Supporting Information for:

Synthesis and Evaluation of Enantiomeric Quinoline-2-carboxamides: Positron Emission Tomography Imaging Agents for the Translocator Protein

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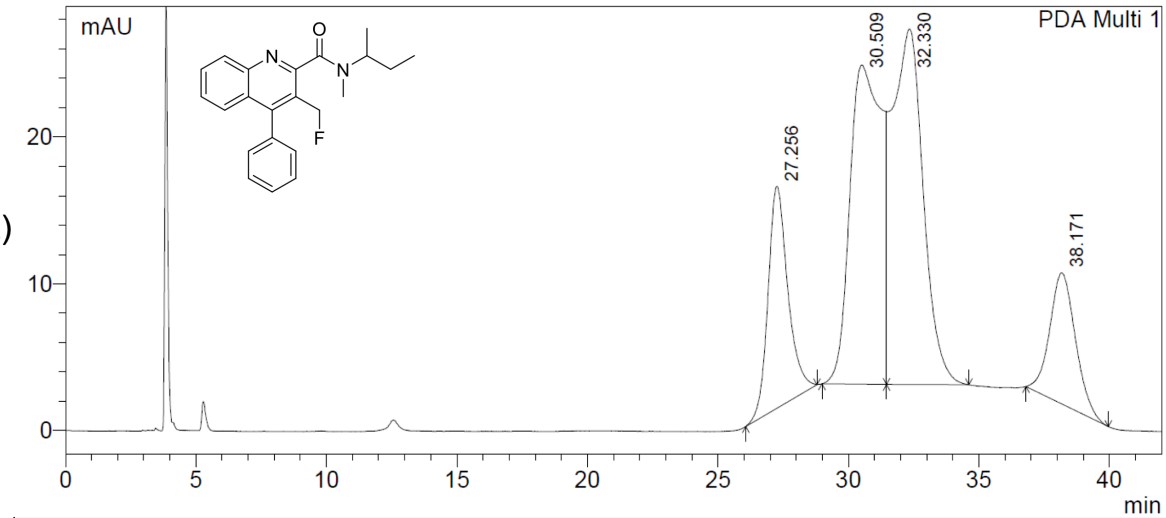
1. Chiral HPLC Trace for (*R*)-LW223.

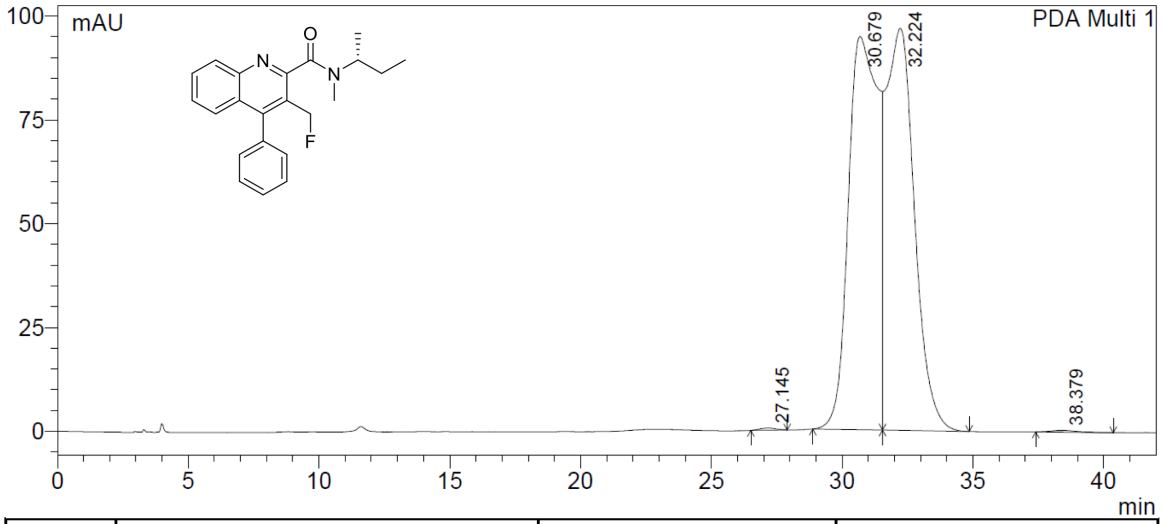
The chiral HPLC method was calibrated with the corresponding racemic mixture and performed using an AD-H column, 2.5% isopropanol in hexane and a 1 mL min^{-1} flow rate. (Note: each enantiomer of LW223 appears as a mixture of amide rotamers by HPLC).

(a)



Peak	Ret. Time	Area	Area%
1	27.256	15118	21.597
2	30.509	21743	31.061
3	32.330	24215	34.593
4	38.171	8925	12.749

(b)

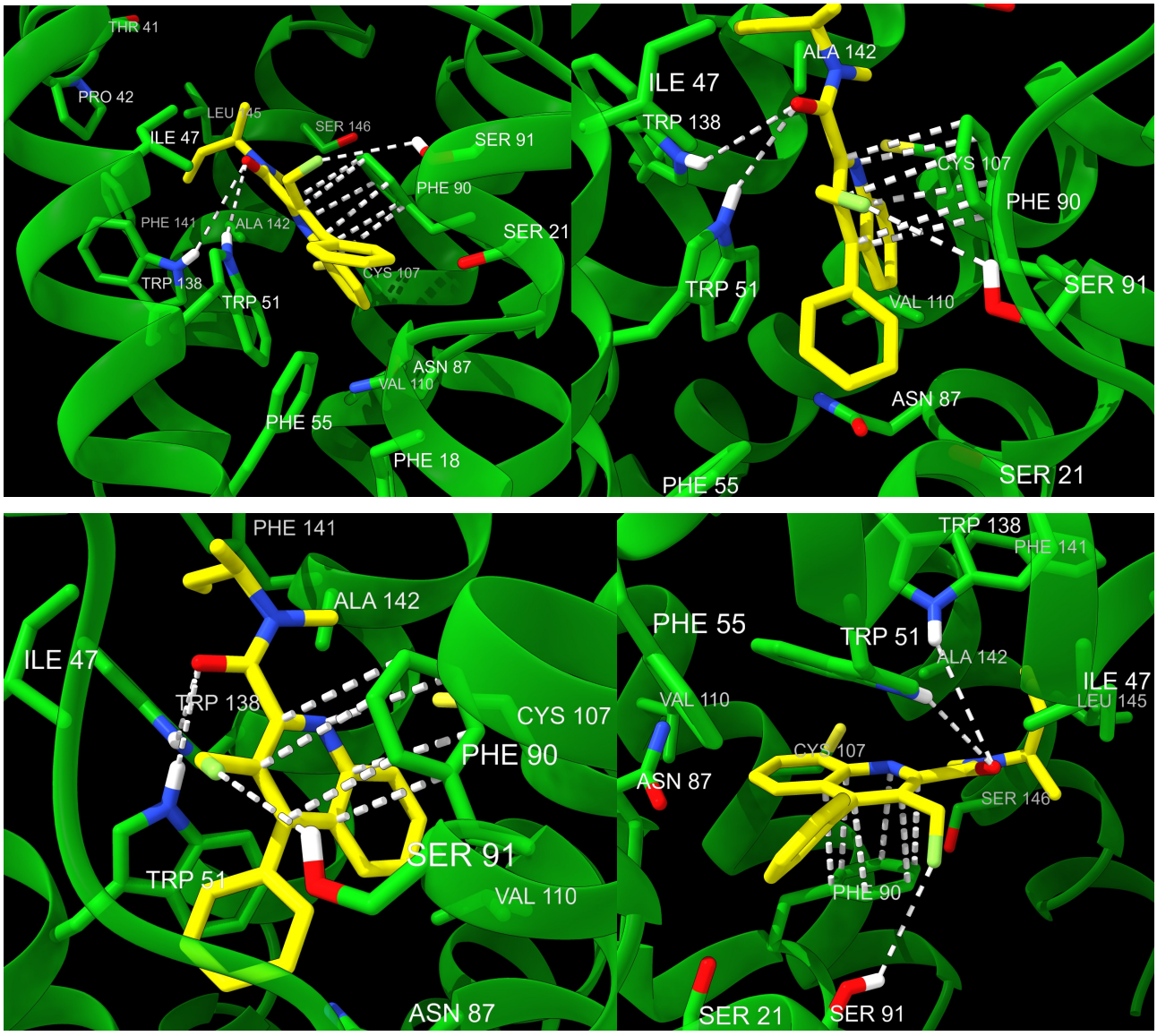


Peak	Ret. Time	Area	Area%
1	27.145	21940	0.264
2	30.679	7486077	49.204
3	32.224	7378647	50.289
4	38.379	29955	0.243

Figure S1: Chiral HPLC of (a) racemic LW223 and (b) (*R*)-LW223 showing a 99.5:0.5 er.

2. Other Docked Views of (*R*)- and (*S*)-LW223.

(*R*)-LW223:



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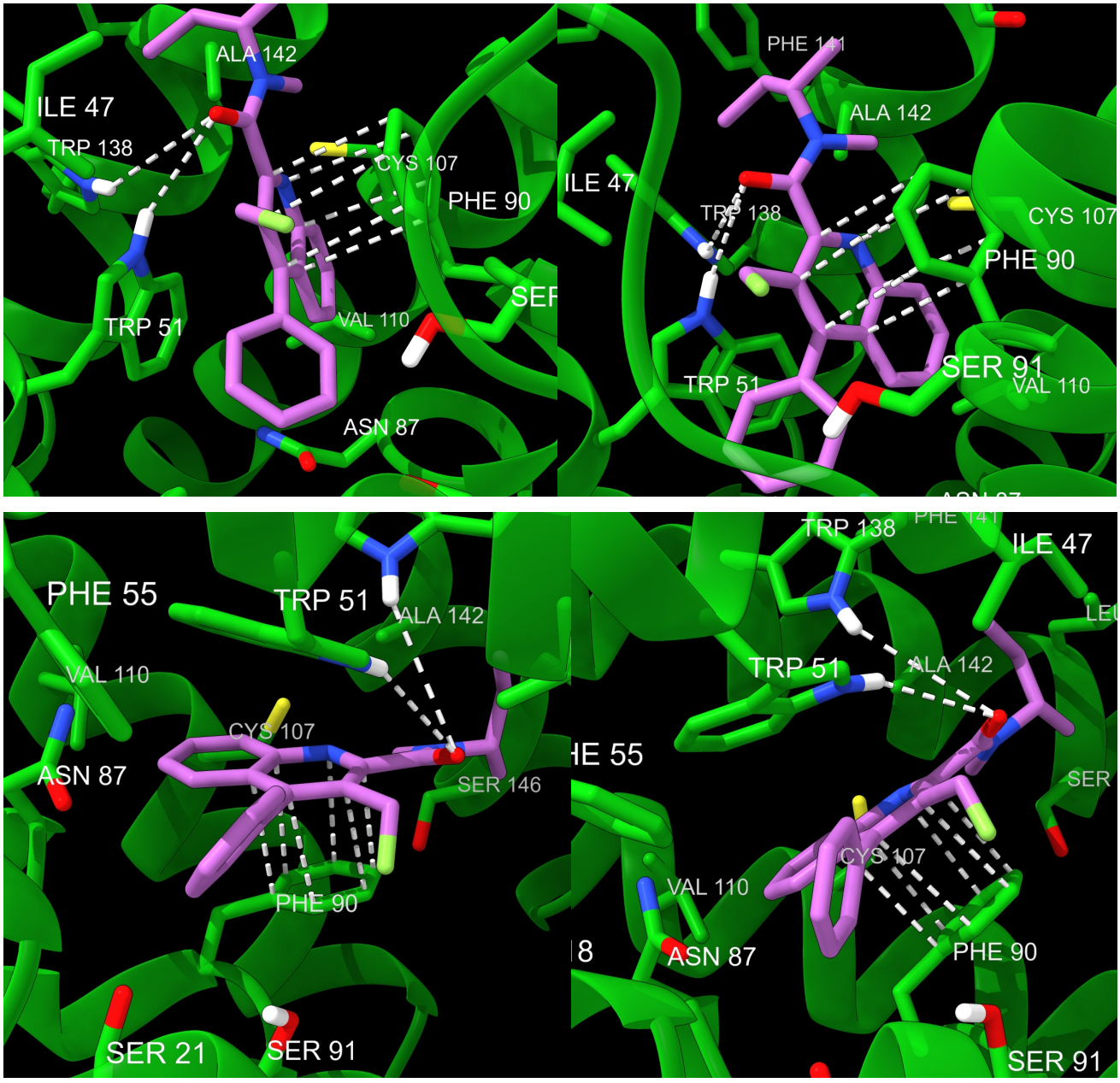
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TRP 138
CYS 107
PHE 90
TRP 51
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ALA 142
ILE 47
TRP 138
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TRP 51
SER 91
VAL 110
PHE 55
TRP 51
ALA 142
VAL 110
CYS 107
ASN 87
SER 146
PHE 90
SER 21
SER 91
TRP 138
ILE 47
TRP 51
ALA 142
CYS 107
VAL 110
ASN 87
PHE 90
SER 91

3. Procedure and Replicates for Physicochemical Data

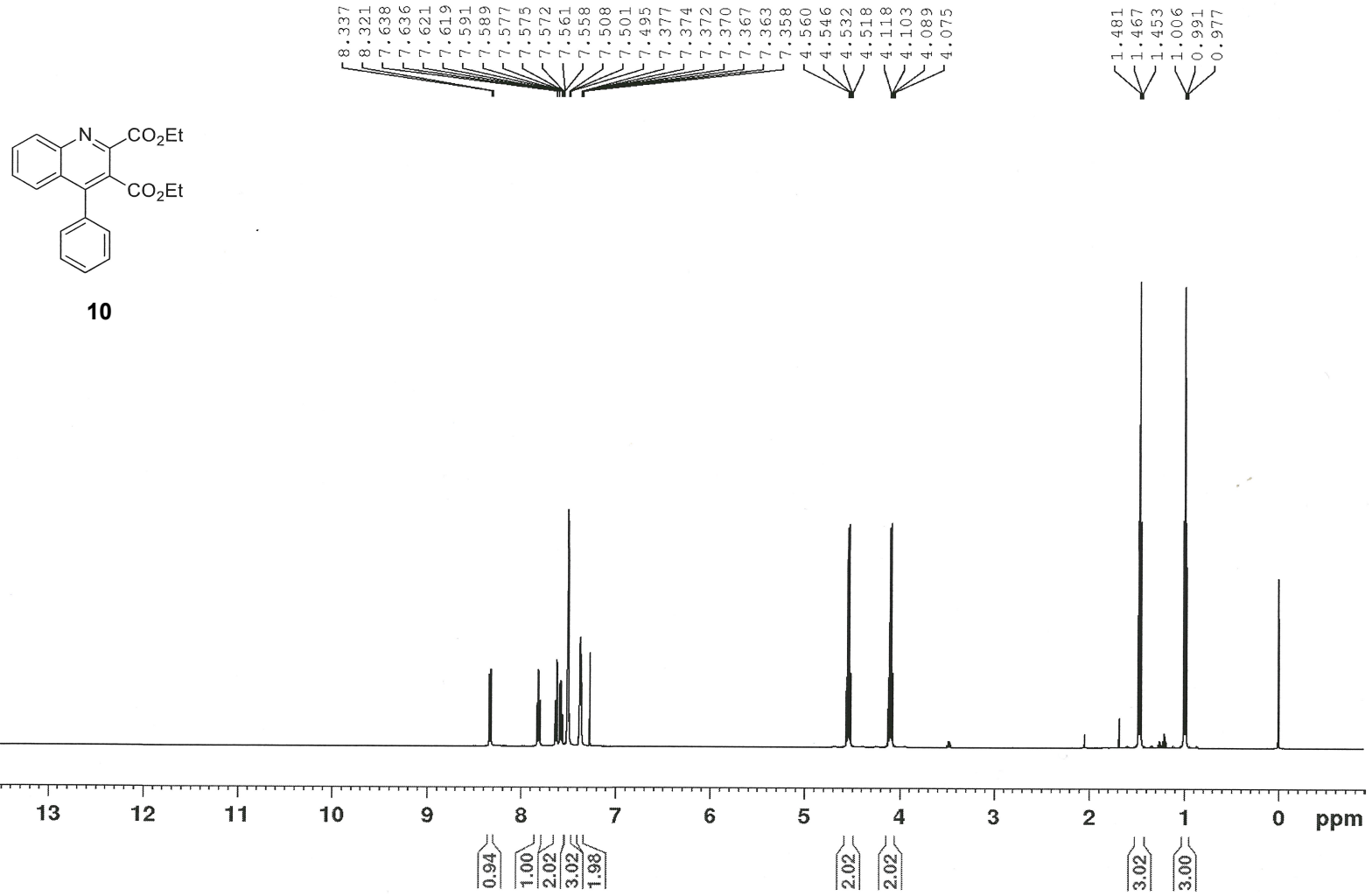
All physicochemical analyses were performed using a Dionex Ultimate 3000 series, and data acquisition and processing performed using Chromeleon 6.8 Chromatography software. Standard and test compounds were dissolved in 1:1 organic/aqueous phases and prepared to a concentration of 0.5 mg/mL. The HPLC system was set to 25 °C, and UV detection achieved using a diode array detector (190–800 nm). Analysis was performed using 5 μL sample injections.

	Log P[a]		P_m[b]			K_m[b]			%PPM[c]		
	1	**2**	**1**	**2**	**3**	**1**	**2**	**3**	**1**	**2**	**3**
PK11195	3.85	4.11	0.54	0.50	0.52	189	186	178	90	94	91
AB5186	3.74	3.73	0.36	0.34	0.35	129	122	120	90	88	91
LW223	4.17	4.09	0.57	0.56	0.54	202	195	188	91	95	89

[a] Determined using C_{18} column. [b] Determined using immobilised artificial membrane (IAM) column. [c] Determined using human serum albumin (HAS) coated column.

4. ^{1}H and ^{13}C NMR Spectra for all Compounds

^{1}H NMR (400 MHz, $CDCl_3$)



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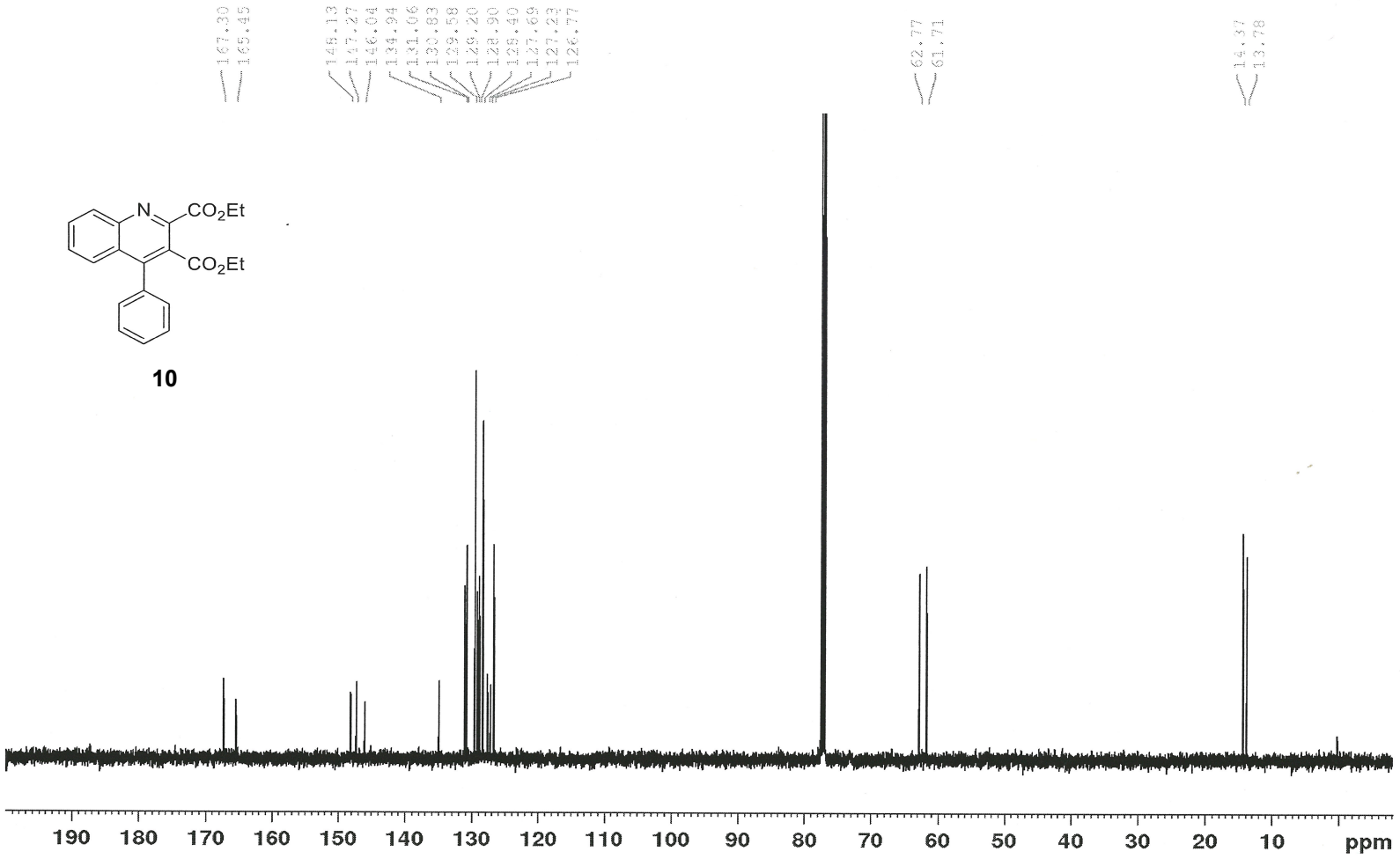
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



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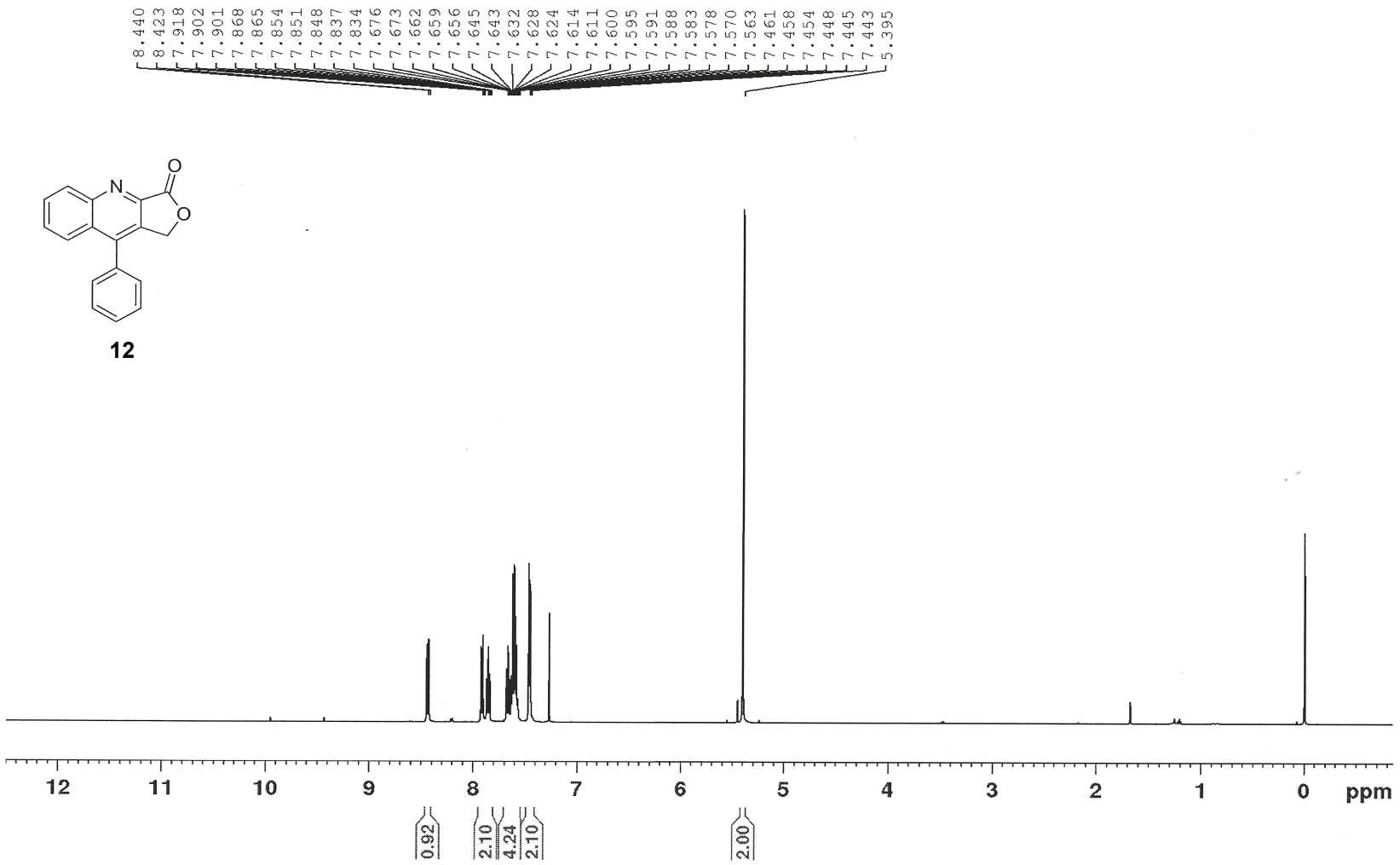

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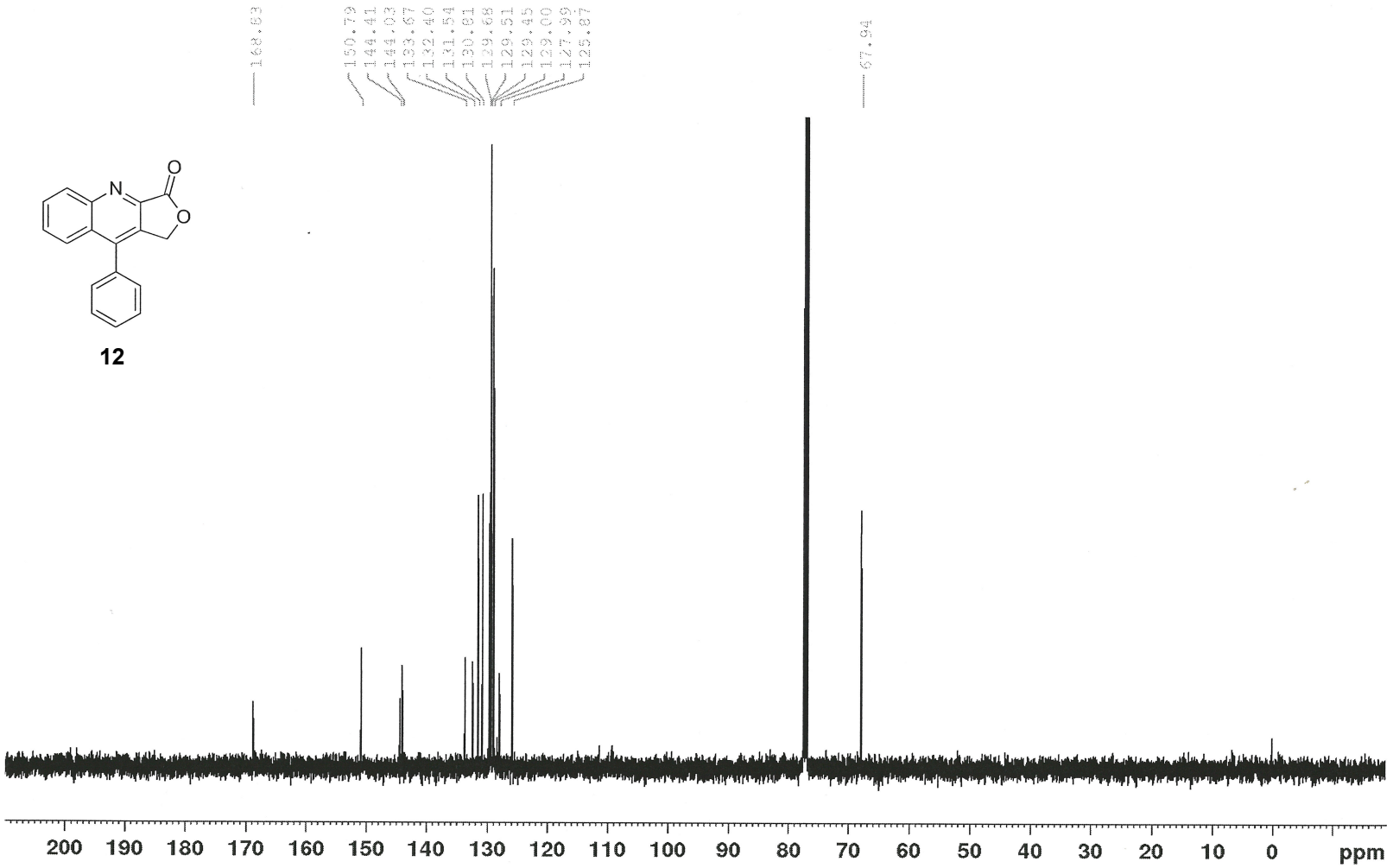

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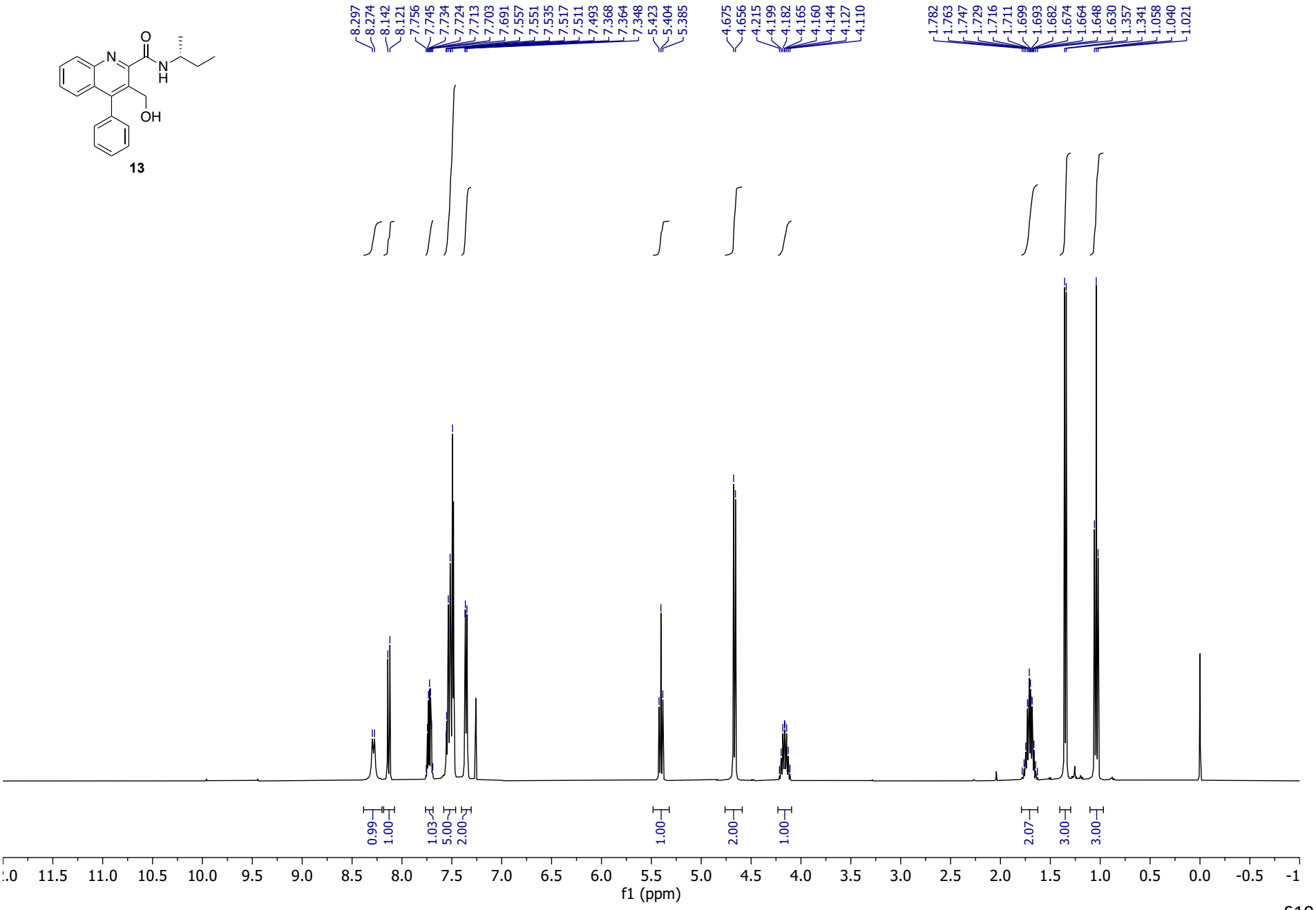

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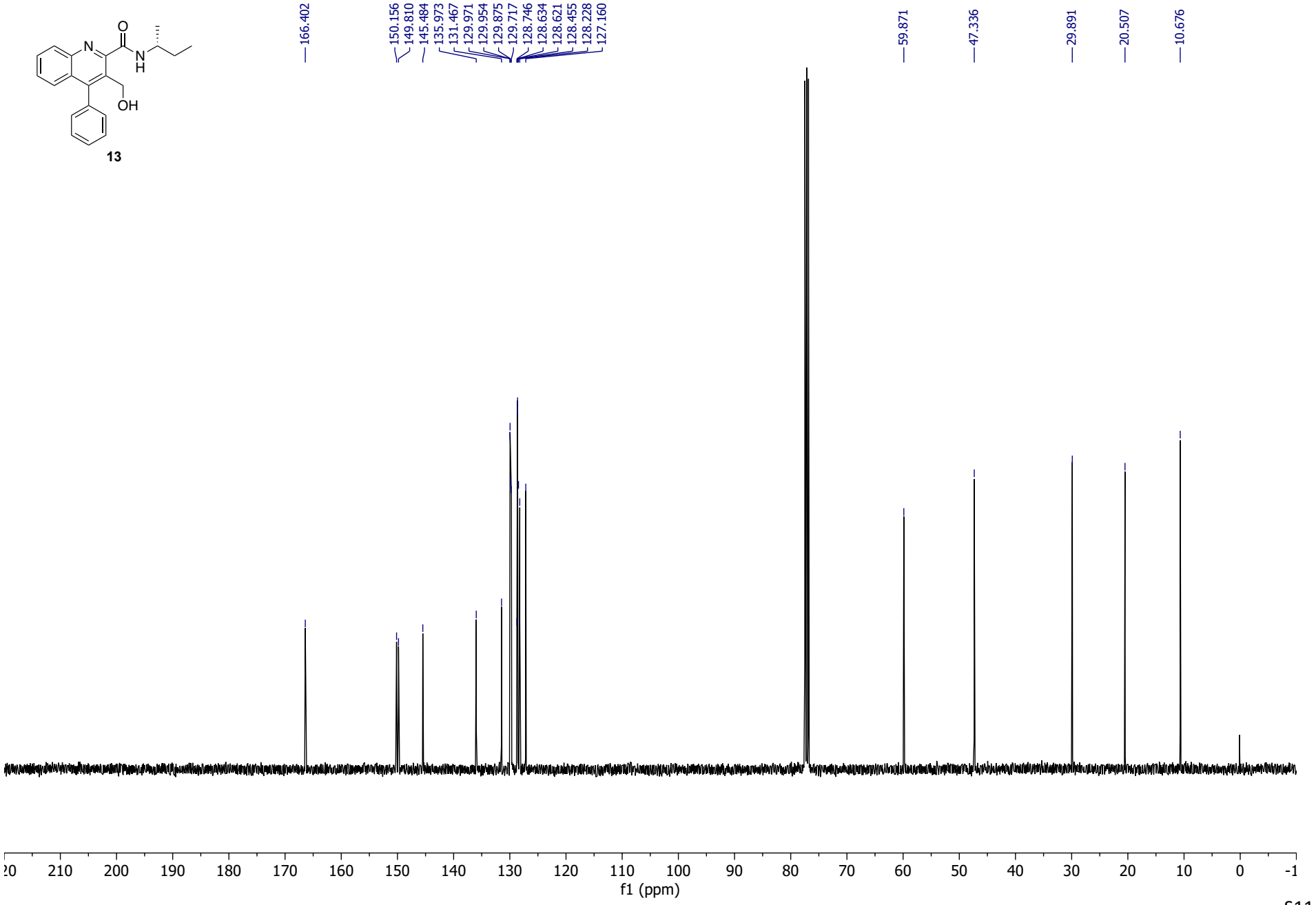

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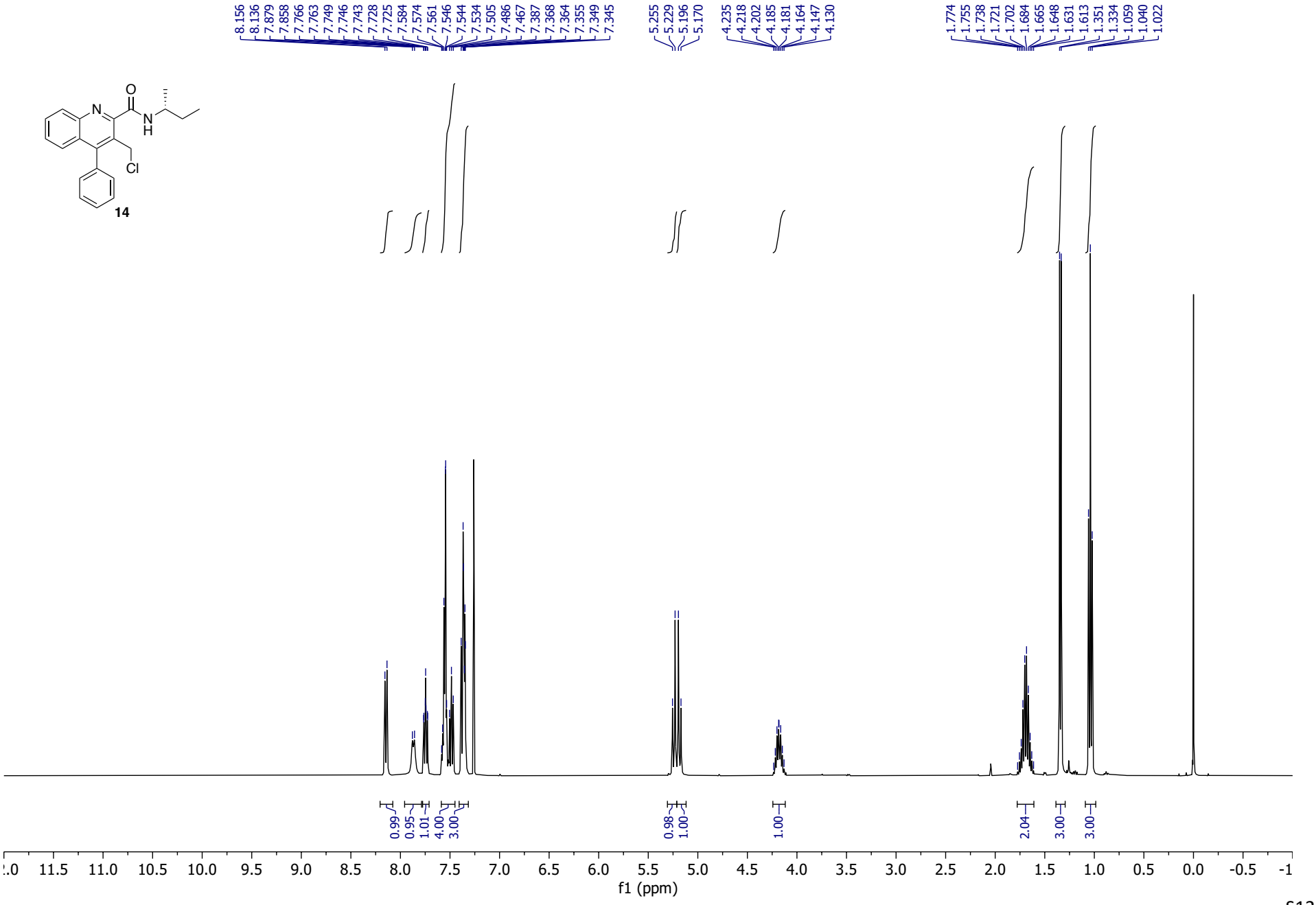

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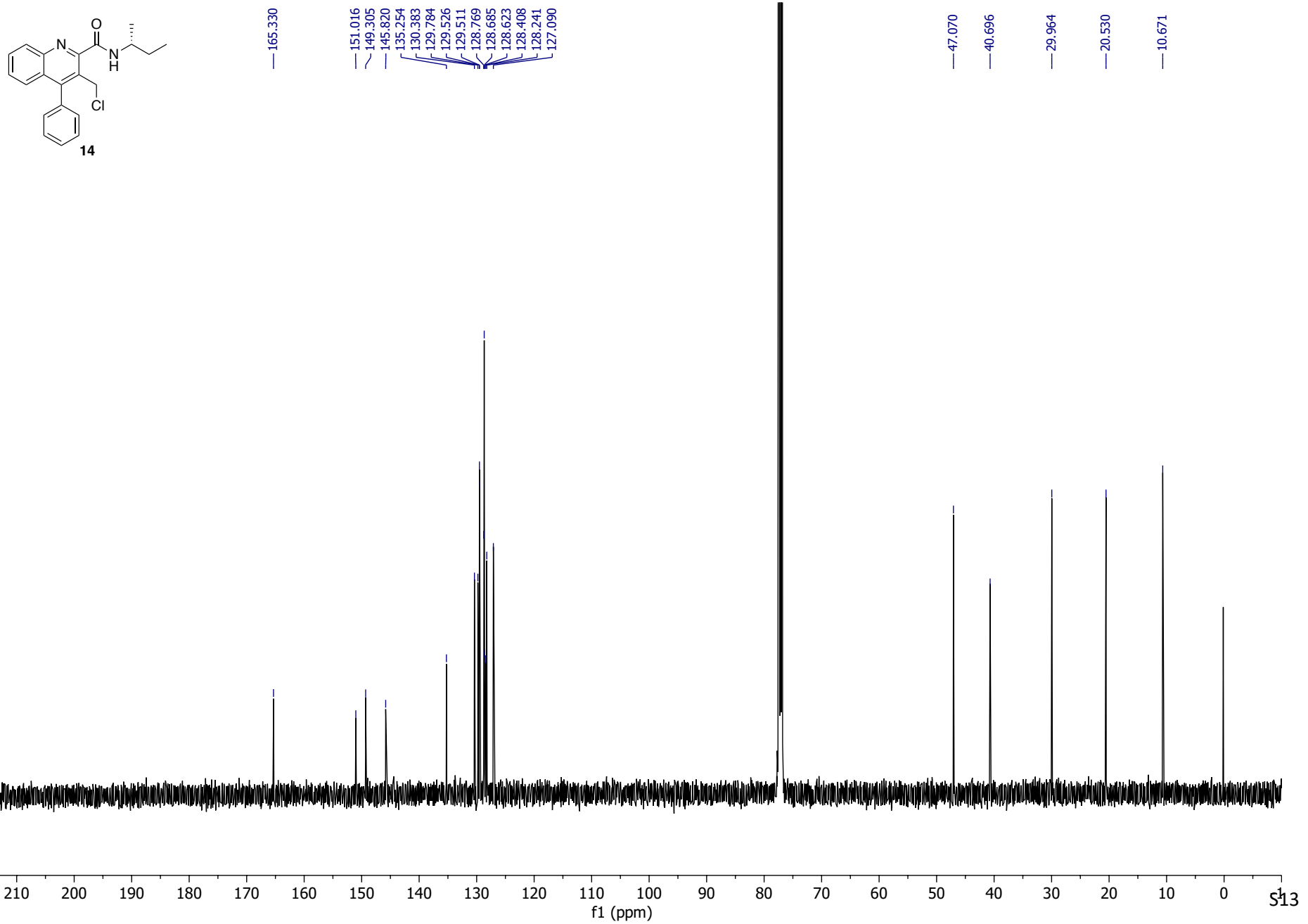

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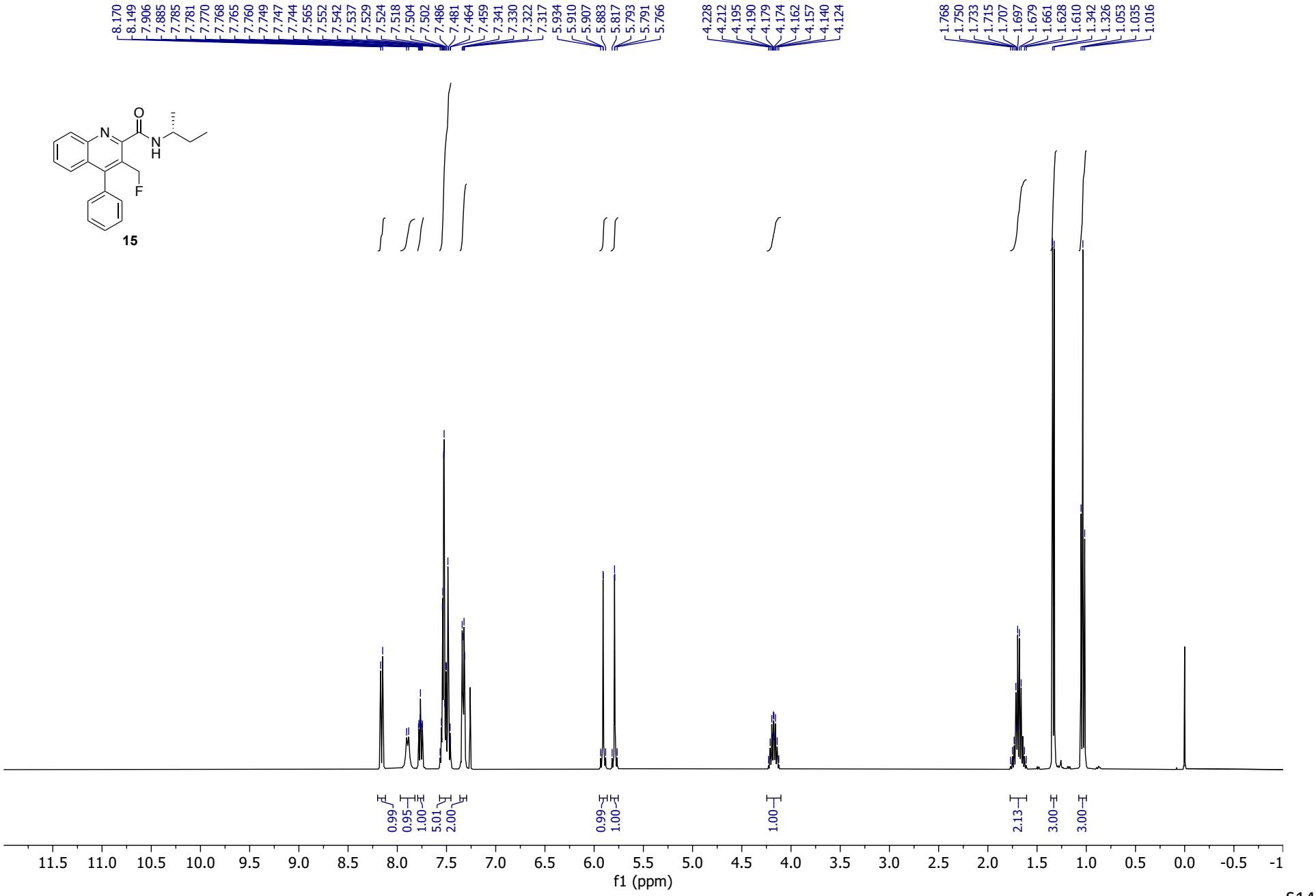

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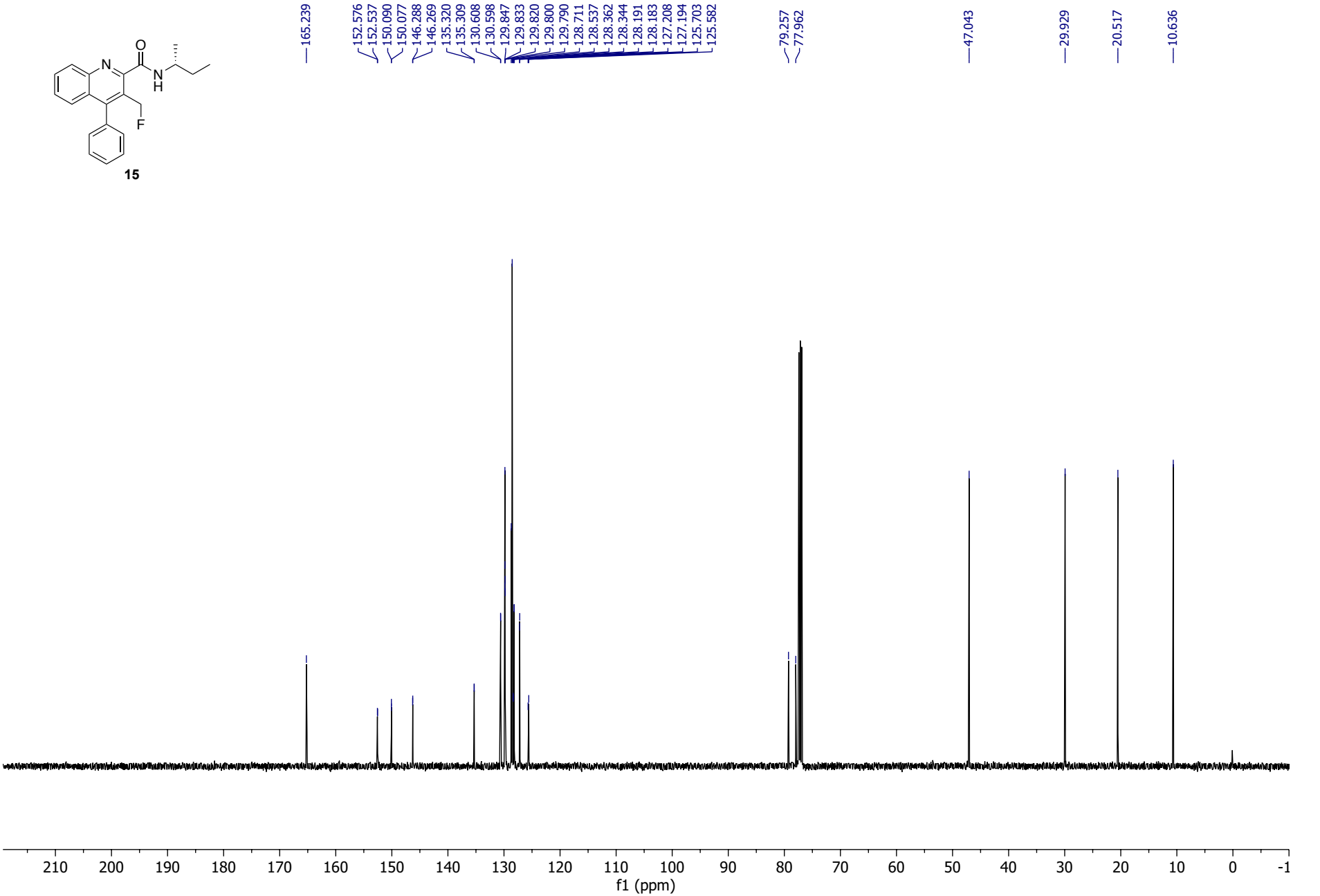

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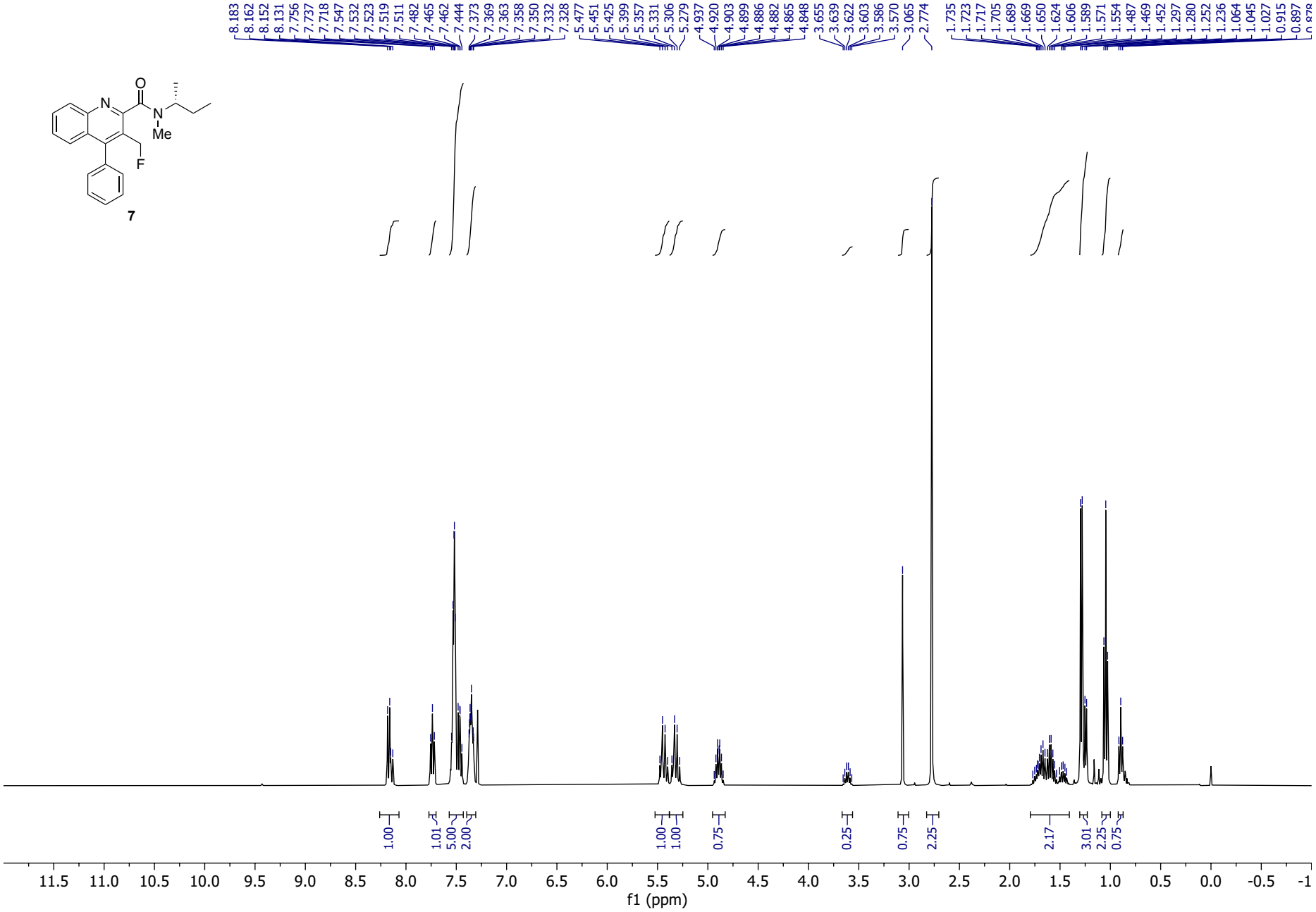

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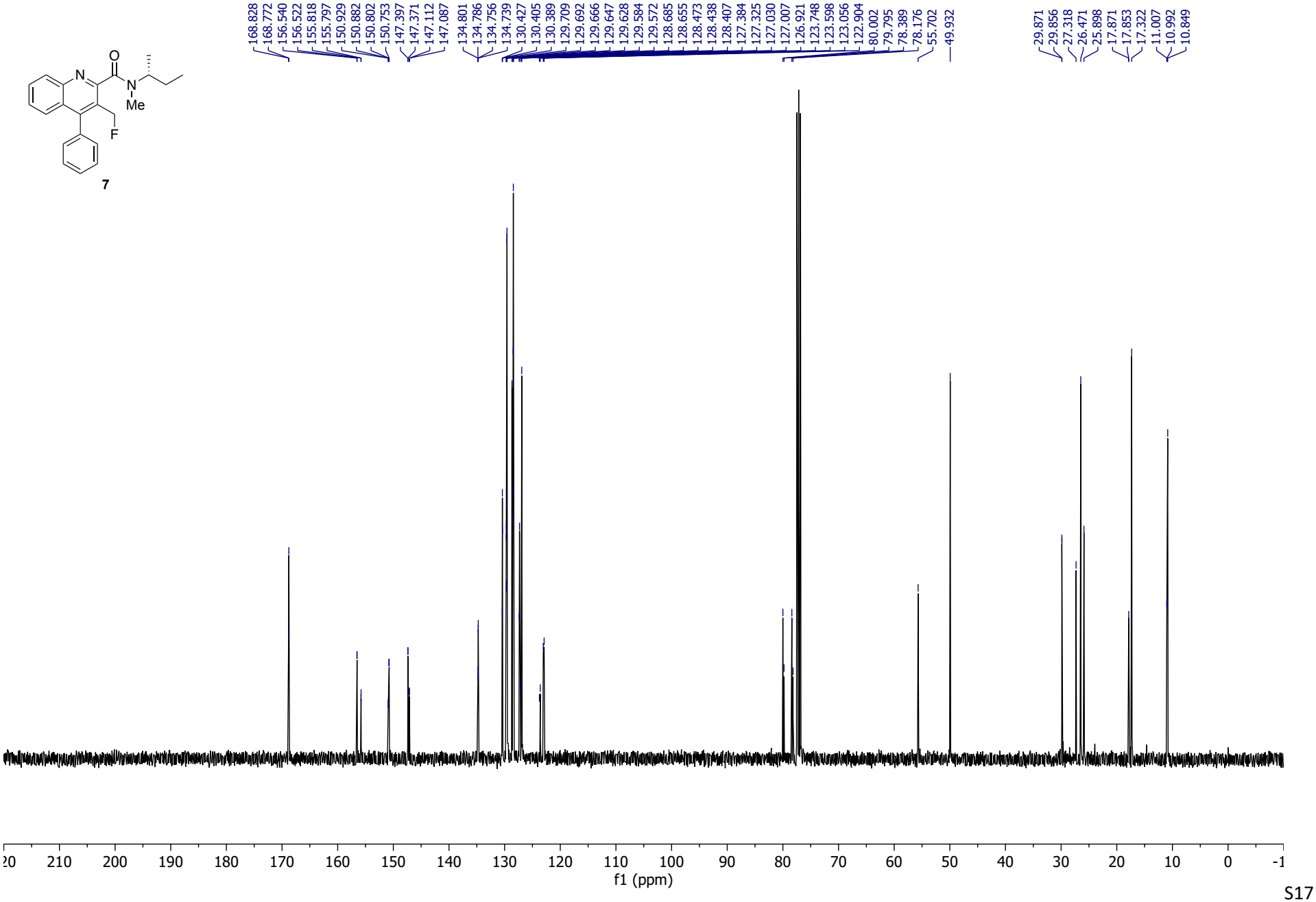

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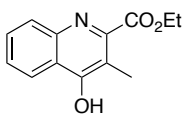

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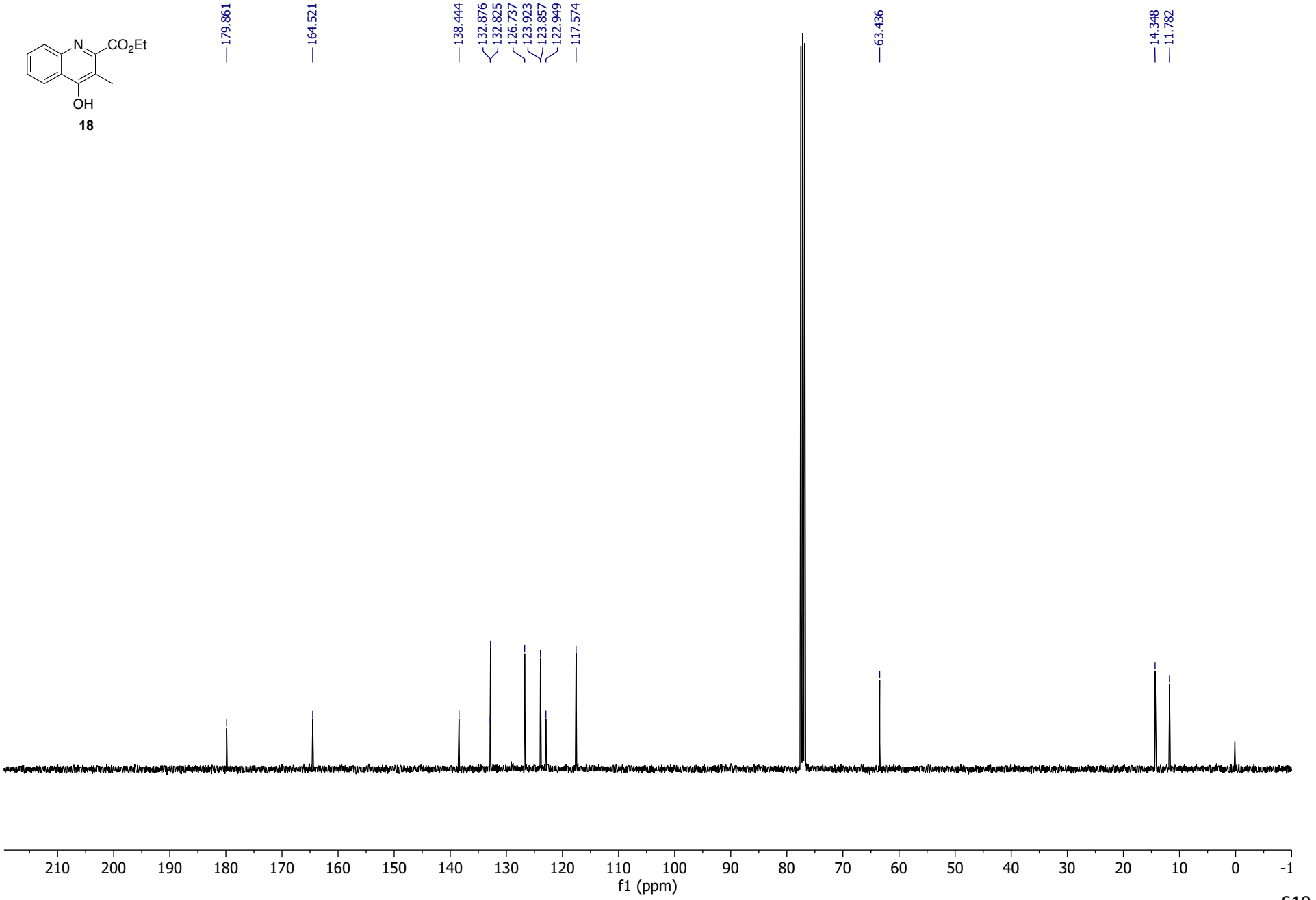

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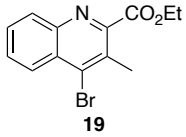

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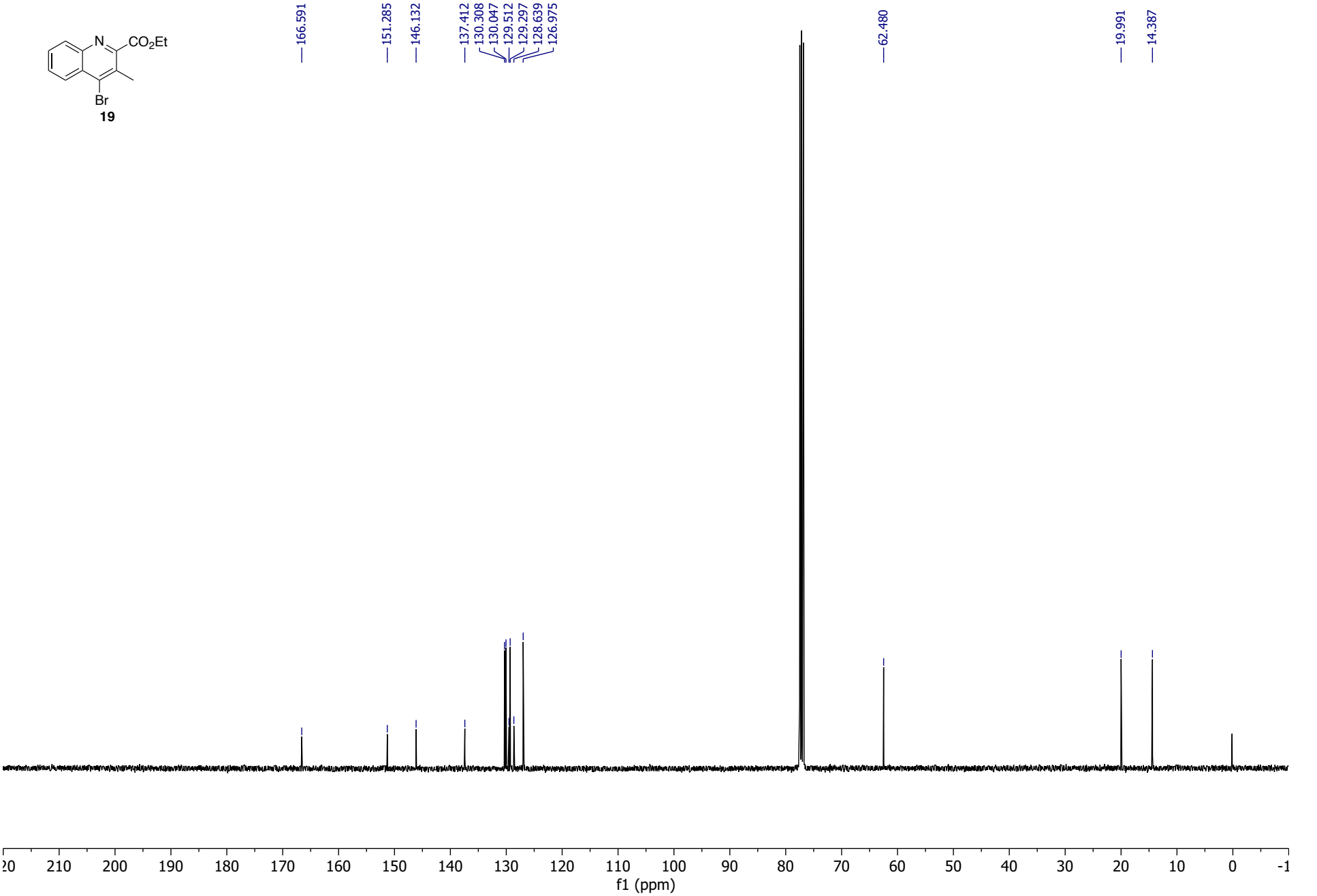

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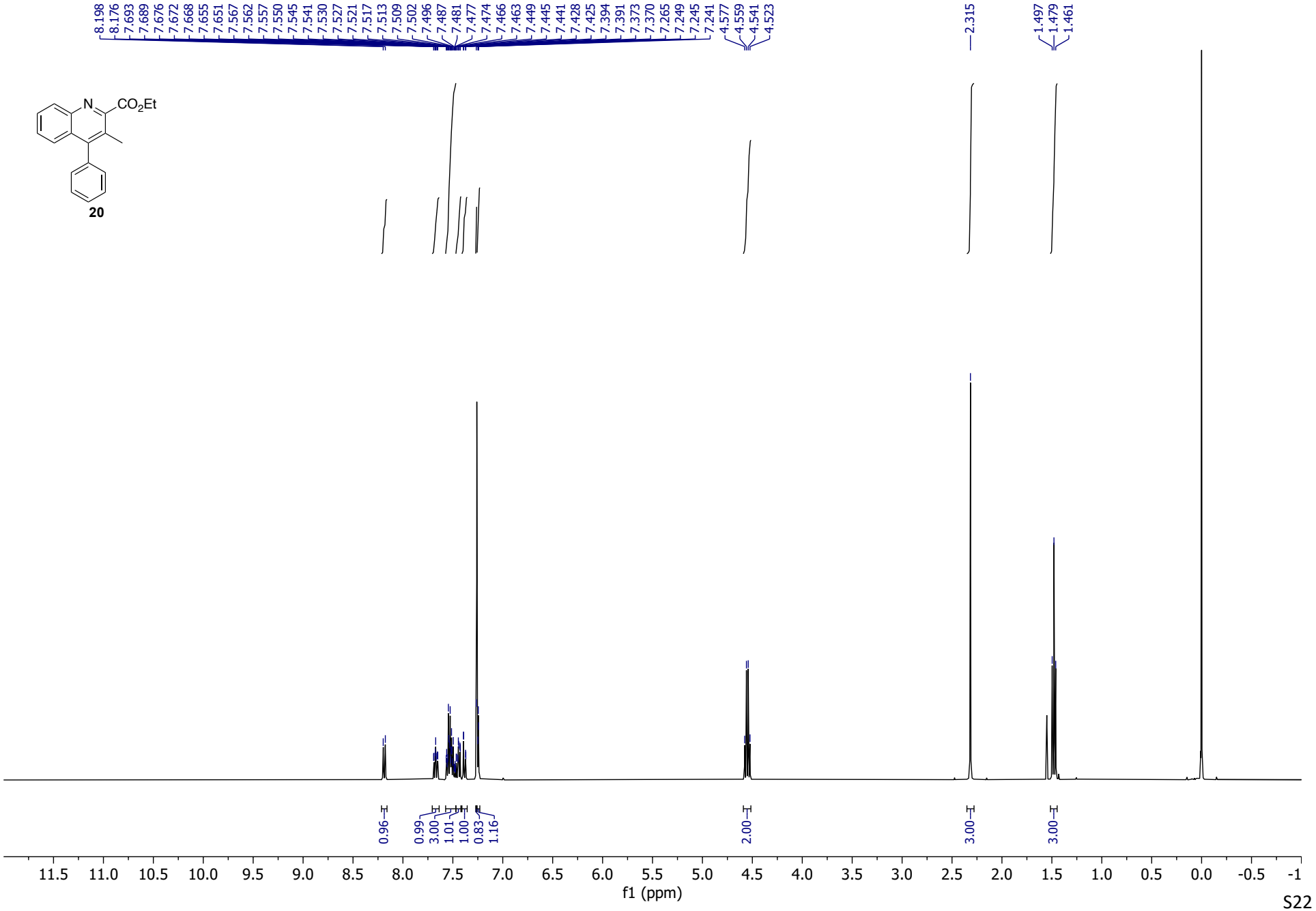

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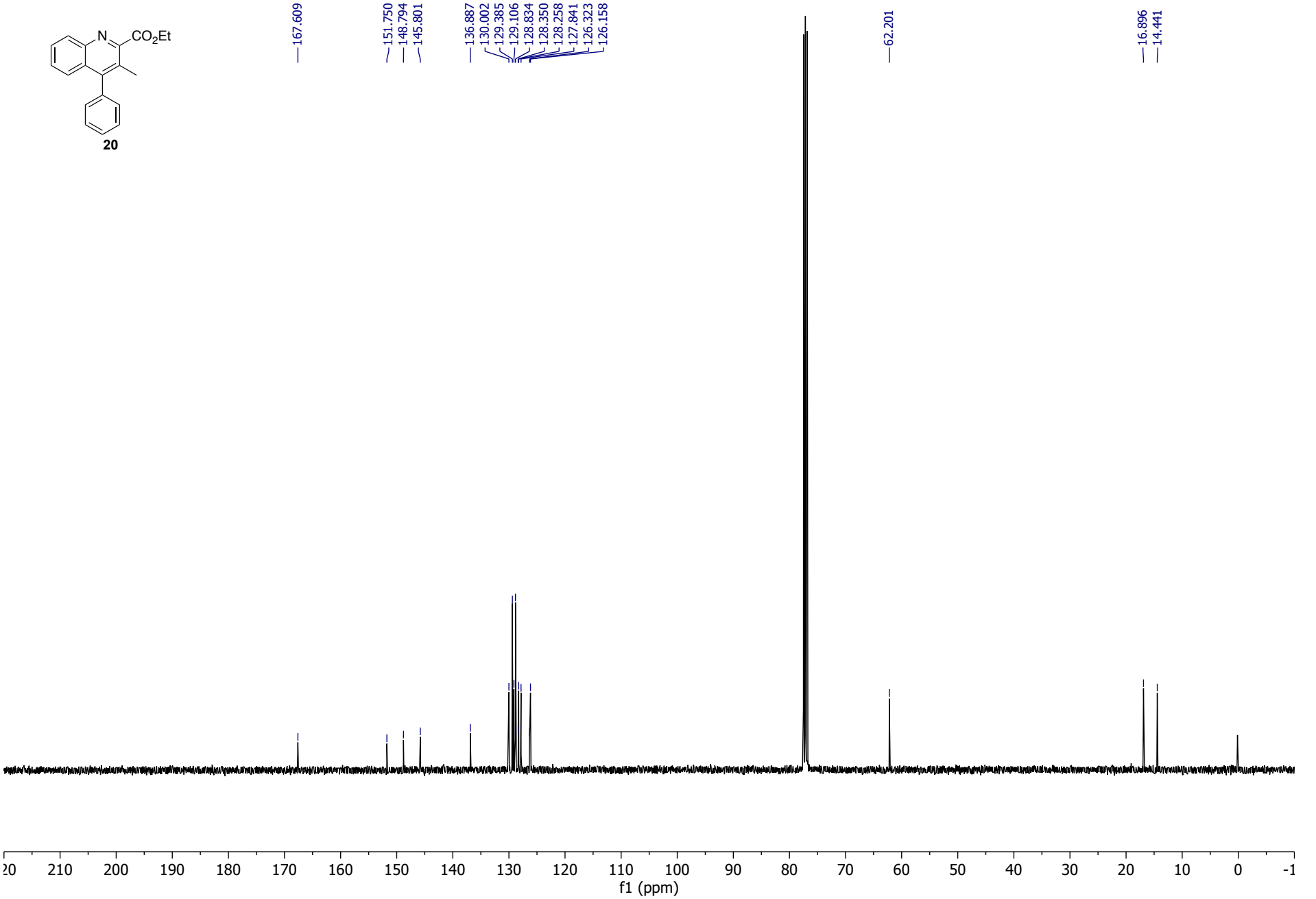

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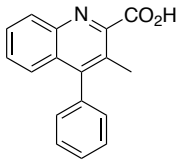

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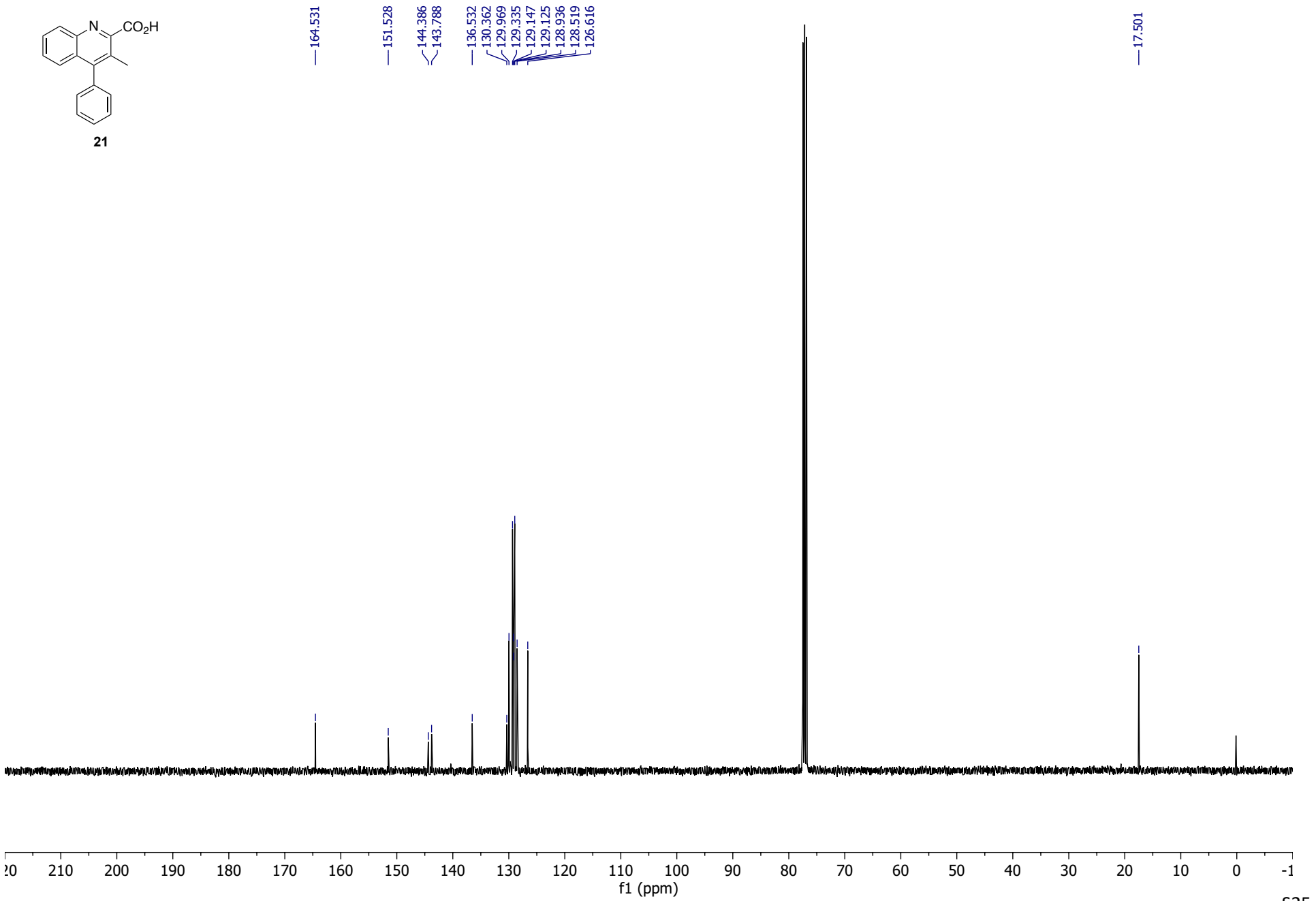

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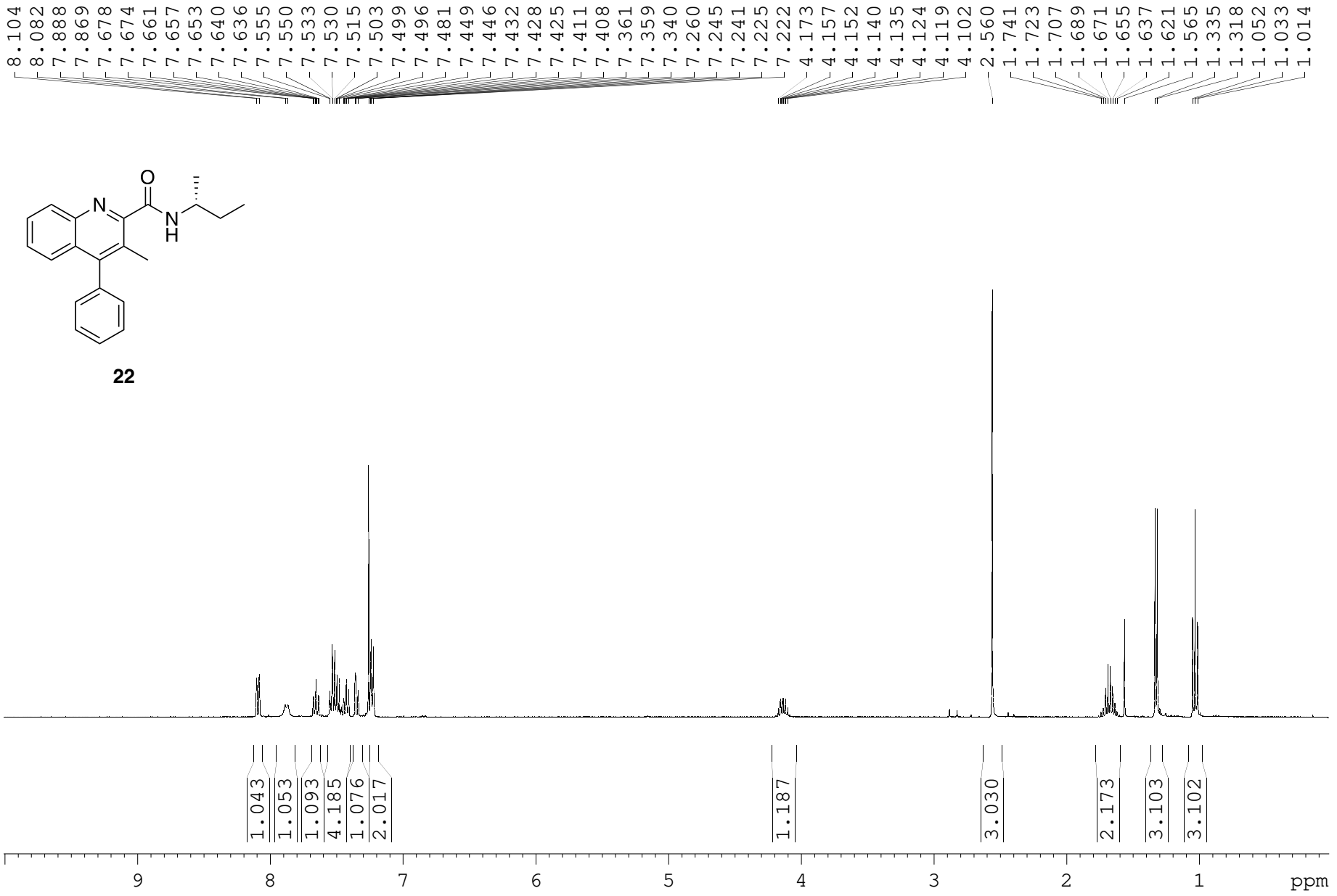

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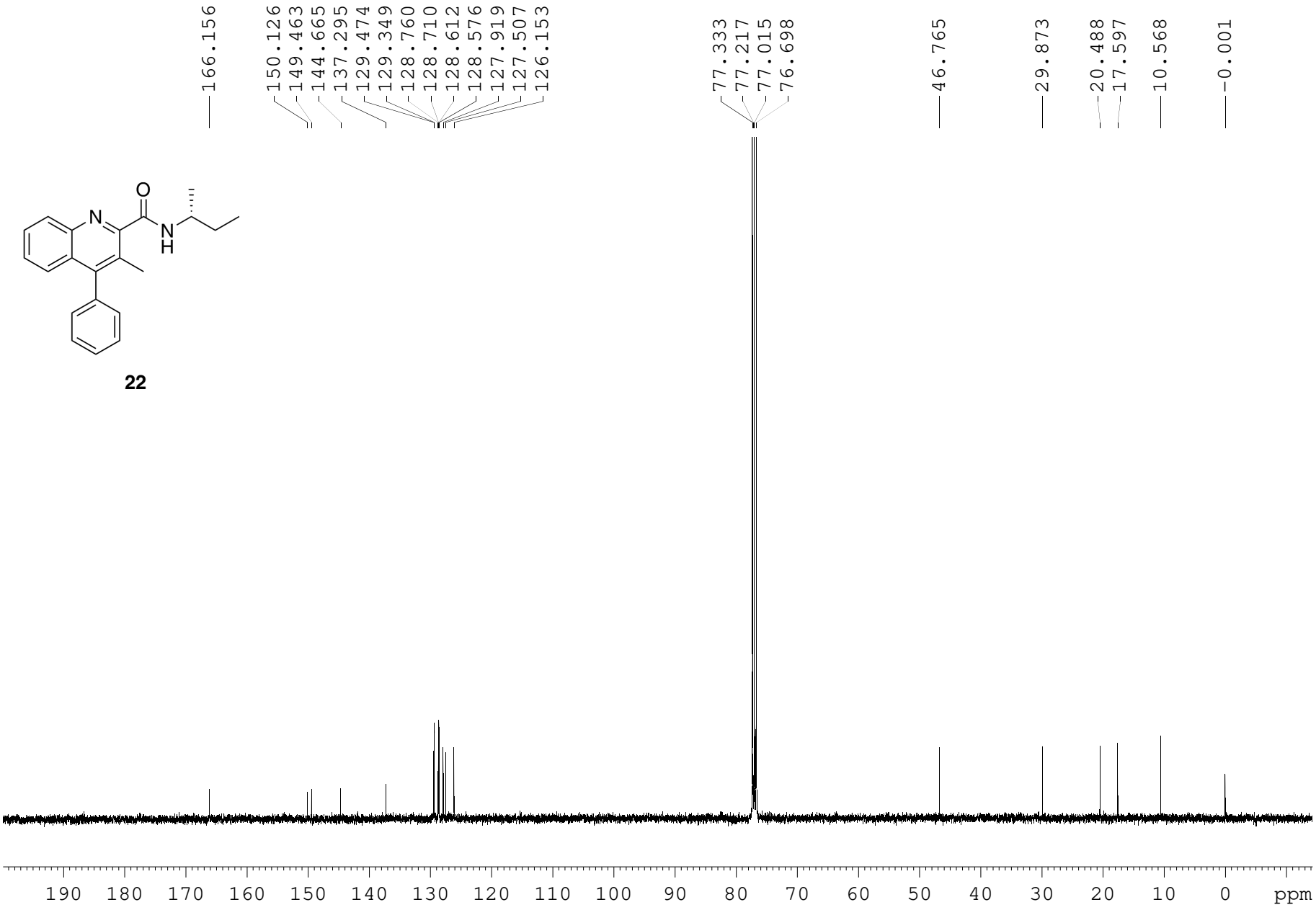

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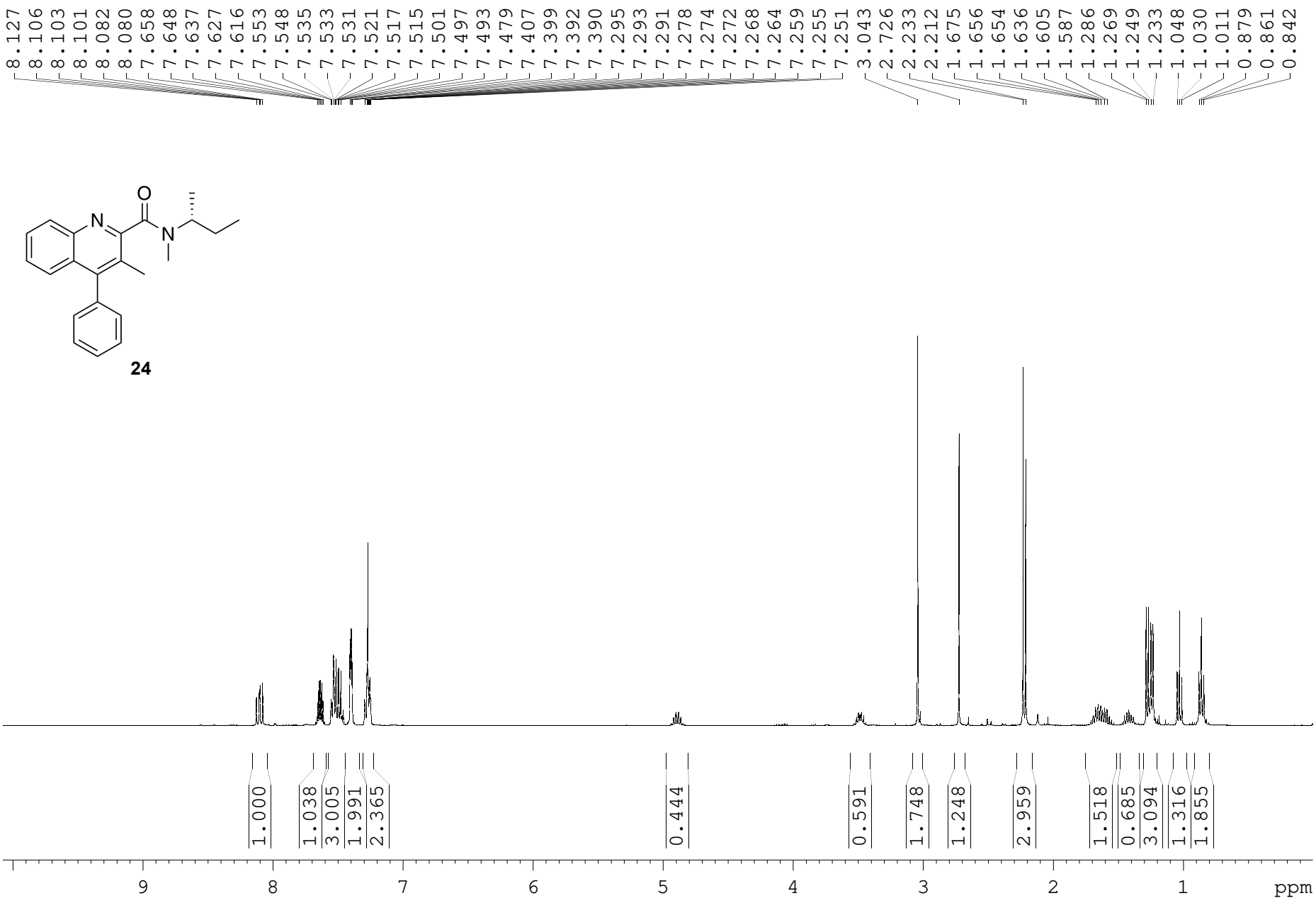

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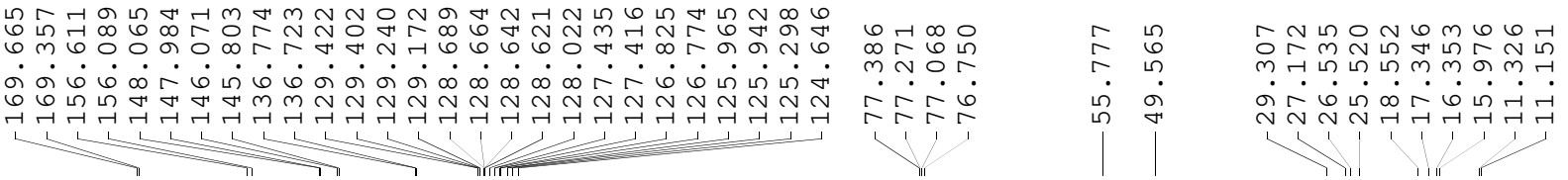

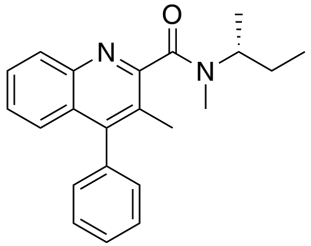

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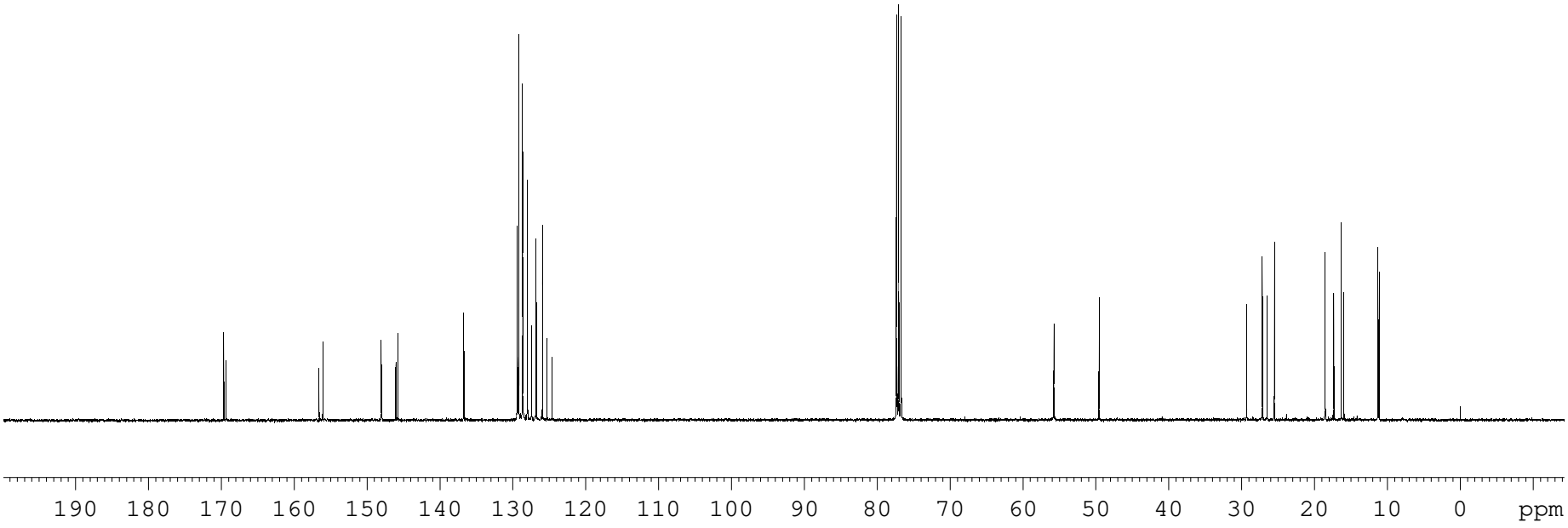

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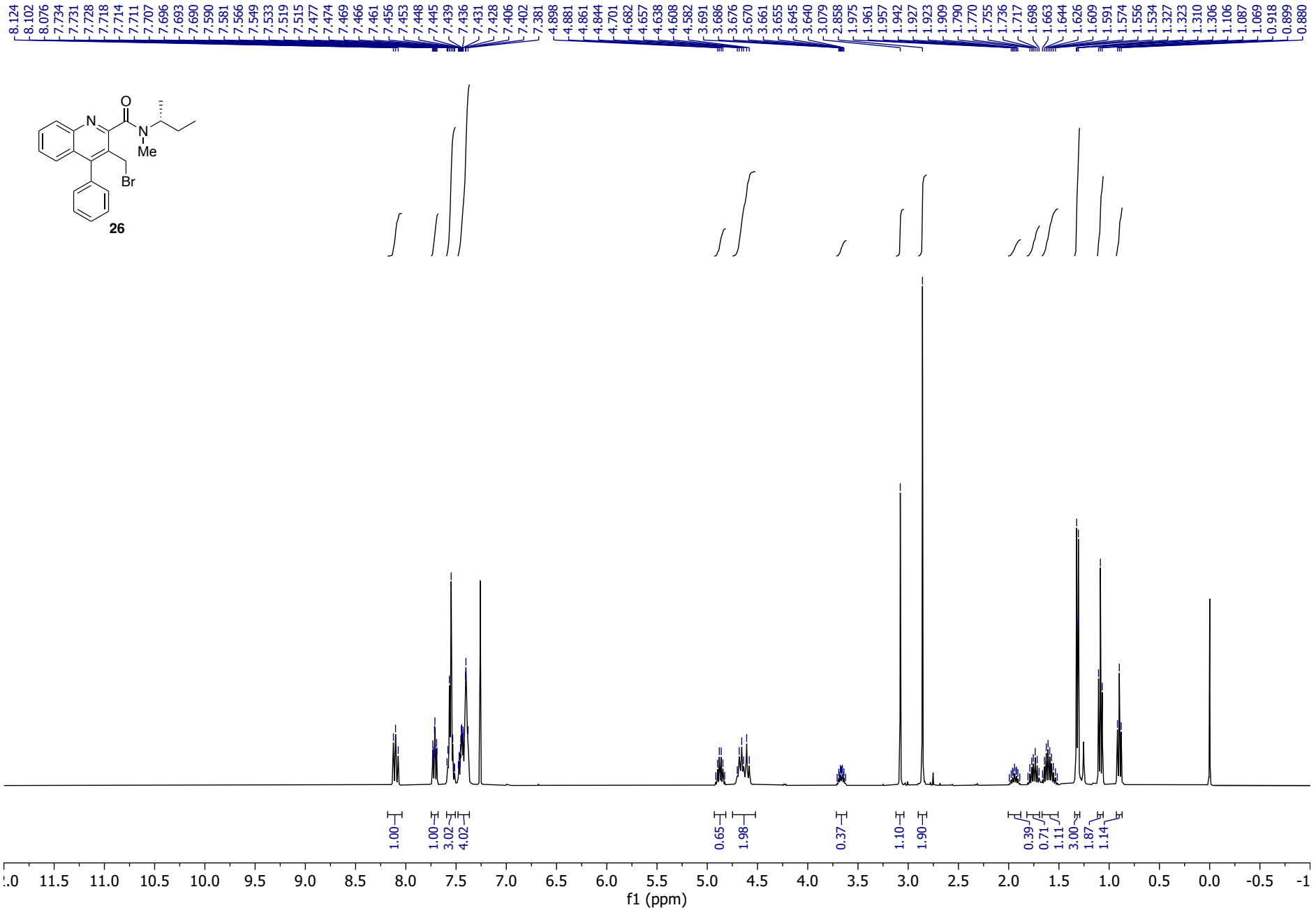

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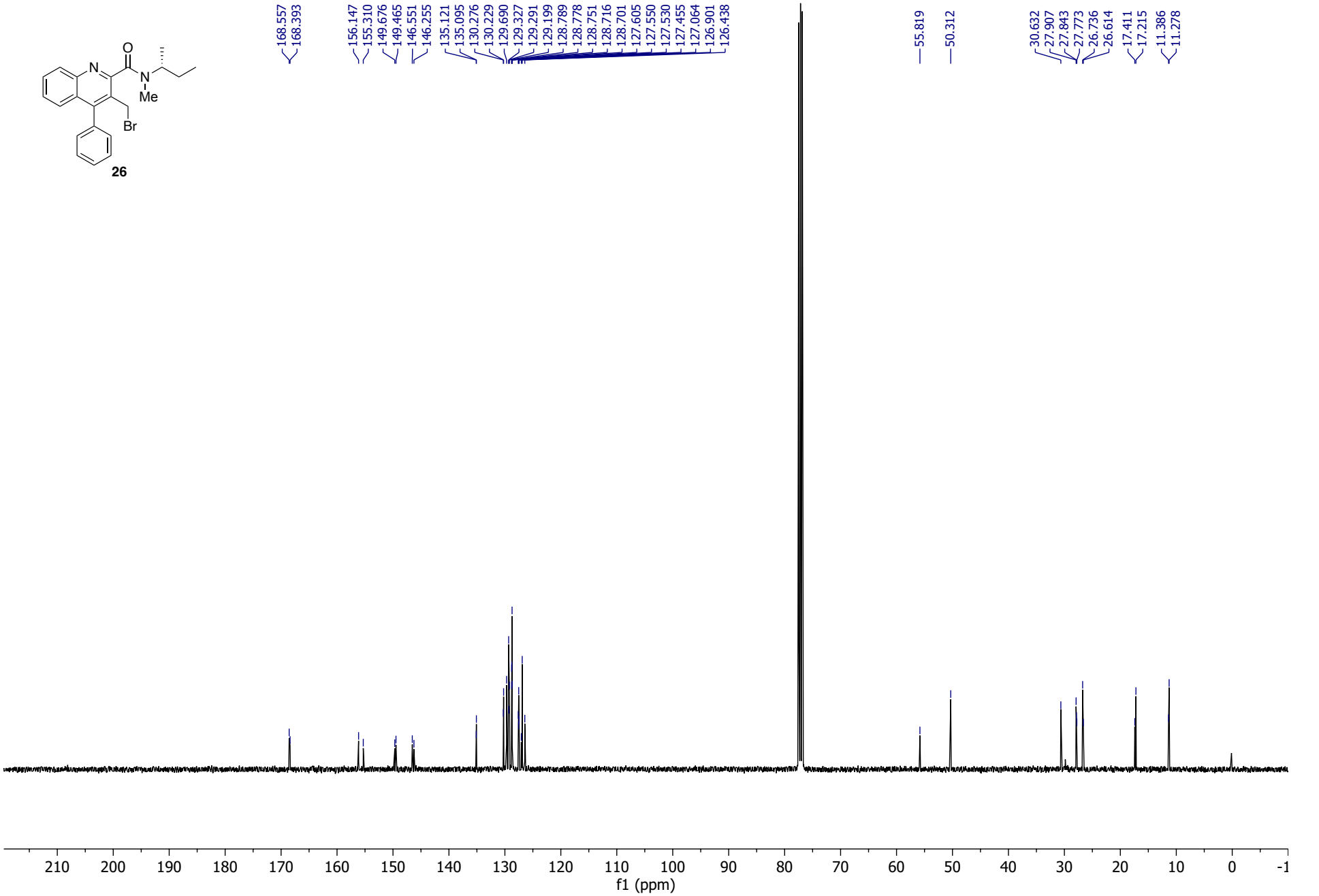

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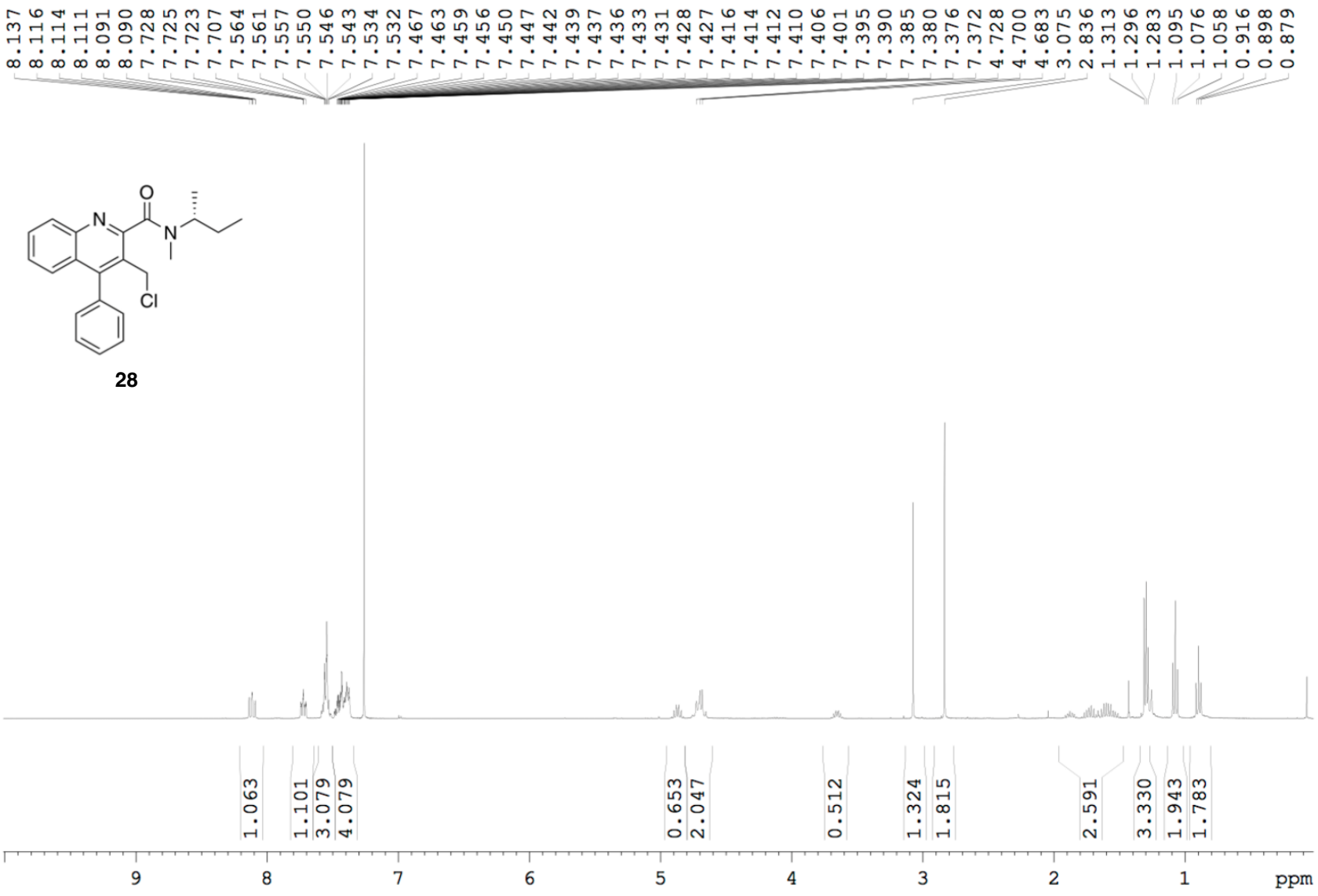

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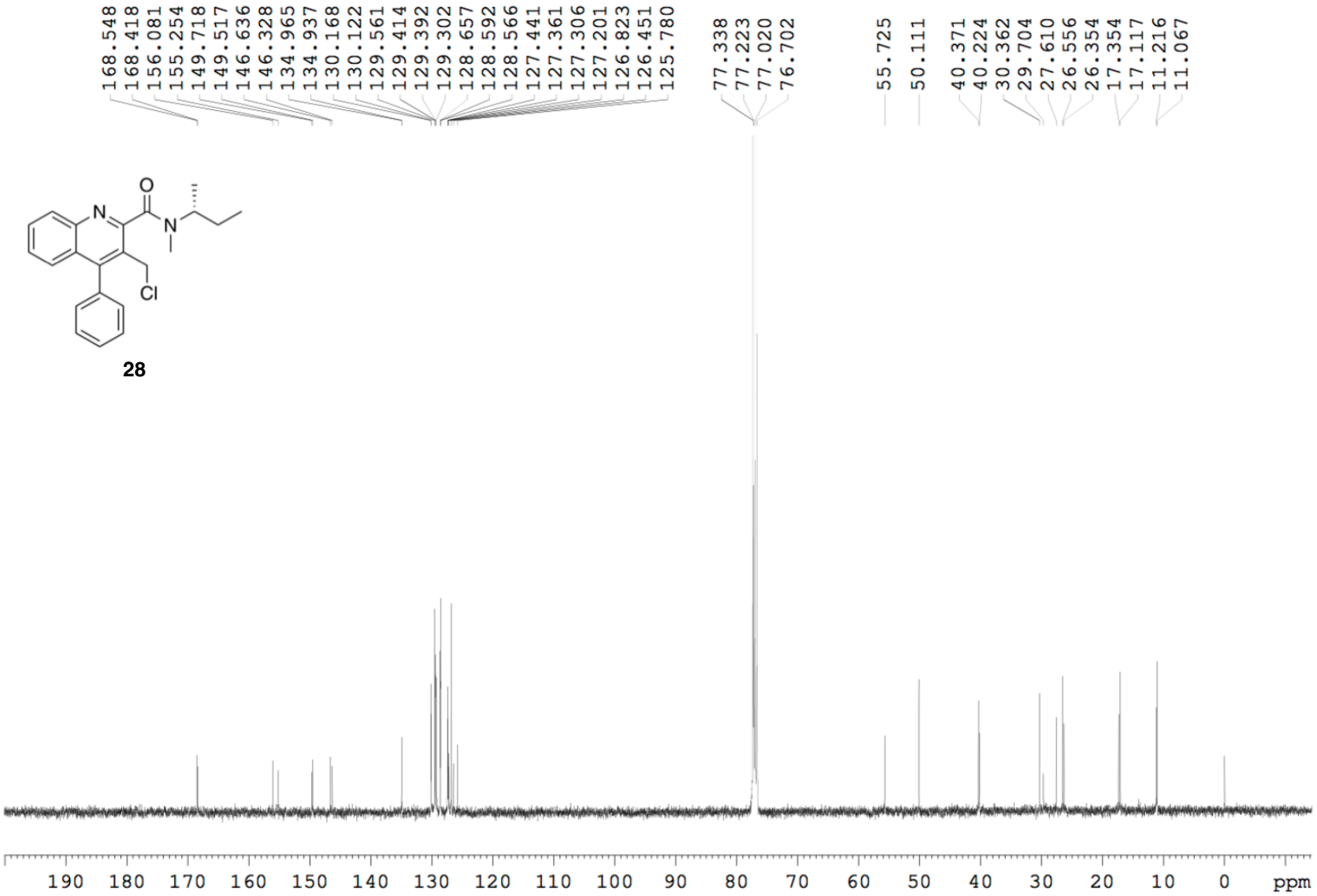

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