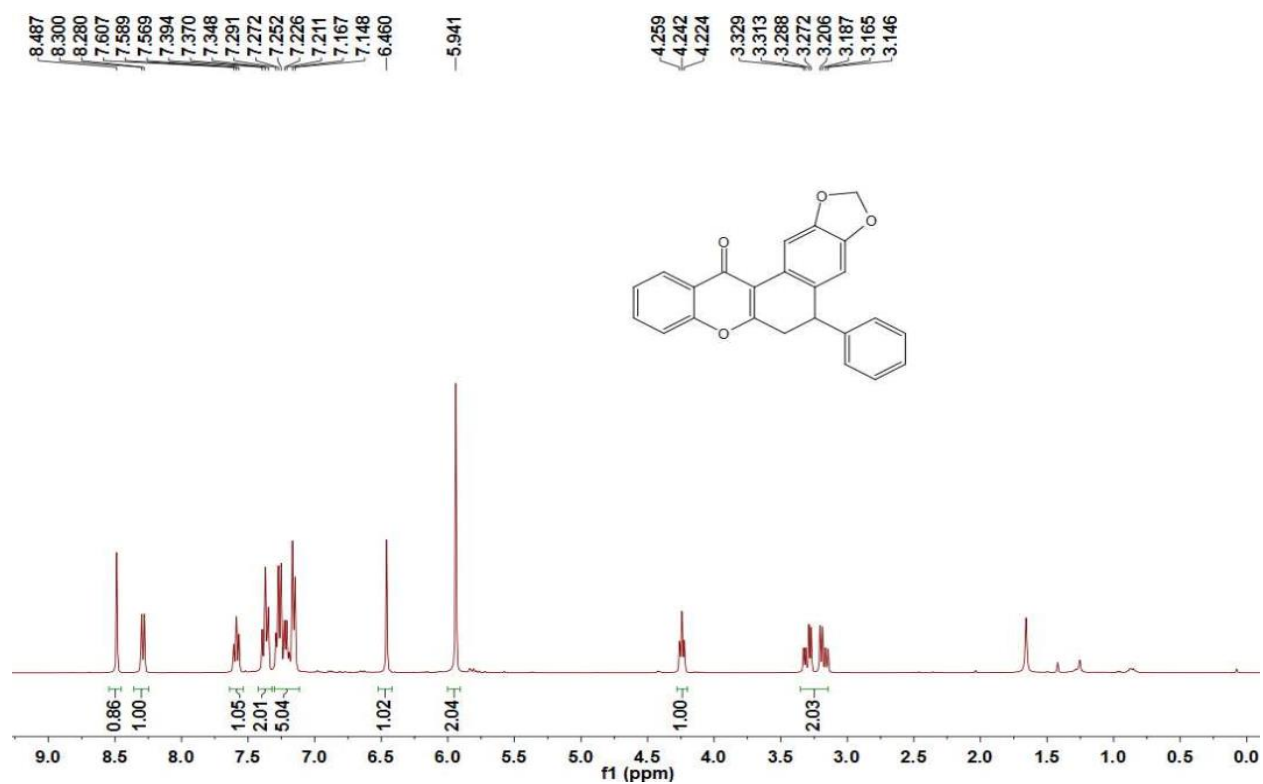
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3a**



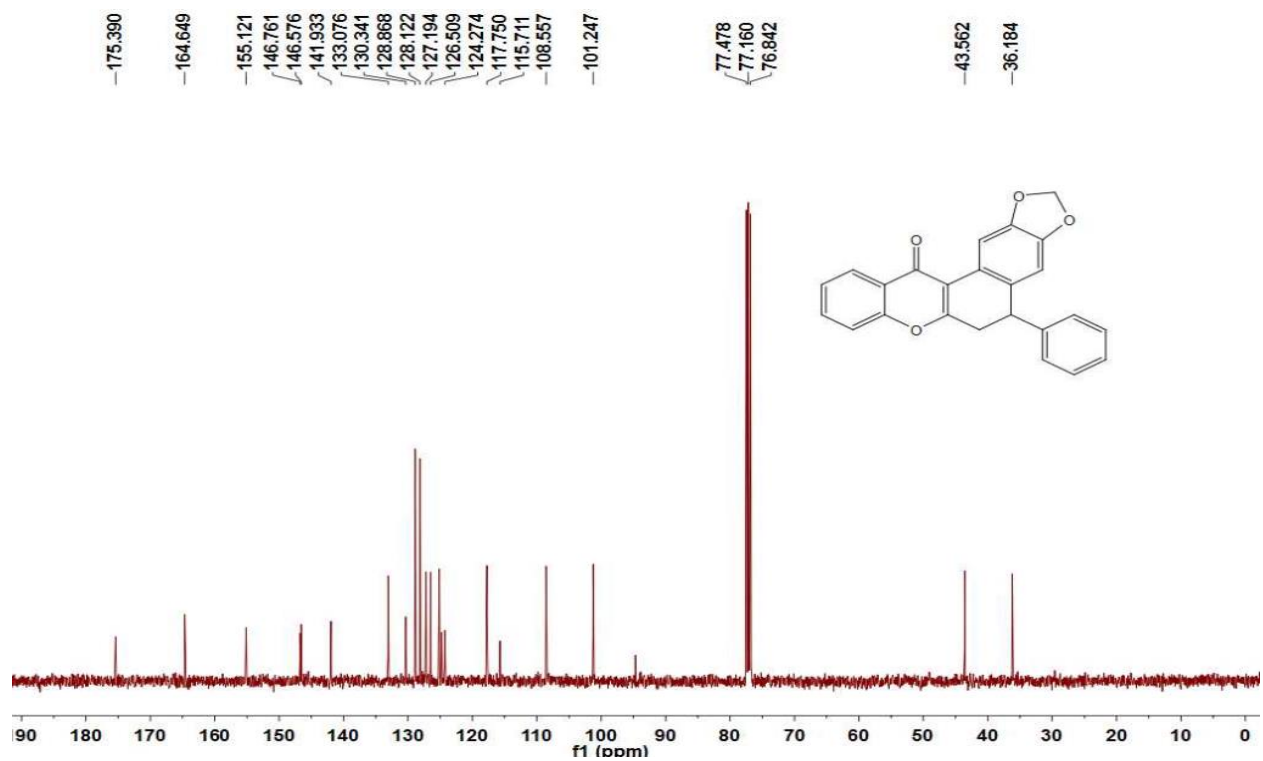
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3a**



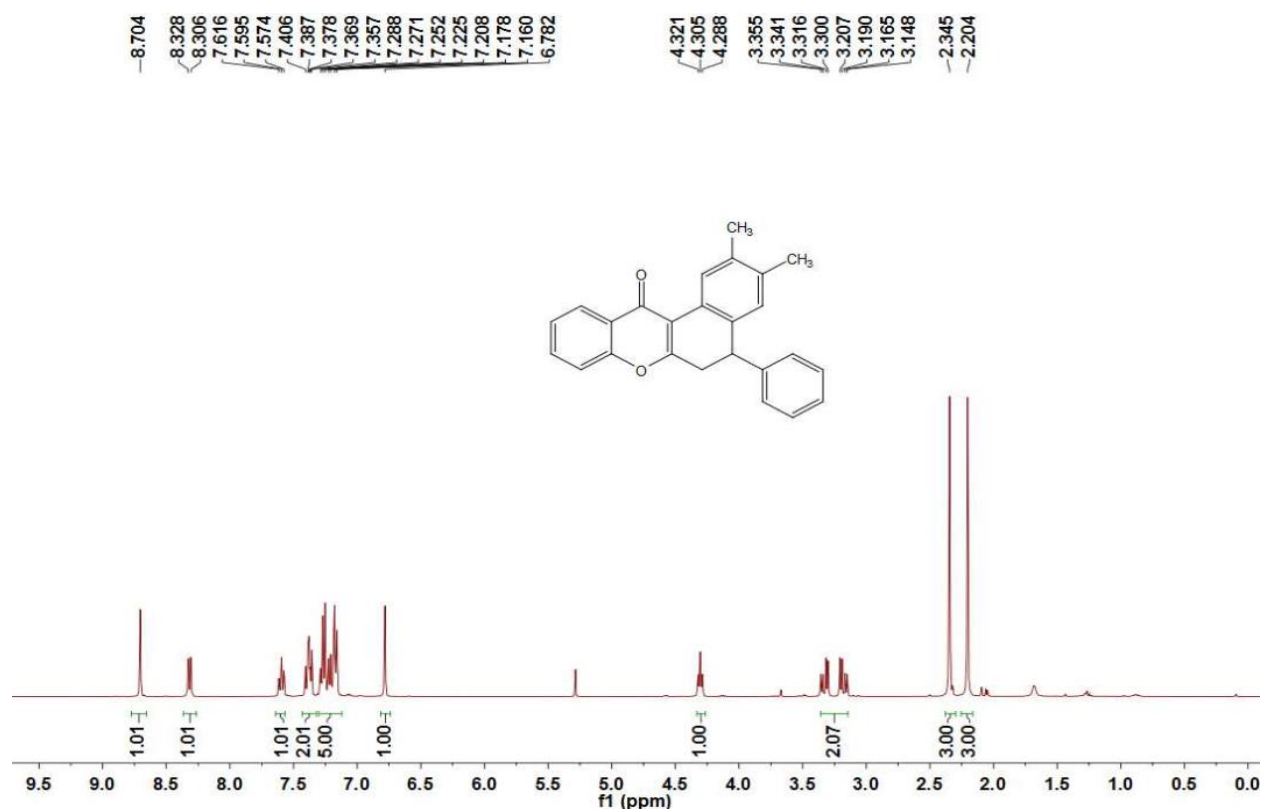
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3b**



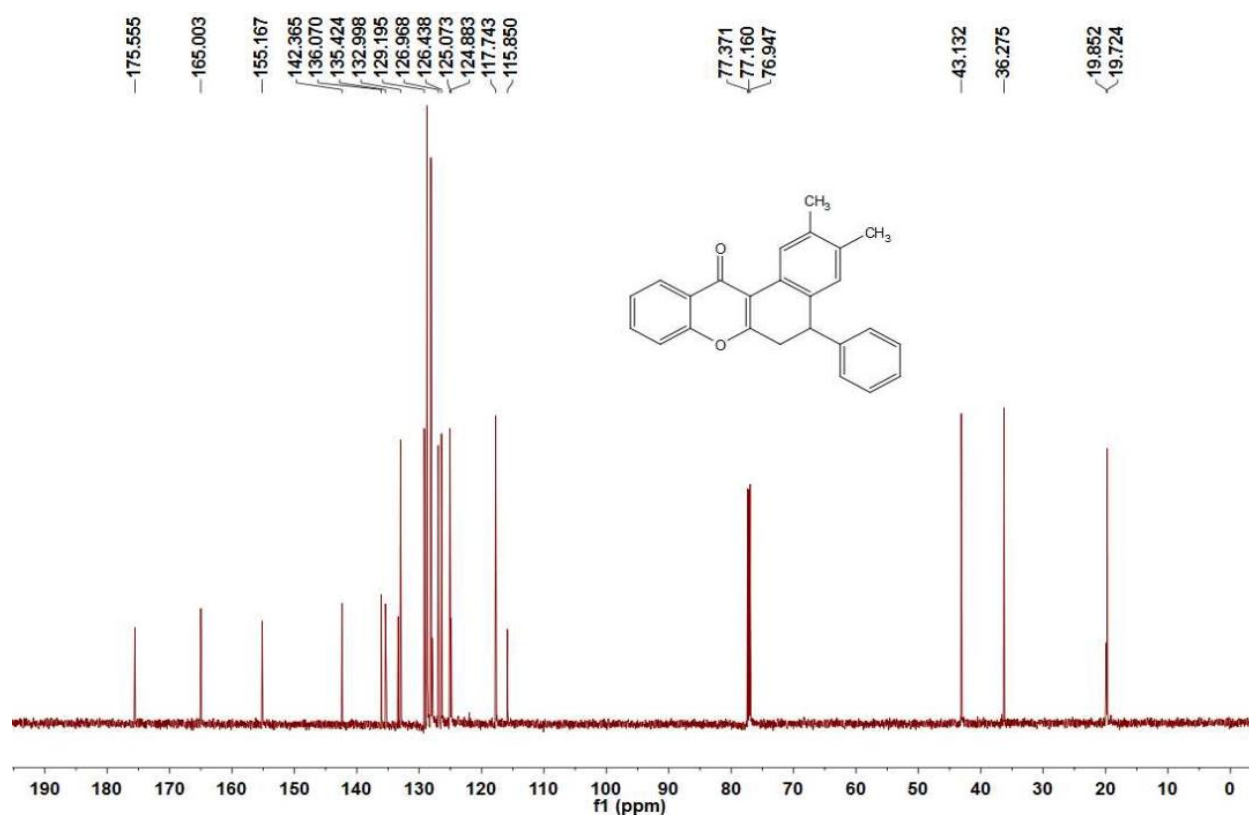
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3b**



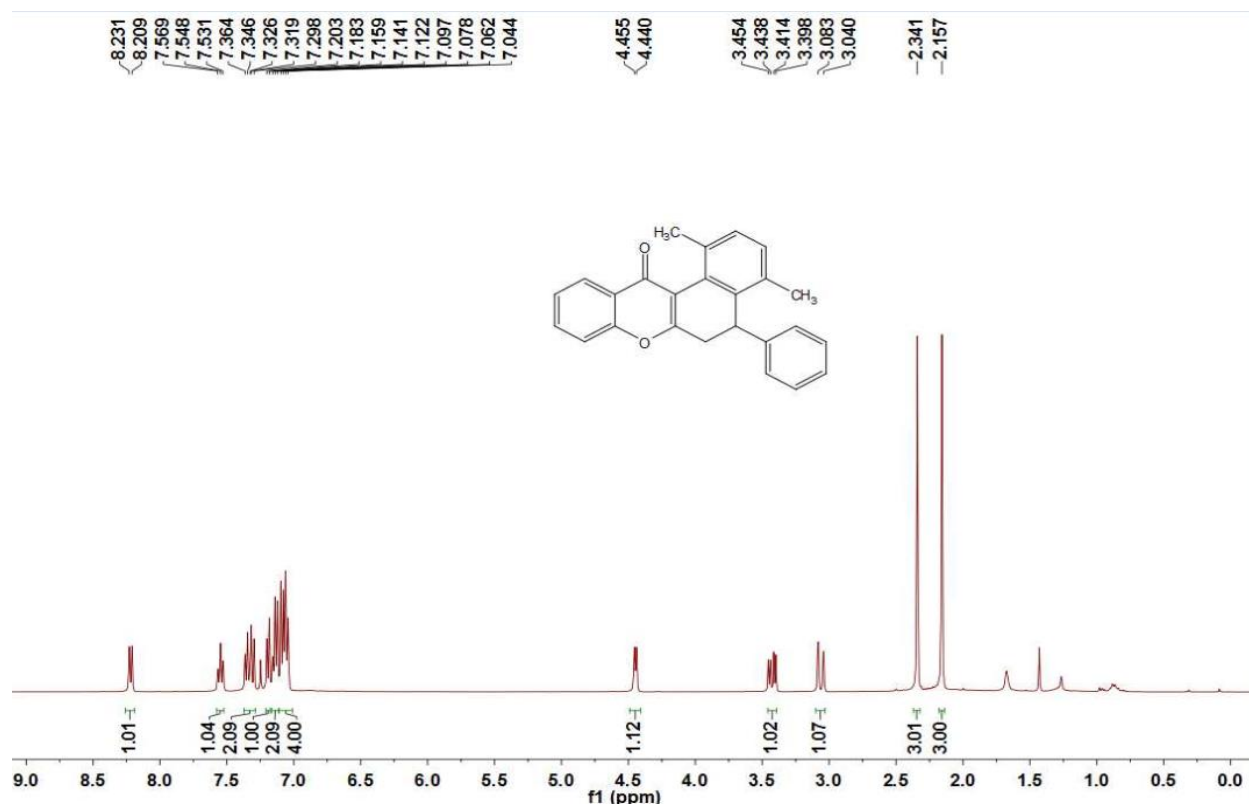
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3c**



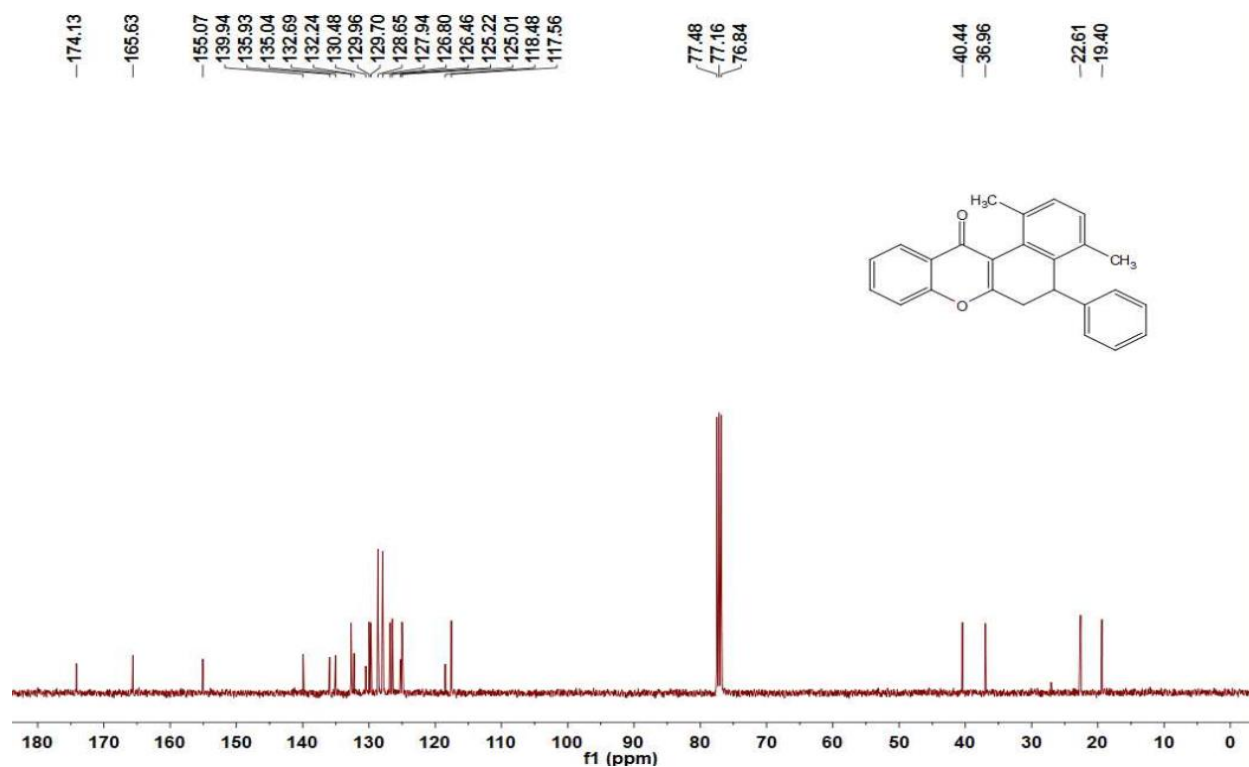
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3c**



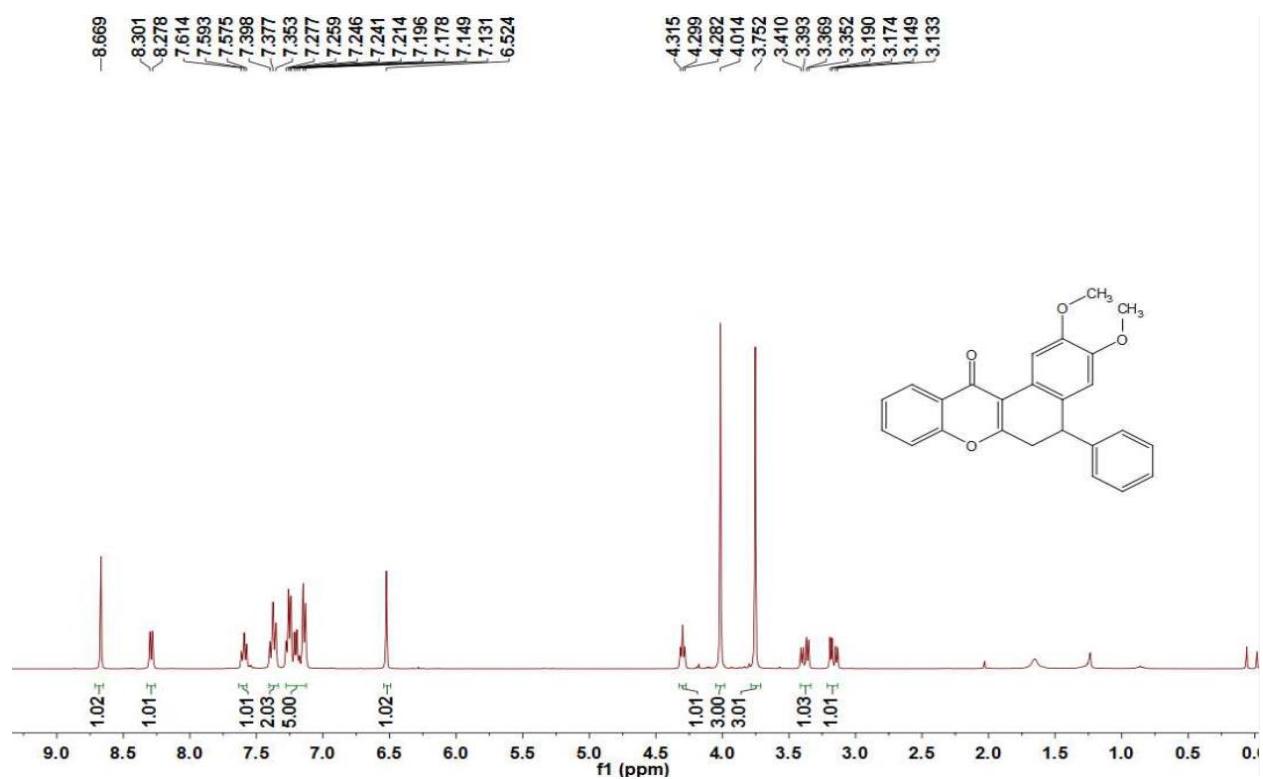
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3d**



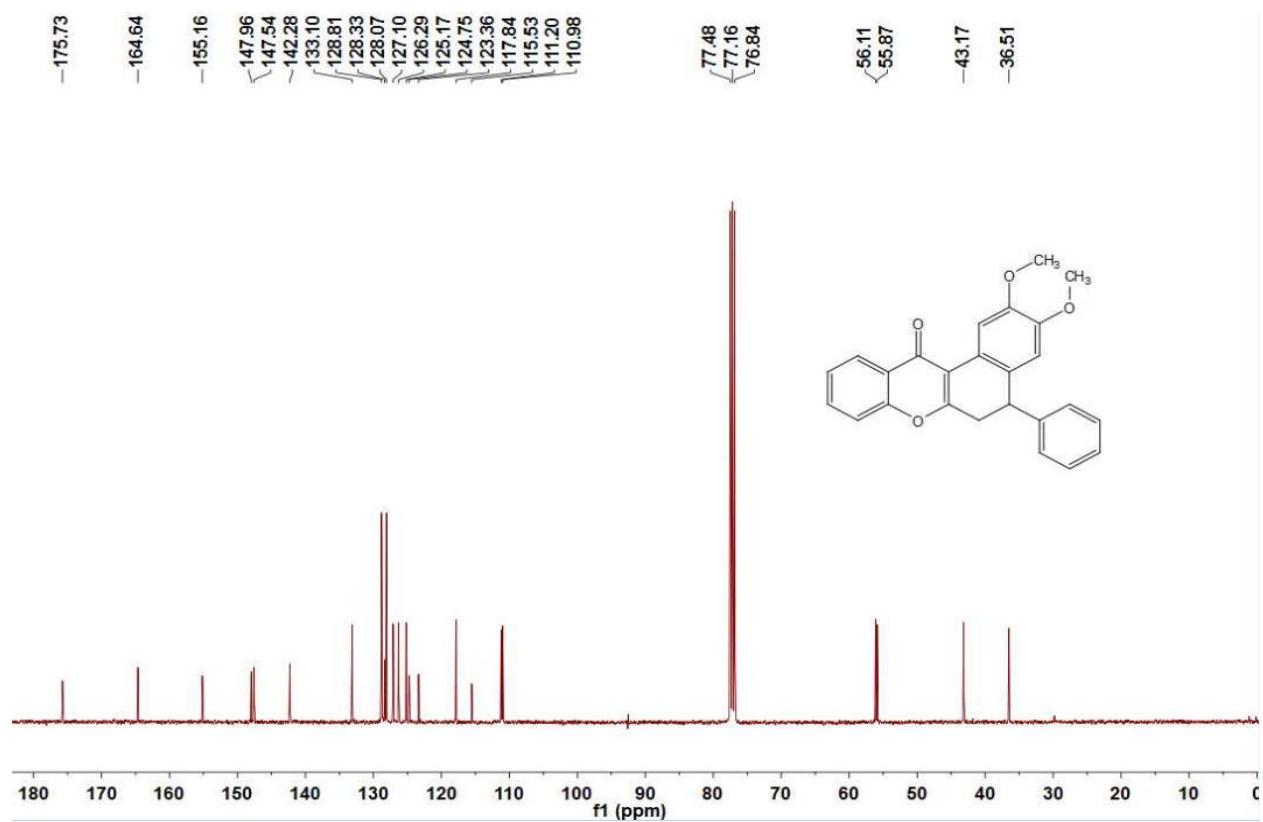
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3d**



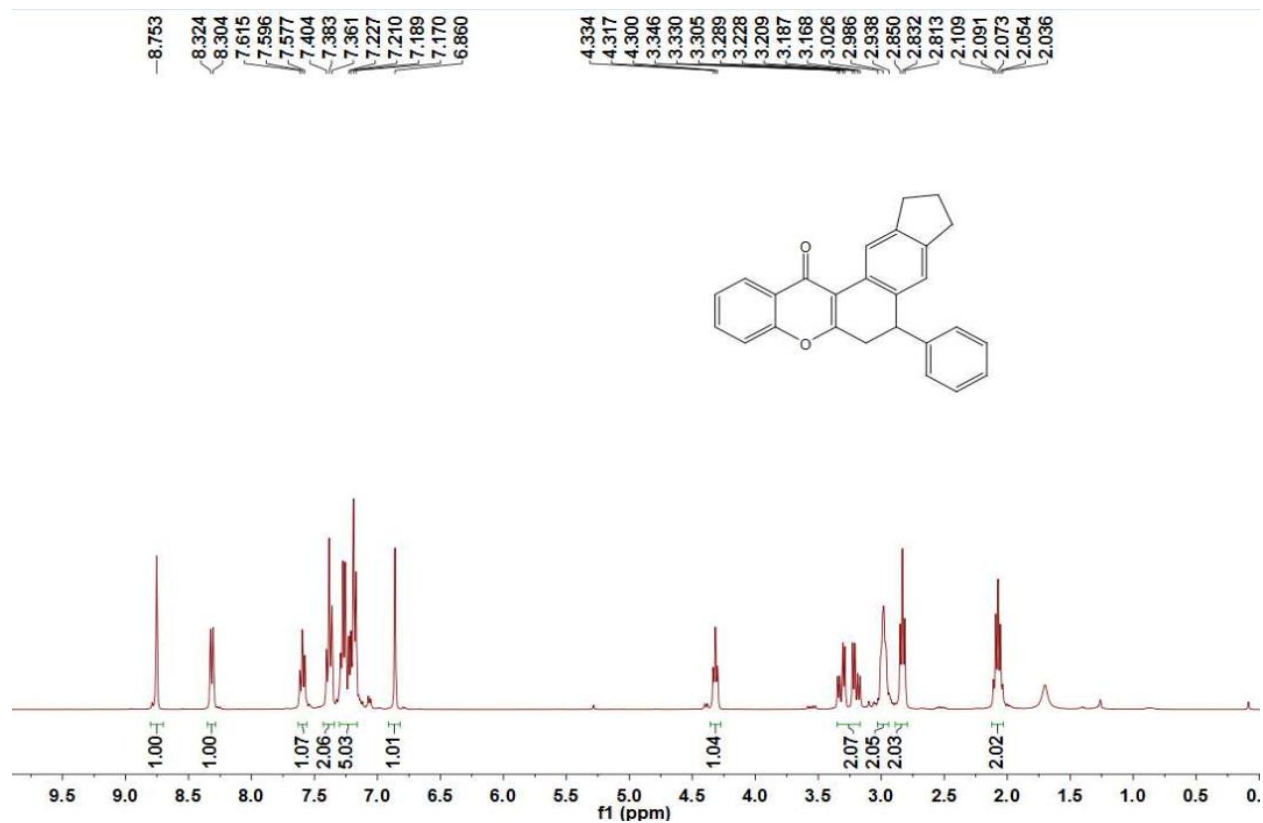
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3e**



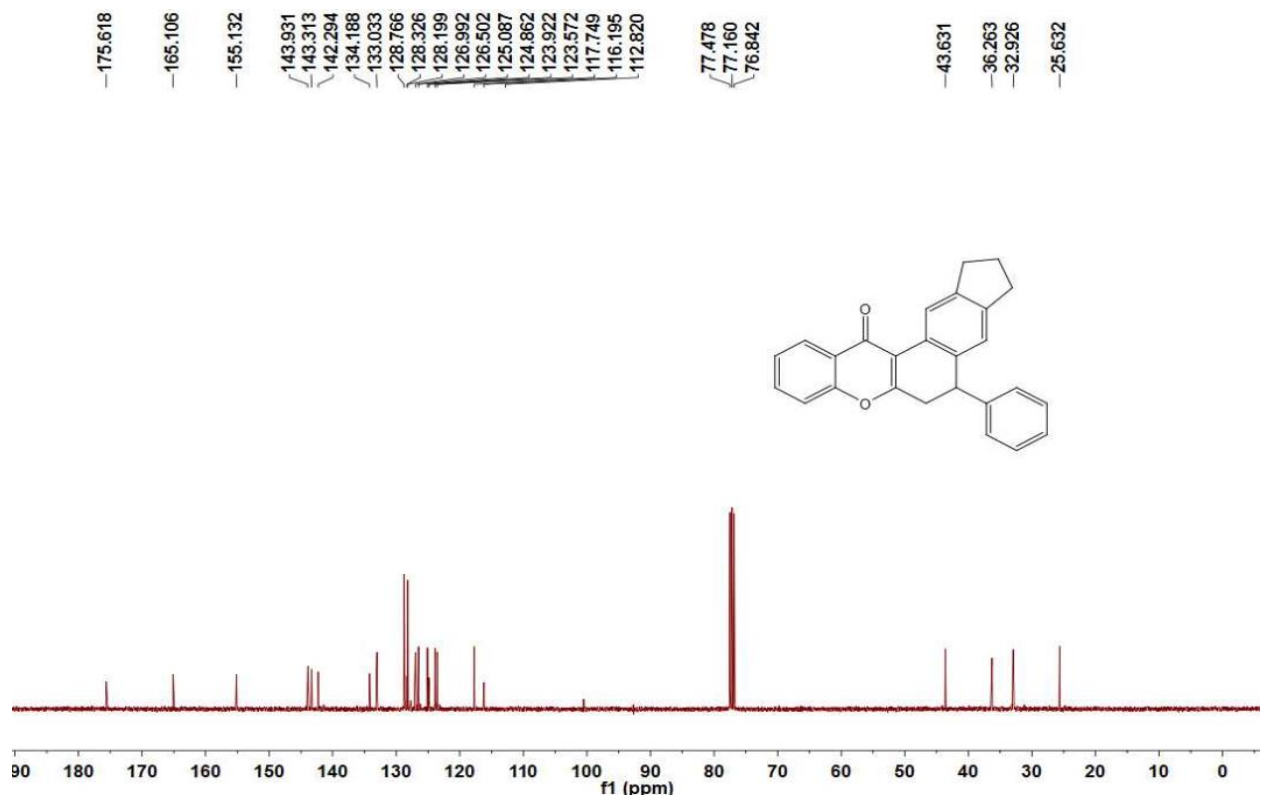
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3e**



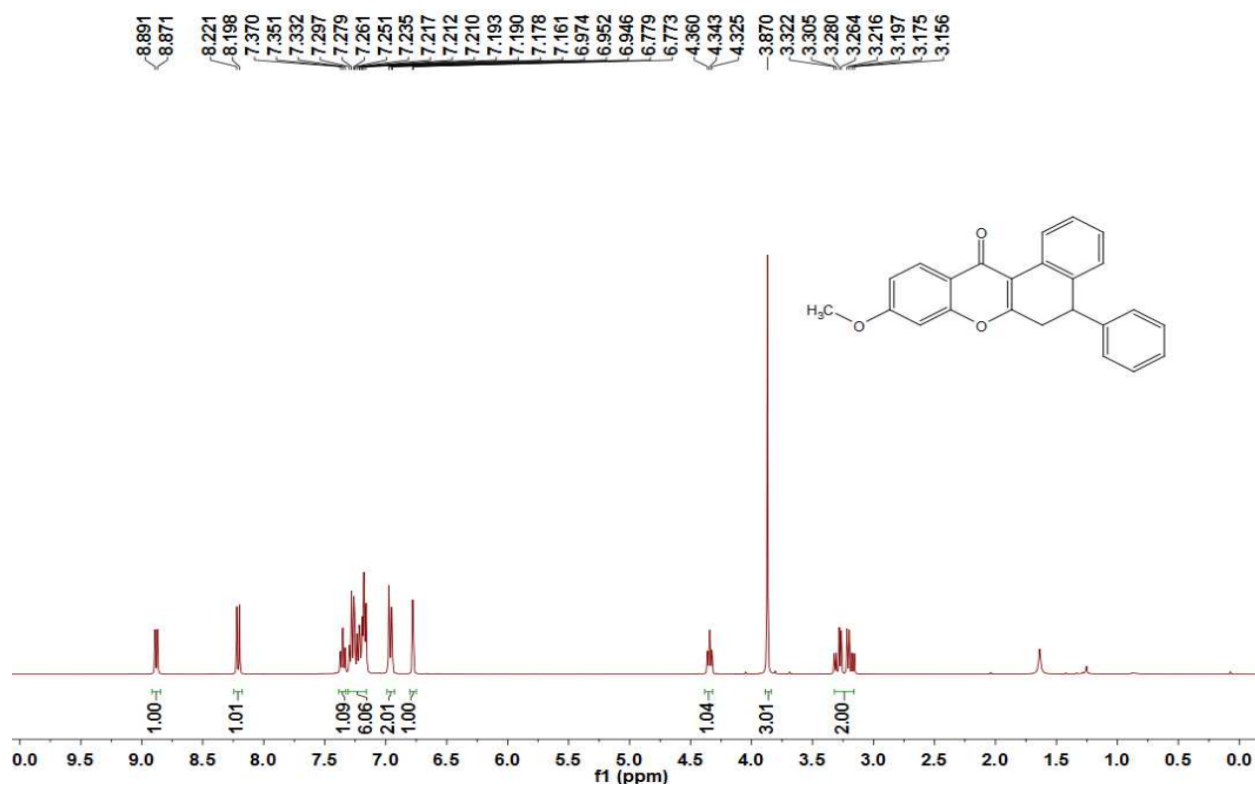
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3f**



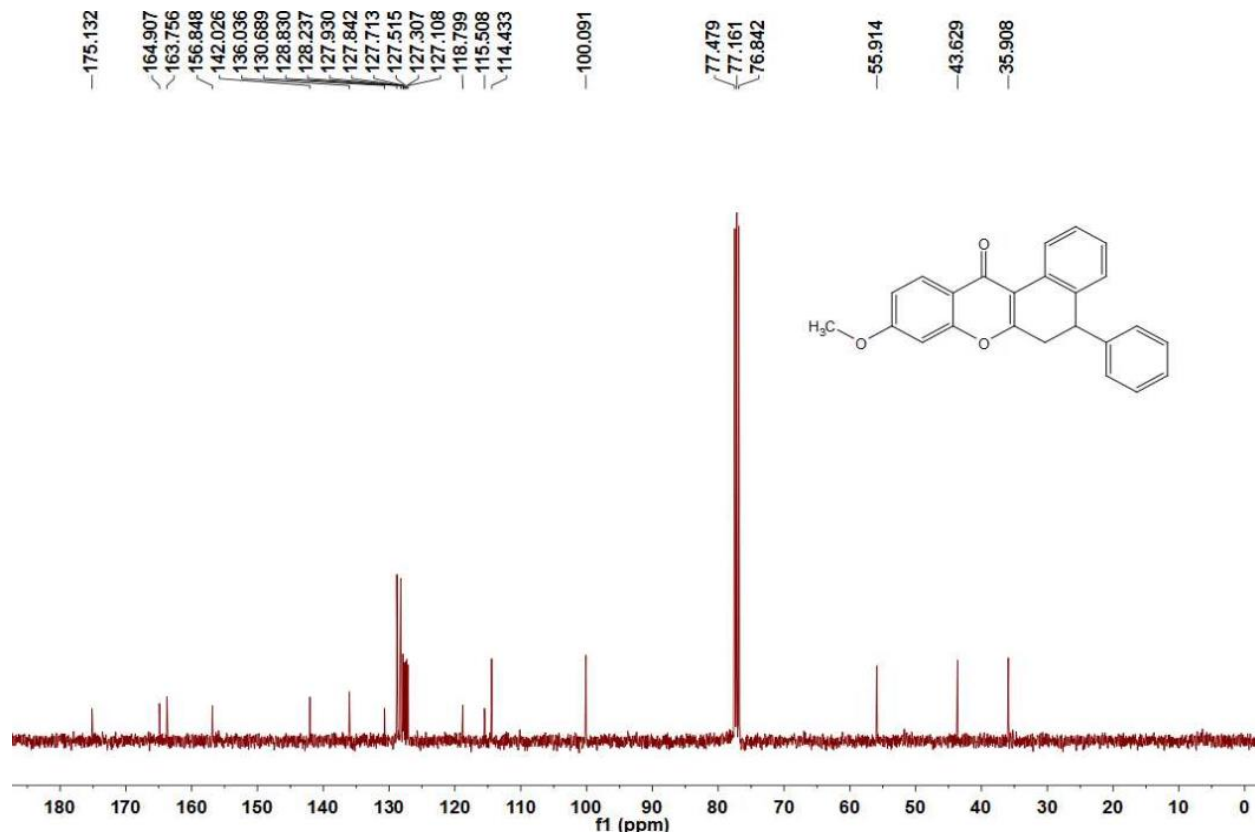
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3f**



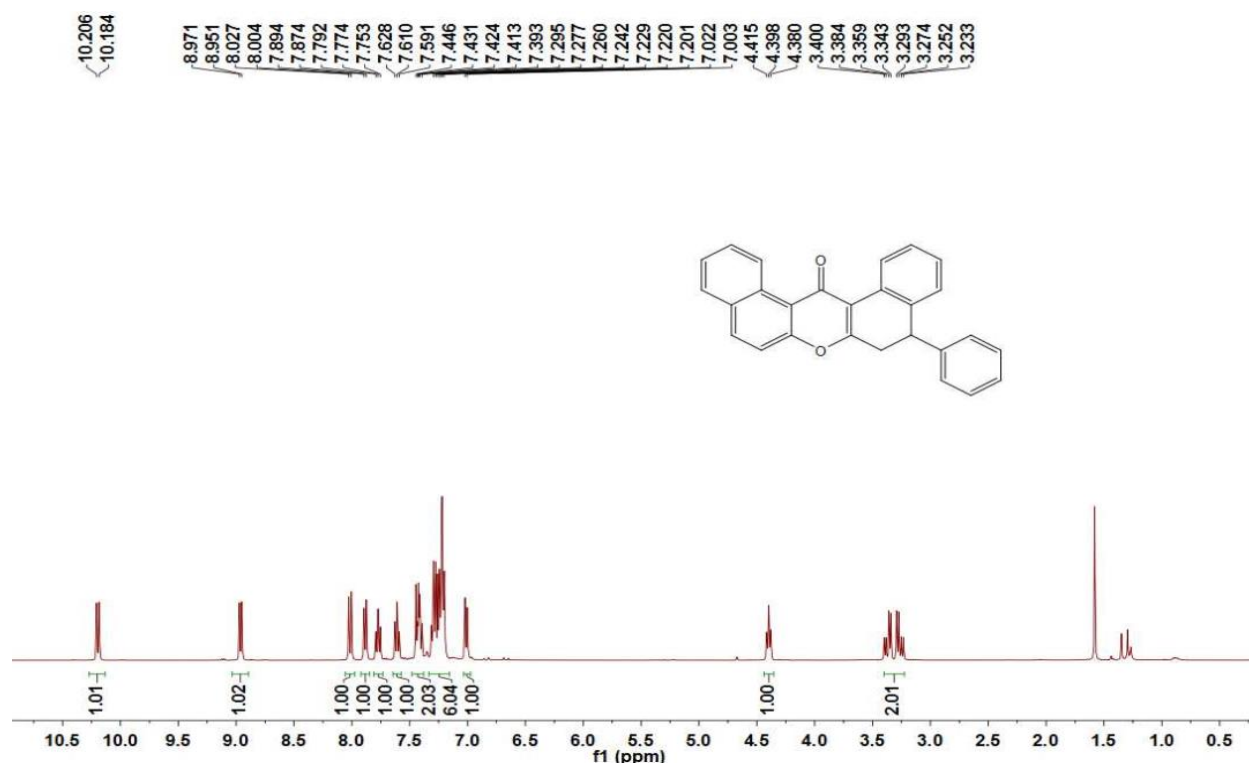
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3g**



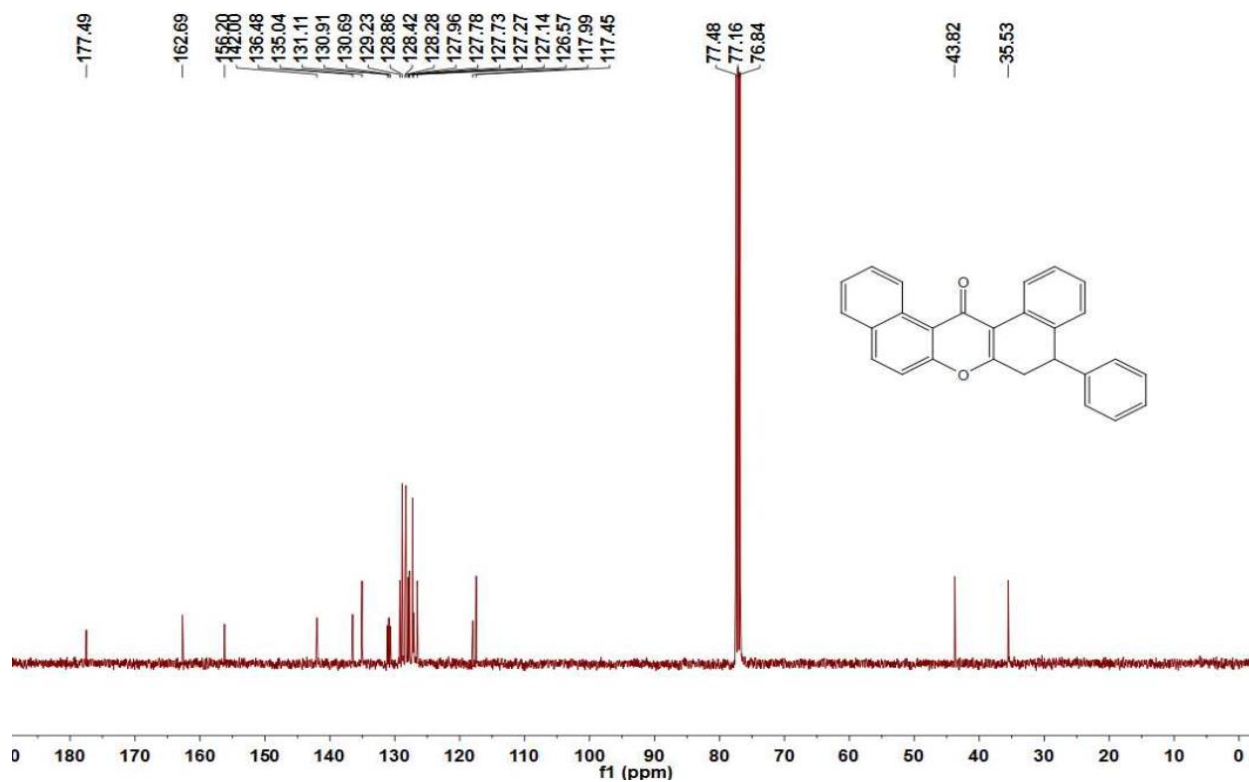
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3g**



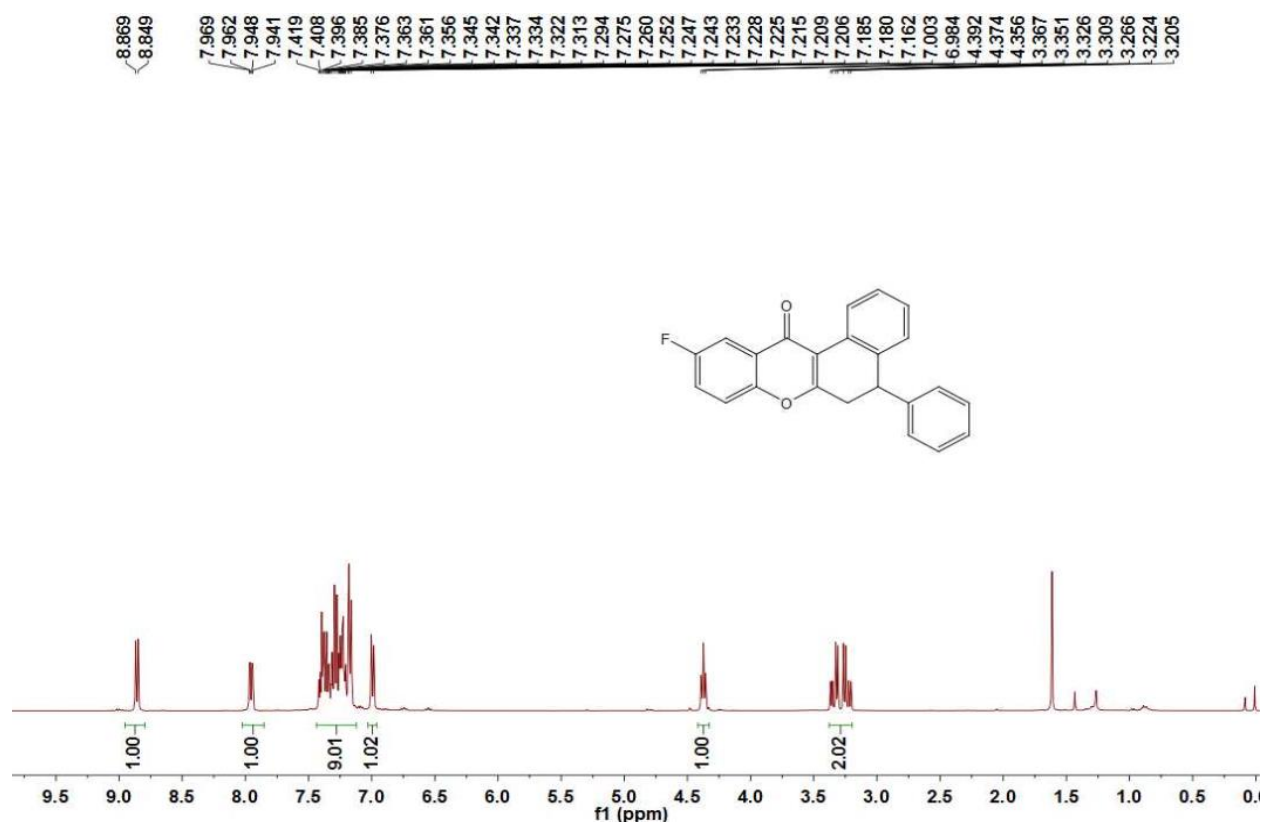
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3h**



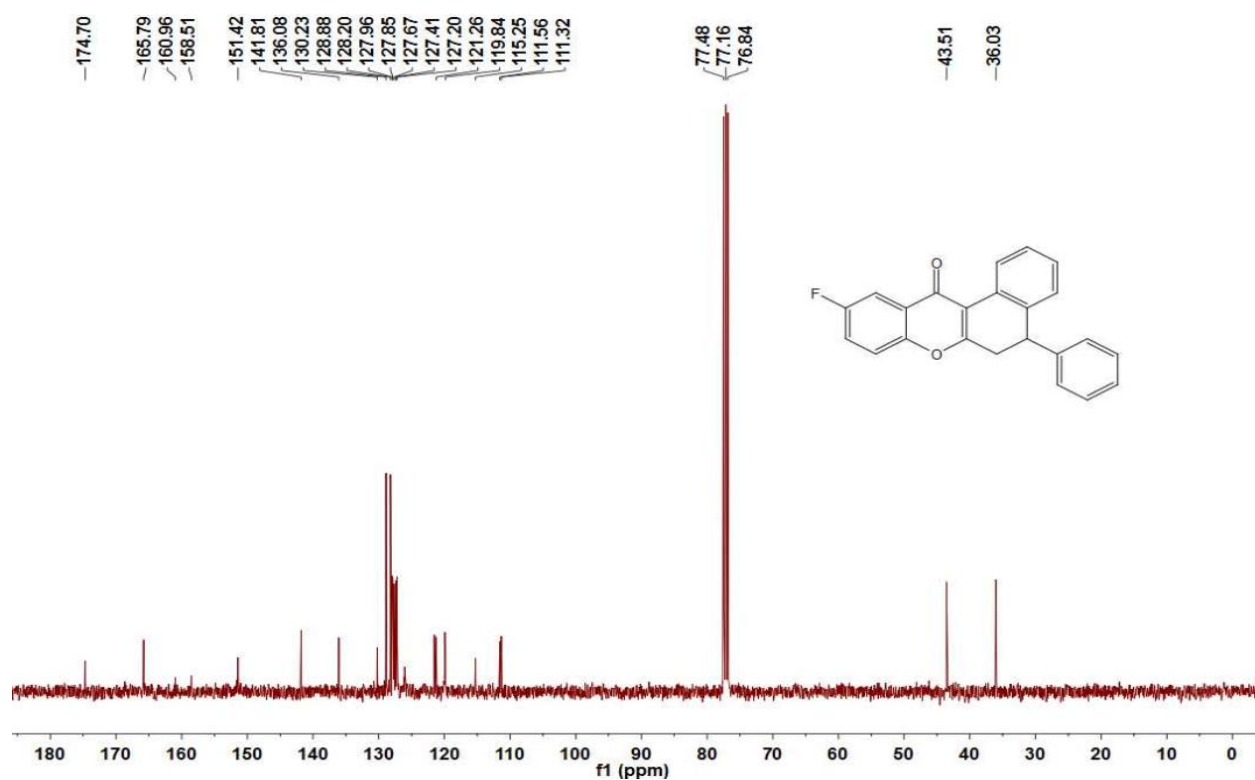
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3h**



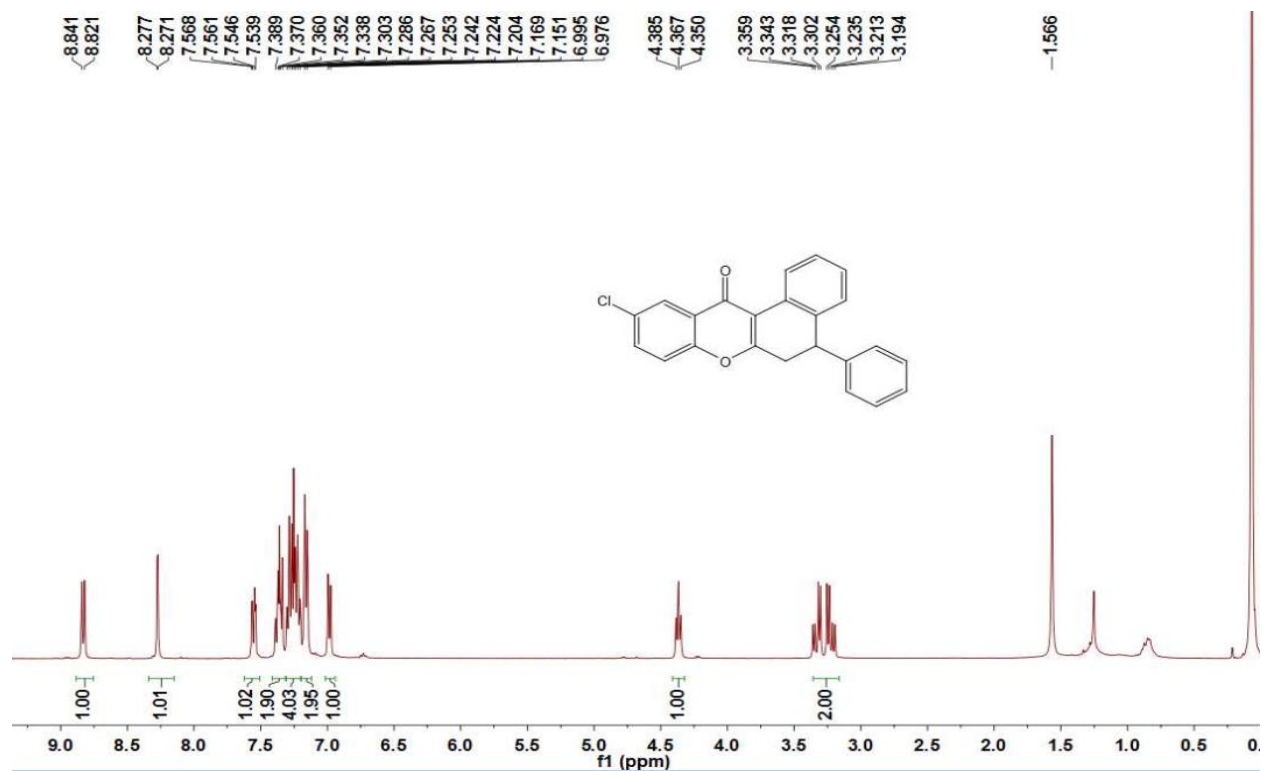
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3i**



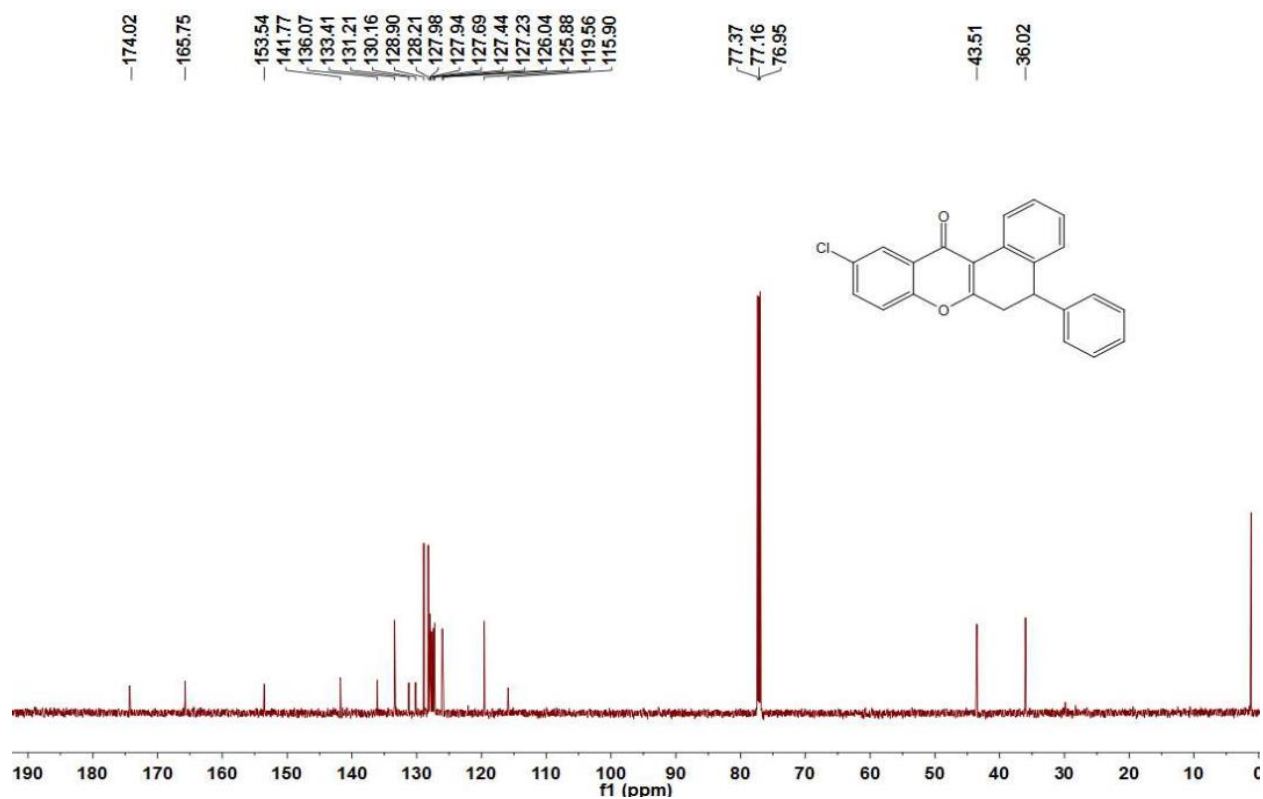
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3i**



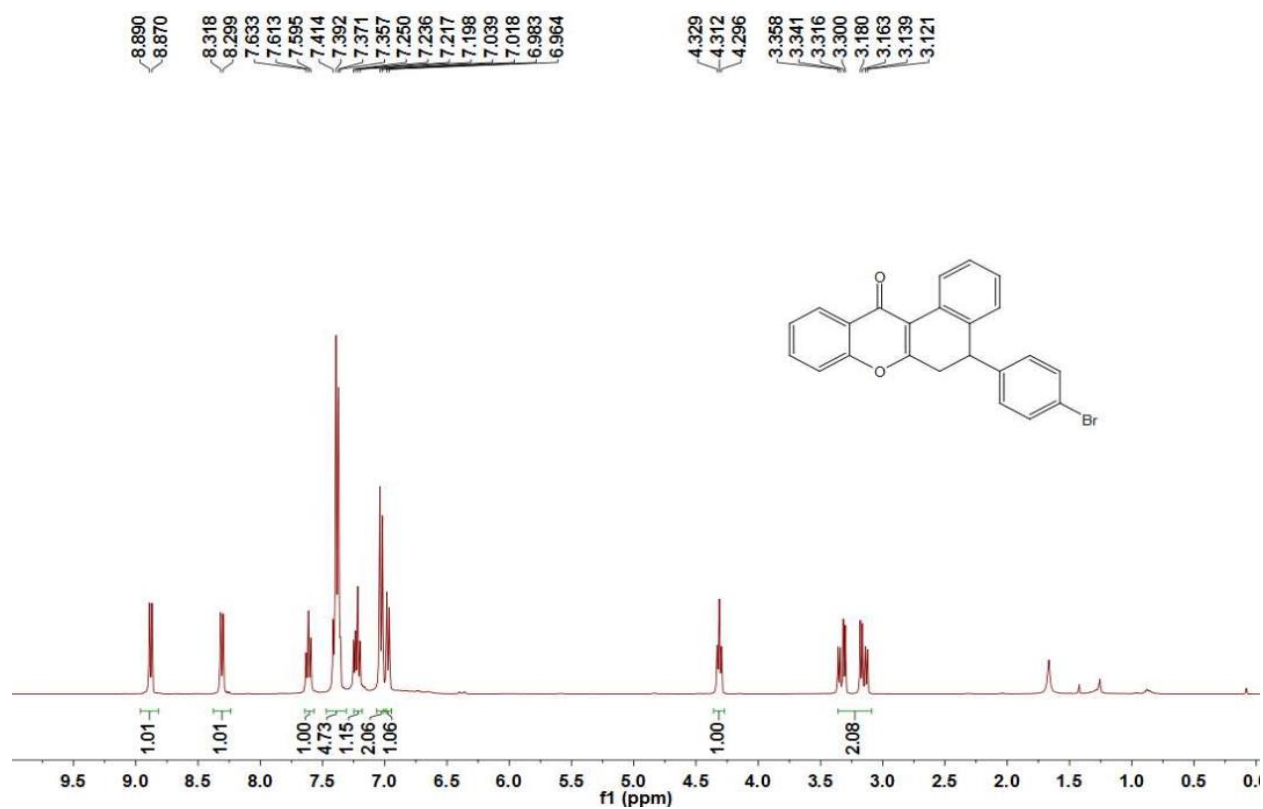
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3j**



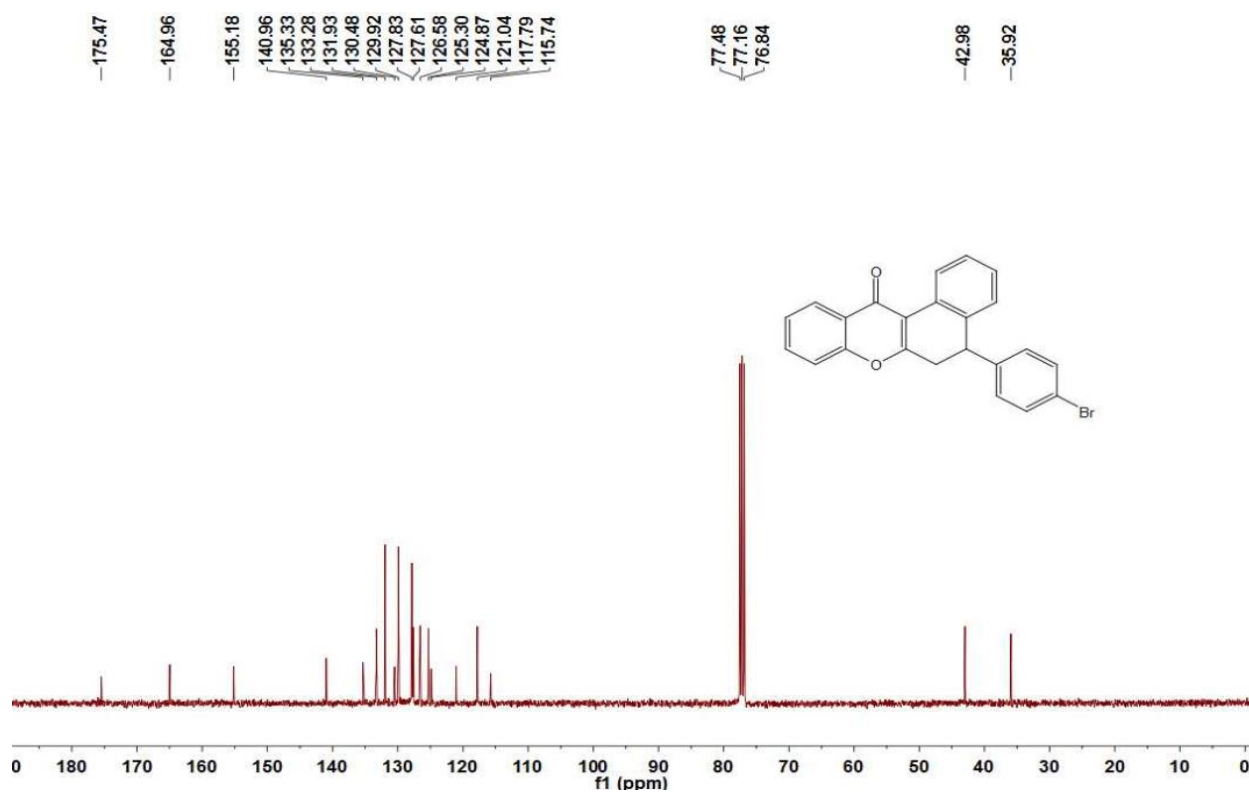
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3j**



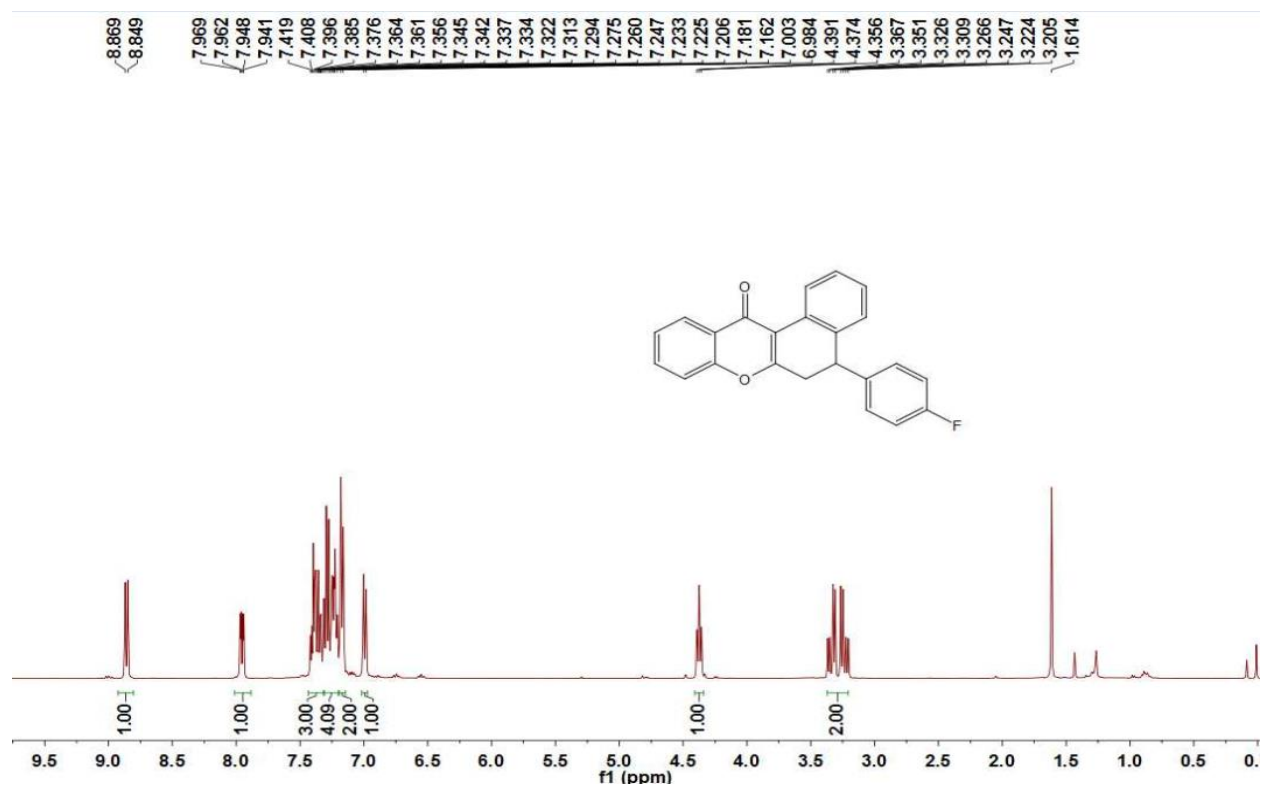
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3k**



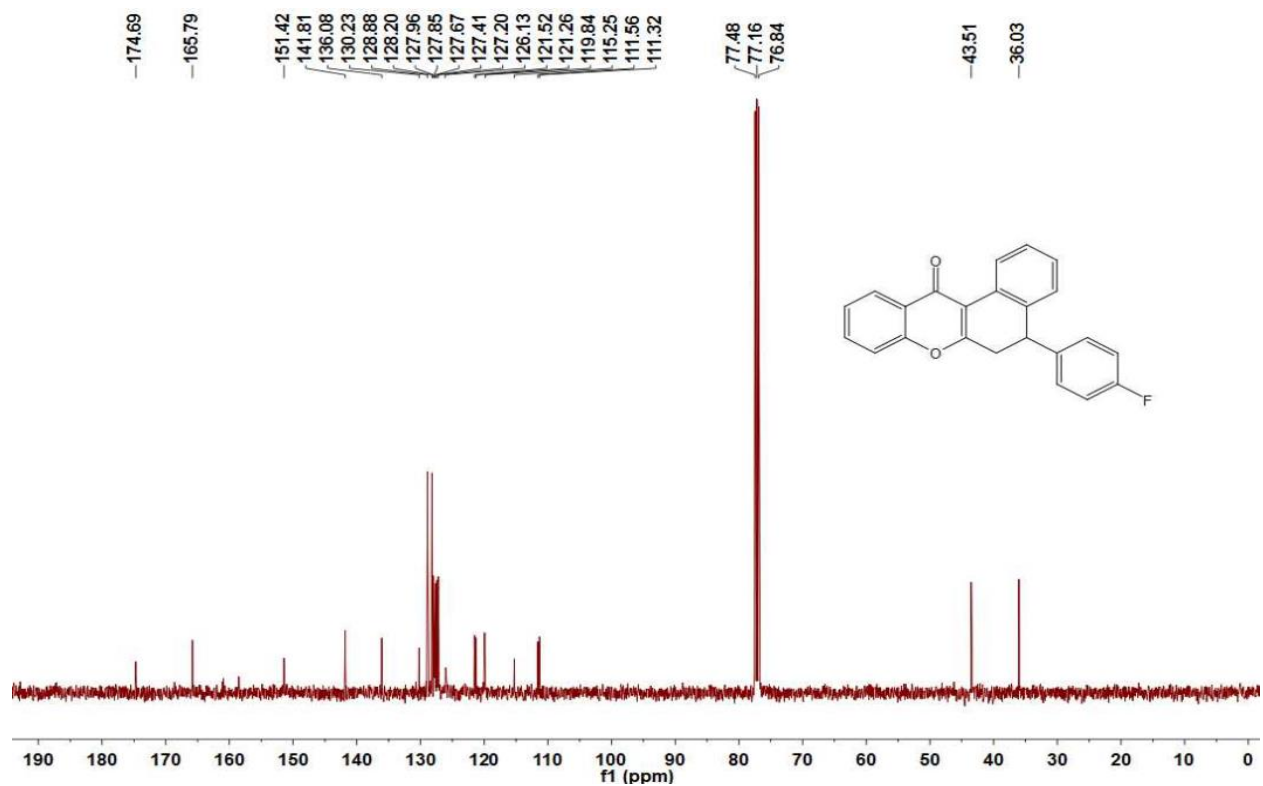
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3k**



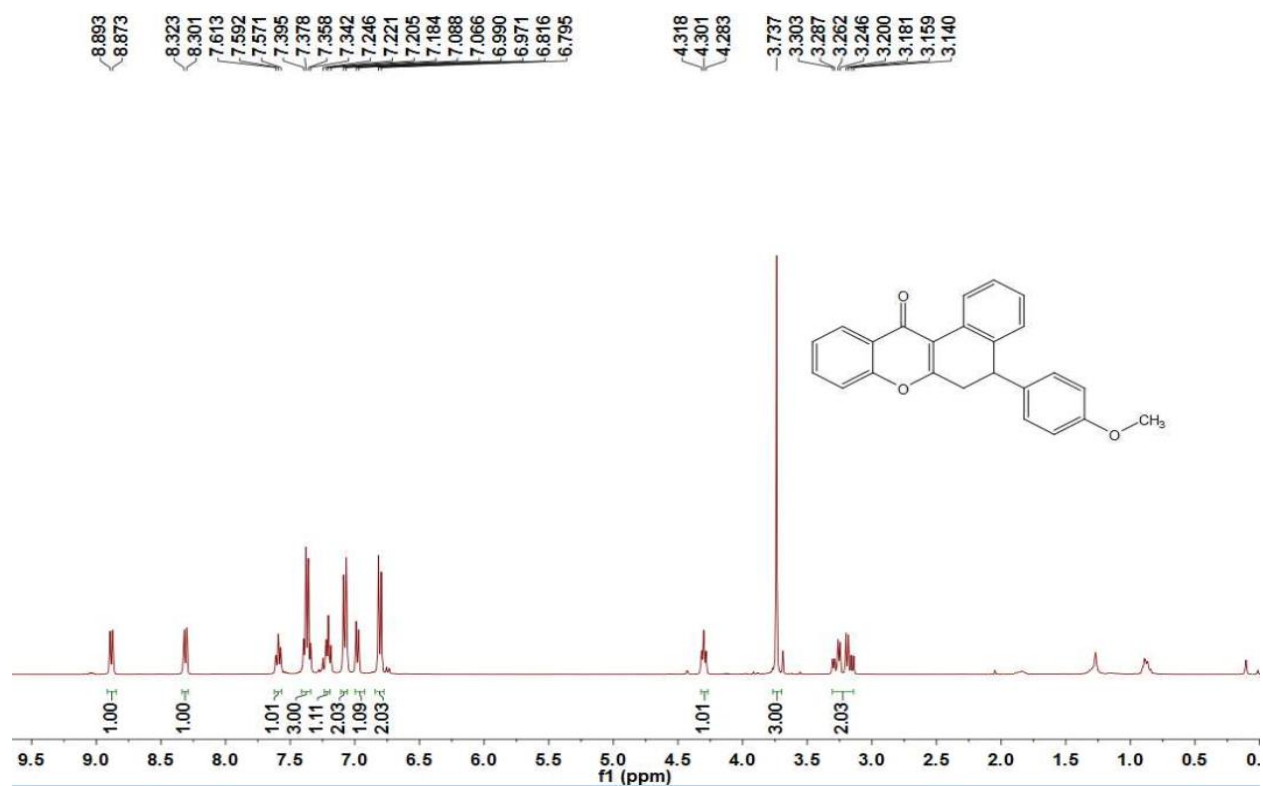
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3l**



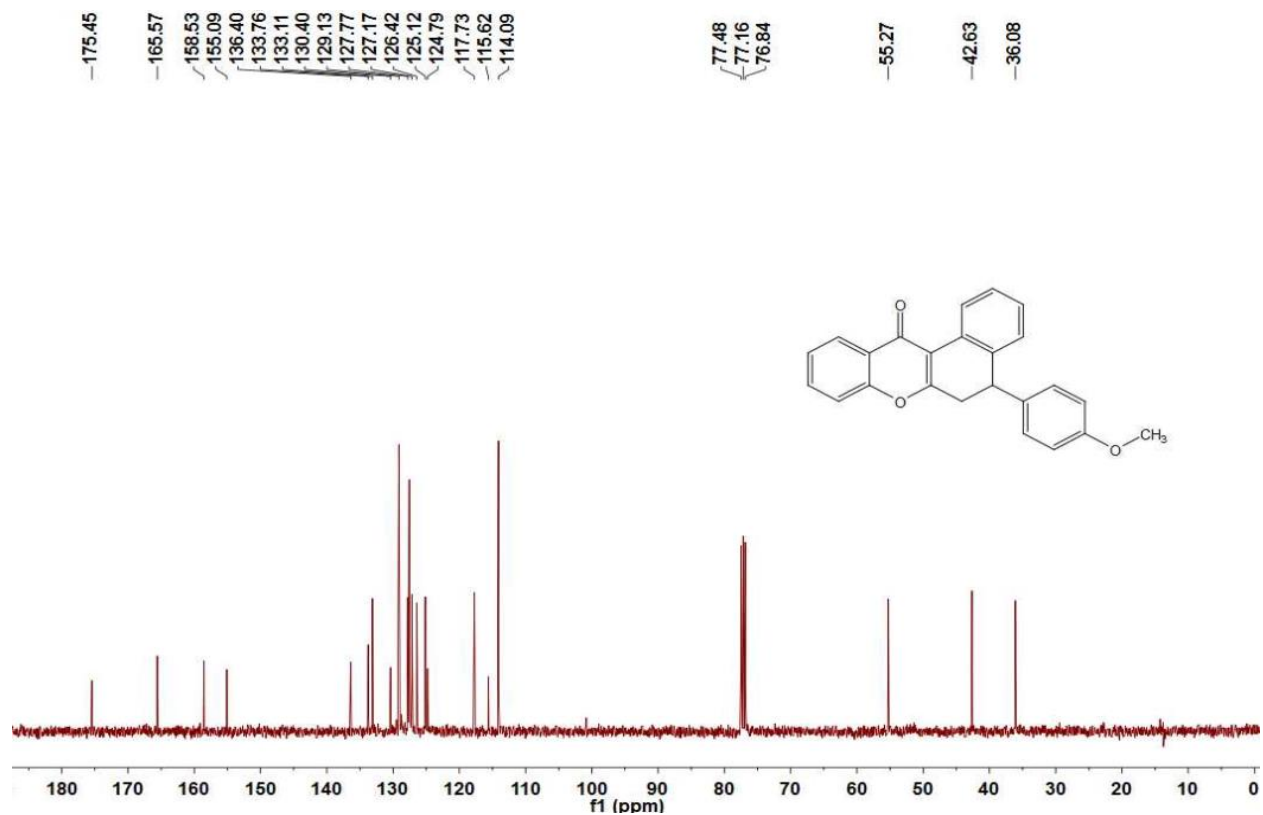
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3l**



^1H NMR spectrum (400 MHz, CDCl_3) of compound **3m**



^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3m**



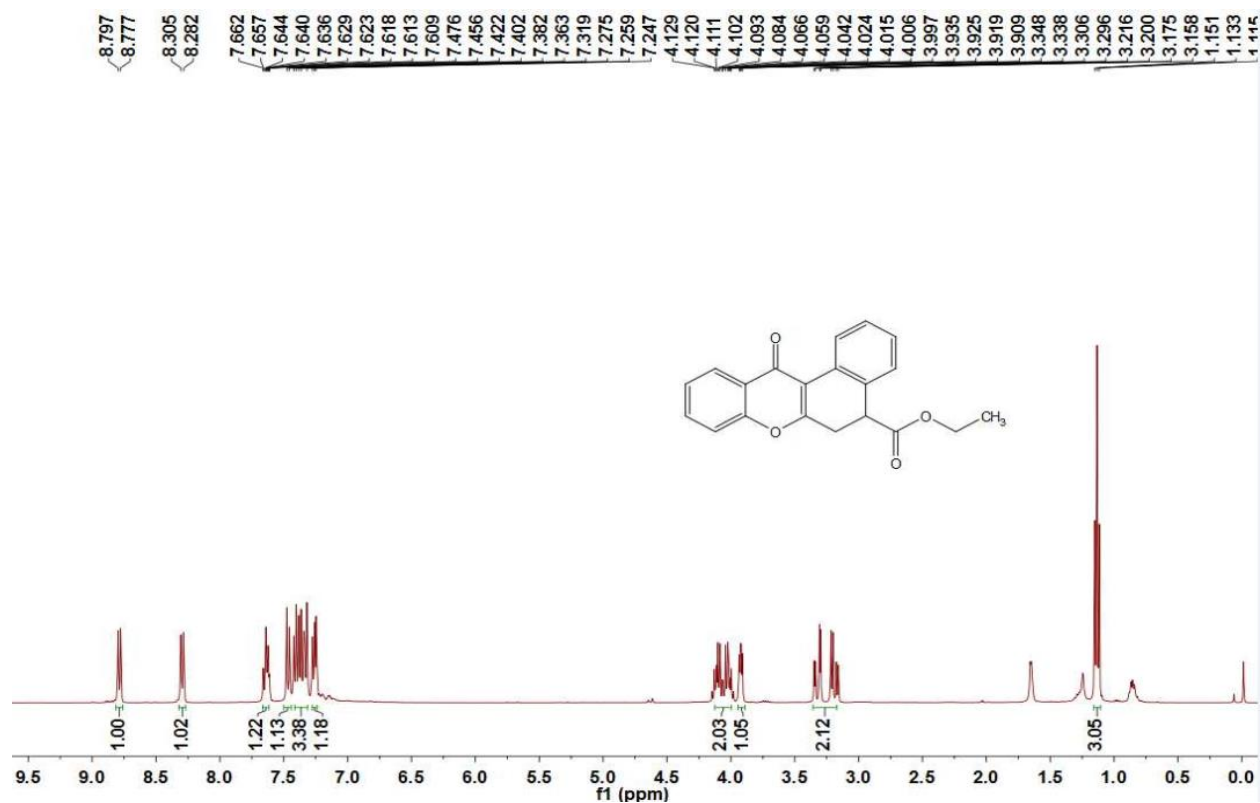
Chemical structure: c1ccc2c(c1)oc(=O)c3ccccc32CCc4ccsc4

¹H NMR spectrum (CDCl₃) data:

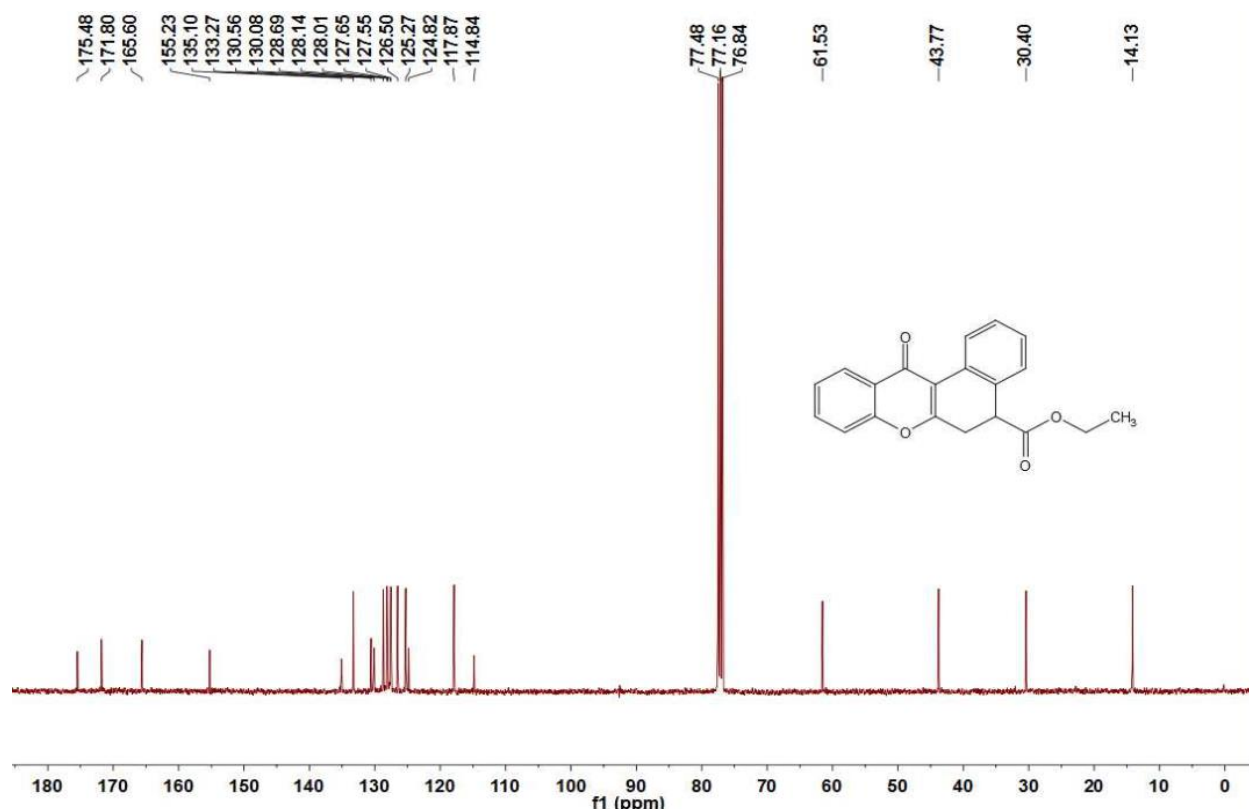
Chemical Shift (ppm)	Integration
8.856, 8.836	1.00
8.311, 8.291	1.01
7.636, 7.618, 7.597	1.06
7.413, 7.394, 7.381	3.01
7.374, 7.362, 7.343	2.03
7.249, 7.231, 7.213	1.03
7.099, 7.081	1.02
6.960, 6.948, 6.846	1.01
4.419, 4.403, 4.387	1.02
3.354, 3.338, 3.313, 3.297, 3.233, 3.217, 3.191, 3.175	1.03, 1.00
1.691	-

Chemical structure of 2-(2-(thiophen-2-yl)ethyl)-2H-chromene-3-carbonyl (10) is shown. The ¹³C NMR spectrum (CDCl₃) displays peaks at 175.512, 165.418, 155.157, 142.508, 136.026, 133.207, 129.976, 127.729, 127.616, 127.593, 127.414, 127.142, 126.521, 126.259, 125.225, 124.831, 122.117, 117.773, 115.534, 77.478, 77.161, 76.842, 39.187, and 35.314 ppm.

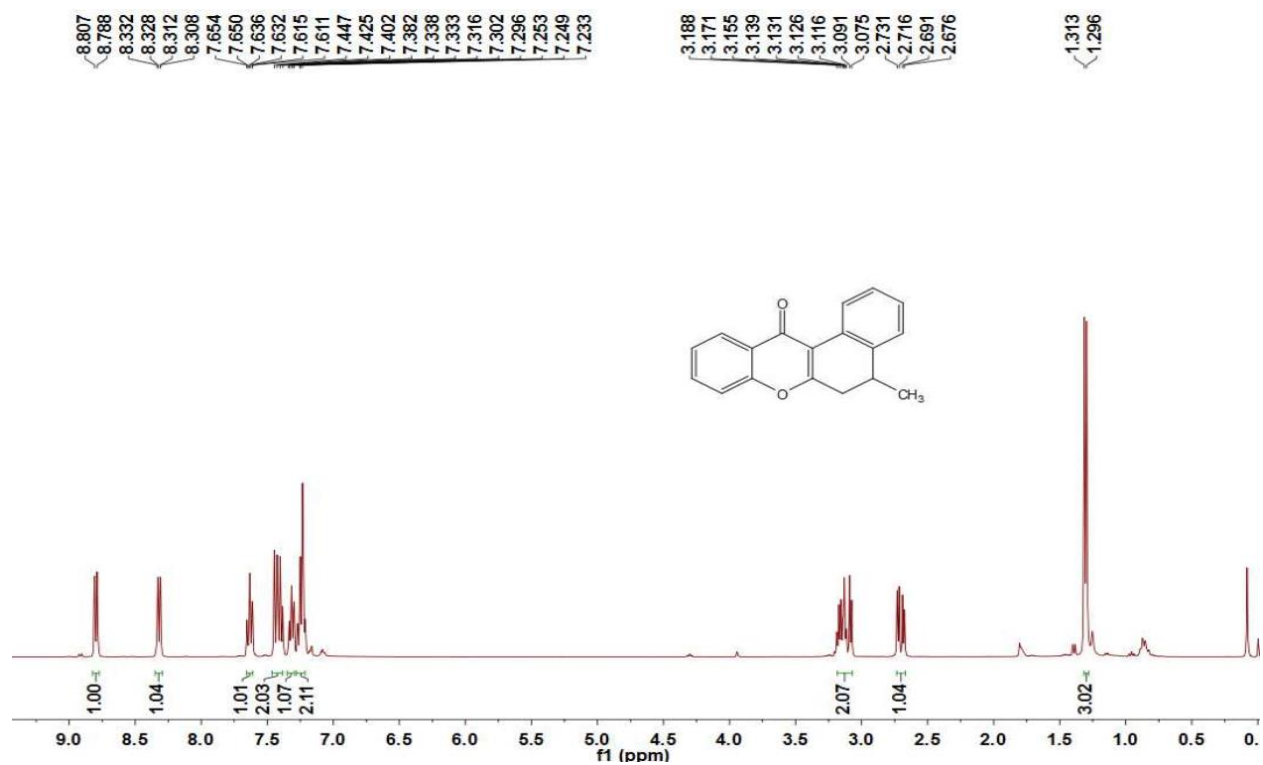
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3o**



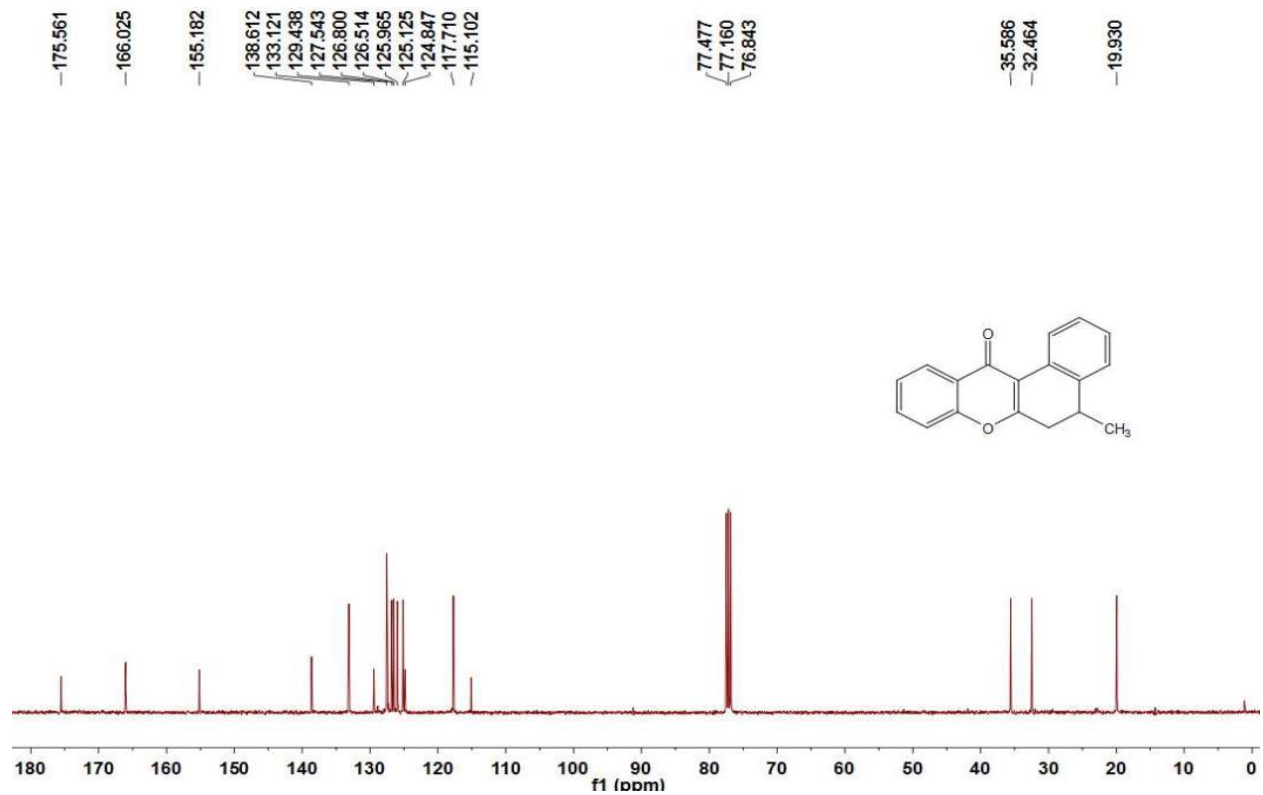
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3o**



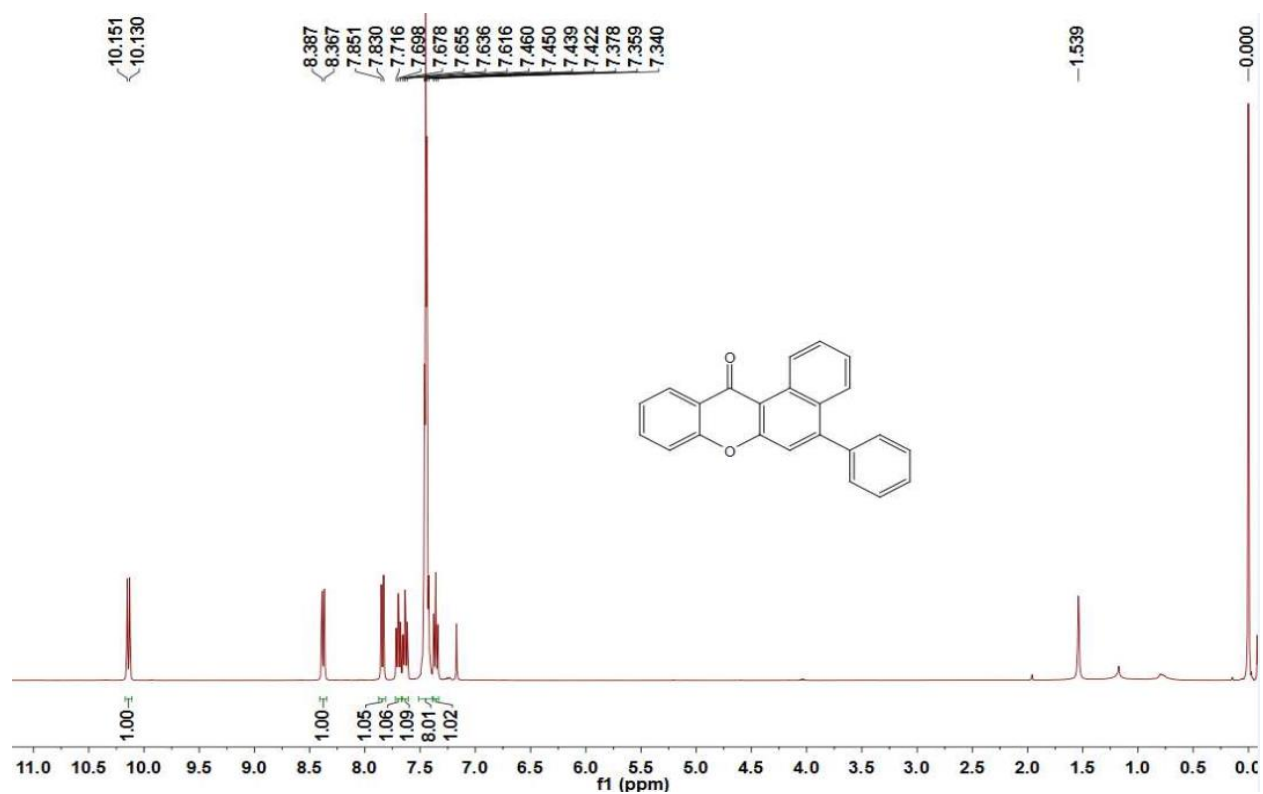
^1H NMR spectrum (400 MHz, CDCl_3) of compound **3p**



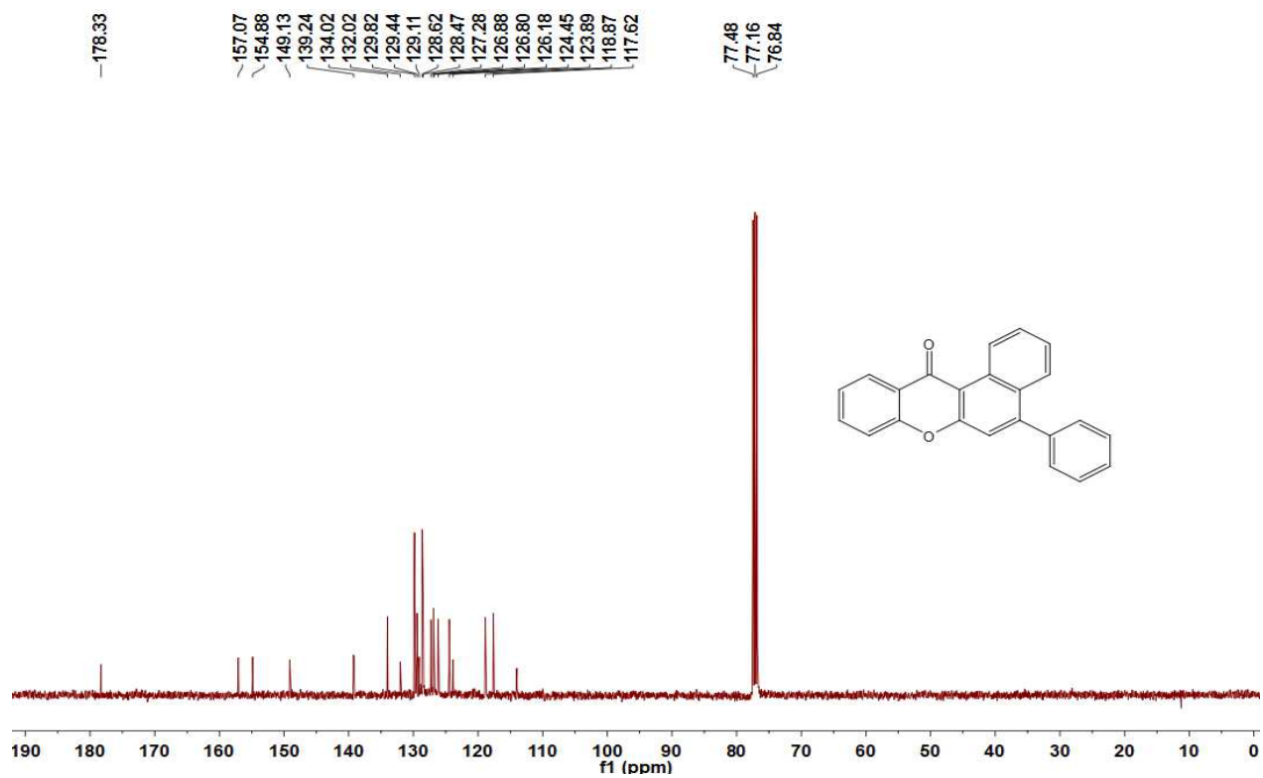
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3p**



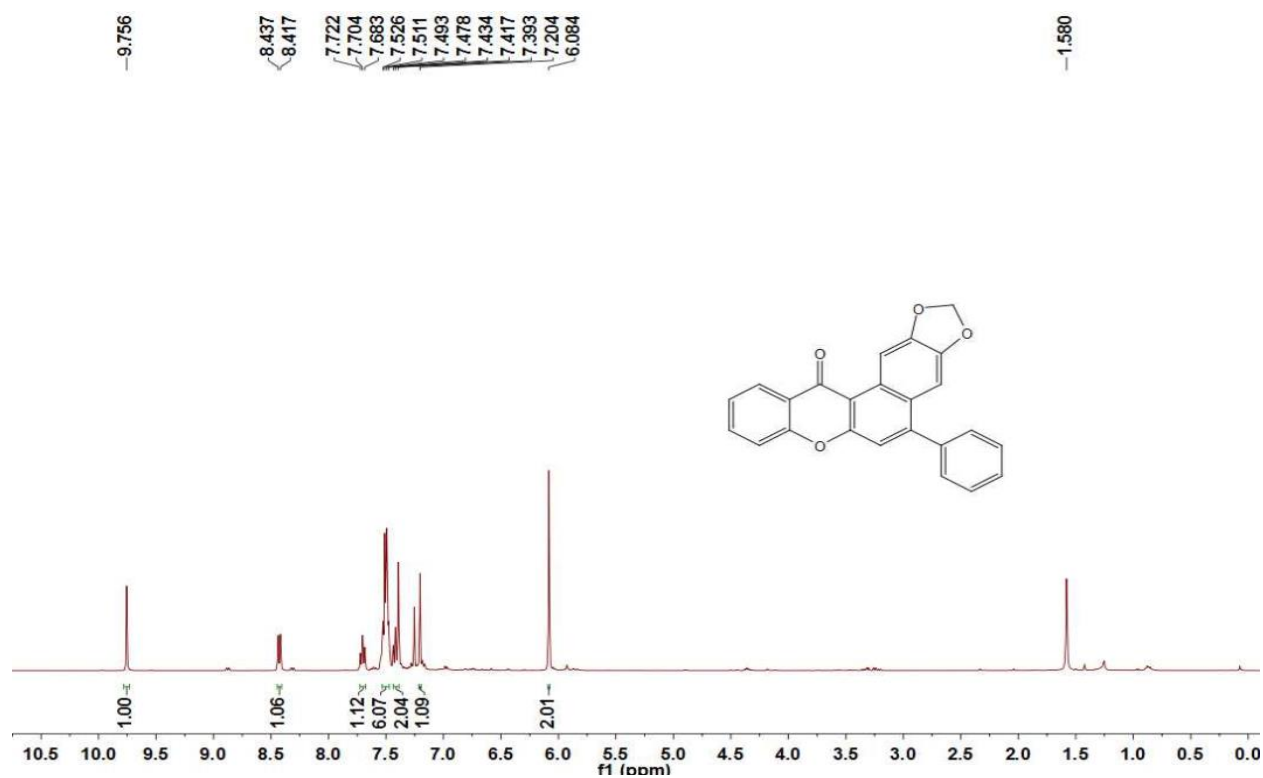
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4a**



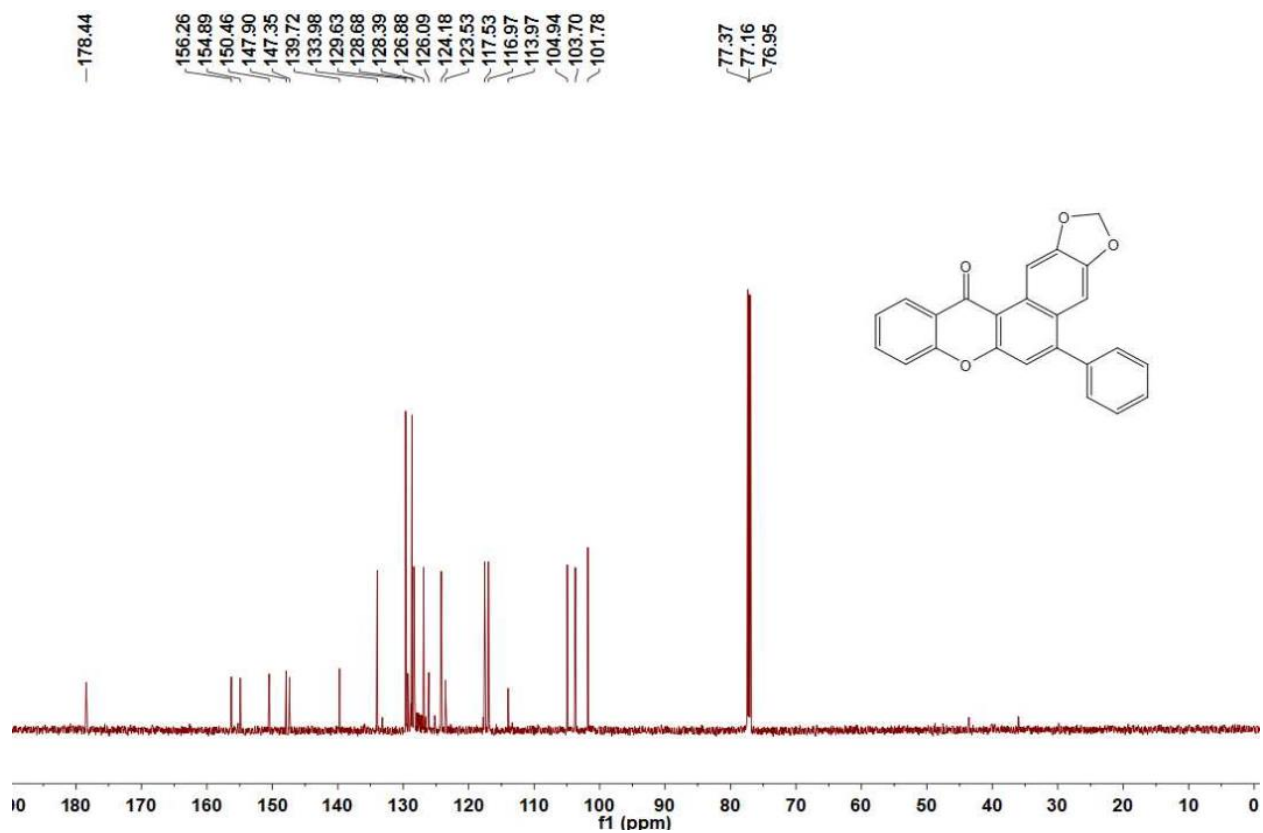
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4a**



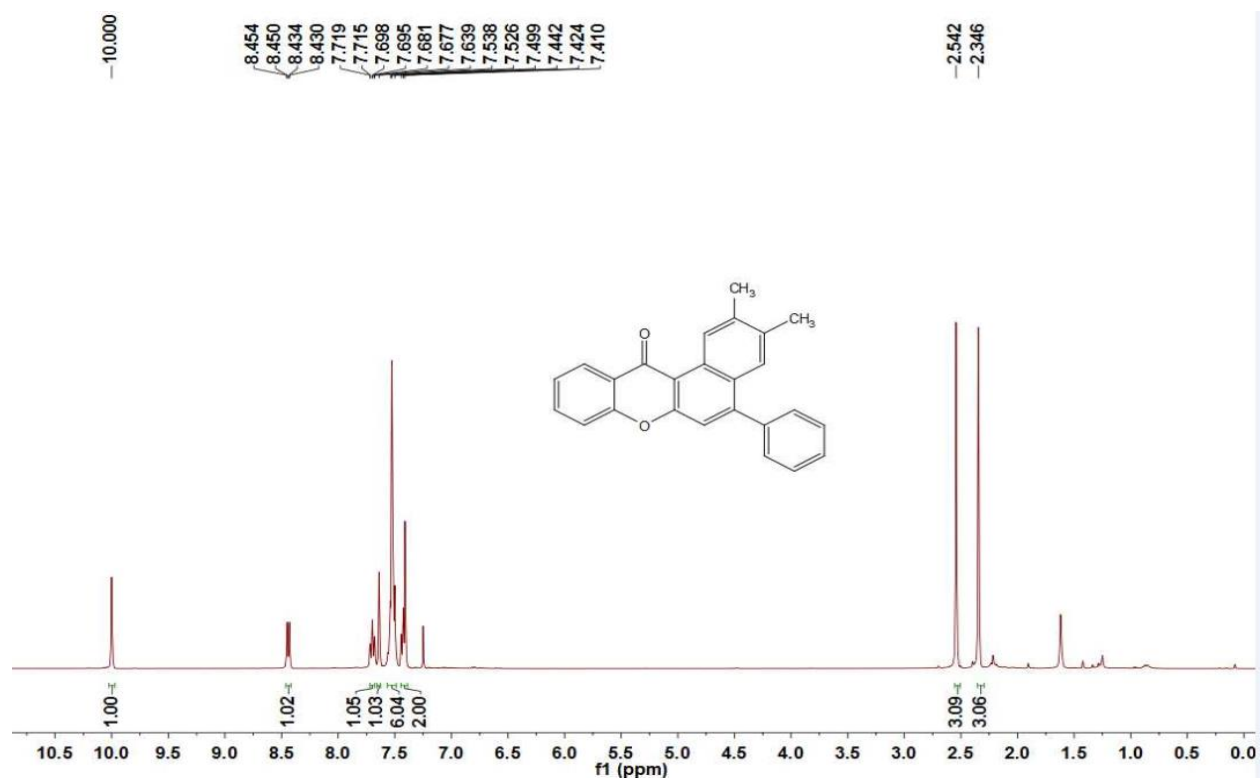
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4b**



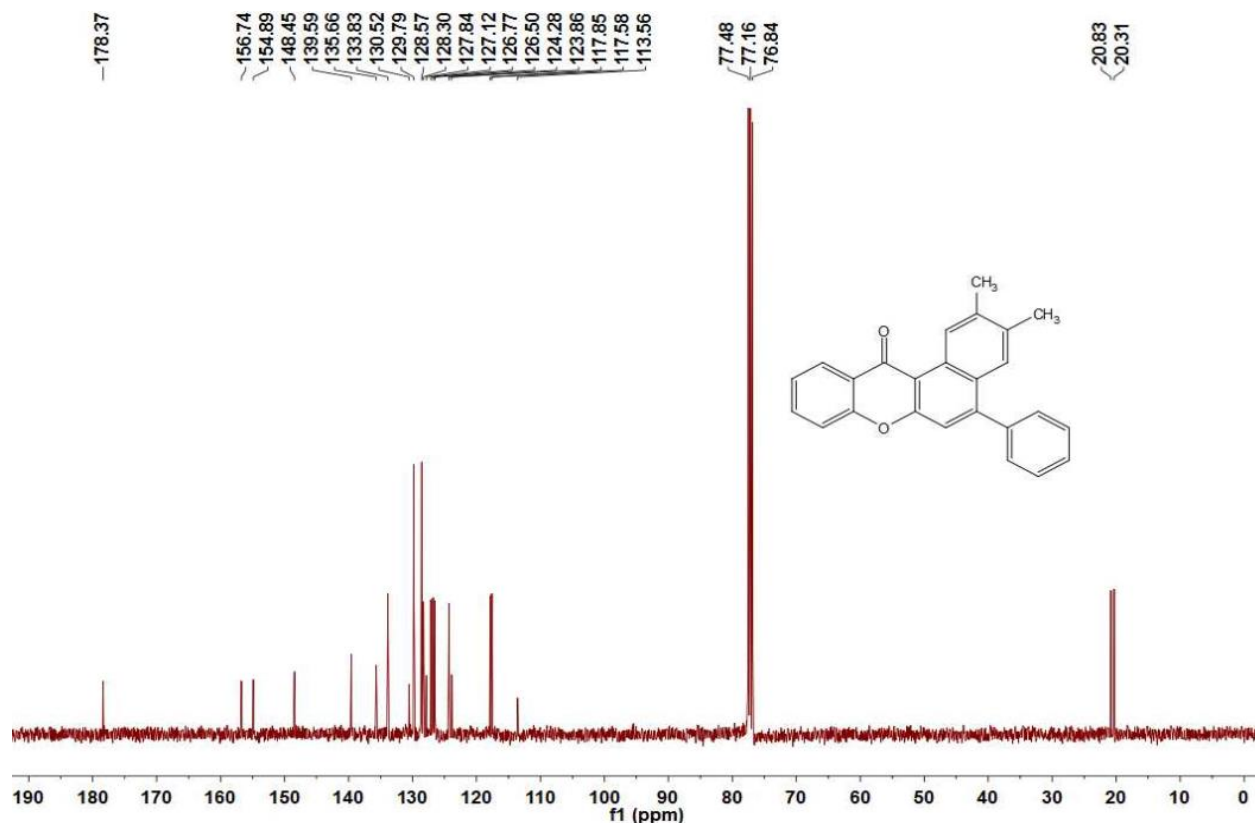
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4b**



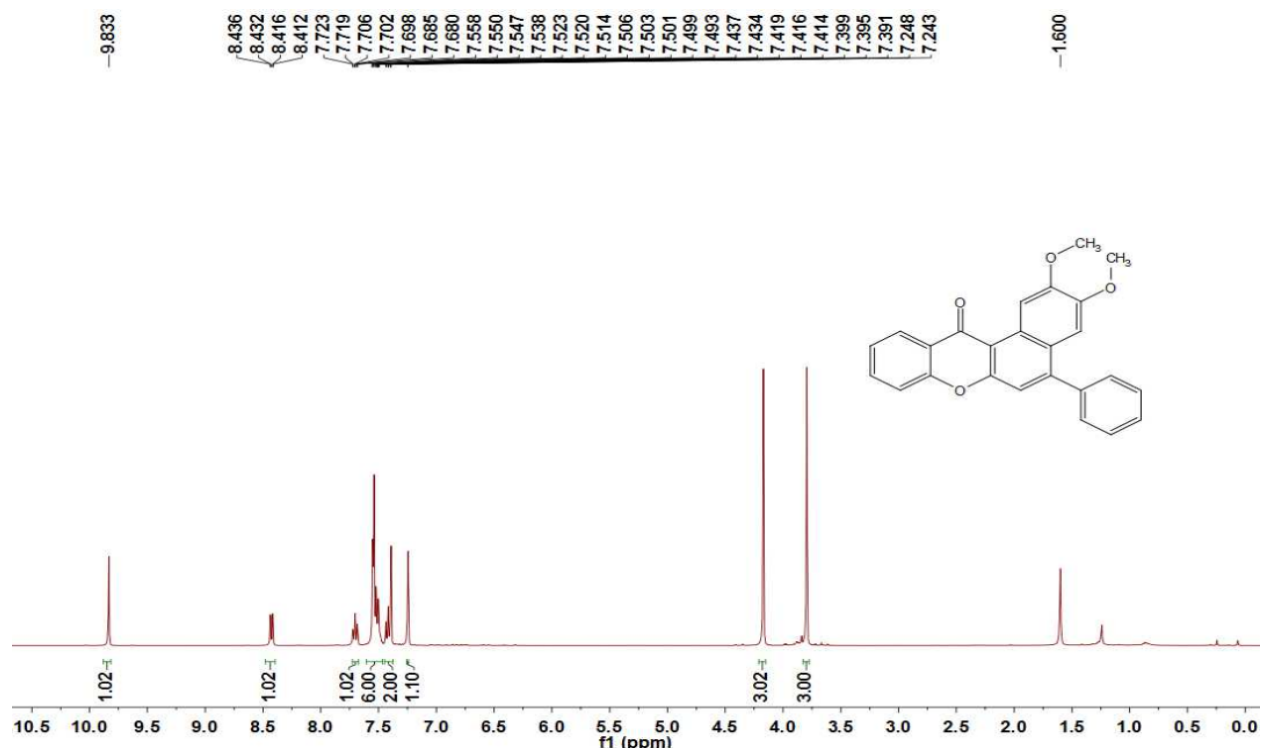
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4c**



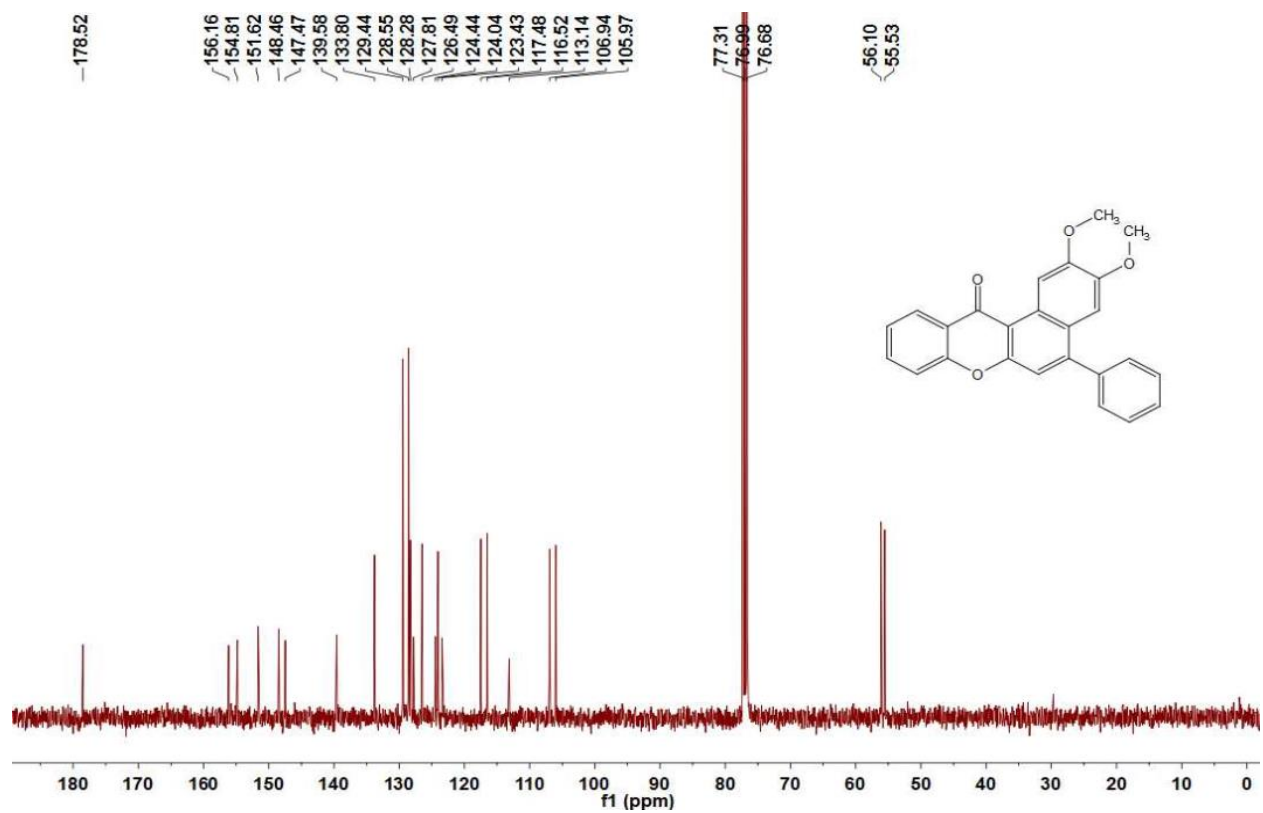
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4c**



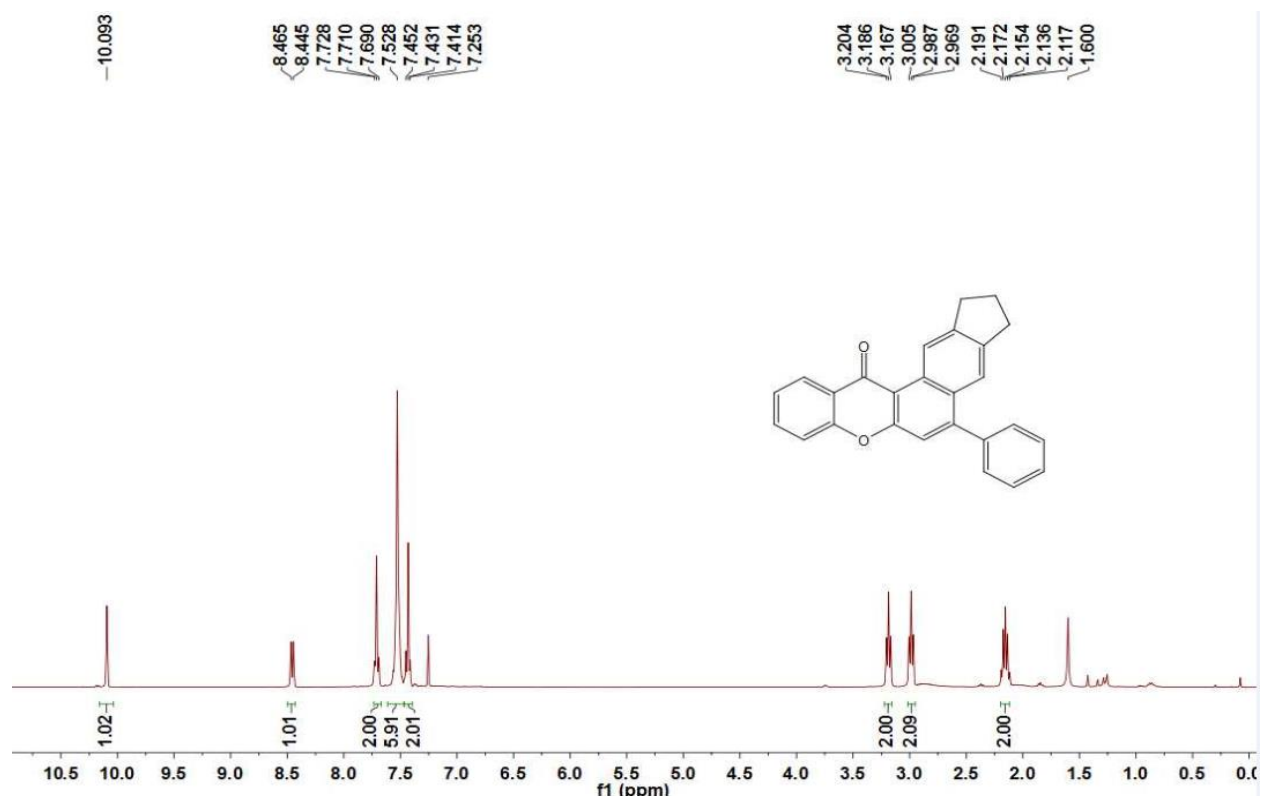
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4d**



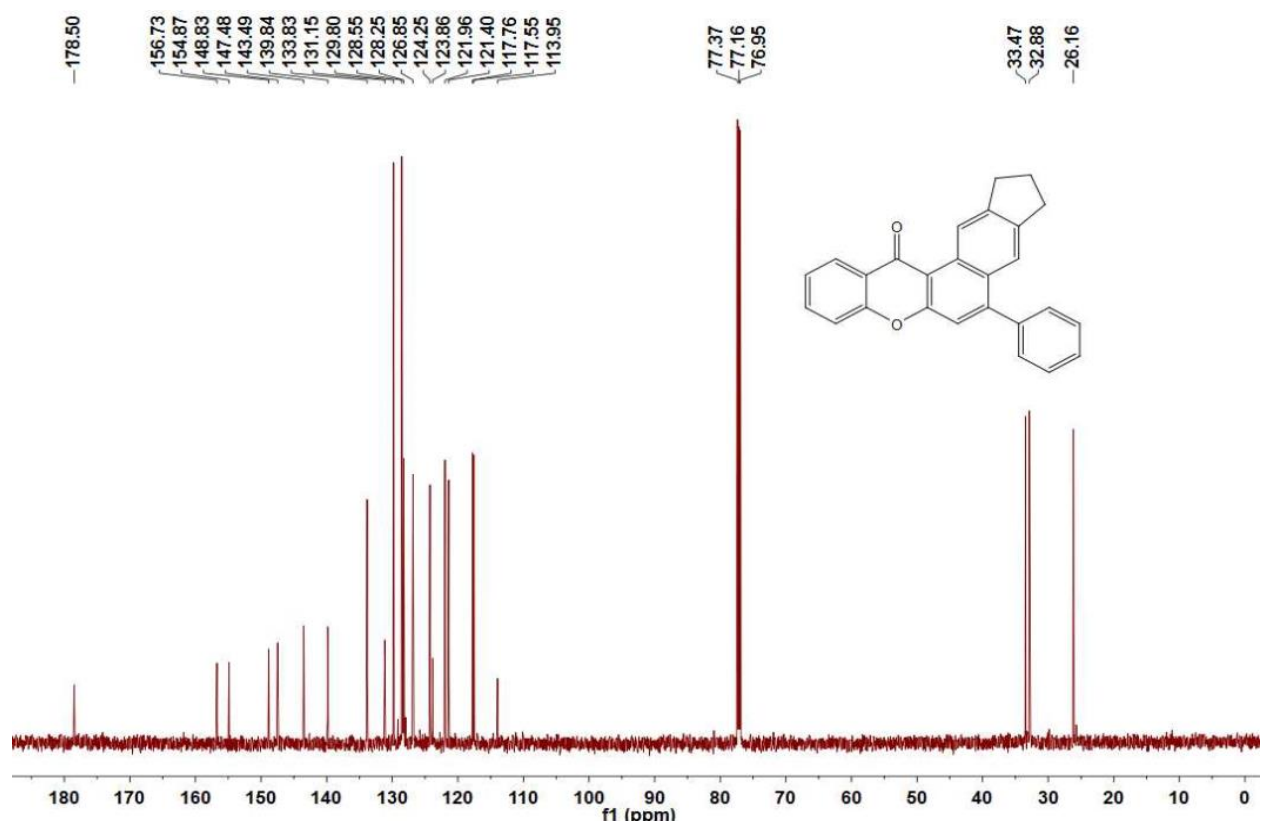
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4d**



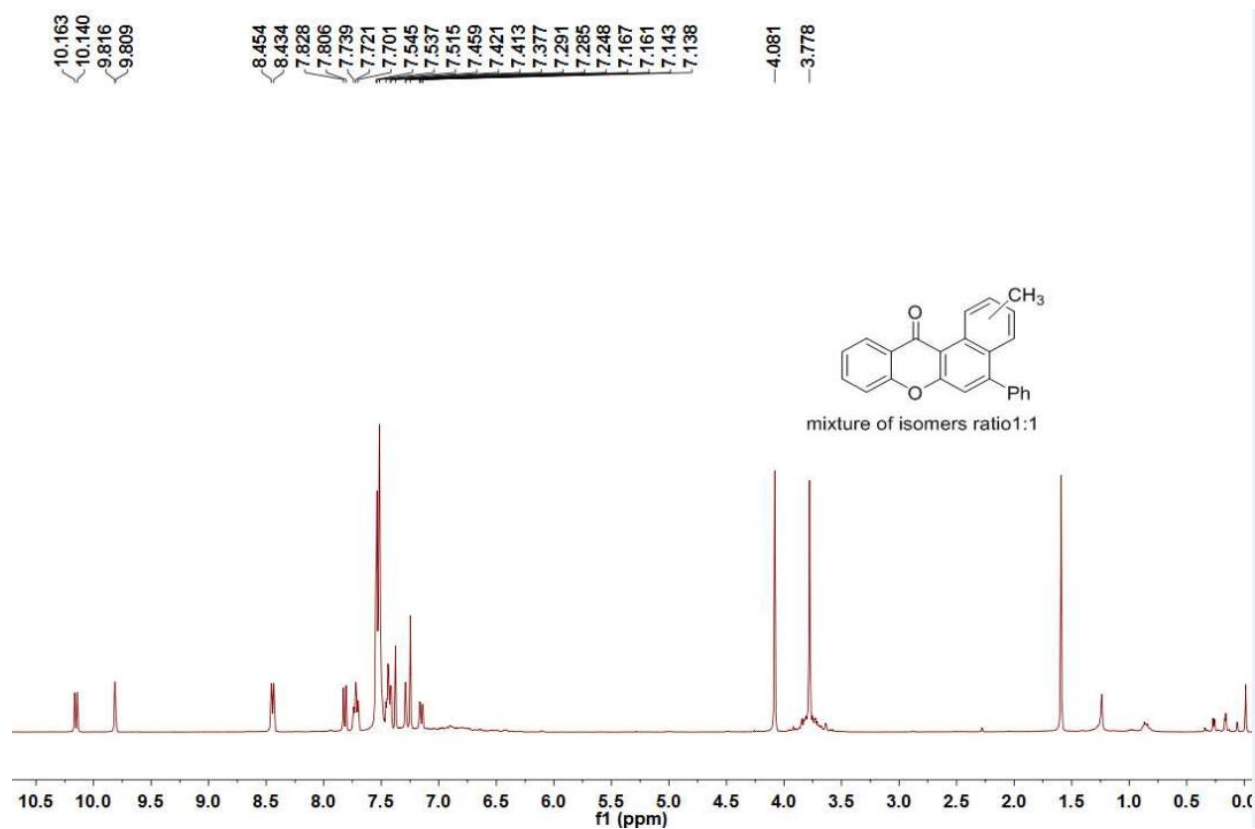
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4e**



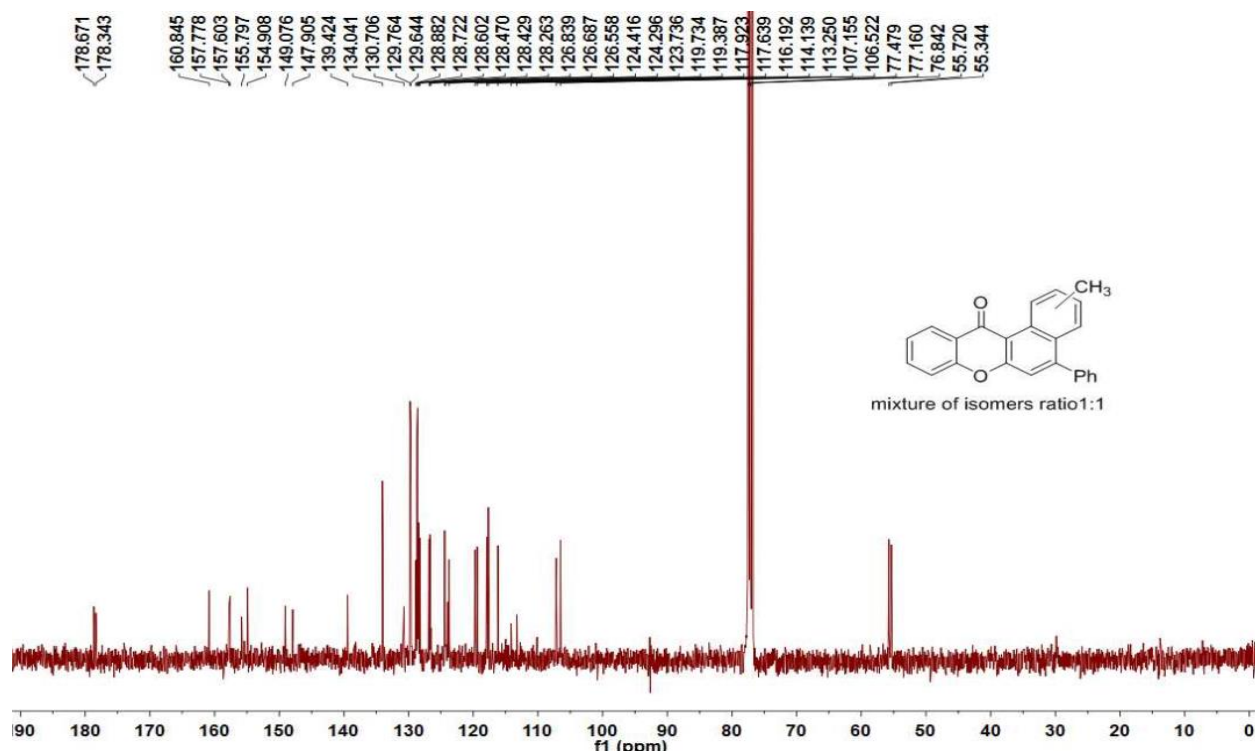
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4e**



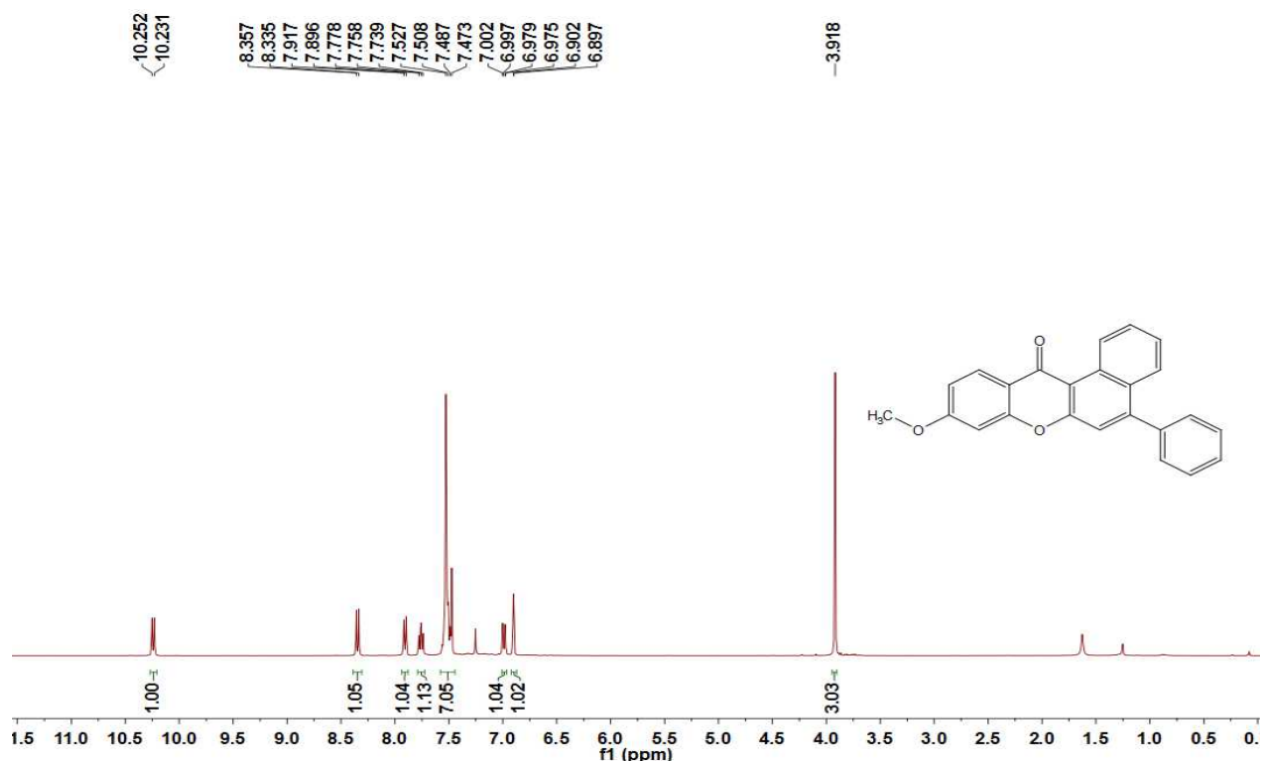
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4f**



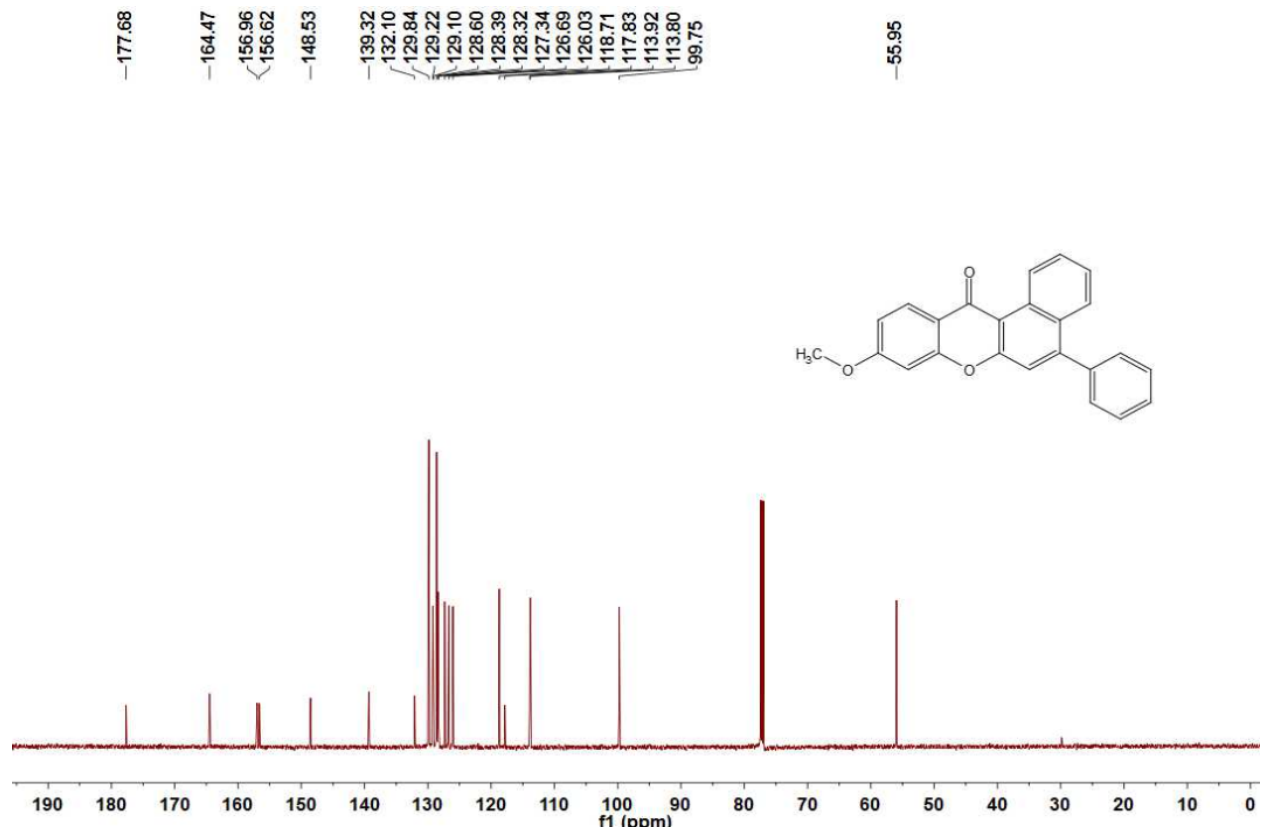
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4f**



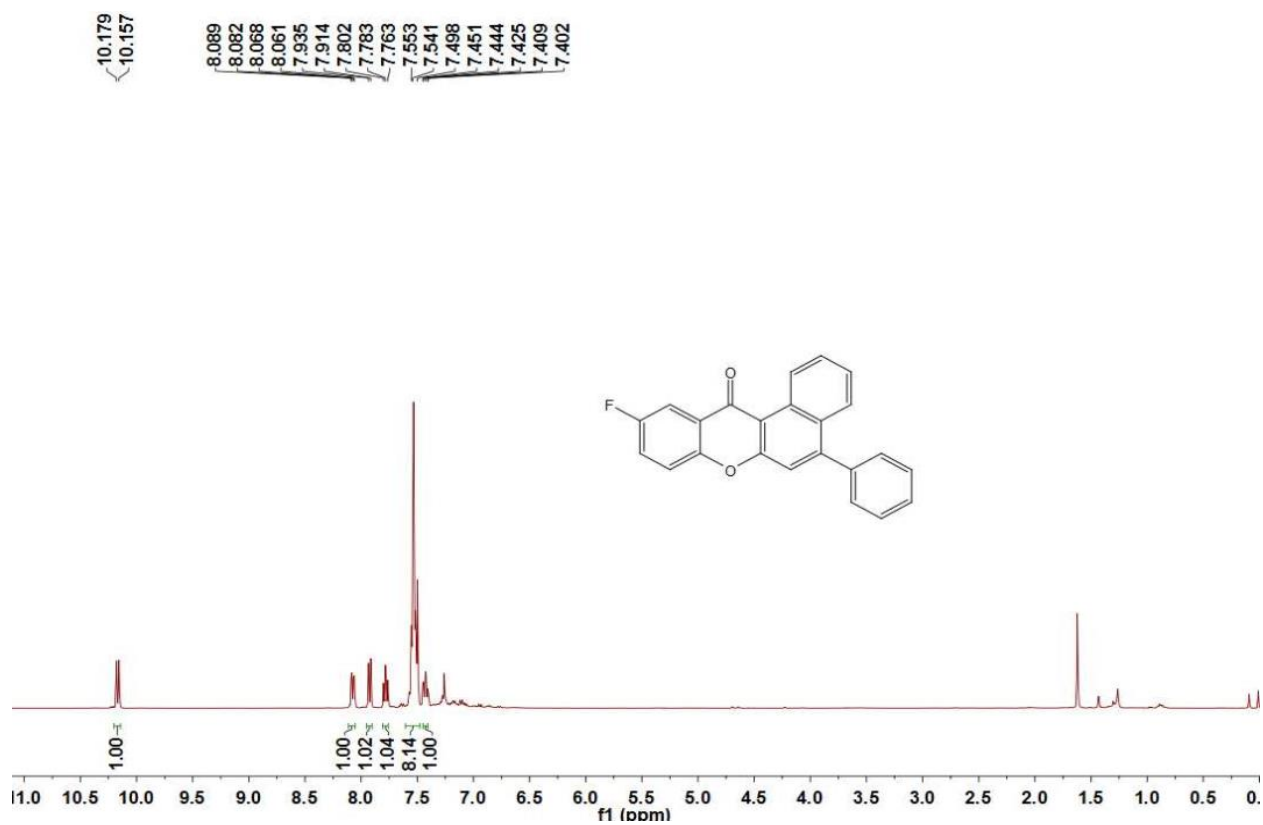
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4g**



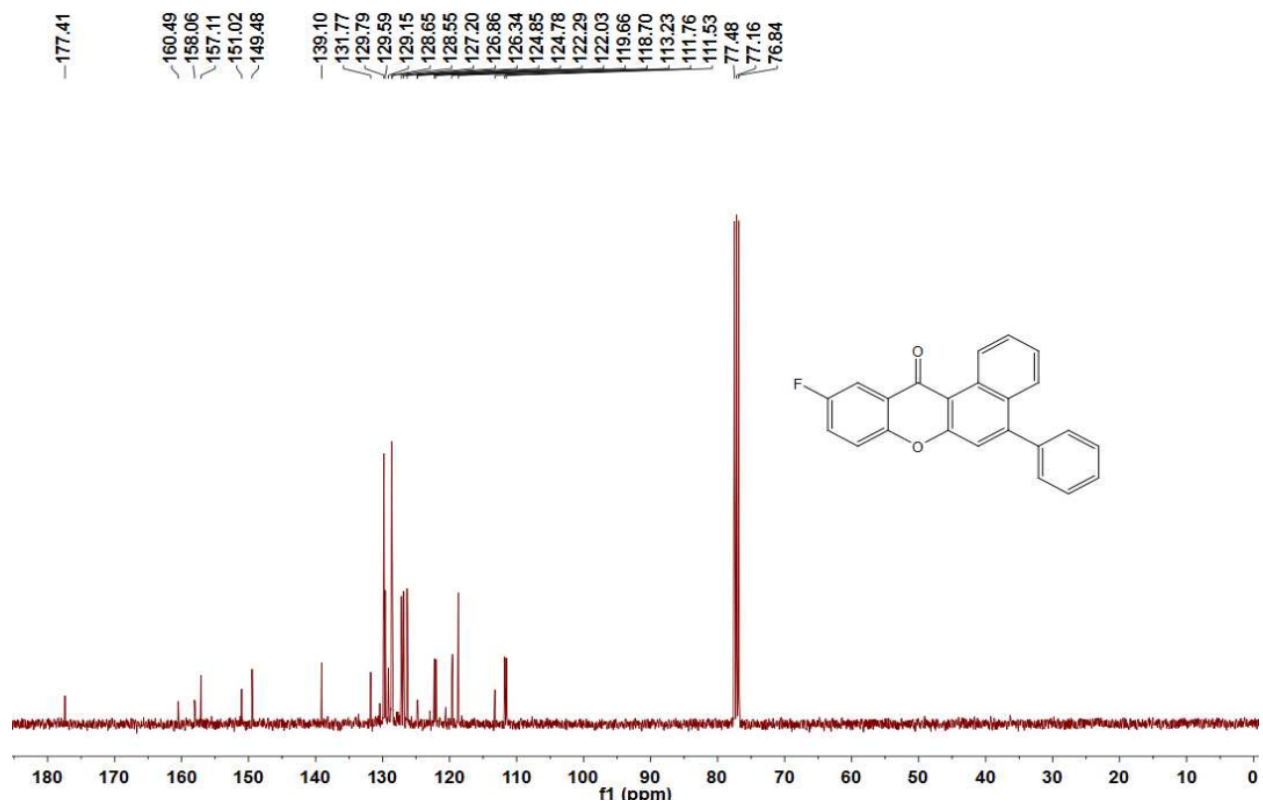
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4g**



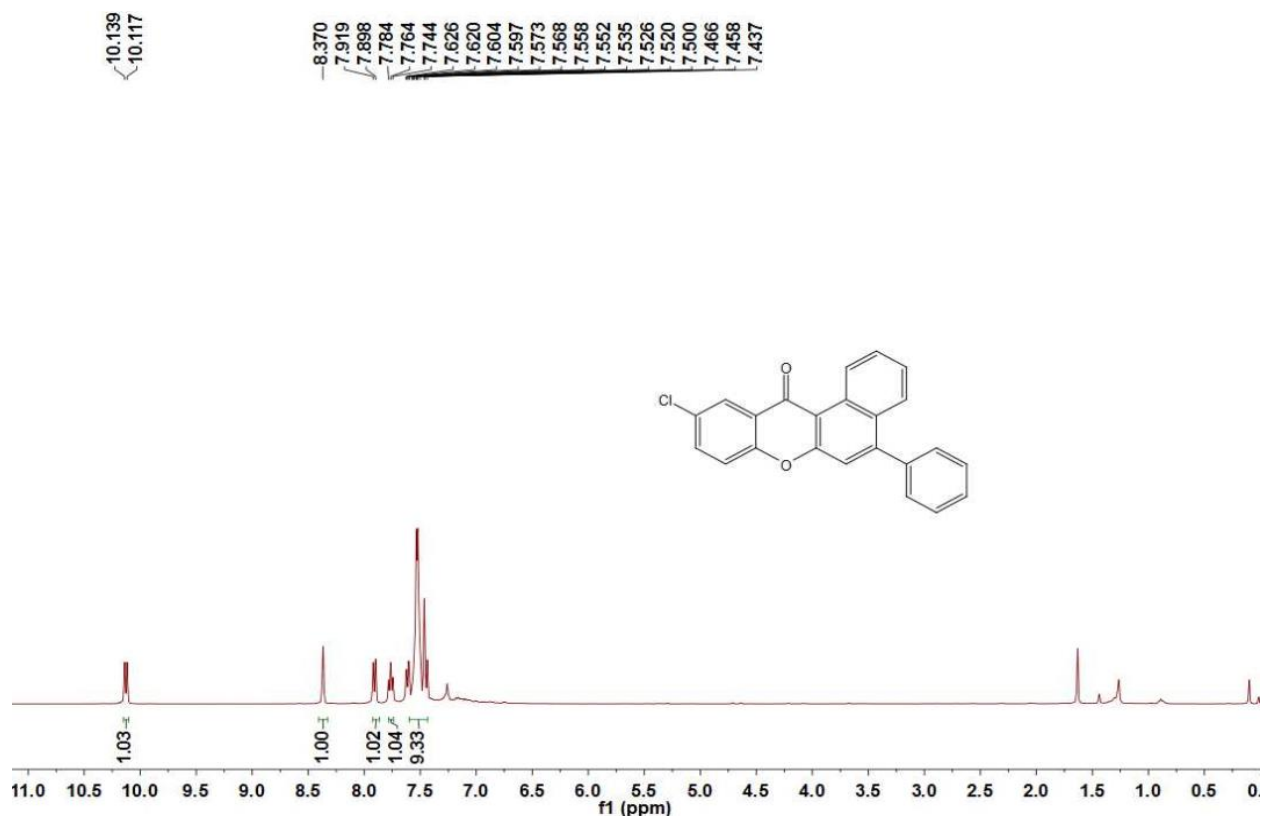
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4h**



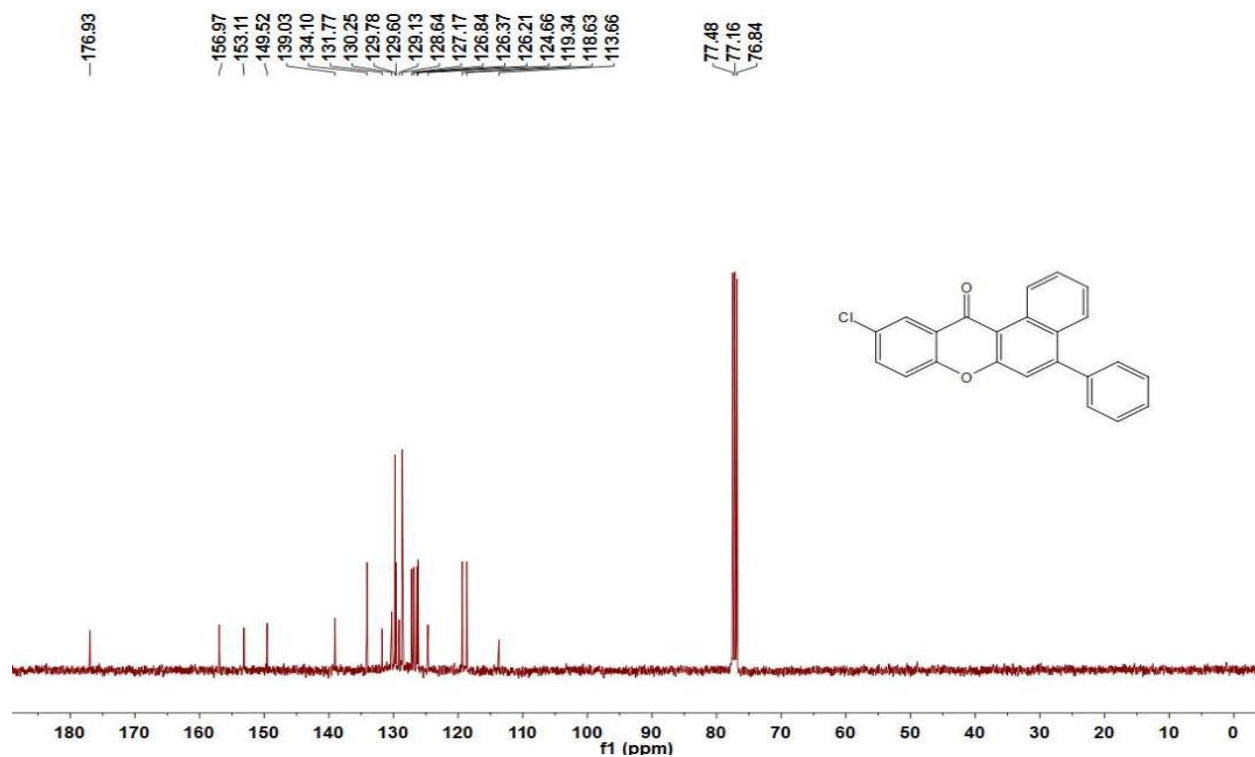
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4h**



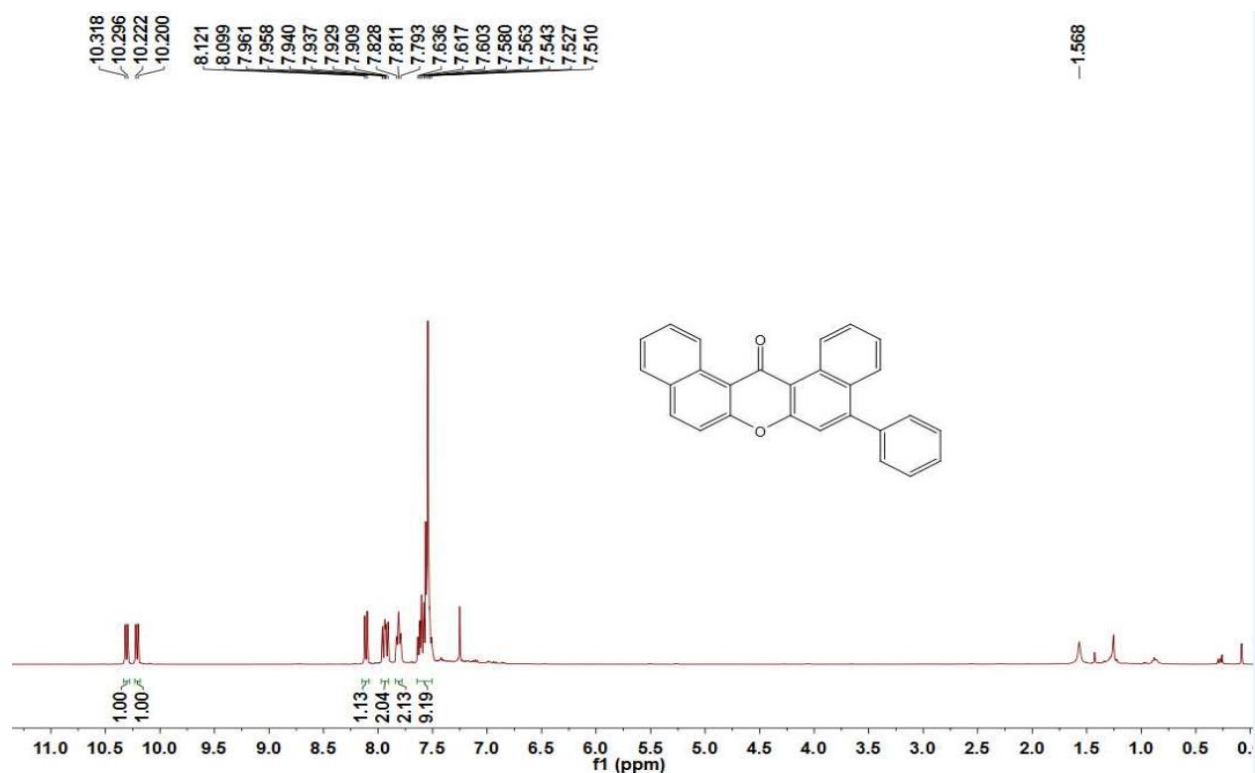
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4i**



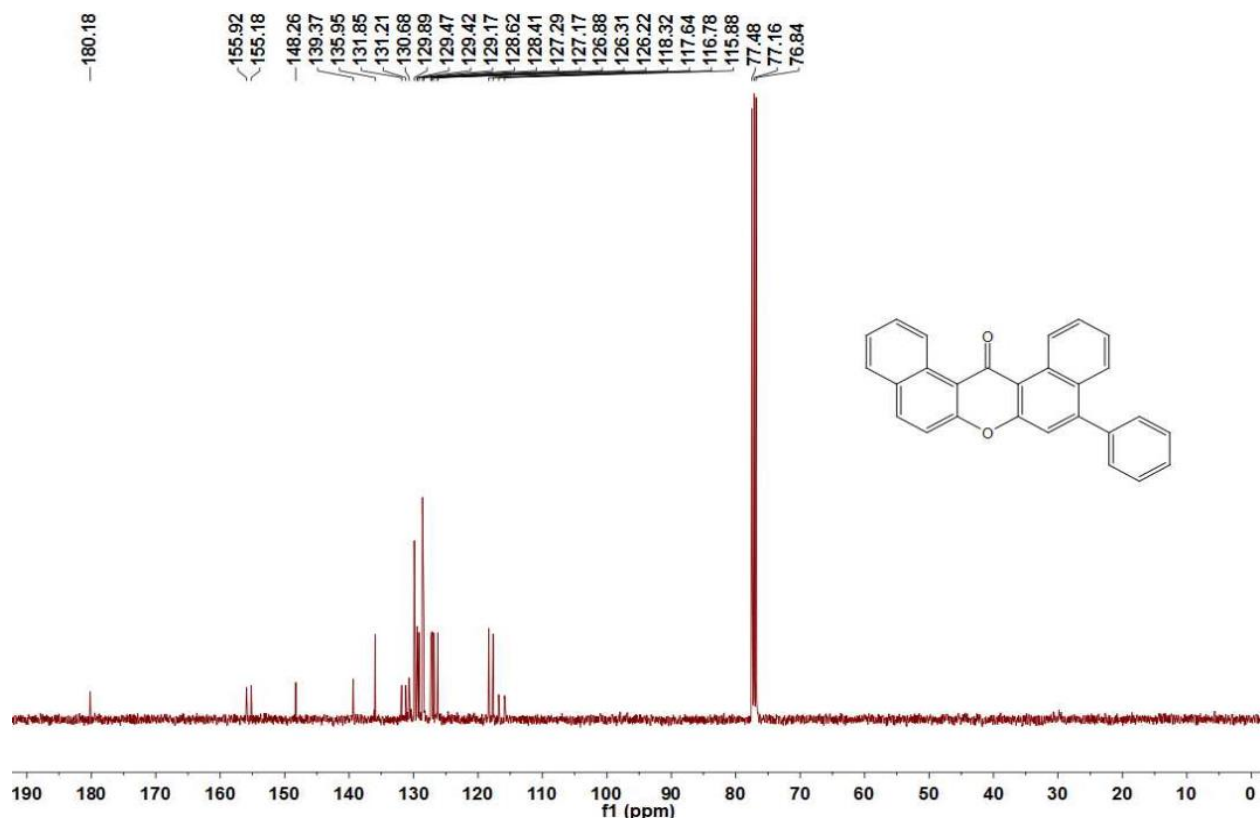
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4i**



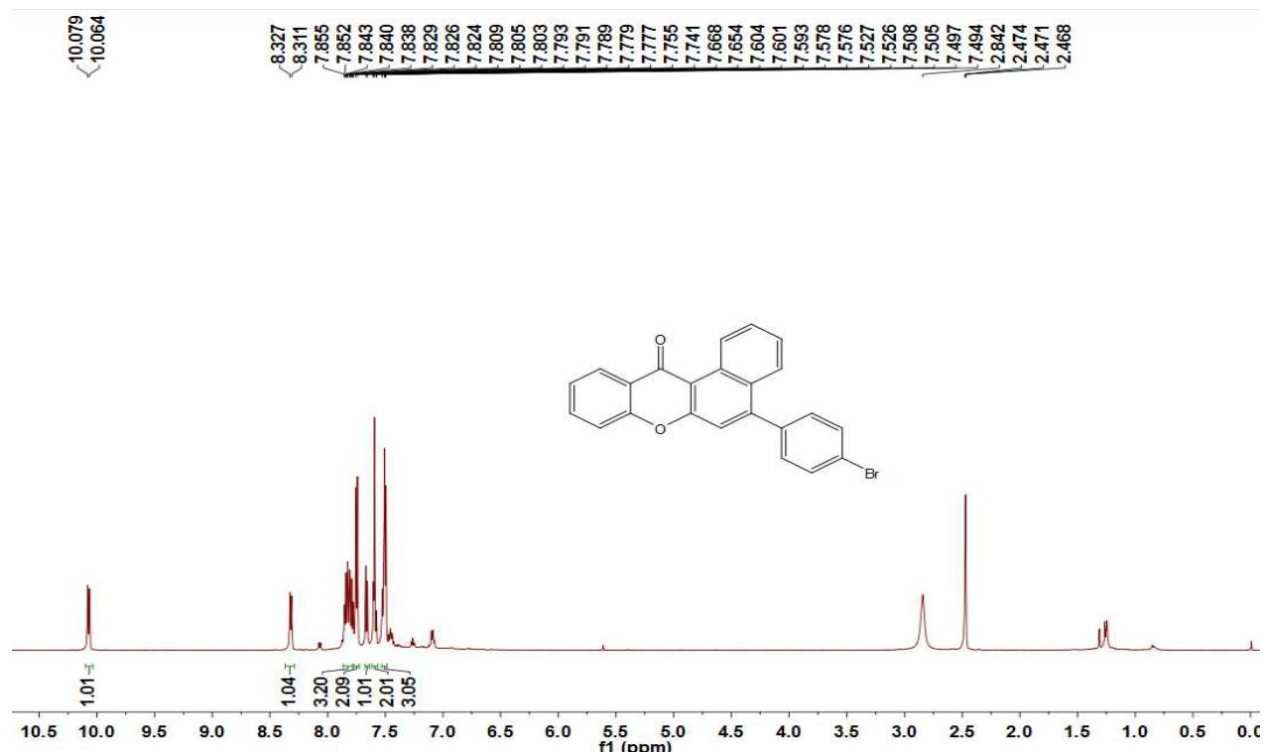
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4j**



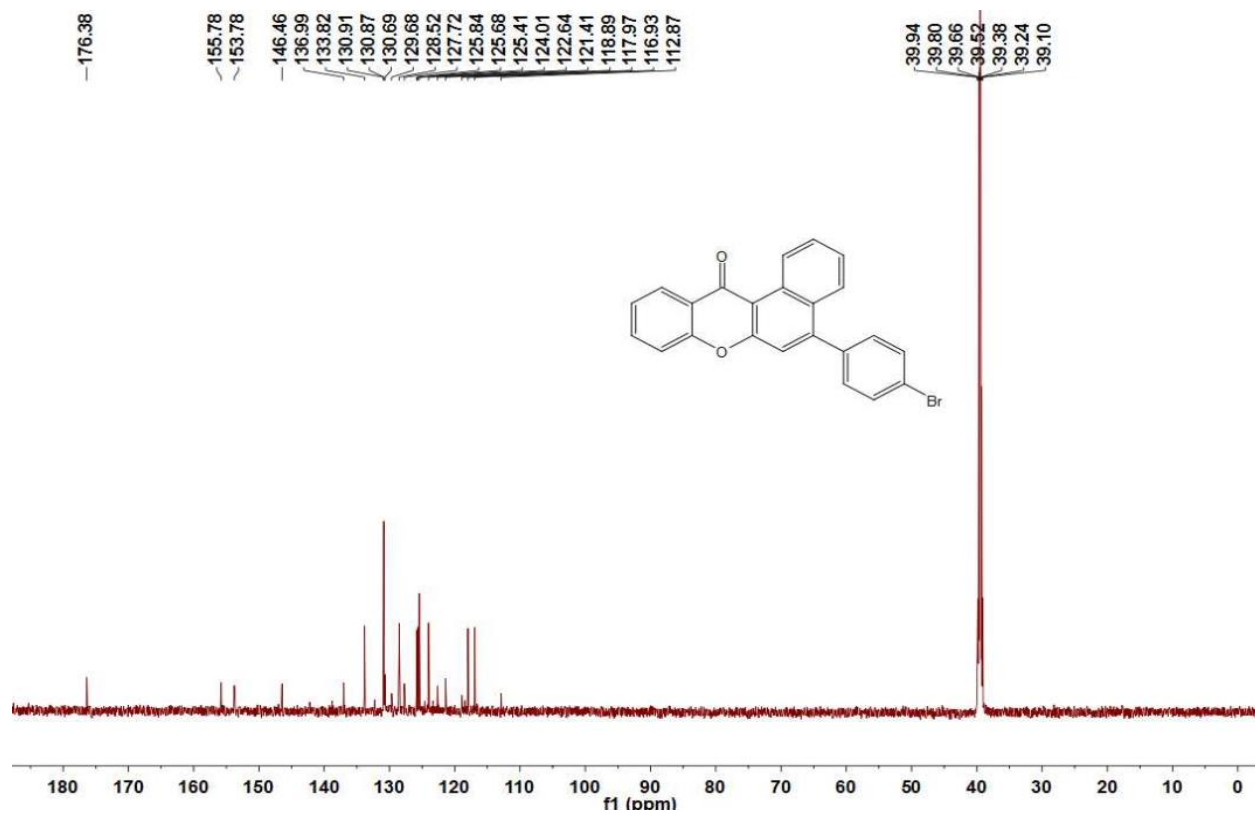
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4j**



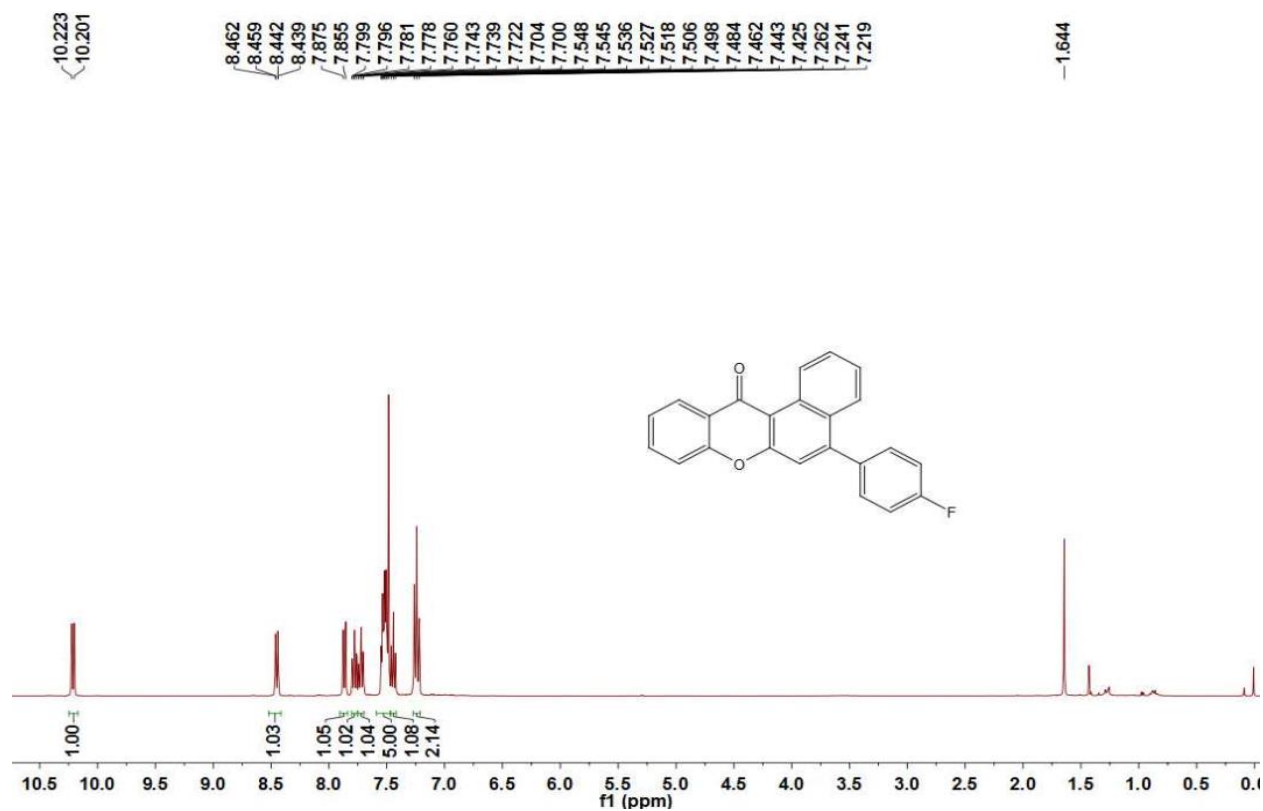
^1H NMR spectrum (400 MHz, $\text{DMSO-}d_6$) of compound **4k**



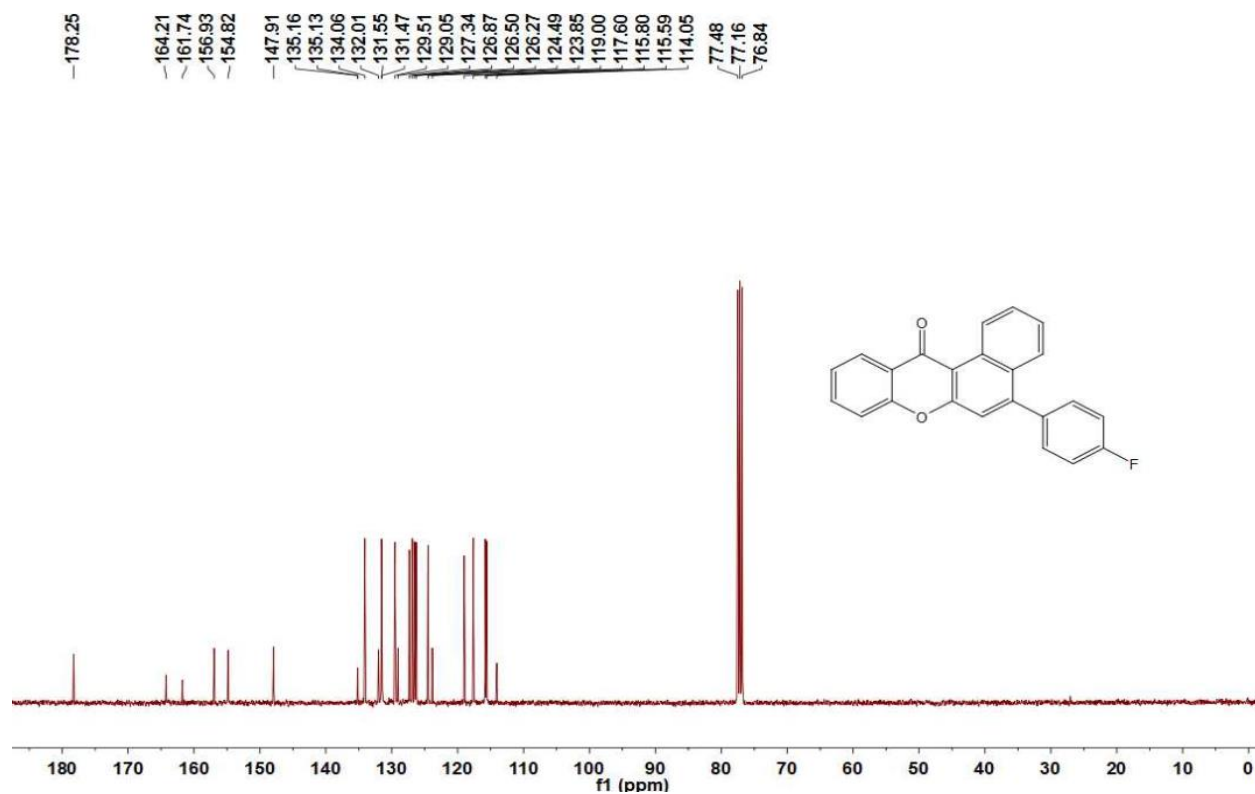
^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of compound **4k**



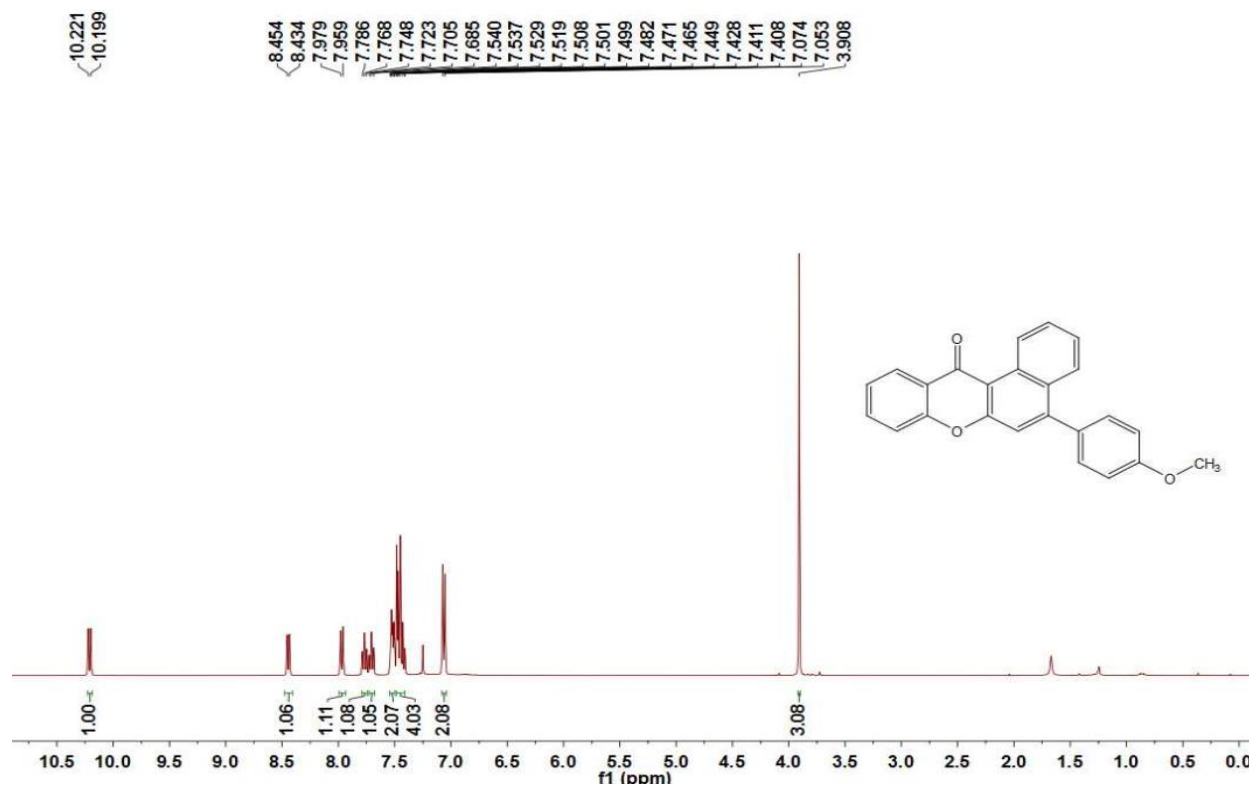
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4l**



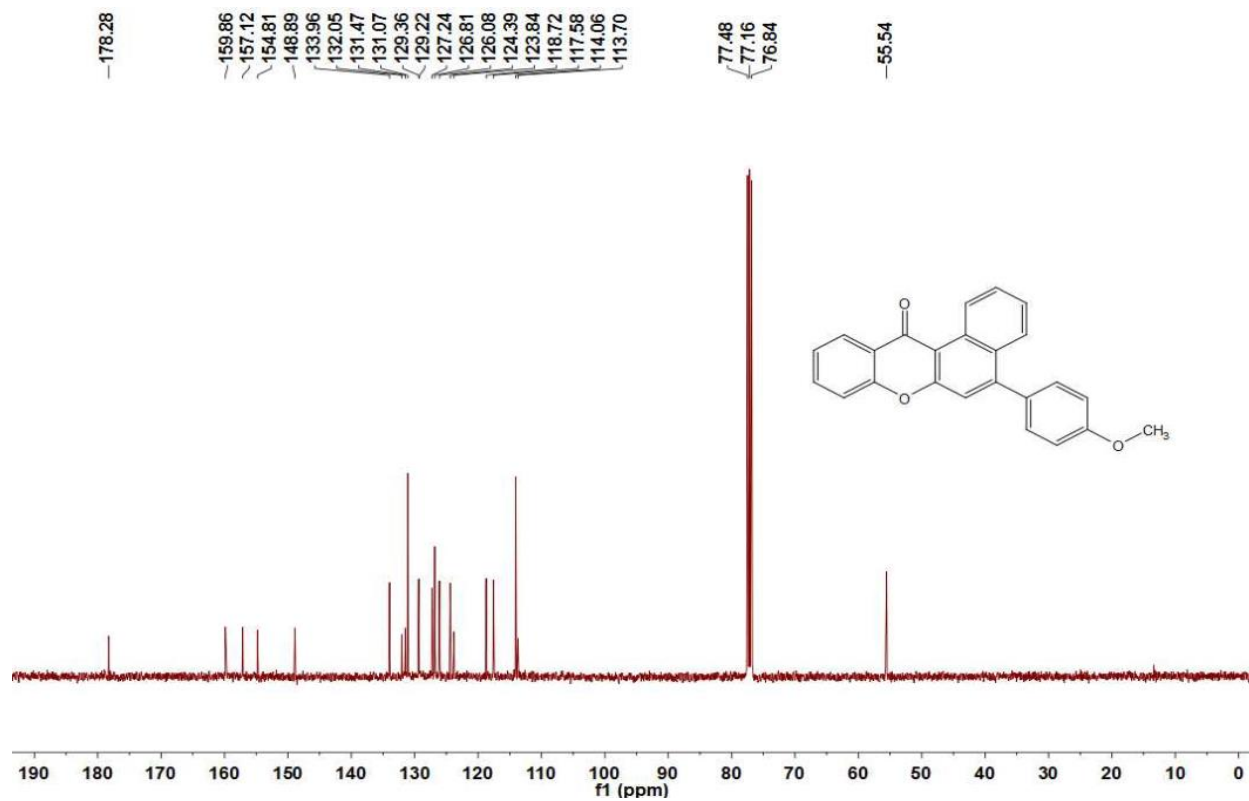
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4l**



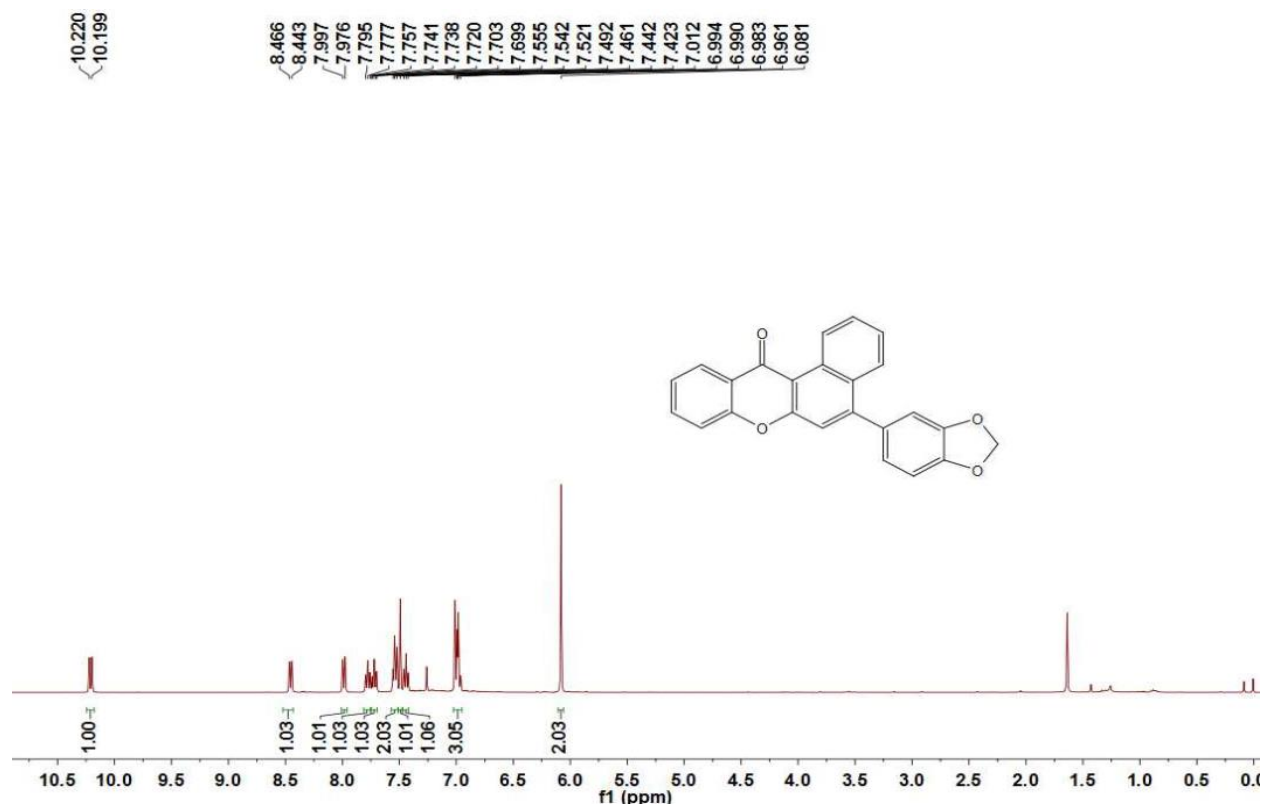
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4m**



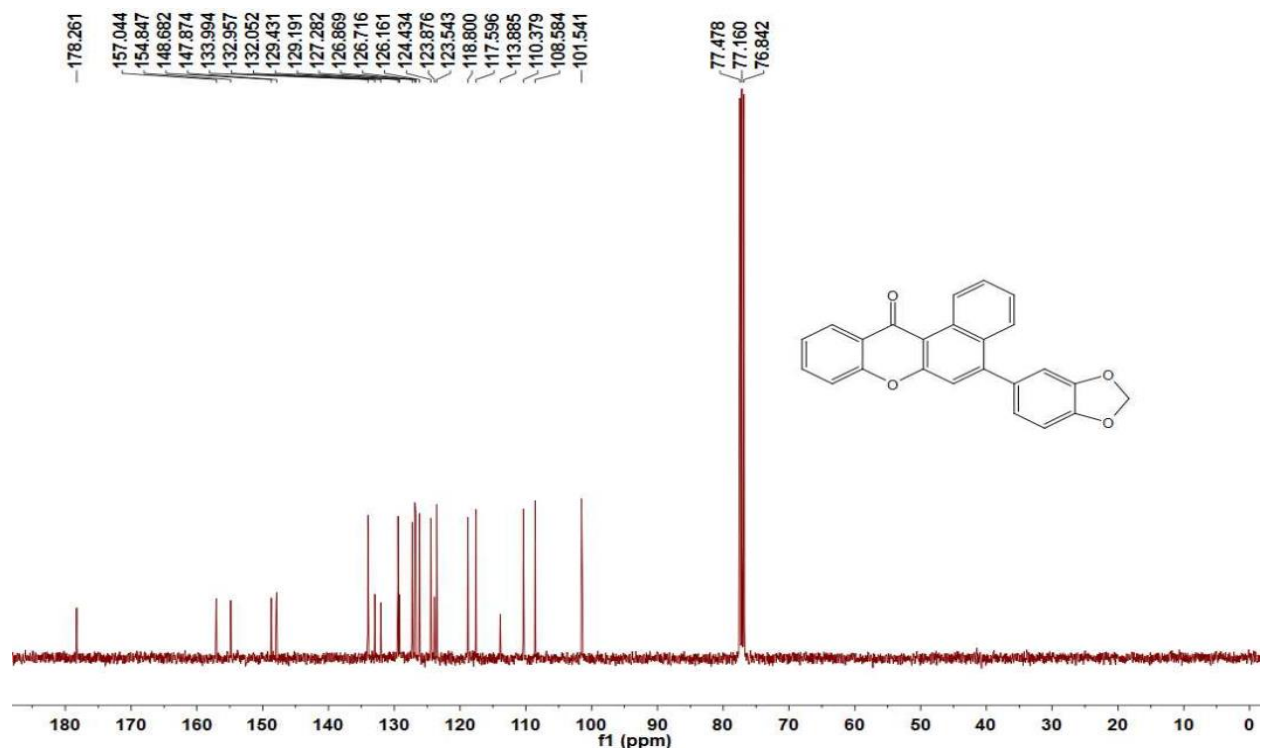
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4m**



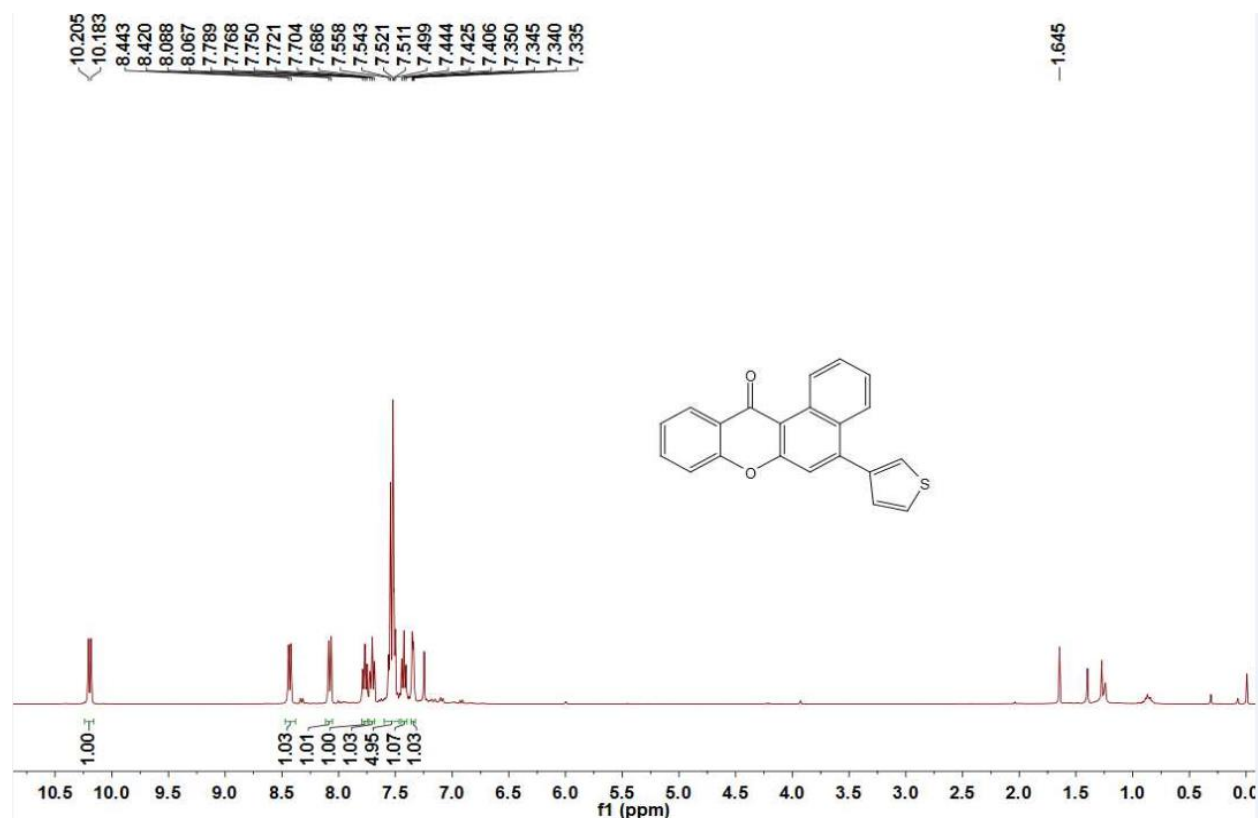
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4n**



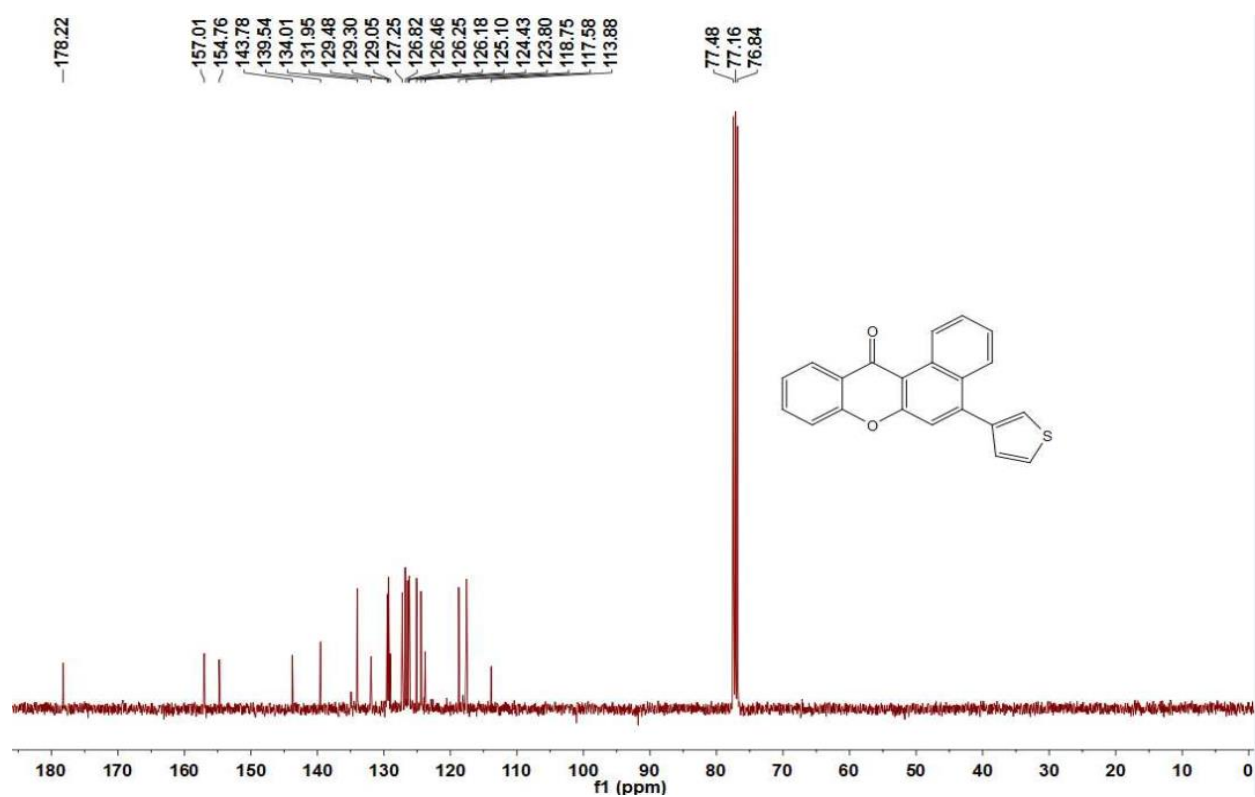
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4n**



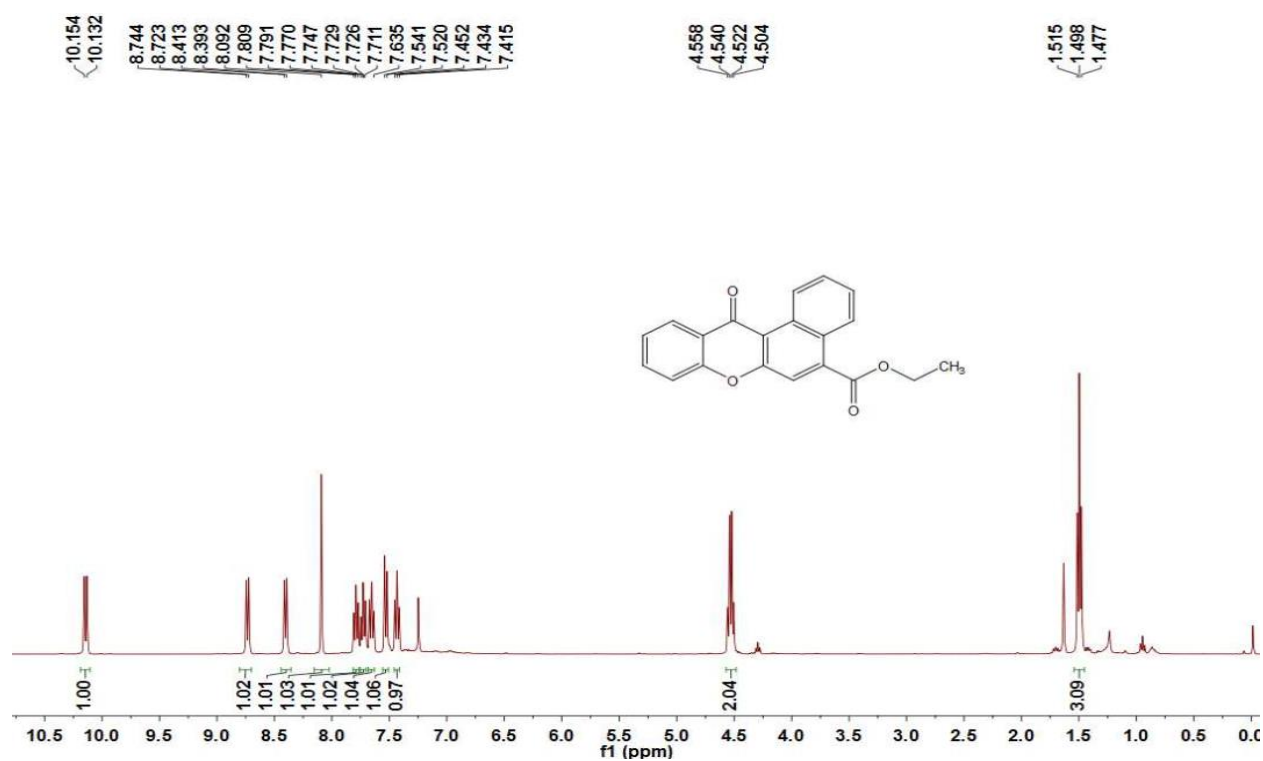
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4o**



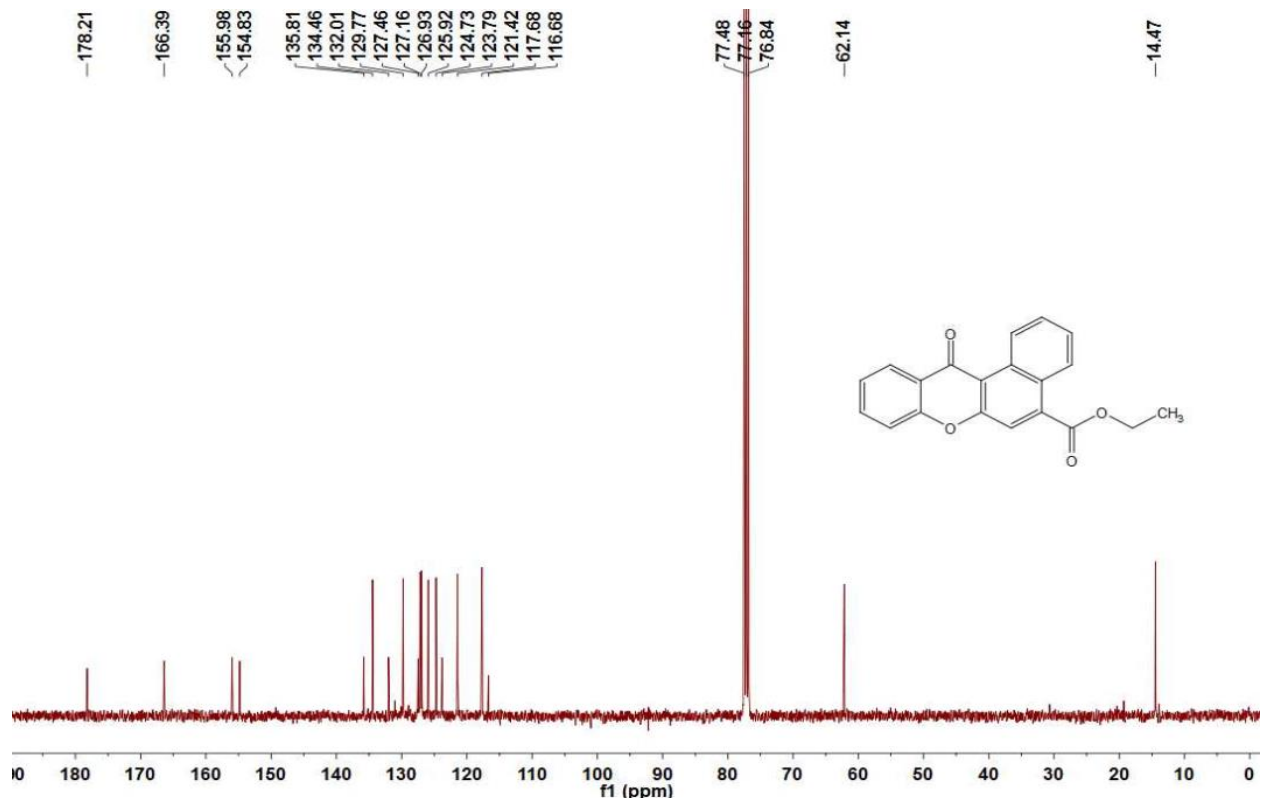
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4o**



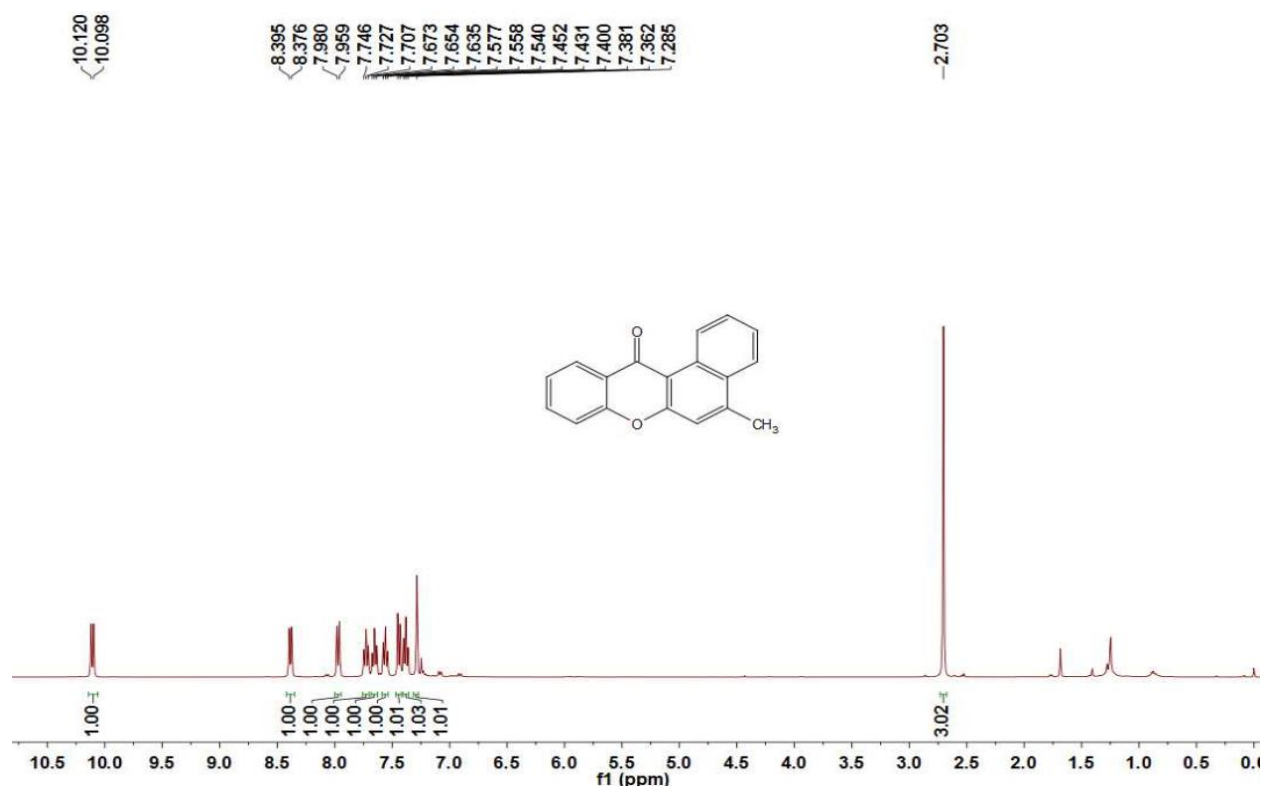
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4p**



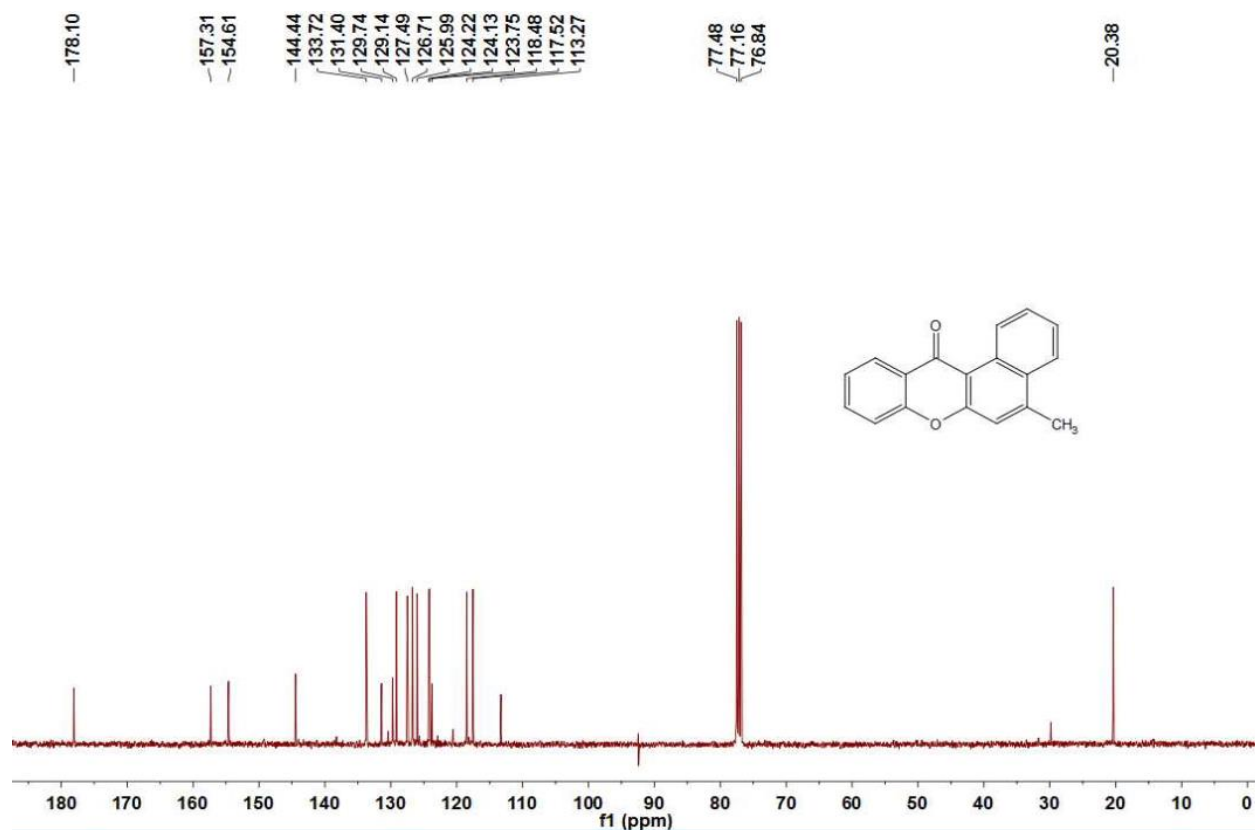
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4p**



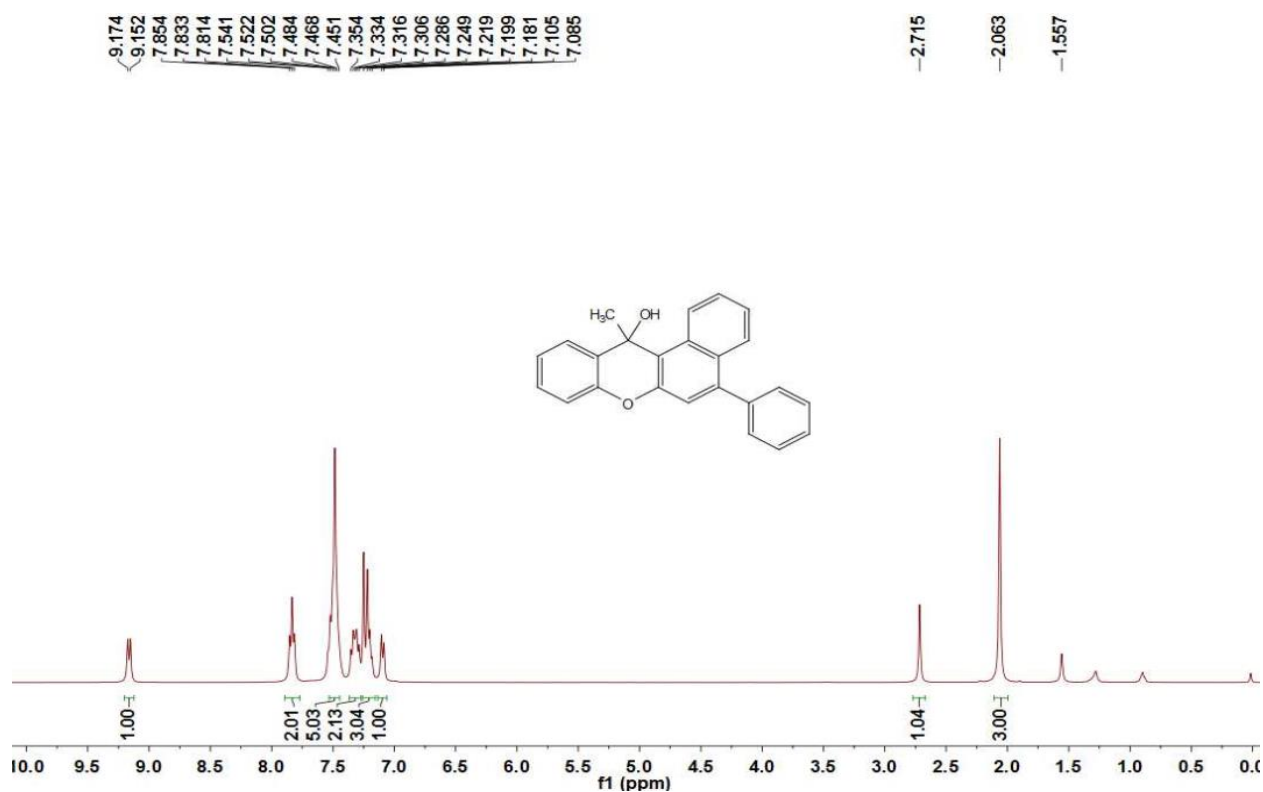
^1H NMR spectrum (400 MHz, CDCl_3) of compound **4q**



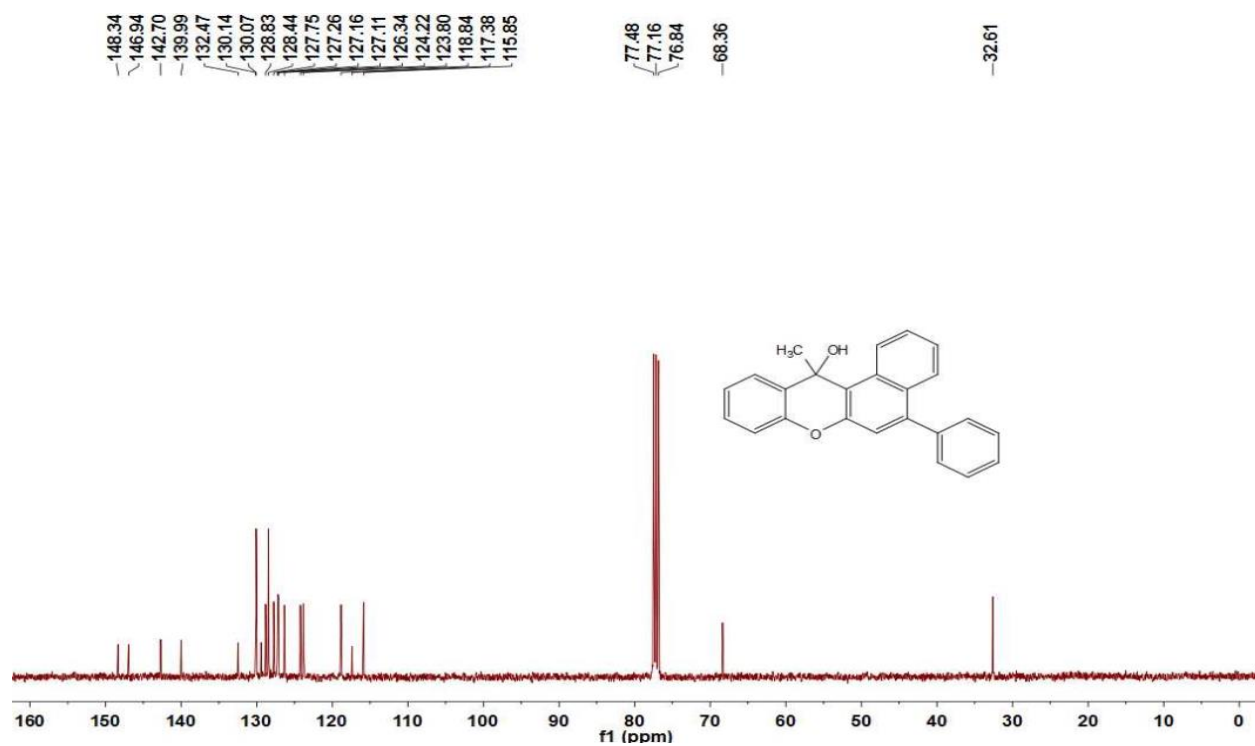
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4q**



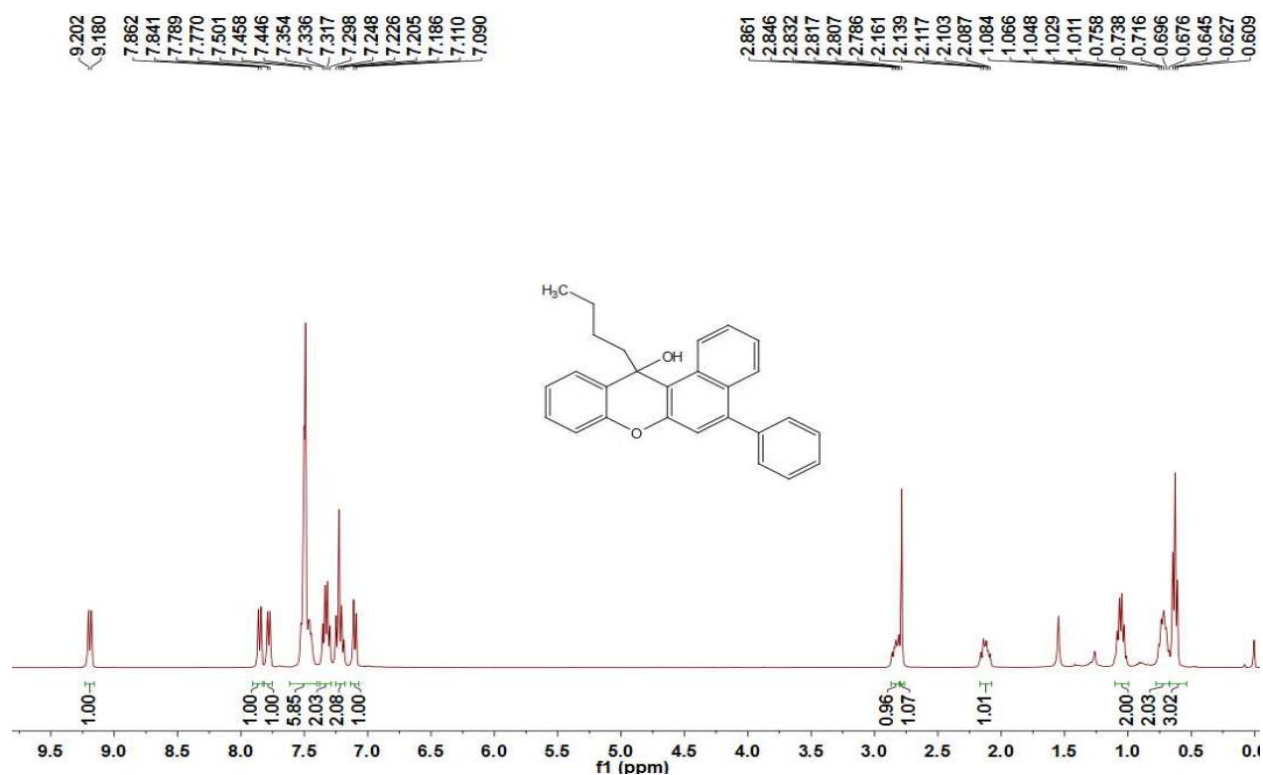
^1H NMR spectrum (400 MHz, CDCl_3) of compound 5



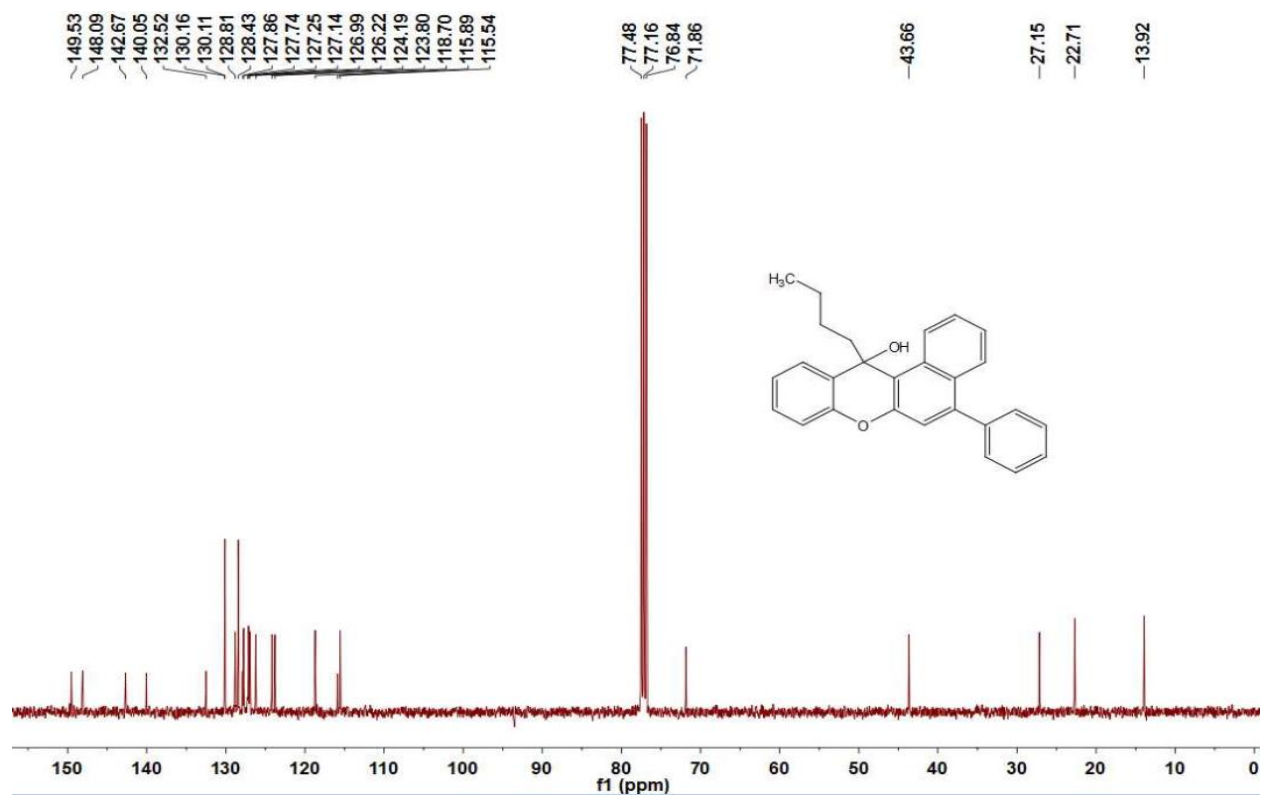
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound 5



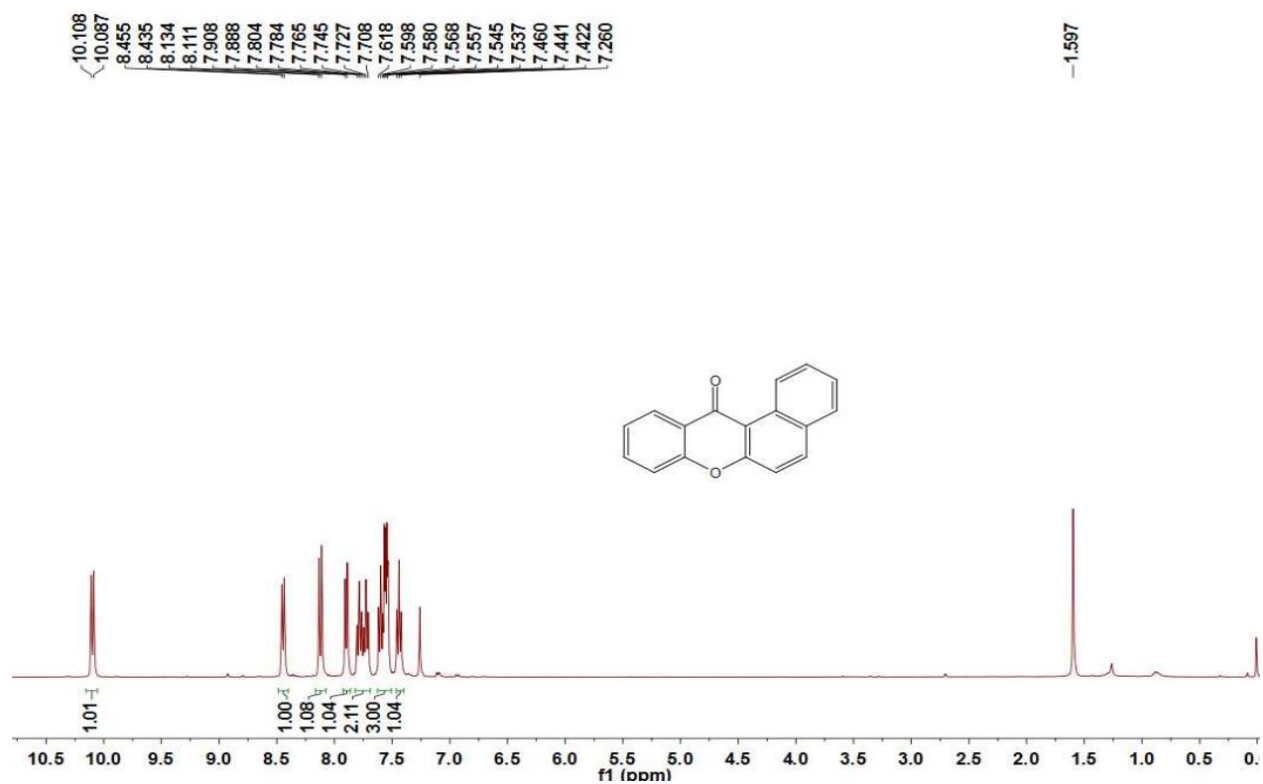
^1H NMR spectrum (400 MHz, CDCl_3) of compound **6**



^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **6**



^1H NMR spectrum (400 MHz, CDCl_3) of compound **8**



^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **8**

