Supporting Information

$PdCl_2$ Catalyzed Efficient Assembly of Organic Azides, CO, and Alcohols under Mild Conditions: A Direct Approach to Carbamates

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General Information

Analytical

Flash Column Chromatography was applied to obtain all reaction yields and performed on silica gel 300-400 mesh. NMR spectra were recorded on a Bruker AVIII-400 spectrometer. ^{1}H-NMR Chemical shifts (δ:) were reported in units parts per million refering to TMS signal by assigning its resonance as 0.00 ppm in $CDCl_3$ or referring to resonance of DMSO as 2.50 ppm in DMSO-d_6. All ^{13}C-NMR Chemical shifts were reported in units ppm by assigning resonance of $CHCl_3$ as 77.16 ppm in $CDCl_3$ or that of DMSO as 39.52 ppm in DMSO-d_6. All coupling constants (J) were reported in Hertz (Hz). High Resolution Mass Spectra were measured by APEX IV Fourier Transform Ion Cyclotron Resonance Mass Spectrometer in ESI Positive (showed a systematic error of about 0.0005). Infrared spectra were recorded on a Nicolet FT-IR Spectrophotometer NEXUS-470. The wave numbers (ν) of recorded IR signals are quoted in cm^{-1}. Thin Layer Chromatograms (TLC) was visualized under UV and via phosphomolybdic acid stain.

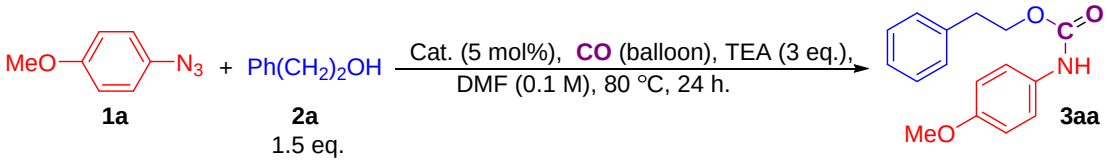
Chemical

All substrates were synthesized in our lab and isolated through Flash Column Chromatography or direct extraction, and the purities were confirmed by NMR. All catalysts were purchased in the high quality and all commercially obtained reagents were used as received. Anhydrous solvents were distilled in small scale with CaH_2 or sodium and stored under Argon. Barring large-scale preparation, reactions were carried in Schlenk tube under given conditions with a magnetic stirrer. Unless otherwise noted, isolated yields were calculated based on quantity of starting material.

Detailed Screen of Reaction Conditions

Reactions were conducted under the given conditions below. **1a** and catalyst were added to a 25 mL schlenk tube. After air-evacuated and refilled with CO, liquid reagents were added via syringe. While reaction completed, the mixture was extracted with ethyl acetate and NaCl aqueous solution. The organic portion was dried, concentrated and afforded product **3aa** via Flash Column Chromatography.

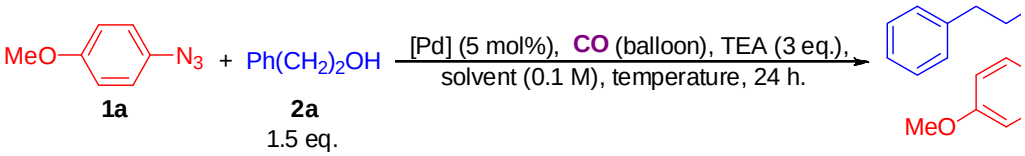
Table S1. Searching For Proper Catalyst.[a]



entry	Cat.	yield of **3aa**
1	$Co(OAc)_2\ 4H_2O$	0
2	$CoCl_2$	0
3	$MnCl_2$	0
4	$Mn(OAc)_2$	0
5	$Ni(OAc)_2$	0
6	$NiCl_2$	0
7	ZnBr	0
8	$AlCl_3$	0
9	$Sc(OTF)_3$	0
10	$FeBr_2$	0
11	$FeCl_3$	0
12	CuCl	0
13	$CuCl_2$	0
14	$Rh(OAc)_2$	< 5%
15	$RuCl_2$(p-cymene)	< 5%
16	AgOAc	0

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), Catalyst (0.01 mmol), TEA= triethylamine (0.6 mmol), DMF (2 mL), 24 h with a CO balloon.

Table S2. Optimation of Reaction Conditions.[a]



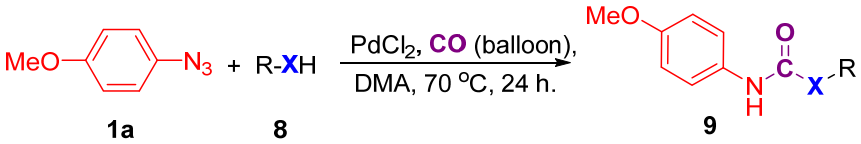
1a **2a** 1.5 eq.

entry	catalyst	solvent	temperature (°C)	yield[b]
1	5 mol% $Pd(cod)Cl_2$	DMF	80	51%
2[c]	5 mol% $Pd(cod)Cl_2$	DMF	80	36%
3	5 mol% $PdCl_2$	DMF	80	52%
4[c]	5 mol% $PdCl_2$	DMF	80	35%
5	5 mol% $Pd(OAc)_2$	DMF	80	< 10%
6	5 mol% $PdBr_2$	DMF	80	50%
7	5 mol% $PdCl_2(PhCN)_2$	DMF	80	51%
8	5 mol% $PdCl_2$	MeCN	50	trace
9	5 mol% $PdCl_2$	dioxane	50	trace
10	5 mol% $PdCl_2$	toluene	50	0
11	5 mol% $PdCl_2$	DCE	50	trace
12	5 mol% $PdCl_2$	THF	50	< 10%
13	5 mol% $PdCl_2$	AcOEt	50	trace
14	5 mol% $PdCl_2$	DMSO	50	44%
15	5 mol% $PdCl_2$	DMA	50	55%
16	5 mol% $PdCl_2$	NMP	50	77%
17	5 mol% $PdCl_2$	DMA	70	90%
18	5 mol% $PdCl_2$	DMA	90	73%
19	5 mol% $PdCl_2$	DMA	100	66%
20	5 mol% $PdCl_2$	NMP	70	61%
21	5 mol% $PdCl_2$	NMP	90	50%
22	1% $PdCl_2$	DMA	70	82%
23[d]	1% $PdCl_2$	DMA	70	76%
24[d]	2% $PdCl_2$	DMA	70	91%
25[d,e]	**2% $PdCl_2$**	**DMA**	**70**	**89%**
26[d,e]	no catalyst	DMA	70	0
27[d,e,f]	2% $PdCl_2$	DMA	70	0

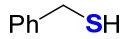
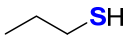
[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), TEA= triethylamine (0.6 mmol), solvent (2 mL), 24 h with a CO balloon. [b] Isolated yields. [c] PPh_3 (20 mol%) was added. [d] 1.2 eq. of **2a** was employed in DMA 0.2 M. [e] without TEA. [f] CO was replaced by Ar. [g] CO was replaced by CO_2.

Supplemental Experiments

Table S3. Reactions with Other Nucleophiles.[a]

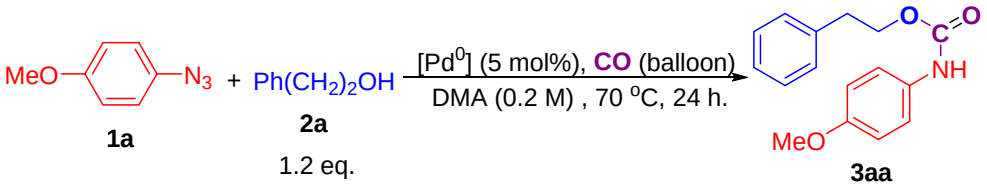


1a **8** **9**

entry	R-XH	yield of **9**
1	PhOH	< 5%
2		0
3		0
4	PhCOOH	0
5	AcOH	0

[a] Reactions were carried under standard conditions: **1a** (0.3 mmol), **8** (0.36 mmol), $PdCl_2$ (0.006 mmol), DMA (1.5 mL), 70 °C, 24 h with a CO balloon.

Table S4. Reactions Catalyzed by Pd(0) Catalysts. [a,b]

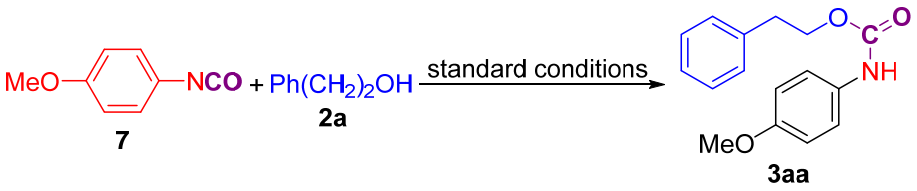


1a **2a** 1.2 eq. **3aa**

entry	[Pd^0]	**3aa**
1	$Pd(PPh_3)_4$	trace
2	10% Pd/C	trace

[a] Reactions conditions: **1a** (0.3 mmol), **2a** (0.36 mmol), Pd(0) Catalyst (0.015 mmol), DMA (1.5 mL), 70 °C, 24 h with a CO balloon. [b] 1,2-bis(4-methoxyphenyl)diazene was detecedas the major product by GC-MS.

Table S5. Several Control Experiments With 1-Isocyanato-4-methoxybenzenea.[a]



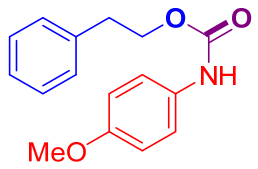
entry	control	yield[b]
1	---	79%
2	CO was changed to Ar	80%
3	carried without $PdCl_2$	63%

[a] Standard conditions: **7**(0.3 mmol), **2a** (0.36 mmol), $PdCl_2$ (0.006 mmol), DMA (1.5 mL), 70 °C, 24 h with a CO balloon. [b] Isolated yields.

In this table, several control experiments were conducted with 1-isocyanato-4-methoxybenzene (**7**) and **2a**to get an insight into the mechanism. The yield of the reaction without CO was almost the same as the yield ofthat under the standard conditions, illustrating that there is no influence from CO in the step of nucleophilic addition (entry 1, 2). Yet, nearly 20% of yield dropped as the reaction carried in the absence $PdCl_2$ (entry 3). This shows $PdCl_2$ promotes the second step of nucleophilic addition, most probably because of the Lewis acidity of $PdCl_2$and absence of usually necessitated basic promotor for a high yield. These results give a possibility that the catalyst did not leave immediately after the formation of isocyanate, but clung on to it to ease the following nucleophilic attack.

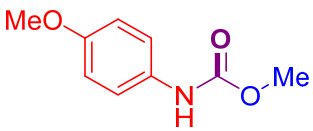
Experimental procedure for syntheses and Characterization Data of carbamates

3aa



Phenethyl 4-methoxyphenylcarbamate (3aa). Typical procedure: **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) were added to a 25 mL schlenk tube equipped with a magnetic stirrer bar. After air-evacuation and refilled with CO for three times or more, **2a** (43.9 mg, 0.36 mmol) and DMA (1.5 mL) were added via syringe. The formed mixture was stirred at 70 ºC for 24 h. The solution was then cooled to room temperature followed by diluting with ethyl acetate (10 mL). After being shaken with saturated NaCl aqueous solution (10 mL), the organic portion was separated. Repeat once and the aqueous portion was extracted with ethyl acetate (5 mL). The organic portions were combined, dried over Na_2SO_4, filtered, and evaporated under vaccum. The residue was purified through Flash Column Chromatography on silica gel (petroleum ether : ethyl acetate = 30:1)to afford **3aa** (72.2 mg, 89% yield). **3aa**: White solid; FT-IR (neat, cm^{-1}): 3436, 1696, 1532, 1414, 1247, 1079, 829, 776;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.36-7.17 (m, 7H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.50 (brs, 1H), 4.37 (t, *J* = 7.2 Hz, 2H), 3.77 (s, 3H), 2.97 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:156.17, 153.97, 137.99, 131.01, 129.05, 128.65, 126.70, 120.82(brs), 114.38, 65.67, 55.62, 35.55 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{16}H_{18}NO_3$ $(M+H)^+$272.1281, found: 272.1278.

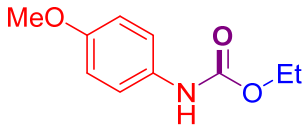
3ab



Methyl 4-methoxyphenylcarbamate (3ab).[1] The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2b** (11.5 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ab** (45.9 mg, 85% yield). **3ab**: White solid; FT-IR (neat, cm^{-1}): 3344, 3003,

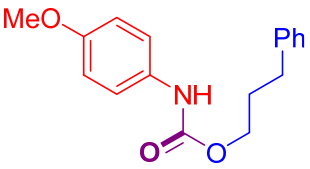
2946, 1738, 1540, 1512, 1444, 1324, 1233, 1188, 1073, 1023, 837, 766;^{1}H NMR (400 MHz, $CDCl_3$) δ:7.28 (d, *J*= 7.2 Hz, 2H), 6.84 (dt, J_1 = 9.2, J_2= 3.2 Hz, 2H), 6.72 (brs, 1H), 3.77 (s, 3H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:156.09, 154.63, 131.05, 120.81(brs), 114.31, 55.56, 52.34 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_9H_{12}NO_3(M+H)^+$182.0812, found: 182.0807.

3ac

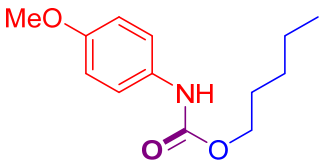


Ethyl 4-methoxyphenylcarbamate (3ac).[2] The reaction of**1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2c** (16.6 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ac** (48.5 mg, 83% yield). **3ac**:White solid; FT-IR (neat, cm^{-1}): 3320, 2983, 2920, 1700, 1539, 1416, 1238, 1074, 1029, 826, 774, 629;^{1}H NMR (400 MHz, $CDCl_3$) δ:7.28 (d, *J* = 7.6 Hz, 2H), 6.88-6.79 (m, 2H), 6.70 (brs, 1H), 4.20 (q, *J* = 7.2 Hz, 2H), 3.77 (s, 3H), 1.29 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:155.99, 154.25, 131.20, 120.81 (brs), 114.29, 61.16, 55.56, 14.66 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{10}H_{14}NO_3(M+H)^+$196.0968, found:196.0962.

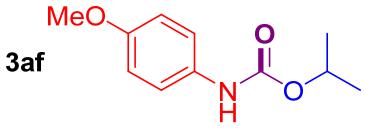
3ad



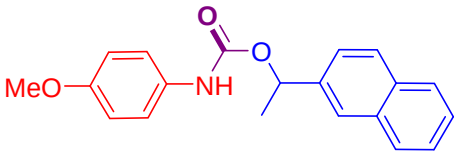
3-Phenylpropyl 4-methoxyphenylcarbamate (3ad). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2d** (49.0 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h,afforded product **3ad** (59.5 mg, 70% yield). **3ad**: White solid; FT-IR (neat, cm^{-1}): 3302, 2963, 2939, 1702, 1536, 1416, 1242, 1090, 1062, 827, 732, 699; ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.35-7.10 (m, 7H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.65 (brs, 1H), 4.16 (t, *J* = 6.6 Hz, 2H), 3.76 (s, 3H), 2.73-2.66 (m, 2H), 2.02-1.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:156.06, 154.16, 141.38, 131.13, 128.53, 128.49, 126.08, 120.83 (brs), 114.34, 64.62, 55.57, 32.25, 30.66 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{17}H_{20}NO_3(M+H)^+$ 286.1438, found: 286.1439.

3ae 

Pentyl 4-methoxyphenylcarbamate (3ae). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2e** (31.7 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ae** (58.2 mg, 82% yield). **3ae**: White solid; FT-IR (neat, cm^{-1}): 3336, 2958, 2934, 2857, 1072, 1599, 1540, 1419, 1227, 1082, 1034, 827, 742;^{1}H NMR (400 MHz, $CDCl_3$) δ:7.28 (d, J = 7.2 Hz, 2H), 6.83 (dt, J_1 = 8.8, J_2= 2.8 Hz, 2H), 6.66 (brs, 1H), 4.14 (t, J = 6.8 Hz, 2H), 3.77 (s, 3H), 1.70-1.61 (m, 2H), 1.42-1.28 (m, 4H), 0.91 (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:156.02 154.31, 131.25, 120.82 (brs), 114.33, 65.40, 55.58, 28.76, 28.11, 22.43, 14.05 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{13}H_{20}NO_3(M+H)^+$ 238.1438, found: 238.1435.

3af 

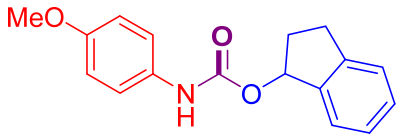
Isopropyl 4-methoxyphenylcarbamate (3af).[3] The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2f** (21.6 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3af** (47.7 mg, 76% yield). **3af**: White solid; FT-IR (neat, cm^{-1}): 3312, 2980, 2933, 2837, 1696, 1537, 1415, 1241, 1113, 1056, 1030, 828, 773, 644;^{1}H NMR (400 MHz, $CDCl_3$) δ:7.28 (d, J = 8.0 Hz, 2H), 6.83 (dt, J_1 = 8.8, J_2= 2.6 Hz, 2H), 6.58 (brs, 1H), 5.00 (hept, 6.2 Hz, 1H), 3.77 (s, 3H), 1.28 (d, J = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:155.94, 153.79, 131.35, 120.74 (brs), 114.33, 68.62, 55.58, 22.21 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{11}H_{16}NO_3(M+H)^+$ 210.1125, found: 210.1124.

3ag 

1-(Naphthalen-2-yl)ethyl 4-methoxyphenylcarbamate (3ag). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2g** (61.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ag** (58.0 mg, 60% yield). **3ag**: White solid; FT-IR (neat, cm^{-1}): 3386, 2933, 1711, 1519, 1415, 1217, 1070, 1029, 823, 752;^{1}H NMR (400 MHz, $CDCl_3$)

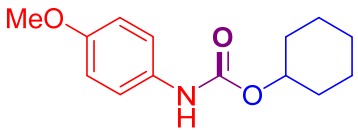
δ:7.85-7.79 (m, 4H), 7.57-7.44 (m, 3H), 7.27 (d, *J* = 8.4 Hz, 2H), 6.85-6.78 (m, 2H), 6.62 (brs, 1H), 6.05 (q, *J* = 6.4 Hz, 1H), 3.75 (s, 3H), 1.67 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:156.11, 153.40, 139.27, 133.36, 133.20, 131.09, 128.51, 128.20, 127.80, 126.34, 126.19, 125.14, 124.22, 120.76 (brs), 114.37, 73.40, 55.61, 22.42 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{20}H_{20}NO_3(M+H)^+$ 322.1438, found: 322.1439.

3ah

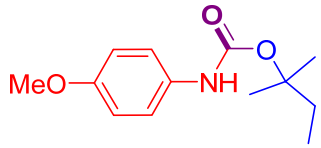


2,3-Dihydro-1H-inden-1-yl 4-methoxyphenylcarbamate (3ah). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2h** (48.2 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ah** (50.4 mg, 60% yield). **3ah**: White solid FT-IR (neat, cm^{-1}): 3302, 2918, 2836, 1691, 1533, 1415, 1241, 1058, 824, 749;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.49 (d, *J* = 7.6 Hz, 1H), 7.38-7.18 (m, 5H), 6.84 (d, *J* = 8.8 Hz, 2H), 6.49 (brs, 1H), 6.22 (dd, J_1 = 6.8, J_2= 3.6 Hz, 1H), 3.78 (s, 3H), 3.19-3.05 (m, 1H), 2.94-2.83 (m, 1H), 2.58-2.47 (m, 1H), 2.22-2.12 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.11, 153.97, 144.51, 141.23, 131.14, 129.14, 126.90, 125.73, 124.98, 120.76 (brs), 114.42, 79.24, 55.57, 32.57, 30.29 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{17}H_{18}NO_3(M+H)^+$ 284.1281, found: 284.1278.

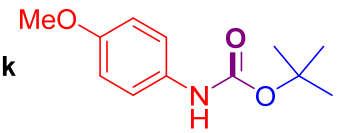
3ai



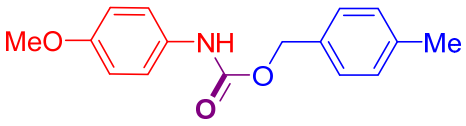
Cyclohexyl 4-methoxyphenylcarbamate (3ai). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2i** (36.0 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h,afforded product **3ai** (45.0 mg, 60% yield). **3ai**: White solid; FT-IR (neat, cm^{-1}): 3338, 2938, 2858, 1699, 1537, 1415, 1234, 1065, 1030, 826, 780, 630;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, *J* = 8.0 Hz, 2H), 6.84 (dt, J_1 = 8.8, J_2= 2.8 Hz, 2H), 6.54 (brs, 1H), 4.83-4.64 (m, 1H), 3.77 (s, 3H), 1.98-1.85 (m, 2H), 1.79-1.67 (m, 2H), 1.61-1.15 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.92, 153.71, 131.38, 120.67 (brs), 114.34, 73.56, 55.60, 32.06, 25.50, 23.89 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{14}H_{20}NO_3(M+H)^+$ 250.1438, found: 250.1437.

3aj 

***tert*-Pentyl 4-methoxyphenylcarbamate (3aj).** The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2j** (31.7 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3aj** (9.8 mg, 14% yield). **3aj**: Transparent colorless liquid; FT-IR (neat, cm^{-1}): 3334, 2965, 2929, 1702, 1516, 1228, 1158, 829;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (d, J = 8.0 Hz, 2H), 6.83 (d, J = 9.2 Hz, 2H), 6.36 (brs, 1H), 3.78 (s, 3H), 1.83 (q, J = 7.5 Hz, 2H), 1.47 (s, 6H), 0.92 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.87, 153.28, 131.61, 120.71 (brs), 114.34, 82.82, 55.66, 33.87, 25.97, 8.44 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{13}H_{19}NNaO_3$ $(M+Na)^+$ 260.1257, found: 260.1252.

3ak 

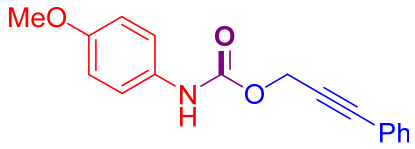
***tert*-Butyl4-methoxyphenylcarbamate (3ak).**[3] The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2k** (26.6 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ak** (10.0 mg, 15% yield). **3ak**: White solid; FT-IR (neat, cm^{-1}): 3338, 2929, 1702, 1517, 1412, 1240, 1162, 829, 724;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (d, J = 8.4 Hz, 2H), 6.83 (dt, J_1 = 9.2, J_2= 2.6 Hz, 2H), 6.35 (brs, 1H), 3.78 (s, 3H), 1.51 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.88, 153.32, 131.60, 120.78 (brs), 114.37, 80.38, 55.66, 28.52 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{12}H_{17}NNaO_3$ $(M+Na)^+$ 246.1101, found: 246.1098.

3al 

4-Methylbenzyl 4-methoxyphenylcarbamate (3al). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2l** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h,afforded product **3al** (57.3 mg, 70% yield). **3al**: White solid; FT-IR (neat, cm^{-1}): 3317, 2959, 2940, 1701, 1534, 1418, 1229, 1067, 1030, 824, 809, 784;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (d,

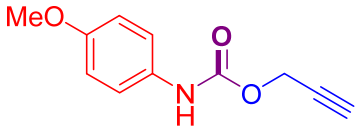
J = 8.0 Hz, 4H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.70 (brs, 1H), 5.12 (s, 2H), 3.75 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.09, 153.96, 138.20, 133.30, 131.04, 129.34, 128.52, 120.80 (brs), 114.32, 66.94, 55.55, 21.26 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{16}H_{18}NO_3(M+H)^+$ 272.1281, found: 272.1285.

3am

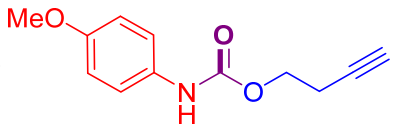


3-Phenylprop-2-ynyl 4-methoxyphenylcarbamate (3am). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2m** (47.5 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3am** (48.4 mg, 57% yield). **3am**: White solid; FT-IR (neat, cm^{-1}): 3322, 2950, 2833, 1880, 1701, 1541, 1414, 1239, 1070, 829, 754, 690, 645;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48-7.41 (m, 2H), 7.34-7.24 (m, 5H), 6.84 (dt, J_1 = 9.2, J_2= 2.8 Hz, 2H), 6.77 (brs, 1H), 5.00 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.29, 153.21, 132.01, 130.71, 128.86, 128.41, 122.27, 120.94 (s), 114.39, 86.66, 83.36, 55.58, 53.63 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{17}H_{16}NO_3(M+H)^+$ 282.1125, found: 282.1124.

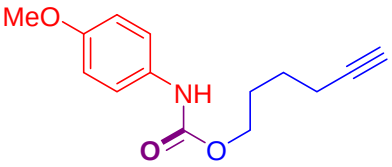
3an



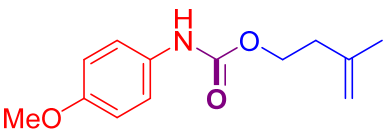
Prop-2-ynyl 4-methoxyphenylcarbamate(3an).[4] The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2n** (20.2 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3an** (30.4 mg, 49% yield). **3an**: White solid; FT-IR (neat, cm^{-1}): 3304, 3254, 2936, 2839, 2130, 1697, 1552, 1514, 1453, 1418, 1225, 1065, 1035, 828, 744, 682; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, *J* = 8.0 Hz, 2H), 6.84 (dt, J_1 = 8.8, J_2= 2.8 Hz, 2H), 6.74 (brs, 1H), 4.76 (d, *J* = 2.4 Hz, 2H), 3.77 (s, 3H), 2.50 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.35, 153.00, 130.57, 120.98 (brs), 114.39, 78.11, 75.04, 55.59, 52.76 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{11}H_{12}NO_3(M+H)^+$ 206.0812, found: 206.0808.

3ao 

But-3-ynyl 4-methoxyphenylcarbamate (3ao). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2o** (25.2 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ao** (44.8 mg, 68% yield). **3ao**: White solid; FT-IR (neat, cm^{-1}): 3352, 3295, 2957, 2907, 2837, 1881, 1694, 1551, 1523, 1419, 1238, 1088, 1033, 832, 750; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, J = 8.0 Hz, 2H), 6.84 (dt, J_1 = 8.8, J_2= 2.6 Hz, 2H), 6.72 (brs, 1H), 4.26 (t, J = 6.6 Hz, 2H), 3.78 (s, 3H), 2.57 (td, J_1 = 6.8, J_2= 2.8 Hz, 2H), 2.03 (t, J = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.20, 153.66, 130.86, 120.86 (brs), 114.38, 80.35, 69.91, 62.92, 55.59, 19.45 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{12}H_{14}NO_3(M+H)^+$ 220.0968, found: 220.0966.

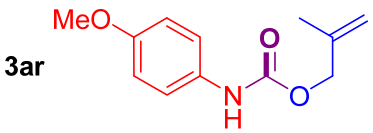
3ap 

Hex-5-ynyl 4-methoxyphenylcarbamate (3ap). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2p** (35.3 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h,afforded product **3ap** (53.2 mg, 72% yield). **3ap**: White solid; FT-IR (neat, cm^{-1}): 3343, 3274, 2942, 2865, 1704, 1545, 1420, 1229, 1029, 833, 815, 744; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, J = 7.2 Hz, 2H), 6.86-6.81 (m, 2H), 6.68 (brs, 1H), 4.17 (t, J = 6.6 Hz, 2H), 3.77 (s, 3H), 2.24 (td, J_1 = 7.2, J_2= 2.4 Hz, 2H), 1.97 (t, J = 2.6 Hz, 1H), 1.83-1.73 (m, 2H), 1.67-1.56 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.05, 154.14, 131.10, 120.79 (brs), 114.33, 84.00, 68.86, 64.66, 55.57, 28.09, 24.96, 18.16 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{14}H_{18}NO_3(M+H)^+$ 248.1281, found: 248.1282.

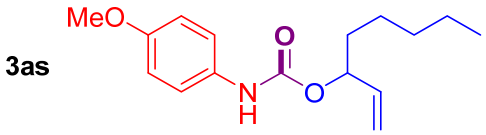
3aq 

3-Methylbut-3-enyl 4-methoxyphenylcarbamate (3aq). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2q** (31.0 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3aq** (54.8 mg, 78% yield). **3aq**: White solid; FT-IR (neat, cm^{-1}):

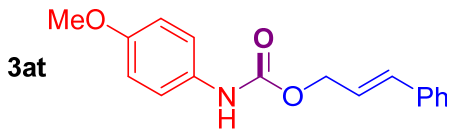
3329, 2961, 2937, 1699, 1526, 1516, 1416, 1228, 1084, 1063, 1027, 827, 772, 521; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, *J* = 6.8 Hz, 2H), 6.83 (d, *J* = 9.2 Hz, 2H), 6.68 (brs, 1H), 4.80 (d, *J* = 21.2 Hz, 2H), 4.26 (t, *J* = 6.8 Hz, 2H), 3.77 (s, 3H), 2.37 (t, *J* = 6.8 Hz, 2H), 1.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.01, 154.06, 141.81, 131.00, 120.71 (brs), 114.29 112.36, 63.31, 55.56, 37.10, 22.53 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{13}H_{18}NO_3(M+H)^+$ 236.1281, found: 236.1282.



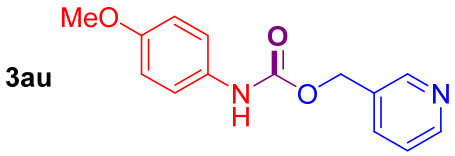
2-Methylallyl 4-methoxyphenylcarbamate (3ar). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2r** (25.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ar** (42.6 mg, 64% yield). **3ar**: White solid; FT-IR (neat, cm^{-1}): 3327, 2925, 2840, 1705, 1532, 1414, 1236, 1086, 1028, 893, 824, 775; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29 (d, *J* = 7.6 Hz, 2H), 6.84 (dt, J_1 = 9.2, J_2= 2.8 Hz, 2H), 6.71 (brs, 1H), 5.01 (s, 1H), 4.93 (s, 1H), 4.57 (s, 2H), 3.77 (s, 3H), 1.78 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.14, 153.86, 140.42, 131.05, 120.80 (brs), 114.35, 112.82, 68.42, 55.58, 19.53 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{12}H_{16}NO_3(M+H)^+$ 222.1125, found: 222.1120.



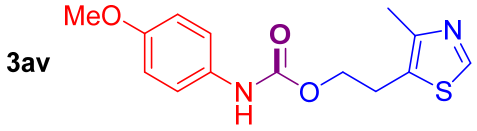
Oct-1-en-3-yl 4-methoxyphenylcarbamate (3as). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2s** (46.1 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3as** (39.0 mg, 47% yield). **3as**: White solid; FT-IR (neat, cm^{-1}): 3314, 2957, 2935, 2857, 1697, 1534, 1414, 1248, 826; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29 (d, *J* = 8.0 Hz, 2H), 6.84 (dt, J_1 = 8.8, J_2= 2.8 Hz, 2H), 6.57 (brs, 1H), 5.88-5.75 (m, 1H), 5.33-5.13 (m, 3H), 3.77 (s, 3H), 1.72-1.55 (m, 2H), 1.42-1.21 (m, 6H), 0.88 (t, *J* = 6.8 Hz, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.09, 153.53, 137.09, 131.22, 120.73 (brs), 116.68, 114.41, 75.89, 55.66, 34.53, 31.74, 24.86, 22.67, 14.13 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{16}H_{23}NNaO_3$ $(M+Na)^+$ 300.1570, found: 300.1574.



Cinnamyl 4-methoxyphenylcarbamate (3at). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2t** (48.2 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3at** (57.8 mg, 68% yield). **3at**: White solid; FT-IR (neat, cm^{-1}): 3332, 2995, 2964, 2936, 2835, 1695, 1530, 1413, 1235, 1059, 1032, 782, 744, 692, 650; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.22 (m, 7H), 6.83 (dt, J_1 = 9.2, J_2= 2.8 Hz, 2H), 6.74-6.61 (m, 2H), 6.31 (dt, J_1 = 15.6, J_2= 6.4 Hz, 1H), 4.80 (dd, J_1 = 6.0, J_2= 1.0 Hz, 2H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.17, 153.89, 136.35, 134.17, 131.00, 128.71, 128.16, 126.74, 123.65, 120.87 (brs), 114.37, 65.78, 55.58 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{17}H_{17}NNaO_3$ $(M+Na)^+$ 306.1101, found: 306.1100.

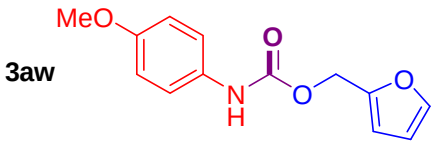


Pyridin-3-ylmethyl 4-methoxyphenylcarbamate (3au). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2u** (39.2 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3au** (38.7 mg, 50% yield). **3au**: White solid; FT-IR (neat, cm^{-1}): 3428, 3233, 3186, 3024, 2976, 2933, 1724, 1514, 1415, 1296, 1228, 1060, 1030, 838, 794; ^1H NMR (400 MHz, DMSO) δ: 9.60 (brs, 1H), 8.65 (s, 1H), 8.55 (d, J = 3.6 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.48-7.28 (m, 3H), 6.86 (d, J = 9.2 Hz, 2H), 5.17 (s, 2H), 3.70 (s, 3H);^{13}C NMR (100 MHz, DMSO) δ: 154.91, 153.40, 149.40, 149.28, 136.04, 132.38, 131.98, 123.61, 119.83 (brs), 114.00, 63.36, 55.18 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{14}H_{15}N_2O_3(M+H)^+$ 259.1077, found: 259.1081.

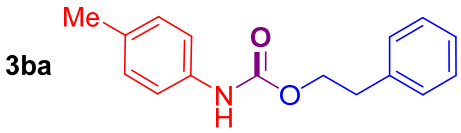


2-(4-Methylthiazol-5-yl)ethyl 4-methoxyphenylcarbamate (3av). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2v** (51.5 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3av** (59.6 mg, 68% yield). **3av**: White solid; FT-IR (neat,

cm^{-1}): 3234, 3108, 3040, 2984, 2936, 2891, 2839, 2065, 1719, 1604, 1552, 1514, 1423, 1298, 1229, 1071, 1035, 922, 840, 753, 567; ^{1}H NMR (400 MHz, DMSO) δ: 9.44 (brs, 1H), 8.84 (s, 1H), 7.37-7.35 (m, 2H), 6.85 (d, *J* = 9.2 Hz, 2H), 4.23 (t, *J* = 6.4 Hz, 2H), 3.70 (s, 3H), 3.12 (t, *J* = 6.4 Hz, 2H), 2.34 (s, 3H);^{13}C NMR (100 MHz, DMSO) δ: 154.84, 153.45, 150.65, 149.40, 132.04, 127.15, 119.92 (brs), 113.91, 64.01, 55.12, 25.58, 14.60 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{14}H_{17}N_2O_3S(M+H)^+$ 293.0954, found: 293.0961.

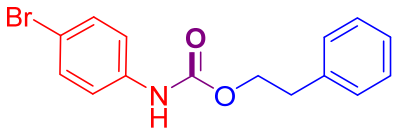


Furan-2-ylmethyl 4-methoxyphenylcarbamate (3aw). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2w** (35.3 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3aw** (38.1 mg, 52% yield). **3aw**: Light yellow solid; FT-IR (neat, cm^{-1}): 3314, 1703, 1540, 1417, 1237, 1063, 1027, 830, 744, 645; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.42 (dd, J_1 = 1.2, J_2= 0.6 Hz, 1H), 7.26 (d, *J* = 9.2 Hz, 2H), 6.86-6.79 (d, *J* = 9.0 Hz, 2H), 6.67 (brs, 1H), 6.43 (d, *J* = 3.2 Hz, 1H), 6.36 (dd, J_1 = 3.2, J_2= 2.0 Hz, 1H), 5.12 (s, 2H), 3.76 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.15, 153.54, 149.83, 143.38, 130.84, 120.86 (brs), 114.34, 110.76, 110.71, 58.71, 55.58 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{13}H_{13}NNaO_4$ $(M+Na)^+$ 270.0737, found: 270.0740.

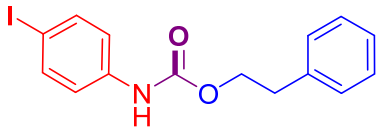


Phenethyl*p*-tolylcarbamate (3ba). The reaction of **1b** (39.9 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ba** (60.9 mg, 80% yield). **3ba**: White solid; FT-IR (neat, cm^{-1}): 3330, 2957, 2936, 1697, 1595, 1531, 1409, 1239, 1083, 818, 735, 698, 507; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37-7.16 (m, 7H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.56 (brs, 1H), 4.37 (t, *J* = 6.8 Hz, 2H), 2.98 (t, *J* = 7.0 Hz, 2H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.72, 137.96, 135.35, 133.16, 129.65, 129.04, 128.66, 126.71, 118.98 (brs), 65.66, 35.53, 20.86 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{16}H_{18}NO_2(M+H)^+$

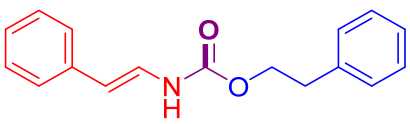
256.1332, found: 256.1331.

3ca 

Phenethyl 4-bromophenylcarbamate (3ca). The reaction of **1c** (59.4 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ca** (83.9 mg, 88% yield). **3ca**: White solid; FT-IR (neat, cm^{-1}): 3322, 2970, 2955, 2937, 2892, 1699, 1590, 1532, 1399, 1236, 1081, 820, 743, 700, 502; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.37 (d, *J* = 8.8 Hz, 2H), 7.32-7.20 (m, 7H), 6.73 (brs, 1H), 4.36 (t, *J* = 7.0 Hz, 2H), 2.96 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 153.43, 137.72, 137.06, 132.03, 128.96, 128.66, 126.76, 120.38 (brs), 116.04, 65.89, 35.40 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{15}H_{15}BrNO_2(M+H)^+$ 320.0281, found: 320.0279.

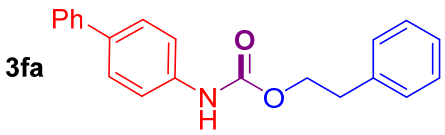
3da 

Phenethyl 4-iodophenylcarbamate (3da). The reaction of **1d** (73.5 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3da** (70.0 mg, 64% yield). **3ba**: White solid; FT-IR (neat, cm^{-1}): 3309, 3026, 2964, 1694, 1590, 1531, 1397, 1310, 1242, 1083, 817, 744, 700, 669, 502; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.55 (d, *J* = 8.8 Hz, 2H), 7.34-7.19 (m, 5H), 7.12 (d, *J* = 6.0 Hz, 2H), 6.69 (brs, 1H), 4.36 (t, *J* = 6.8 Hz, 2H), 2.96 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.35, 137.98, 137.77, 137.71, 128.97, 128.67, 126.76, 120.68 (brs), 86.43, 65.89, 35.30 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{15}H_{15}INO_2(M+H)^+$ 368.0142, found: 368.0153.

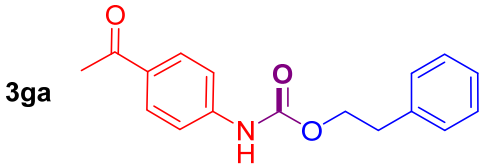
3ea 

(*E*)-Phenethylstyrylcarbamate (3ea). The reaction of **1e** (43.5 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h,

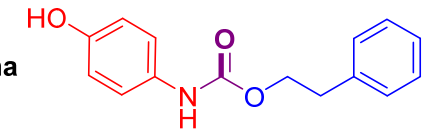
afforded product **3ea** (70.1 mg, 87% yield). **3ea**: Light yellow solid; FT-IR (neat, cm^{-1}): 3385, 2935, 1718, 1654, 1515, 1469, 1307, 1226, 1078, 964, 752, 694, 574; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.36-7.08 (m, 11H), 6.72 (d, *J* = 10.8 Hz, 1H), 5.92 (d, *J* = 14.4 Hz, 1H), 4.35 (t, *J* = 6.8 Hz, 2H), 2.94 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.74, 137.71, 136.35, 128.98, 128.74, 128.65, 126.74, 126.40, 125.37, 124.09, 110.88, 66.08, 35.42 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{17}H_{18}NO_2(M+H)^+$ 268.1332, found: 268.1337.



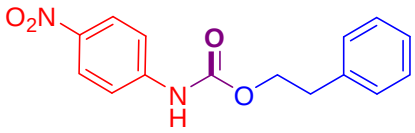
Phenethyl biphenyl-4-ylcarbamate (3fa). The reaction of **1f** (58.5 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3fa** (61.3 mg, 65% yield). **3fa**: White solid; FT-IR (neat, cm^{-1}): 3329, 3029, 2933, 2893, 1714, 1591, 1533, 1318, 1235, 1080, 833, 748, 699, 619, 498; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.59-7.49 (m, 4H), 7.41 (t, *J* = 7.6 Hz, 4H), 7.35-7.19 (m, 6H), 6.68 (brs, 1H), 4.40 (t, *J* = 7.0 Hz, 2H), 3.00 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.57, 140.64, 137.89, 137.26, 136.50, 129.04, 128.90, 128.69, 127.80, 127.14, 126.91, 126.75, 119.14 (brs), 65.82, 35.51 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{21}H_{20}NO_2(M+H)^+$ 318.1489, found: 318.1496.



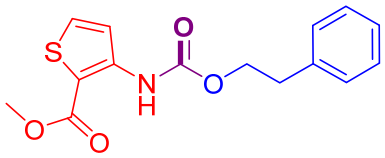
Phenethyl 4-acetylphenylcarbamate (3ga). The reaction of **1g** (48.3 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ga** (79.3 mg, 94% yield). **3ga**: White solid; FT-IR (neat, cm^{-1}): 3348, 2971, 2919, 1707, 1673, 1607, 1528, 1229, 1083, 830, 755, 703, 624, 603, 493; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 3H), 7.33-7.16 (m, 5H), 4.38 (t, *J* = 7.0 Hz, 2H), 2.96 (t, *J* = 7.0 Hz, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 197.30, 153.25, 142.78, 137.60, 132.01, 129.89, 128.89, 128.60, 126.70, 117.76, 65.93, 35.29, 26.36 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{17}H_{18}NO_3(M+H)^+$ 284.1281, found: 284.1280.

3ha 

Phenethyl 4-hydroxyphenylcarbamate (3ha). The reaction of **1h** (40.5 mg, 0.3 mmol), $PdCl_2$(1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ha** (59.7 mg, 78% yield). **3ha**: White solid; FT-IR (neat, cm^{-1}): 3337, 2959, 2895, 1696, 1538, 1311, 1234, 834, 736, 696, 638, 498; ^{1}H NMR (400 MHz, DMSO) δ: 9.28 (brs, 1H), 9.10 (s, 1H), 7.49-7.10 (m, 7H), 6.69 (d, J = 8.4 Hz, 2H), 4.27 (t, J = 6.8 Hz, 2H), 2.93 (t, J = 6.7 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ: 153.74, 152.88, 138.23, 130.67, 128.91, 128.40, 126.36, 120.19 (brs), 115.16, 64.49, 34.87 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{15}H_{16}NO_3(M+H)^+$ 258.1125, found: 258.1119.

3ia 

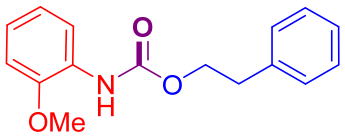
Phenethyl 4-nitrophenylcarbamate (3ia). The reaction of **1i** (49.2 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ia** (71.4 mg, 83% yield). **3ia**: White solid; FT-IR (neat, cm^{-1}): 3378, 3087, 3028, 2954, 1740, 1599, 1550, 1514, 1333, 1216, 1111, 1065, 852, 749, 694, 624; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.17 (dt, J_1 = 9.2, J_2= 2.4 Hz 2H), 7.52 (d, J = 8.8 Hz, 2H), 7.36-7.20 (m, 5H), 7.13 (brs, 1H), 4.43 (t, J = 7.0 Hz, 2H), 3.00 (t, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.90 144.05, 143.06, 137.48, 128.94, 128.72, 126.87, 125.29, 117.88, 66.38, 35.23 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{15}H_{15}N_2O_4(M+H)^+$ 287.1026, found: 287.1031.

3ja 

Methyl 3-(phenethoxycarbonylamino)thiophene-2-carboxylate (3ja). The reaction of **1j** (55.0 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ja** (79.5 mg, 87% yield). **3ja**: Light yellow solid;

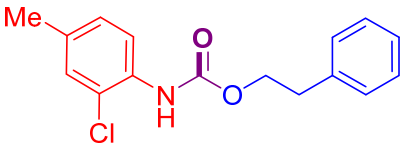
FT-IR (neat, cm^{-1}): 3331, 3114, 2949, 1730, 1678, 1578, 1446, 1285, 1220, 1095, 999, 779, 705, 637, 506; ^1H NMR (400 MHz, $CDCl_3$) δ: 9.50 (s, 1H), 7.86 (s, 1H), 7.40 (d, J = 5.2 Hz, 1H), 7.34-7.19 (m, 5H), 4.38 (t, J = 7.2 Hz, 2H), 3.85 (s, 3H), 2.99 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.56, 152.94, 145.10, 137.60, 131.60, 128.97, 128.61, 126.67, 121.31, 108.79, 66.19, 51.89, 35.36ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{15}H_{16}NO_4S(M+H)^+$ 306.0795, found: 306.0793.

3ka



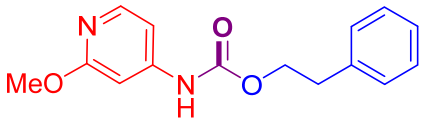
Phenethyl 2-methoxyphenylcarbamate (3ka). The reaction of **1k** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ka** (48.9 mg, 60% yield). **3ka**: Transparent colorless liquid; FT-IR (neat, cm^{-1}): 3432, 3028, 2956, 2838, 2101, 1733, 1064, 1536, 1461, 1434, 1229, 1210, 1066, 1028, 748, 700, 570; ^1H NMR (400 MHz, $CDCl_3$) δ: 8.08 (brs, 1H), 7.36-7.16 (m, 6H), 7.02-6.90 (m, 2H), 6.83 (dd, J_1 = 8.0, J_2= 1.8 Hz, 1H), 4.38 (t, J = 7.2 Hz, 2H), 3.82 (s, 3H), 2.99 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.47, 147.69, 137.93, 129.01, 128.61, 127.69, 126.64, 122.84, 121.18, 118.32 (brs), 110.07, 65.62, 55.68, 35.52 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{16}H_{18}NO_3(M+H)^+$ 272.1281, found: 272.1278.

3la

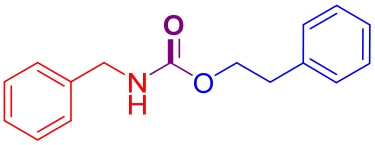


Phenethyl 2-chloro-4-methylphenylcarbamate (3la). The reaction of **1l** (50.1 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3la** (81.6 mg, 94% yield). **3la**: White solid; FT-IR (neat, cm^{-1}): 3429, 3287, 2919, 1696, 1533, 1417, 1242, 1090, 813, 737, 698; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.86 (s, 1H), 7.24-7.18 (m, 2H), 7.14 (d, J = 7.2 Hz, 3H), 7.12-7.06 (m, 1H), 6.97 (s, 1H), 6.67 (dd, J_1 = 8.1, J_2= 1.4 Hz, 1H), 4.29 (t, J = 7.2 Hz, 2H), 2.90 (t, J = 7.0 Hz, 2H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.18, 137.94, 137.65, 134.29, 128.98, 128.67, 128.65, 126.72, 124.64, 120.63, 119.21, 65.99, 35.43, 21.38 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{16}H_{17}ClNO_2(M+H)^+$ 290.0942, found:

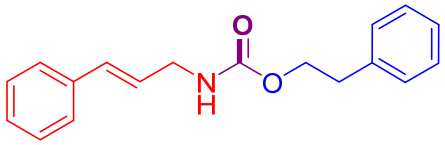
290.0943.

3ma 

Phenethyl 2-methoxypyridin-4-ylcarbamate (3ma). The reaction of **1m** (45.0 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **3ma** (66.4 mg, 81% yield). **3ma**: Transparent colorless liquid; FT-IR (neat, cm^{-1}): 3319, 3028, 2950, 1742, 1603, 1528, 1399, 1220, 1072, 1042, 860, 824, 769, 747, 700, 496, 466; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.97 (d, *J* = 5.6 Hz, 1H), 7.48 (s, 1H), 7.33-7.15 (m, 5H), 6.93-6.85 (m, 2H), 4.37 (t, *J* = 6.8 Hz, 2H), 3.88 (s, 3H), 2.95 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.49, 153.02, 147.63, 147.46, 137.55, 128.90, 128.64, 126.74, 107.39, 98.24, 66.07, 53.63, 35.24 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{15}H_{17}N_2O_3(M+H)^+$ 273.1234, found: 273.1240.

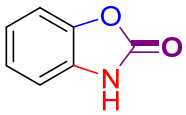
3na 

Phenethylbenzylcarbamate (3na). The reaction of **1n** (39.9 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 90 ºC, under CO (1 atm), 24 h, afforded product **3na** (28.3 mg, 37% yield). **3na**: White solid; FT-IR (neat, cm^{-1}): 3334, 2932, 1688, 1535, 1455, 1252, 1147, 1074, 749, 699, 660; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.39-7.14 (m, 10H), 5.00 (brs, 1H), 4.43-4.25 (m, 4H), 2.93 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.63, 138.63, 138.12, 129.05, 128.79, 128.59, 127.63, 127.60, 126.60, 65.54, 45.15, 35.66 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{16}H_{18}NO_2(M+H)^+$ 256.1332, found: 256.1334.

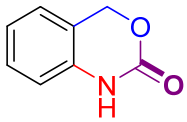
3oa 

Phenethylcinnamylcarbamate (3oa). The reaction of **1o** (47.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and **2a** (43.9 mg, 0.36 mmol) in DMA (1.5 mL), at 90 ºC, under CO (1 atm), 24 h, afforded product **3oa** (10.0 mg, 12% yield). **3oa**: White solid; FT-IR (neat, cm^{-1}): 3331, 3028, 1693,

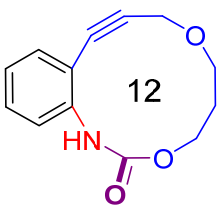
1537, 1255, 1144, 985, 966, 745, 695; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50-7.18 (m, 10H), 6.50 (d, *J* = 15.6 Hz, 1H), 6.27-6.05 (m, 1H), 4.79 (s, 1H), 4.32 (t, *J* = 6.8 Hz, 2H), 3.96 (s, 2H), 2.95 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.49, 138.16, 136.69, 131.89, 129.07, 128.73, 128.62, 127.85, 126.63, 126.54, 126.04, 65.56, 43.21, 35.68 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{18}H_{20}NO_2(M+H)^+$ 282.1489, found: 282.1493.

5a 

Benzo[*d*]oxazol-2(3*H*)-one (5a).[5] The reaction of **4a** (40.5 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **5a** (32.3 mg, 81% yield). **5a**: White solid; FT-IR (neat, cm^{-1}): 3223, 1772, 1736, 1480, 1398, 1253, 942, 894, 741, 720, 697, 574; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.03 (brs, 1H), 7.24-7.08 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.57, 144.02, 129.60, 124.35, 122.84, 110.44, 110.24 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_7H_5NNaO_2$ $(M+Na)^+$ 158.0212, found: 158.0206.

5b 

1*H*-Benzo[*d*][1,3]oxazin-2(4*H*)-one (5b).[6] The reaction of **4b** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **5b** (45.5 mg, 99% yield). **5b**: White solid; FT-IR (neat, cm^{-1}): 3213, 3160, 3000, 2942, 1710, 1604, 1417, 1297, 1064, 888, 744; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.45 (brs, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.11-7.01 (m, 2H), 6.91 (d, *J* = 8.0 Hz, 1H), 5.33 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.25, 135.68, 129.28, 124.19, 123.38, 117.87, 114.49, 68.81 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_8H_7NNaO_2$ $(M+Na)^+$ 172.0369, found: 172.0370.

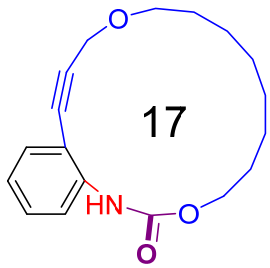
5c 

(5c)

The reaction of **4c** (69.3 mg, 0.3 mmol), $PdCl_2$ (2.7 mg, 0.015mmol, 5mol%) in DMA (6 mL), at

70 ºC, under CO (1 atm), 24 h, afforded product **5c** (30.3 mg, 43% yield). **5c**: White solid; FT-IR (neat, cm^{-1}): 3313, 2947, 2923, 2873, 1702, 1504, 1489, 1444, 1225, 1111, 1040, 768, 750; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.41 (dd, J_1 = 7.6, J_2= 1.6 Hz, 1H), 7.30 (td, J_1 = 7.6, J_2= 1.6 Hz, 1H), 7.26-7.17 (m, 2H), 6.44 (brs, 1H), 4.46 (t, J = 5.6 Hz, 2H), 4.32 (s, 2H), 3.78 (t, J = 5.2 Hz, 2H), 1.93(p, J = 5.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.72, 138.65, 131.37, 129.09, 127.74, 127.25, 122.62, 92.65, 83.29, 64.15, 61.17, 58.97, 29.87 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{13}H_{14}NO_3(M+H)^+$ 232.0968, found: 232.0968.

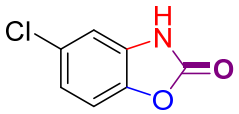
5d



(5d)

The reaction of **4d** (90.3 mg, 0.3 mmol), $PdCl_2$ (2.7 mg, 0.015mmol, 5mol%) in DMA (6 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **5d** (36.5 mg, 40% yield). **5d**: Transparent colorless liquid; FT-IR (neat, cm^{-1}): 3397, 2932, 2857, 1739, 1581, 1523, 1452, 1232, 1210, 1098, 836, 757; ^1H NMR (400 MHz, $CDCl_3$) δ:8.16 (d, J = 8.0 Hz, 1H), 7.49 (brs, 1H), 7.36-7.29 (m, 2H), 6.96 (td, J_1 = 7.6, J_2= 1.2 Hz, 1H), 4.39 (s, 2H), 4.20 (t, J = 5.4 Hz, 2H), 3.60 (t, J = 6.0 Hz, 2H), 1.72-1.58 (m, 4H), 1.57-1.36 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.40, 139.48, 131.02, 129.77, 122.32, 117.46, 110.84, 93.15, 81.22, 70.97, 65.39, 59.03, 28.95, 26.86 (overlap, 2C), 26.47, 24.43, 23.93 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{18}H_{24}NO_3(M+H)^+$ 302.1751, found: 302.1755.

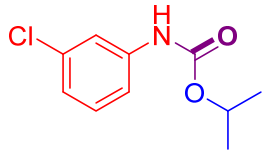
6a



Chlorzoxazone (6a).[7] The reaction of **1p** (50.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **6a** (42.3 mg, 84% yield). **6a**: Light yellow solid; FT-IR (neat, cm^{-1}): 3468, 3158, 3086, 3054, 2978, 1773, 1620, 1480, 1151, 963, 804, 723, 713; ^1H NMR (400 MHz, DMSO) δ: 11.82 (s, 1H), 7.28 (d, J = 8.8 Hz, 1H), 7.14-7.05 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ: 154.30, 142.13, 131.71, 127.79, 121.51, 110.78, 109.83 ppm;

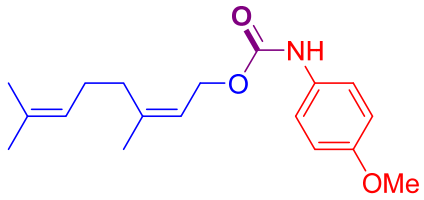
HR-MS (ESI, positive): *m/z* calculated for $C_7H_4ClNNaO_2$ $(M+Na)^+$ 191.9823, found: 191.9822.

6b



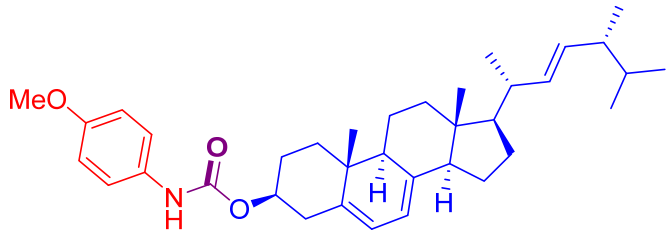
Chlorpropham (6b).[8] The reaction of **1q** (45.9 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and *i*-PrOH (180.0 mg, 3.0mmol, 10equiv) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **6b** (60.0 mg, 94% yield). **6b**: Transparent colorless liquid; Transparent colorless liquid; FT-IR (neat, cm^{-1}): 3319, 3124, 3085, 2982, 2167, 1733, 1595, 1537, 1424, 1221, 1111, 1047, 901, 873, 830, 774, 682, 555, 440; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.51 (s, 1H), 7.25-7.15 (m, 2H), 7.04-6.98 (m, 1H), 6.76 (brs, 1H), 5.02 (hept, *J* = 6.3 Hz, 1H), 1.29 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.16, 139.48, 134.81, 130.07, 123.34, 118.76, 116.68, 69.22, 22.13 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{10}H_{12}ClNNaO_2$ $(M+Na)^+$ 236.0449, found: 236.0446.

6c



(*Z*)-3,7-Dimethylocta-2,6-dienyl 4-methoxyphenylcarbamate (6c). The reaction of **1a** (44.7 mg, 0.3 mmol), $PdCl_2$ (1.1 mg, 0.006 mmol) and Nerol (55.4 mg, 0.36mmol) in DMA (1.5 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **6c** (76.0 mg, 84% yield). **6c**: Transparent colorless liquid; FT-IR (neat, cm^{-1}): 3323, 2965, 2931, 1702, 1537, 1515, 1443, 1415, 1222, 1033, 828, 766; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.27 (d, *J* = 8.0 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.63 (s, 1H), 5.39 (t, *J* = 7.0 Hz, 1H), 5.10 (t, *J* = 6.4 Hz, 1H), 4.64 (d, *J* = 6.8 Hz, 2H), 3.76 (s, 3H), 2.17-2.03 (m, 4H), 1.77 (s, 3H), 1.68 (s, 3H), 1.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.98, 154.12, 142.65, 132.25, 131.19, 123.69, 120.75 (brs), 119.55, 114.30, 61.74, 55.55, 32.27, 26.76, 25.76, 23.60, 17.73 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{18}H_{25}NNaO_3$ $(M+Na)^+$ 326.1727, found: 326.1733.

6d

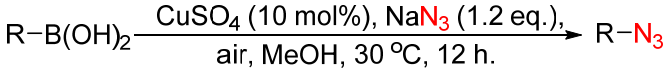


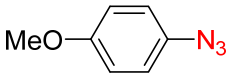
(3*S*,9*S*,10*R*,13*R*,14*R*,17*R*)-17-((2*R*,5*R*,*E*)-5,6-Dimethylhept-3-en-2-yl)-10,13-dimethyl-2,3,4,9,10,11,12,13,14,15,16,17-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 4-methoxyphenylcarbamate (6d). The reaction of **1a** (59.6 mg, 0.4mmol), $PdCl_2$ (1.4 mg, 0.008mmol) and Ergosterol (39.7 mg, 0.1mmol, 0.25equiv) in DMA (2.0 mL), at 70 ºC, under CO (1 atm), 24 h, afforded product **6d** (31.4 mg, 57% yield based on Ergosterol). **6d**: Light yellow solid; FT-IR (neat, cm^{-1}): 3337, 2958, 2870, 1695, 1528, 1414, 1228, 1062, 1035, 829, 768; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, J = 8.4 Hz, 2H), 6.84 (dt, J_1 = 9.2, J_2= 3.7 Hz, 2H), 6.49 (s, 1H), 5.58 (dd, J_1 = 5.6, J_2= 2.4 Hz, 1H), 5.41-5.35 (m, 1H), 5.29-5.11 (m, 2H), 4.76-4.63 (m, 1H), 3.77 (s, 3H), 2.59 (ddd, J_1 = 14.4, J_2= 4.8, J_3= 2.4 Hz, 1H), 2.38 (t, J = 12.4 Hz, 1H), 2.12-1.95 (m, 4H), 1.95-1.82 (m, 3H), 1.82-1.18 (m, 11H), 1.04 (d, J = 6.4 Hz, 3H), 0.96 (s, 3H), 0.92 (d, J = 6.8 Hz, 3H), 0.83 (t, J = 6.4 Hz, 6H), 0.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.05, 153.59, 141.62, 138.73, 135.72, 132.14, 131.26, 120.79 (brs), 120.39, 116.49, 114.39, 73.75, 55.88, 55.62, 54.68, 46.19, 42.97, 40.56, 39.18, 38.07, 37.23, 37.16, 33.23, 28.62, 28.42, 23.13, 21.24, 21.20, 20.08, 19.78, 17.74, 16.34, 12.20 ppm; HR-MS (ESI, positive): *m/z* calculated for $C_{36}H_{52}NO_3(M+H)^+$ 546.3942, found: 546.3942.

Syntheses and Characterization Data of Organic Azides

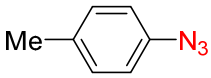
Method A

The organic azides from boronic acids were prepared according to the procedure reported by Tao, C.-Z. et al.[9]

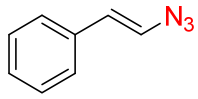


1a 

1-Azido-4-methoxybenzene (1a).[9] Light yellow crystal, 94% yield; FT-IR (neat, cm^{-1}): 2957, 2836, 2105, 1584, 1504, 1292, 1246, 1035, 824, 745;^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.97-6.92 (m, 2H), 6.90-6.85 (m, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.12, 132.46, 120.10, 115.24, 55.66 ppm.

1b 

1-Azido-4-methylbenzene (1b).[9] Light yellow liquid, 90% yield; FT-IR (neat, cm^{-1}): 3222, 3030, 2924, 2420, 2105, 1506, 1298, 1128, 809, 630, 497;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.14 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 8.4 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.35, 134.77, 130.49, 119.00, 20.94 ppm.

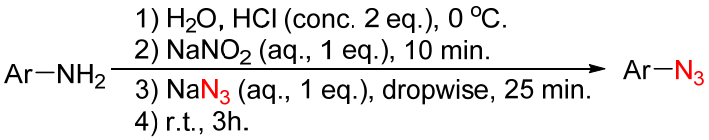
1e 

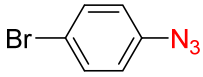
(*E*)-(2-Azidovinyl)benzene (1e).[9] Yellow liquid, 50% yield; FT-IR (neat, cm^{-1}): 3026, 2925, 2279, 2101, 1637, 1330, 1285, 1259, 930, 748, 692;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34-7.17 (m, 5H), 6.59 (d, J = 14.0 Hz, 1H), 6.26 (d, J = 14.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 135.15, 128.89, 127.52, 126.80, 125.95, 119.92 ppm.

Method B

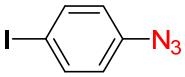
Aryl azides from aromatic amines were synthesied according to the procedure reported by Kwok,

S. W. et al.[10]

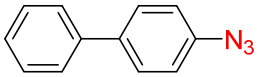


1c 

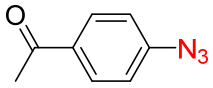
1-Azido-4-bromobenzene (1c).[11] Yellowgreen solid, 93% yield; FT-IR (neat, cm^{-1}): 3243, 2415, 2129, 1584, 1483, 1294, 1072, 1010, 821, 530, 492;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48-7.42 (m, 2H), 6.93-6.87 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 139.37, 132.93, 120.81, 117.89 ppm.

1d 

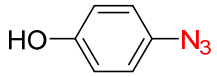
1-Azido-4-iodobenzene(1d).[12] Brown solid, 98% yield; FT-IR (neat, cm^{-1}): 2414, 2126, 1480, 1292, 1129, 1006, 818, 490;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.64 (d, J = 8.4 Hz, 2H), 6.78 (d, J = 8.8 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.12, 138.84, 121.17, 88.35 ppm.

1f 

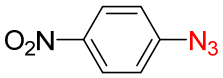
4-Azidobiphenyl (1f).[13] Light yellow solid, 30% yield; FT-IR (neat, cm^{-1}): 2921, 2125, 1680, 1484, 1293, 912, 835, 763, 743, 691;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.57 (t, J = 8.4 Hz, 4H), 7.44 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.10 (d, J = 8.4 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.30, 139.31, 138.17, 129.02, 128.60, 127.52, 127.02, 119.55 ppm.

1g 

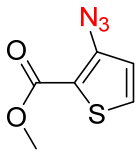
1-(4-Azidophenyl)ethanone(1g).[13] Yellow solid, 62% yield; FT-IR (neat, cm^{-1}): 2925, 2099, 1682, 1597, 1359, 1269, 1180, 834, 721, 589, 540;^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00-7.93 (m, 2H), 7.13-7.05 (m, 2H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 196.64, 145.01, 133.95, 130.37, 119.07, 26.57 ppm.

1h 

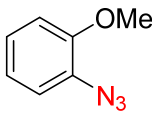
4-Azidophenol (1h).[14] Yellow solid, 85% yield; FT-IR (neat, cm^{-1}): 3333, 2115, 1596, 1507, 1238, 828, 776, 636, 511;^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.95-6.87 (m, 2H), 6.86-6.79 (m, 2H), 5.13 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.86, 132.71, 120.33, 116.76 ppm.

1i 

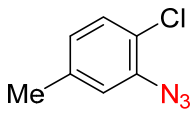
1-Azido-4-nitrobenzene (1i).[15] Light yellow solid, 99% yield; FT-IR (neat, cm^{-1}): 3112, 3079, 3023, 2927, 2130, 1605, 1520, 1344, 1290, 1109, 848, 749, 683, 559, 531, 486;^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.28-8.22 (m, 2H), 7.18-7.11 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.02, 144.80, 125.77, 119.54 ppm.

1j 

Methyl 3-azidothiophene-2-carboxylate (1j). Light yellow solid, 60% yield; FT-IR (neat, cm^{-1}): 3399, 3104, 2958, 2367, 2224, 2136, 1789, 1707, 1538, 1440, 1390, 1250, 1106, 1080, 927, 798, 742, 671, 635, 463;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48 (d, J = 5.6 Hz, 1H), 6.92 (d, J = 5.6 Hz, 1H), 3.88 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.44, 142.34, 131.28, 122.21, 117.28, 52.22 ppm.

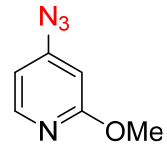
1k 

1-Azido-2-methoxybenzene (1k).[9] Light yellow liquid, 76% yield; FT-IR (neat, cm^{-1}): 3067, 2940, 2839, 2114, 1592, 1497, 1456, 1304, 1244, 1102, 1028, 746, 660;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.09 (td, J_1 = 8.0, J_2= 1.6 Hz, 1H), 7.01 (dd, J_1 = 8.0, J_2= 1.6 Hz, 1H), δ: 6.96-6.86 (m, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.99, 128.41, 125.76, 121.39, 120.39, 112.17, 55.98 ppm.

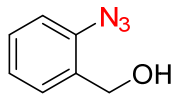
1l 

2-Azido-1-chloro-4-methylbenzene (1l). Yellow liquid, 93% yield; FT-IR (neat, cm^{-1}): 2955, 2925,

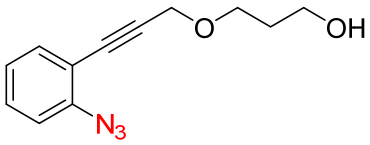
2856, 2125, 1576, 1488, 1402, 1311, 1137, 1049, 808, 760, 672, 566;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.22 (d, *J* = 8.4 Hz, 1H), 6.95 (s, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.31, 136.75, 130.41, 126.65, 121.98, 120.26, 21.02 ppm.

1m 

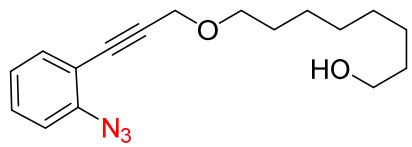
4-Azido-2-methoxypyridine (1m). Light yellow liquid, 67% yield; FT-IR (neat, cm^{-1}): 2985, 2950, 2112, 1601, 1566, 1478, 1400, 1258, 1223, 1041, 839, 798;^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.08 (d, *J* = 5.6 Hz, 1H), 6.55 (dd, J_1 = 5.6, J_2= 2.0 Hz, 1H), 6.37 (d, *J* = 1.6 Hz, 1H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.73, 150.89, 148.32, 108.37, 100.29, 53.78 ppm.

4a 

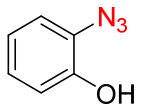
(2-Azidophenyl)methanol (4a)[16] Light yellow solid, 73% yield; FT-IR (neat, cm^{-1}): 3325, 2929, 2130, 1704, 1514, 1297, 1224, 1034, 913, 828, 743;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.32 (m, 2H), 7.21-7.11 (m, 2H), 4.64 (d, *J* = 6.0 Hz, 2H), 2.09 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.00, 132.01, 129.40, 129.24, 125.10, 118.18, 61.80 ppm.

4b 

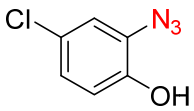
3-(3-(2-Azidophenyl)prop-2-ynyloxy)propan-1-ol (4b). Yellow thick liquid, 64% yield; FT-IR (neat, cm^{-1}): 3393, 2946, 2876, 2131, 1570, 1487, 1442, 1304, 1095, 755, 650;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (dd, J_1 = 7.8, J_2= 1.4 Hz, 1H), 7.33 (td, J_1 = 8.0, J_2= 1.6 Hz, 1H), 7.12-7.06 (m, 2H), 4.42 (s, 2H), 3.78 (td, J_1 = 5.8, J_2= 4.0 Hz, 4H), 2.59 (brs, 1H), 1.89 (p, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.17, 133.85, 129.81, 124.65, 118.64, 114.64, 91.09, 81.94, 68.50, 61.02, 59.07, 32.15 ppm.

4c 

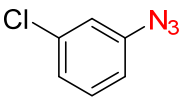
8-(3-(2-Azidophenyl)prop-2-ynyloxy)octan-1-ol (4c). Light yellow liquid, 74% yield; FT-IR (neat, cm^{-1}): 3387, 2930, 2856, 2130, 1570, 1488, 1303, 1097, 817, 755;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (dd, J_1 = 7.8, J_2= 1.4 Hz, 1H), 7.33 (td, J_1 = 8.0, J_2= 1.6 Hz, 1H), 7.14-7.05 (m, 2H), 4.40 (s, 2H), 3.65-3.56 (m, 4H), 1.83 (brs, 1H), 1.68-1.51 (m, 4H), 1.44-1.29 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.25, 133.98, 129.78, 124.71, 118.77, 114.99, 91.70, 81.66, 70.44, 63.12, 58.90, 32.82, 29.63, 29.47, 29.44, 26.16, 25.76 ppm.

4d 

2-Azidophenol(4d).[17] Brown solid, 31% yield; FT-IR (neat, cm^{-1}): 3372, 2955, 2925, 2853, 2118, 1594, 1495, 1458, 1296, 1248, 746;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.10-7.02 (m, 2H), 6.97-6.90 (m, 2H), 5.31 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.38, 126.21, 126.06, 121.34, 118.39, 116.09 ppm.

1p 

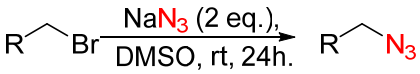
2-Azido-4-chlorophenol (1p). Brown solid, 91% yield; FT-IR (neat, cm^{-1}): 3519, 3425, 2926, 2122, 1592, 1493, 1351, 1295, 1203, 1106, 889, 850, 813, 719, 659;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.05 (d, J = 2.4 Hz, 1H), 7.01 (dd, J_1 = 8.4, J_2= 2.4 Hz, 1H), 6.85 (d, J = 8.4 Hz, 1H), 5.35 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.07, 127.17, 126.13, 125.82, 118.39, 117.07 ppm.

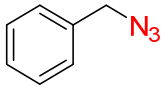
1q 

1-Azido-3-chlorobenzene(1q).[18] Yellow liquid, 67% yield; FT-IR (neat, cm^{-1}): 3066, 2424, 2106, 1591, 1476, 1286, 1140, 874, 853, 774, 726, 675;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.27 (t, J = 8.2 Hz, 1H), 7.13-7.09 (m, 1H), 7.02 (t, J = 2.0 Hz, 1H), 6.91 (ddd, J_1 = 8.0, J_2= 2.4, J_3= 0.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.63, 135.60, 130.82, 125.23, 119.48, 117.41 ppm.

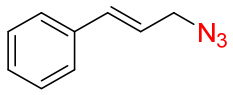
Method C

For alkyl azides synthesis from alkyl bromides, the method was refered to the Alvarez procedure.[19]



1n 

(Azidomethyl)benzene (1n).[19] Light yellow liquid, 75% yield; FT-IR (neat, cm^{-1}): 3455, 2956, 2915, 2851, 2099, 1736, 1456, 1365, 1218, 1089, 1026, 746, 528;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43-7.28 (m, 5H), 4.32 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 135.50, 128.96, 128.43, 128.34, 54.91 ppm.

1o 

(*E*)-(3-Azidoprop-1-enyl)benzene (1o).[19] Brown liquid, 98% yield; FT-IR (neat, cm^{-1}): 3029, 2957, 2923, 2852, 2097, 1448, 1261, 1025, 965, 882, 800, 744, 691;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43-7.23 (m, 5H), 6.64 (d, J = 15.6 Hz, 1H), 6.23 (dt, J_1 = 15.6, J_2= 6.7 Hz, 1H), 3.93 (d, J = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 136.12, 134.67, 128.79, 128.31, 126.76, 122.52, 53.12 ppm.

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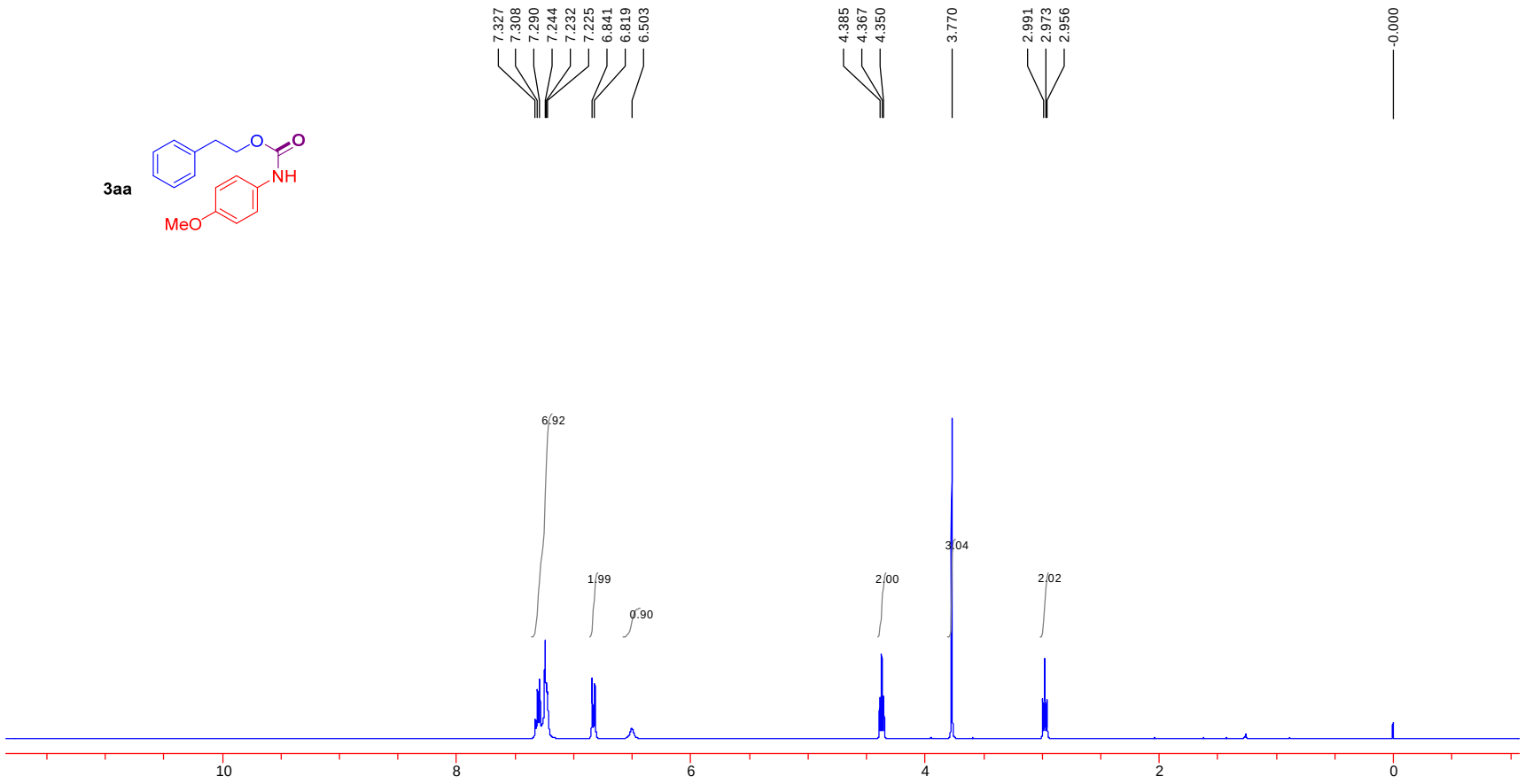
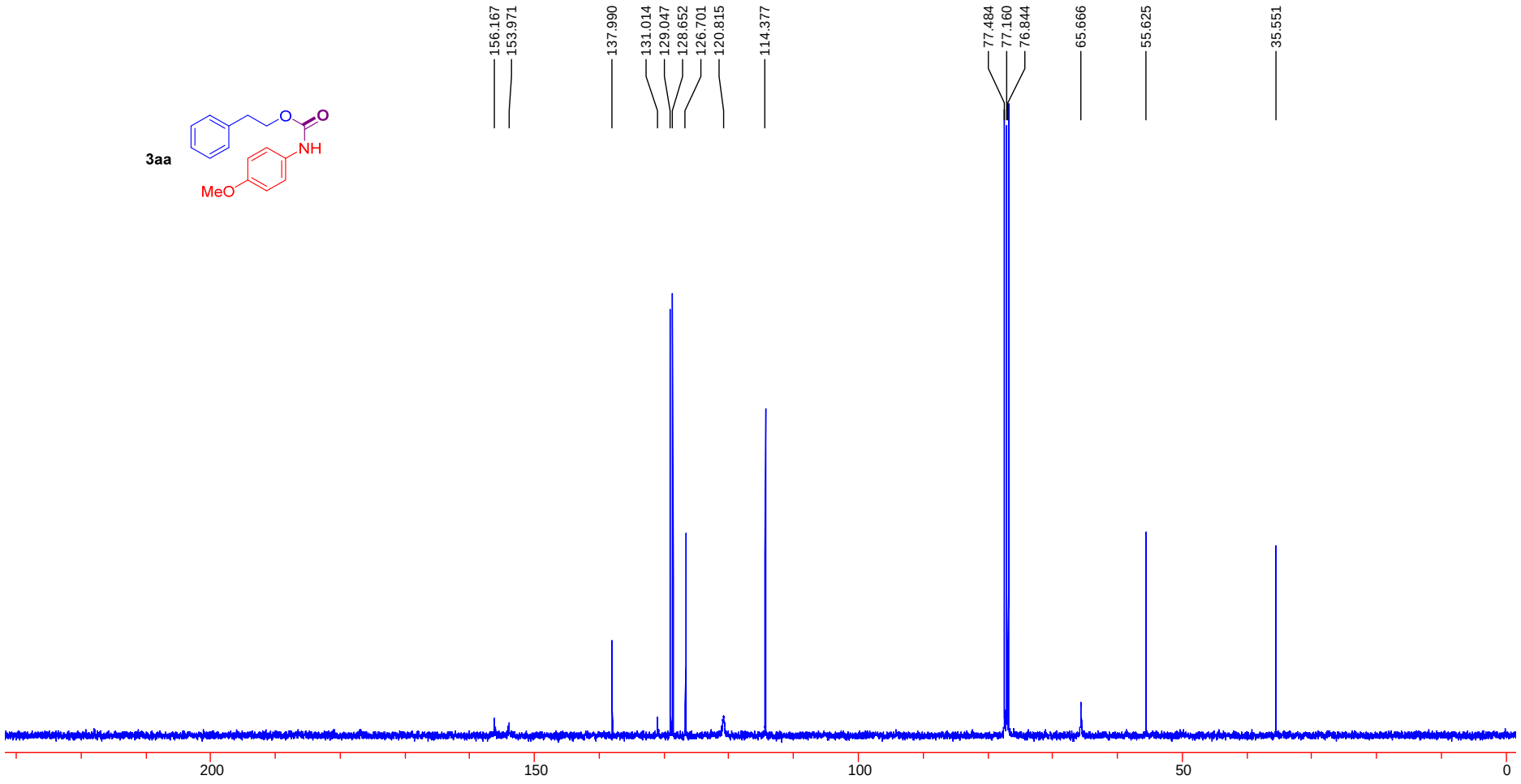
Copies of NMR Spectra

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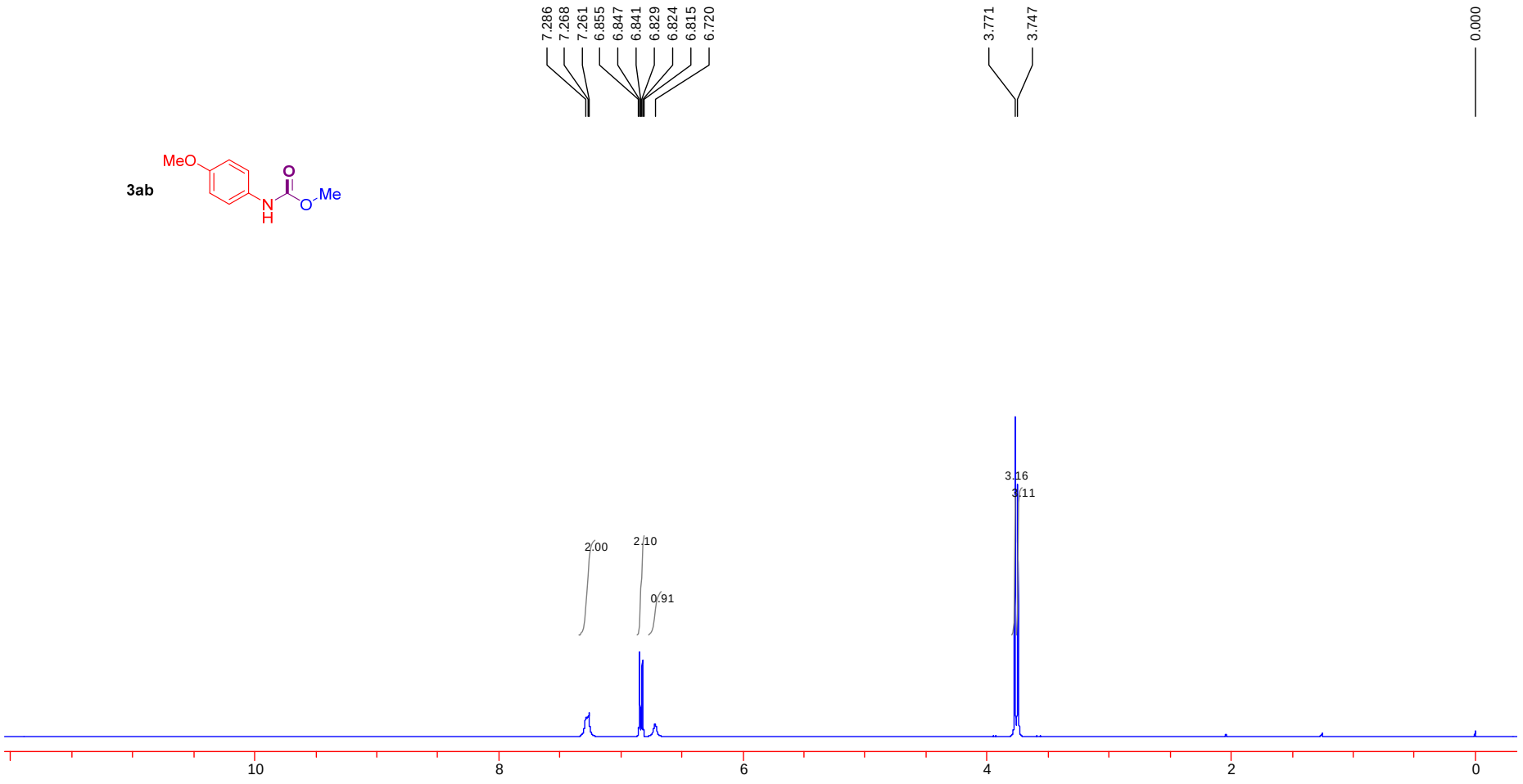
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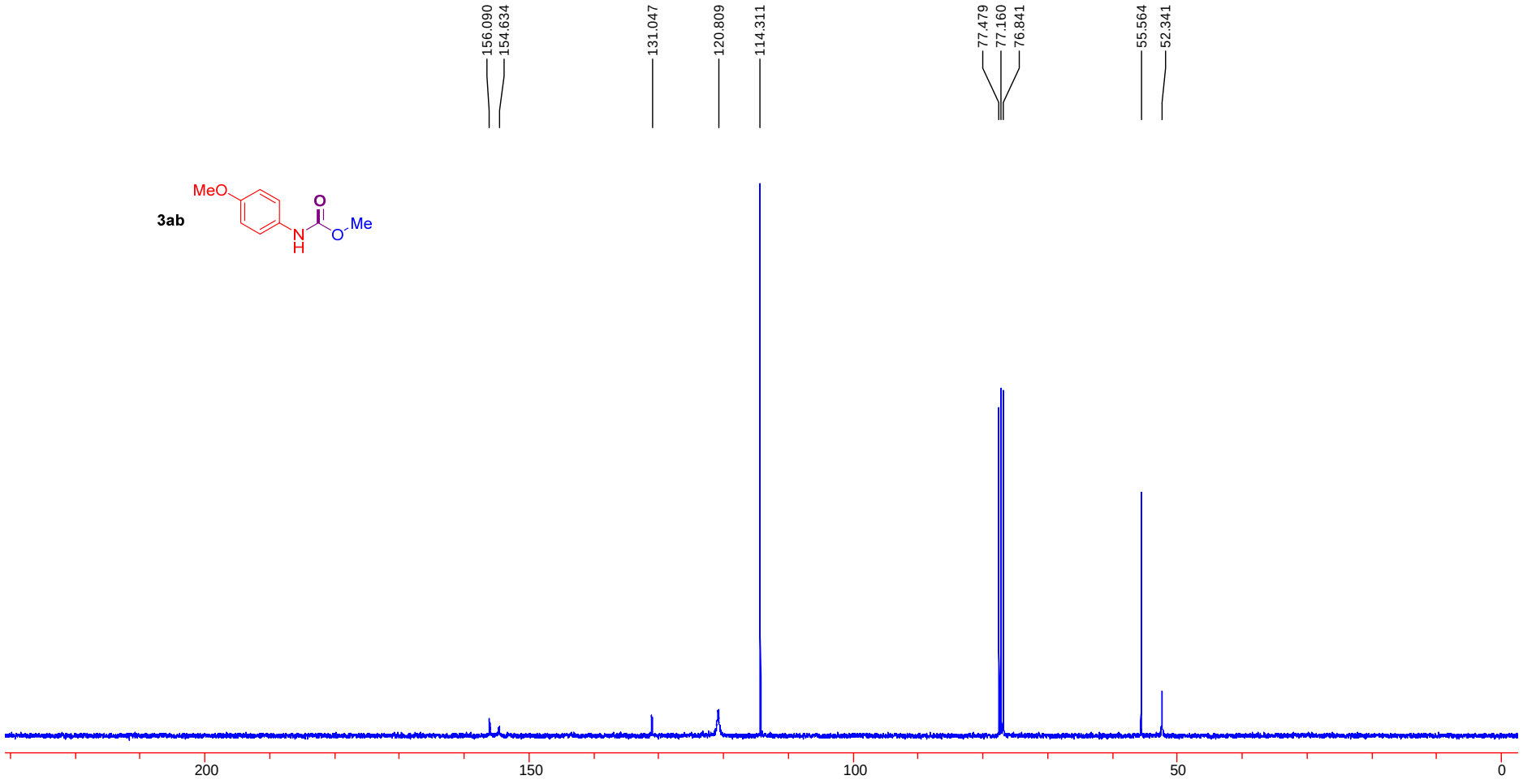
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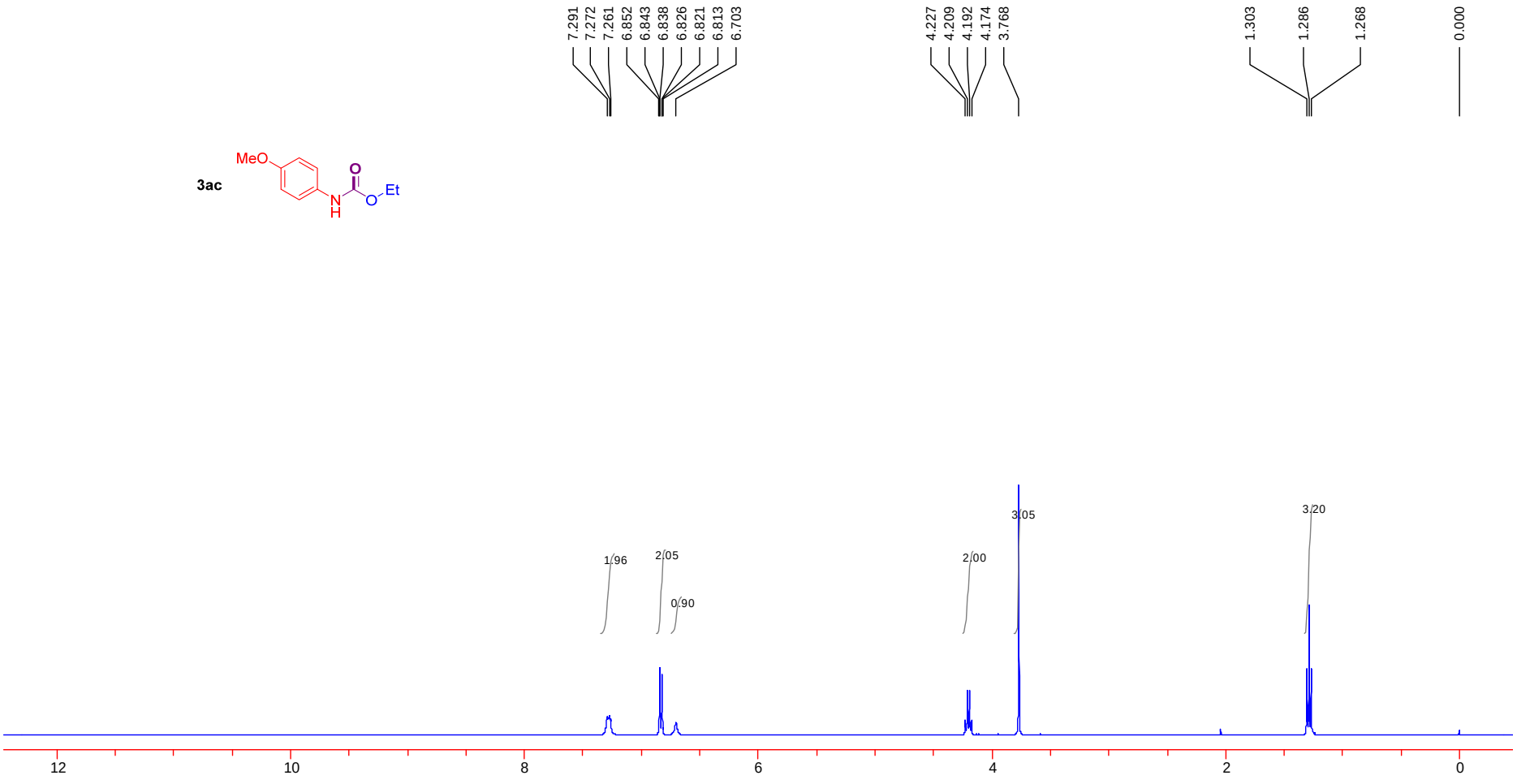
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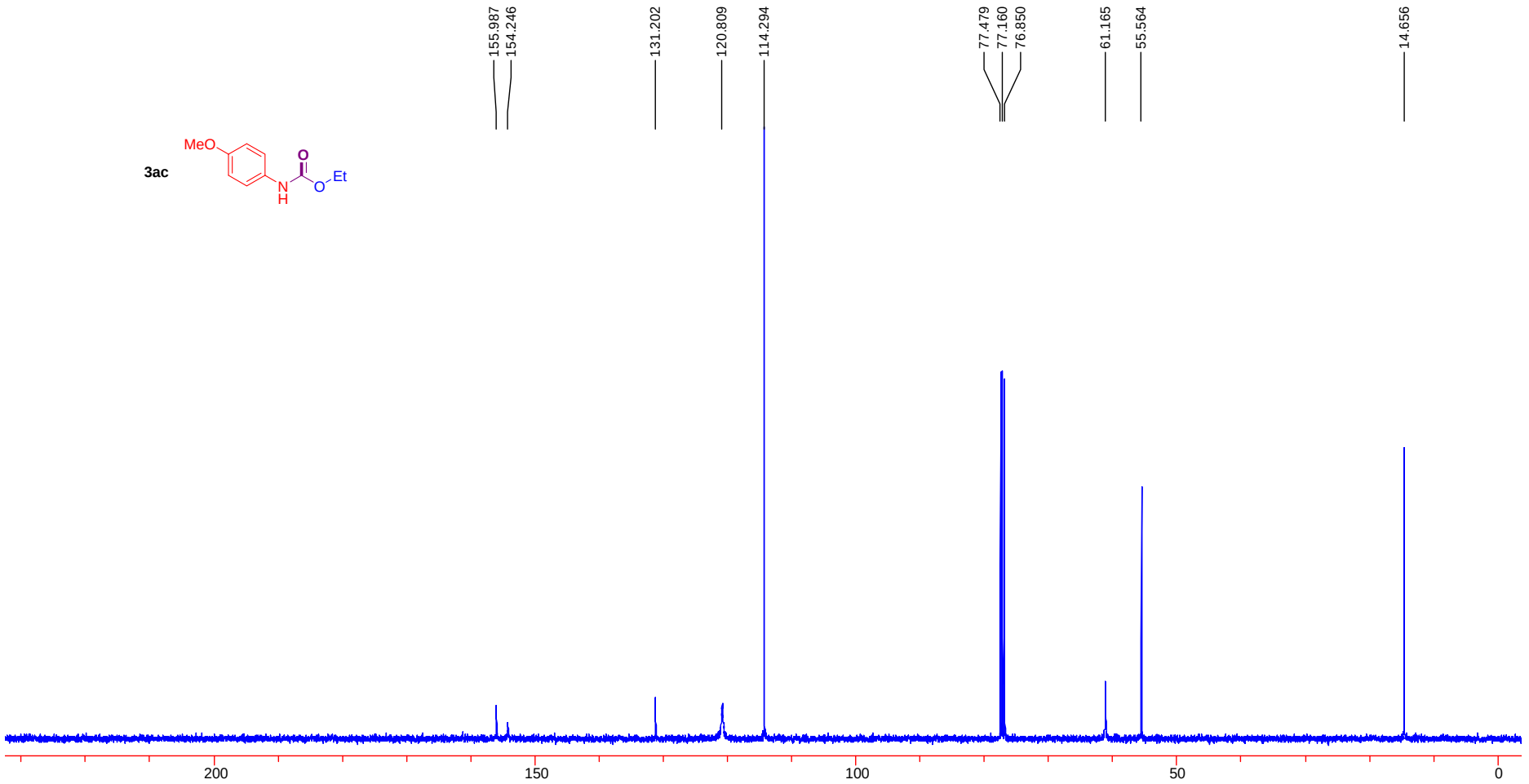
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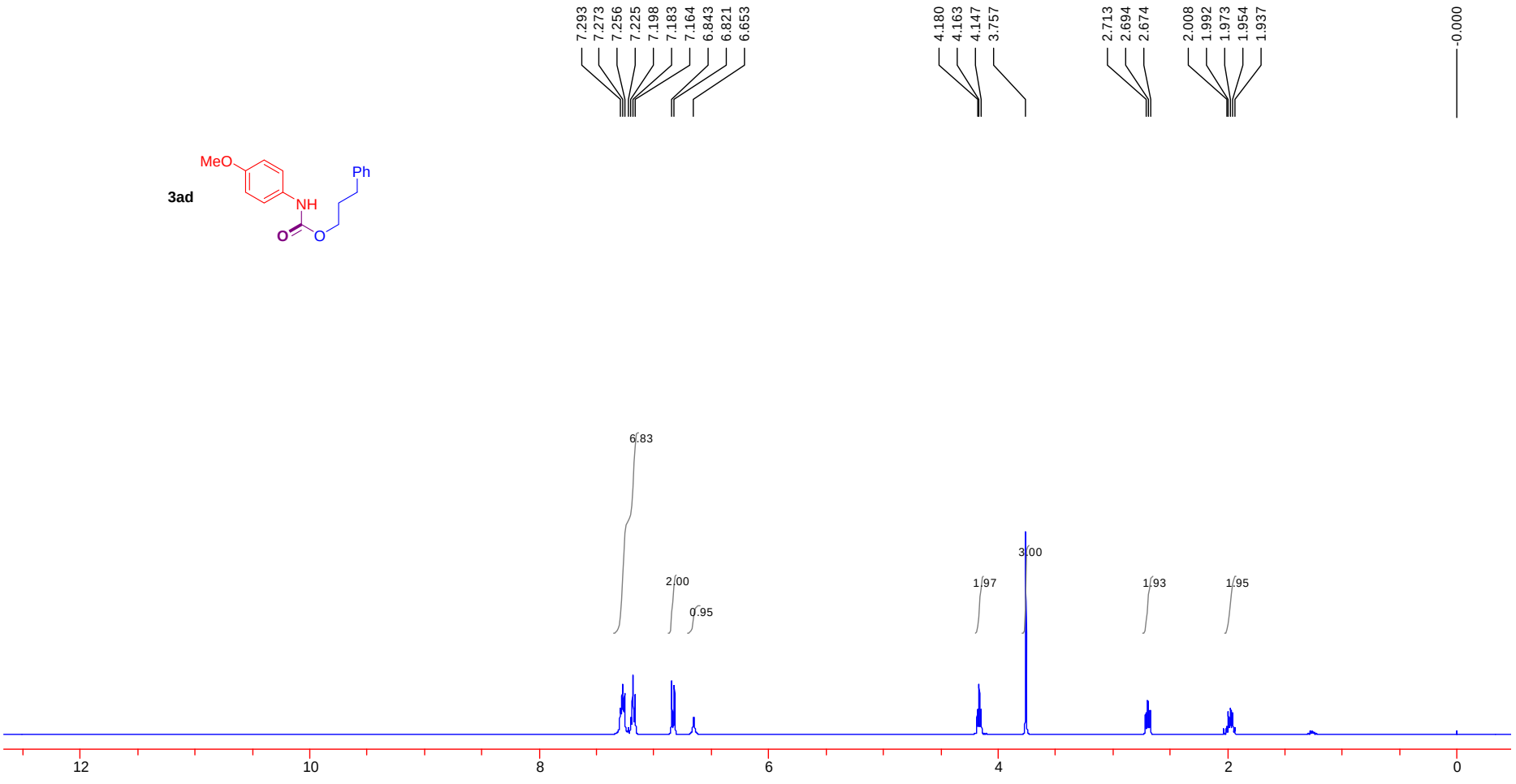
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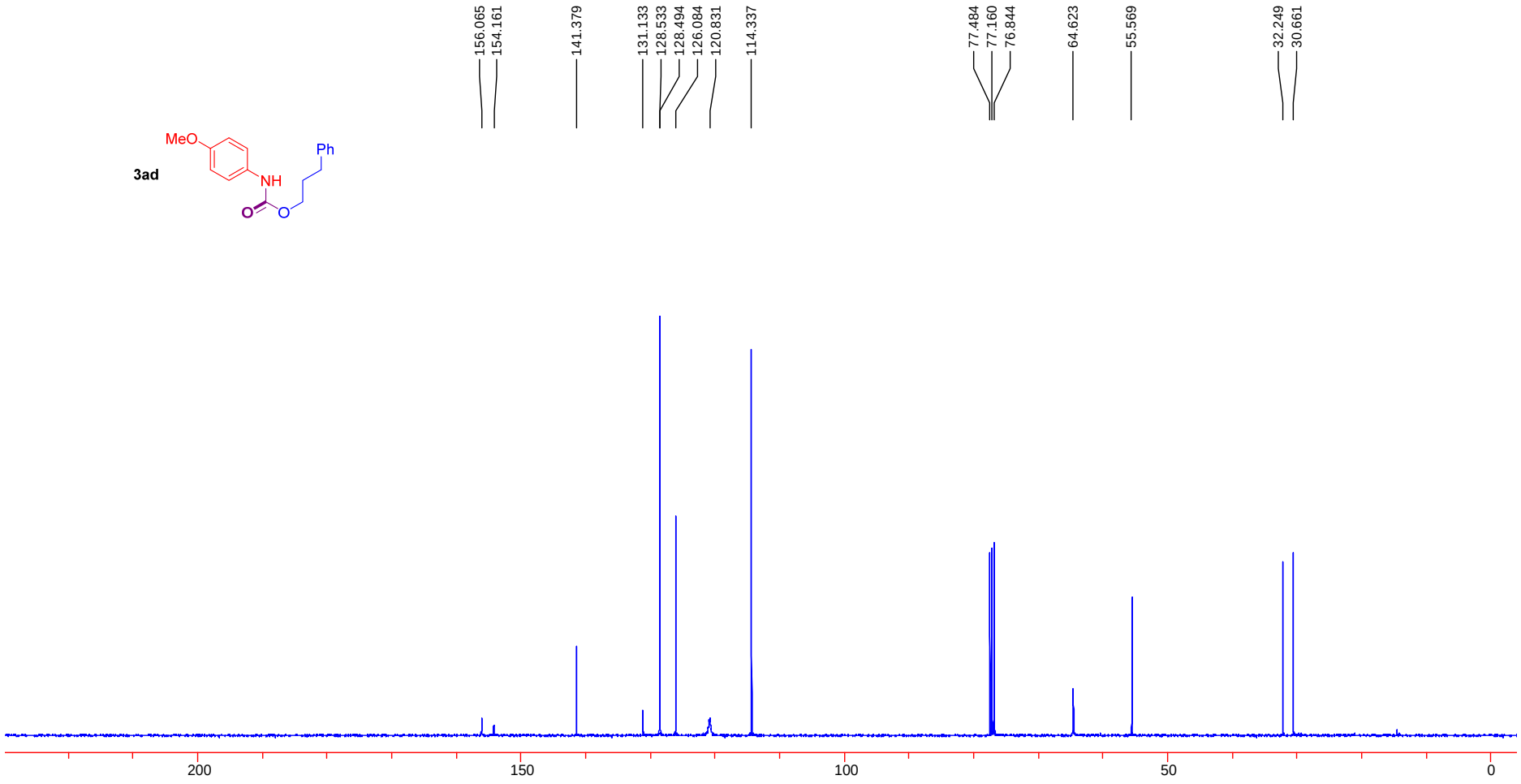
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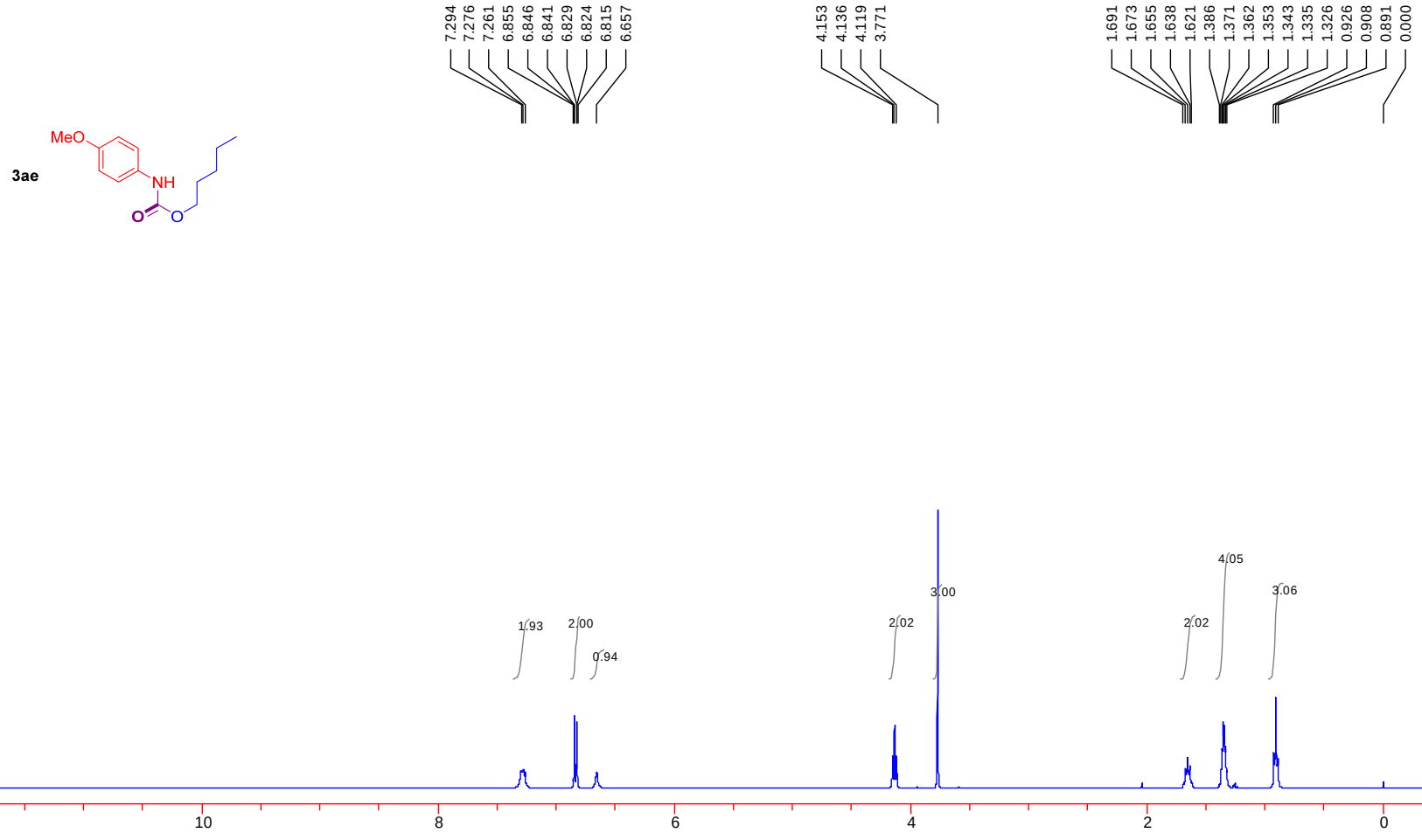
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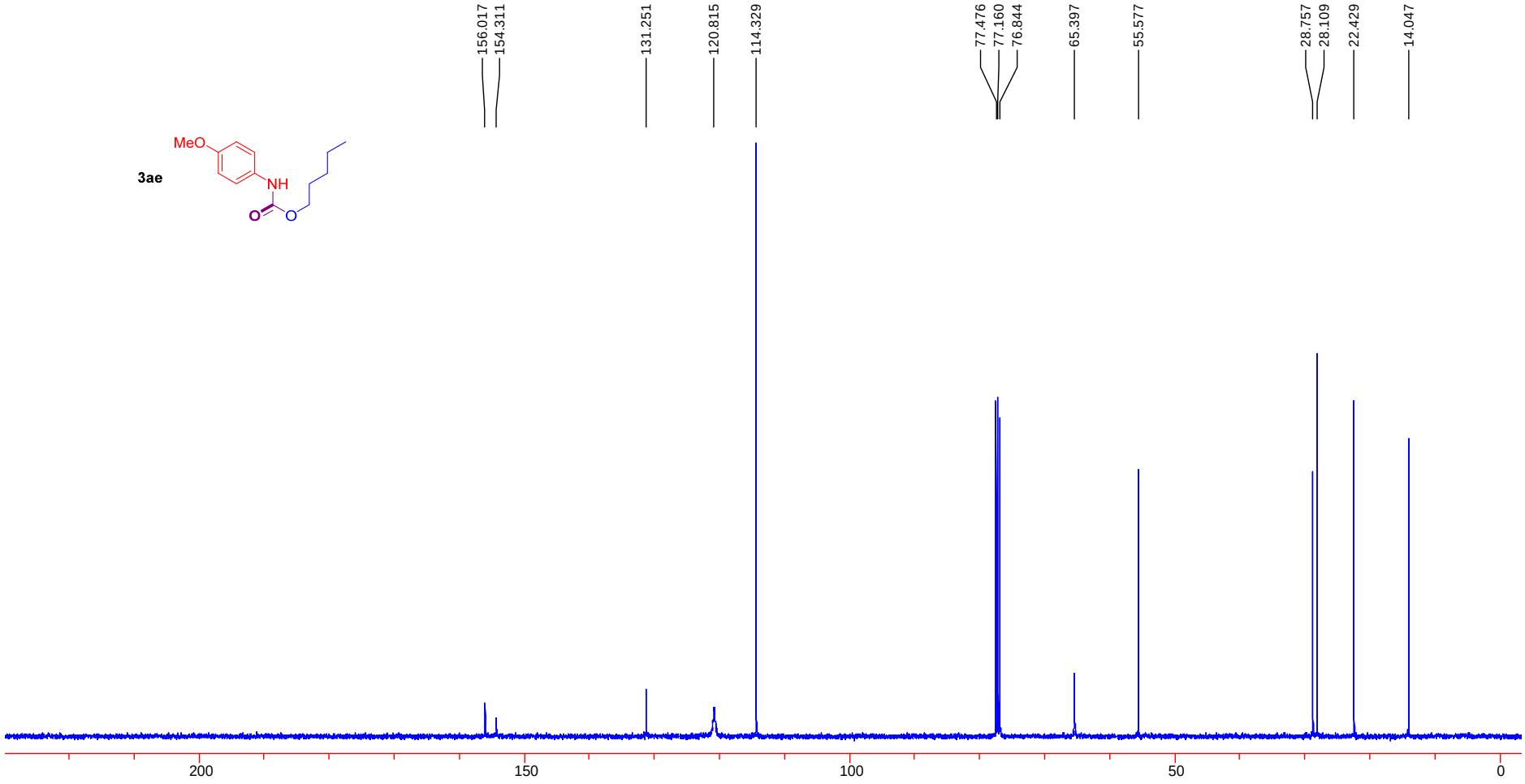
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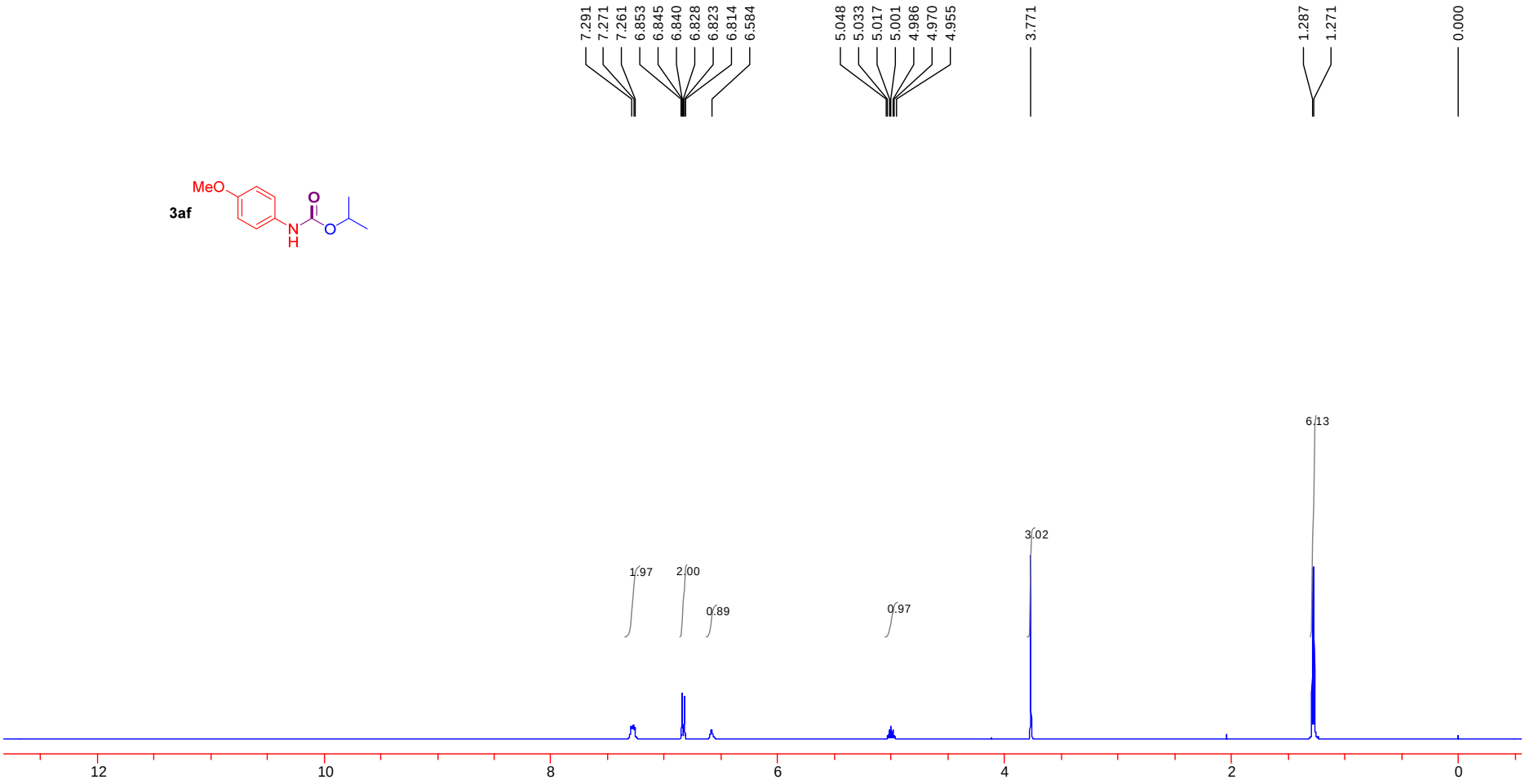
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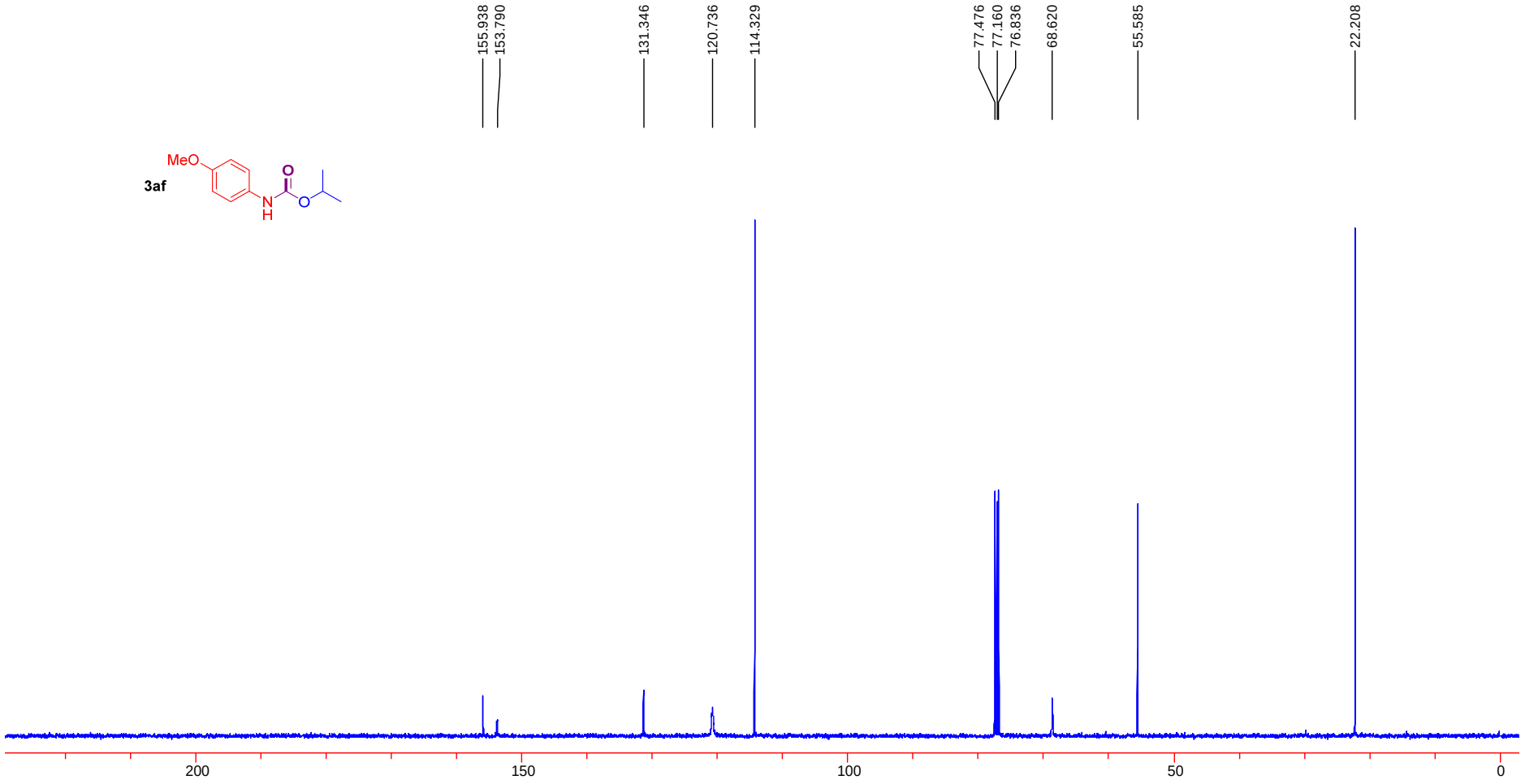
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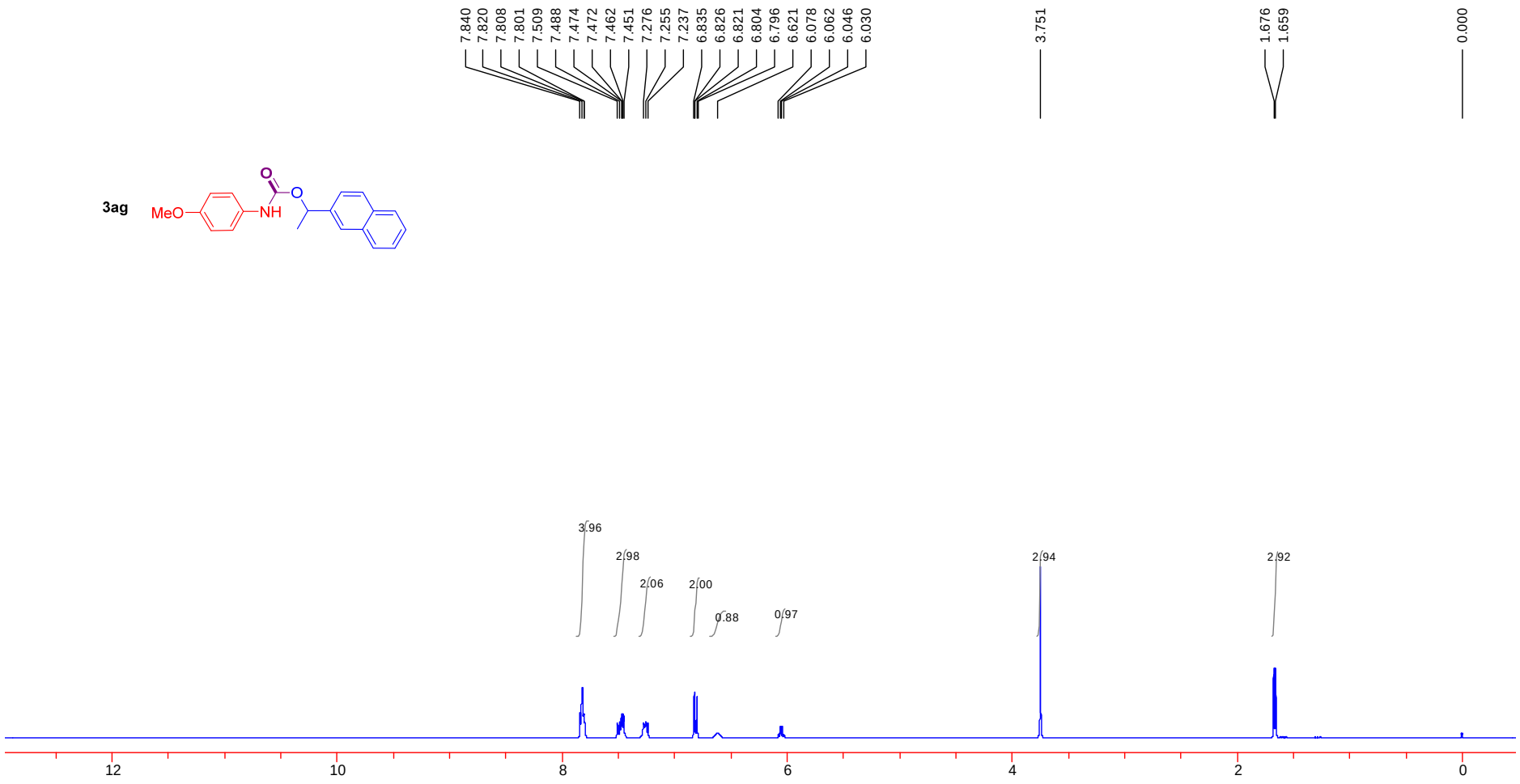
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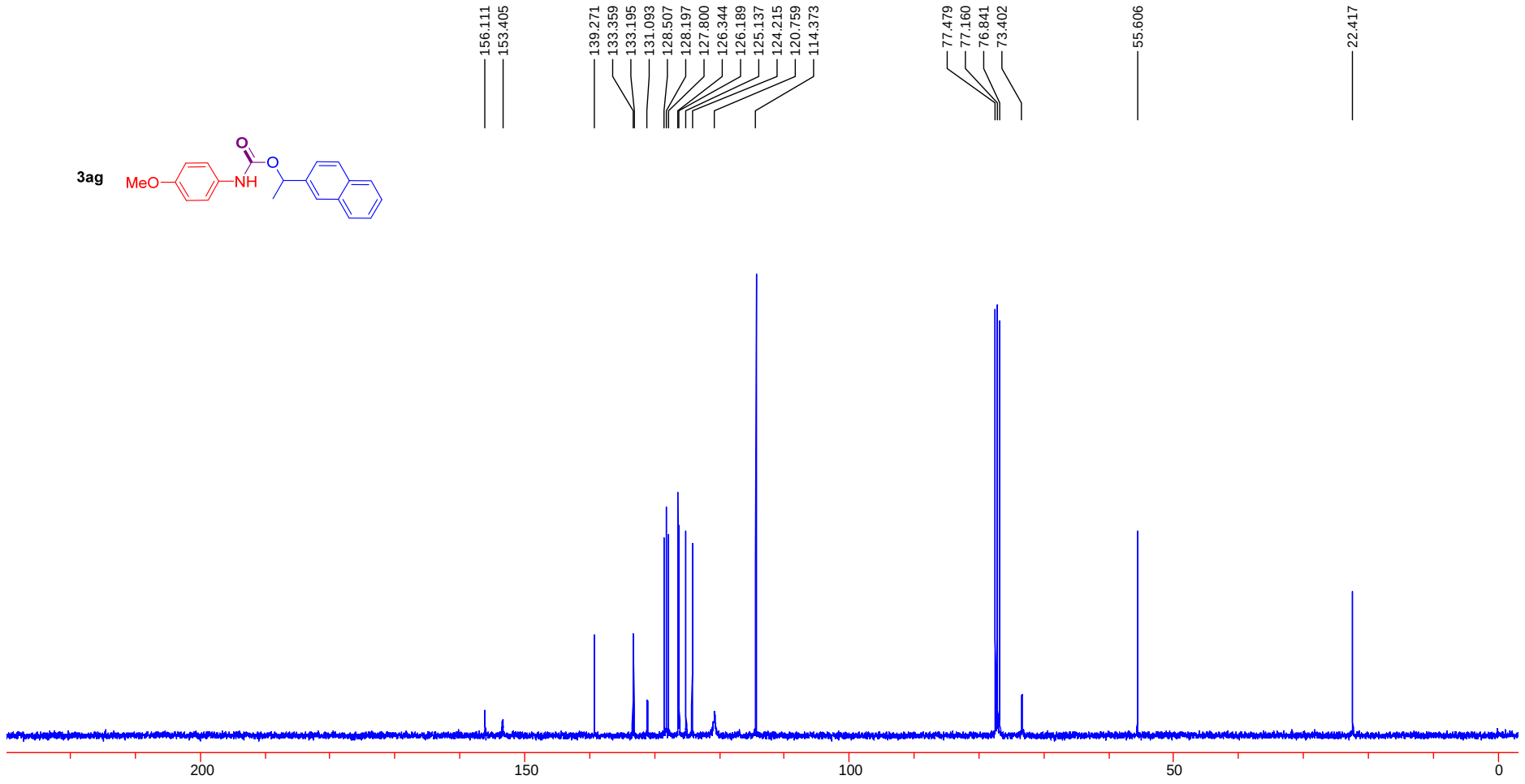
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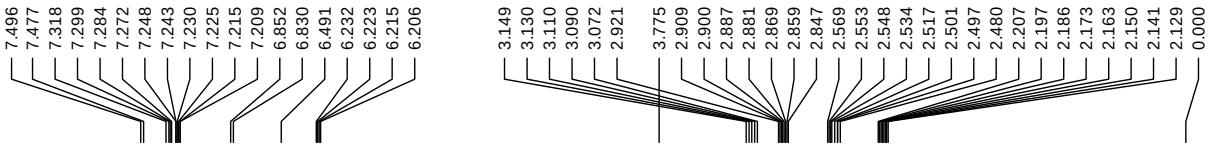
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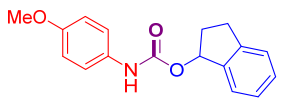
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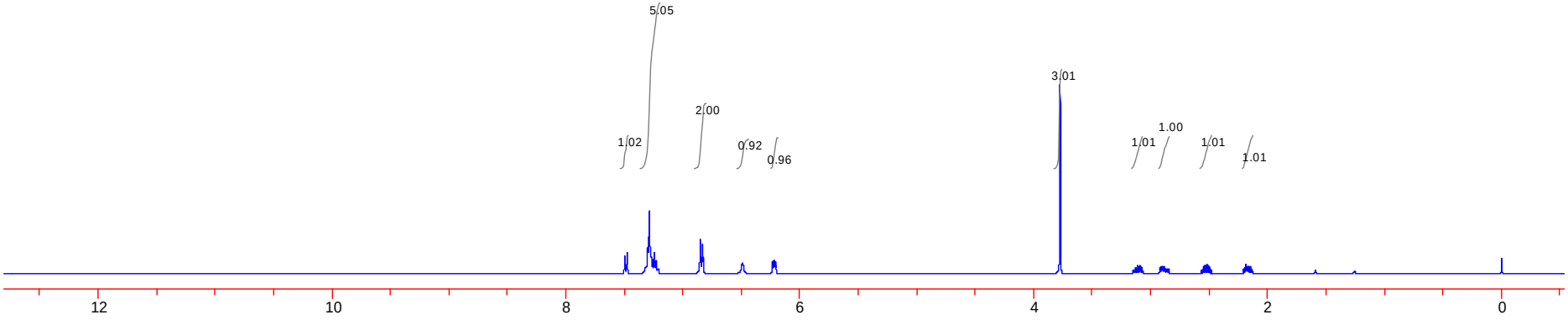
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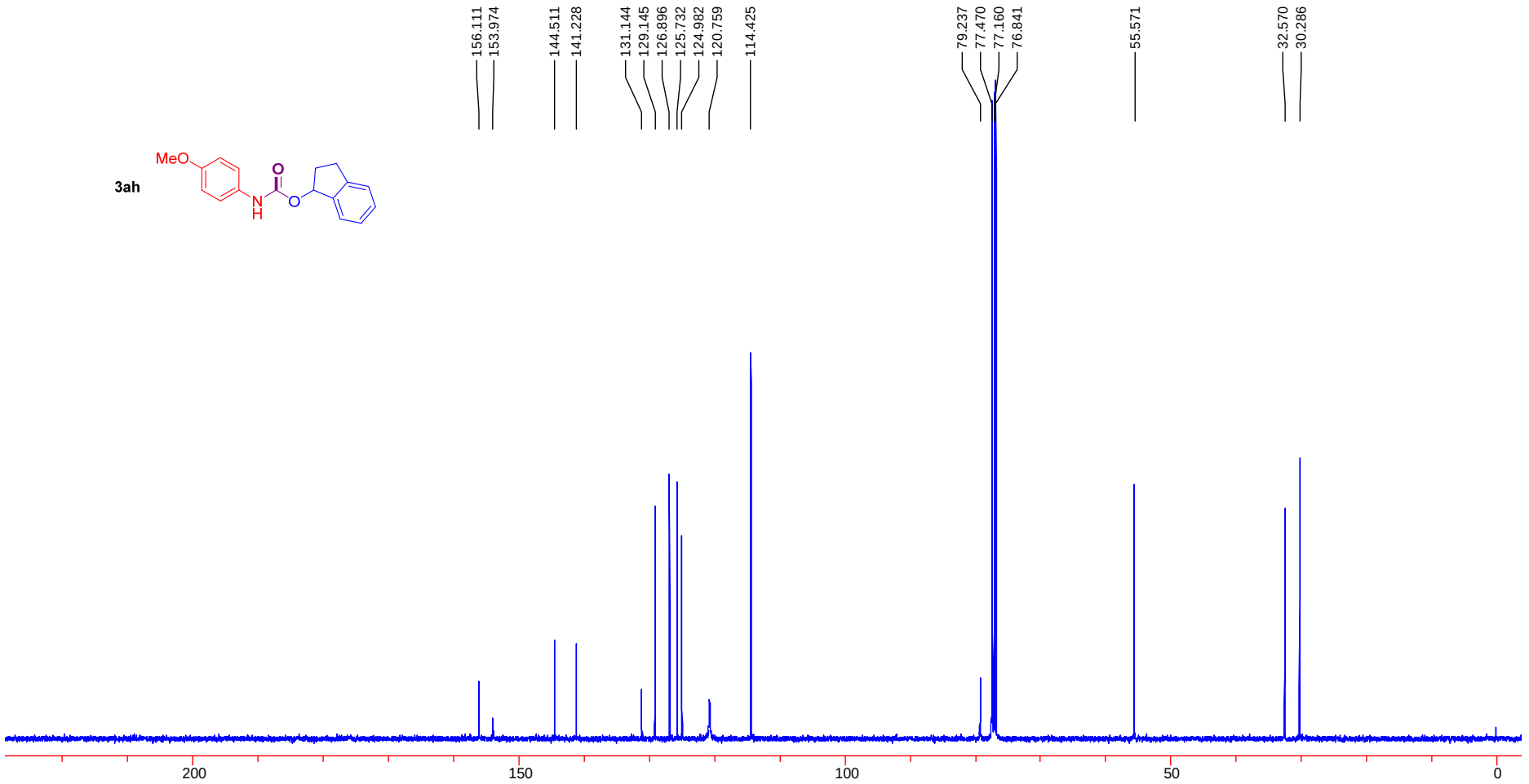
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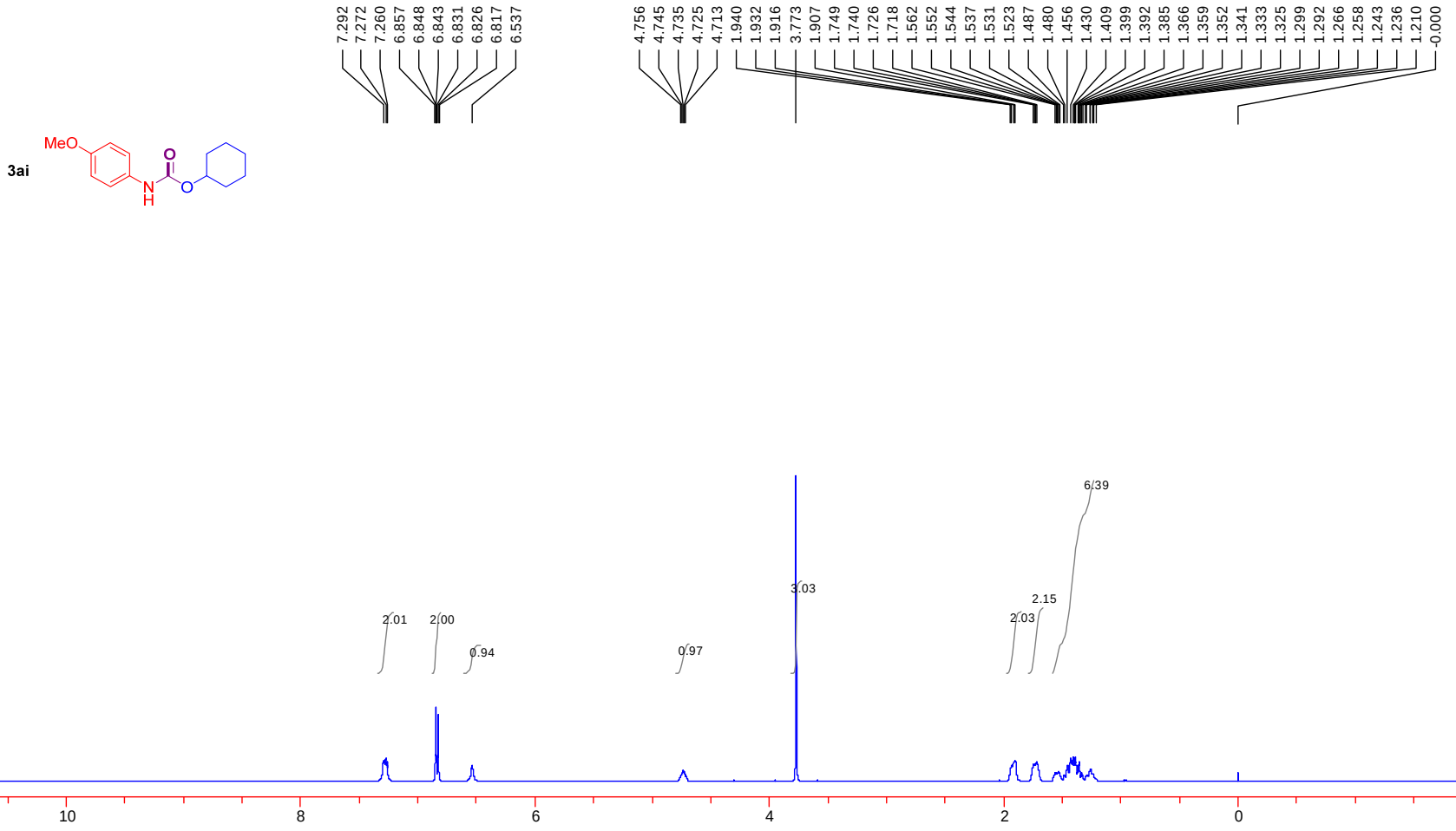
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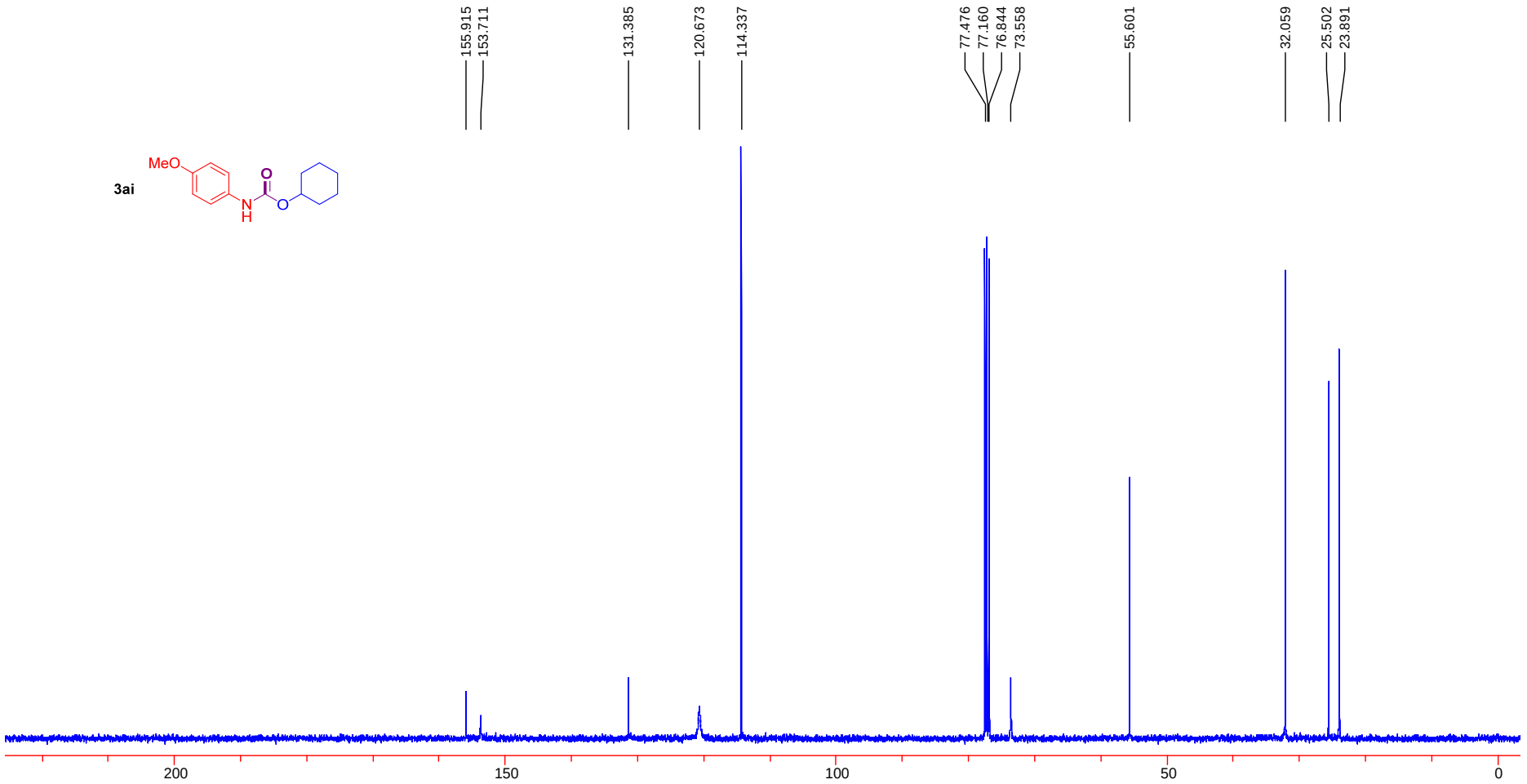
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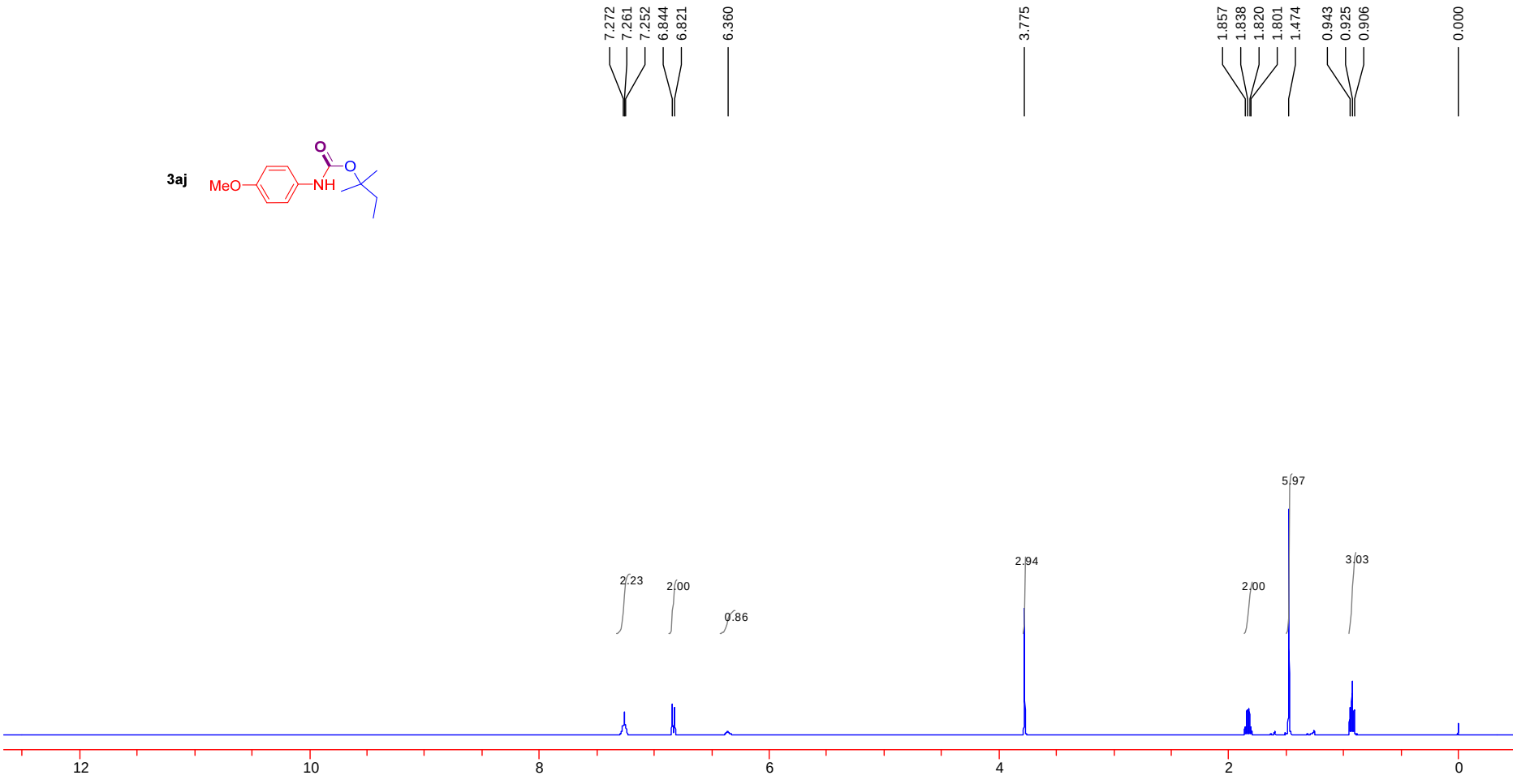
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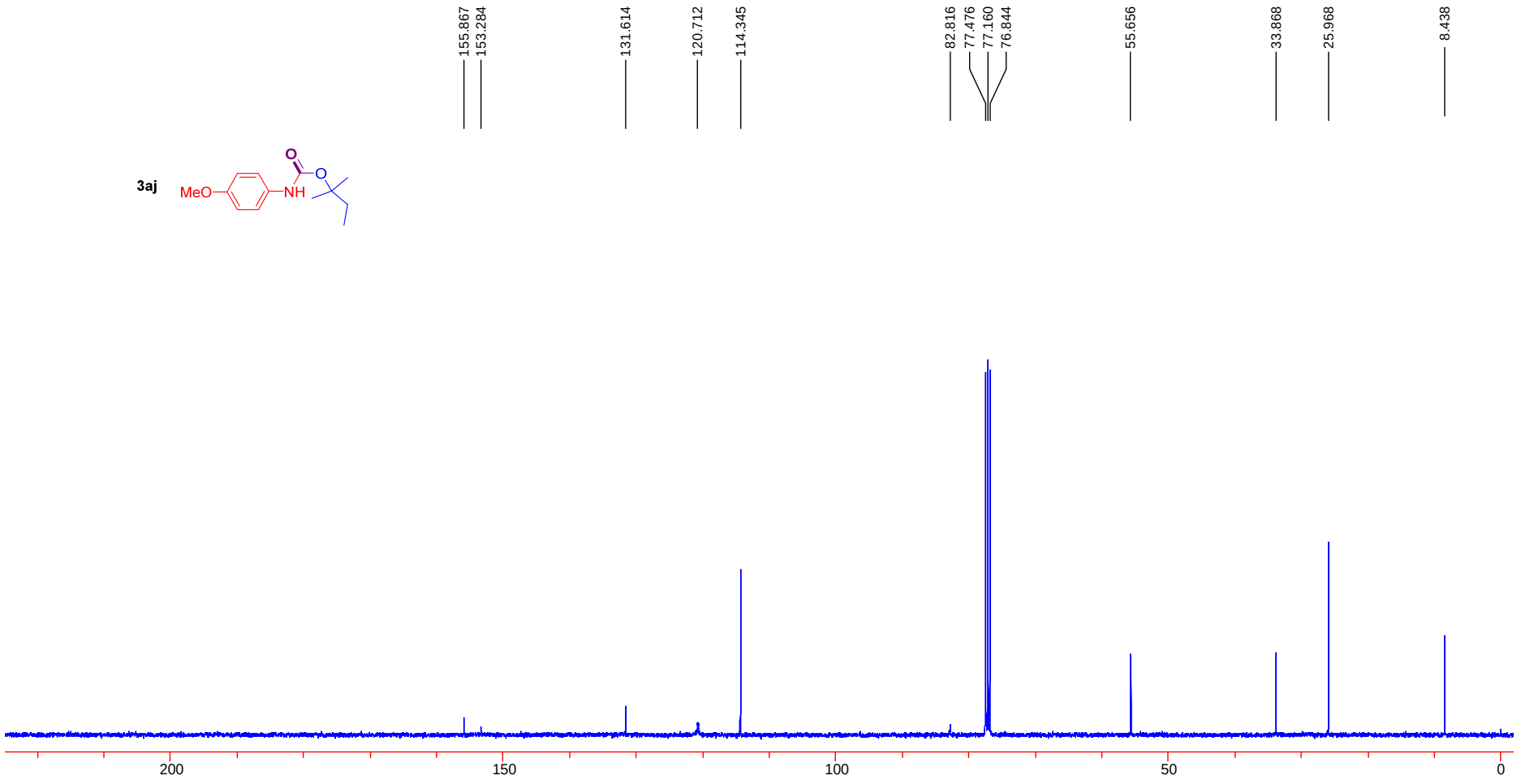
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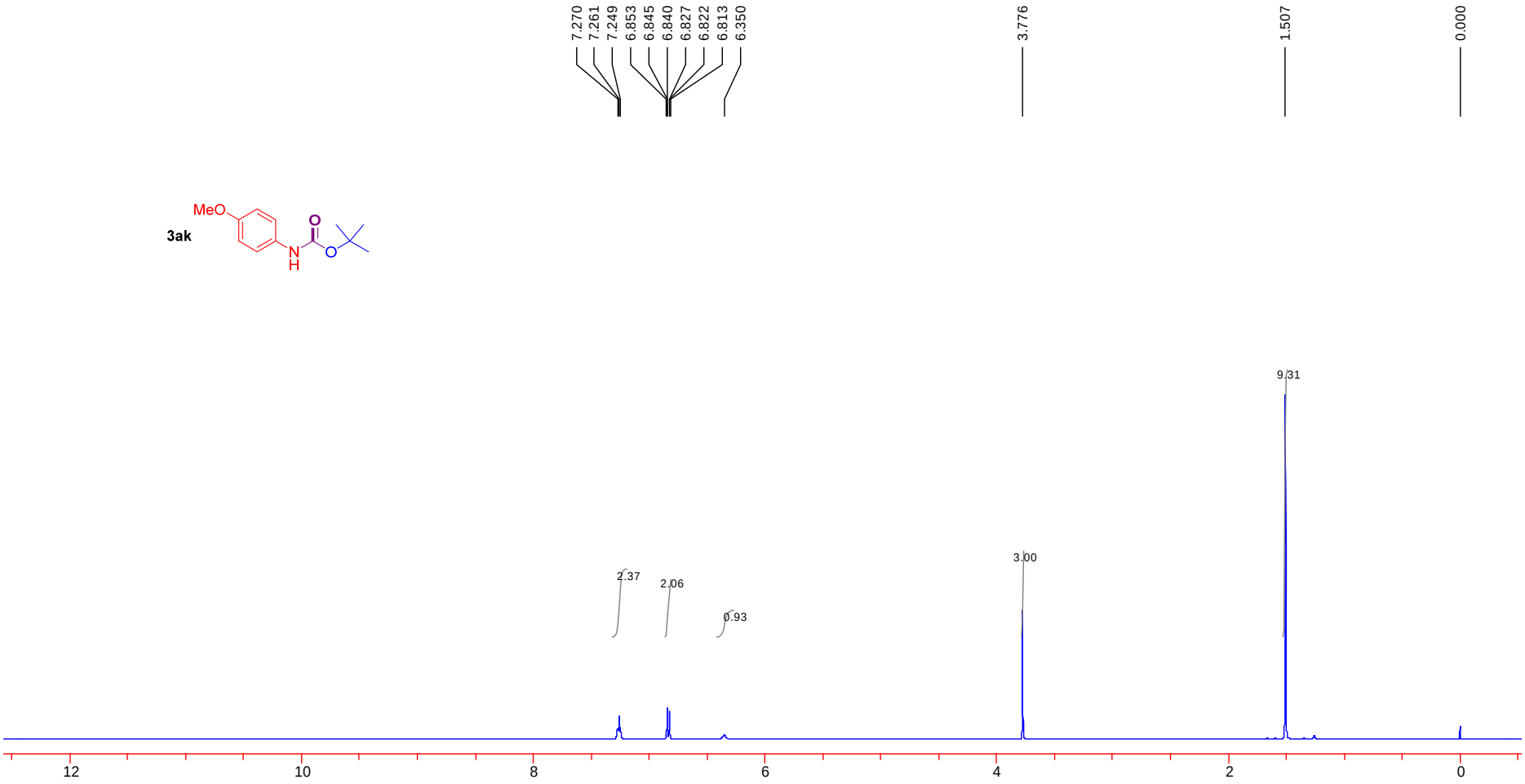
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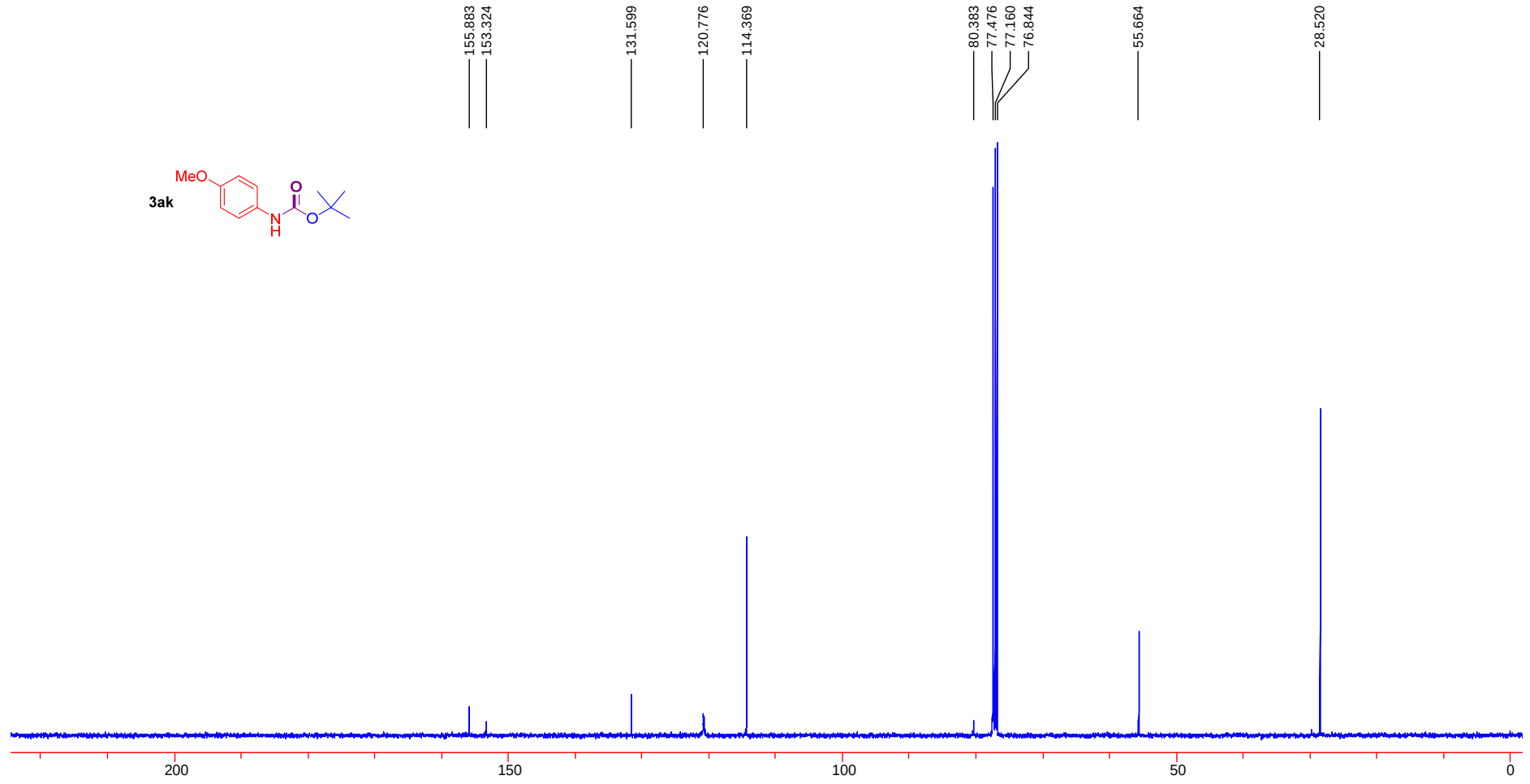
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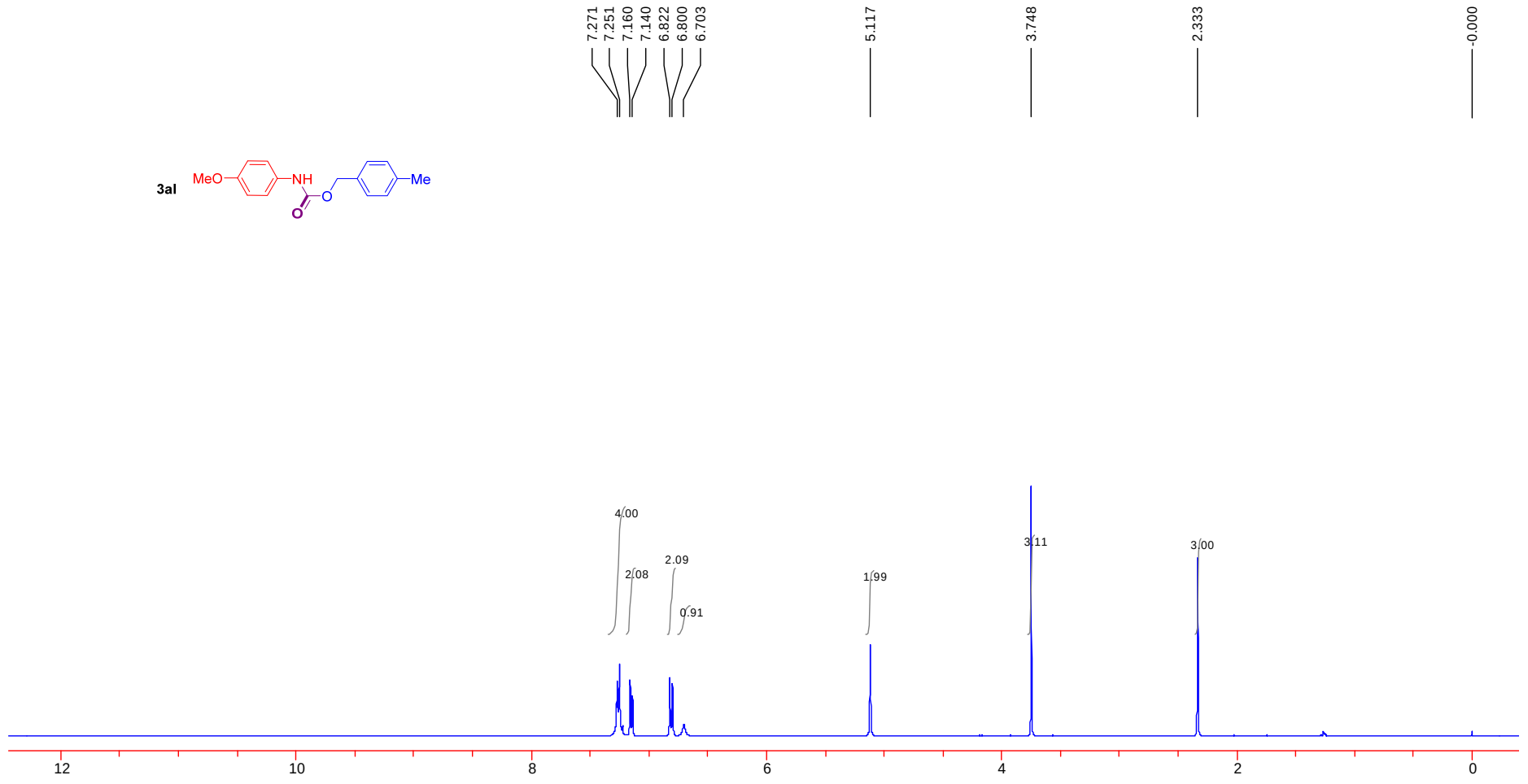
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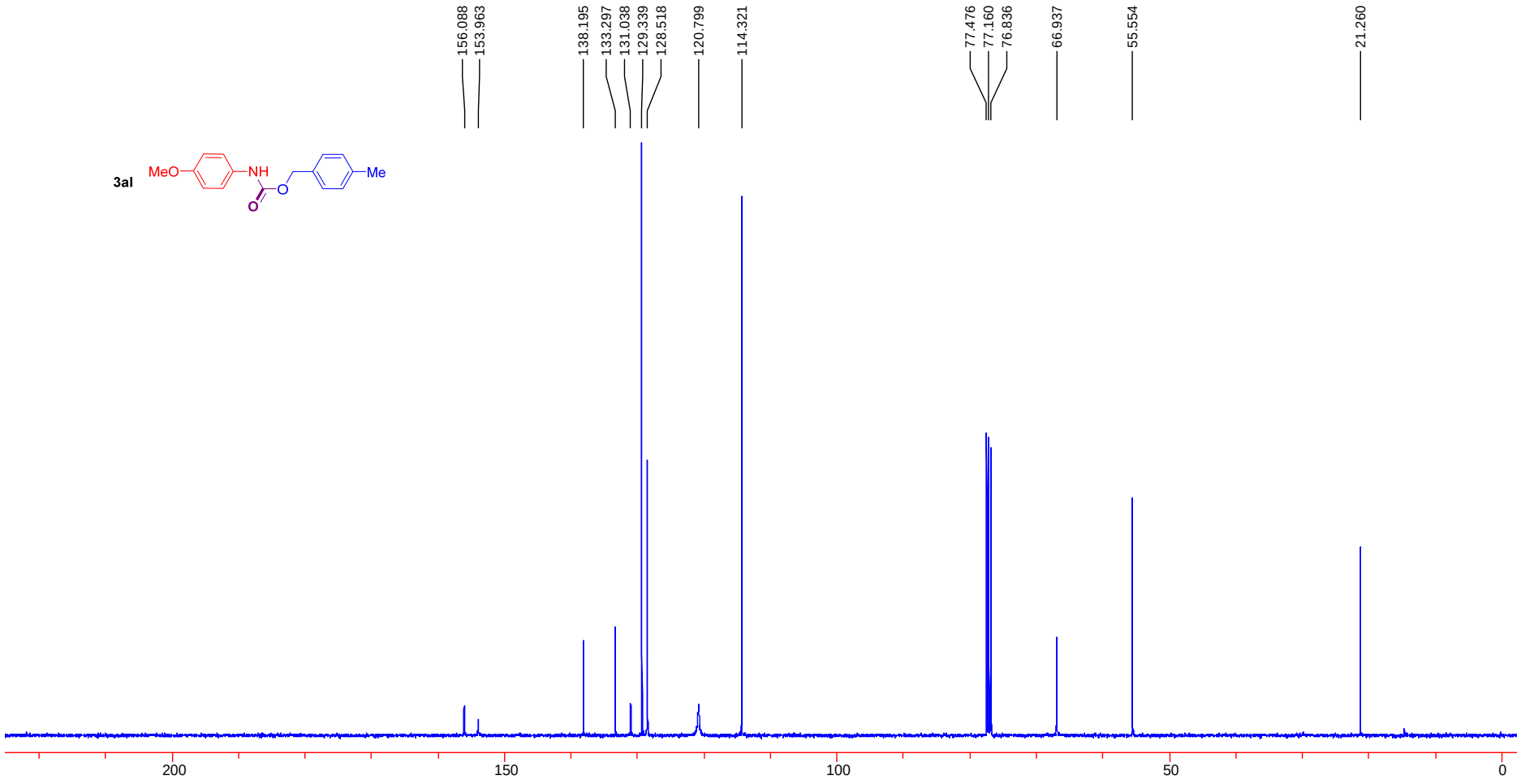
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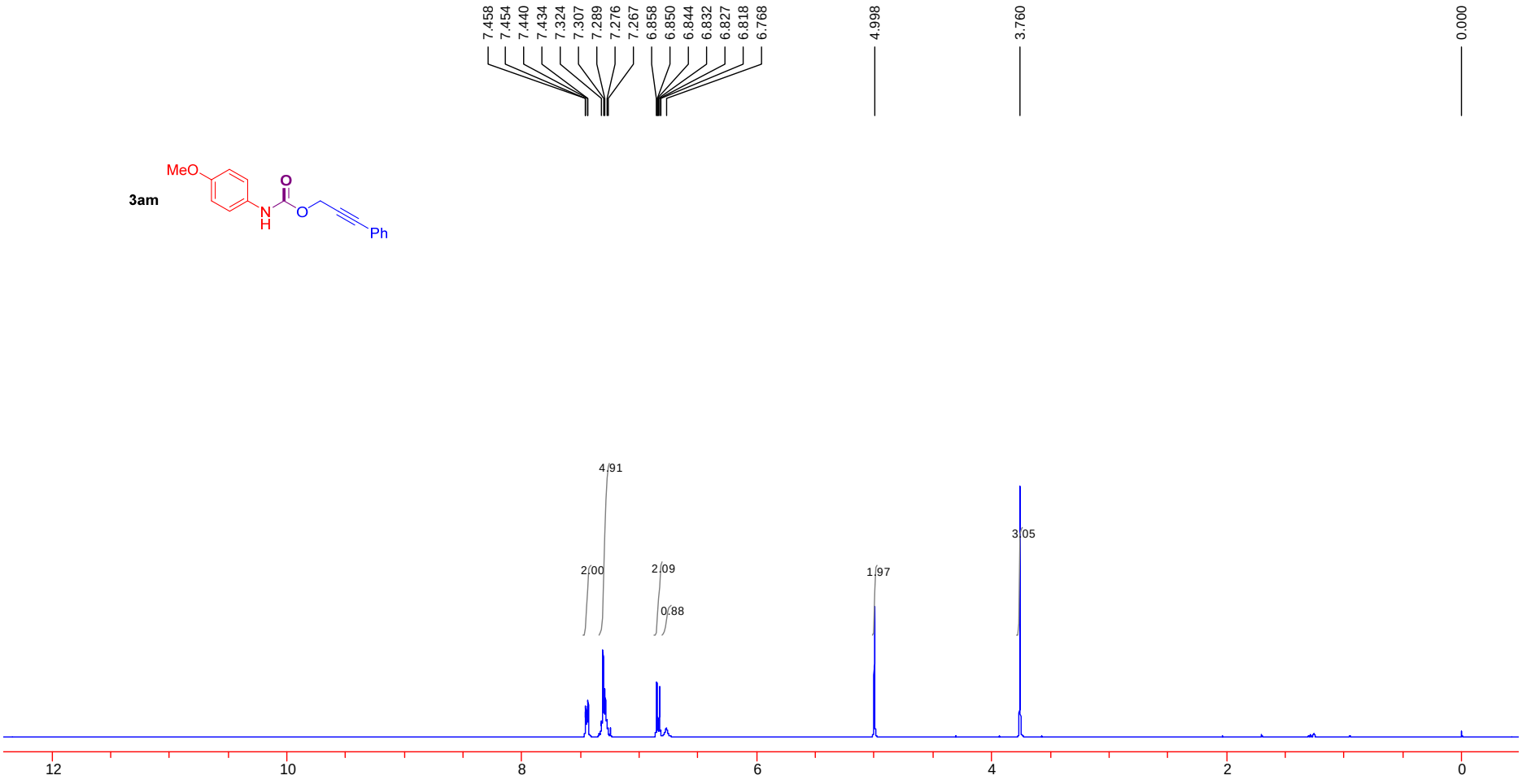
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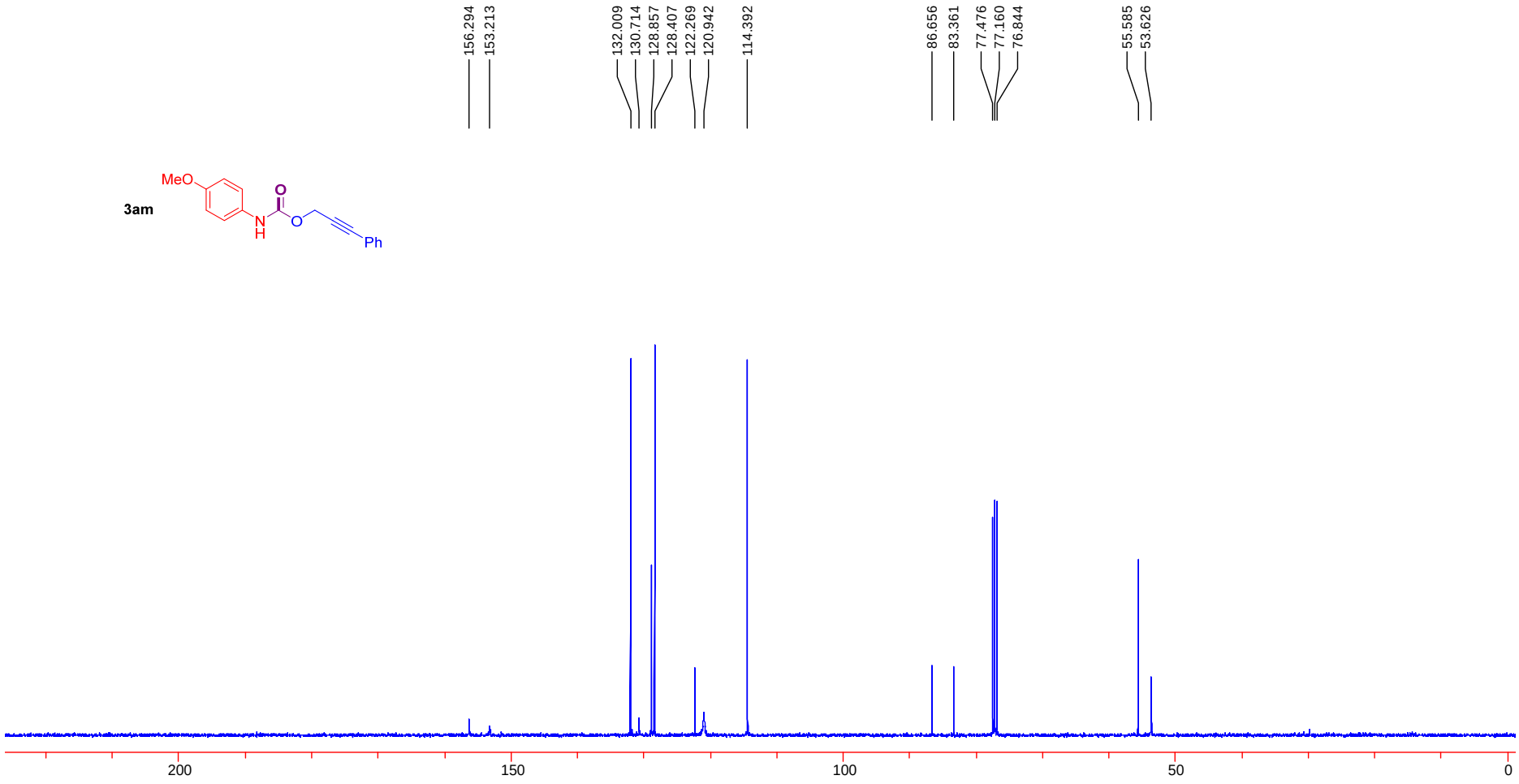
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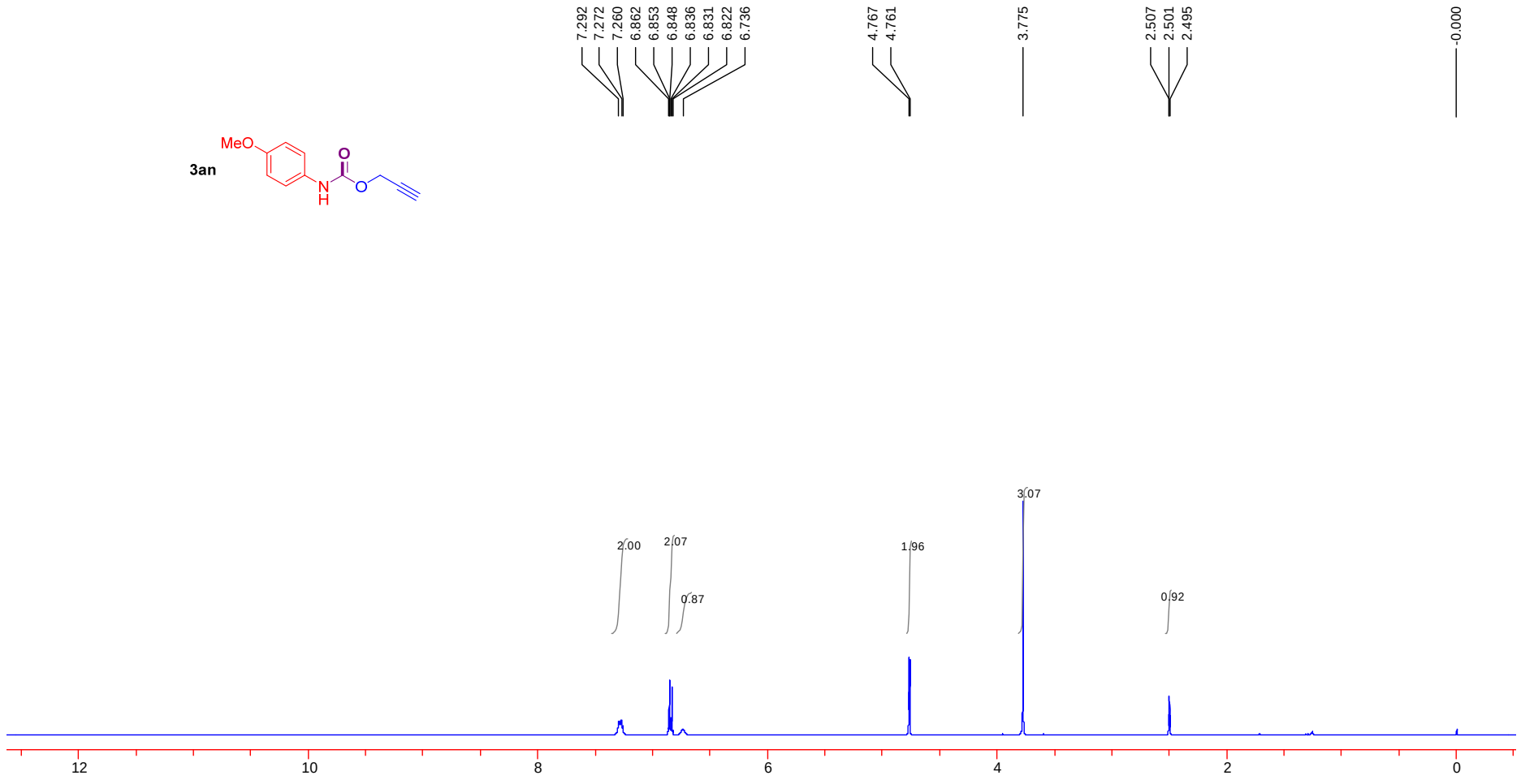
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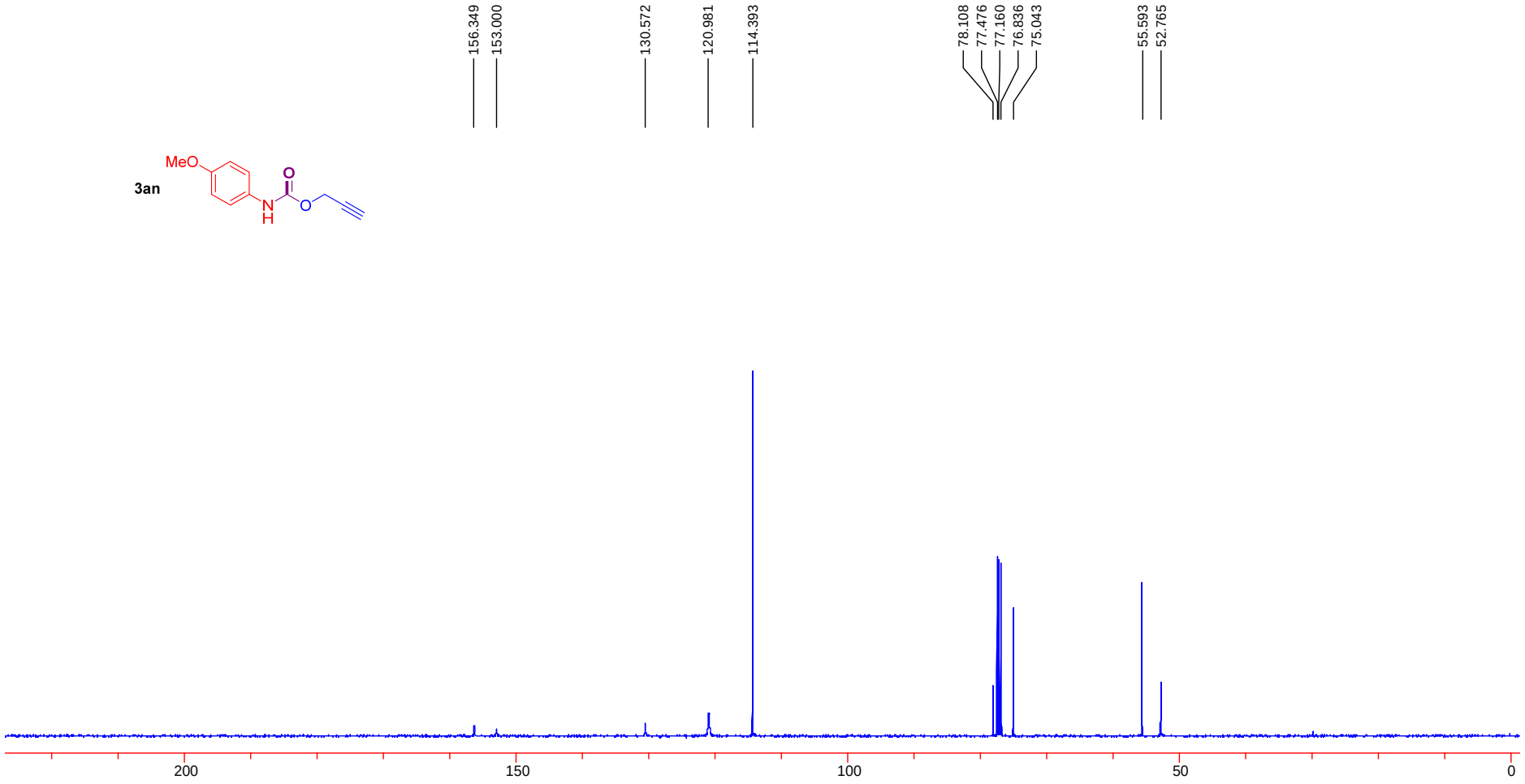
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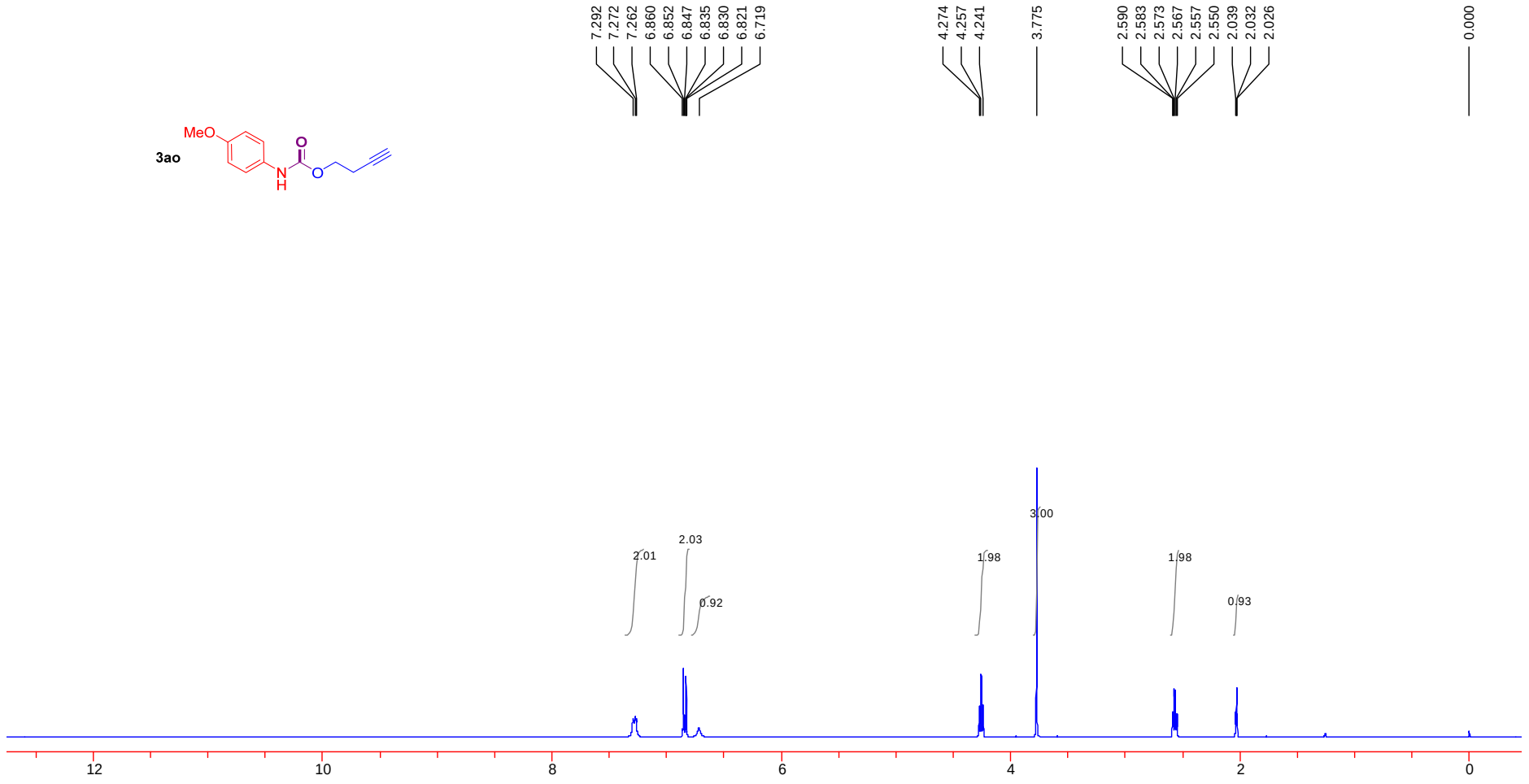
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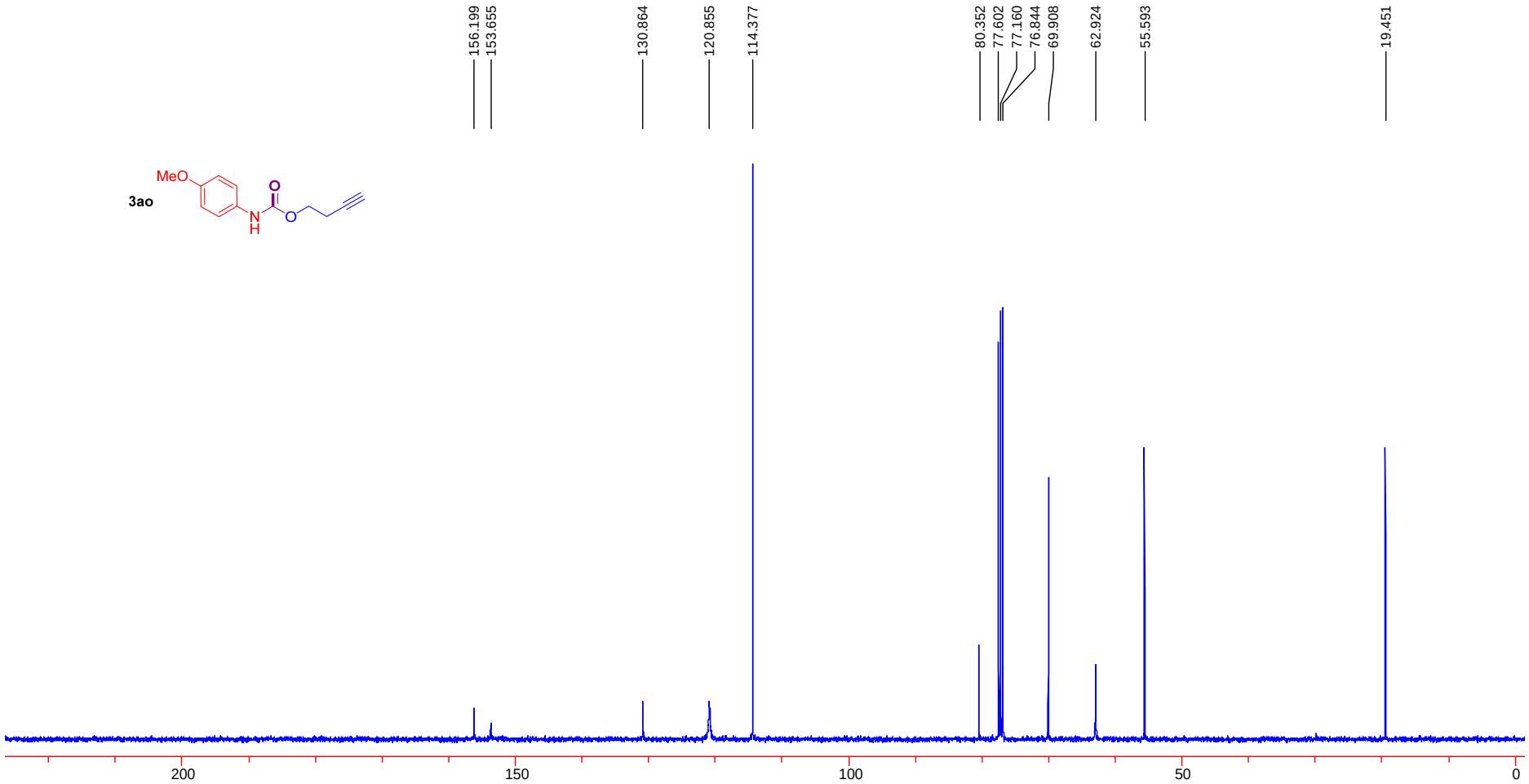
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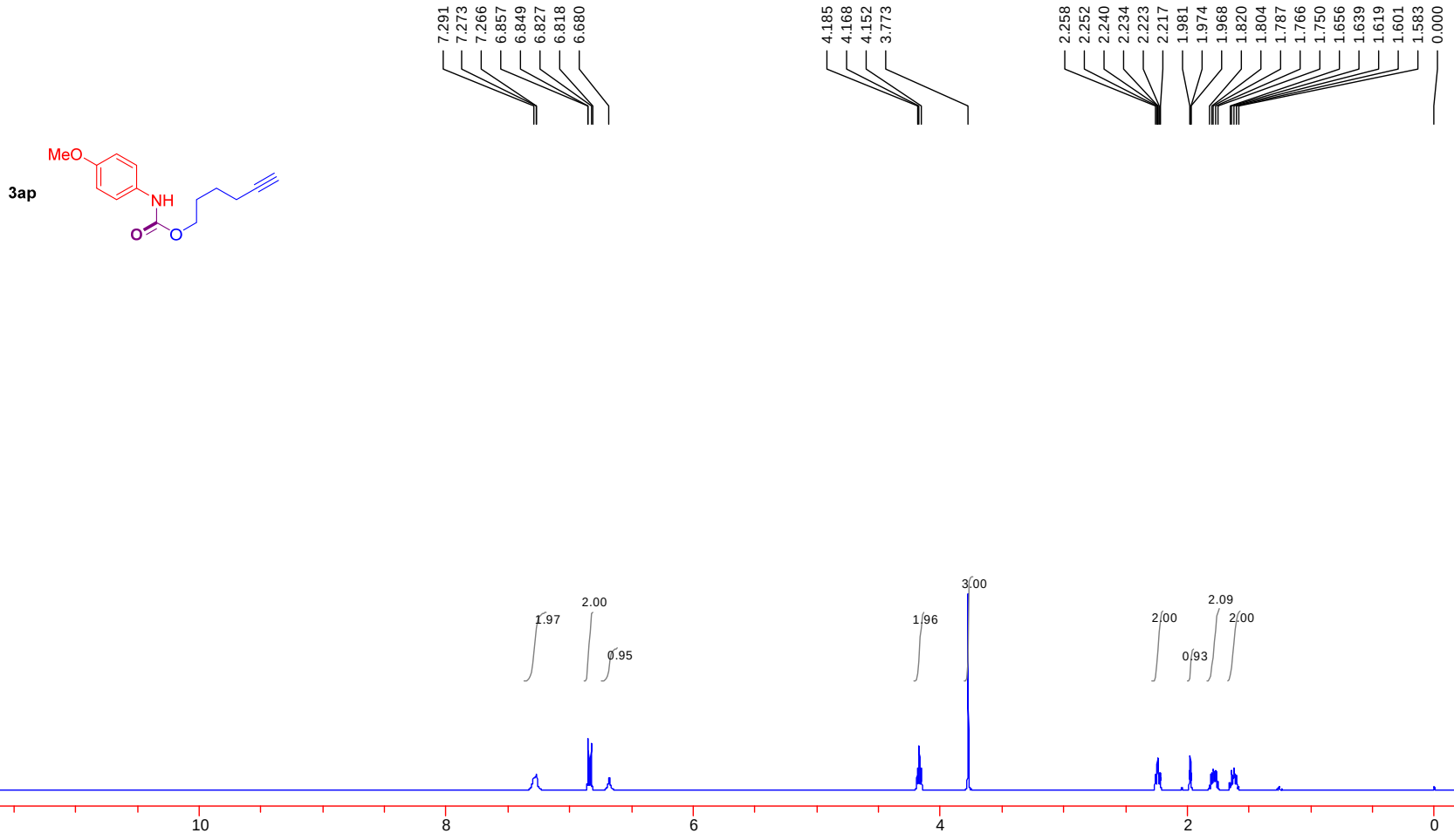
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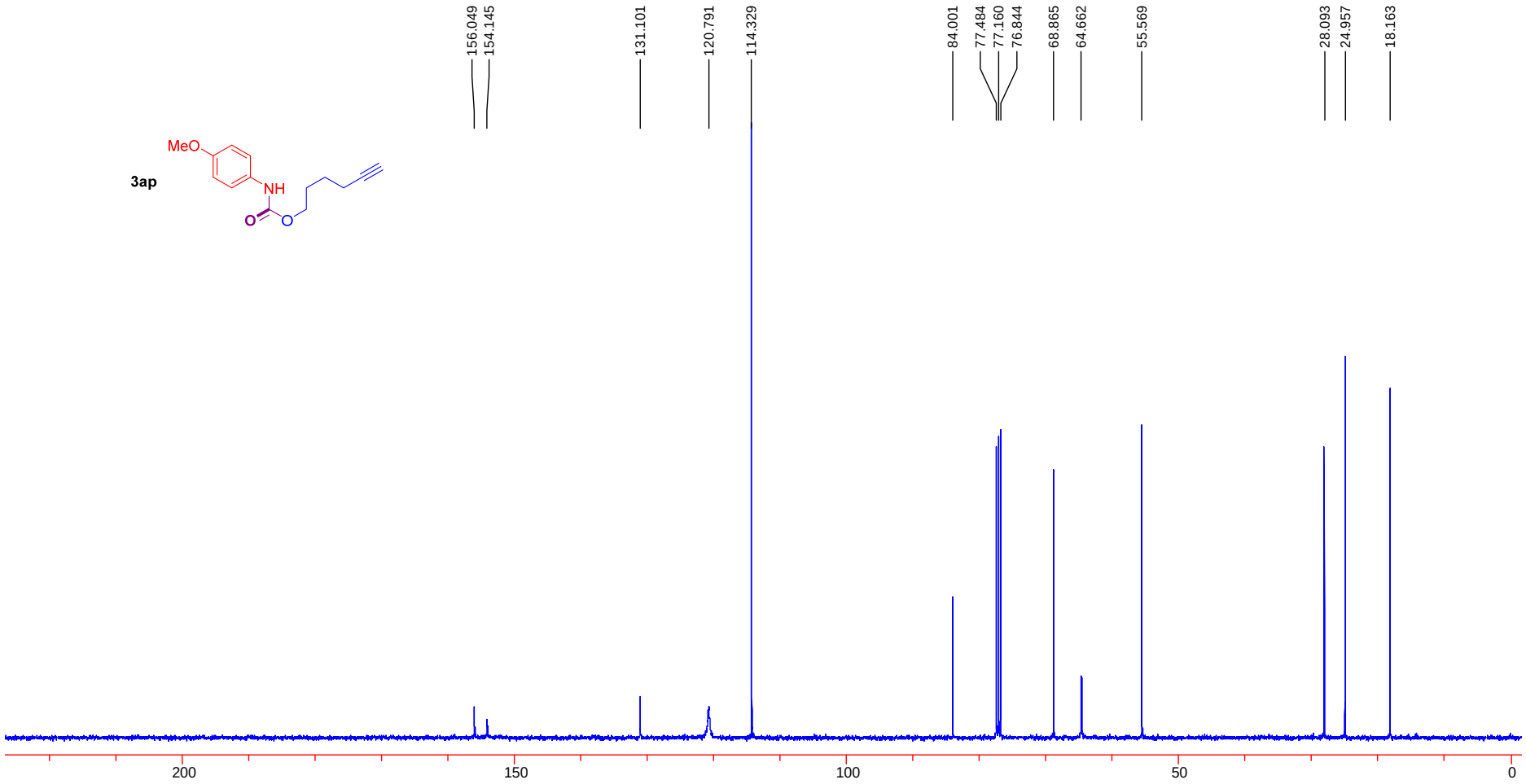
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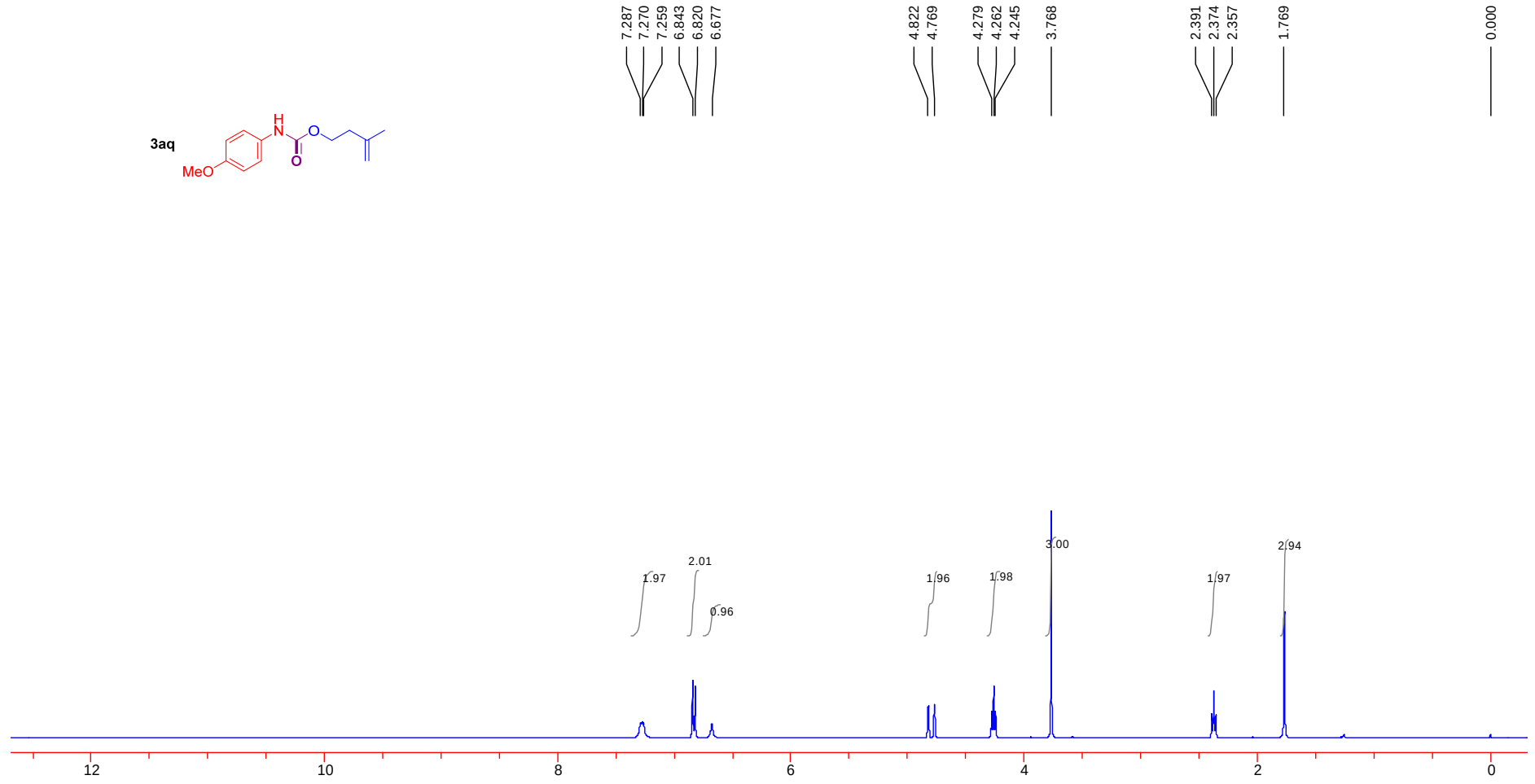
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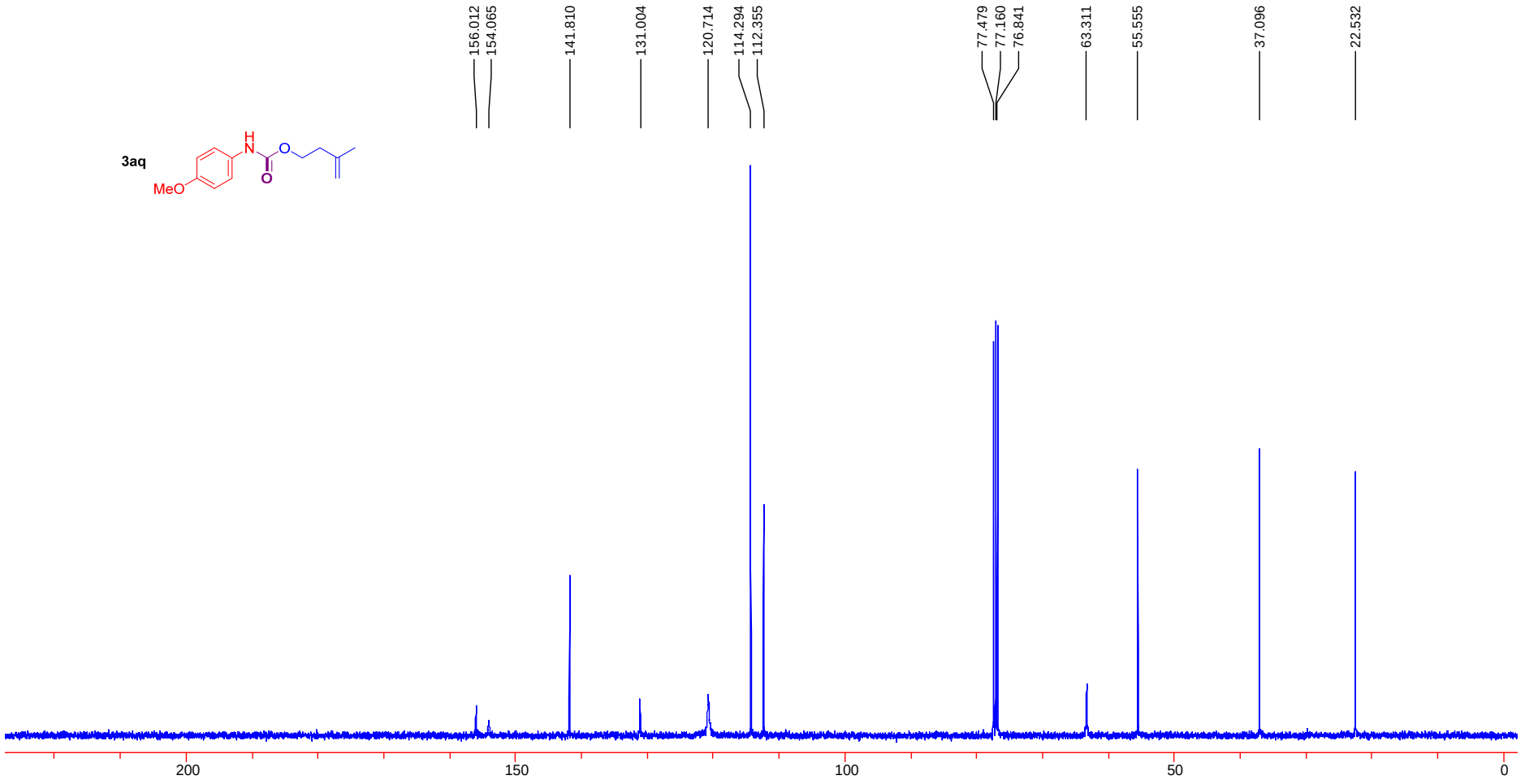
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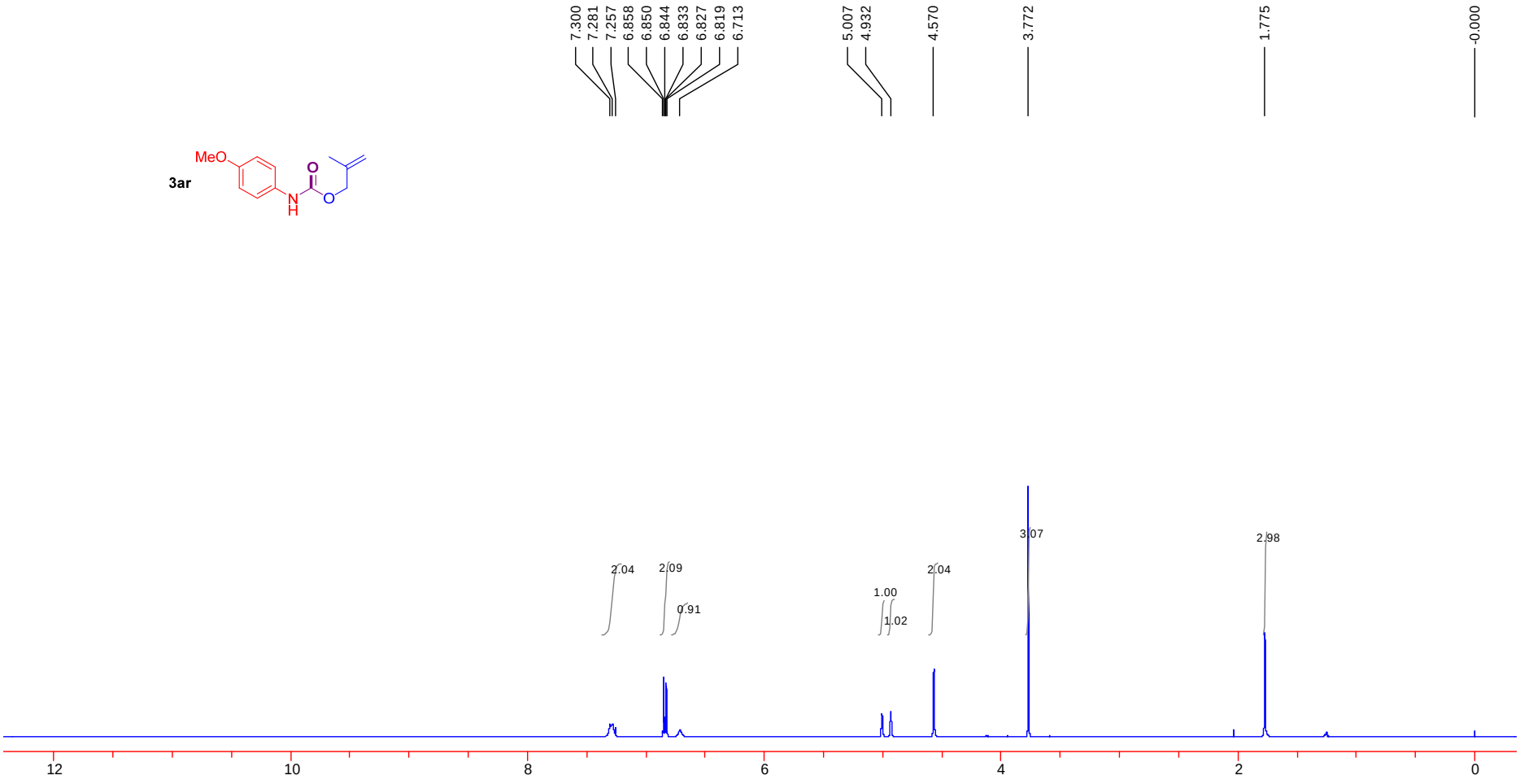
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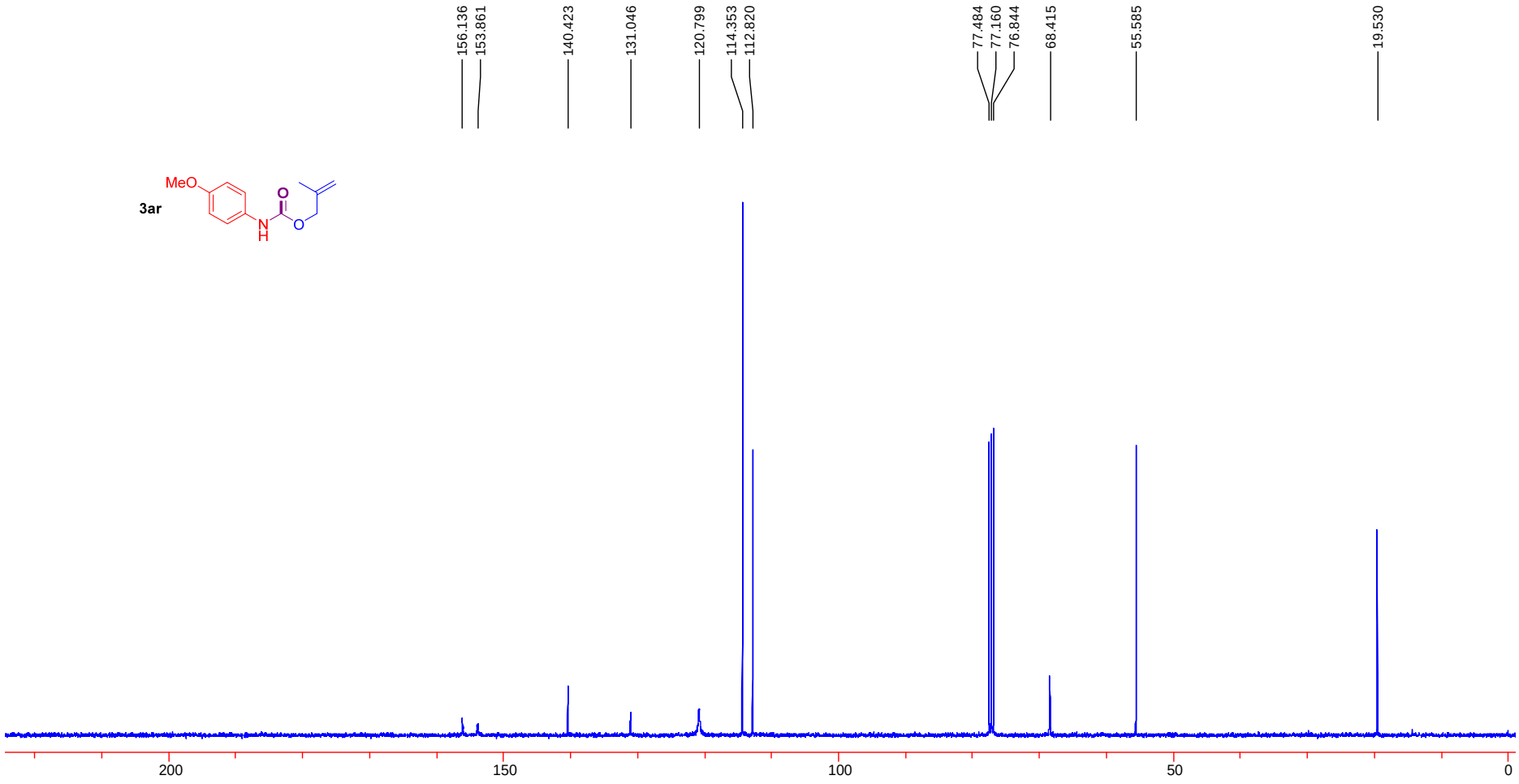
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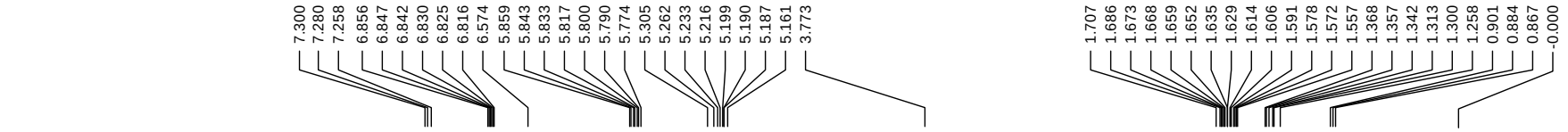
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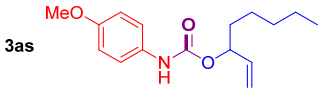
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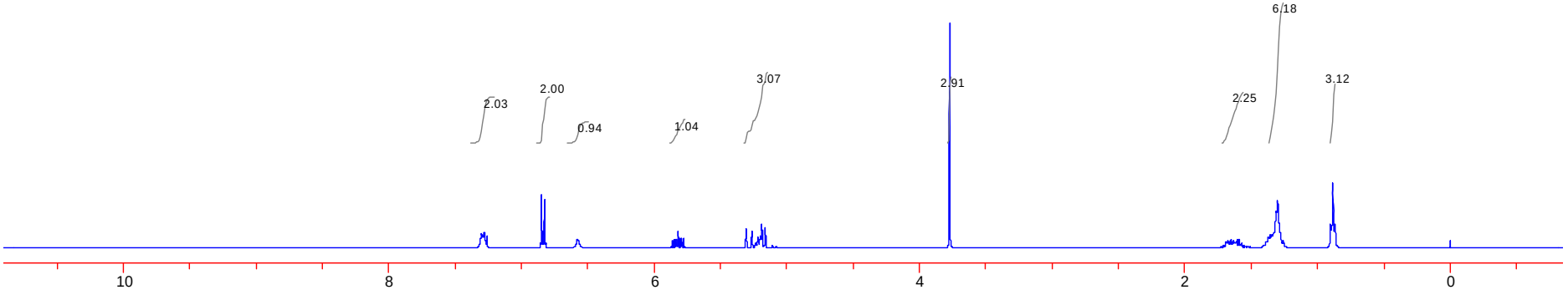
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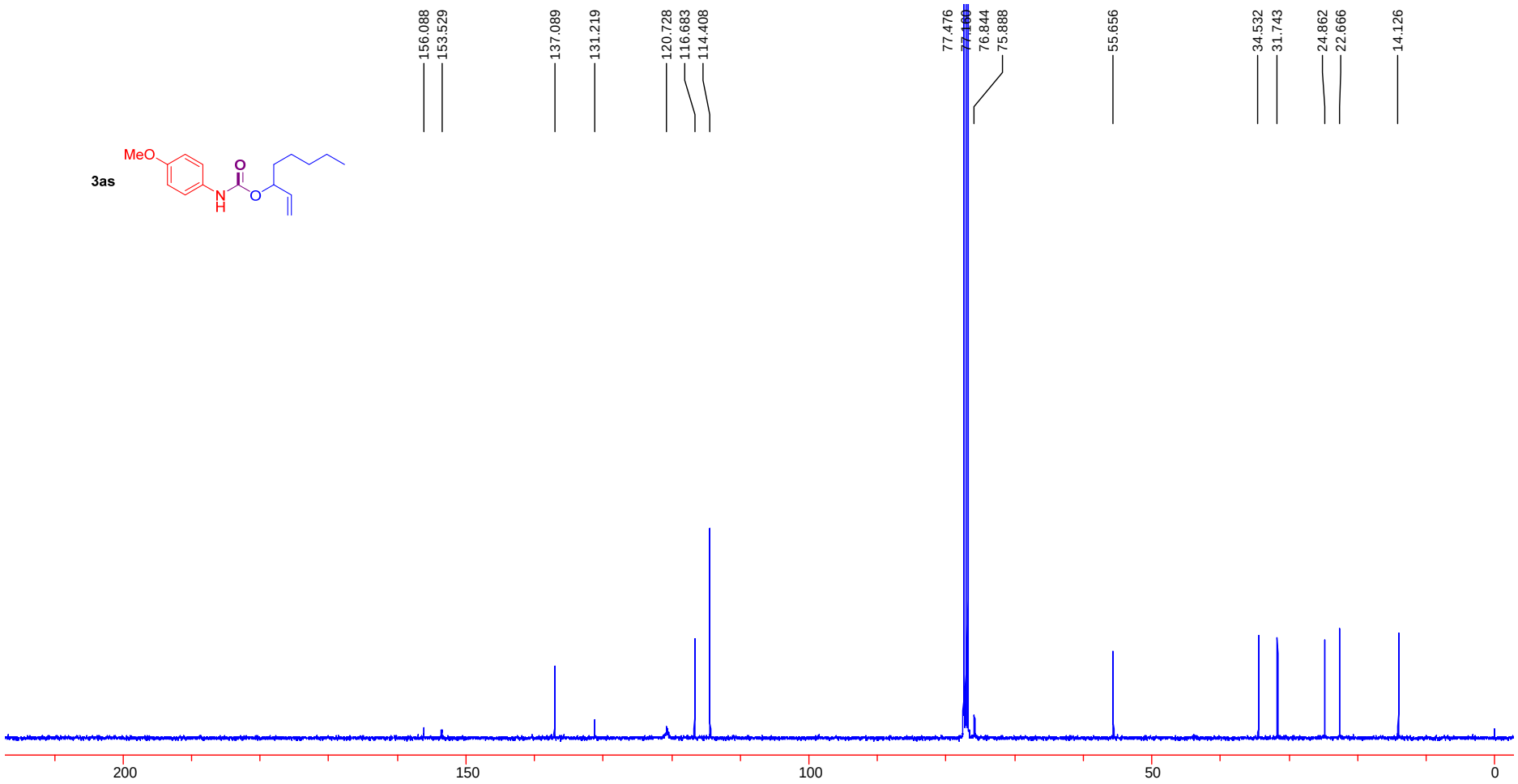
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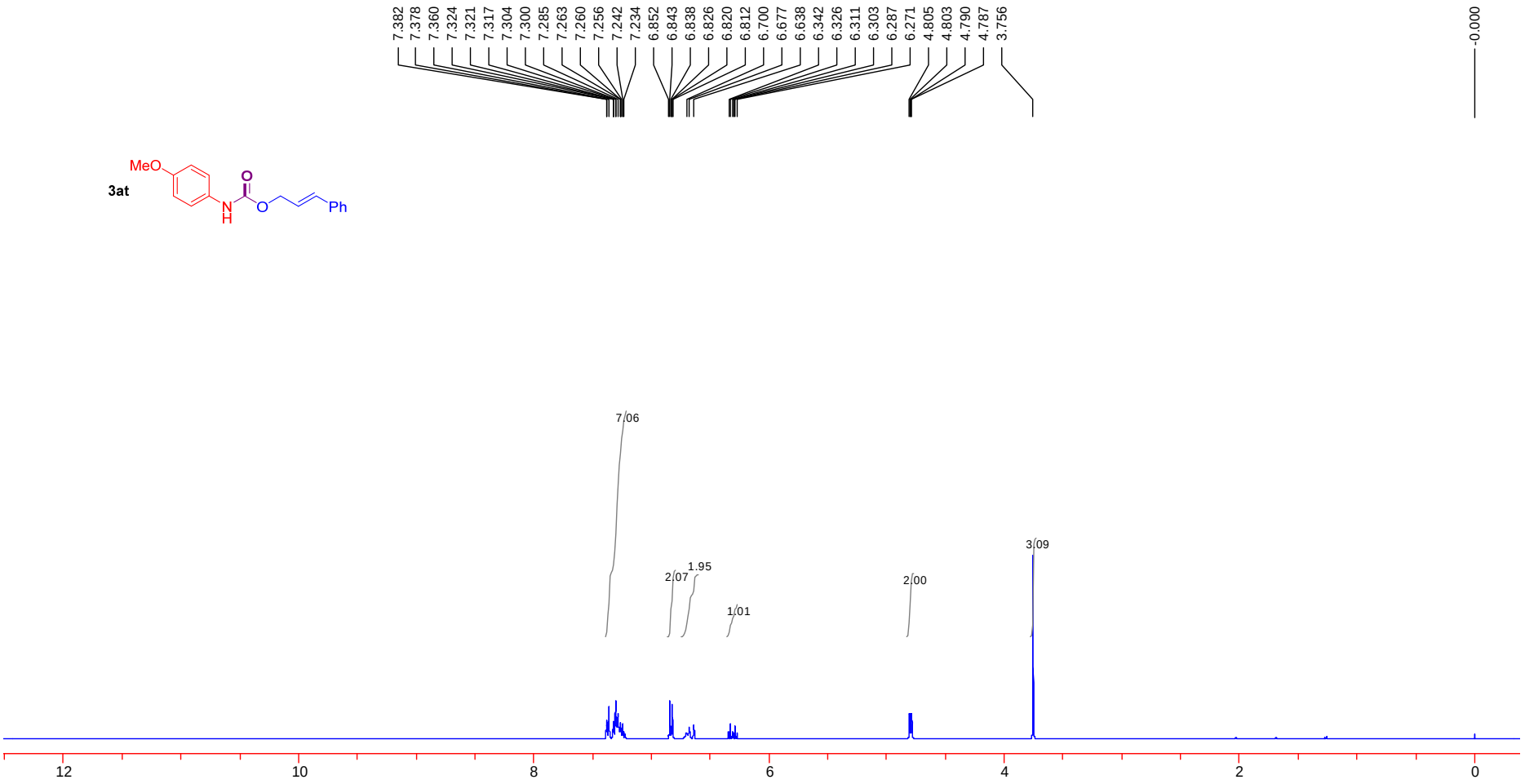
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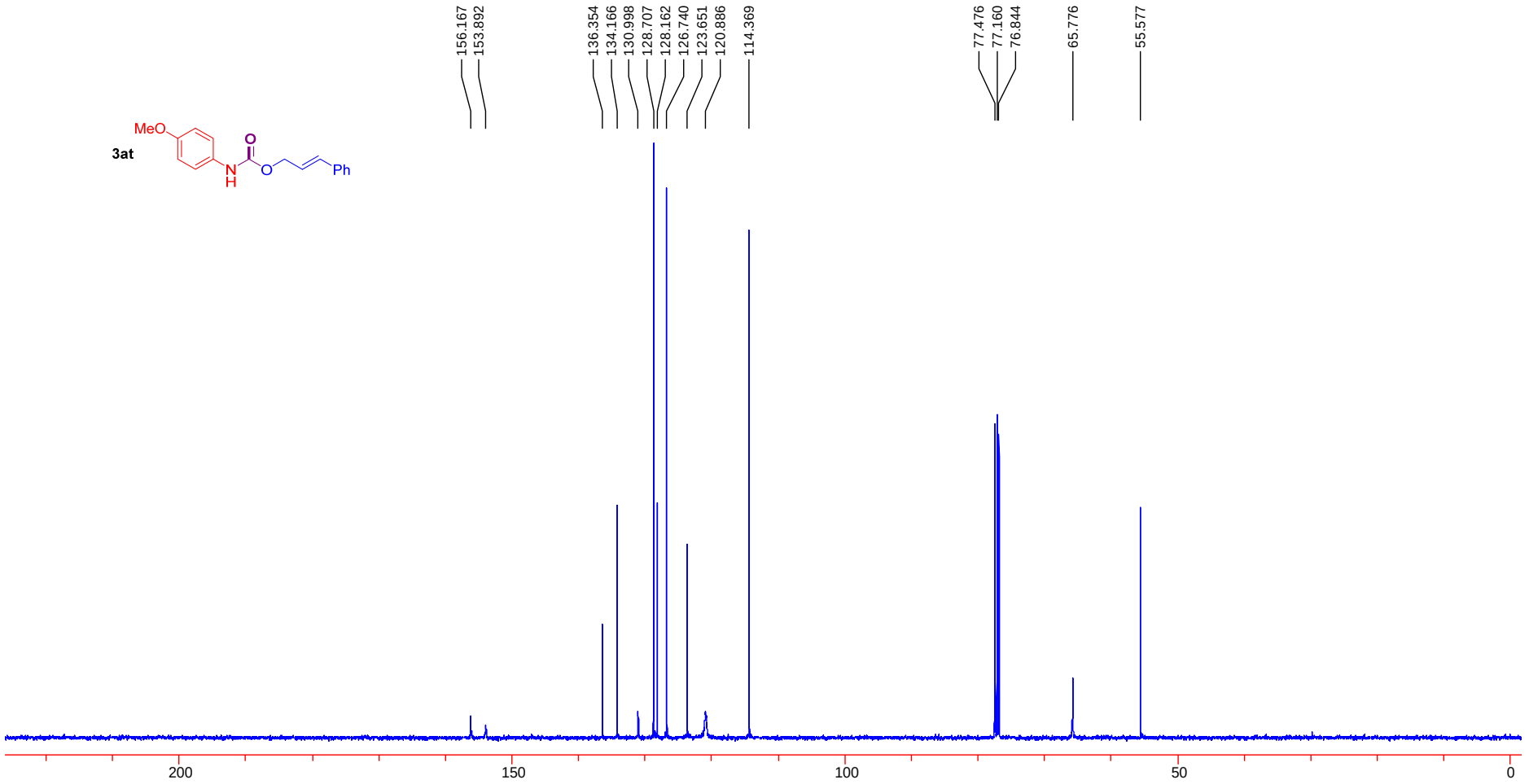
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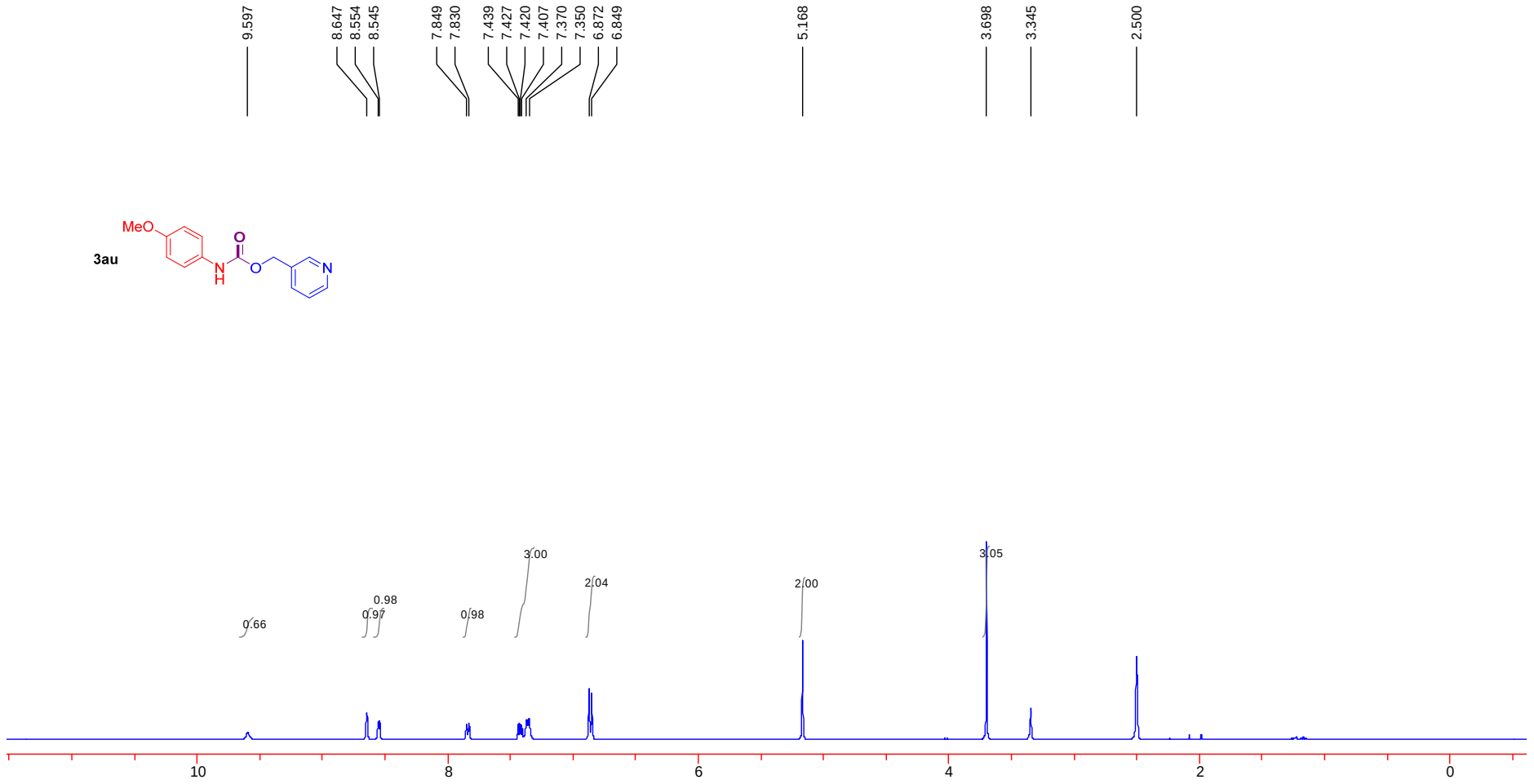
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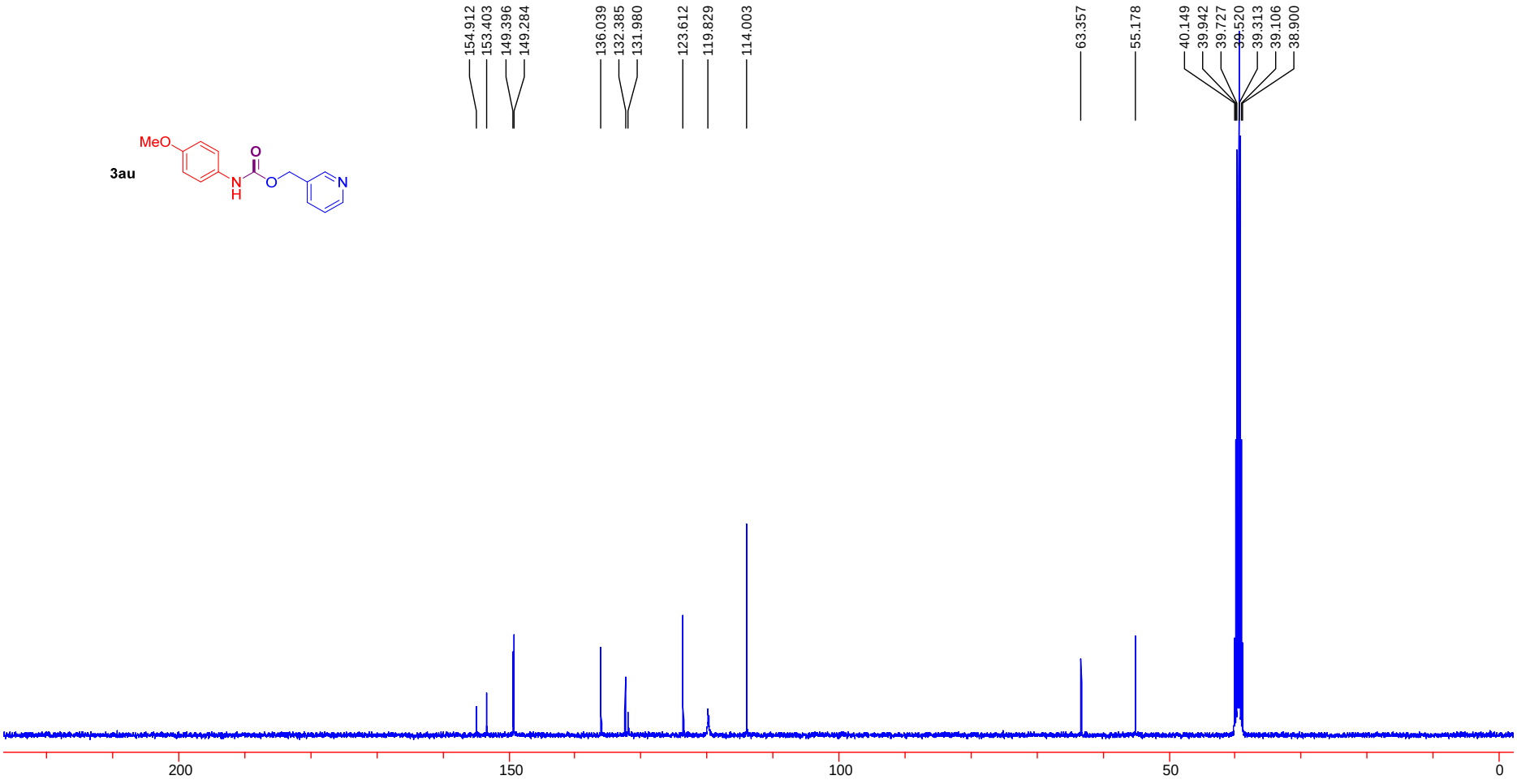
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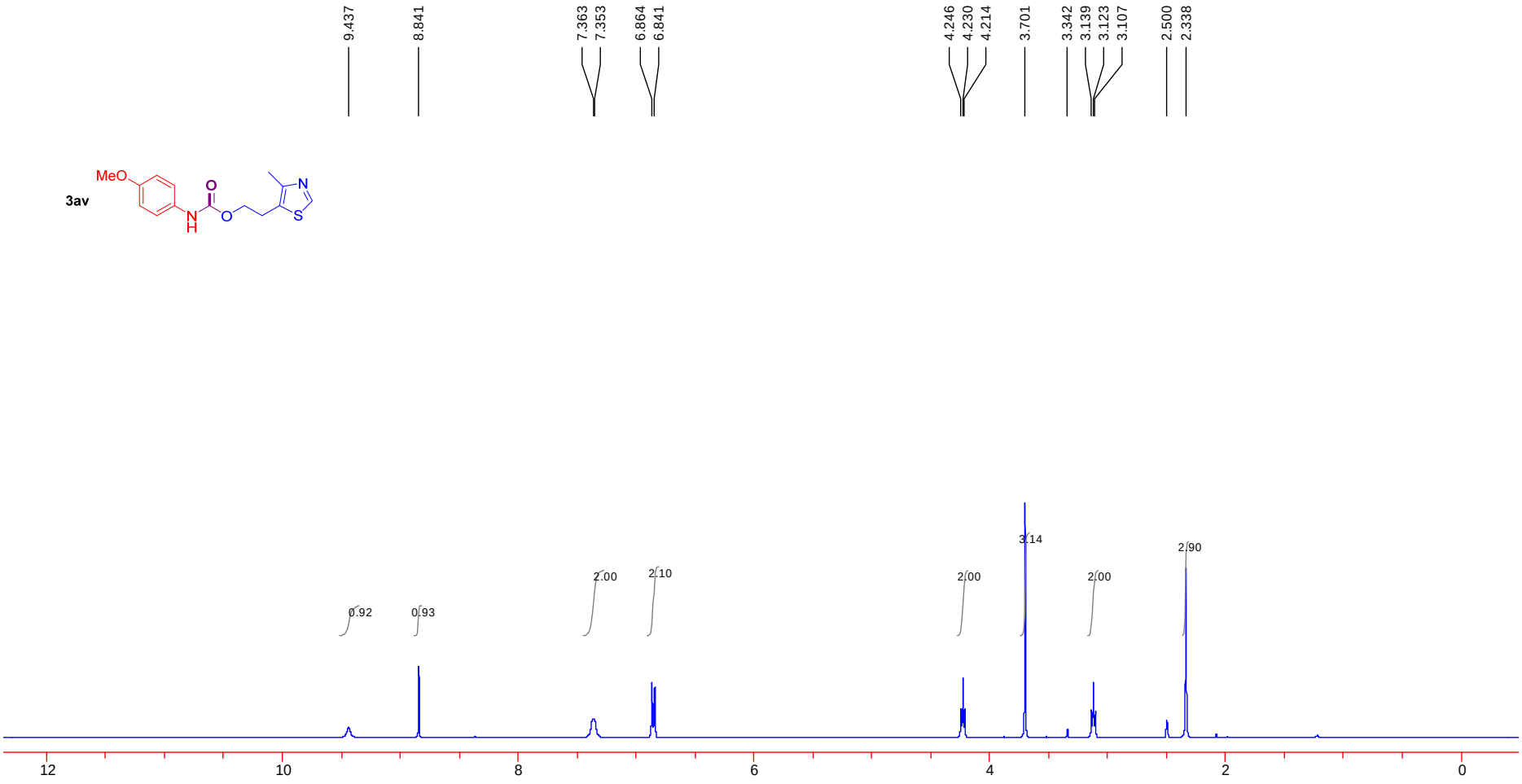
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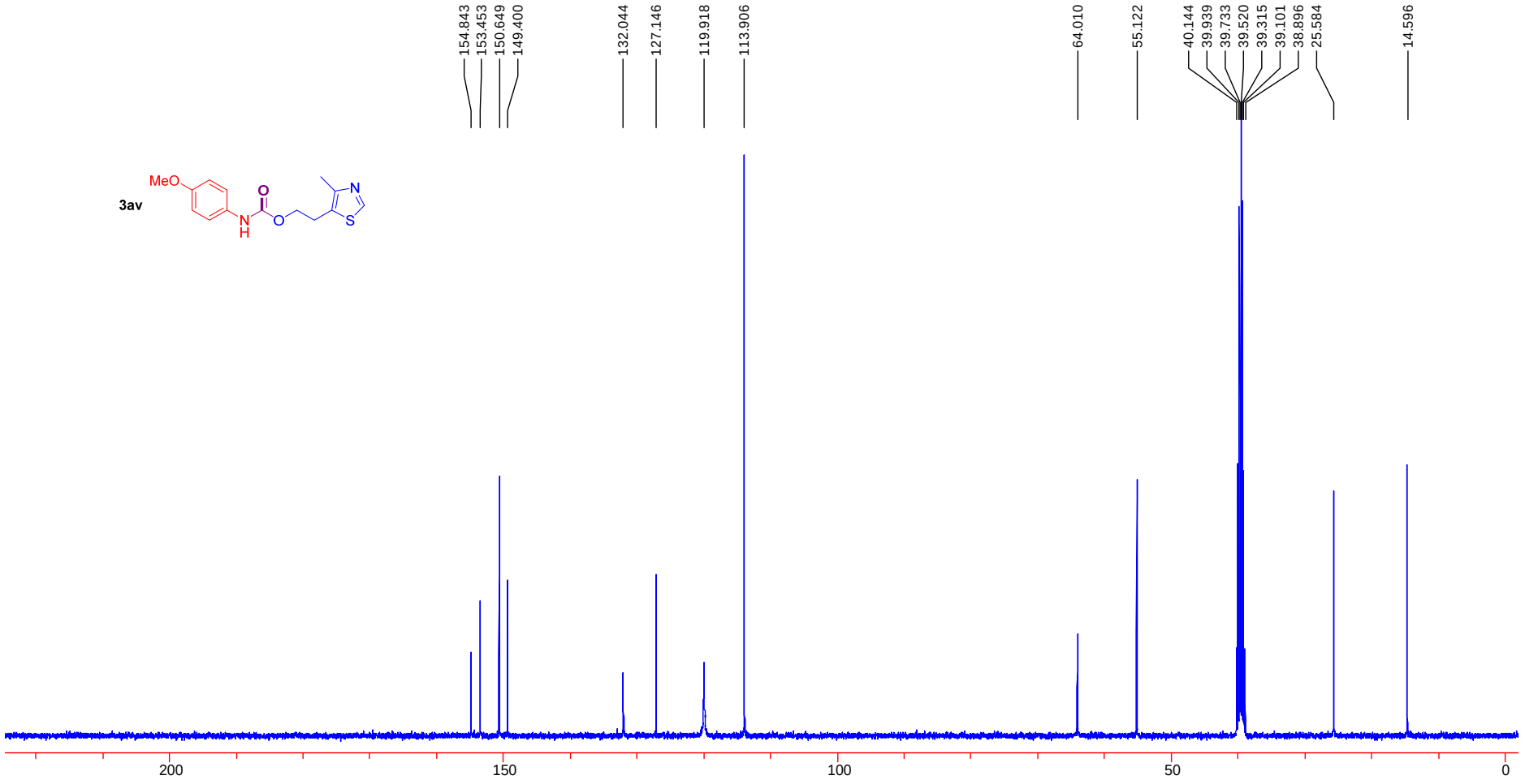
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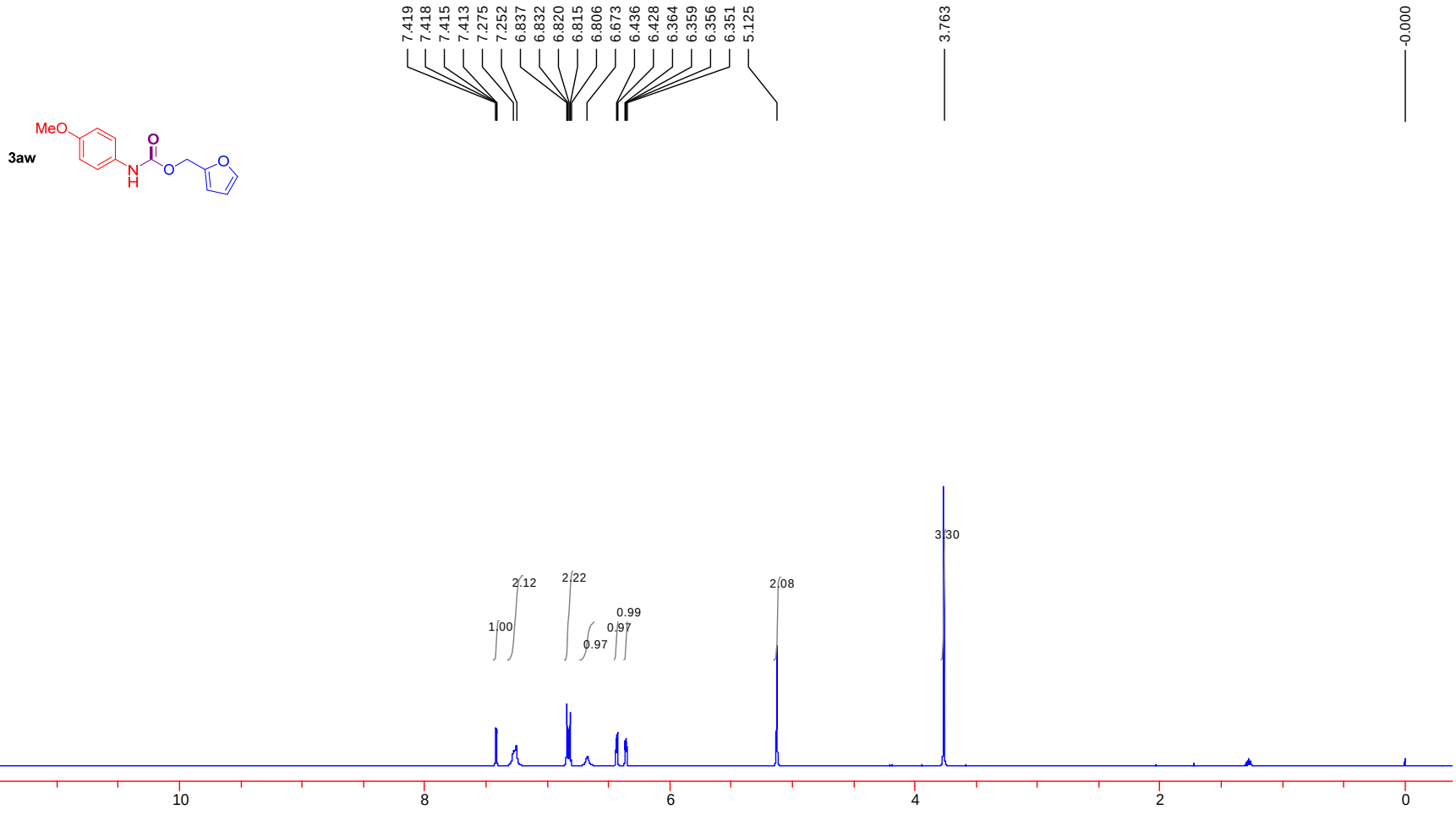
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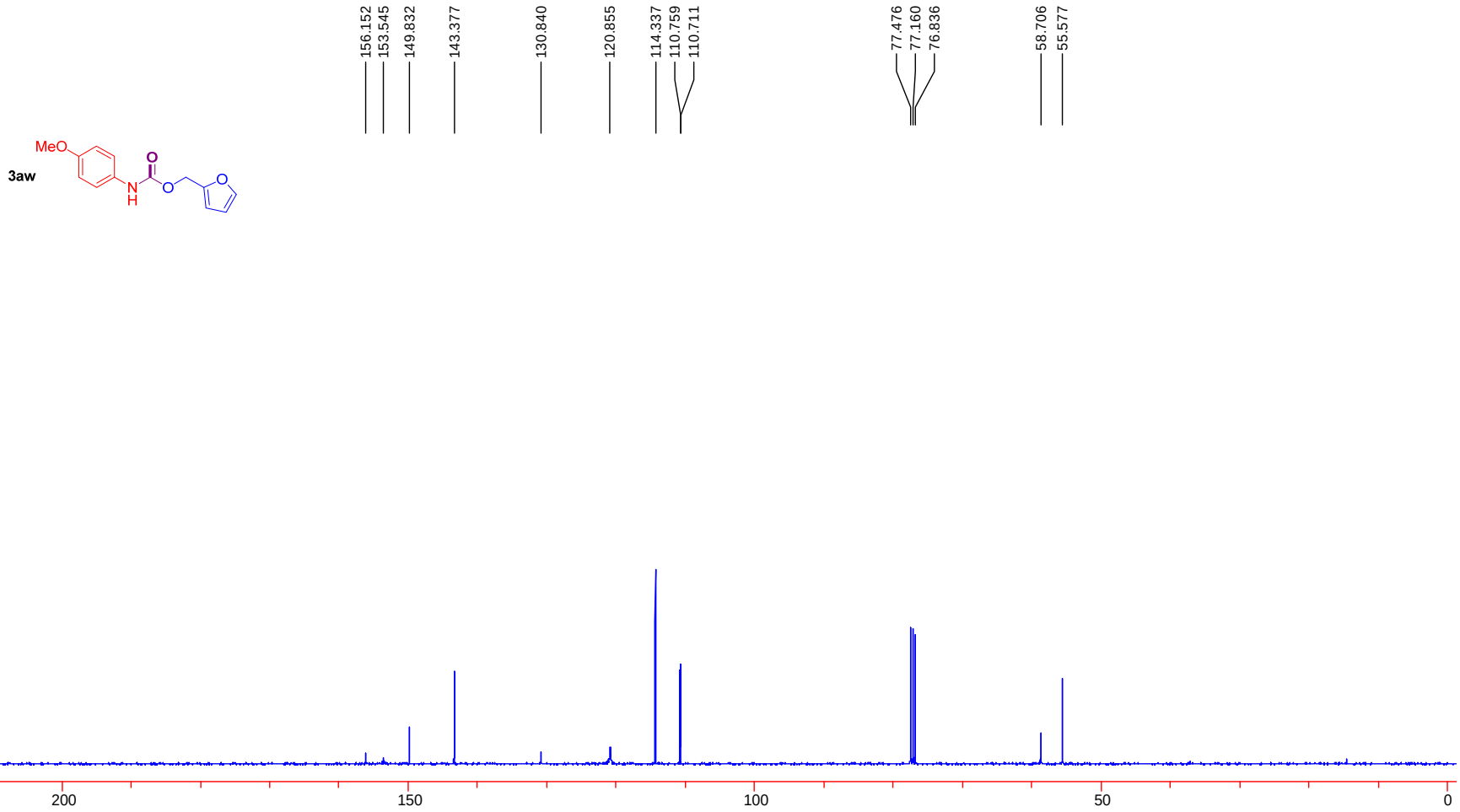
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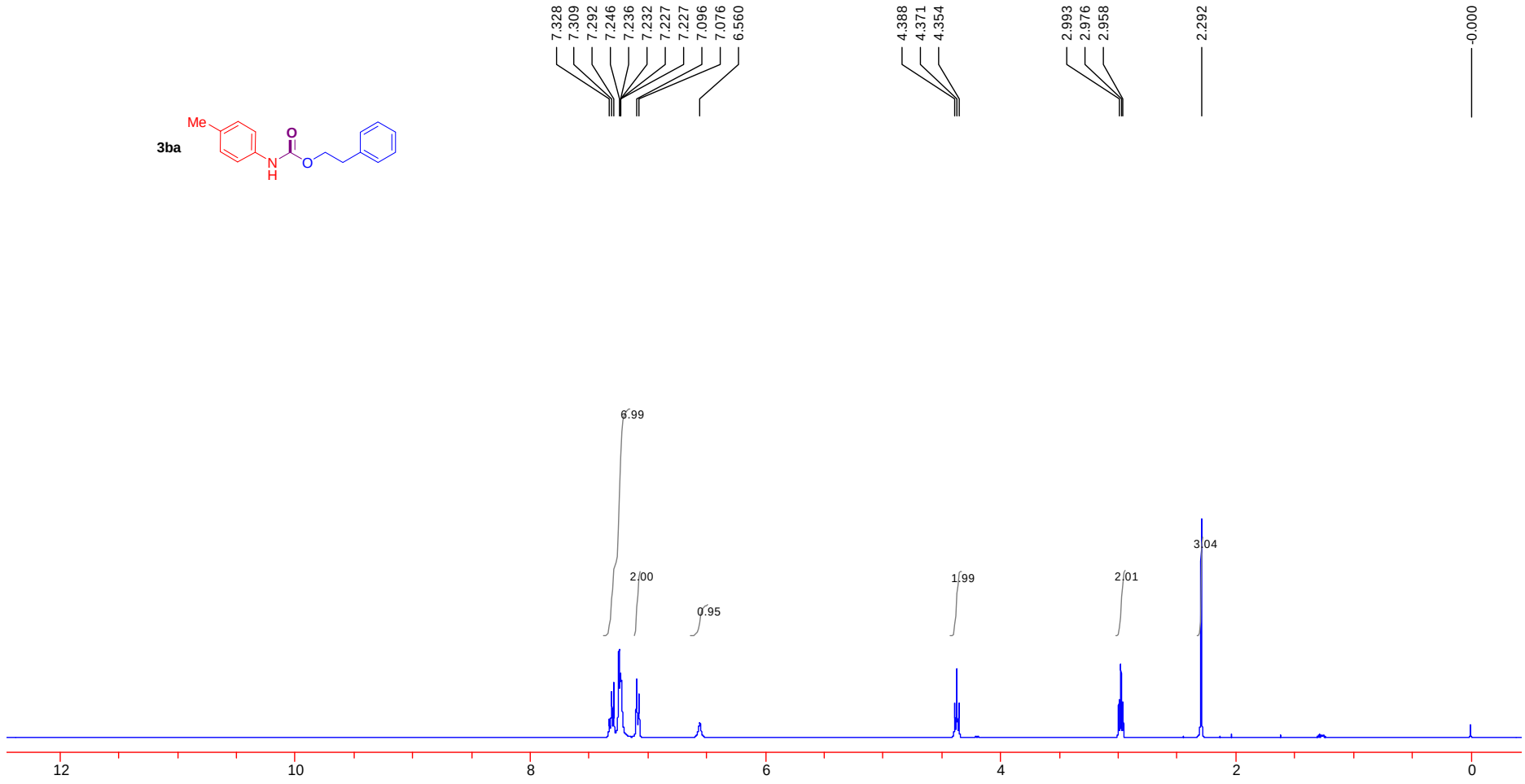
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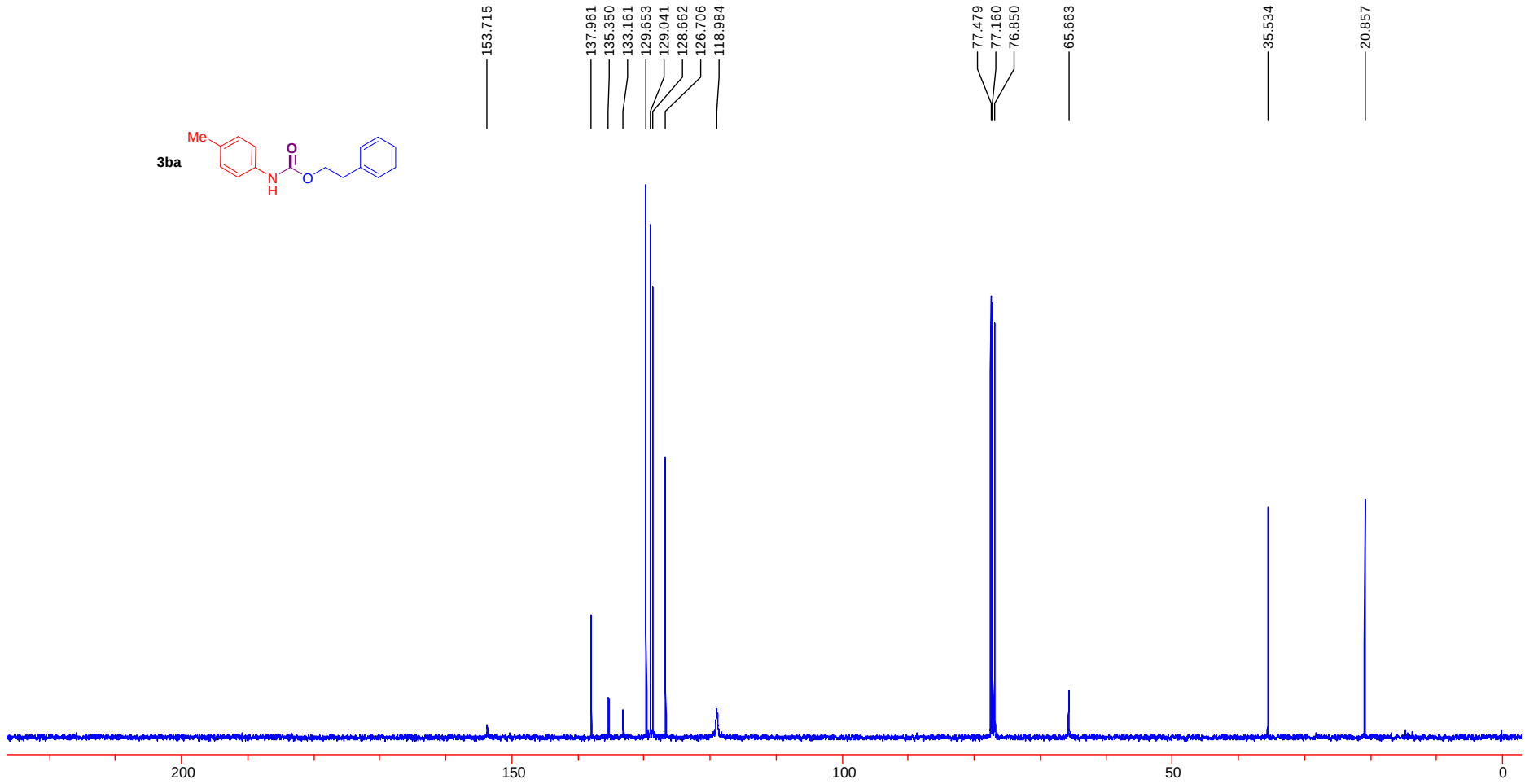
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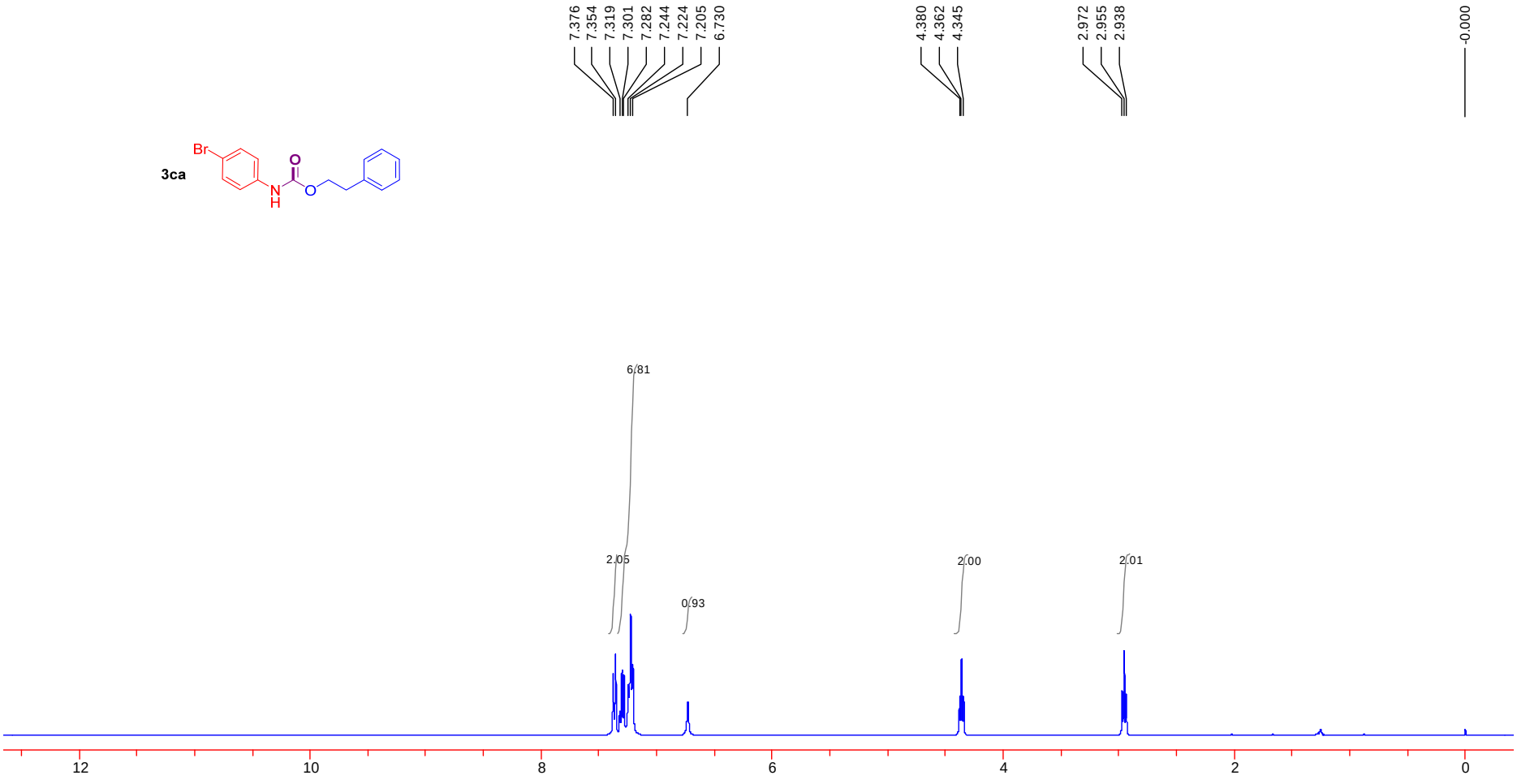
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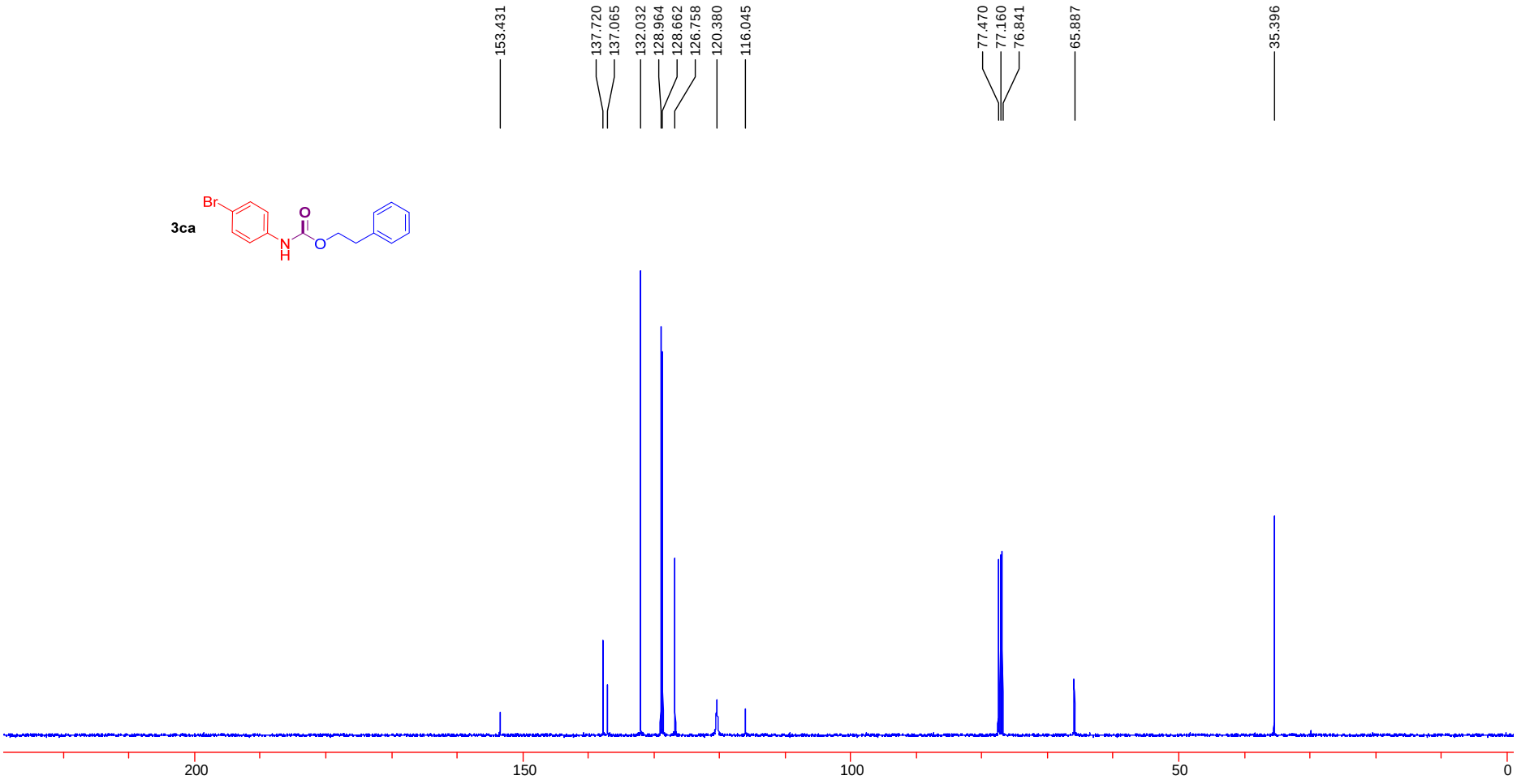
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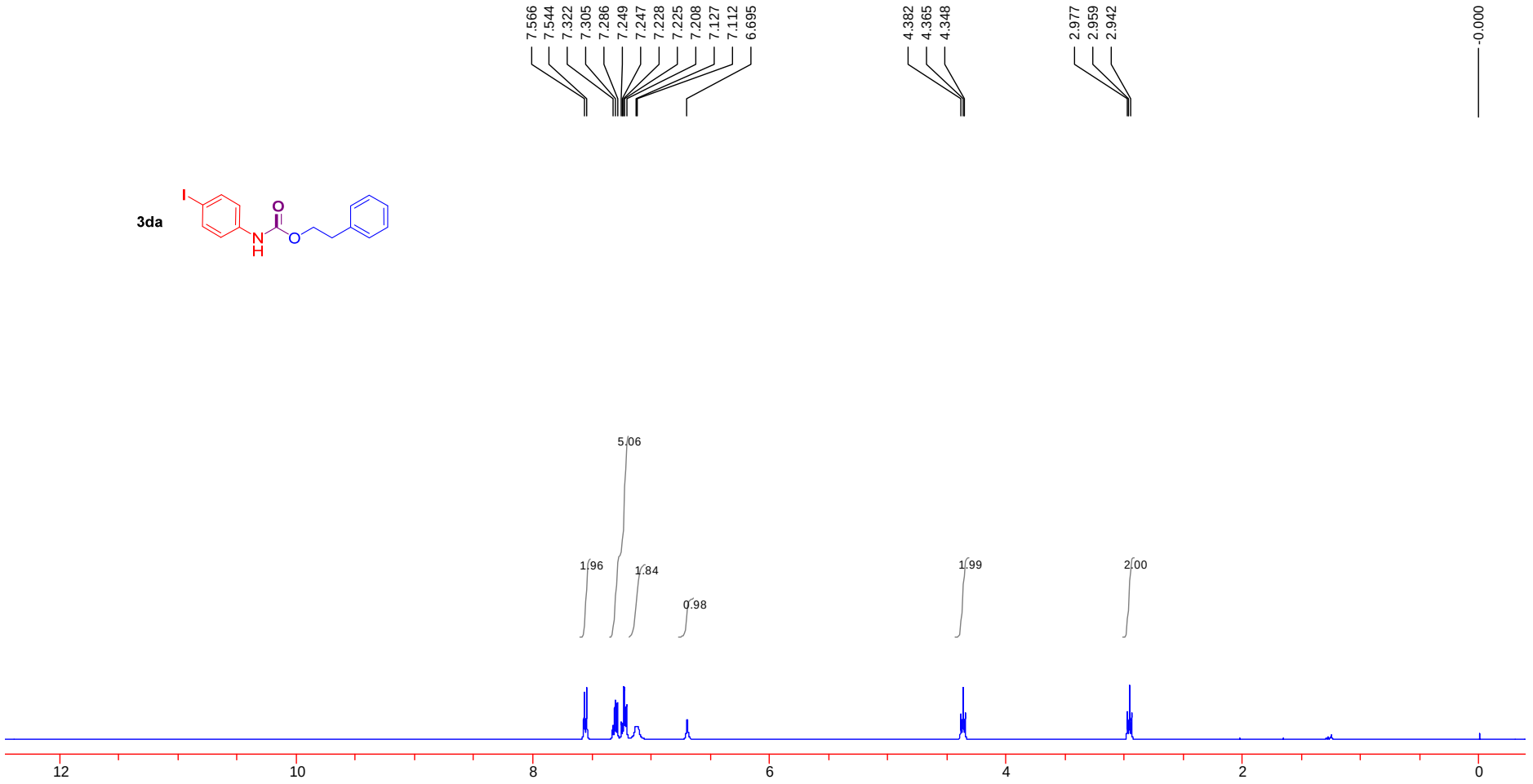
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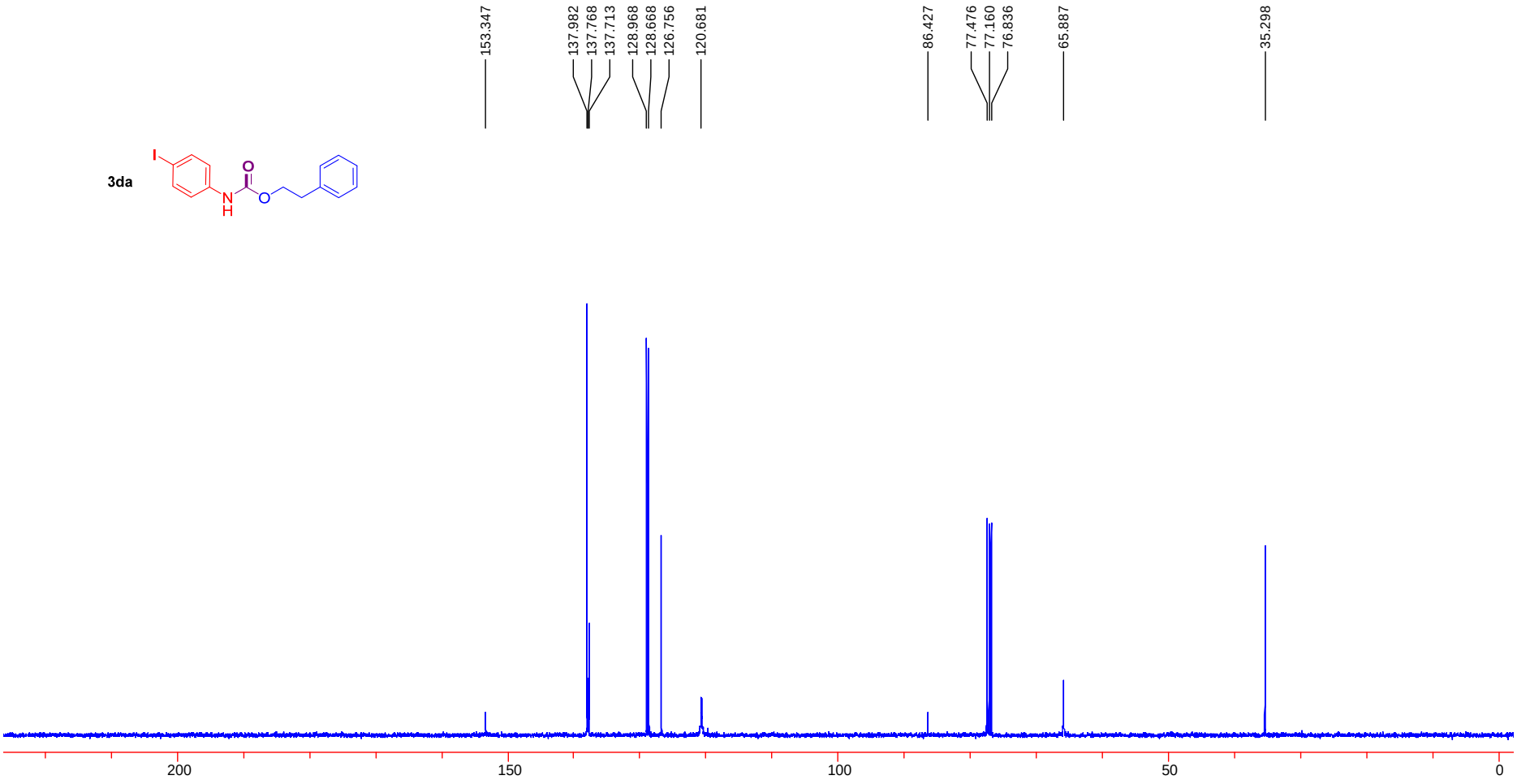
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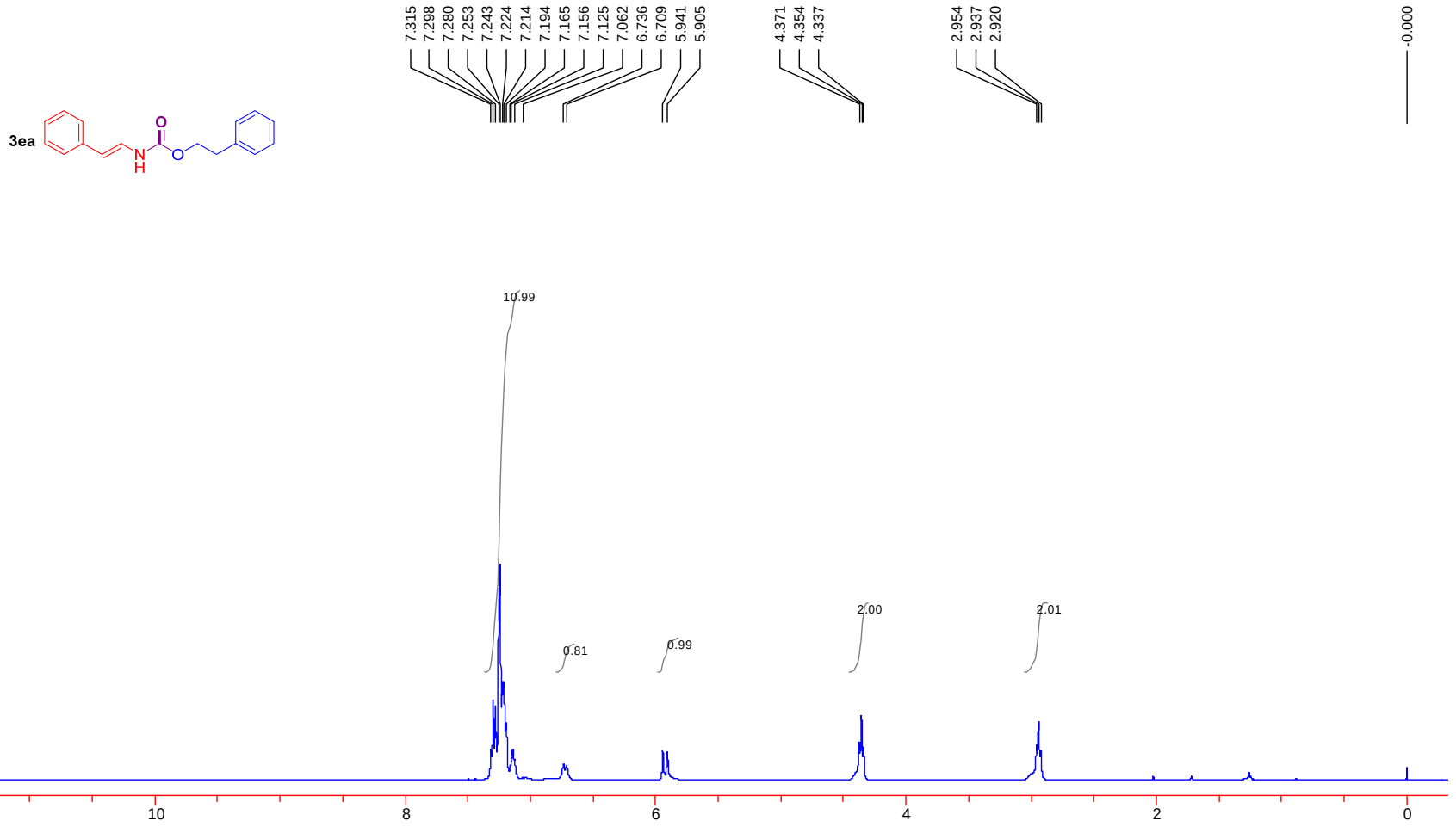
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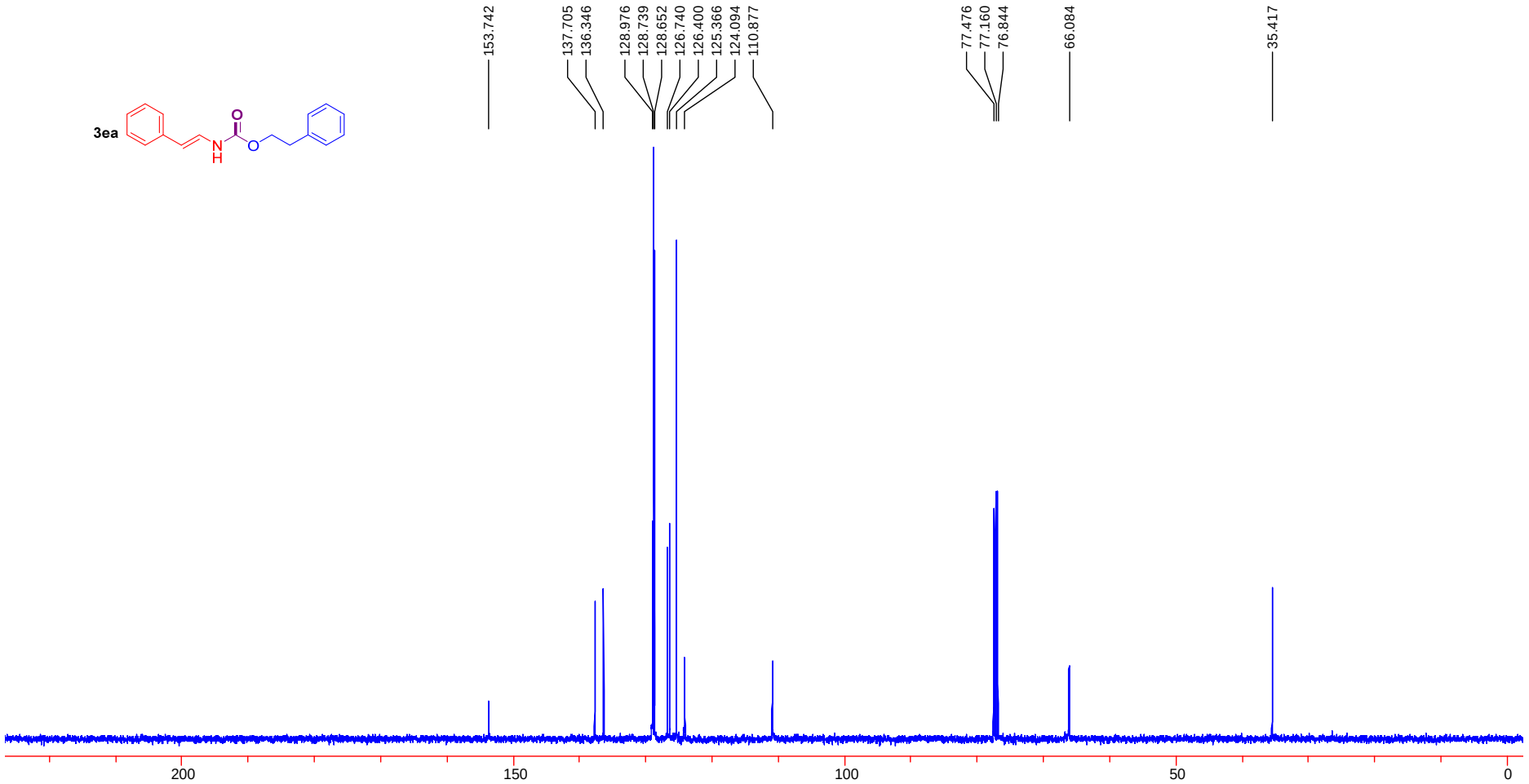
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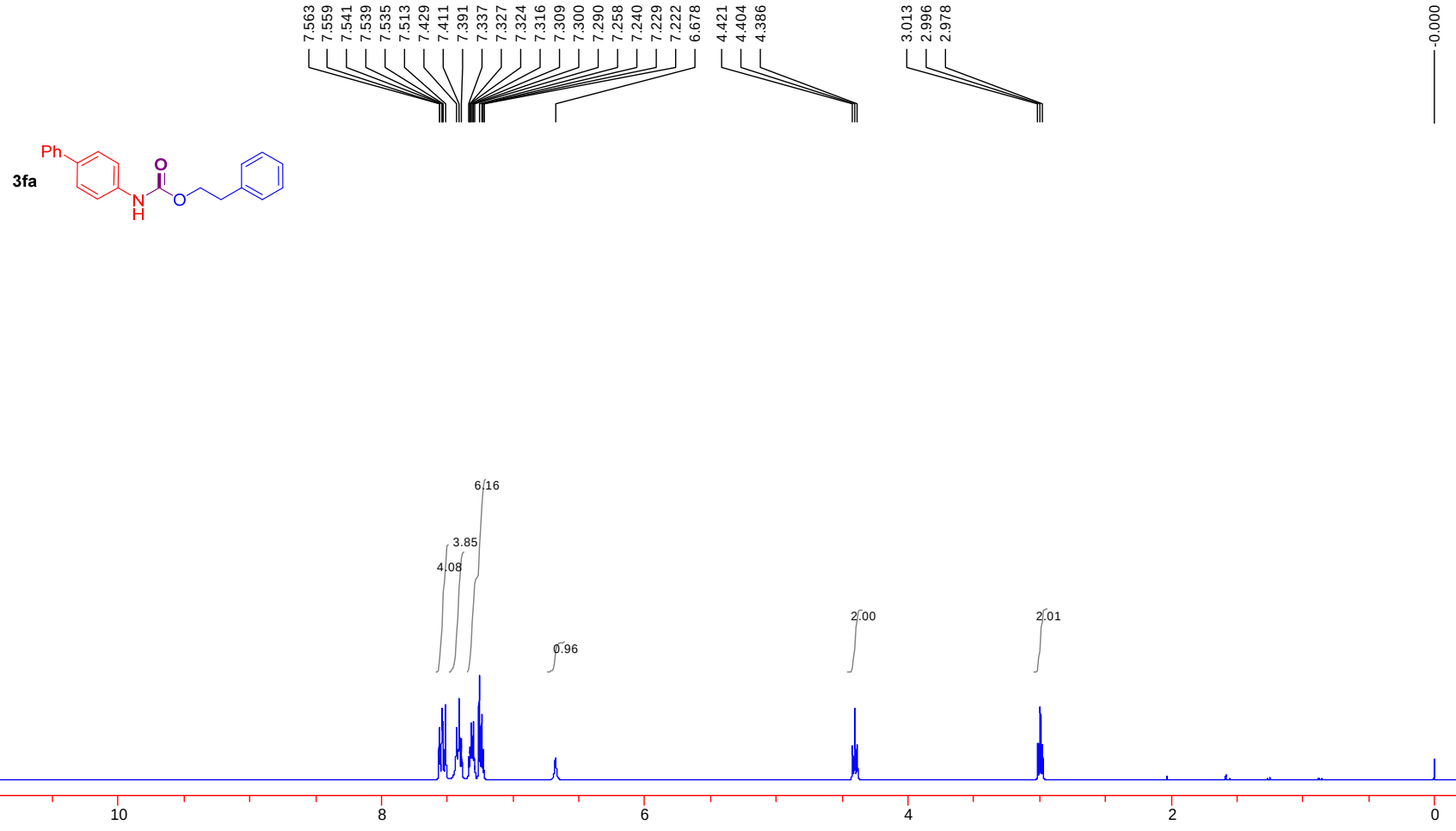
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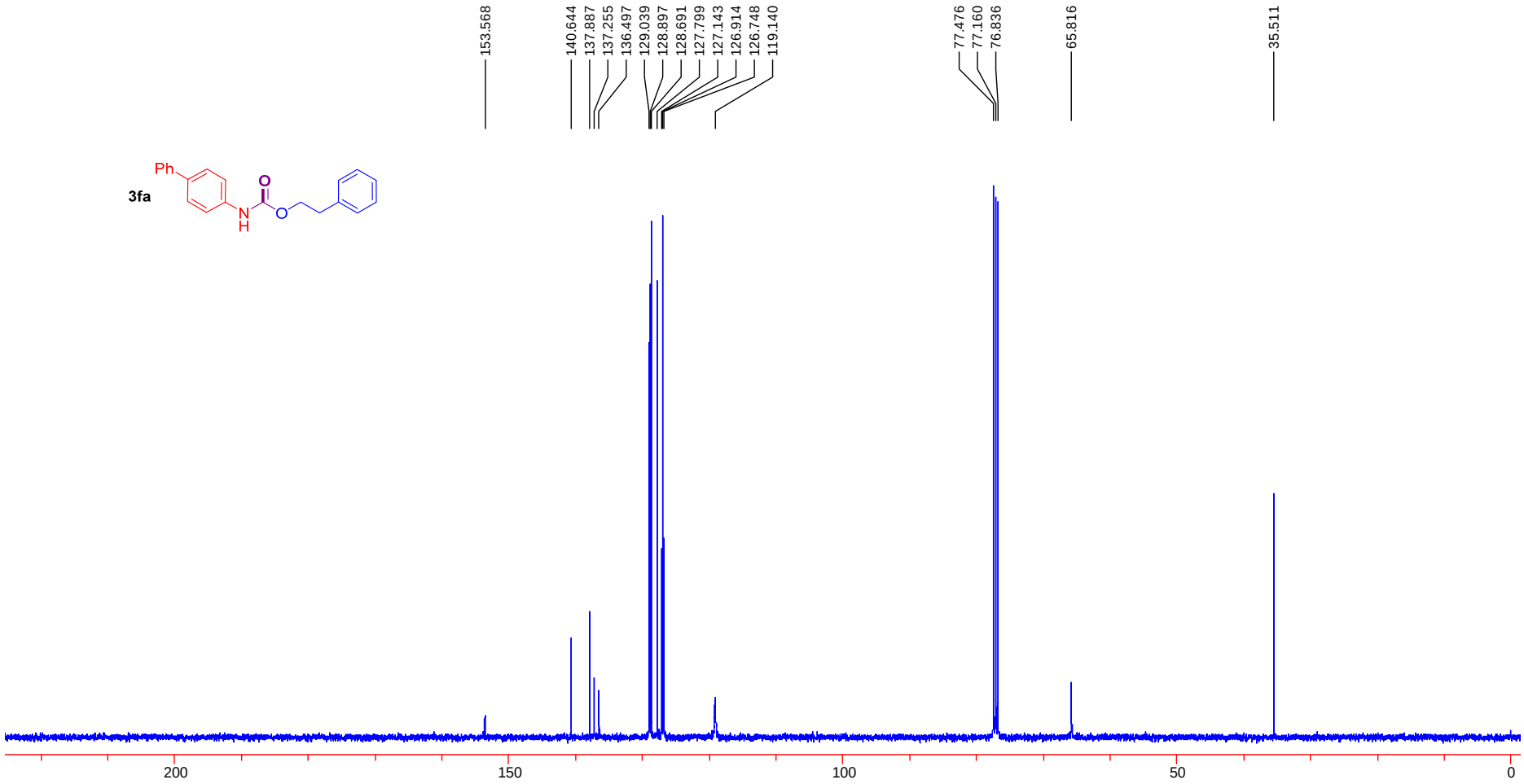
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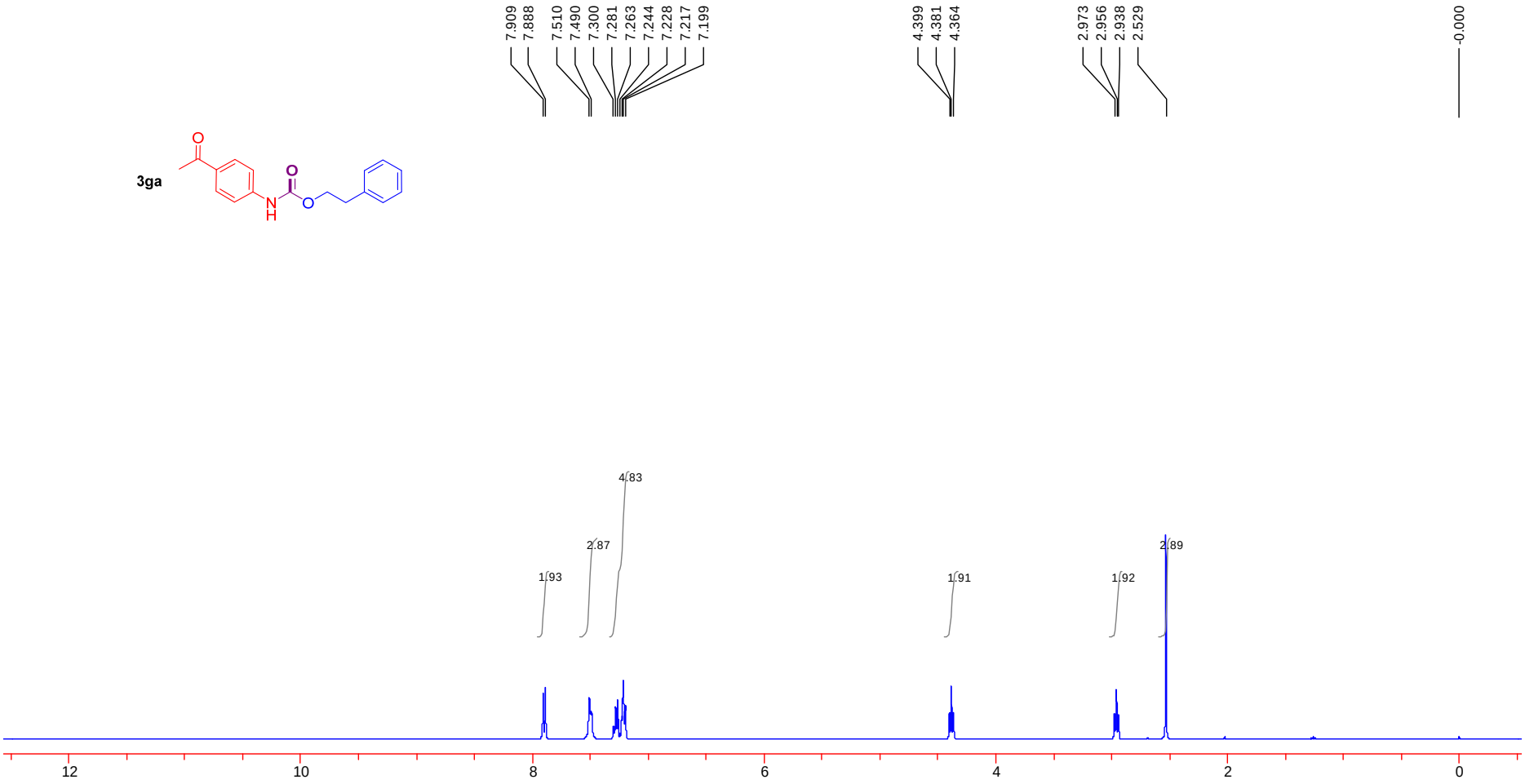
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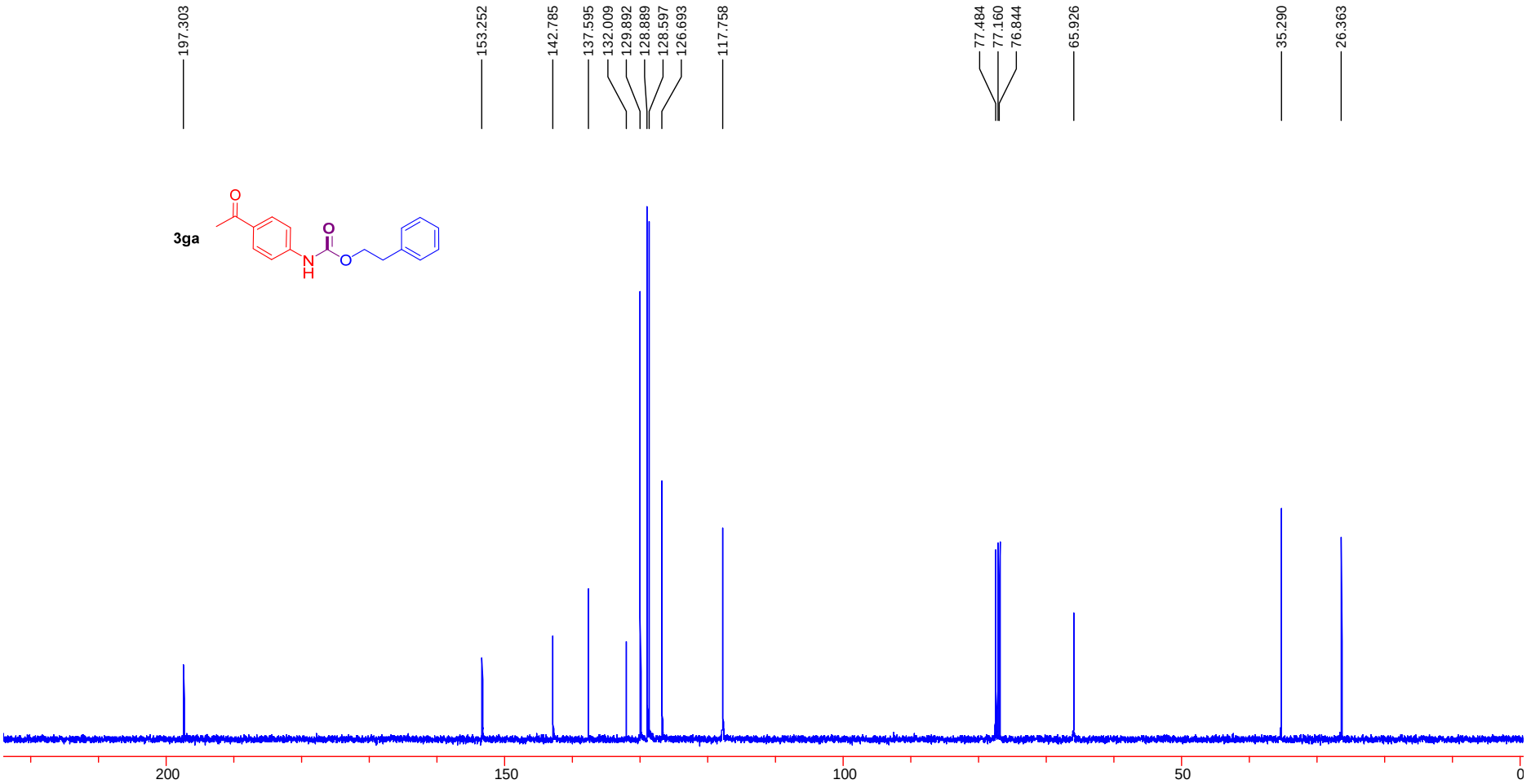
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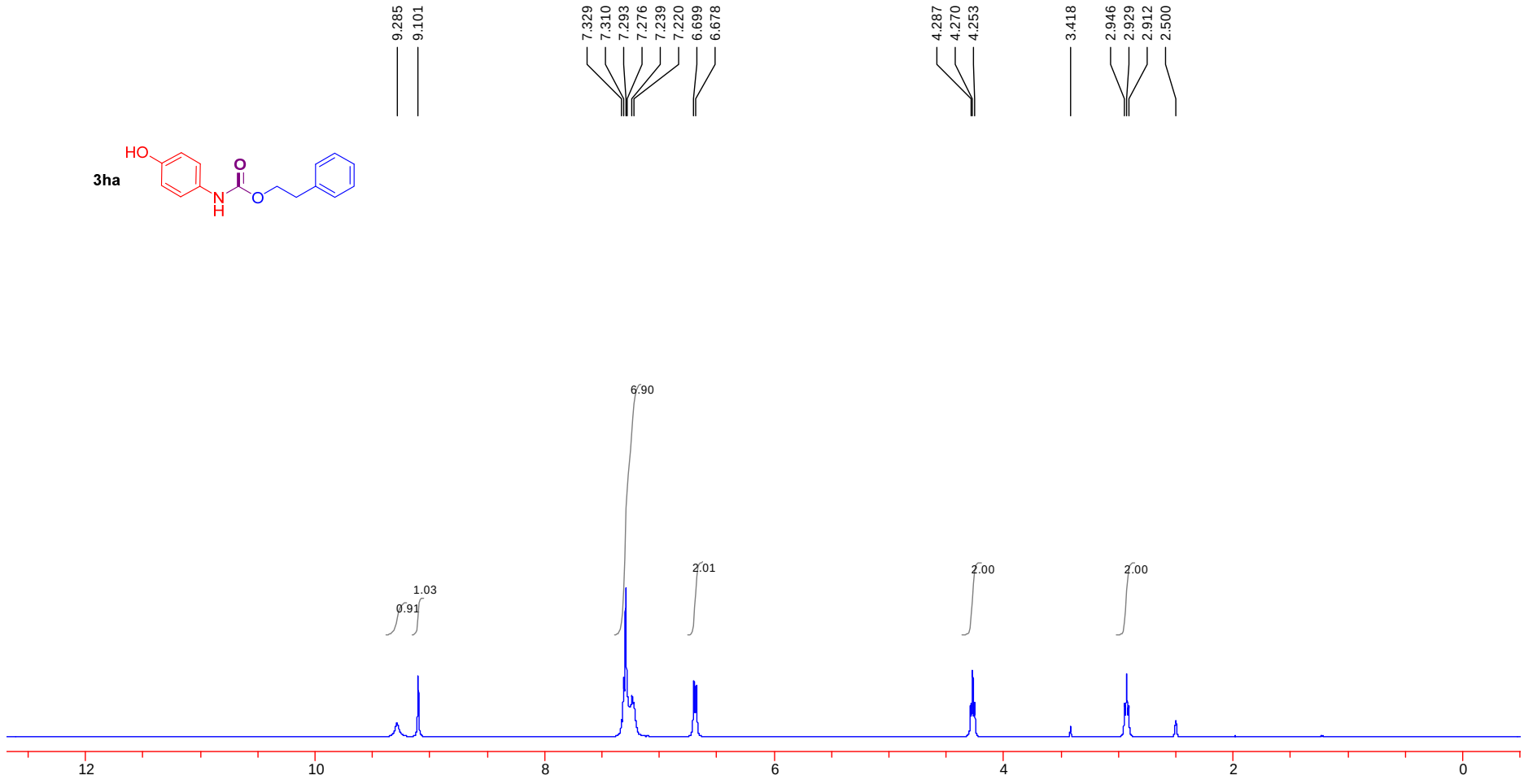
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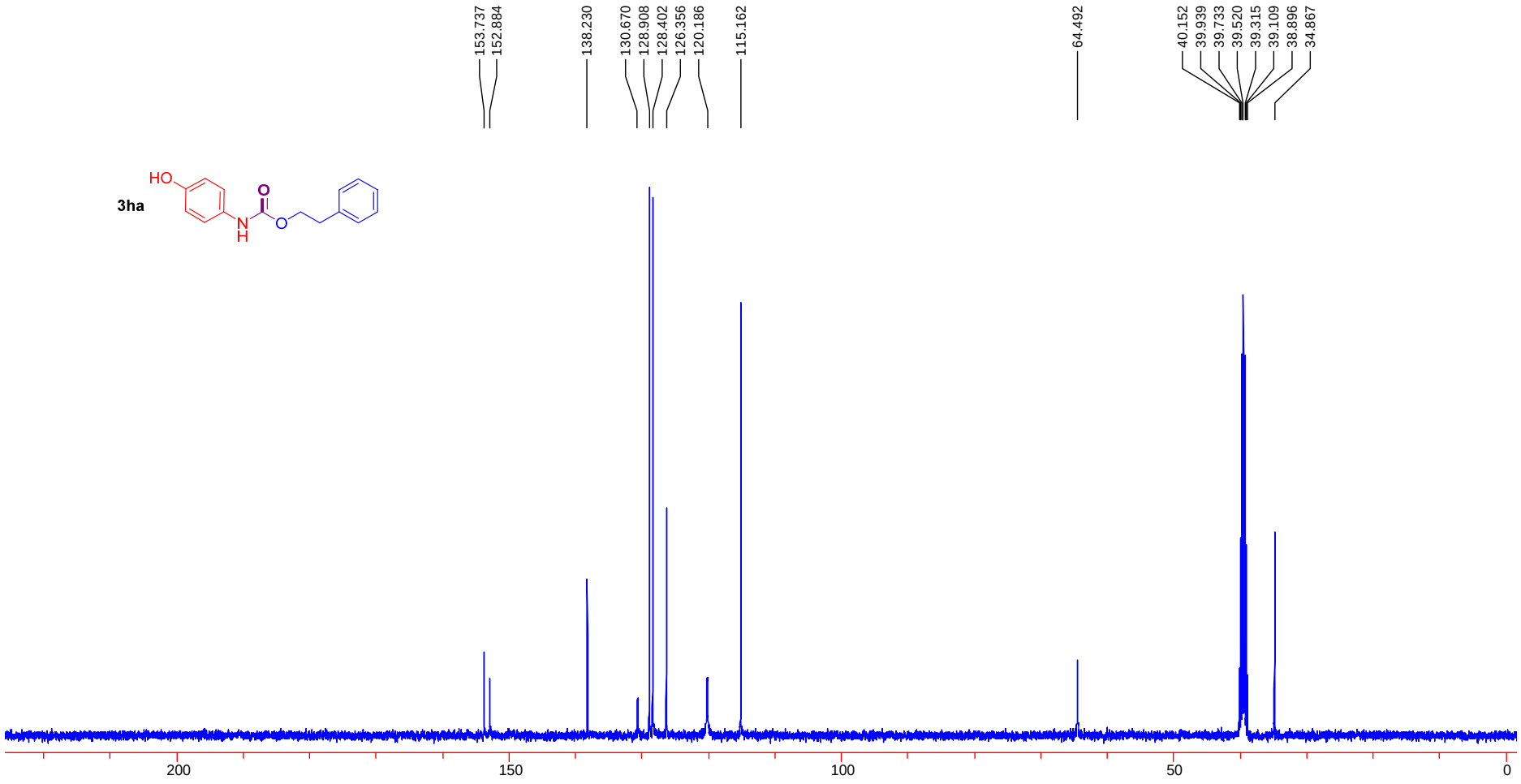
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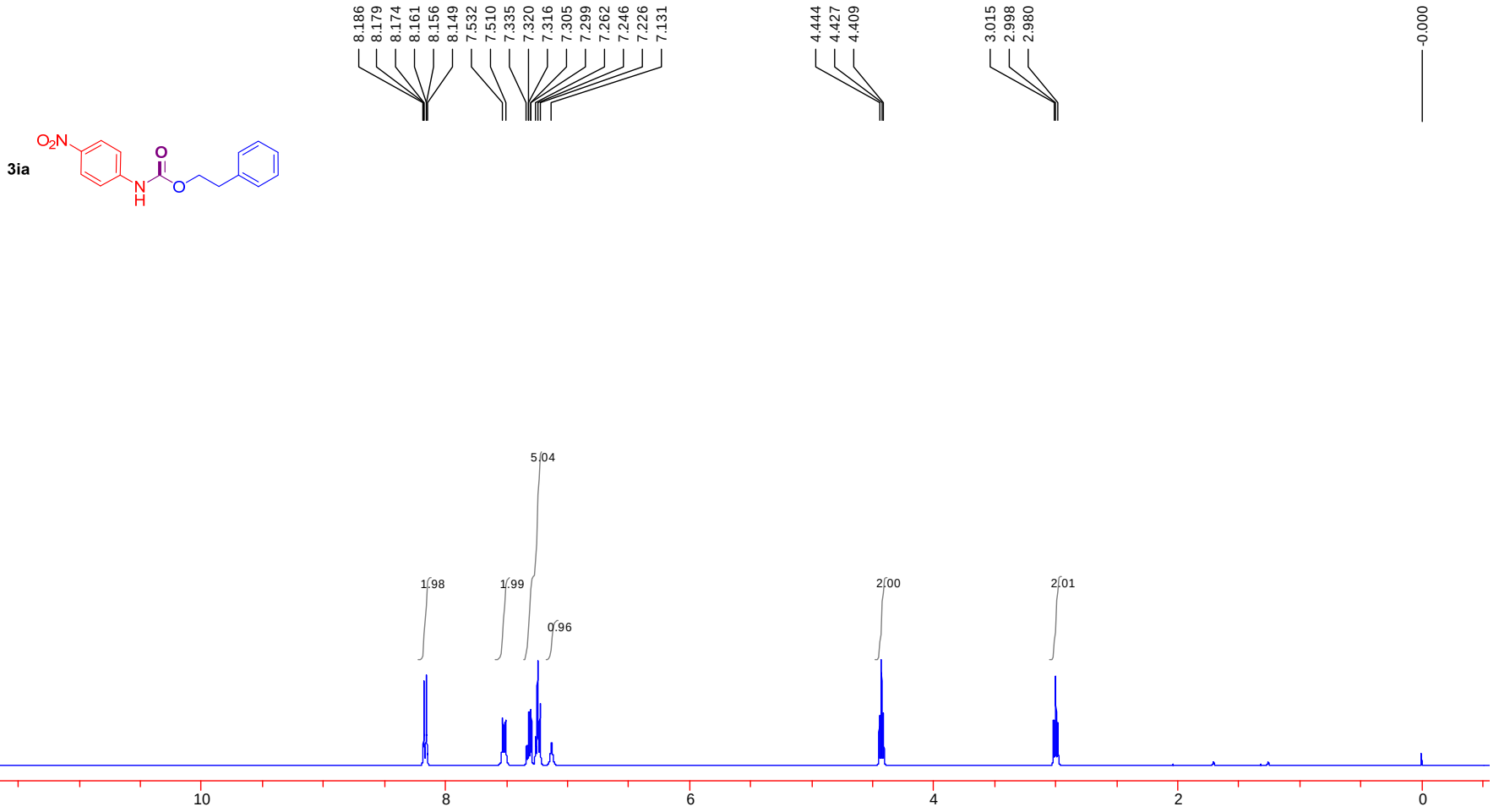
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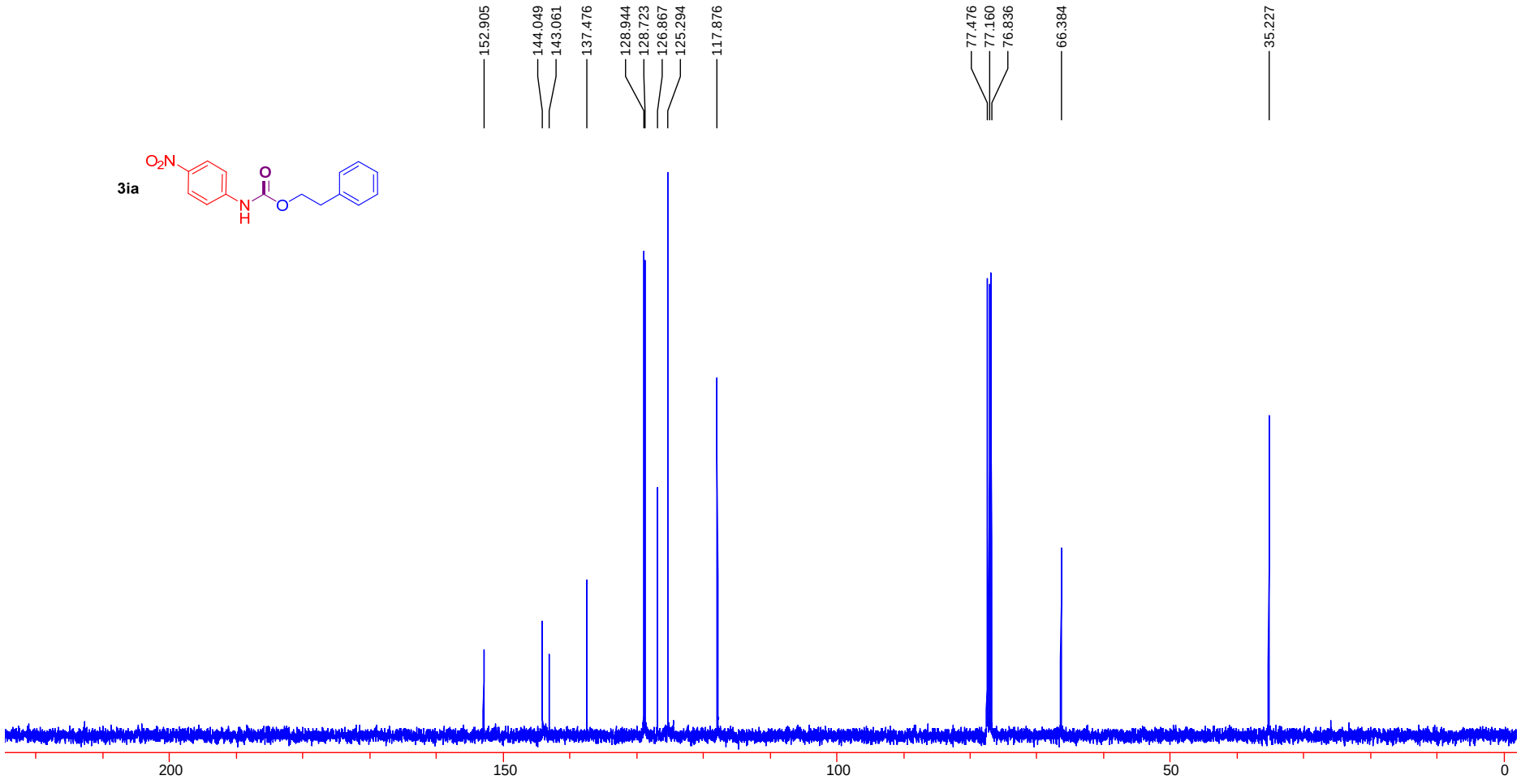
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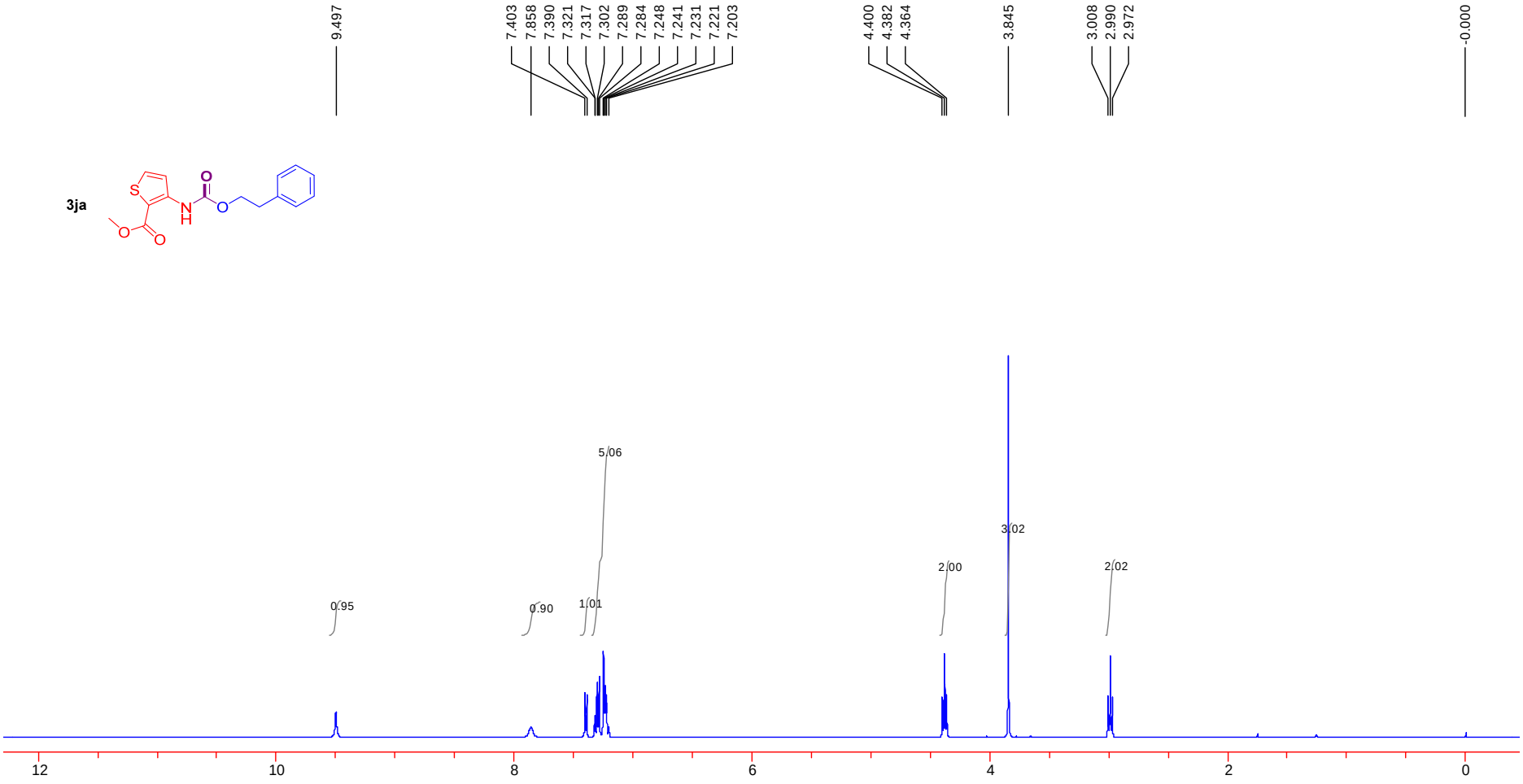
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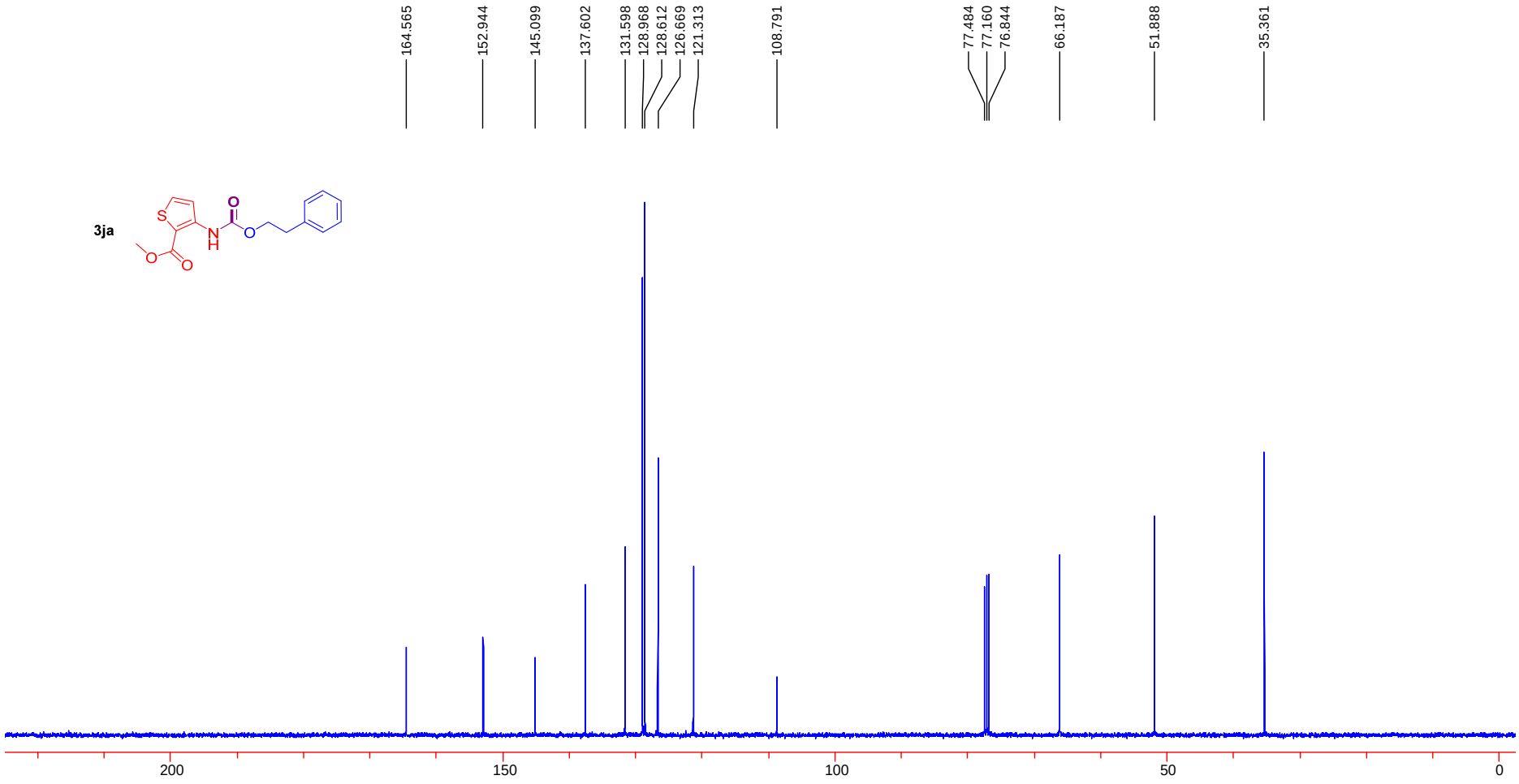
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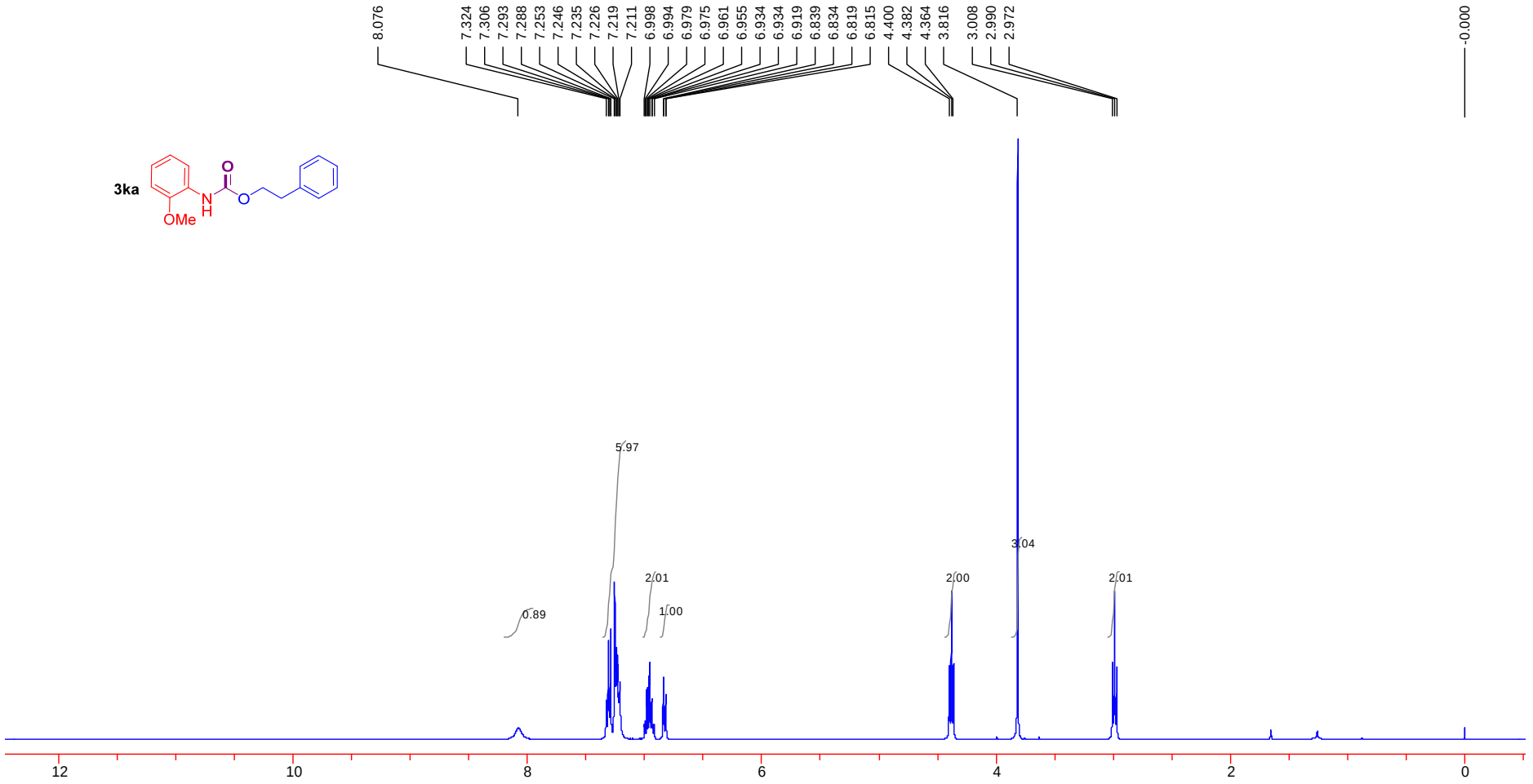
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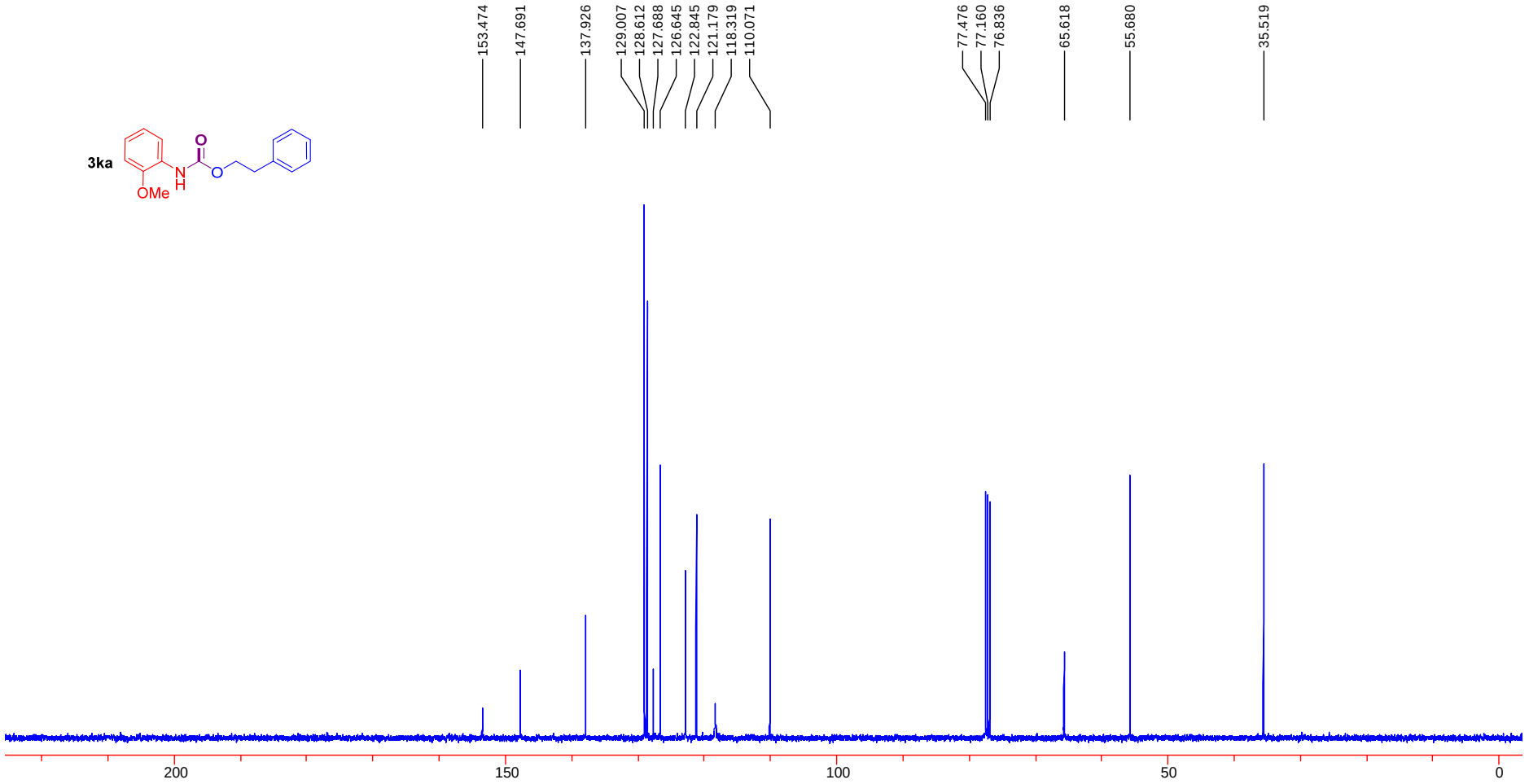
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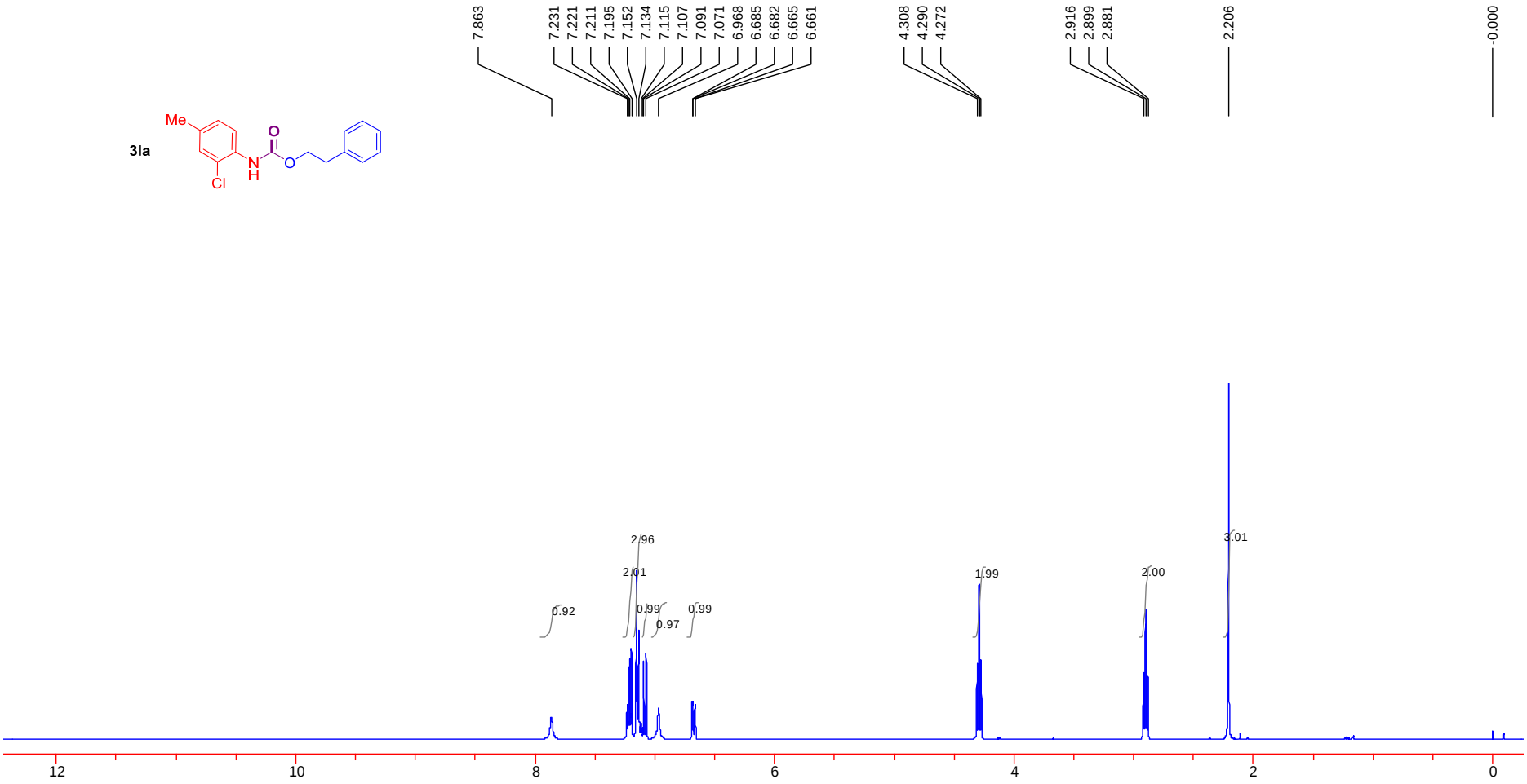
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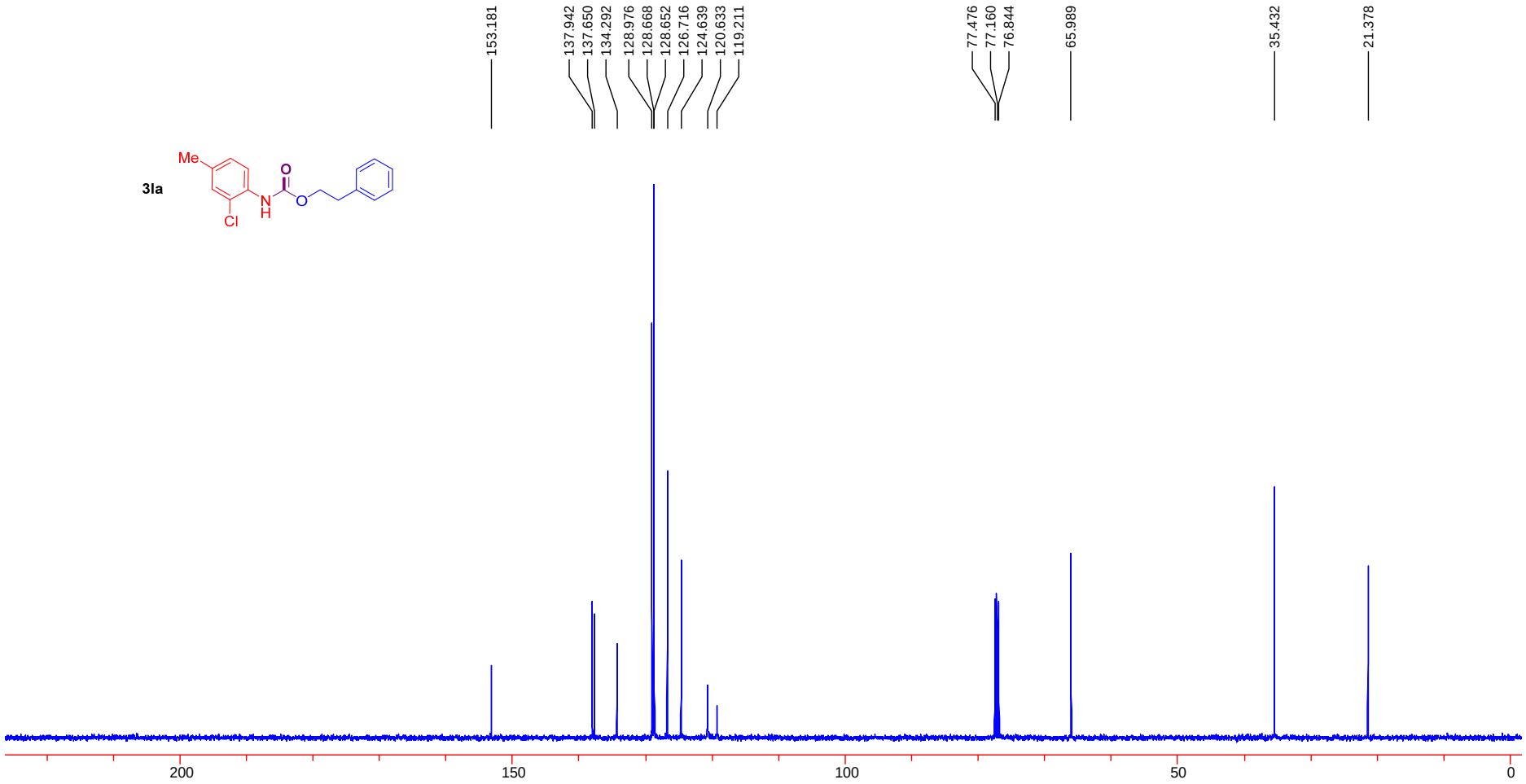
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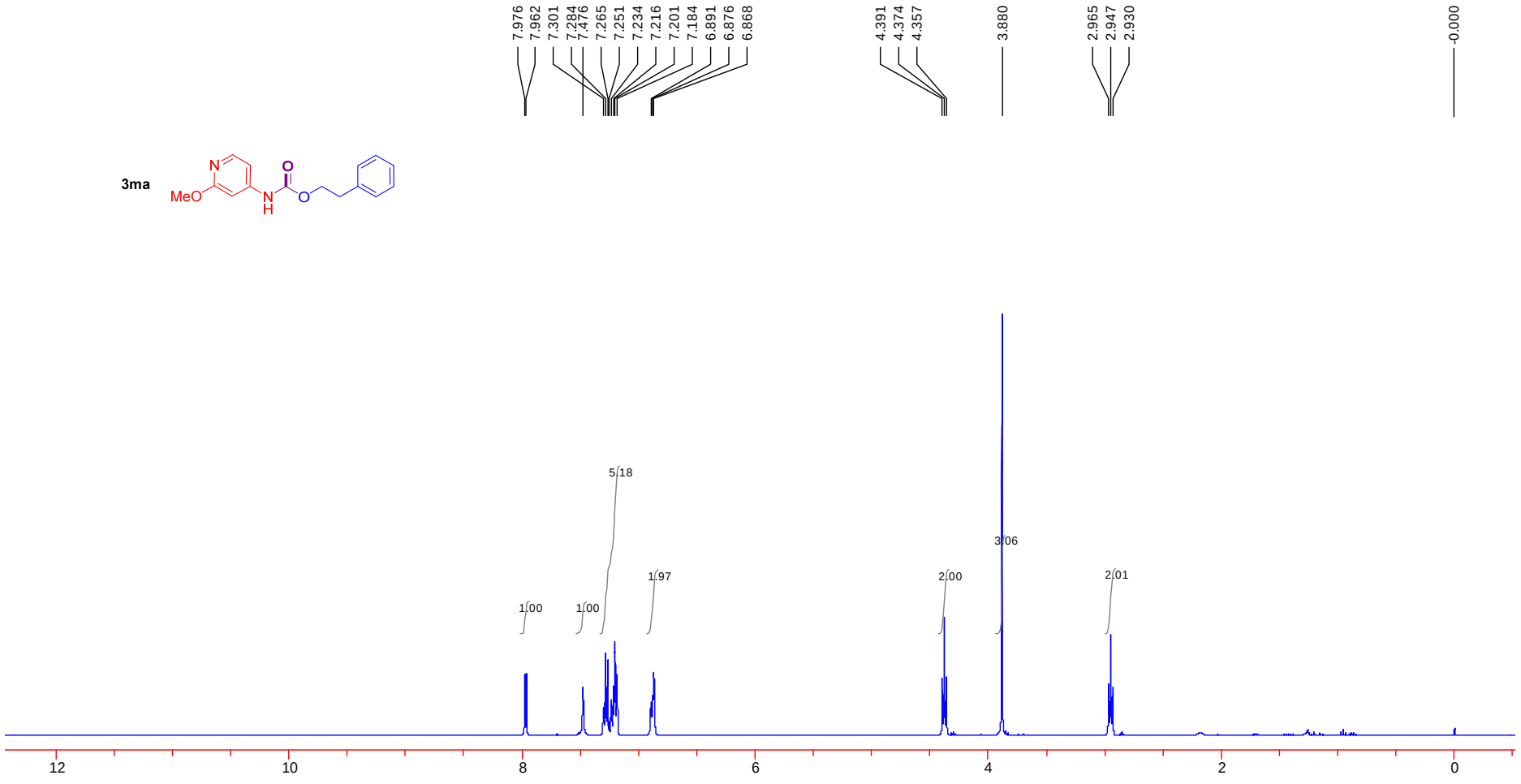
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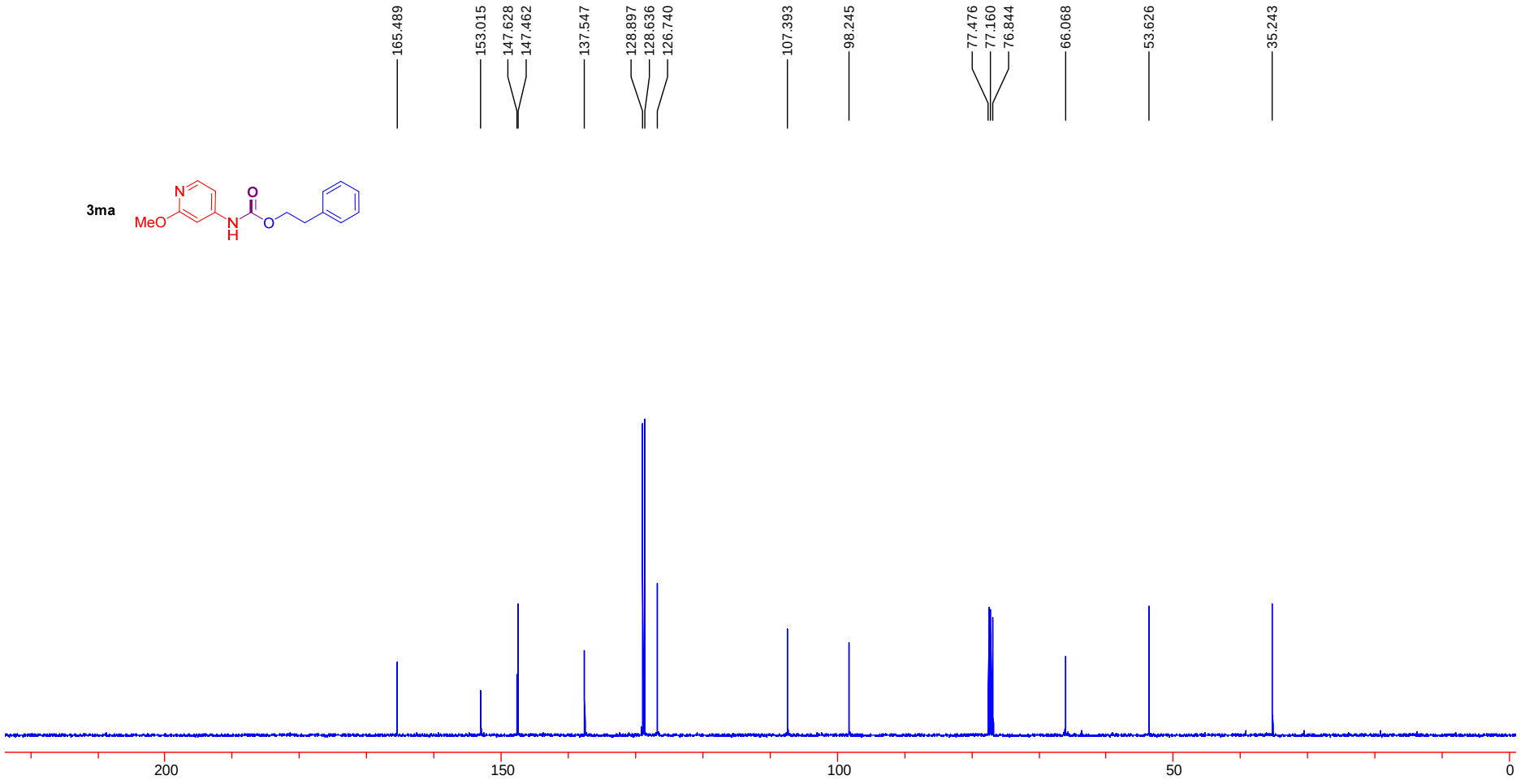
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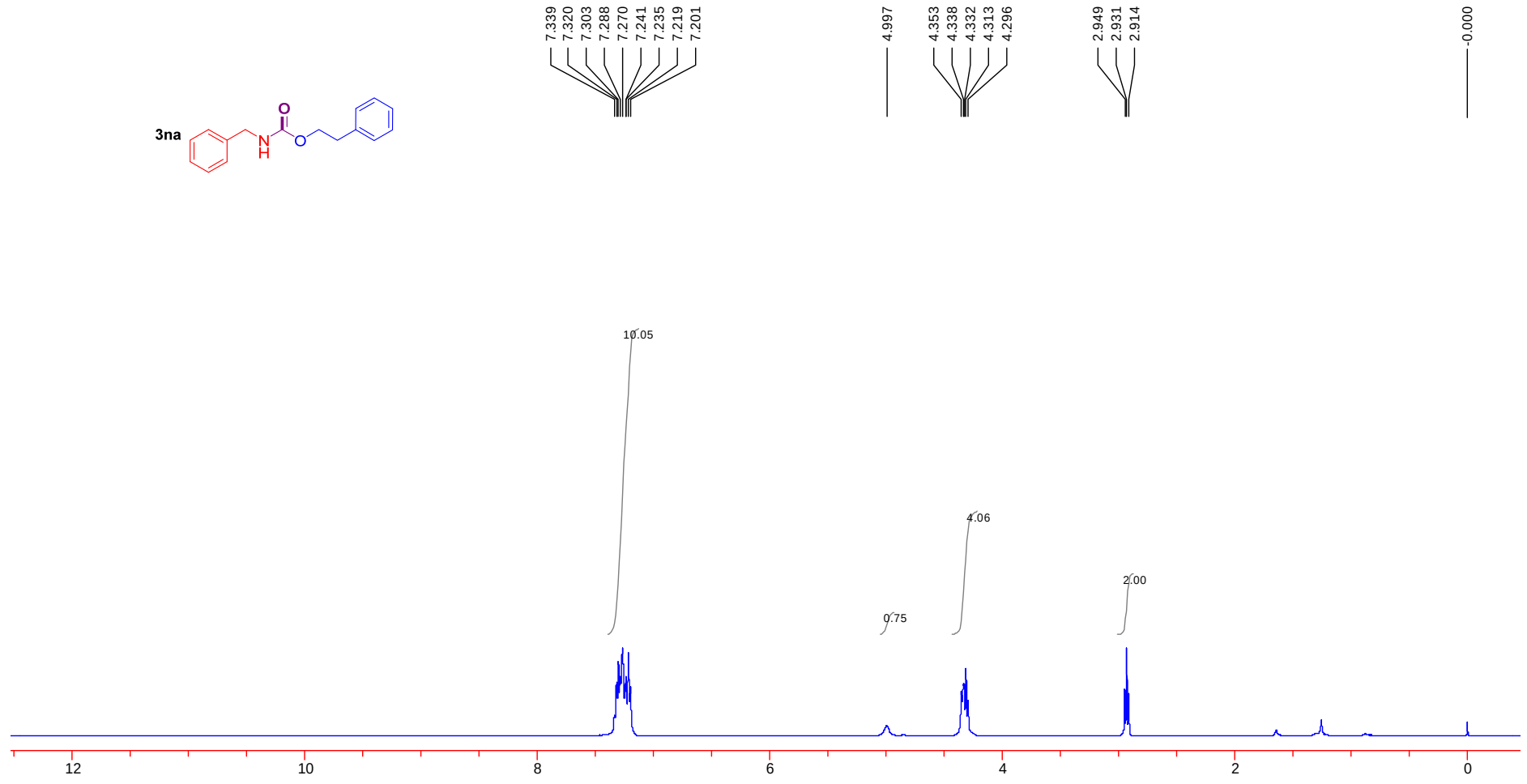
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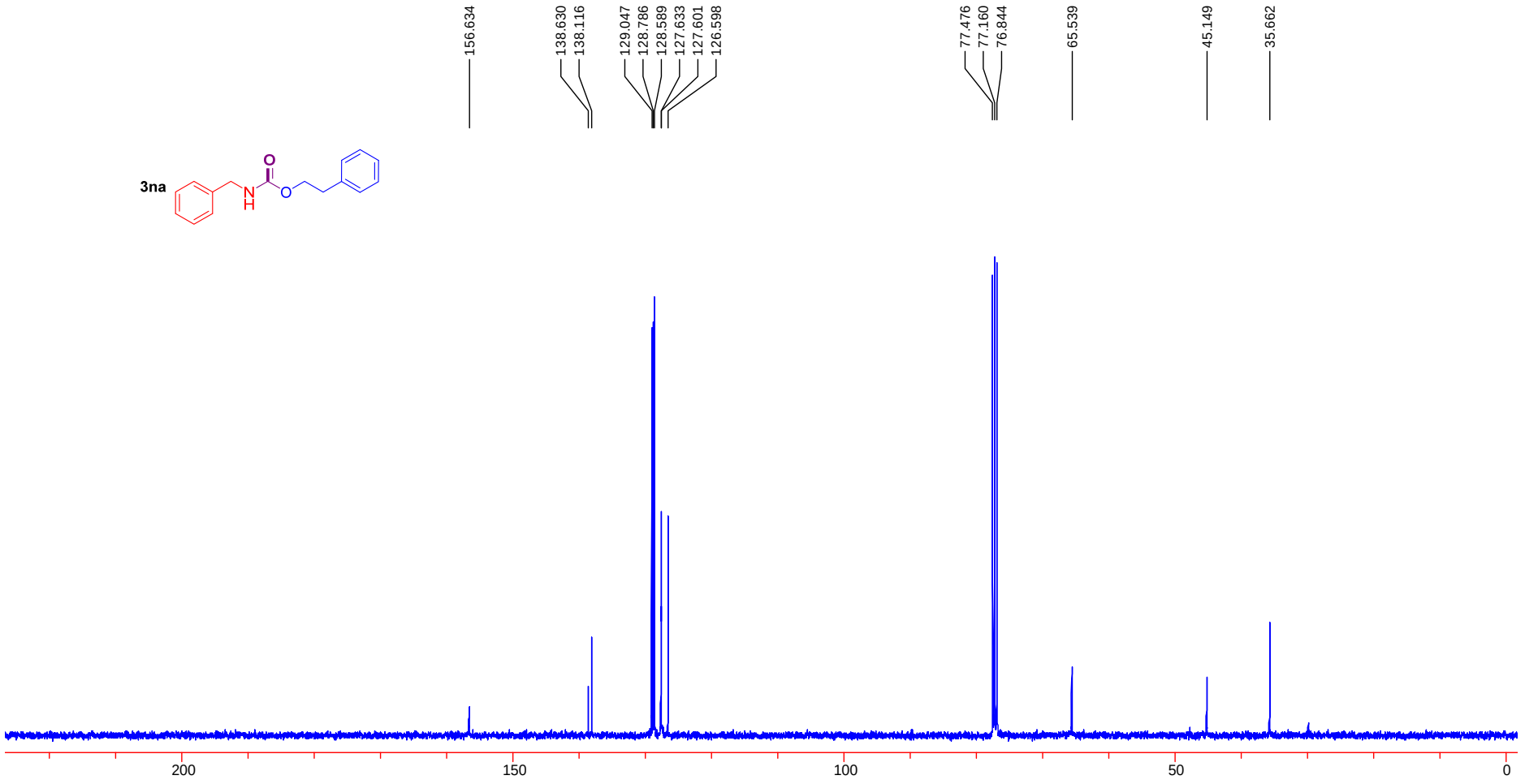
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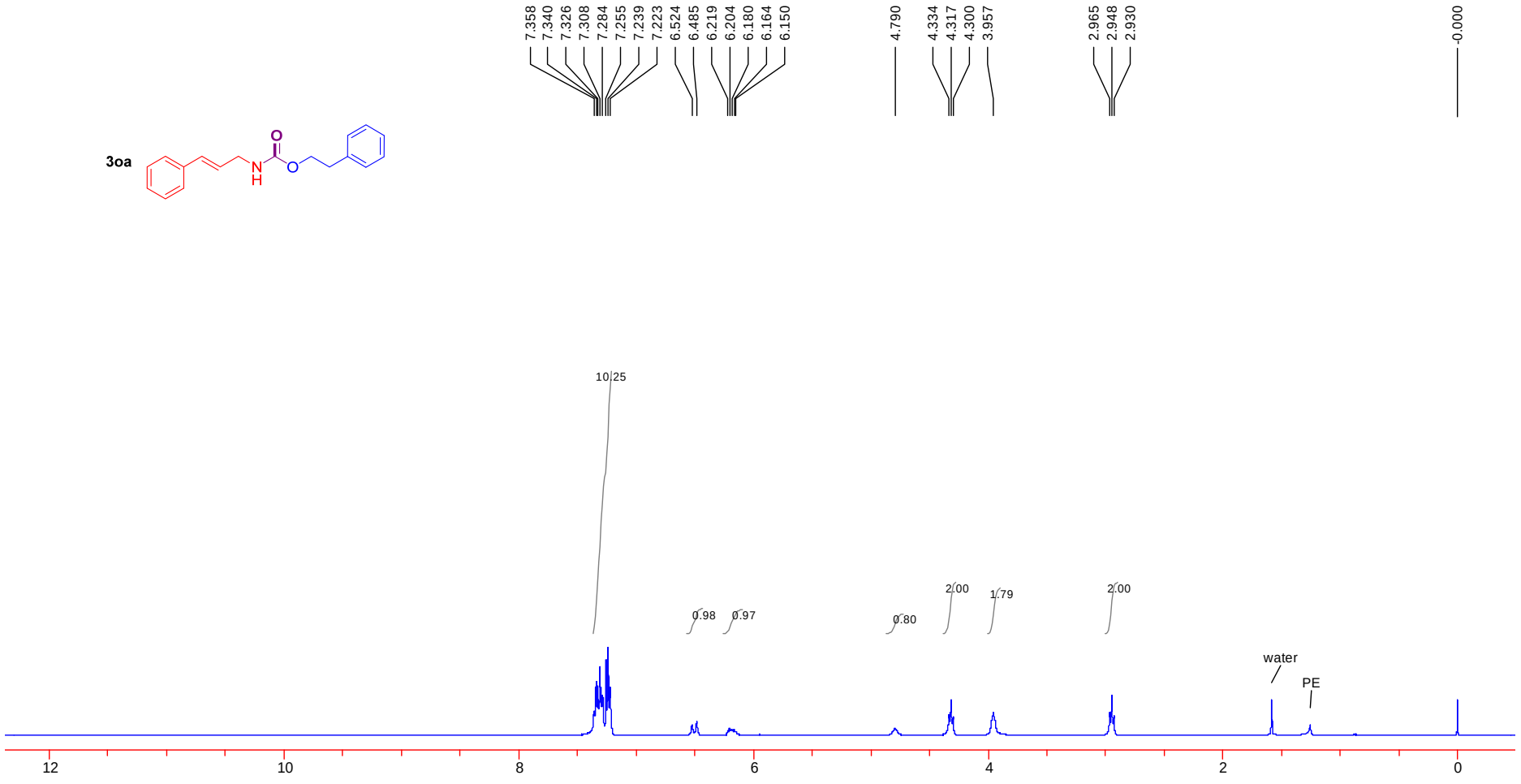
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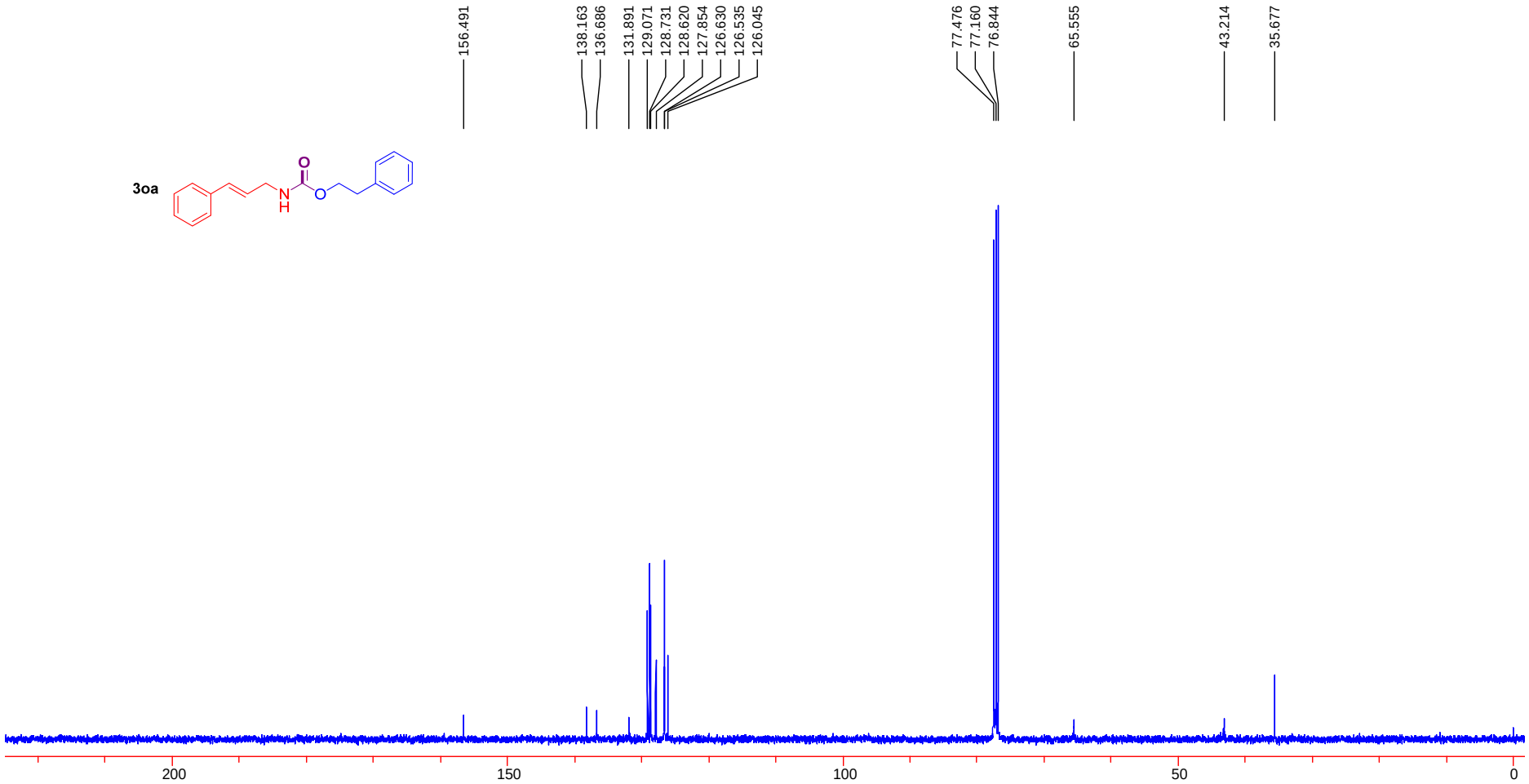
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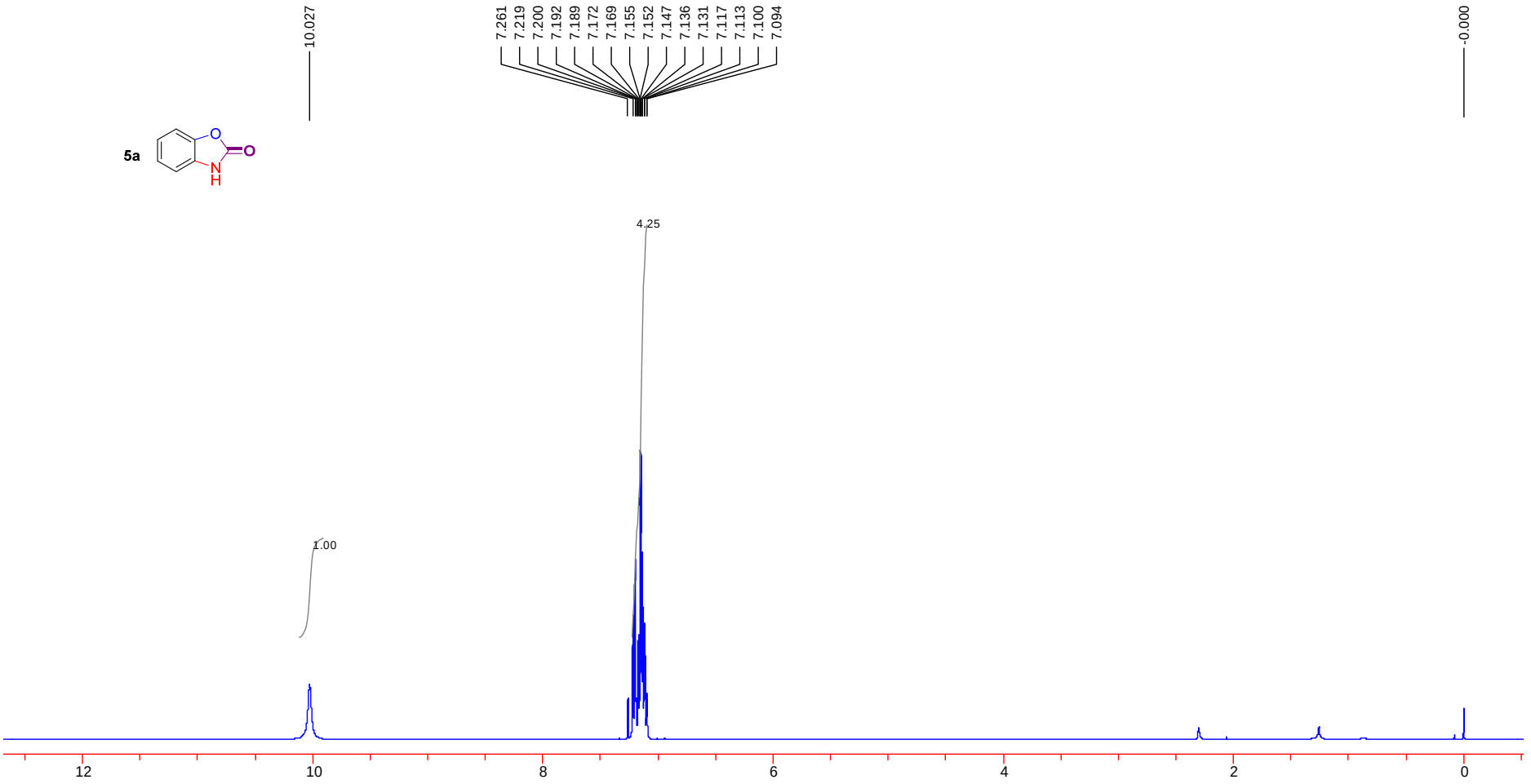
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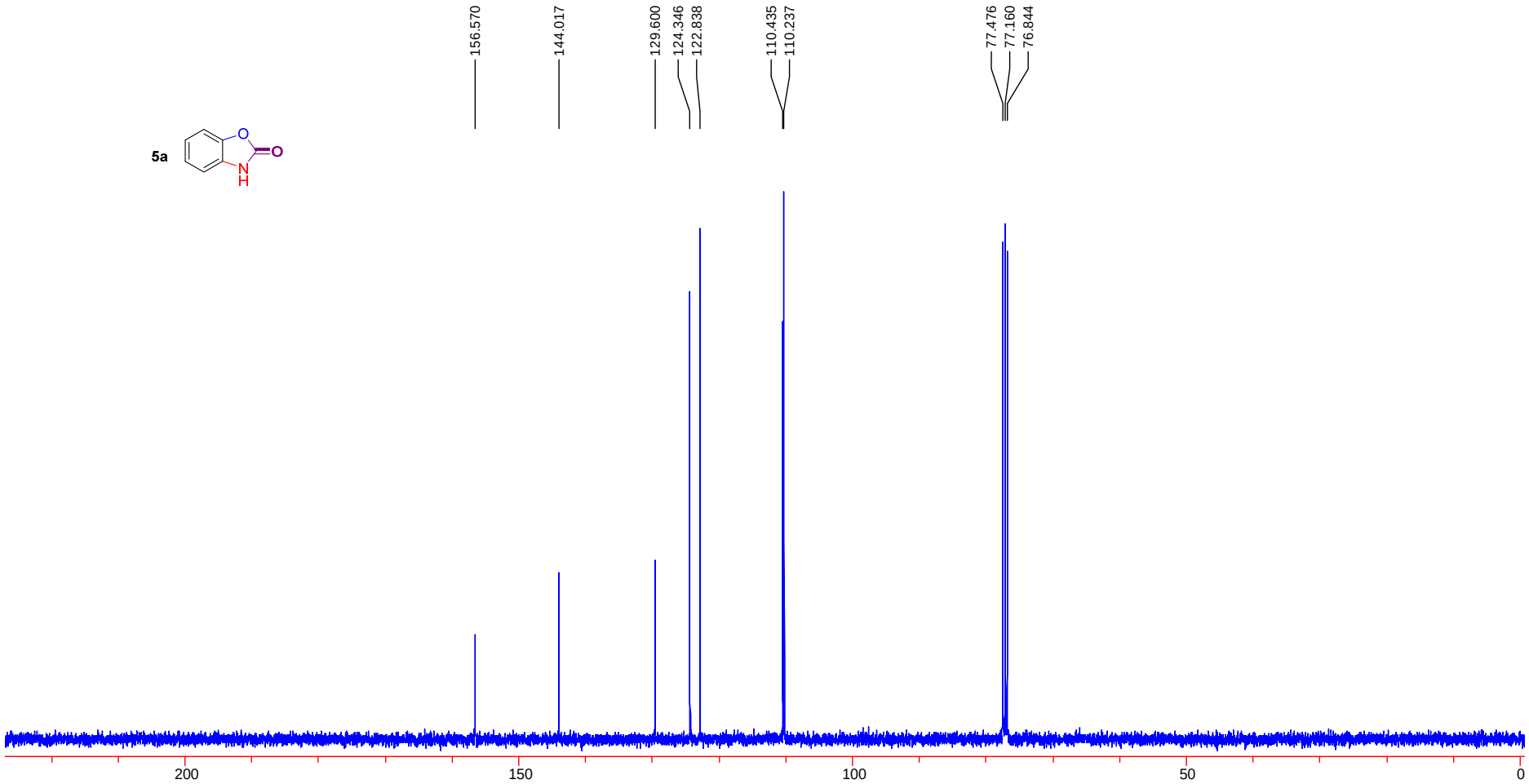
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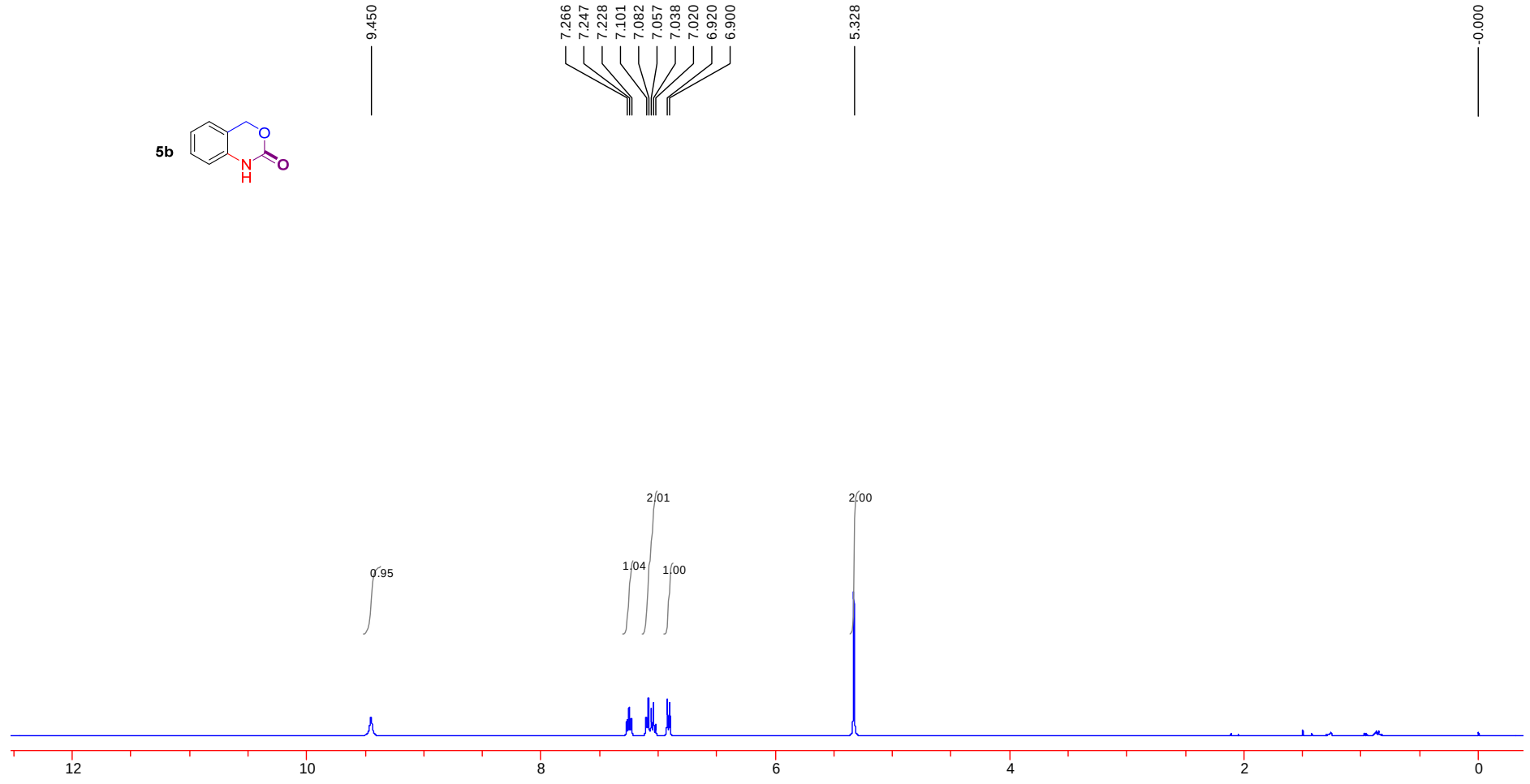
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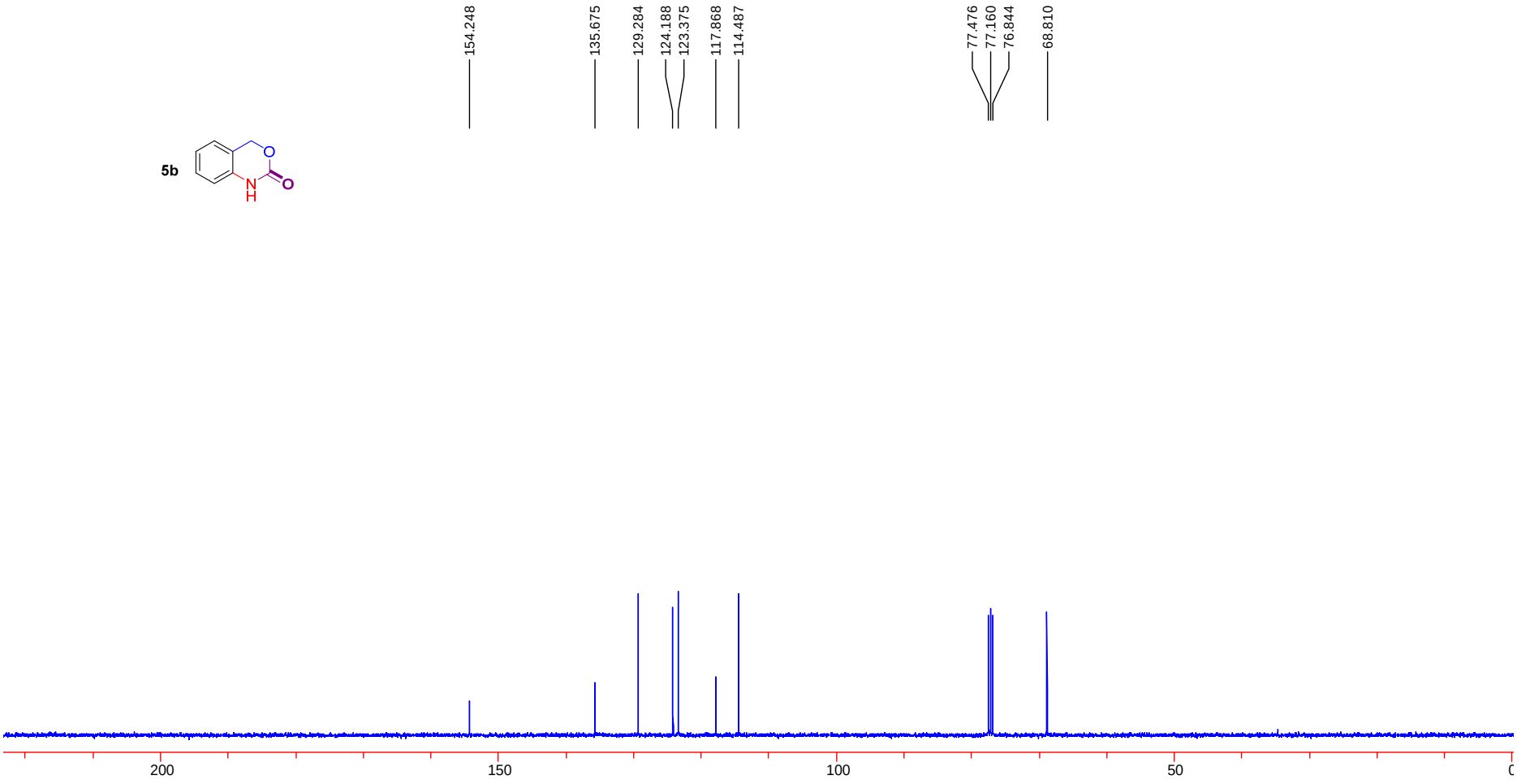
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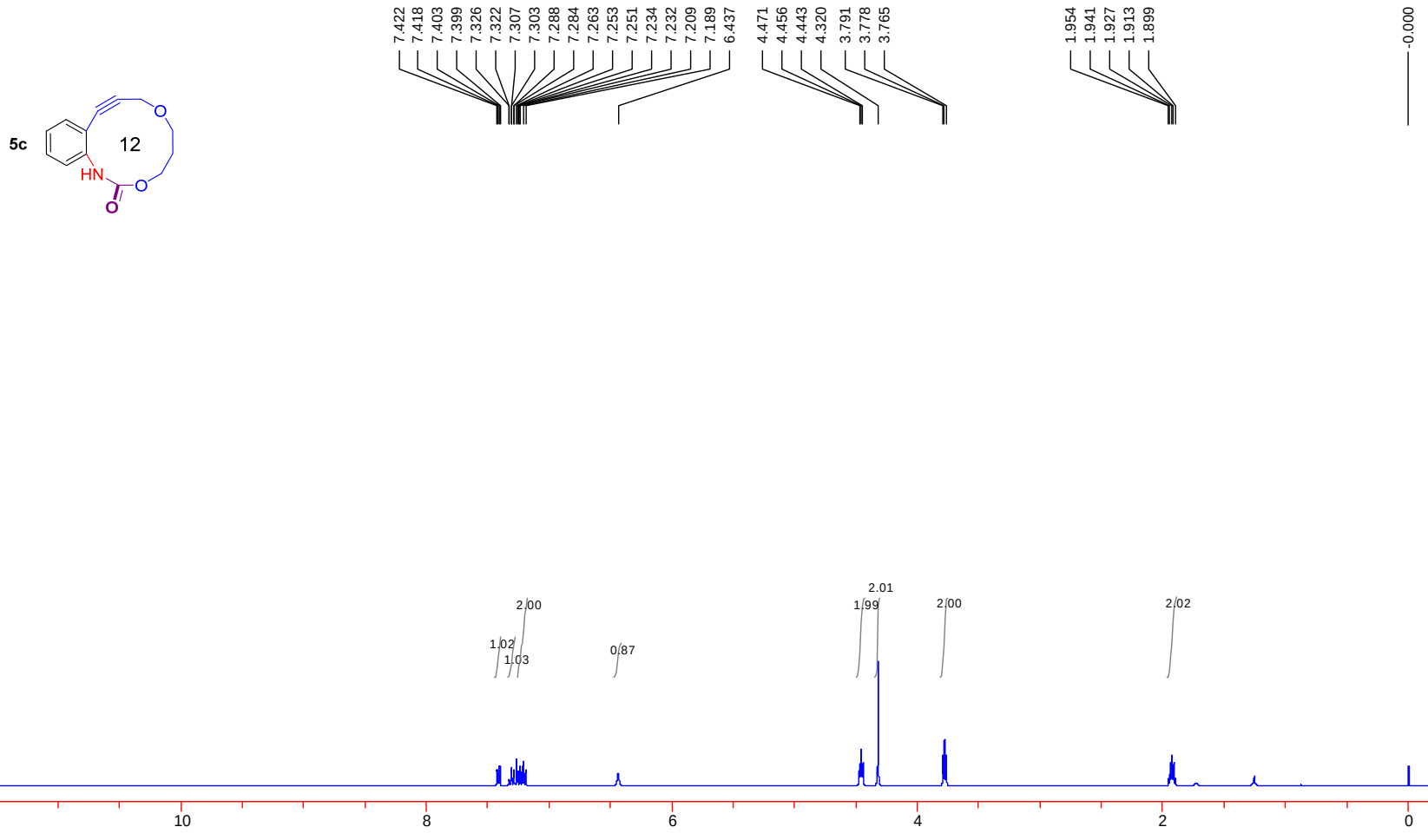
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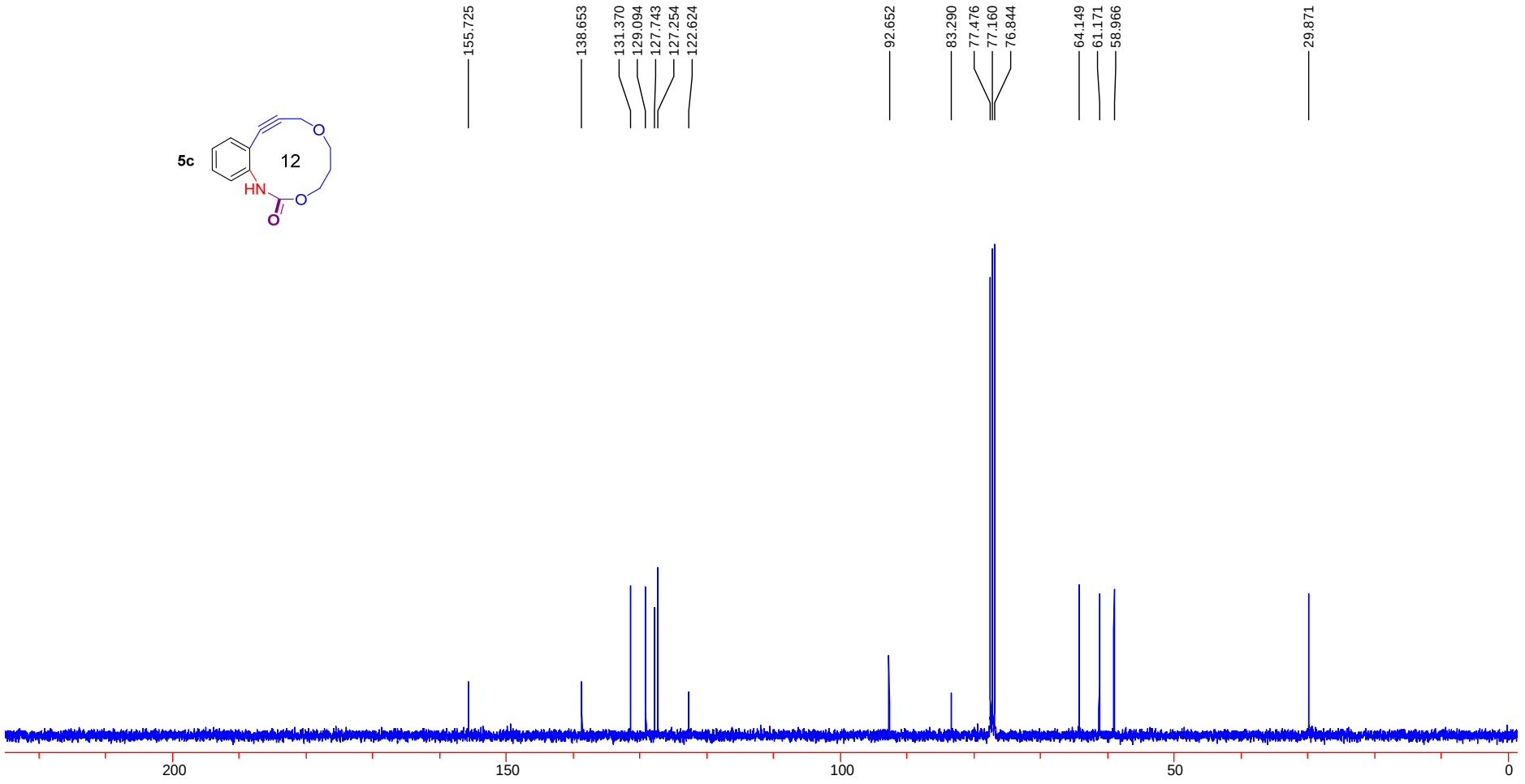
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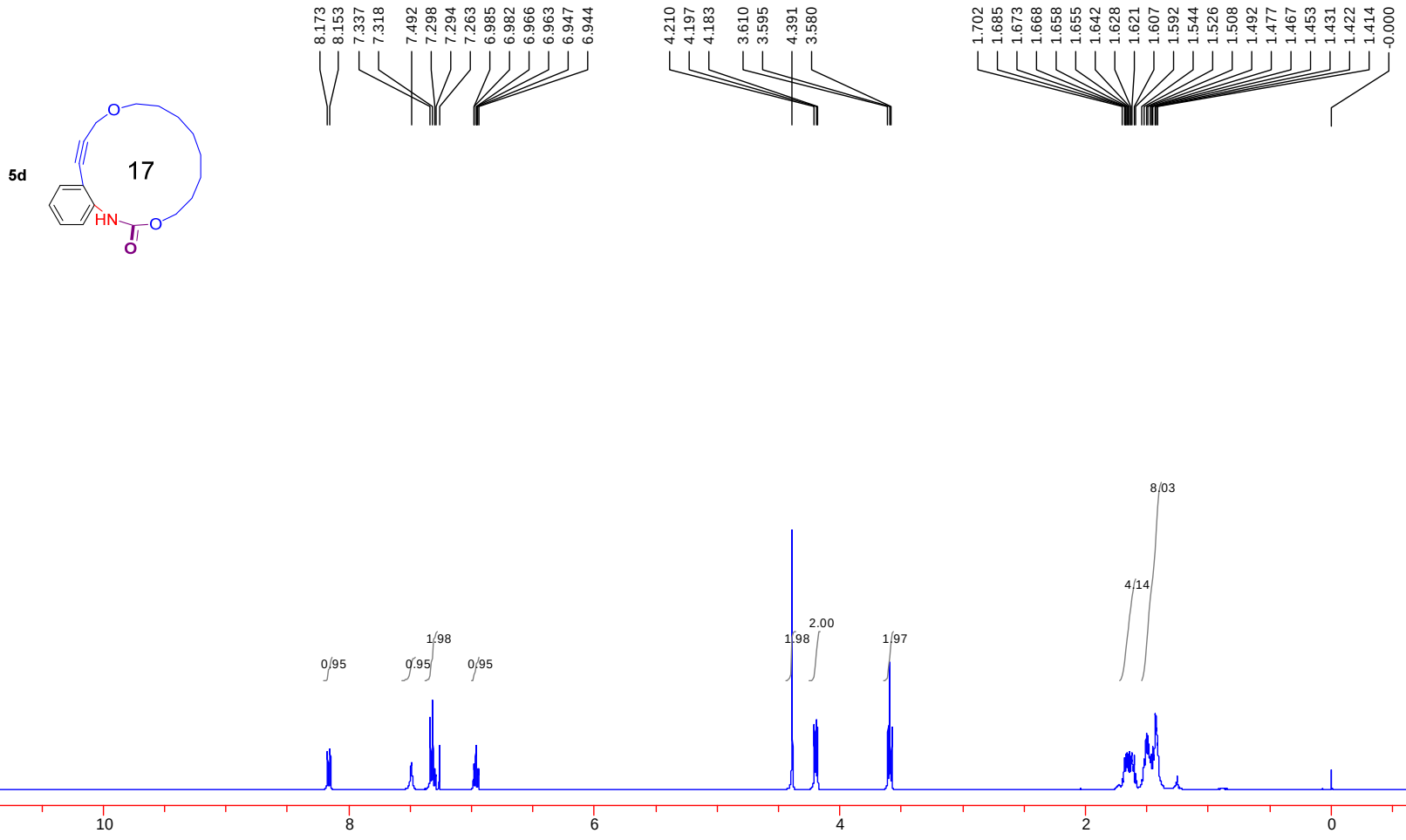
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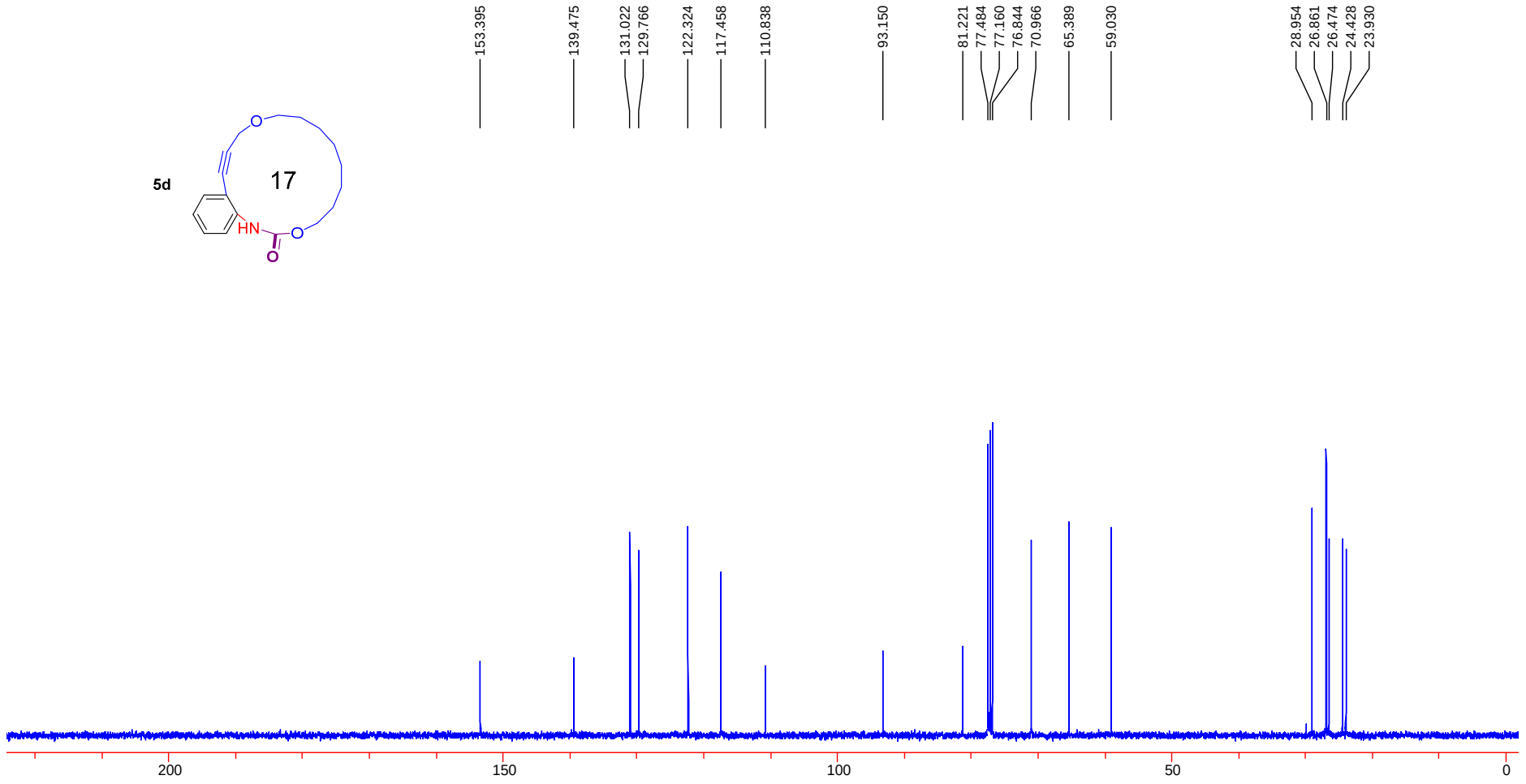
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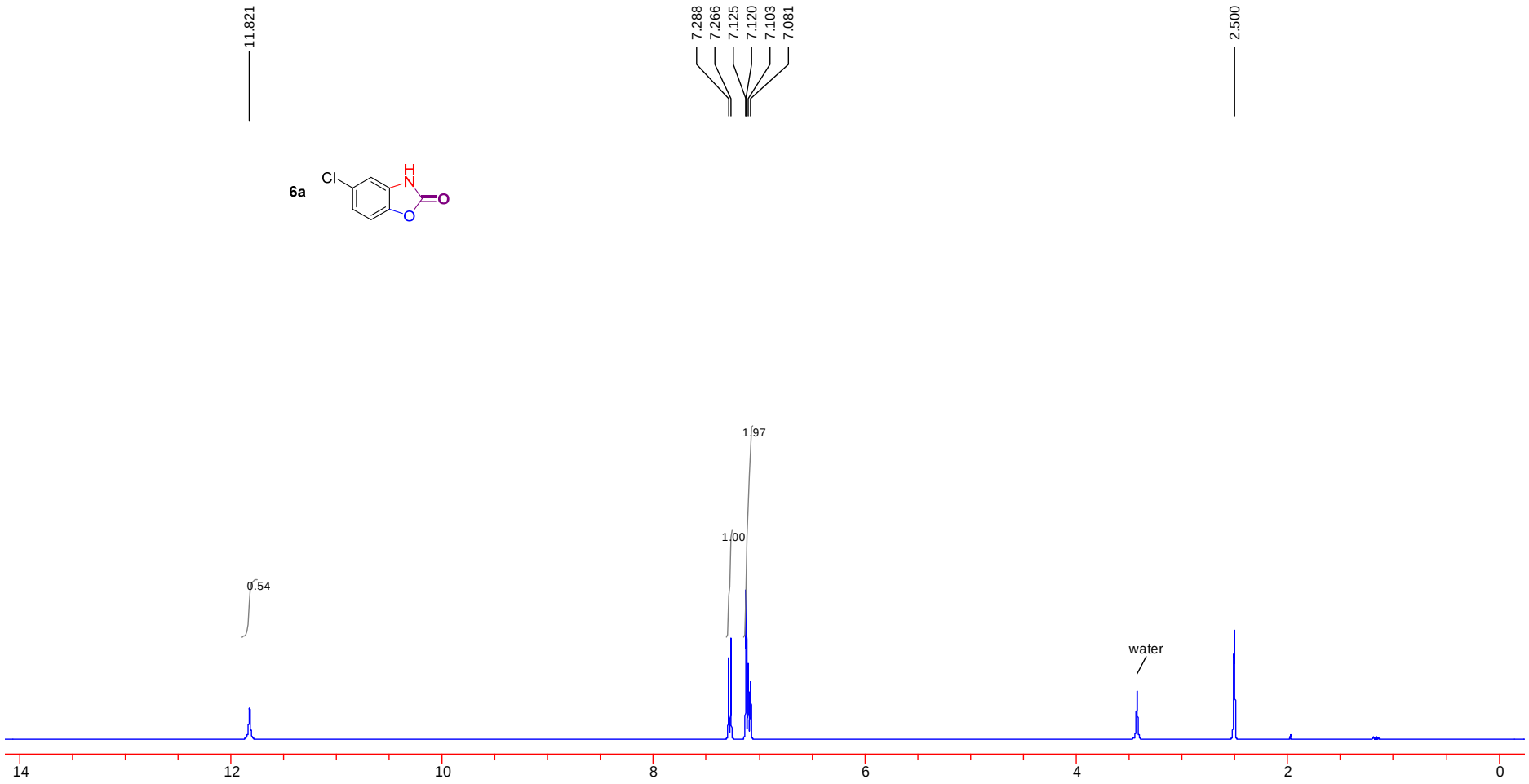
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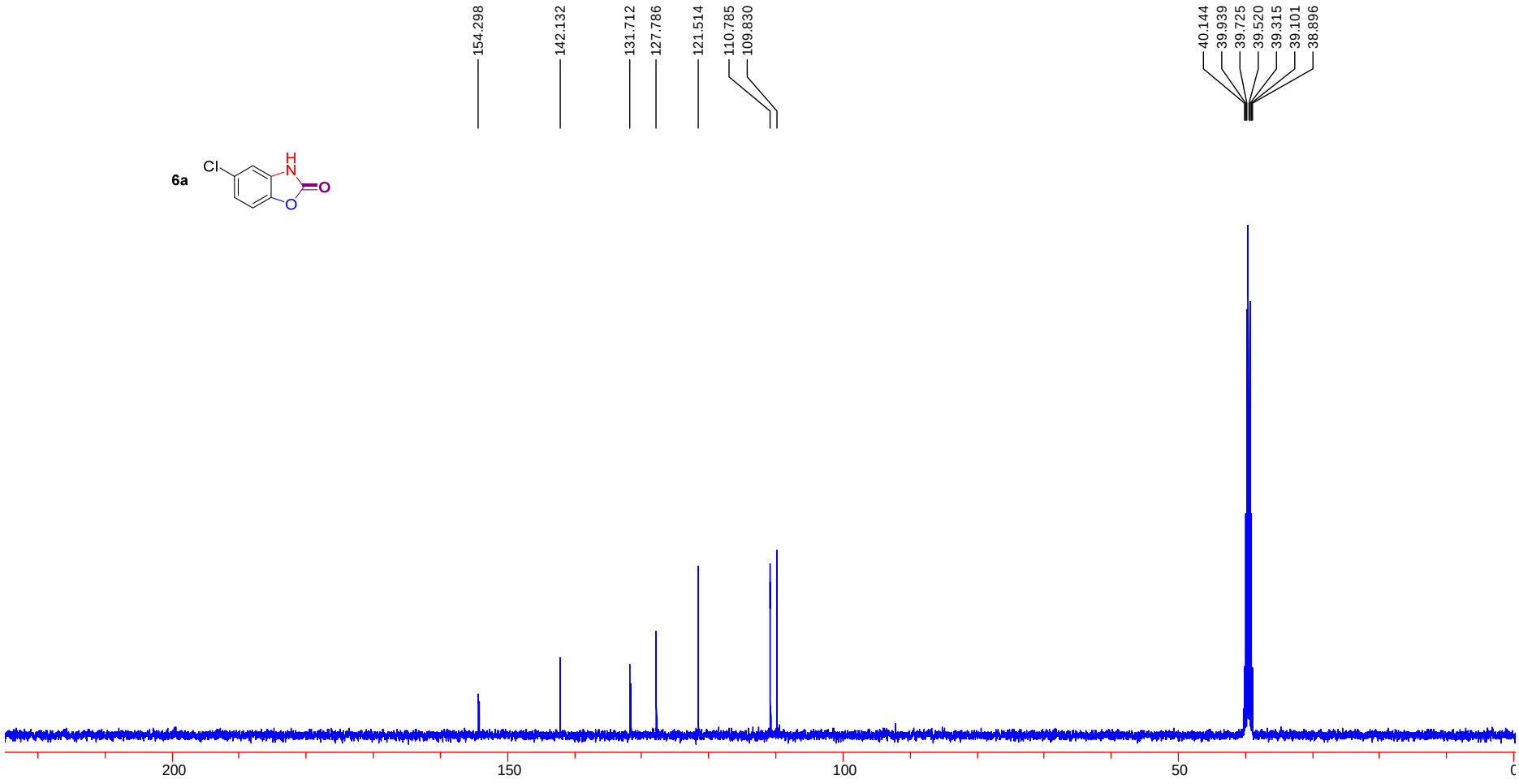
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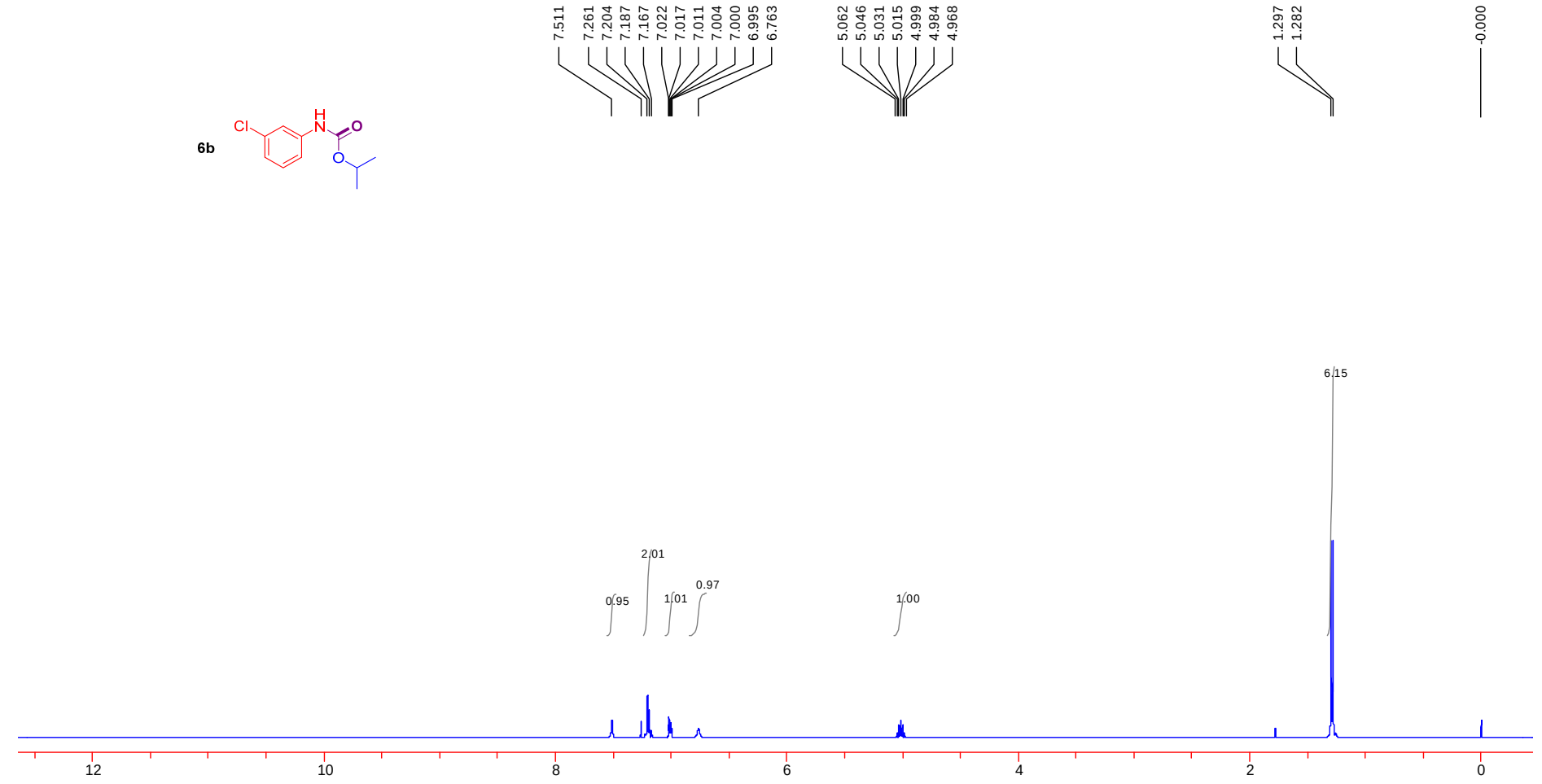
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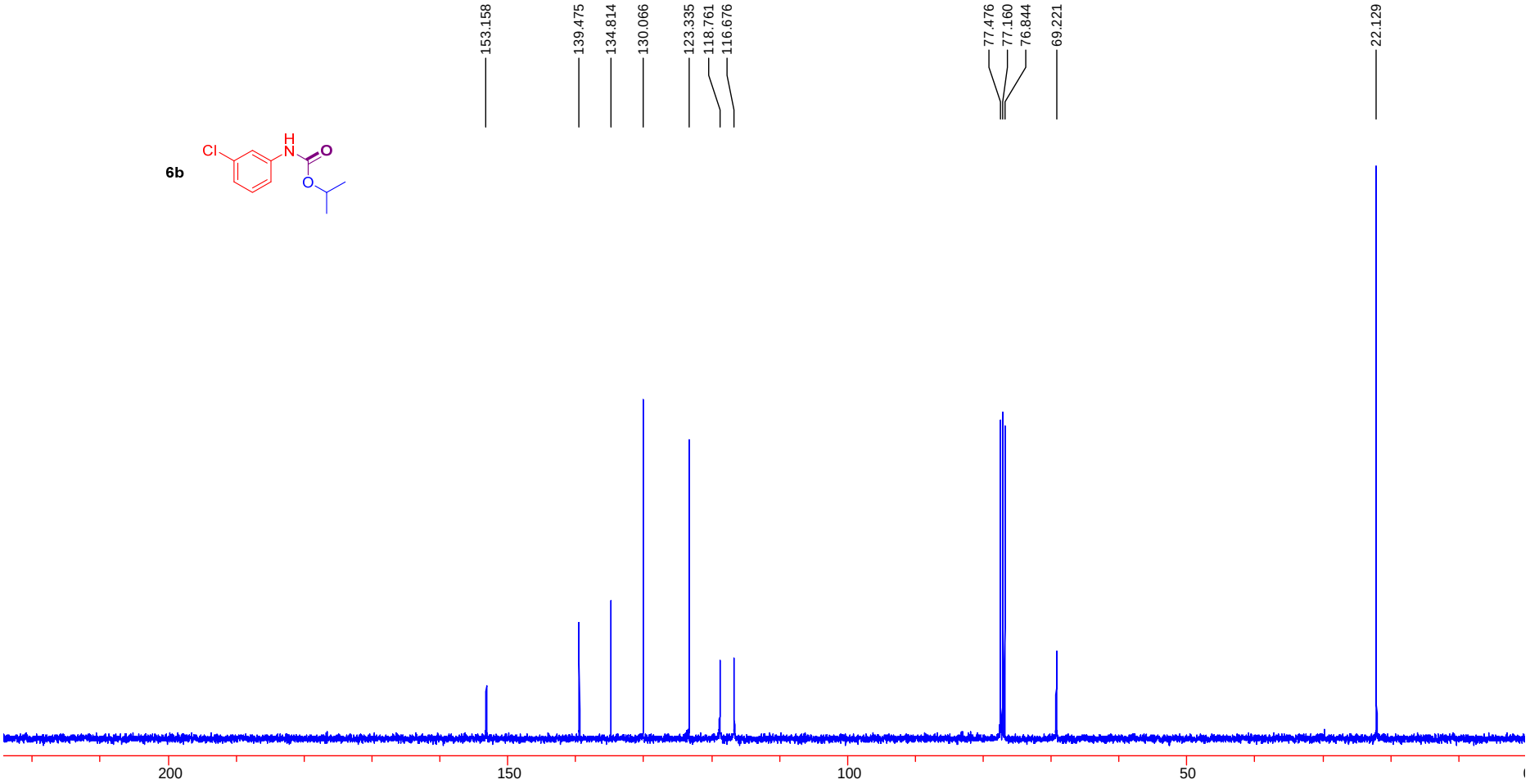
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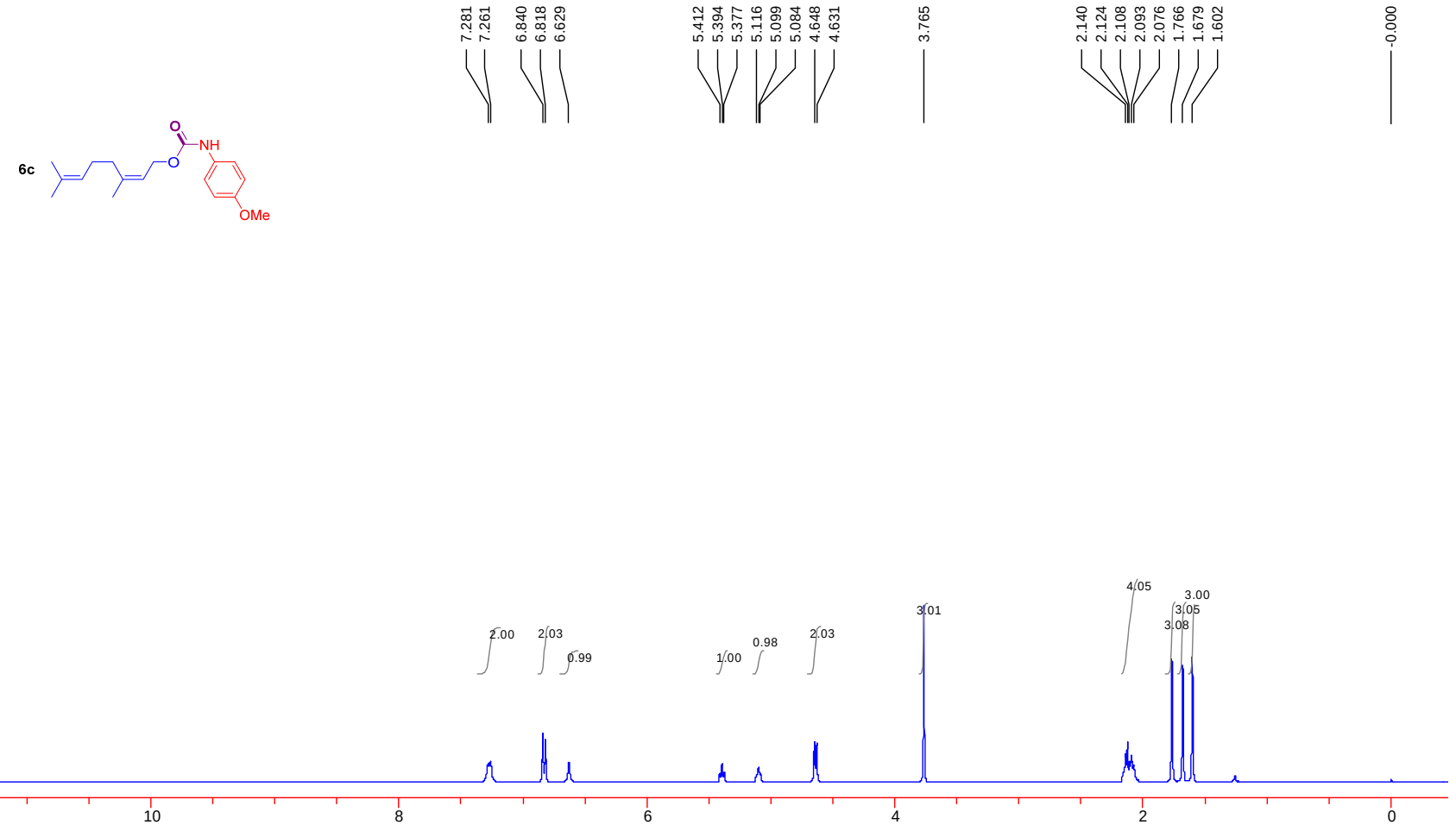
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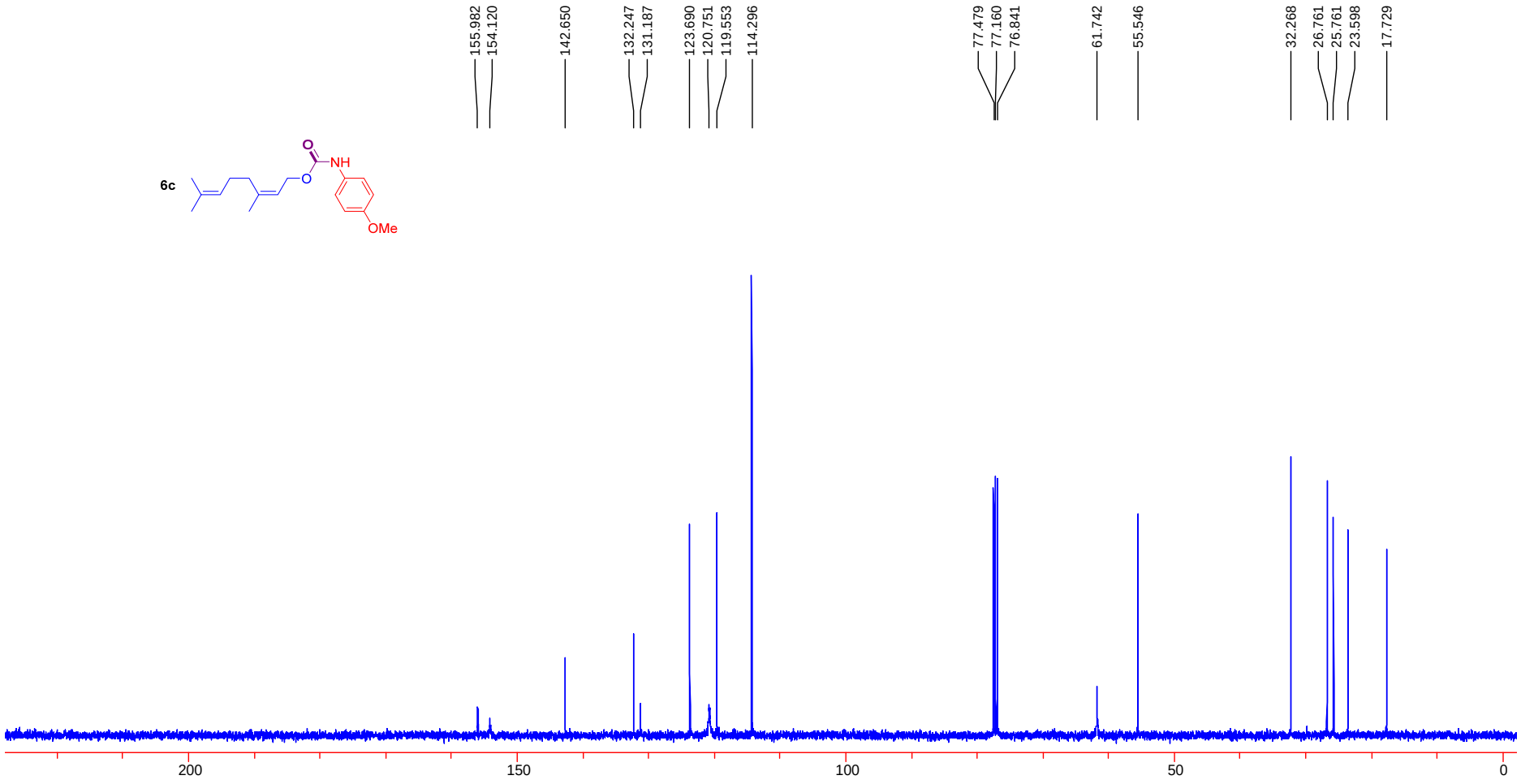
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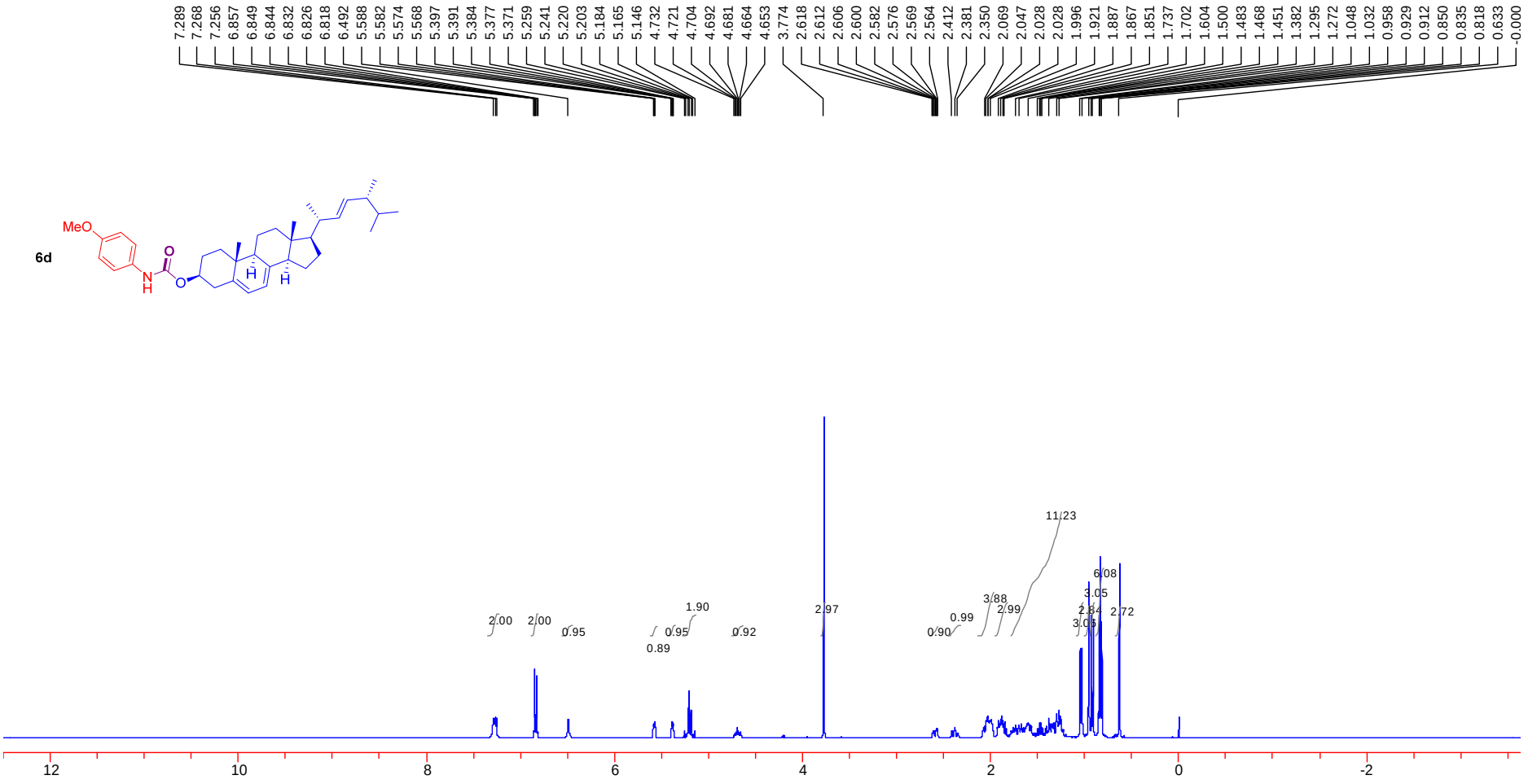
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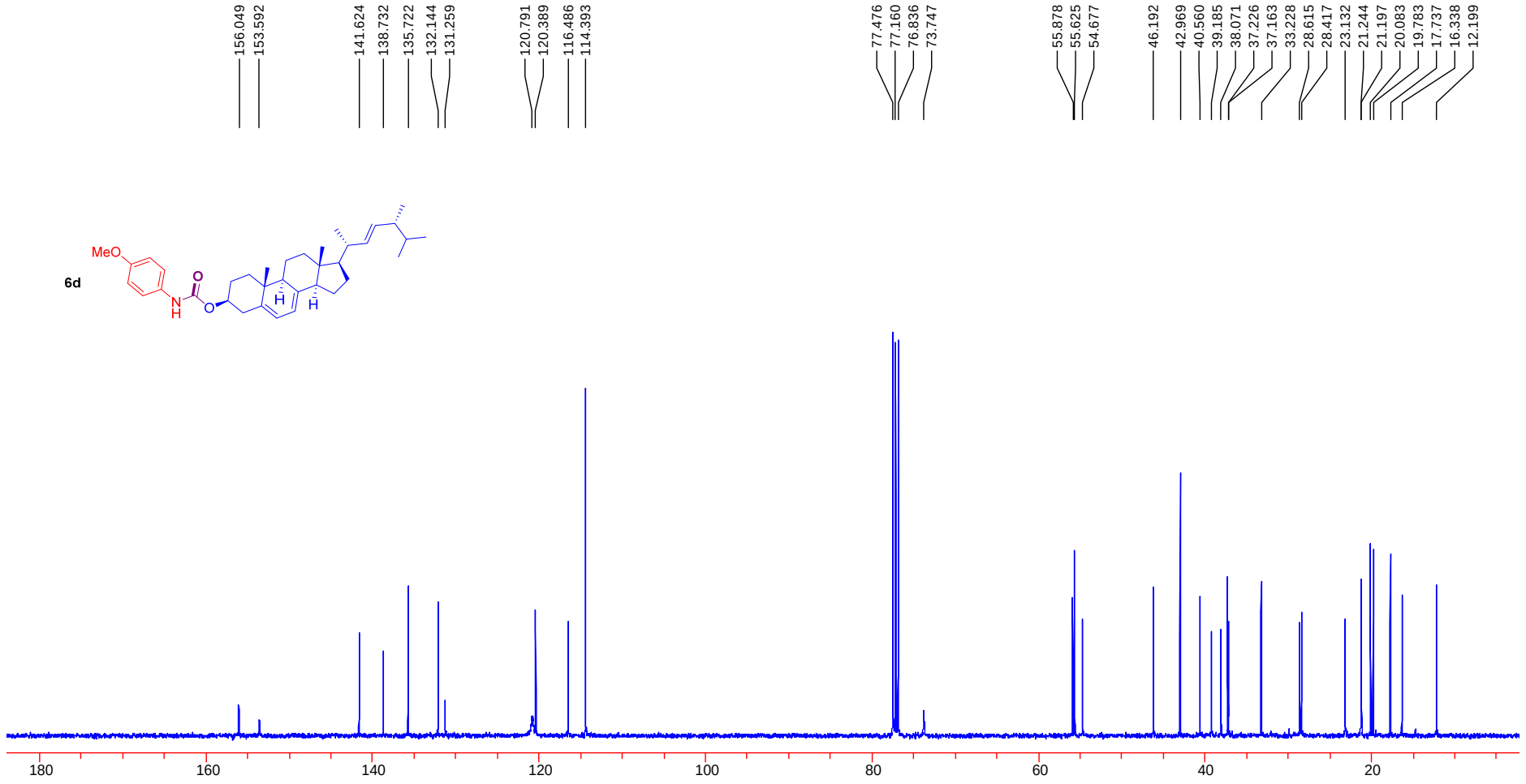
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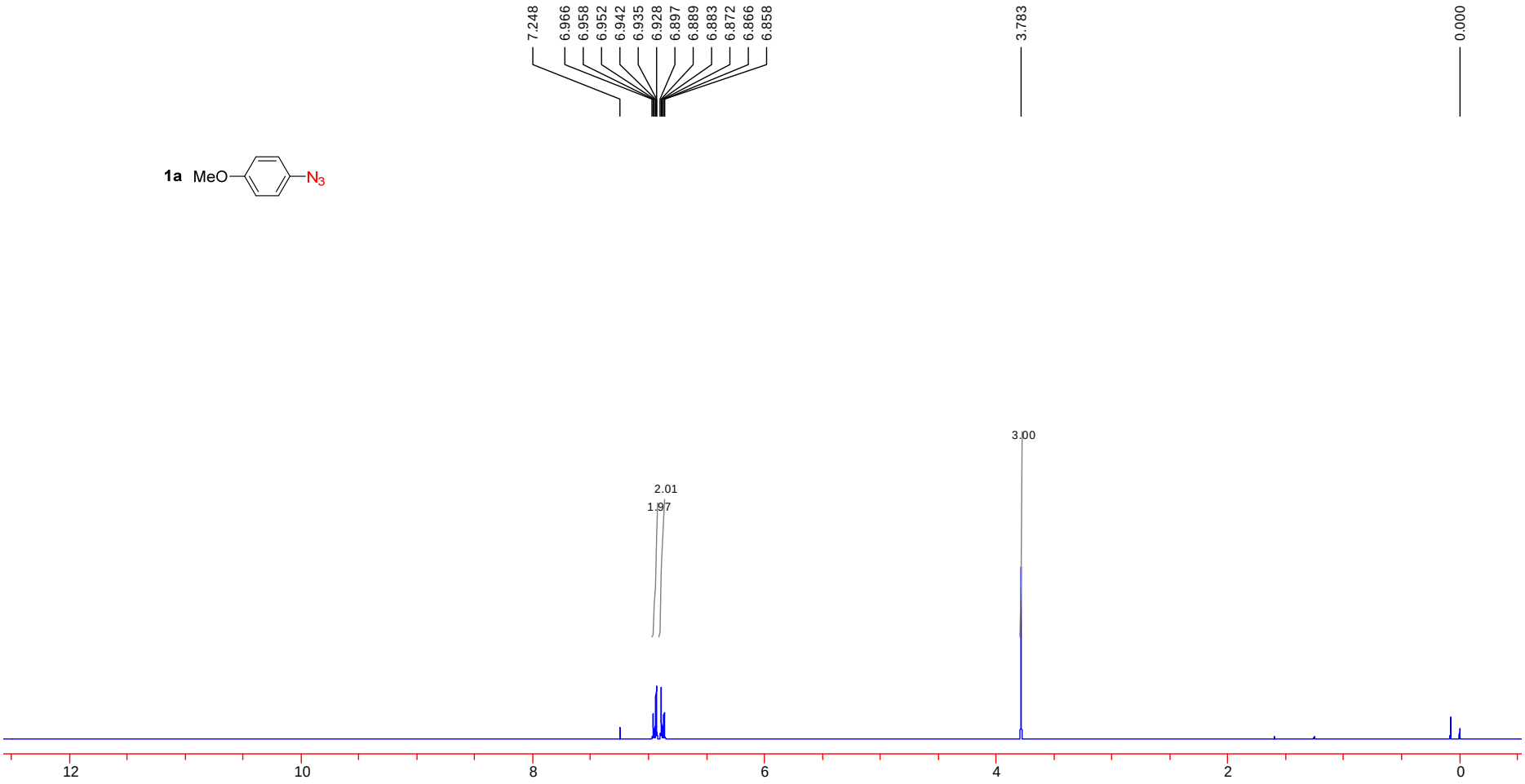
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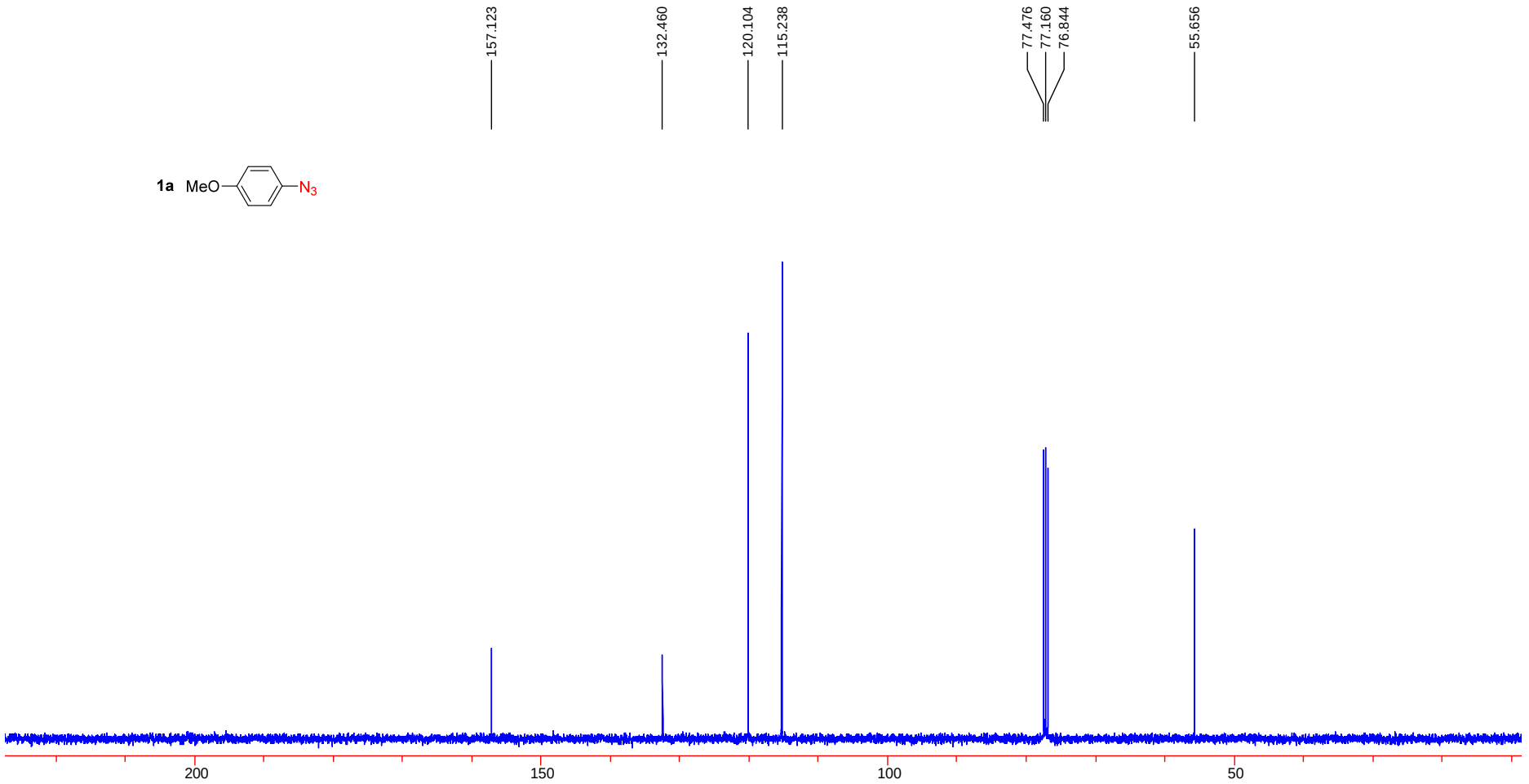
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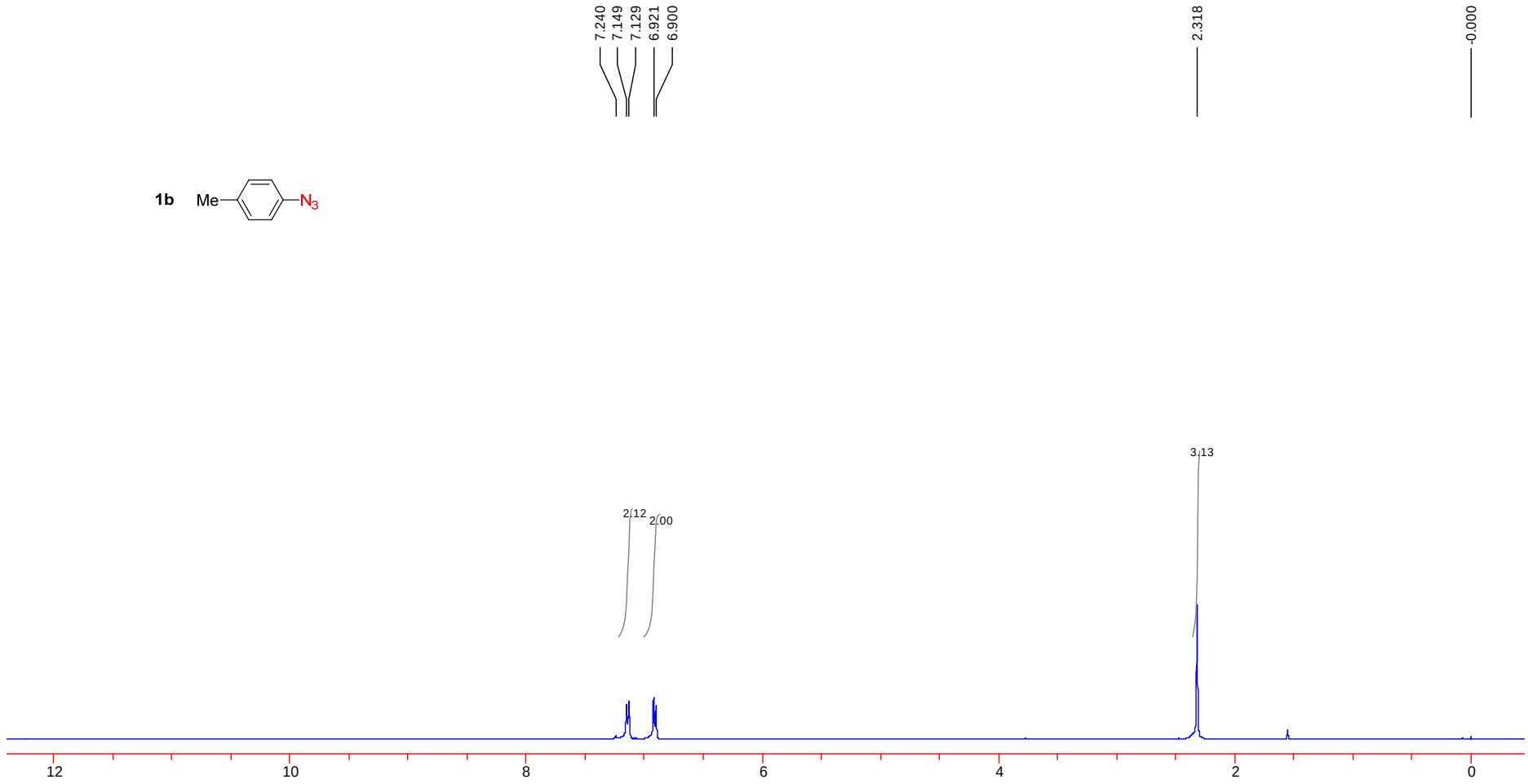
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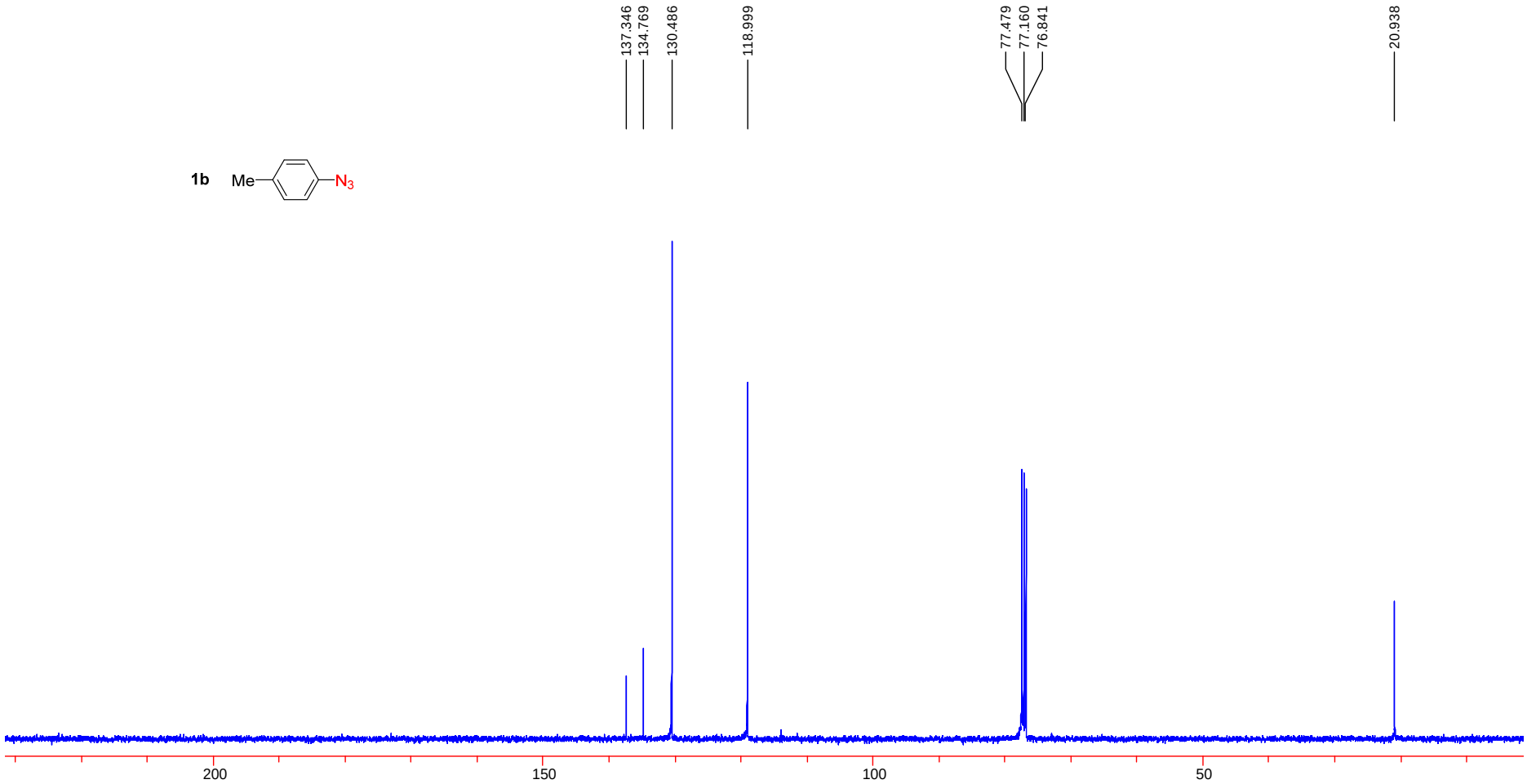
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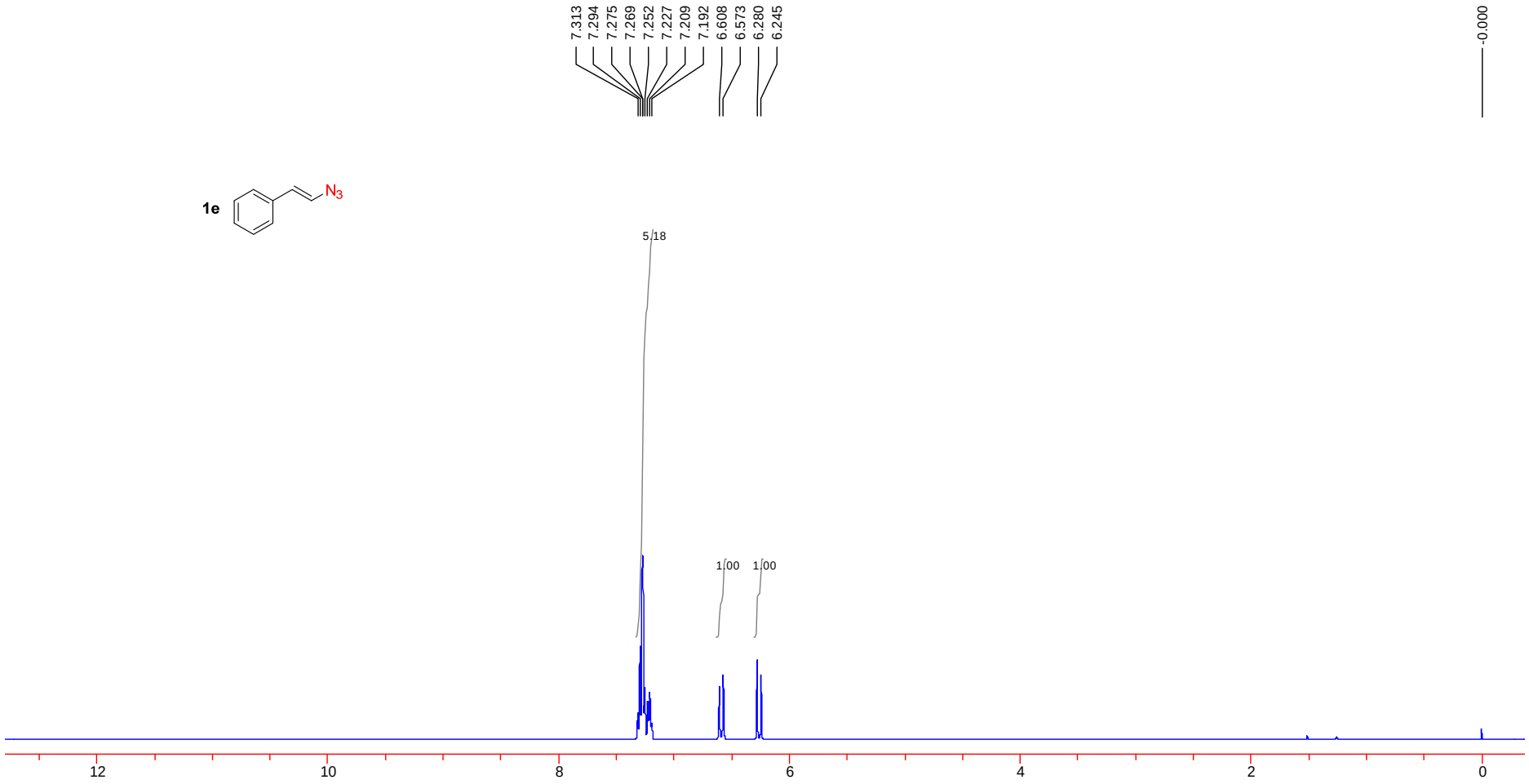
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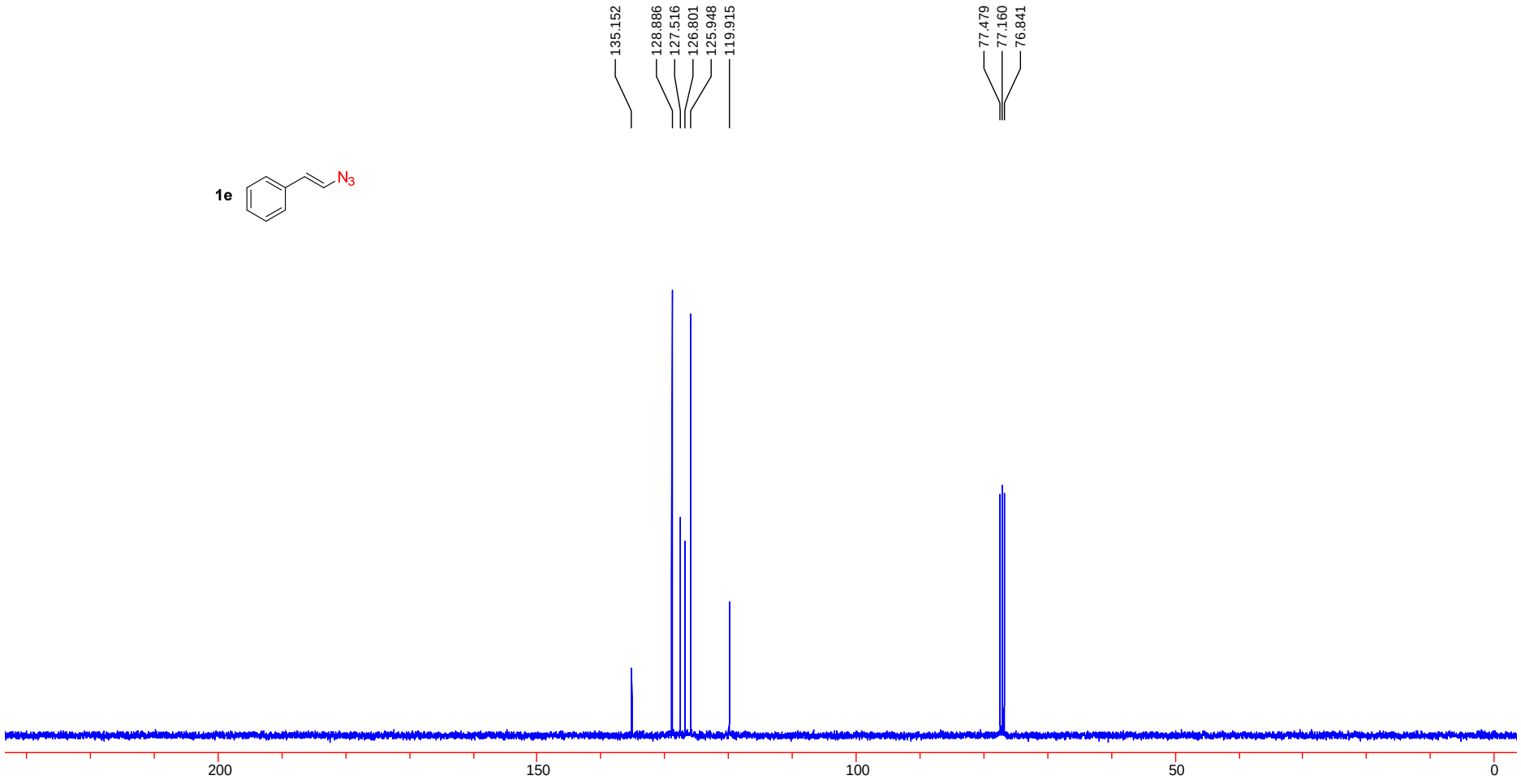
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77.160
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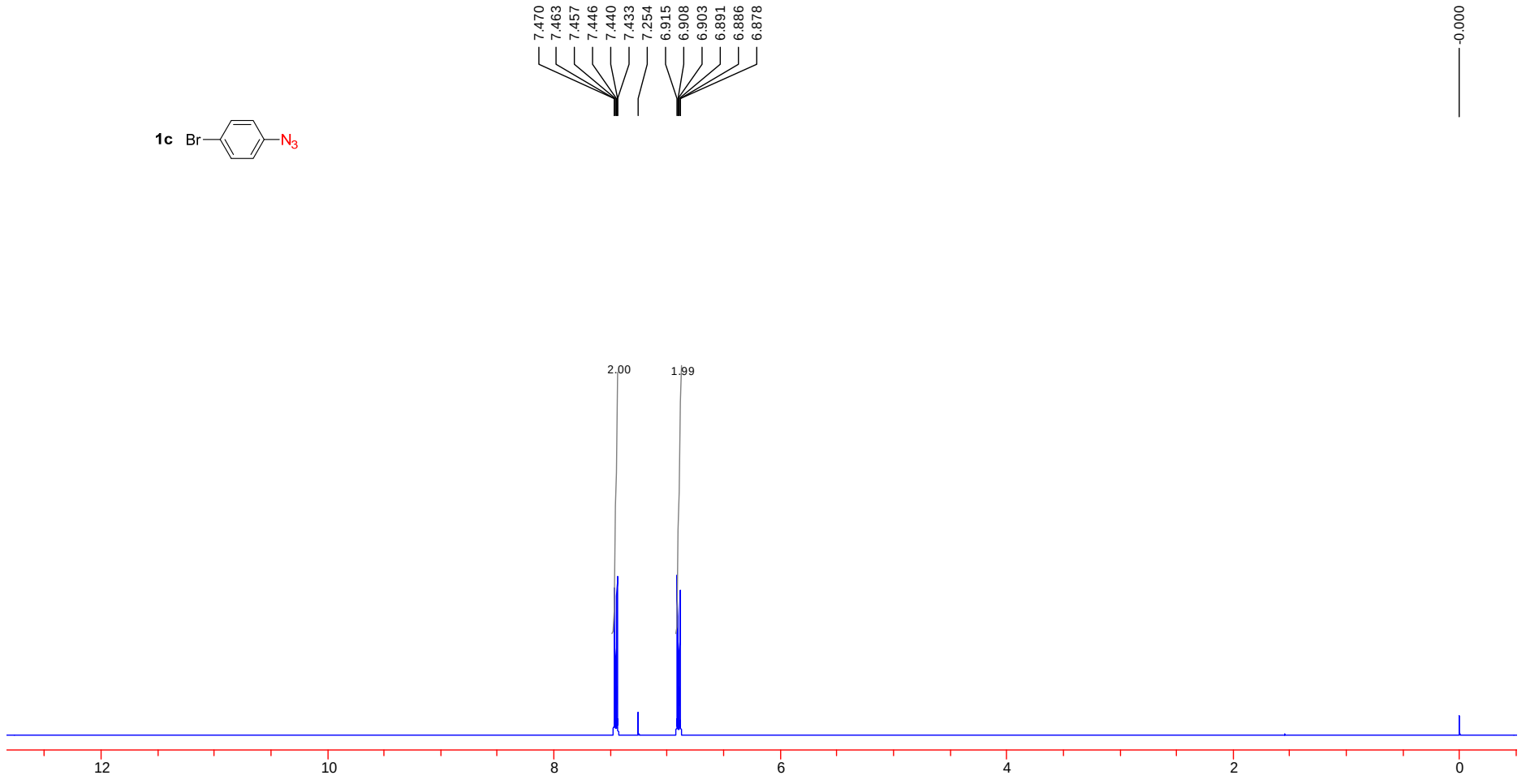
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6.915
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6.903
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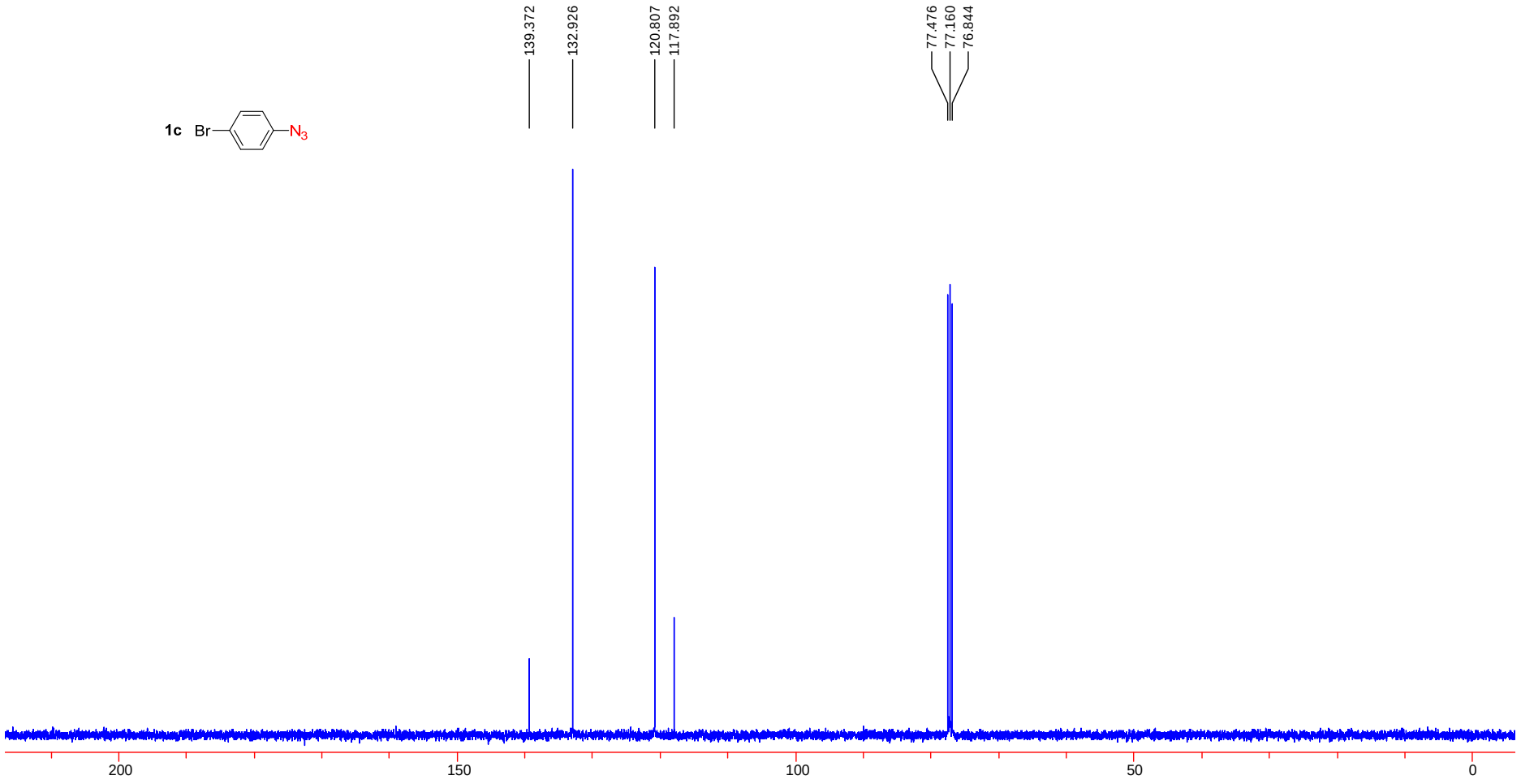
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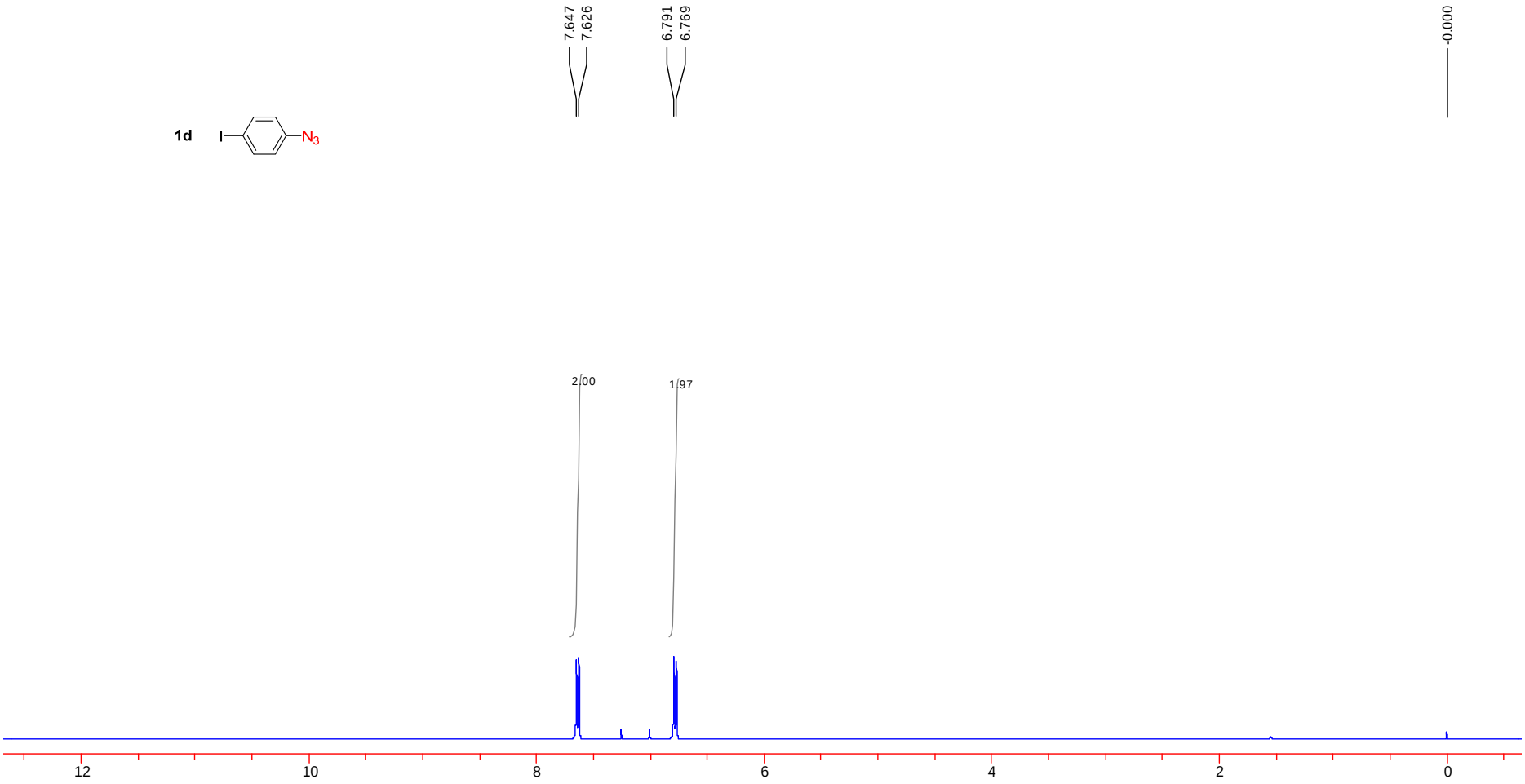
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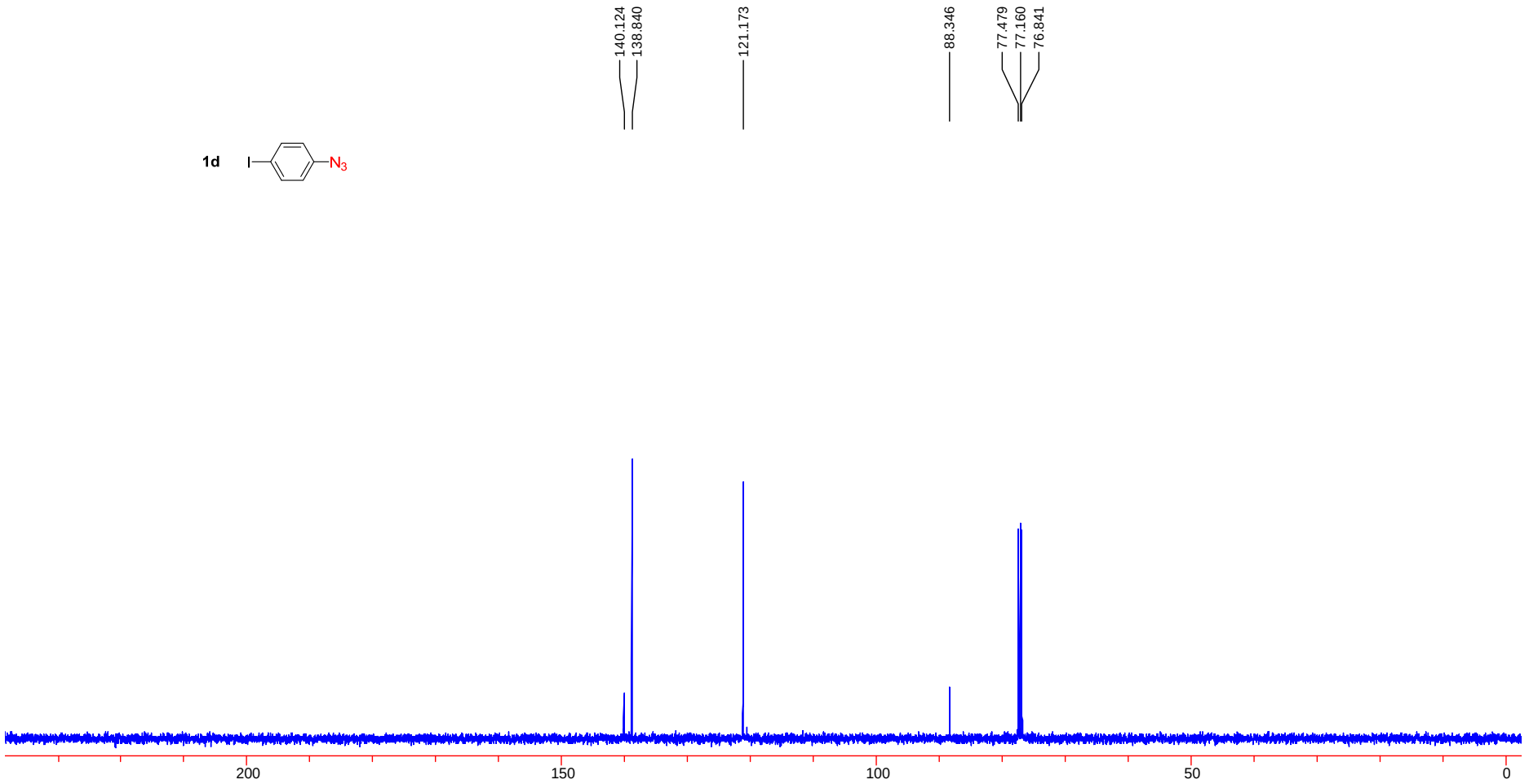
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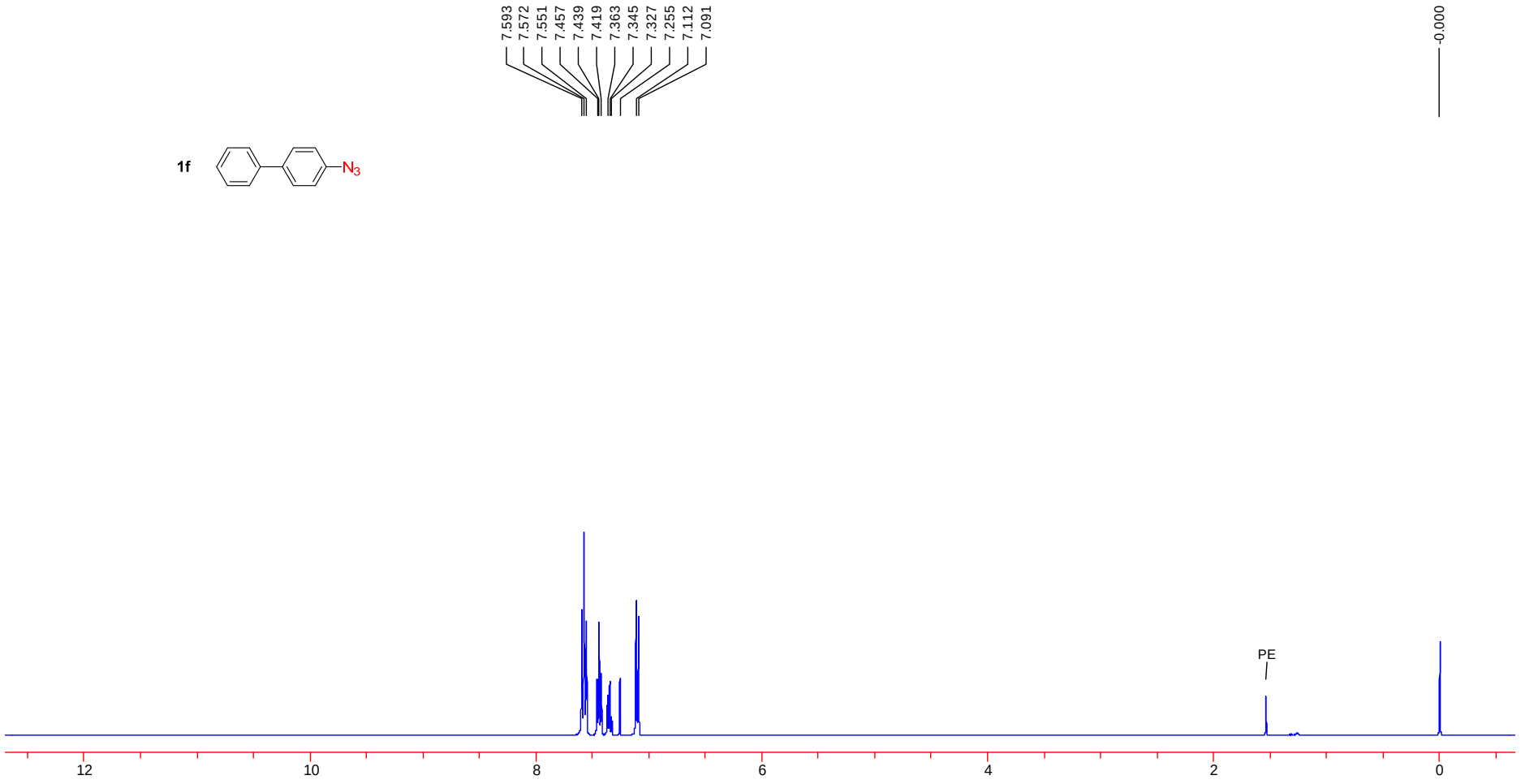
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PE
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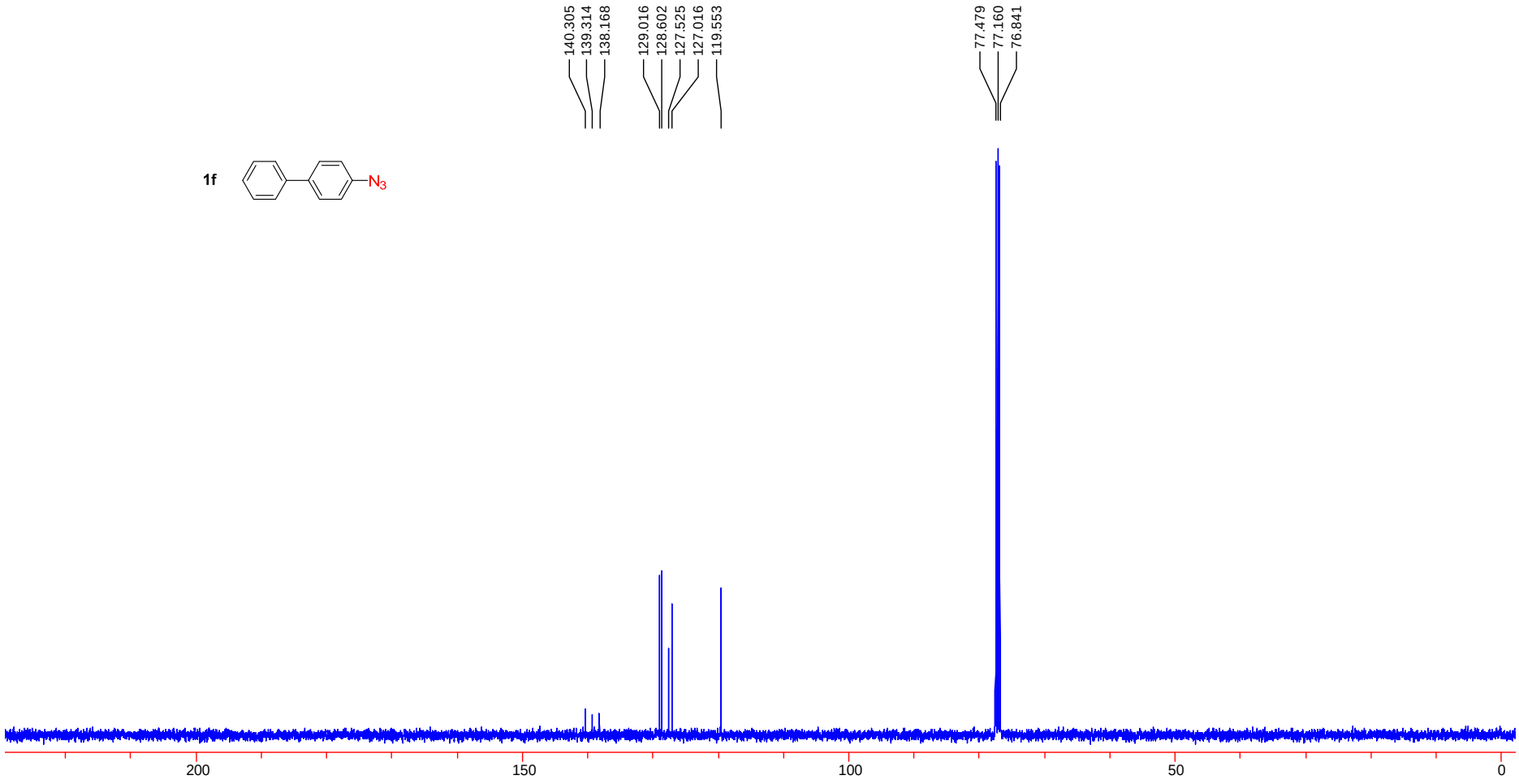
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1f
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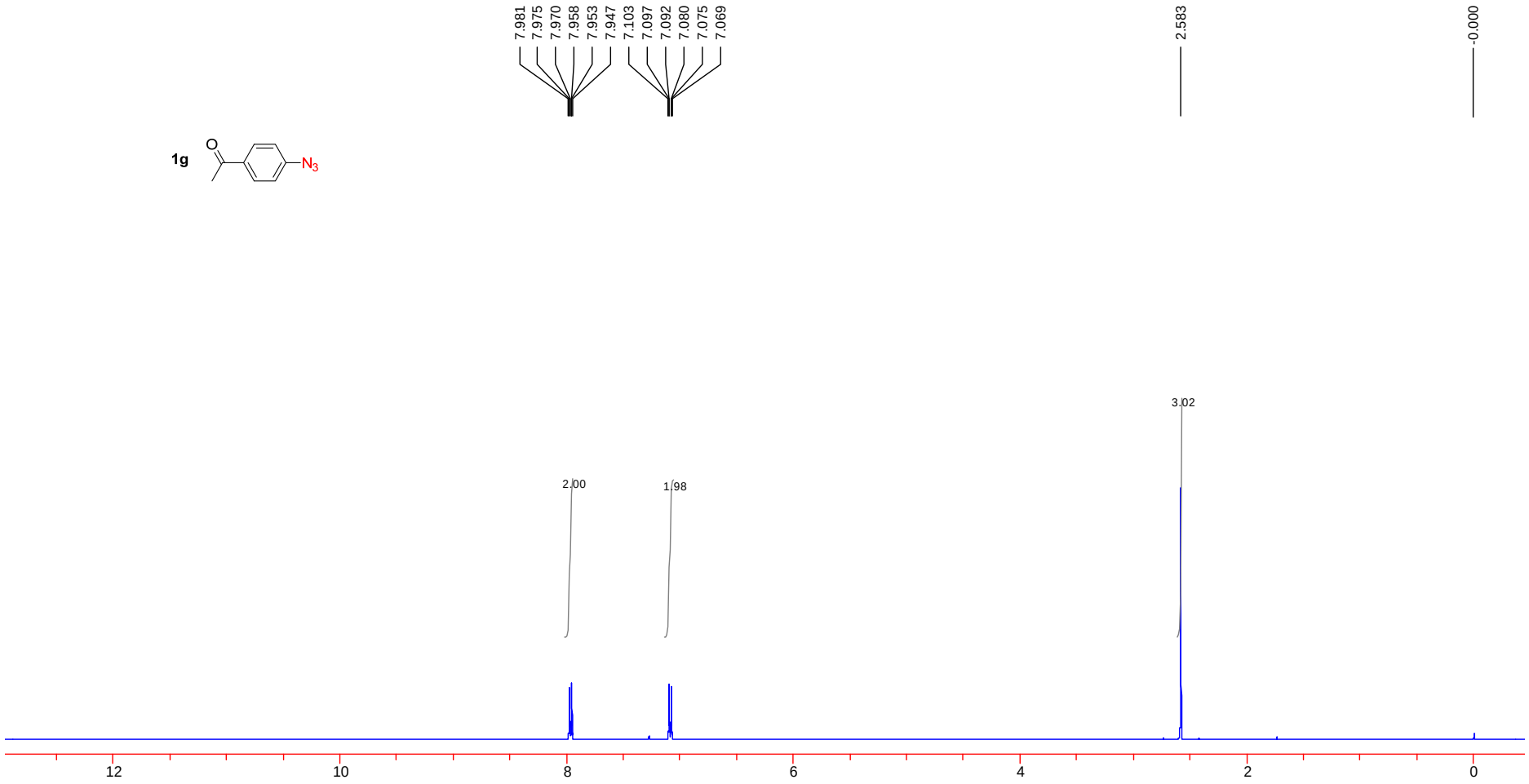
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7.103
7.097
7.092
7.080
7.075
7.069
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O
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2
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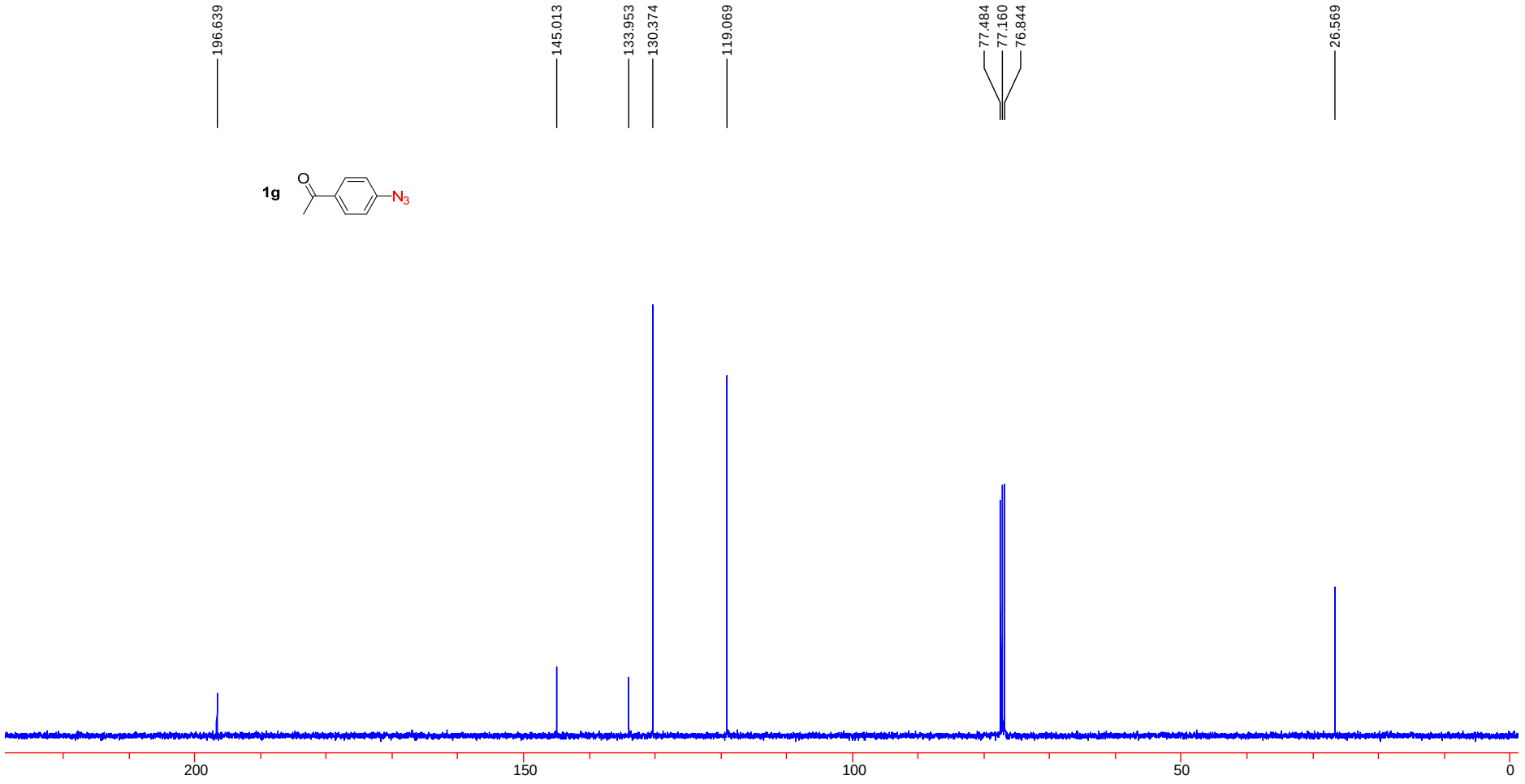
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76.844
26.569
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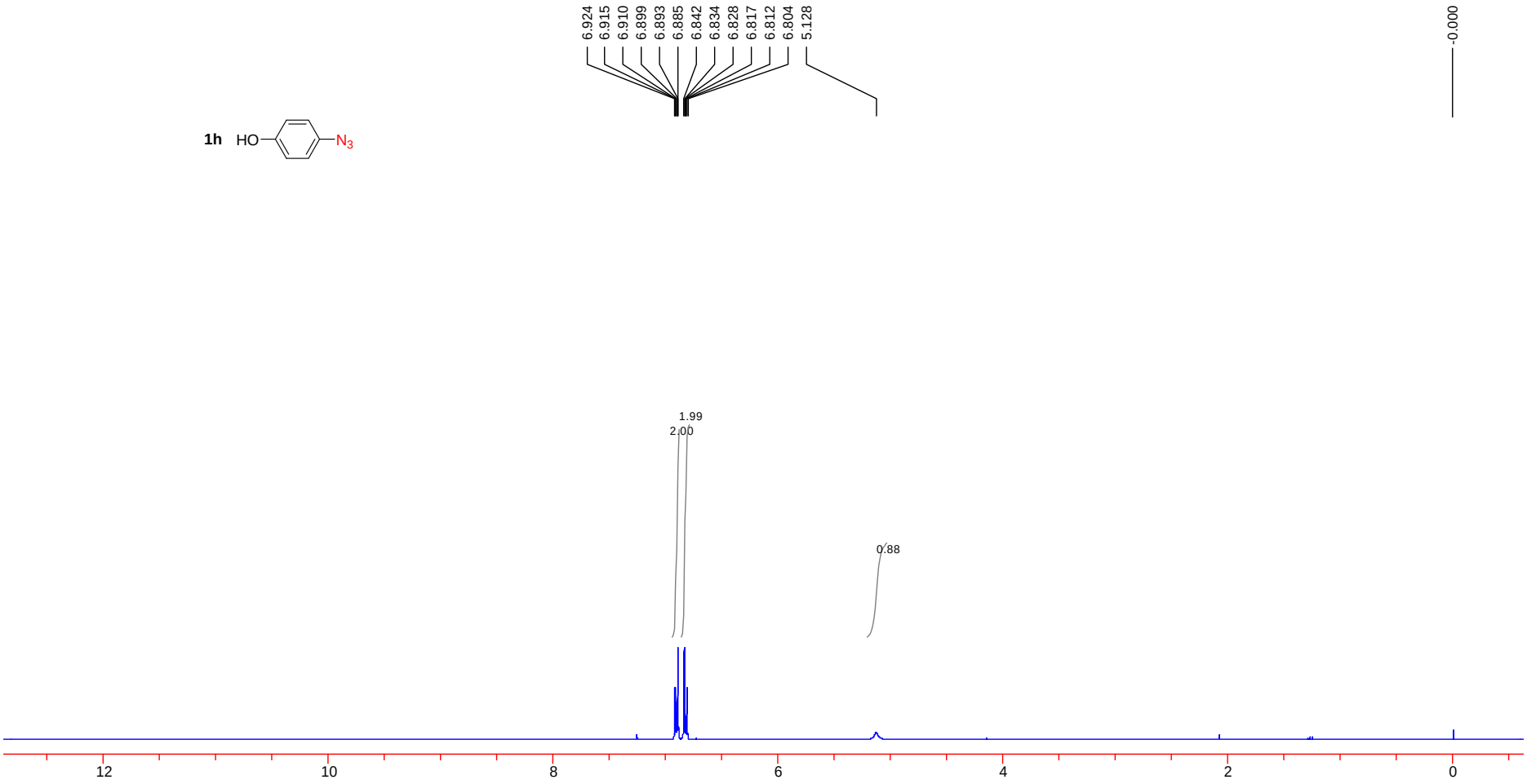
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6.817
6.812
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1h
HO
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2
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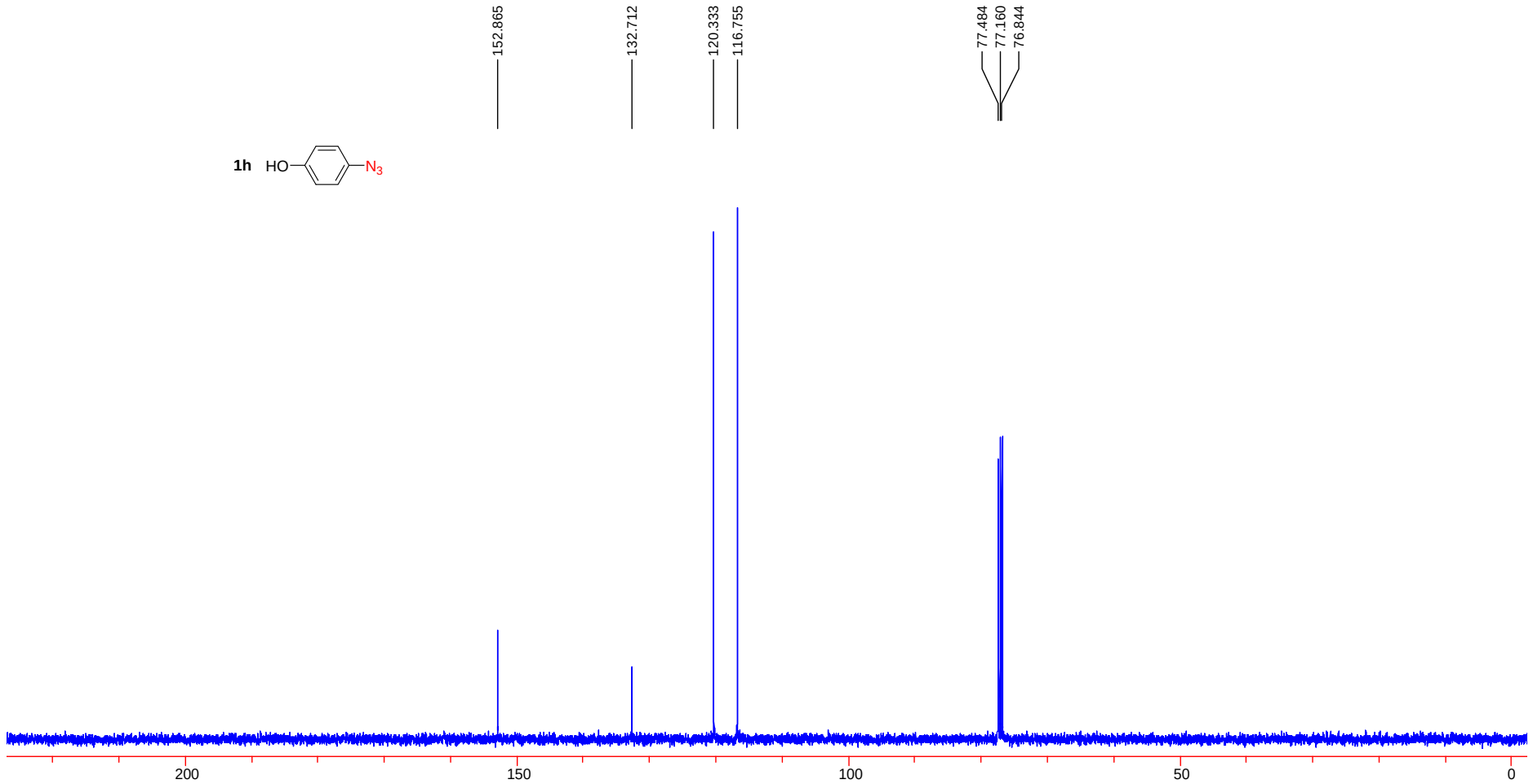
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1h
HO
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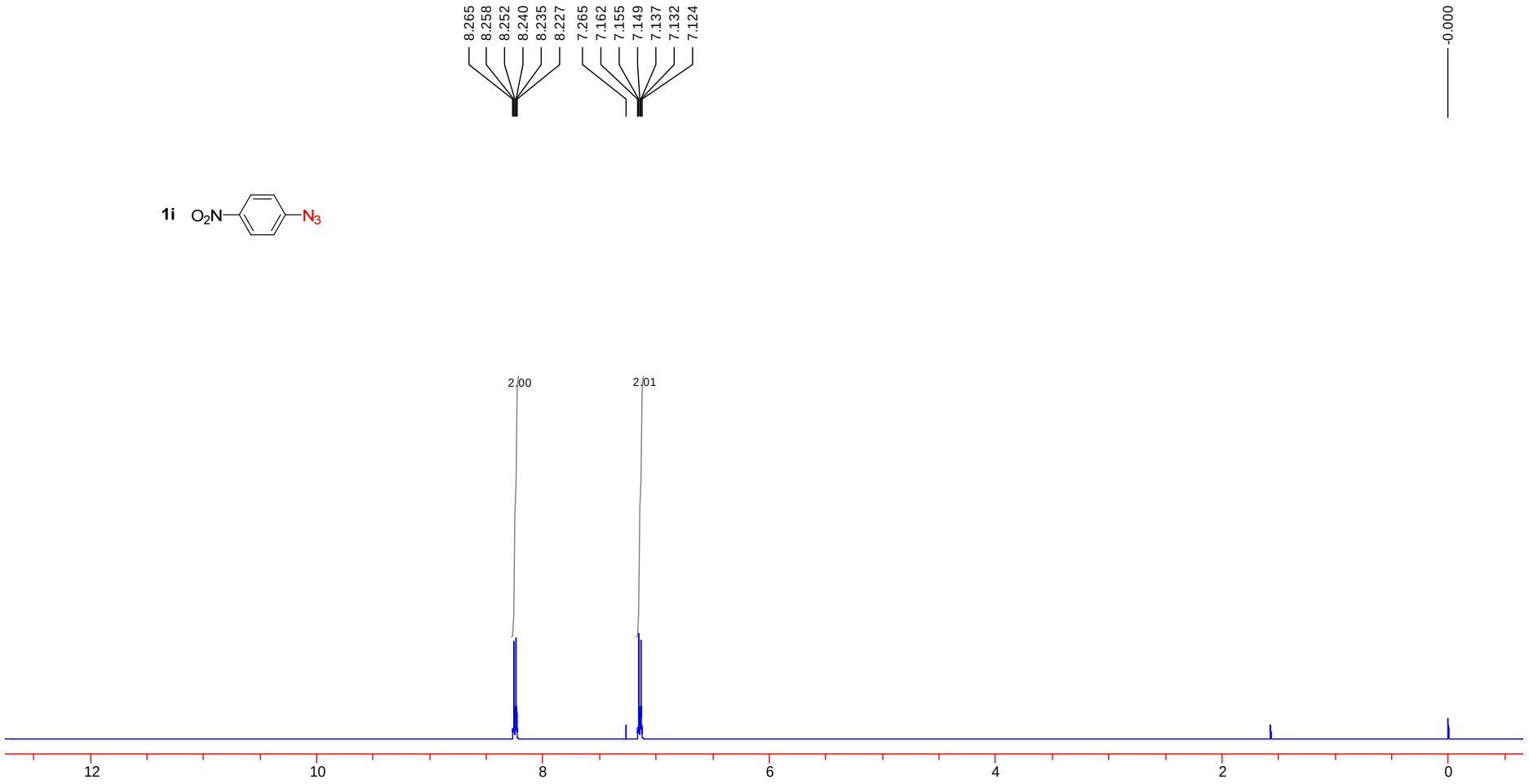
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8.252
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8.227
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7.162
7.155
7.149
7.137
7.132
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-0.000
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N3
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2.01
12
10
8
6
4
2
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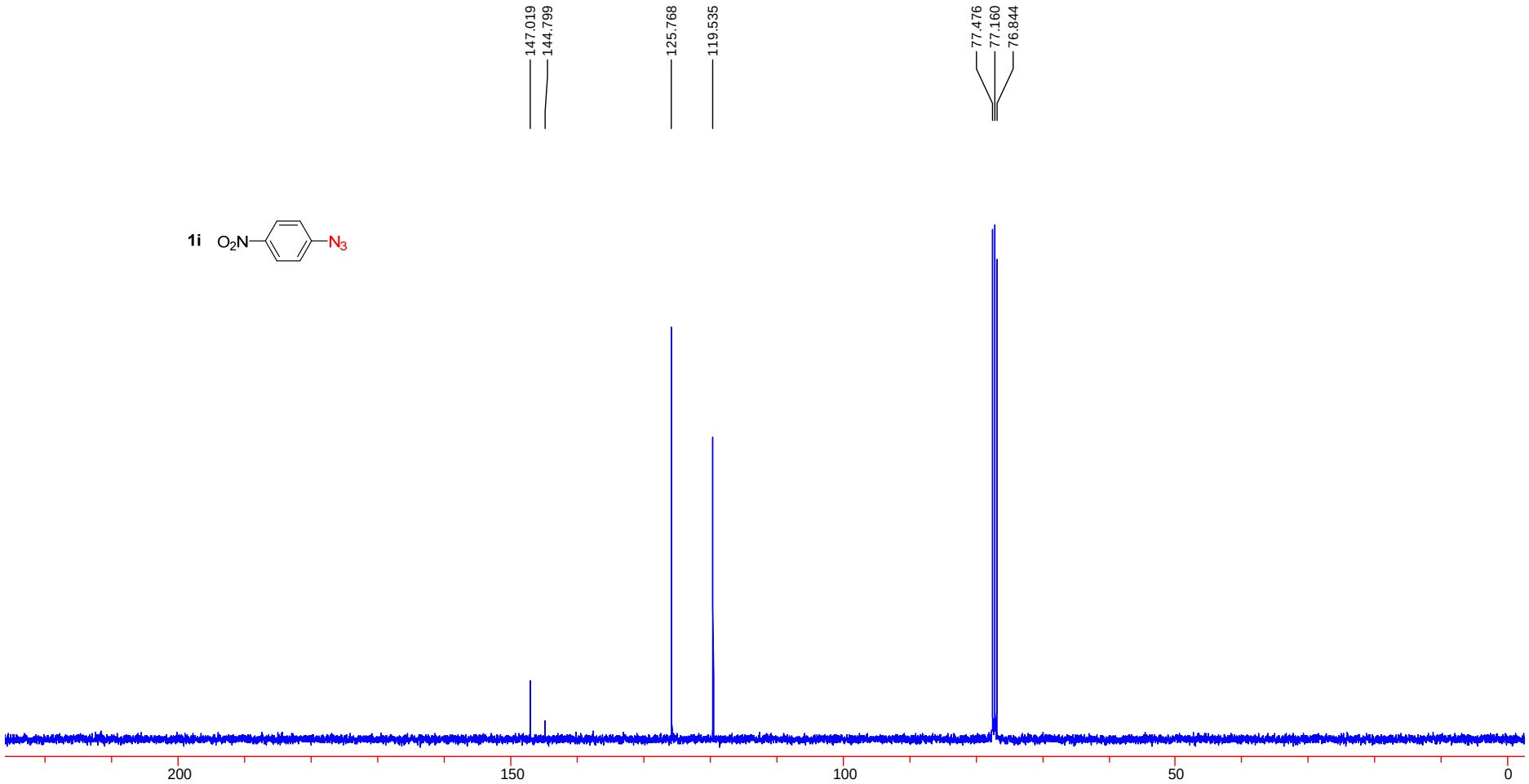
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76.844
1i
O2N
N3
200
150
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50
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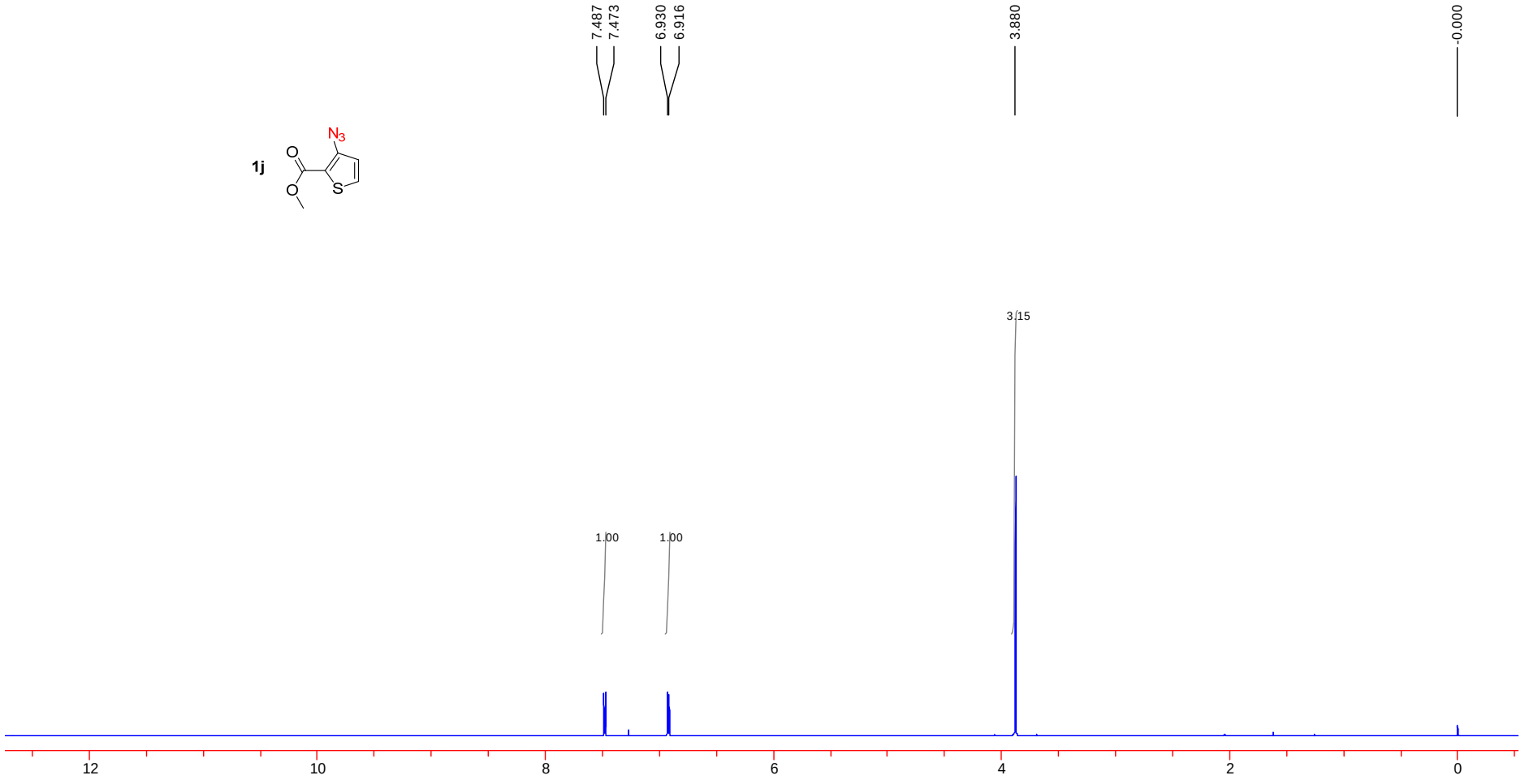
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6.916
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1.00
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10
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2
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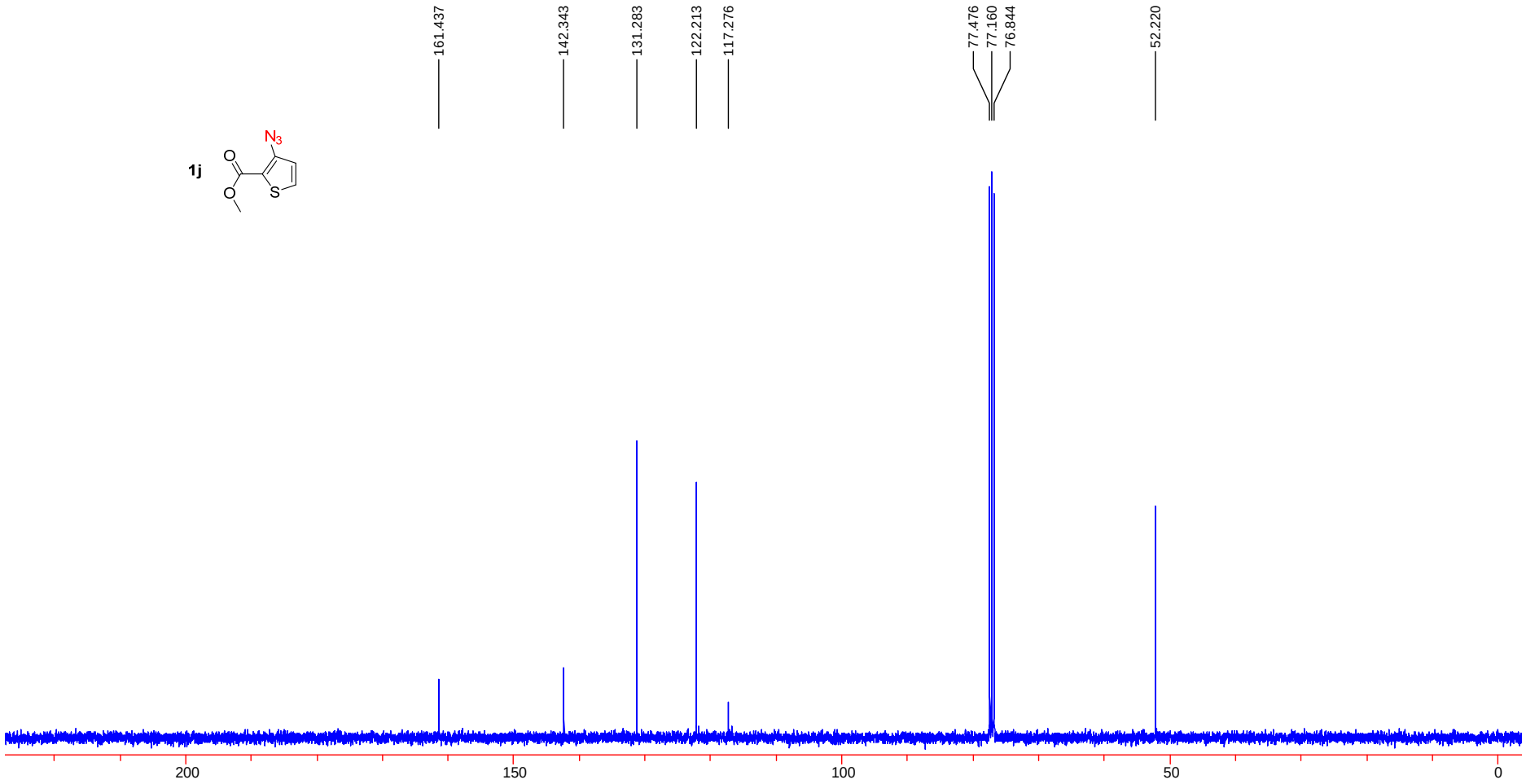
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52.220
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O
O
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150
100
50
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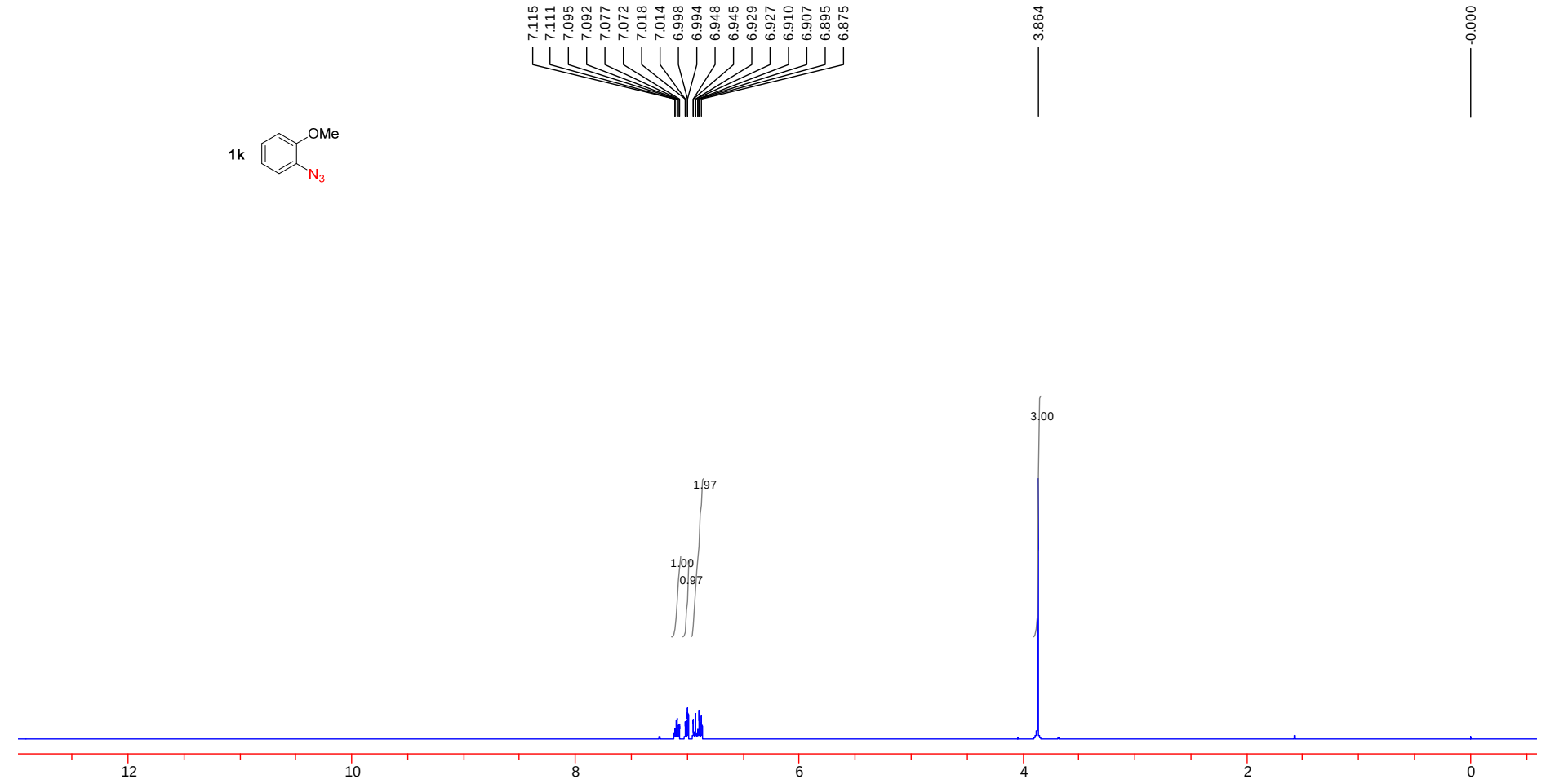
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7.095
7.092
7.077
7.072
7.018
7.014
6.998
6.994
6.948
6.945
6.929
6.927
6.910
6.907
6.895
6.875
3.864
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OMe
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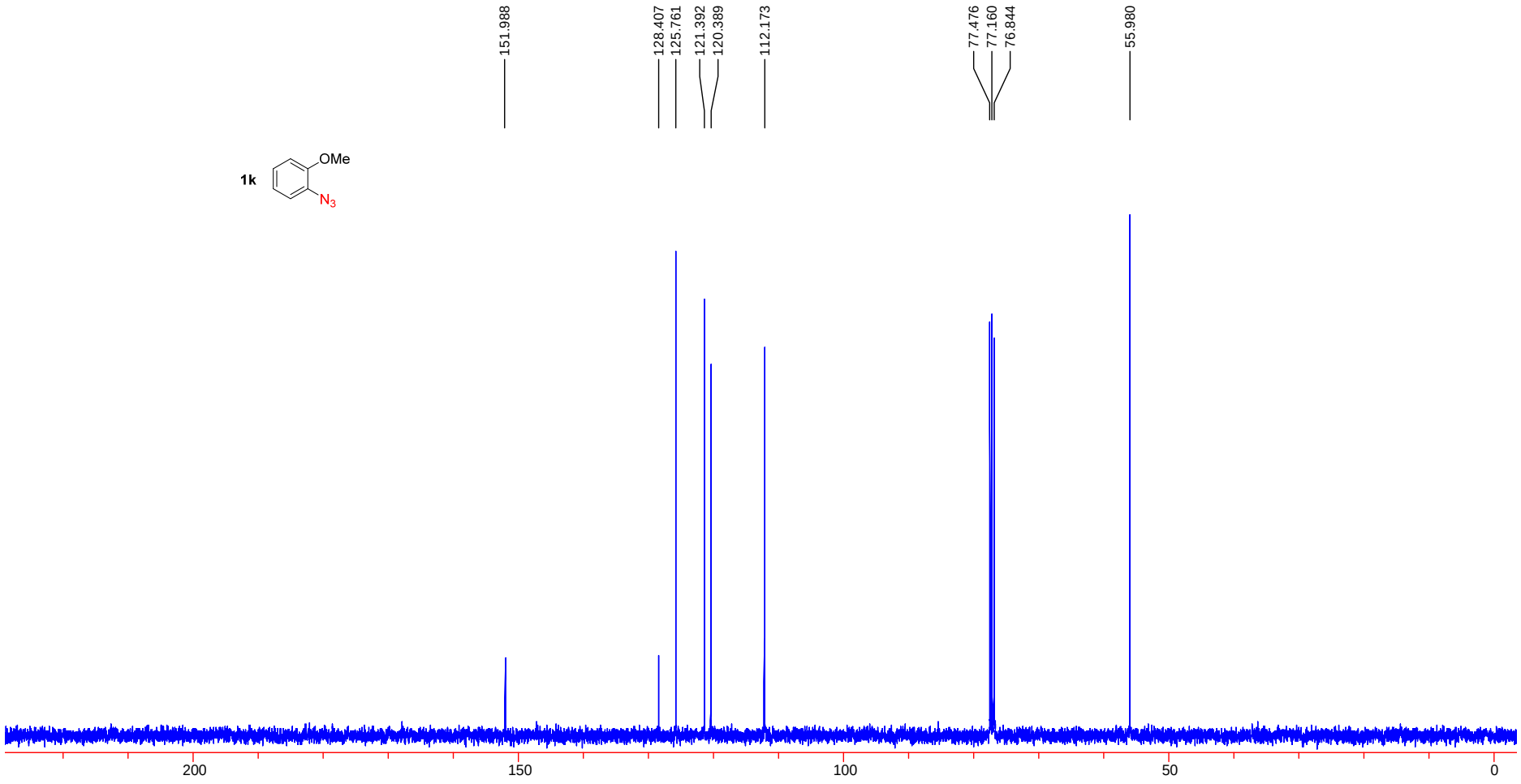
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N3
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100
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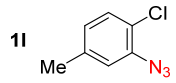
0

1l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Me
N3

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1.00
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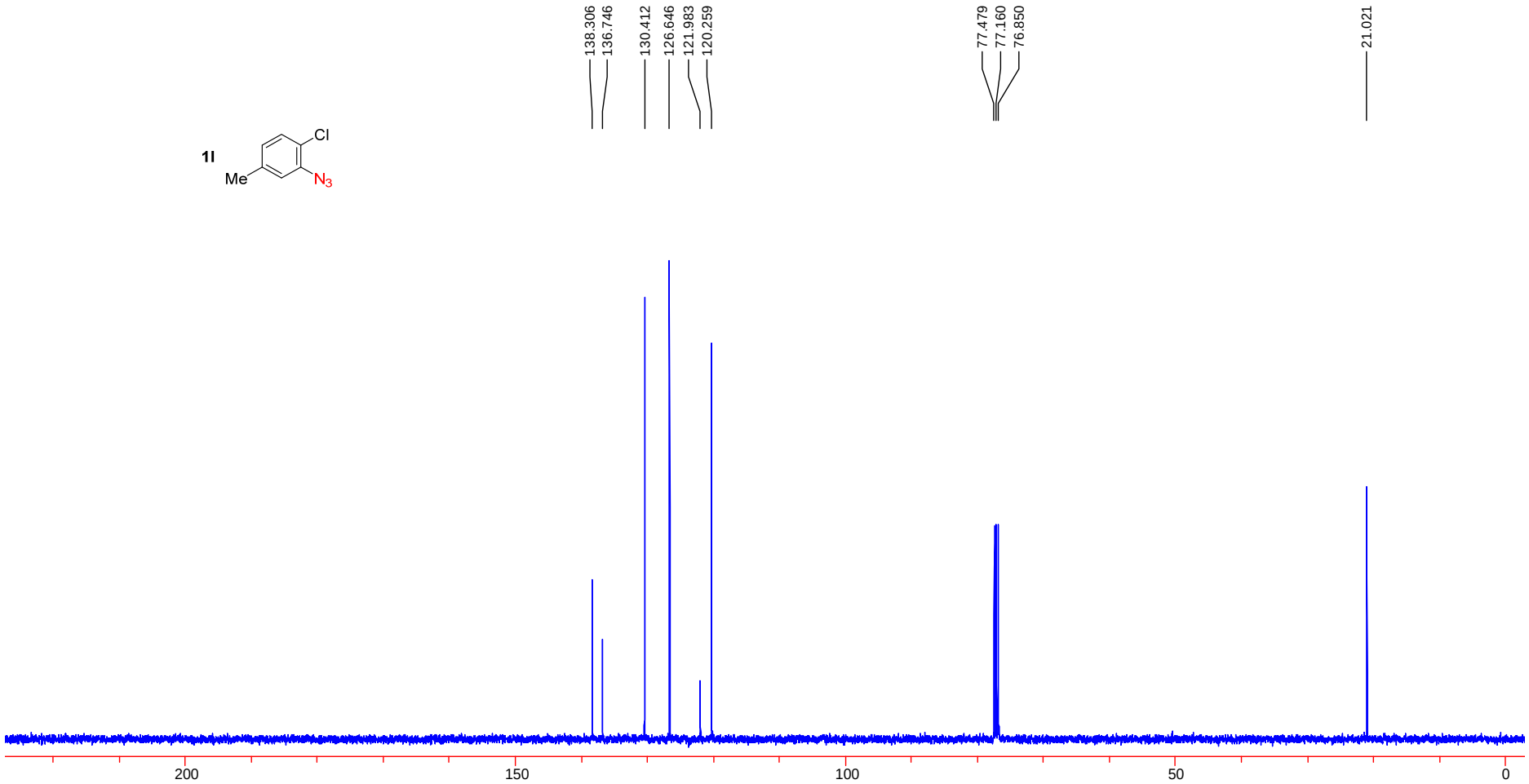
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126.646
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77.160
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Me
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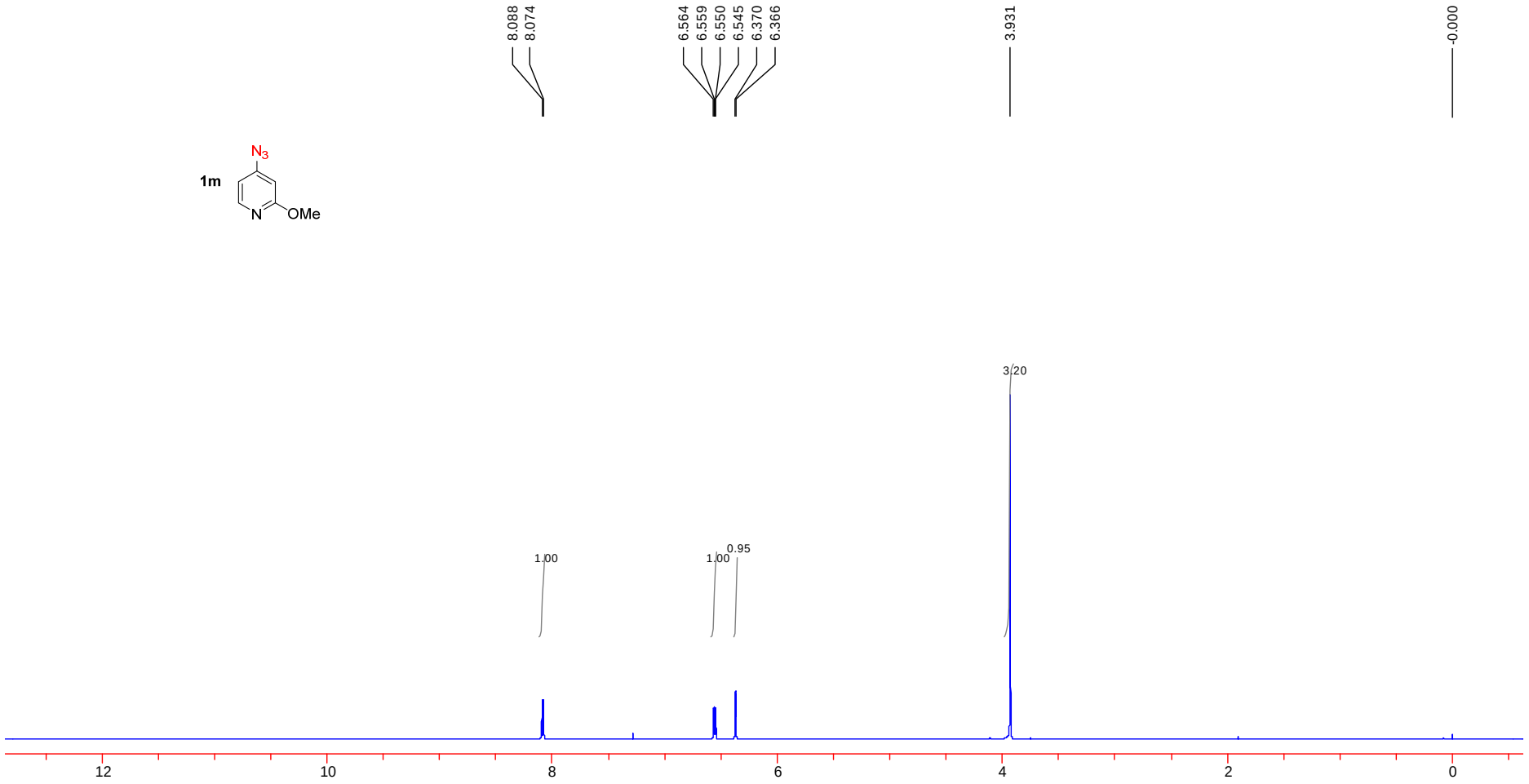
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6.545
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6.366
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N
OMe
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2
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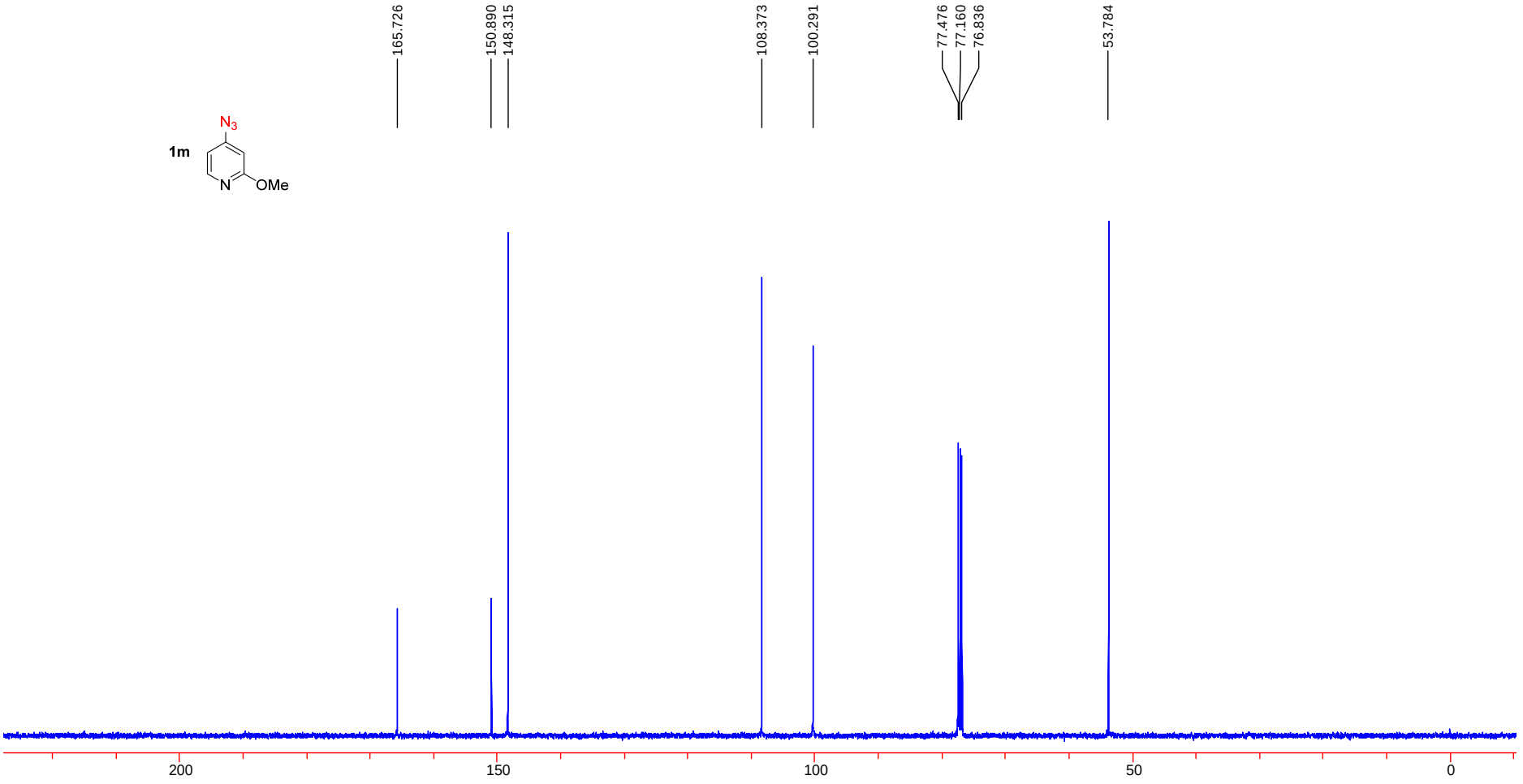
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N
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50
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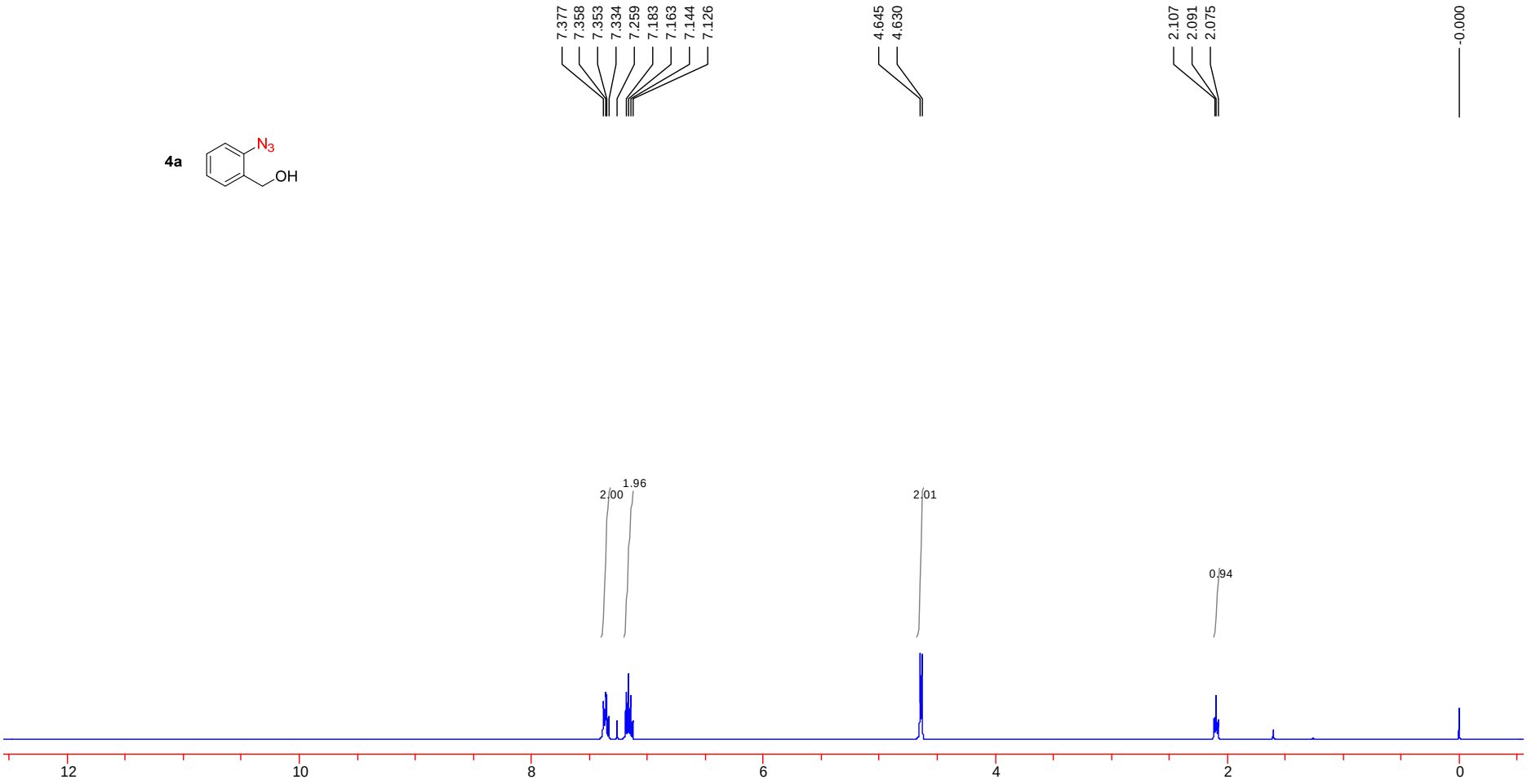
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4.630
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2.091
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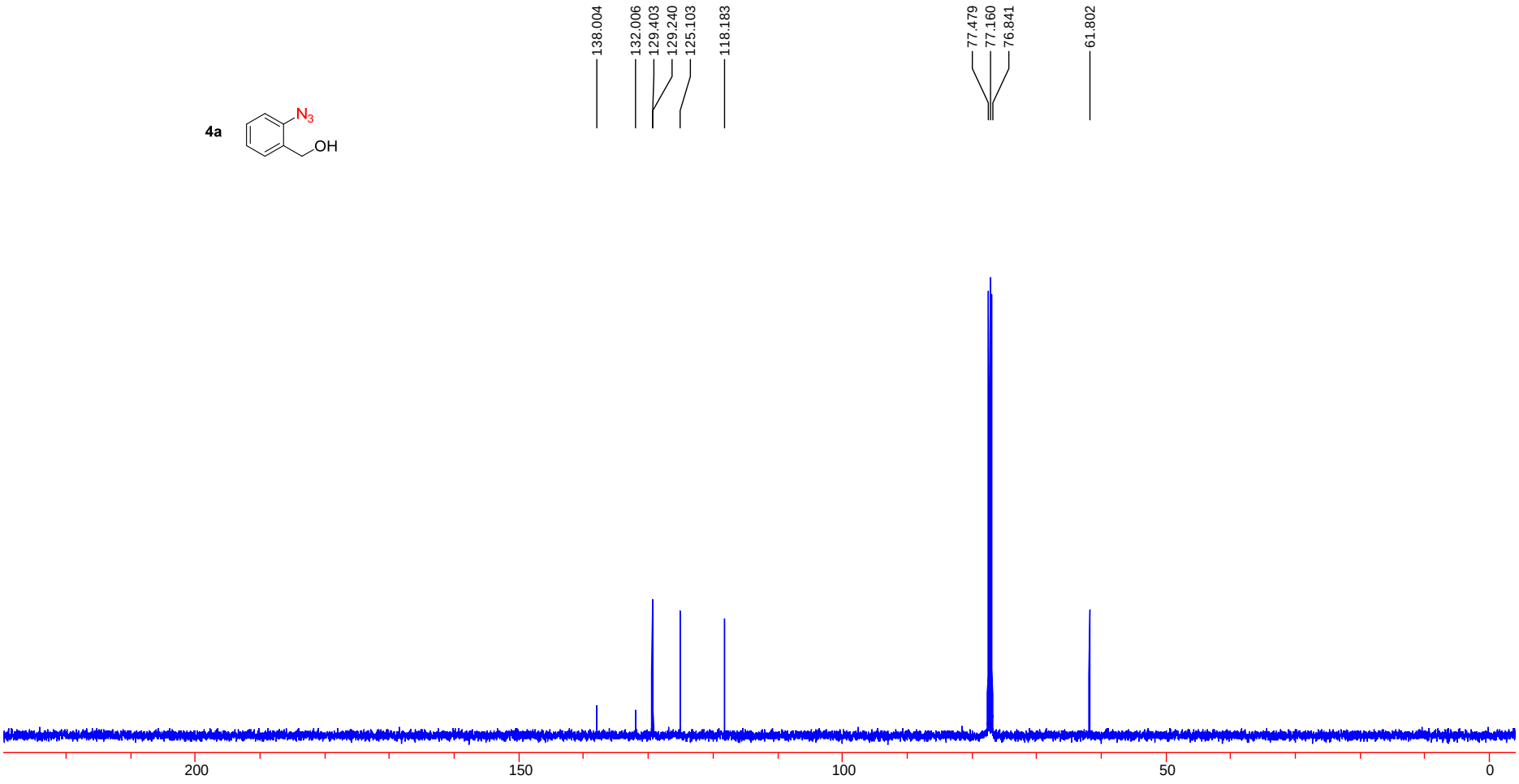
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77.160
76.841
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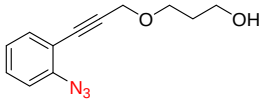
100
50
0

4b


O
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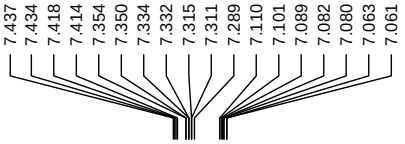
N3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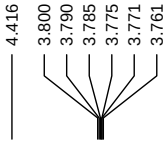
7.089
7.082
7.080
7.063
7.061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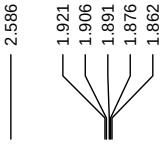
3.771
3.761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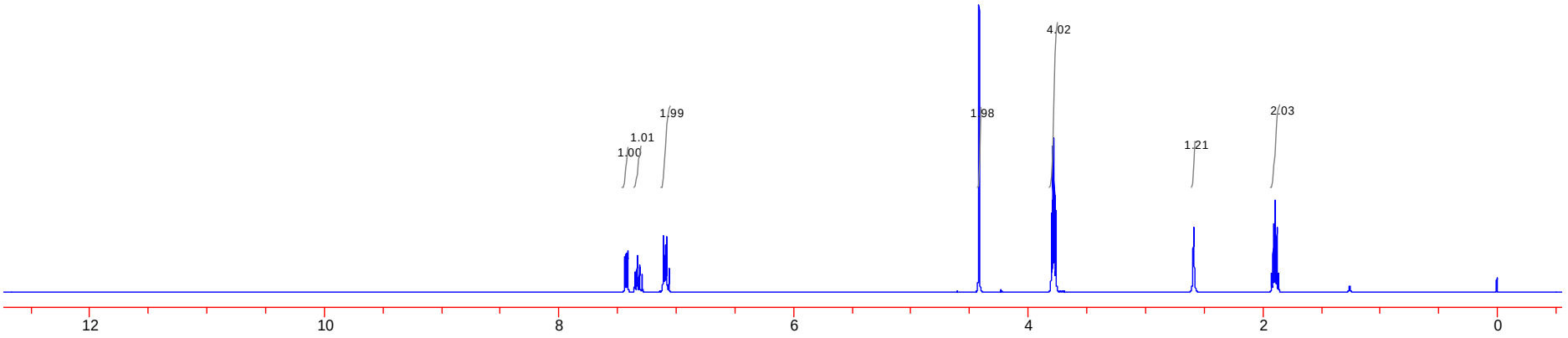
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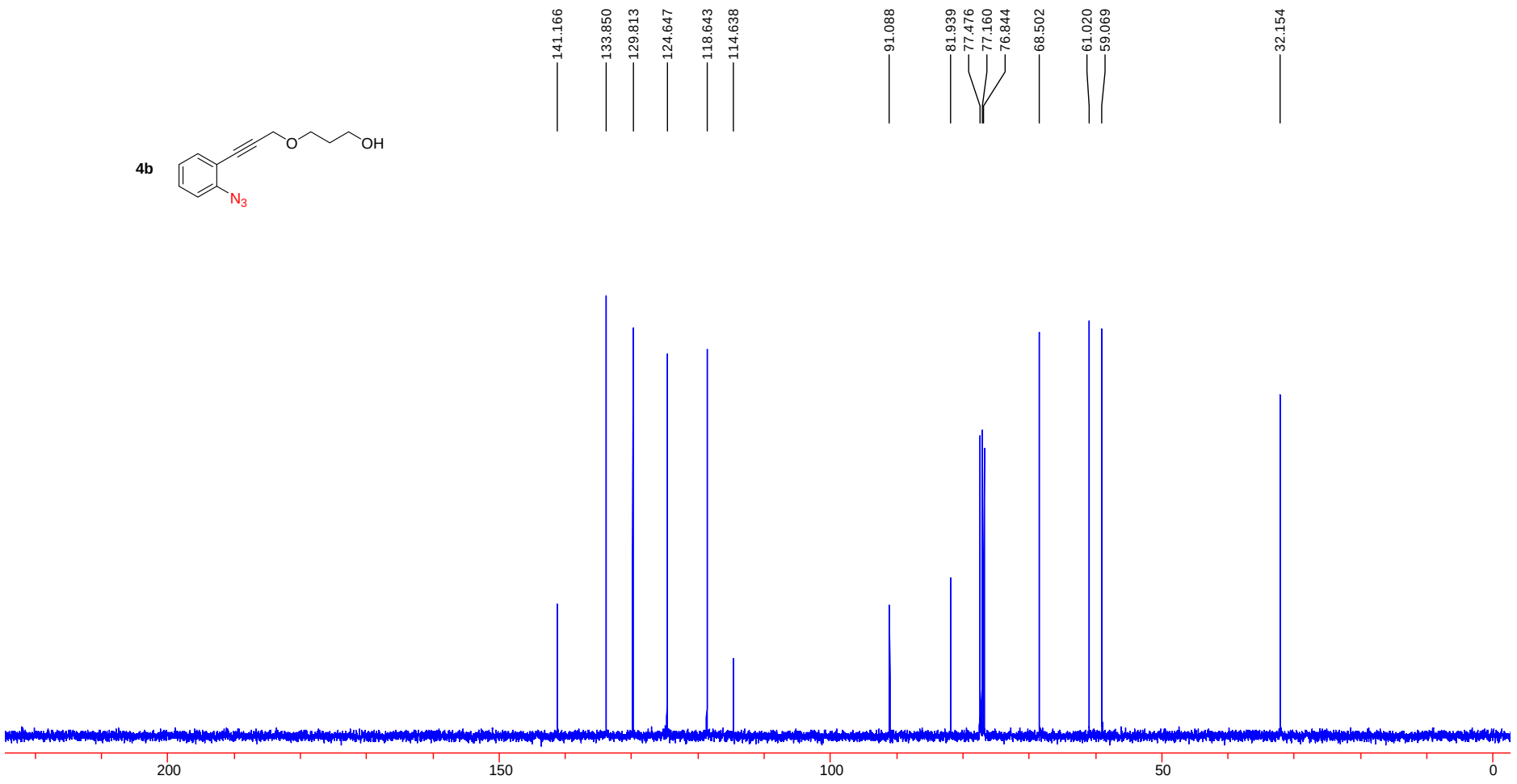
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61.020
59.069
32.154
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O
OH
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50
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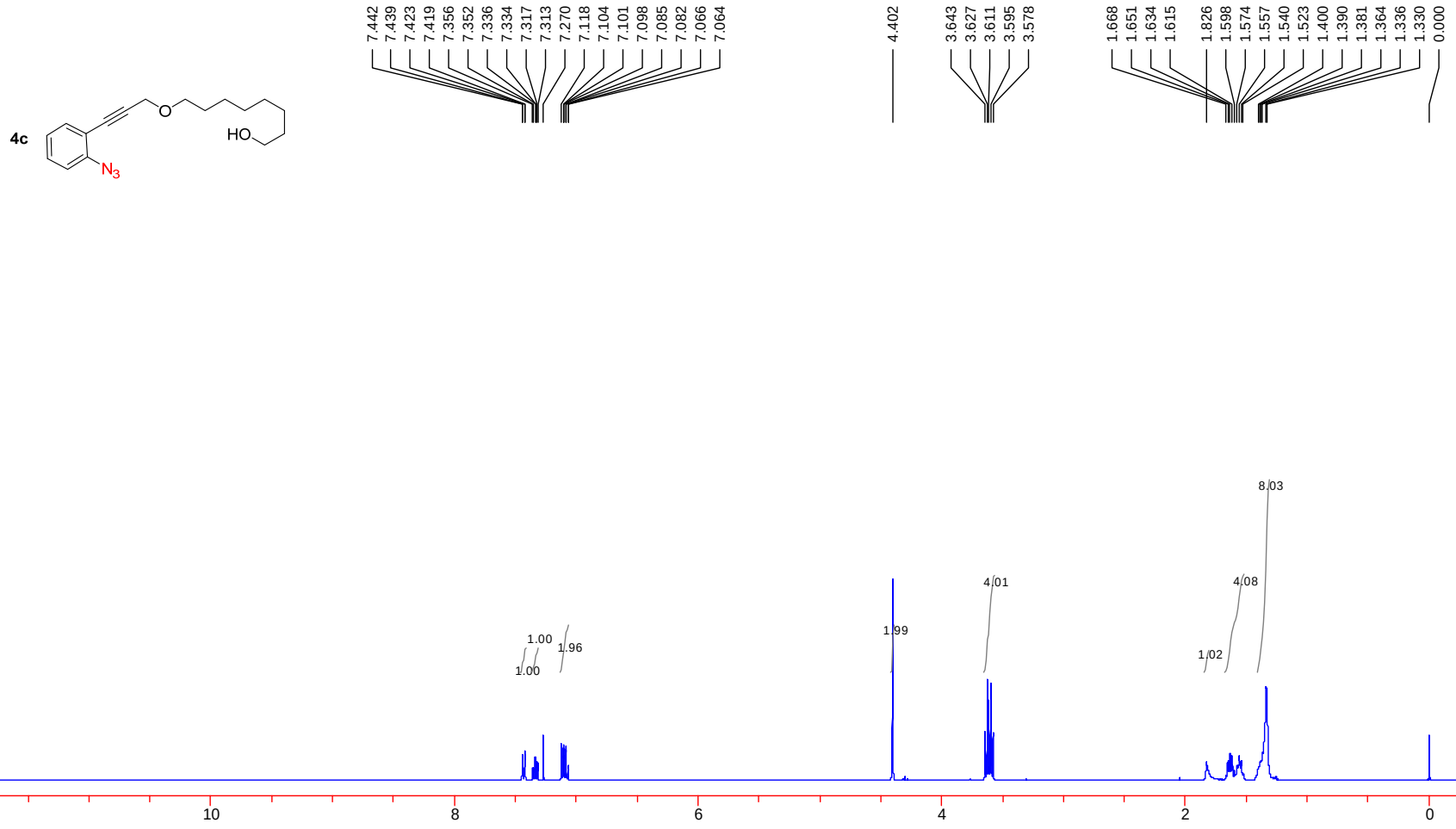
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HO
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1.381
1.364
1.336
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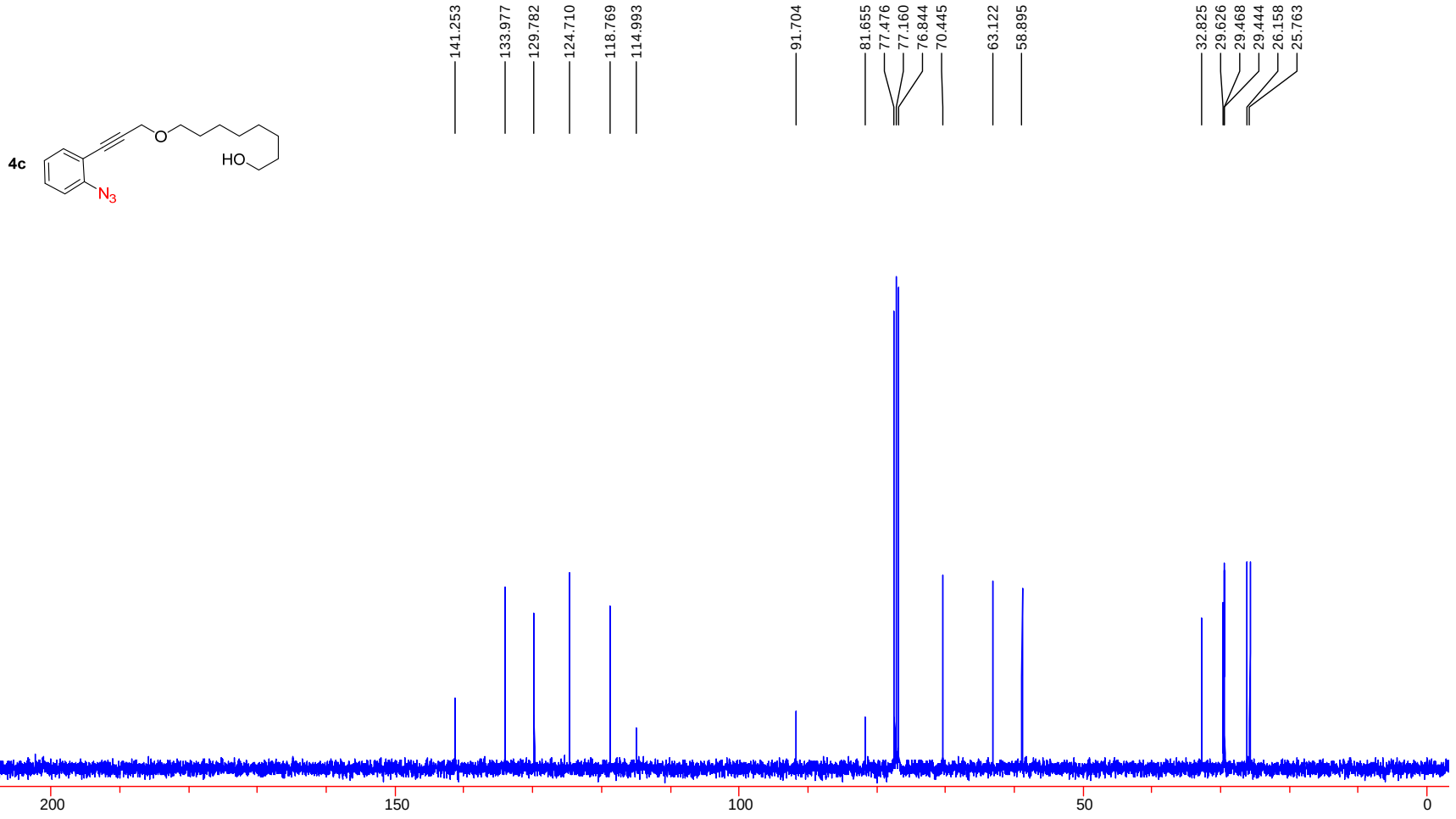
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HO
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77.160
76.844
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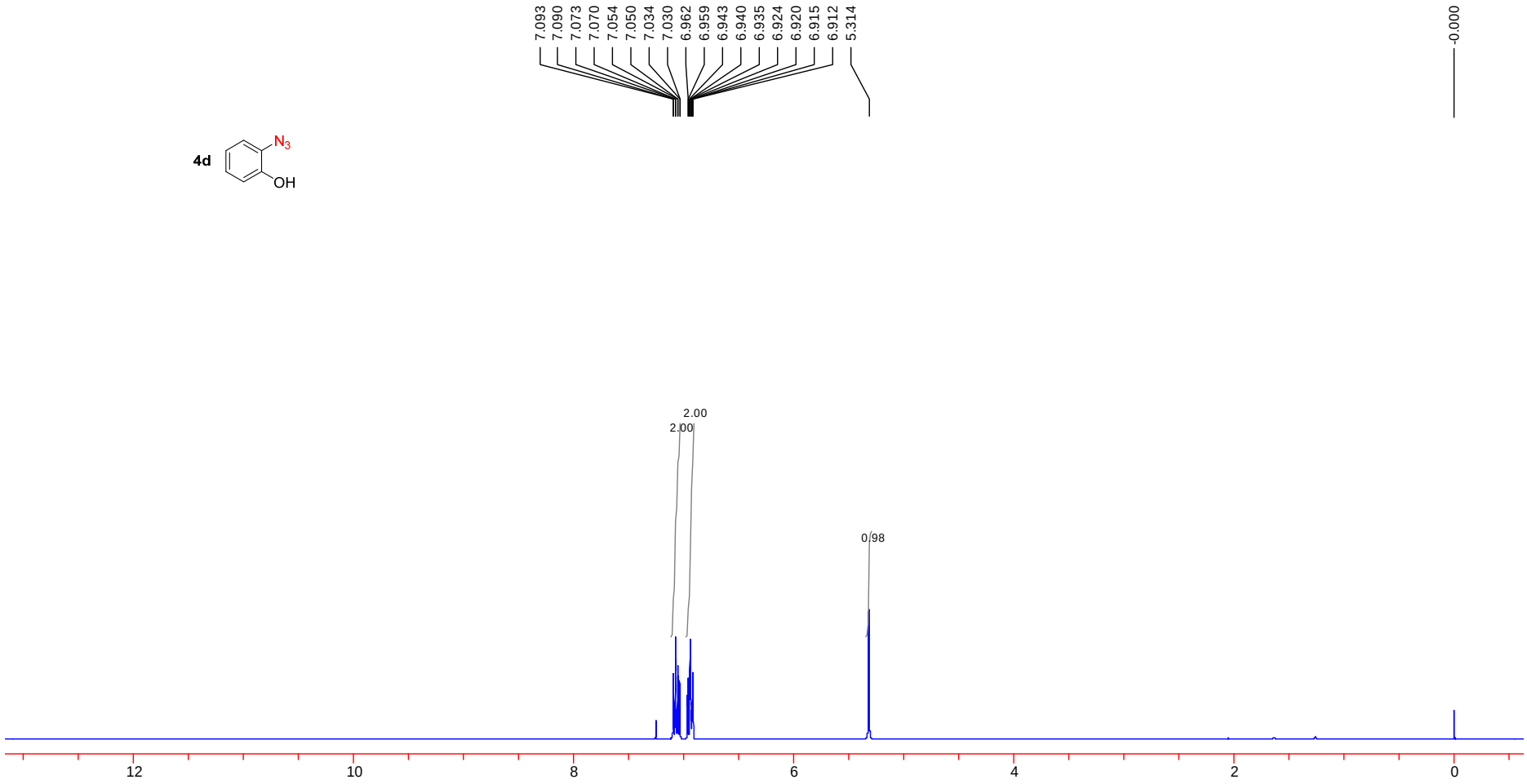
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6.920
6.915
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4d
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2.00
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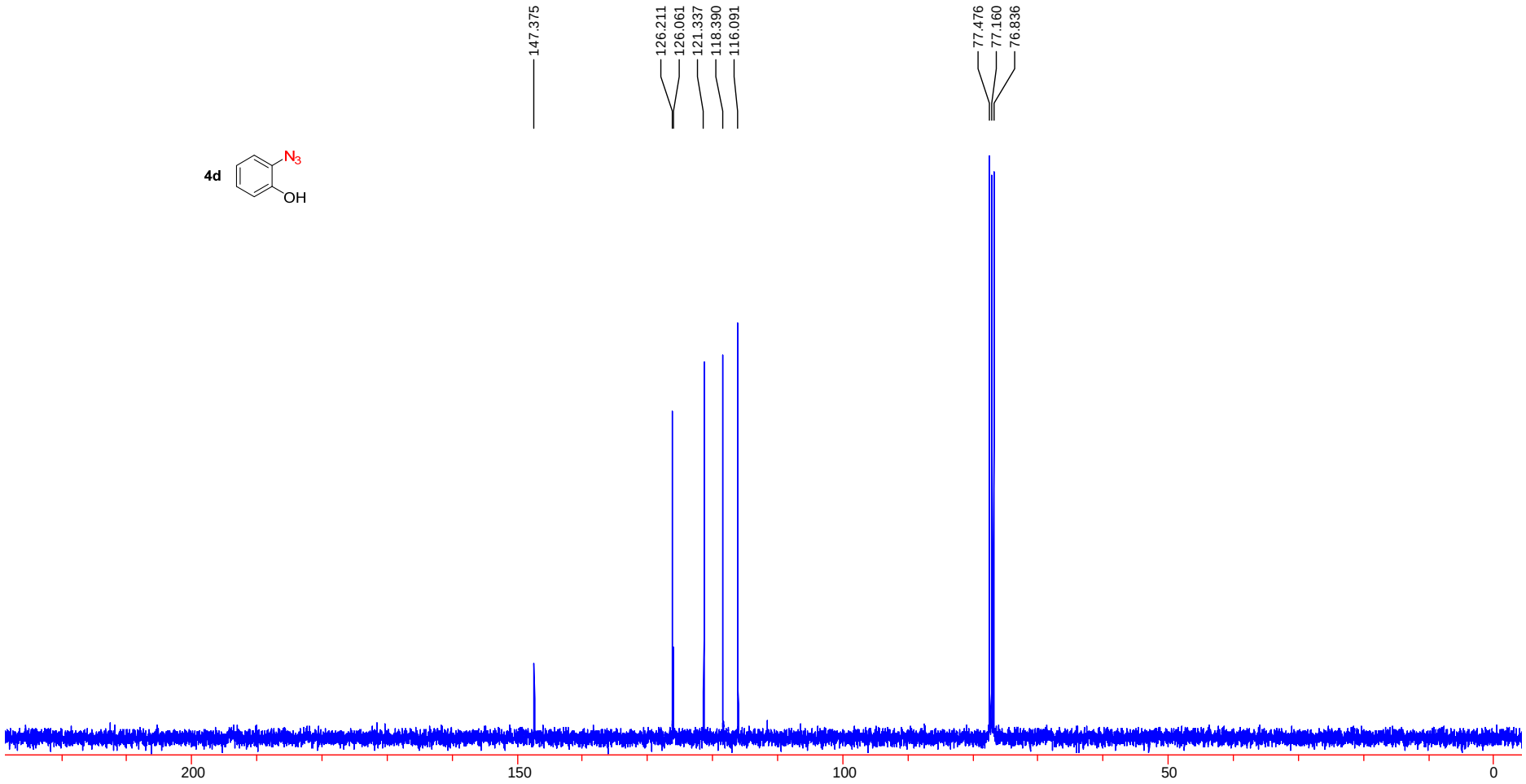
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4d
N3
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150
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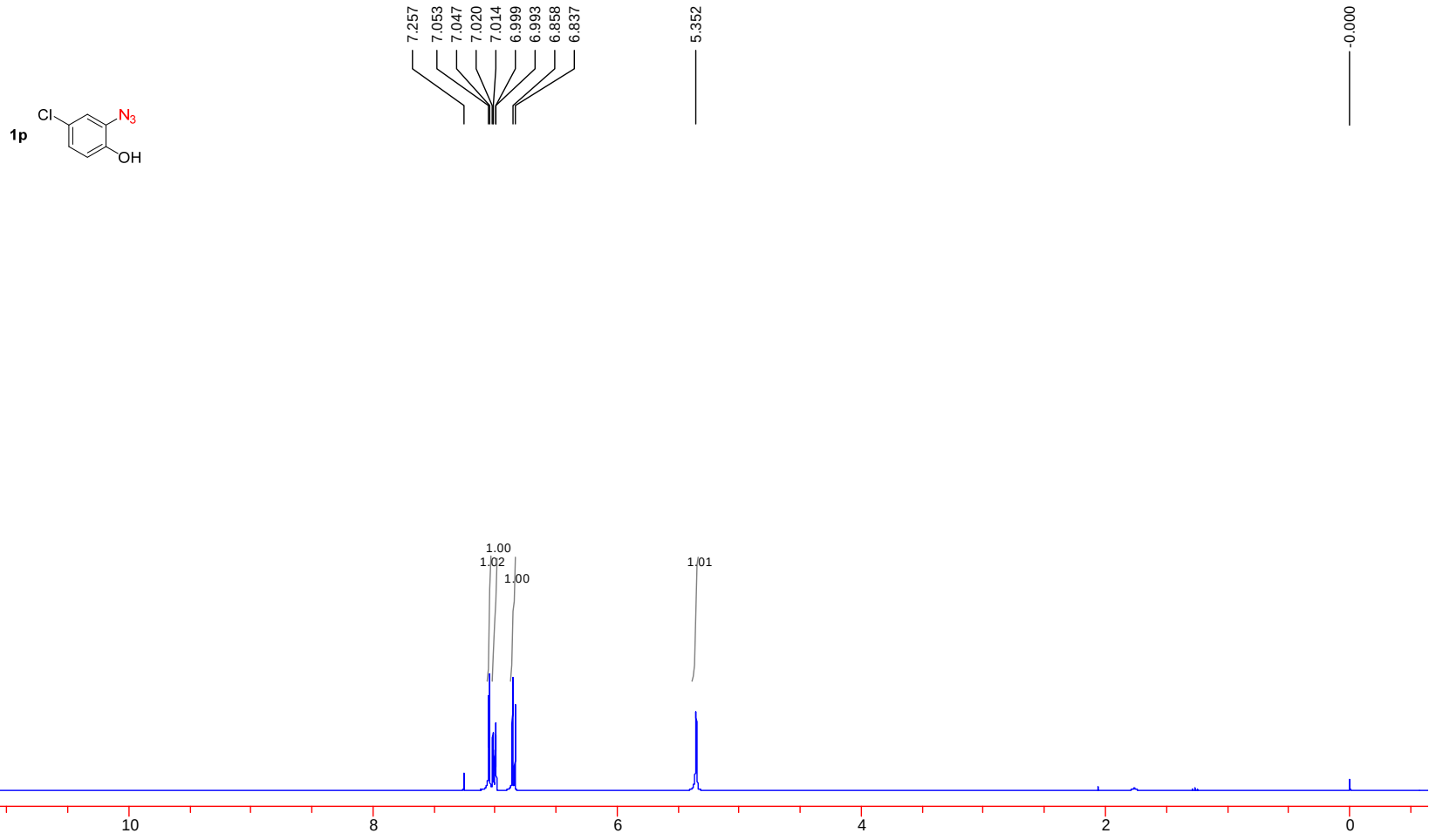
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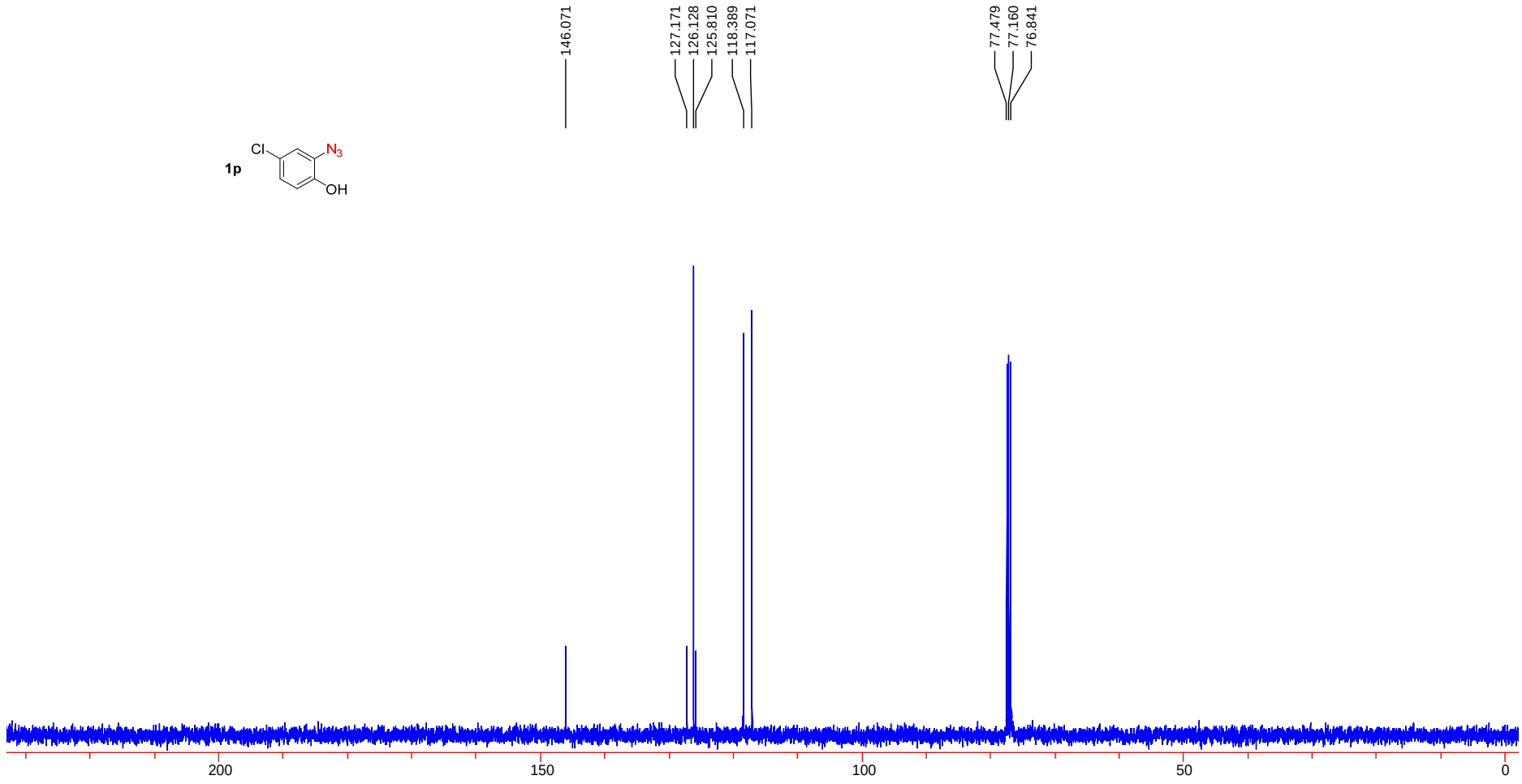
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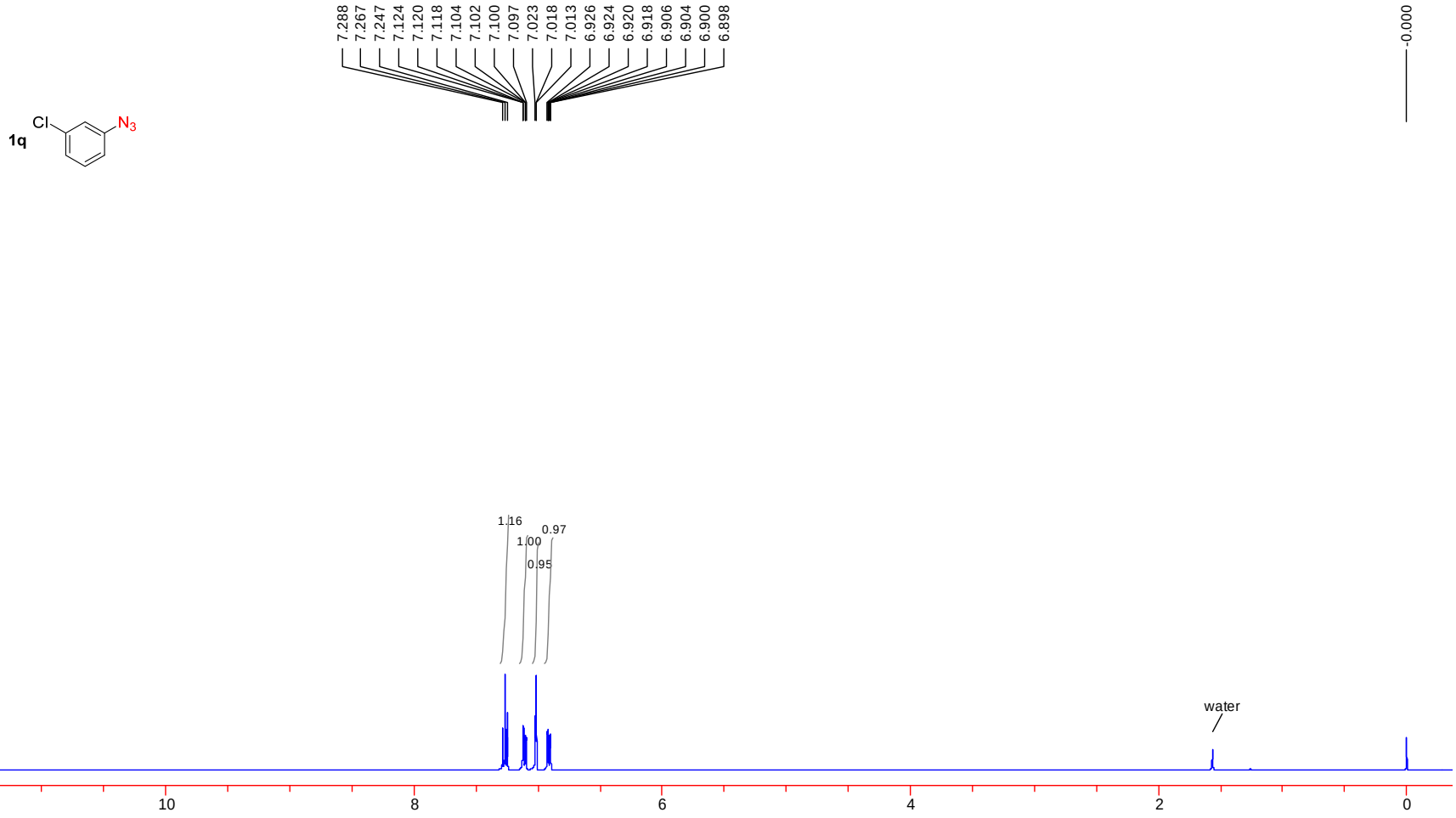
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7.013
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6.920
6.918
6.906
6.904
6.900
6.898
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Cl
N3
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0.95
0.97
water
12
10
8
6
4
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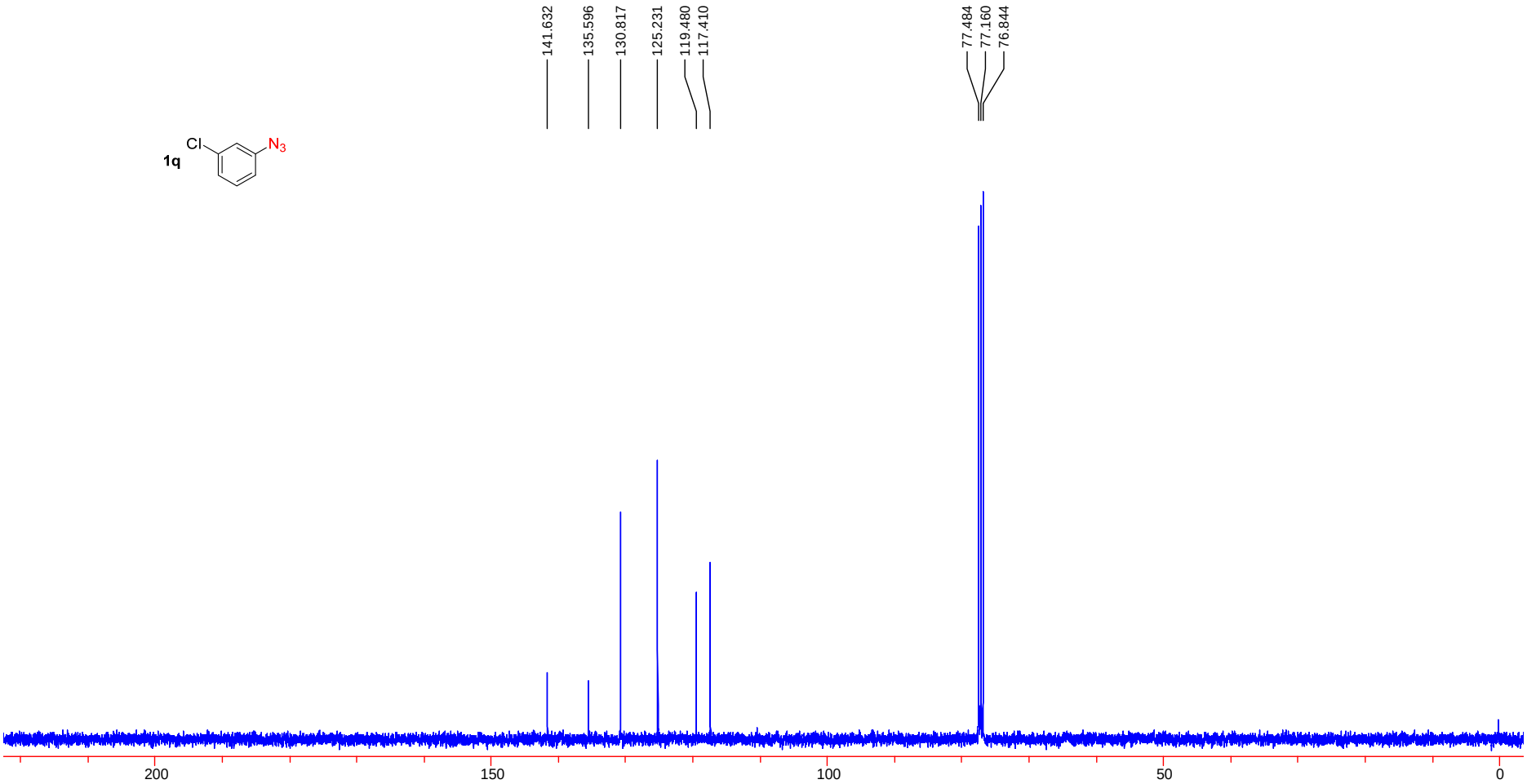
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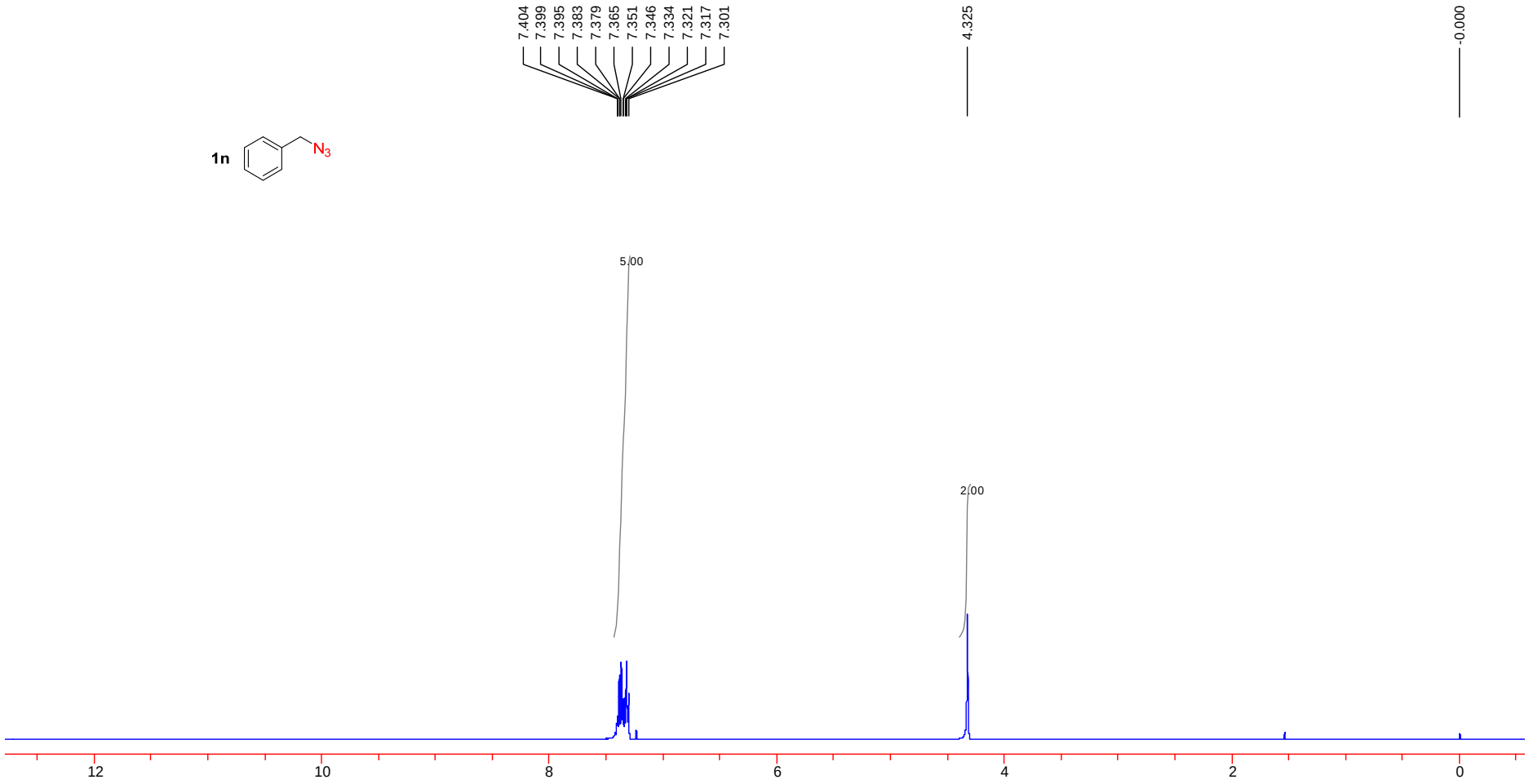
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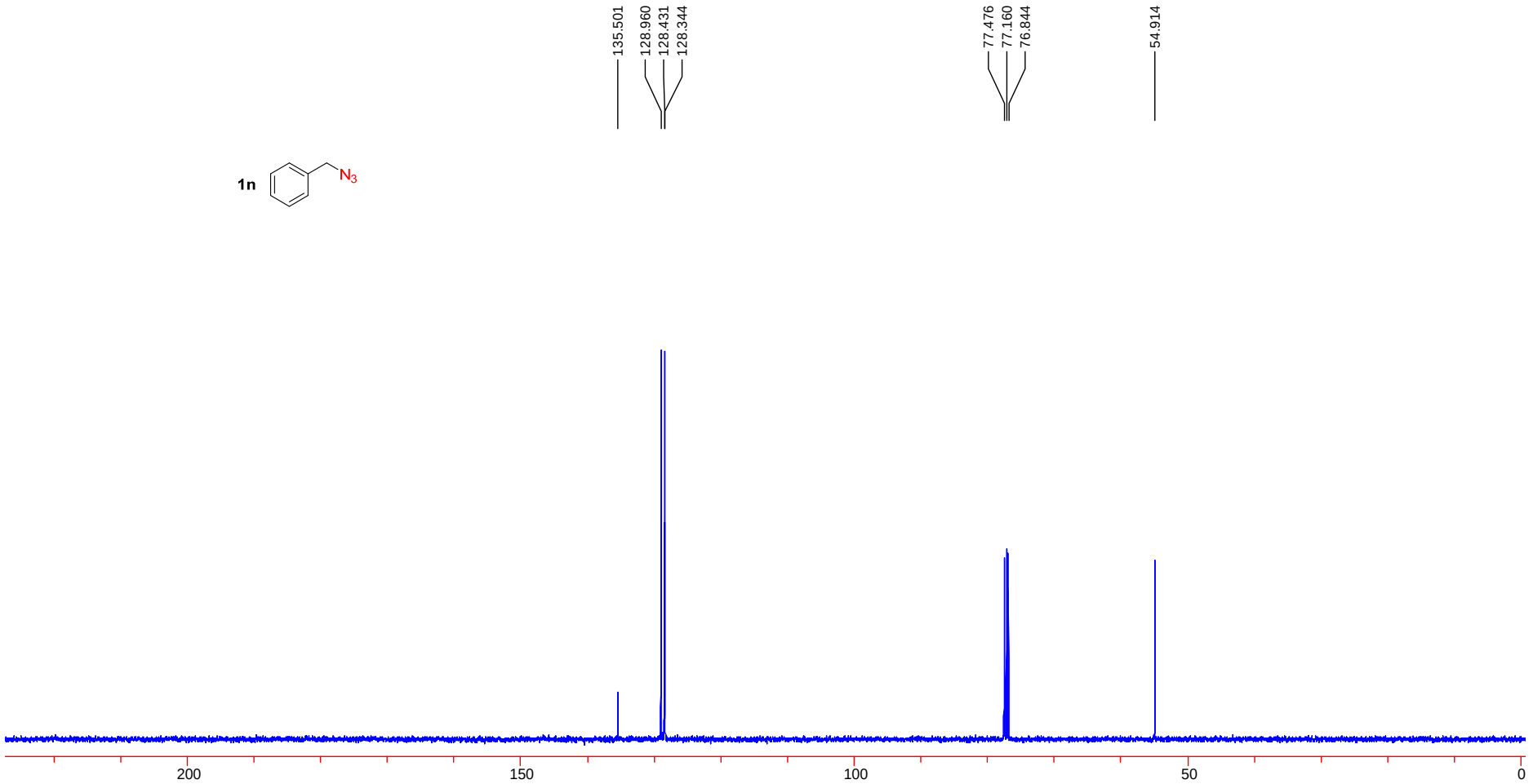
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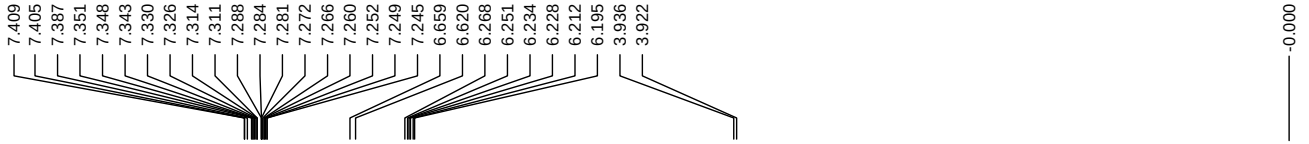
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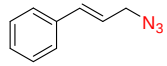
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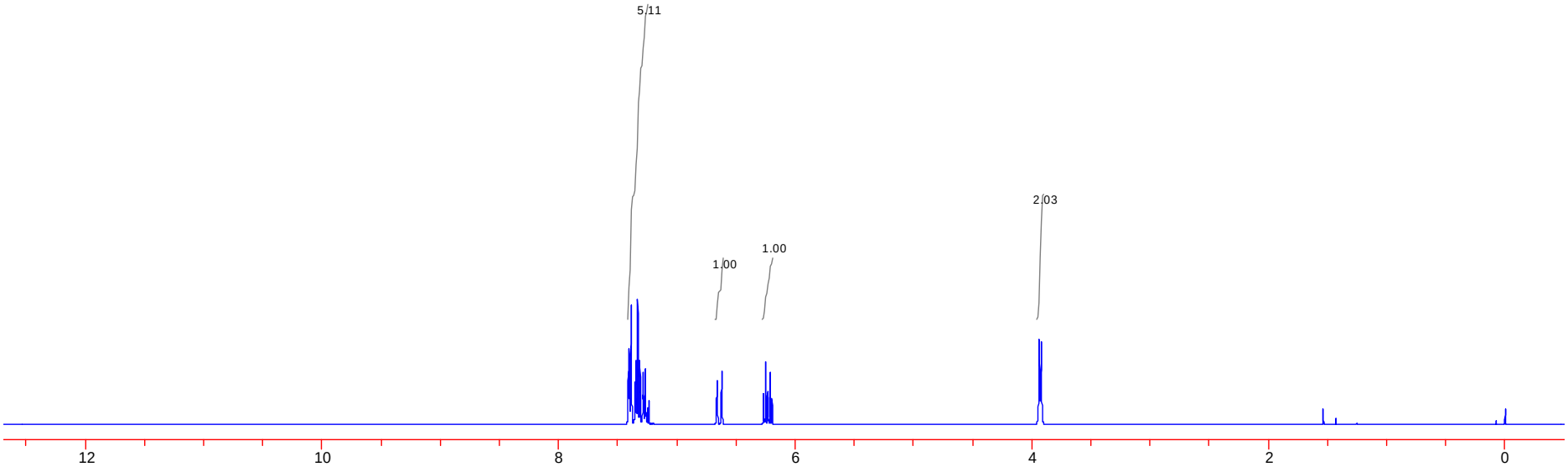
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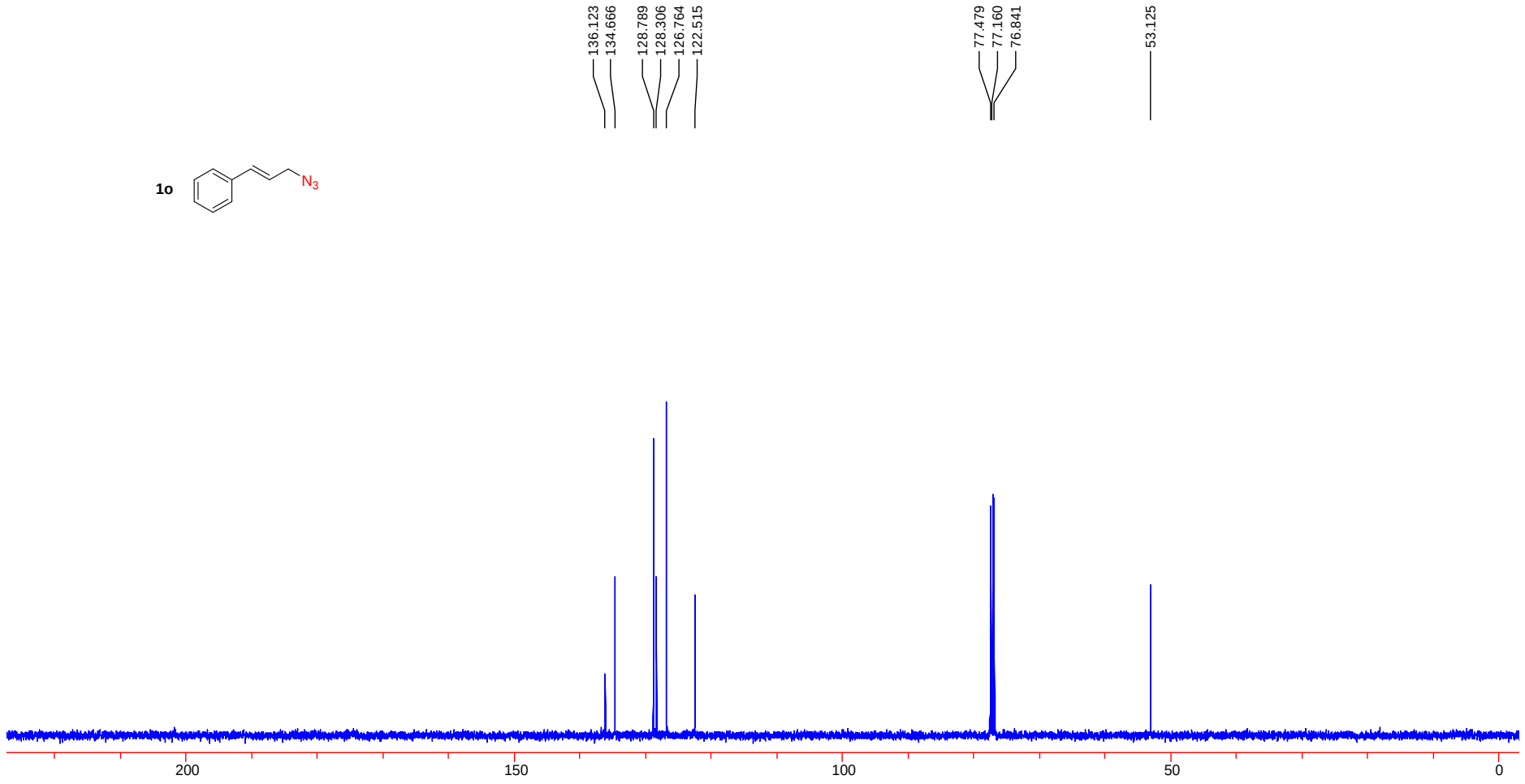
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150
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50
0