Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Highly *α*-position regioselective ring-opening of epoxides catalyzed by halohydrin dehalogenase from *Ilumatobacter coccineus*: a biocatalytic approach to 2-azido-2-aryl-1-ols

Authors:

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1. General experimental information

Column chromatography was performed on silica gel (200-400 mesh). TLC was performed on silica gel. ^{1}H NMR (400 MHz) chemical shifts were reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard. Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublets, dq = doublet of quartets, qd = quartet of doublets, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR (100 MHz) chemical shifts were reported in ppm (δ) from tetramethylsilane (TMS) with the solvent resonance as the internal standard.

Chemicals epoxides **1a**, **1f**, **1g**, **1h** were purchased from J&K Chemical (Shanghai, China). The other epoxides were prepared from olefins according to the reported procedures.[1] Isopropyl-β-D-thiogalactopyranoside (IPTG, >99%) and kanamycin sulfate salt (>99%) were purchased from Solarbio (Beijing, China). All the other biological, chemical reagents and solvents were obtained from commercial suppliers and used without further purification.

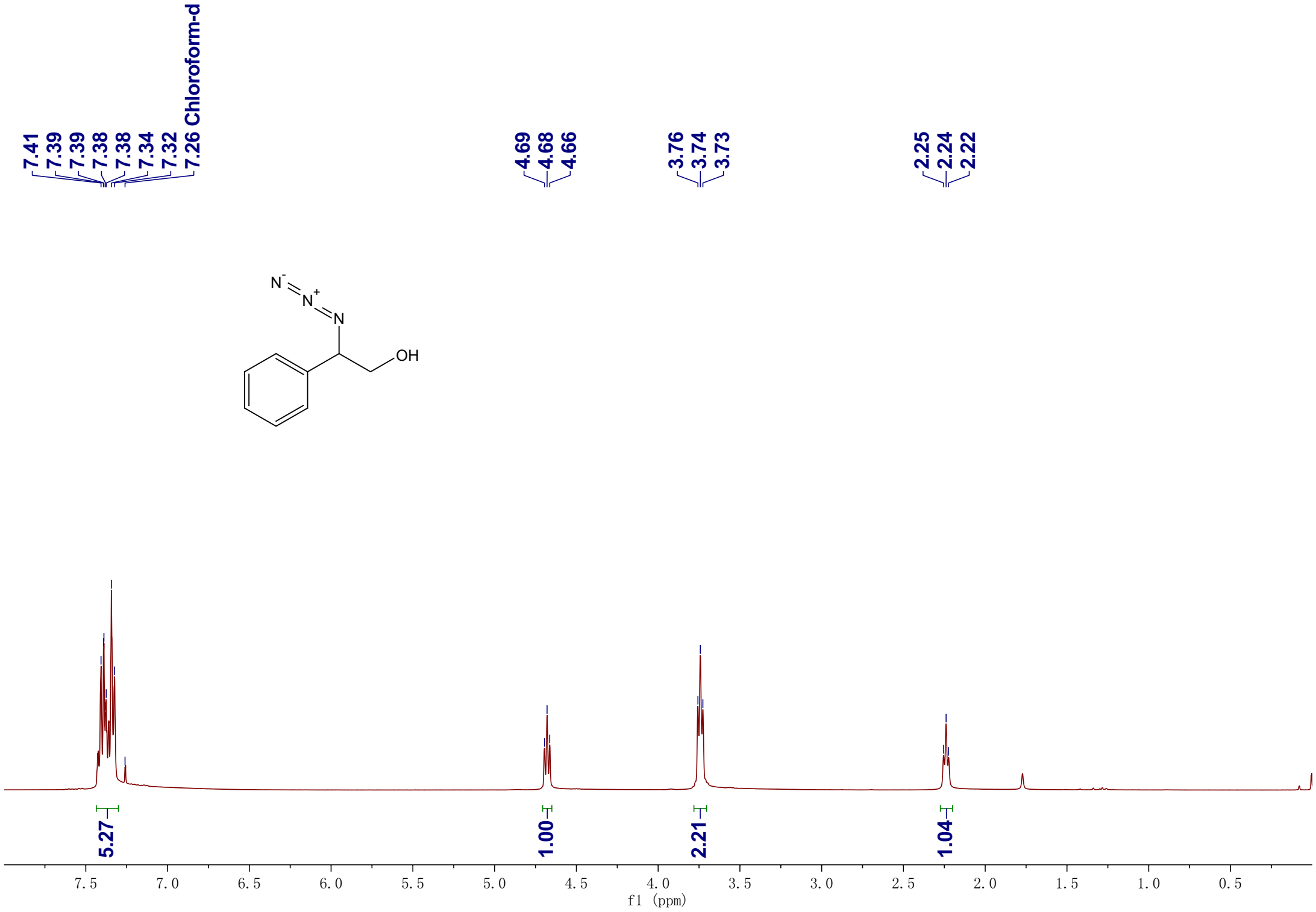
2. HPLC analysis method

The HPLC analysis was performed on SPD-M20A equipped with Chiralcel OJ-H chiral column (4.6 mmΦ×250 mmL) purchased from Daicel Chemical Industries. Analysis method for (*R*, *S*)-**2a**: 2-propanol:hexane = 5:95, 0.5 mL/min, 220 nm. The retention times for (*S*)-**2a** and (*R*)-**2a** were 25.5 min and 26.3 min, respectively.

3. Reference

1. Bernasconi S, Orsini F, Sello G, et al. Bacterial monooxygenase mediated preparation of nonracemic chiral oxiranes: study of the effects of substituent nature and position. Tetrahedron: Asymmetry, 2004, 15(10): 1603-1606.

4. NMR spectra of 2a-2k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3.74
3.73
2.25
2.24
2.22
N
N
N
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2.21
1.04
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7.0
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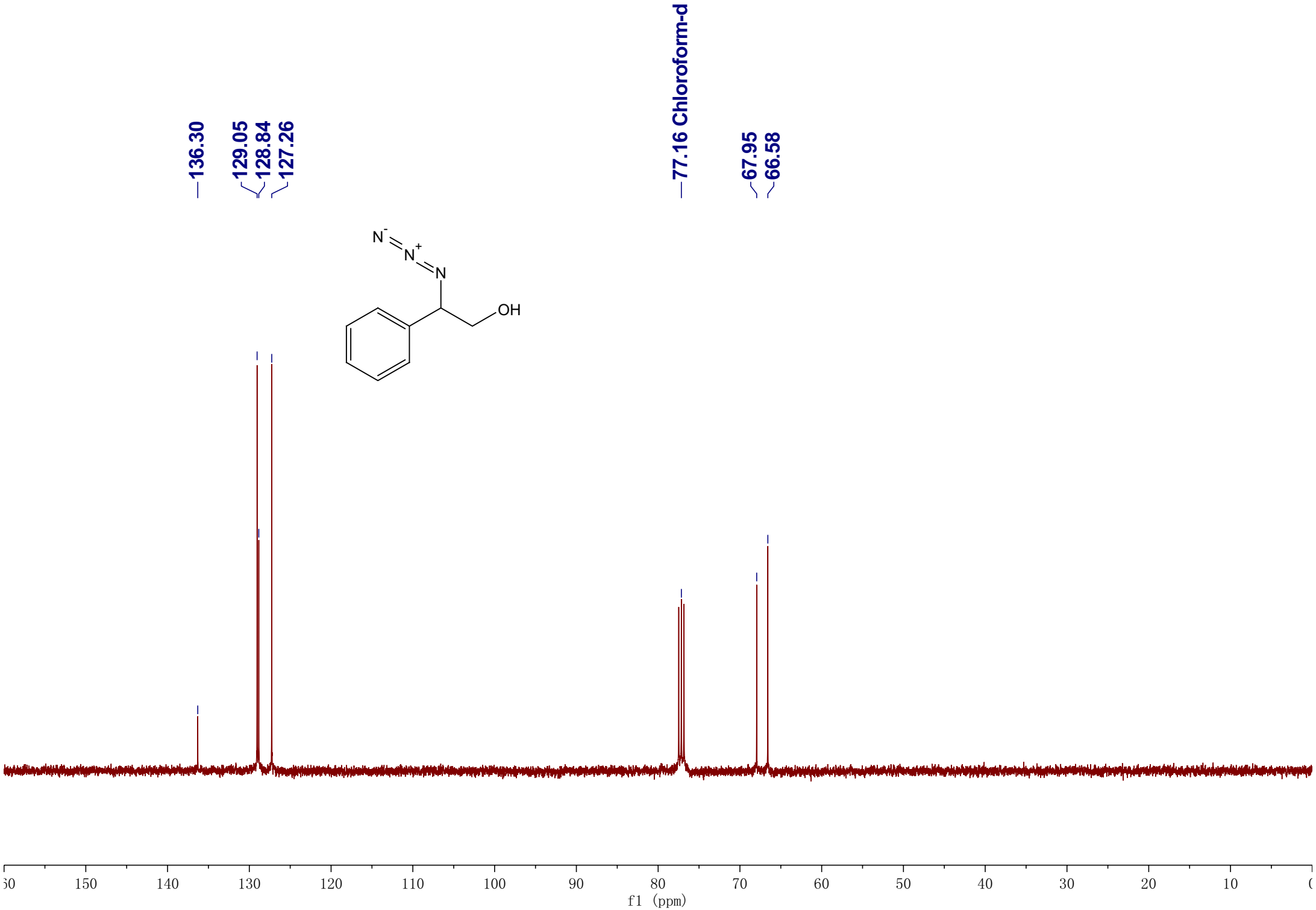
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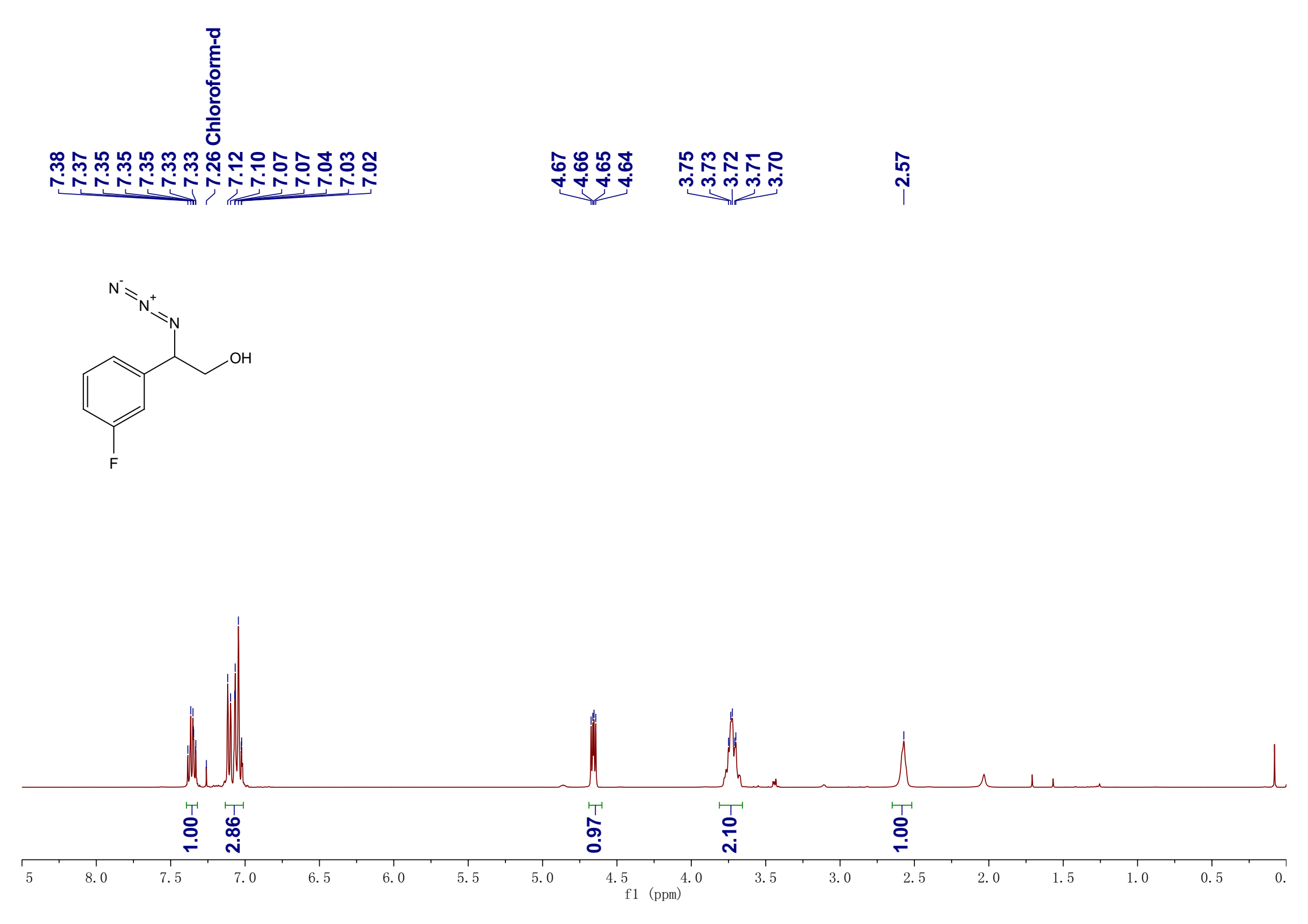
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7.04
7.03
7.02
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4.65
4.64
3.75
3.73
3.72
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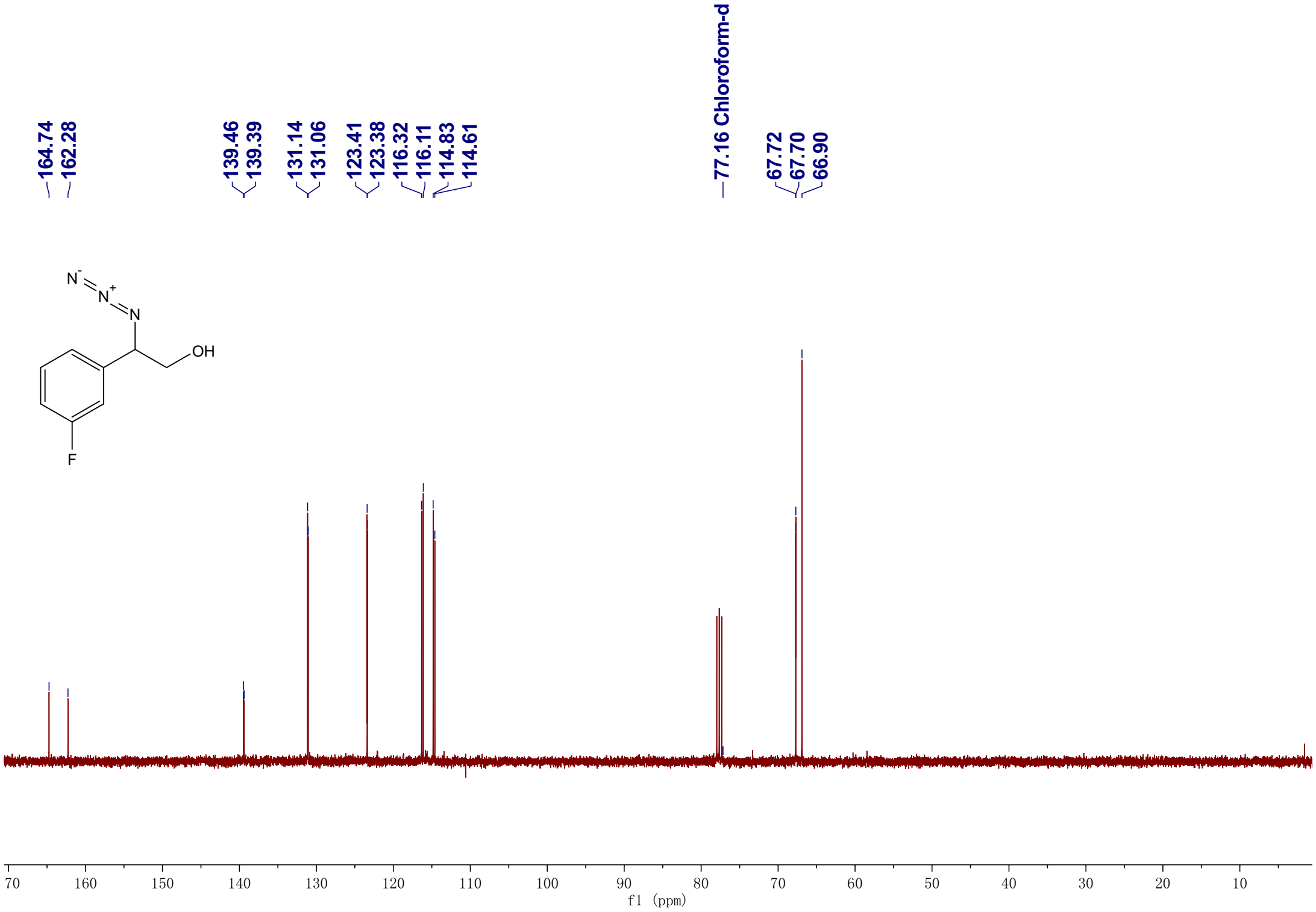
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67.72
67.70
66.90
N
N+
N
OH
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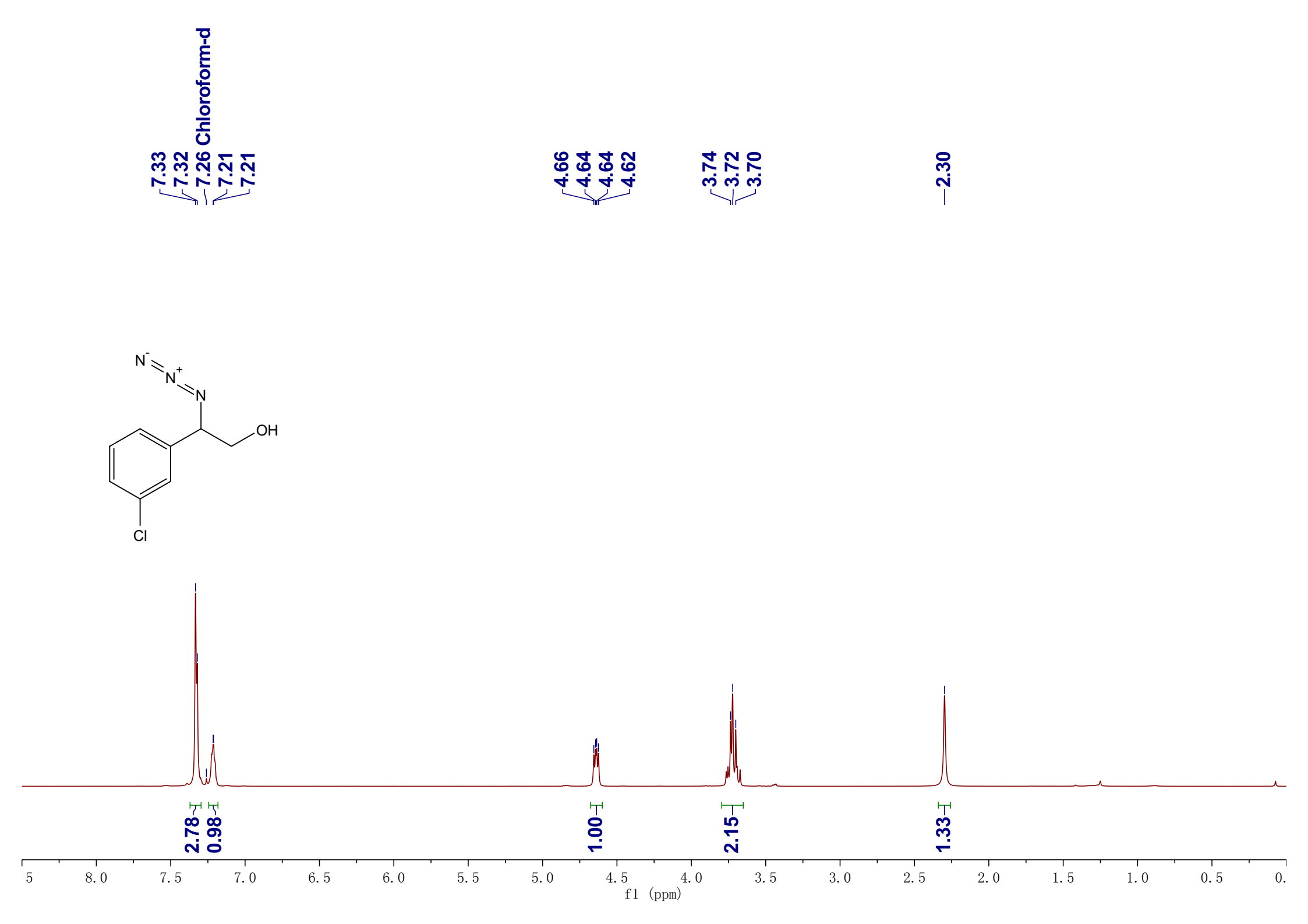
f1 (ppm)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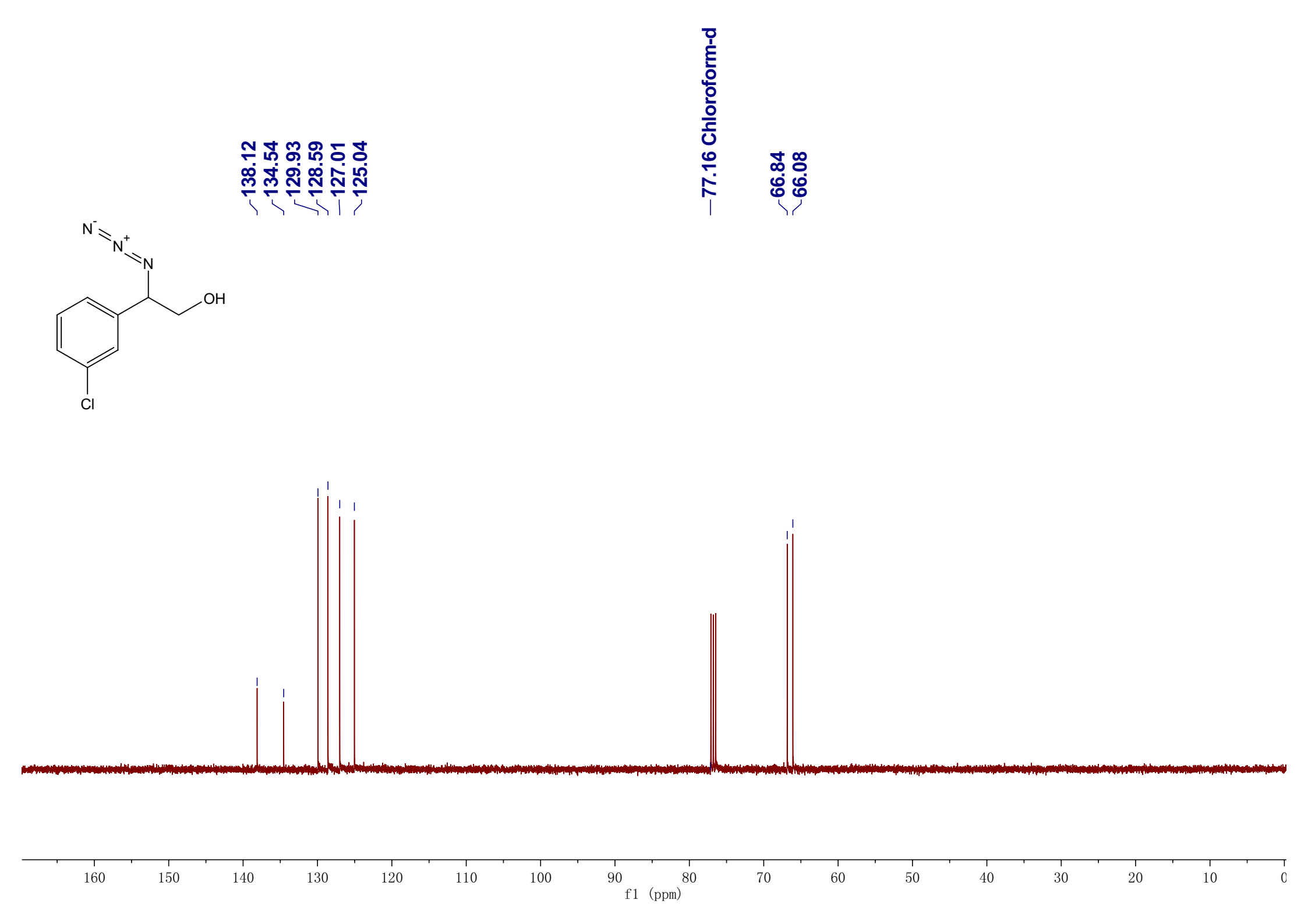
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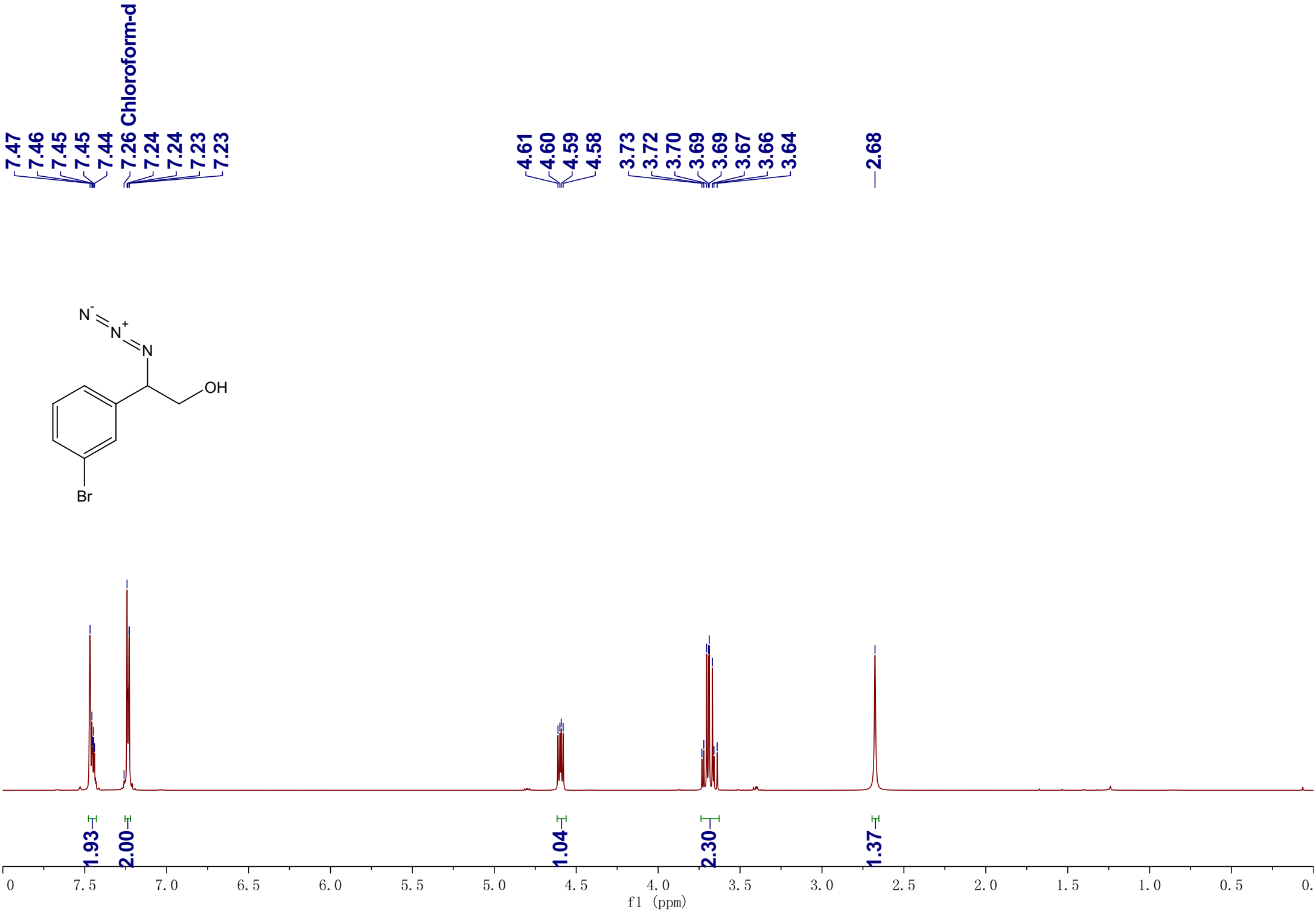
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3.72
3.70
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3.67
3.66
3.64
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OH
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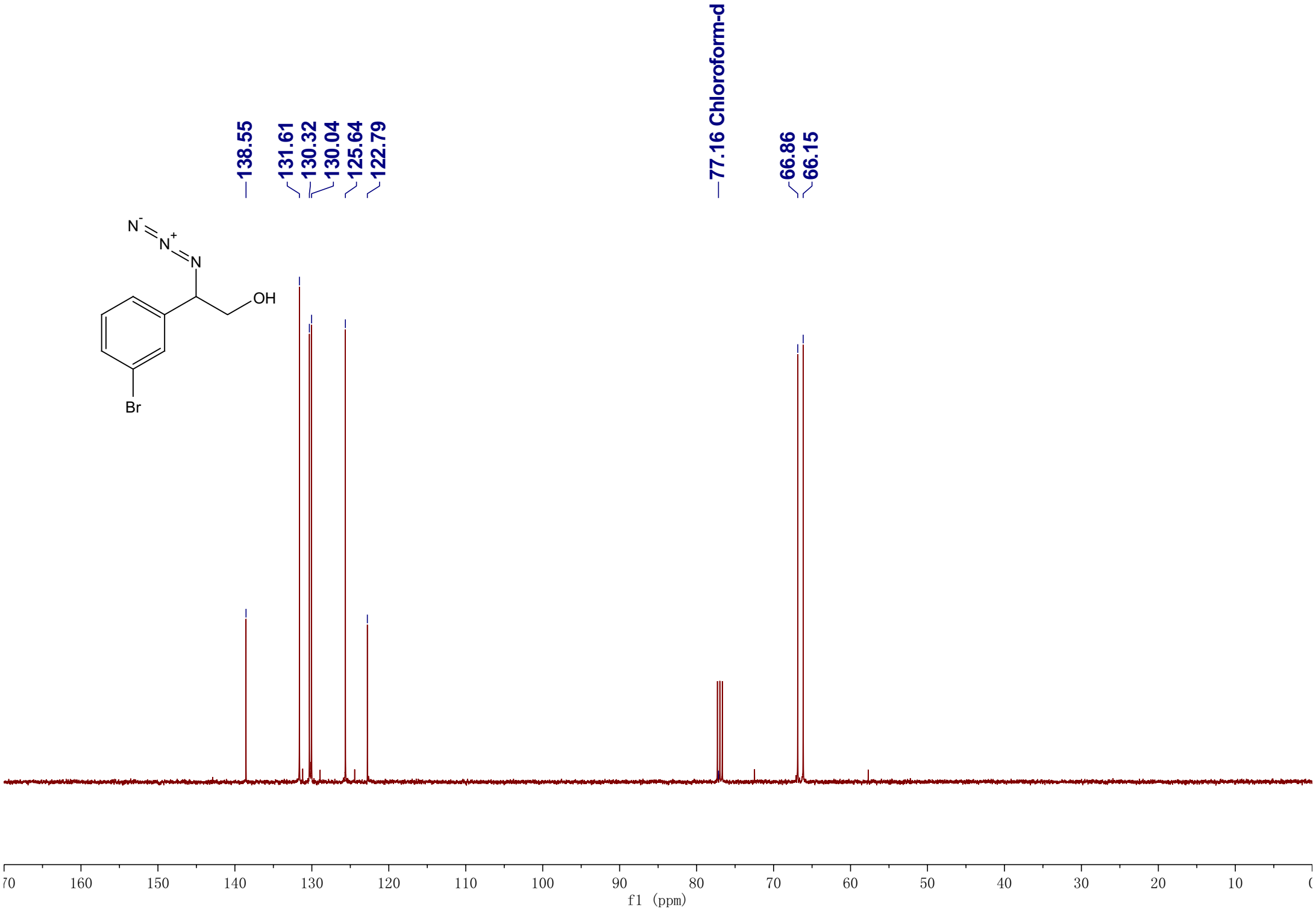
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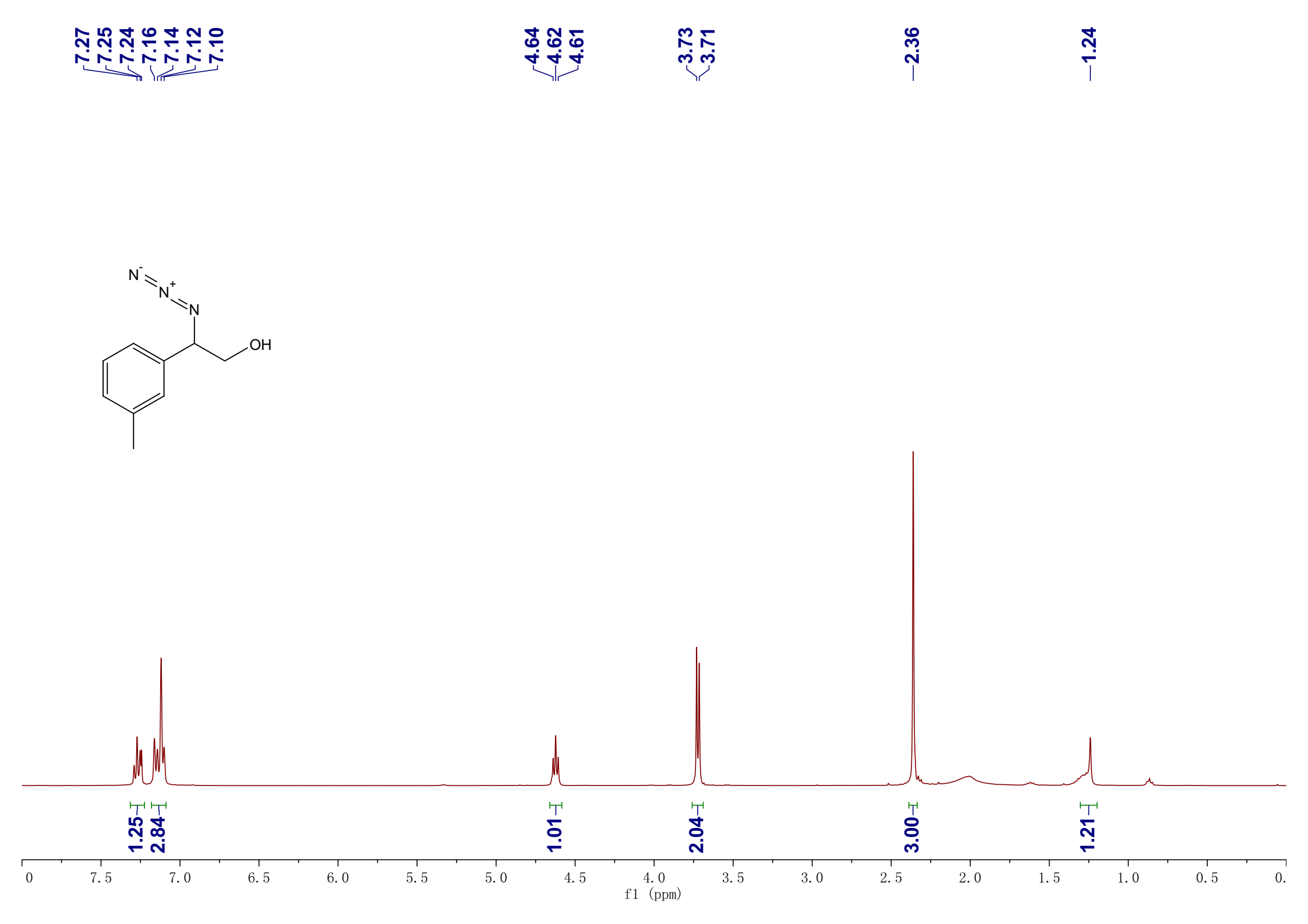
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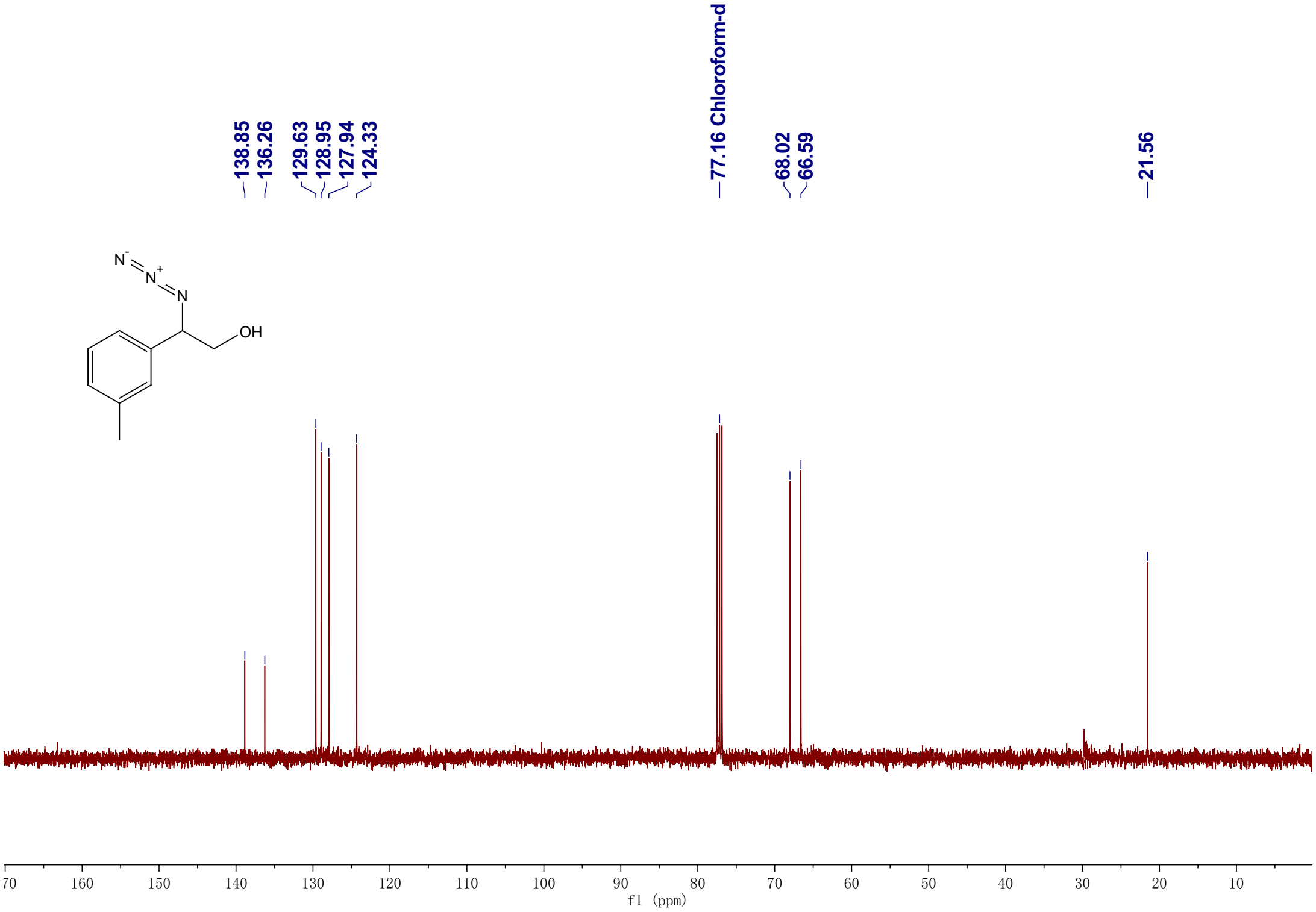
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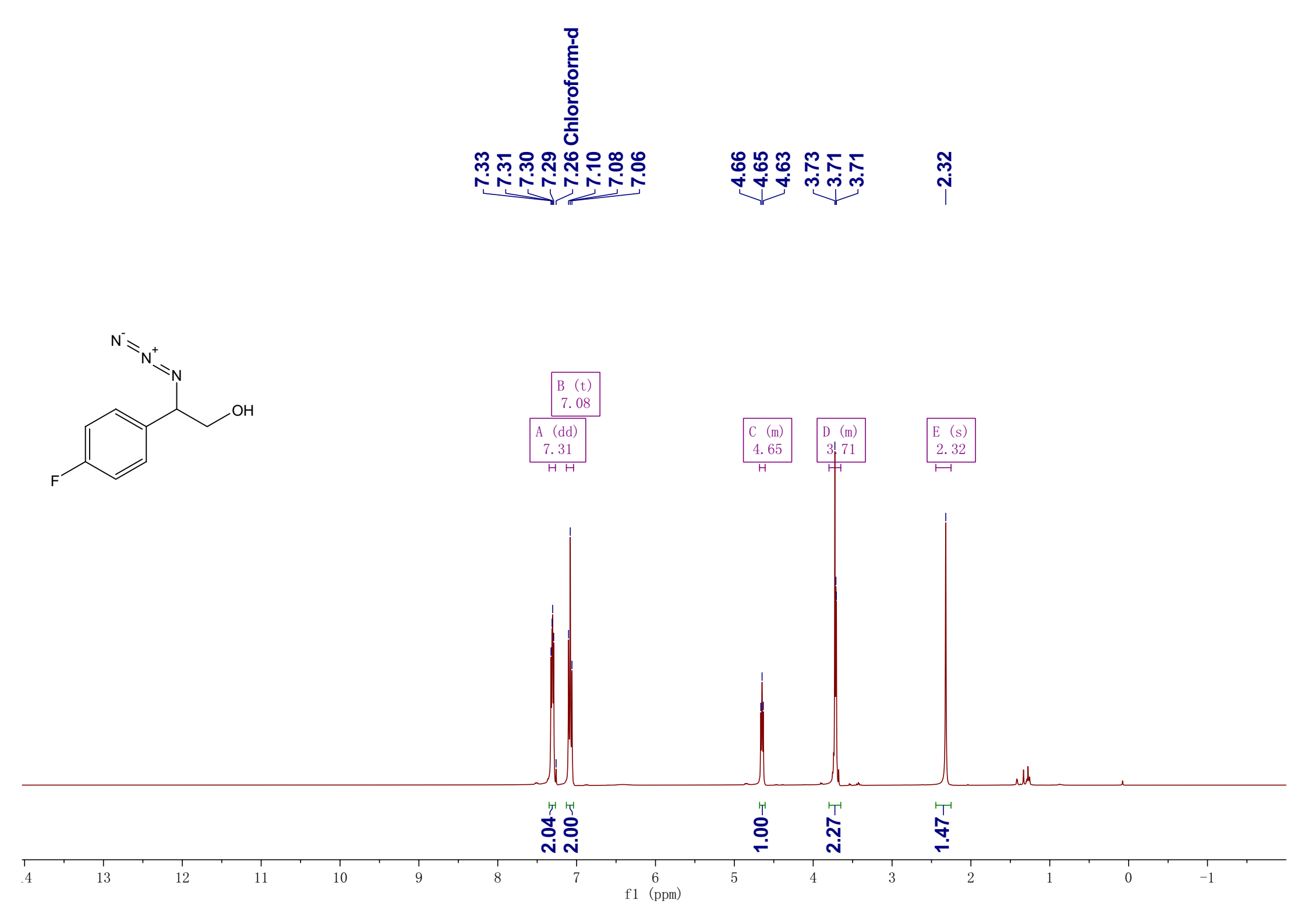
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3.73
3.71
3.71
2.32
B (t)
7.08
A (dd)
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C (m)
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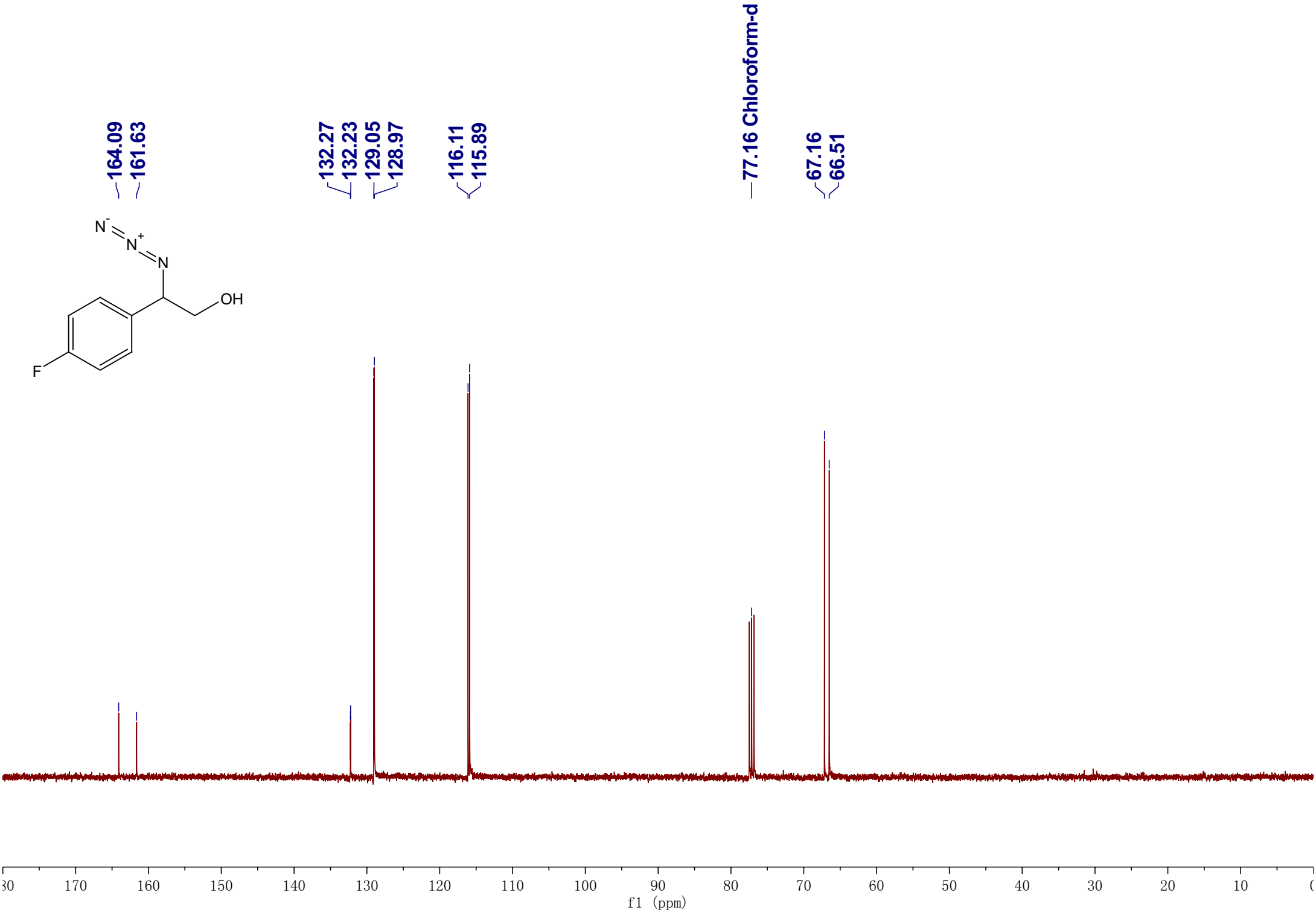
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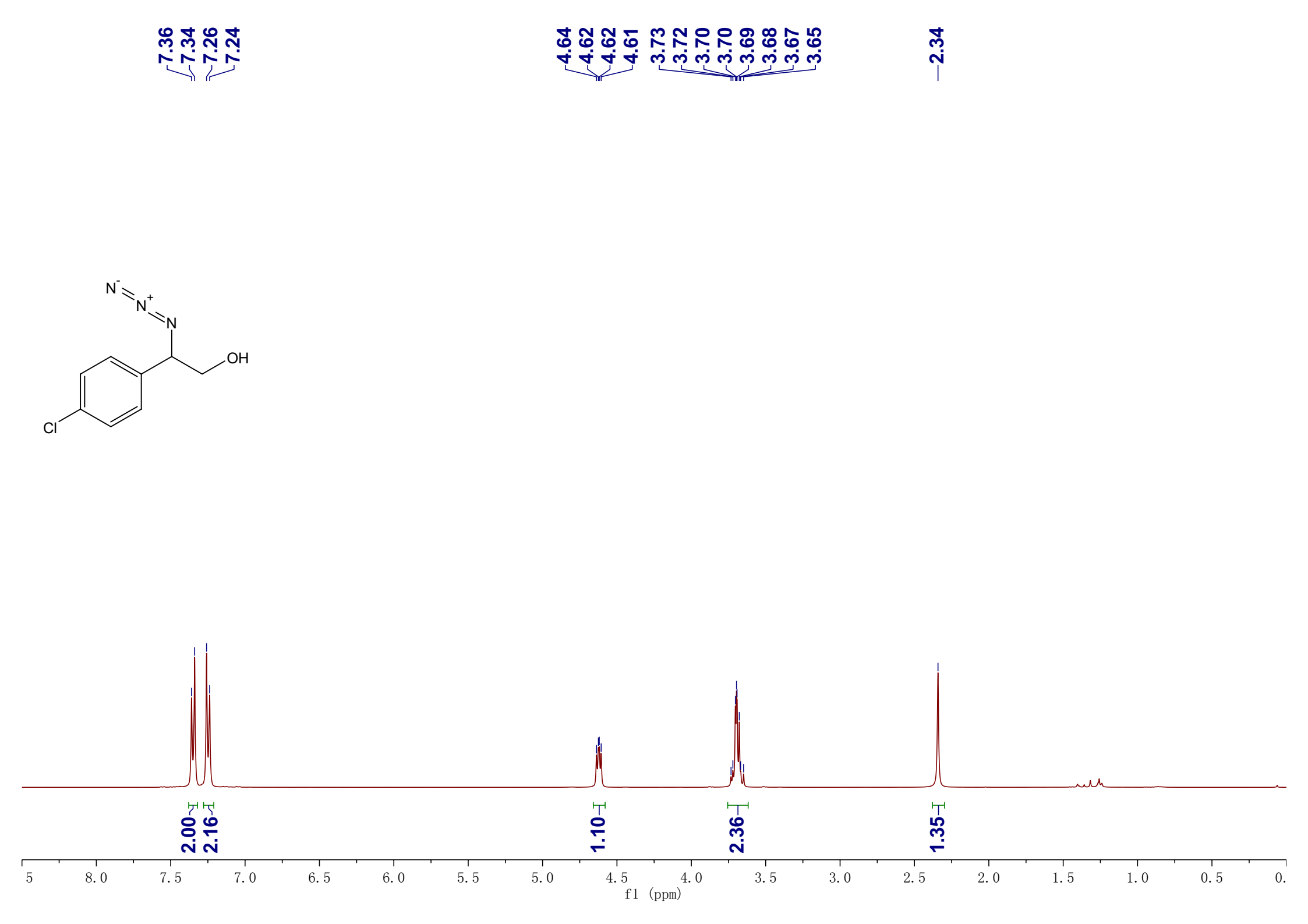
OH
F
f1 (ppm)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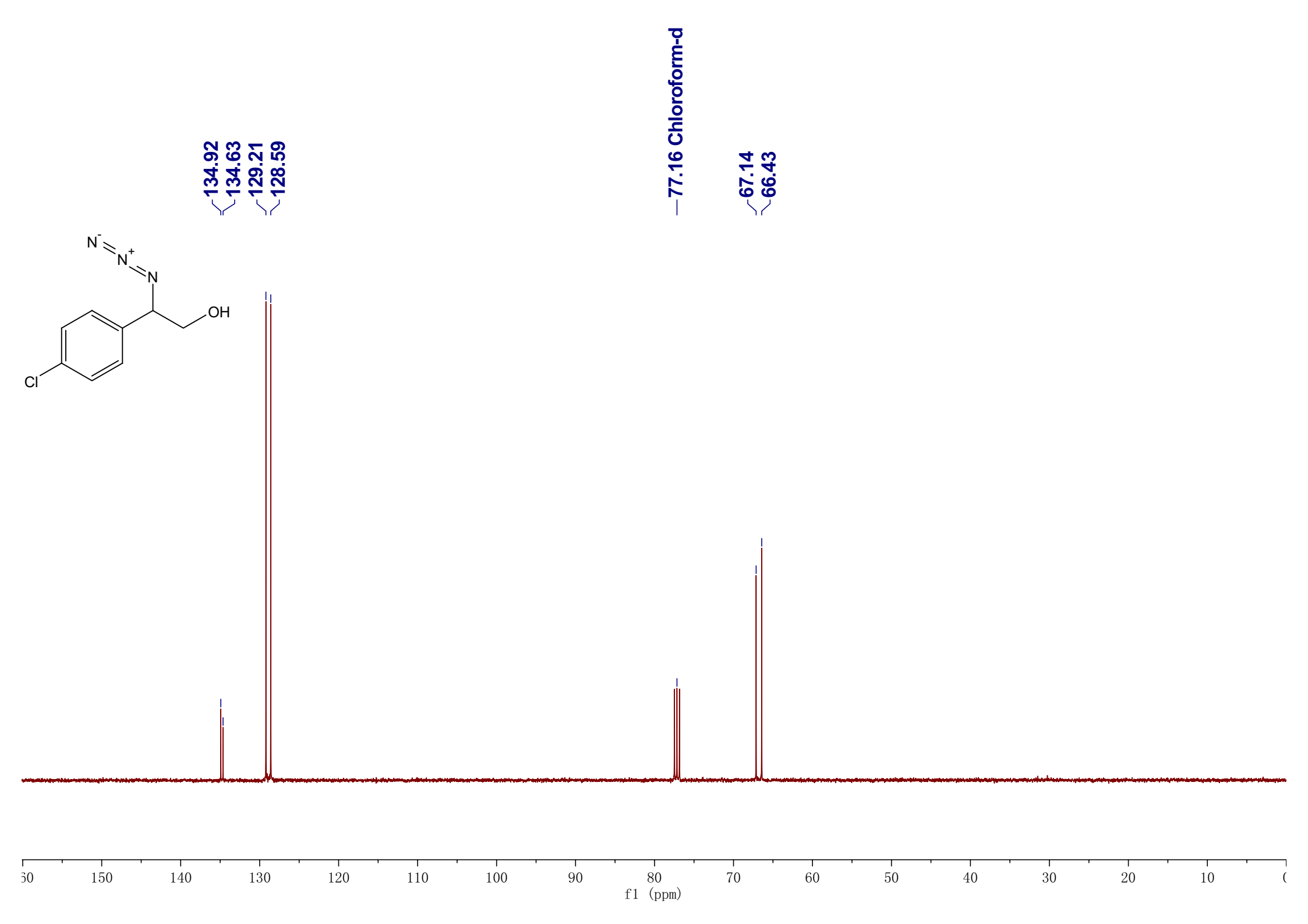
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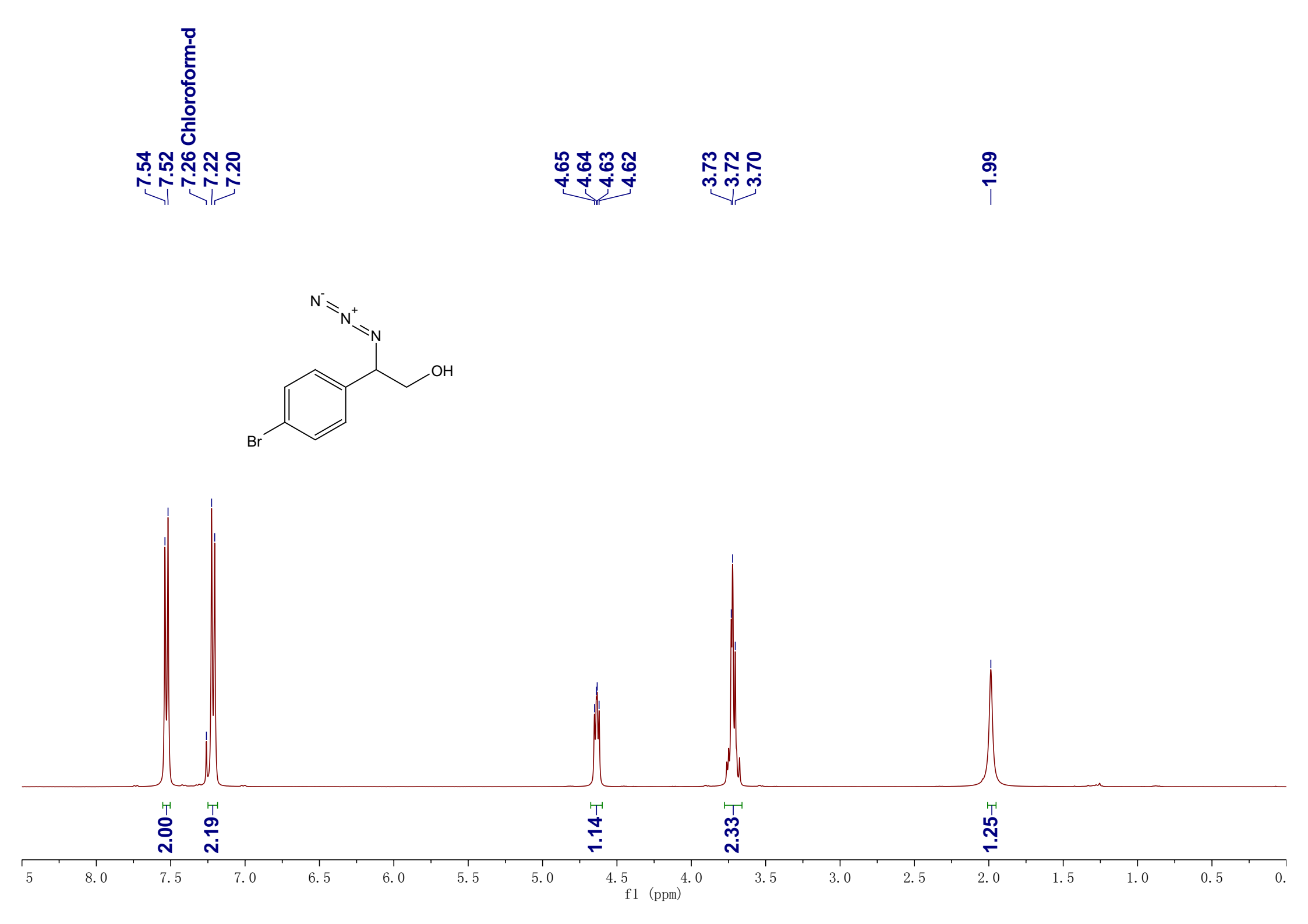
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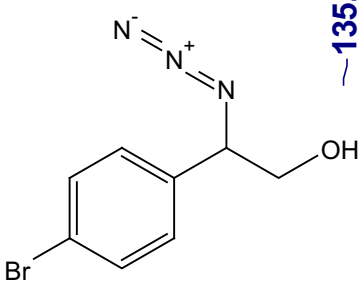

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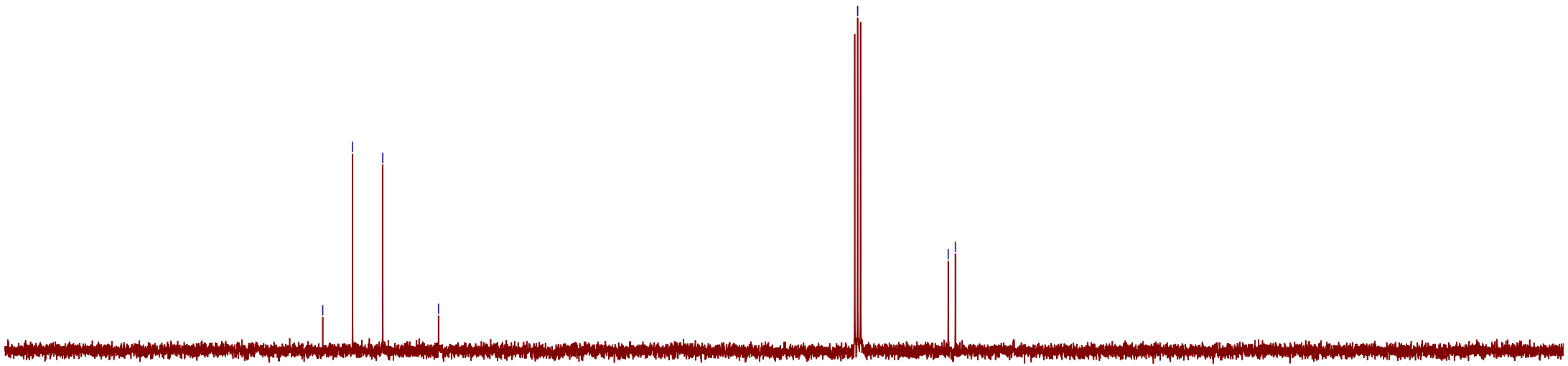

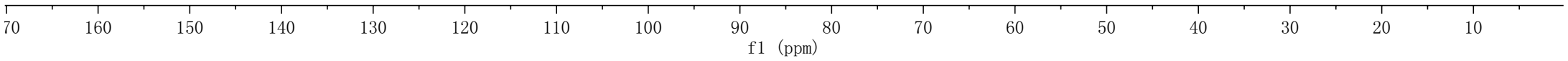

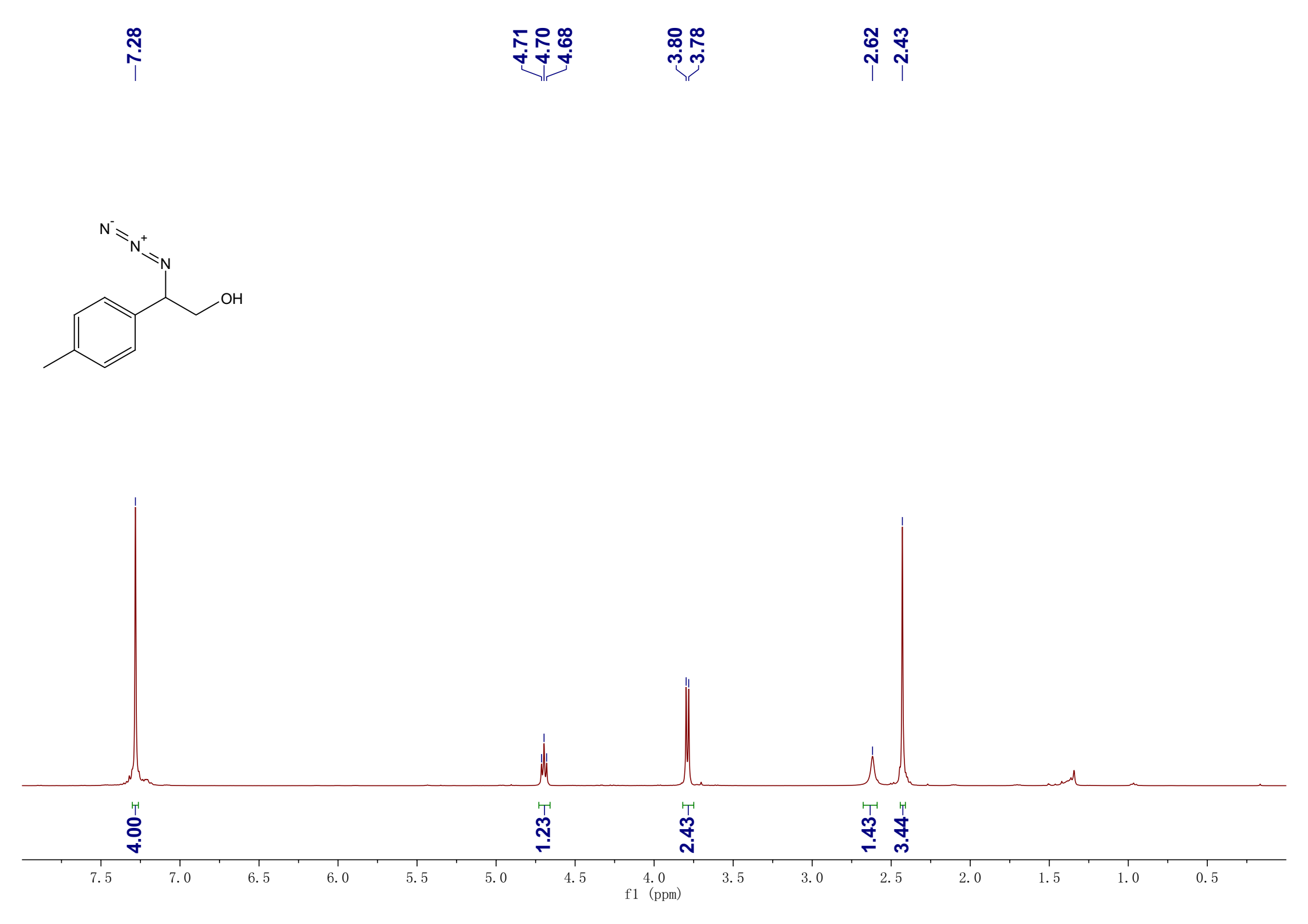
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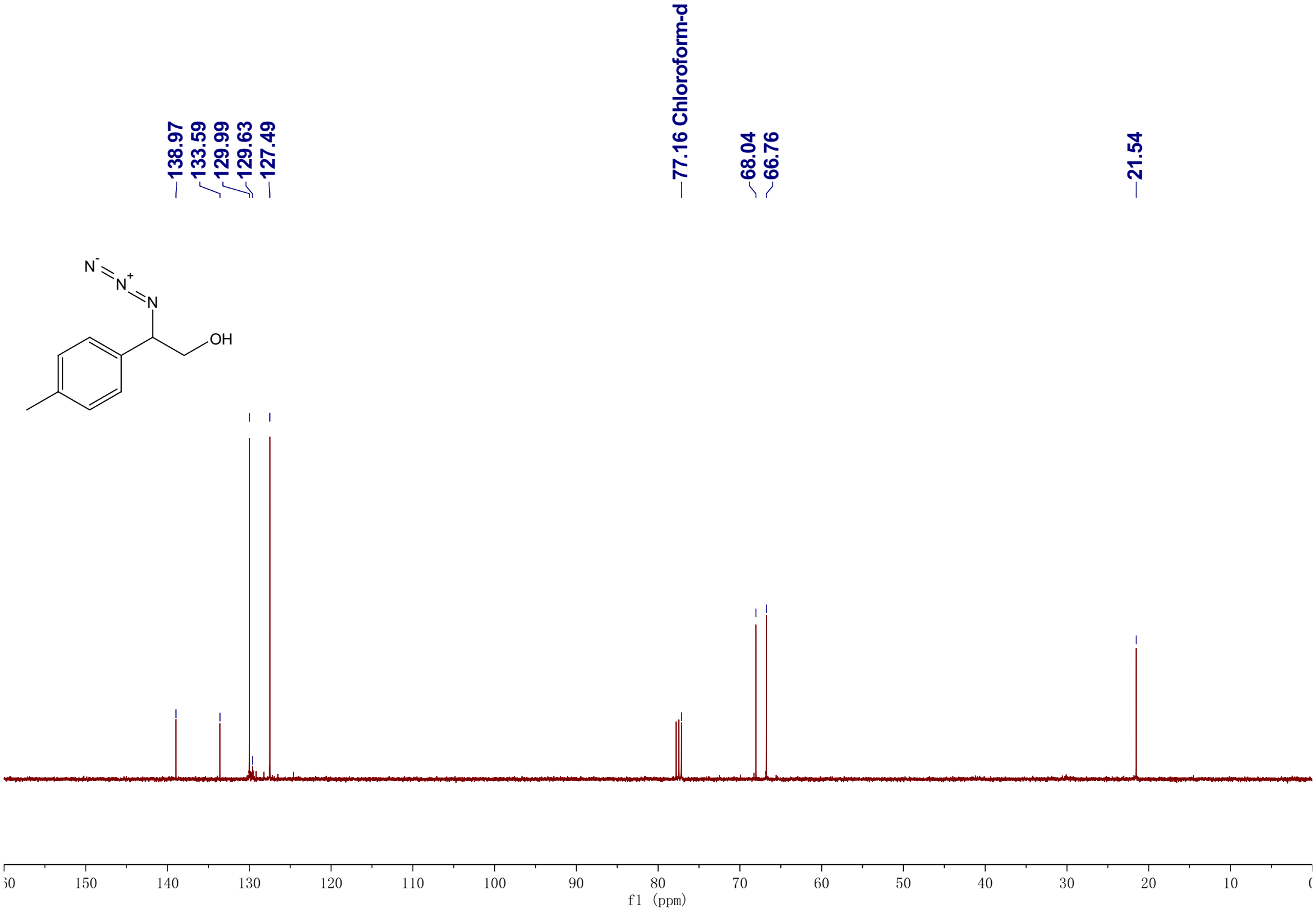
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10
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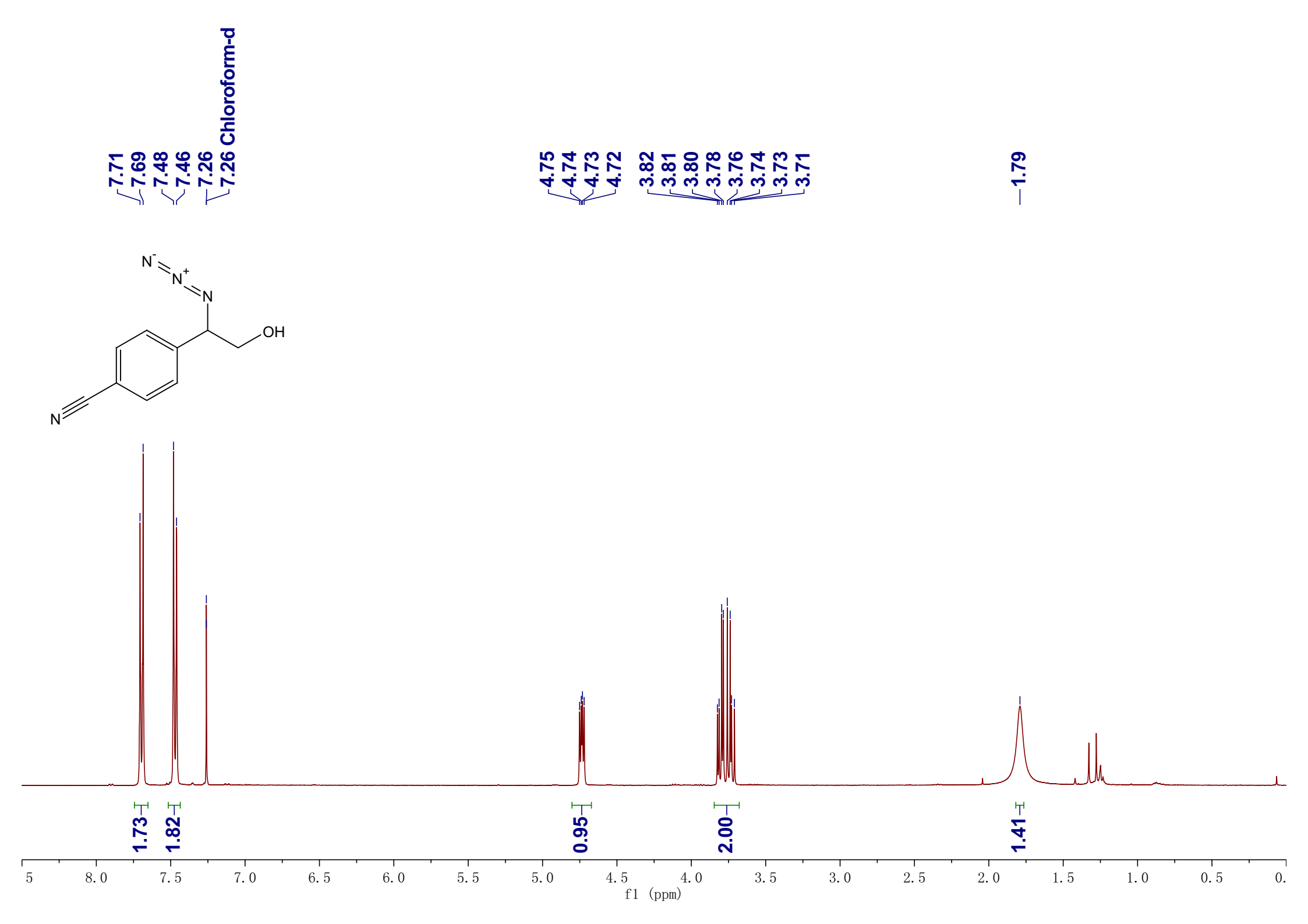
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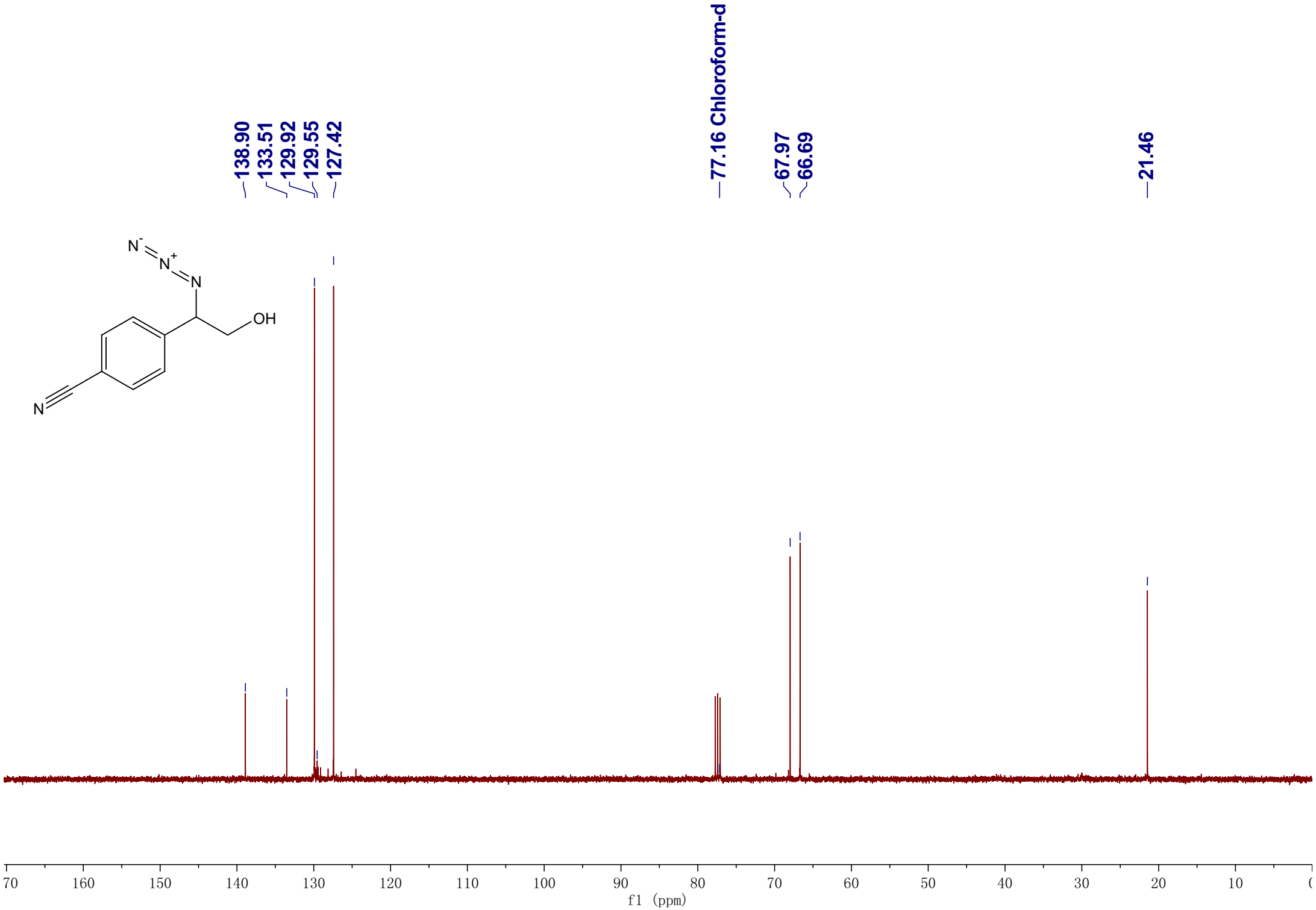
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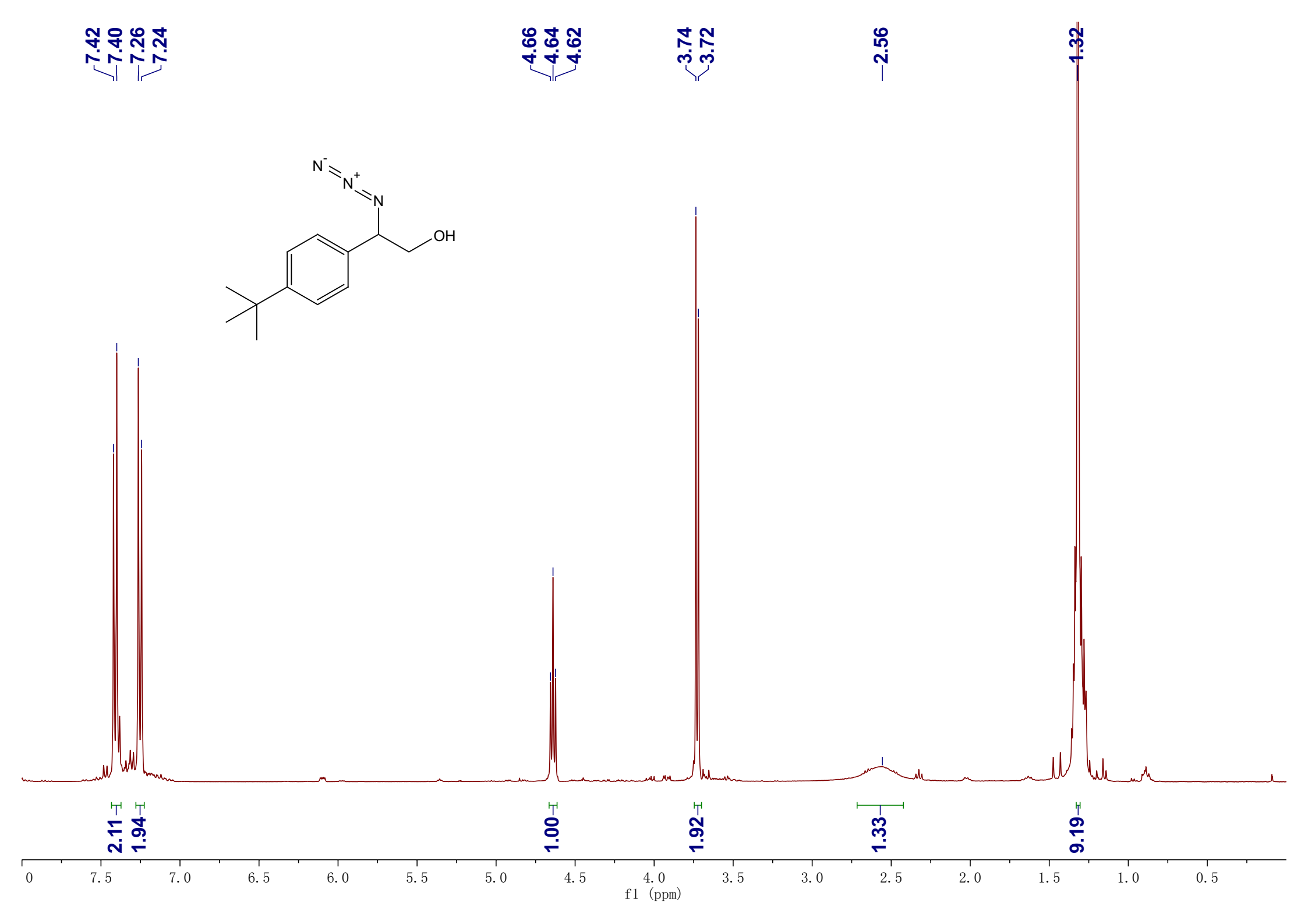
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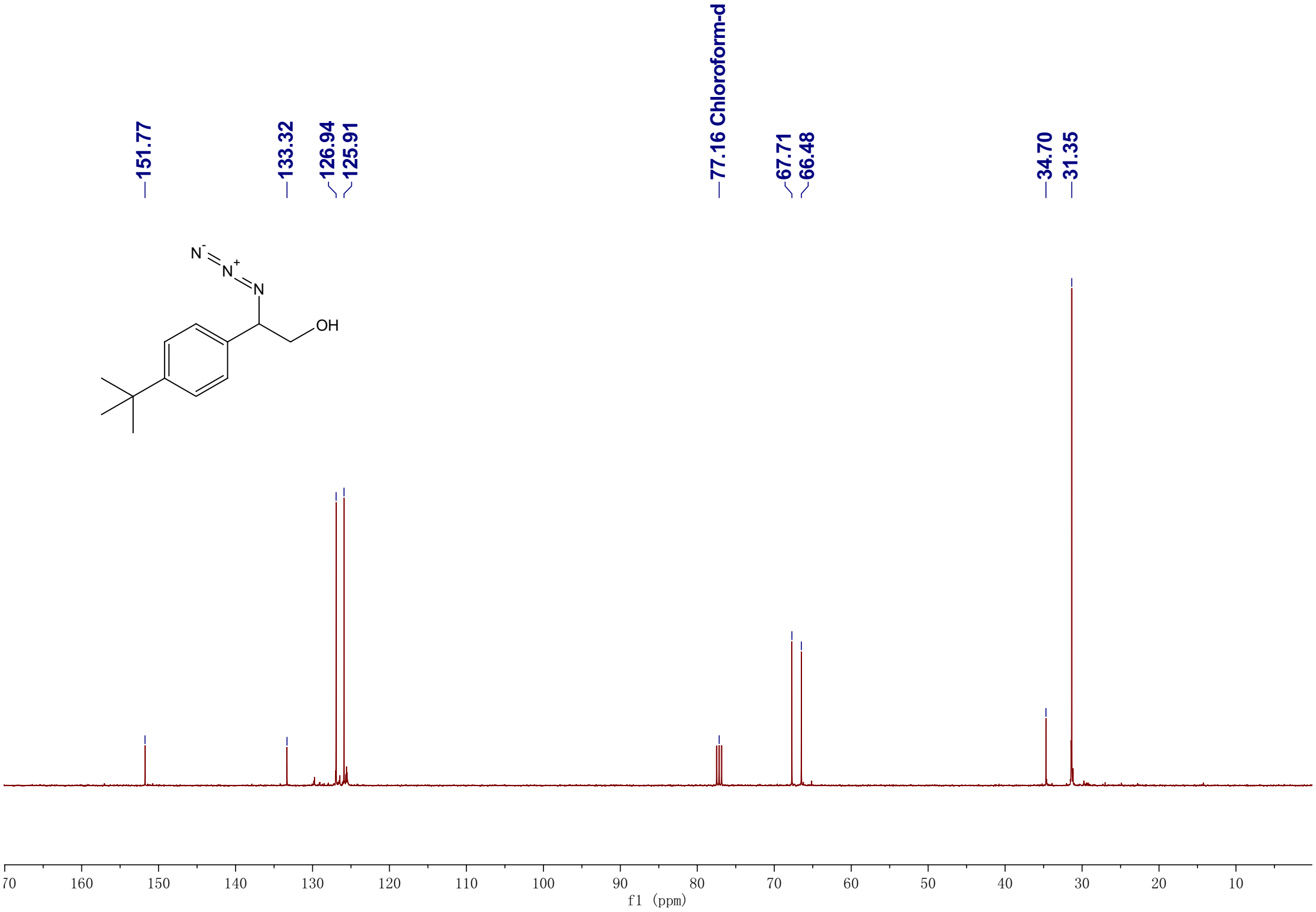
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f1 (ppm)