

“Annulated Isoxazoles via [3+2] Cycloaddition of Alkenyl Bromides and Oximoyl Chlorides and Ag(I) Promoted Elimination”

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1. Solid State Molecular Structures

Table 1. X-ray crystallography data for compounds **6a** and **7b**.

Compound	6a	7b
Formula	C ₁₃ H ₁₁ NO ₂	C ₁₄ H ₁₅ NO ₃
Formula weight	213.23	245.27
Color, habit	Colorless, blade	Yellow, tablet
Crystal size (mm)	0.03 x 0.10 x 0.29	0.15 x 0.24 x 0.29
Crystal system	Orthorhombic	Monoclinic
Lattice type	Primitive	Primitive
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (#19)	<i>P</i> 2 ₁ / <i>c</i> (#14)
a(Å)	7.6193	7.7658
b(Å)	10.9707	11.9846
c(Å)	11.8577	13.1138
α(deg)	90	90
β(deg)	90	94.745
γ(deg)	90	90
V(Å ³)	991.2	1216.3
Z	4	4
D _{calc} (g/cm ³)	1.429	1.339
F ₀₀₀	448.00	520.00
μ (MoKα) (cm ⁻¹)	7.90	0.95
2 θ _{max} (deg)	132.8	60.2
Total no. reflections	8924	21539
No. unique reflections	1725	3563
Residuals (F ² , all data) R1;wR2	0.048; 0.119	0.047; 0.108
Residuals (F) R1;wR2	0.046; 0.116	0.039; 0.103
Goodness of fit indicator	1.07	1.03

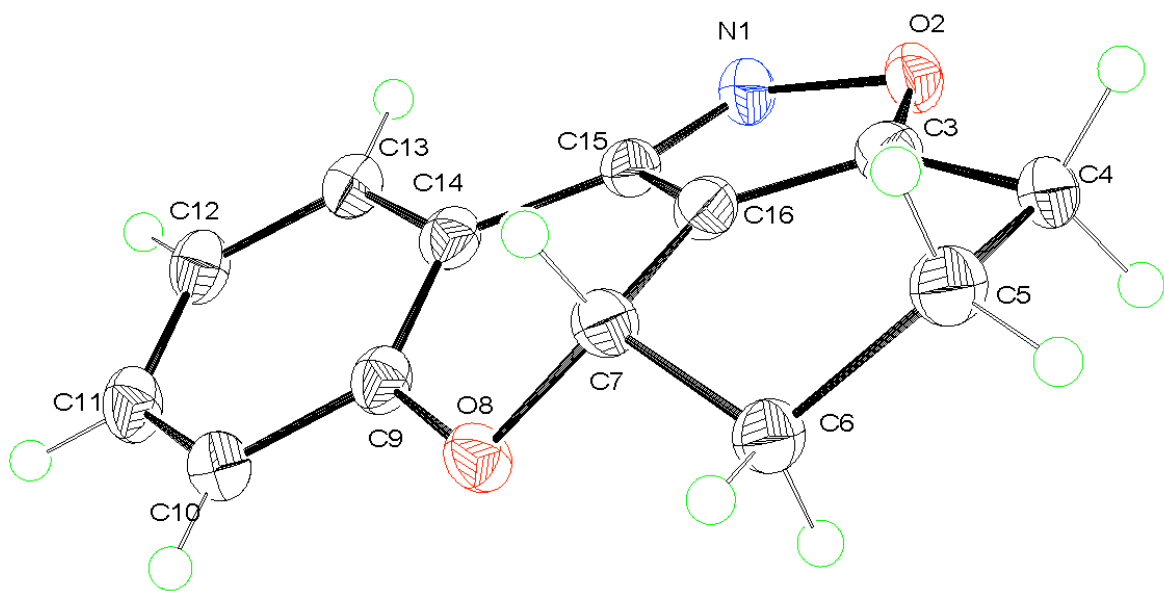


Figure 1. Solid state molecular structure of compound **6a**.

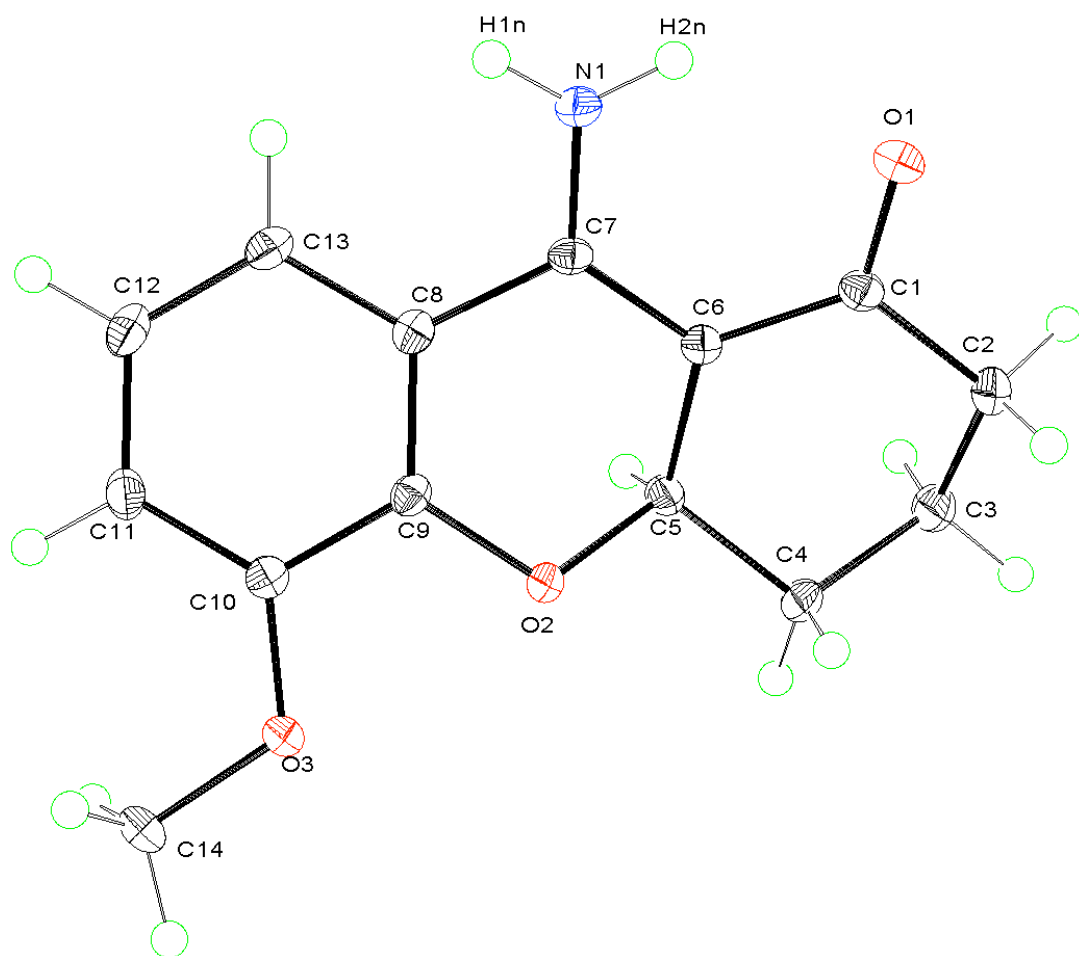


Figure 2. Solid state molecular structure of compound **7b**.

2. NMR spectra

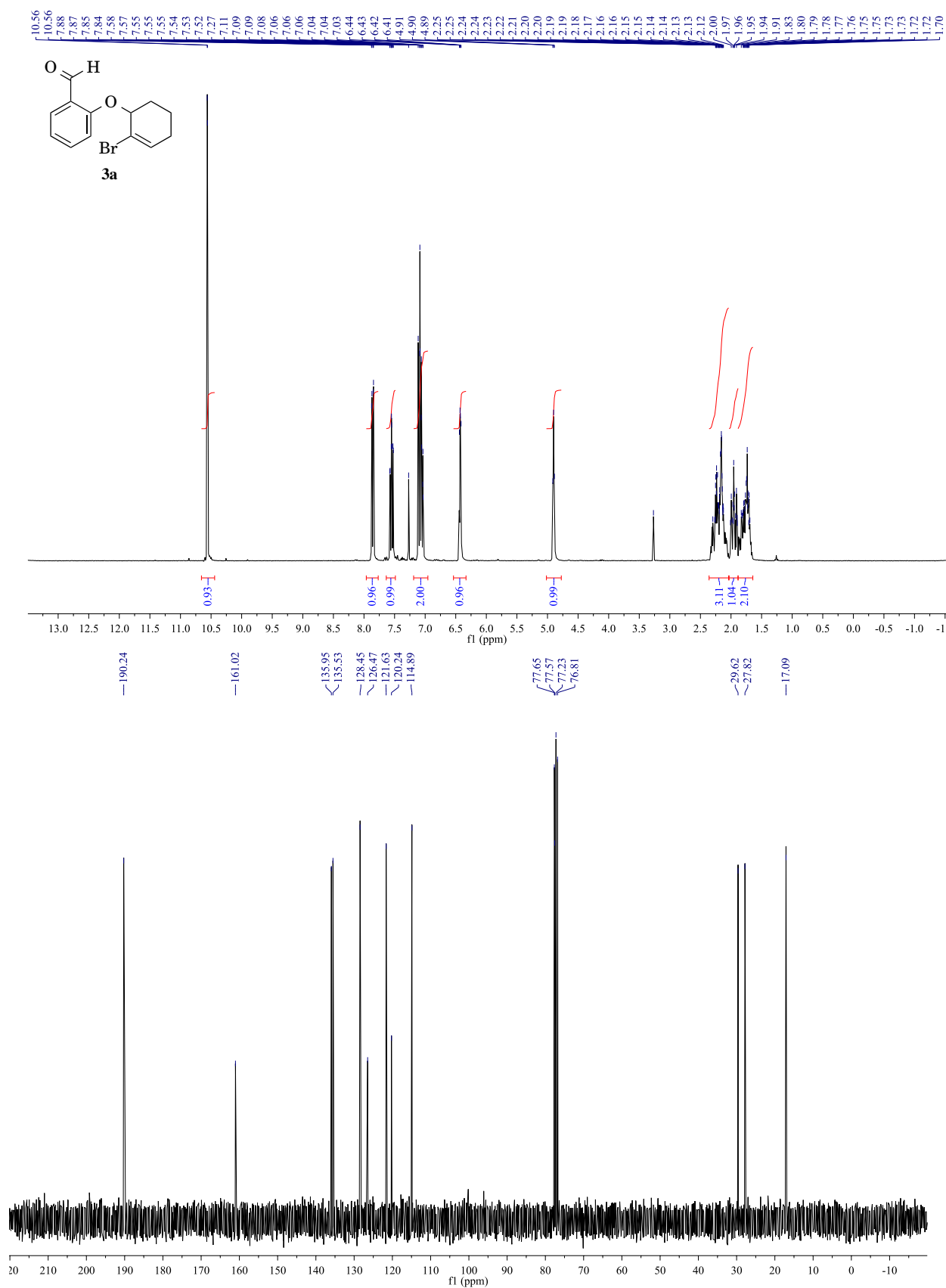


Figure 1: NMR spectra for compound **3a**

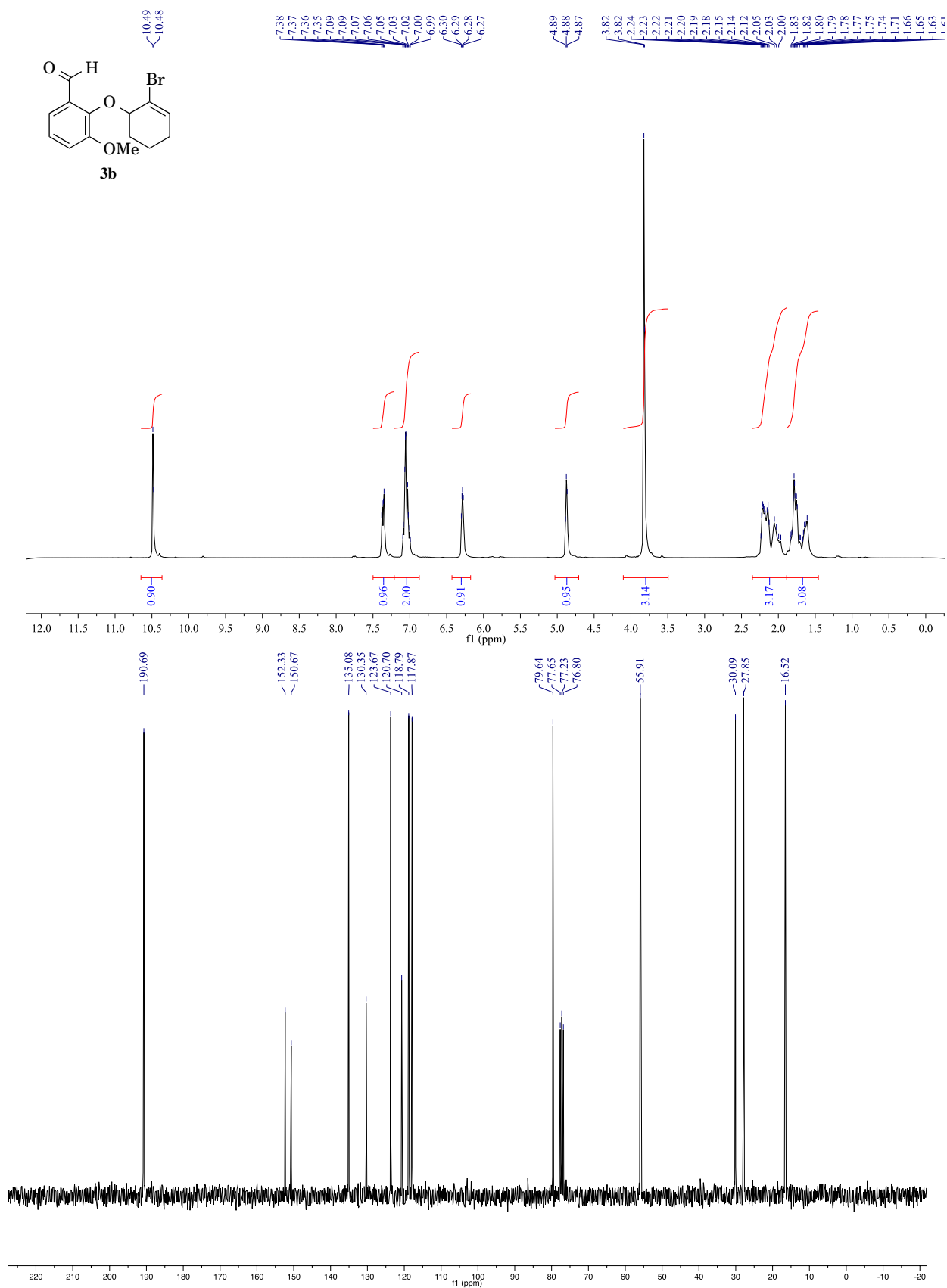


Figure 2: NMR spectra for compound **3b**

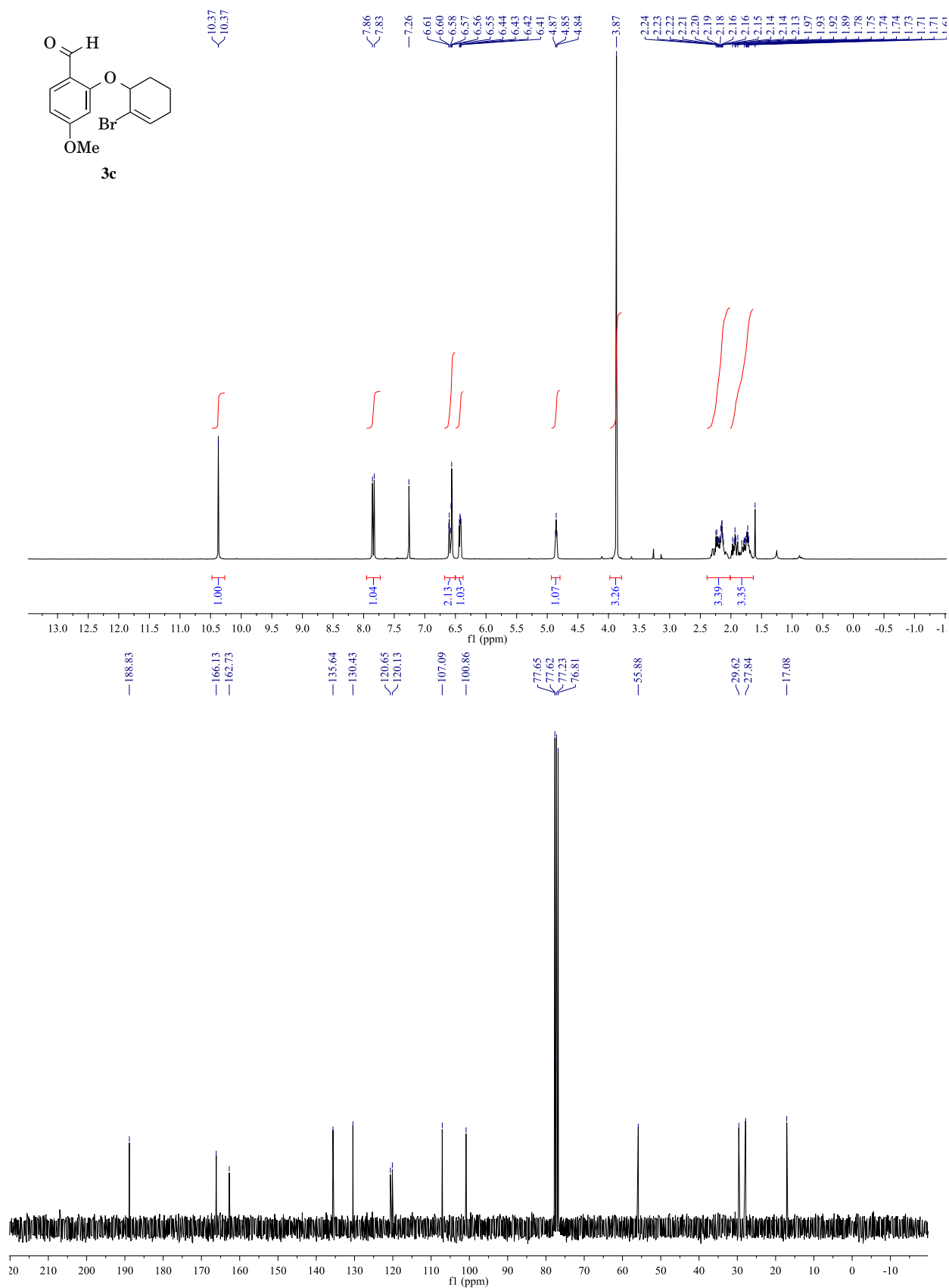


Figure 3: NMR spectra for compound **3c**

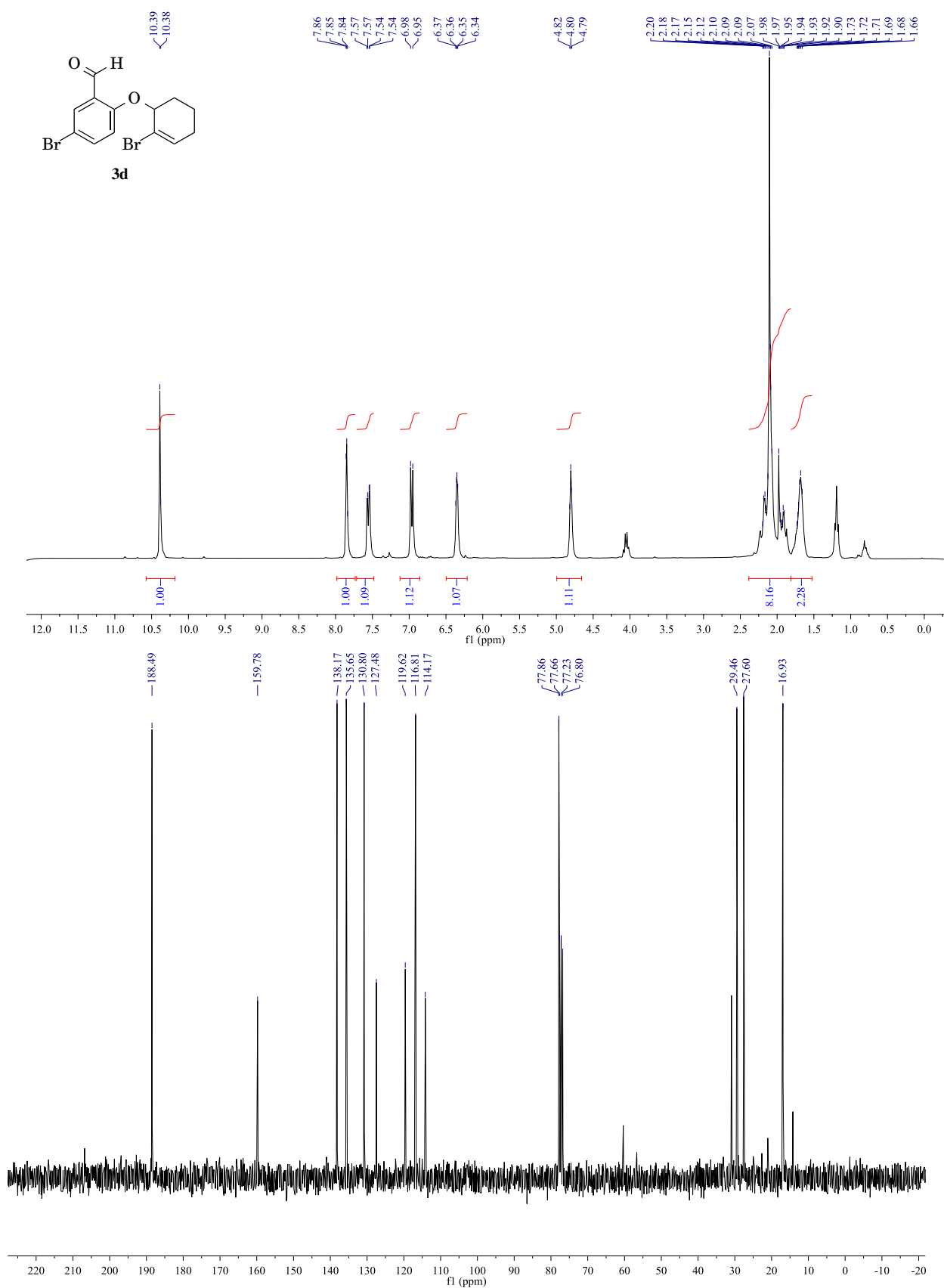


Figure 4: NMR spectra for compound **3d**

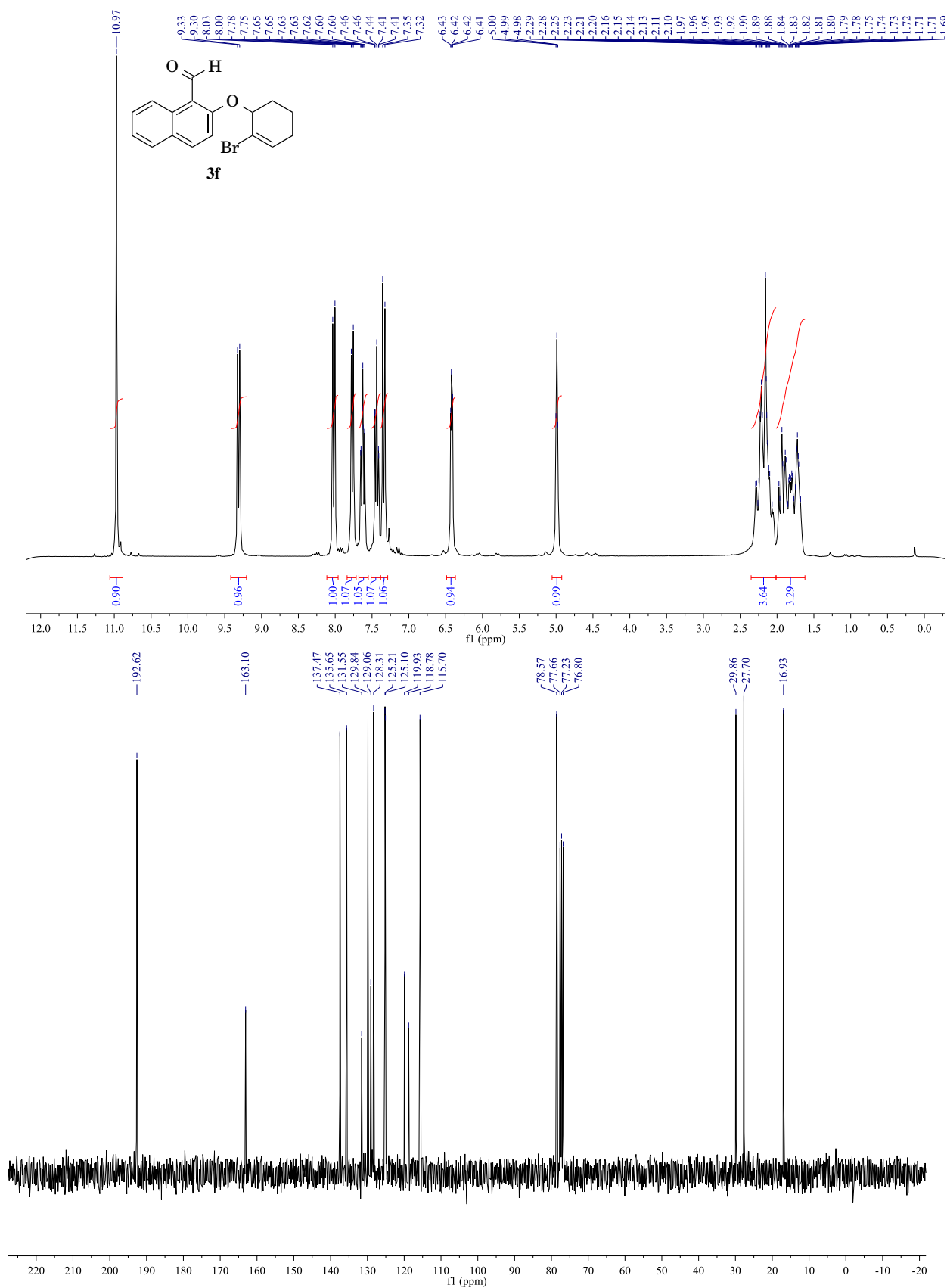


Figure 6: NMR spectra for compound **3f**

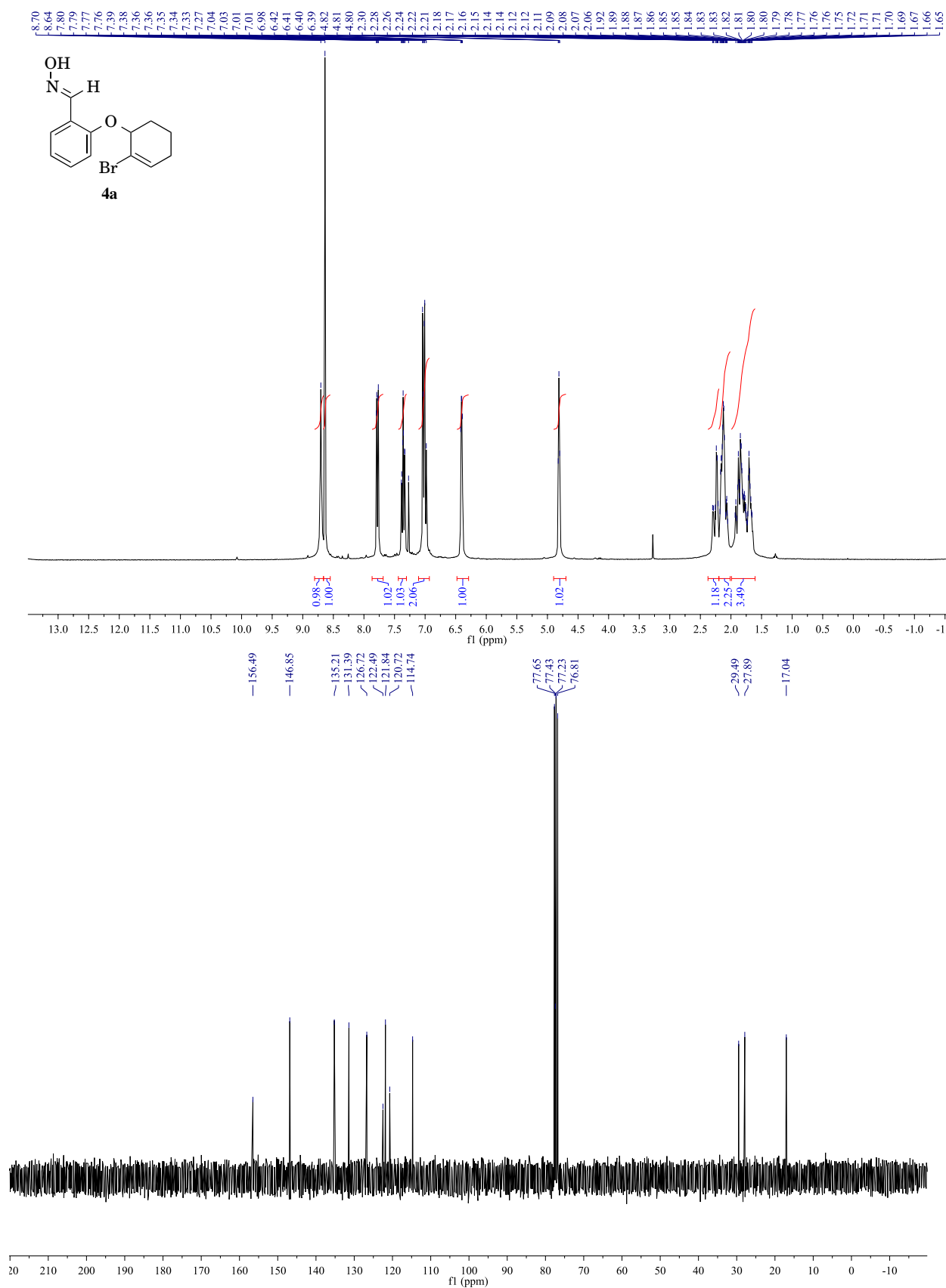


Figure 7: NMR spectra for compound **4a**

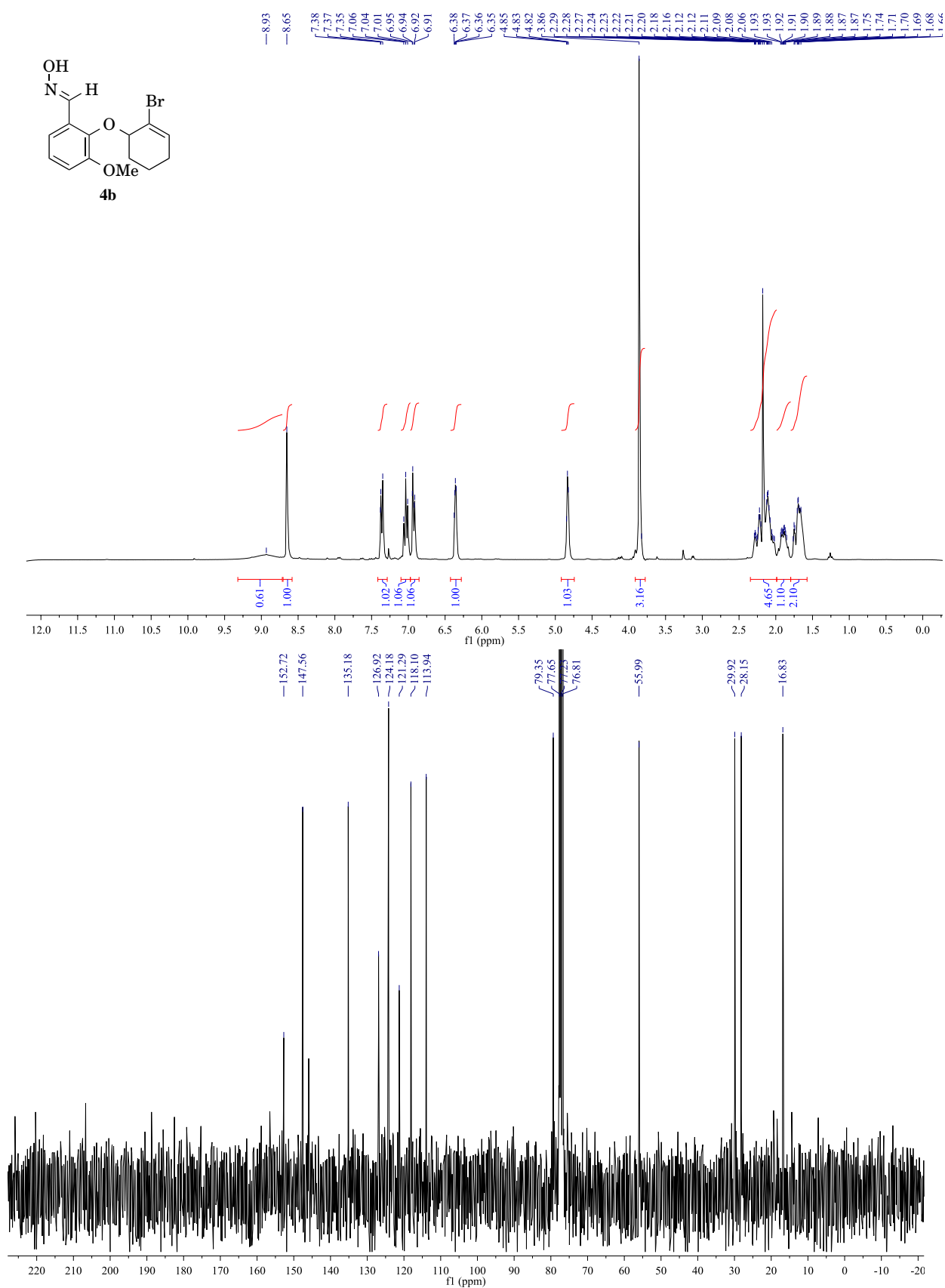


Figure 8: NMR spectra for compound **4b**

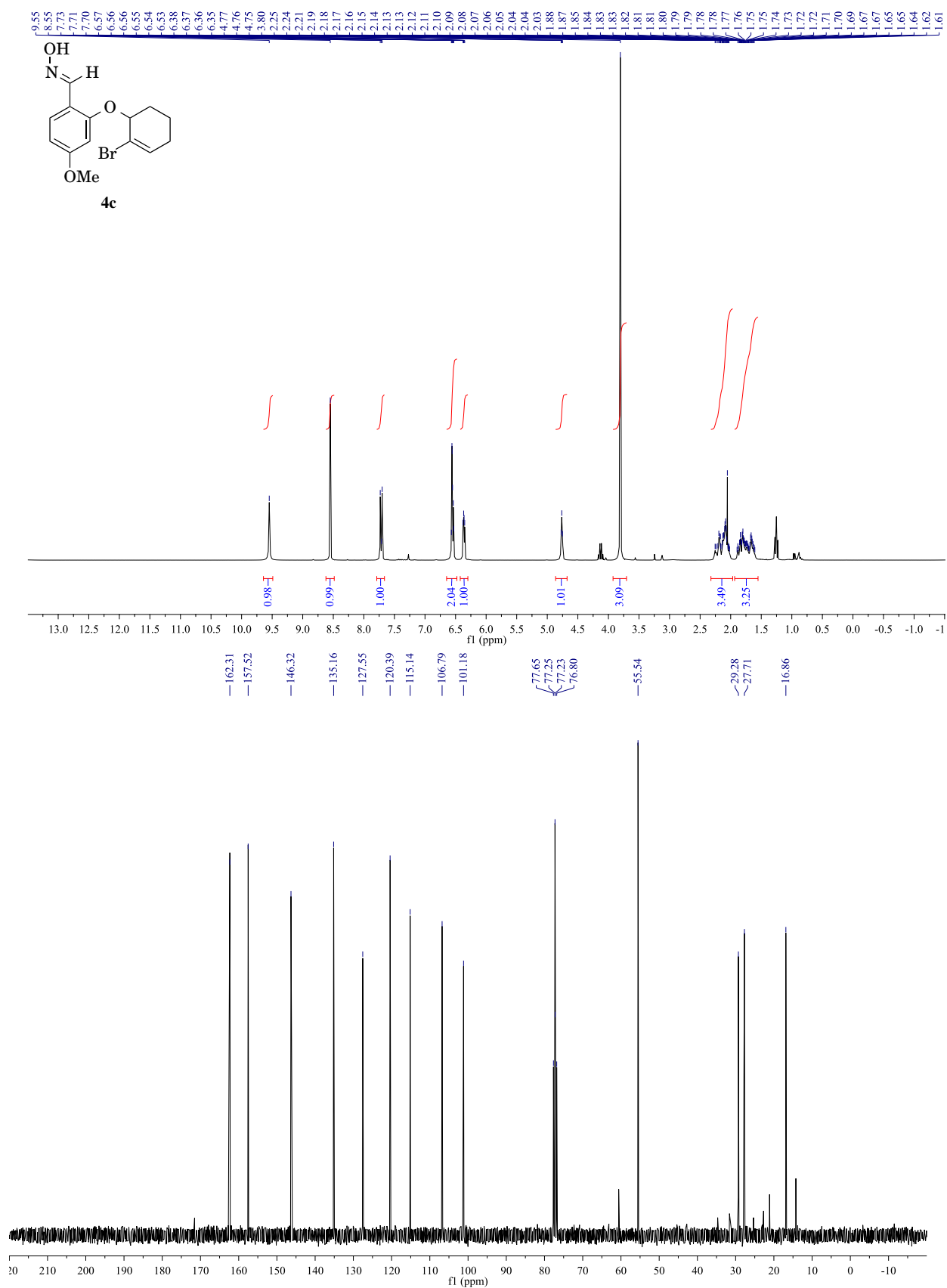


Figure 9: NMR spectra for compound **4c**

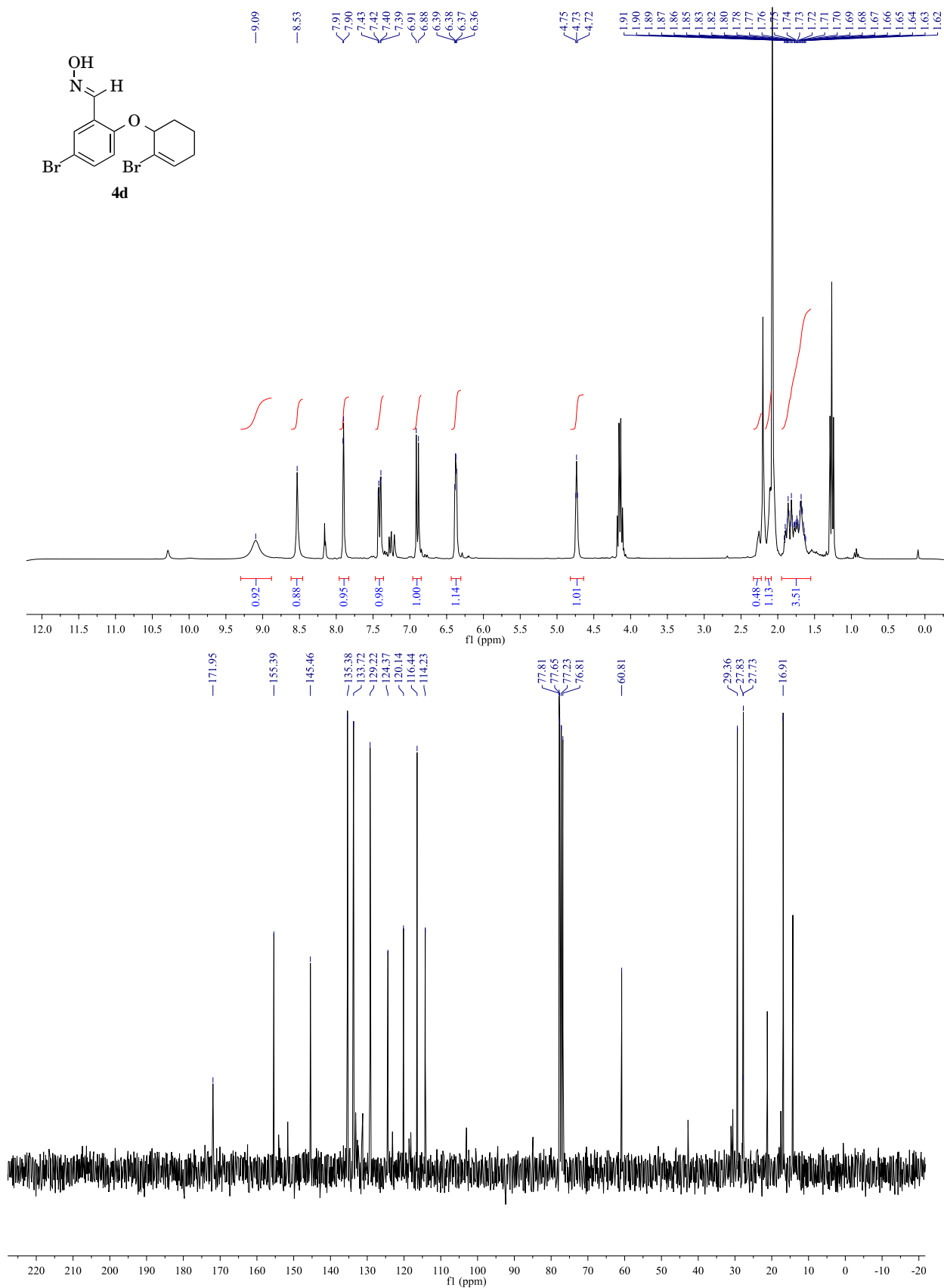


Figure 10: NMR spectra for compound **4d**

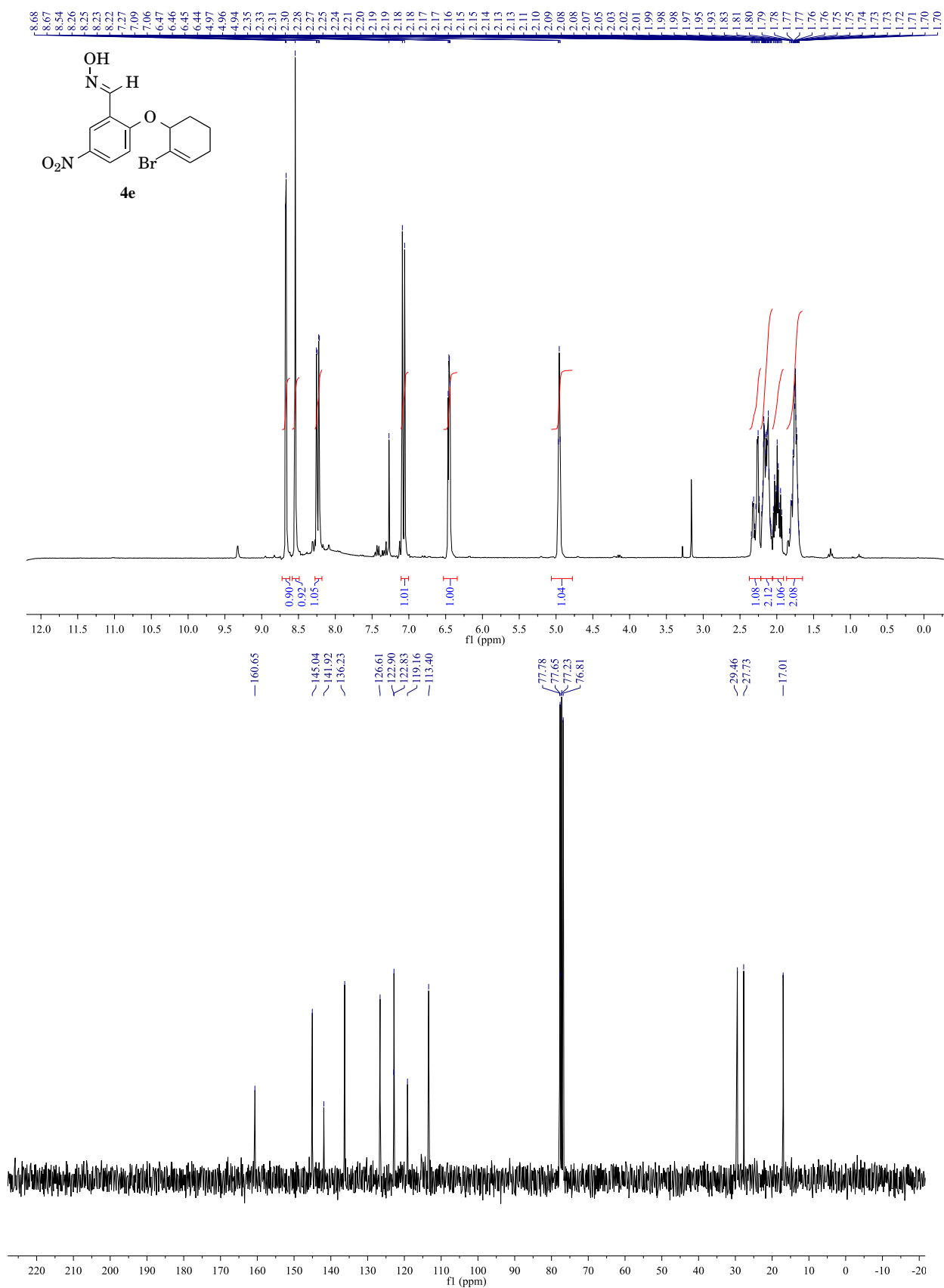


Figure 11: NMR spectra for compound **4e**

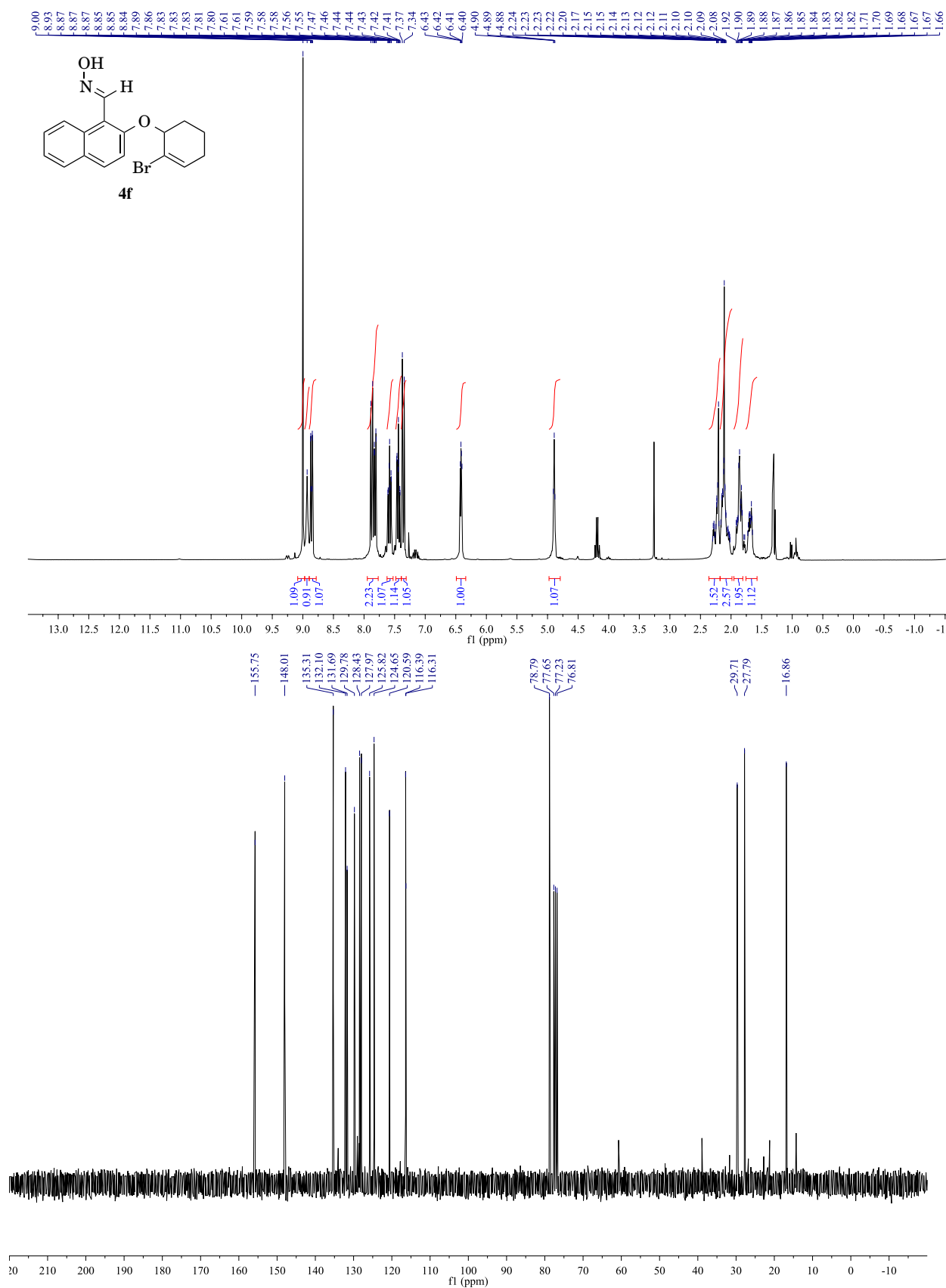


Figure 12: NMR spectra for compound **4f**

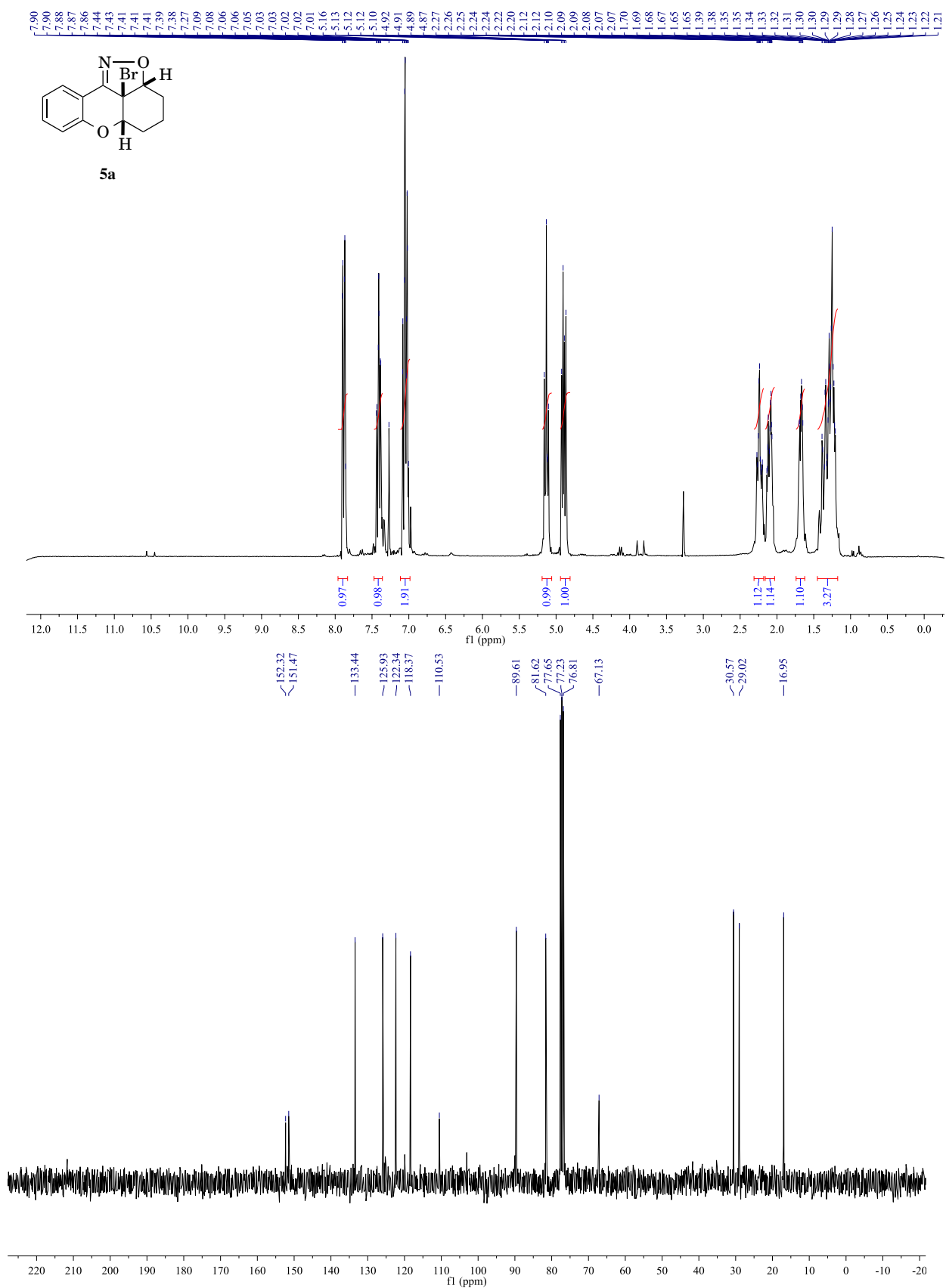


Figure 13: NMR spectra for compound **5a**

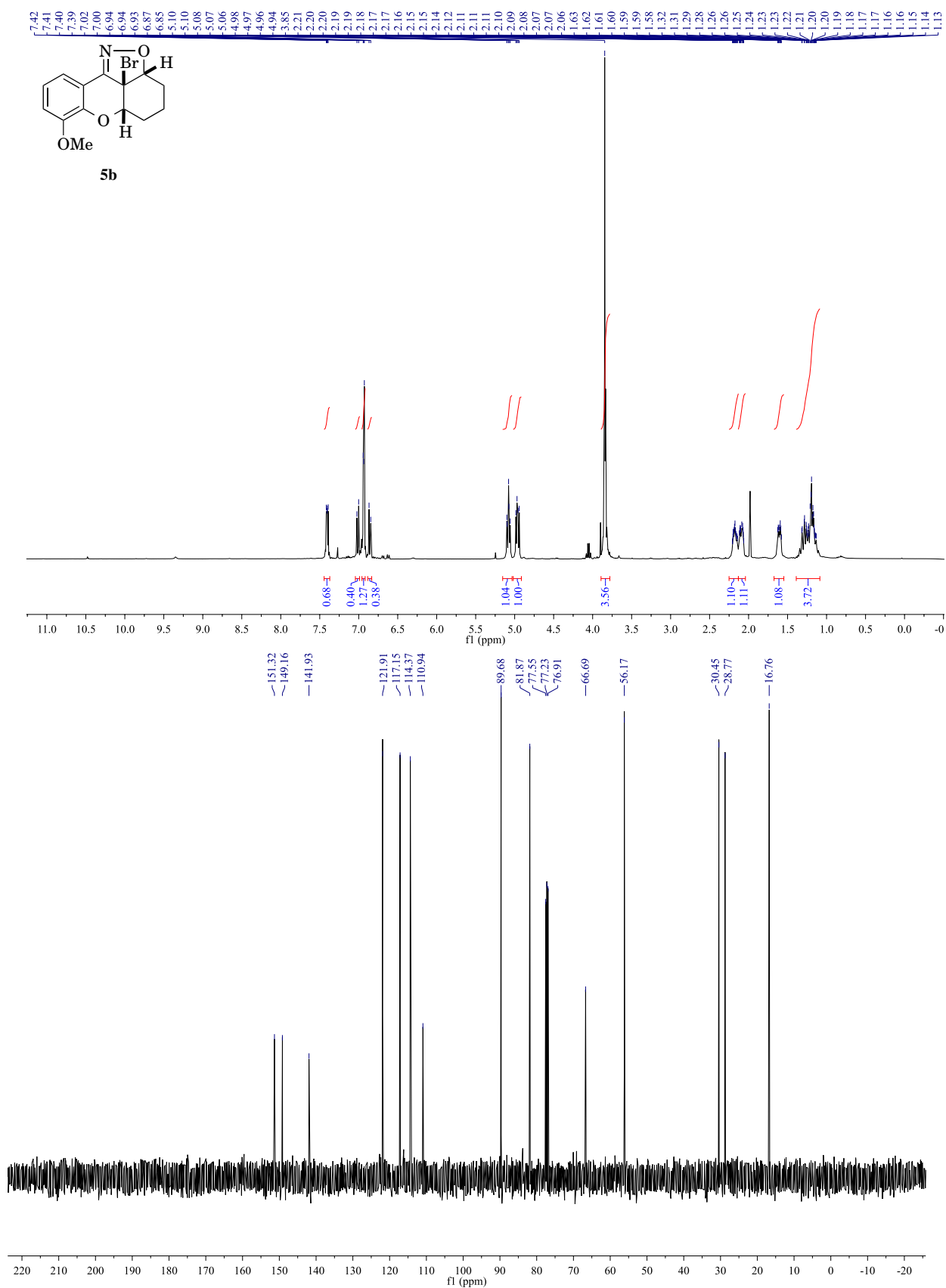


Figure 14: NMR spectra for compound **5b**

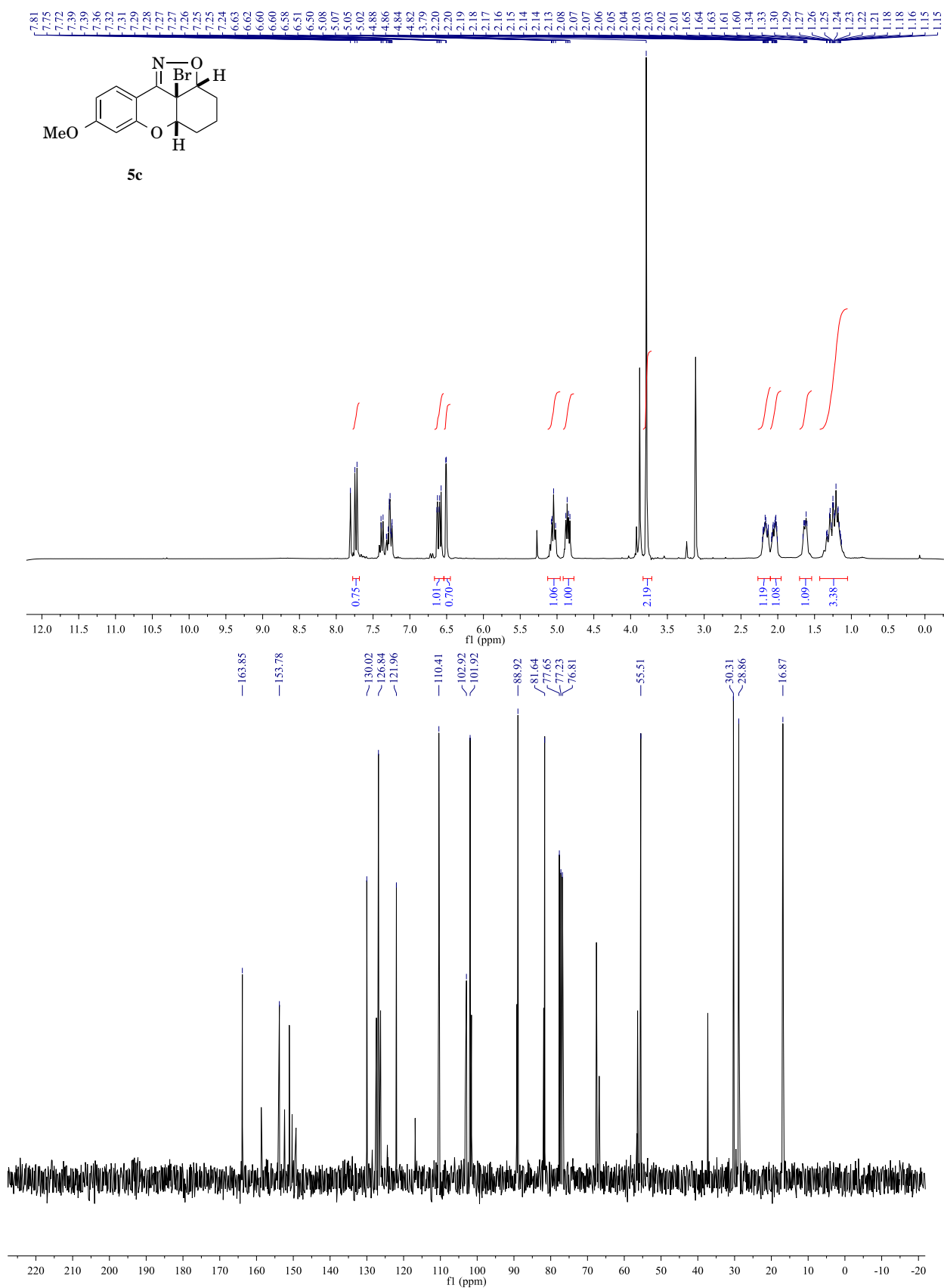


Figure 15: NMR spectra for compound **5c**

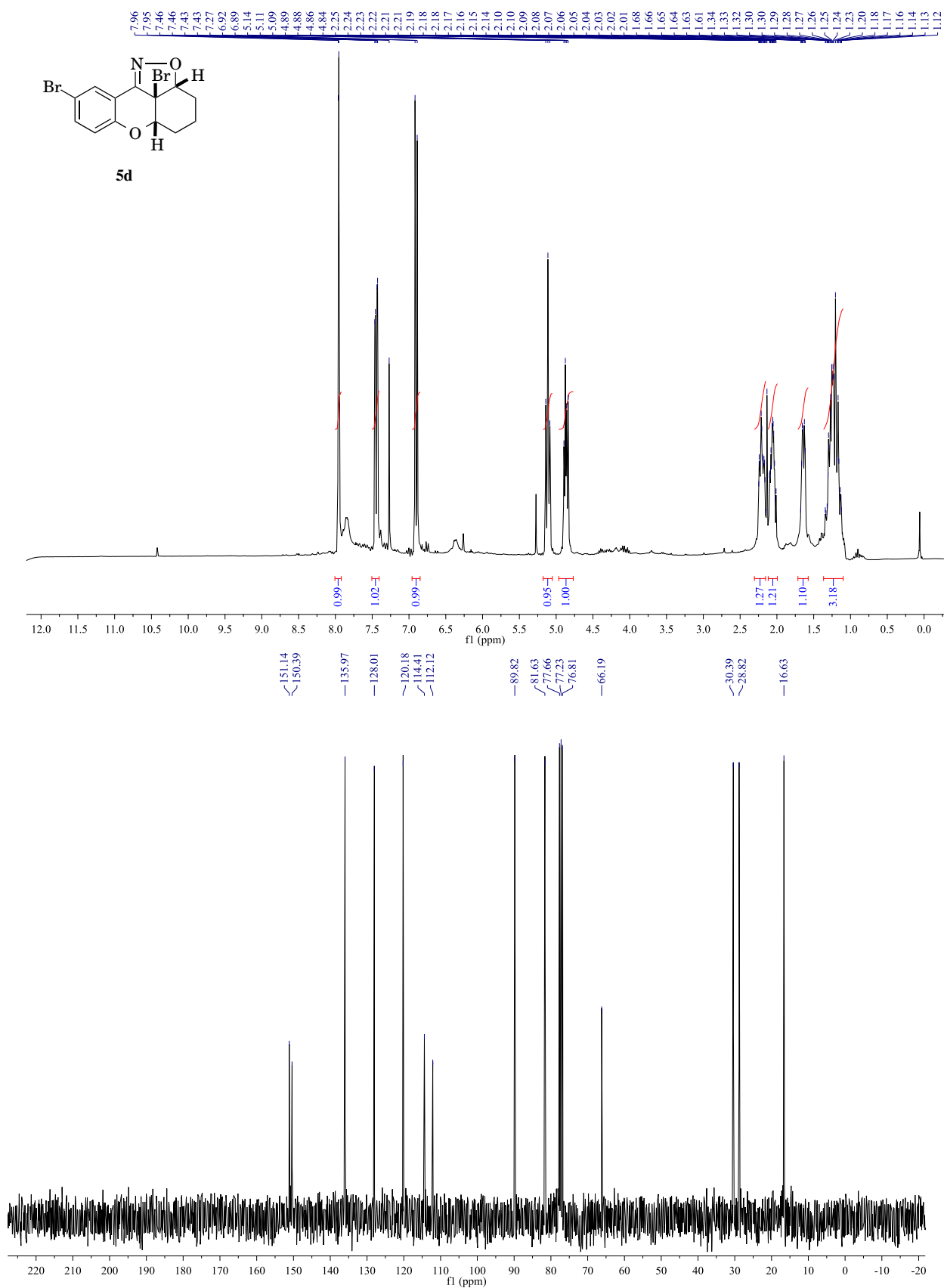


Figure 16: NMR spectra for compound **5d**

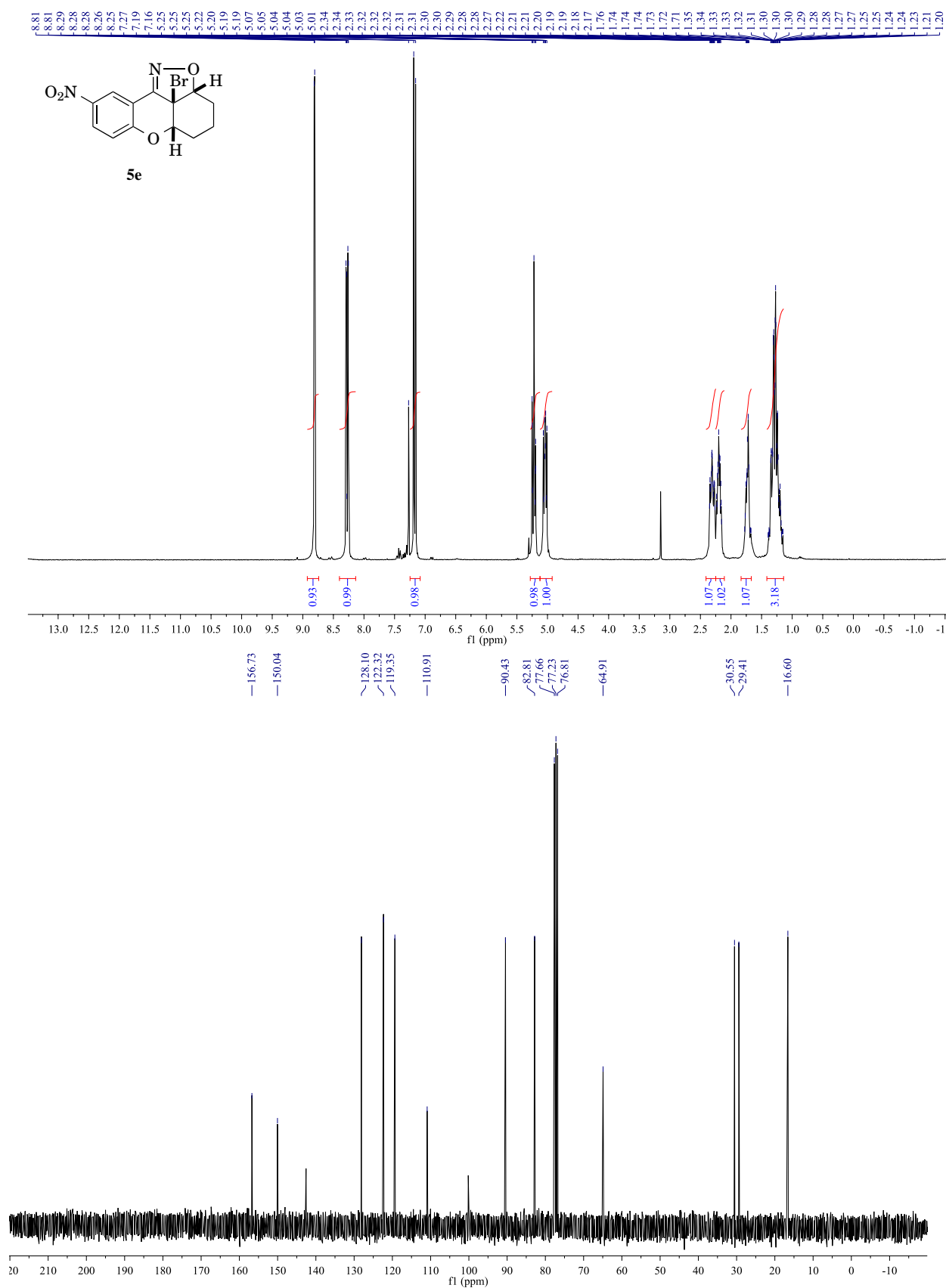


Figure 17: NMR spectra for compound **5e**

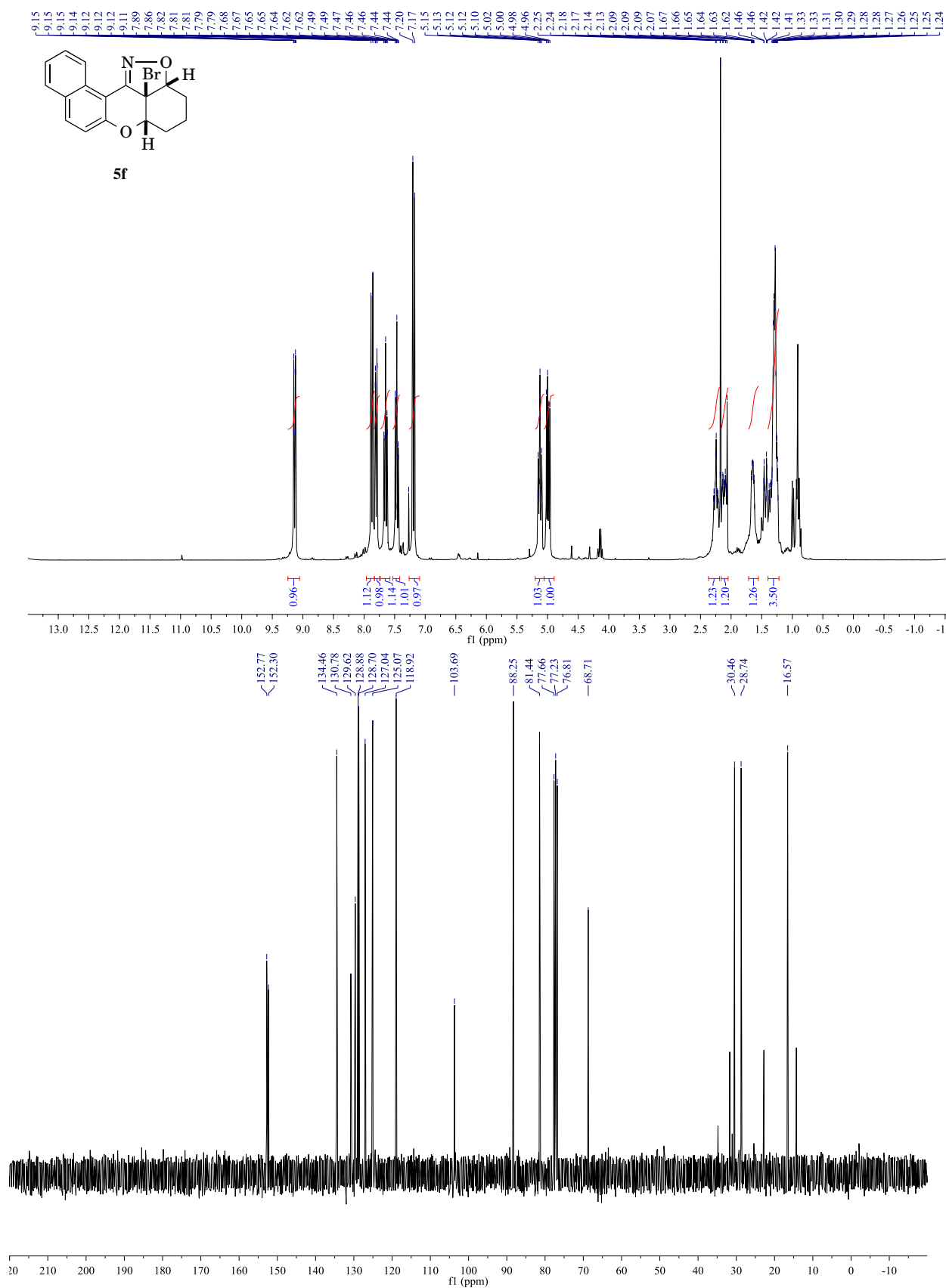


Figure 18: NMR spectra for compound **5f**

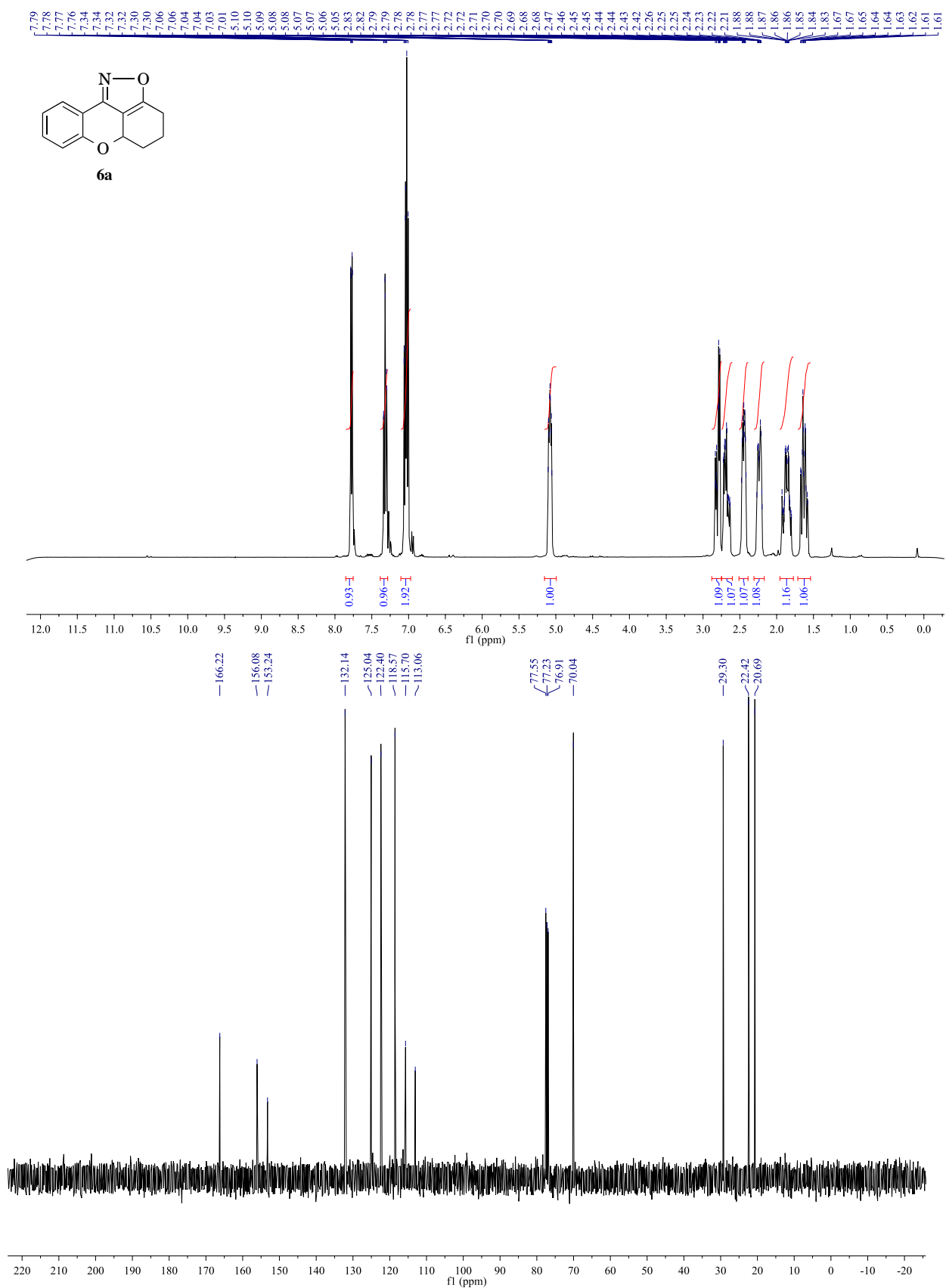


Figure 19: NMR spectra for compound **6a**

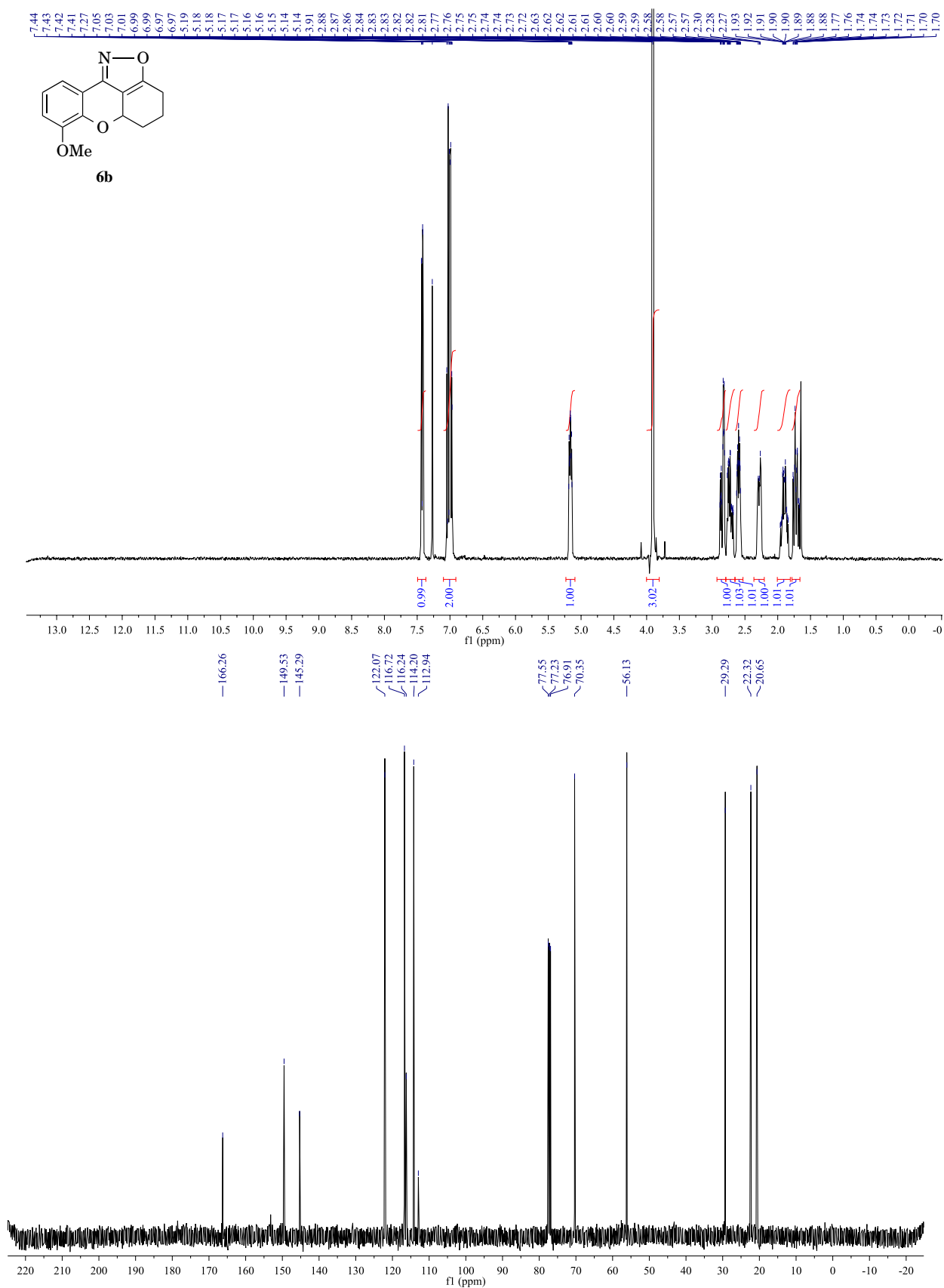


Figure 20: NMR spectra for compound **6b**

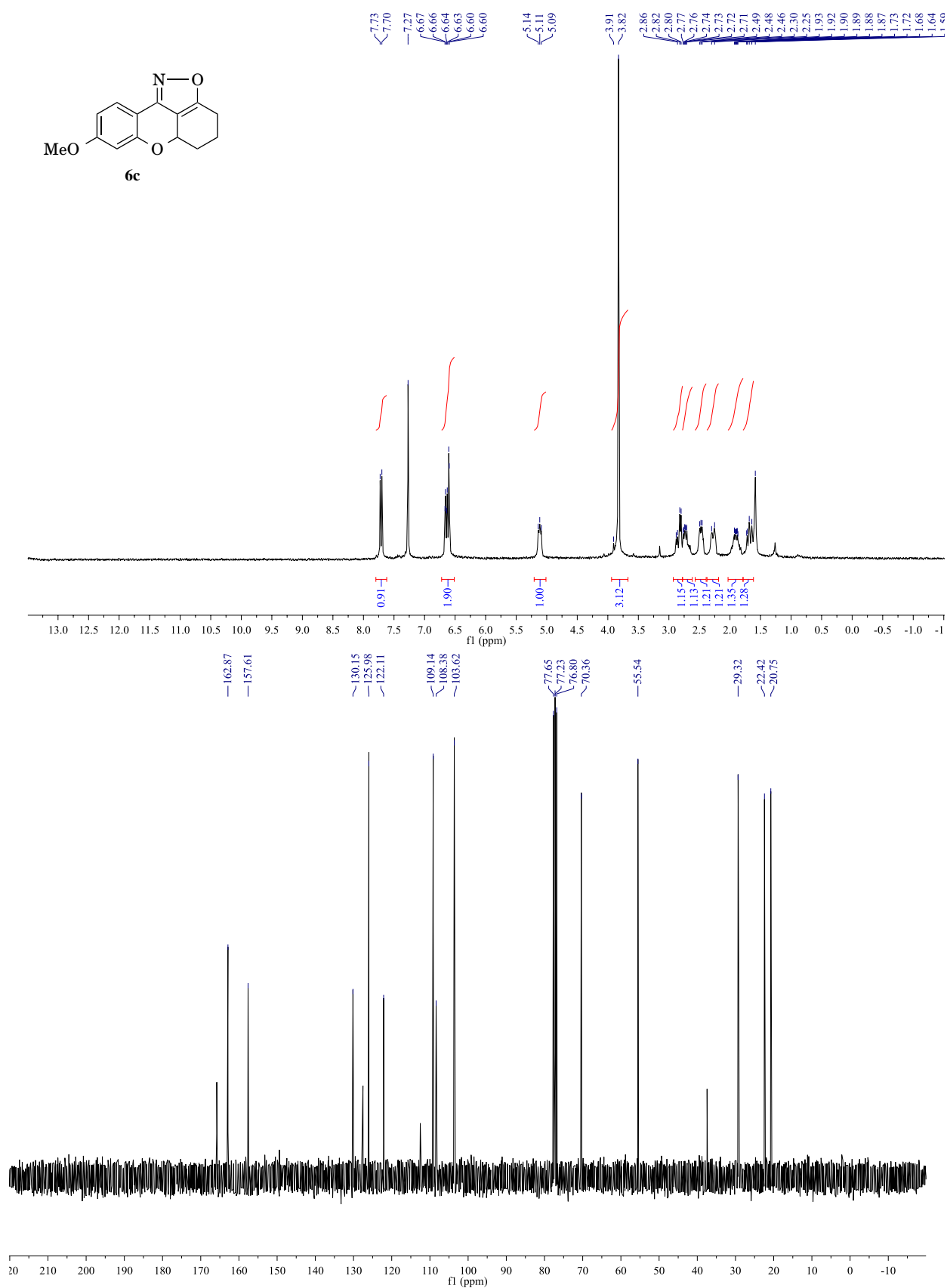


Figure 21: NMR spectra for compound **6c**

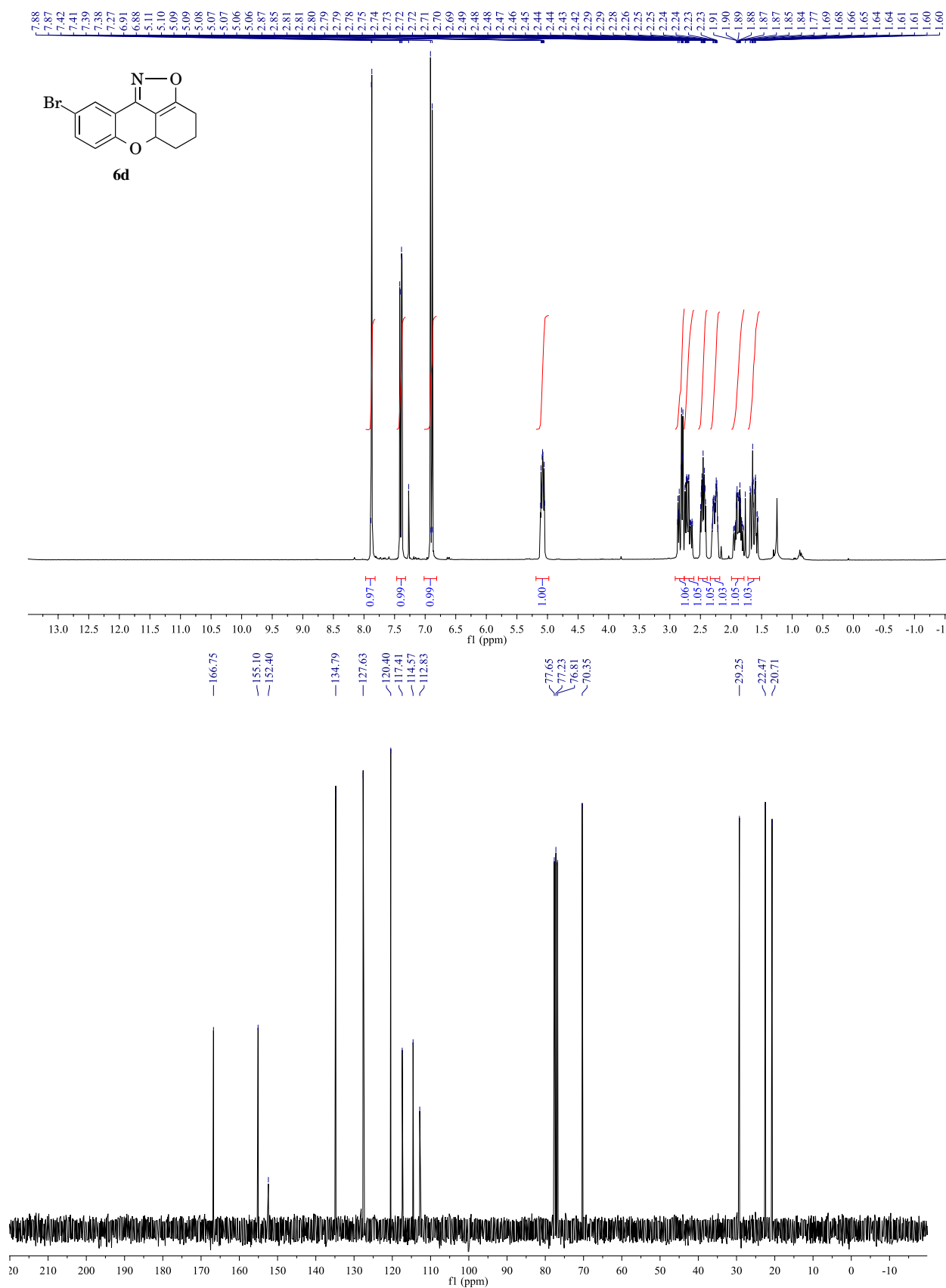


Figure 22: NMR spectra for compound **6d**

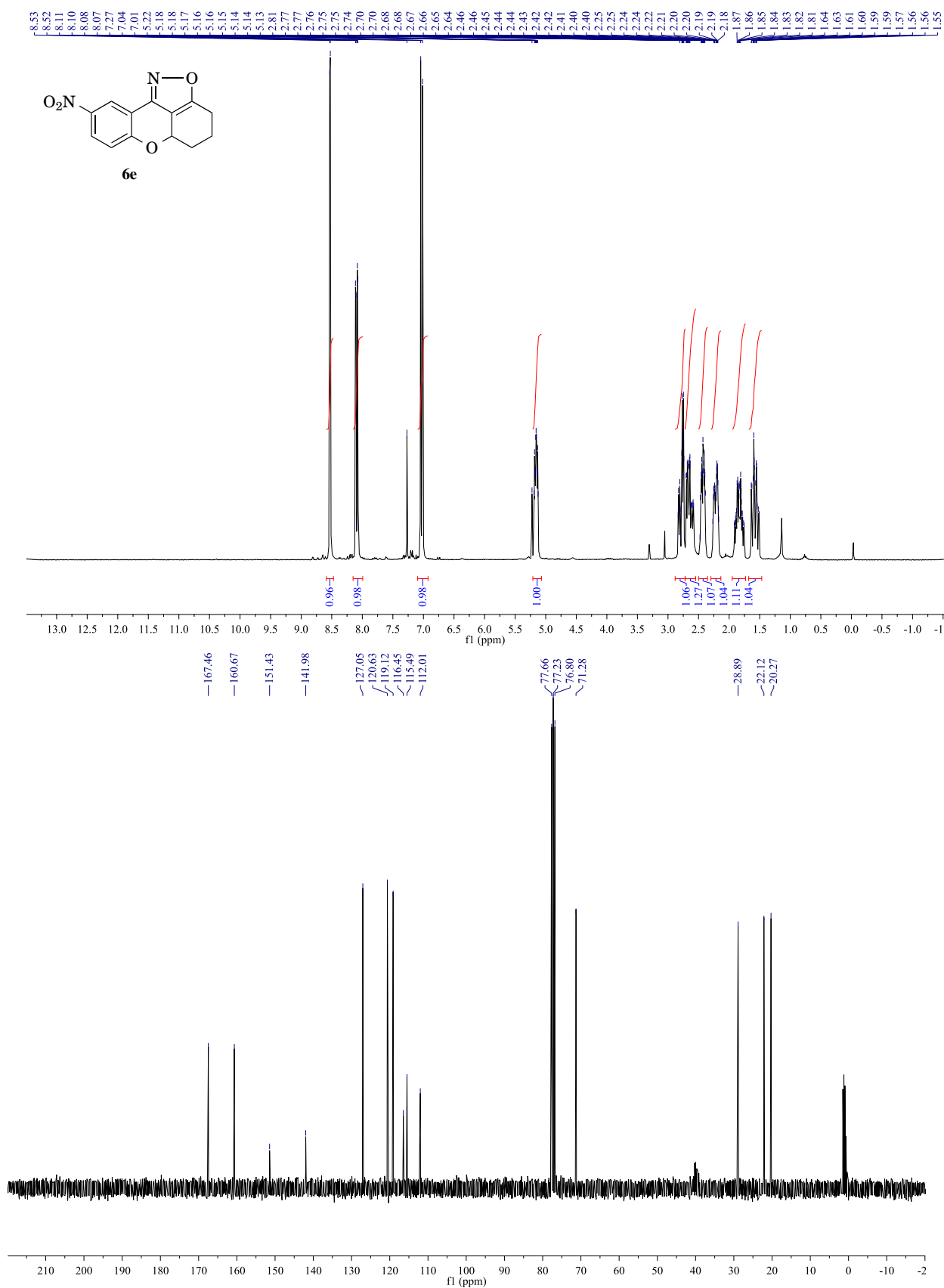


Figure 23: NMR spectra for compound **6e**

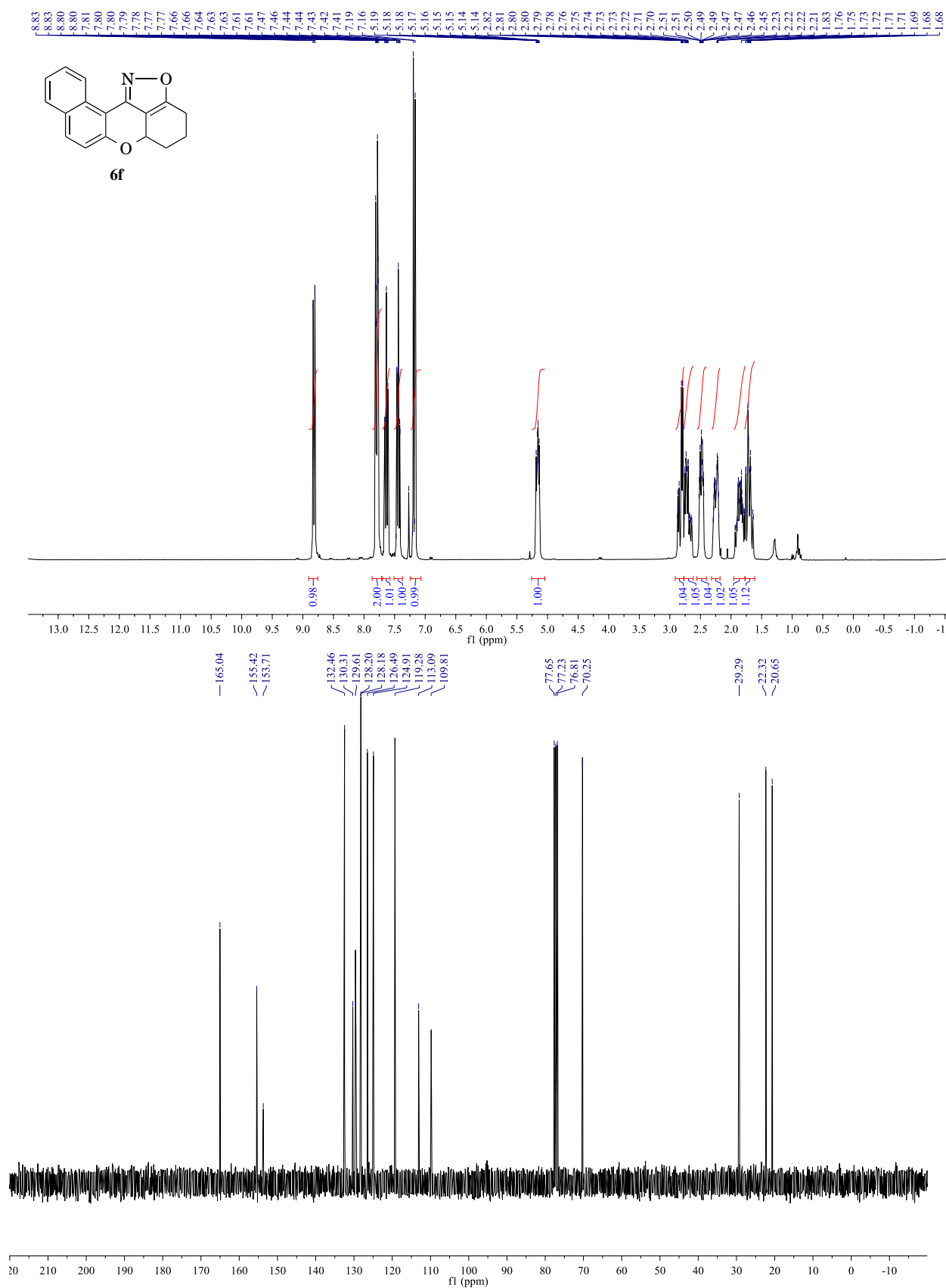


Figure 24: NMR spectra for compound **6f**

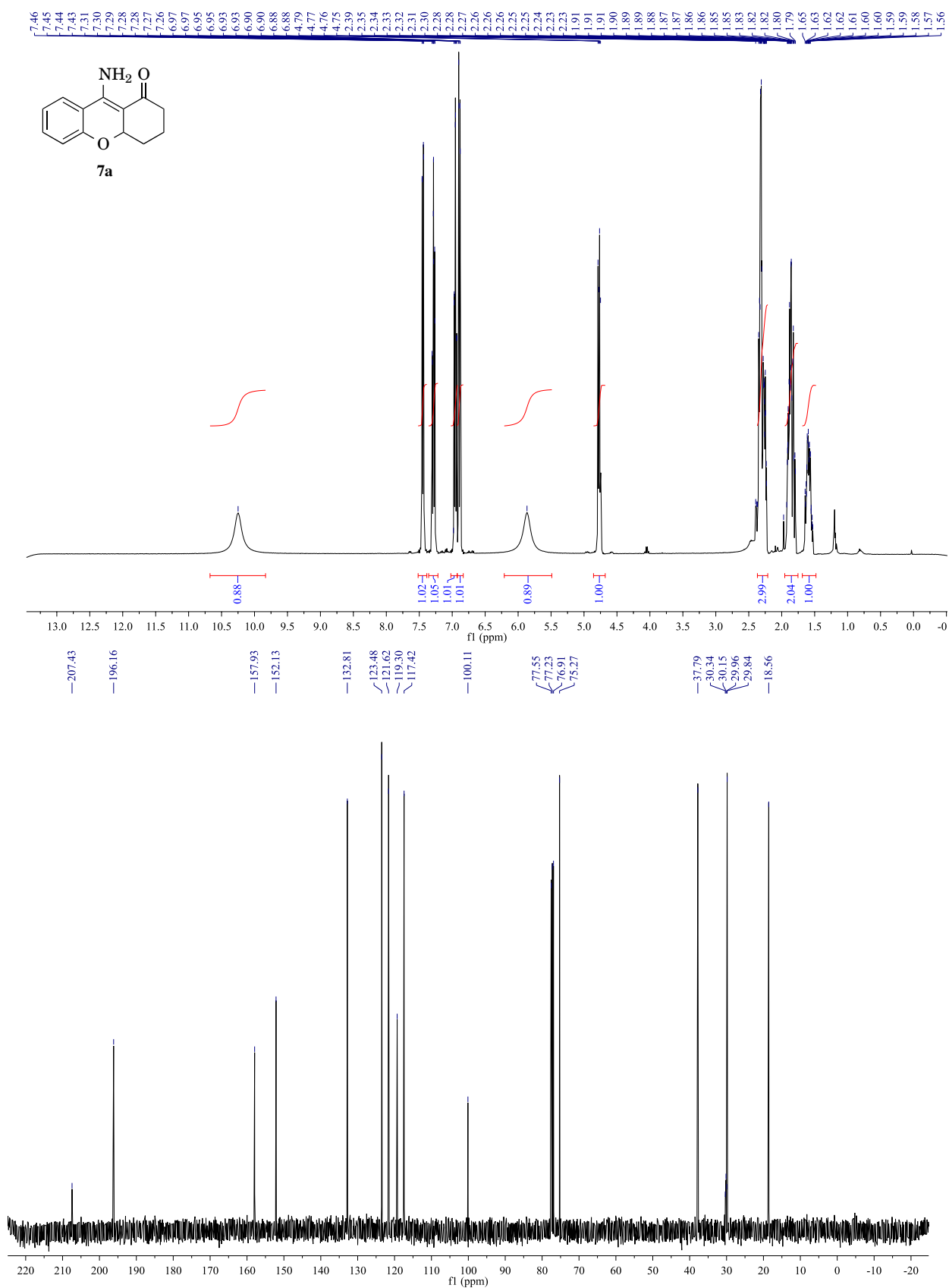


Figure 25: NMR spectra for compound **7a**

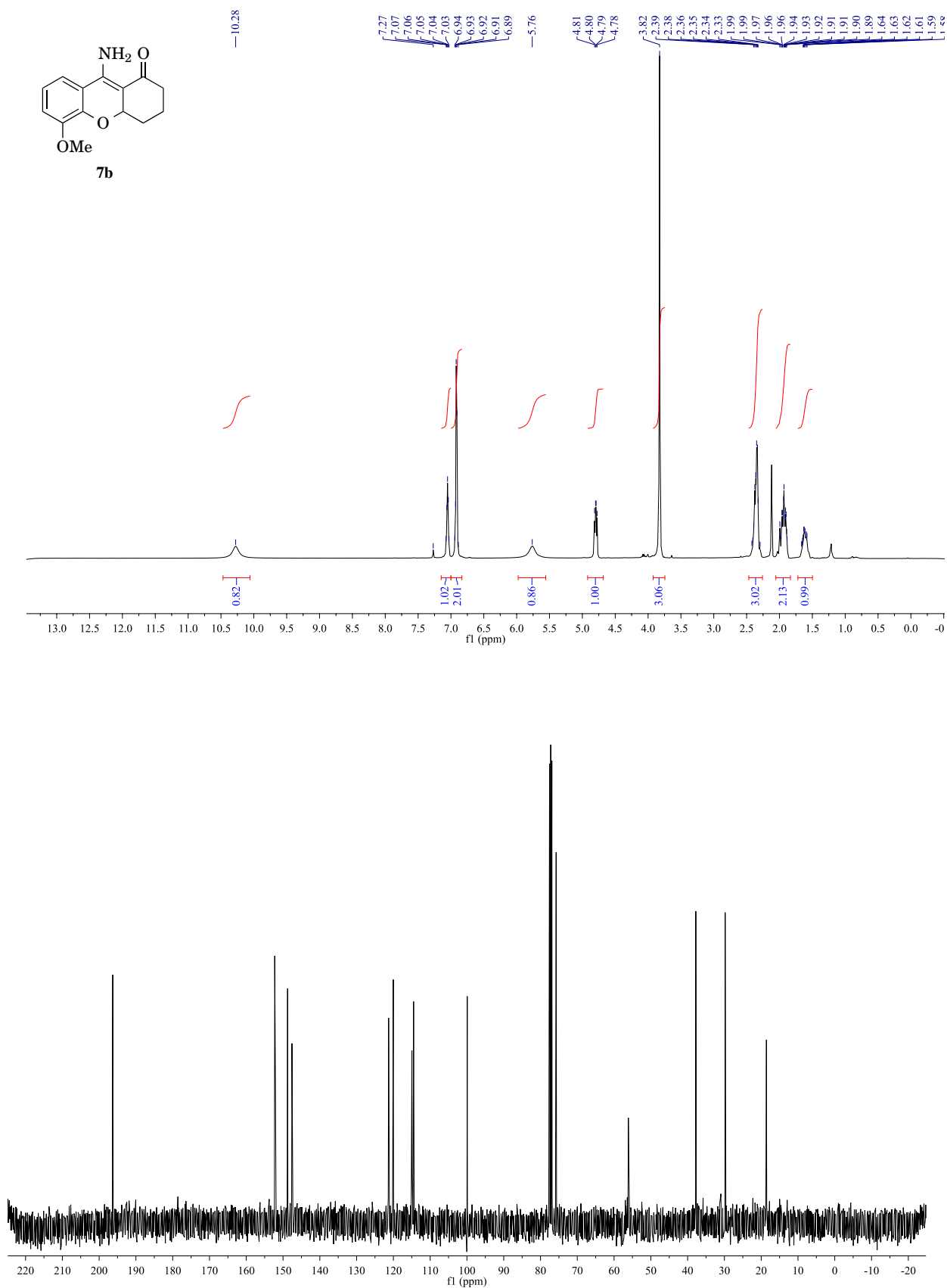


Figure 26: NMR spectra for compound **7b**