

Supporting Information for

1-(2*H*-Azirine-2-carbonyl)benzotriazoles: Preparation and Use as *N*-Heterocyclic

Building Blocks

Ekaterina E. Galenko, Firuza M. Shakirova, Vladimir A. Bodunov, Mikhail S. Novikov, Alexander F. Khlebnikov*

St. Petersburg State University, Institute of Chemistry, 7/9 Universitetskaya nab, St. Petersburg, 199034, Russia

E-mail: a.khlebnikov@spbu.ru

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X-RAY DIFFRACTION EXPERIMENTS

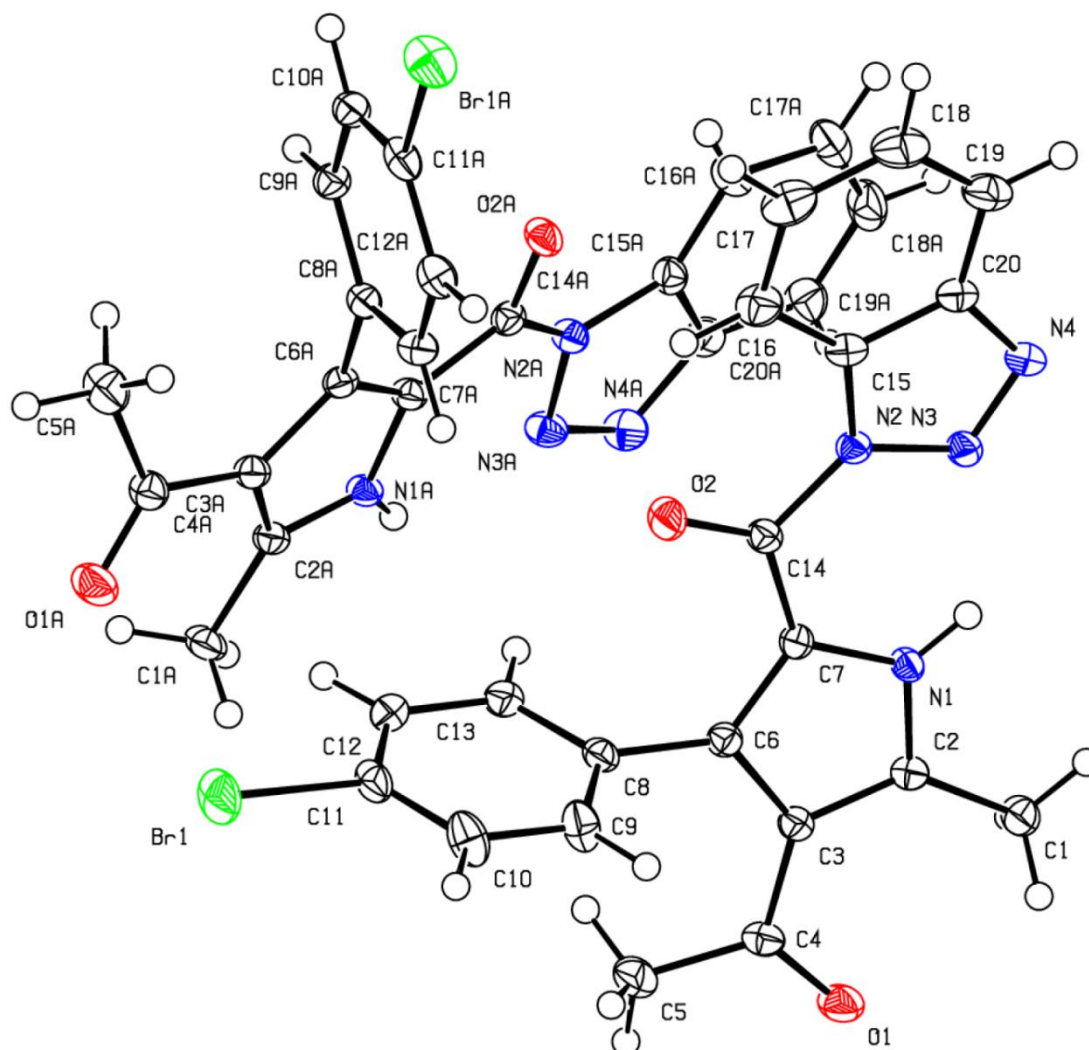
Crystal structure of **6d** was determined by single crystal X-ray diffraction analysis. Suitable crystals were selected and fixed on micro-amounts and the diffraction data were collected on a diffractometer. The crystals **6d** were measured at a temperature of 100(2) K, using monochromated CuK α radiation. The unit cell parameters and refinement characteristics of the crystal structure of **6d** is given below. Using Olex2[1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimization.

References

1. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, 42, 339.
2. Sheldrick, G. M. *Acta Cryst.* **2015**, A71, 3.
3. Sheldrick, G. M. *Acta Cryst.* **2015**, C71, 3.

1-(5-(1*H*-Benzo[d][1,2,3]triazole-1-carbonyl)-4-(4-bromophenyl)-2-methyl-1*H*-pyrrole-3-yl)ethanone **6d**

Single crystals of **6d** were obtained by slow evaporation of acetonitrile solution at room temperature. (CCDC 1974787)



Molecular structure of compound **6d**, displacement parameters are drawn at 50% probability level.

Table S1. Crystal data and structure refinement for 6d

Identification code	6d (7060-11415)
Empirical formula	C ₄₀ H ₃₀ Br ₂ N ₈ O ₄
Formula weight	846.54
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	16.09300(10)
b/Å	13.15410(10)
c/Å	16.98630(10)
α/°	90
β/°	99.8840(10)
γ/°	90
Volume/Å ³	3542.44(4)
Z	4
ρ _{calc} /g/cm ³	1.587
μ/mm ⁻¹	3.367
F(000)	1712.0
Crystal size/mm ³	0.25 × 0.20 × 0.10
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	6.992 to 144.944
Index ranges	-19 ≤ h ≤ 19, -16 ≤ k ≤ 16, -21 ≤ l ≤ 21
Reflections collected	24540
Independent reflections	7008 [R _{int} = 0.0354, R _{sigma} = 0.0280]
Data/restraints/parameters	7008/0/491
Goodness-of-fit on F ²	1.033
Final R indexes [I>=2σ (I)]	R ₁ = 0.0327, wR ₂ = 0.0875
Final R indexes [all data]	R ₁ = 0.0349, wR ₂ = 0.0891
Largest diff. peak/hole / e Å ⁻³	0.36/-0.81

Table S2. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 6d U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
Br _{1A}	9550.3(2)	8653.2(2)	4962.4(2)	31.74(8)
Br ₁	6204.7(2)	8503.8(2)	389.1(2)	35.39(8)
O _{2A}	6096.0(8)	6864.5(11)	5291.3(7)	20.5(3)
O ₂	6024.1(8)	10165.8(11)	3631.3(8)	24.5(3)
O ₁	1937.8(9)	10634.8(12)	2141.4(8)	27.0(3)
O _{1A}	6295.4(9)	5769.2(13)	1543.7(8)	29.8(3)
N _{1A}	4928.0(9)	5820.3(11)	3439.5(8)	15.7(3)
N ₁	3975.1(9)	11030.3(11)	3981.3(9)	15.6(3)
N _{2A}	4764.3(10)	6270.8(11)	5147.3(9)	16.2(3)
N ₂	5774.1(9)	11004.0(12)	4727.3(9)	16.0(3)
N _{3A}	4033.7(10)	5902.4(12)	4689.7(9)	19.4(3)
N ₄	5665.5(10)	11741.9(13)	5853.3(9)	20.5(3)
N ₃	5232.2(10)	11367.9(12)	5209.3(9)	18.0(3)

N _{4A}	3440.8(10)	5909.3(13)	5114.3(10)	22.6(3)
C _{11A}	8537.9(11)	7938.1(15)	4569.8(11)	20.3(4)
C ₂₀	6513.4(12)	11640.8(14)	5814.3(11)	19.1(4)
C ₃	3343.4(11)	10508.3(14)	2784.8(10)	16.8(3)
C _{2A}	5211.1(11)	5691.7(14)	2746.0(10)	16.9(4)
C ₇	4596.9(11)	10590.3(13)	3623.6(10)	15.9(3)
C ₂	3225.4(11)	11001.7(14)	3492.9(10)	16.2(3)
C ₆	4217.2(11)	10249.9(14)	2872.1(10)	16.2(3)
C _{14A}	5514.5(11)	6480.9(13)	4832.5(11)	16.0(4)
C ₈	4672.5(11)	9792.9(14)	2267.4(10)	17.8(4)
C _{3A}	6053.9(11)	6017.6(14)	2854.7(10)	16.8(3)
C _{10A}	8439.5(12)	6951.3(15)	4824.2(11)	20.3(4)
C _{6A}	6266.3(11)	6371.8(13)	3653.5(11)	15.8(4)
C _{7A}	5559.7(11)	6232.5(14)	4011.3(10)	15.7(3)
C _{9A}	7697.1(12)	6437.2(14)	4536.3(11)	18.2(4)
C _{8A}	7057.4(11)	6908.4(14)	4002.6(10)	15.9(3)
C ₄	2638.4(12)	10267.3(15)	2135.6(11)	19.6(4)
C ₁₄	5490.8(11)	10548.8(14)	3960.9(10)	16.8(4)
C _{15A}	4615.1(12)	6521.6(13)	5898.5(11)	17.5(4)
C _{13A}	7166.1(12)	7908.1(14)	3769.7(11)	19.5(4)
C ₁	2463.7(12)	11427.1(15)	3762.2(12)	22.2(4)
C _{16A}	5116.9(13)	6906.1(15)	6593.5(11)	22.2(4)
C _{1A}	4668.2(12)	5262.9(16)	2023.3(11)	22.0(4)
C ₁₅	6597.2(12)	11166.8(14)	5098.4(11)	18.3(4)
C _{12A}	7910.9(13)	8428.9(15)	4052.0(11)	21.3(4)
C _{20A}	3766.6(13)	6291.5(14)	5868.5(11)	20.7(4)
C ₁₃	4941.9(13)	8783.0(15)	2311.8(11)	22.3(4)
C ₁₁	5565.9(12)	9012.9(16)	1146.1(11)	23.1(4)
C ₉	4844.6(14)	10393.9(15)	1642.3(12)	26.3(4)
C ₁₉	7216.2(13)	11953.4(16)	6369.9(12)	26.5(4)
C _{4A}	6599.1(12)	5886.3(15)	2247.7(11)	20.1(4)
C ₁₂	5382.2(13)	8386.1(16)	1745.4(12)	24.5(4)
C ₁₀	5298.4(14)	10014.4(16)	1083.4(12)	28.5(5)
C _{19A}	3369.4(14)	6446.1(16)	6531.0(13)	27.2(4)
C _{18A}	3853.1(15)	6833.4(17)	7208.0(12)	29.2(5)
C ₁₆	7388.4(12)	10975.7(16)	4893.8(12)	25.1(4)
C _{17A}	4711.3(14)	7055.2(16)	7235.5(12)	27.6(4)
C ₅	2774.2(13)	9563.1(18)	1474.0(12)	29.6(5)
C ₁₈	7993.7(13)	11749.6(18)	6170.9(14)	31.7(5)
C _{5A}	7541.3(13)	5835.7(19)	2510.9(13)	31.0(5)
C ₁₇	8074.0(13)	11272.2(17)	5448.1(14)	30.8(5)

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 6d. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[\mathbf{h}^2\mathbf{a}^{*2}\mathbf{U}_{11}+2\mathbf{h}\mathbf{k}\mathbf{a}^*\mathbf{b}^*\mathbf{U}_{12}+\dots]$.

Atom	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
Br _{1A}	18.85(12)	43.00(15)	33.38(13)	-8.93(9)	4.48(9)	-12.27(9)
Br ₁	25.56(13)	52.82(17)	30.92(13)	-10.63(10)	13.69(10)	3.43(10)
O _{2A}	15.3(6)	28.3(7)	17.4(6)	-6.5(5)	1.7(5)	-1.8(5)
O ₂	16.7(6)	34.6(8)	22.9(7)	-6.4(6)	5.5(5)	2.2(6)
O ₁	17.5(7)	42.9(9)	19.9(6)	-2.0(6)	0.7(5)	3.0(6)
O _{1A}	26.2(7)	46.9(9)	17.0(7)	-2.0(6)	5.3(6)	3.4(7)
N _{1A}	11.7(7)	21.0(8)	13.9(7)	-0.6(6)	0.8(5)	-0.5(6)
N ₁	14.1(7)	19.3(7)	13.4(7)	-2.2(6)	2.9(6)	-0.8(6)
N _{2A}	15.2(8)	19.0(7)	14.4(7)	-0.3(6)	2.2(6)	-1.5(6)
N ₂	13.0(7)	20.2(7)	14.8(7)	0.2(6)	2.1(6)	1.2(6)
N _{3A}	14.9(7)	24.9(8)	17.8(7)	0.7(6)	1.3(6)	-2.8(6)
N ₄	20.6(8)	23.9(8)	15.5(7)	0.4(6)	-0.9(6)	1.5(6)
N ₃	17.6(8)	22.5(8)	14.3(7)	0.2(6)	3.7(6)	1.9(6)
N _{4A}	18.4(8)	28.3(9)	21.8(8)	2.6(7)	5.7(6)	-1.8(7)
C _{11A}	14.3(9)	29.3(10)	18.8(8)	-7.5(8)	6.7(7)	-6.4(7)
C ₂₀	18.7(9)	19.4(9)	18.0(8)	2.6(7)	-0.5(7)	-0.2(7)
C ₃	17.4(9)	18.3(9)	14.7(8)	0.2(7)	2.5(7)	0.5(7)
C _{2A}	16.1(9)	20.3(9)	14.0(8)	1.0(7)	1.8(7)	1.5(7)
C ₇	14.7(8)	17.5(8)	15.7(8)	-0.2(7)	3.4(7)	0.4(7)
C ₂	14.6(8)	18.4(8)	15.7(8)	1.4(7)	2.5(7)	-1.6(7)
C ₆	16.8(9)	16.7(8)	15.3(8)	1.2(7)	3.1(7)	0.5(7)
C _{14A}	13.5(9)	17.5(8)	17.0(8)	0.3(7)	2.9(7)	1.5(6)
C ₈	15.6(8)	23.0(9)	14.2(8)	-2.9(7)	0.9(7)	-0.5(7)
C _{3A}	15.3(8)	19.6(9)	15.2(8)	0.6(7)	1.7(7)	0.7(7)
C _{10A}	14.9(9)	28.7(10)	17.3(8)	-2.4(7)	2.4(7)	2.7(7)
C _{6A}	13.7(9)	17.8(8)	15.3(8)	1.0(7)	1.2(7)	1.8(6)
C _{7A}	14.1(8)	18.7(8)	13.9(8)	-0.2(7)	0.9(7)	-0.4(7)
C _{9A}	15.7(9)	21.2(9)	17.8(8)	0.1(7)	2.9(7)	1.3(7)
C _{8A}	12.3(8)	20.7(9)	15.0(8)	-2.2(7)	3.5(6)	-1.4(7)
C ₄	18.5(9)	24.2(9)	15.5(8)	2.6(7)	1.3(7)	-1.0(7)
C ₁₄	17.2(9)	18.9(9)	14.3(8)	0.3(7)	2.7(7)	0.5(7)
C _{15A}	21.5(9)	15.9(8)	15.9(8)	0.8(7)	5.4(7)	0.9(7)
C _{13A}	18.7(9)	21.8(9)	17.4(8)	0.8(7)	1.1(7)	-0.2(7)
C ₁	16.1(9)	30.7(10)	20.3(9)	-4.2(8)	4.1(7)	0.8(7)
C _{16A}	26.4(10)	22.1(9)	18.0(9)	-1.2(7)	3.4(8)	-3.7(8)
C _{1A}	17.6(9)	32.7(10)	14.6(8)	-3.6(8)	-0.5(7)	-0.9(8)
C ₁₅	15.7(9)	19.7(9)	18.3(8)	3.5(7)	-0.2(7)	-1.3(7)
C _{12A}	23.2(10)	22.2(9)	19.7(9)	-1.4(7)	6.9(8)	-4.1(7)
C _{20A}	21.9(10)	20.7(9)	20.2(9)	3.2(7)	5.3(7)	0.8(7)
C ₁₃	23.0(10)	27.0(10)	16.7(9)	1.5(7)	2.9(7)	5.6(8)
C ₁₁	15.4(9)	35.1(11)	19.7(9)	-8.2(8)	5.5(7)	-0.4(8)
C ₉	38.2(12)	19.4(9)	23.8(10)	-2.9(8)	12.1(9)	-1.9(8)
C ₁₉	25.9(10)	26.4(10)	23.9(10)	0.8(8)	-5.0(8)	-3.0(8)
C _{4A}	18.7(9)	23.5(9)	18.7(9)	-0.2(7)	4.7(7)	-0.6(7)

C ₁₂	23.0(10)	28.7(10)	21.1(9)	-1.3(8)	1.5(8)	8.5(8)
C ₁₀	36.7(12)	27.6(10)	24.8(10)	-4.5(8)	15.5(9)	-8.2(9)
C _{19A}	25.8(11)	32.3(11)	26.4(10)	4.3(8)	12.2(9)	3.5(8)
C _{18A}	39.3(12)	29.9(11)	21.8(9)	0.3(8)	14.8(9)	4.3(9)
C ₁₆	17.0(9)	32.1(11)	26.5(10)	1.7(8)	4.6(8)	-0.8(8)
C _{17A}	40.2(12)	24.7(10)	18.6(9)	-3.6(8)	6.8(8)	-2.2(9)
C ₅	24.1(10)	38.0(12)	24.0(10)	-10.1(9)	-3.4(8)	1.6(9)
C ₁₈	20.7(10)	35.1(12)	35.2(11)	1.1(10)	-6.9(9)	-7.5(9)
C _{5A}	17.8(10)	48.5(13)	28.4(10)	-8.9(10)	9.1(8)	-3.0(9)
C ₁₇	15.2(10)	37.0(12)	39.7(12)	4.8(10)	3.2(9)	-2.5(8)

Table S4. Bond Lengths for 6d.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br _{1A}	C _{11A}	1.9002(18)	C ₇	C ₁₄	1.455(2)
Br ₁	C ₁₁	1.9008(18)	C ₂	C ₁	1.489(2)
O _{2A}	C _{14A}	1.220(2)	C ₆	C ₈	1.487(2)
O ₂	C ₁₄	1.212(2)	C _{14A}	C _{7A}	1.447(2)
O ₁	C ₄	1.228(2)	C ₈	C ₁₃	1.395(3)
O _{1A}	C _{4A}	1.221(2)	C ₈	C ₉	1.389(3)
N _{1A}	C _{2A}	1.345(2)	C _{3A}	C _{6A}	1.420(2)
N _{1A}	C _{7A}	1.390(2)	C _{3A}	C _{4A}	1.474(2)
N ₁	C ₇	1.383(2)	C _{10A}	C _{9A}	1.387(3)
N ₁	C ₂	1.342(2)	C _{6A}	C _{7A}	1.390(3)
N _{2A}	N _{3A}	1.381(2)	C _{6A}	C _{8A}	1.487(2)
N _{2A}	C _{14A}	1.429(2)	C _{9A}	C _{8A}	1.395(3)
N _{2A}	C _{15A}	1.378(2)	C _{8A}	C _{13A}	1.393(3)
N ₂	N ₃	1.380(2)	C ₄	C ₅	1.501(3)
N ₂	C ₁₄	1.434(2)	C _{15A}	C _{16A}	1.405(3)
N ₂	C ₁₅	1.383(2)	C _{15A}	C _{20A}	1.391(3)
N _{3A}	N _{4A}	1.291(2)	C _{13A}	C _{12A}	1.392(3)
N ₄	N ₃	1.290(2)	C _{16A}	C _{17A}	1.378(3)
N ₄	C ₂₀	1.384(2)	C ₁₅	C ₁₆	1.399(3)
N _{4A}	C _{20A}	1.392(3)	C _{20A}	C _{19A}	1.401(3)
C _{11A}	C _{10A}	1.386(3)	C ₁₃	C ₁₂	1.391(3)
C _{11A}	C _{12A}	1.380(3)	C ₁₁	C ₁₂	1.381(3)
C ₂₀	C ₁₅	1.393(3)	C ₁₁	C ₁₀	1.384(3)
C ₂₀	C ₁₉	1.405(3)	C ₉	C ₁₀	1.386(3)
C ₃	C ₂	1.408(2)	C ₁₉	C ₁₈	1.377(3)
C ₃	C ₆	1.430(2)	C _{4A}	C _{5A}	1.507(3)
C ₃	C ₄	1.475(2)	C _{19A}	C _{18A}	1.371(3)
C _{2A}	C _{3A}	1.404(2)	C _{18A}	C _{17A}	1.404(3)
C _{2A}	C _{1A}	1.490(2)	C ₁₆	C ₁₇	1.378(3)
C ₇	C ₆	1.391(2)	C ₁₈	C ₁₇	1.405(3)

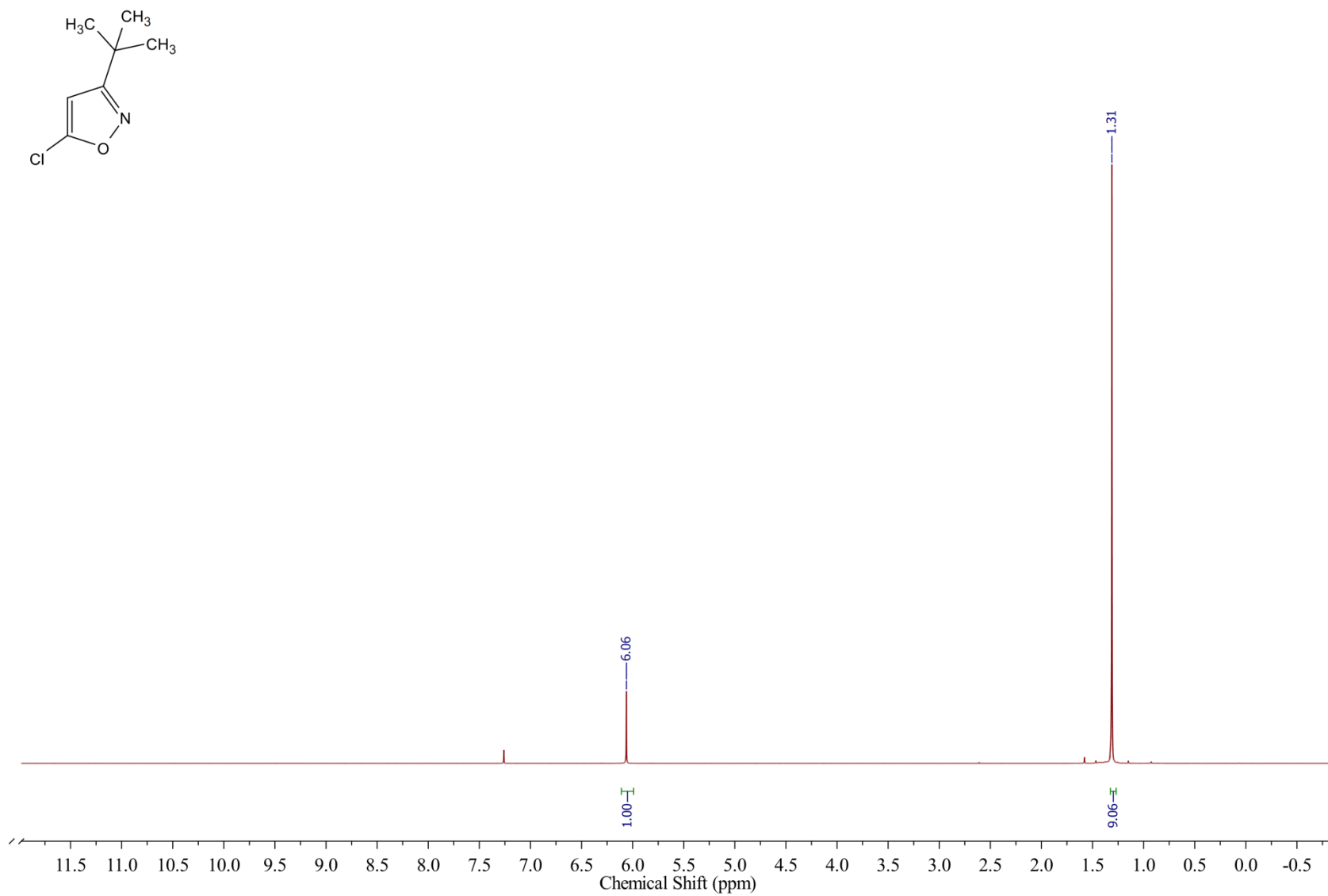
Table S5. Bond Angles for 6d.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2A	N1A	C7A	110.12(15)	C7A	C6A	C3A	107.08(16)
C2	N1	C7	110.98(15)	C7A	C6A	C8A	126.64(16)
N3A	N2A	C14A	123.34(15)	N1A	C7A	C14A	127.60(16)
C15A	N2A	N3A	109.77(15)	N1A	C7A	C6A	107.52(15)
C15A	N2A	C14A	126.36(16)	C6A	C7A	C14A	124.89(16)
N3	N2	C14	123.26(15)	C10A	C9A	C8A	120.49(18)
N3	N2	C15	109.22(14)	C9A	C8A	C6A	122.28(17)
C15	N2	C14	127.51(15)	C13A	C8A	C6A	118.39(16)
N4A	N3A	N2A	108.82(15)	C13A	C8A	C9A	119.31(17)
N3	N4	C20	108.46(15)	O1	C4	C3	119.92(17)
N4	N3	N2	109.32(15)	O1	C4	C5	120.05(17)
N3A	N4A	C20A	108.60(16)	C3	C4	C5	120.02(16)
C10A	C11A	Br1A	119.42(15)	O2	C14	N2	116.93(16)
C12A	C11A	Br1A	118.77(15)	O2	C14	C7	124.35(16)
C12A	C11A	C10A	121.79(17)	N2	C14	C7	118.71(15)
N4	C20	C15	109.20(16)	N2A	C15A	C16A	134.24(18)
N4	C20	C19	128.80(18)	N2A	C15A	C20A	103.88(16)
C15	C20	C19	122.00(18)	C20A	C15A	C16A	121.87(17)
C2	C3	C6	107.19(15)	C12A	C13A	C8A	120.62(17)
C2	C3	C4	122.60(16)	C17A	C16A	C15A	115.74(19)
C6	C3	C4	130.04(16)	N2	C15	C20	103.80(16)
N1A	C2A	C3A	108.14(15)	N2	C15	C16	134.47(18)
N1A	C2A	C1A	122.04(16)	C20	C15	C16	121.72(18)
C3A	C2A	C1A	129.83(16)	C11A	C12A	C13A	118.78(18)
N1	C7	C6	107.50(15)	N4A	C20A	C19A	129.78(19)
N1	C7	C14	125.70(16)	C15A	C20A	N4A	108.93(16)
C6	C7	C14	126.72(16)	C15A	C20A	C19A	121.29(19)
N1	C2	C3	107.59(15)	C12	C13	C8	120.69(18)
N1	C2	C1	119.98(16)	C12	C11	Br1	119.83(16)
C3	C2	C1	132.41(17)	C12	C11	C10	121.46(18)
C3	C6	C8	128.10(16)	C10	C11	Br1	118.70(15)
C7	C6	C3	106.73(15)	C10	C9	C8	121.07(19)
C7	C6	C8	124.96(16)	C18	C19	C20	116.0(2)
O2A	C14A	N2A	116.48(16)	O1A	C4A	C3A	120.88(17)
O2A	C14A	C7A	123.34(17)	O1A	C4A	C5A	119.87(17)
N2A	C14A	C7A	120.18(16)	C3A	C4A	C5A	119.15(16)
C13	C8	C6	122.19(17)	C11	C12	C13	119.00(19)
C9	C8	C6	118.97(17)	C11	C10	C9	118.90(19)
C9	C8	C13	118.83(17)	C18A	C19A	C20A	117.1(2)
C2A	C3A	C6A	107.13(16)	C19A	C18A	C17A	121.24(19)
C2A	C3A	C4A	123.35(16)	C17	C16	C15	115.8(2)
C6A	C3A	C4A	129.22(17)	C16A	C17A	C18A	122.74(19)
C11A	C10A	C9A	118.98(17)	C19	C18	C17	121.69(19)
C3A	C6A	C8A	125.87(16)	C16	C17	C18	122.7(2)

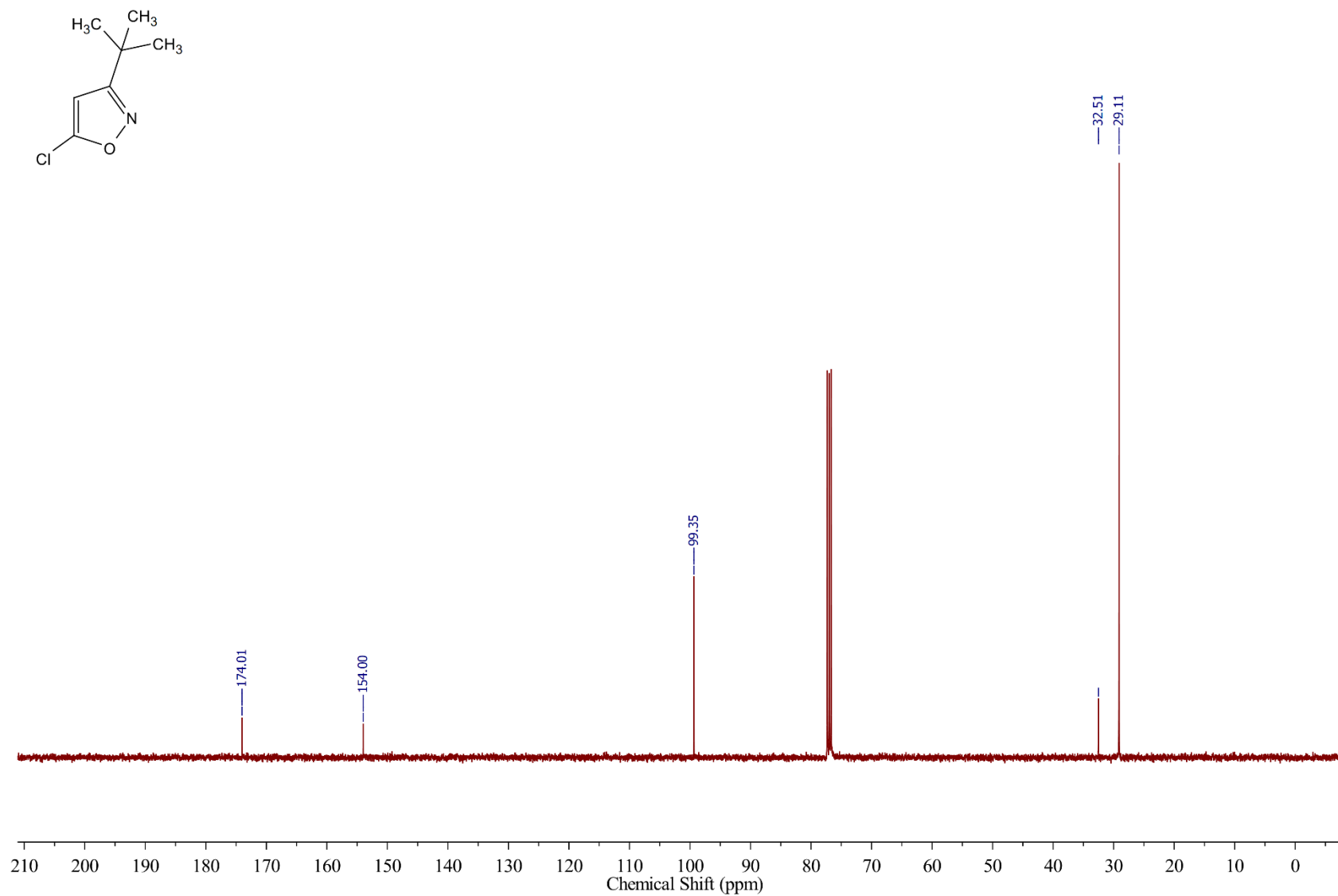
Table S6. Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for 6d.

Atom	x	y	z	U(eq)
H _{1A}	4417.06	5665.91	3519.68	19
H ₁	4059.79	11293.81	4464.6	19
H _{10A}	8873.89	6631.97	5190.22	24
H _{9A}	7623.74	5758.9	4703.89	22
H _{13A}	6727.9	8237.73	3414.97	23
H _{1B}	2090.47	10870.34	3861.57	33
H _{1C}	2164.48	11874.97	3346.75	33
H _{1D}	2634.9	11815.84	4255.56	33
H _{16A}	5698.72	7053.86	6619.11	27
H _{1AA}	4175.34	4932.01	2178.84	33
H _{1AB}	4990.91	4763.02	1772	33
H _{1AC}	4481.43	5811.65	1643.84	33
H _{12A}	7985.99	9109.6	3891.04	26
H ₁₃	4823.22	8362.18	2733.36	27
H ₉	4648.19	11076.01	1597.16	32
H ₁₉	7158.71	12285.62	6854.24	32
H ₁₂	5554	7694.23	1770.4	29
H ₁₀	5423.76	10434.66	664.24	34
H _{19A}	2790.03	6289.42	6512.01	33
H _{18A}	3603.09	6953.89	7666.9	35
H ₁₆	7449.27	10661.32	4403.39	30
H _{17A}	5025.25	7319.01	7716.89	33
H _{5A}	2227.62	9321.98	1190.9	44
H _{5B}	3114.67	8981.23	1699.19	44
H _{5C}	3069.02	9926.35	1100.05	44
H ₁₈	8488.41	11936.75	6531.77	38
H _{5AA}	7802.42	5554.49	2077.96	46
H _{5AB}	7672.53	5399.06	2983.35	46
H _{5AC}	7761.59	6520.71	2642.54	46
H ₁₇	8623.79	11148.44	5336.73	37

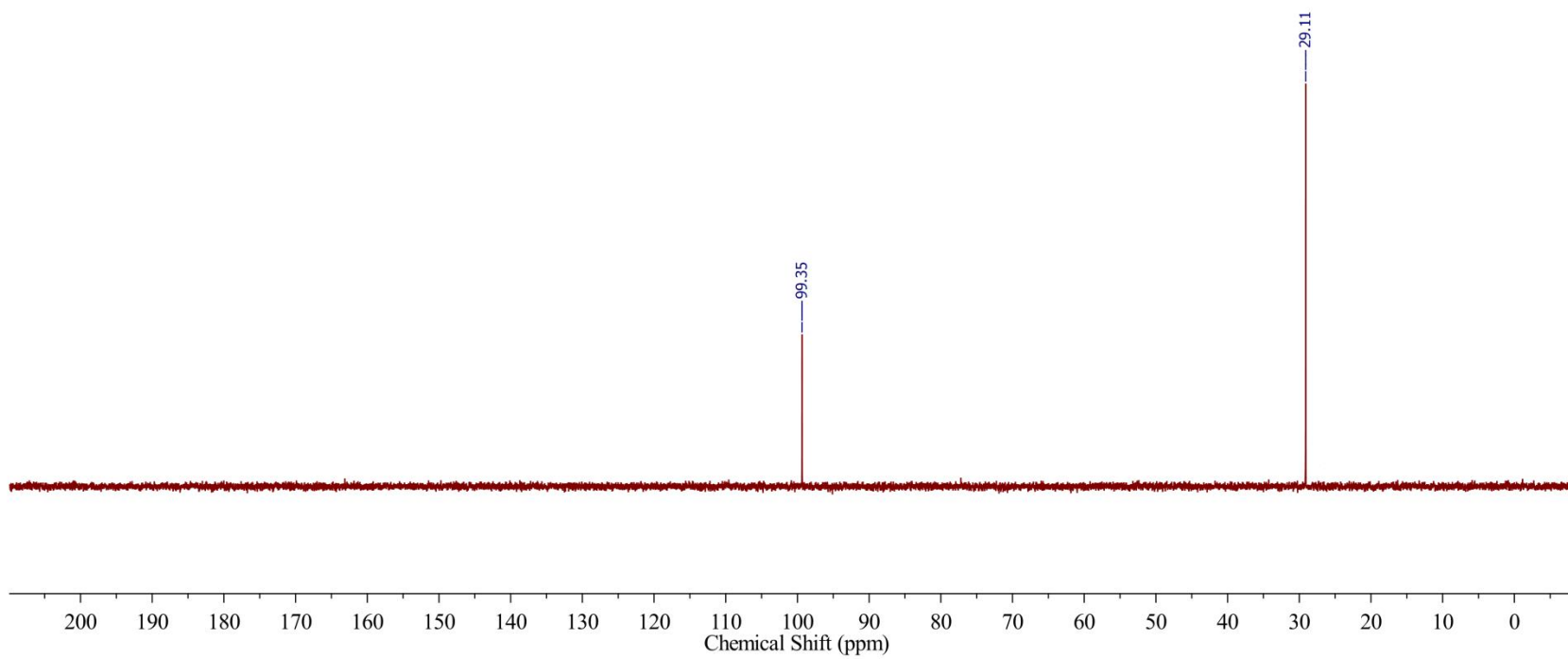
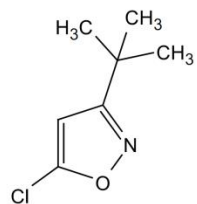
3-(*tert*-Butyl)-5-chloroisoxazole 3j, ^1H NMR, CDCl_3 , 400 MHz



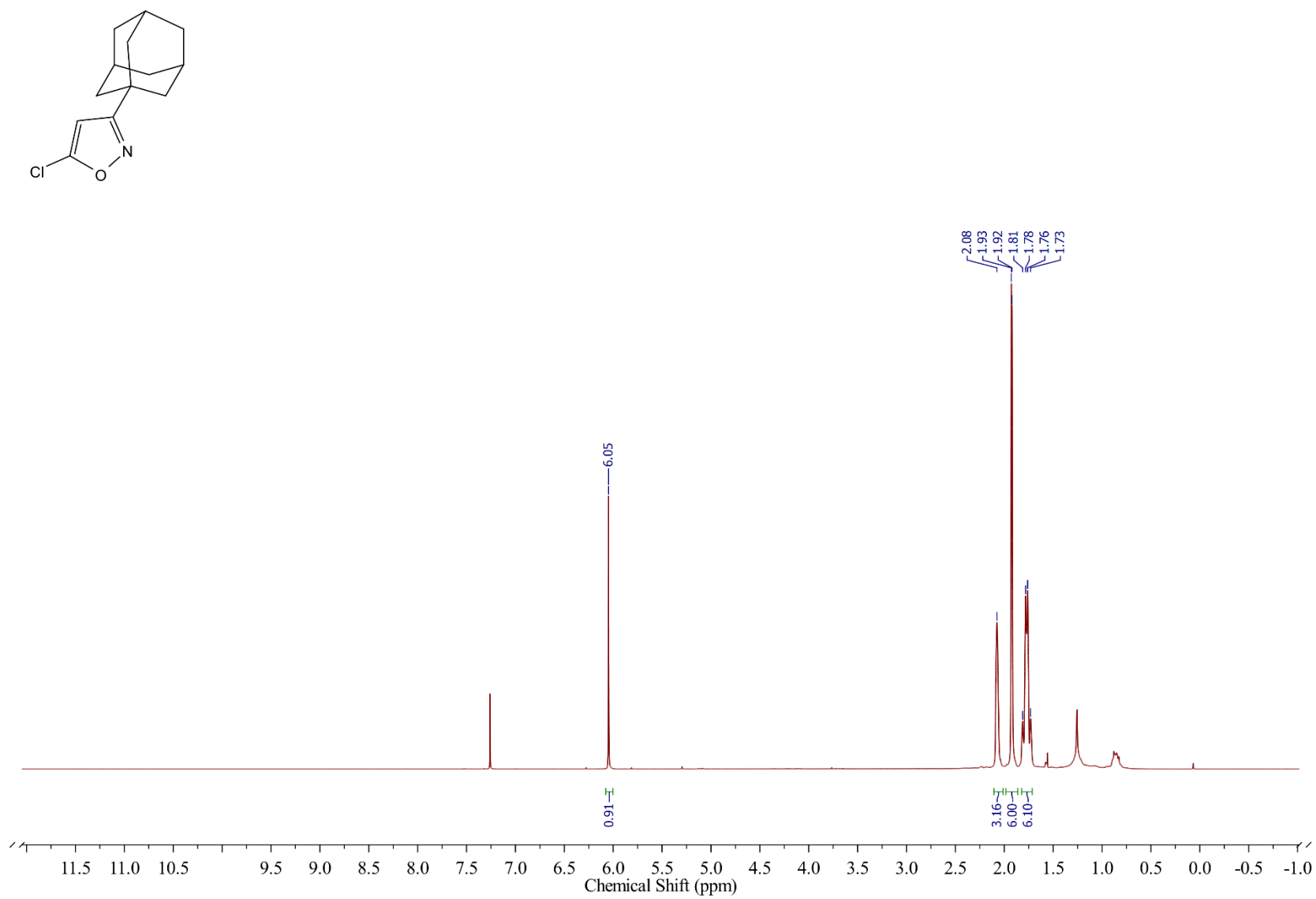
3-(*tert*-Butyl)-5-chloroisoxazole 3j, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



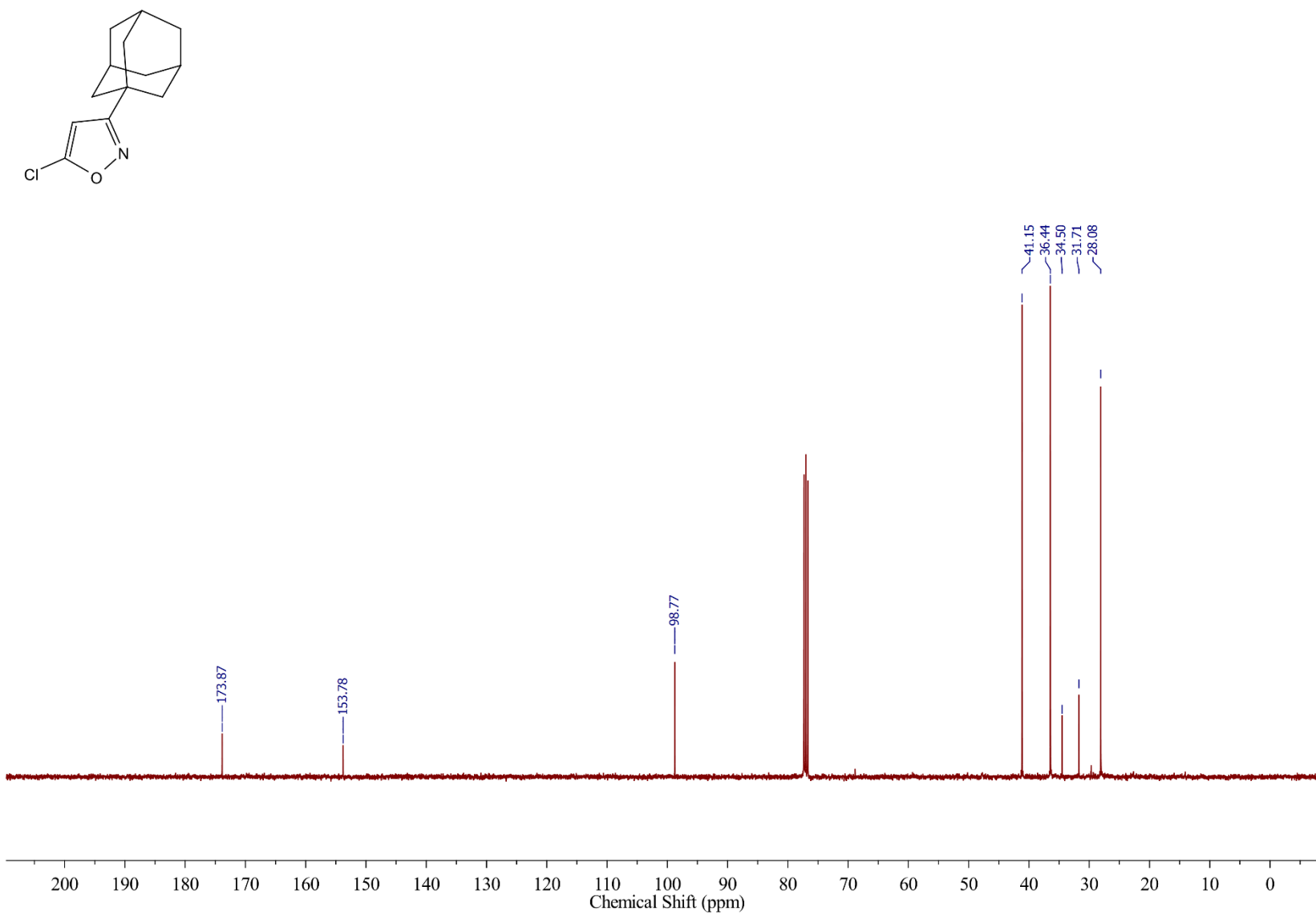
3-(*tert*-Butyl)-5-chloroisoxazole 3j, DEPT, CDCl₃, 100 MHz



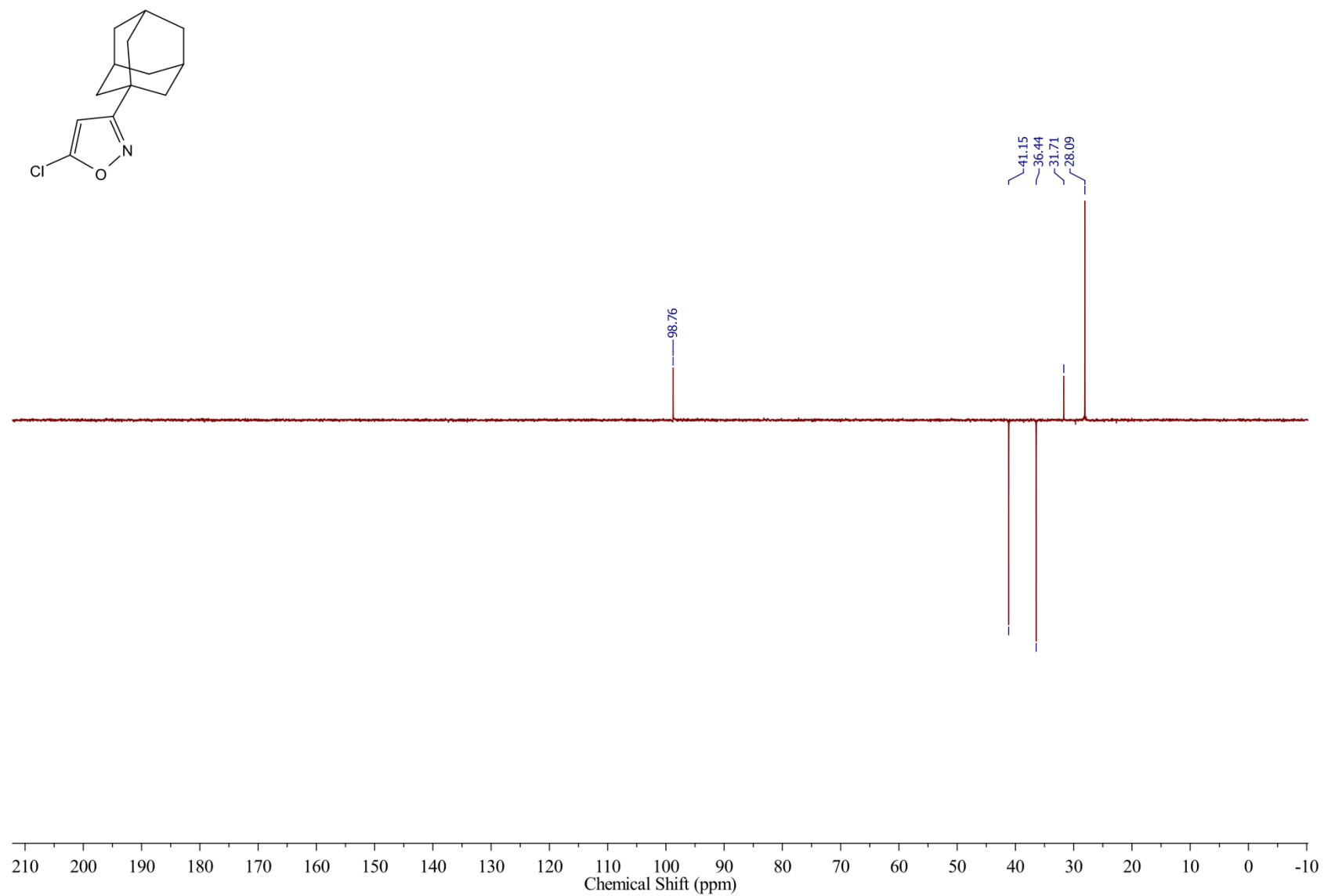
3-(Adamantan-1-yl)-5-chloroisoxazole 3k, ^1H NMR, CDCl_3 , 400 MHz



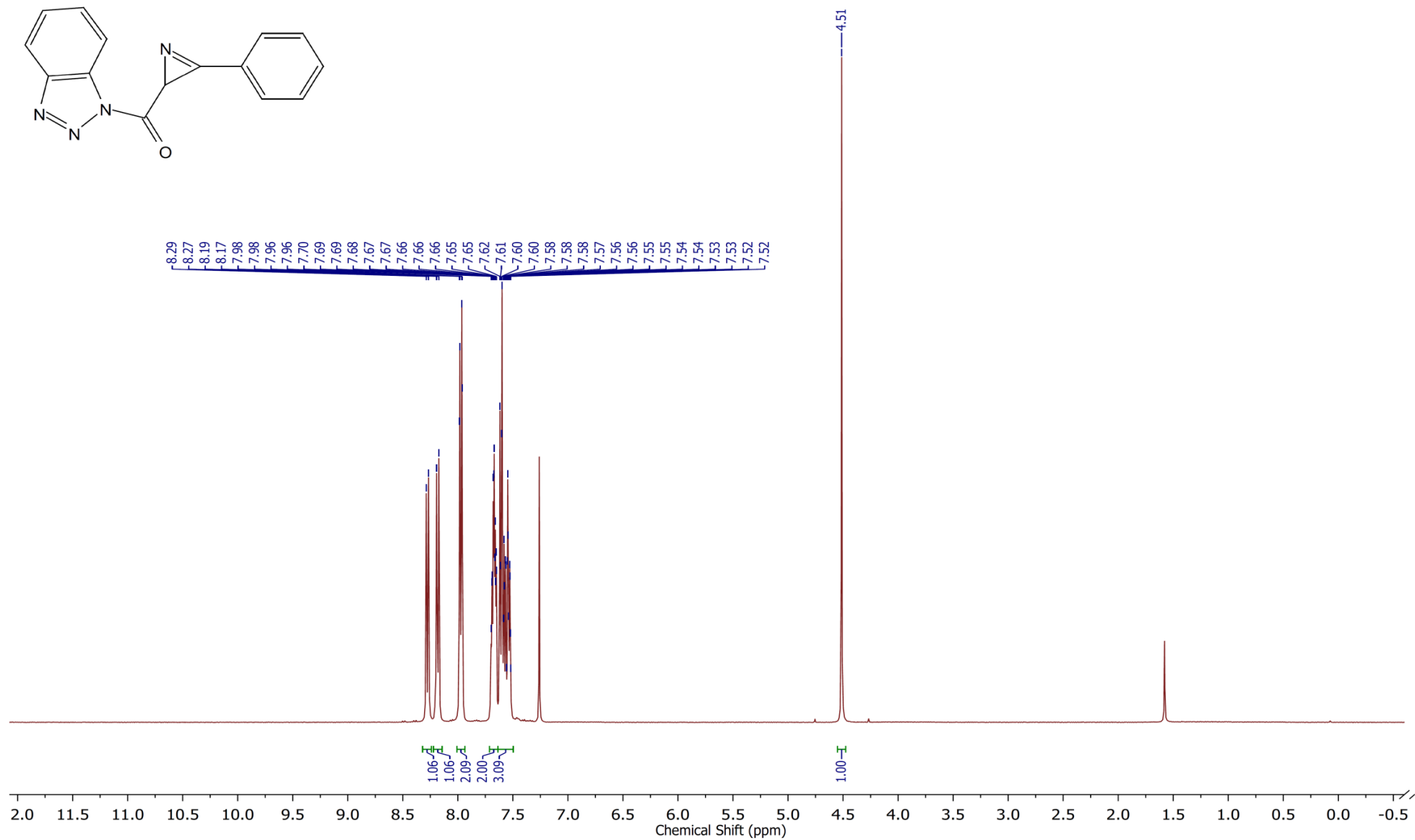
3-(Adamantan-1-yl)-5-chloroisoxazole 3k, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



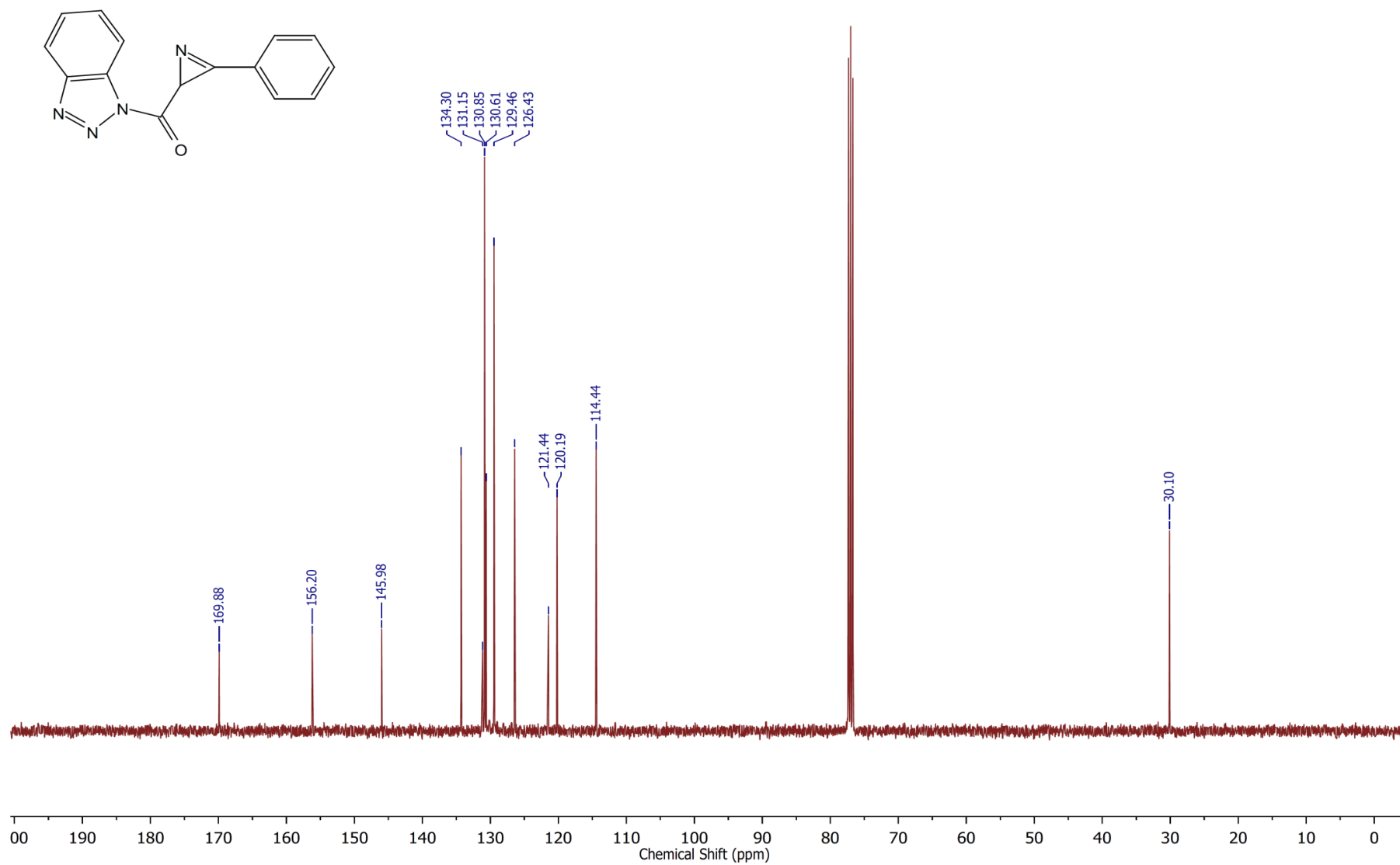
3-(Adamantan-1-yl)-5-chloroisoxazole 3k, DEPT, CDCl₃, 100 MHz



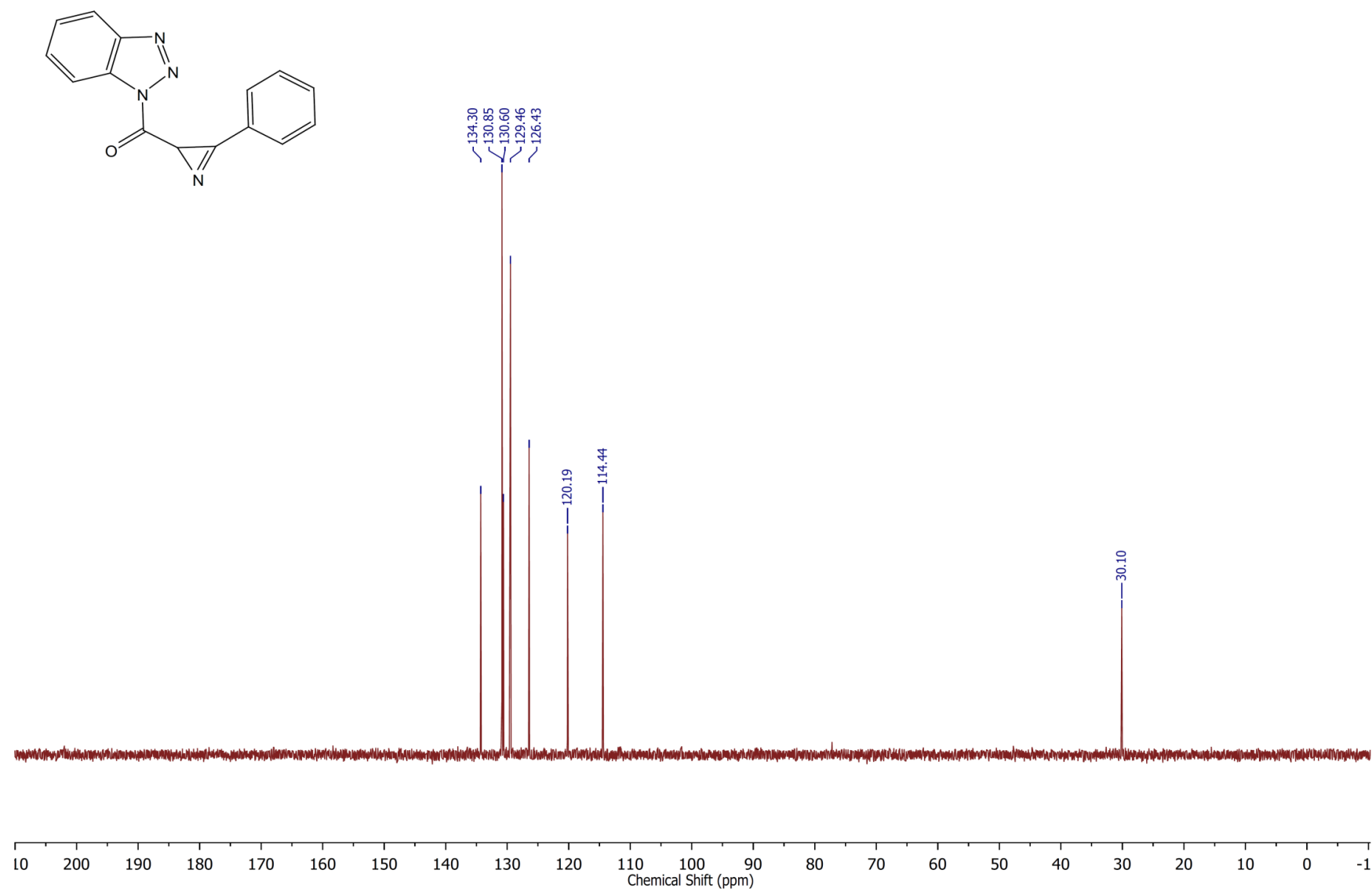
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone 1a, ¹H NMR, CDCl₃, 400 MHz



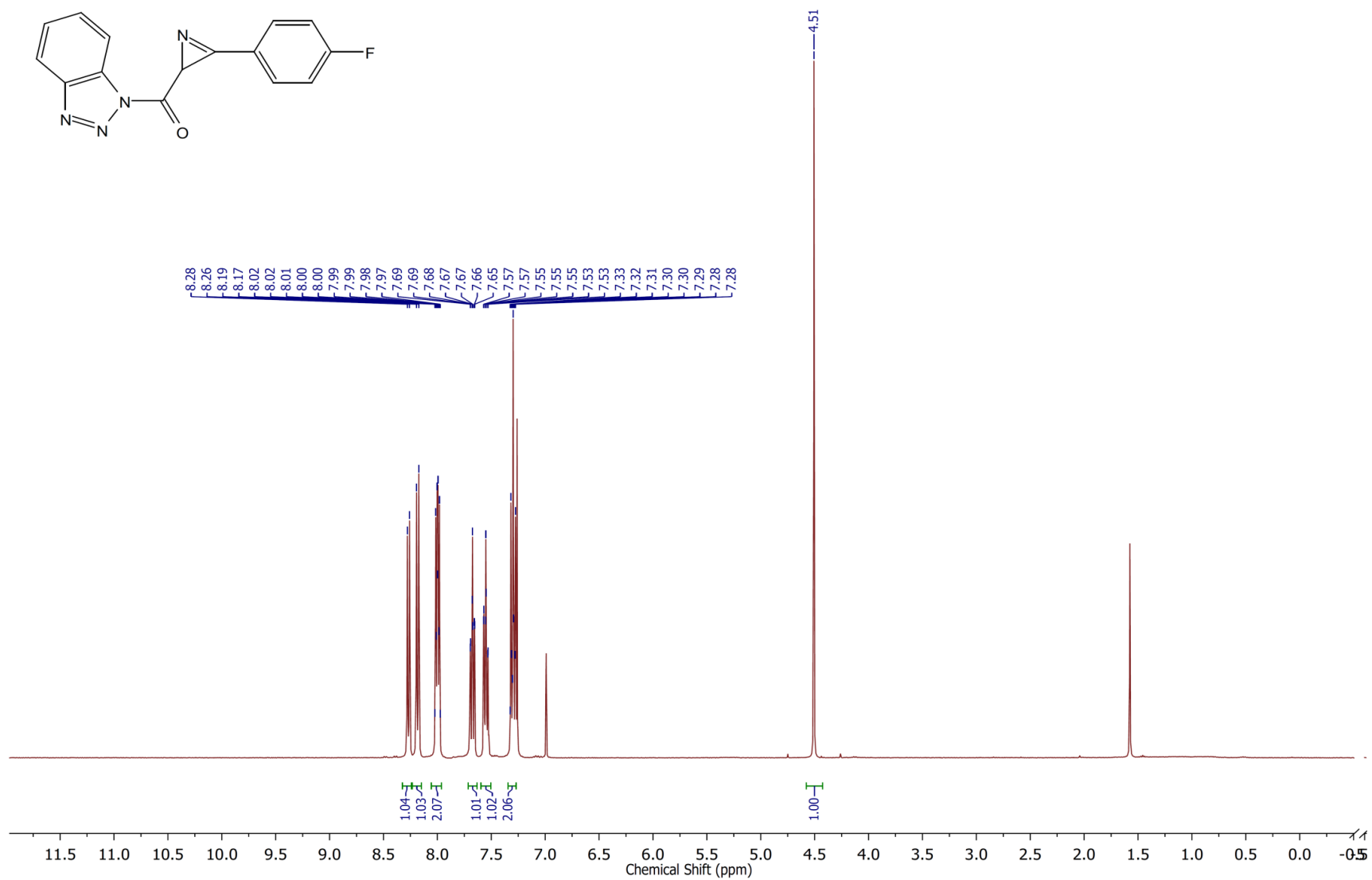
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone 1a, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



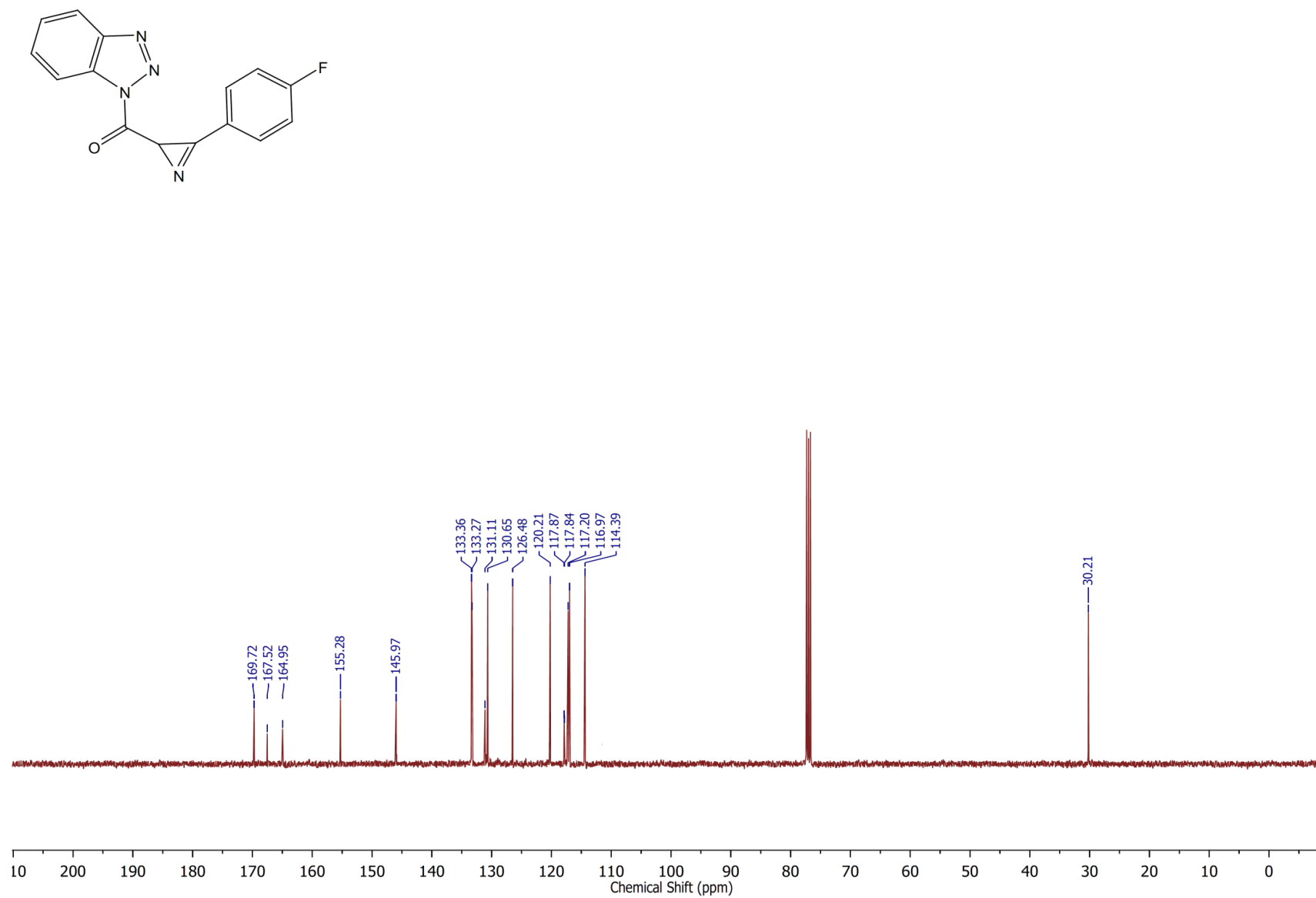
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone 1a, DEPT, CDCl₃, 100 MHz



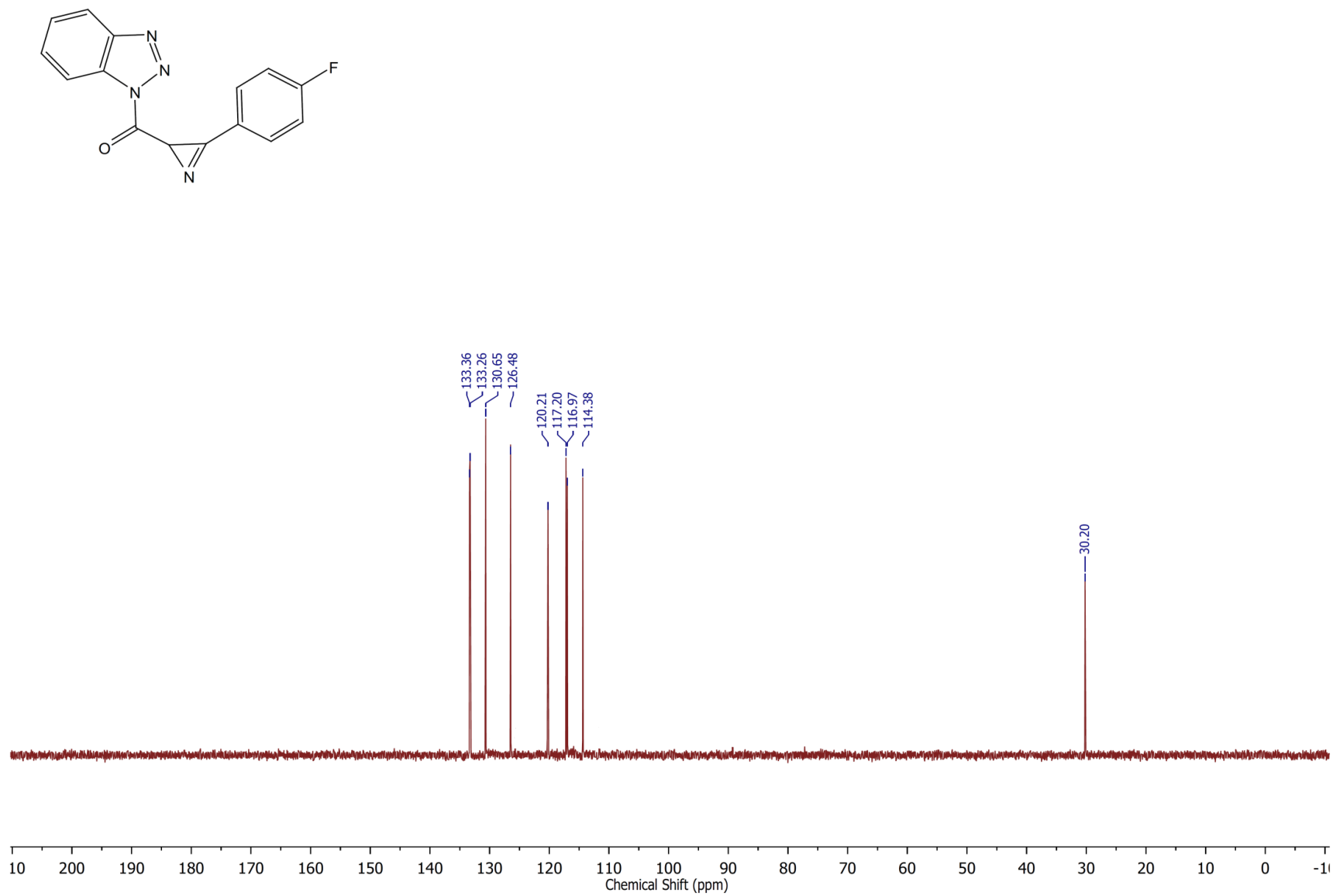
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-fluorophenyl)-2*H*-azirin-2-yl)methanone 1b, ¹H NMR, CDCl₃, 400 MHz



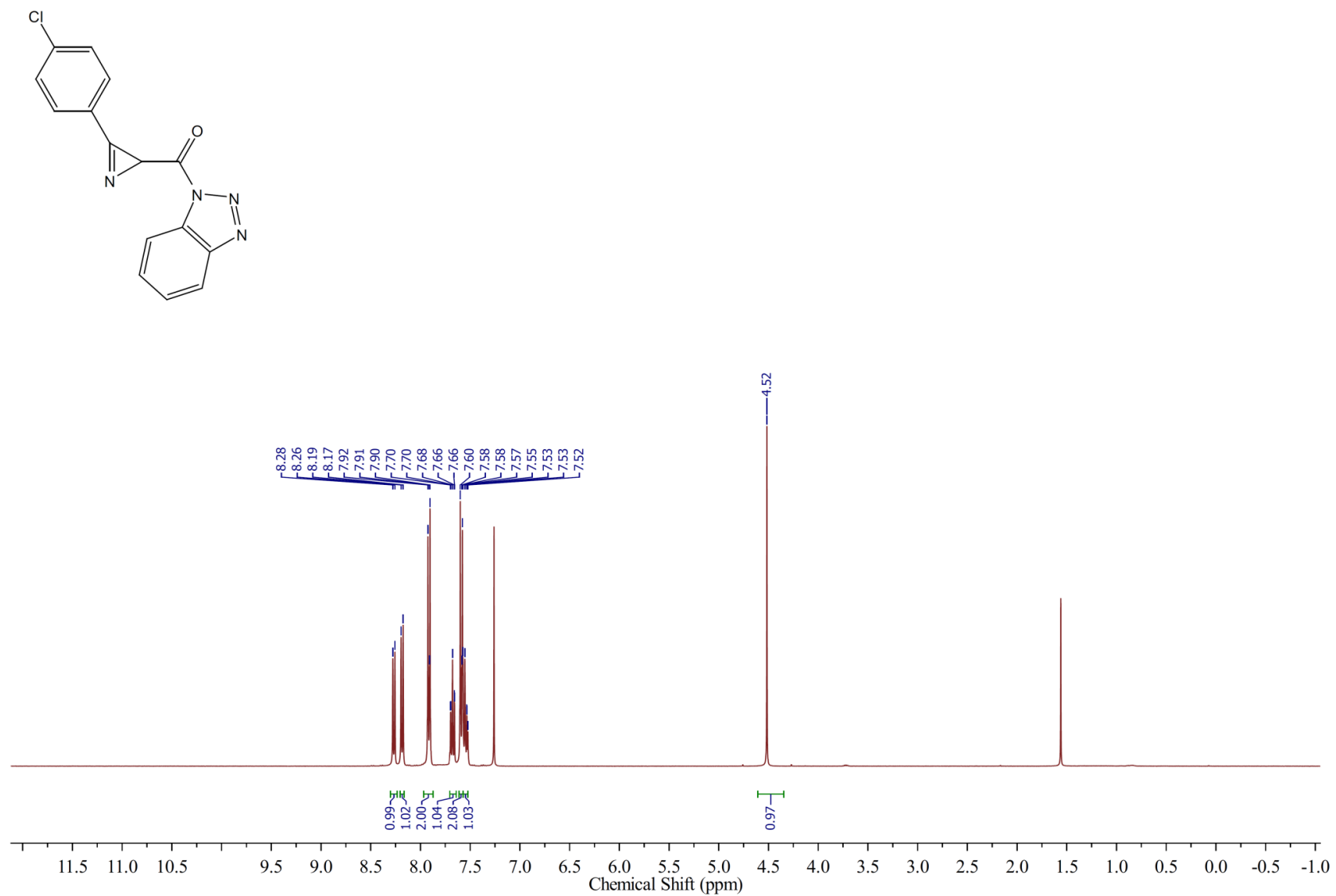
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-fluorophenyl)-2*H*-azirin-2-yl)methanone 1b, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



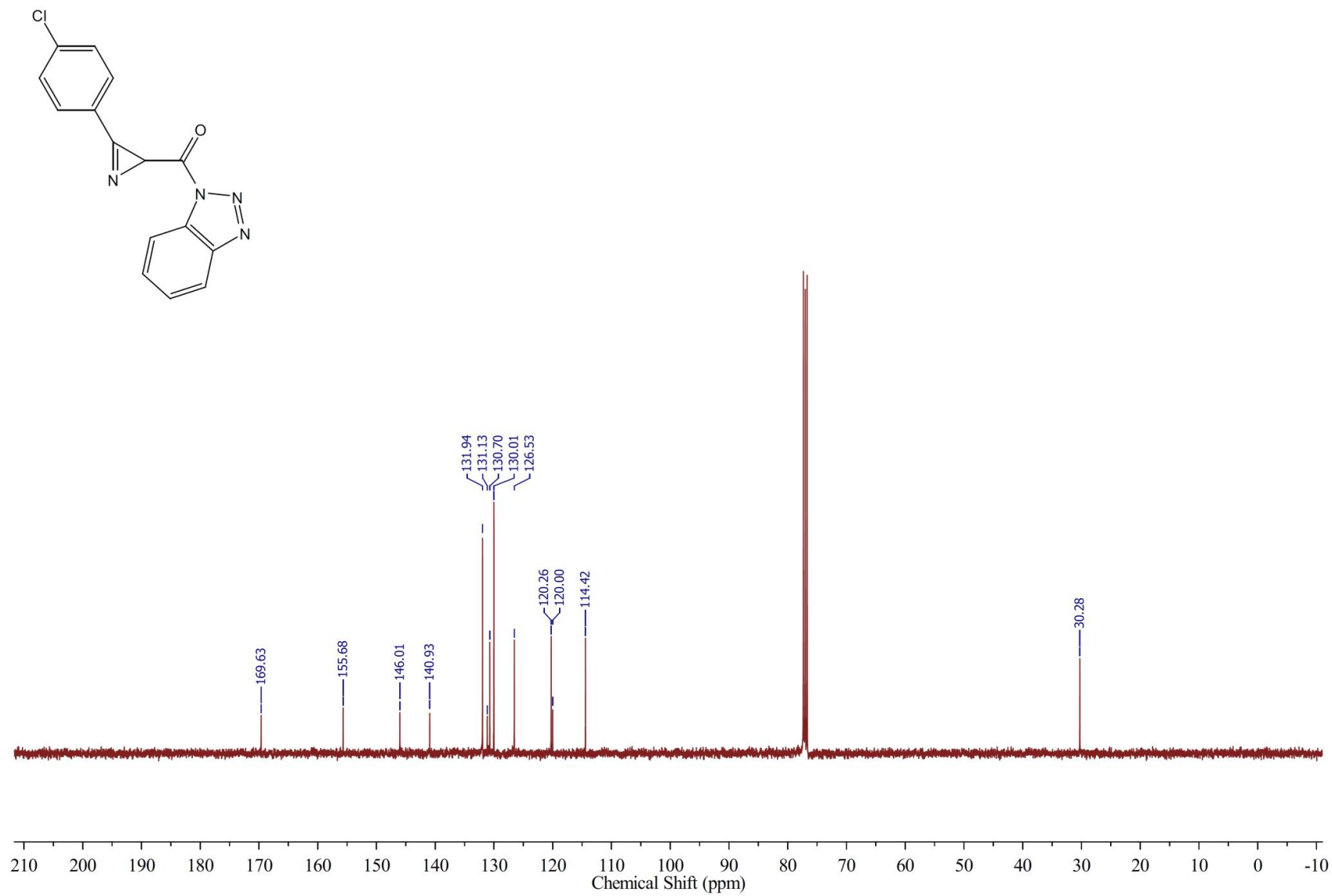
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-fluorophenyl)-2*H*-azirin-2-yl)methanone 1b, DEPT, CDCl₃, 100 MHz



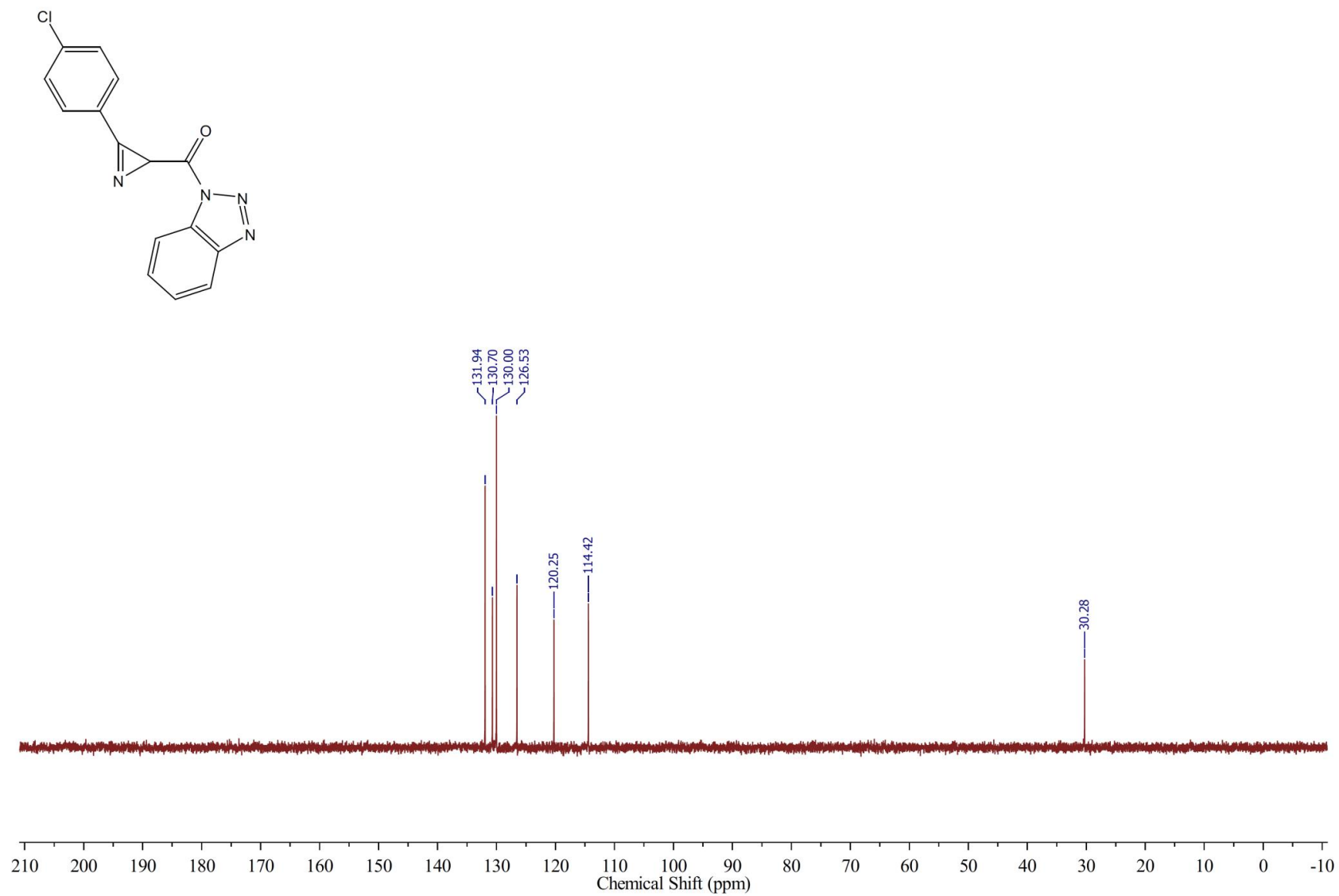
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-chlorophenyl)-2*H*-azirin-2-yl)methanone 1c, ¹H NMR, CDCl₃, 400 MHz



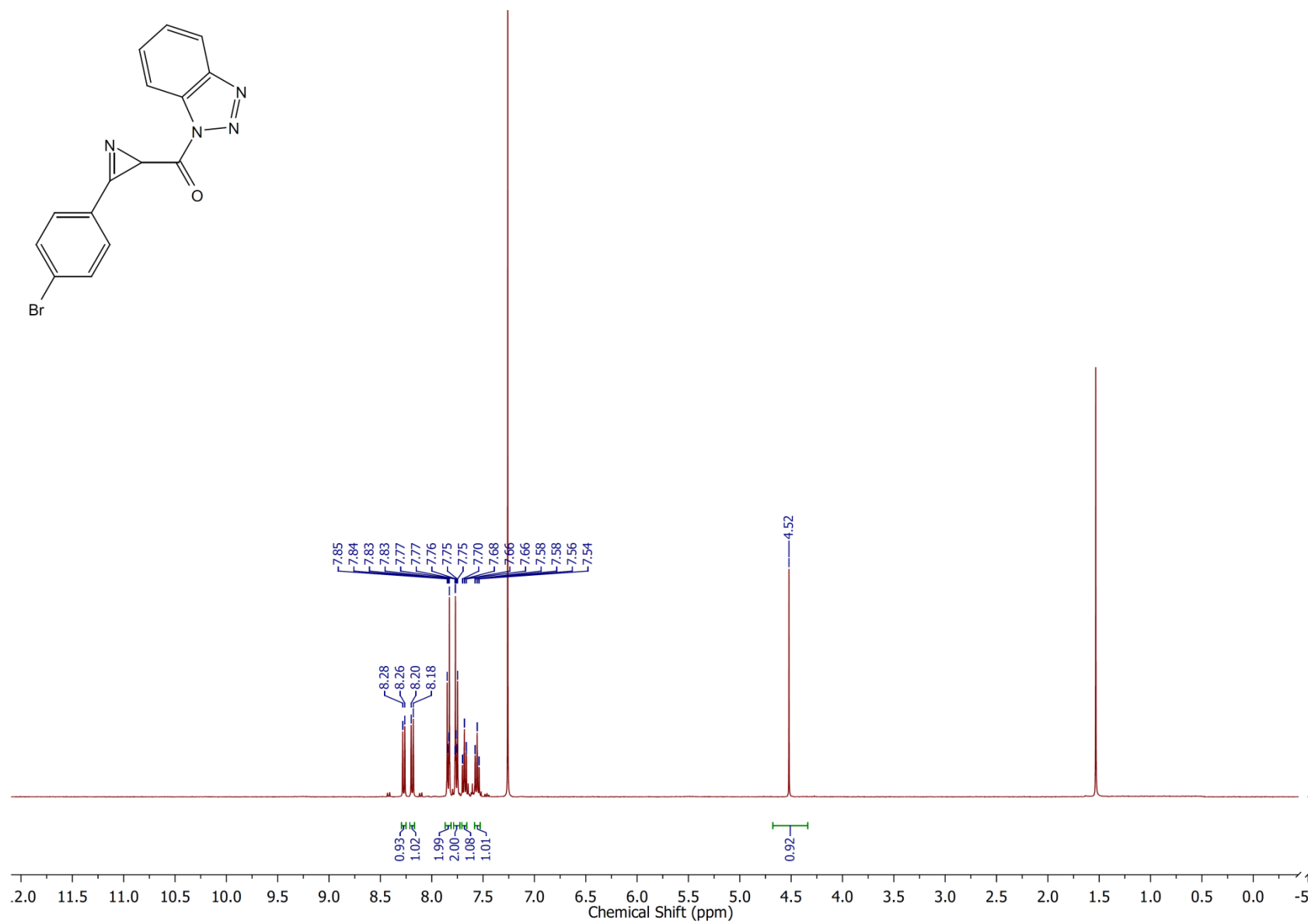
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-chlorophenyl)-2*H*-azirin-2-yl)methanone 1c, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



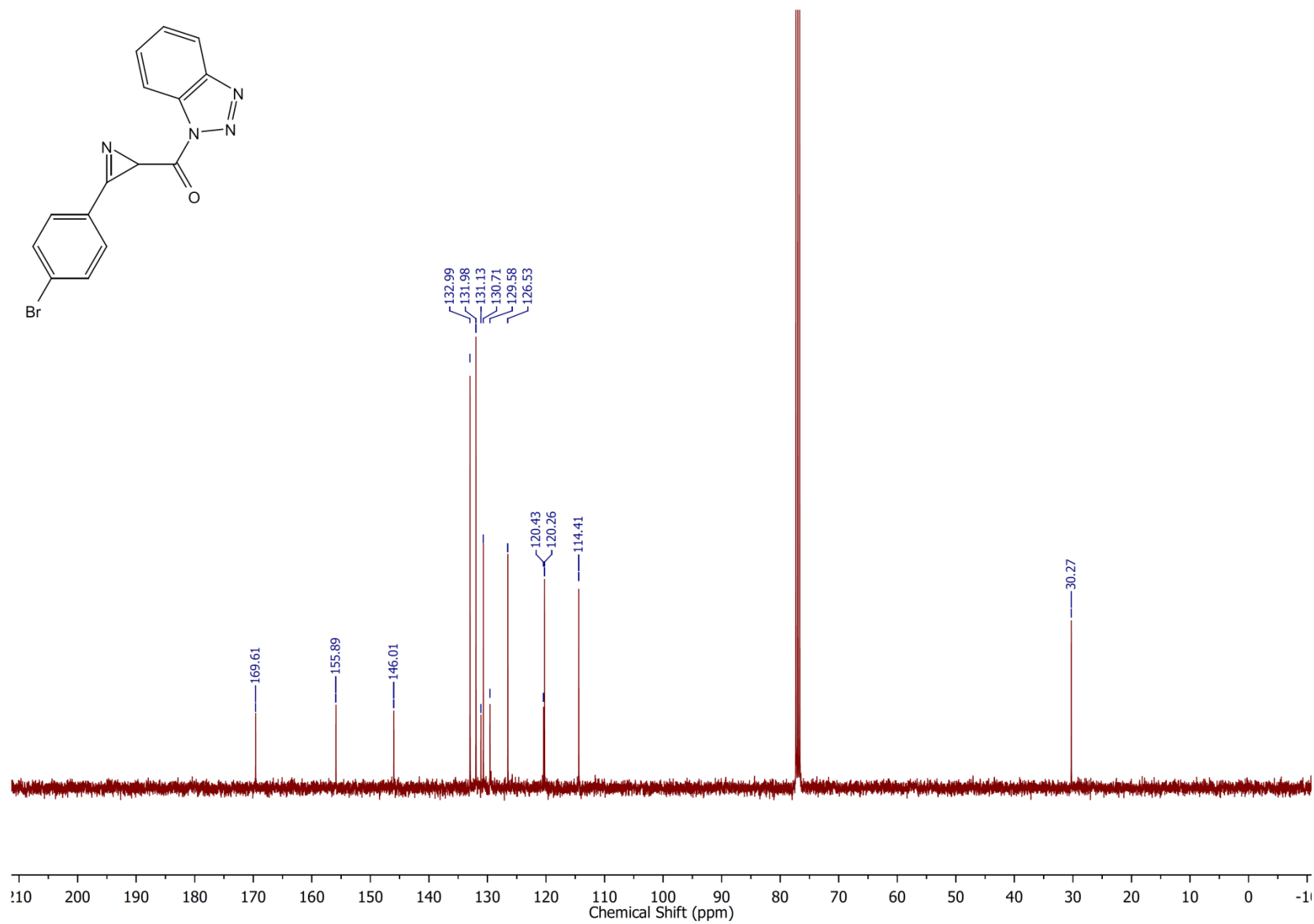
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-chlorophenyl)-2*H*-azirin-2-yl)methanone 1c, DEPT, CDCl₃, 100 MHz



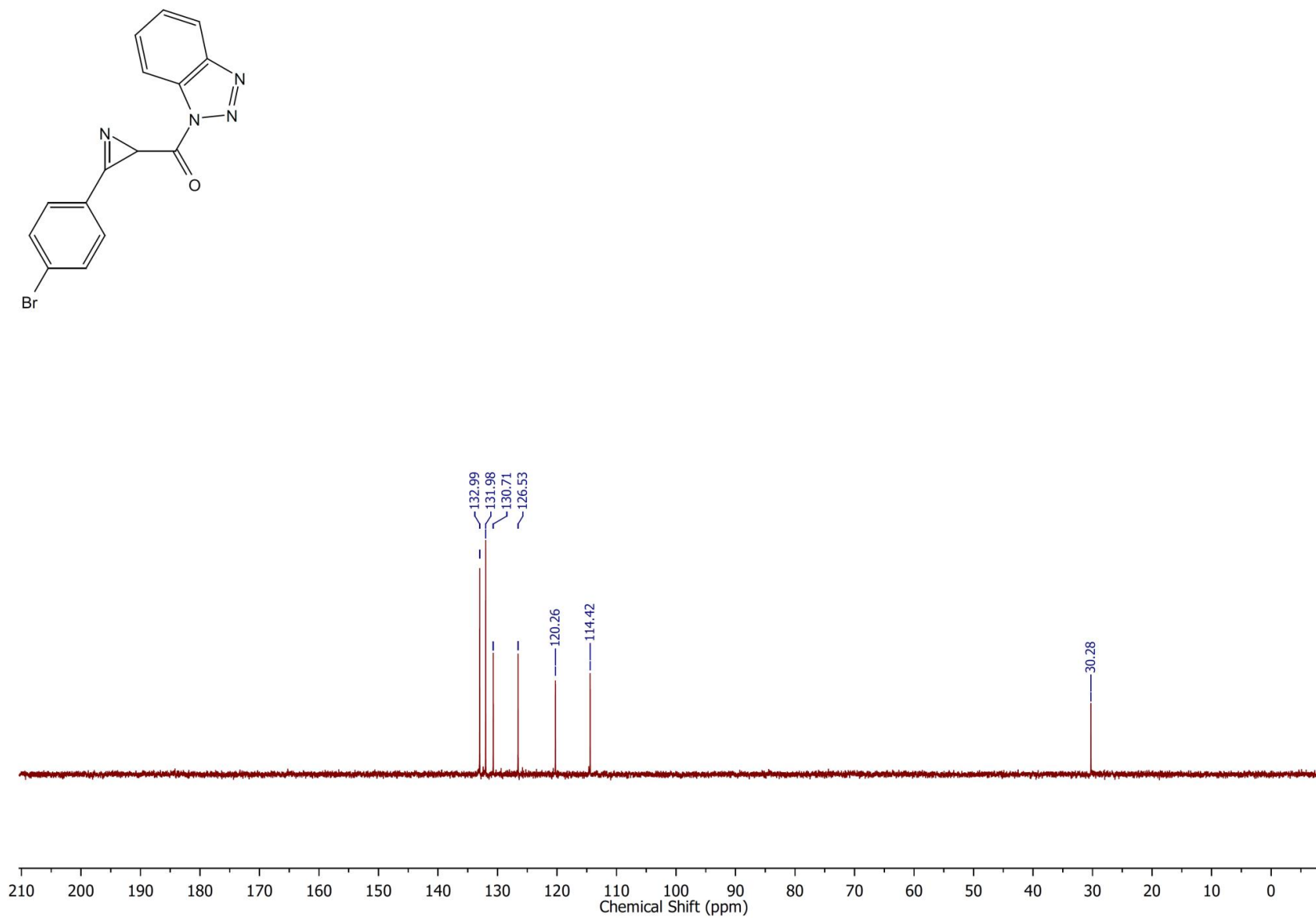
((1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-bromophenyl)-2*H*-azirin-2-yl)methanone 1d, ¹H NMR, CDCl₃, 400 MHz



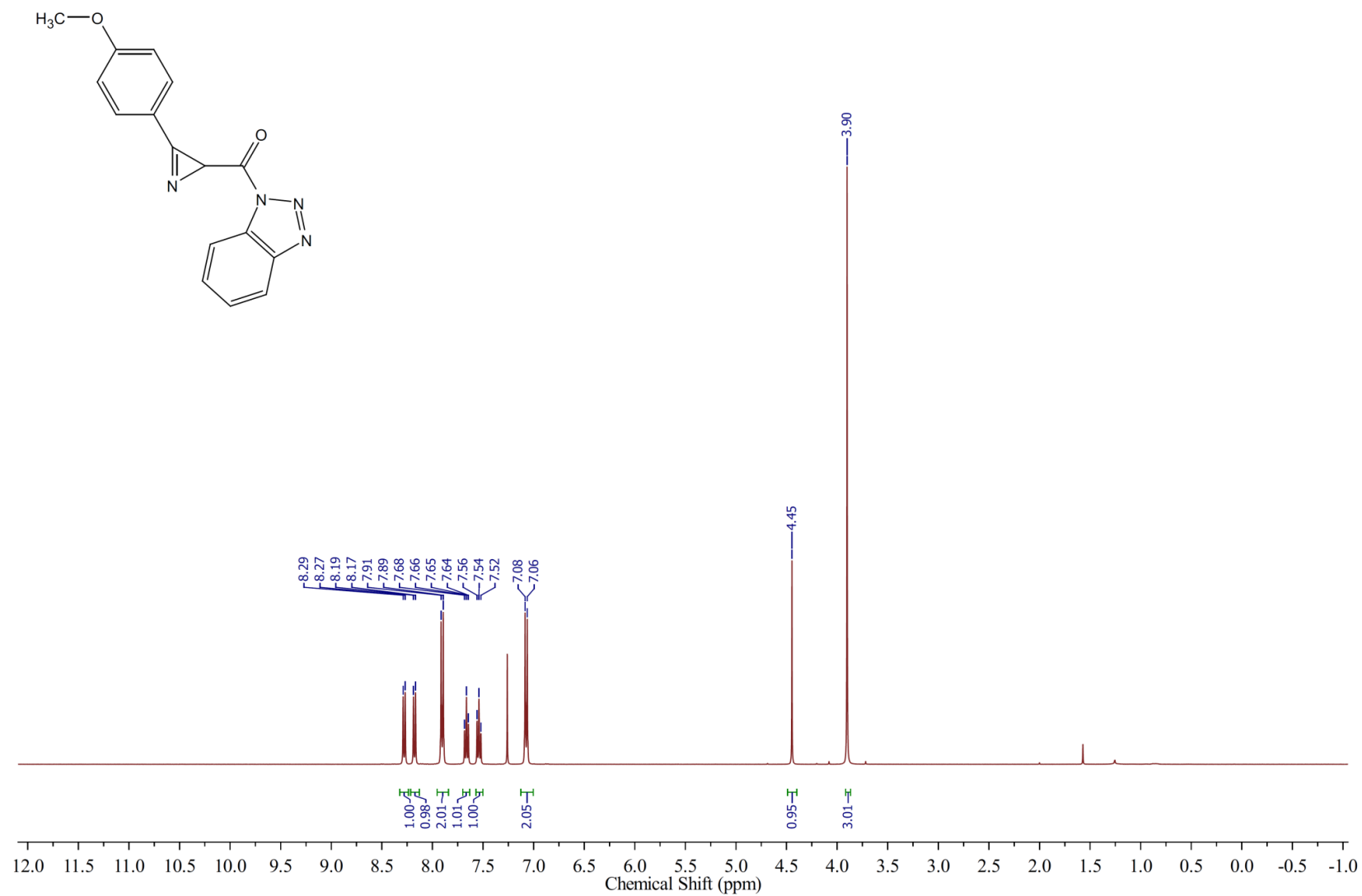
((1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-bromophenyl)-2*H*-azirin-2-yl)methanone 1d, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



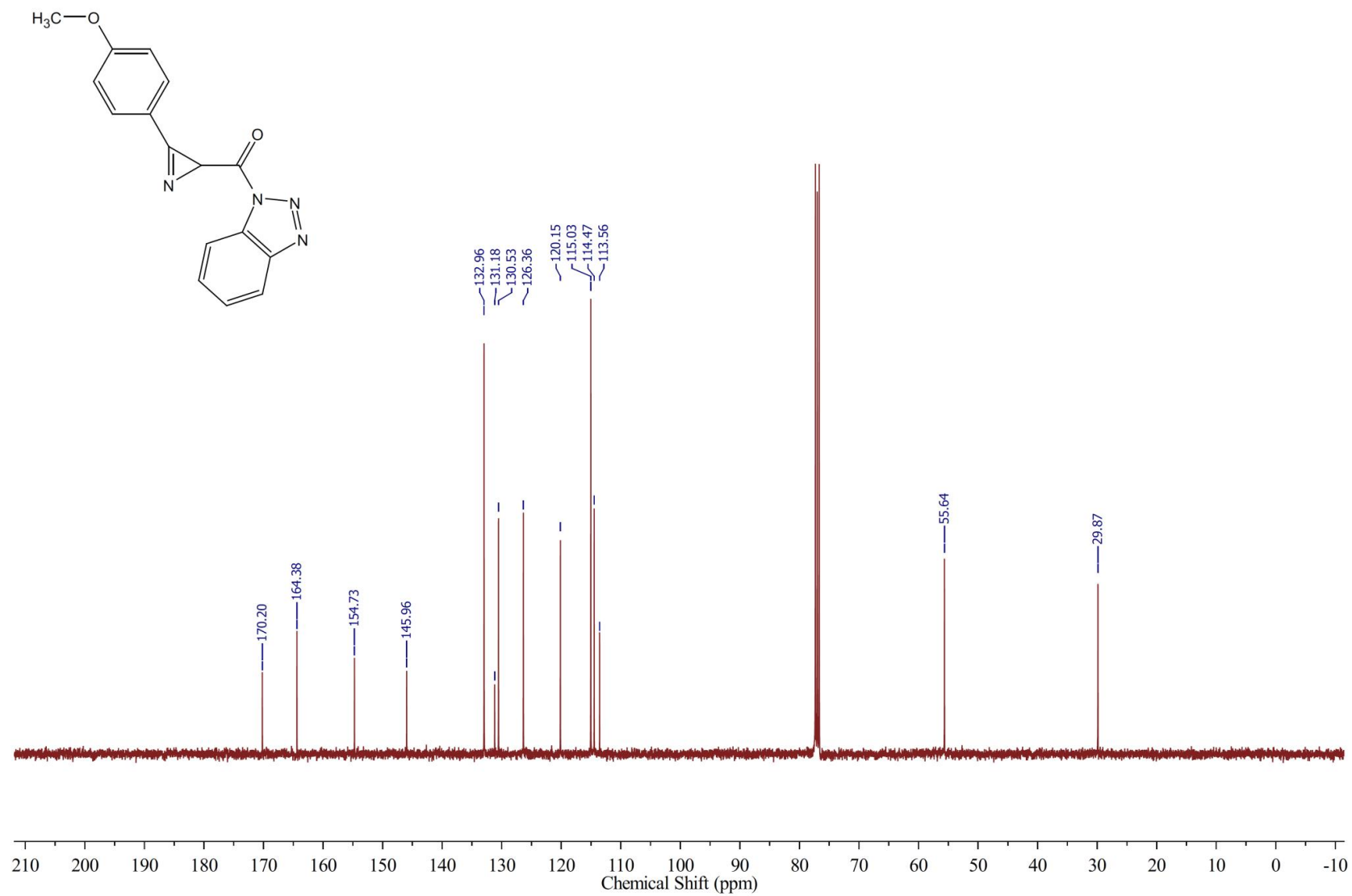
((1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-bromophenyl)-2*H*-azirin-2-yl)methanone 1d, DEPT, CDCl₃, 100 MHz



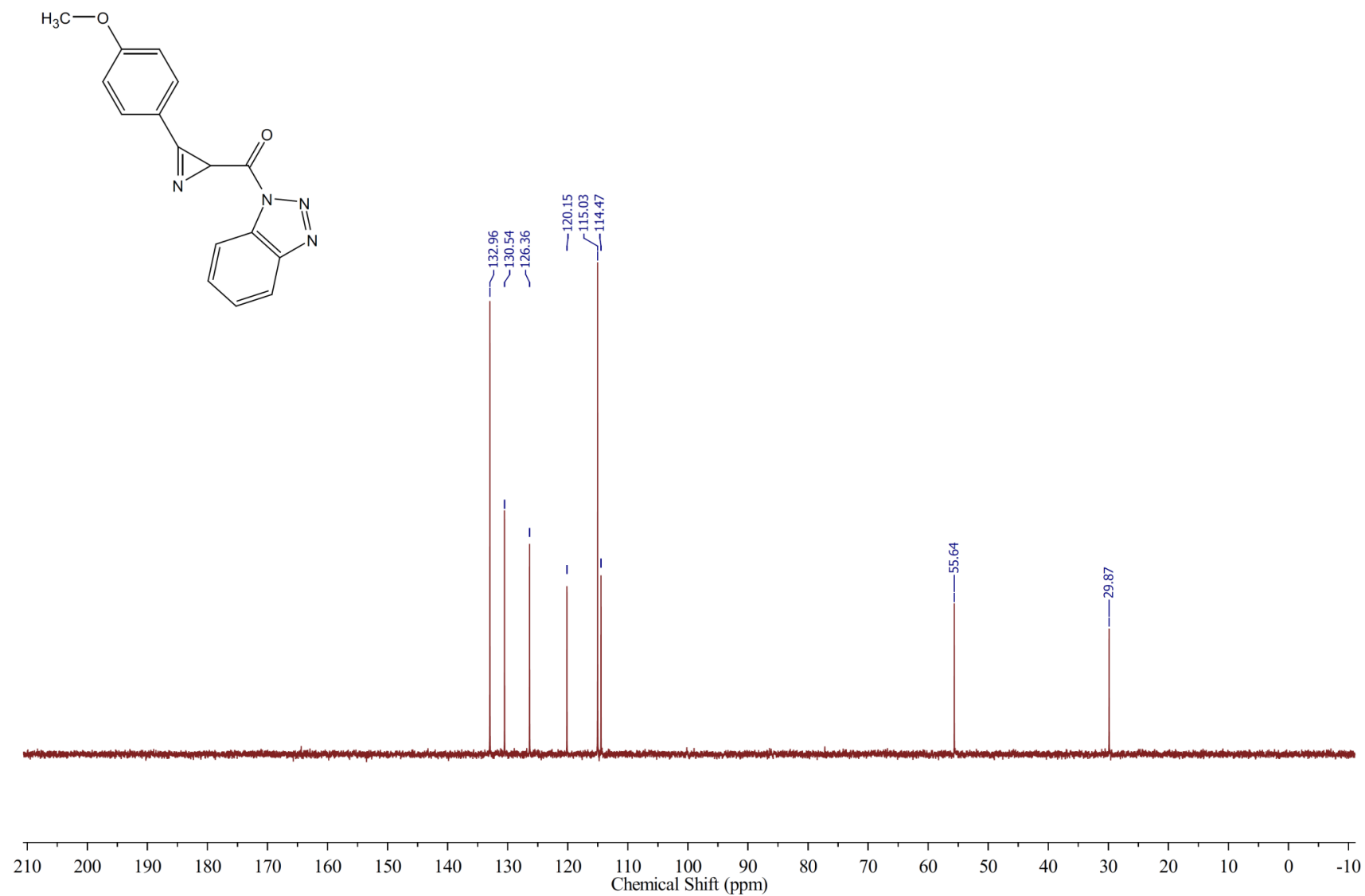
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-methoxyphenyl)-2*H*-azirin-2-yl)methanone 1e, ¹H NMR, CDCl₃, 400 MHz



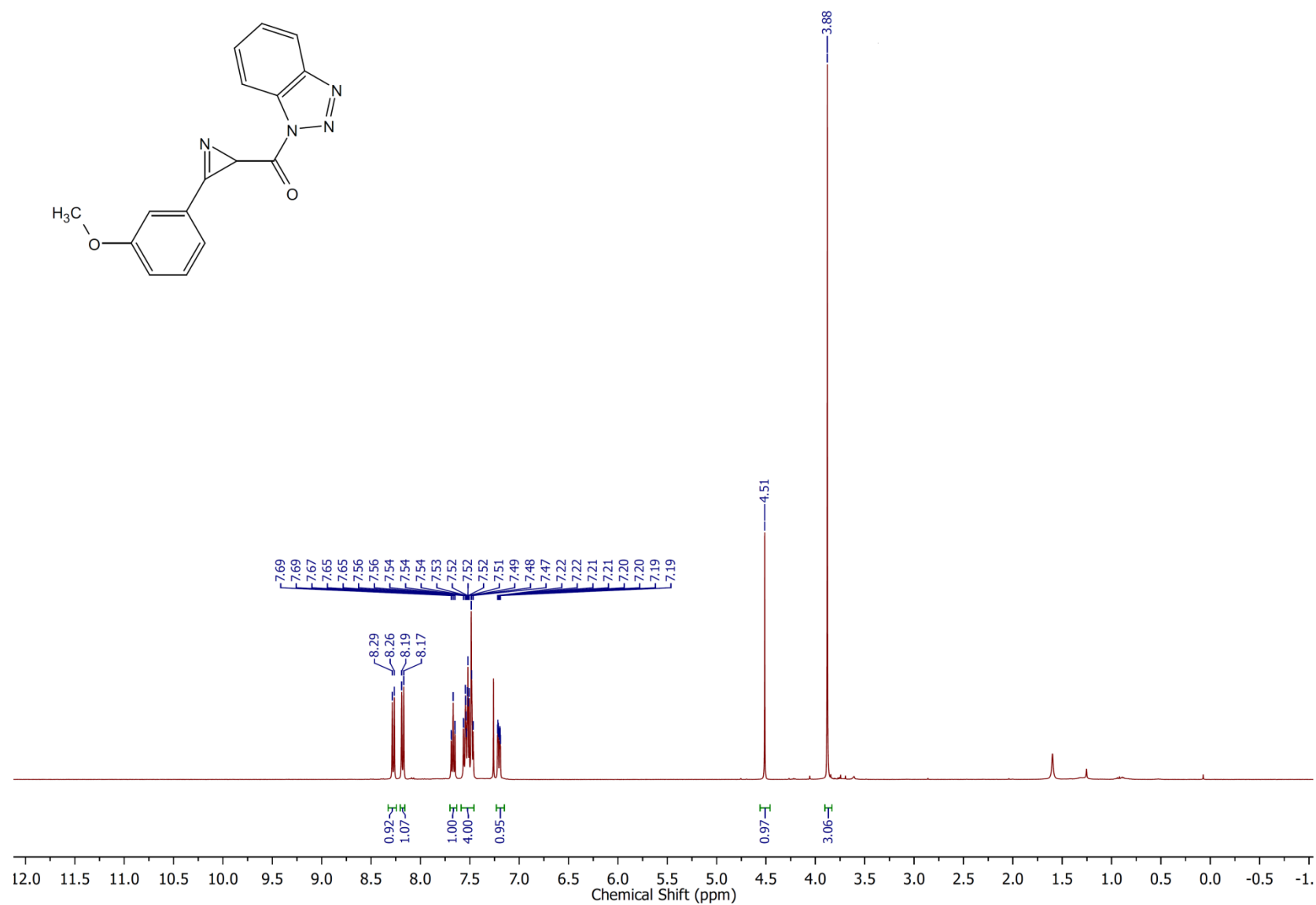
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-methoxyphenyl)-2*H*-azirin-2-yl)methanone **1e**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



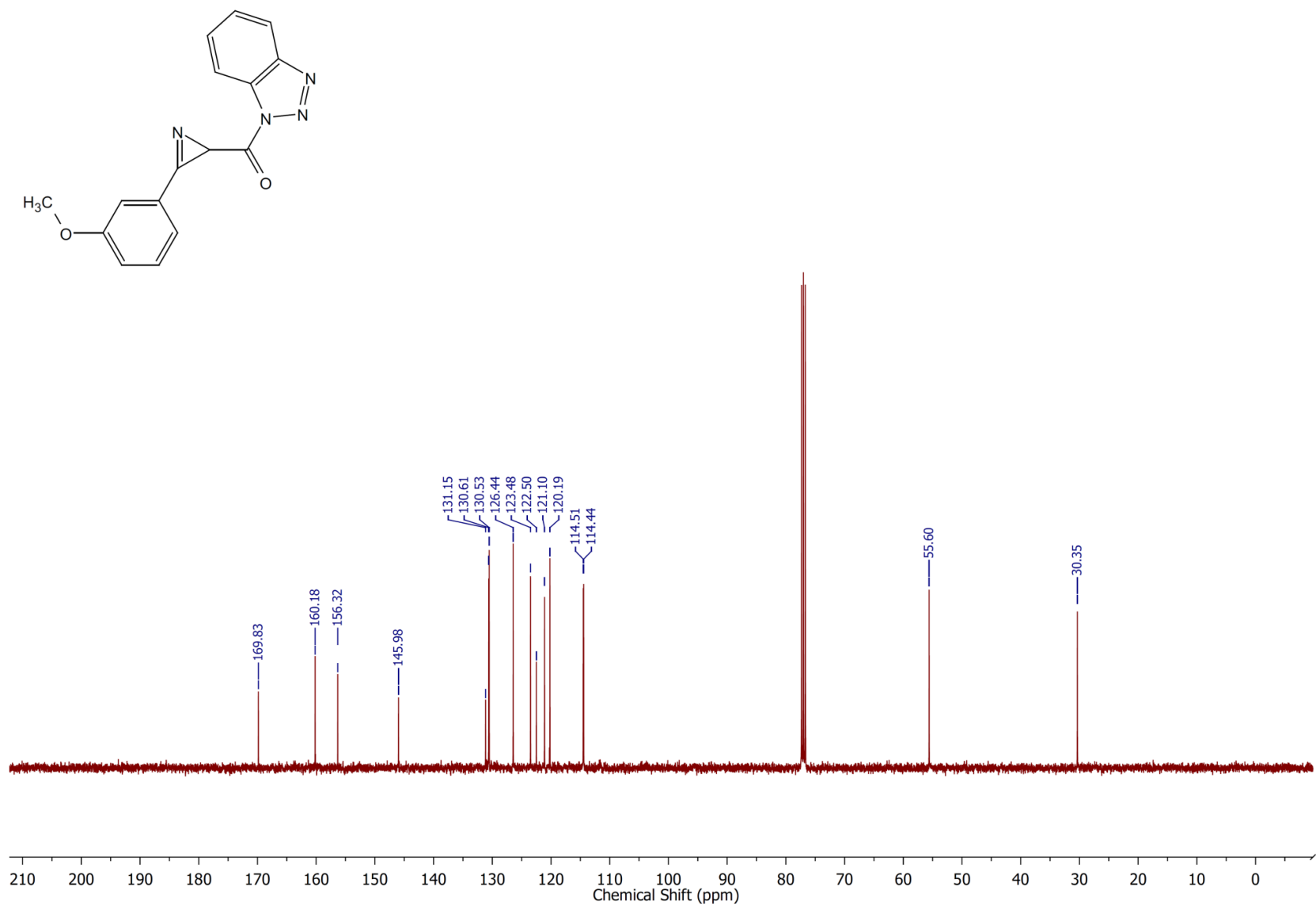
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(4-methoxyphenyl)-2*H*-azirin-2-yl)methanone 1e, DEPT, CDCl₃, 100 MHz



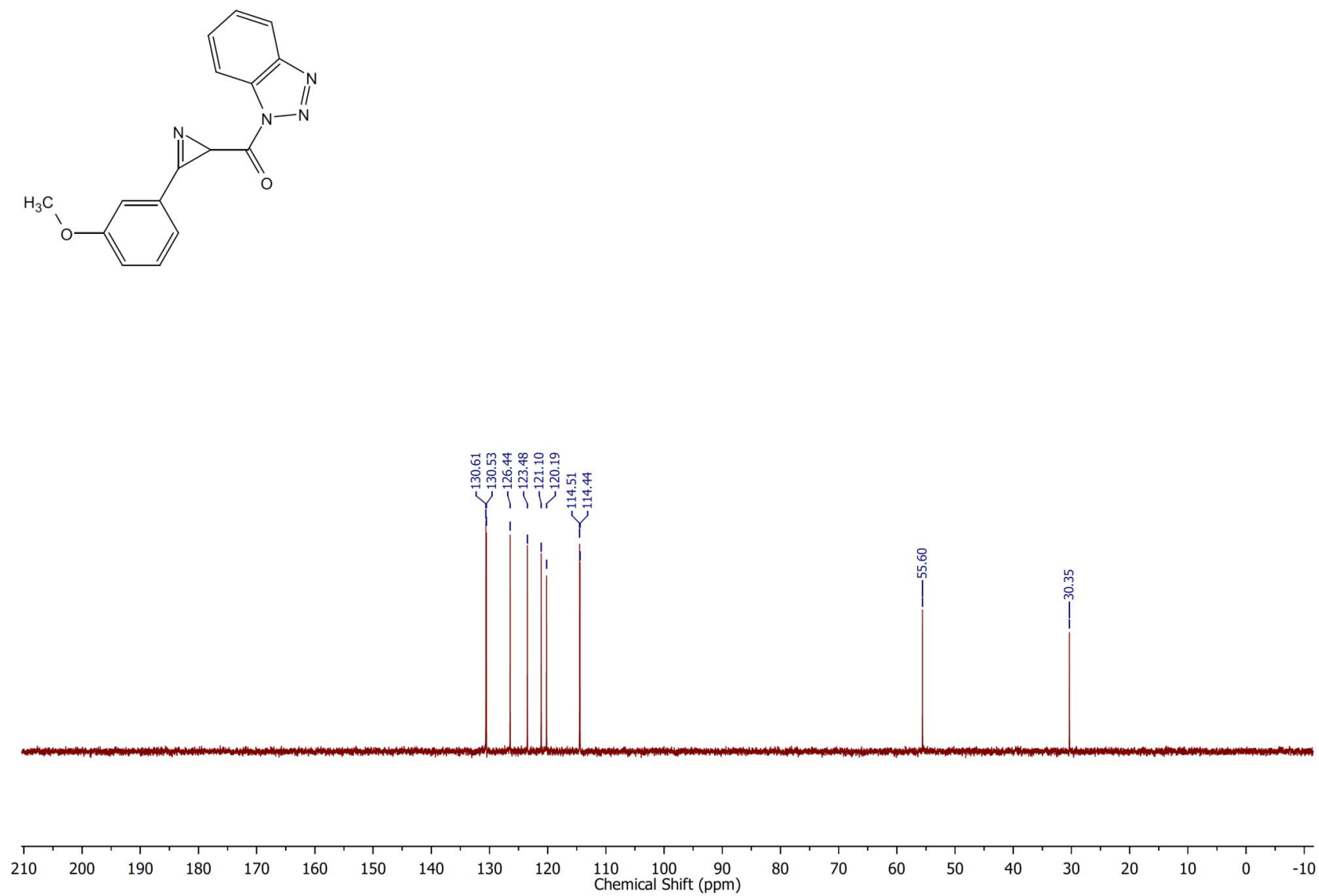
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(3-methoxyphenyl)-2*H*-azirin-2-yl)methanone 1f, ¹H NMR, CDCl₃, 400 MHz



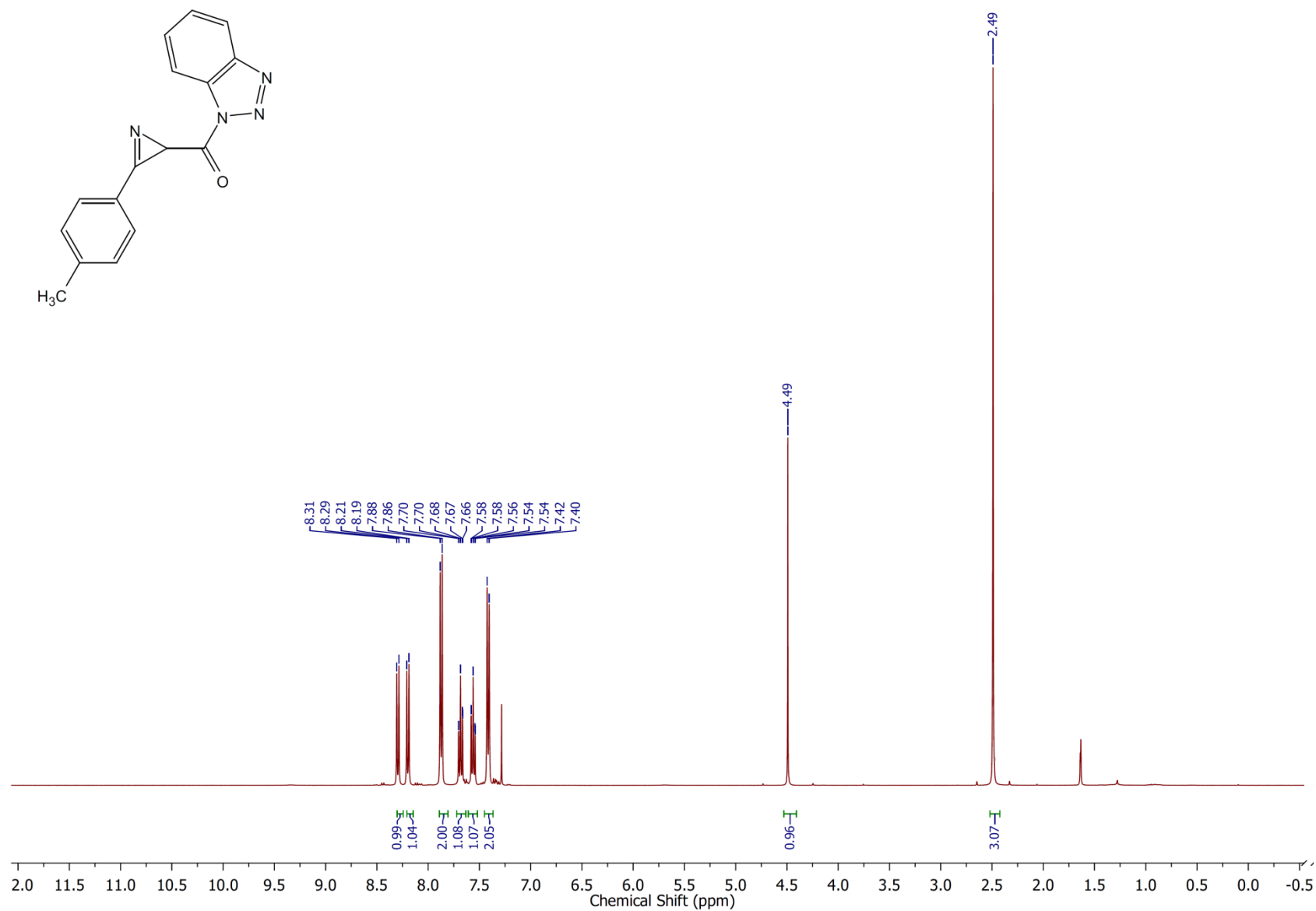
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(3-methoxyphenyl)-2*H*-azirin-2-yl)methanone 1f, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



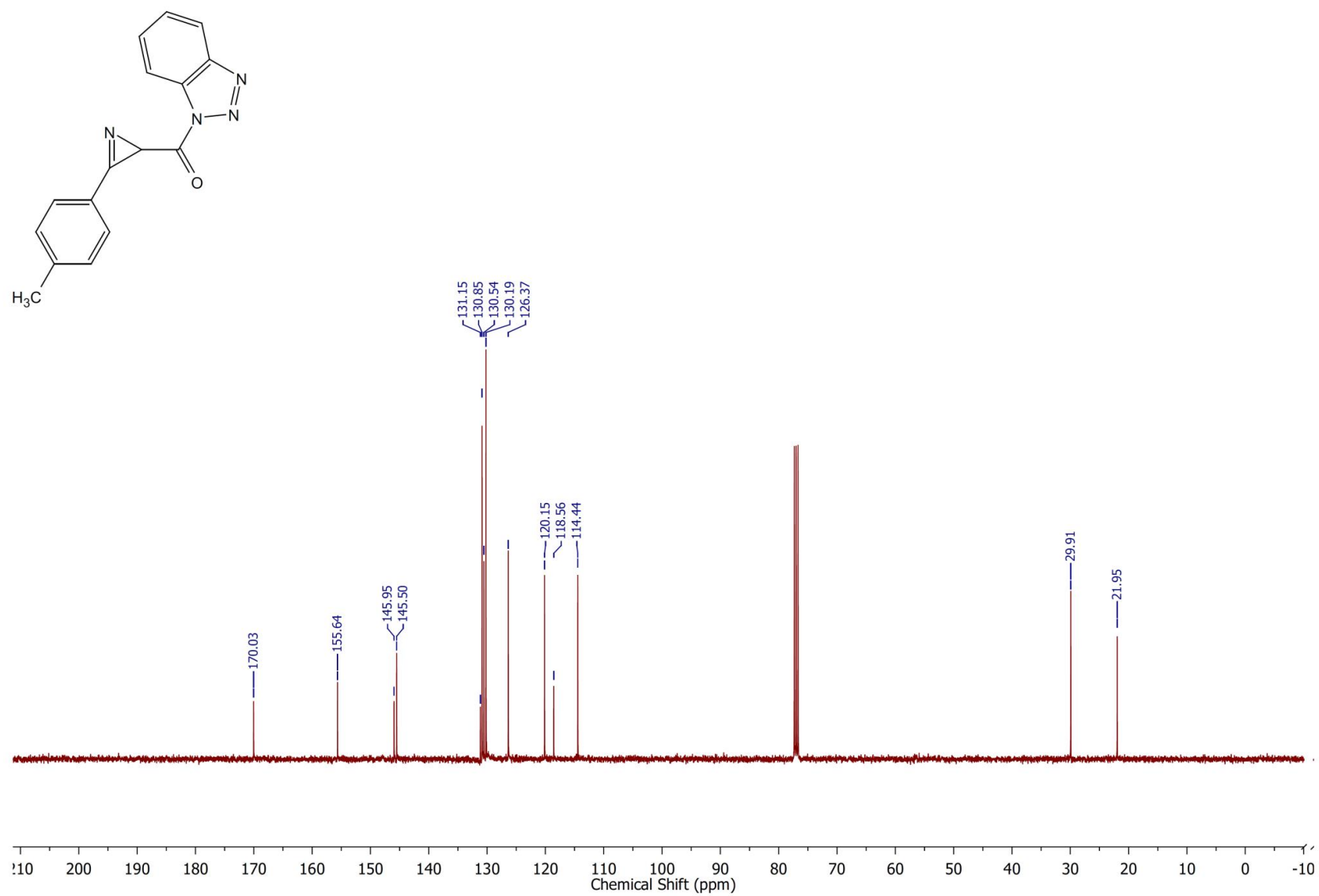
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(3-methoxyphenyl)-2*H*-azirin-2-yl)methanone 1f, DEPT, CDCl₃, 100 MHz



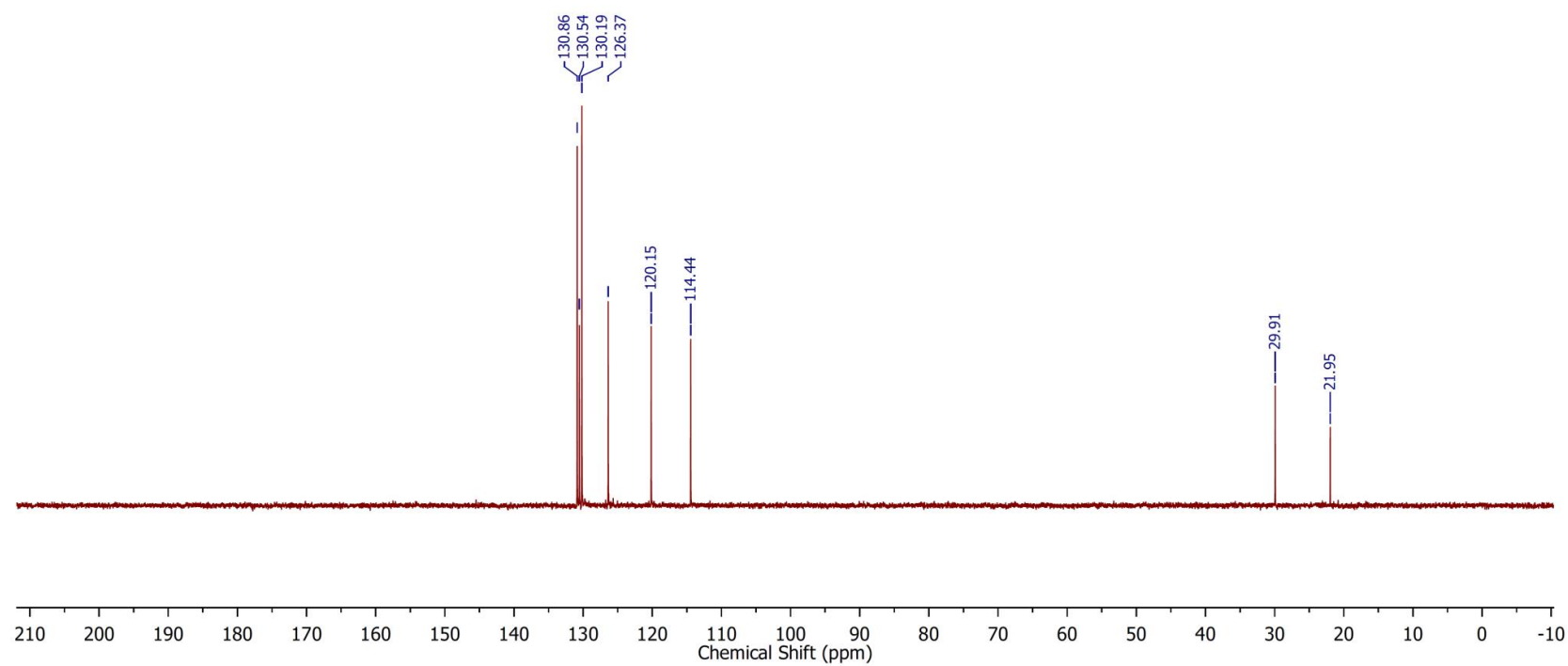
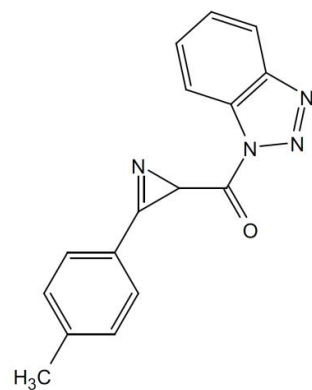
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(*p*-tolyl)-2*H*-azirin-2-yl)methanone 1g, ¹H NMR, CDCl₃, 400 MHz



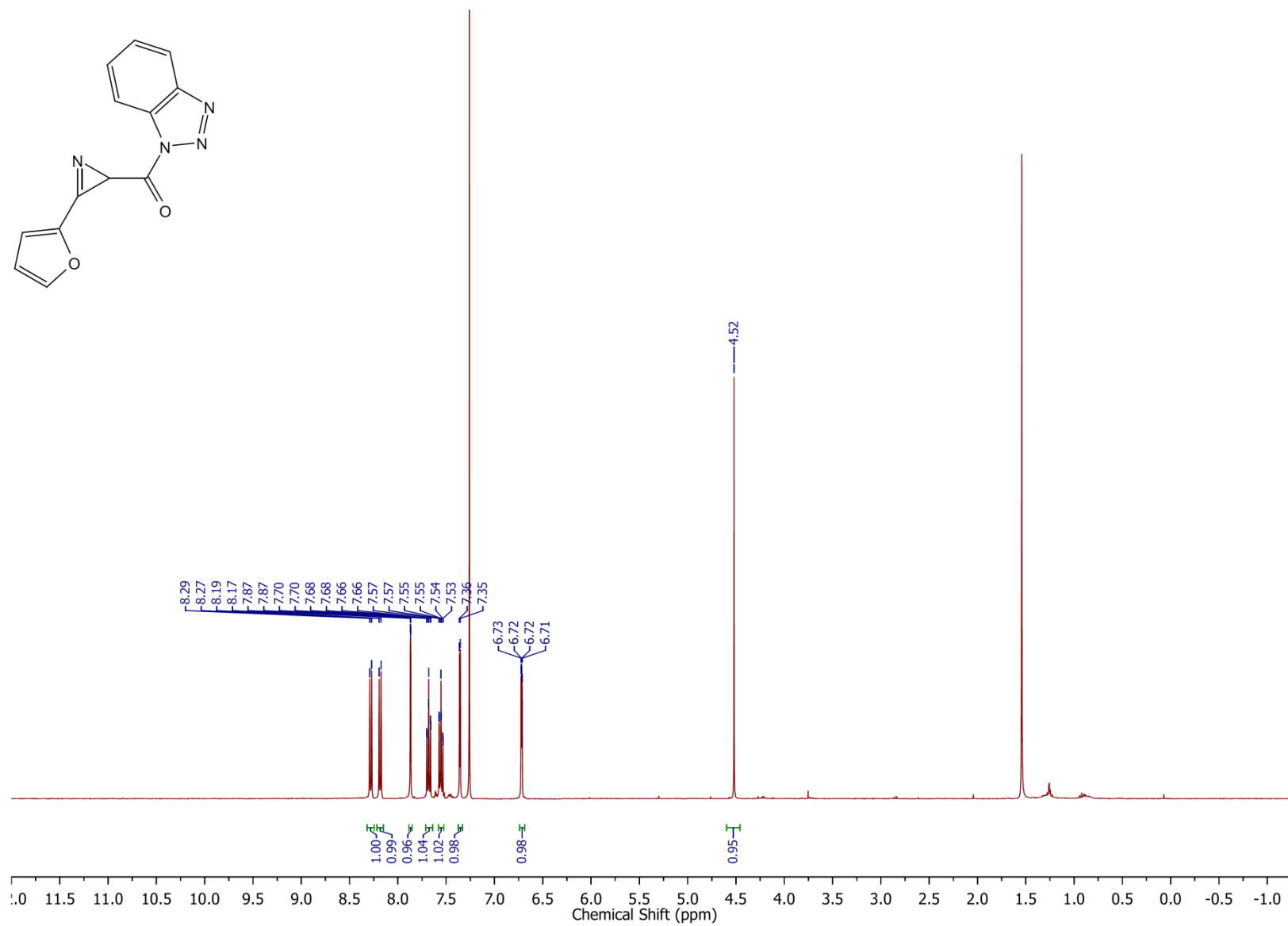
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(*p*-tolyl)-2*H*-azirin-2-yl)methanone **1g**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



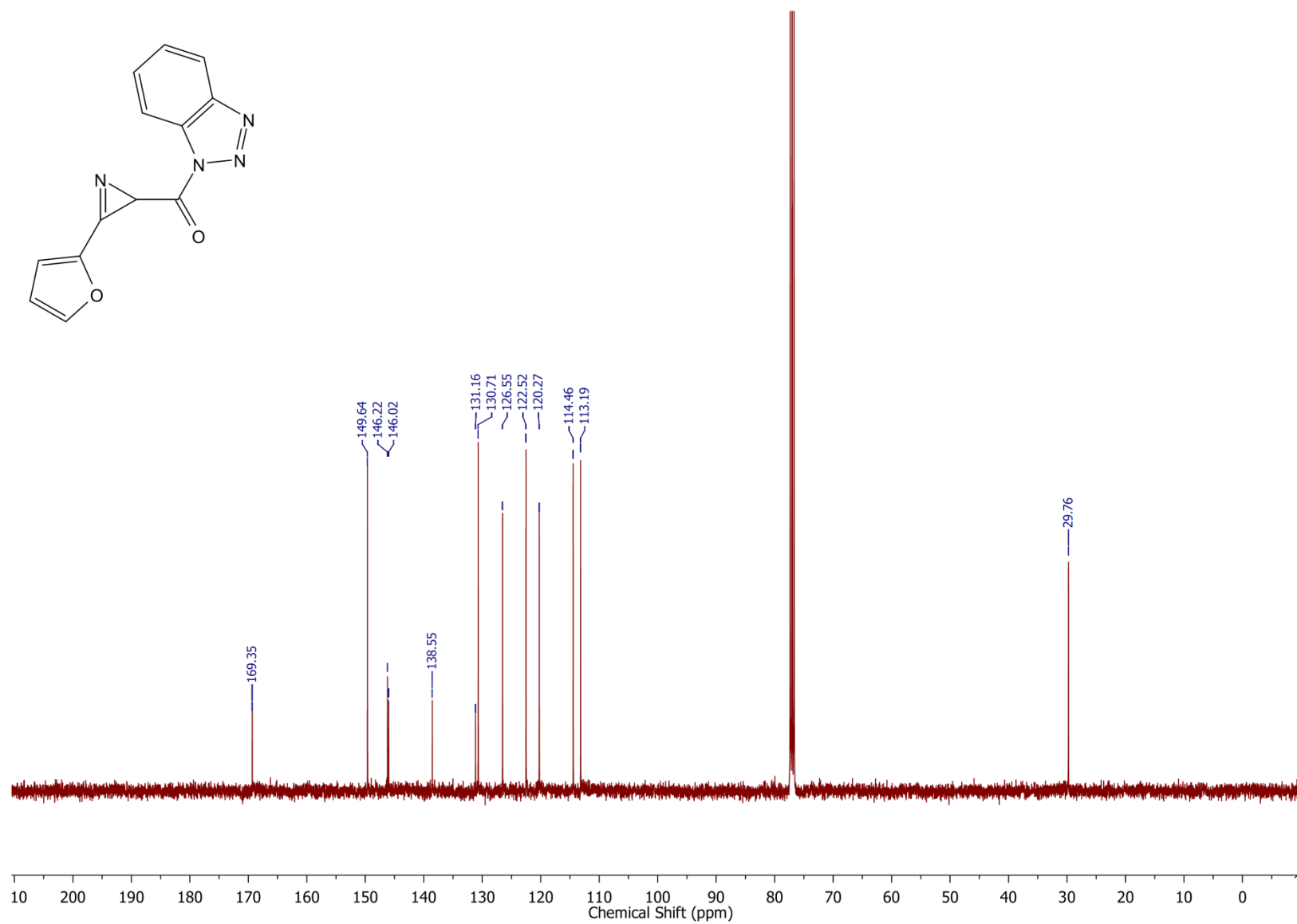
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(*p*-tolyl)-2*H*-azirin-2-yl)methanone 1g, DEPT, CDCl₃, 100 MHz



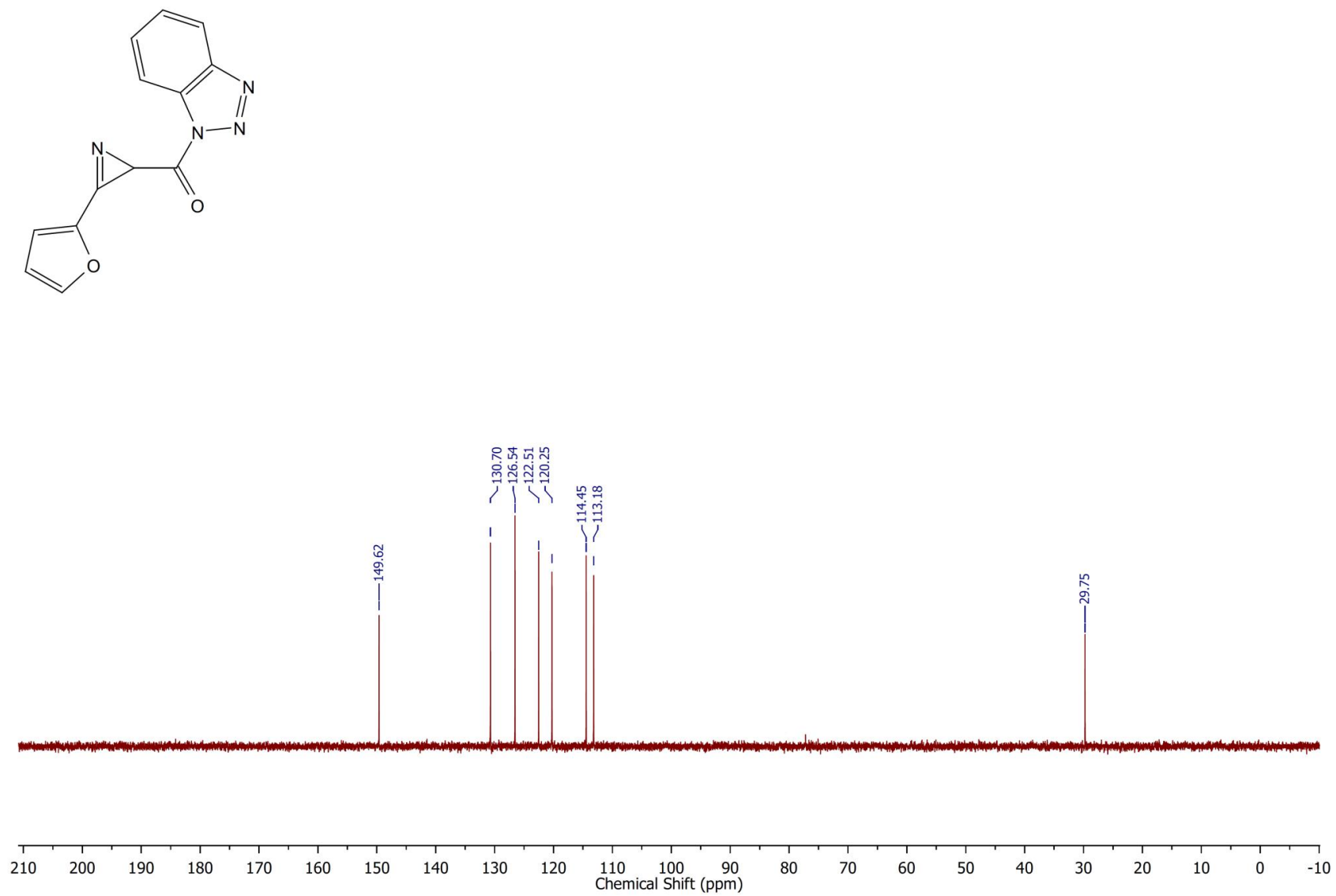
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)((furan-2-yl)-2*H*-azirin-2-yl)methanone 1h, ¹H NMR, CDCl₃, 400 MHz



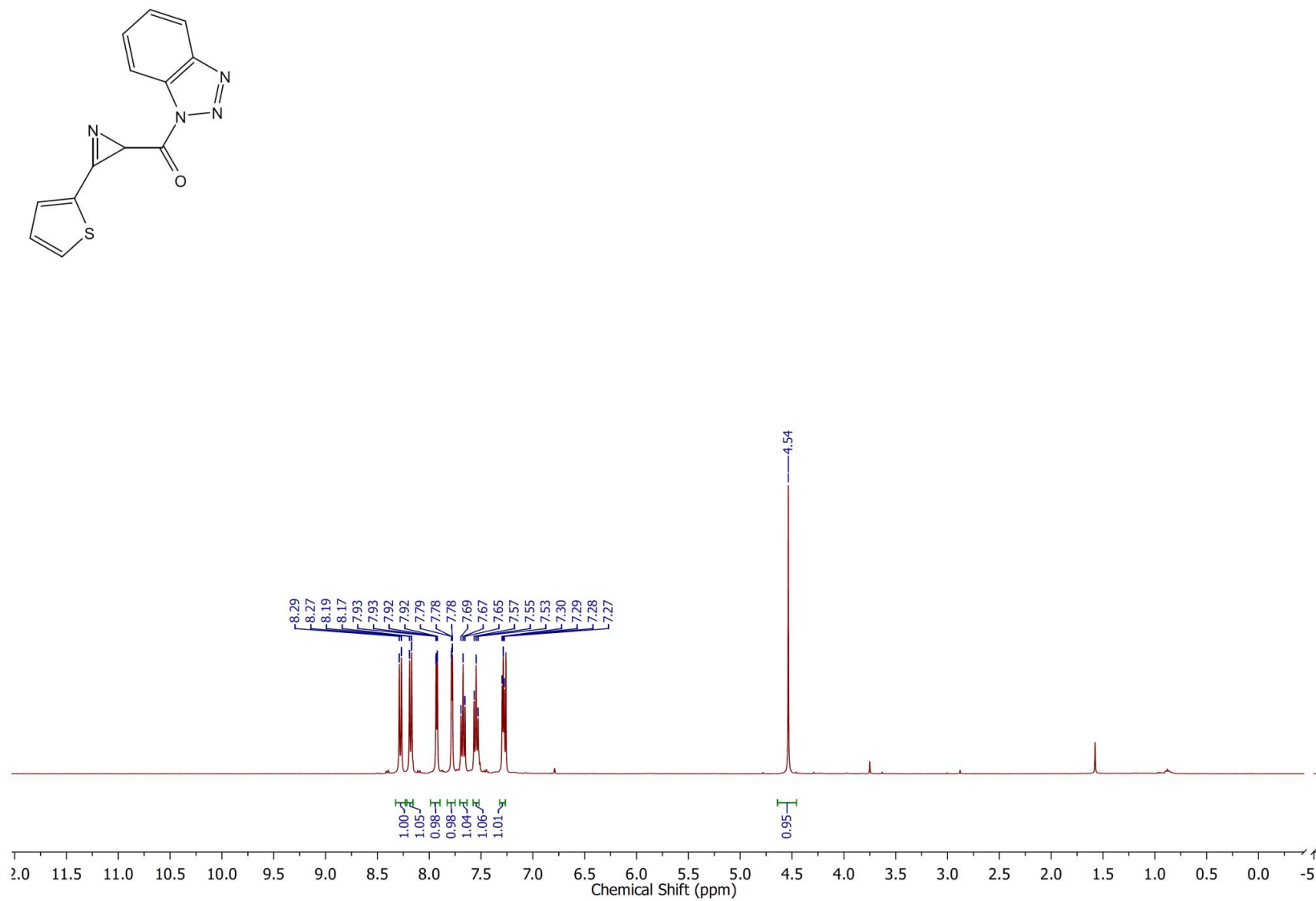
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)((furan-2-yl)-2*H*-azirin-2-yl)methanone **1h**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



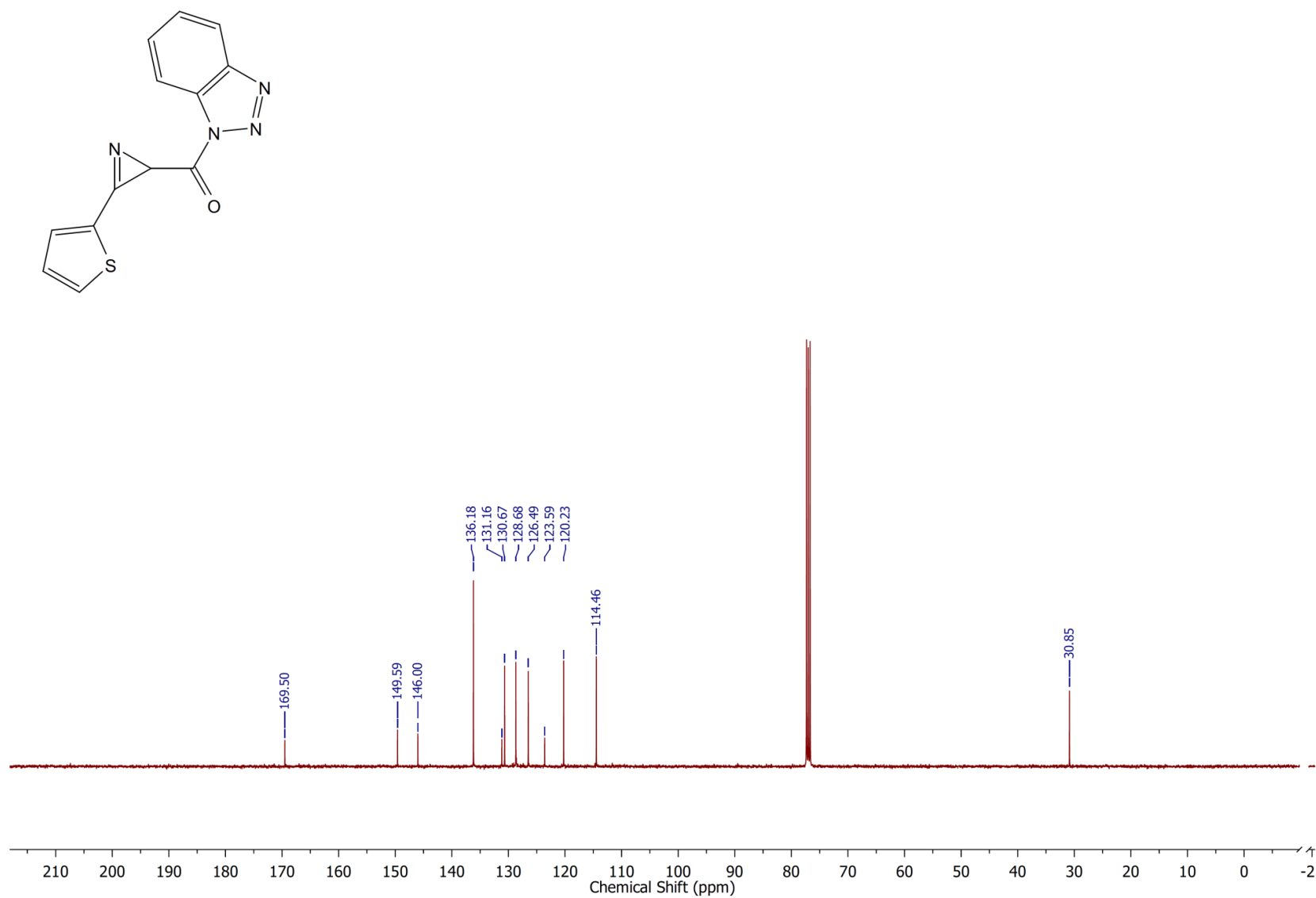
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)((furan-2-yl)-2*H*-azirin-2-yl)methanone 1h, DEPT, CDCl₃, 100 MHz



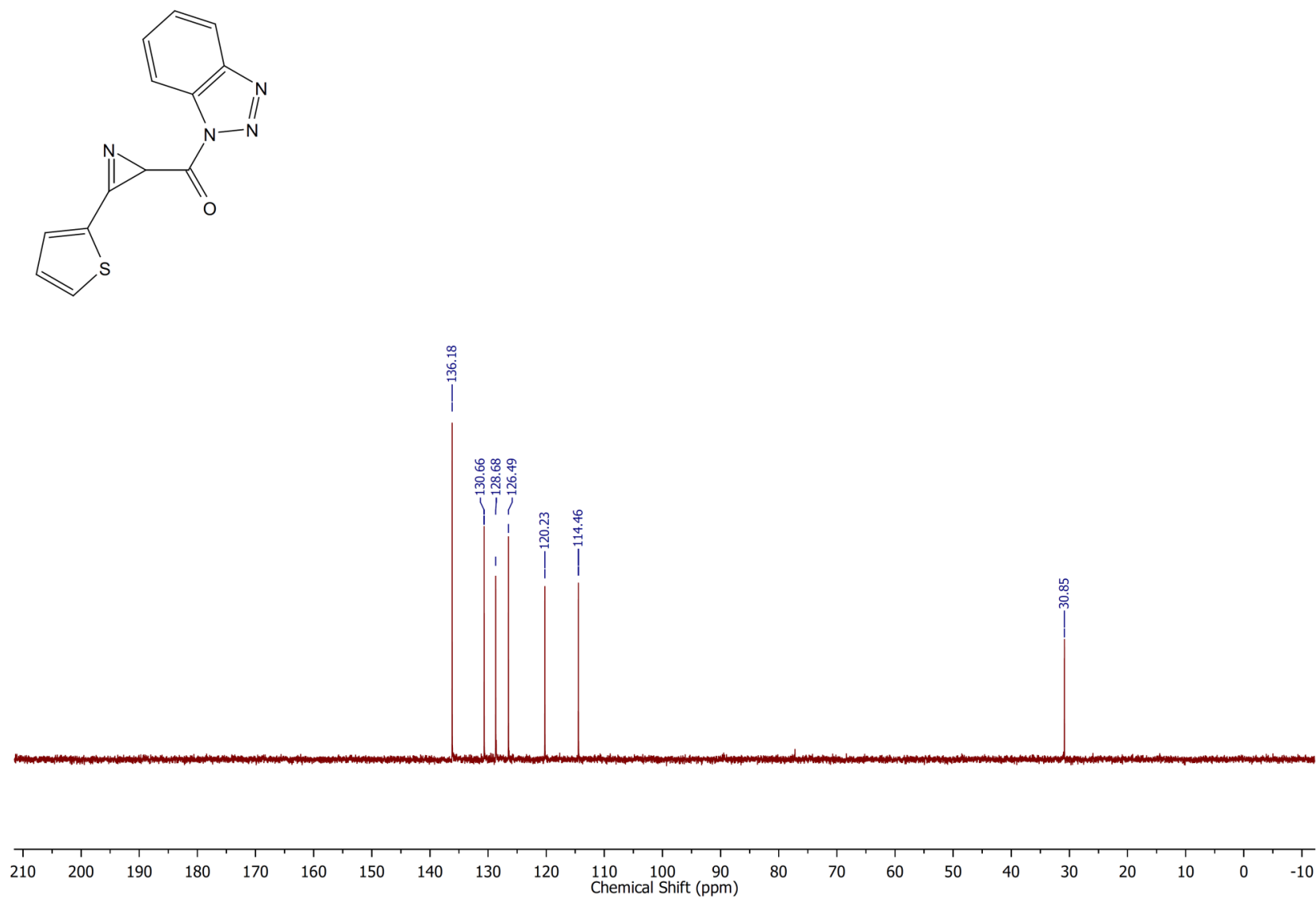
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)((thiophen-2-yl)-2*H*-azirin-2-yl)methanone **1i**, ^1H NMR, CDCl_3 , 400 MHz



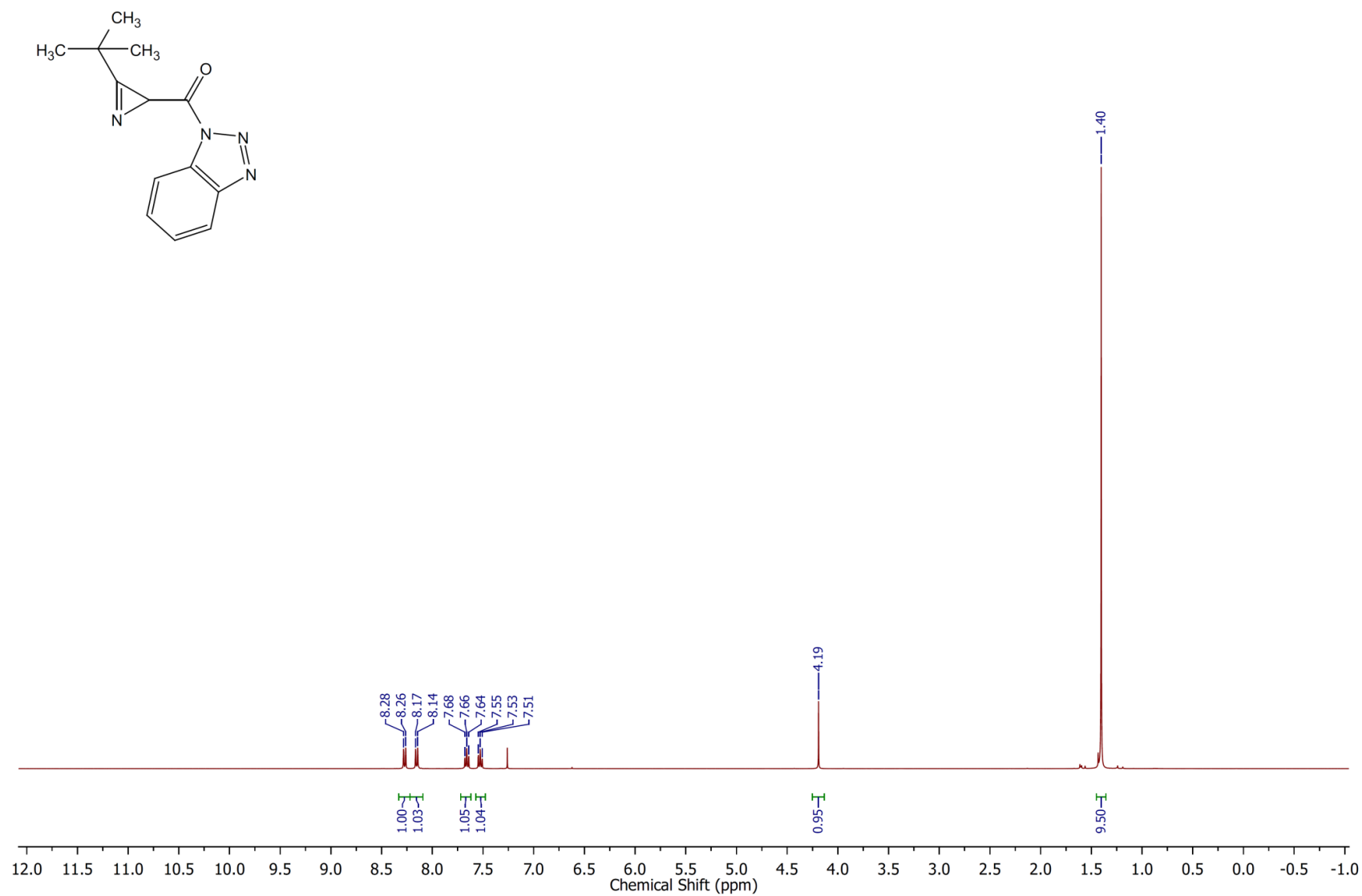
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)((thiophen-2-yl)-2*H*-azirin-2-yl)methanone **1i**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



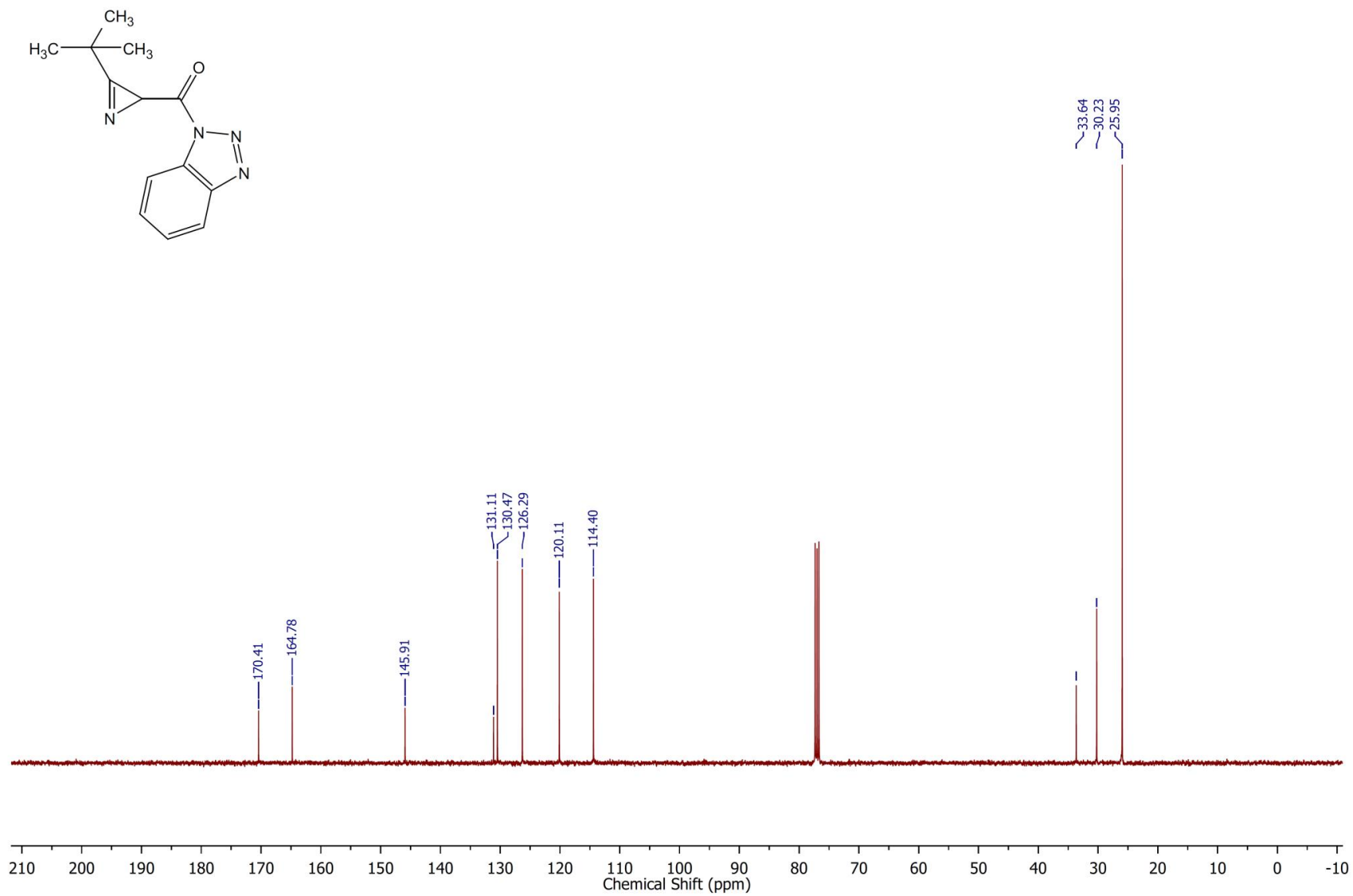
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)((thiophen-2-yl)-2*H*-azirin-2-yl)methanone 1i, DEPT, CDCl₃, 100 MHz



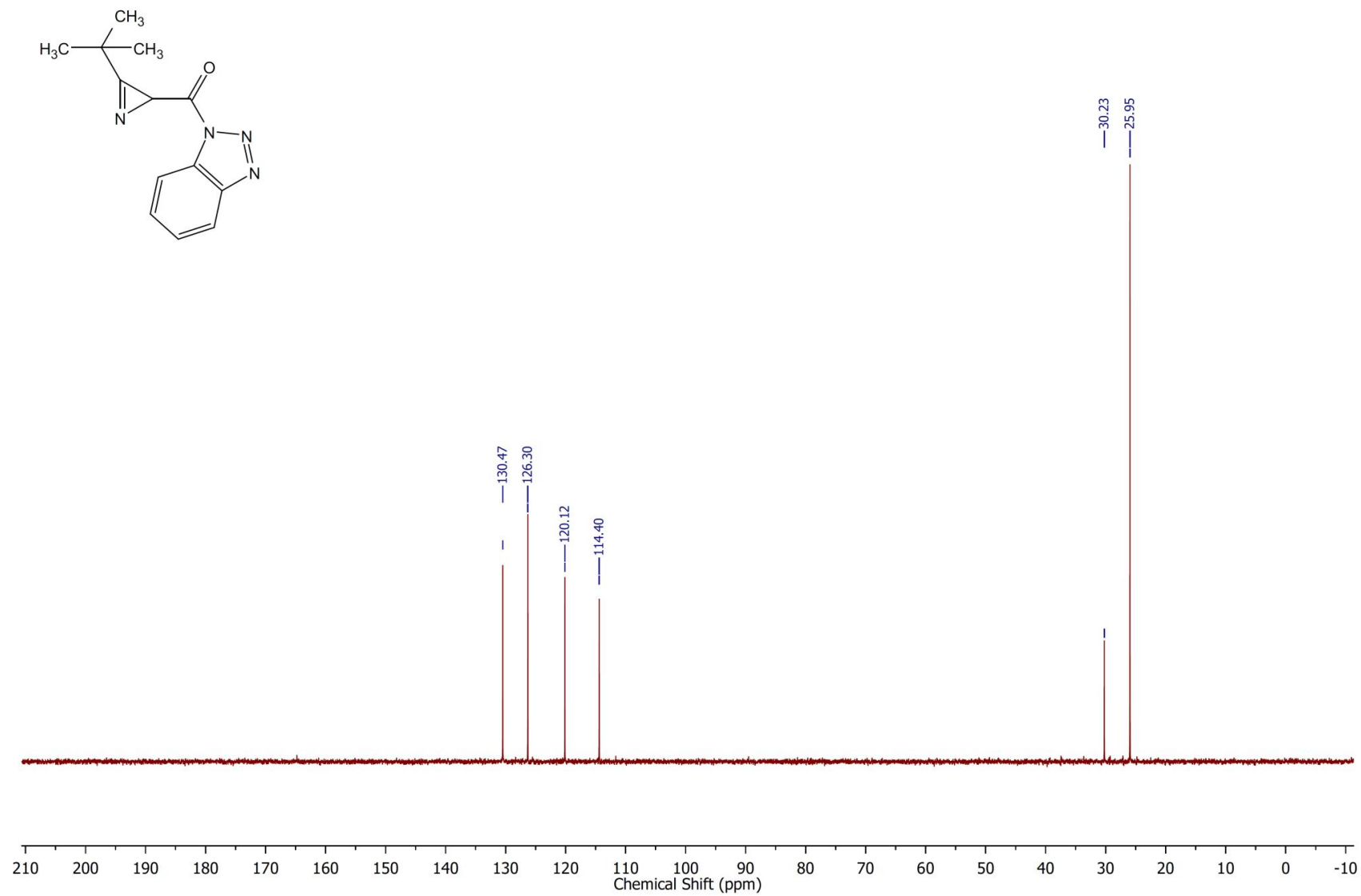
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(*tert*-butyl)-2*H*-azirin-2-yl)methanone 1j, ¹H NMR, CDCl₃, 400 MHz



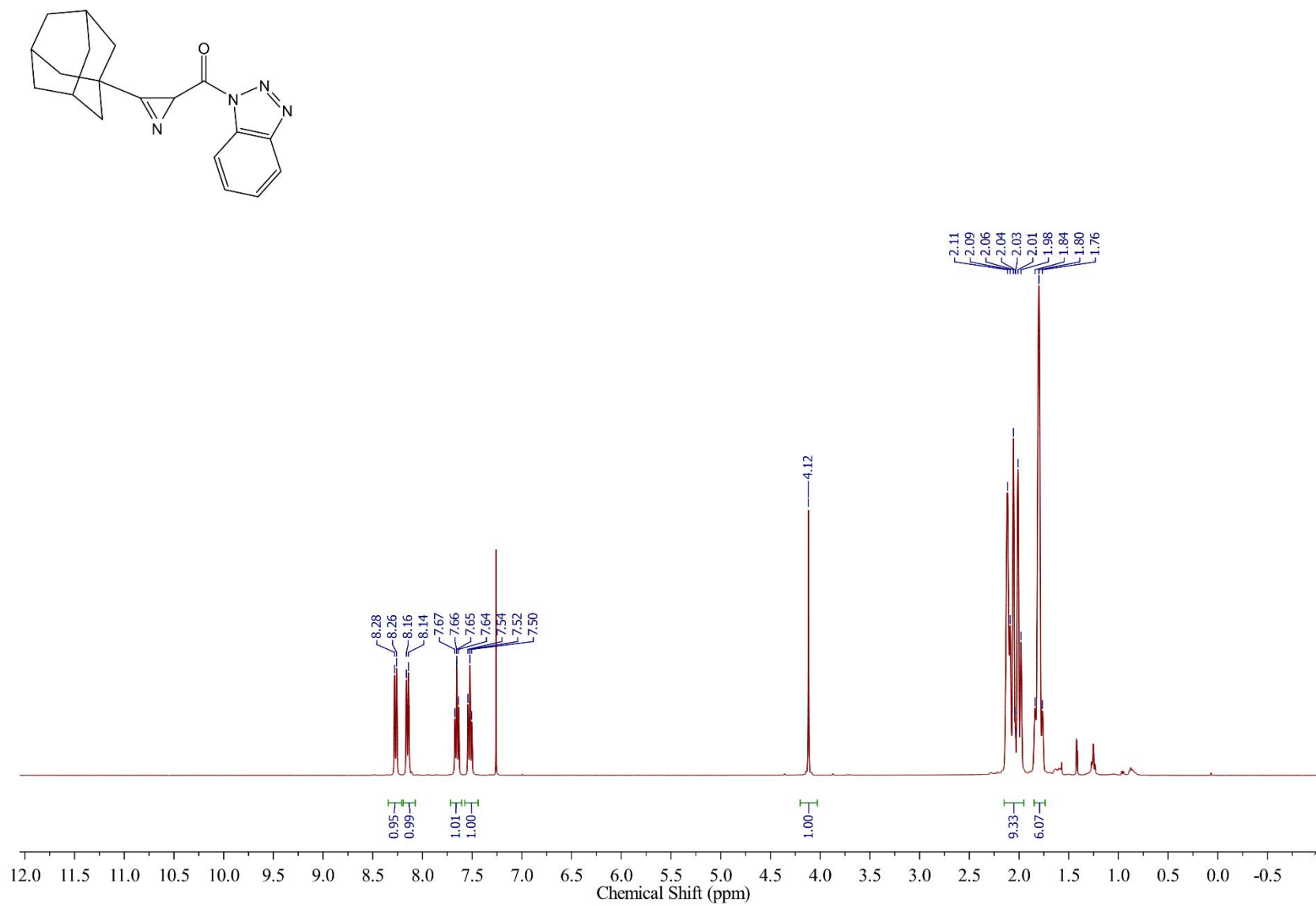
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(*tert*-butyl)-2*H*-azirin-2-yl)methanone **1j**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



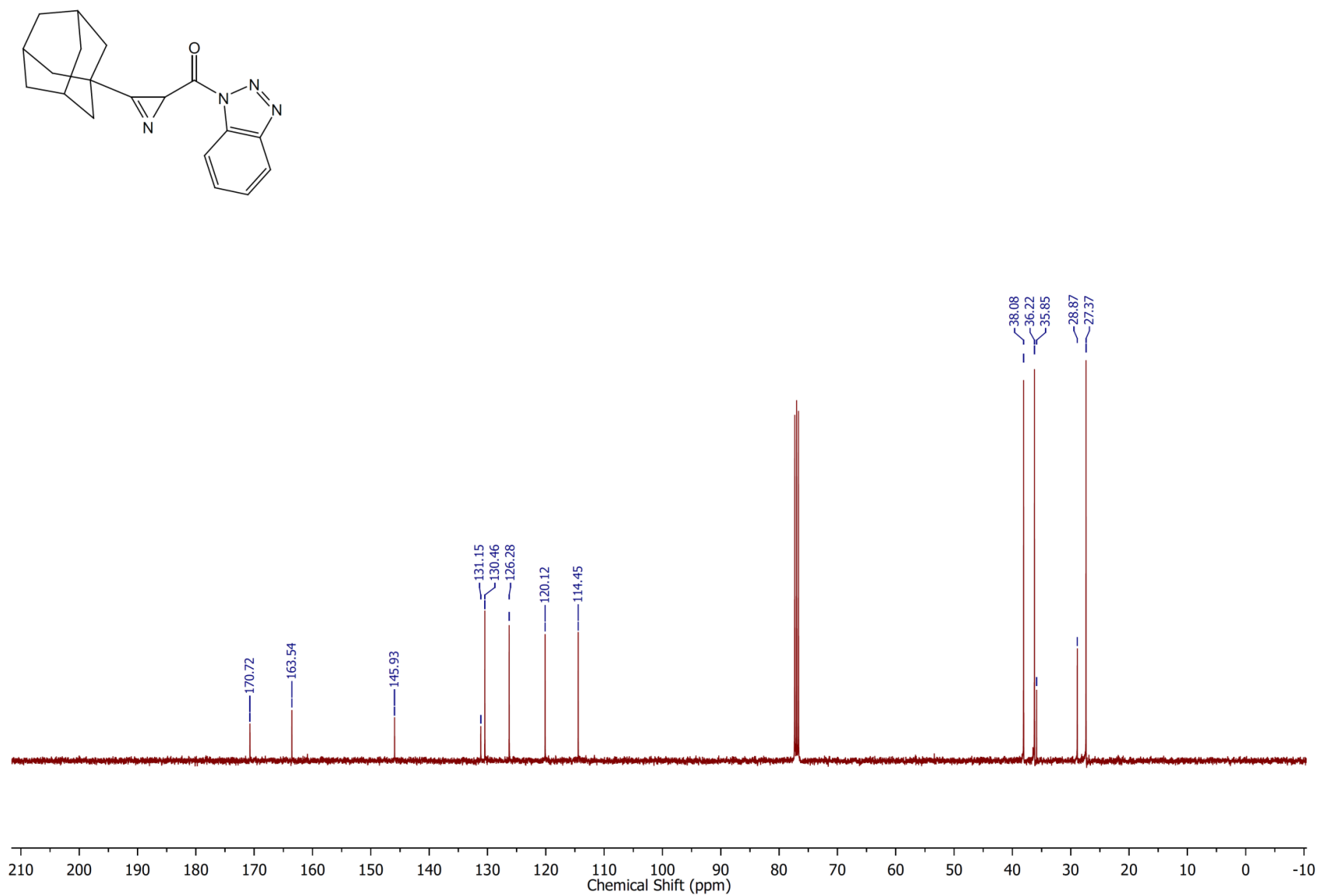
(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)(3-(*tert*-butyl)-2*H*-azirin-2-yl)methanone 1j, DEPT, CDCl₃, 100 MHz



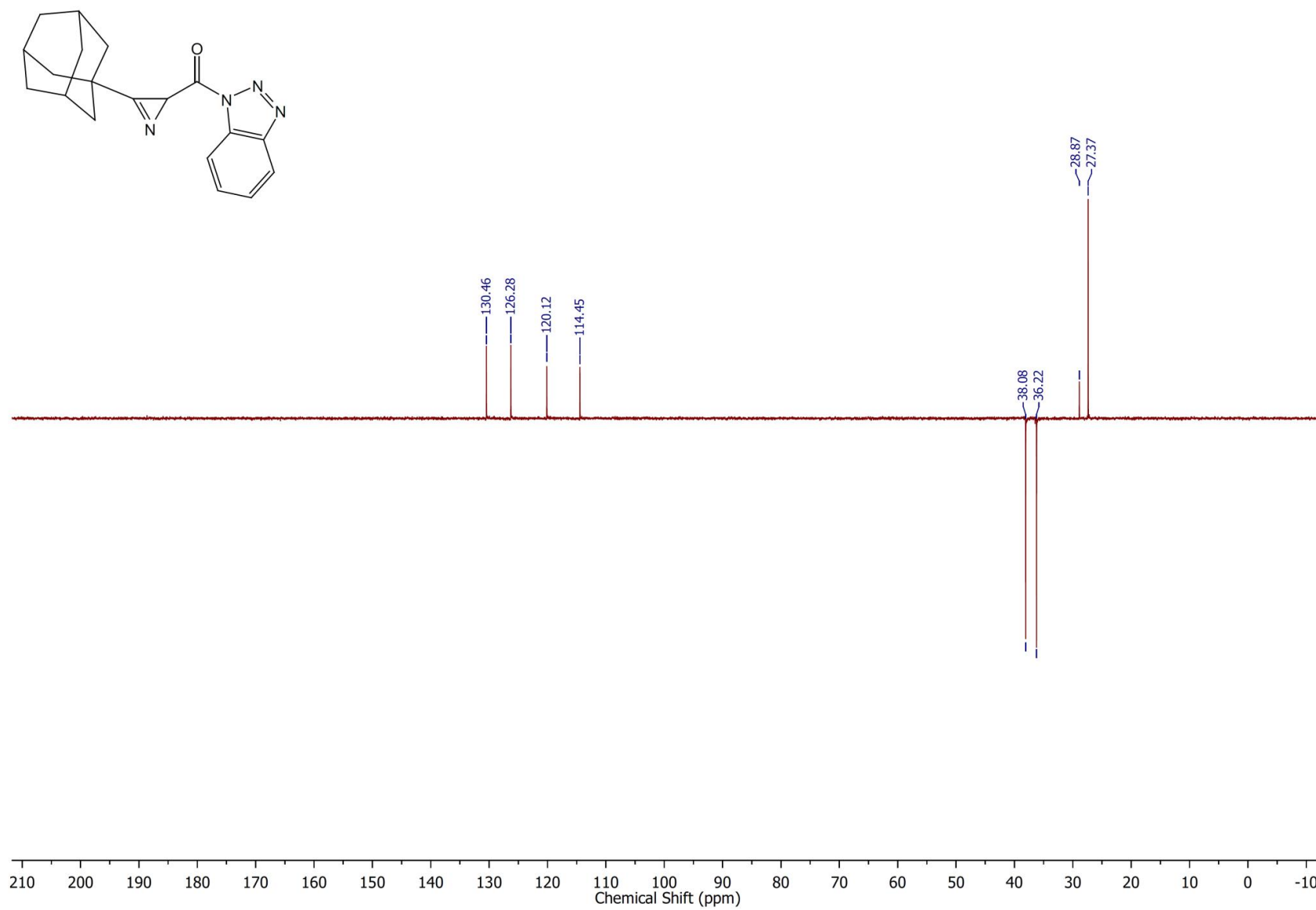
(3-(Adamantan-1-yl)-2*H*-azirin-2-yl)(1*H*-benzo[*d*][1,2,3]triazol-1-yl)methanone 1k, ¹H NMR, CDCl₃, 400 MHz



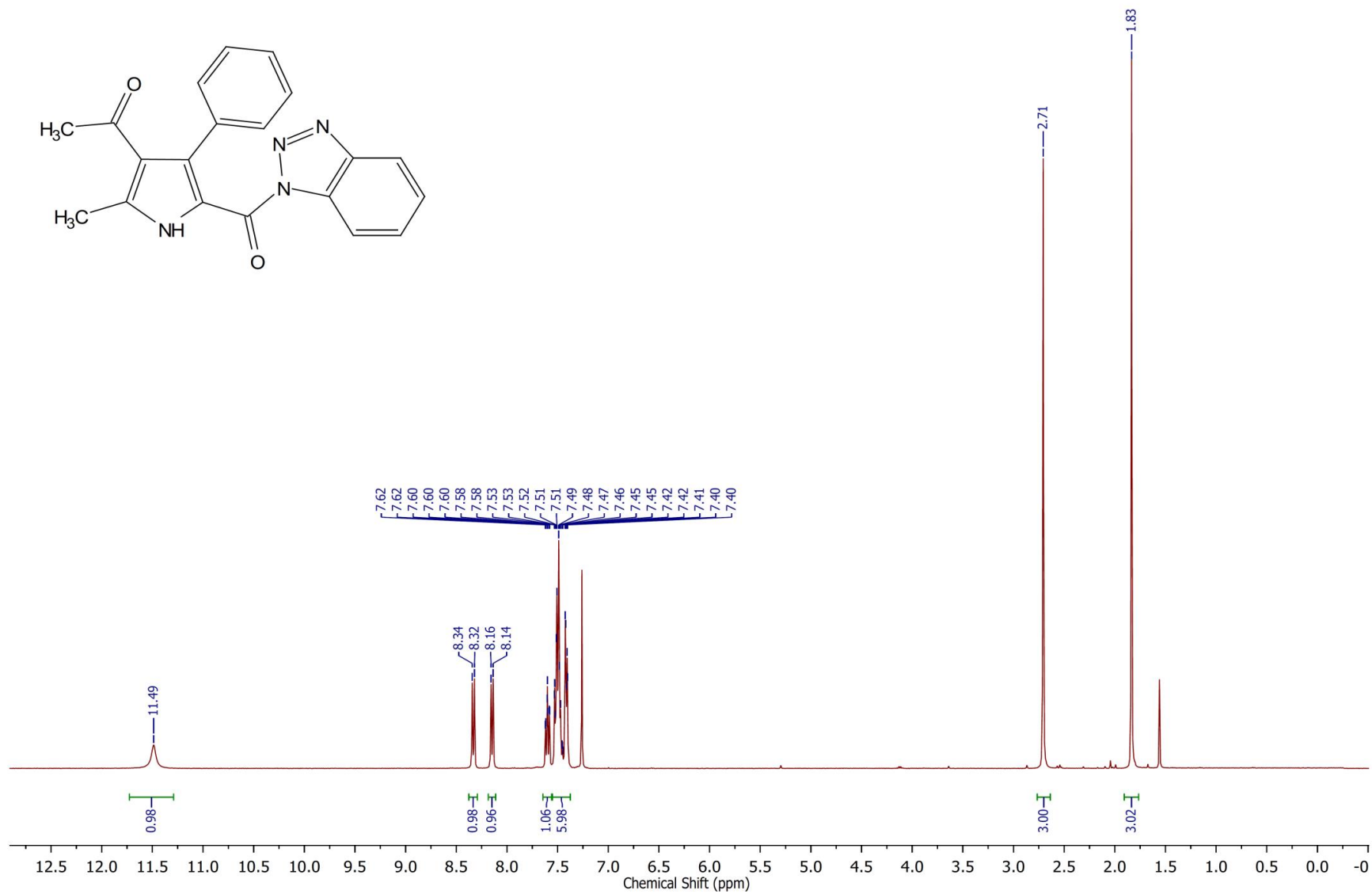
(3-(Adamantan-1-yl)-2*H*-azirin-2-yl)(1*H*-benzo[*d*][1,2,3]triazol-1-yl)methanone 1k, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



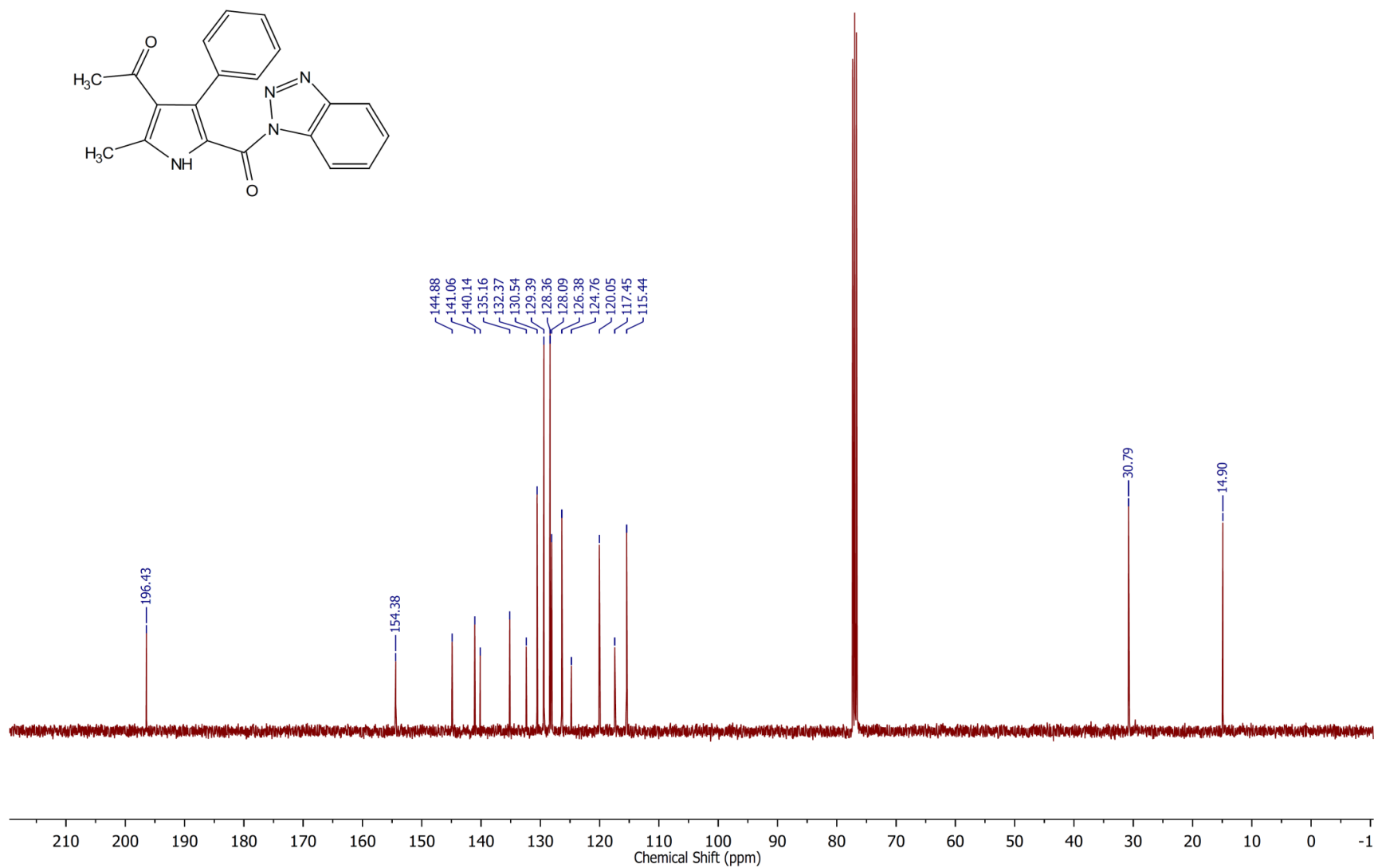
(3-(Adamantan-1-yl)-2*H*-azirin-2-yl)(1*H*-benzo[*d*][1,2,3]triazol-1-yl)methanone 1k, DEPT, CDCl₃, 100 MHz



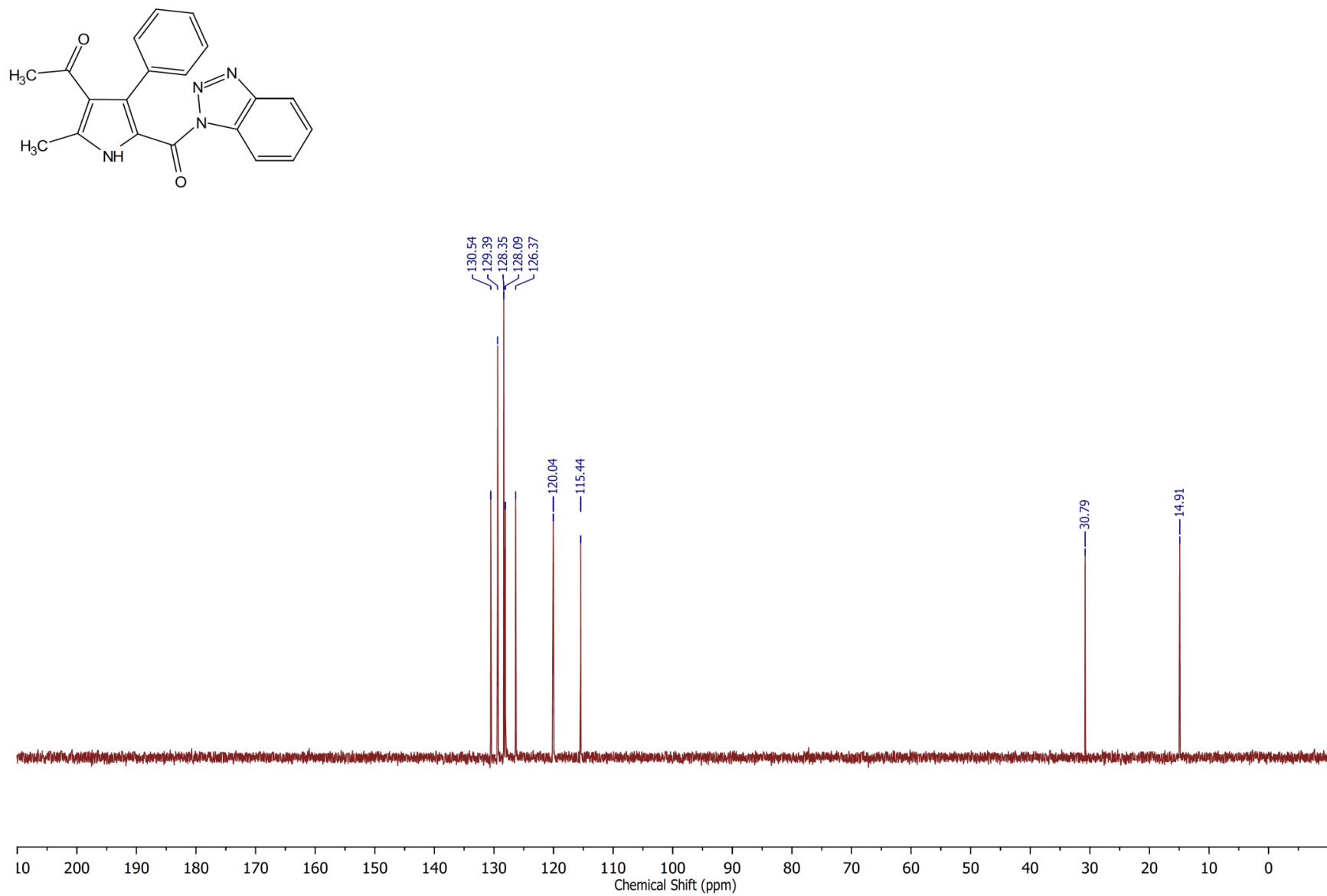
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethan-1-one 6a, ¹H NMR, CDCl₃, 400 MHz



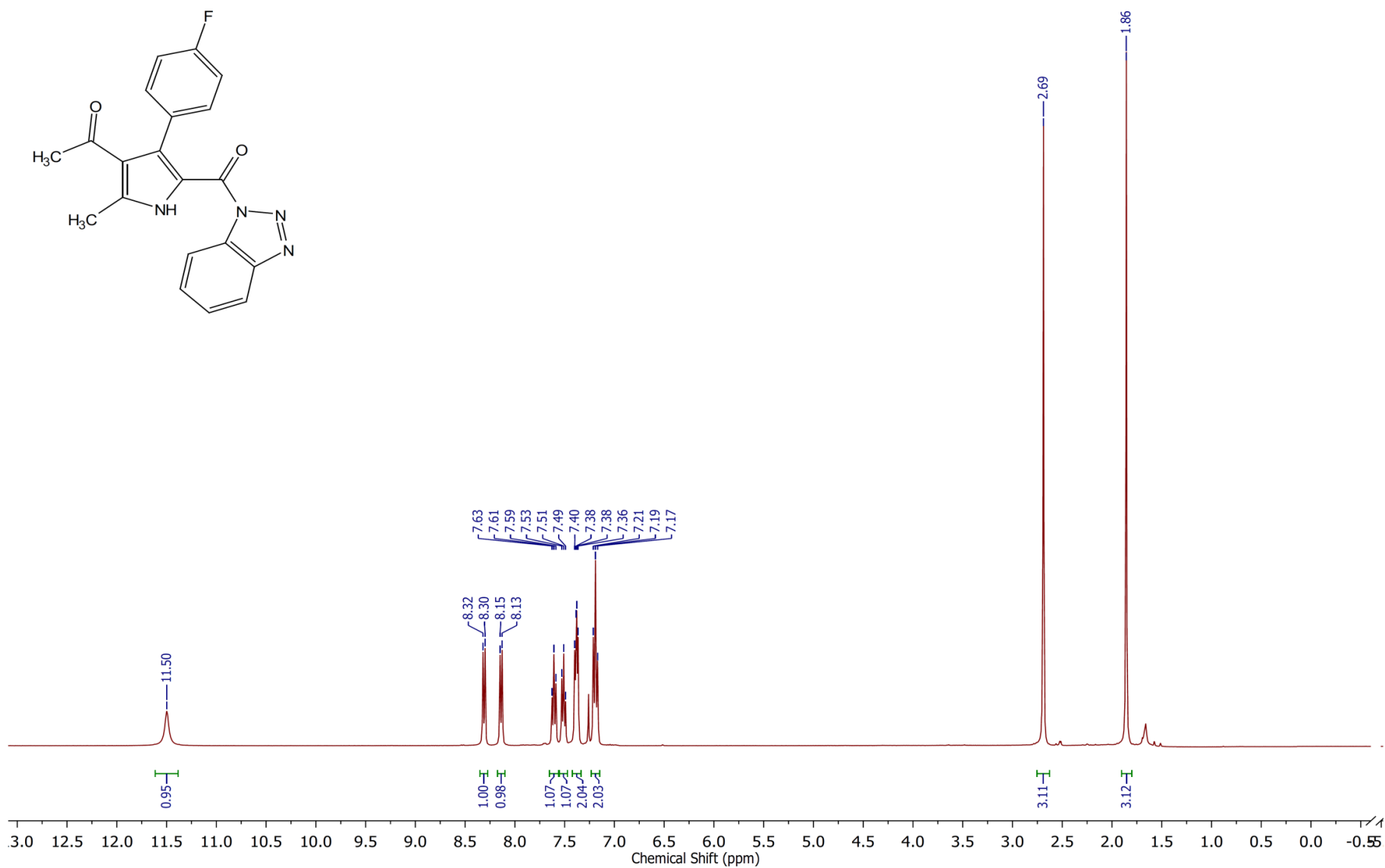
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethan-1-one 6a, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



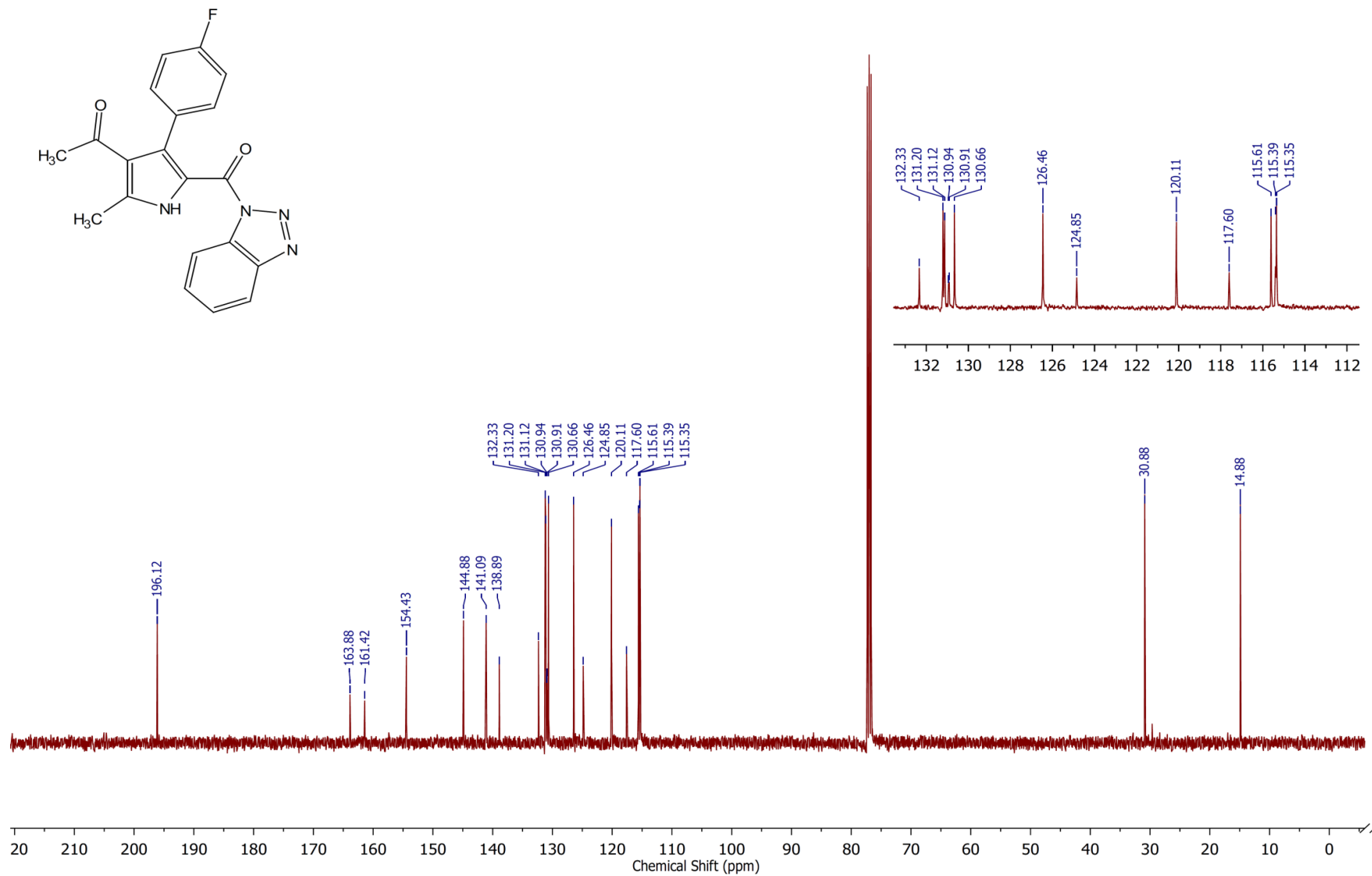
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethan-1-one 6a, DEPT, CDCl₃, 100 MHz



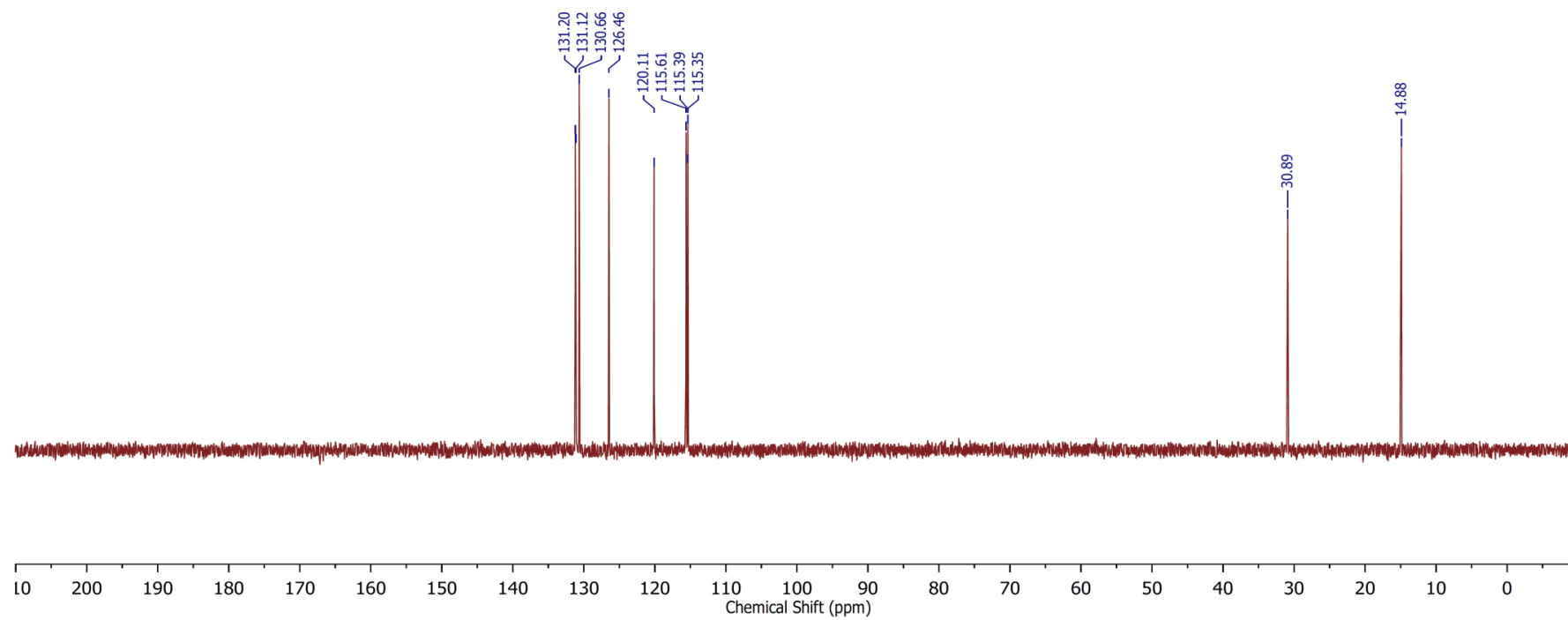
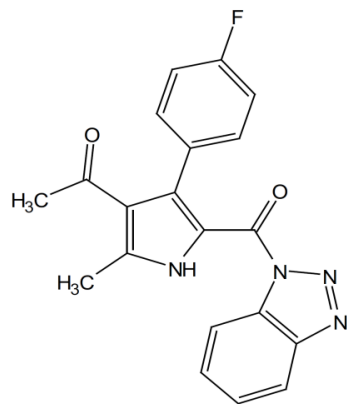
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-fluorophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6b, ¹H NMR, CDCl₃, 400 MHz



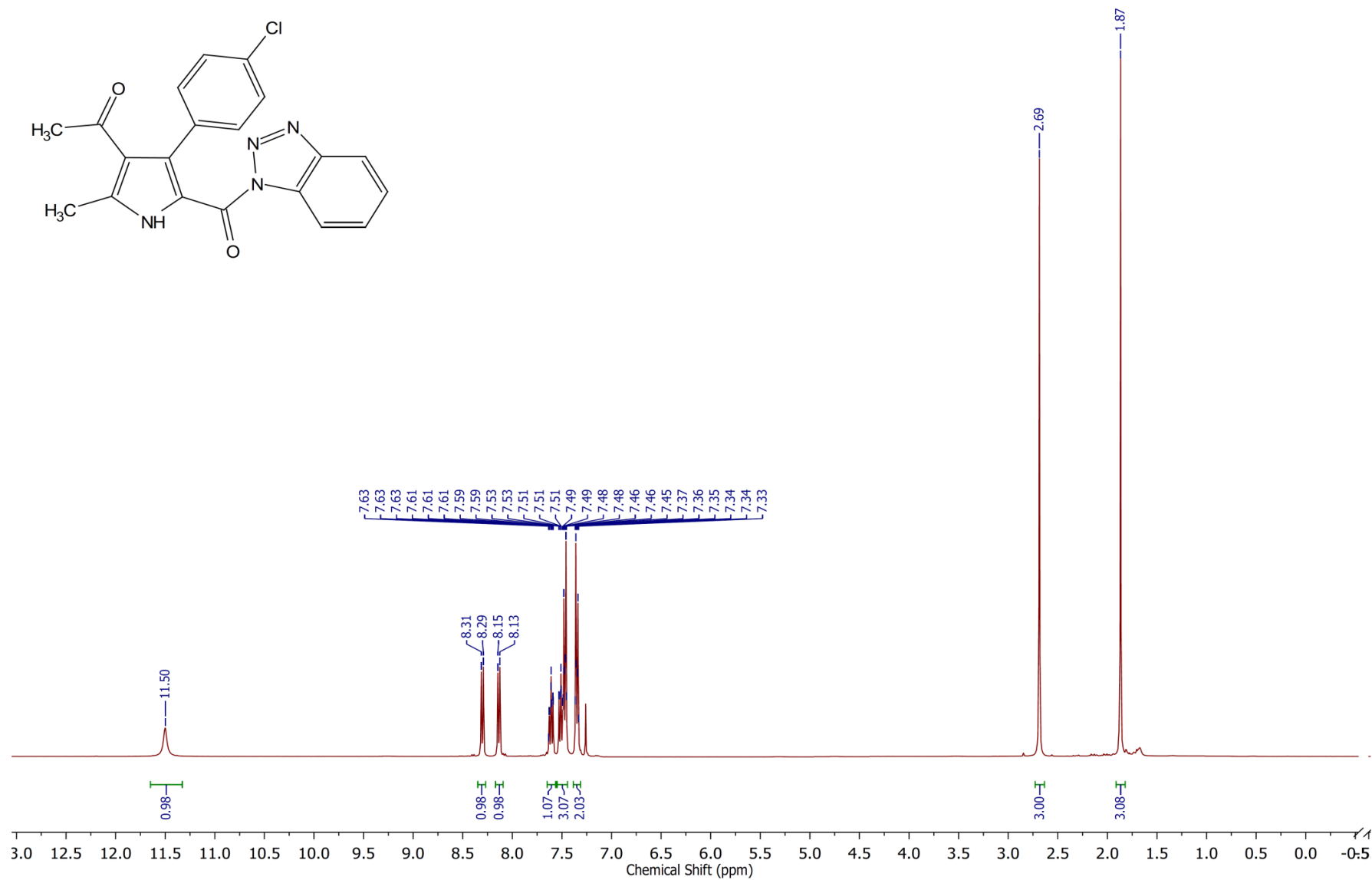
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-fluorophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6b, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



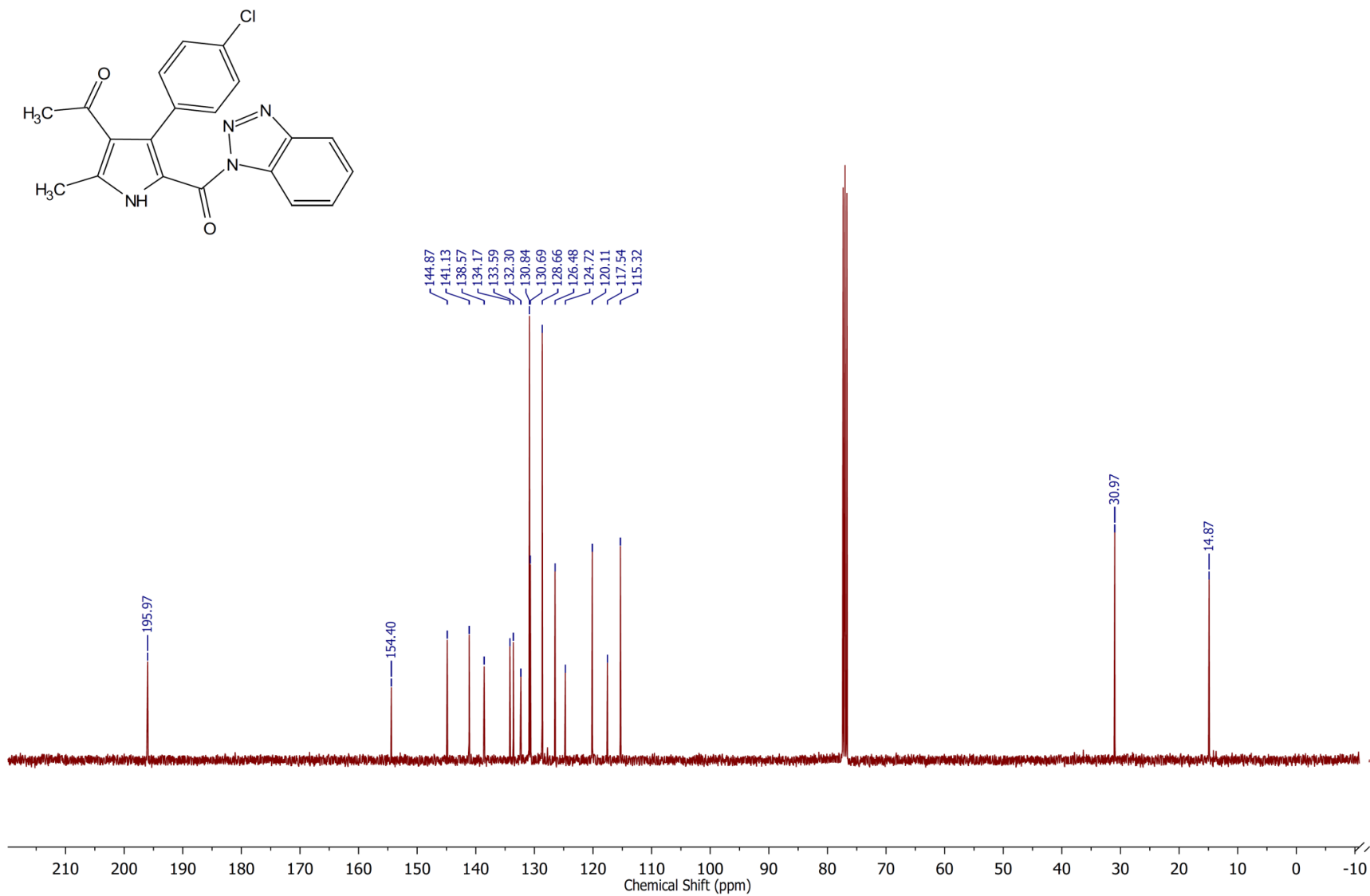
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-fluorophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6b, DEPT, CDCl₃, 100 MHz



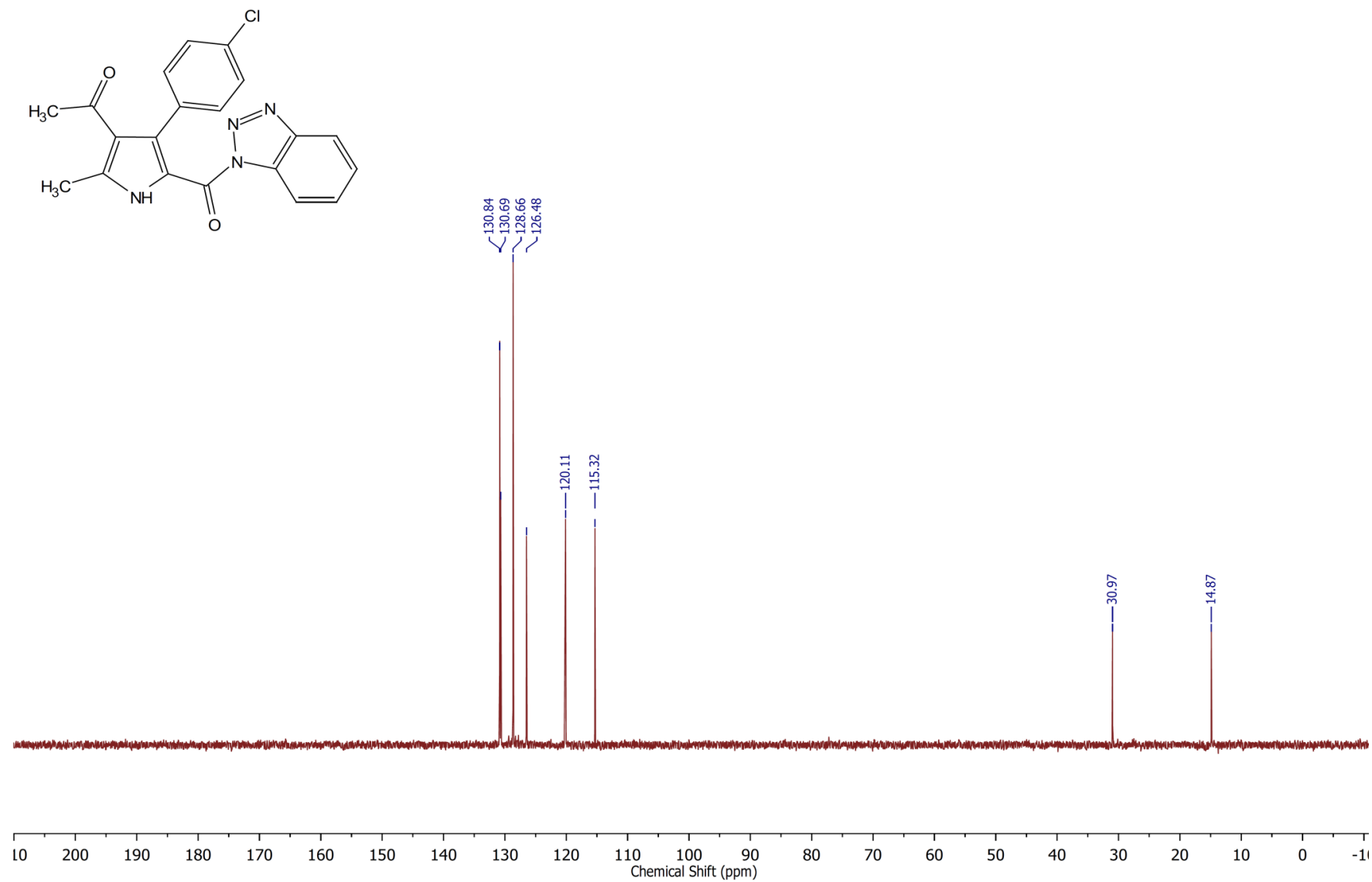
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-chlorophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6c, ¹H NMR, CDCl₃, 400 MHz



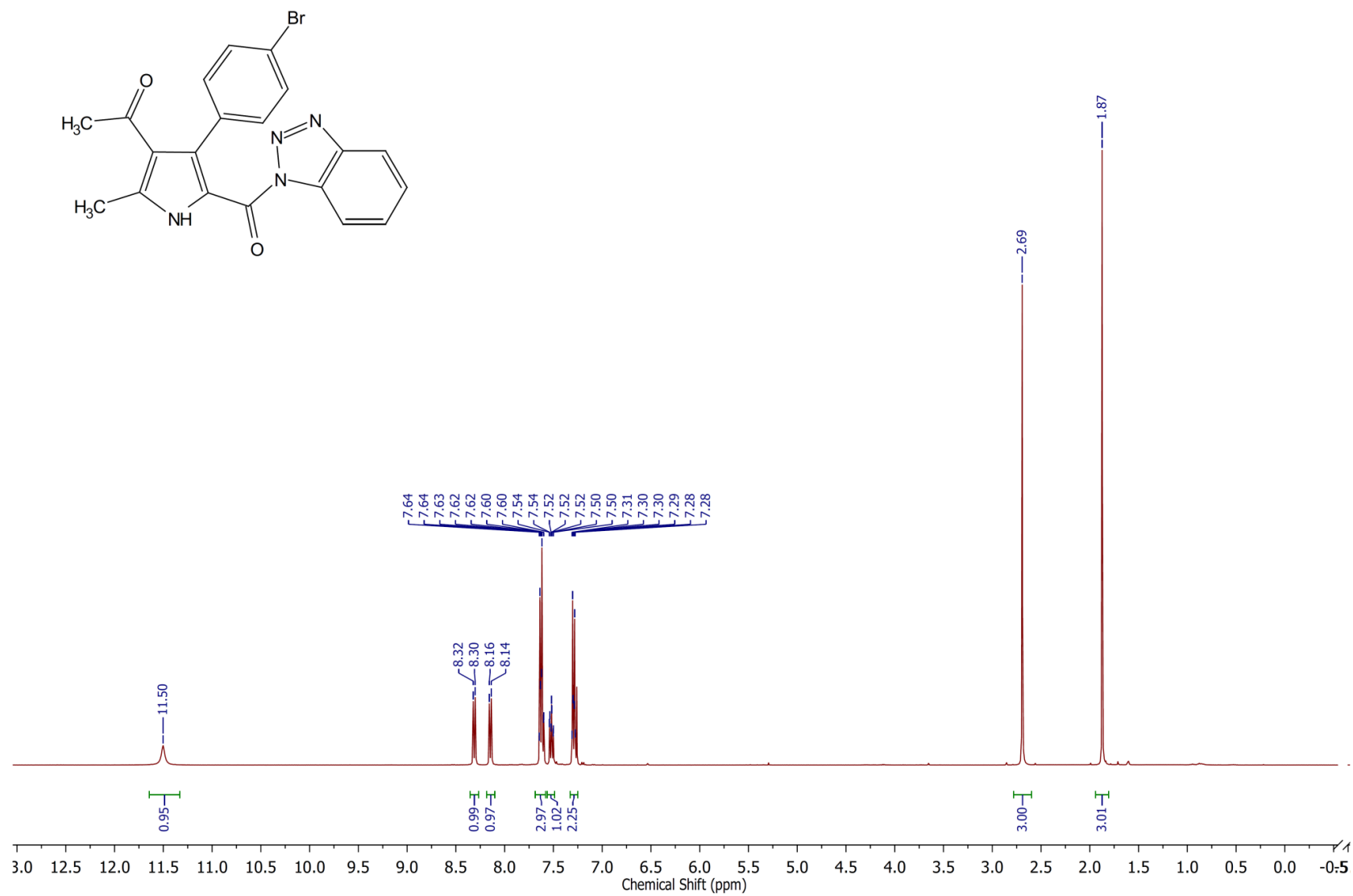
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-chlorophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6c, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



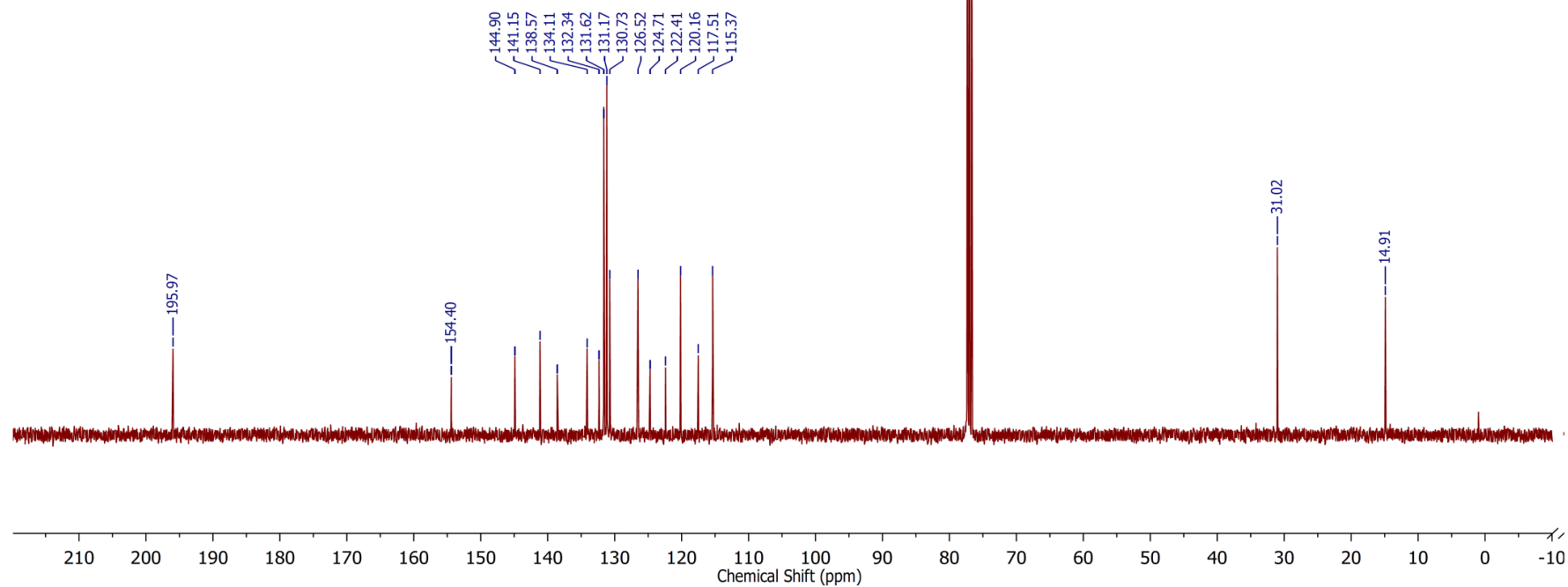
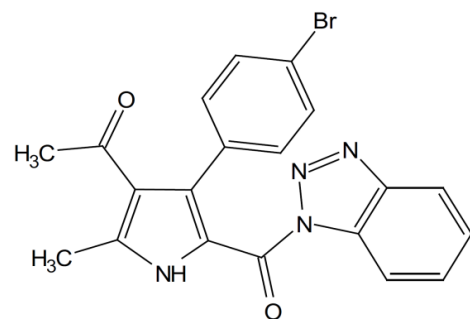
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-chlorophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6c, DEPT, CDCl₃, 100 MHz



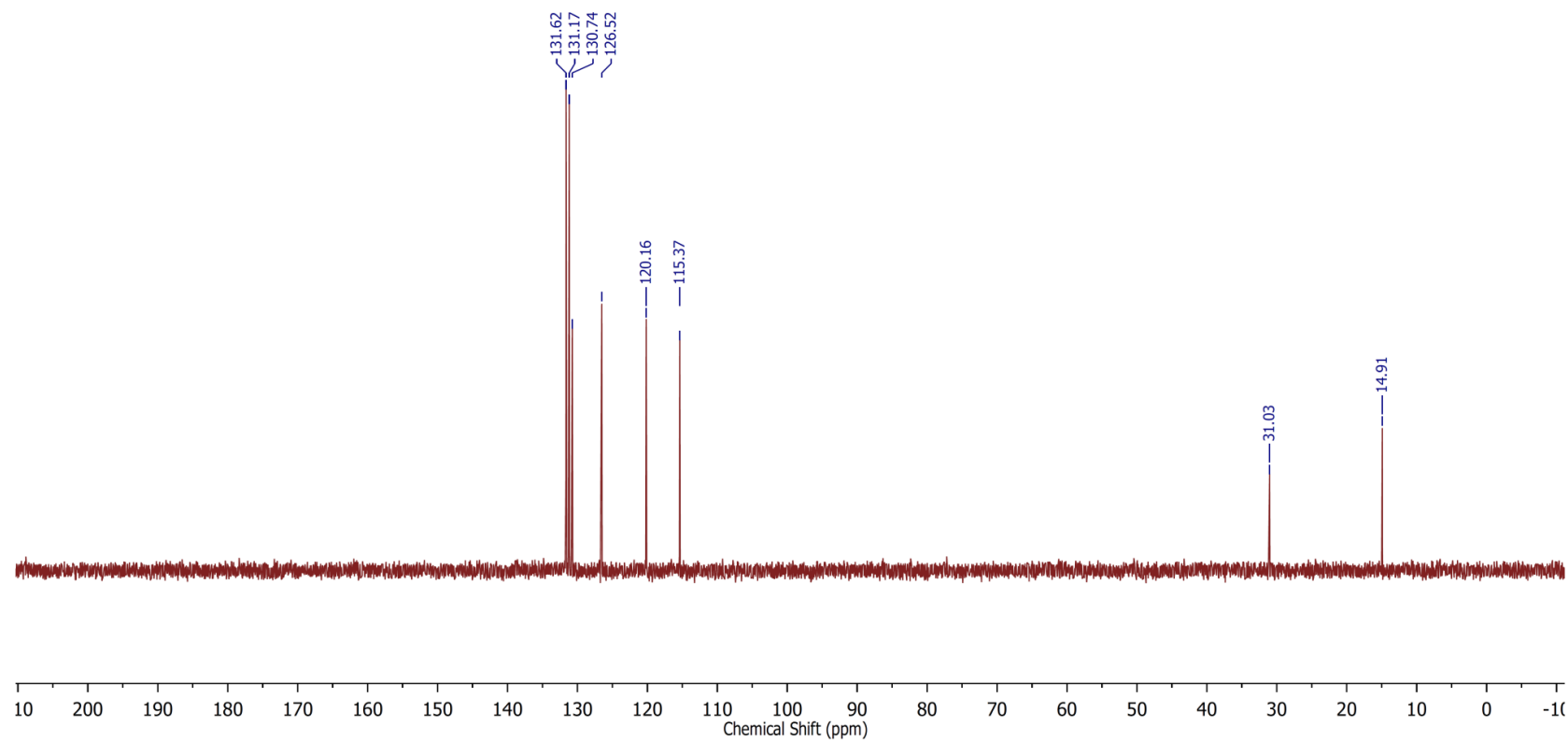
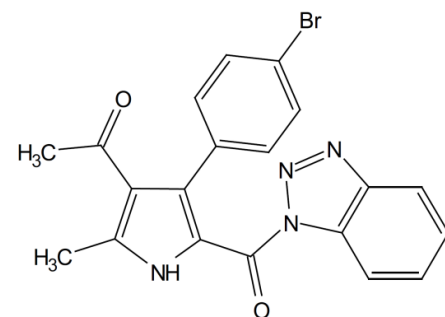
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-bromophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6d, ¹H NMR, CDCl₃, 400 MHz



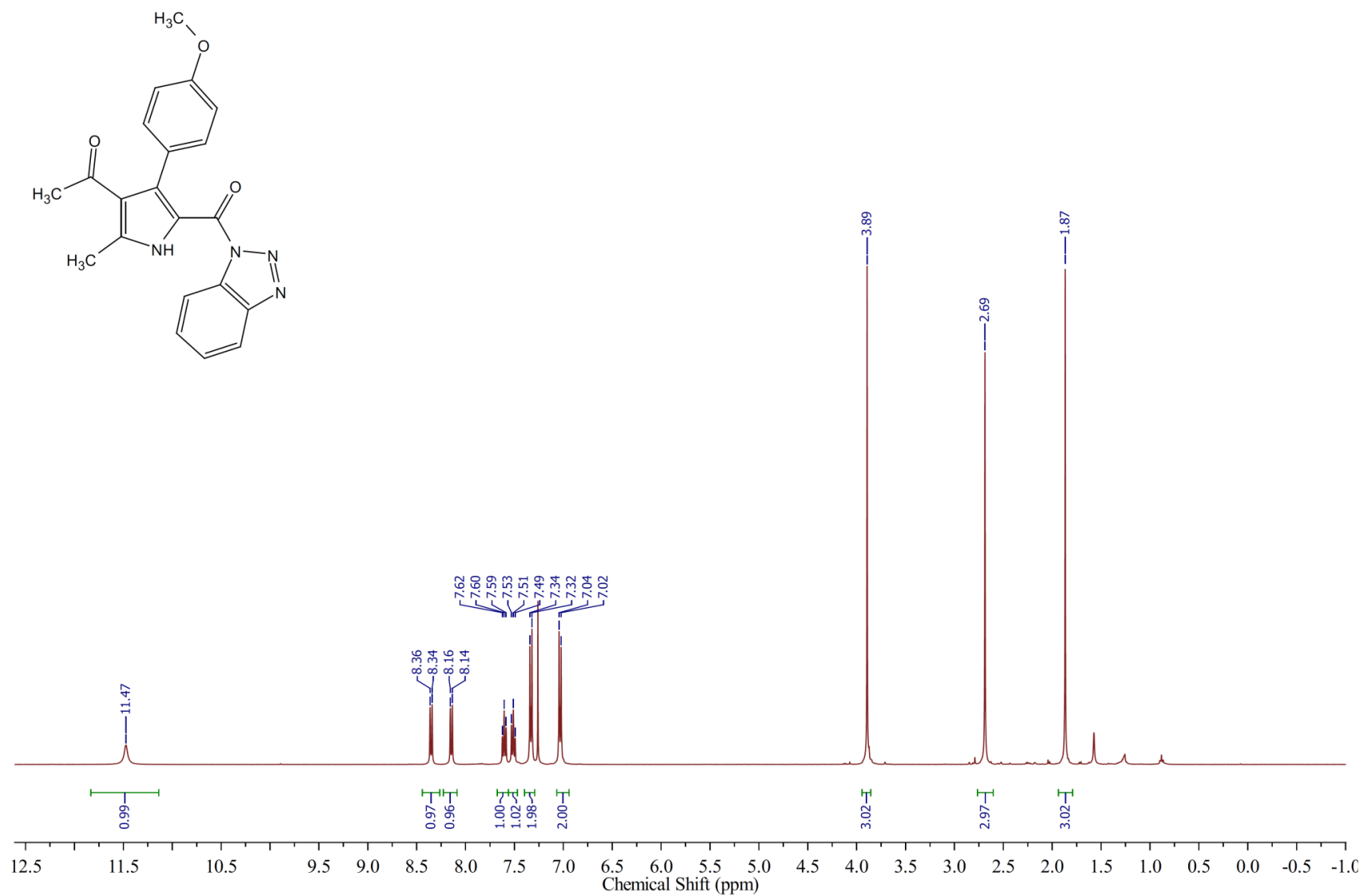
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-bromophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6d, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



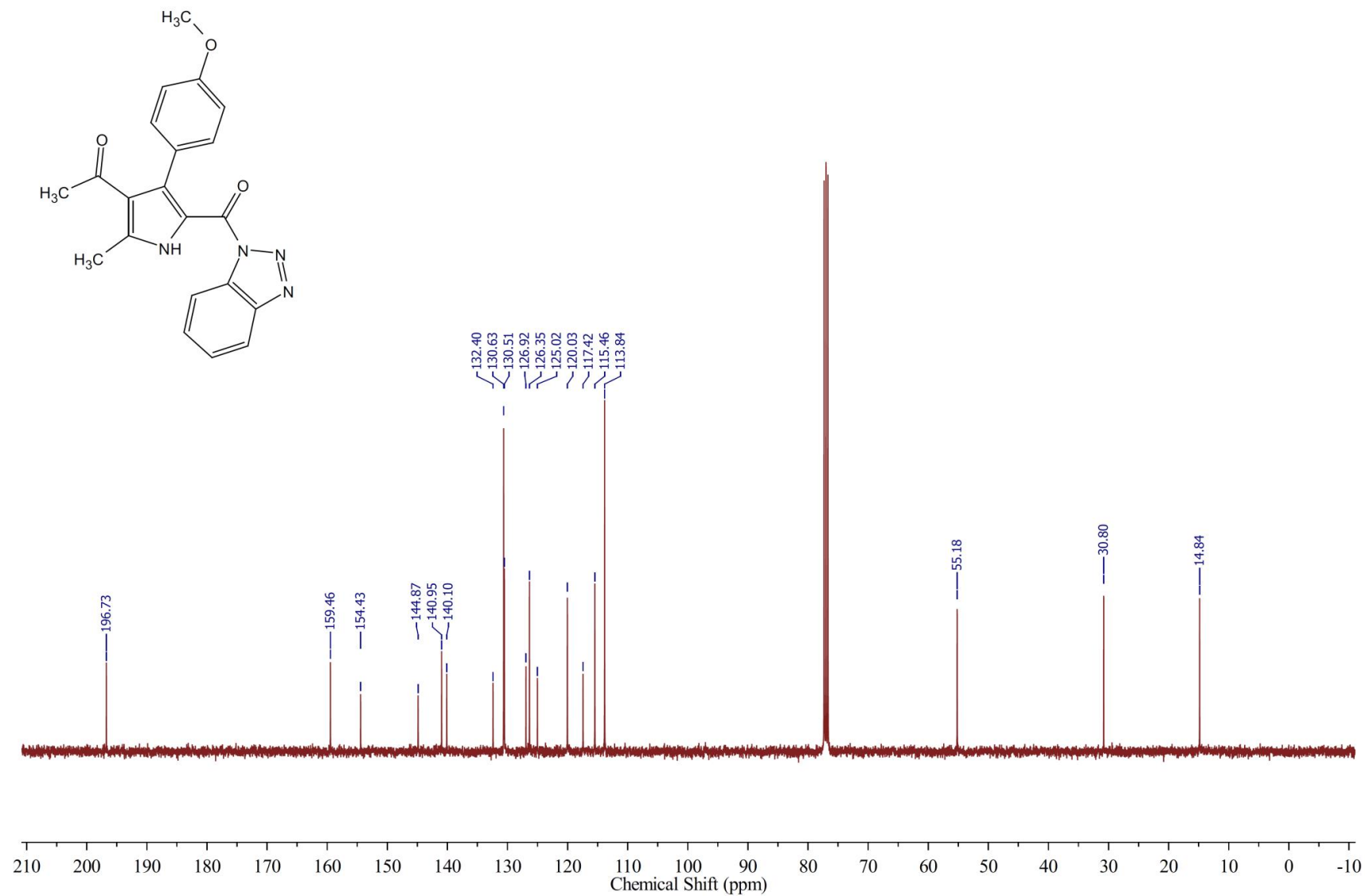
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-bromophenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6d, DEPT, CDCl₃, 100 MHz



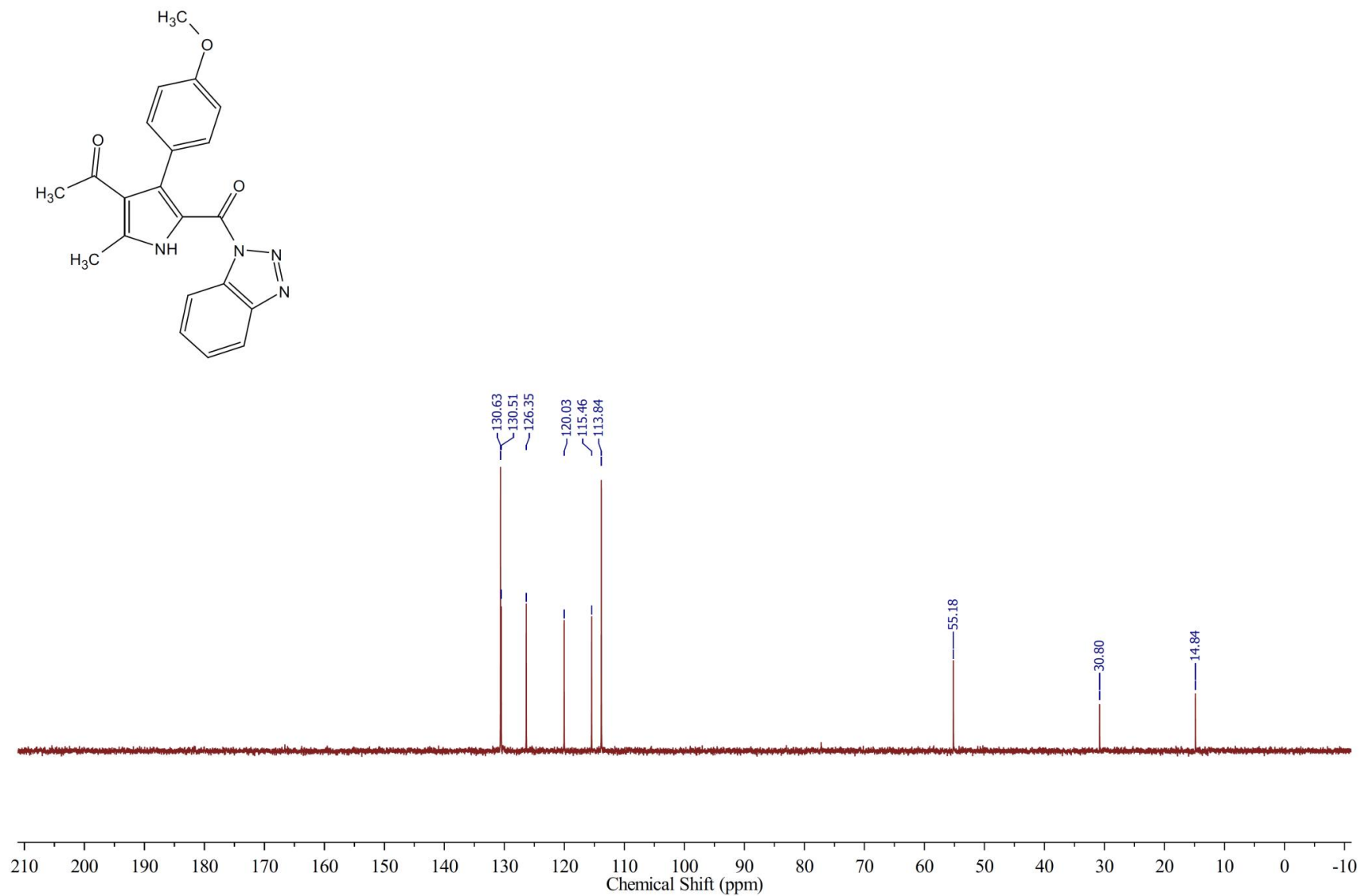
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6e, ¹H NMR, CDCl₃, 400 MHz



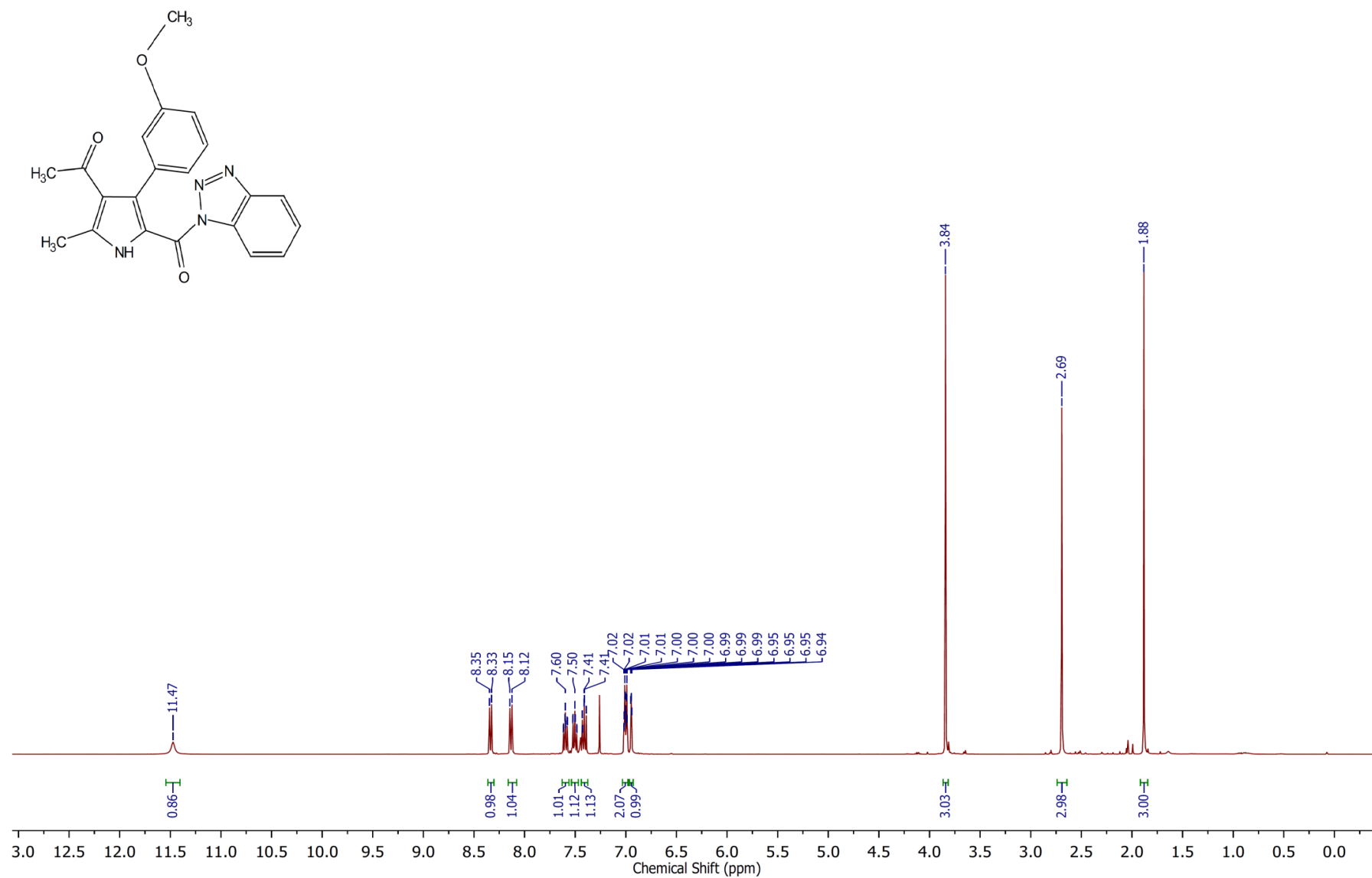
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6e, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



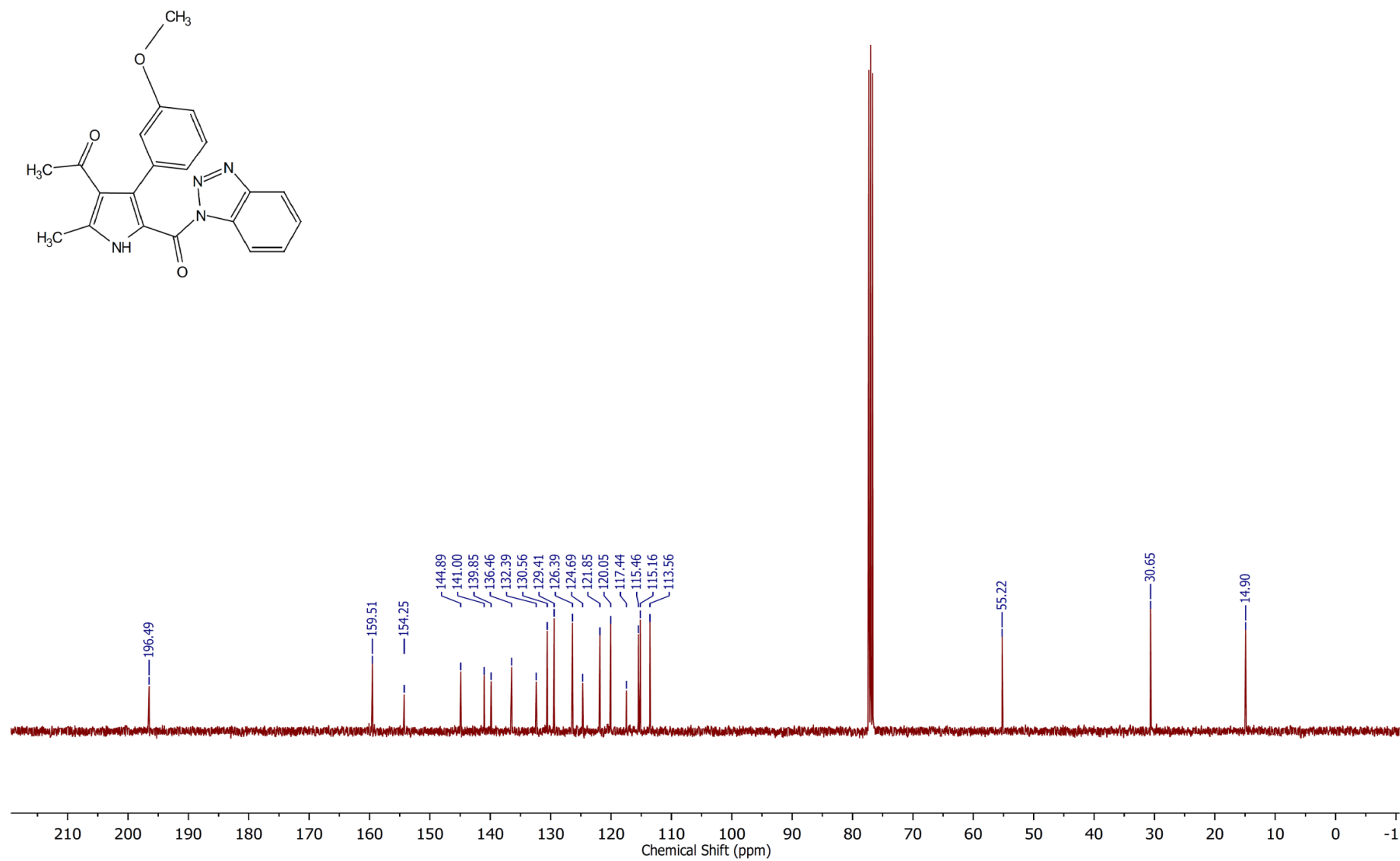
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6e, DEPT, CDCl₃, 100 MHz



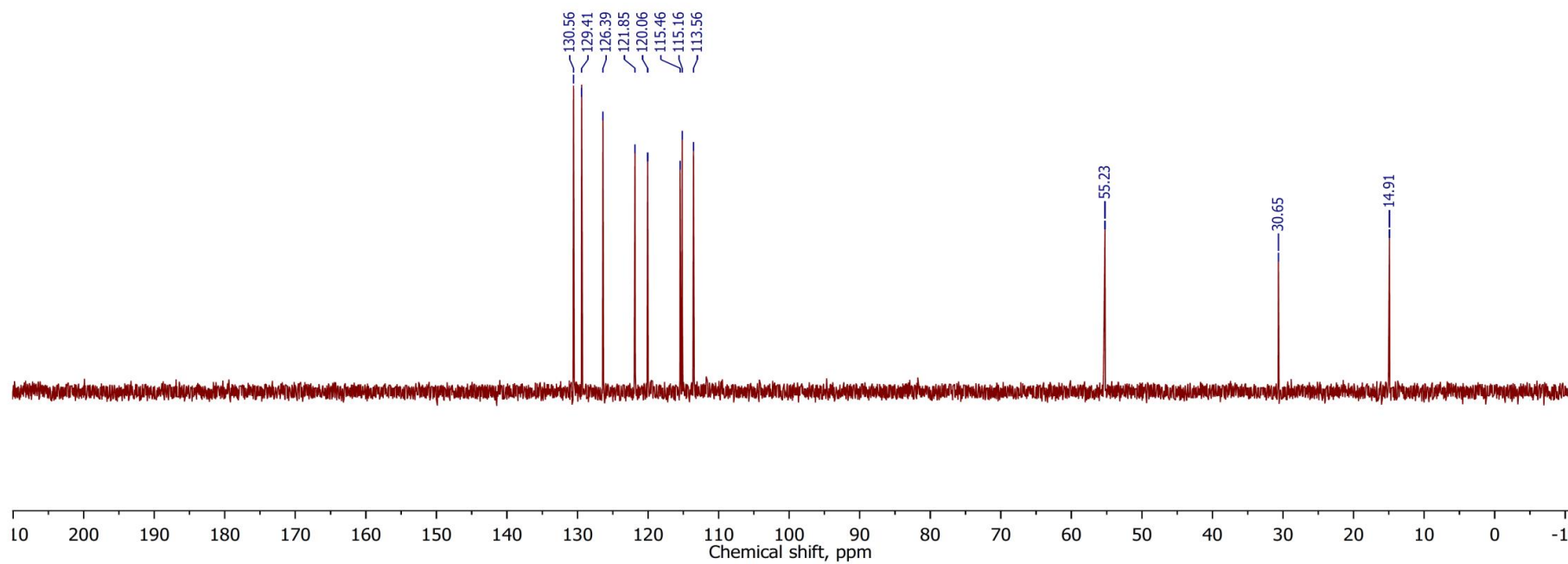
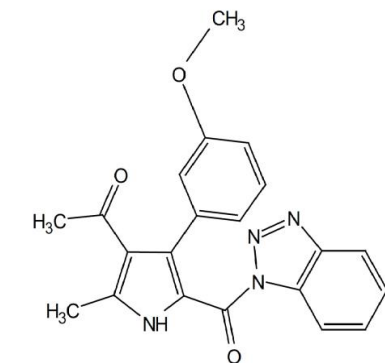
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(3-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6f, ¹H NMR, CDCl₃, 400 MHz



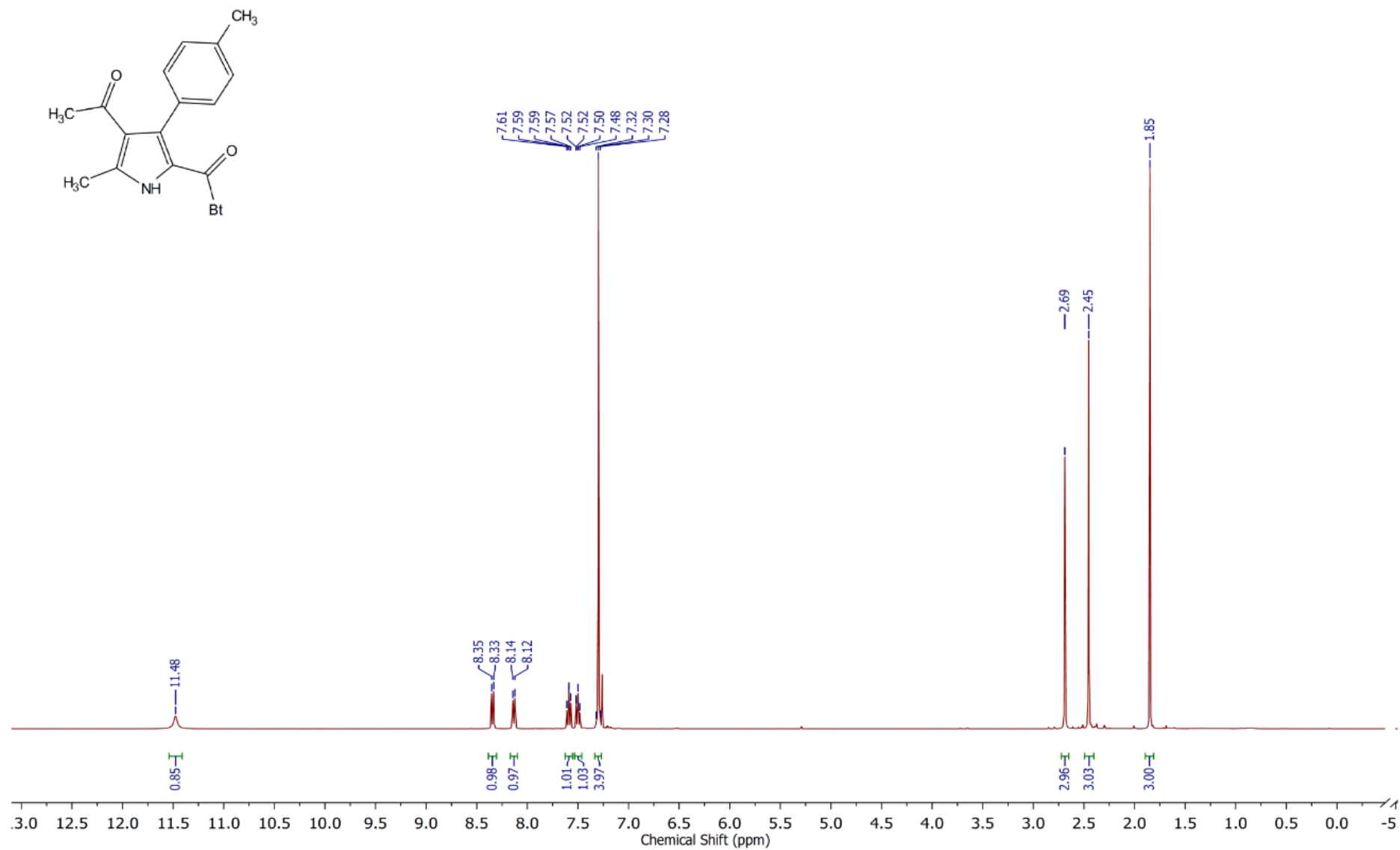
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(3-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6f, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



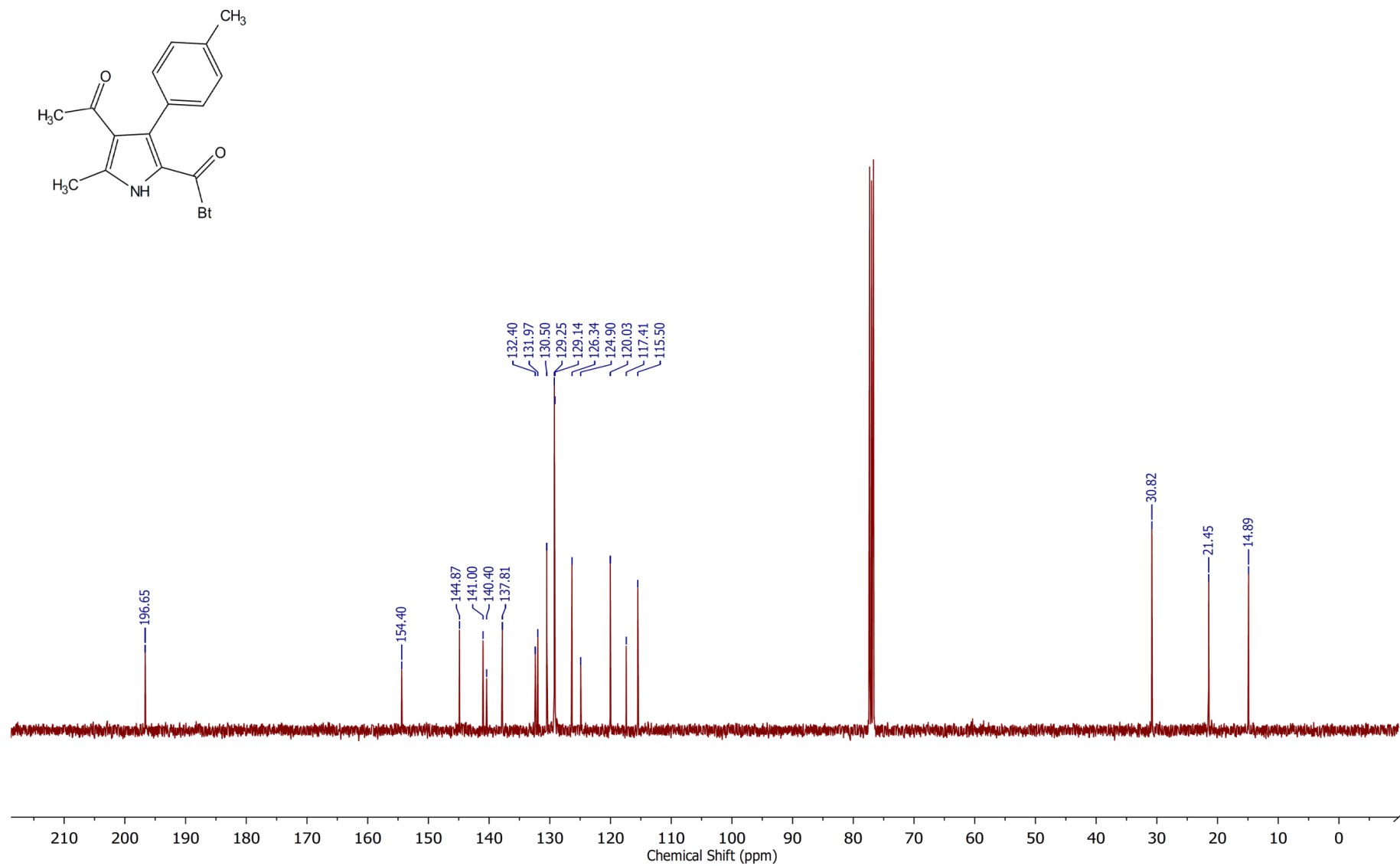
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(3-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6f, DEPT, CDCl₃, 100 MHz



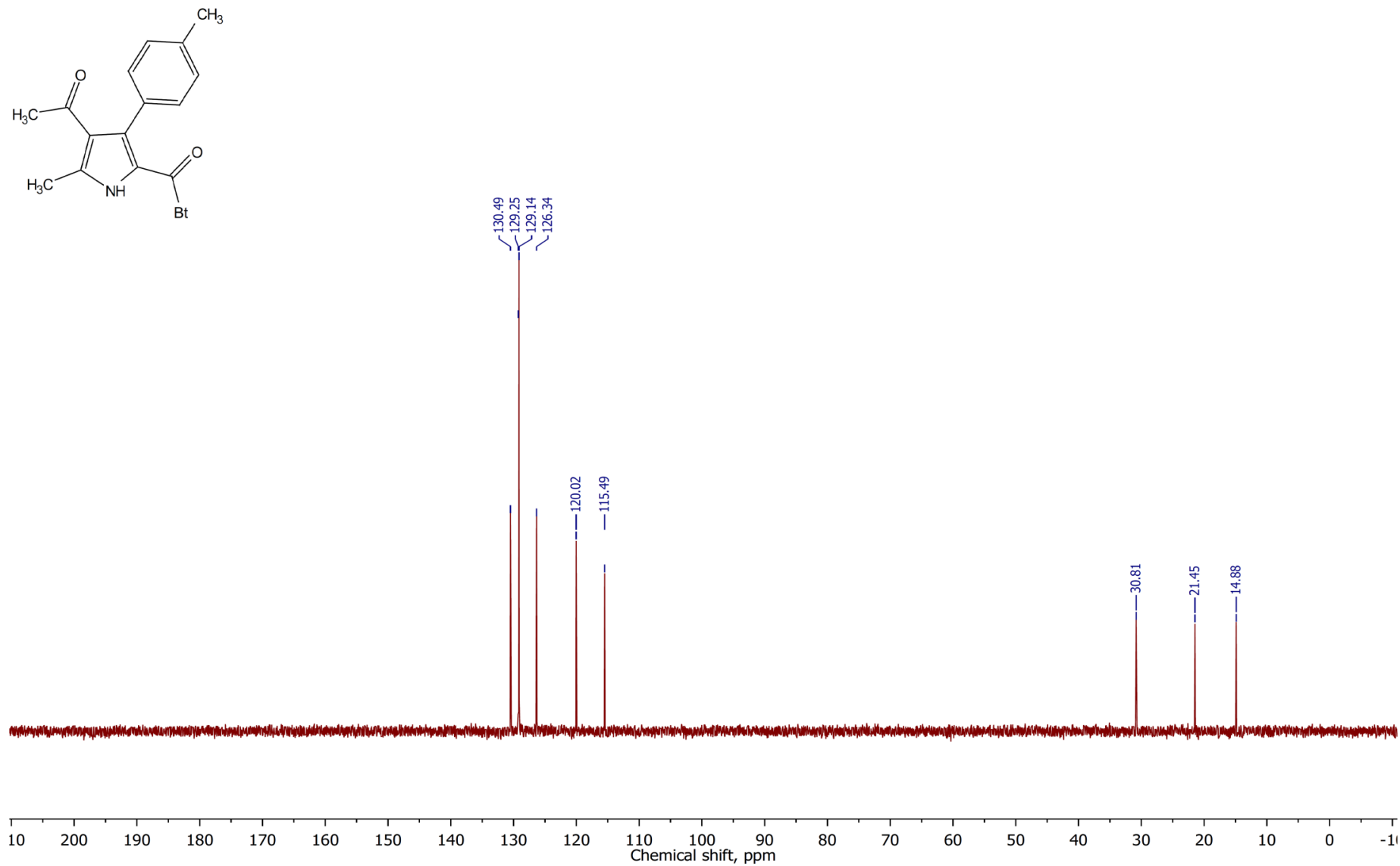
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-(*p*-tolyl)-1*H*-pyrrol-3-yl)ethan-1-one 6g, ¹H NMR, CDCl₃, 400 MHz



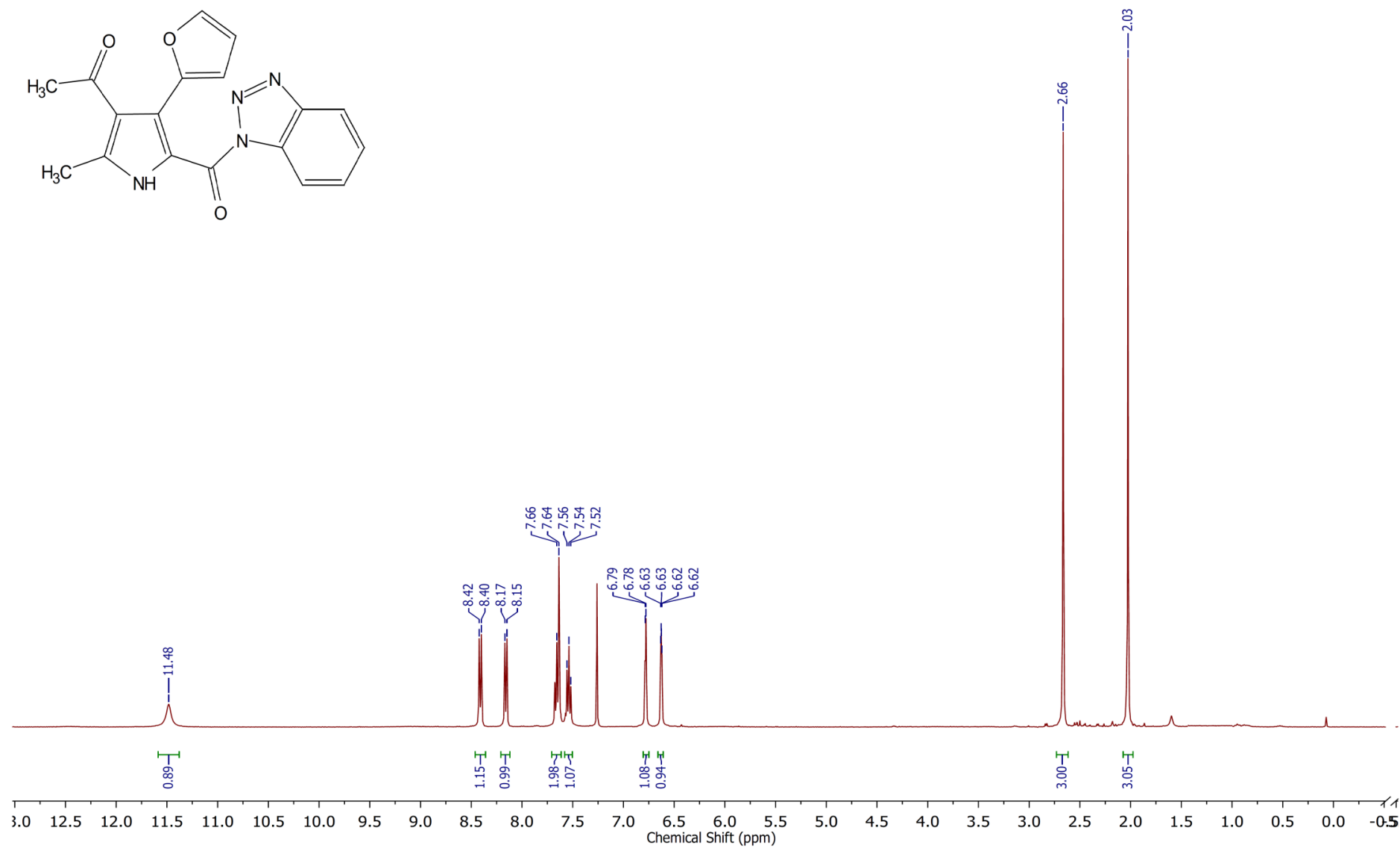
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-(*p*-tolyl)-1*H*-pyrrol-3-yl)ethan-1-one **6g**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



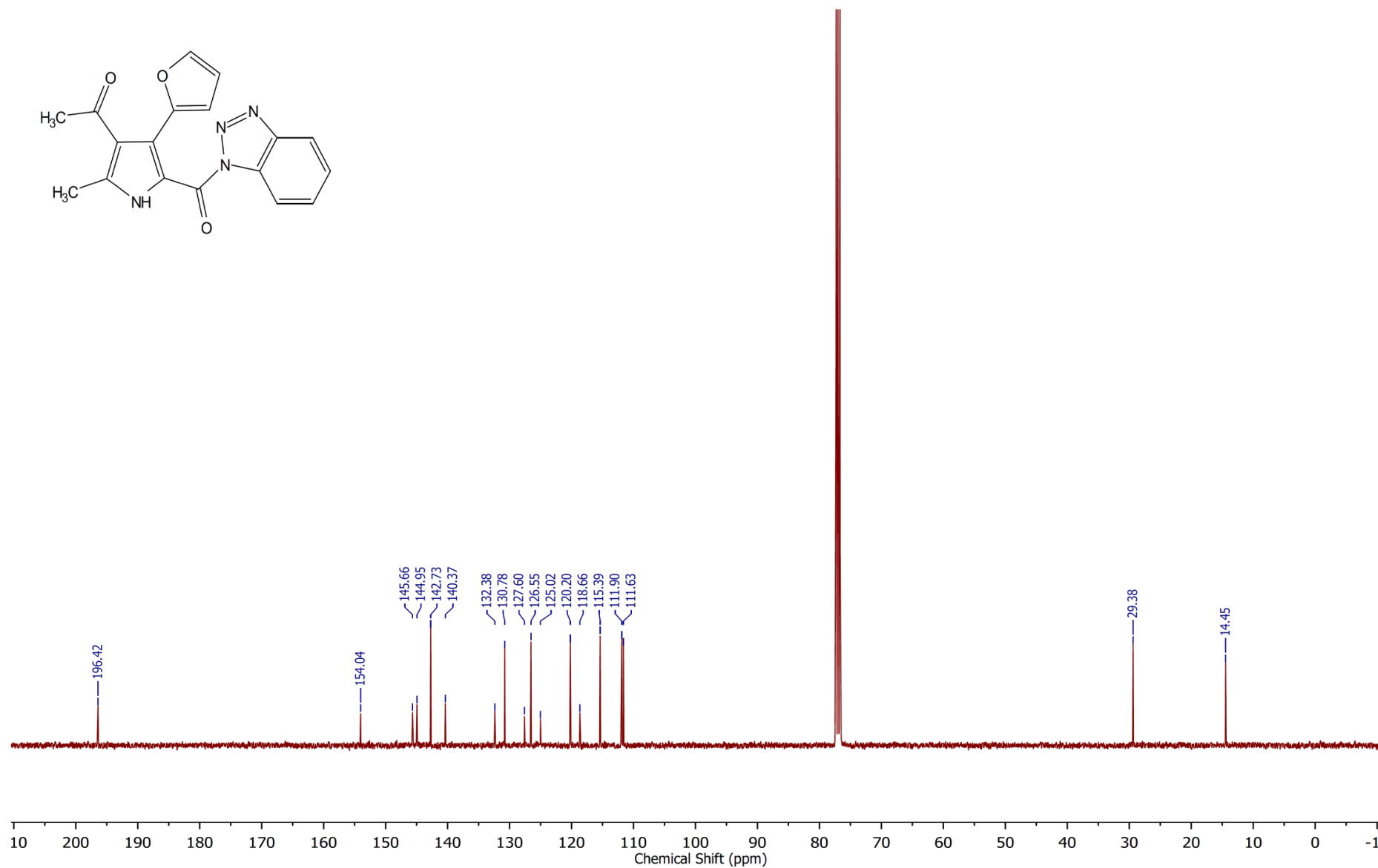
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-(*p*-tolyl)-1*H*-pyrrol-3-yl)ethan-1-one 6g, DEPT, CDCl₃, 100 MHz



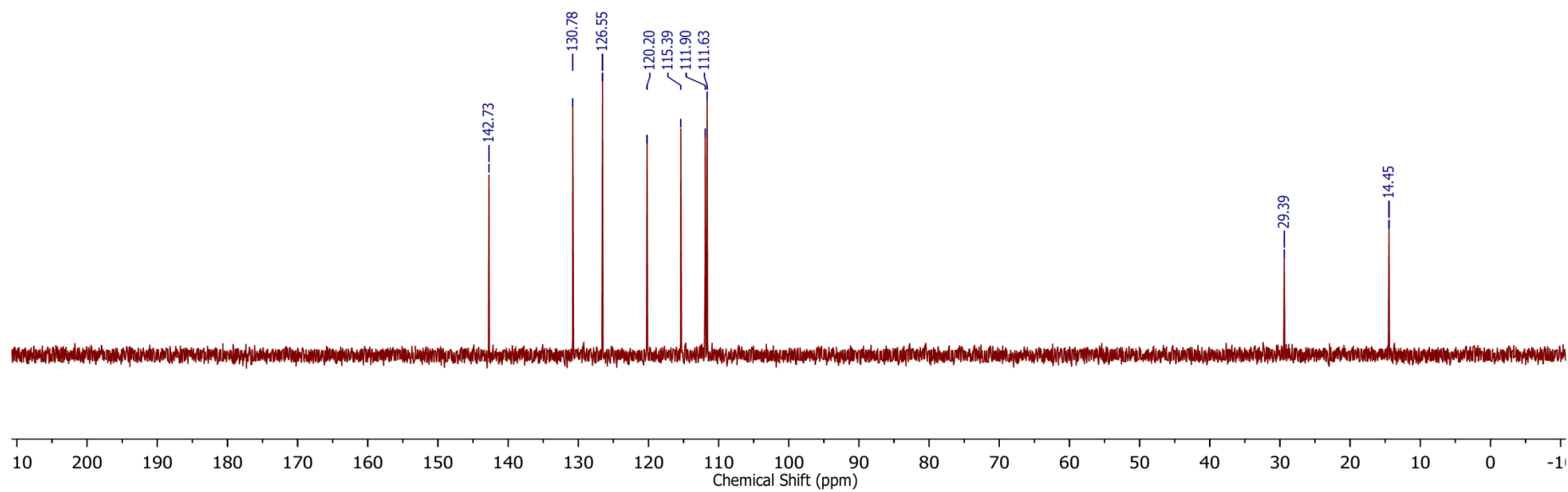
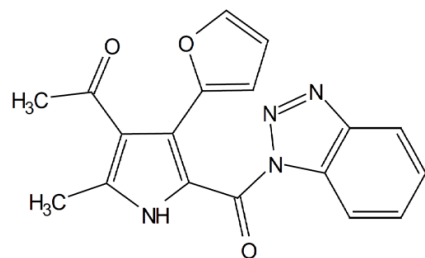
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(furan-2-yl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6h, ¹H NMR, CDCl₃, 400 MHz



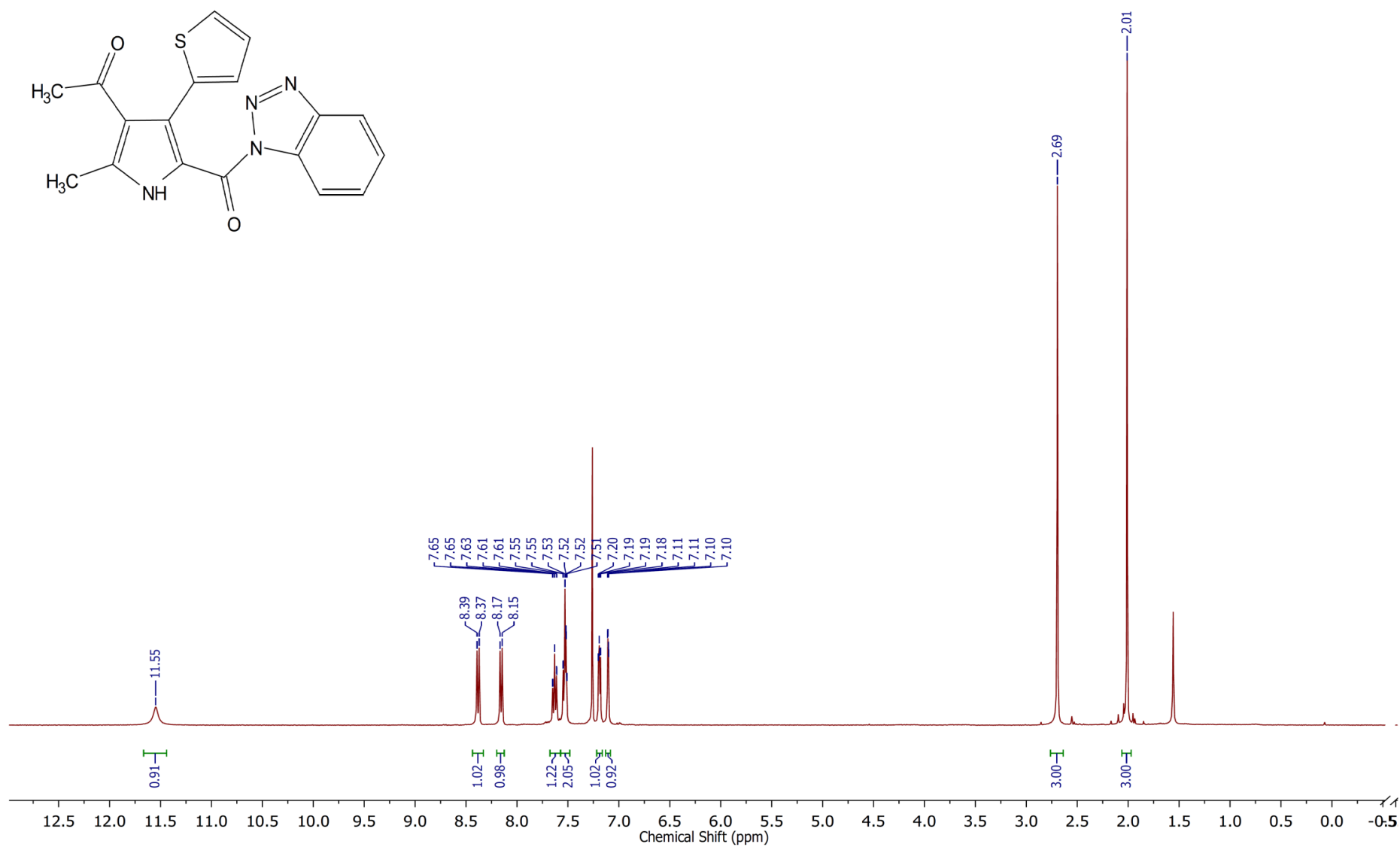
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(furan-2-yl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6h, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



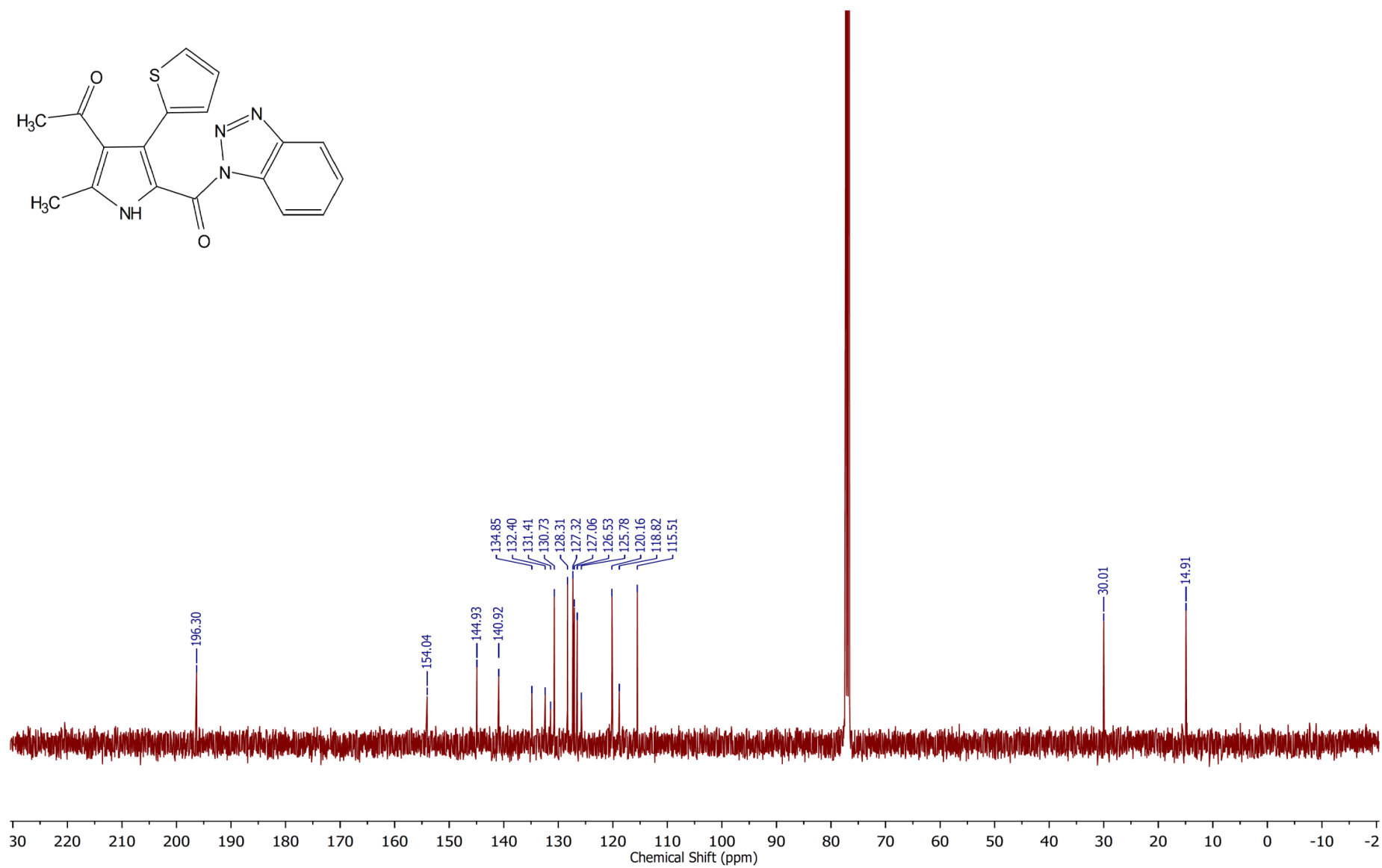
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-(furan-2-yl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one 6h, DEPT, CDCl₃, 100 MHz



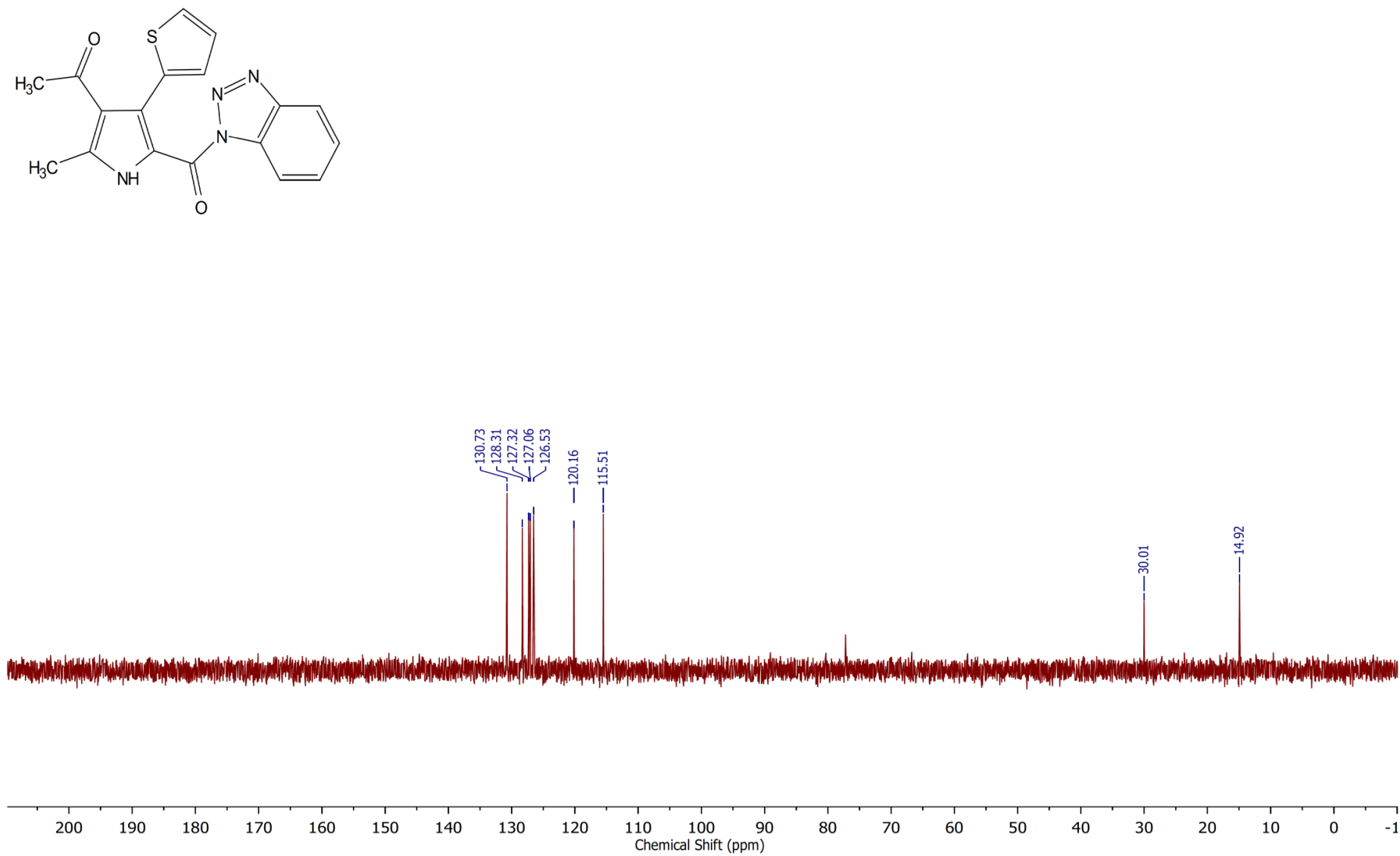
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-(thiophen-2-yl)-1*H*-pyrrol-3-yl)ethan-1-one 6i, ¹H NMR, CDCl₃, 400 MHz



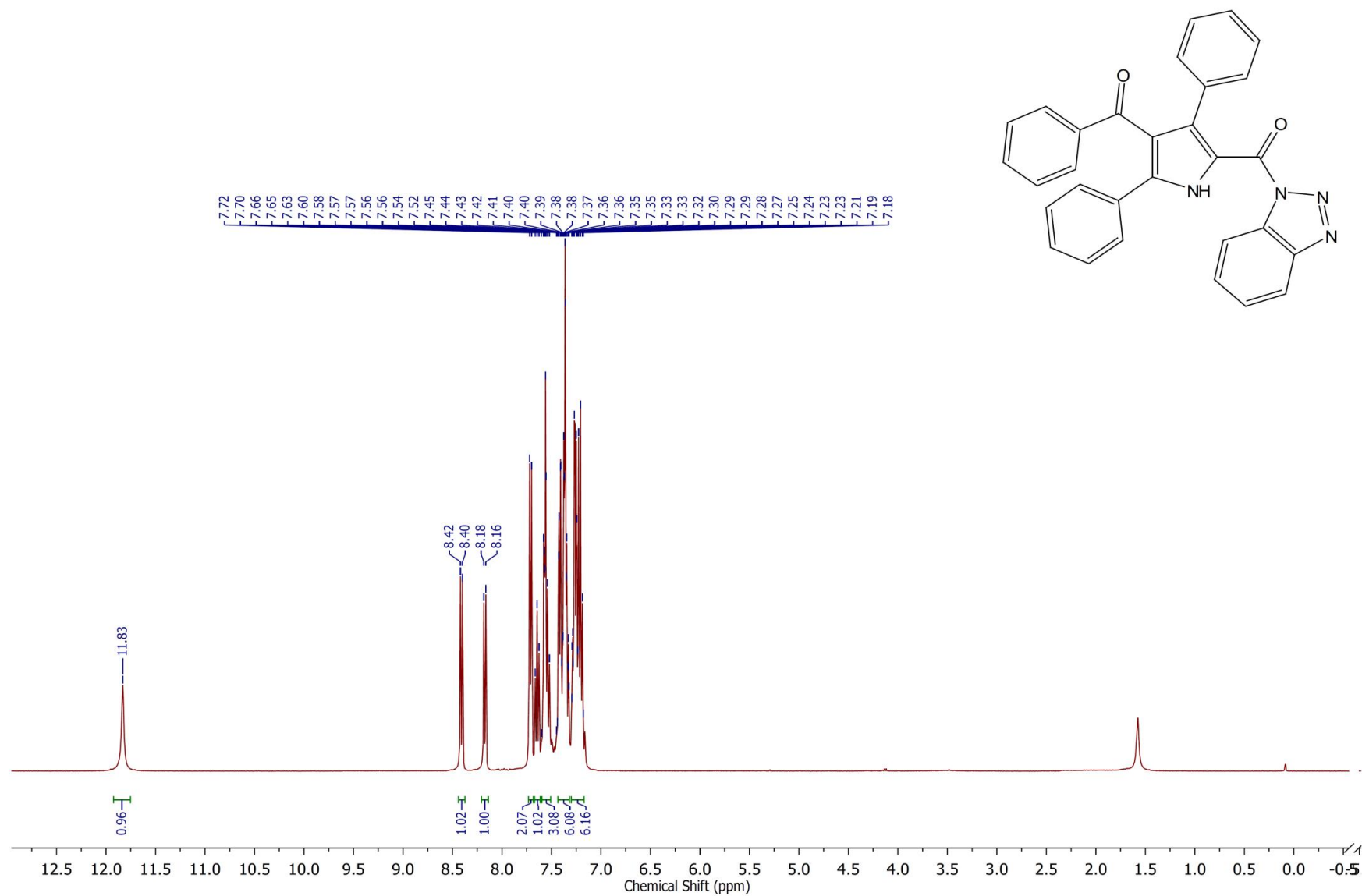
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-(thiophen-2-yl)-1*H*-pyrrol-3-yl)ethan-1-one **6i**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



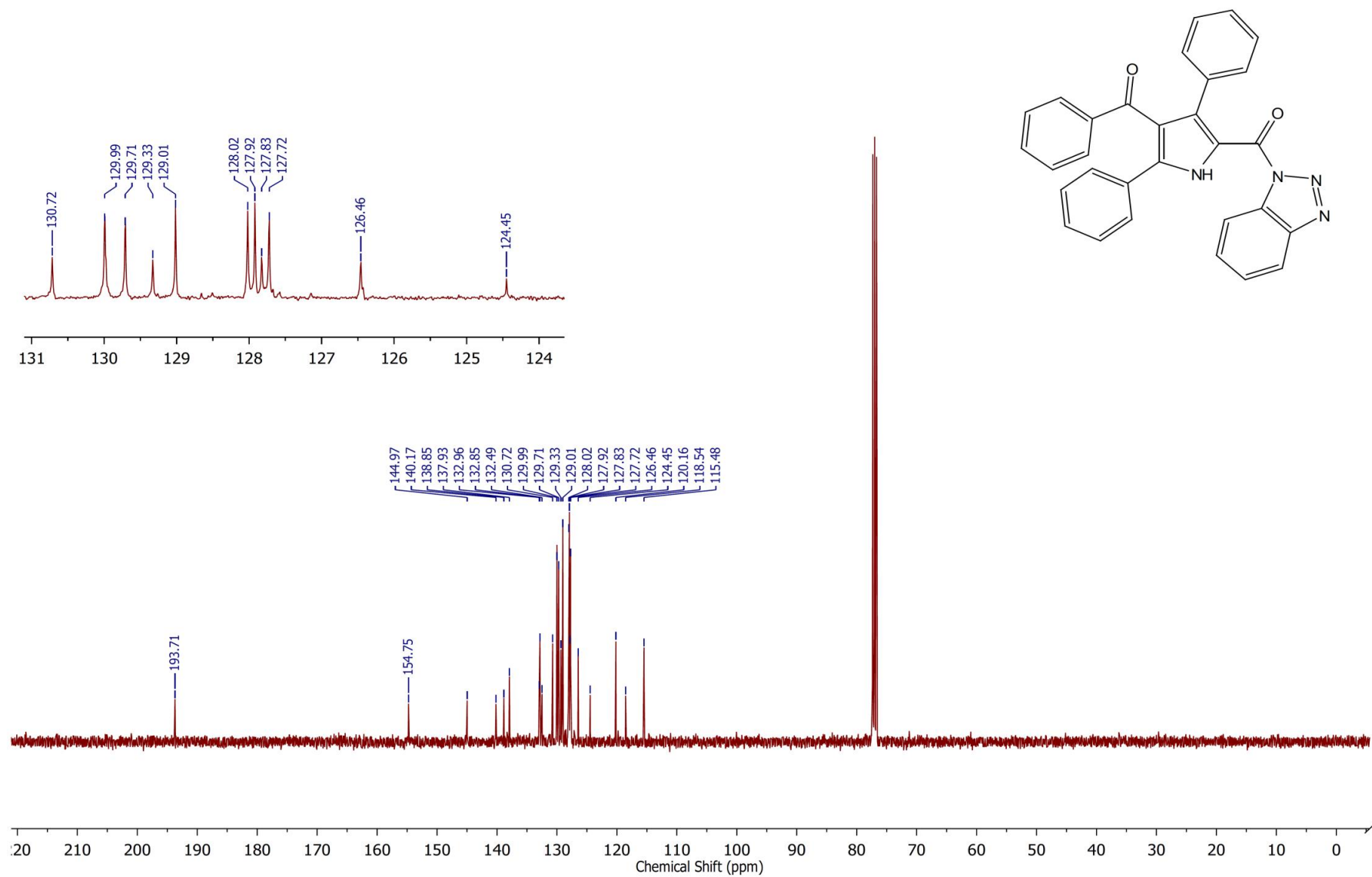
1-(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-methyl-4-(thiophen-2-yl)-1*H*-pyrrol-3-yl)ethan-1-one 6i, DEPT, CDCl₃, 100 MHz



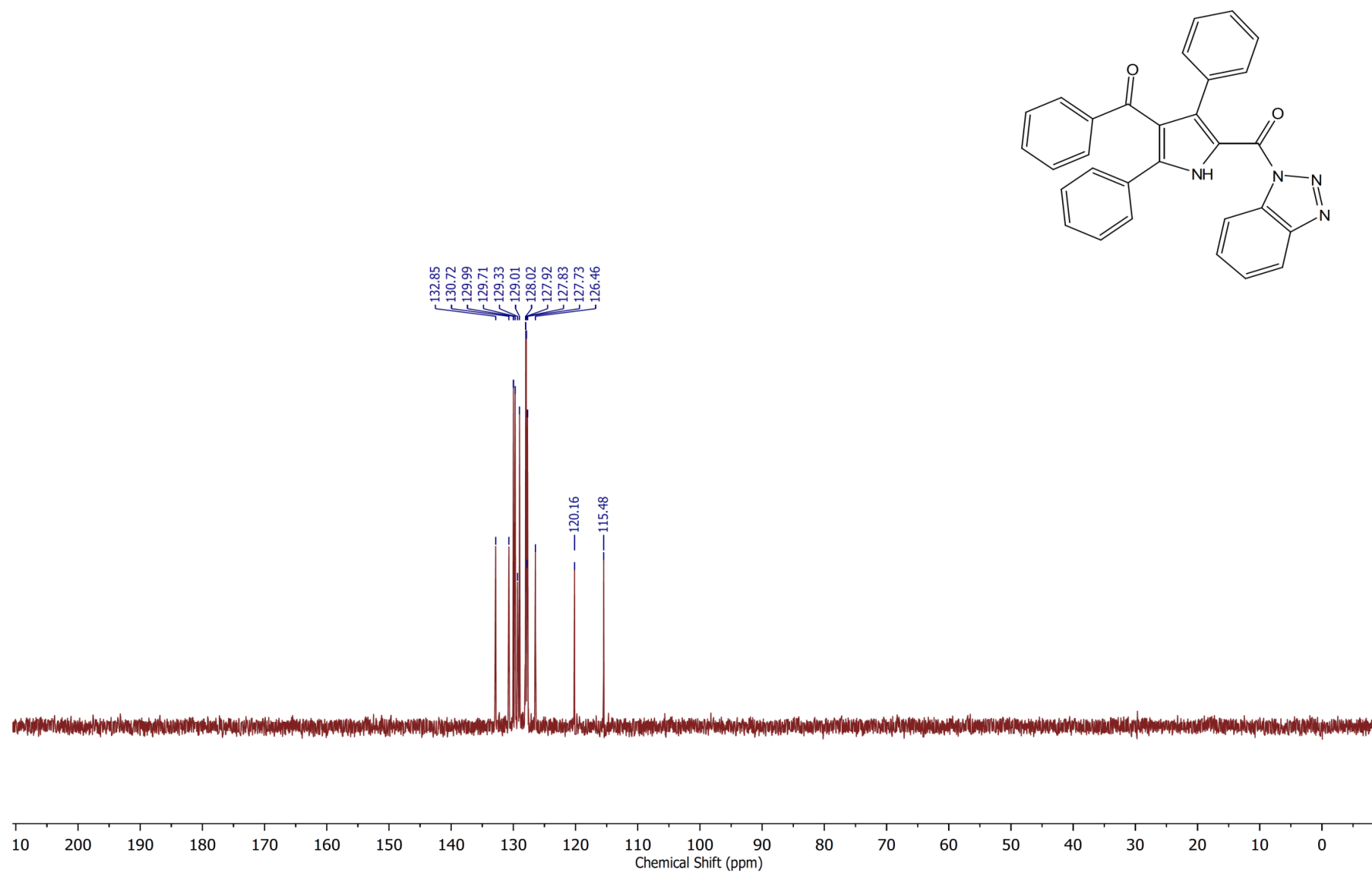
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)(phenyl)methanone **6j**, ^1H NMR, CDCl_3 , 400 MHz



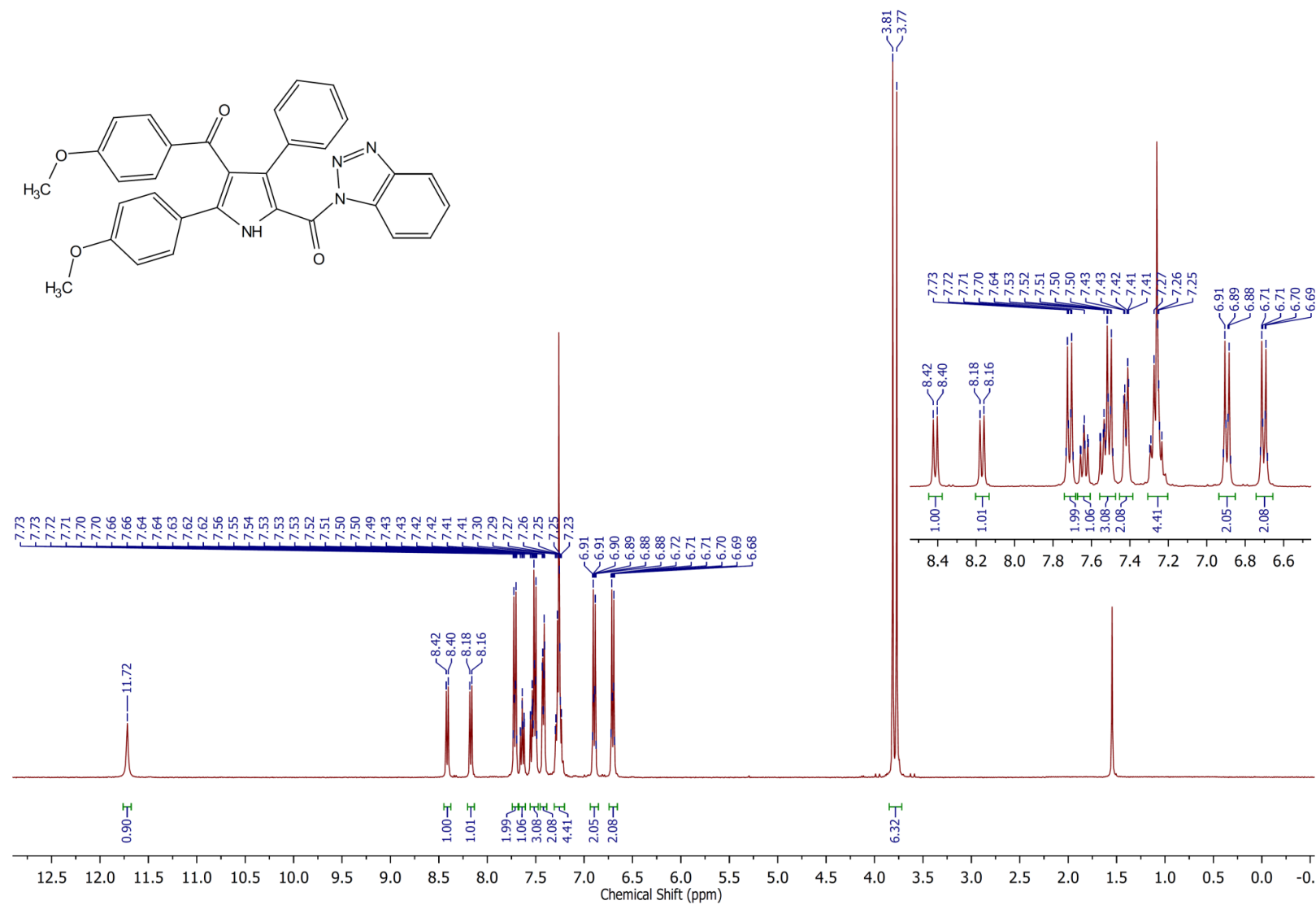
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)(phenyl)methanone **6j**, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



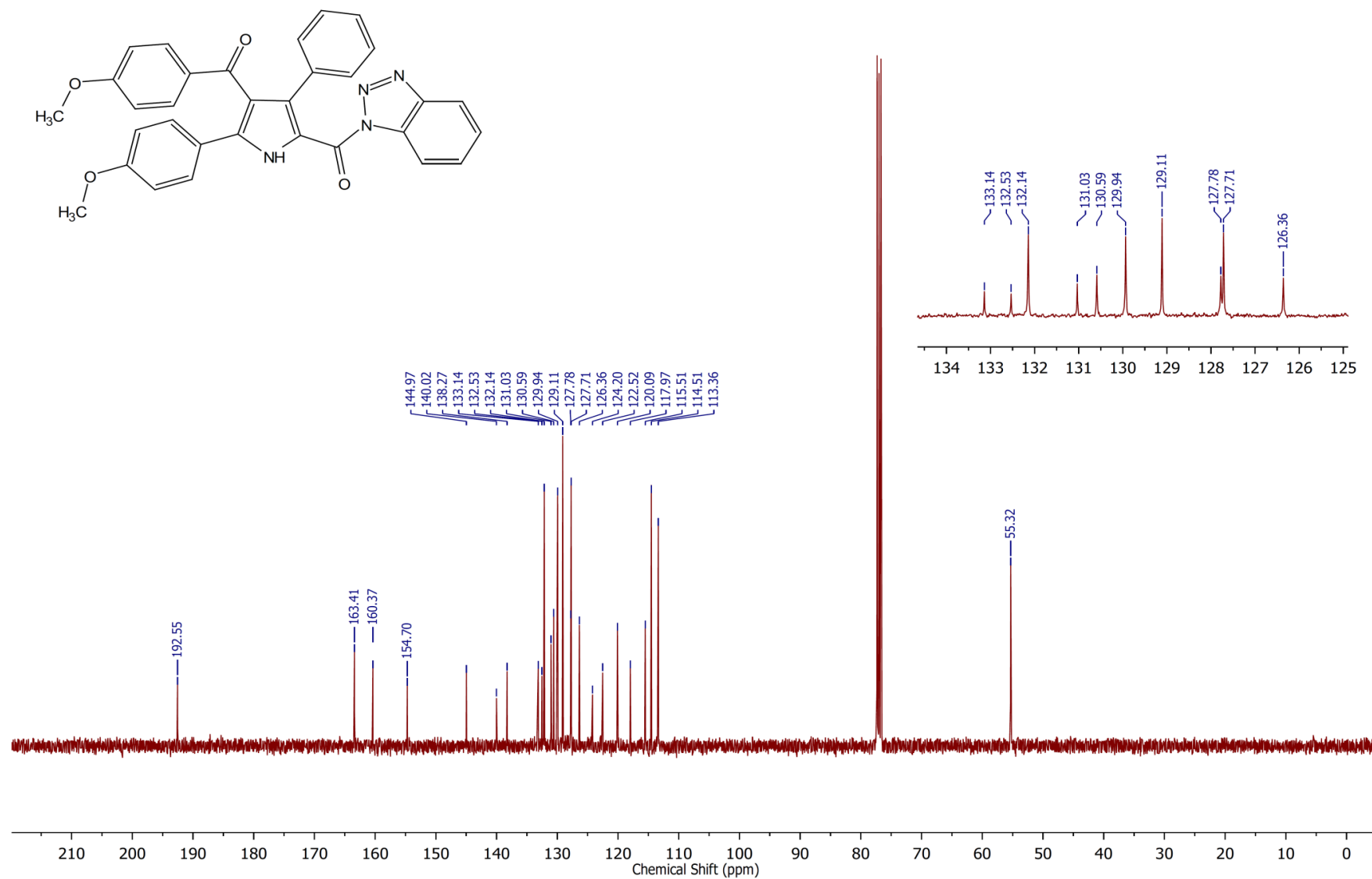
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)(phenyl)methanone 6j, DEPT, CDCl₃, 100 MHz



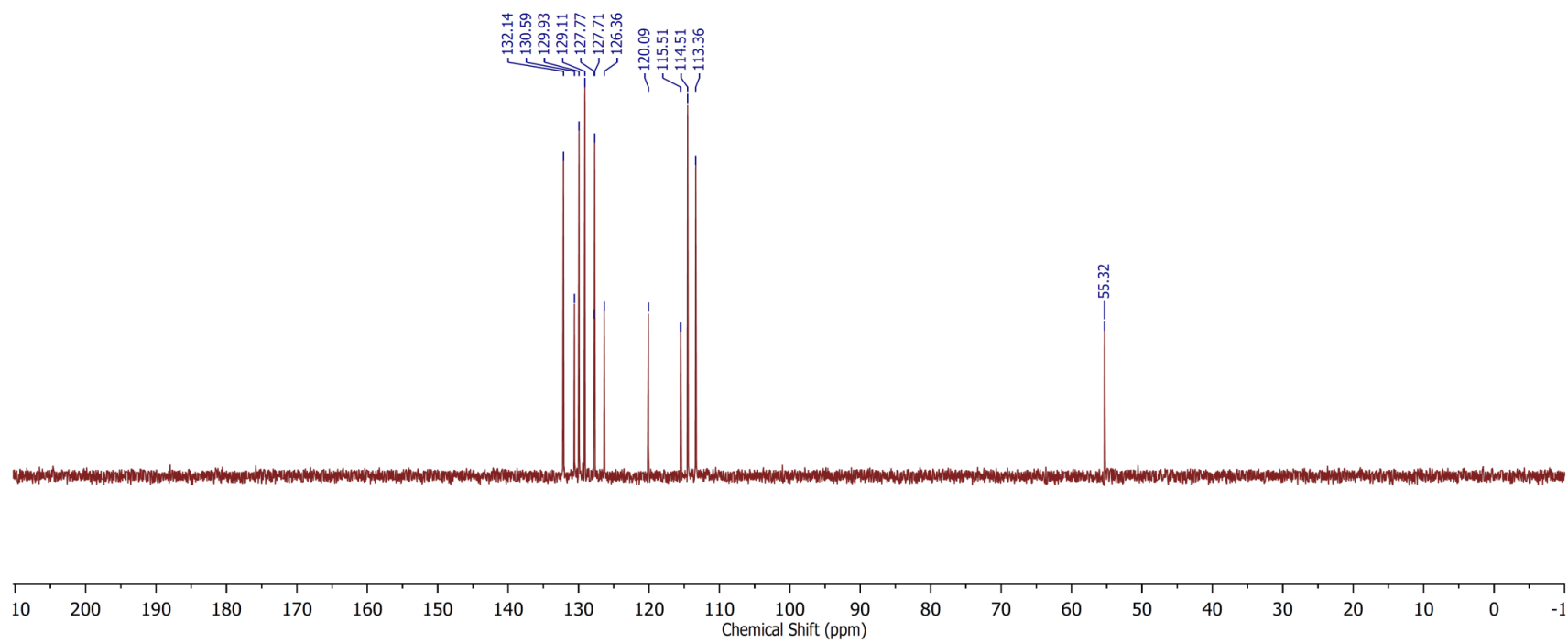
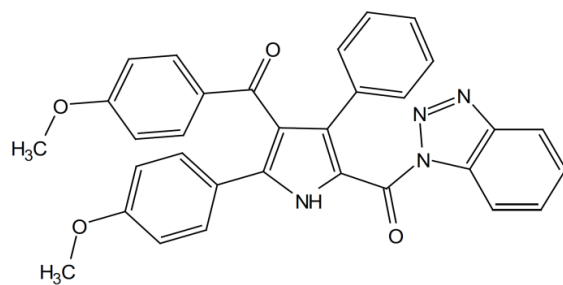
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)(4-methoxyphenyl)methanone 6k, ¹H NMR, CDCl₃, 400 MHz



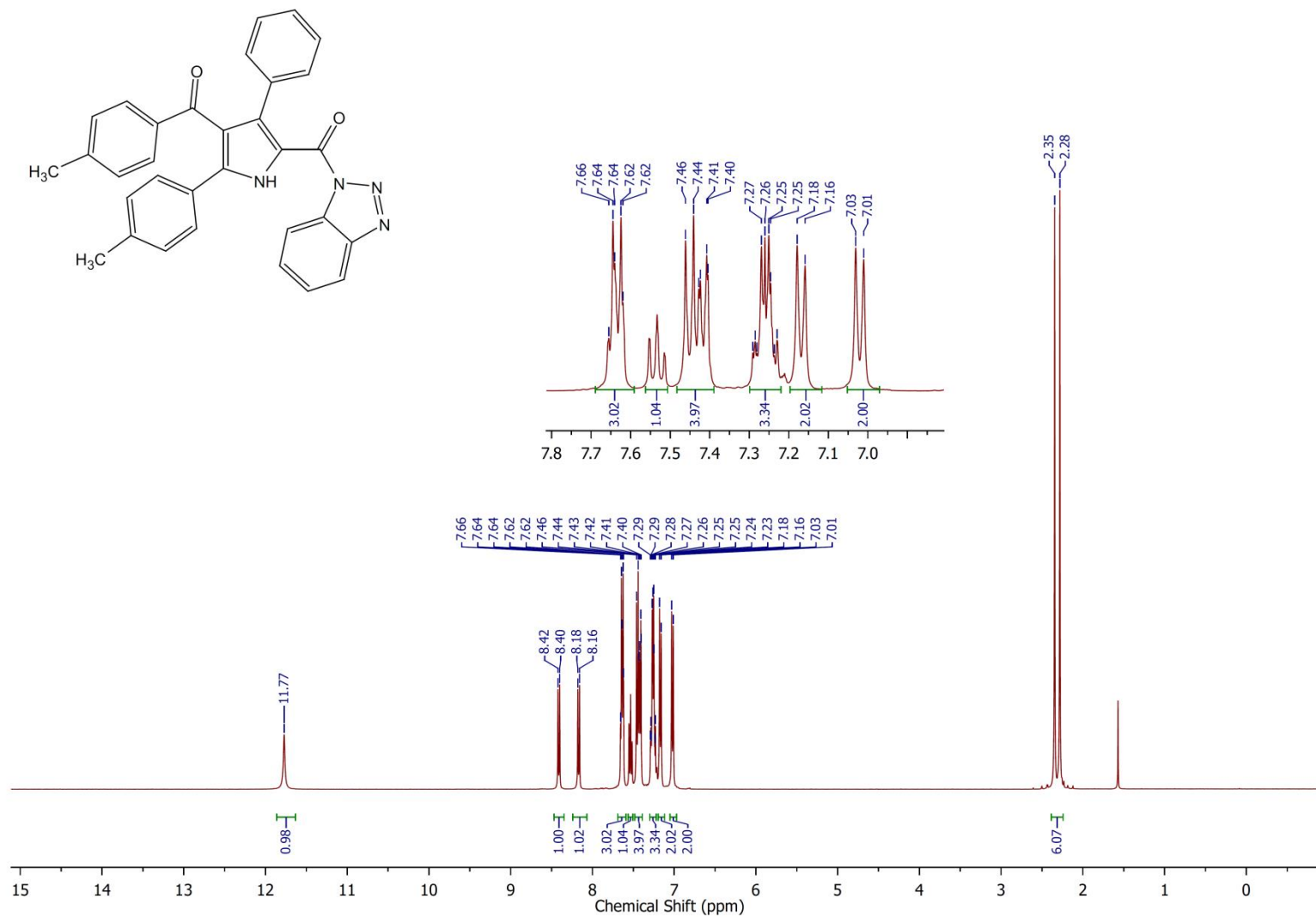
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)(4-methoxyphenyl)methanone 6k, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



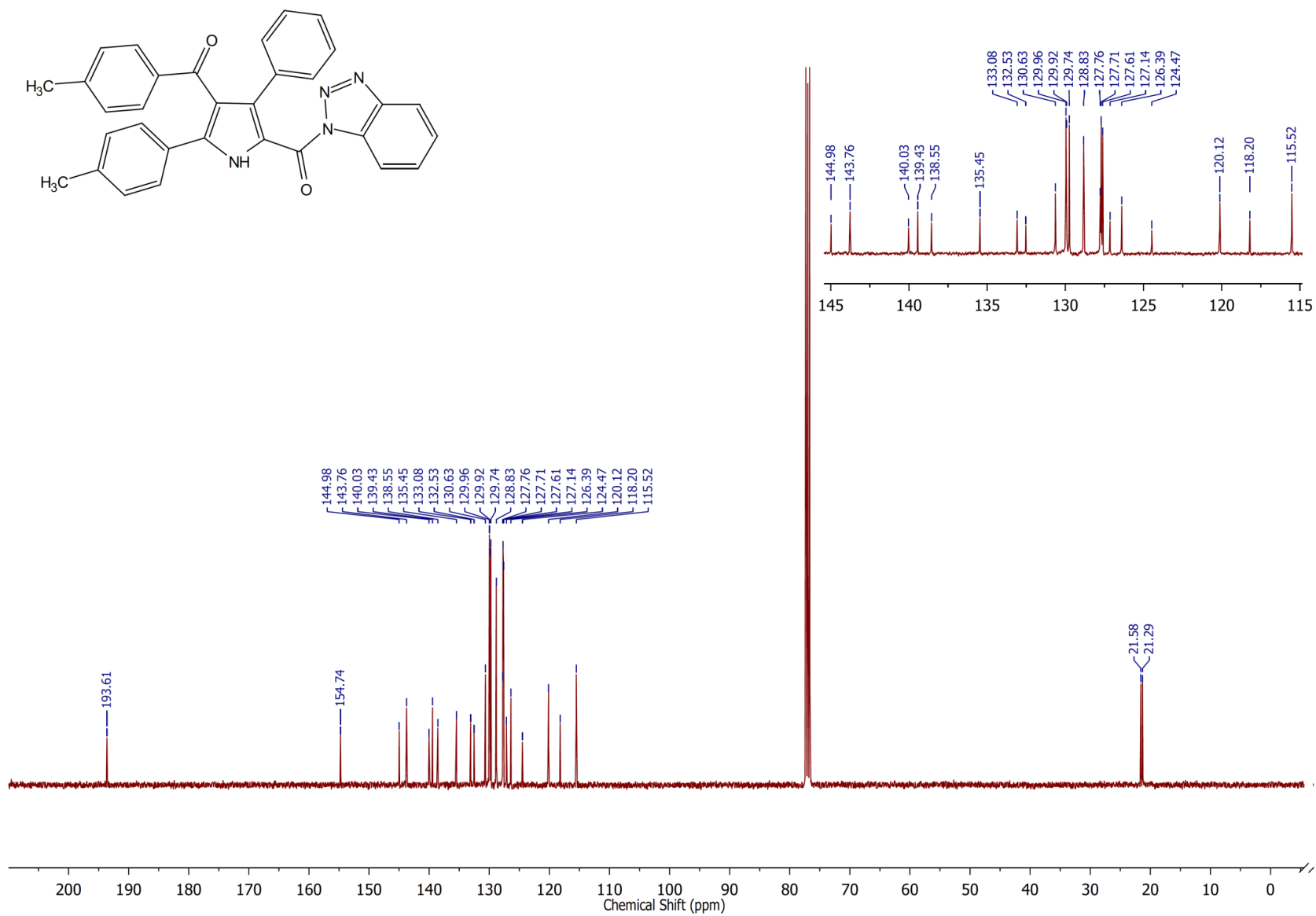
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)(4-methoxyphenyl)methanone 6k, DEPT, CDCl₃, 100 MHz



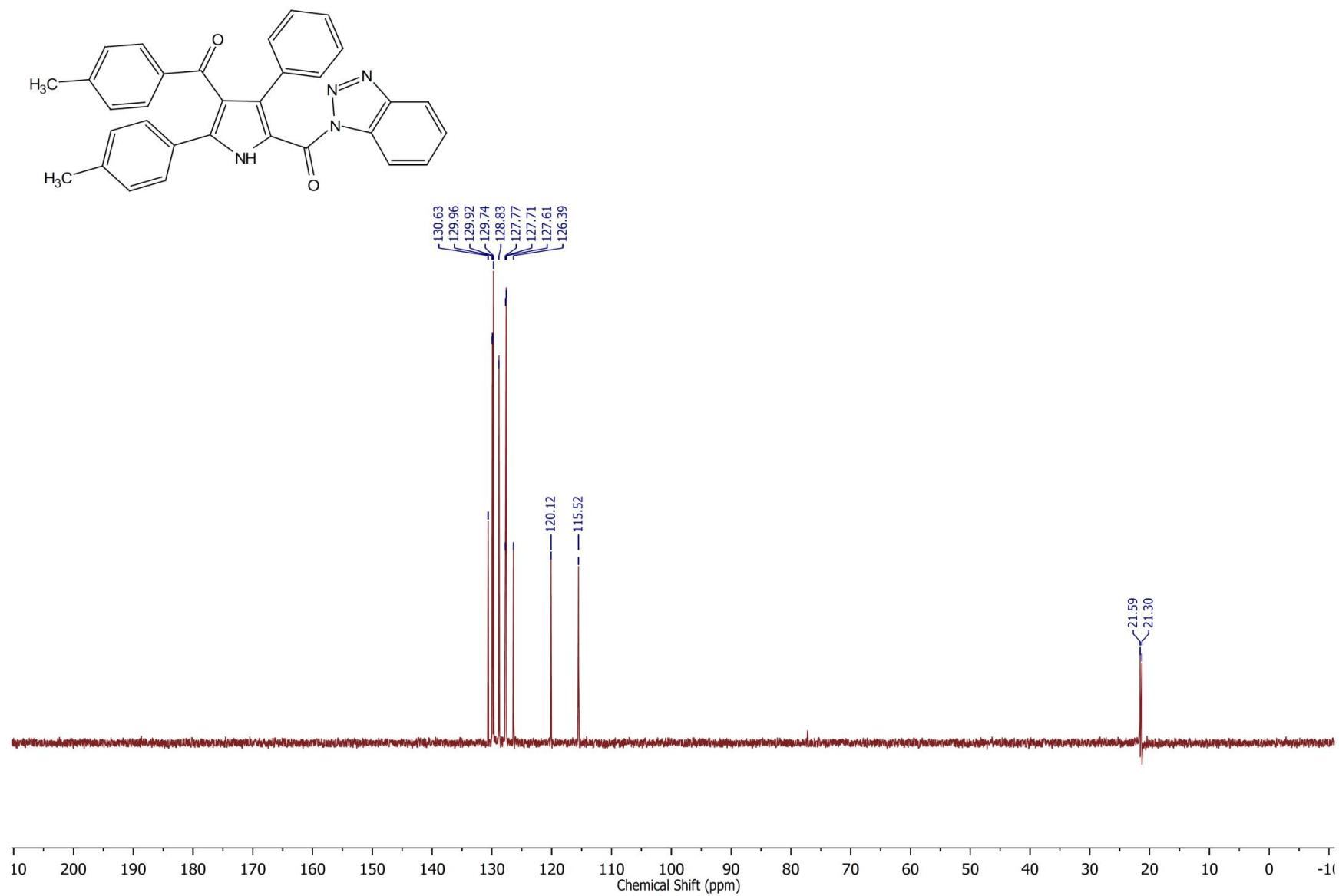
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-phenyl-2-(*p*-tolyl)-1*H*-pyrrol-3-yl)(*p*-tolyl)methanone 6l, ¹H NMR, CDCl₃, 400 MHz



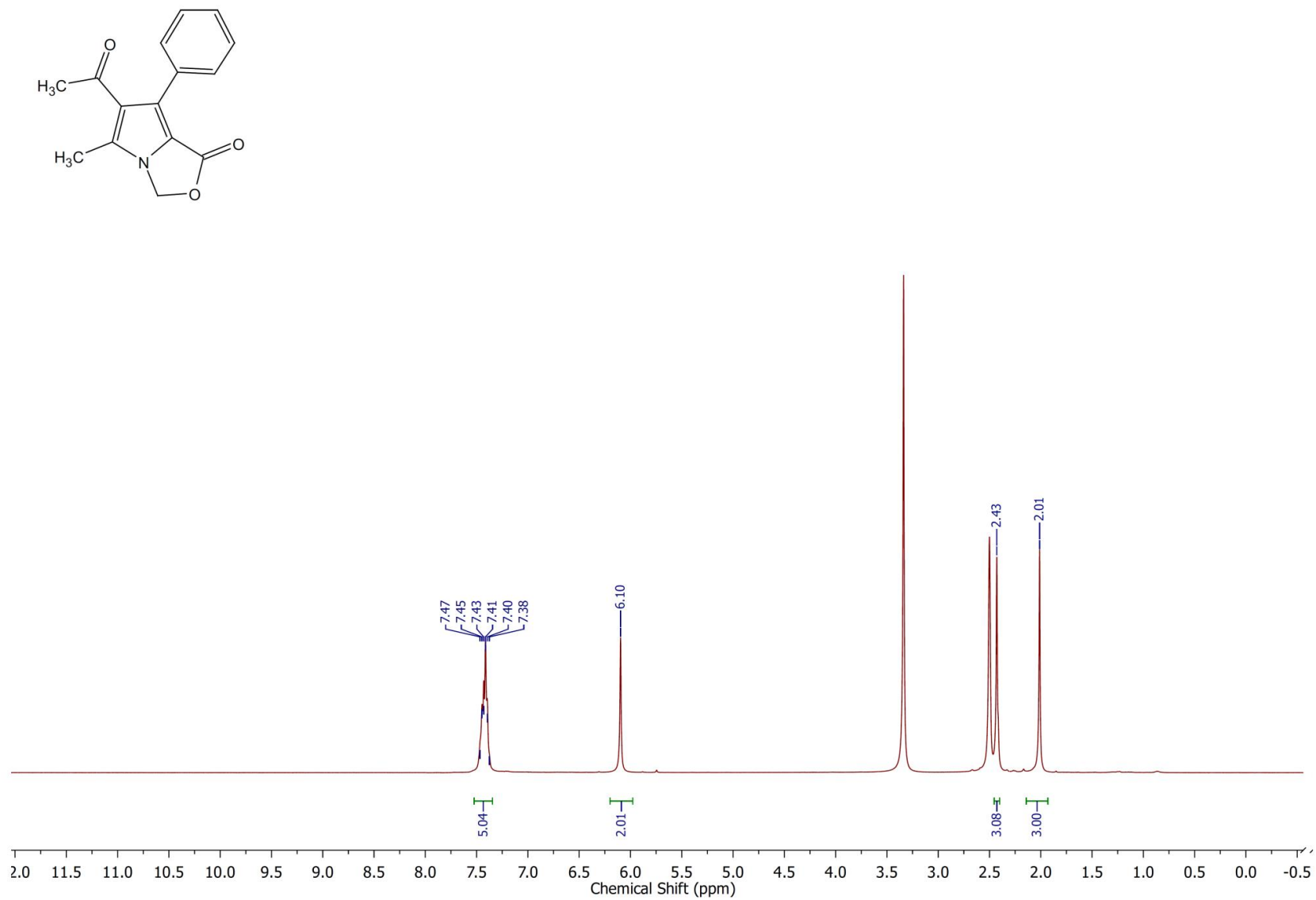
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-phenyl-2-(*p*-tolyl)-1*H*-pyrrol-3-yl)(*p*-tolyl)methanone 6l, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



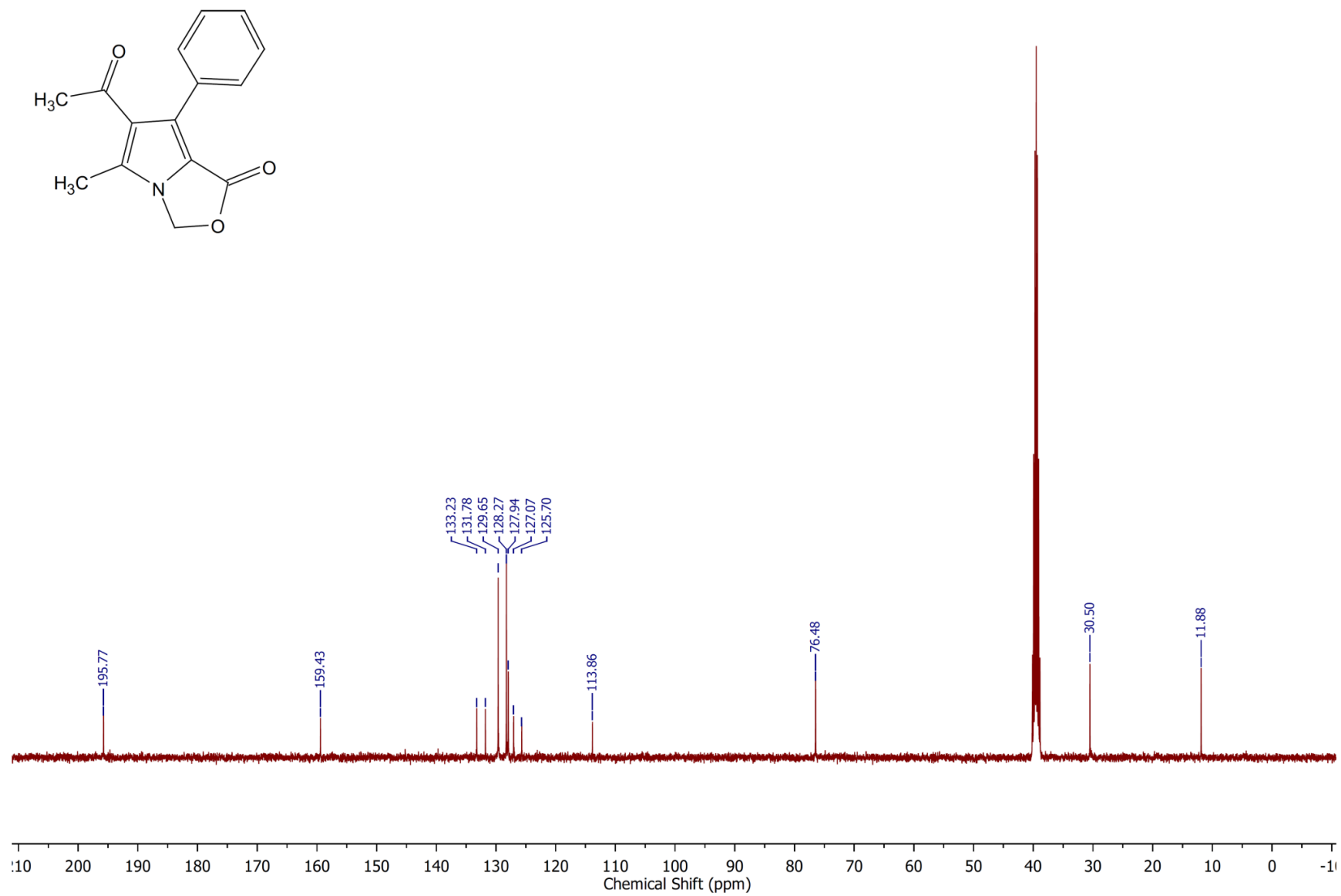
(5-(1*H*-Benzo[*d*][1,2,3]triazole-1-carbonyl)-4-phenyl-2-(*p*-tolyl)-1*H*-pyrrol-3-yl)(*p*-tolyl)methanone 6l, DEPT, CDCl₃, 100 MHz



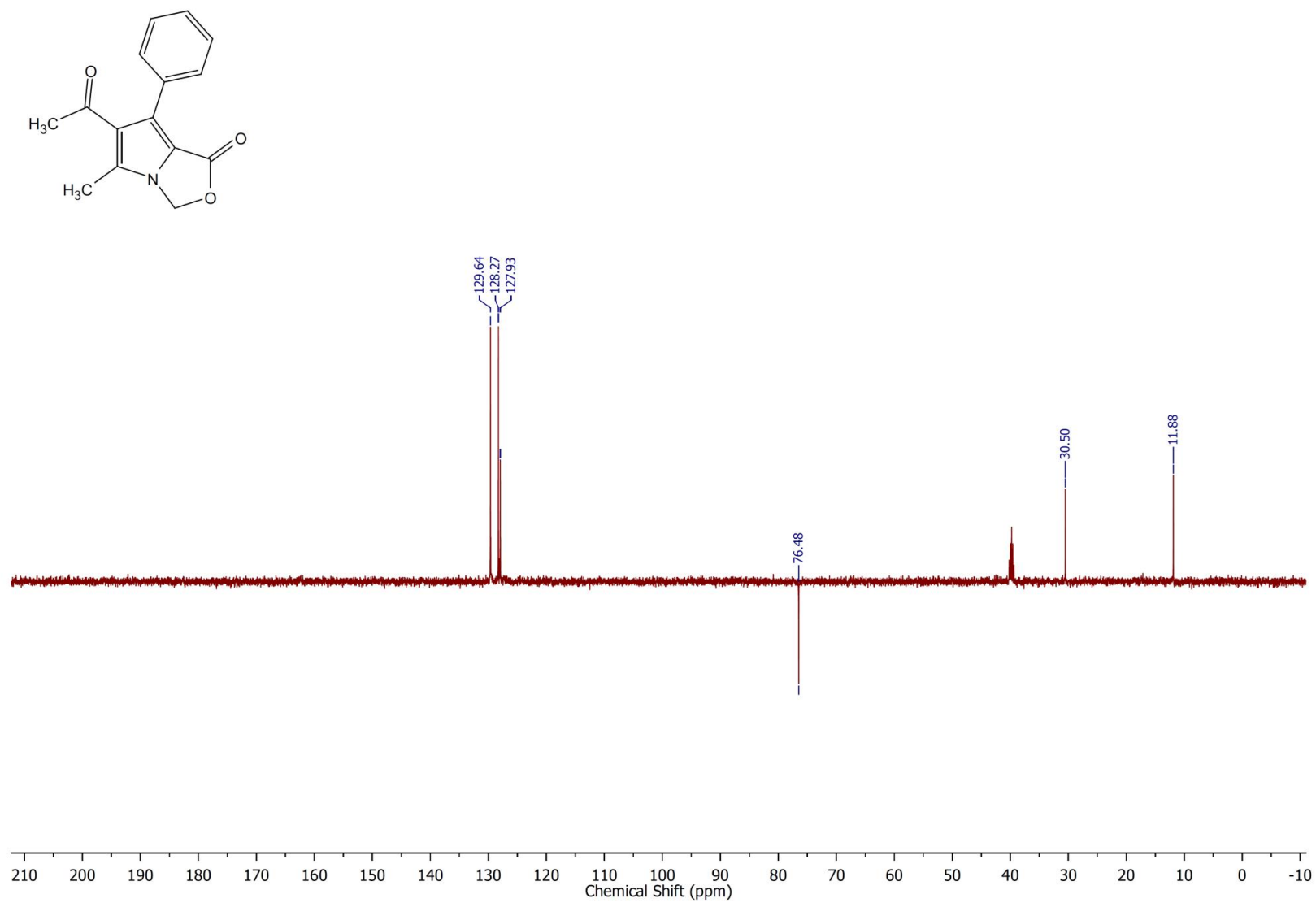
6-Acetyl-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8a, ¹H NMR, DMSO-*d*₆, 400 MHz



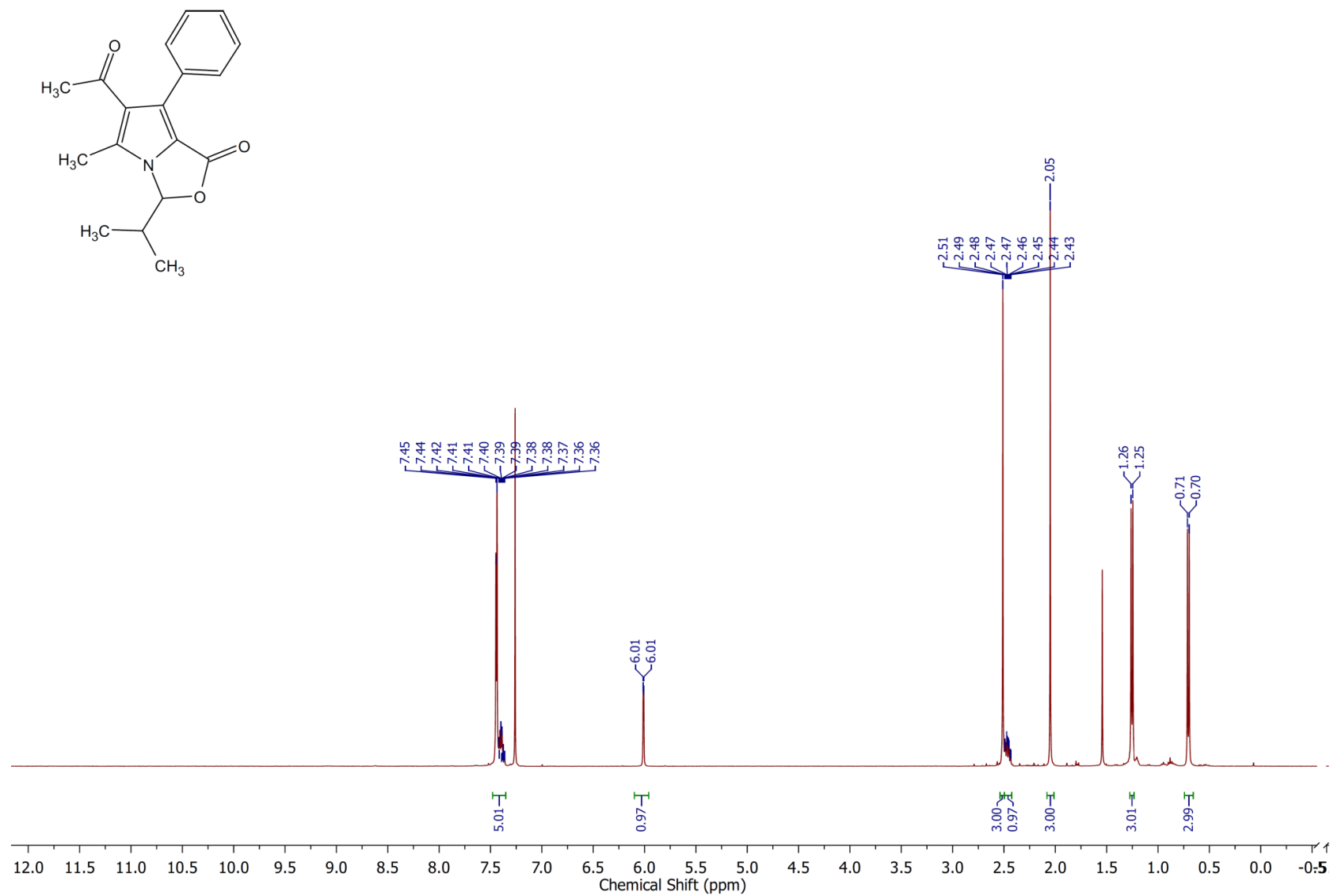
6-Acetyl-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8a, $^{13}\text{C}\{^1\text{H}\}$ NMR, DMSO- d_6 , 100 MHz



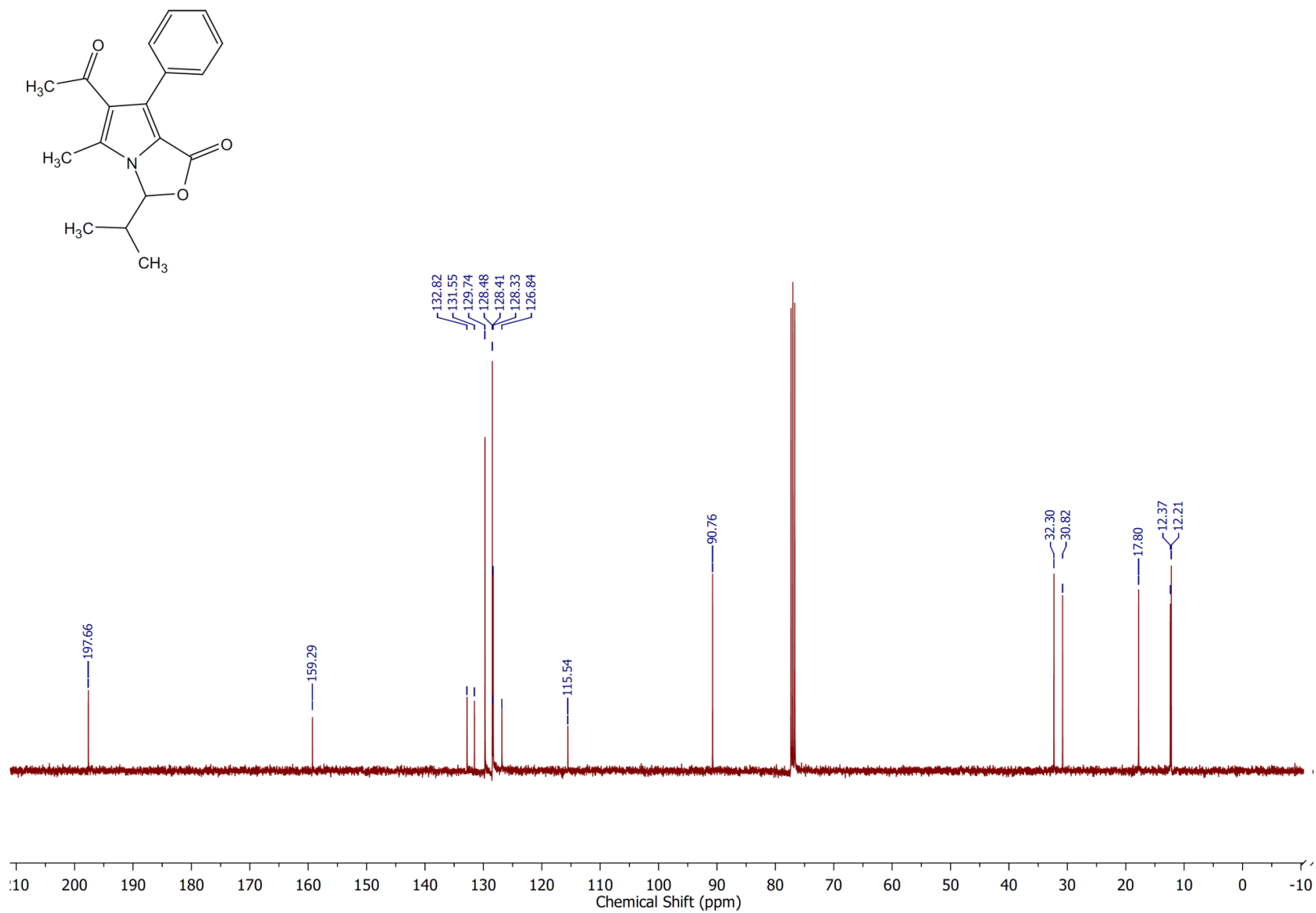
6-Acetyl-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8a, DEPT,DMSO-*d*₆, 100 MHz



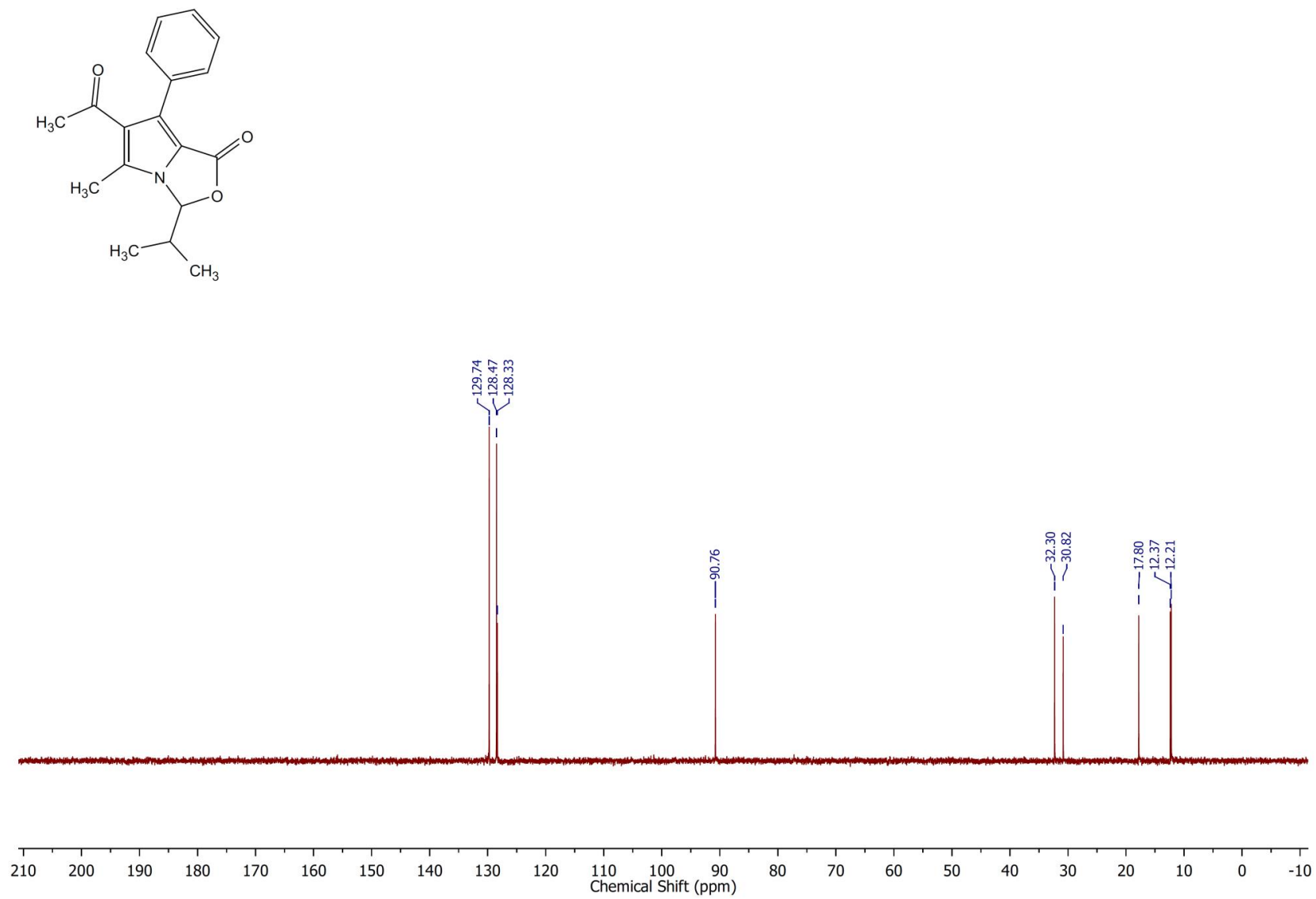
6-Acetyl-3-isopropyl-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8b, ¹H NMR, CDCl₃, 400 MHz



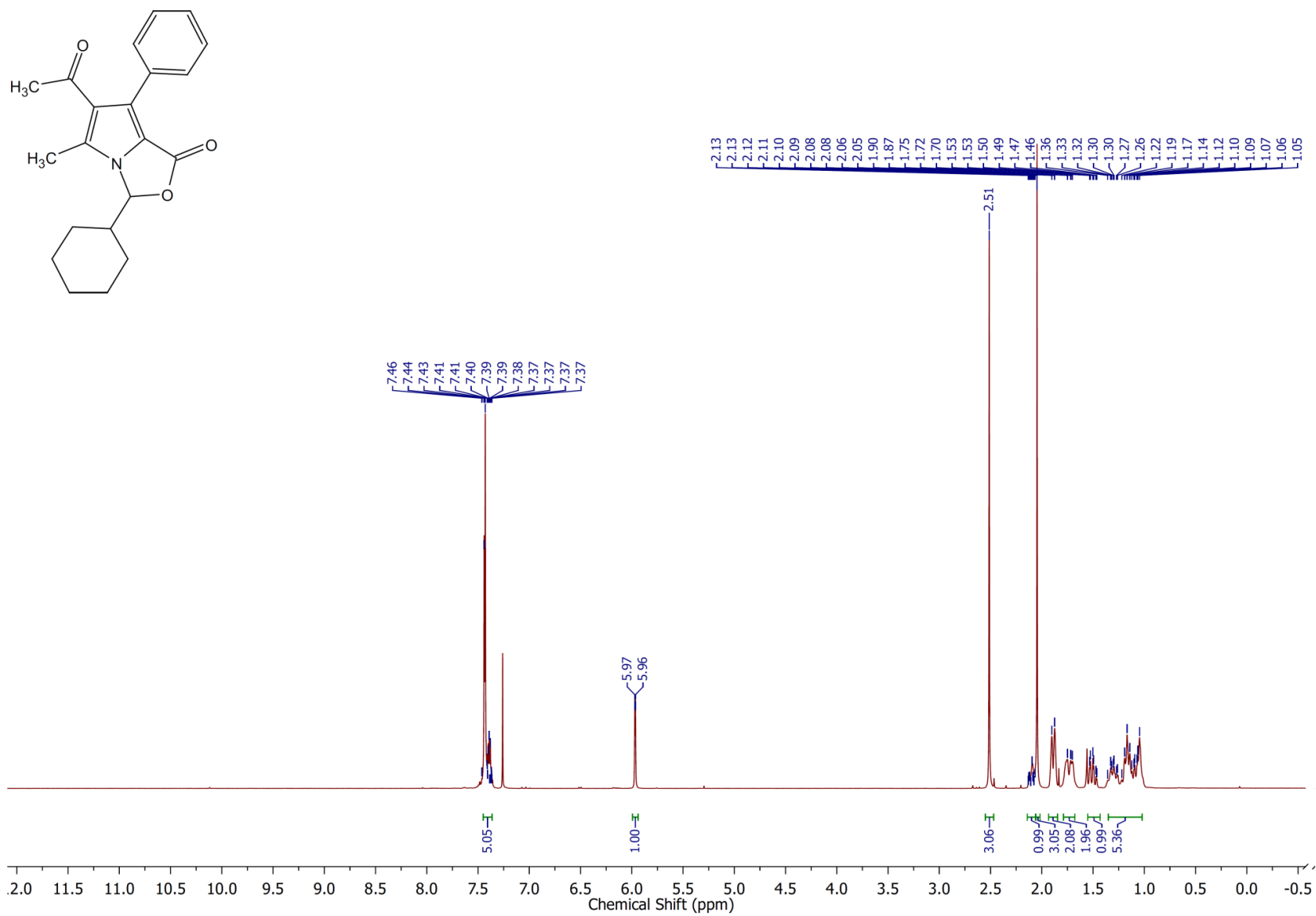
6-Acetyl-3-isopropyl-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8b, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



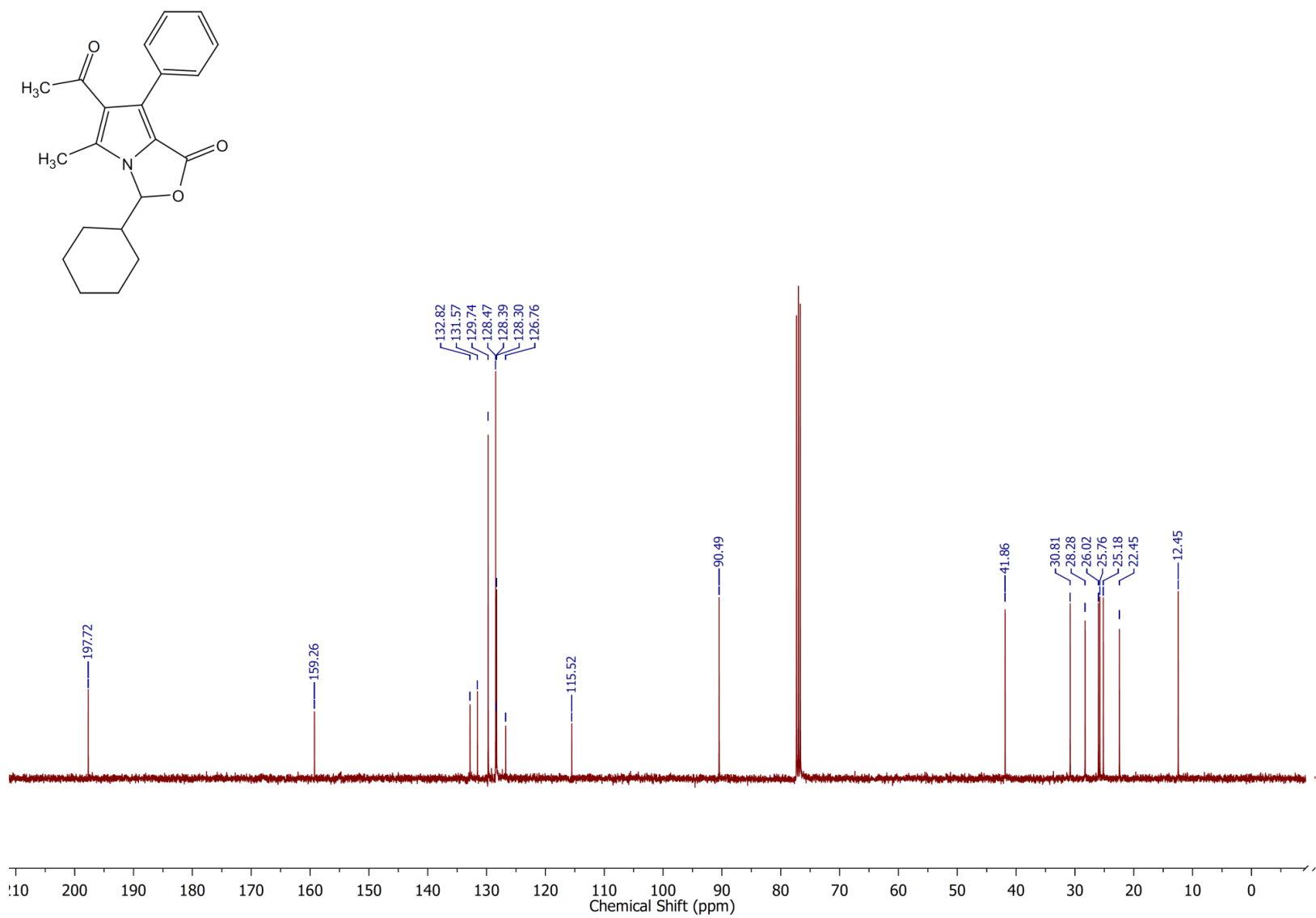
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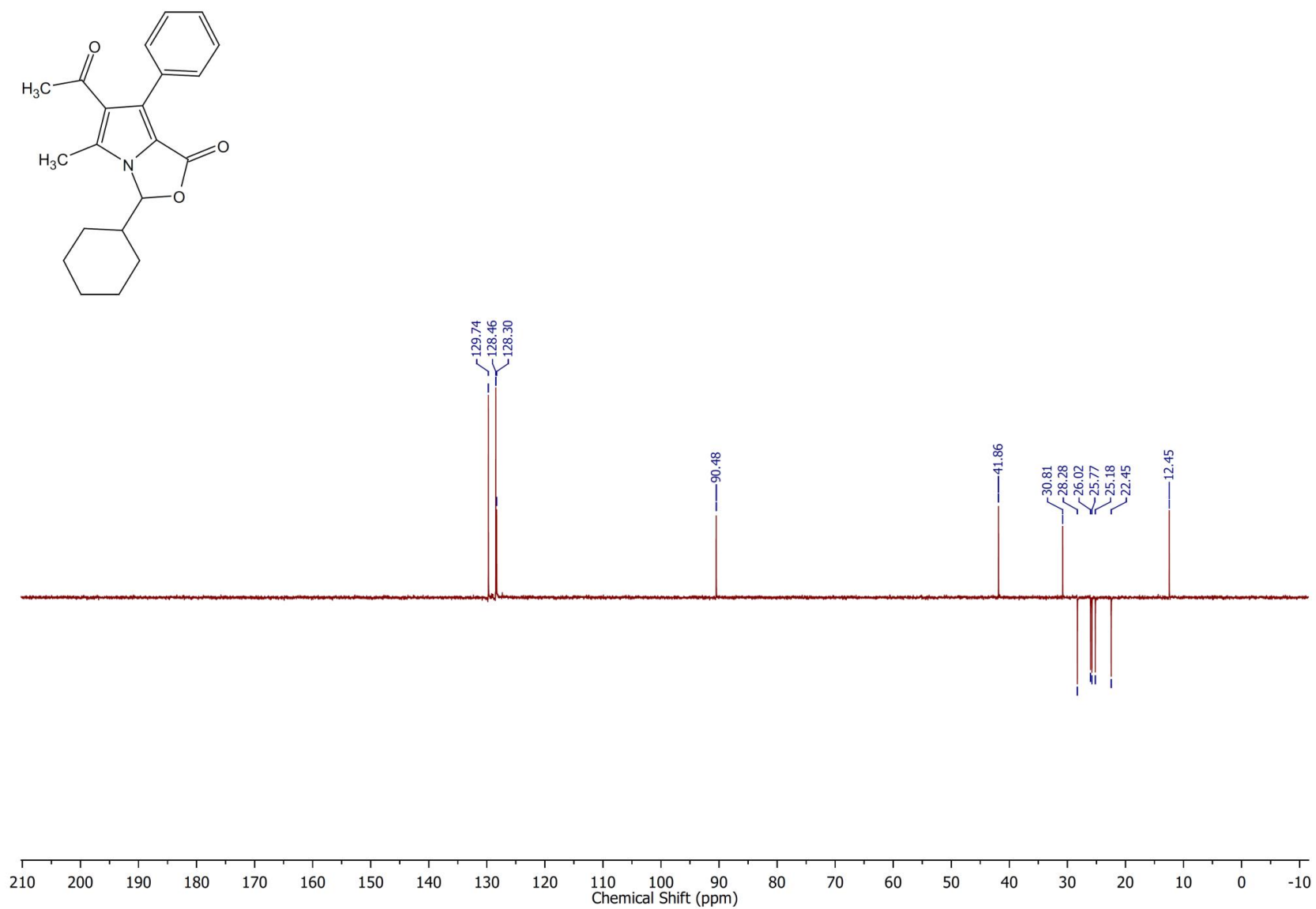
6-Acetyl-3-cyclohexyl-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8c, ¹H NMR, CDCl₃, 400 MHz



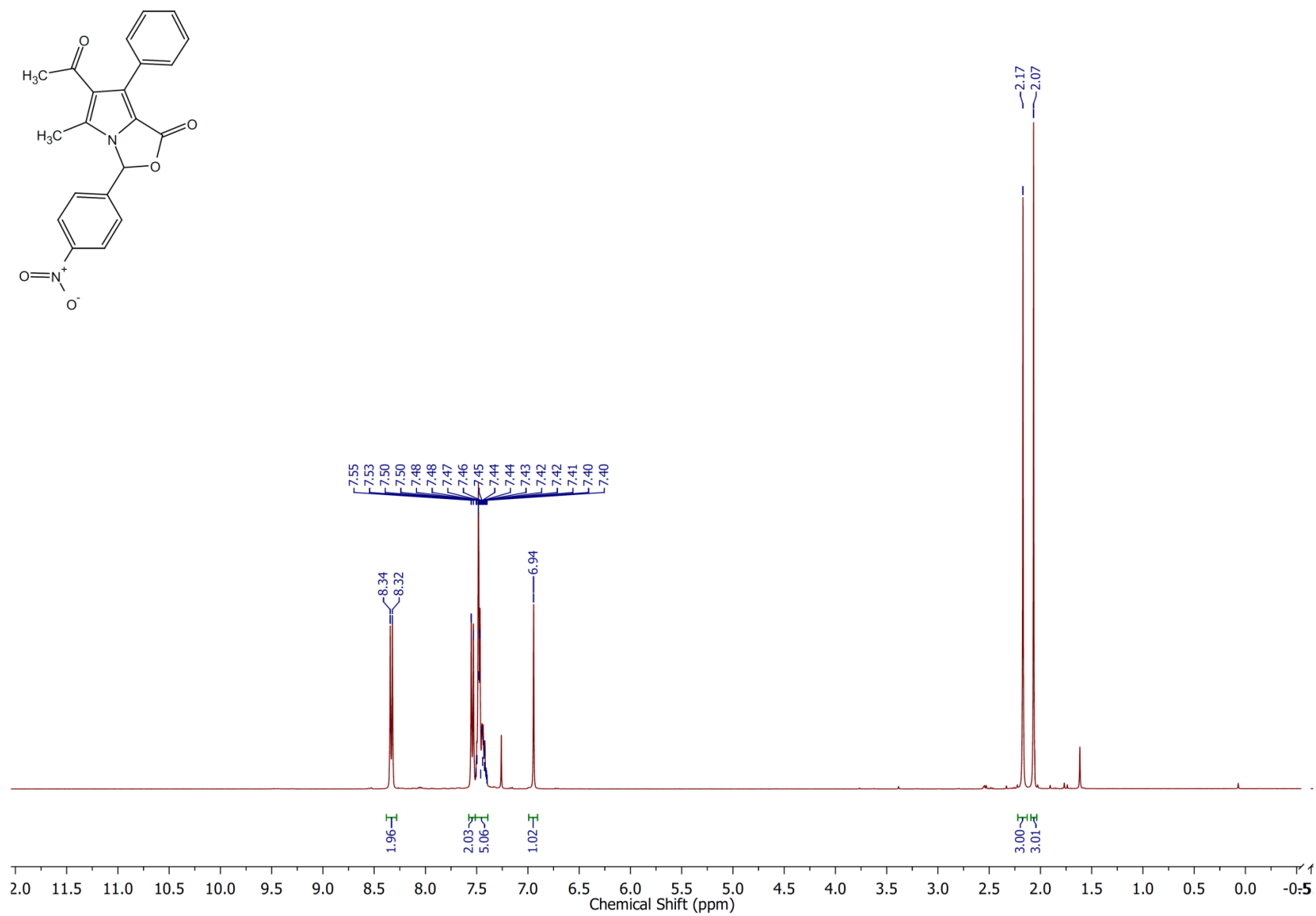
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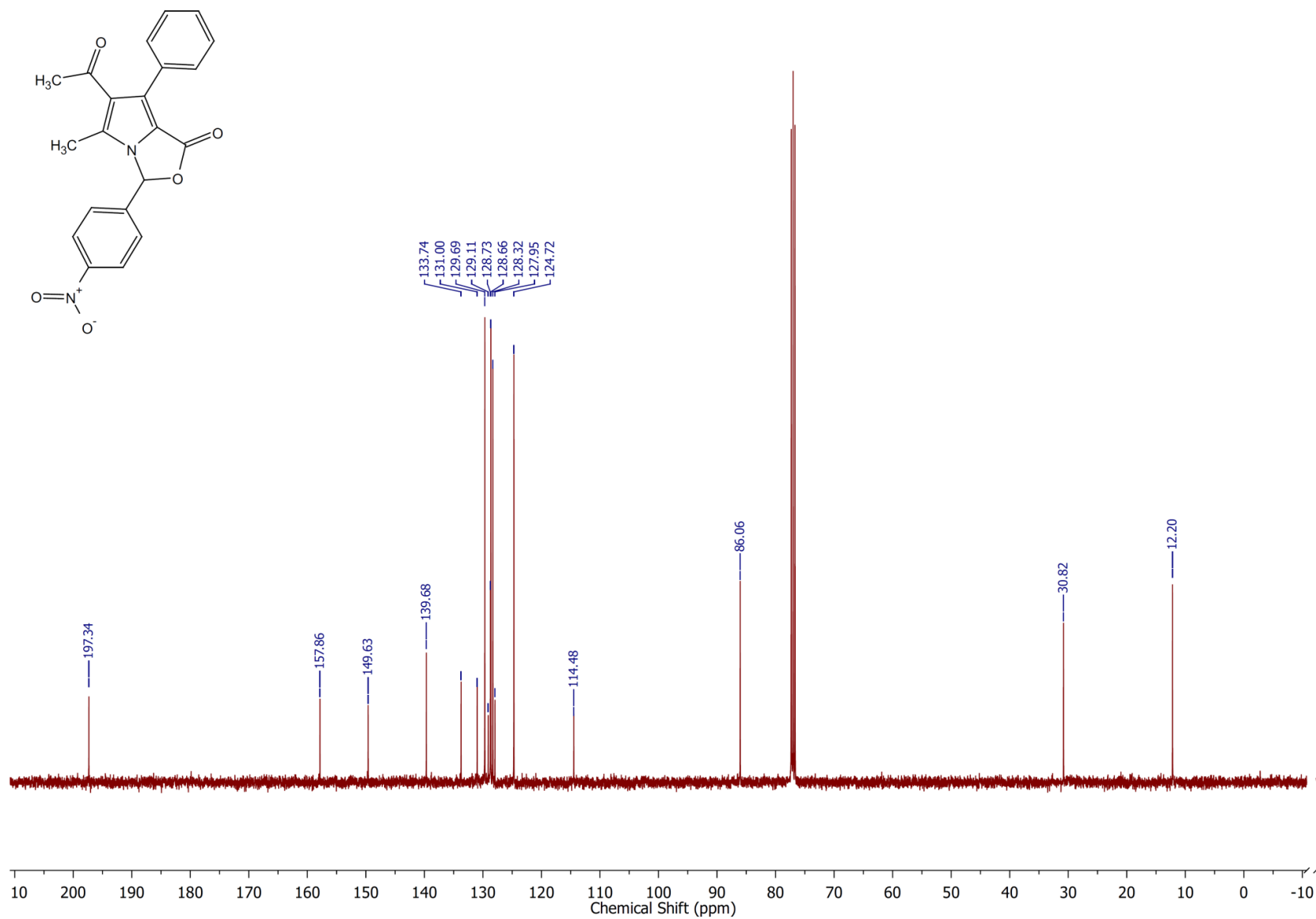
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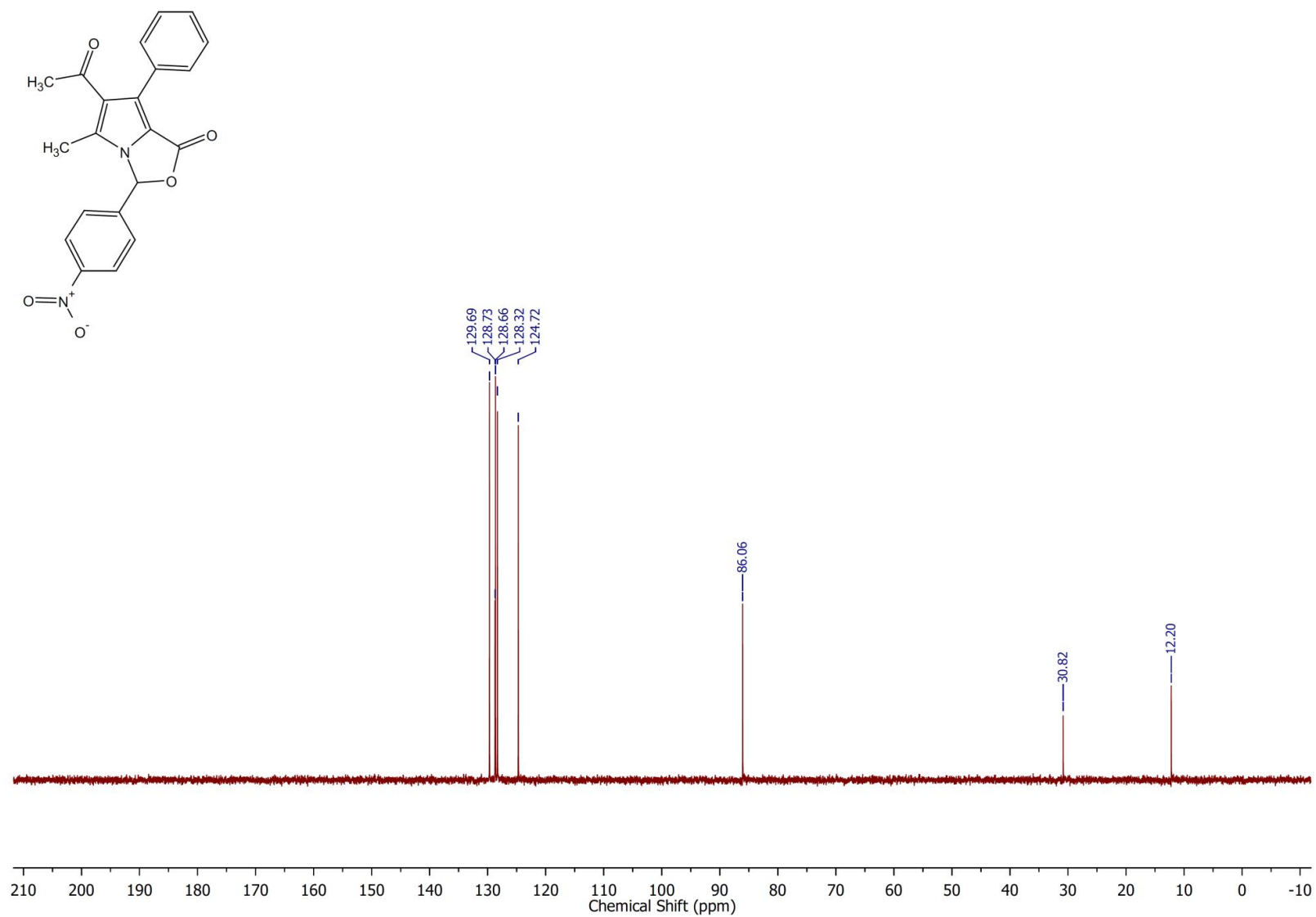
6-Acetyl-5-methyl-3-(4-nitrophenyl)-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8d, ¹H NMR, CDCl₃, 400 MHz



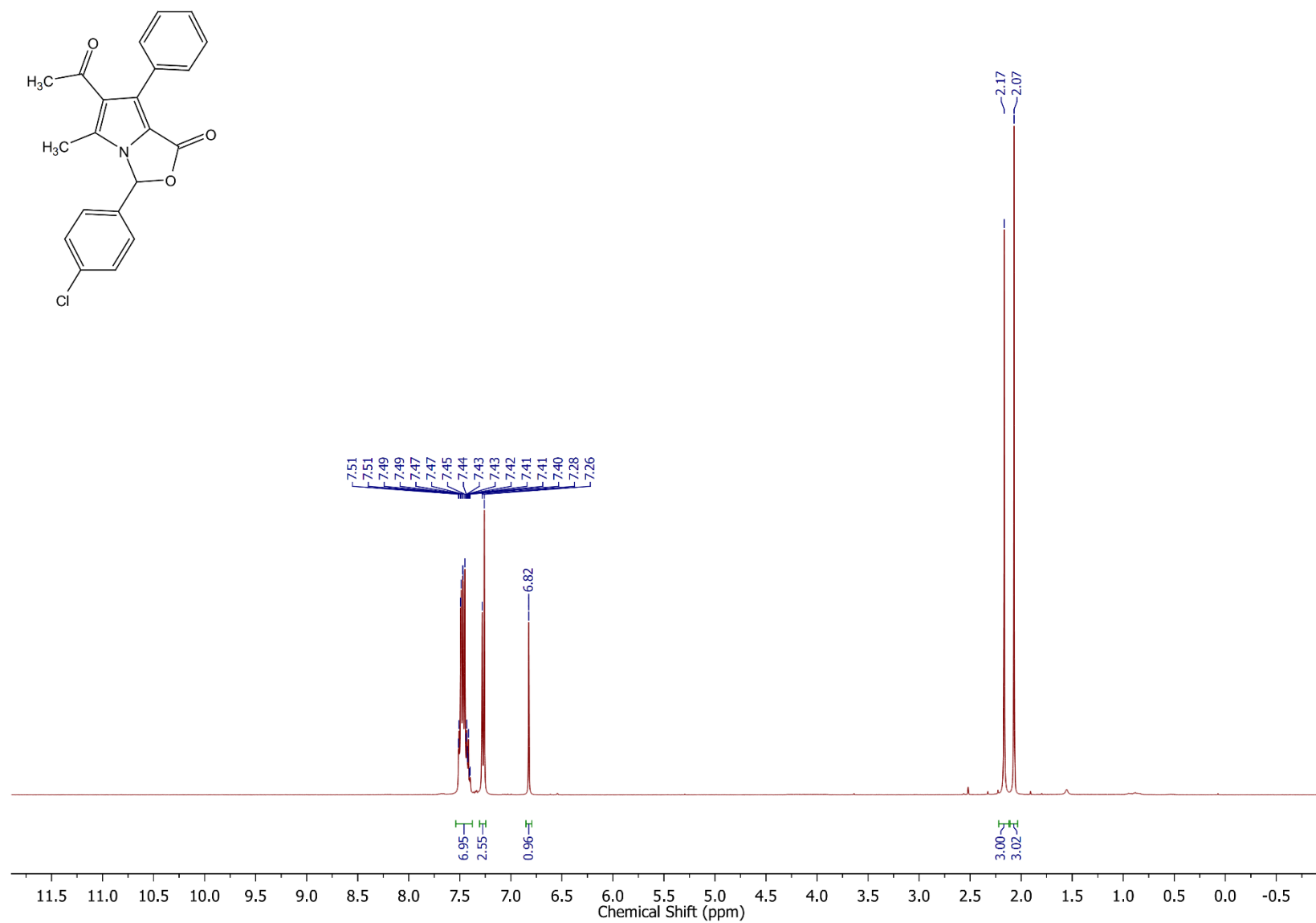
6-Acetyl-5-methyl-3-(4-nitrophenyl)-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8d, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



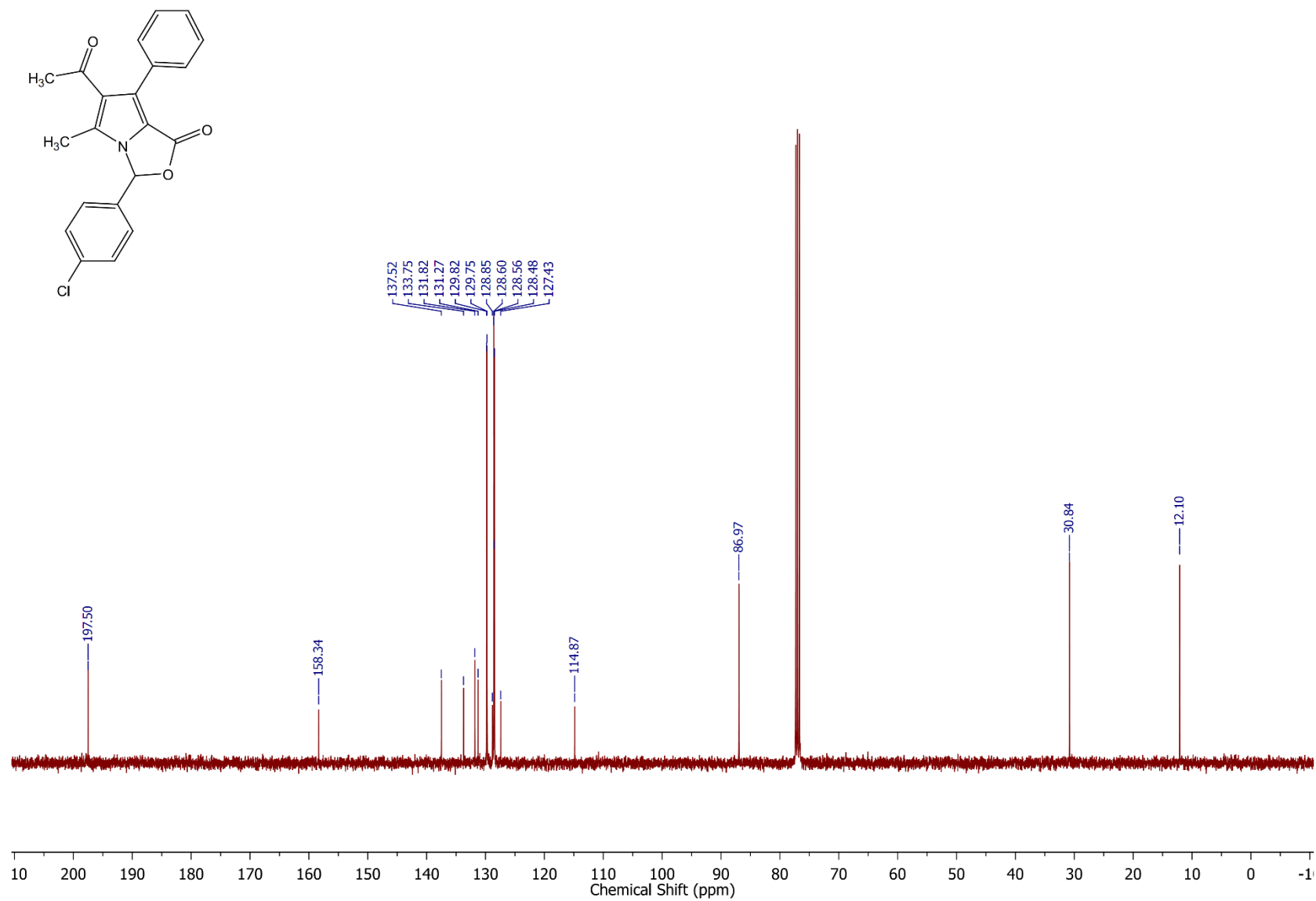
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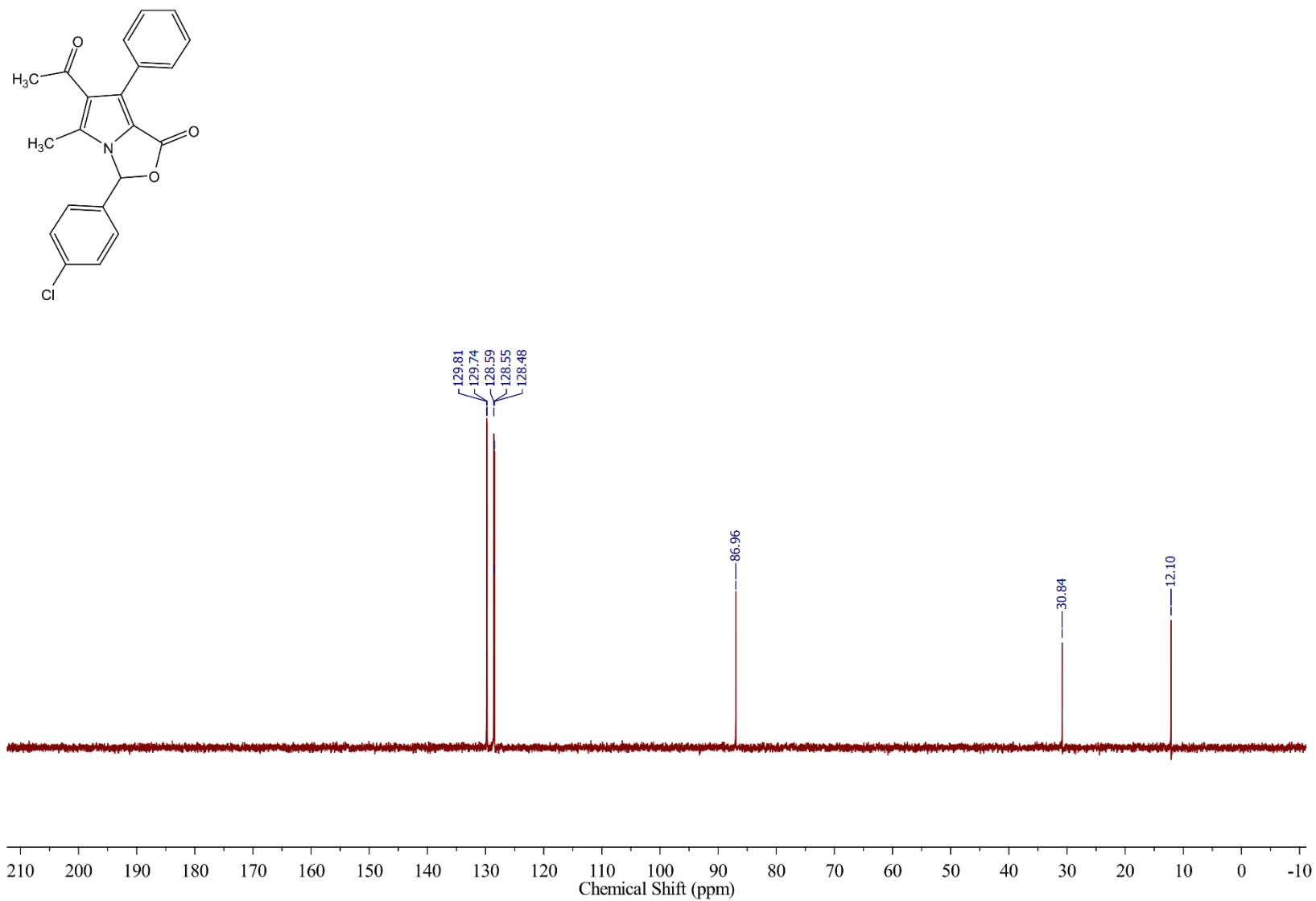
6-Acetyl-3-(4-chlorophenyl)-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8e, ¹H NMR, CDCl₃, 400 MHz



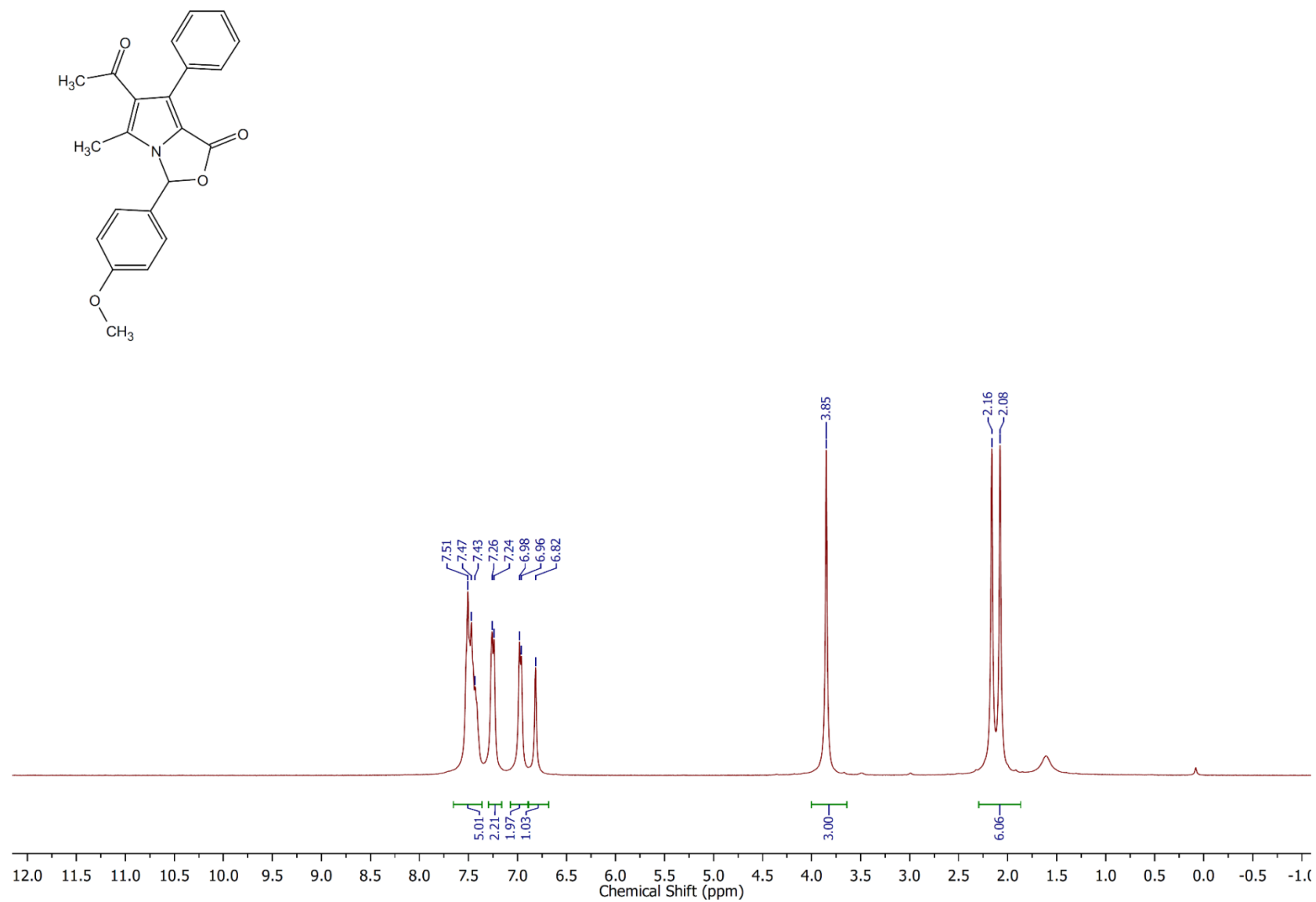
6-Acetyl-3-(4-chlorophenyl)-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8e, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



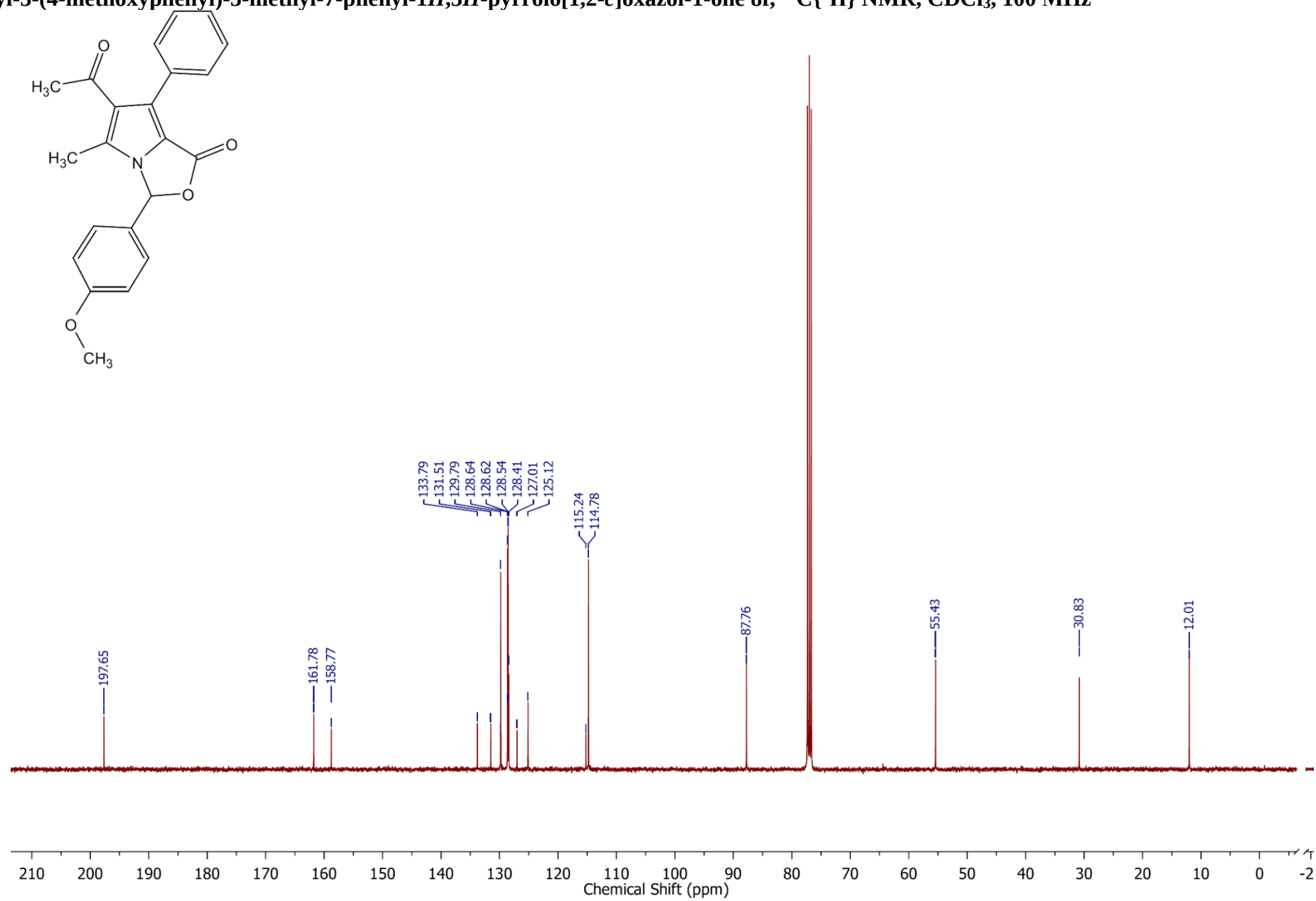
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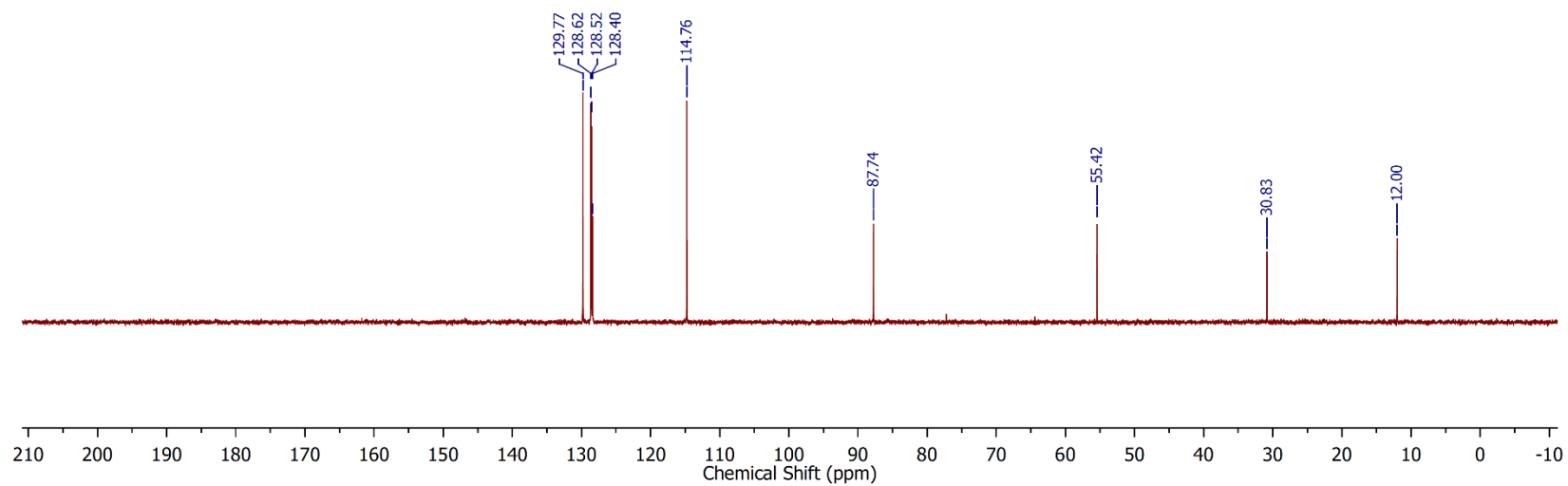
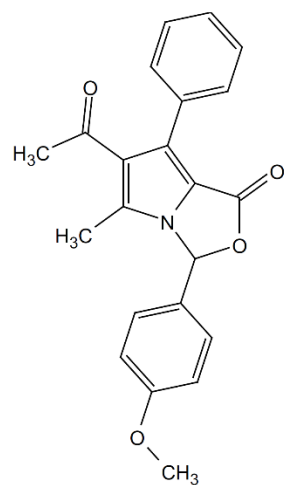
6-Acetyl-3-(4-methoxyphenyl)-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8f, ¹H NMR, CDCl₃, 400 MHz



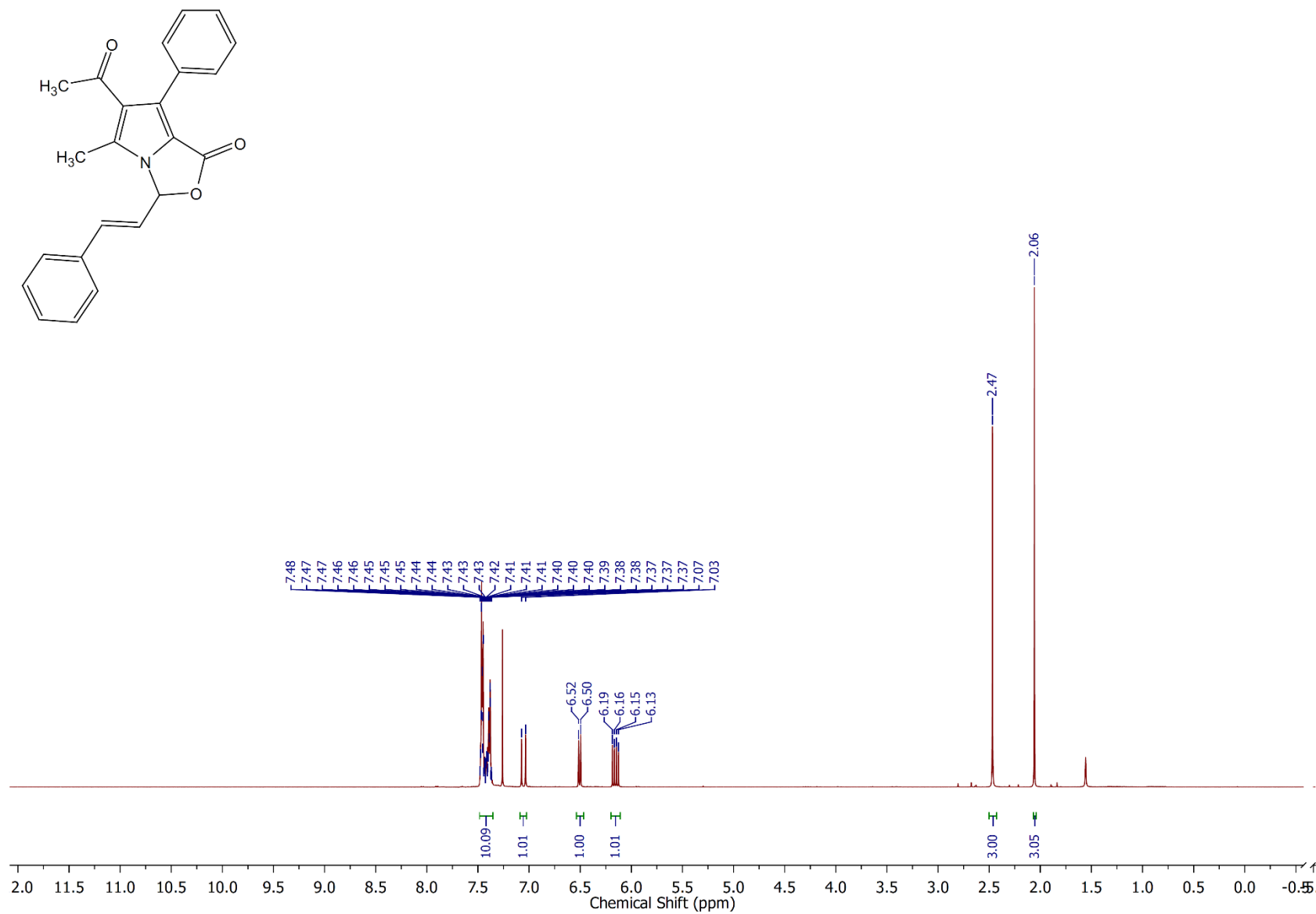
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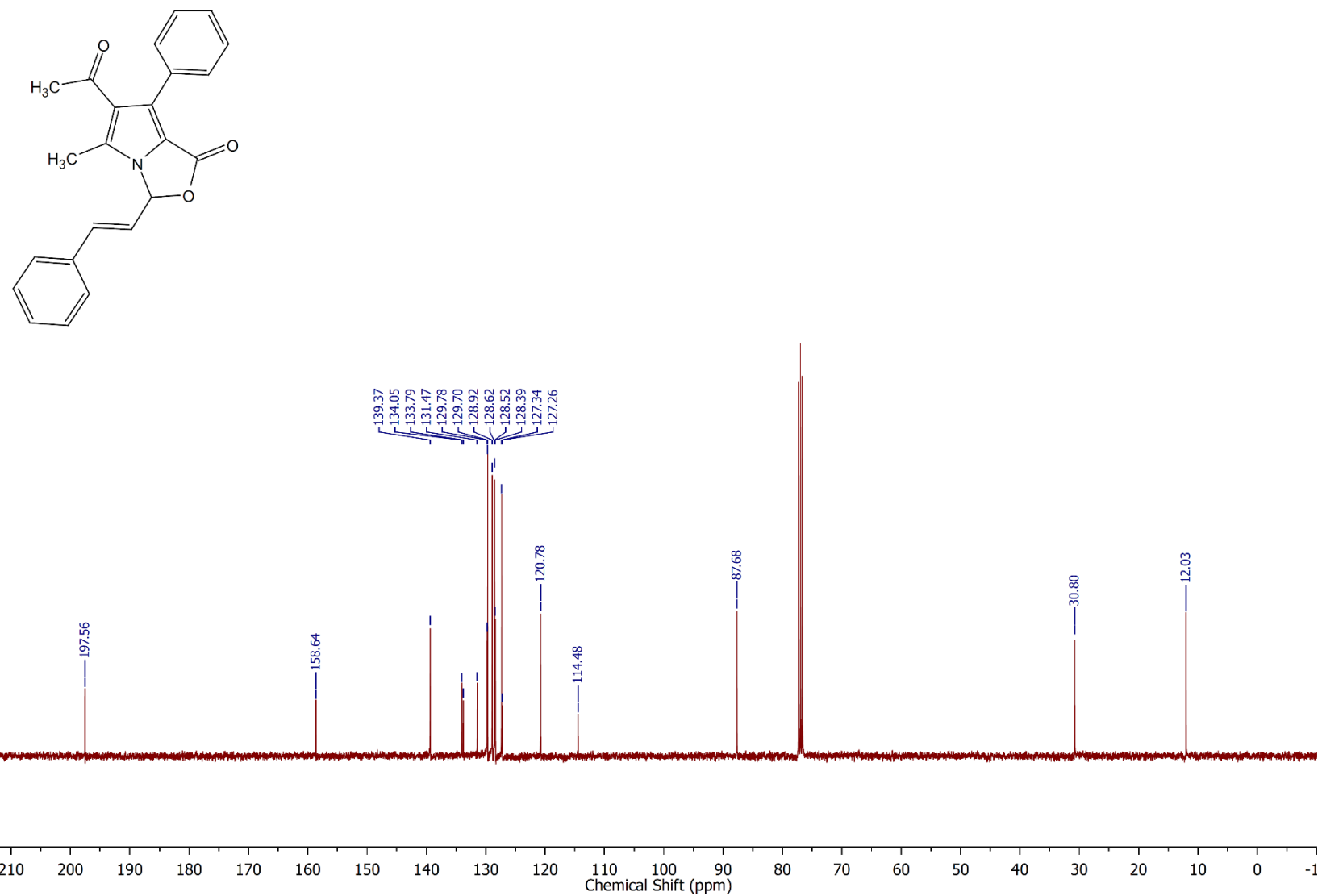
6-Acetyl-3-(4-methoxyphenyl)-5-methyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8f, DEPT, CDCl₃, 100 MHz



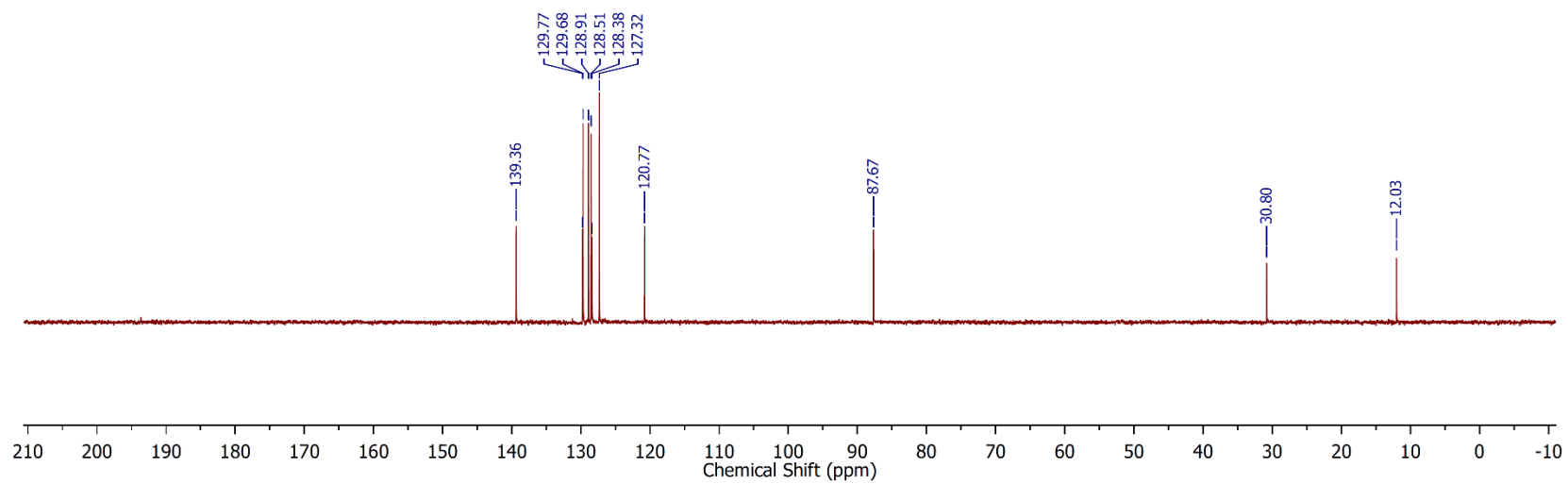
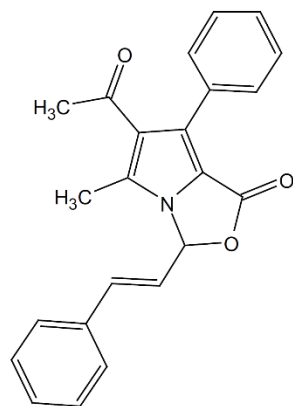
(E)-6-Acetyl-5-methyl-7-phenyl-3-styryl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8g, ¹H NMR, CDCl₃, 400 MHz



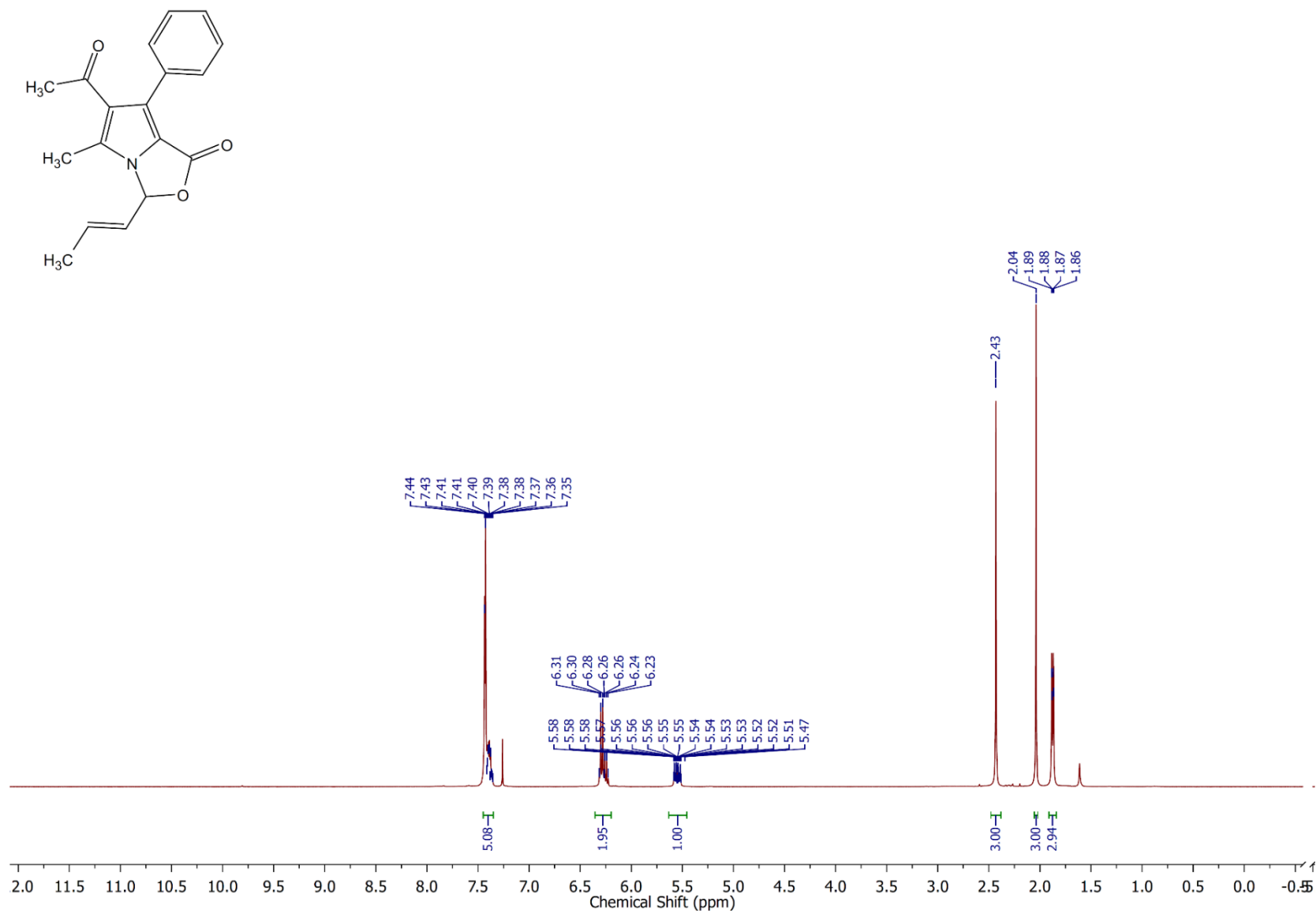
(E)-6-Acetyl-5-methyl-7-phenyl-3-styryl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8g, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



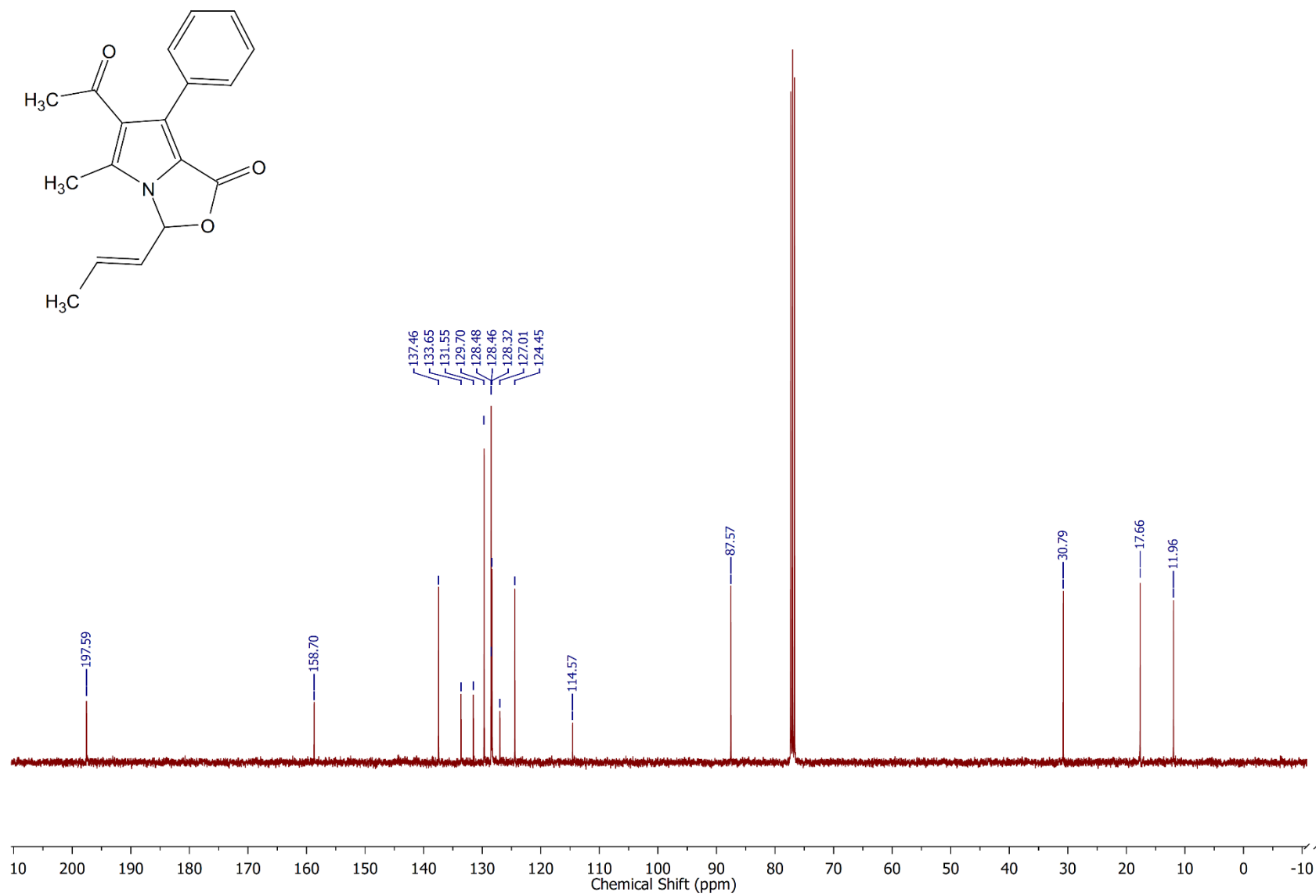
(E)-6-Acetyl-5-methyl-7-phenyl-3-styryl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8g, DEPT, CDCl₃, 100 MHz



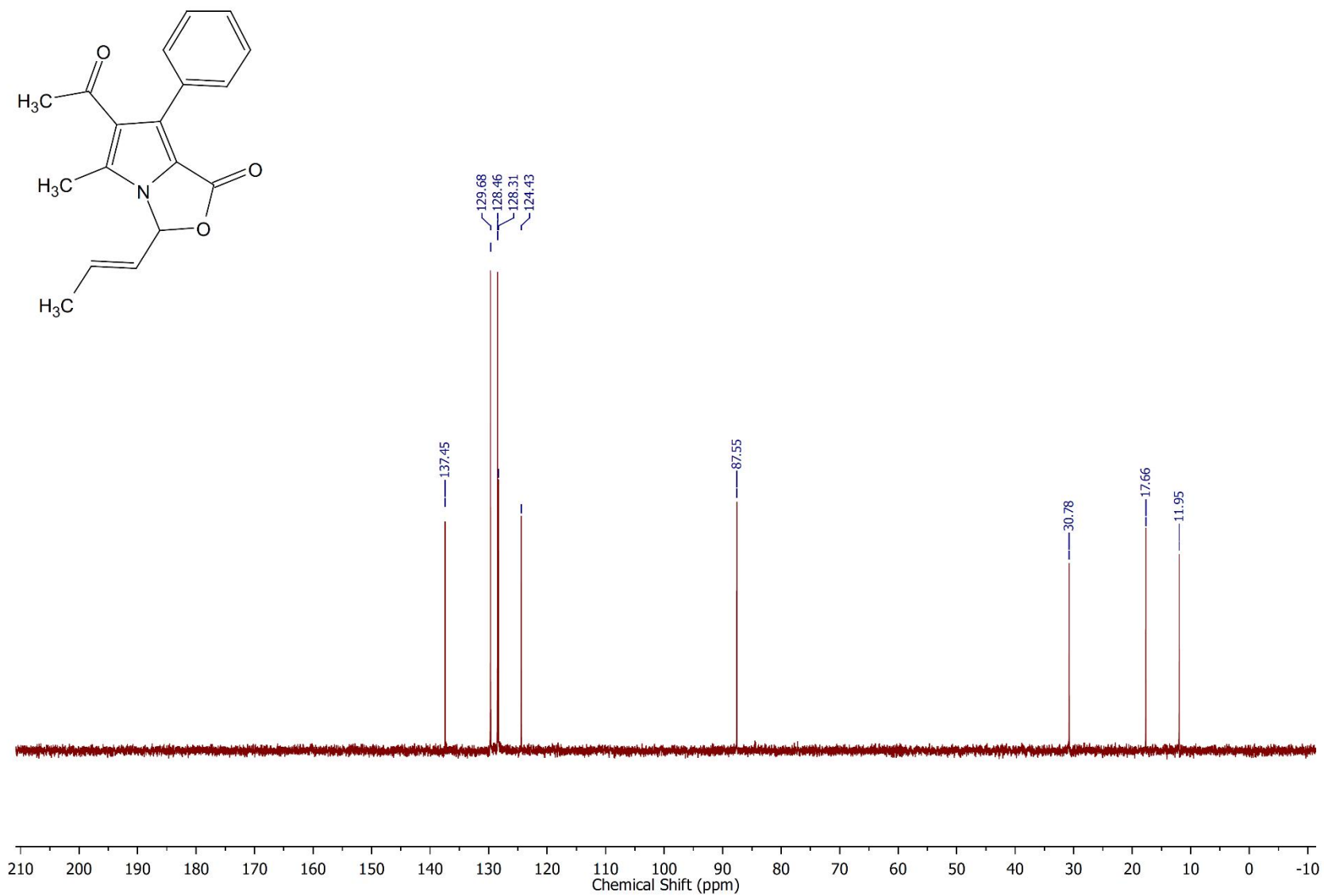
(E)-6-Acetyl-5-methyl-7-phenyl-3-(prop-1-en-1-yl)-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8h, ¹H NMR, CDCl₃, 400 MHz



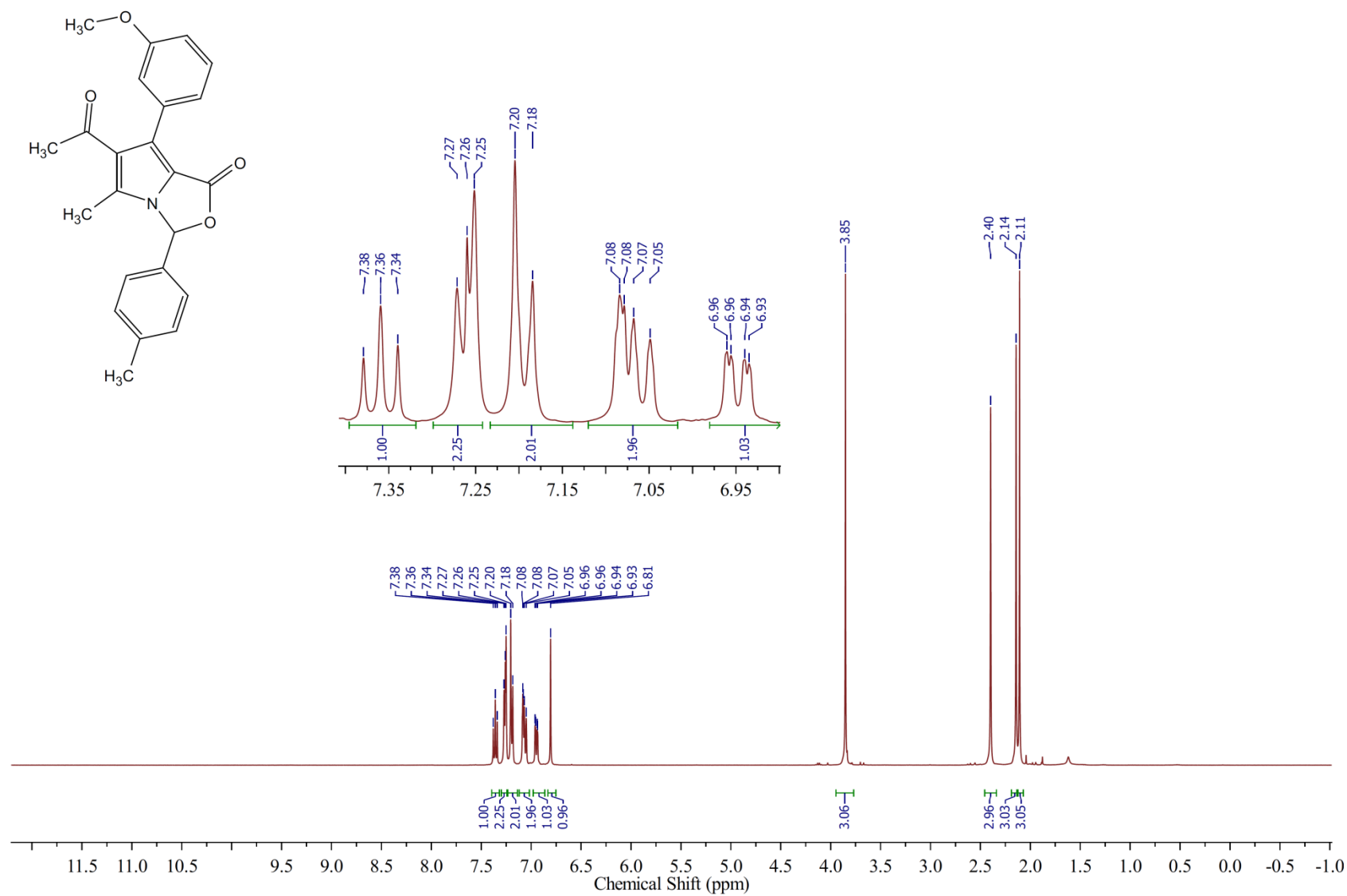
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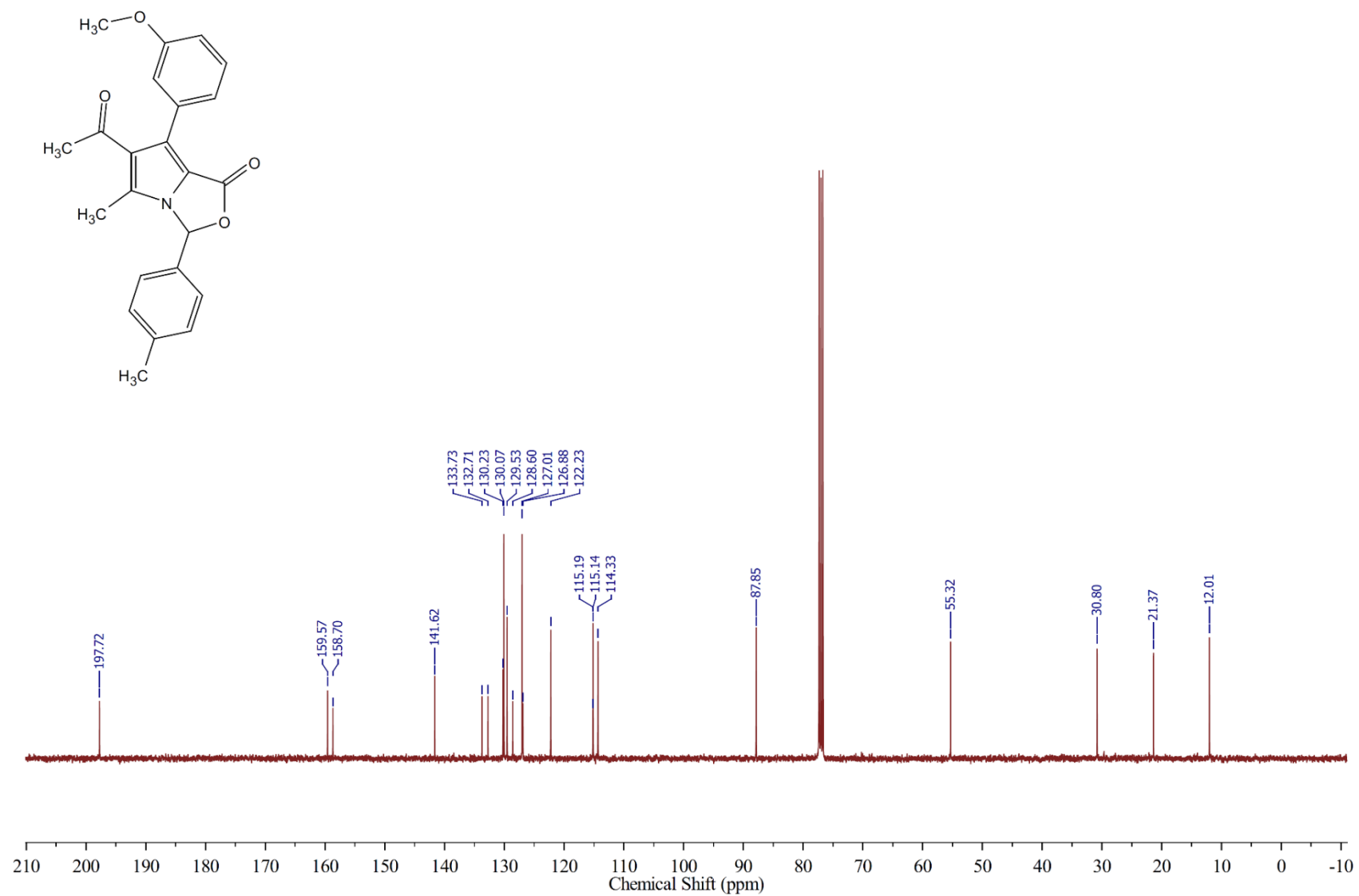
(E)-6-Acetyl-5-methyl-7-phenyl-3-(prop-1-en-1-yl)-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8h, DEPT, CDCl₃, 100 MHz



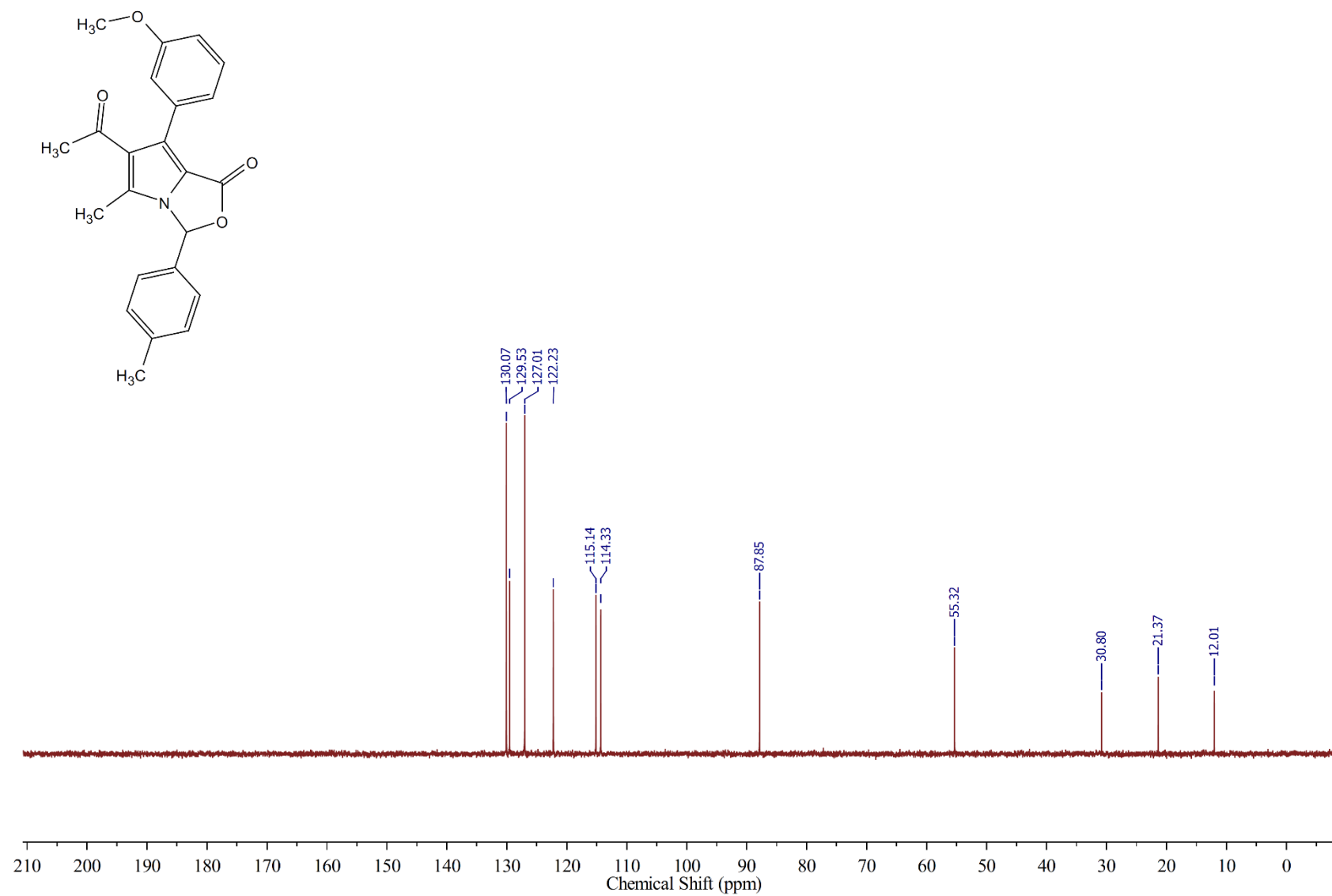
6-Acetyl-7-(3-methoxyphenyl)-5-methyl-3-(*p*-tolyl)pyrrolo[1,2-*c*]oxazol-1(3*H*)-one 8i, ^1H NMR, CDCl_3 , 400 MHz



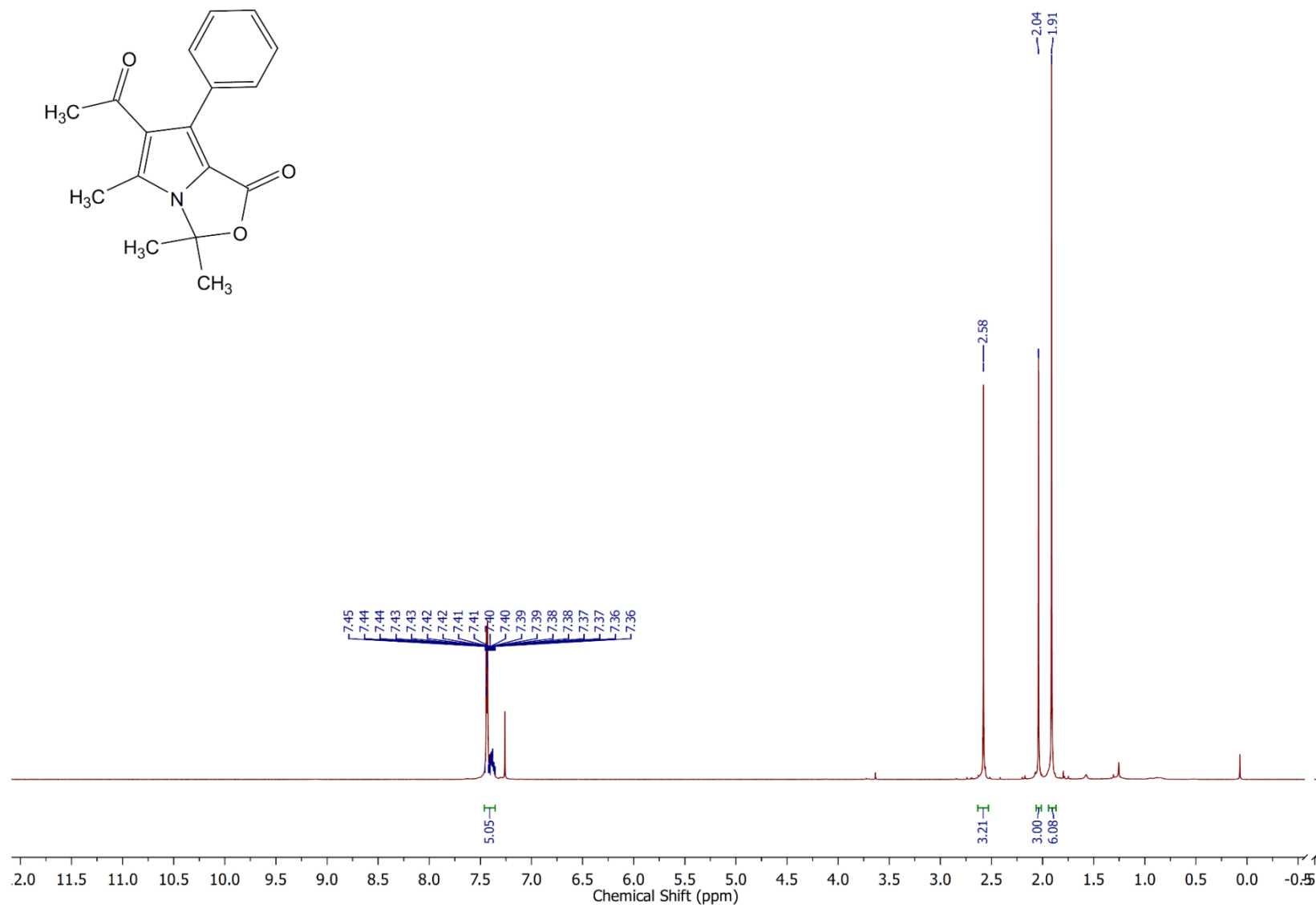
6-Acetyl-7-(3-methoxyphenyl)-5-methyl-3-(*p*-tolyl)pyrrolo[1,2-*c*]oxazol-1(3*H*)-one 8i, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



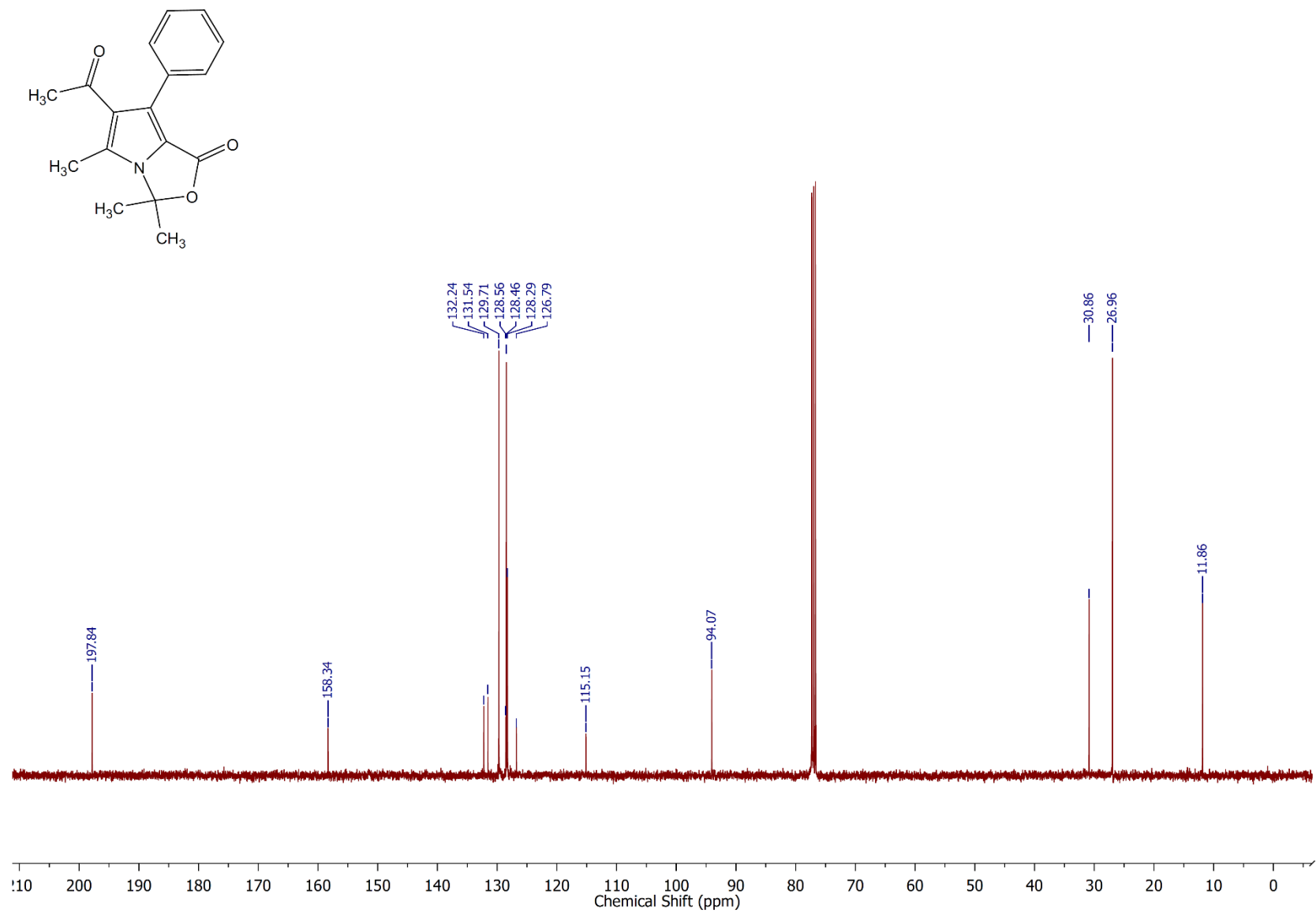
6-Acetyl-7-(3-methoxyphenyl)-5-methyl-3-(*p*-tolyl)pyrrolo[1,2-*c*]oxazol-1(3*H*)-one 8i, DEPT, CDCl₃, 100 MHz



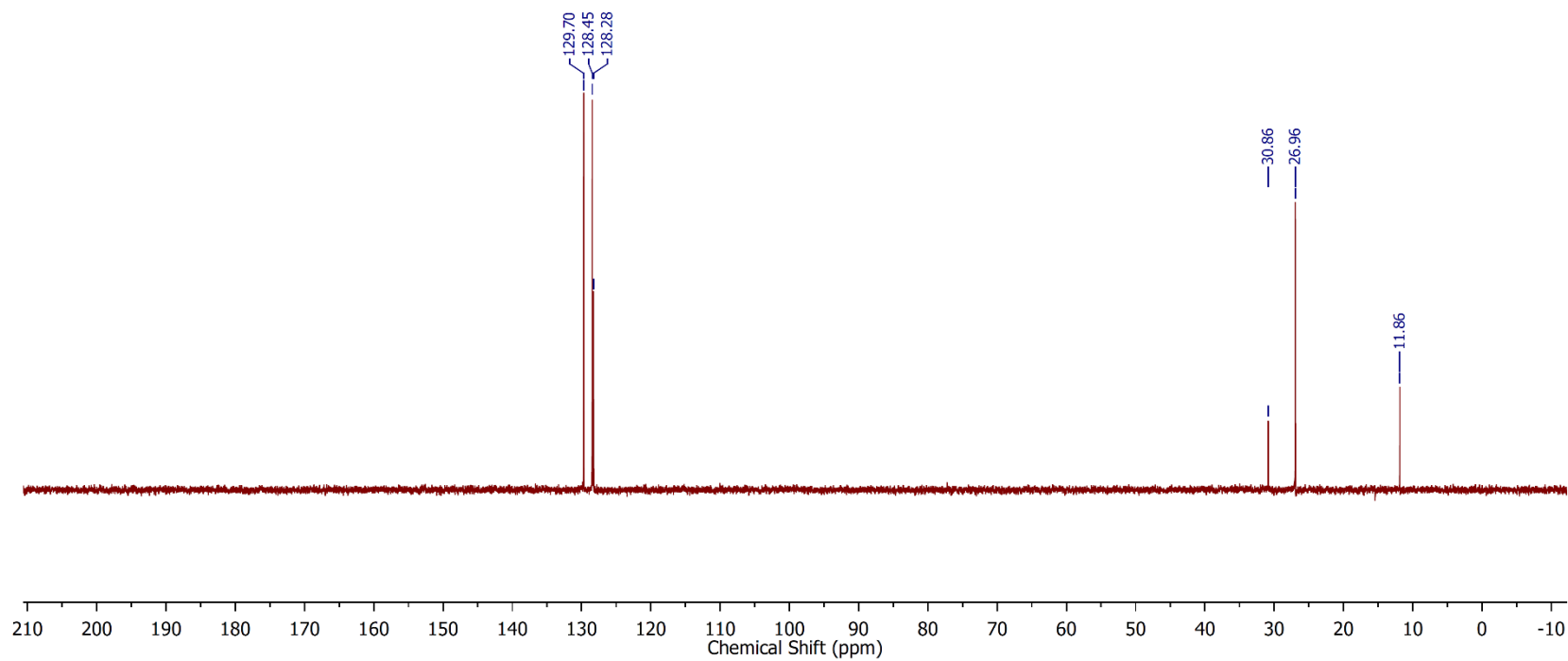
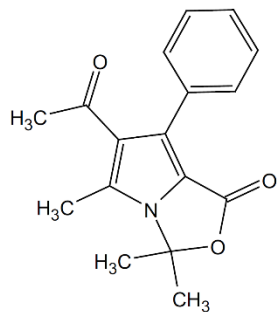
6-Acetyl-3,3,5-trimethyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8j, ¹H NMR, CDCl₃, 400 MHz



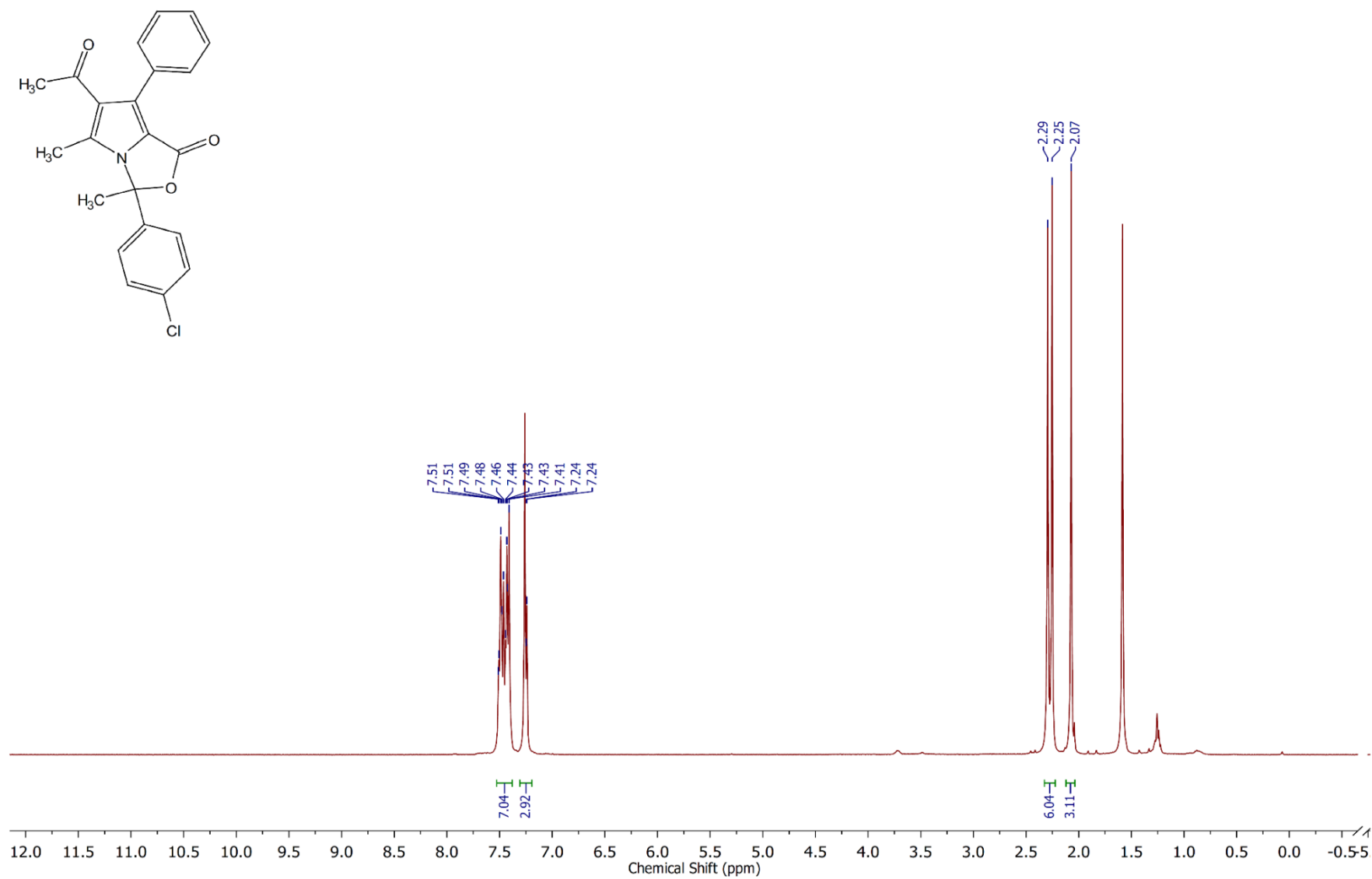
6-Acetyl-3,3,5-trimethyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8j, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



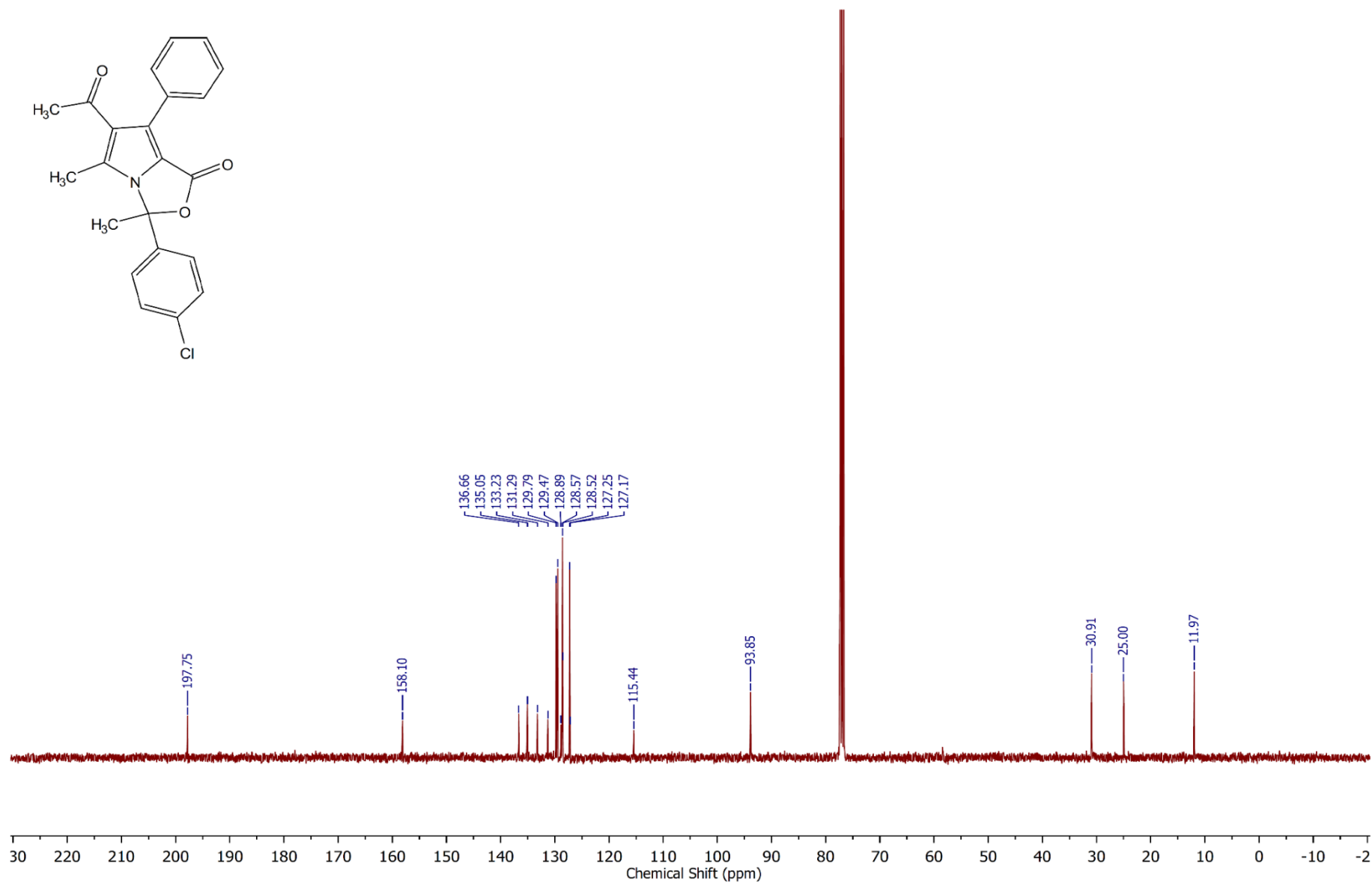
6-Acetyl-3,3,5-trimethyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8j, DEPT, CDCl₃, 100 MHz



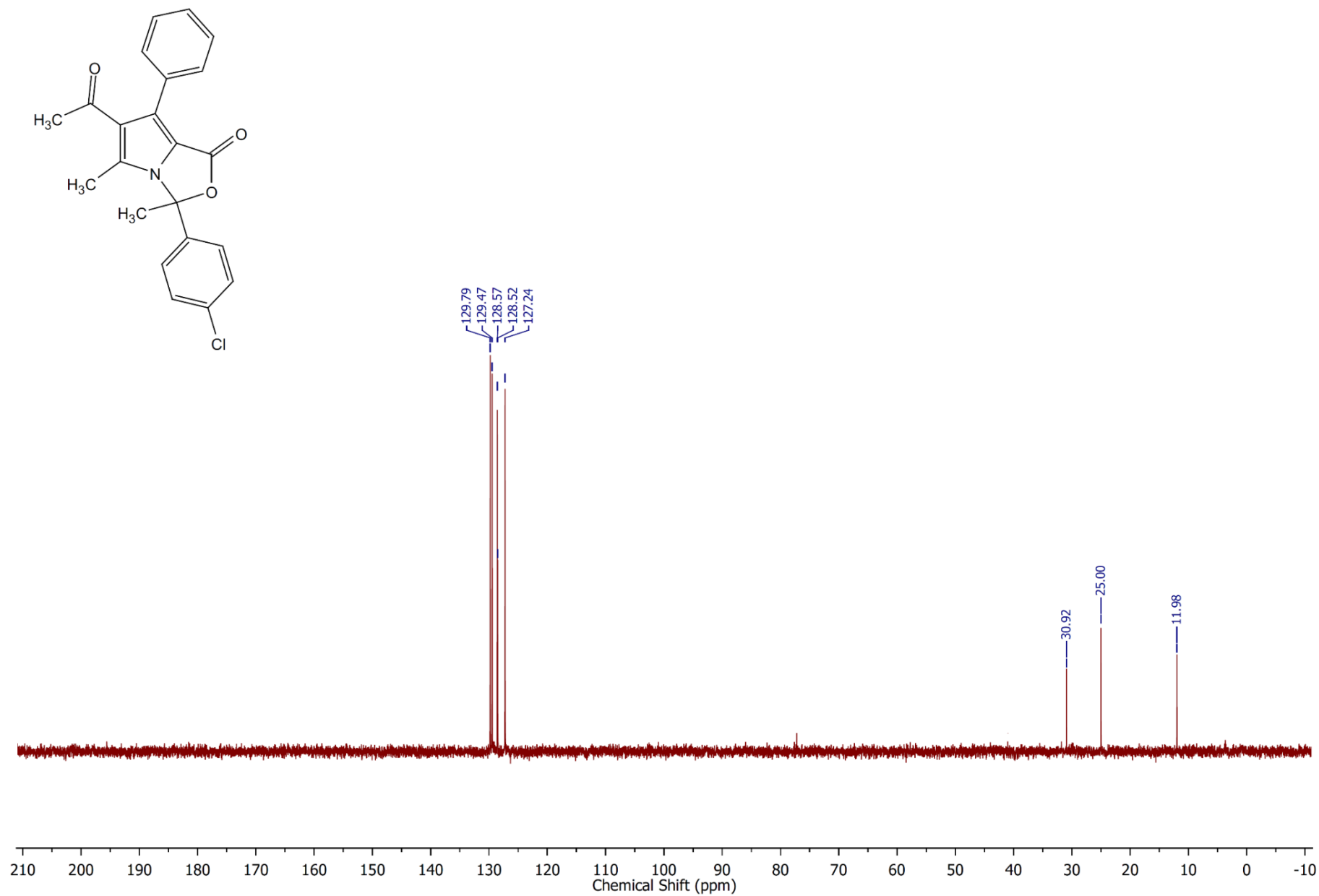
6-Acetyl-3-(4-chlorophenyl)-3,5-dimethyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8k, ¹H NMR, CDCl₃, 400 MHz



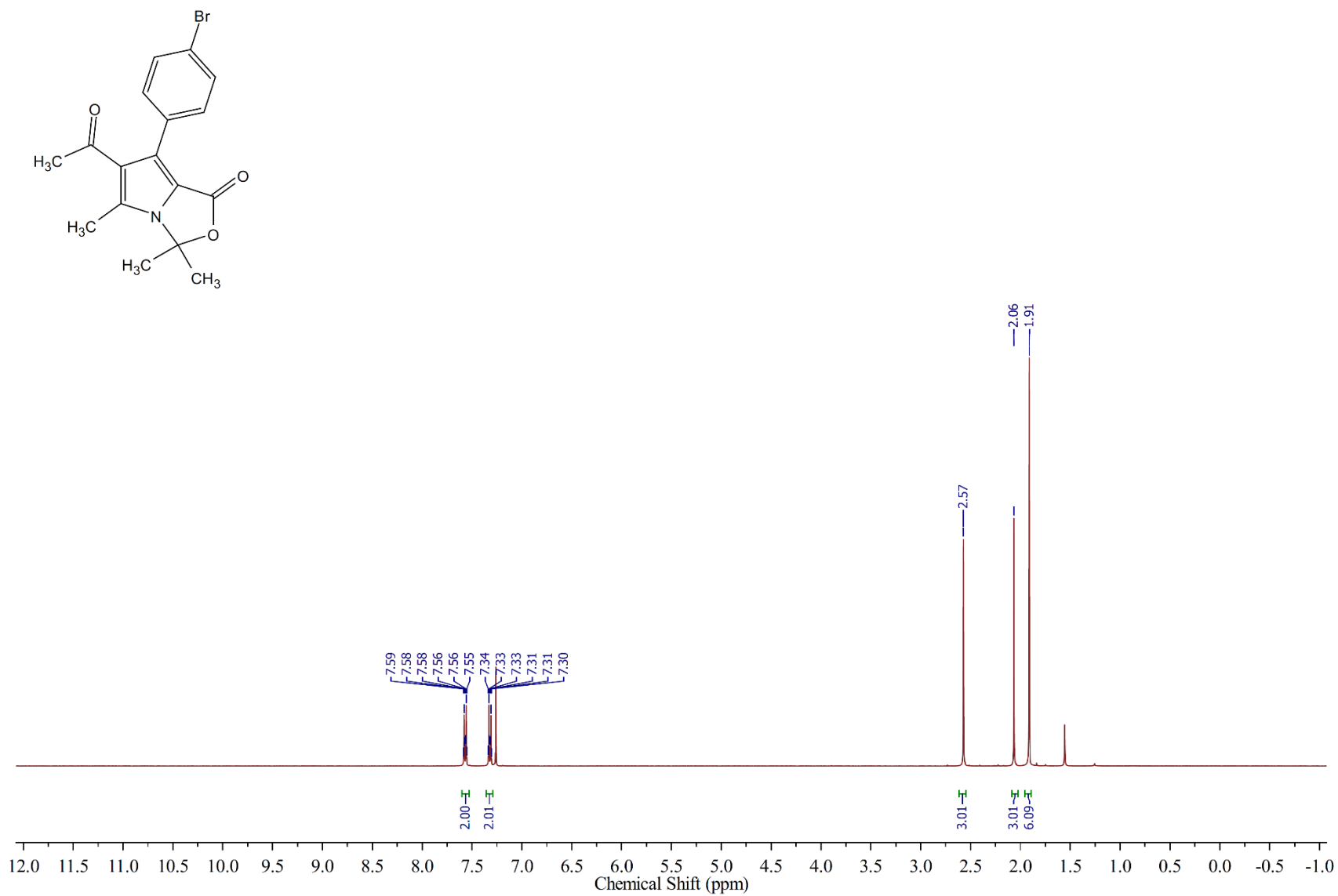
6-Acetyl-3-(4-chlorophenyl)-3,5-dimethyl-7-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]oxazol-1-one 8k, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



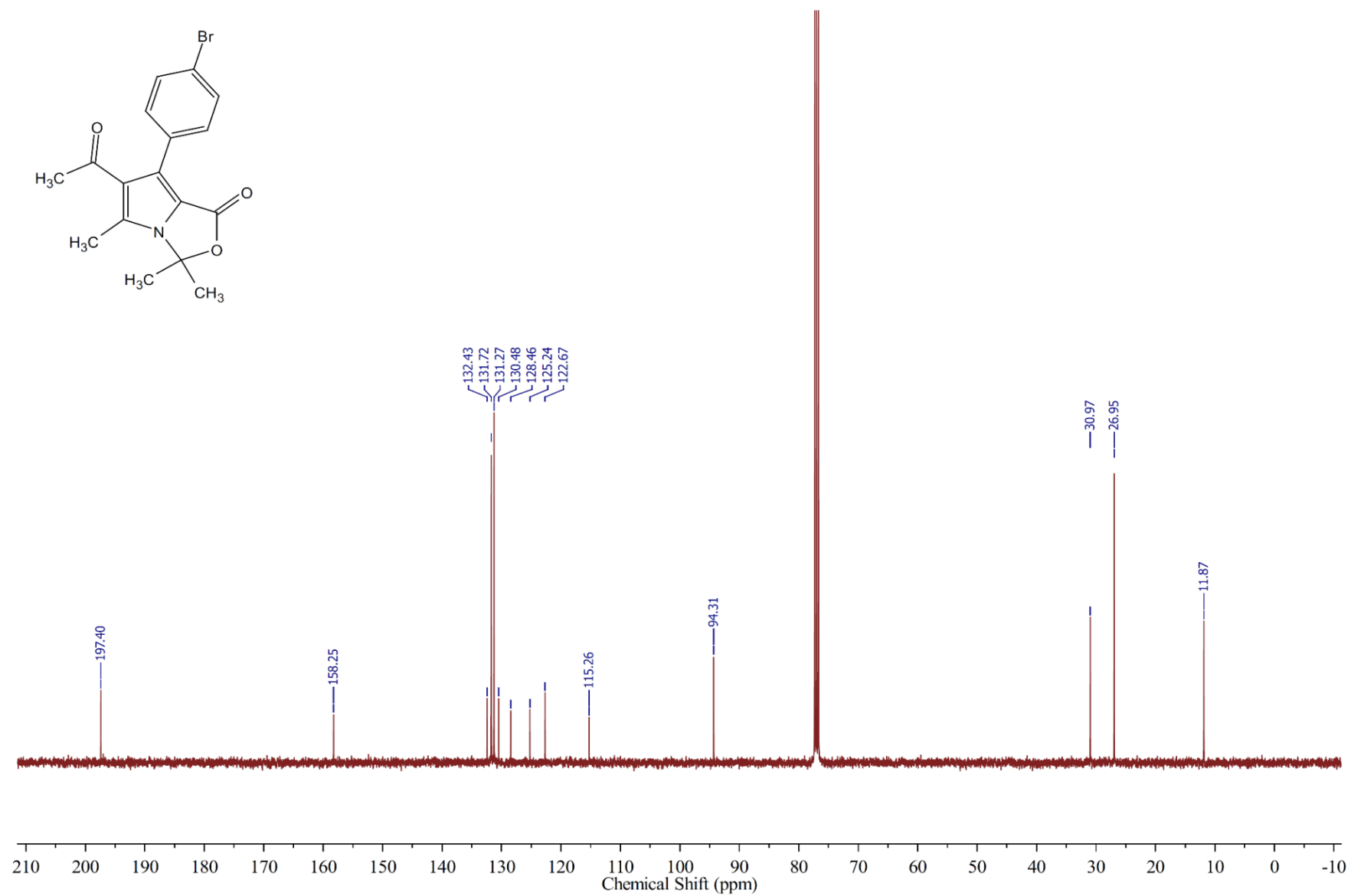
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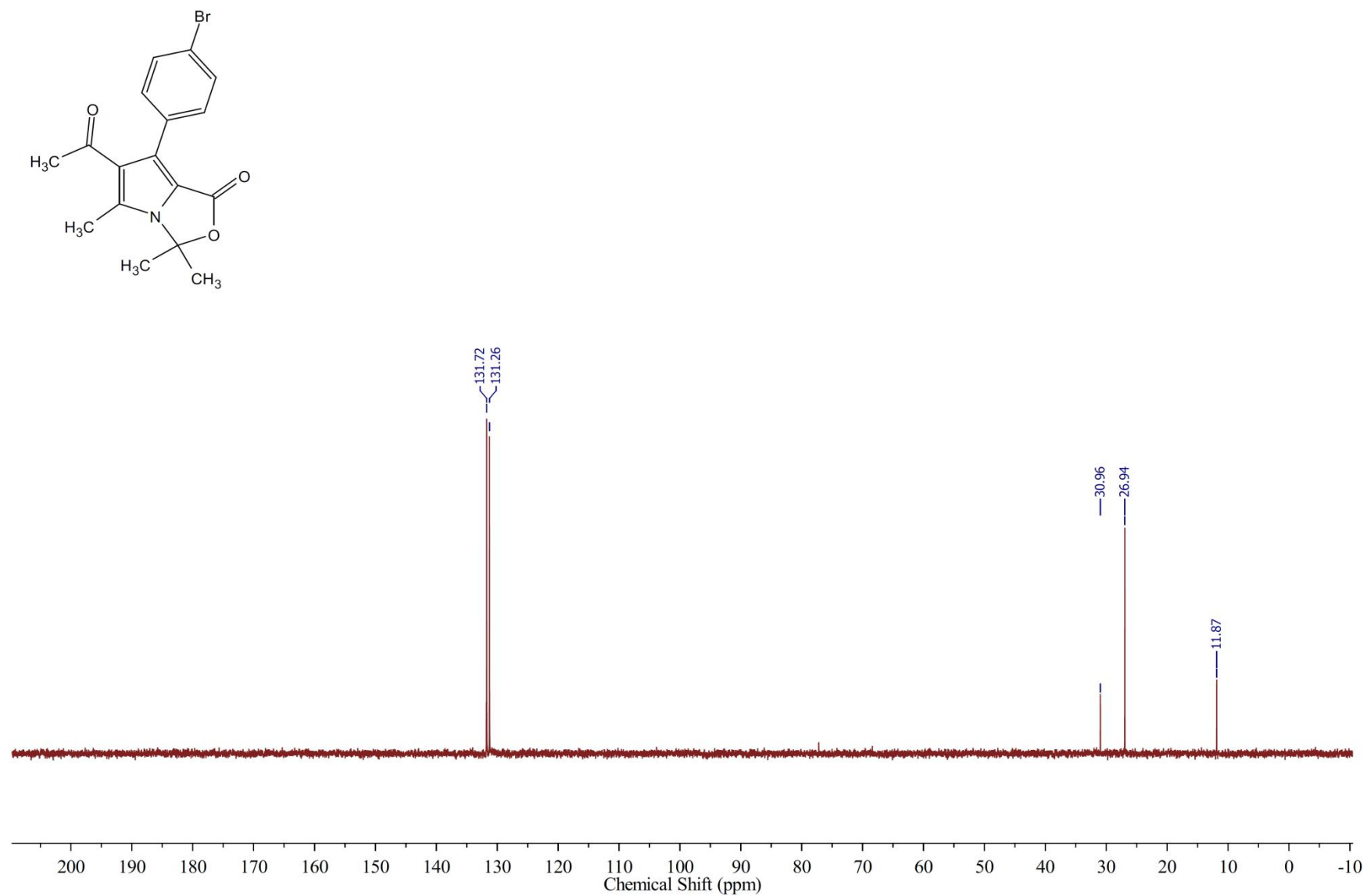
6-Acetyl-7-(4-bromophenyl)-3,3,5-trimethylpyrrolo[1,2-*c*]oxazol-1(3*H*)-one 8l, ^1H NMR, CDCl_3 , 400 MHz



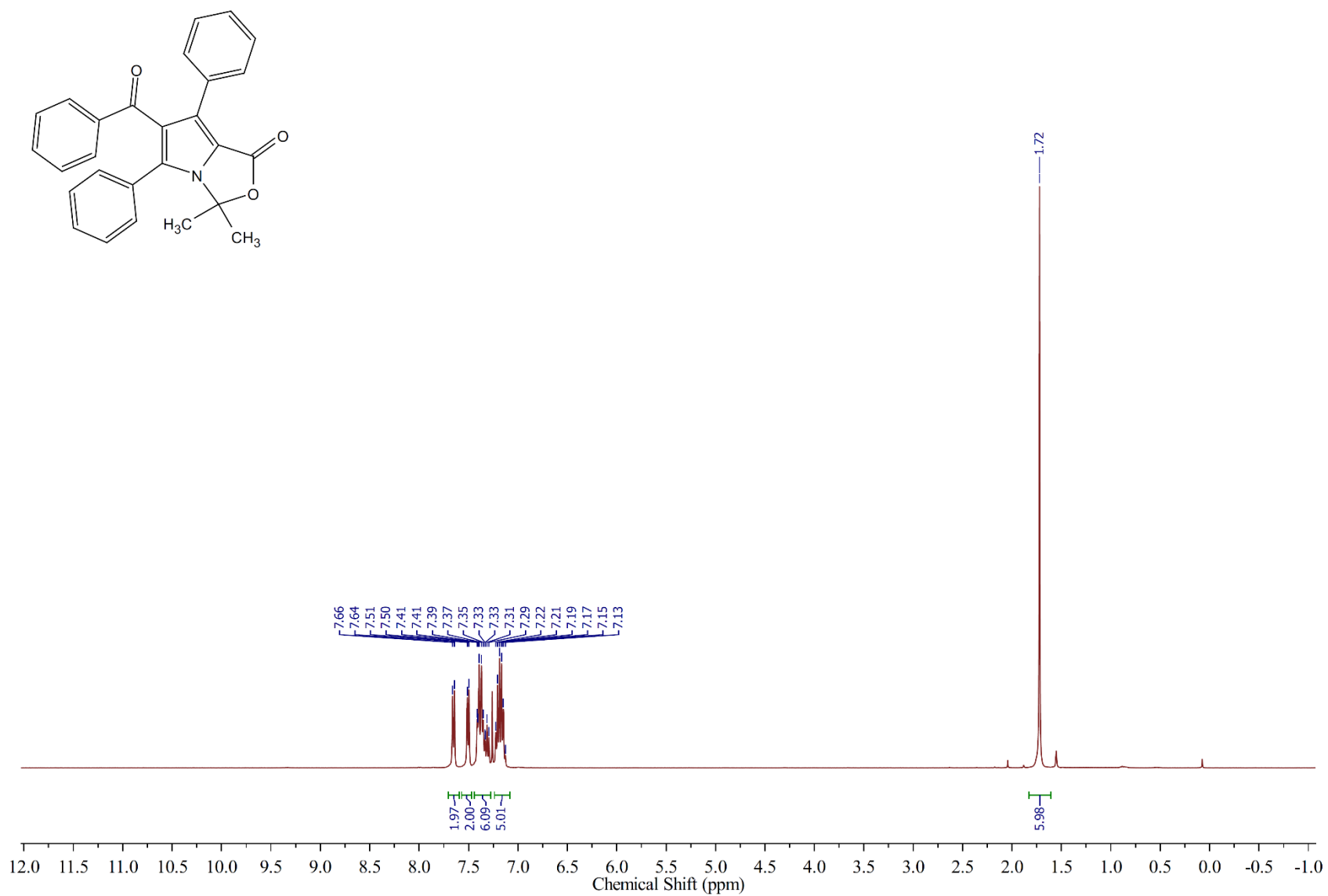
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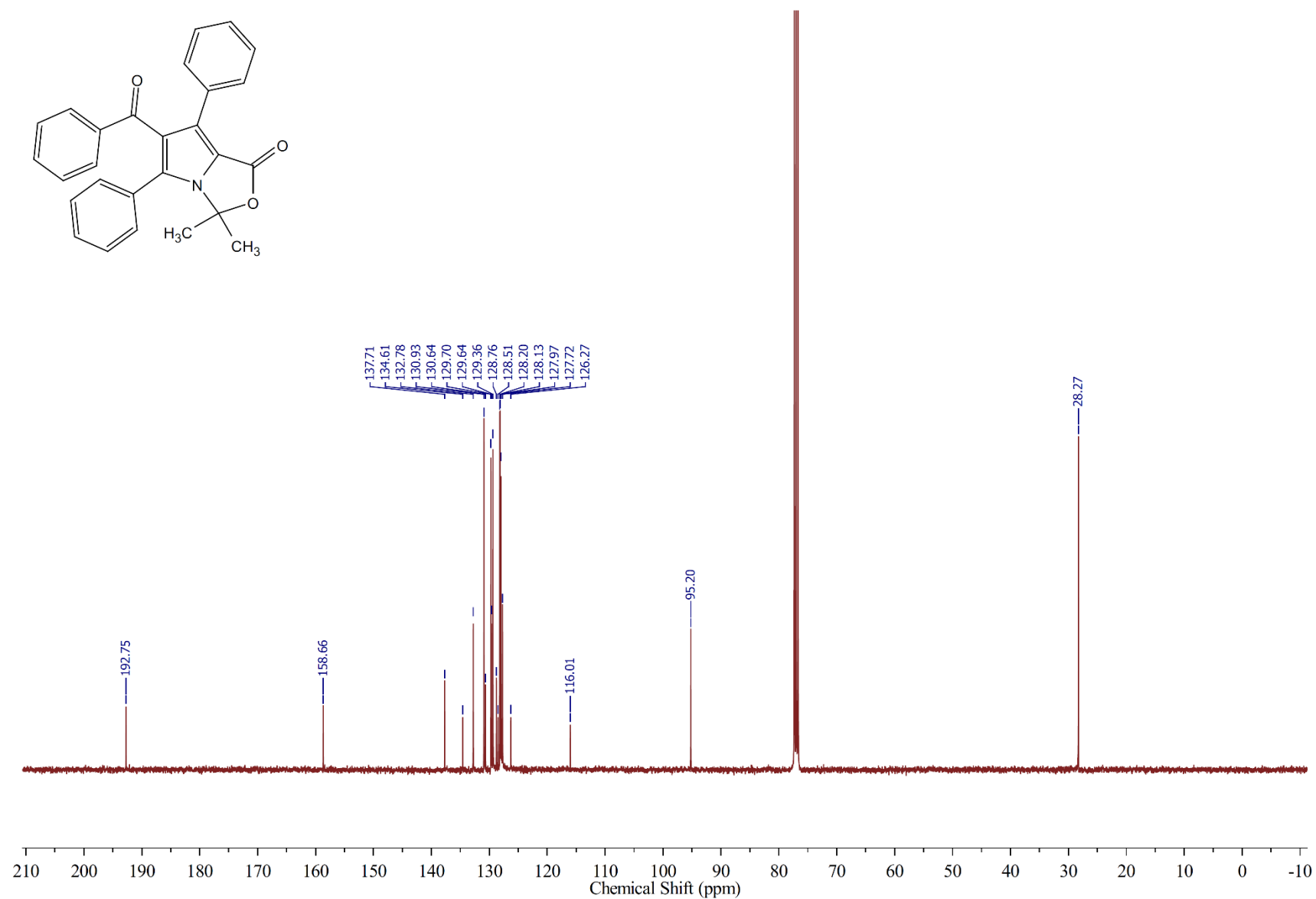
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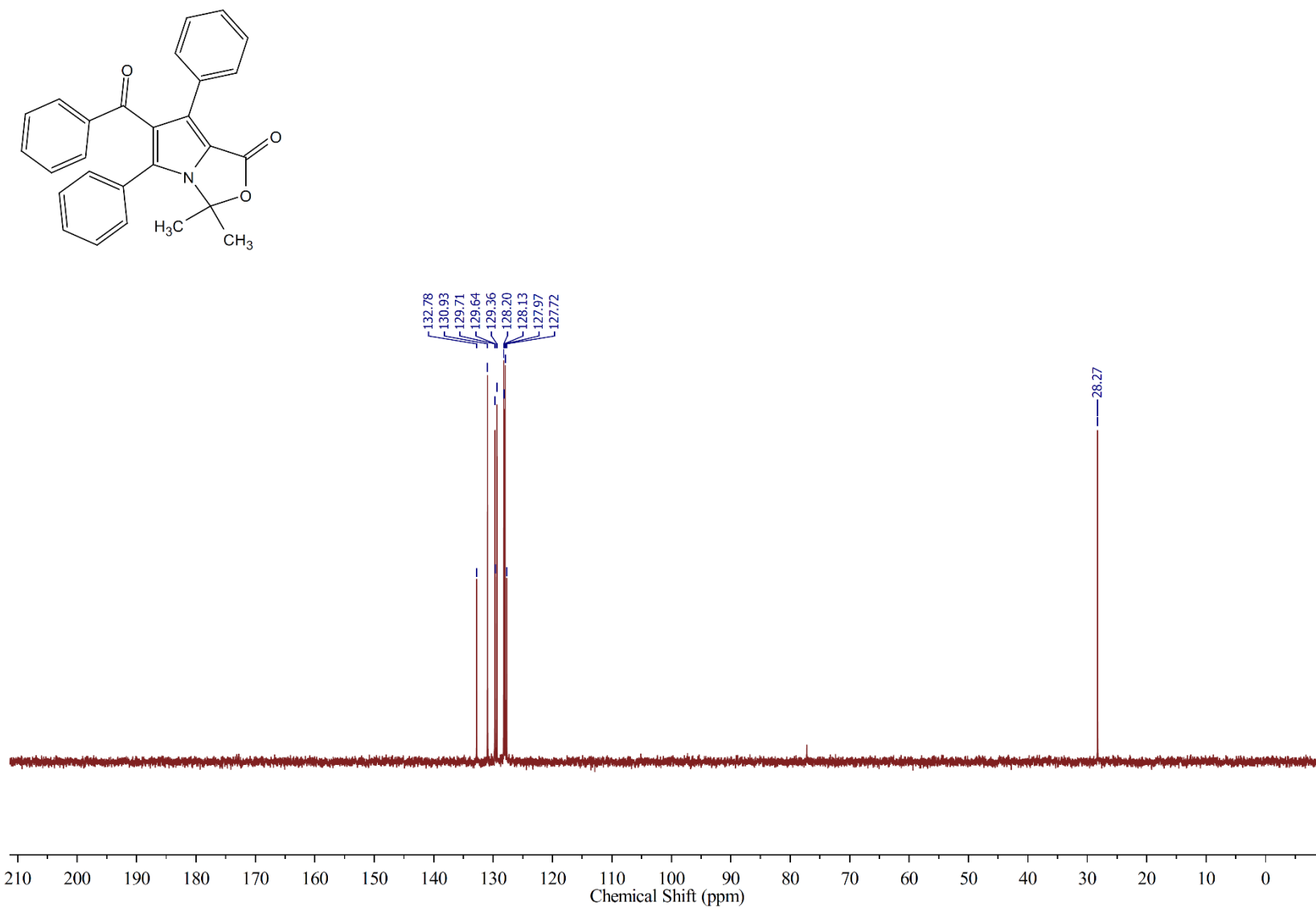
6-Benzoyl-3,3-dimethyl-5,7-diphenylpyrrolo[1,2-*c*]oxazol-1(3*H*)-one 8m, ^1H NMR, CDCl_3 , 400 MHz



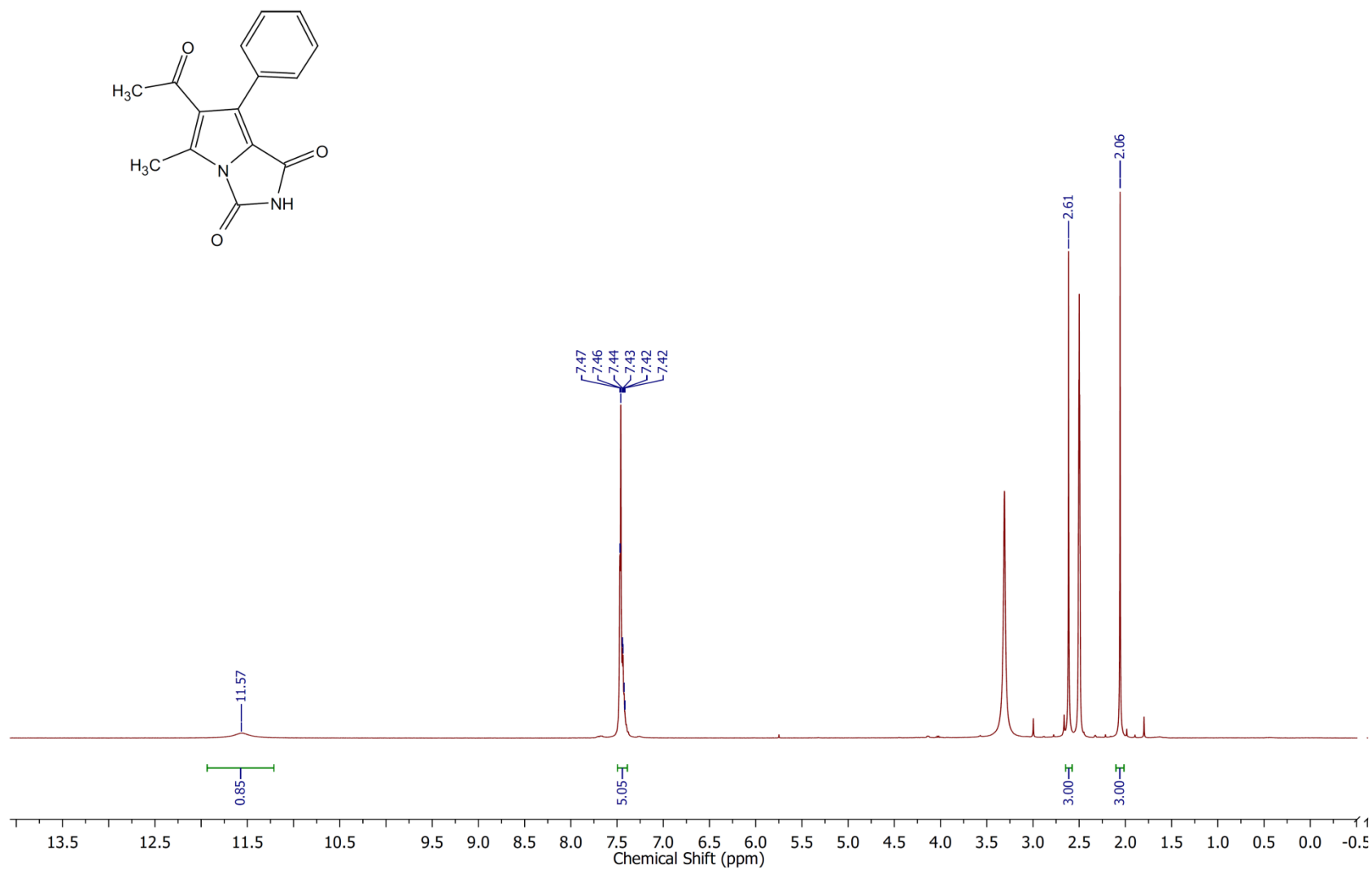
6-Benzoyl-3,3-dimethyl-5,7-diphenylpyrrolo[1,2-*c*]oxazol-1(3*H*)-one 8m, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



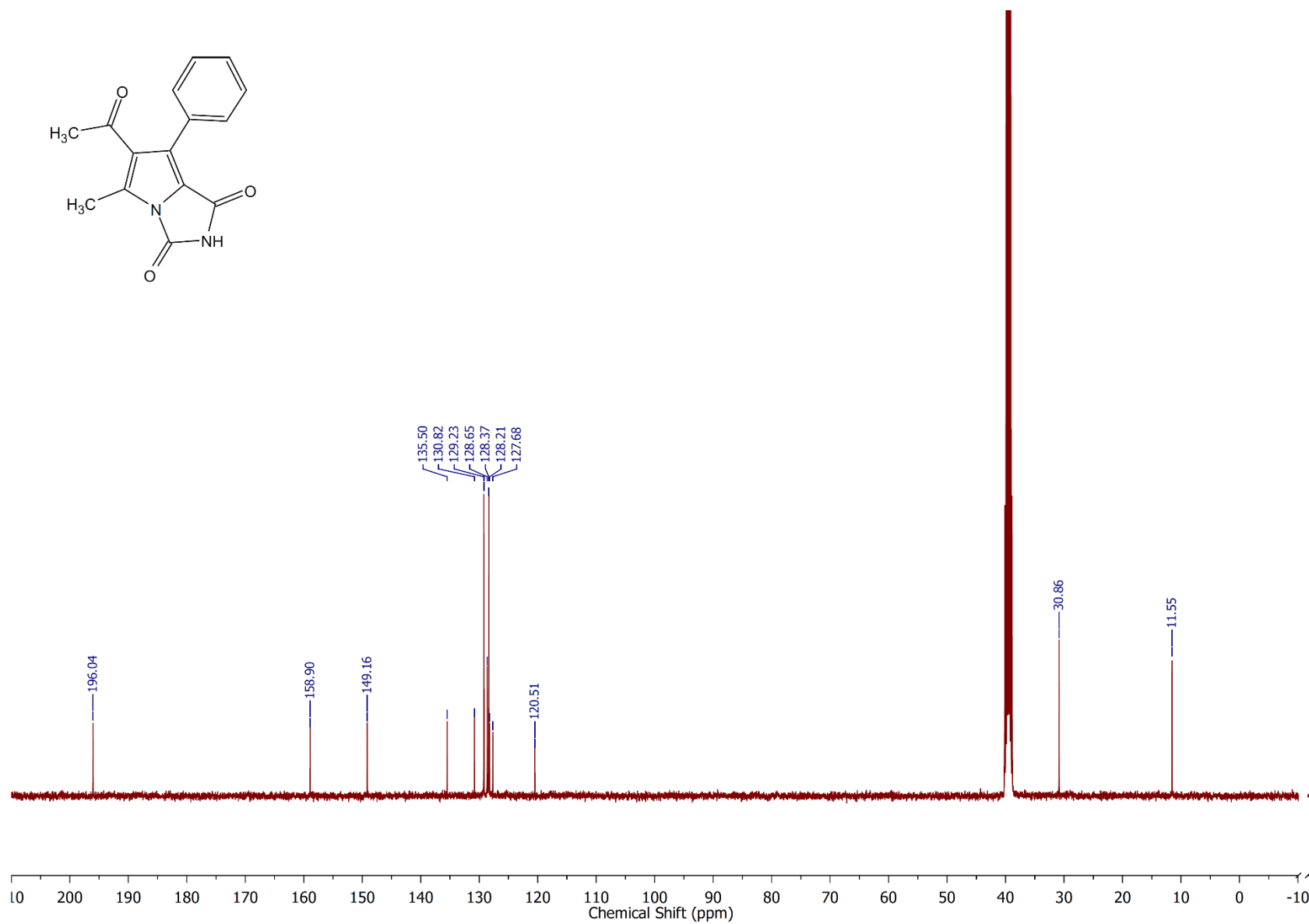
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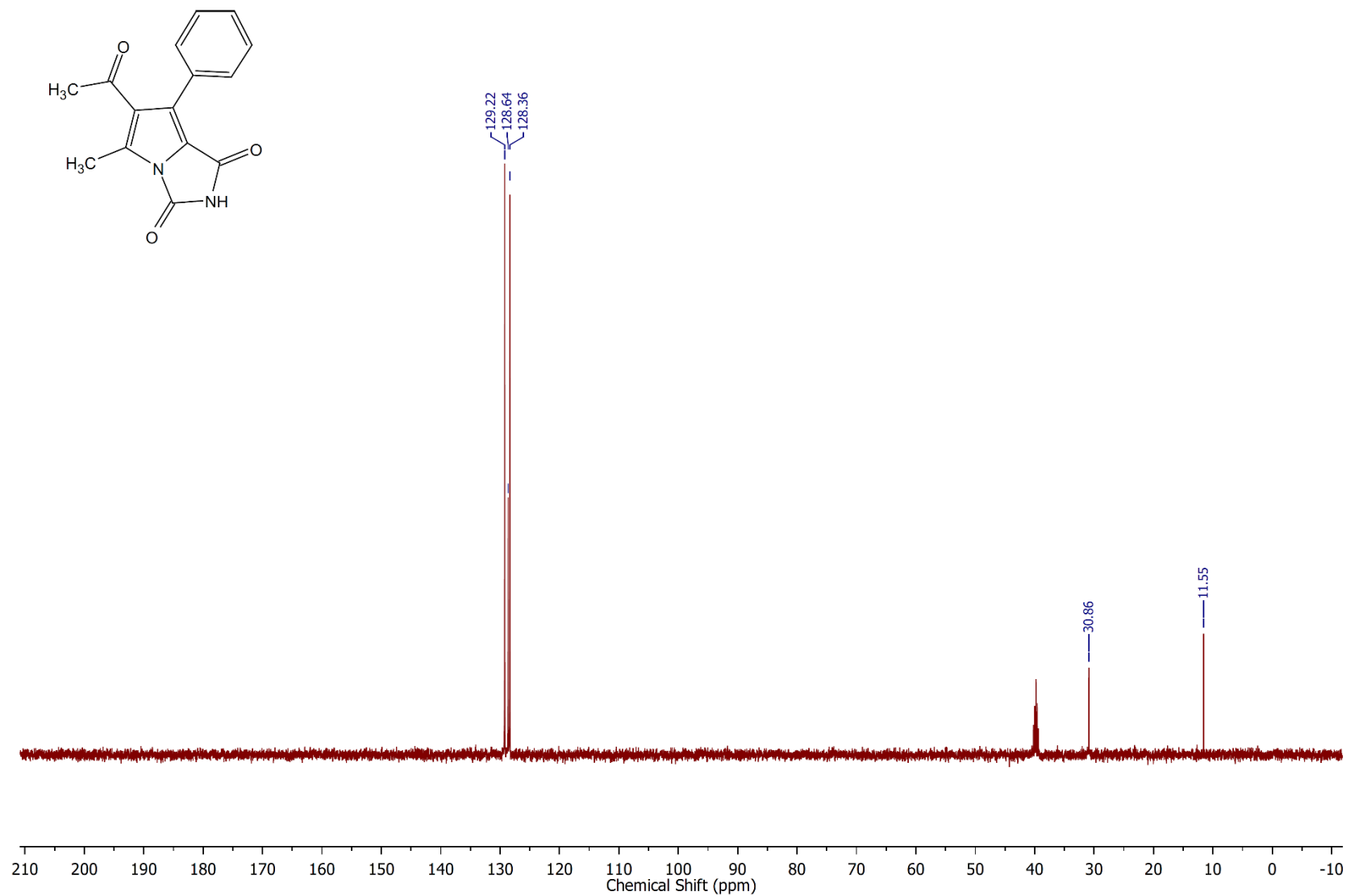
6-Acetyl-5-methyl-7-phenyl-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 10a, ¹H NMR, DMSO-*d*₆, 400 MHz



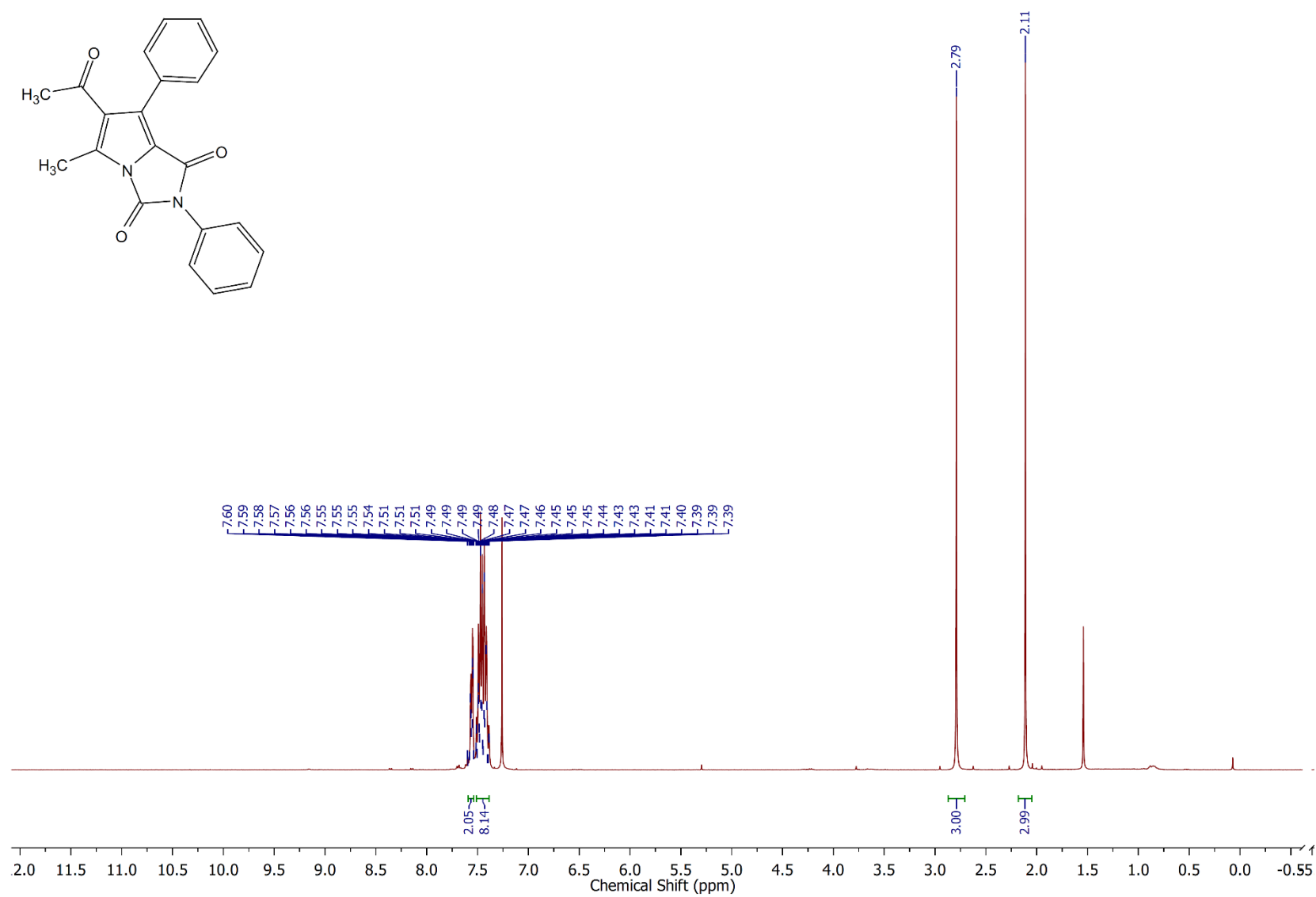
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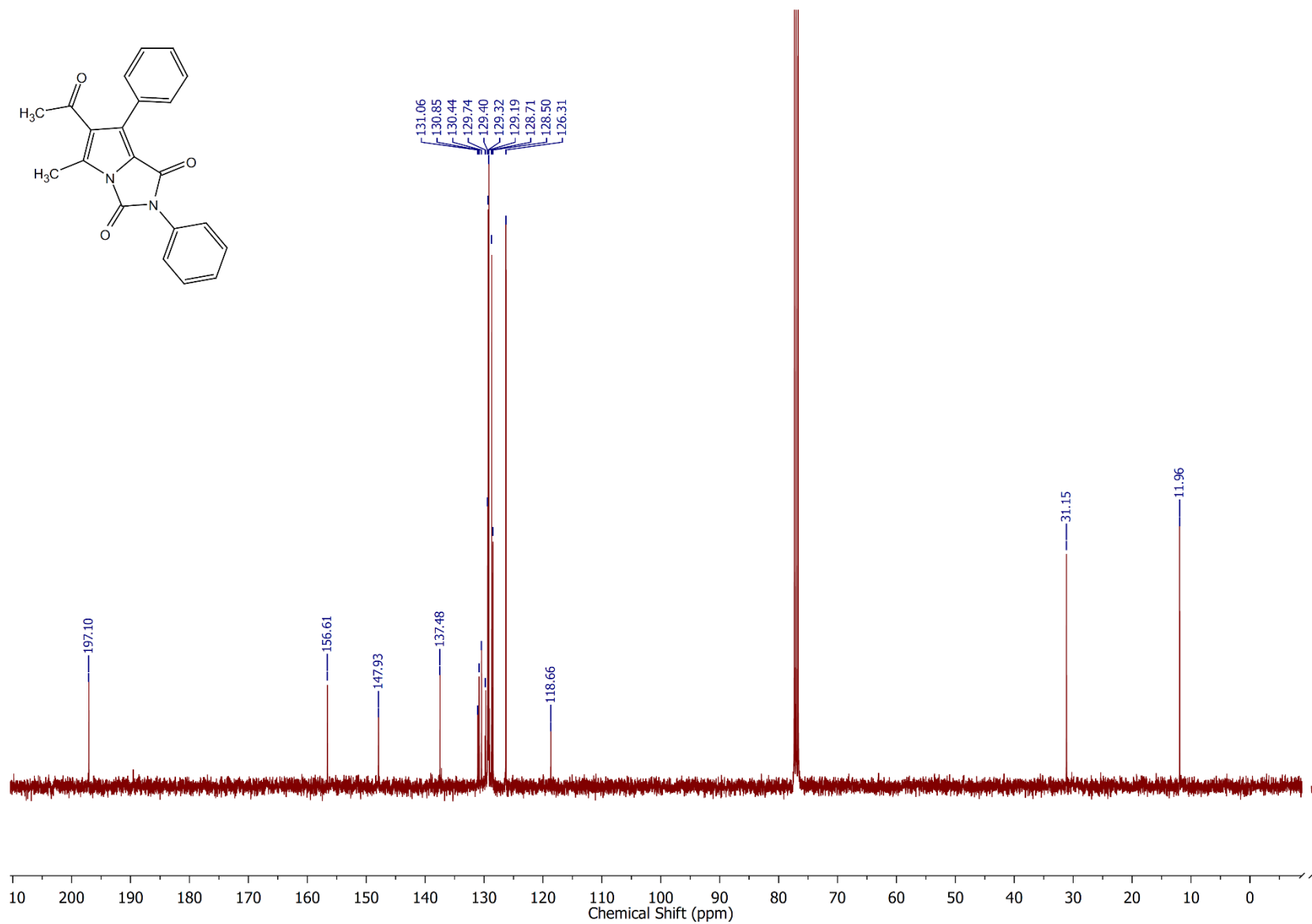
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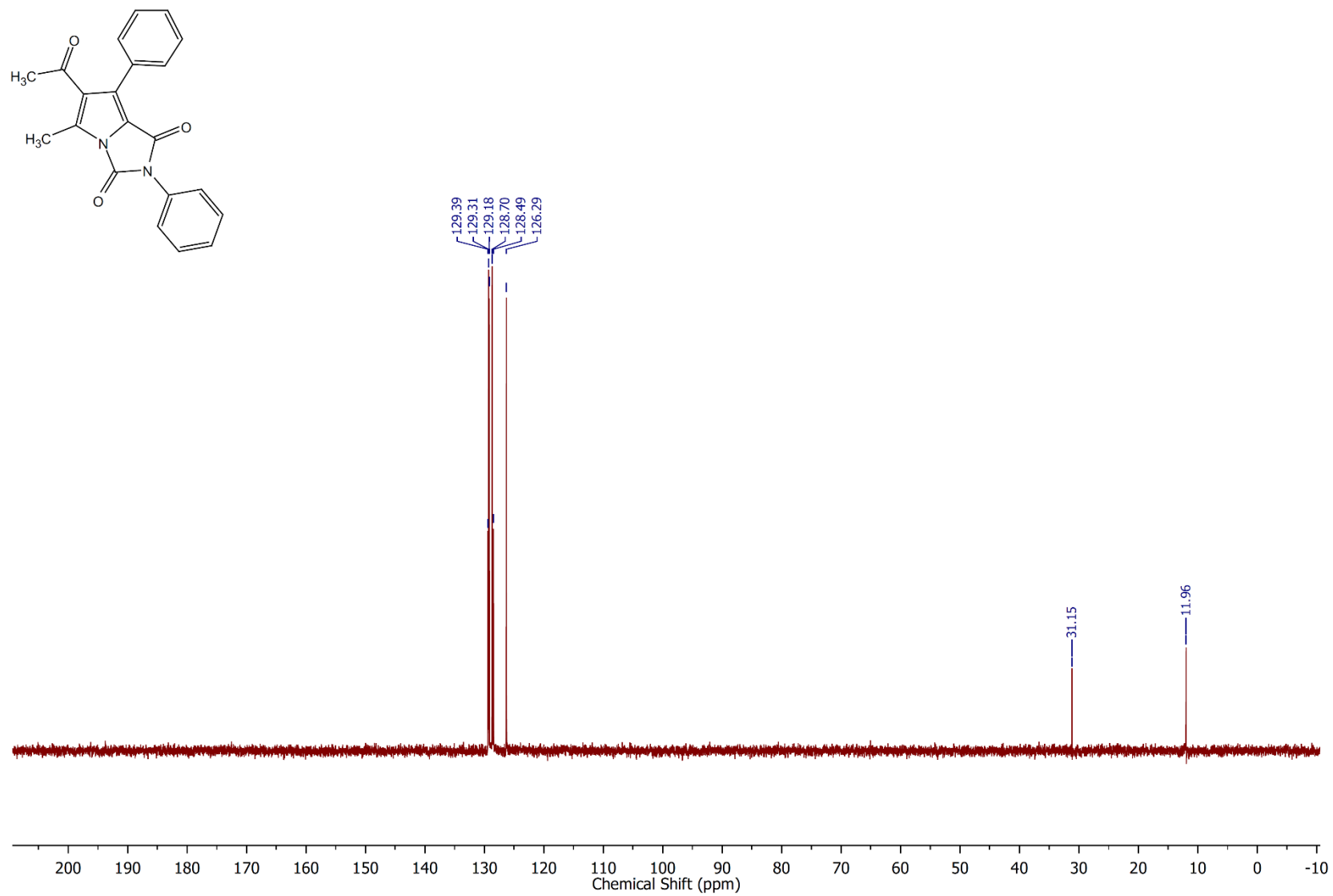
6-Acetyl-5-methyl-2,7-diphenyl-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 10b, ¹H NMR, CDCl₃, 400 MHz



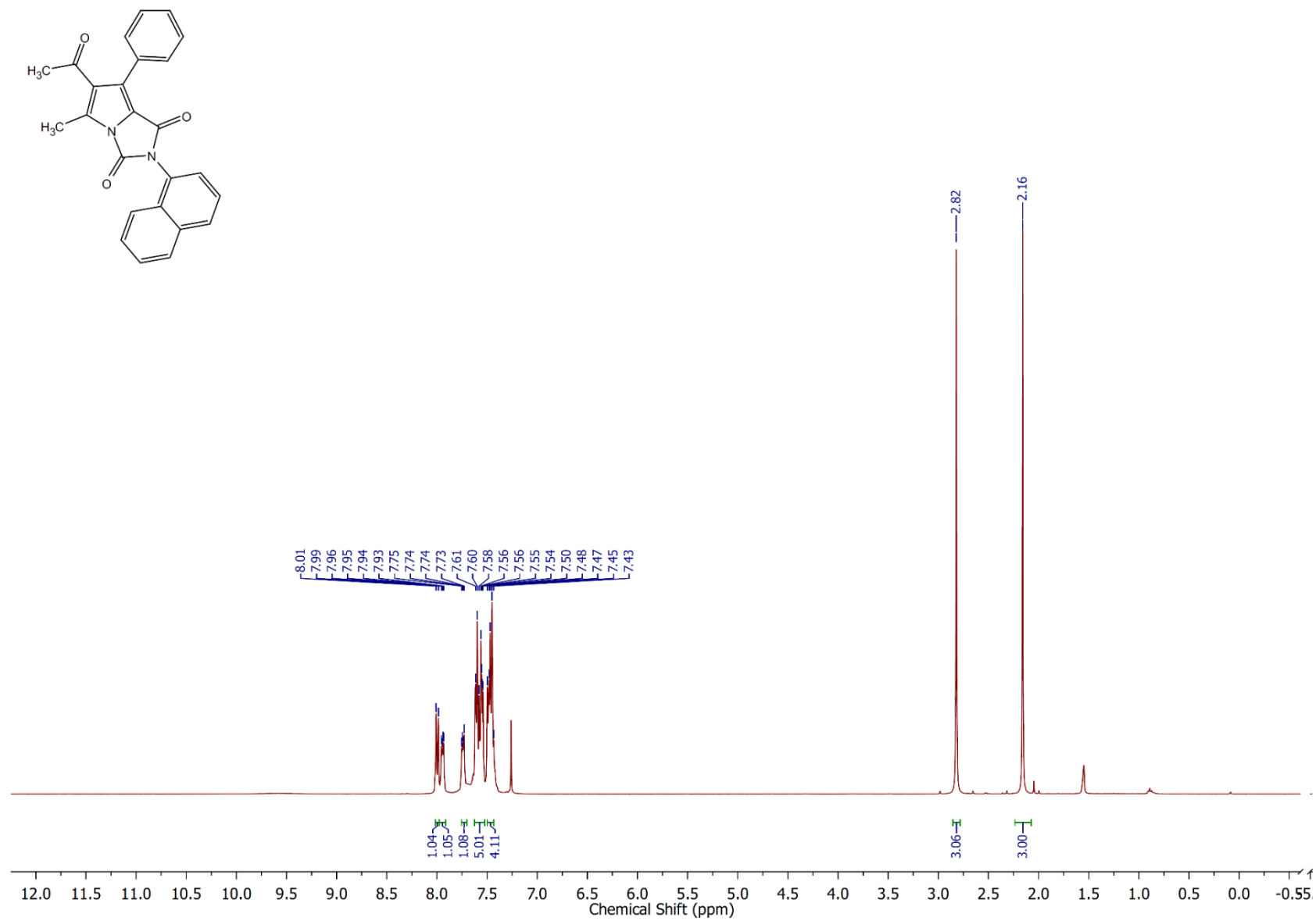
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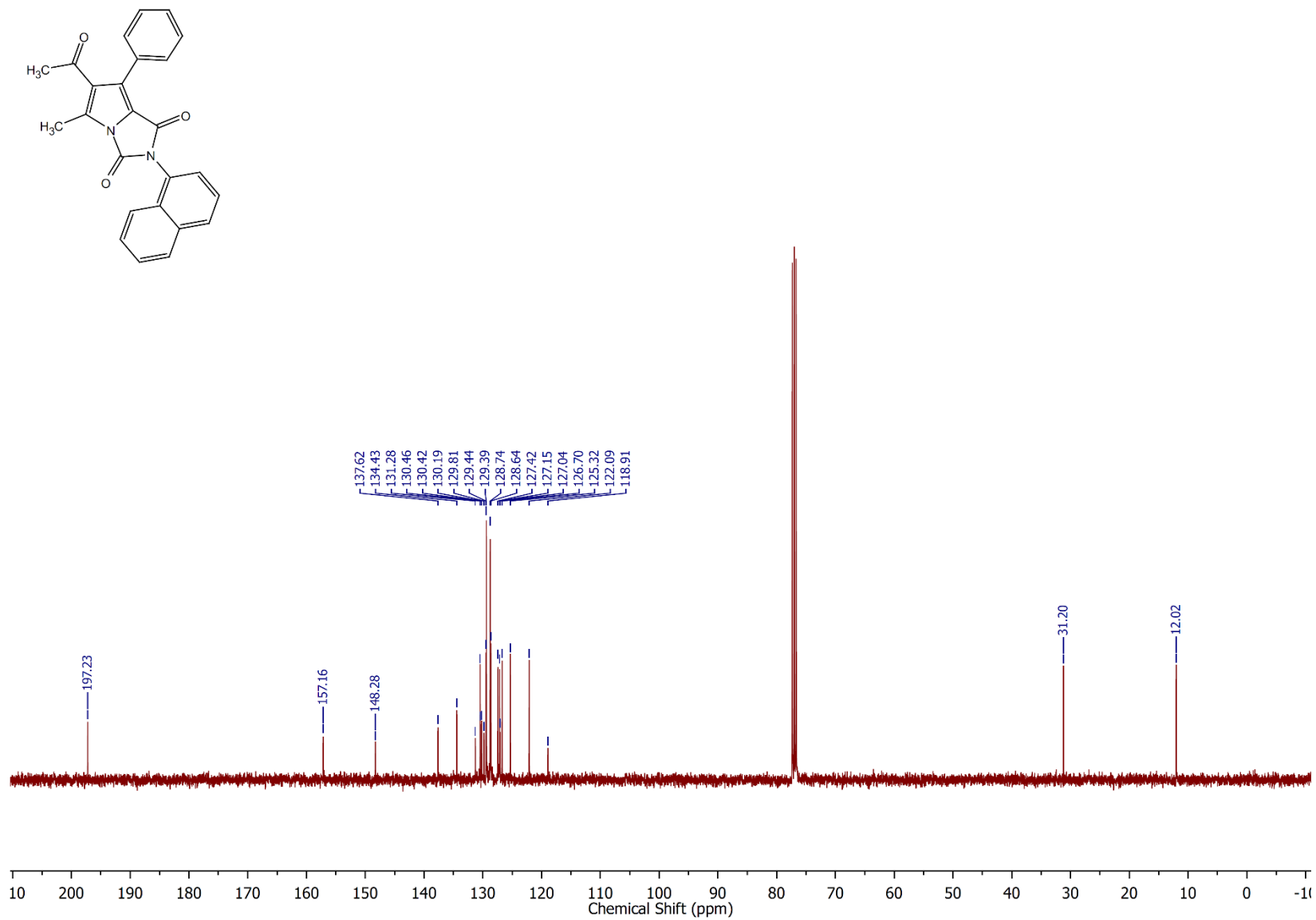
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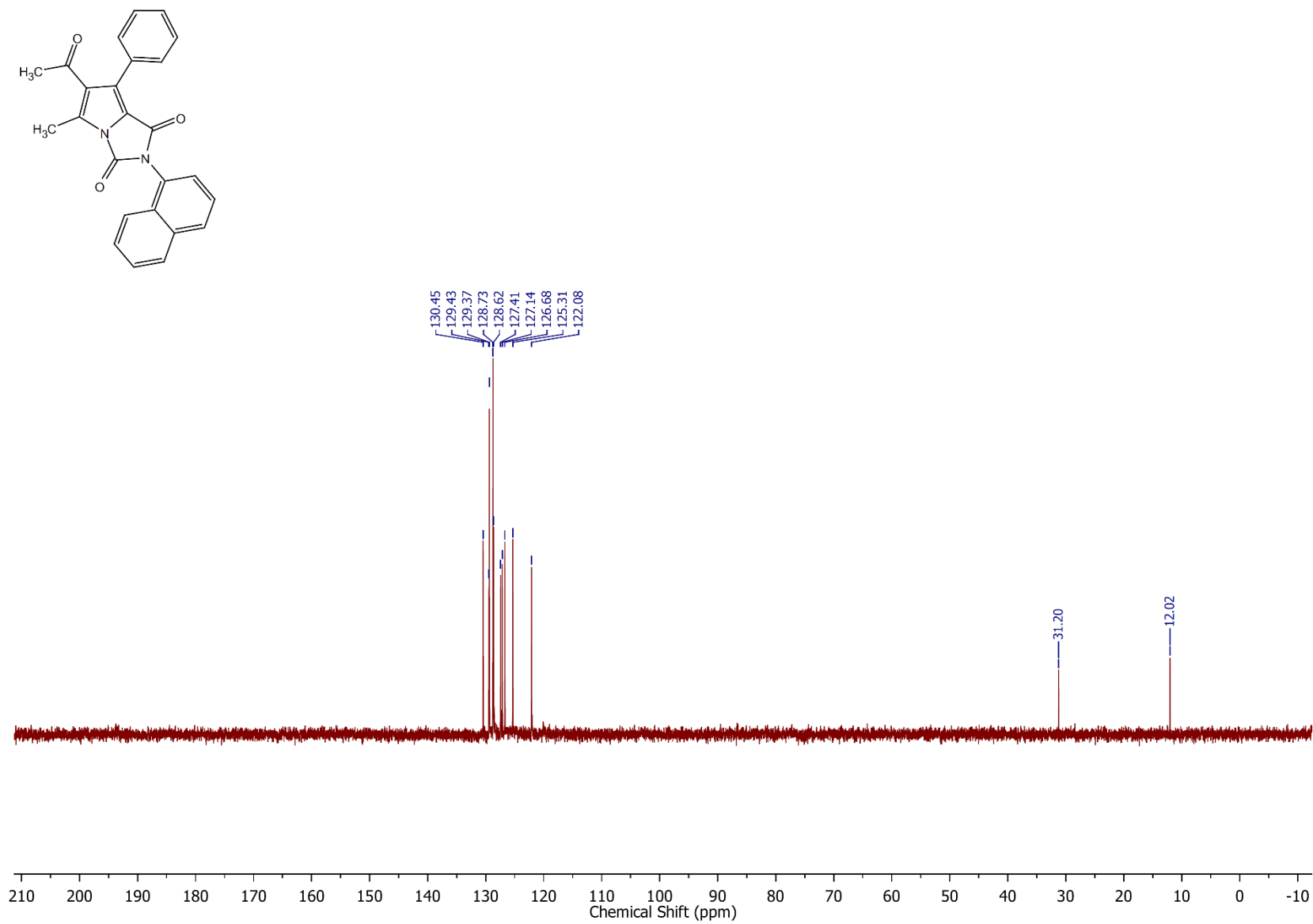
6-Acetyl-5-methyl-2-(naphthalen-1-yl)-7-phenyl-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 10c, ¹H NMR, CDCl₃, 400 MHz



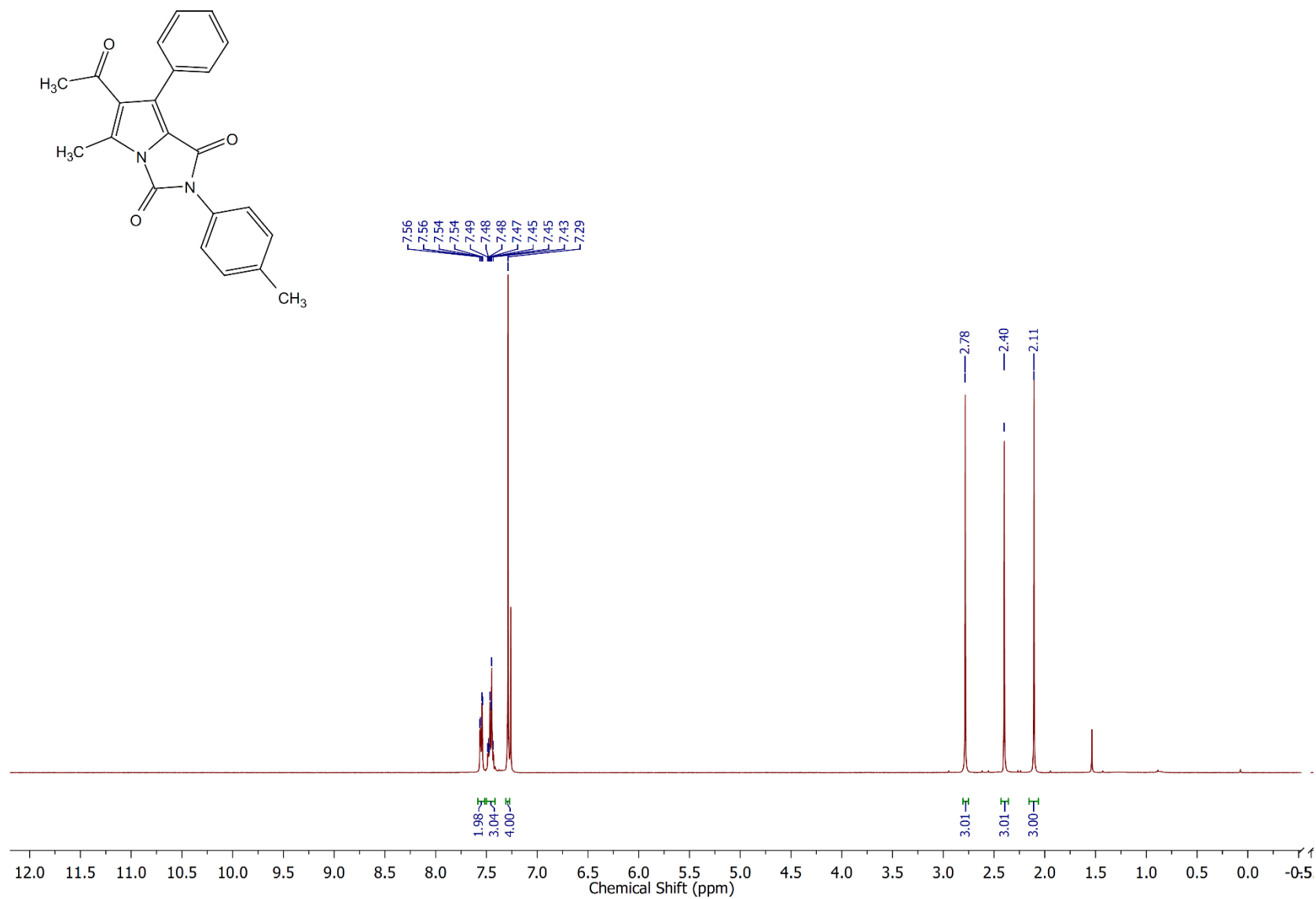
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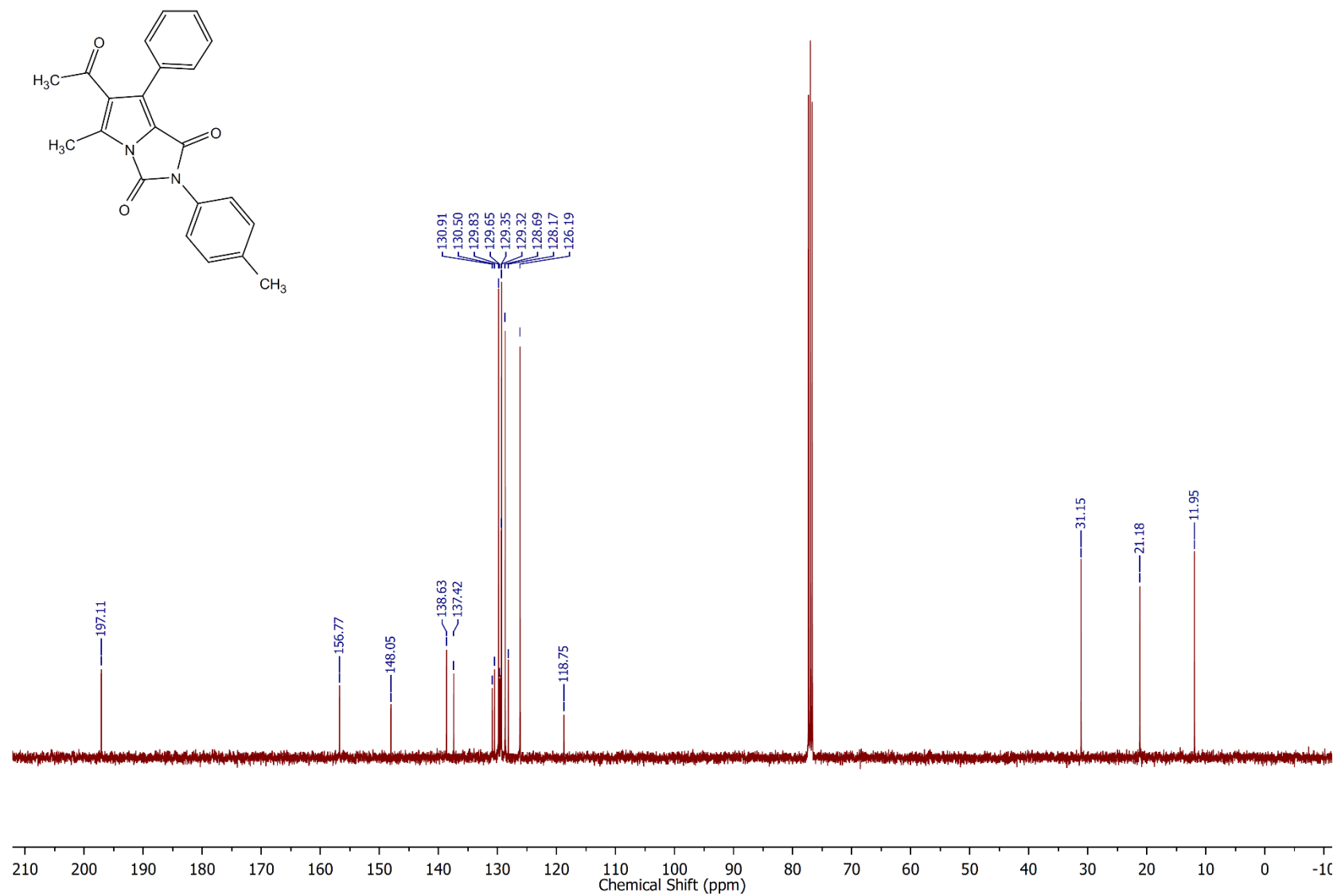
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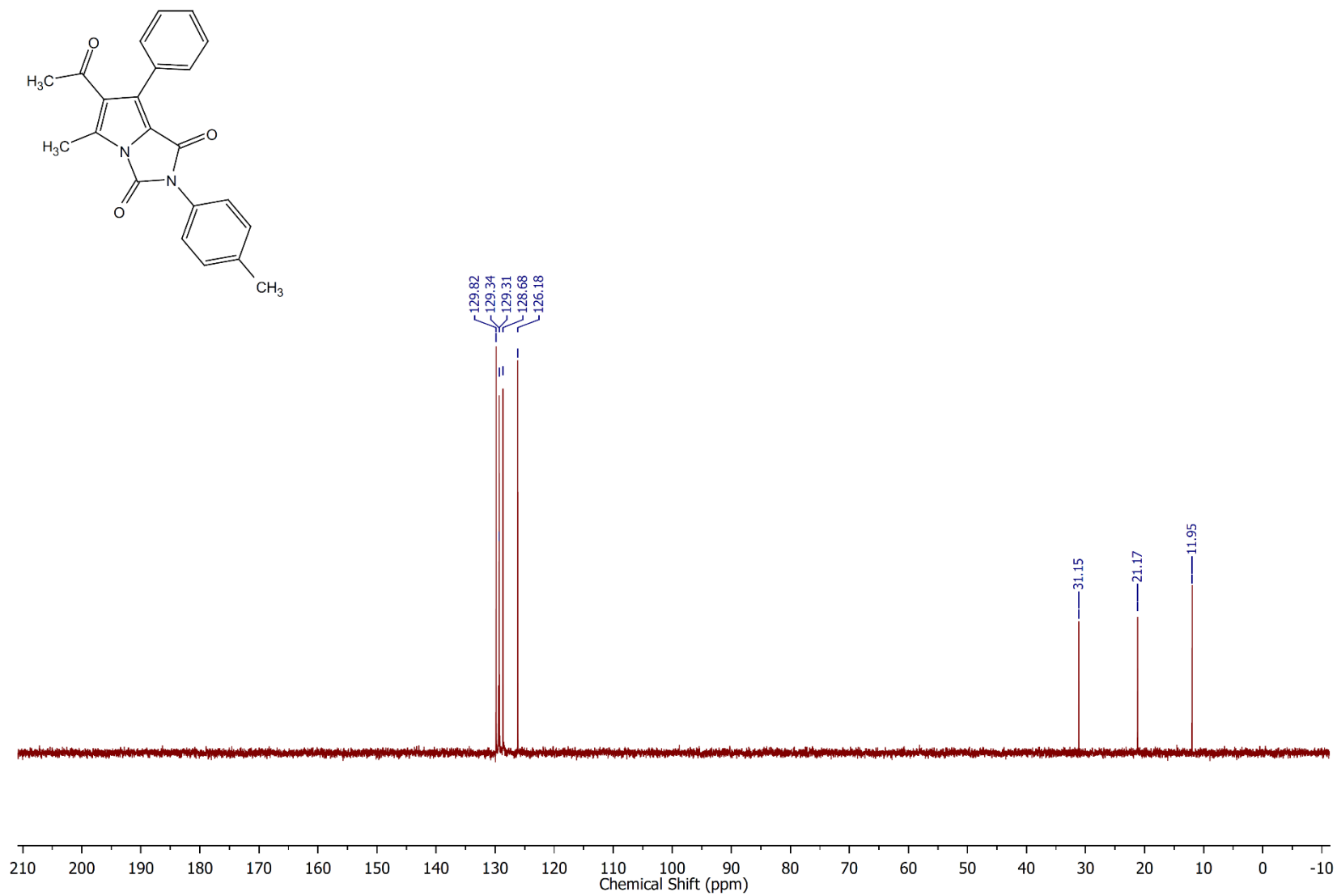
6-Acetyl-5-methyl-7-phenyl-2-(*p*-tolyl)-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 10d, ^1H NMR, CDCl_3 , 400 MHz



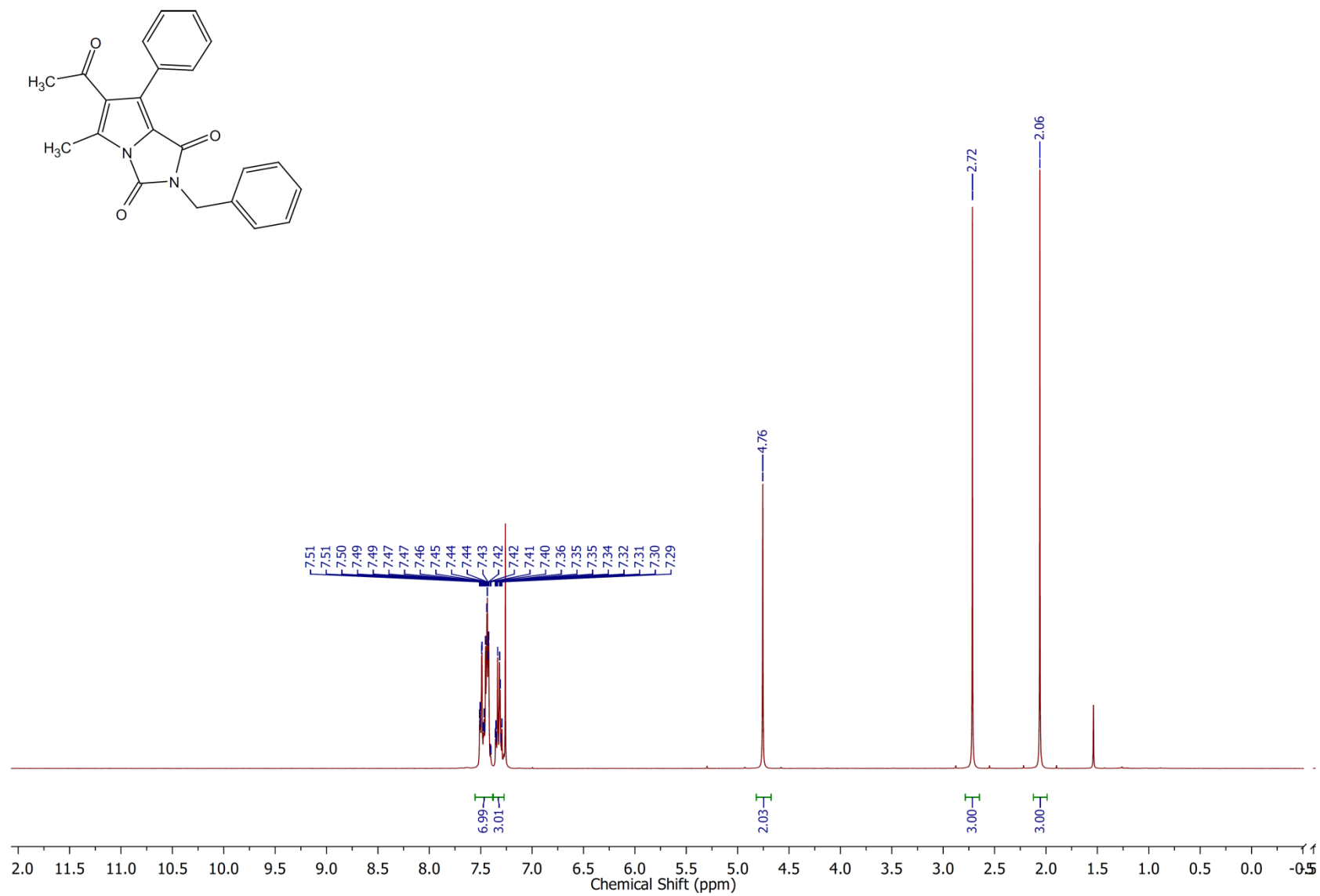
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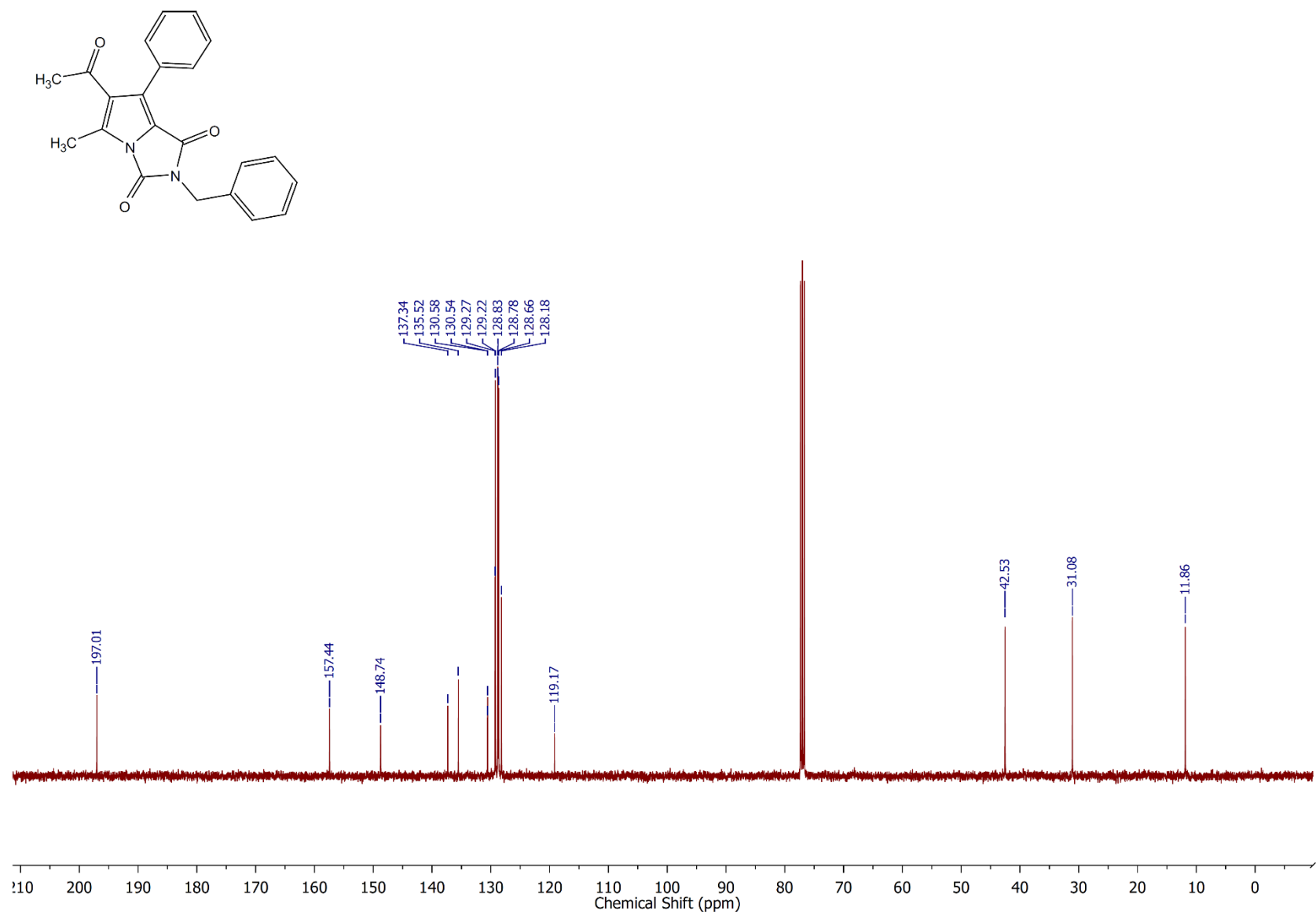
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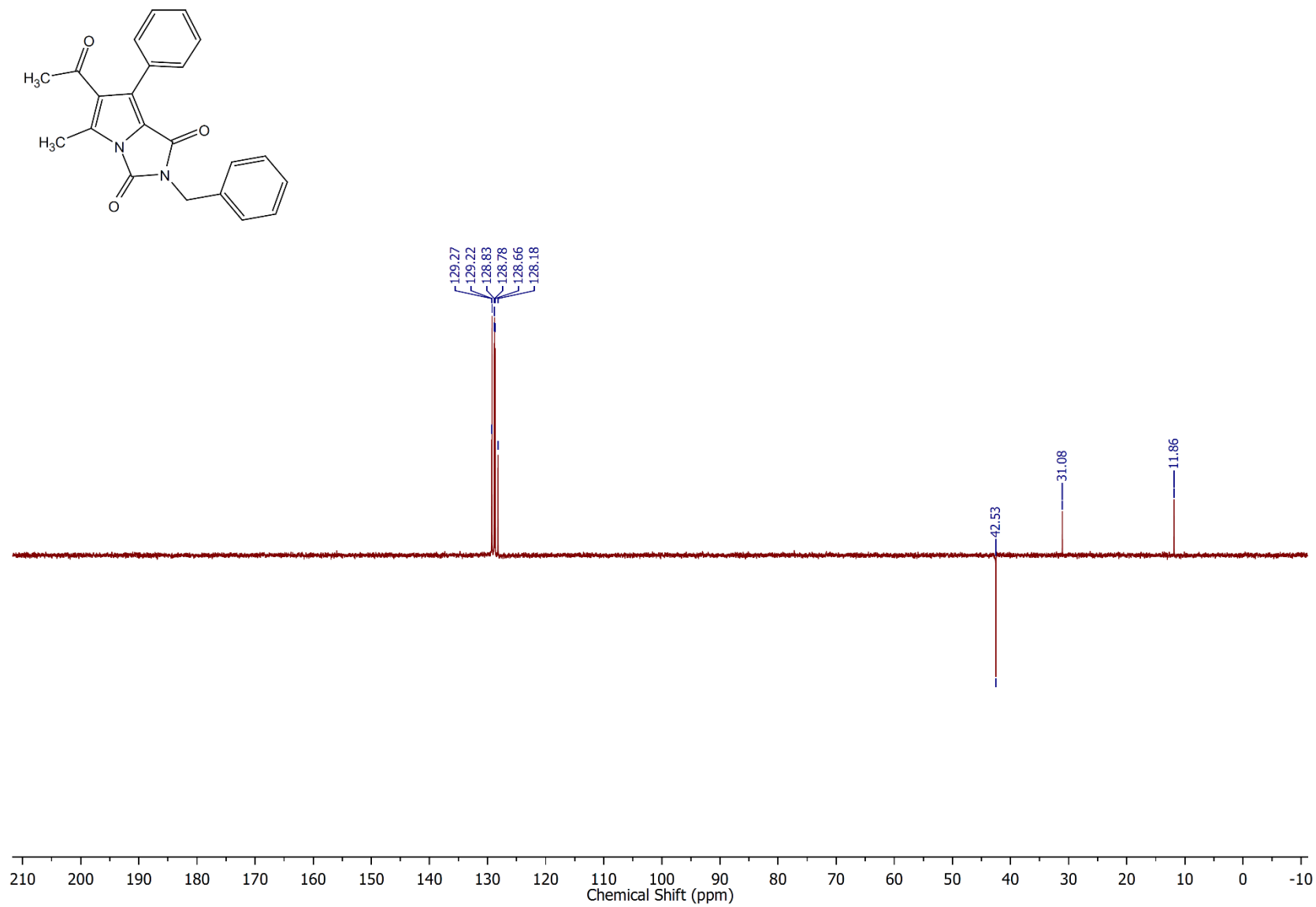
6-Acetyl-2-benzyl-5-methyl-7-phenyl-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 10e, ¹H NMR, CDCl₃, 400 MHz



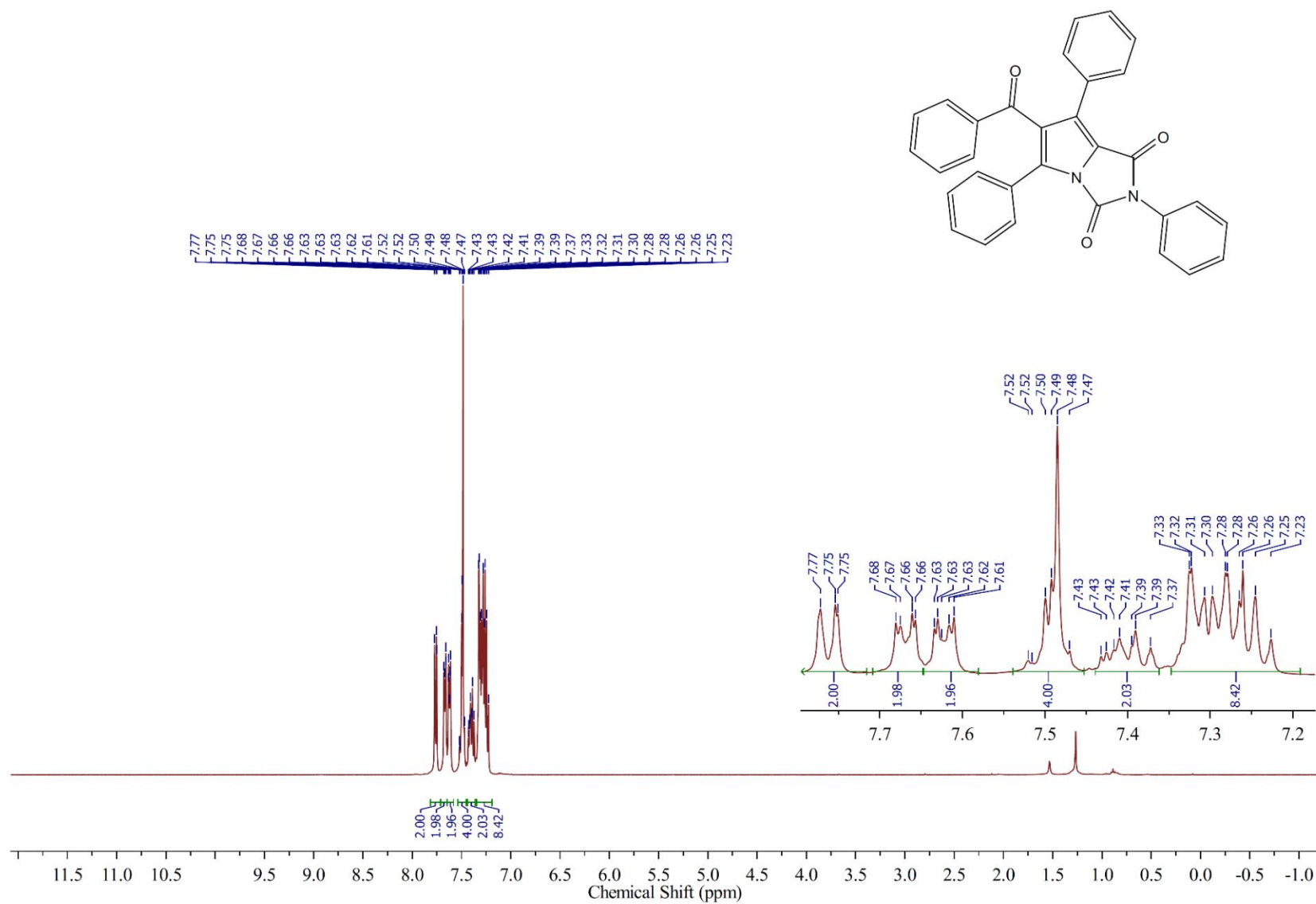
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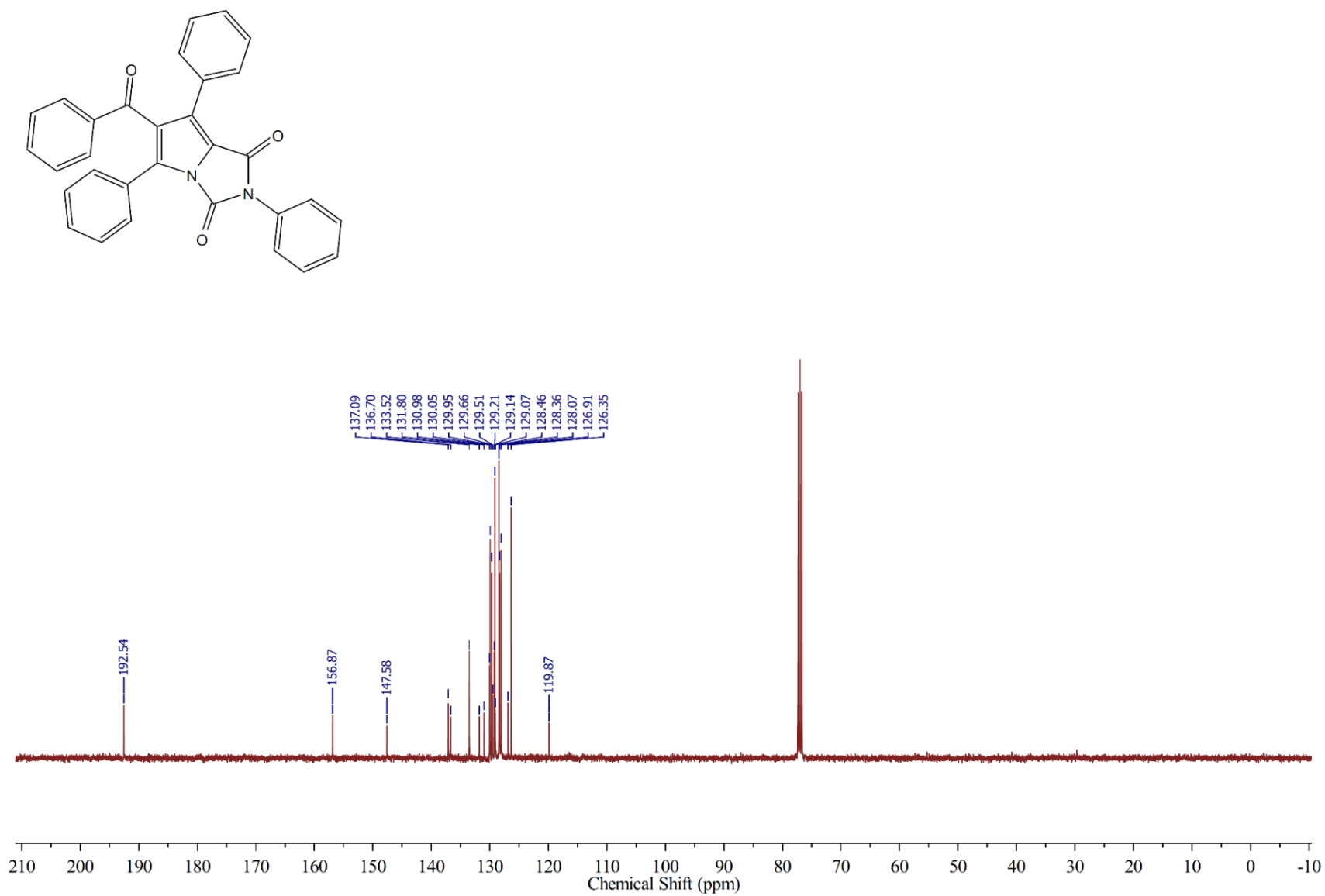
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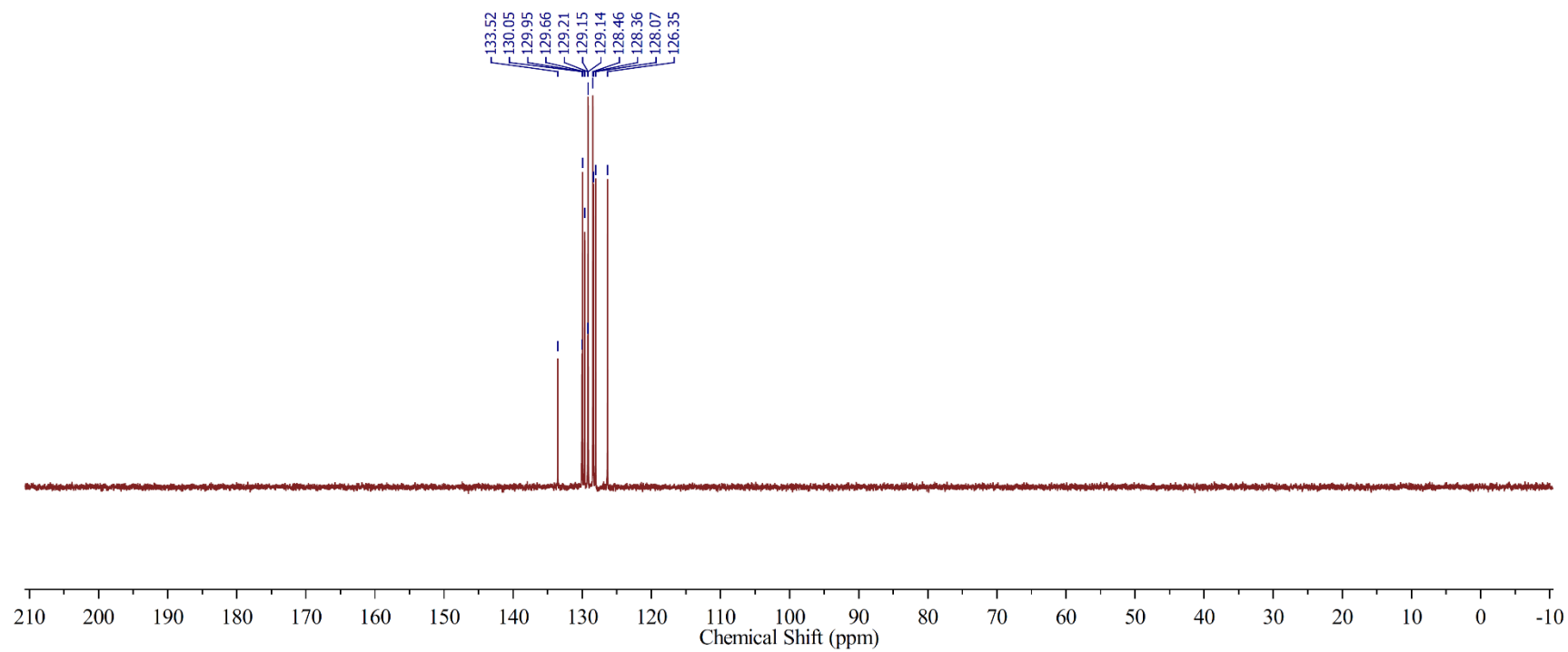
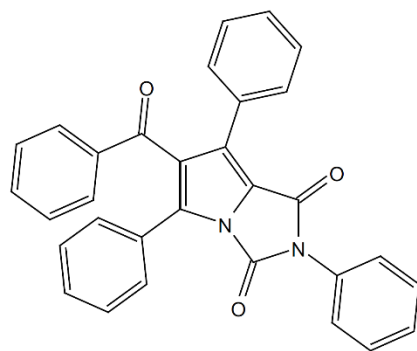
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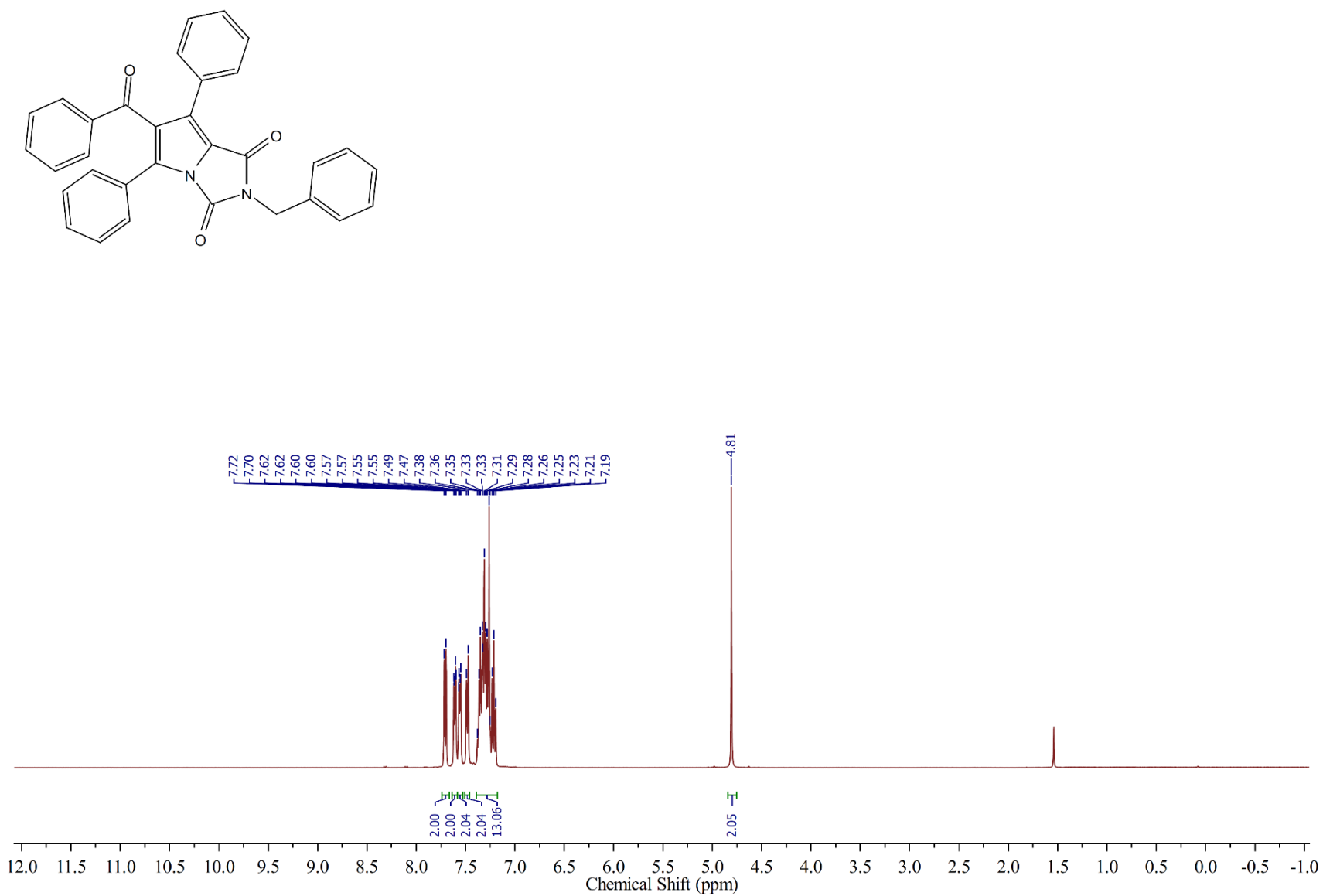
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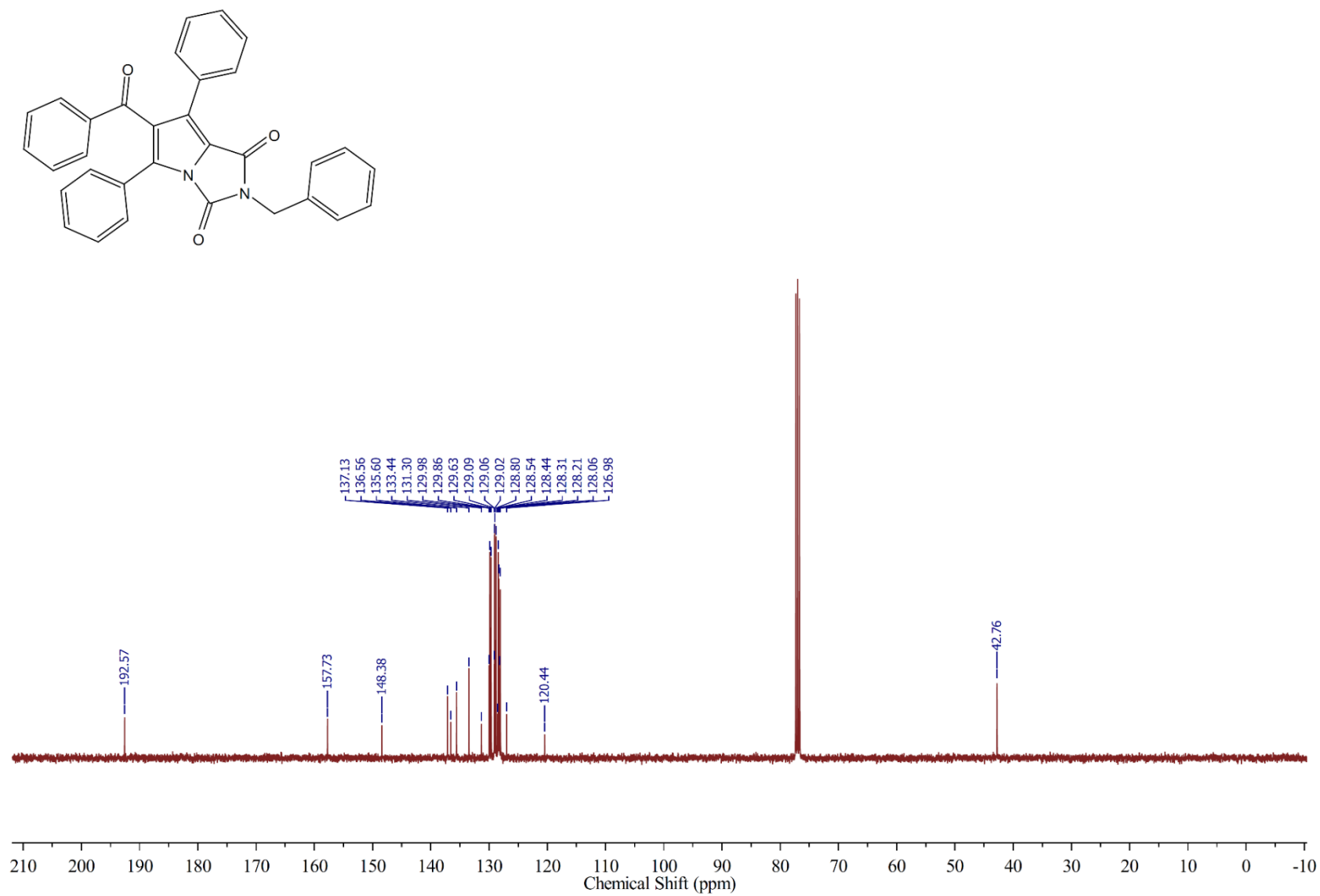
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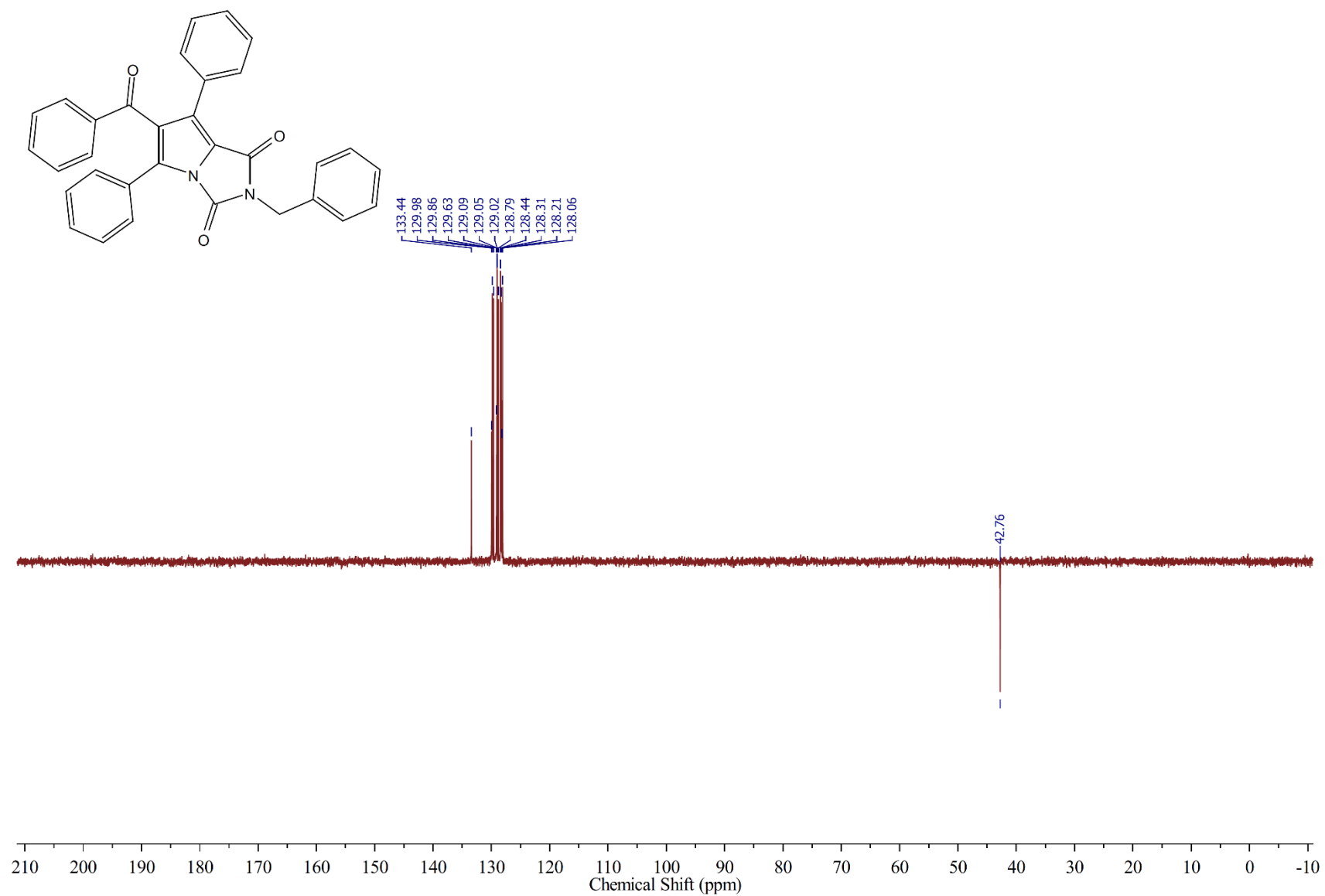
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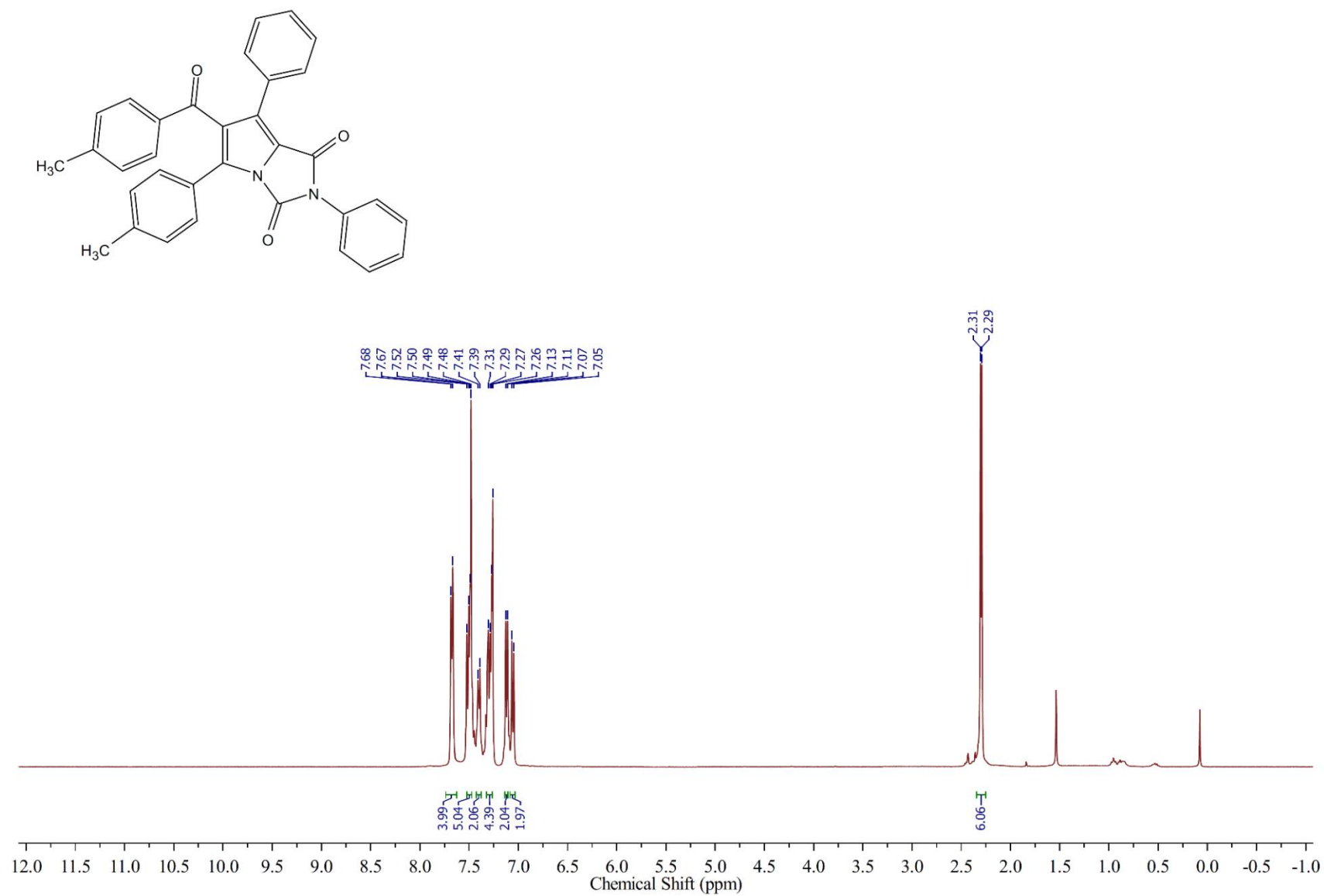
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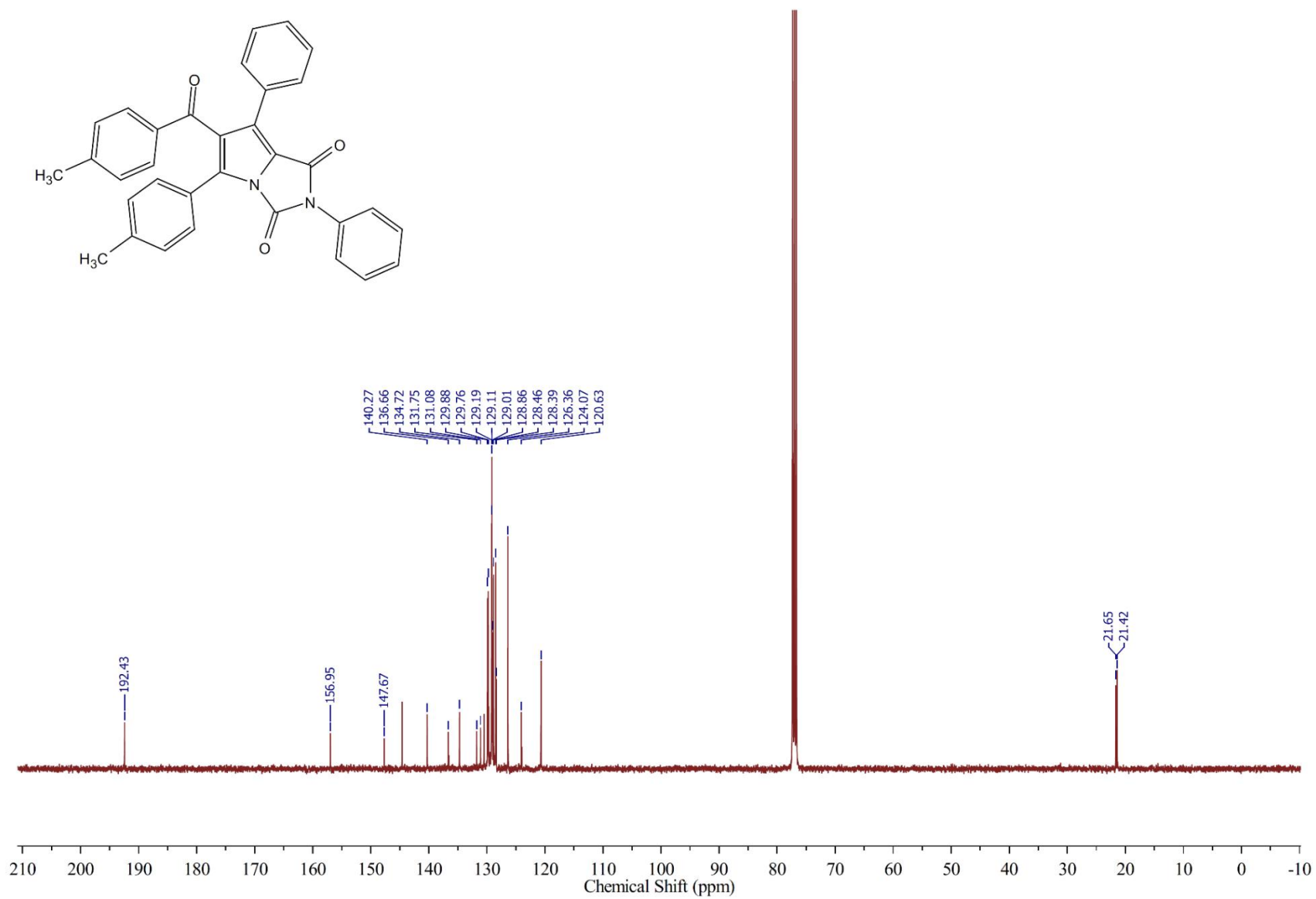
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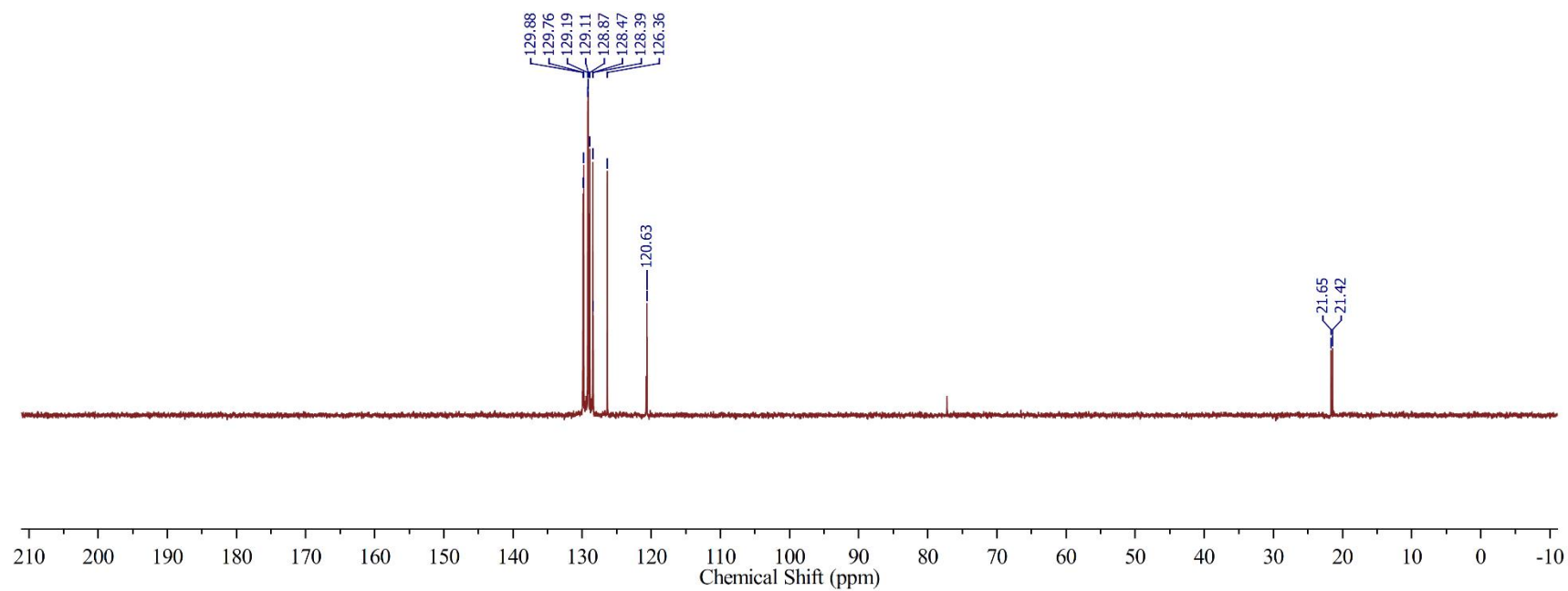
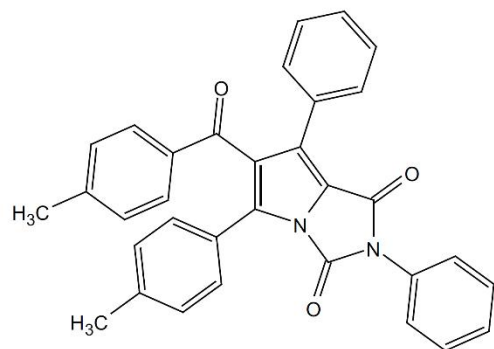
6-(4-Methylbenzoyl)-2,7-diphenyl-5-(*p*-tolyl)-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 10h, ¹H NMR, CDCl₃, 400 MHz



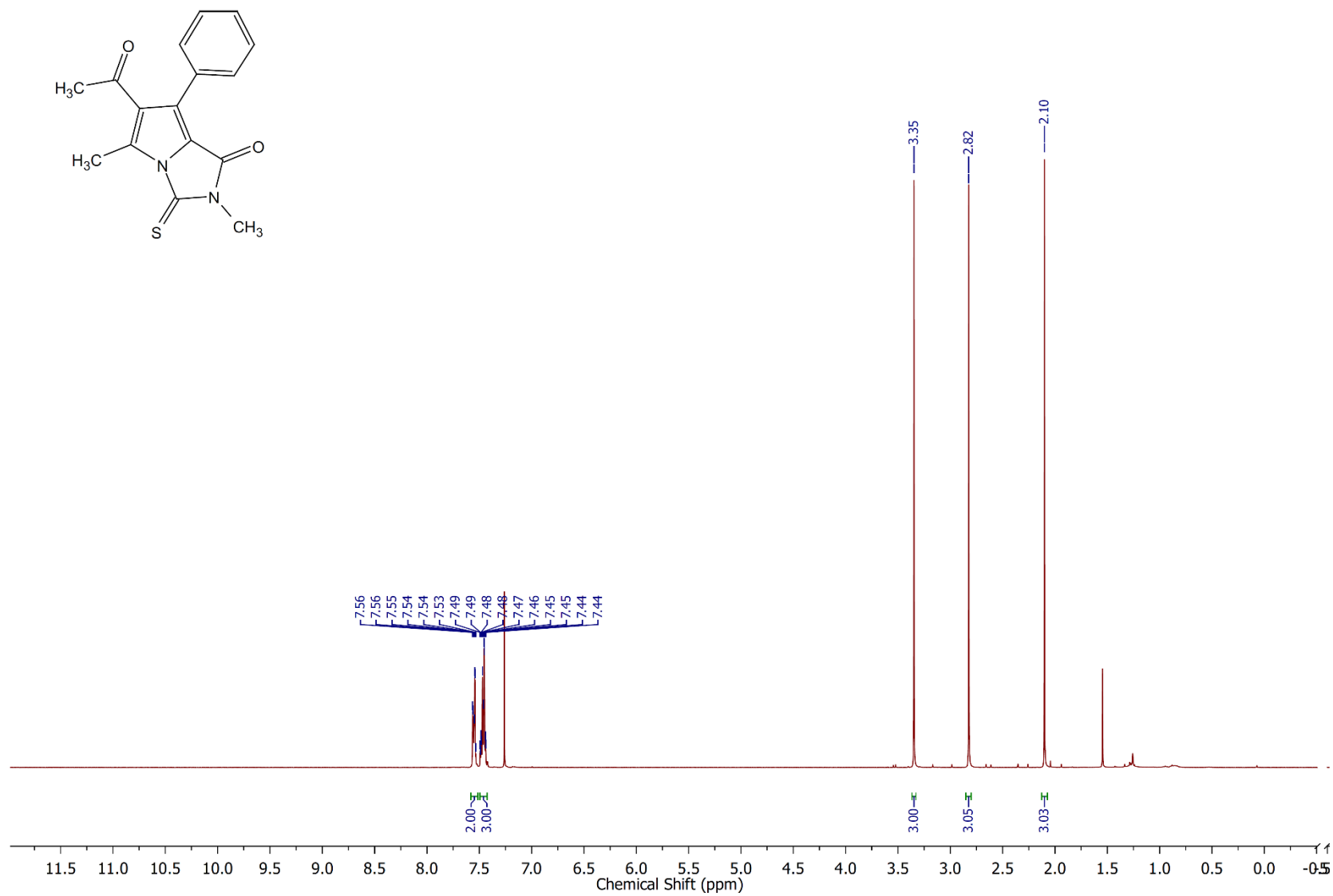
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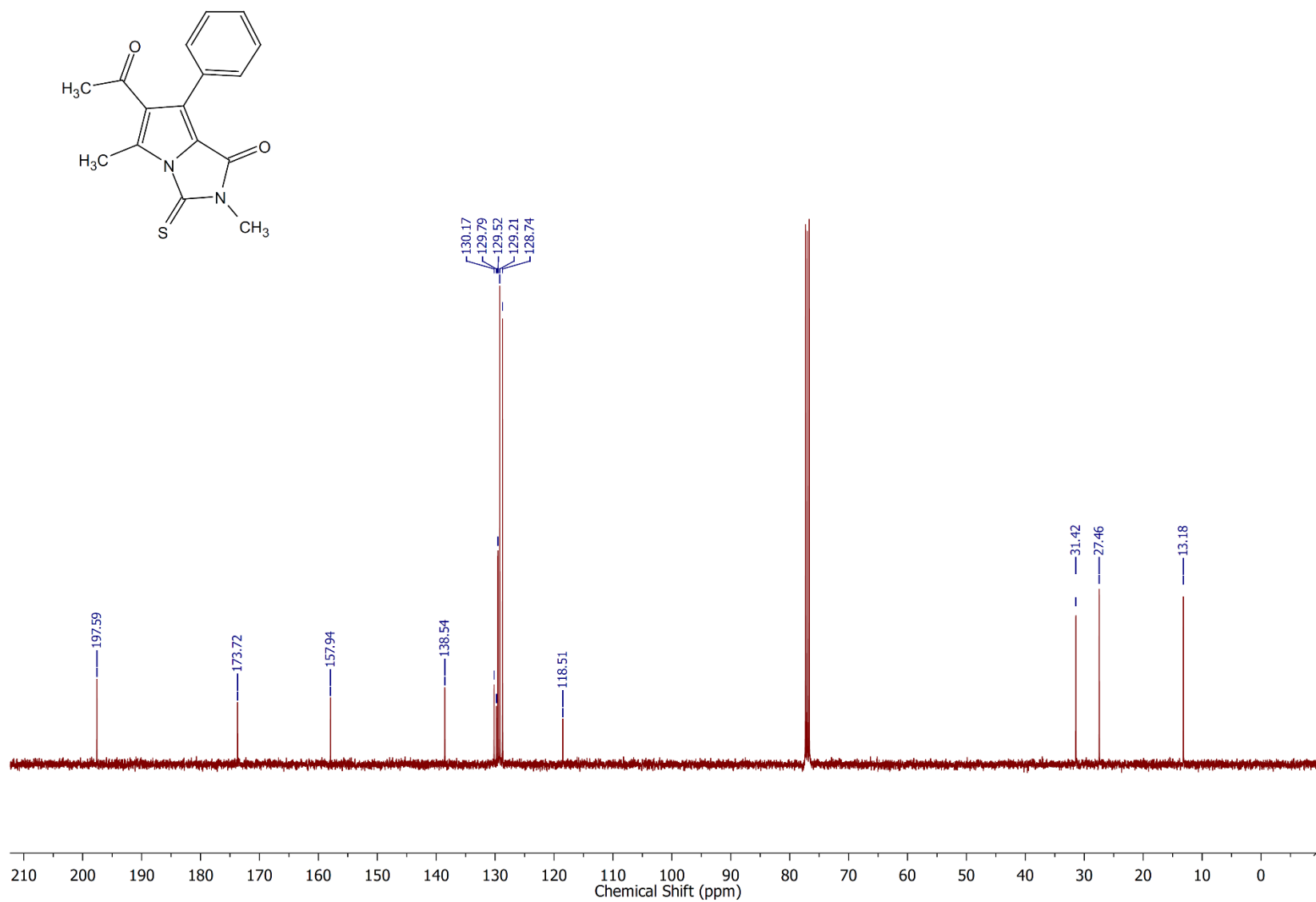
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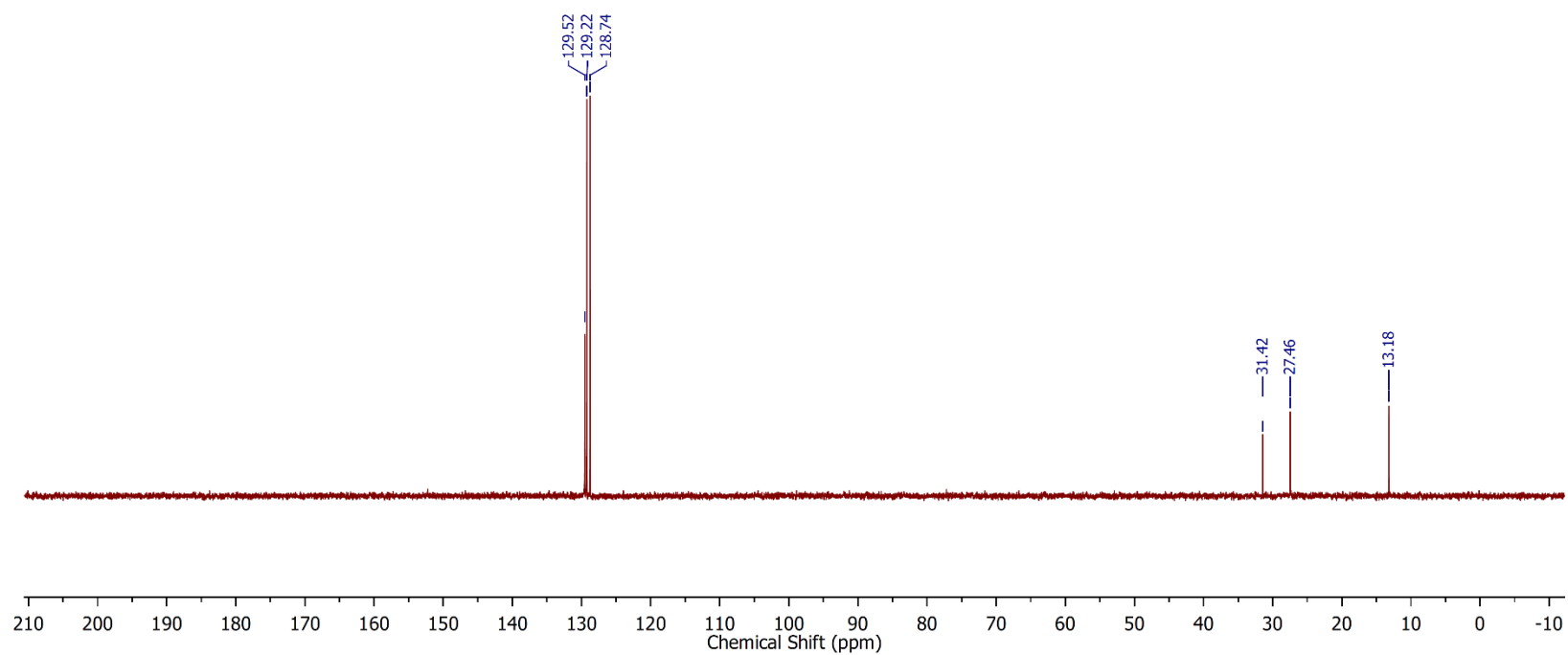
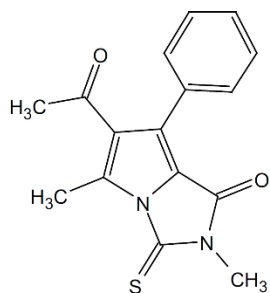
6-Acetyl-2,5-dimethyl-7-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10i, ^1H NMR, CDCl_3 , 400 MHz



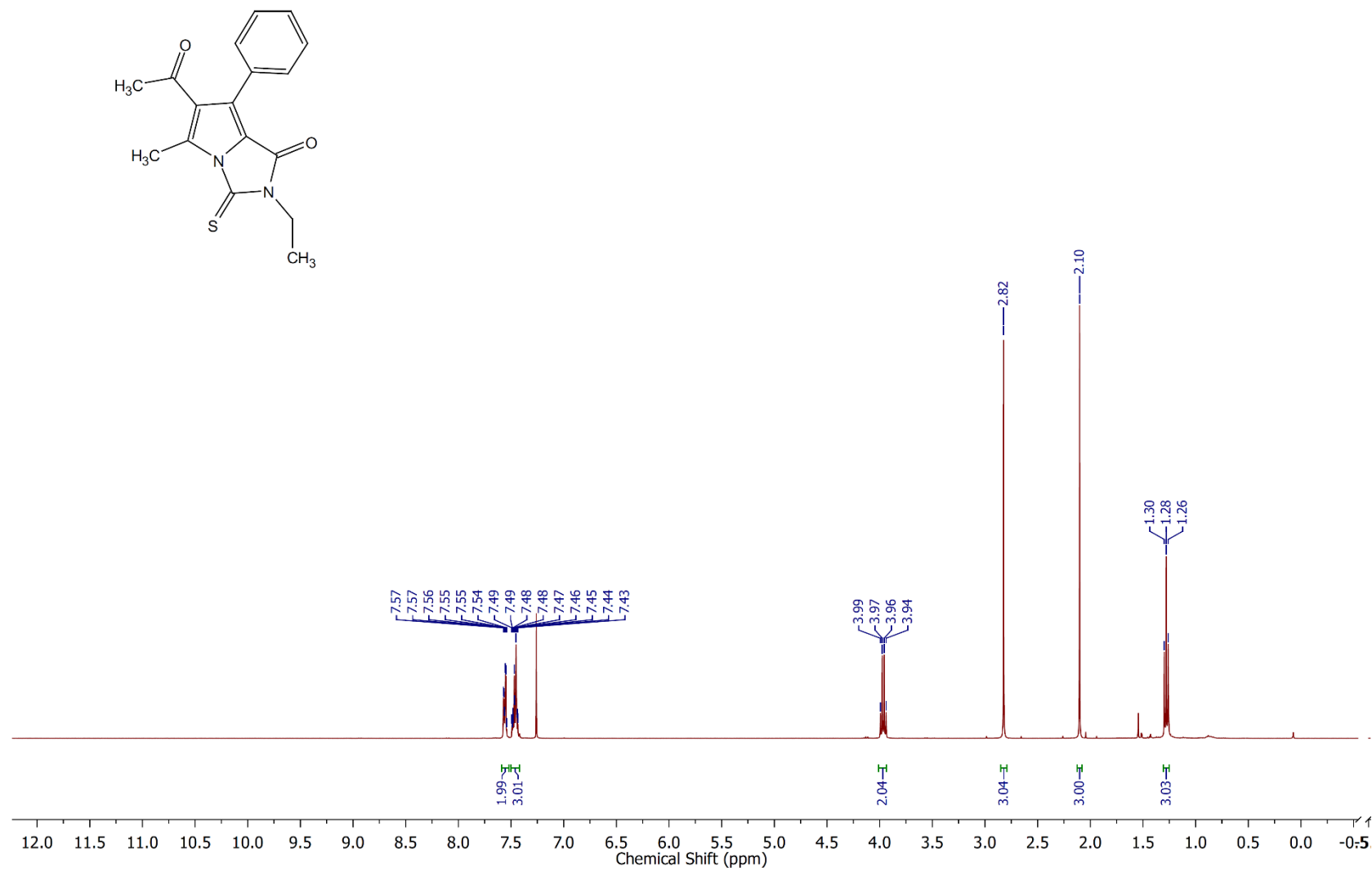
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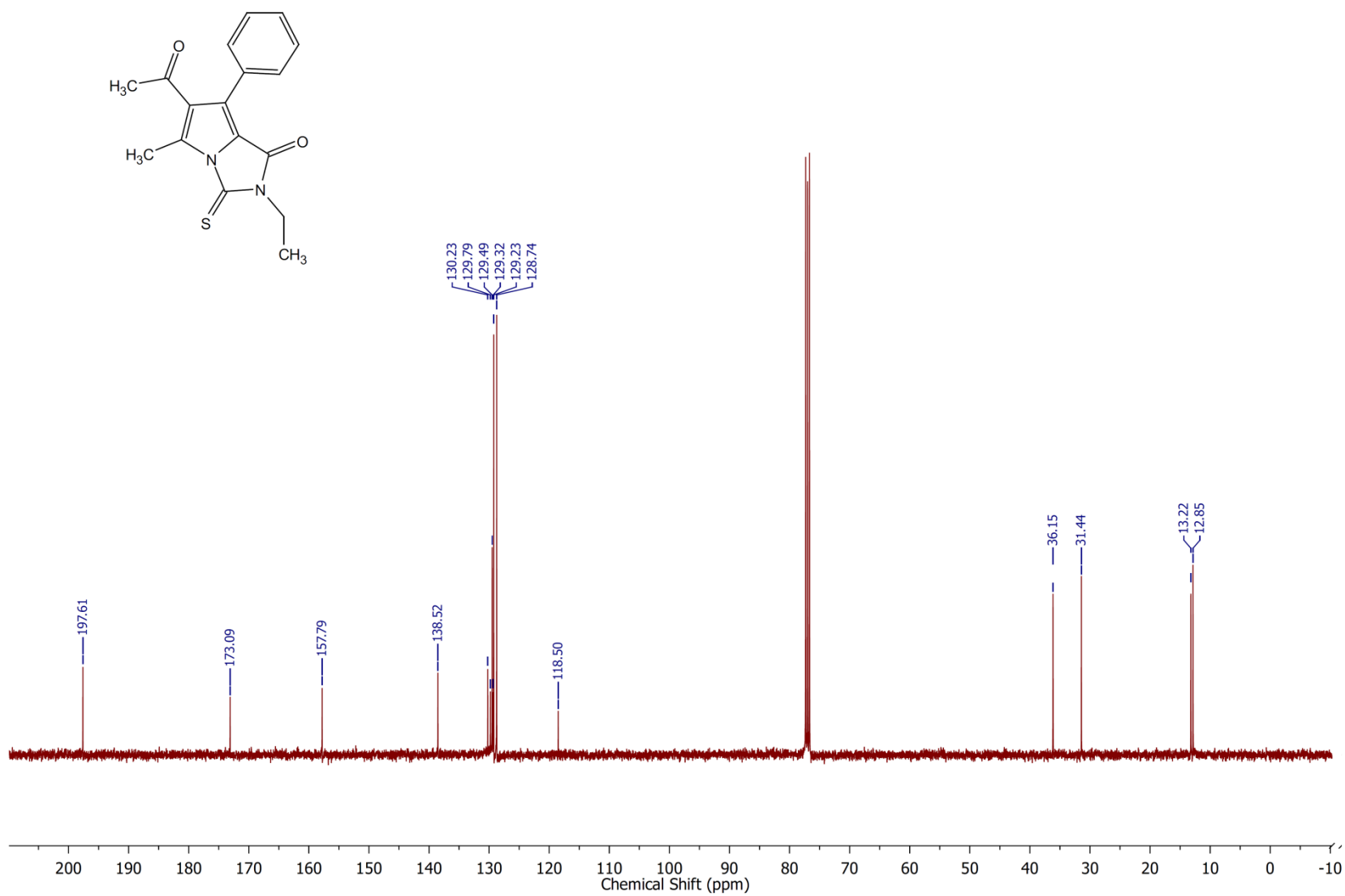
6-Acetyl-2,5-dimethyl-7-phenyl-3-thioxo-2,3-dihydro-1*H*-pyrrolo[1,2-*c*]imidazol-1-one 10i, DEPT, CDCl₃, 100 MHz



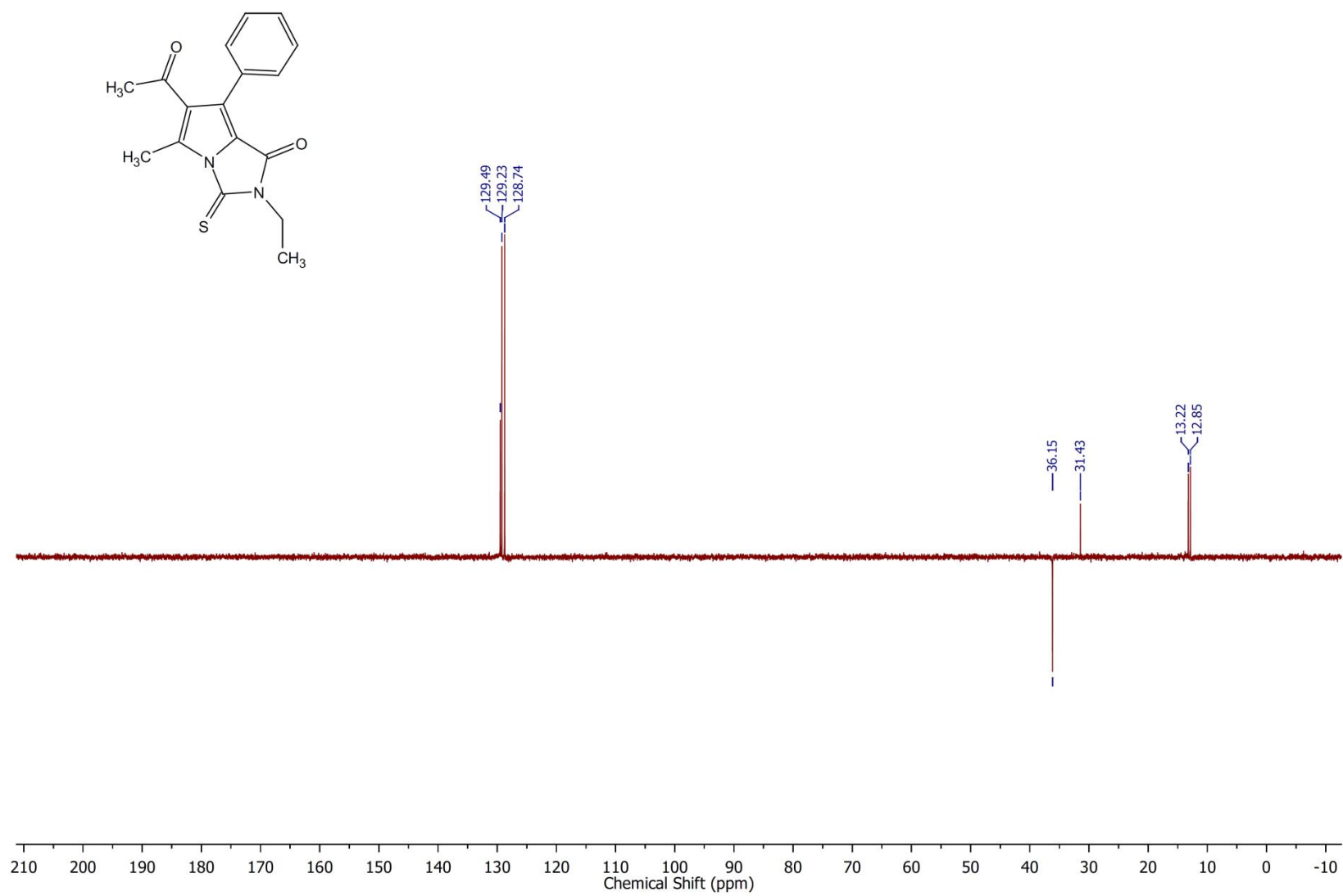
6-Acetyl-2-ethyl-5-methyl-7-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10j, ^1H NMR, CDCl_3 , 400 MHz



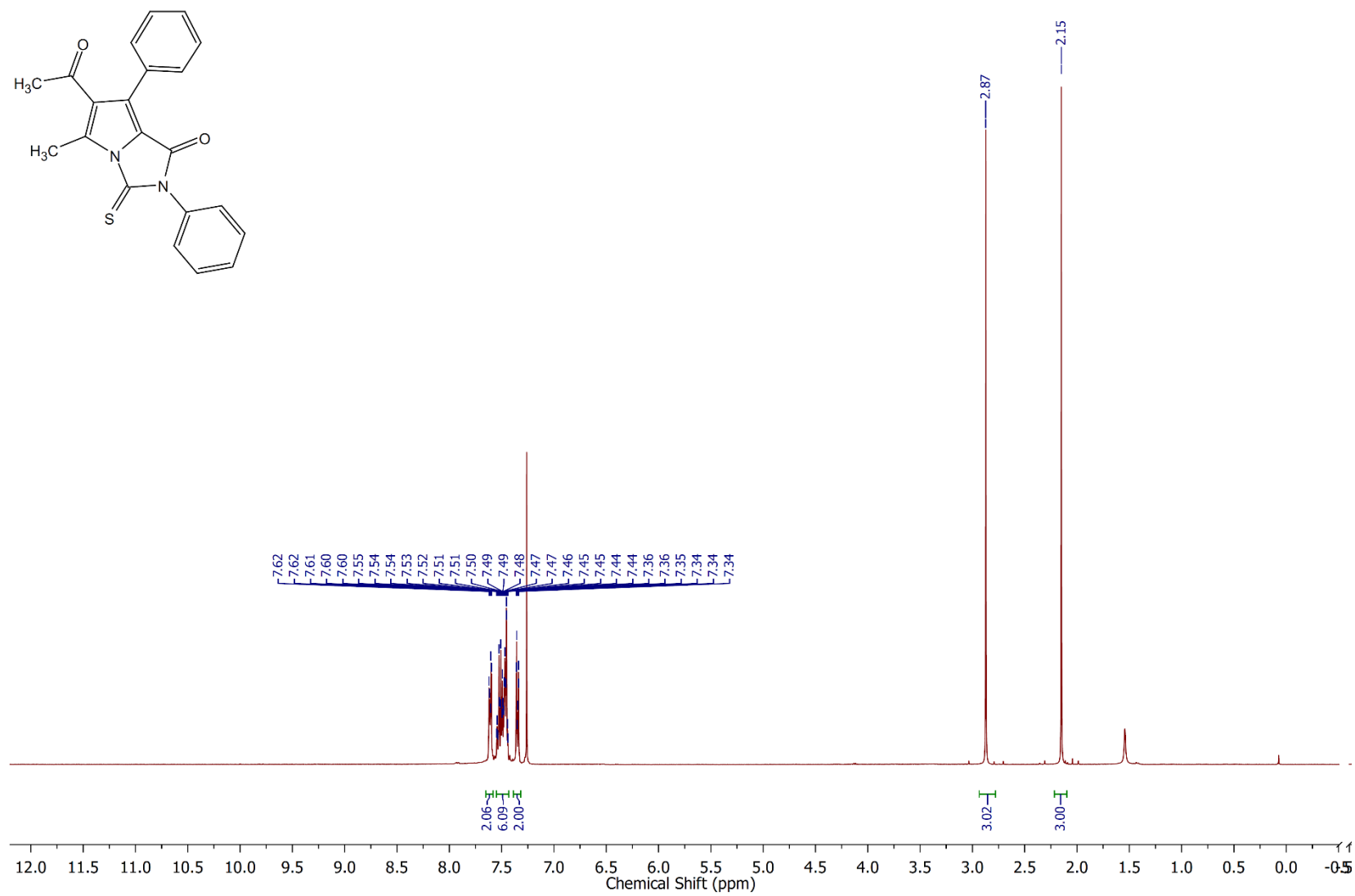
6-Acetyl-2-ethyl-5-methyl-7-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10j, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



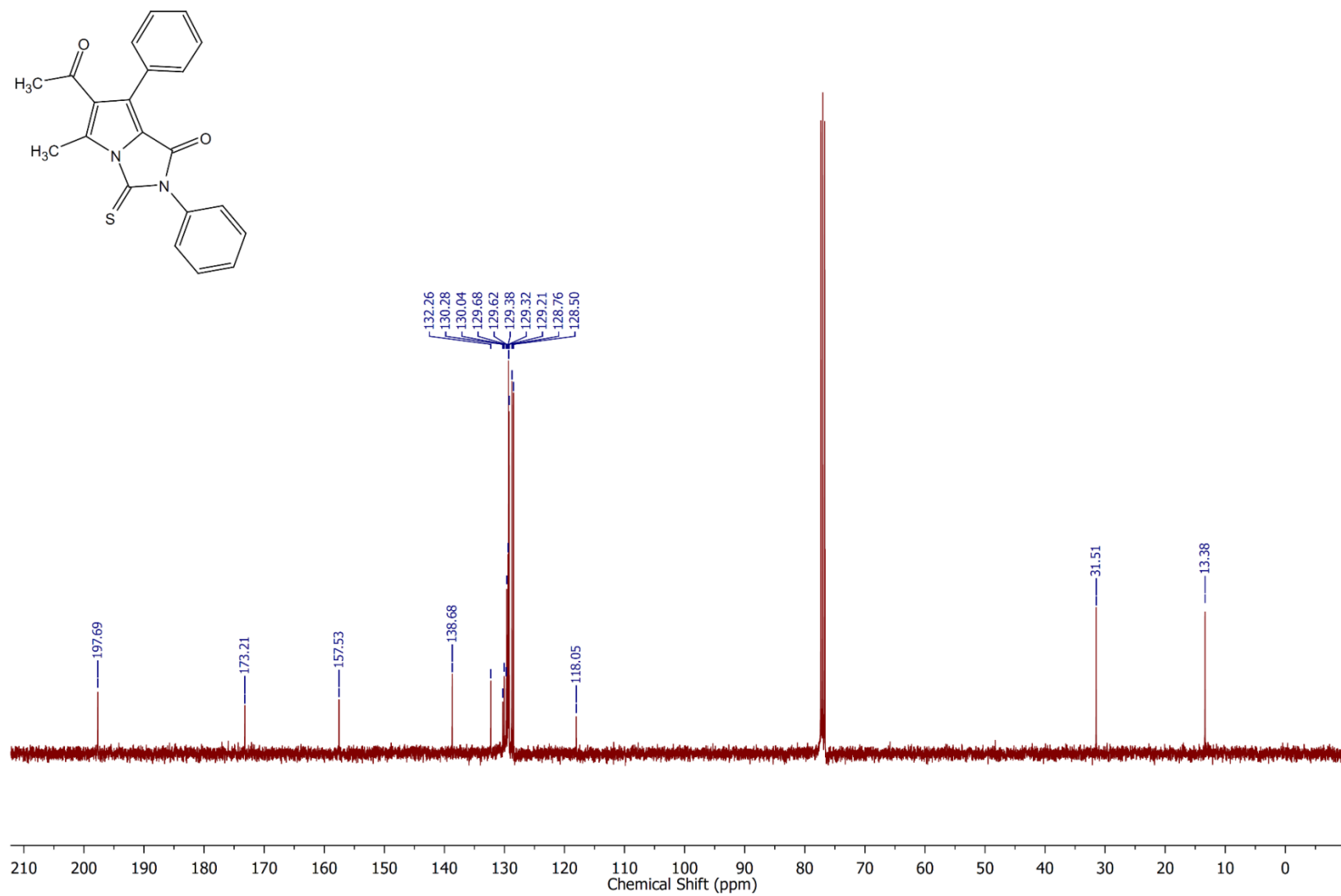
6-Acetyl-2-ethyl-5-methyl-7-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10j, DEPT, CDCl₃, 100 MHz



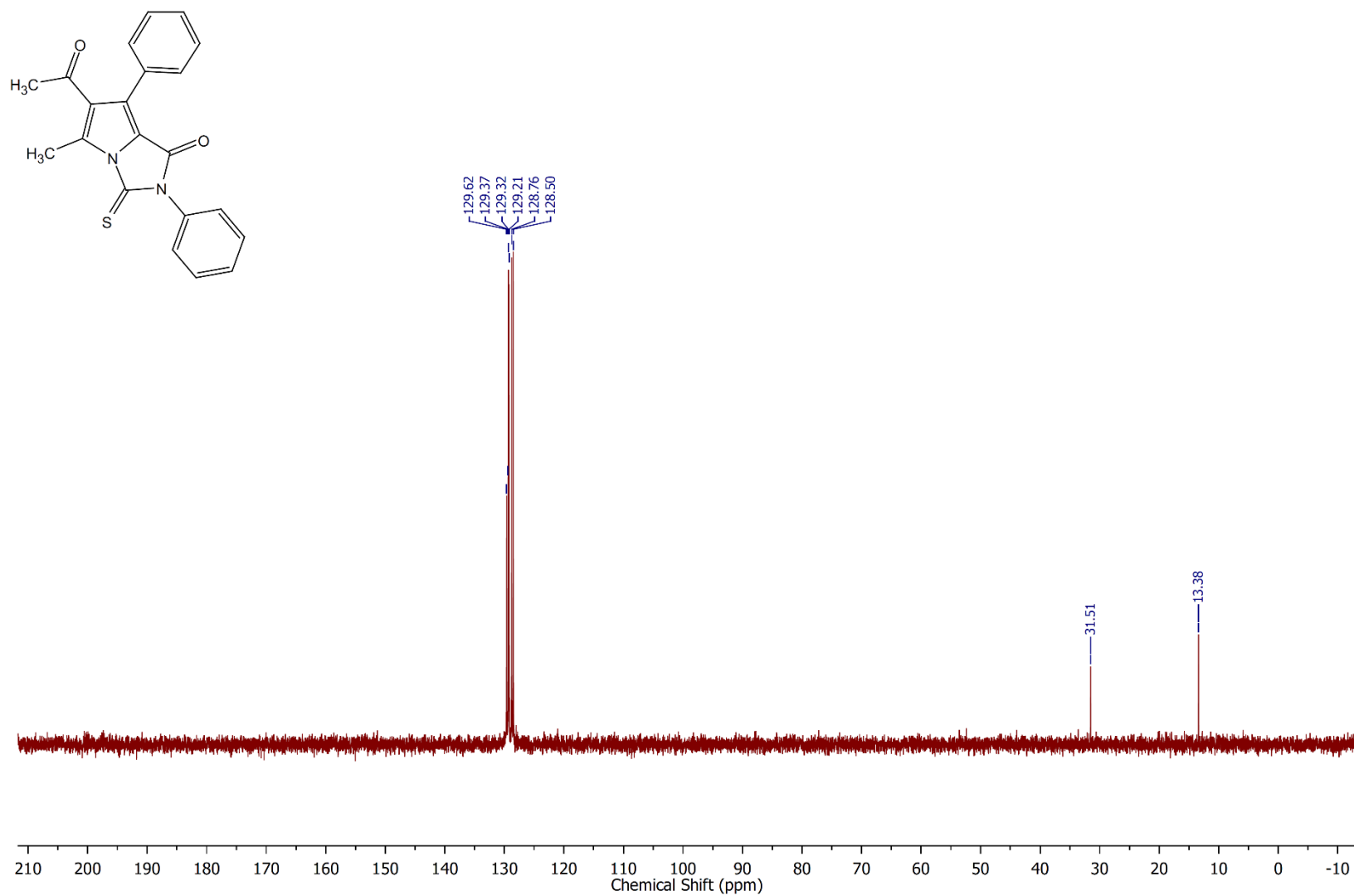
6-Acetyl-5-methyl-2,7-diphenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10k, ^1H NMR, CDCl_3 , 400 MHz



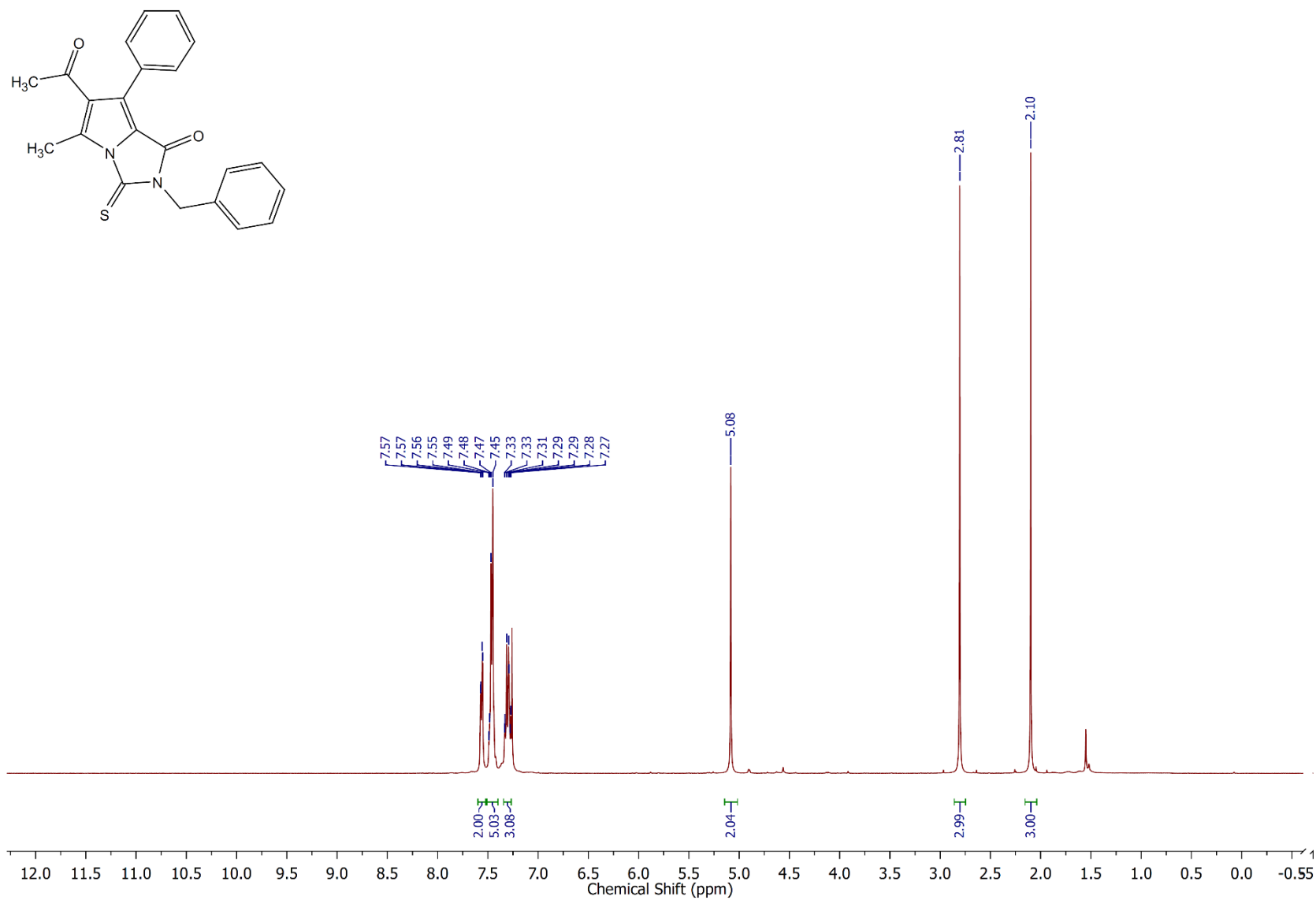
6-Acetyl-5-methyl-2,7-diphenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10k, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



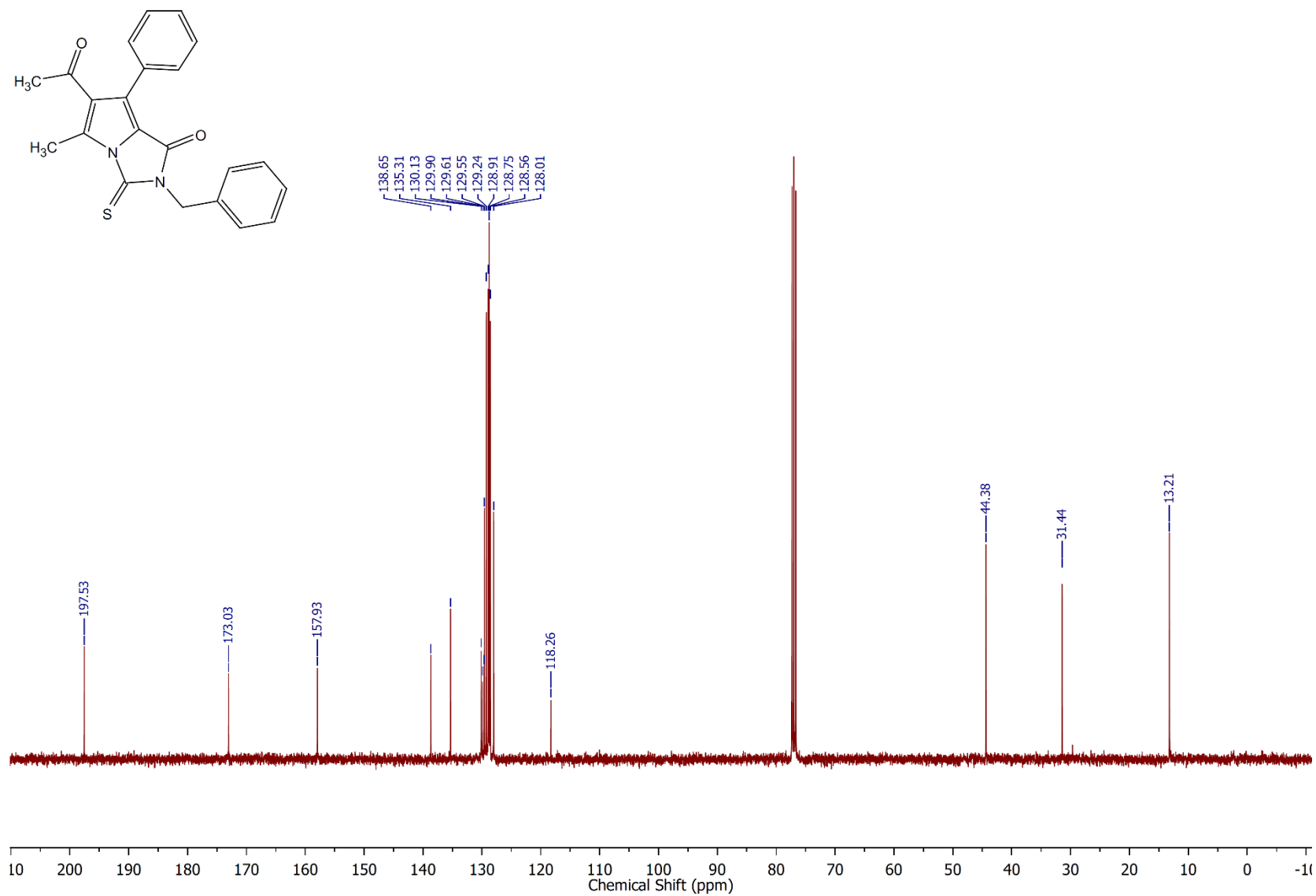
6-Acetyl-5-methyl-2,7-diphenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10k, DEPT, CDCl₃, 100 MHz



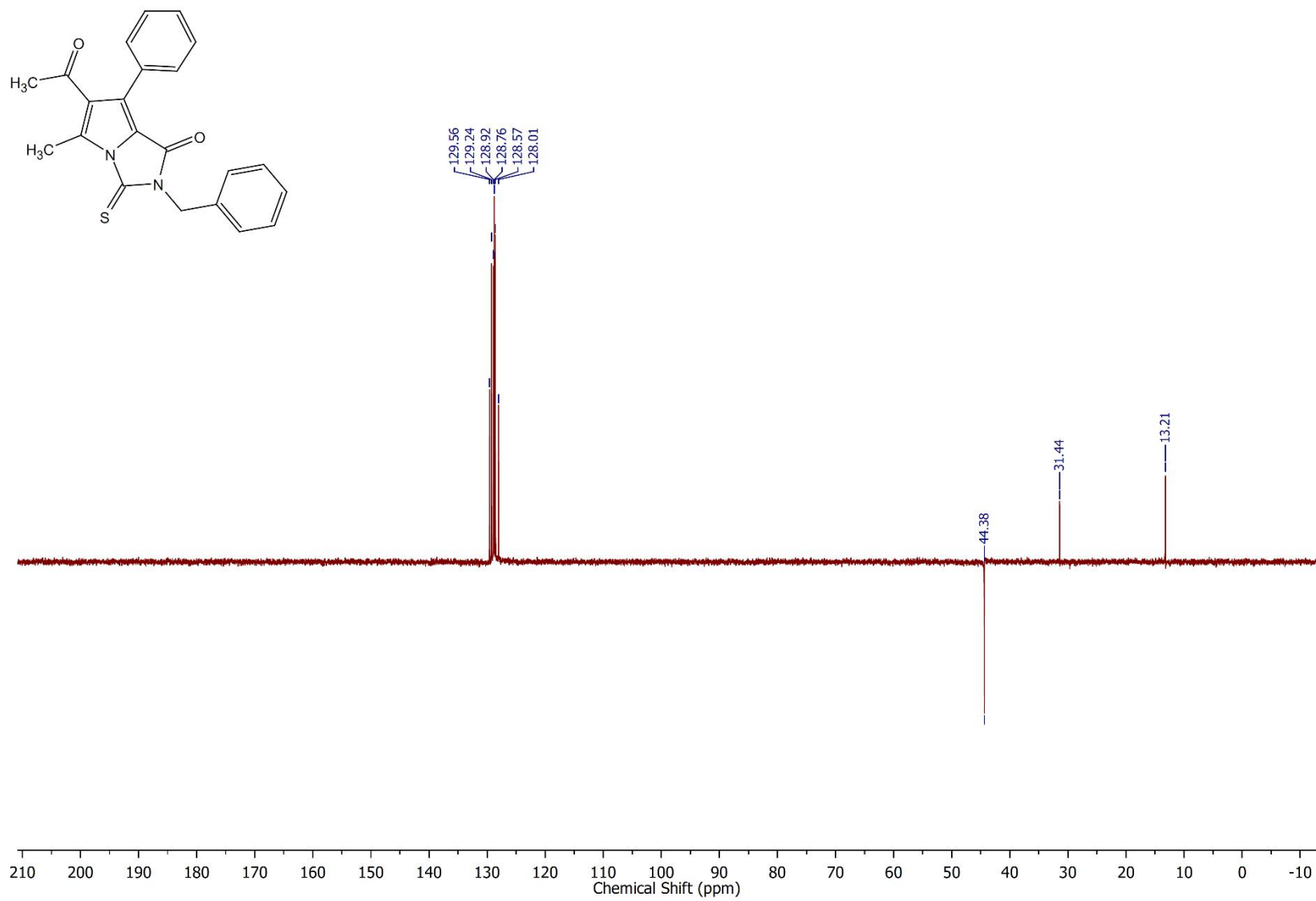
6-Acetyl-2-benzyl-5-methyl-7-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10l, ^1H NMR, CDCl_3 , 400 MHz



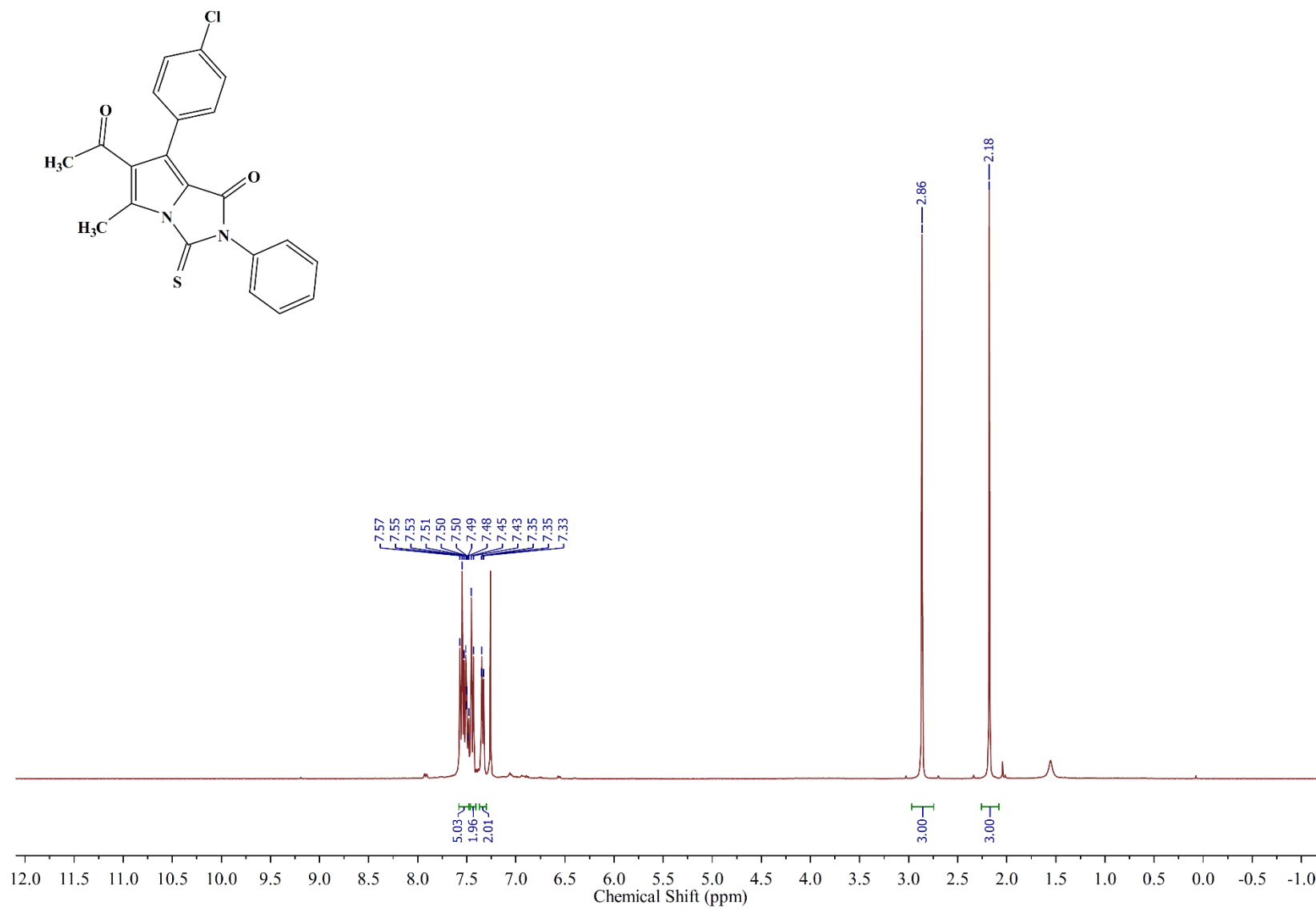
6-Acetyl-2-benzyl-5-methyl-7-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10l, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



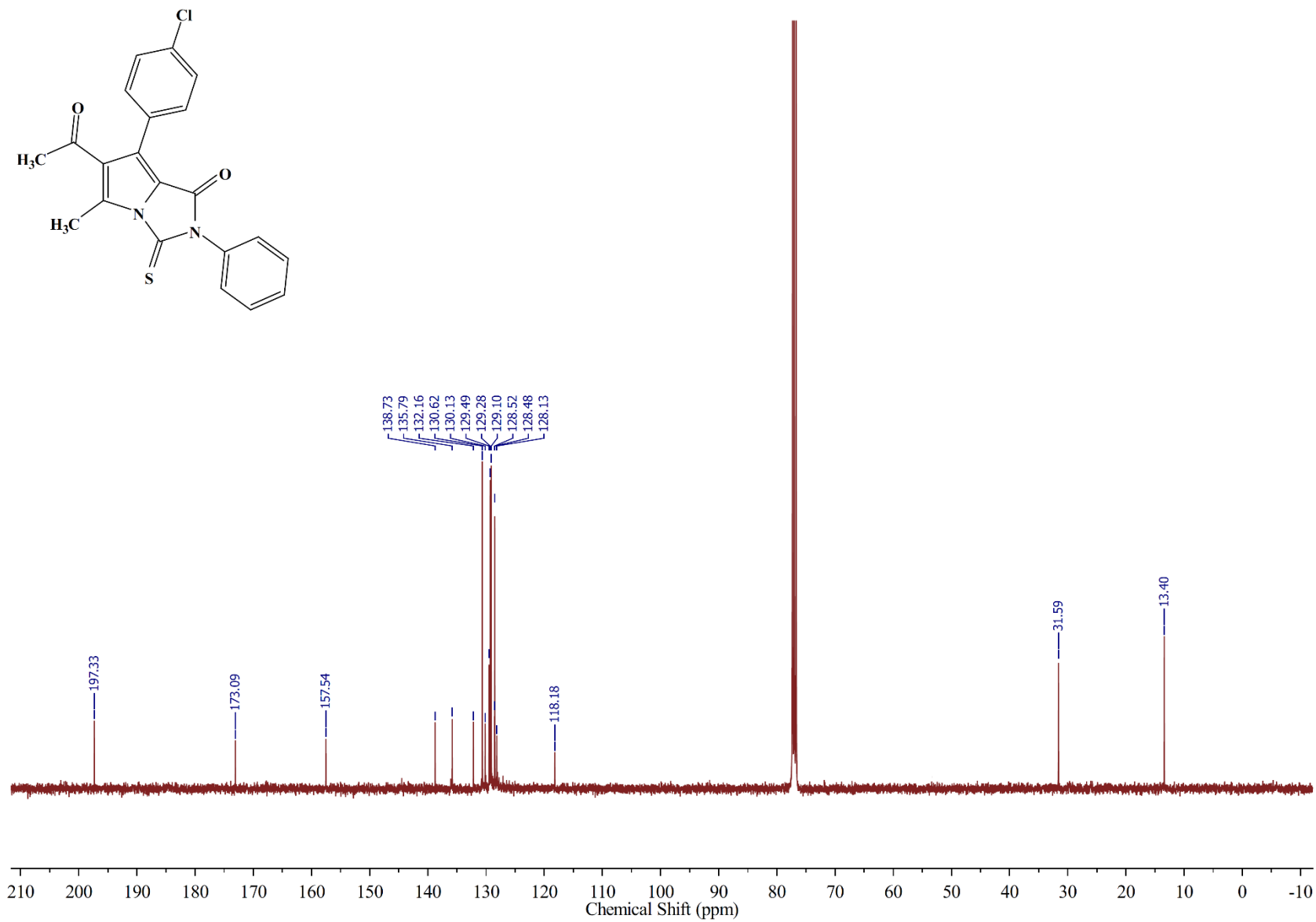
6-Acetyl-2-benzyl-5-methyl-7-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10l, DEPT, CDCl₃, 100 MHz



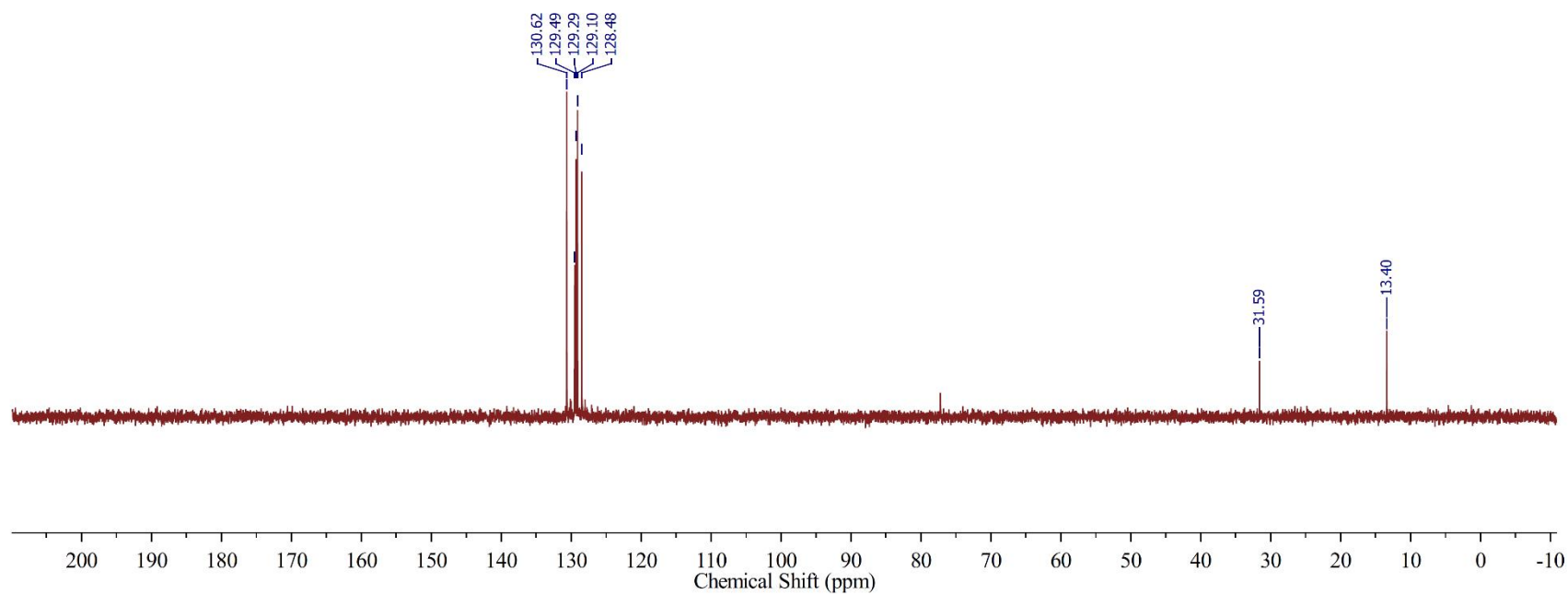
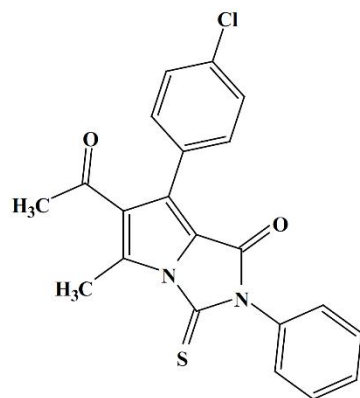
6-Acetyl-7-(4-chlorophenyl)-5-methyl-2-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10m, ^1H NMR, CDCl_3 , 400 MHz



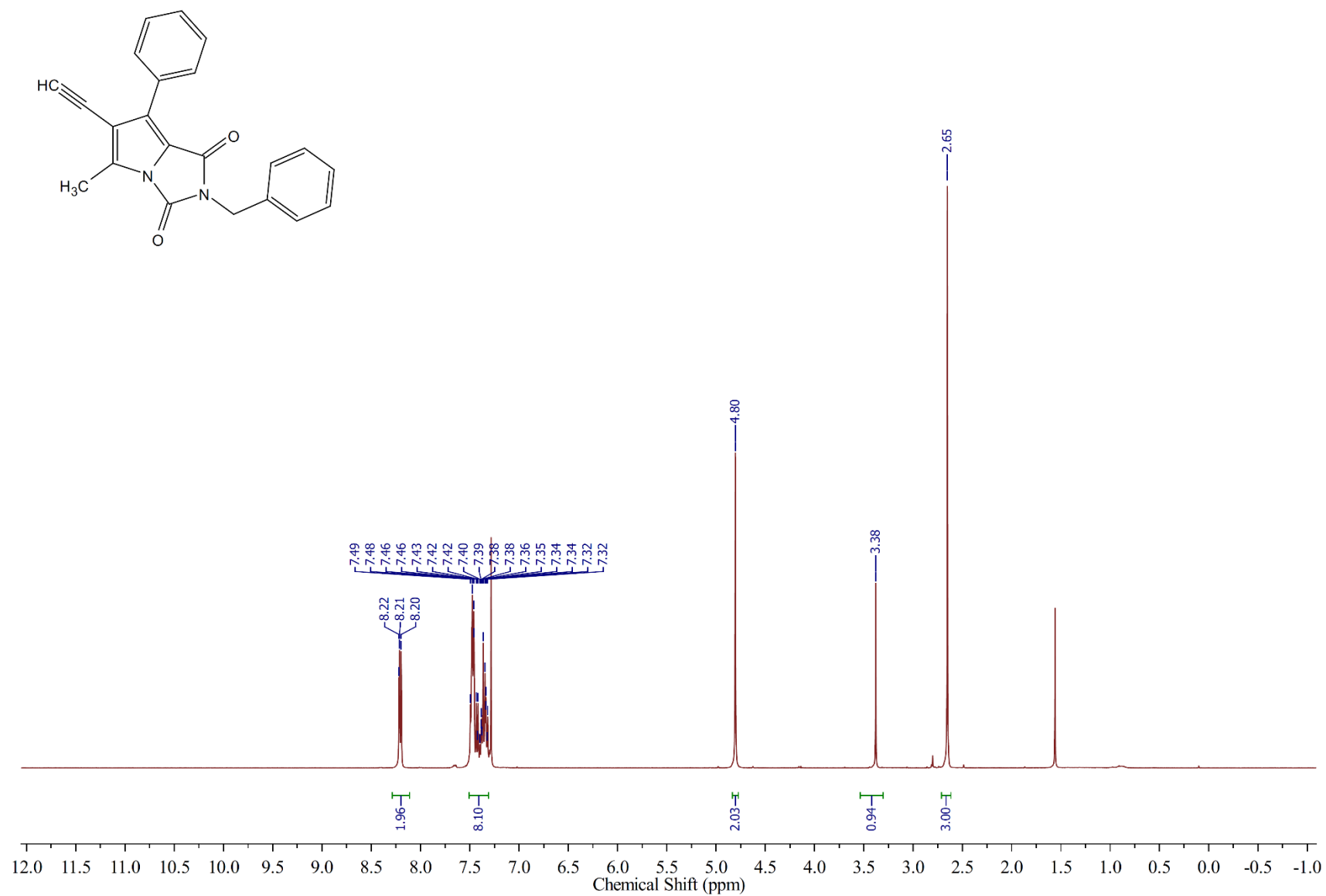
6-Acetyl-7-(4-chlorophenyl)-5-methyl-2-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10m, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



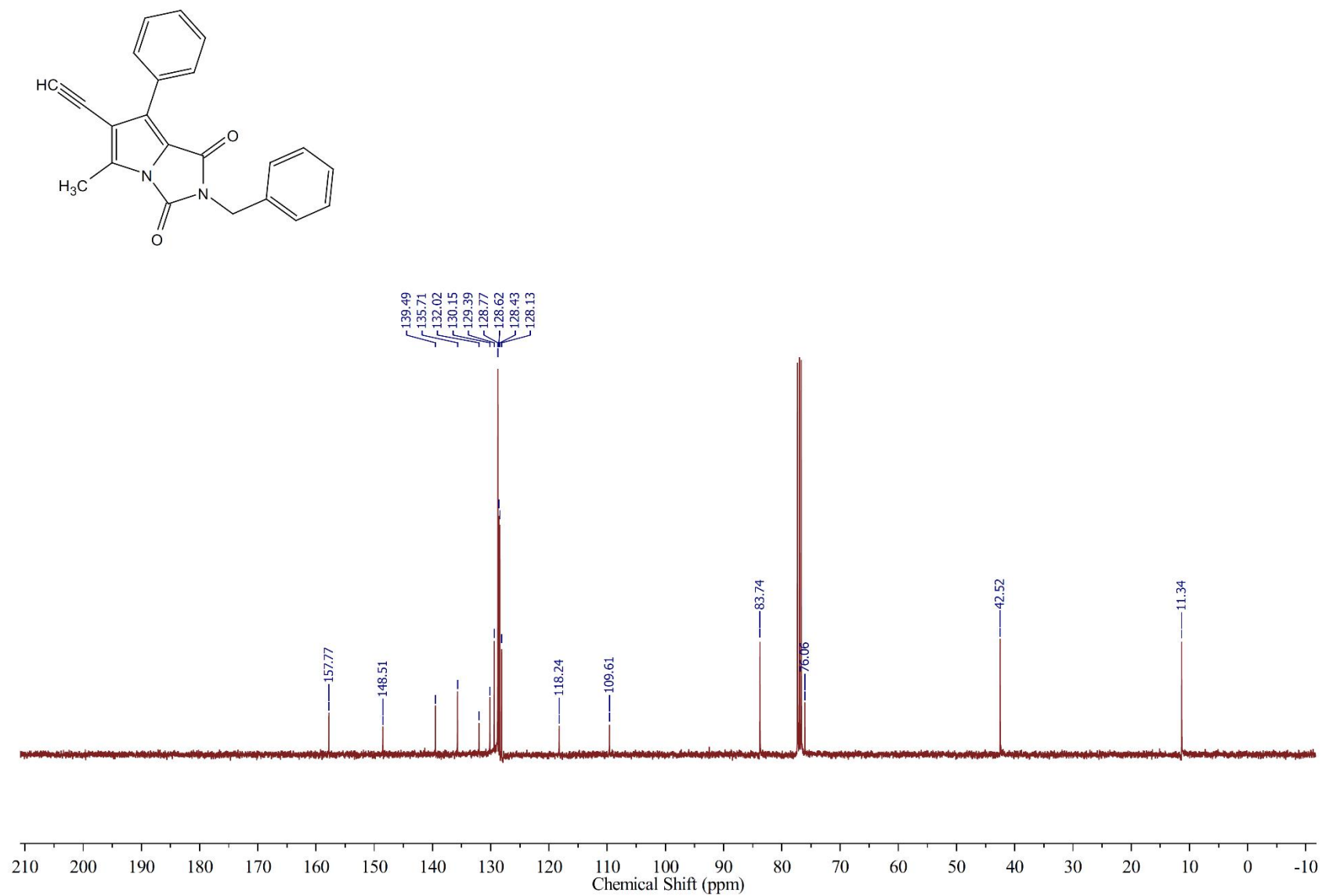
6-Acetyl-7-(4-chlorophenyl)-5-methyl-2-phenyl-3-thioxo-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-one 10m, DEPT, CDCl₃, 100 MHz



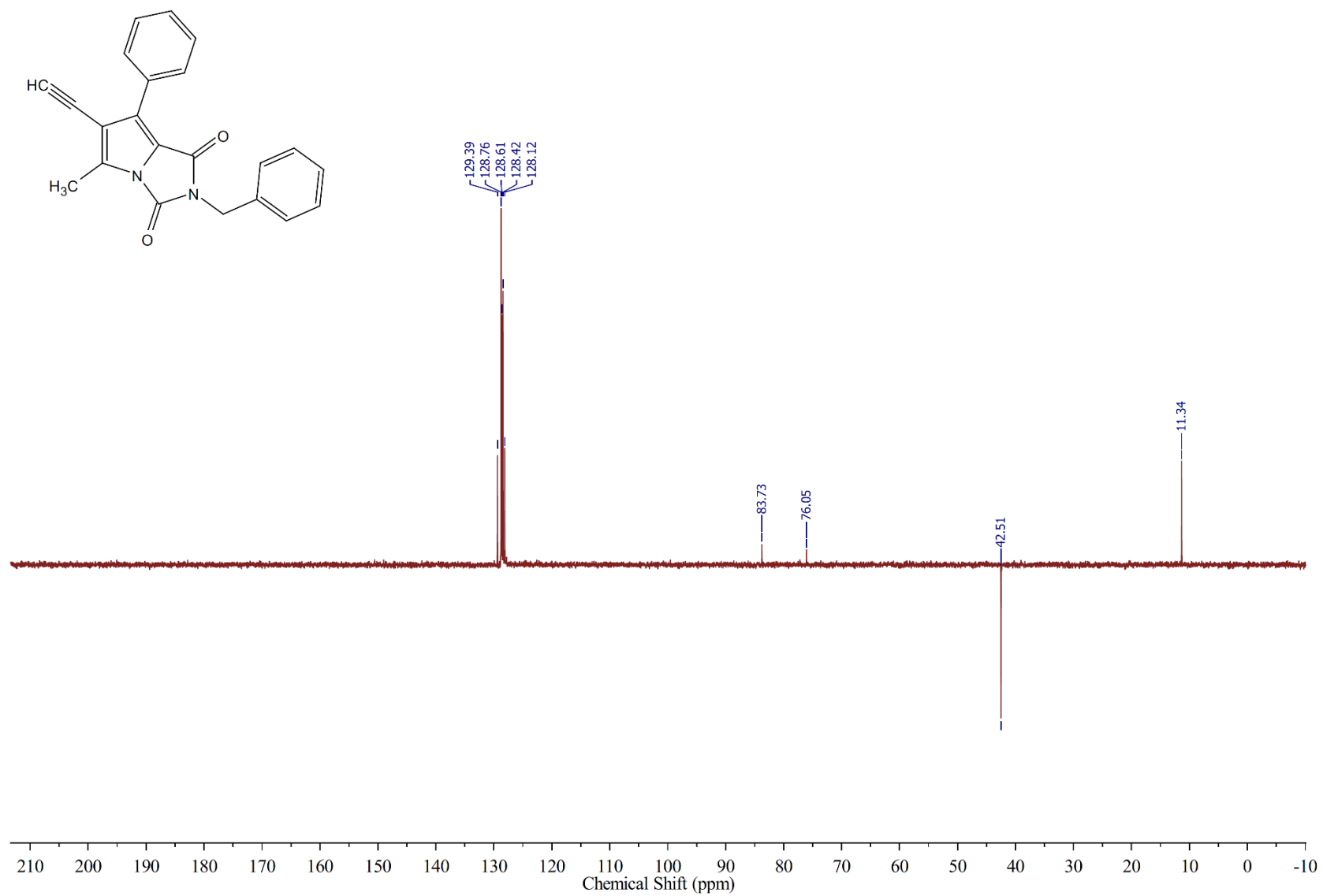
2-Benzyl-6-ethynyl-5-methyl-7-phenyl-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 11, ¹H NMR, CDCl₃, 400 MHz



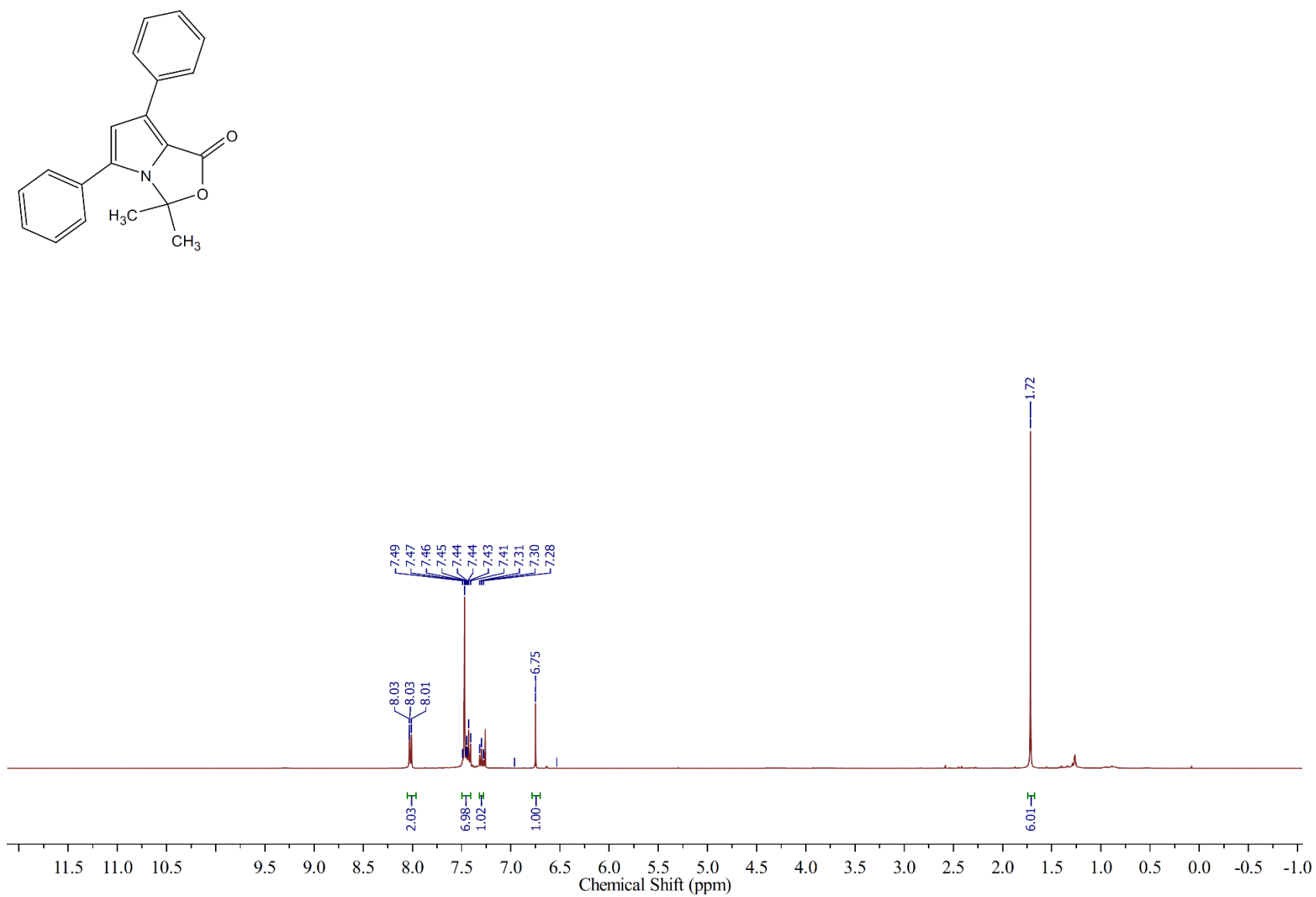
2-Benzyl-6-ethynyl-5-methyl-7-phenyl-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 11, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



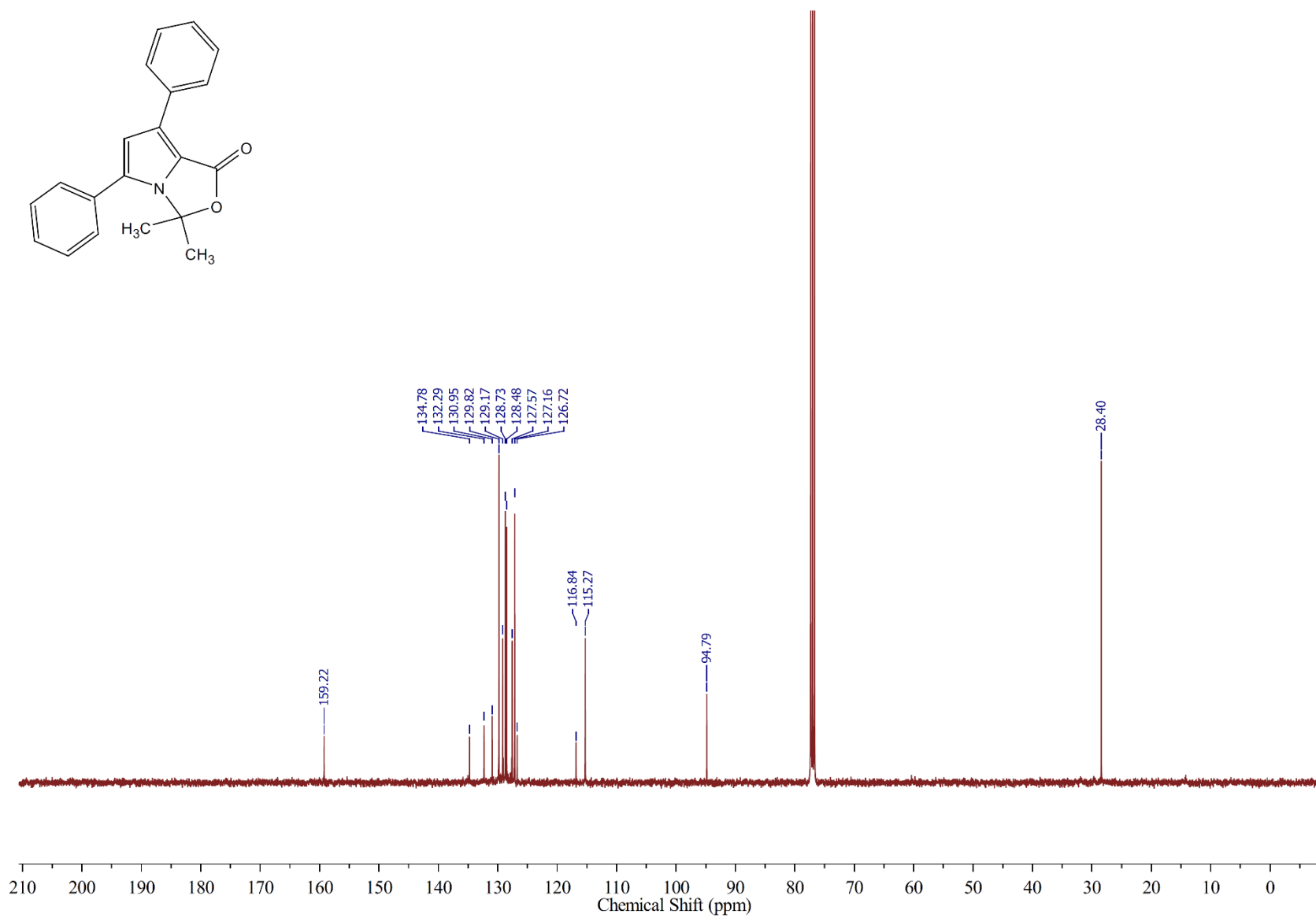
2-Benzyl-6-ethynyl-5-methyl-7-phenyl-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 11, DEPT, CDCl₃, 100 MHz



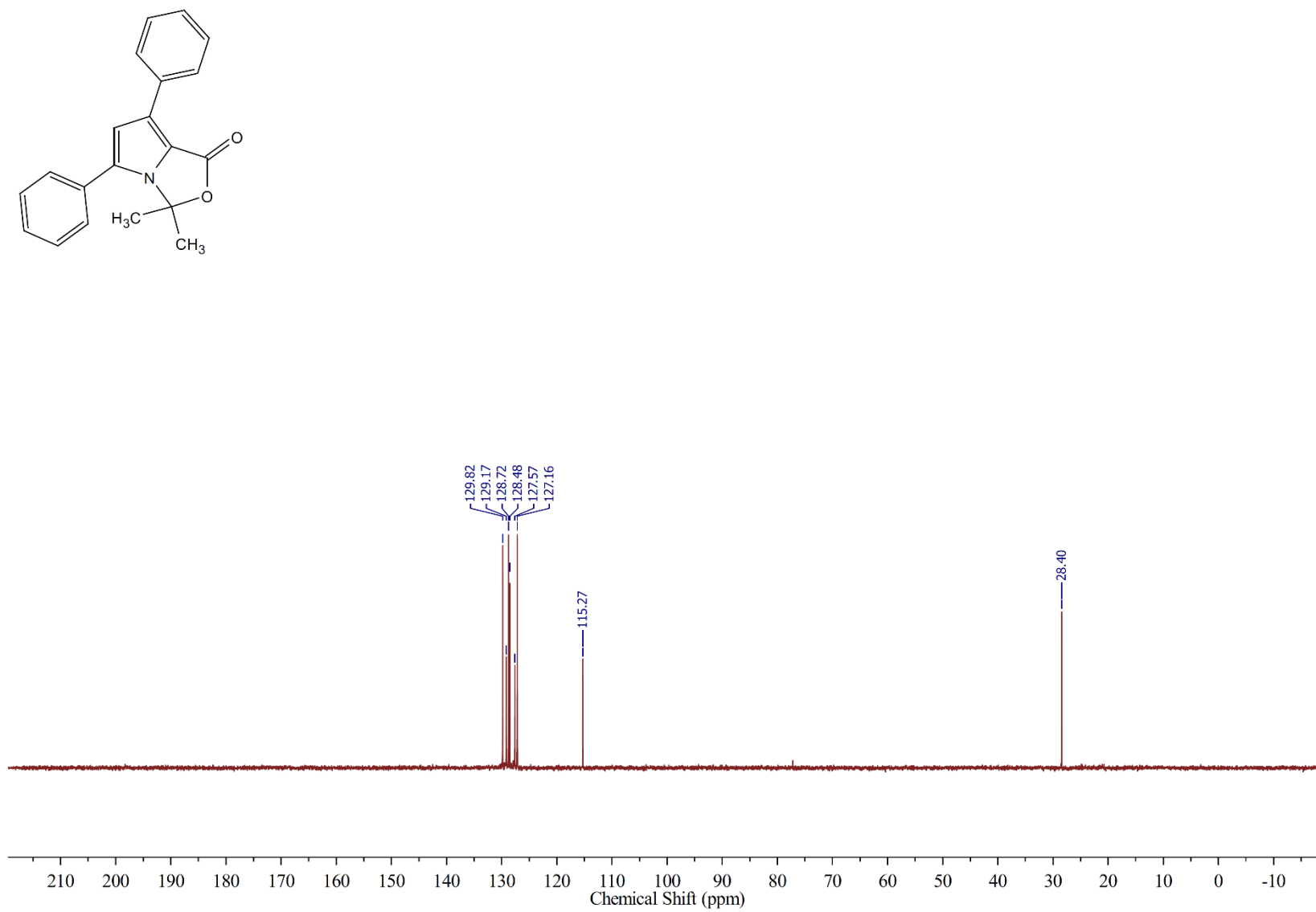
3,3-Dimethyl-5,7-diphenylpyrrolo[1,2-c]oxazol-1(3H)-one 12, ^1H NMR, CDCl_3 , 400 MHz



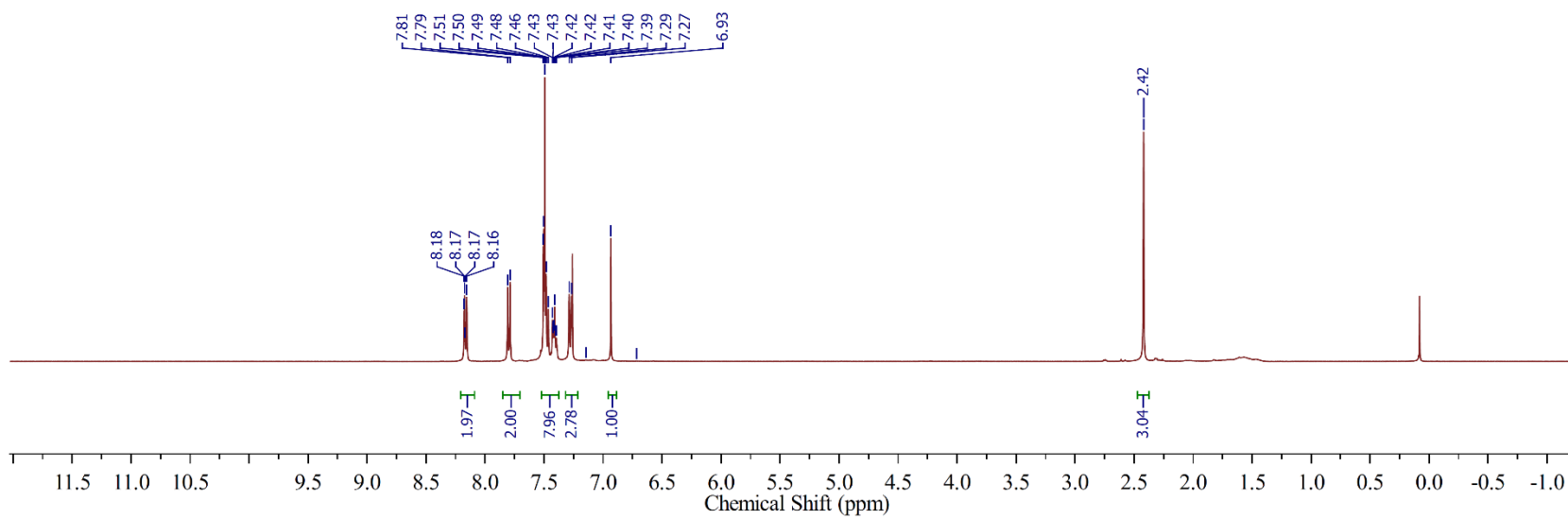
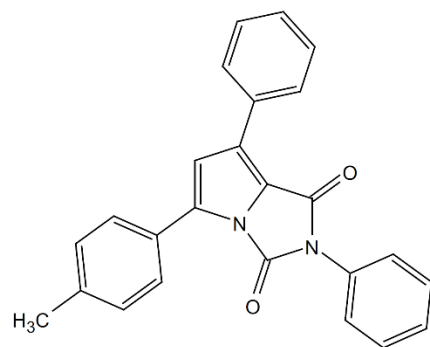
3,3-Dimethyl-5,7-diphenylpyrrolo[1,2-*c*]oxazol-1(3*H*)-one 12, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



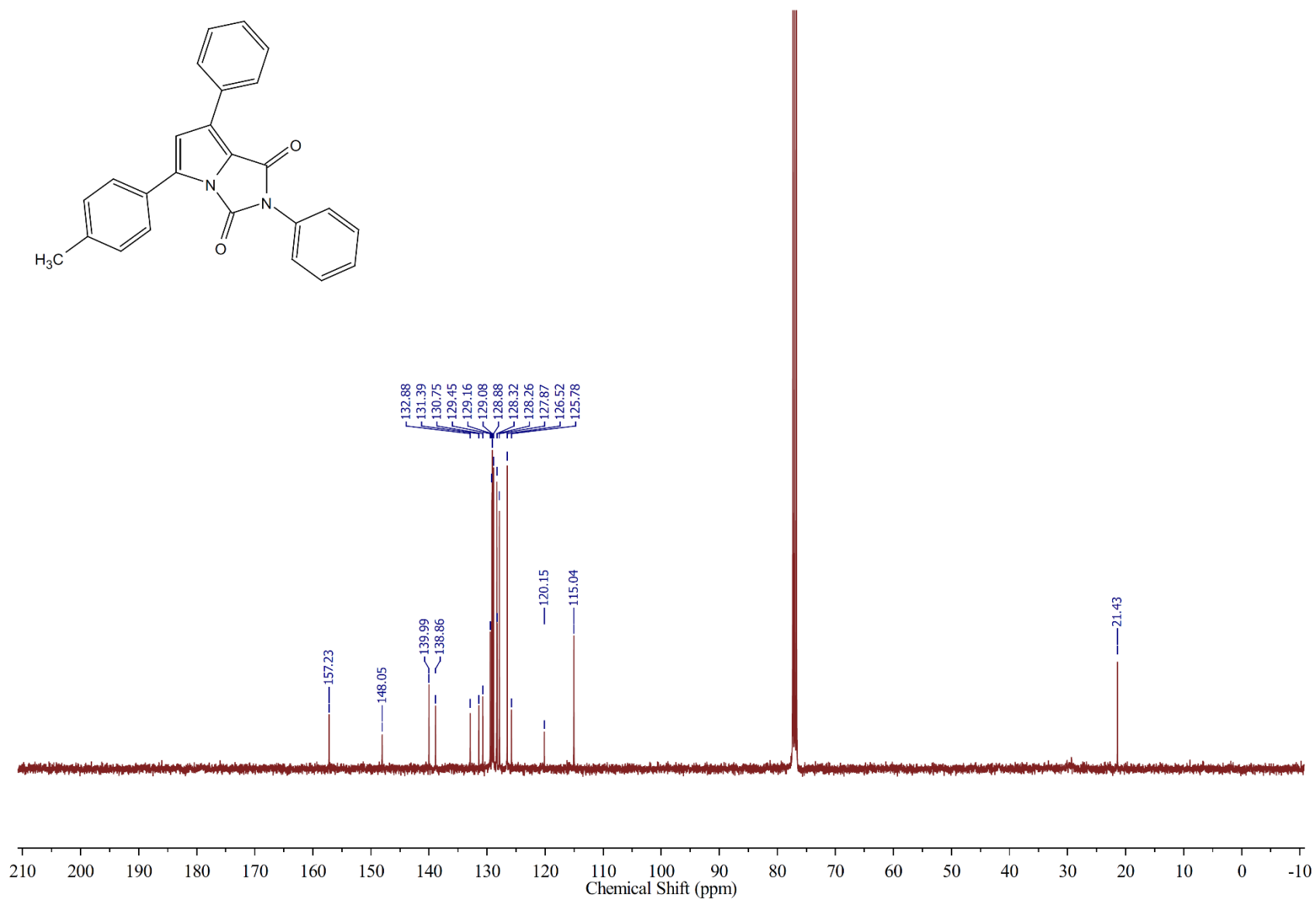
3,3-Dimethyl-5,7-diphenylpyrrolo[1,2-*c*]oxazol-1(3*H*)-one 12, DEPT, CDCl₃, 100 MHz



2,7-Diphenyl-5-(*p*-tolyl)-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 13, ¹H NMR, CDCl₃, 400 MHz



2,7-Diphenyl-5-(*p*-tolyl)-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 13, $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3 , 100 MHz



2,7-Diphenyl-5-(*p*-tolyl)-1*H*-pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 13, DEPT, CDCl₃, 100 MHz

