

Supplimentary Material

Synthesis and evaluation of new coumarin derivatives as antioxidant, antimicrobial, and anti-inflammatory agents

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Contents:

- 1- NMR spectra of compounds (**2a**, **4a**, **5c**, **6b**, **8e**, **9f**)
- 2- X-ray Crystallographic data of Compound **2a**

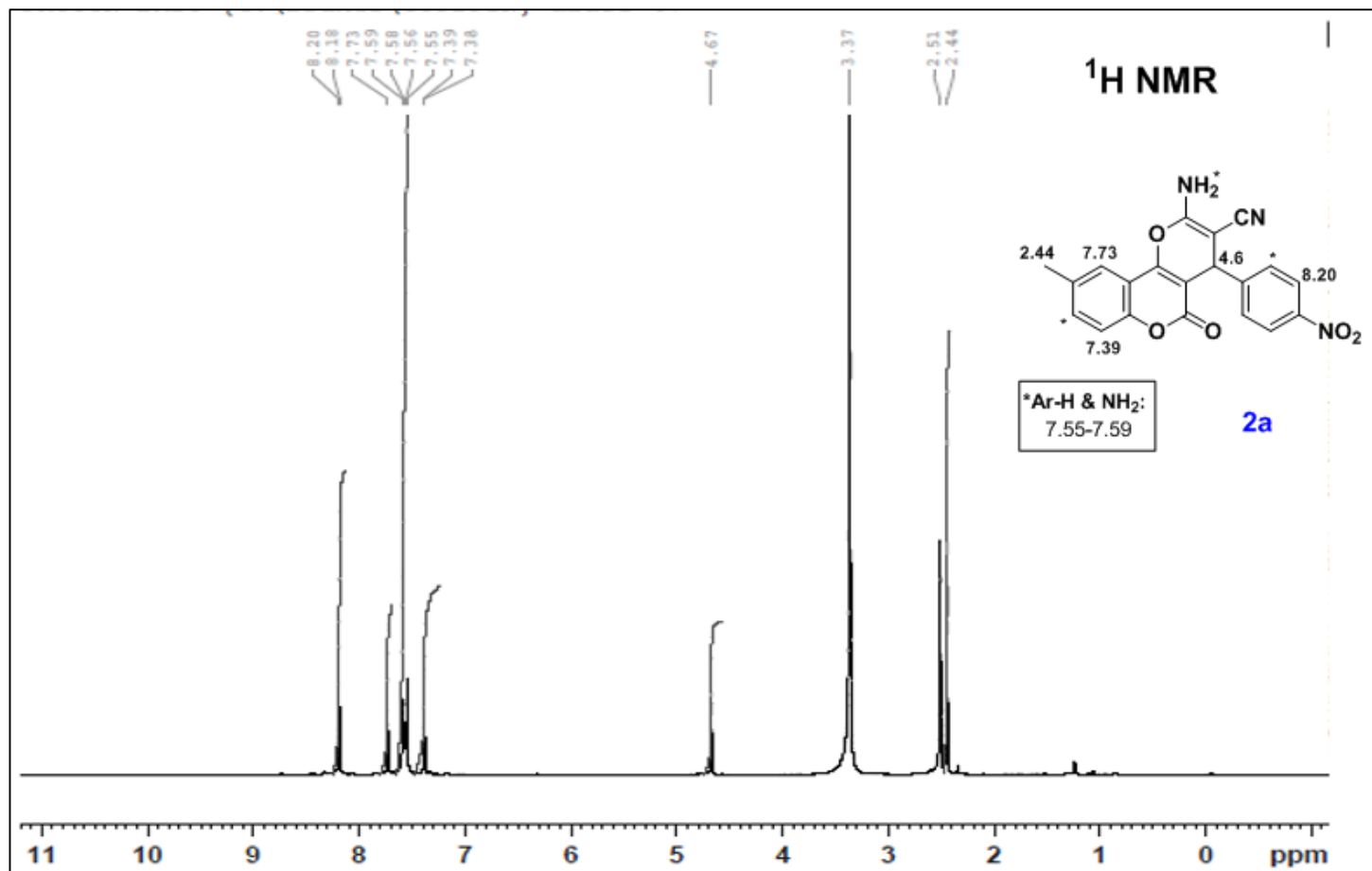


Figure S1: ¹H-NMR spectrum of compound **2a** in DMSO-d₆ (700 MHz).

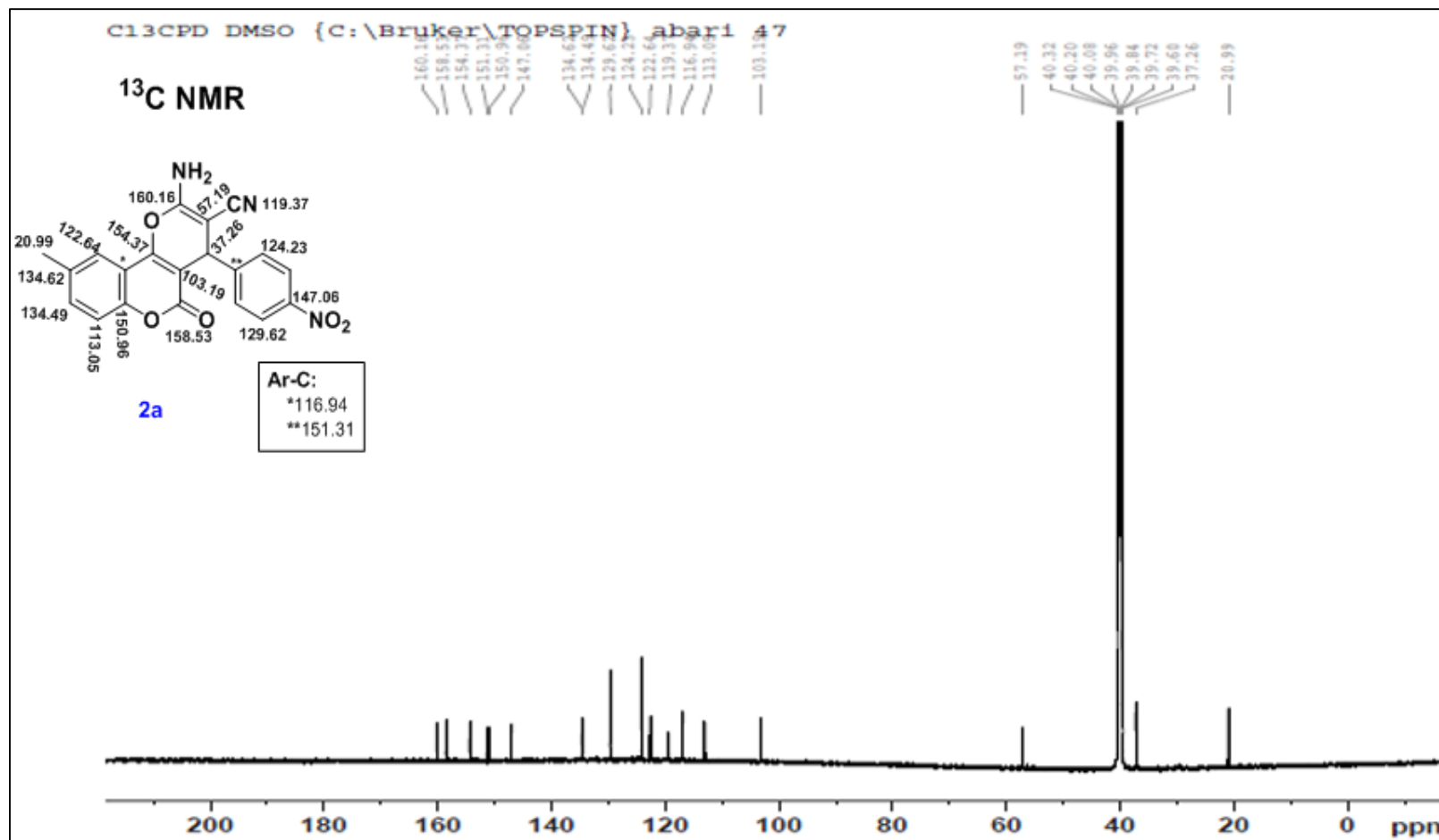


Figure S2: ¹³C-NMR spectrum of compound **2a** in DMSO-d₆ (176 MHz).

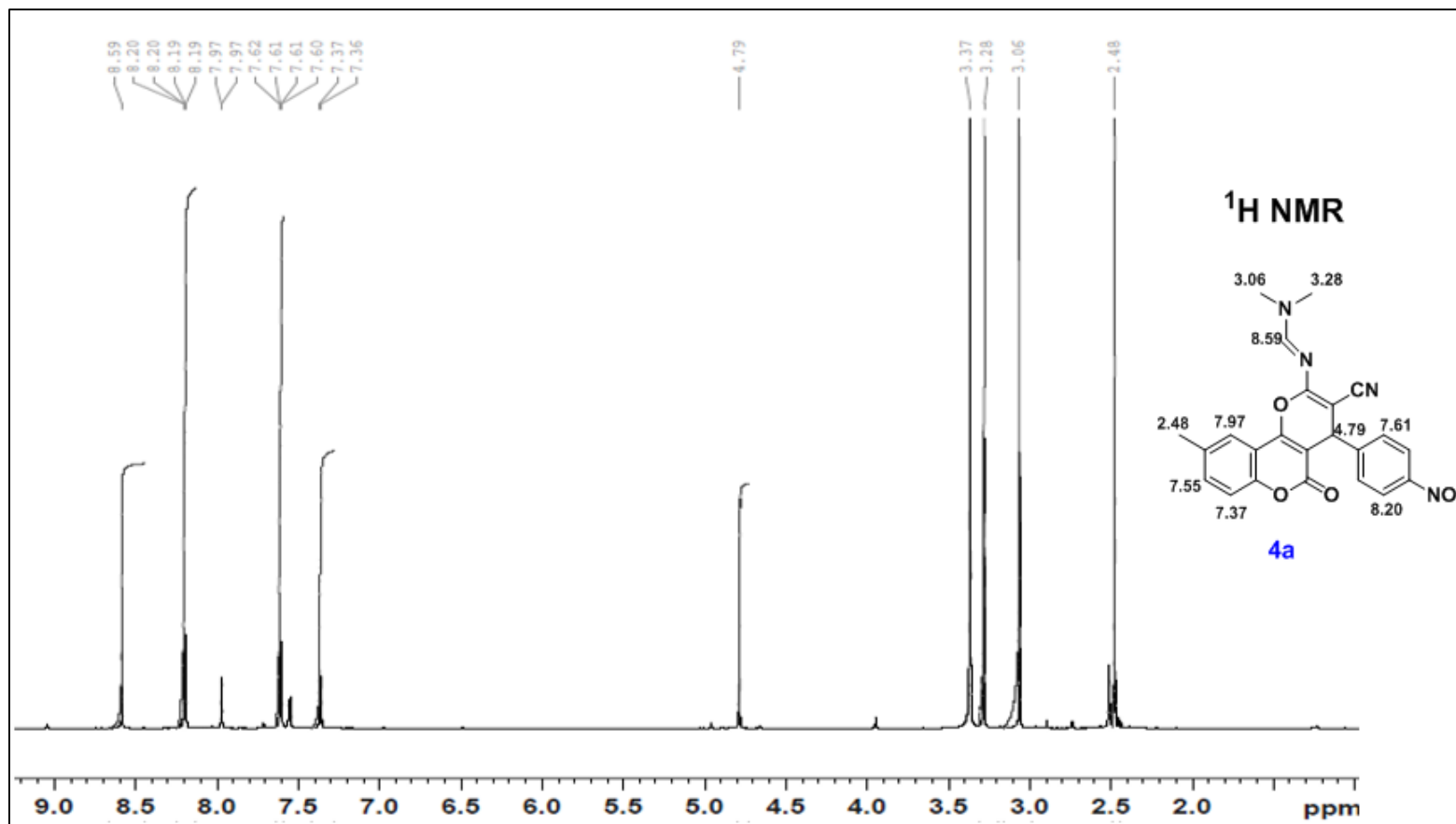


Figure S3: ¹H-NMR spectrum of compound **4a** in DMSO-d₆ (700 MHz).

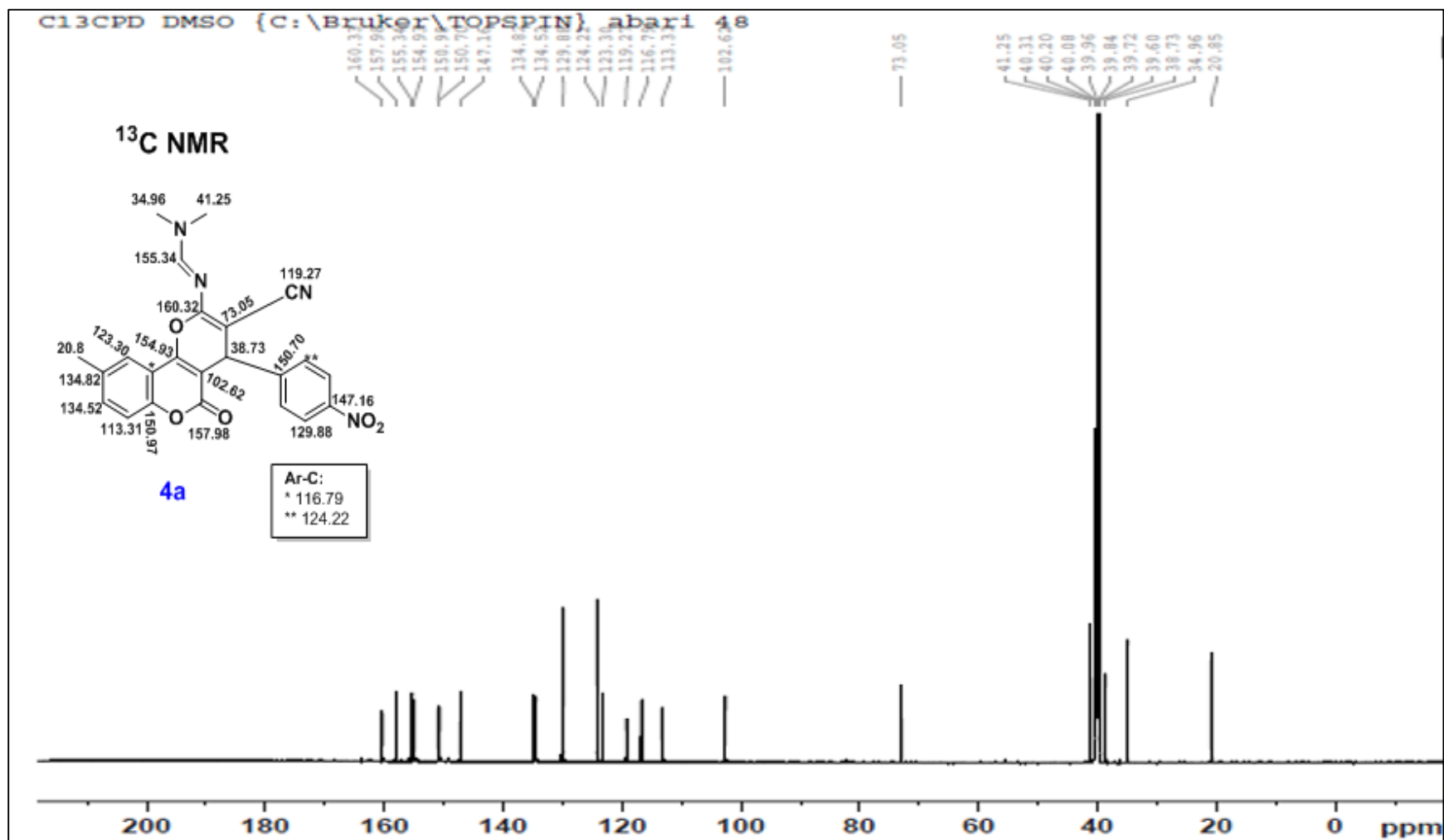


Figure S4: ¹³C-NMR spectrum of compound **4a** in DMSO-d₆ (176 MHz).

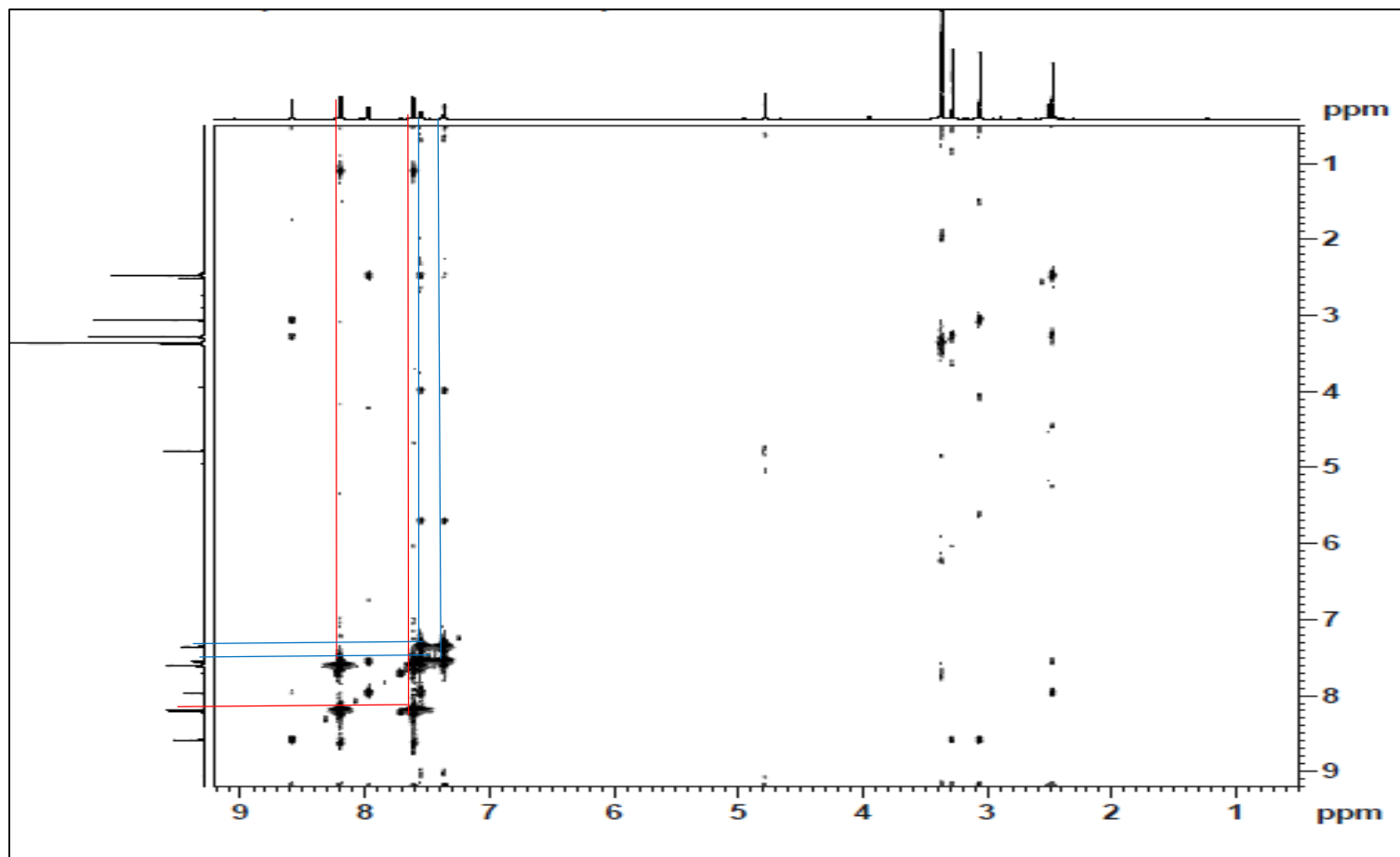


Figure S5: ^1H - ^1H -Homomuclear COSY NMR spectrum of compound **4a** in DMSO-d_6 (700 MHz).

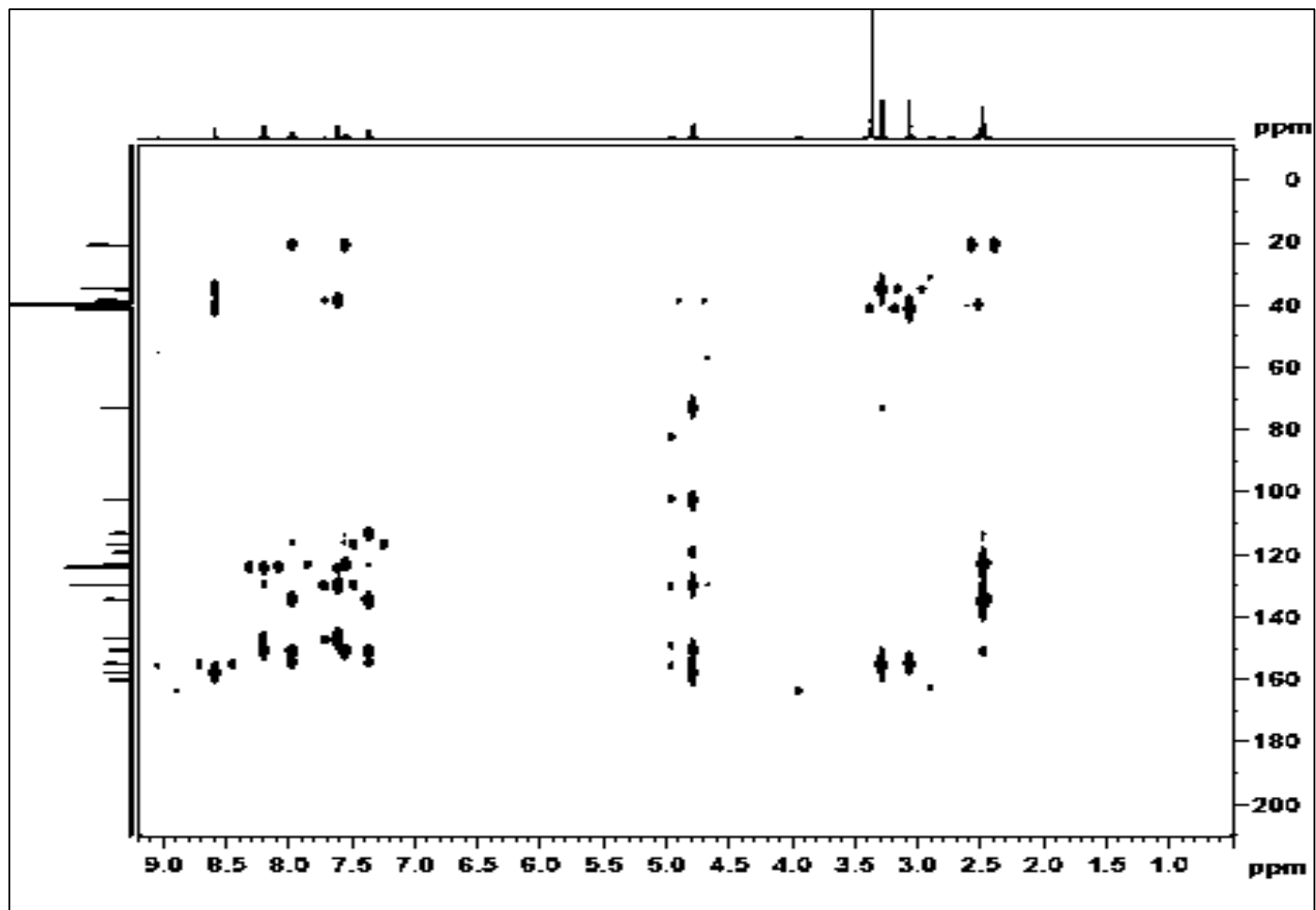


Figure S6: ^1H - ^{13}C -Heteronuclear COSY (HMBC) NMR spectrum of compound **4a** in DMSO- d_6 (700/176 MHz).

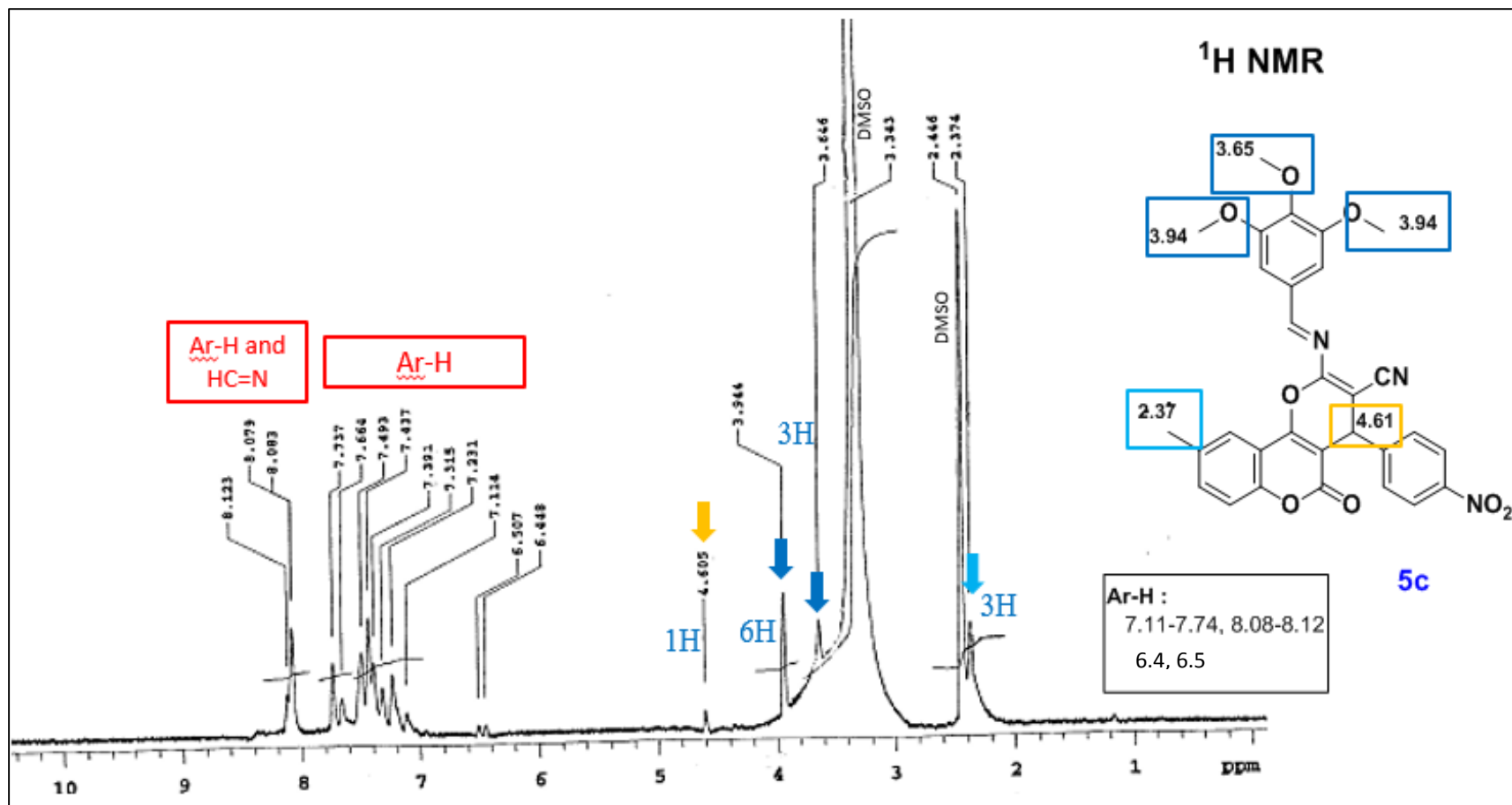


Figure S7: ¹H-NMR spectrum of compound **5c** in DMSO-d₆ (600 MHz).

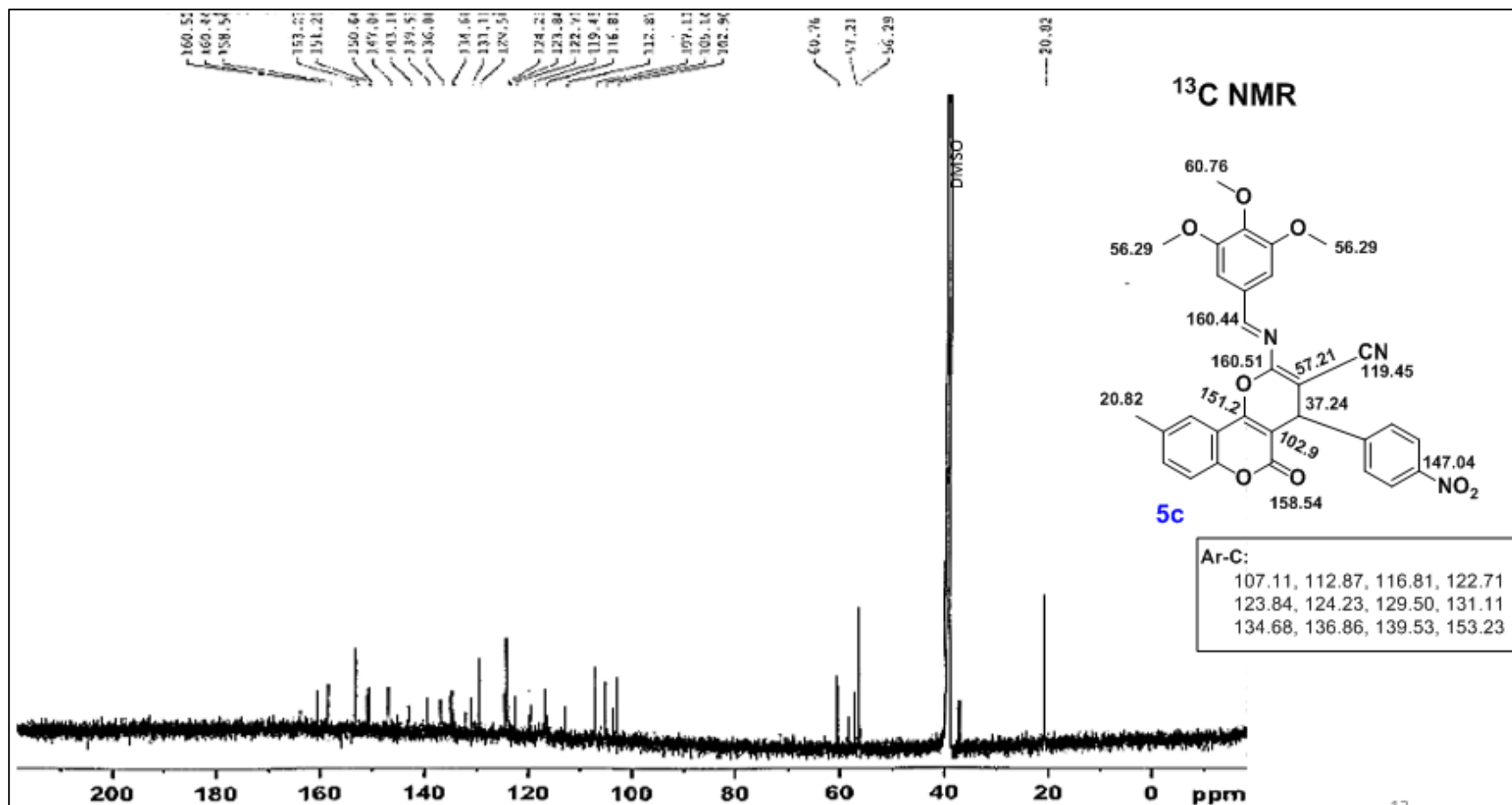


Figure S8: ¹³C-NMR spectrum of compound **5c** in DMSO-d₆ (176 MHz).

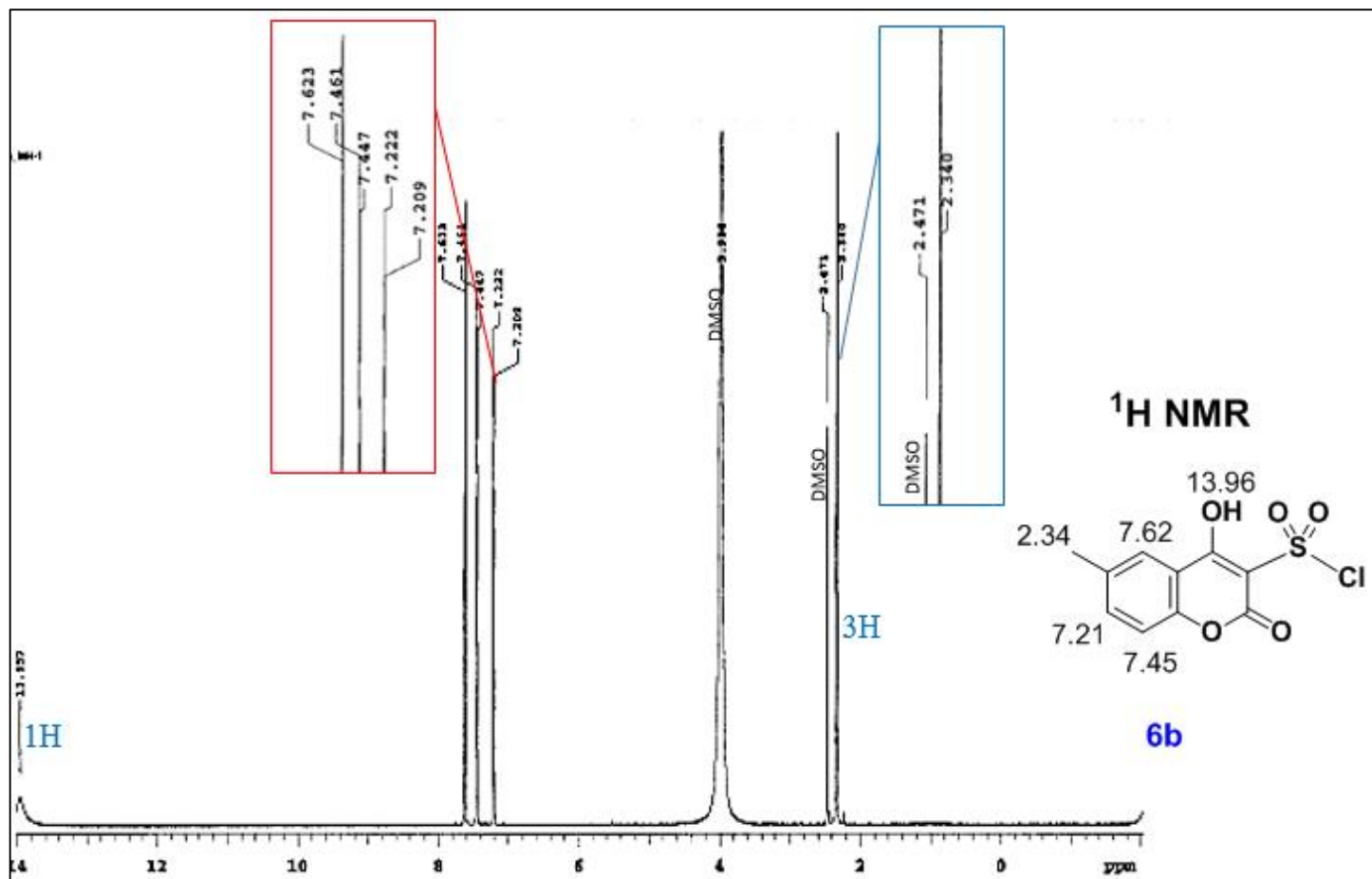


Figure S9: ¹H-NMR spectrum of compound **6b** in DMSO-d₆ (600 MHz).

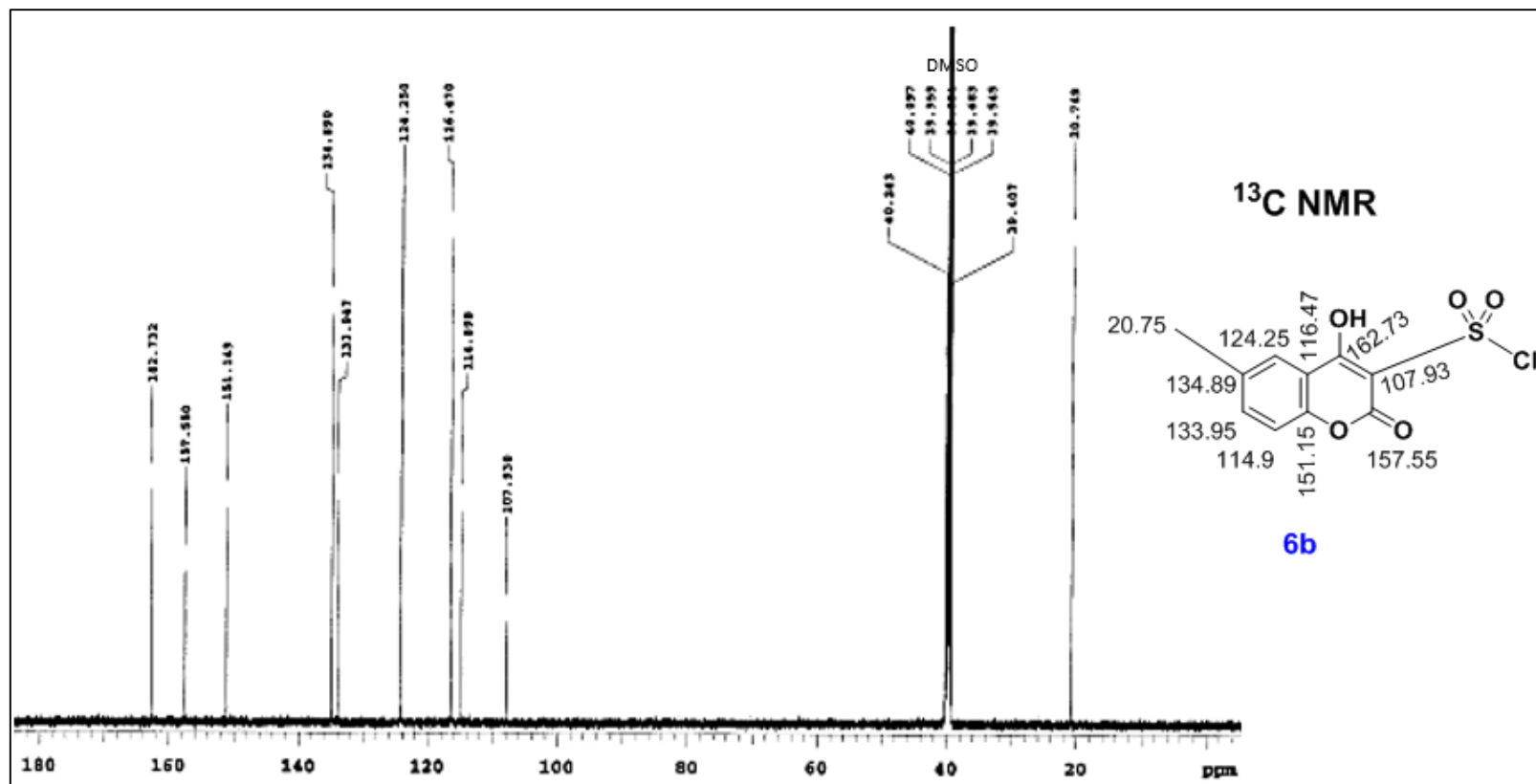


Figure S10a: ¹³C-NMR spectrum of compound **6b** in DMSO-d₆ (154 MHz).

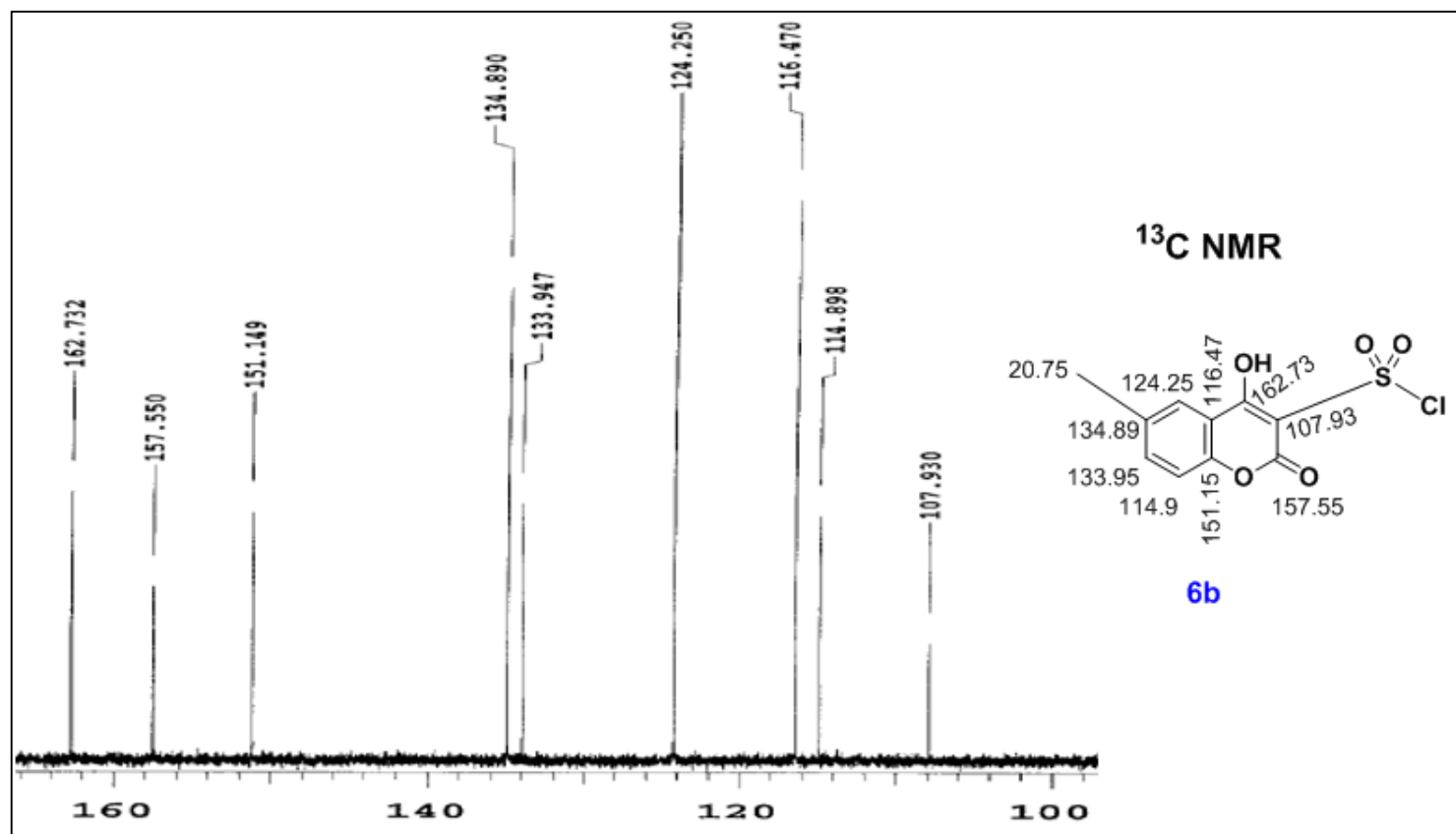


Figure S10b: ¹³C-NMR spectrum of compound **6b** in DMSO-d₆ (154 MHz).

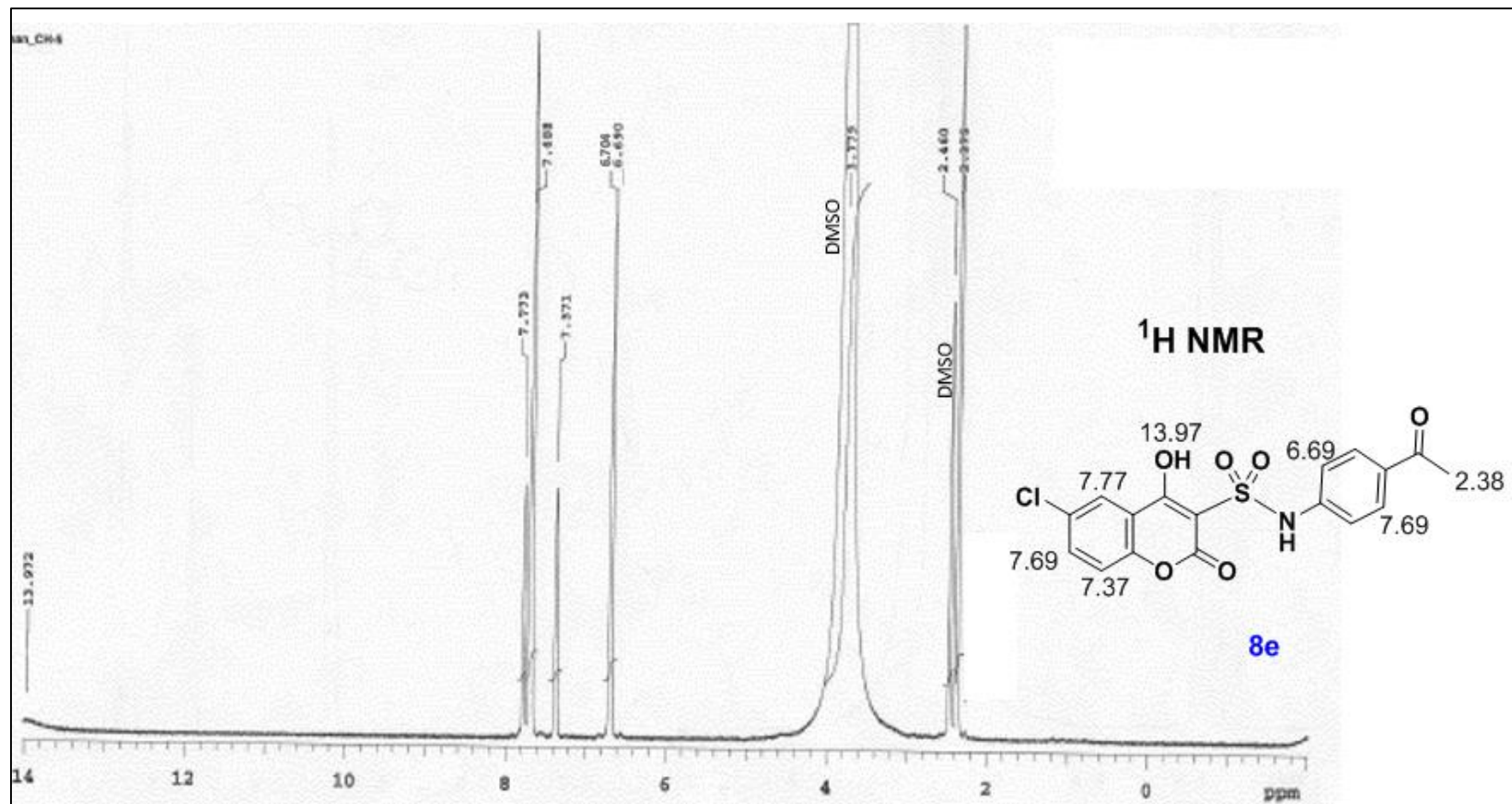


Figure S11: ¹H-NMR spectrum of compound **8e** in DMSO-d₆ (600 MHz).

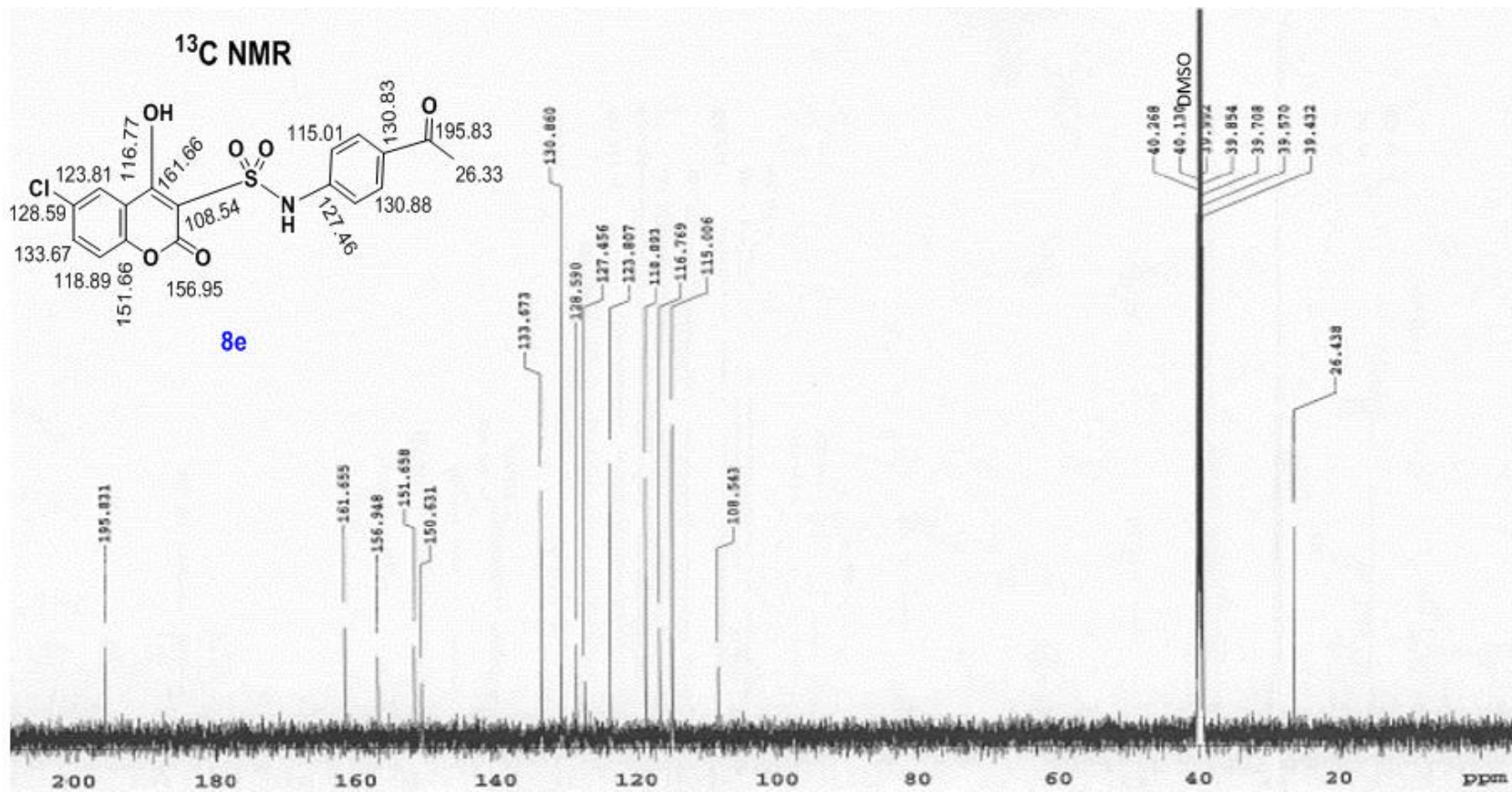


Figure S12: ¹³C-NMR spectrum of compound **8e** in DMSO-d₆ (154 MHz).

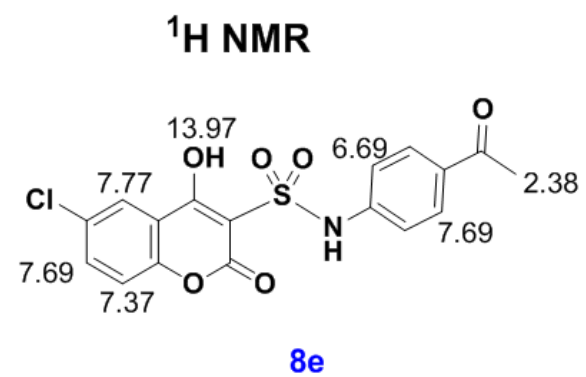
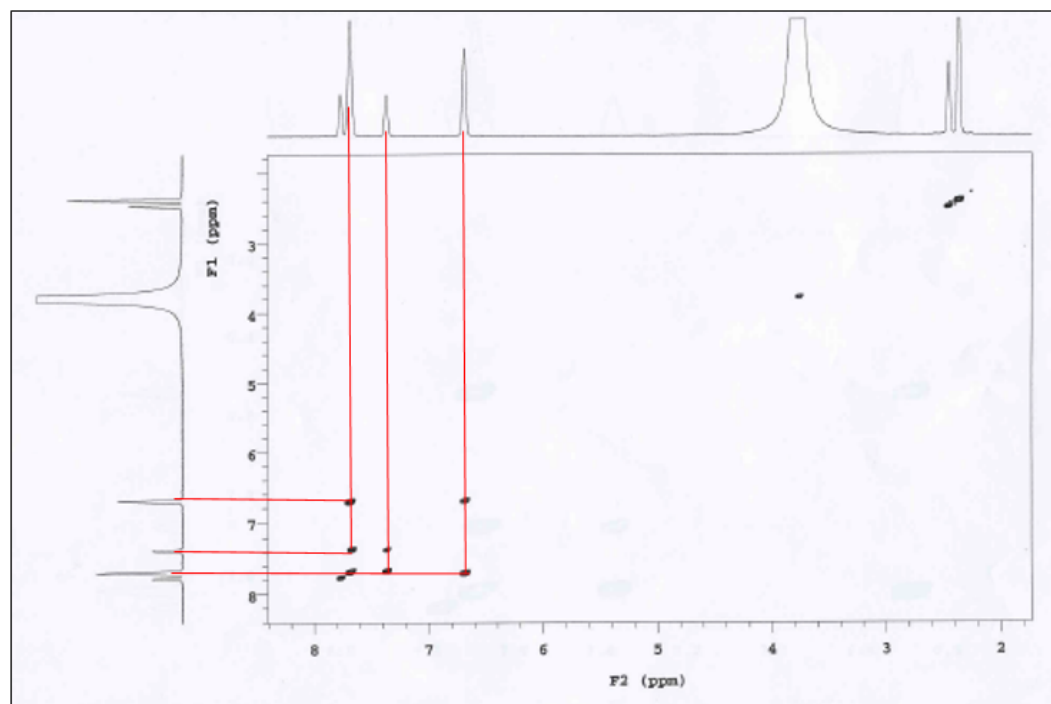


Figure S13: ^1H - ^1H -Homomuclear COSY NMR spectrum of compound **8e** in DMSO- d_6 (600 MHz).

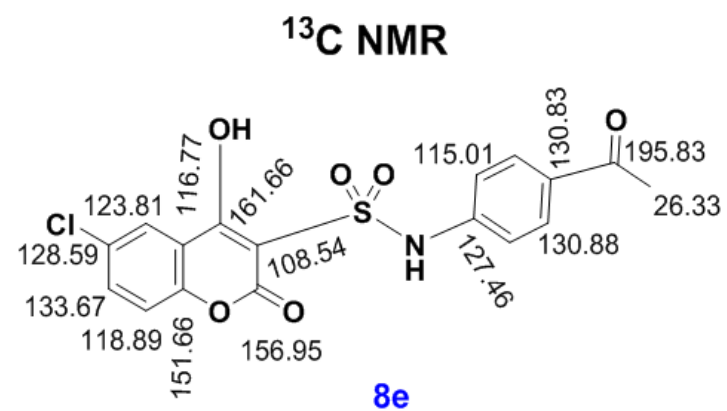
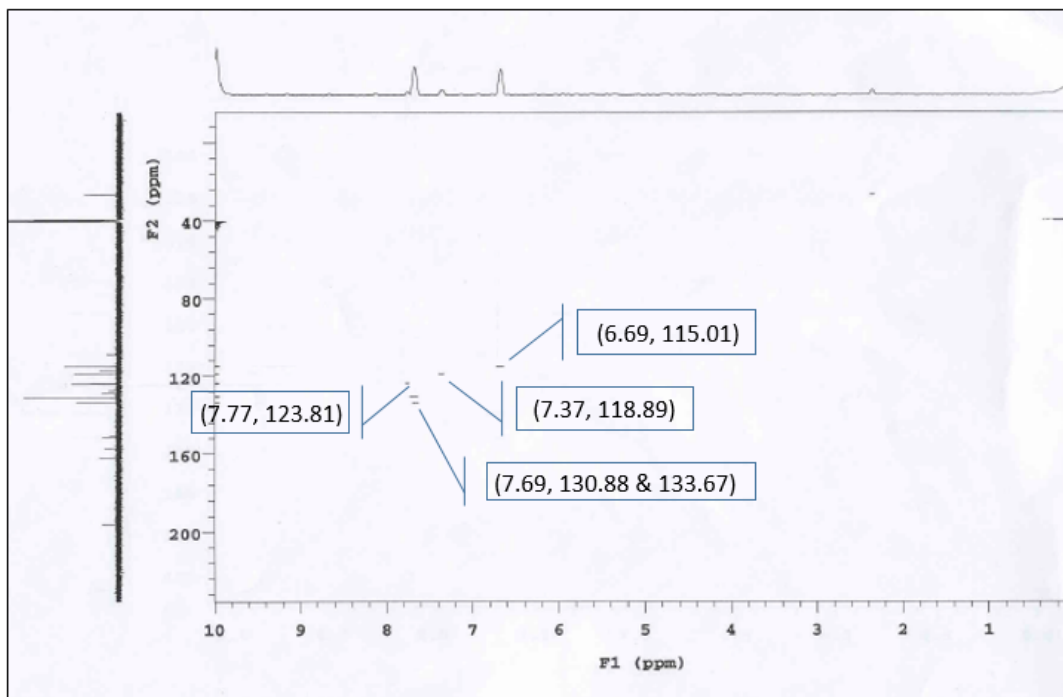
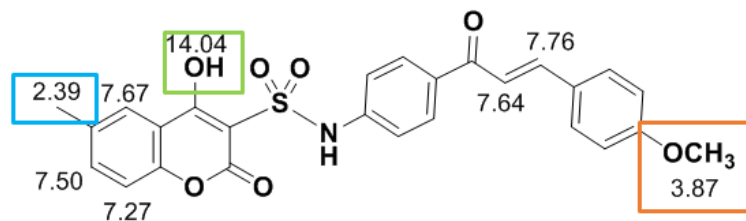


Figure S14: ^1H - ^{13}C -Heteronuclear COSY NMR spectrum of compound **8e** in DMSO-d_6 (600/154 MHz).



Ar-H:
6.83, 7.01, 7.82, 8.00

9f

¹H NMR

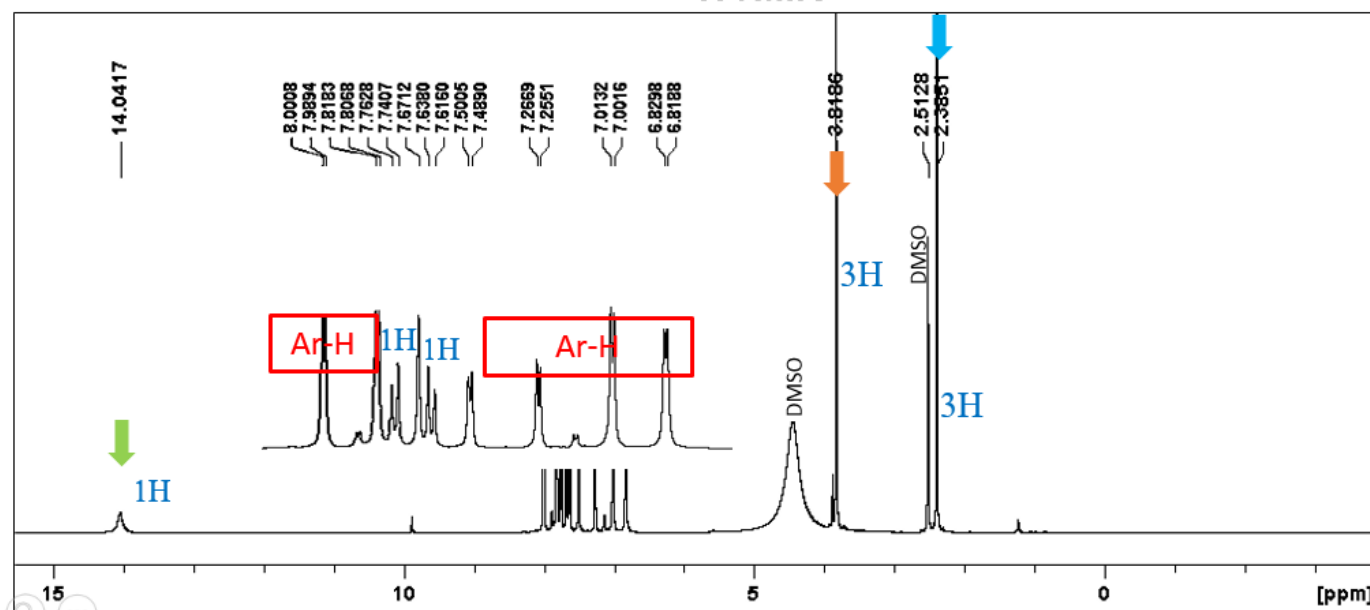
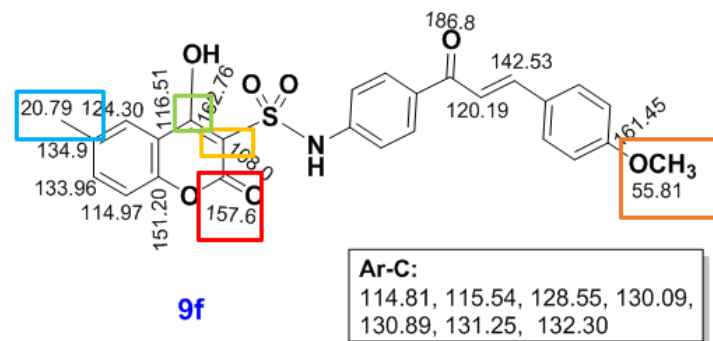


Figure S15: ¹H-NMR spectrum of compound **9f** in DMSO-d₆ (700 MHz).



9f

^{13}C NMR

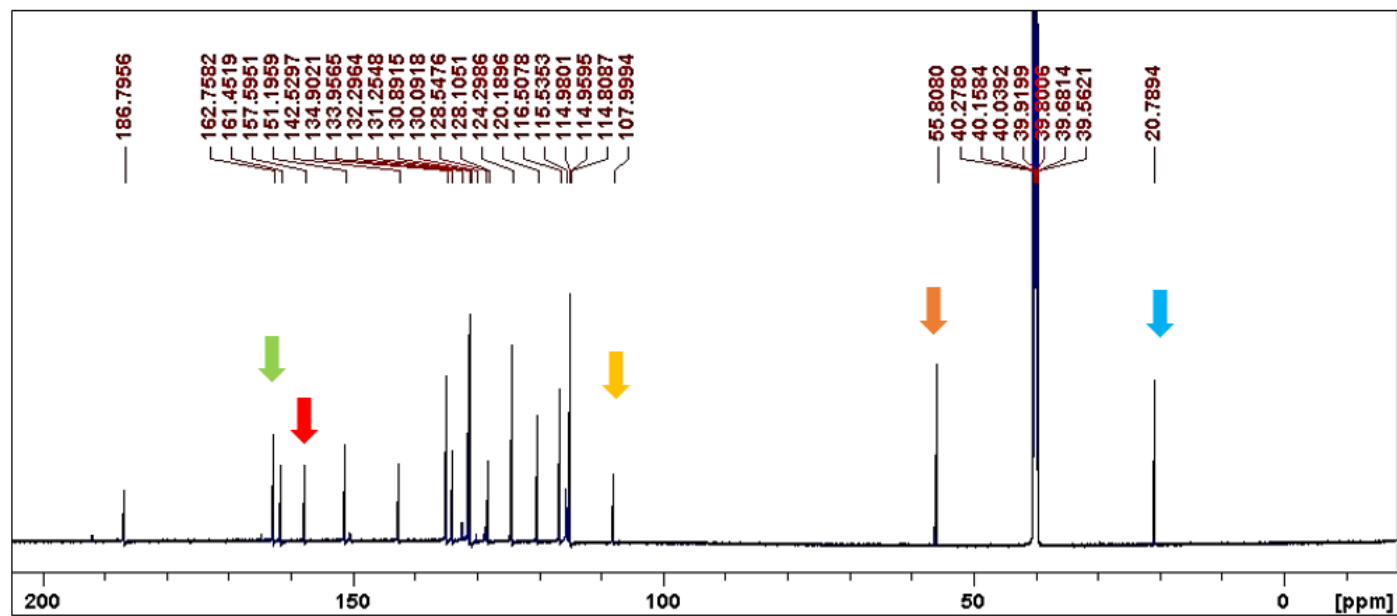


Figure S16: ^{13}C -NMR spectrum of compound 9f in DMSO- d_6 (176 MHz).

Table S1: X-ray Crystallographic data of Compound **2a**: Bond precision: C-C = 0.0020 Å, Wavelength=0.71073, Cell: a=6.1640(4) b=20.1792(14) c=13.4613(9) °=90, °=95.956(2), °=90, Temperature: 123 K, Correction method= # Reported T Limits: Tmin=0.721 Tmax=0.746, AbsCorr = MULTI-SCAN, Data completeness= 1.000, Theta(max)= 29.998, R(reflections)= 0.0478(3442), wR2(reflections)= 0.1142(4853), S = 1.017, Npar= 262.

	Calculated	Reported
Volume	1665.34(19)	1665.34(19)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C ₂₀ H ₁₃ N ₃ O ₅	C ₂₀ H ₁₃ N ₃ O ₅
Sum formula	C ₂₀ H ₁₃ N ₃ O ₅	C ₂₀ H ₁₃ N ₃ O ₅
Mr	375.33	375.33
Dx,g cm-3	1.497	1.497
Z	4	4
Mu (mm-1)	0.110	0.110
F000	776.0	776.0
F000'	776.41	
h,k,lmax	8,28,18	8,28,18
Nref	4855	4853
Tmin,Tmax	0.991,0.995	0.721,0.746
Tmin'	0.970	