Electronic Supplementary Information for:

TEMP and Copper Cocatalyzed Oxygenation of Ketones with Molecular Oxygen: Chemoselective Synthesis of α-Ketoesters

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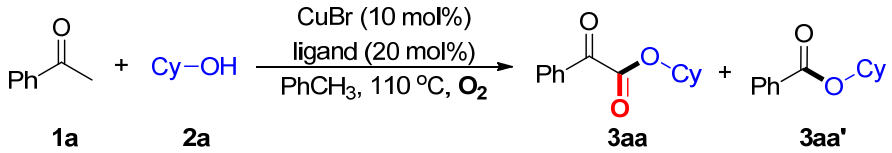
General Remarks

1a-1v, **2a-2q**, **2s**, ^{n}BuOH, α/β-Ionone, Nopol, β-Citronellol, Borneol, Menthol, Diacetone-*D*-Glucose, Cholesterol, **5a-5b**, **6**, and **7** are commercially available which are purchased from Sigma-Aldrich, Alfa-Aesar, Acros, Beijing Ouhe and Beijing Chemical Works, Ltd. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. **2r** was prepared through nucleophilic substitution of NaN_3 with 6-bromohexan-1-ol according to literature.[1] **1o-D_3** was prepared according to literature.[2]

Gas chromatography (GC) was performed on an Agilent Technologies 6820 chromatograph equipped with a HP-5 column (30 m × 0.32 mm, film thickness 0.25 μm). Analysis of crude reaction mixture was done on an Agilent 7890 GC System with an Agilent 5975 Mass Selective Detector. Products were purified by flash chromatography on silica gel. ^{1}H-NMR spectra were recorded on Bruker AVANCE III-400 spectrometers. Chemical shifts (in ppm) were referenced TMS in $CDCl_3$ (0 ppm). ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.00 ppm). Mass spectra were recorded using a PE SCLEX QSTAR spectrometer. High resolution mass spectra were obtained with a Bruker APEX IV Fourier transform ion cyclotron resonance mass spectrometer.

Screening of Reaction Parameters

Table S1. Screening of Ligands.[a]

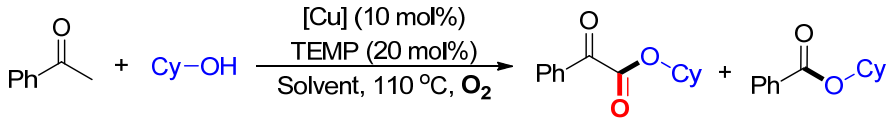


1a **2a** **3aa** **3aa'**

Entry	Ligand	Yield of **3aa** (%)[b]	Yield of **3aa'** (%)[b]
1	Py	27	3
2	**TEMP**	**75 (70)**	**2**
3	piperidine	0	0
4	pyrrole	0	0
5	$(^{i}Pr)_2NH$	9	0
6	$(Cy)_2NH$	6	1
7	1,10-phen	0	0
8	2,2'-Bpy	4	0
9	*L*-proline	0	0
10	pyrrolidine	0	0
11	$CyNH_2$	0	0
12	DMAP	25	33
13	2,6-dimethylpyridine	22	1
14	2,6-di-*tert*-butylpyridine	0	0
15	1,2-diaminocyclohexane	0	0

[a] Reaction conditions: **1a** (0.40 mmol), **2a** (0.80 mmol), CuBr (0.04 mmol), and ligand (0.08 mmol) in $PhCH_3$ (2.0 mL) under O_2 (balloon) was stirred at 110 °C for 10 h. [b] GC yields, isolated yield was listed in parentheses. Py = pyridine; TEMP = 2,2,6,6-tetramethylpiperidine; DMAP = *N*,*N*-dimethyl-4-aminopyridine; 1,10-Phen = phenanthroline; 2,2'-Bpy = 2,2'-bipyridine.

Table S2. Screening of Copper Salts and Solvents.[a]



1a **2a** **3aa** **3aa'**

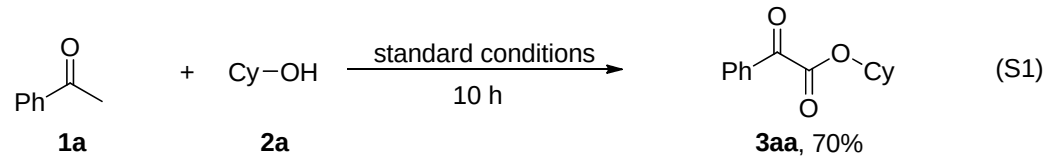
Entry	[Cu]	Solvent	Yield of **3aa** (%)[b]	Yield of **3aa'** (%)[b]
1	**CuBr**	**$PhCH_3$**	**75 (70)**	**2**
2	CuCl	$PhCH_3$	60	4
3	CuI	$PhCH_3$	3	0
4	$CuBr_2$	$PhCH_3$	47	6
5	$CuCl_2$	$PhCH_3$	31	10
6	$Cu(OAc)_2$	$PhCH_3$	13	0
7	CuBr	PhCl	48	2
8	CuBr	xylene	50	1
9	CuBr	DMF	5	2
10	CuBr	DMSO	0	0

[a] Reaction conditions: **1a** (0.40 mmol), **2a** (0.80 mmol), [Cu] (0.04 mmol), and TEMP (0.08 mmol) in Solvent (2.0 mL) under O_2 (balloon) was stirred at 110 °C for 10 h. [b] GC yields, isolated yield was listed in parentheses.

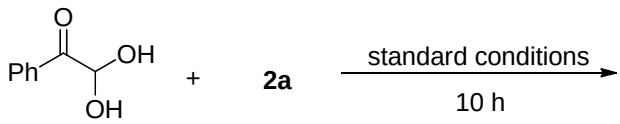
Control Experiments

（1）Investigation on potential intermediates:

Some potential intermediates were subjected to the reaction system. The results, listed in eqn (S1)-(S6), imply phenylglyoxal monohydrate might be a intermediate in this transformation. The reasonable fisrt step is the formation of phenylglyoxal intermediate via copper-catalyzed aerobic oxidation of methyl ketones. Subsequent dehydrogenative coupling of alcohol and phenylglyoxal would generate α-ketoester. Furthermore, copper catalsyst, *N*-ligand and molecular oxygen are essential to the dehydrogenative coupling of alcohol and phenylglyoxal monohydrate (eqn (S2)).

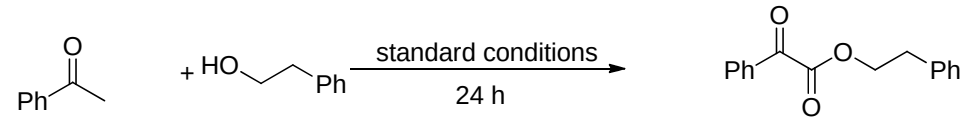


1a **2a** **3aa**, 70% (S1)

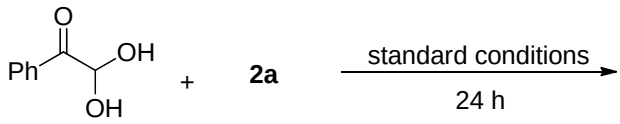


5a **2a** **3aa**, 89% (S2)

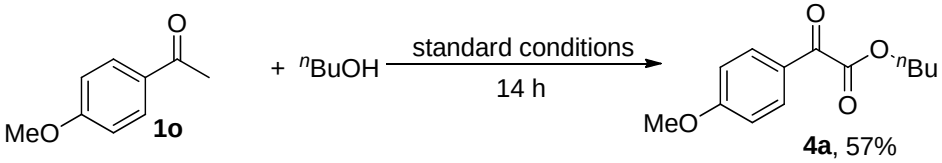
without CuBr: 0%
without TEMP: 0%
Ar instead of O_2: 0%



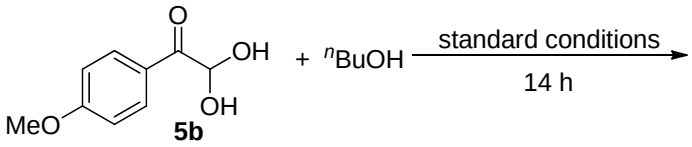
1a **2b** **3ab**, 75% (S3)



5a **2a** **3ab**, 71% (S4)

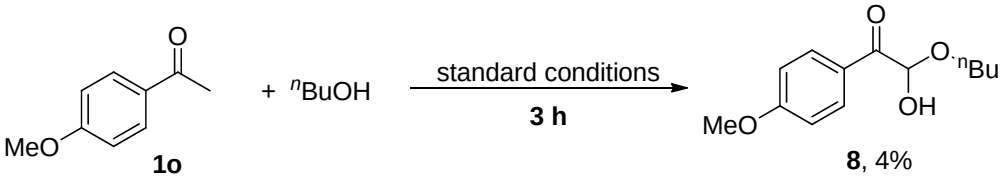


1o **4a**, 57% (S5)

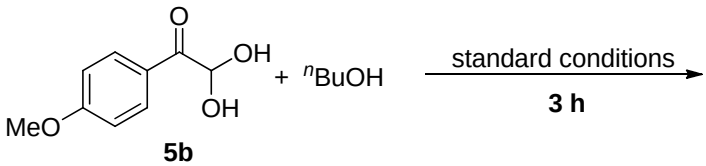


5b **4a**, 81% (S6)

（2）Isolation of 8:



1o **8**, 4% (S7)

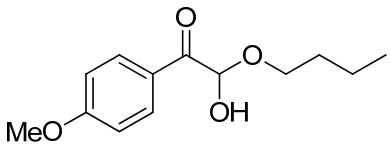


5b **8**, 46% (S8)

Eqn (S7): Mix **1o** (60.1 mg, 0.40 mmol), ^{n}BuOH (59.4 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under

O_2 (balloon). The reaction mixture was stirred at 110 ^oC for ***3h***, the mixture was cooled to room temperature and concentrated in vacuum. The residue was purified by flash chromatography on a short silica gel (eluent: petroleum ether/ethyl acetate = 10/1) to afford 4.1 mg (4%) of **8** (eqn (S7)). Besides, the reaction of **5b** and ^{n}BuOH under the above conditions, could afford 44.3 mg (46%) of **8** (eqn (S8)).

Based on these results (eqn (S5)-(S8)), we postulate that α-hydroxyl ester, generating from the addition of alcohol to phenylglyoxal monohydrate, might be a key intermediate in the process.



2-Butoxy-2-hydroxy-1-(4-methoxyphenyl)ethanone (8):

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 87.32 (d, *J* = 8.4 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 5.10 (d, *J* = 5.6 Hz, 1H), 4.22-4.08 (m, 2H), 3.80 (s, 3H), 3.48 (d, *J* = 5.6, 1H), 1.60-1.51 (m, 2H), 1.32-1.20 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 173.9, 159.6, 130.7, 127.7, 113.9, 72.4, 65.8, 55.2, 30.3, 18.8, 13.5 ppm;

HRMS *m/z* (ESI) calcd for $C_{13}H_{18}NaO_4$ $(M + Na)^+$, 261.1097, found 261.1096.

Radical Trapping Experiments

When employing TEMPO (2,2,6,6-tetramethyl-piperidinooxy), or BHT (2,6-di-*tert*-4-methylphenol) as radical trapper, the reactions were mostly inhibited (eqn (S9)-(S10)), which suggested radical species might involves during the reaction. Yield of **3aa** was determined by GC:

1a **2a** **3aa**, 0% (S9)

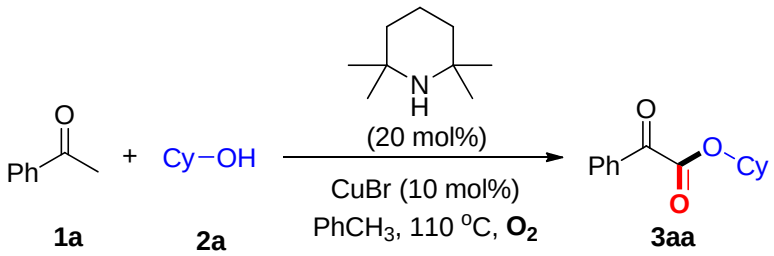
1a **2a** **3aa**, 0% (S10)

EPR Spectra

EPR spectra were recorded at room temperature on a Bruker ESP-300 spectrometer operating at 9.7 GHz and a cavity equipped with a Bruker Aquax liquid sample cell. Typical spectrometer parameters were: Receiver Gain = $1.00*10^5$; Phase = 60 deg; Harmonic = 1; Mod. Frequency = 100 KHz; Mod. Amplitude = 2 G; Center Field = 3430 G; Sweep width = 120 G; Resolution = 1024 points; Conversion = 40.960 ms; Time const = 20.480 m; Sweep time = 41.943 s; Power = 10 mW.

DMPO (5,5-dimethyl-1-pyrroline *N*-oxide) was employed as the radical trap agent. The EPR results are summarized in Table S3:

Table S3. The EPR Results of Different Conditions.



1a **2a** **3aa**

Entry	Variation from S.C.	Yield of **3aa** (%)	EPR signals	Figure No.
1	none	72%	hydroxyl radical	Figure S1
2	SC +SOD	--	hydroxyl radical (much weaker)	Figure S2
3	without **1a**	0	TEMPO radical	Figure S3
4	without **2a**	0	none	Figure S4
5	without CuBr	0	TEMPO radical	Figure S5
6	without TMP	0	nearly none	Figure S6
7	Ar instead of O_2	0	none	Figure S7

Discussions：1) These results imply a hydroxyl radical might be generated during

the transformation. It is known that half-life of hydroxyl radical ($HO^{\bullet}$) is much longer than superoxide radical anion ($O^{\bullet-}$). And a few of $HO^{\bullet}$ that derives from superoxide radical anion might exist in reation systems before the addition of SOD, leading to the results of entry 2. (2) TEMP could be oxidized to TEMPO under aerobic condition,[3] which have been captured by EPR (entries 3, and 5). However, it is not clear yet why no TEMPO signals was observed under conditions of entry 4.

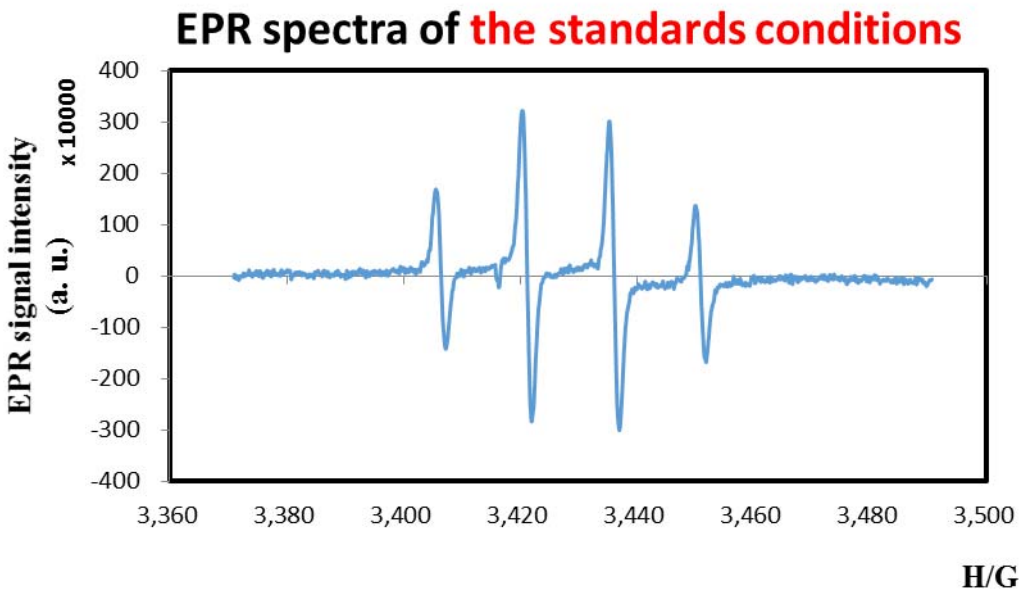


Figure S1. EPR spectra (X band, 9.7 GHz, RT) of the standard conditions: **1a** (0.40 mmol), **2a** (0.80 mmol), CuBr (0.04 mmol), and TEMP (0.08 mmol) in $PhCH_3$ (2.0 mL) under O_2 was stirred at 110 ^{o}C for 1h. 0.01 mL of this reaction solution was taken out into a small tube, followed by the addition of 0.01 mL DMPO (0.9 M). Then, this mixture was analysed by EPR. Signals corresponding to hydroxyl radical were observed.

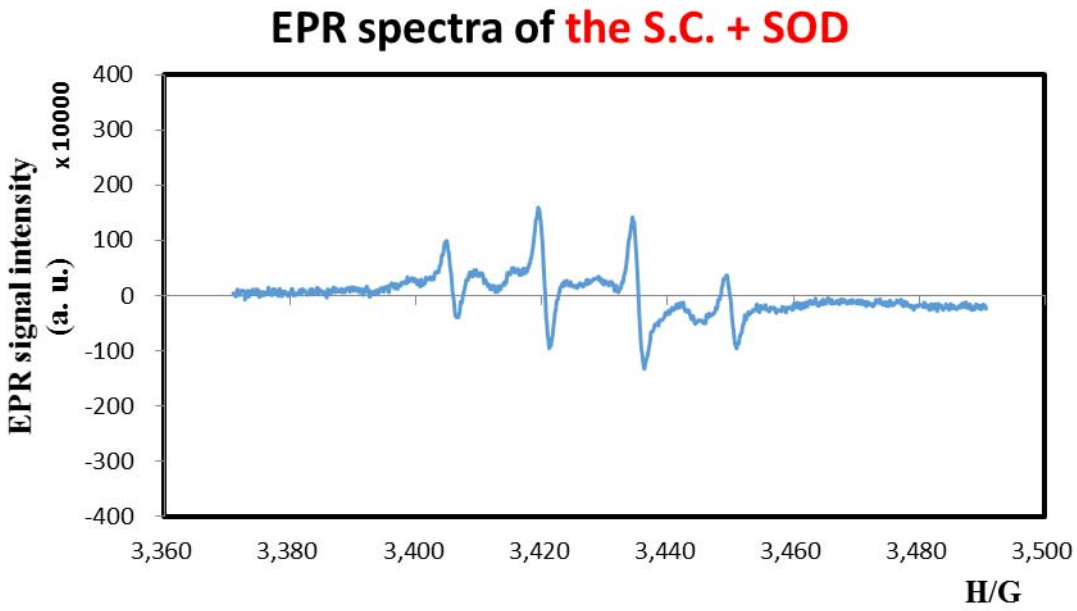


Figure S2. EPR spectra (X band, 9.7 GHz, RT) of the standard conditions + SOD: **1a** (0.40 mmol), **2a** (0.80 mmol), CuBr (0.04 mmol), and TEMP (0.08 mmol) in $PhCH_3$ (2.0 mL) under O_2 was stirred at 110 ^oC for 1h. 0.01 mL of this reaction solution was taken out into a small tube, mixed well with 0.02 mL SOD solvent (1 M) followed by the addition of 0.01 mL DMPO (0.9 M). Then, this mixture was analysed by EPR.

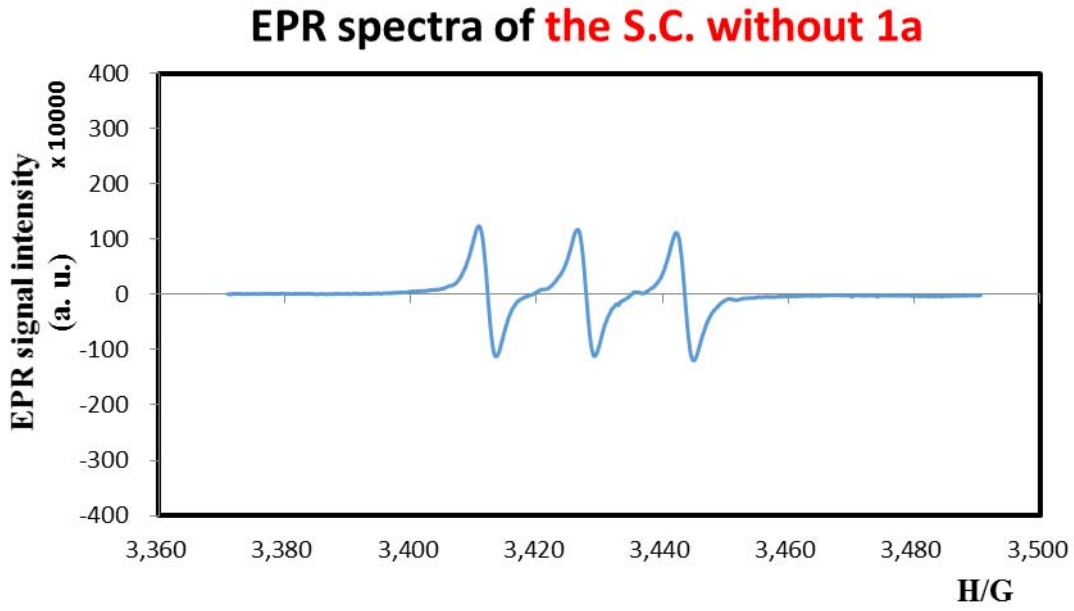


Figure S3. EPR spectra (X band, 9.7 GHz, RT) of the S.C. without **1a**: **2a** (0.80 mmol), CuBr (0.04 mmol), and TEMP (0.08 mmol) in $PhCH_3$ (2.0 mL) under O_2 was stirred at 110 ^oC for 1h. 0.01 mL of this reaction solution was taken out into a small tube, followed by the addition of 0.01 mL DMPO (0.9 M). Then, this mixture was analysed by EPR.

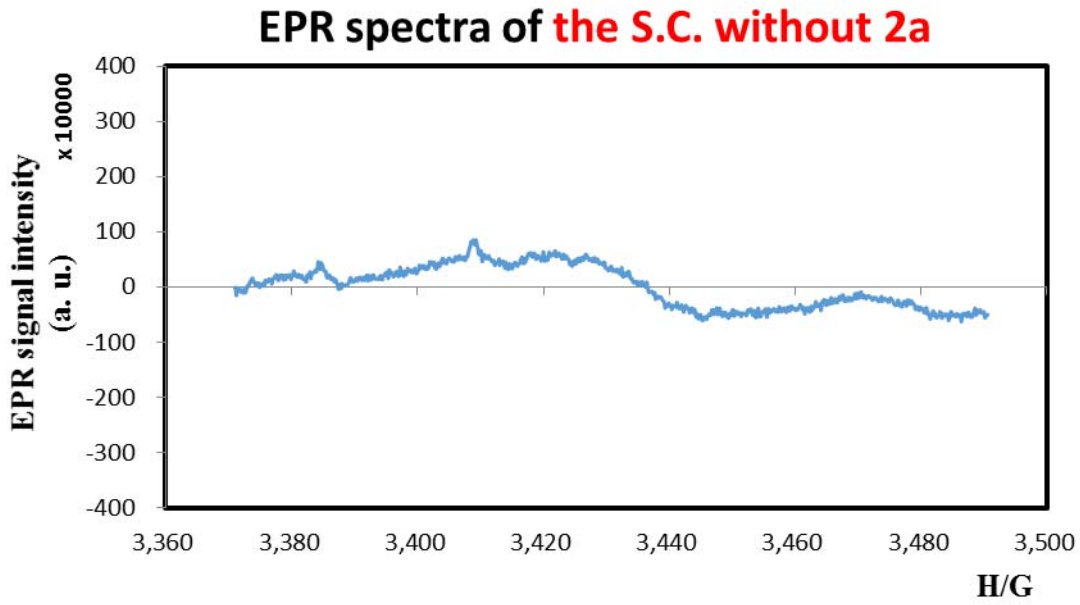


Figure S4. EPR spectra (X band, 9.7 GHz, RT) of the S.C. without **2a**: **1a** (0.40 mmol), CuBr (0.04 mmol), and TEMP (0.08 mmol) in $PhCH_3$ (2.0 mL) under O_2 was stirred at 110 ^oC for 1h. 0.01 mL of this reaction solution was taken out into a small tube, followed by the addition of 0.01 mL DMPO (0.9 M). Then, this mixture was analysed by EPR.

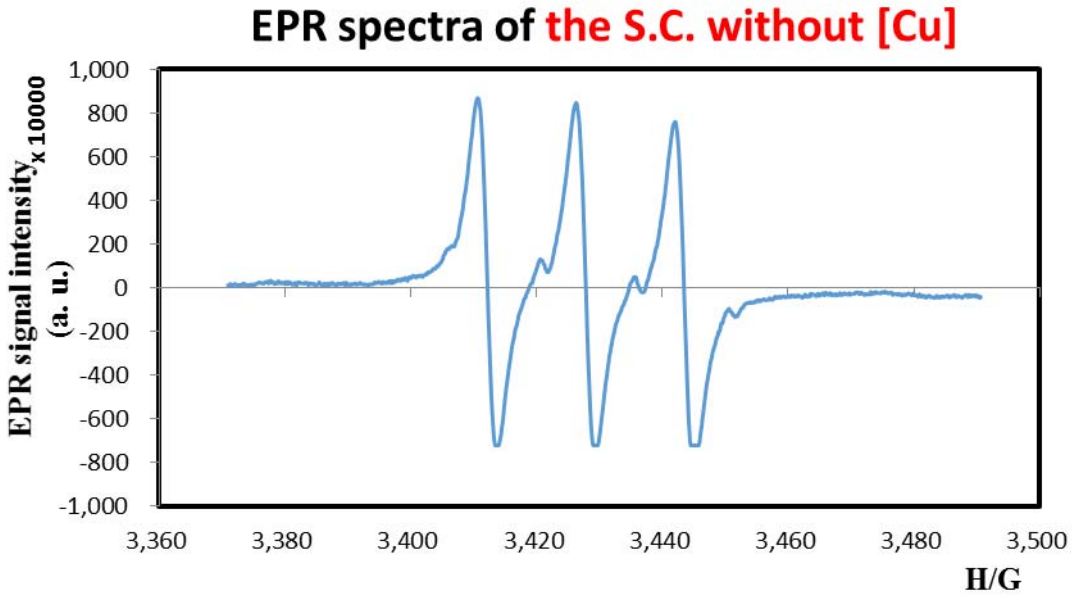


Figure S5. EPR spectra (X band, 9.7 GHz, RT) of the S.C. without [Cu]: **1a** (0.40 mmol), **2a** (0.80 mmol), and TEMP (0.08 mmol) in $PhCH_3$ (2.0 mL) under O_2 was stirred at 110 ^oC for 1h. 0.01 mL of this reaction solution was taken out into a small tube, followed by the addition of 0.01 mL DMPO (0.9 M). Then, this mixture was analysed by EPR.

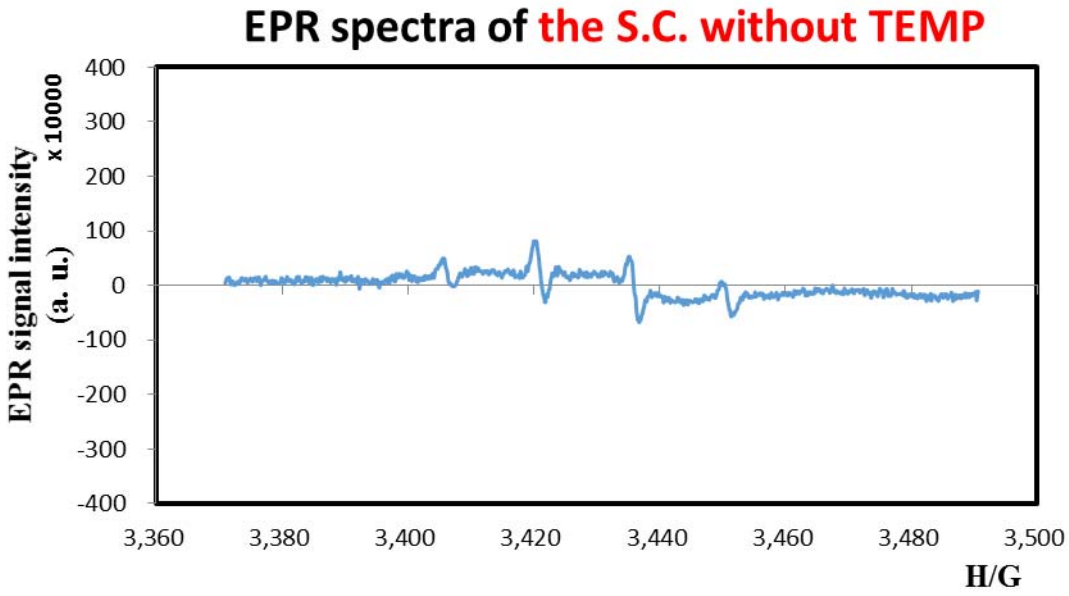


Figure S6. EPR spectra (X band, 9.7 GHz, RT) of the S.C. without TEMP: **1a** (0.40 mmol), **2a** (0.80 mmol), and CuBr (0.04 mmol) in $PhCH_3$ (2.0 mL) under O_2 was stirred at 110 ^oC for 1h. 0.01 mL of this reaction solution was taken out into a small tube, followed by the addition of 0.01 mL DMPO (0.9 M). Then, this mixture was analysed by EPR.

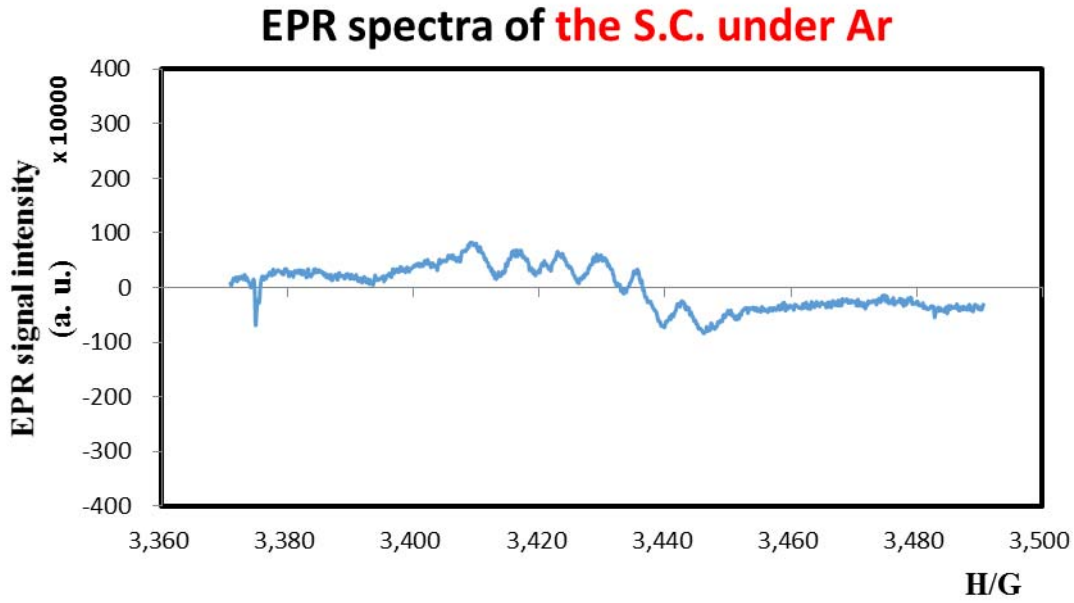
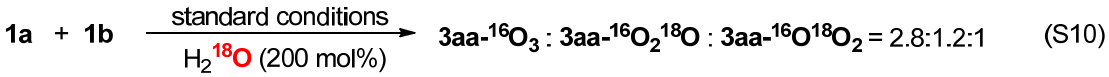


Figure S7. EPR spectra (X band, 9.7 GHz, RT) of the S.C. under Ar: **1a** (0.40 mmol), **2a** (0.80 mmol), CuBr (0.04 mmol), and TEMP (0.08 mmol) in $PhCH_3$ (2.0 mL) under Ar was stirred at 110 ^oC for 1h. 0.01 mL of this reaction solution was taken out into a small tube, followed by the addition of 0.01 mL DMPO (0.9 M). Then, this mixture was analysed by EPR.

Labeling Experiments

（1） ^{18}O labelling experiment with $H_2{}^{18}O$



Mix acetophenone **1a** (48.1 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), TEMP (11.3 mg, 0.080 mmol), and $\mathbf{H_2{}^{18}O}$ (16.0 mg, 0.80 mmol) in $PhCH_3$ (2.00 mL) under $^{16}O_2$ (balloon). The reaction mixture was stirred at 110 ^{o}C for 10 h, After cooling down to room temperature, the mixture was measured by GC-MS (m/z = 107 is detected, Figure S8) and HRMS (**3aa-$^{16}O_3$** : **3aa-$^{16}O_2{}^{18}O$** : **3aa-$^{16}O{}^{18}O_2$** = 2.8:1.2:1, Figure S9). The ^{18}O labelling at keto-carbonyl group of product supports the reversible condensation of ketone with amine, as well as the hydrolysis of **E** (Scheme 4 of text). The observation of **3aa-$^{16}O{}^{18}O_2$** might be reasonably accounted by the equilibrium between $\mathbf{F^1}$ and $\mathbf{F^2}$ (Scheme 4 of text).

Furthermore, no product could be obtained adding 4Å MS into the standard conditions. All these results demonstrate that water is participated in organocatalytic cycle and oxygen atom exchange of H_2O with ketones, phenylglyoxal monohydrate intermediates might occur during the transformation.

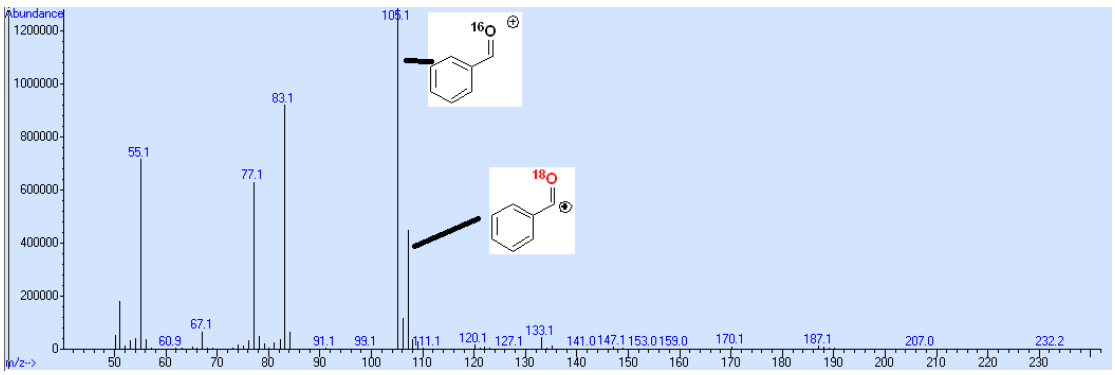


Figure S8. GC-MS Analysis of the Mixture of Labelling Experiment under $H_2{}^{18}O$.

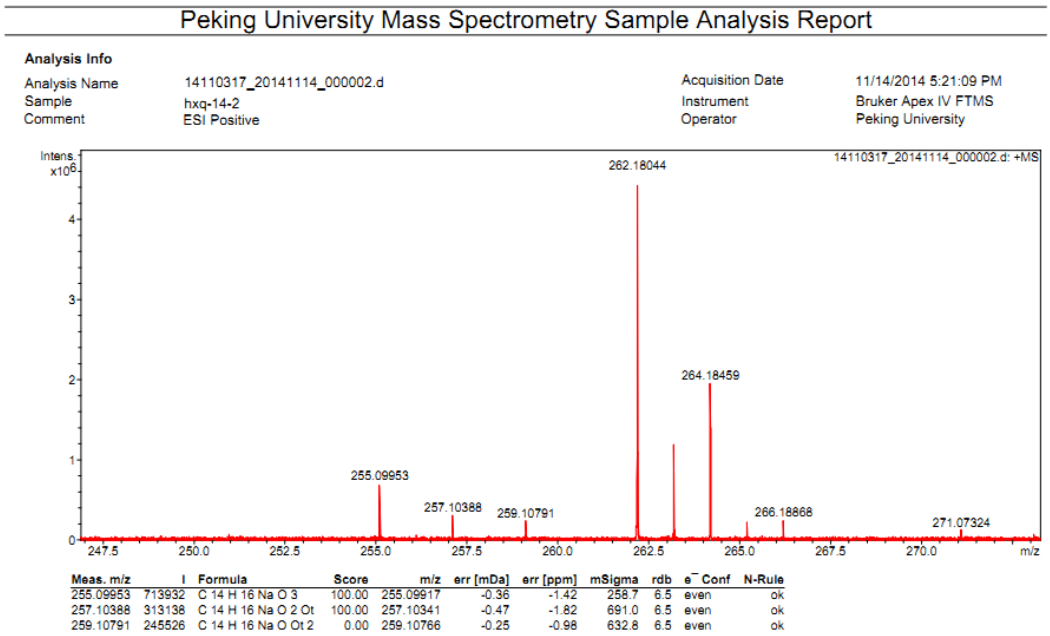


Figure S9. HRMS Analysis of the Mixture of Labelling Experiment under $H_2{}^{18}O$.

（2） ^{18}O labeling experiment with $^{18}O_2$

Because $H_2{}^{18}O$ would be generated from molecular $^{18}O_2$ under the standard conditions, labelling experiment with $^{18}O_2$ would not give solid proof about the O-source of new forming ester-carbonyl group.

We performed the reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), TEMP (11.3 mg, 0.080 mmol), in $PhCH_3$ (2.00 mL) under $^{18}O_2$. The reaction mixture was stirred at 110 ^oC for 10 h, After cooling down to room temperature, the mixture was measured by GC-MS (Figure S10). m/z = 107 peak was ovserved too. Notably, the abundance of m/z = 107 is higher than m/z = 105. (cf. Fogure S8).

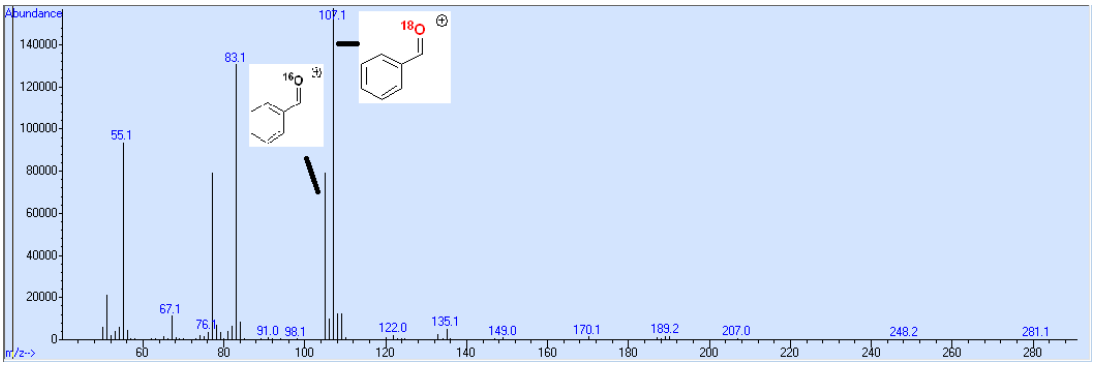
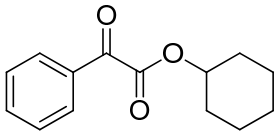


Figure S10. GC-MS Analysis of the Mixture of Labelling Experiment under $^{18}O_2$.

Experimental Procedure and Characterization Data for Products

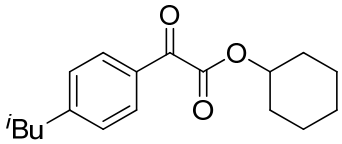


01) **3aa**

Cyclohexyl 2-oxo-2-phenylacetate (3aa):[4]

Typical procedure: Mix acetophenone **1a** (48.1 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (2,2,6,6-tetramethylpiperidine, 11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon). The reaction mixture was stirred at 110 ^oC. After the disappearance of **1a** (TLC detection, 10 h for **3aa**), the mixture was cooled to room temperature and concentrated in vacuum. The residue was purified by flash chromatography on a short silica gel (eluent: petroleum ether/ethyl acetate = 100/1) to afford 65.4 mg (70%) of **3aa**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.02-7.96 (m, 2H), 7.65 (tt, J_1 = 7.4 Hz, J_2 = 1.2 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 5.14-5.05 (m, 1H), 2.03-1.98 (m, 2H), 1.82-1.75 (m, 2H), 1.67-1.54 (m, 3H), 1.49-1.24 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.8, 163.6, 134.7, 132.5, 129.9, 128.8, 75.4, 31.4, 25.1, 23.6 ppm.



02)

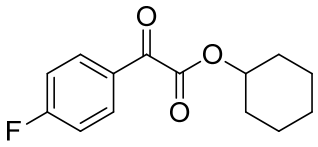
Cyclohexyl 2-(4-isobutylphenyl)-2-oxoacetate (3ba):

The reaction of 1-(4-isobutylphenyl)ethanone **1b** (70.5 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 24 h, afforded 99.9 mg (82%) of **3ba**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.91 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 5.13-5.05 (m, 1H), 2.56 (d, J = 7.2 Hz, 2H), 2.03-1.96 (m, 2H), 1.95-1.86 (m, 1H), 1.85-1.73 (m, 2H), 1.66-1.54 (m, 3H), 1.49-1.24 (m, 3H), 0.91 (d, J = 6.8 Hz, 6H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ

= 186.5, 163.9, 149.8, 130.3, 129.9, 129.6, 75.3, 45.5, 31.4, 30.0, 25.1, 23.6, 22.3 ppm;

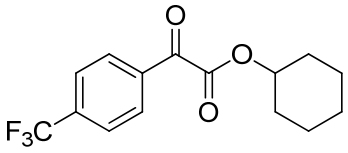
HRMS *m/z* (ESI) calcd for $C_{18}H_{24}NaO_3$ $(M + Na)^+$, 311.1618, found 311.1620.

03) 

Cyclohexyl 2-(4-fluorophenyl)-2-oxoacetate (3ca):[5]

The reaction of 1-(4-fluorophenyl)ethanone **1c** (55.3 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 13 h, afforded 77.7 mg (78%) of **3ca**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.09-8.02 (m, 2H), 7.28-7.15 (m, 2H), 5.13-5.05 (m, 1H), 2.04-1.96 (m, 2H), 1.84-1.74 (m, 2H), 1.66-1.54 (m, 3H), 1.49-1.24 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.9, 166.7 (d, *J* = 256.4 Hz), 163.2, 132.8 (d, *J* = 9.0 Hz), 129.1 (d, *J* = 3.6 Hz), 116.2 (d, *J* = 21.4 Hz), 75.6, 31.4, 25.1, 23.6 ppm.

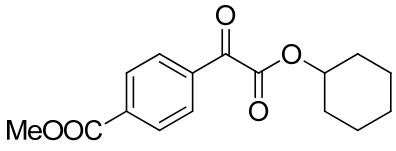
04) 

Cyclohexyl 2-oxo-2-(4-(trifluoromethyl)phenyl)acetate (3da):

The reaction of 1-(4-(trifluoromethyl)phenyl)ethanone **1d** (75.3 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 16 h, afforded 78.7 mg (66%) of **3da**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.14 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.4 Hz, 2H), 5.15-5.07 (m, 1H), 2.05-1.96 (m, 2H), 1.85-1.75 (m, 2H), 1.68-1.55 (m, 3H), 1.50-1.25 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.4, 162.6, 135.7 (q, *J* = 31.7 Hz), 135.4, 130.3, 125.9 (q, *J* = 3.1 Hz), 123.3 (q, *J* = 271.7 Hz), 76.0, 31.4, 25.1, 23.6 ppm;

HRMS *m/z* (ESI) calcd for $C_{15}H_{15}F_3NaO_3$ $(M + Na)^+$, 323.0866, found 323.0871.

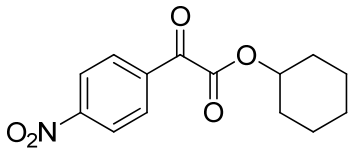
05) 

Methyl 4-(2-(cyclohexyloxy)-2-oxoacetyl)benzoate (3ea):

The reaction of methyl 4-acetylbenzoate **1e** (71.3 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 16 h, afforded 70.0 mg (60%) of **3ea**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.19-8.14 (m, 2H), 8.10-8.04 (m, 2H), 5.15-5.07 (m, 1H), 3.96 (s, 3H), 2.05-1.96 (m, 2H), 1.84-1.75 (m, 2H), 1.68-1.55 (m, 3H), 1.51-1.25 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.9, 165.8, 162.9, 135.7, 135.2, 129.9, 129.8, 75.7, 52.5, 31.3, 25.1, 23.5 ppm;

HRMS *m/z* (ESI) calcd for $C_{16}H_{18}NaO_5$ $(M + Na)^+$, 313.1046, found 313.1051.

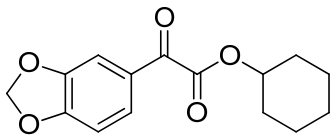
06) 

Cyclohexyl 2-(4-nitrophenyl)-2-oxoacetate (3fa):

The reaction of 1-(4-nitrophenyl)ethanone **1f** (66.1 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 16 h, afforded 69.3 mg (62%) of **3fa**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.36 (dt, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 2H), 8.22 (dt, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 2H), 5.15-5.07 (m, 1H), 2.05-1.97 (m, 2H), 1.85-1.75 (m, 2H), 1.70-1.55 (m, 3H), 1.52-1.25 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.5, 162.0, 151.0, 137.1, 131.0, 123.9, 76.2, 31.3, 25.0, 23.5 ppm;

HRMS *m/z* (ESI) calcd for $C_{14}H_{15}NNaO_5$ $(M + Na)^+$, 300.0842, found 300.0845.

07) 

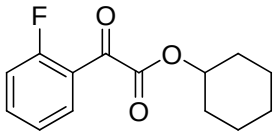
Cyclohexyl 2-(benzo[*d*][1,3]dioxol-5-yl)-2-oxoacetate (3ga):

The reaction of 1-(benzo[*d*][1,3]dioxol-5-yl)ethanone **1g** (65.7 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 15 h, afforded 66.2 mg (60%) of **3ga**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.58 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.45 (d, J = 1.2 Hz, 1H), 6.89 (d, J = 8.0 Hz, 1H), 6.08 (s, 2H), 5.11-5.04 (m, 1H), 2.05-1.94 (m, 2H), 1.84-1.74 (m,

2H), 1.65-1.53 (m, 3H), 1.49-1.24 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.9, 163.8, 153.4, 148.4, 127.6, 127.2, 108.5, 108.2, 102.2, 75.3, 31.3, 25.1, 23.6 ppm;

HRMS *m/z* (ESI) calcd for $C_{15}H_{16}NaO_5$ $(M + Na)^+$, 299.0890, found 299.0890.

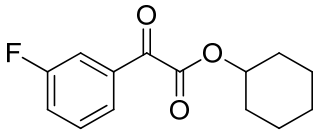
08) 

Cyclohexyl 2-(2-fluorophenyl)-2-oxoacetate (3ha):

The reaction of 1-(2-fluorophenyl)ethanone **1h** (55.3 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 80.2 mg (80%) of **3ha**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.94 (td, J_1 = 7.4 Hz, J_2 = 1.6 Hz, 1H), 7.68-7.60 (m, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.20-7.12 (m, 1H), 5.11-5.02 (m, 1H), 2.04-1.94 (m, 2H), 1.84-1.74 (m, 2H), 1.68-1.53 (m, 3H), 1.48-1.22 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.3, 163.8, 162.7 (d, J = 256.5 Hz), 136.6 (d, J = 8.1 Hz), 130.8, 124.8 (d, J = 4.3 Hz), 121.7 (d, J = 10.3 Hz), 116.5 (d, J = 21.3 Hz), 75.5, 31.2, 25.1, 23.6 ppm;

HRMS *m/z* (ESI) calcd for $C_{14}H_{15}FNaO_3$ $(M + Na)^+$, 273.0897, found 273.0899.

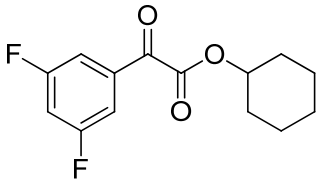
09) 

Cyclohexyl 2-(3-fluorophenyl)-2-oxoacetate (3ia):

The reaction of 1-(3-fluorophenyl)ethanone **1i** (55.3 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 68.0 mg (68%) of **3ia**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.80 (d, J = 8.0 Hz, 1H), 7.71 (dt, J_1 = 9.2 Hz, J_2 = 2.0 Hz, 1H), 7.55-7.46 (m, 1H), 7.71 (td, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 1H), 5.14-5.05 (m, 1H), 2.04-1.96 (m, 2H), 1.85-1.74 (m, 2H), 1.68-1.54 (m, 3H), 1.50-1.25 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.3 (d, J = 1.7 Hz) 162.9, 162.7 (d, J = 247.7 Hz), 134.6 (d, J = 7.3 Hz), 130.6 (d, J = 7.7 Hz) 125.9 (d, J = 2.7 Hz), 121.9 (d, J = 22.2 Hz), 116.4 (d, J = 22.6 Hz), 75.8, 31.4, 25.1, 23.6 ppm;

HRMS *m/z* (ESI) calcd for $C_{14}H_{15}FNaO_3$ $(M + Na)^+$, 273.0897, found 273.0898.

10) 

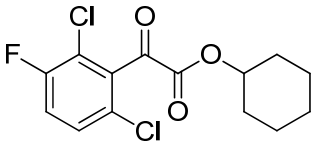
Cyclohexyl 2-(3,5-difluorophenyl)-2-oxoacetate (3ja):

The reaction of 1-(3,5-difluorophenyl)ethanone **1j** (62.5 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 16 h, afforded 60.9 mg (57%) of **3ja**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.60-7.52 (m, 2H), 7.11 (tt, J_1 = 8.4 Hz, J_2 = 2.2 Hz, 1H), 5.13-5.05 (m, 1H), 2.05-1.95 (m, 2H), 1.86-1.74 (m, 2H), 1.68-1.53 (m, 3H), 1.49-1.24 (m, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 183.8 (t, J = 2.7 Hz), 163.0 (dd, J_1 = 250.5 Hz, J_2 = 12.1 Hz), 162.1, 135.4 (t, J = 8.5 Hz), 112.9 (dd, J_1 = 19.2 Hz, J_2 = 6.8 Hz), 110.1 (t, J = 25.2 Hz), 76.1, 31.3, 25.1, 23.6 ppm;

HRMS *m/z* (ESI) calcd for $C_{14}H_{14}F_2NaO_3$ $(M + Na)^+$, 291.0803, found 291.0806.

11) 

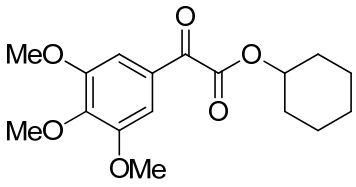
Cyclohexyl 2-(2,6-dichloro-3-fluorophenyl)-2-oxoacetate (3ka):

The reaction of 1-(2,6-dichloro-3-fluorophenyl)ethanone **1k** (82.8 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 24 h, afforded 105.8 mg (83%) of **3ka**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.33 (dd, J_1 = 8.8 Hz, J_2 = 4.4 Hz, 1H), 7.28-7.20 (m, 1H), 5.05-4.96 (m, 1H), 1,96-1.86 (m, 2H), 1.76-1.67 (m, 2H), 1.64-1.50 (m, 3H), 1.47-1.24 (m, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 183.6, 158.6, 156.9 (d, J = 250.1 Hz), 136.9, 129.1 (d, J = 7.2 Hz), 126.9 (d, J = 3.8 Hz), 120.0 (d, J = 19.8 Hz), 118.9 (d, J = 23.4 Hz), 76.4, 31.0, 25.1, 23.4 ppm;

HRMS *m/z* (ESI) calcd for $C_{14}H_{13}Cl_2FNaO_3$ $(M + Na)^+$, 341.0118, found 341.0123.

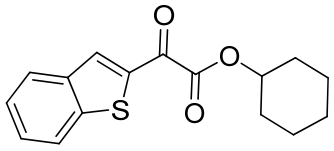
12) 

Cyclohexyl 2-oxo-2-(3,4,5-trimethoxyphenyl)acetate (3la):

The reaction of 1-(3,4,5-trimethoxyphenyl)ethanone **1l** (84.1 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 69.9 mg (54%) of **3la**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.27 (s, 2H), 5.15-5.06 (m, 1H), 3.95 (s, 3H), 3.91 (s, 6H), 2.06-1.96 (m, 2H), 1.85-1.75 (m, 2H), 1.68-1.55 (m, 3H), 1.50-1.24 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.5, 163.7, 153.2, 144.2, 127.4, 107.3, 75.3, 61.0, 56.2, 31.4, 25.1, 23.6 ppm;

HRMS *m/z* (ESI) calcd for $C_{17}H_{22}NaO_6$ $(M + Na)^+$, 345.1309, found 345.1314.

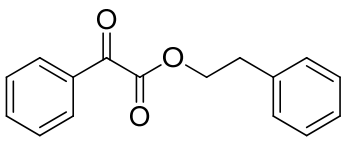
13) 

Cyclohexyl 2-(benzo[*b*]thiophen-2-yl)-2-oxoacetate (3ma):

The reaction of 1-(benzo[*b*]thiophen-2-yl)ethanone **1m** (70.5 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 15 h, afforded 67.4 mg (58%) of **3ma**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.38 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H)，7.54-7.48 (m, 1H), 7.46-7.40 (m, 1H), 5.12-5.04 (m, 1H), 2.05-1.98 (m, 2H), 1.86-1.78 (m, 2H), 1.71-1.58 (m, 3H), 1.50-1.24 (m, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 178.8, 161.2, 143.8, 139.0, 138.9, 134.9, 128.6, 126.8, 125.4, 123.0, 76.1, 31.4, 25.2, 23.7 ppm;

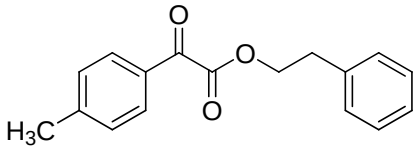
HRMS *m/z* (ESI) calcd for $C_{16}H_{16}NaO_3S$ $(M + Na)^+$, 311.0712, found 311.0715.

14) 

Phenethyl 2-oxo-2-phenylacetate (3ab):[6]

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 24 h, afforded 76.5 mg (75%) of **3ab**.

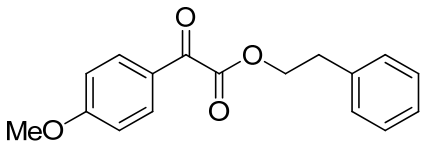
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.76 (d, *J* = 7.2 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.25-7.14 (m, 5H), 4.52 (t, *J* = 7.0 Hz, 2H), 2.99 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.2, 163.8, 136.9, 134.8, 132.3, 129.9, 128.9, 128.8, 128.6, 126.8, 66.3, 34.9 ppm.

15) 

Phenethyl 2-oxo-2-(*p*-tolyl)acetate (3nb):[6]

The reaction of 1-(*p*-tolyl)ethanone **1n** (53.7 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 18 h, afforded 62.7 mg (58%) of **3nb**.

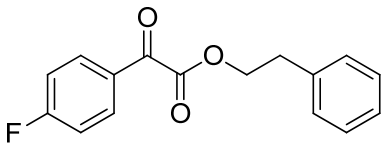
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.76 (d, *J* = 8.0 Hz, 2H), 7.35-7.21 (m, 7H), 4.61 (t, *J* = 7.2 Hz, 2H), 3.08 (t, *J* = 7.0 Hz, 2H), 3.42 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.9, 163.9, 146.2, 137.0, 130.1, 129.9, 129.5, 129.0, 128.6, 126.8, 66.2, 34.9, 21.8 ppm.

16) 

Phenethyl 2-(4-methoxyphenyl)-2-oxoacetate (3ob):[6]

The reaction of 1-(4-methoxyphenyl)ethanone **1o** (60.1 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 61.6 mg (54%) of **3ob**.

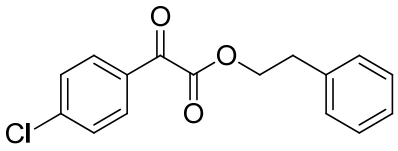
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.88-7.83 (m, 2H), 7.36-7.23 (m, 5H), 6.95-6.89 (m, 2H), 4.60 (t, *J* = 7.0 Hz, 2H), 3.89 (s, 3H), 3.09 (t, *J* = 6.8 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.7, 165.0, 164.0, 137.0, 132.6, 129.0, 128.7, 126.8, 125.4, 114.2, 66.2, 55.6, 34.9 ppm.

17) 

Phenethyl 2-(4-fluorophenyl)-2-oxoacetate (3cb):[6]

The reaction of 1-(4-fluorophenyl)ethanone **1c** (55.3 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 18 h, afforded 76.4 mg (70%) of **3cb**.

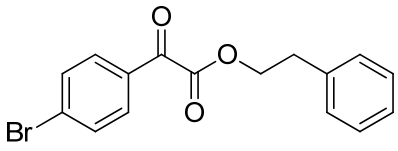
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.92-7.85 (m, 2H), 7.35-7.22 (m, 5H), 7.10 (t, *J* = 8.6 Hz, 2H), 4.62 (t, *J* = 7.2 Hz, 2H), 3.08 (t, *J* = 6.8 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.4, 166.7 (d, *J* = 256.6 Hz), 163.3, 136.9, 132.9 (d, *J* = 8.9 Hz), 129.0, 128.9 (d, *J* = 2.9 Hz), 128.7, 126.9, 116.2 (d, *J* = 22.1 Hz), 66.4, 34.9 ppm.

18) 

Phenethyl 2-(4-chlorophenyl)-2-oxoacetate (3pb):[6]

The reaction of 1-(4-chlorophenyl)ethanone **1p** (61.8 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 18 h, afforded 73.9 mg (64%) of **3pb**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.89 (d, *J* = 8.8 Hz, 2H), 7.42 (d, *J* = 8.8 Hz, 2H), 7.35-7.23 (m, 5H), 4.62 (t, *J* = 7.0 Hz, 2H), 3.09 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.8, 163.1, 141.7, 136.9, 131.4, 130.7, 129.2, 129.0, 128.7, 126.9, 66.5, 34.9 ppm.

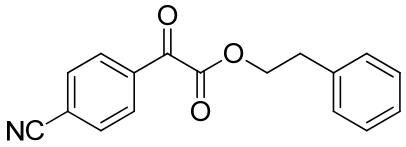
19) 

Phenethyl 2-(4-bromophenyl)-2-oxoacetate (3qb):[6]

The reaction of 1-(4-bromophenyl)ethanone **1q** (79.6 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 14 h, afforded 77.7 mg (58%) of **3qb**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.74-7.67 (m, 2H), 7.62-7.55 (m, 2H), 7.35-7.23 (m, 5H), 4.62

(t, *J* = 7.0 Hz, 2H), 3.08 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.0, 163.1, 136.9, 132.2, 131.4, 131.2, 130.5, 129.0, 128.7, 126.9, 66.5, 34.9 ppm.

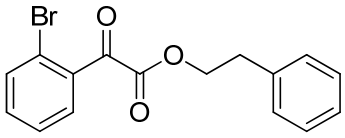
20) 

Phenethyl 2-(4-cyanophenyl)-2-oxoacetate (3rb):

The reaction of 1-(4-bromophenyl)ethanone **1r** (58.1 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 18 h, afforded 67.9 mg (61%) of **3rb**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.99-7.94 (m, 2H), 7.78-7.73 (m, 2H), 7.38-7.25 (m, 5H), 4.68 (t, *J* = 7.0 Hz, 2H), 3.13 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.4, 162.3, 136.8, 135.4, 132.5, 130.4, 129.0, 128.8, 127.0, 117.9, 117.5, 66.8, 34.9 ppm;

HRMS *m/z* (ESI) calcd for $C_{17}H_{13}NNaO_3$ $(M + Na)^+$, 302.0788, found 302.0792.

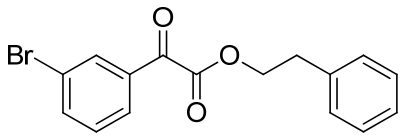
21) 

Phenethyl 2-(2-bromophenyl)-2-oxoacetate (3sb):

The reaction of 1-(2-bromophenyl)ethanone **1s** (79.6 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 11 h, afforded 85.9 mg (64%) of **3sb**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.61-7.54 (m, 2H), 7.42-7.36 (m, 2H), 7.30-7.18 (m, 5H), 4.54 (t, *J* = 7.0 Hz, 2H), 3.05 (t, *J* = 7.2 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 187.1, 162.2, 137.0, 135.5, 133.9, 133.7, 131.7, 129.0, 128.6, 127.6, 126.8, 121.6, 67.1, 34.7 ppm;

HRMS *m/z* (ESI) calcd for $C_{16}H_{13}BrNaO_3$ $(M + Na)^+$, 354.9940, found 354.9947.

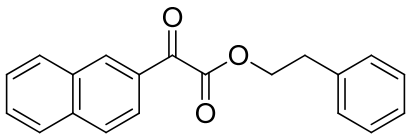
22) 

Phenethyl 2-(3-bromophenyl)-2-oxoacetate (3tb)

The reaction of 1-(3-bromophenyl)ethanone **1t** (79.6 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 11 h, afforded 72.2 mg (56%) of **3tb**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8,08 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.37-7.23 (m, 6H), 4.62 (t, *J* = 7.0 Hz, 2H), 3.09 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.6, 162.8, 137.7, 136.8, 134.1, 132.6, 130.4, 128.9, 128.7, 126.9, 123.1, 66.6, 34.9 ppm;

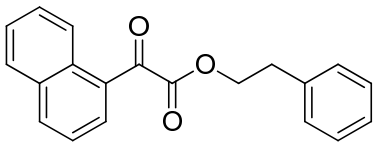
HRMS *m/z* (ESI) calcd for $C_{16}H_{13}BrNaO_3$ $(M + Na)^+$, 354.9940, found 354.9947.

23) 

Phenethyl 2-(naphthalen-2-yl)-2-oxoacetate (3ub):[6]

The reaction of 1-(naphthalen-2-yl)ethanone **1u** (68.1 mg, 0.40 mmol), 2-phenylethanol **2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 85.8 mg (70%) of **3ub**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.36 (s, 1H), 7.99-7.94 (m, 1H), 7.91-7.84 (m, 3H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.35-7.23 (m, 5H), 4.67 (t, *J* = 7.0 Hz, 2H), 3.12 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.2, 163.8, 137.0, 136.3, 133.5, 132.2, 130.0, 129.7, 129.5, 129.0, 128.9, 128.7, 127.9, 127.1, 126.9, 123.9, 66.5, 34.9 ppm.

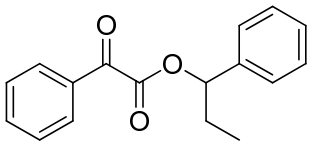
24) 

Phenethyl 2-(naphthalen-1-yl)-2-oxoacetate (3vb):[6]

The reaction of 1-(naphthalen-1-yl)ethanone **1v** (68.1 mg, 0.40 mmol), **2-phenylethanol 2b** (97.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 80.2 mg (66%) of **3vb**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.03 (d, *J* = 8.8 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.70-7.64 (m, 2H), 7.61-7.54 (m, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.35-7.23 (m, 5H), 4.65 (t, *J* = 6.8 Hz, 2H), 3.10 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 188.6, 164.5, 137.0, 135.7, 134.1, 133.9, 130.9, 129.2, 129.0, 128.7, 128.6, 128.0, 127.0, 126.8, 125.6, 124.3,

66.4, 34.9 ppm.

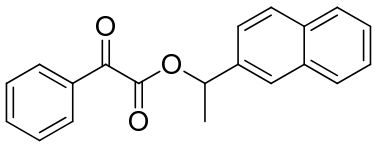
25) 

1-Phenylpropyl 2-oxo-2-phenylacetate (3ac):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 1-phenylpropan-1-ol **2c** (109.0 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 11 h, afforded 74.8 mg (70%) of **3ac**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.93-7.87 (m, 2H), 7.66-7.60 (m, 1H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.43-7.30 (m, 5H), 5.95 (t, *J* = 6.8 Hz, 1H), 2,15-2.04 (m, 1H), 2.02-1.90 (m, 1H), 0.97 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.4, 163.5, 139.1, 134.8, 132.4, 129.9, 128.8, 128.6, 128.4, 126.7, 79.8, 29.2, 9.9 ppm;

HRMS *m/z* (ESI) calcd for $C_{17}H_{16}NaO_3$ $(M + Na)^+$, 291.0992, found 291.0993.

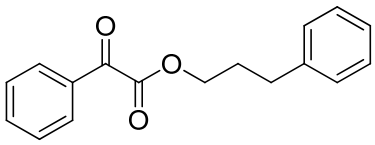
26) 

1-(Naphthalen-2-yl)ethyl 2-oxo-2-phenylacetate (3ad):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 1-(naphthalen-2-yl)ethanol **2d** (137.8 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 13 h, afforded 69.6 mg (57%) of **3ad**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.94-7.87 (m, 3H), 7.86-7.79 (m, 3H), 7.60-7.44 (m, 4H), 7.41 (t, *J* = 8.4 Hz, 2H), 6.33 (q, *J* = 6.5 Hz, 1H), 1.77 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.3, 163.3, 137.5, 134.8, 133.2, 133.0, 132.4, 129.9, 128.8, 128.6, 128.0, 127.6, 126.4, 126.3, 125.4, 123.8, 74.9, 22.1 ppm;

HRMS *m/z* (ESI) calcd for $C_{20}H_{16}NaO_3$ $(M + Na)^+$, 327.0992, found 327.0996.

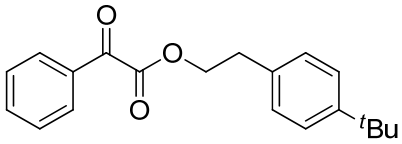
27) 

3-Phenylpropyl 2-oxo-2-phenylacetate (3ae):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 3-phenylpropan-1-ol **2e** (109.0 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 10 h, afforded 77.2 mg (72%) of **3ae**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.01 (d, *J* = 7.6 Hz, 2H), 7.69-7.62 (m, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.32-7.26 (m, 2H), 7.23-7.16 (m, 3H), 4.39 (t, *J* = 6.6 Hz, 2H), 2.75 (t, *J* = 7.8 Hz, 2H), 2.16-2.05 (m, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.3, 163.9, 140.6, 134.9, 132.4, 130.0, 128.9, 128.5, 128.4, 126.1, 65.4, 31.8, 29.9 ppm;

HRMS *m/z* (ESI) calcd for $C_{17}H_{16}NaO_3$ $(M + Na)^+$, 291.0992, found 291.0991.

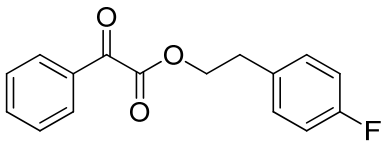
28) 

4-(*tert*-Butyl)phenethyl 2-oxo-2-phenylacetate (3af):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(4-(*tert*-butyl)phenyl)ethanol **2f** (142.6 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 11 h, afforded 93.0 mg (75%) of **3af**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.93-7.87 (m, 2H), 7.68-7.60 (m, 1H), 7.50-7.43 (m, 2H), 7.38-7.23 (m, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 4.61 (t, *J* = 7.0 Hz, 2H), 3.06 (t, *J* = 7.0 Hz, 2H), 1.32 (s, 9H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.3, 163.7, 149.7, 134.8, 133.8, 132.4, 130.0, 128.8, 128.7, 125.6, 66.5, 34.41, 34.36, 31.3 ppm;

HRMS *m/z* (ESI) calcd for $C_{20}H_{22}NaO_3$ $(M + Na)^+$, 333.1461, found 333.1466.

29) 

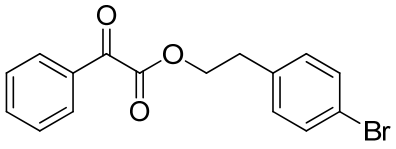
4-Fluorophenethyl 2-oxo-2-phenylacetate (3ag)

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(4-fluorophenyl)ethanol **2g** (112.1 mg,

0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 13 h, afforded 75.2 mg (69%) of **3ag**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.88-7.83 (m, 2H), 7.66-7.60 (m, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.24-7.17 (m, 2H), 7.03-6.94 (m, 2H), 4.59 (t, *J* = 6.8 Hz, 2H), 3.05 (t, *J* = 6.8 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.1, 163.6, 161.8 (d, *J* = 243.1 Hz), 134.9, 132.6 (d, *J* = 3.2 Hz), 132.2, 130.4 (d, *J* = 7.9 Hz), 129.9, 128.8, 115.4 (d, *J* = 21.5 Hz), 66.2, 34.1 ppm;

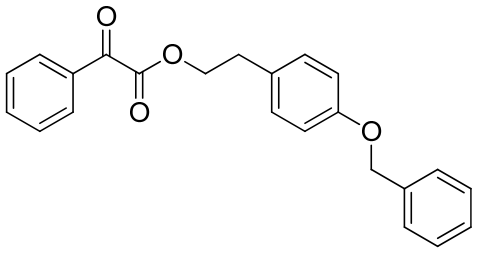
HRMS *m/z* (ESI) calcd for $C_{16}H_{13}FNaO_3$ $(M + Na)^+$, 295.0741, found 295.0744.

30) 

4-Bromophenethyl 2-oxo-2-phenylacetate (3ah):[6]

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(4-bromophenyl)ethanol **2h** (160.8 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 89.8 mg (67%) of **3ah**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.85-7.80 (m, 2H), 7.68-7.61 (m, 1H), 7.50-7.41 (m, 4H), 7.16-7.10 (m, 2H), 4.59 (t, *J* = 6.8 Hz, 2H), 3.04 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.1, 163.6, 136.0, 135.0, 132.2, 131.7, 130.8, 130.0, 128.9, 120.8, 65.9, 34.3 ppm.

31) 

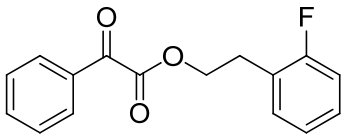
4-(Benzyloxy)phenethyl 2-oxo-2-phenylacetate (3ai):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(4-(benzyloxy)phenyl)ethanol **2i** (182.7 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 100.8 mg (70%) of **3ai**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.88-7.84 (m, 2H), 7.64-7.58 (m, 1H), 7.46-7.41 (m, 4H), 7.40-7.35 (m, 2H), 7.34-7.29 (m, 1H), 7.19-7.14 (m, 2H), 6.95-6.90 (m, 2H), 5.04 (s, 2H), 4.57 (t, *J* = 7.0 Hz, 2H), 3.02 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.3, 163.7, 157.7,

137.0, 134.8, 132.3, 130.0, 129.2, 128.8, 128.5, 127.9, 127.4, 115.0, 70.0, 66.5, 34.0 ppm;

HRMS *m/z* (ESI) calcd for $C_{23}H_{20}NaO_4$ $(M + Na)^+$, 383.1254, found 383.1259.

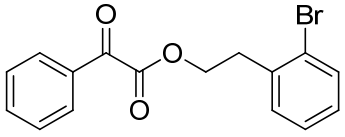
32) 

2-Fluorophenethyl 2-oxo-2-phenylacetate (3aj):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(2-fluorophenyl)ethanol **2j** (112.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 75.2 mg (69%) of **3aj**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.92-7.86 (m, 2H), 7.67-7.60 (m, 1H), 7.50-7.42 (m, 2H), 7.28-7.20 (m, 2H), 7.10-7.01 (m, 2H), 4.62 (t, *J* = 7.0 Hz, 2H), 3.14 (t, *J* = 7.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.1, 163.6, 161.3 (d, *J* = 244.7 Hz), 134.9, 132.3 131.3 (d, *J* = 5.1 Hz), 130.0, 128.8, 128.7 (d, *J* = 7.6 Hz), 124.2 (d, *J* = 2.9 Hz), 123.8 (d, *J* = 16.2 Hz), 115.4 (d, *J* = 21.3 Hz), 65.1 (d, *J* = 1.7 Hz), 28.5 (d, *J* = 2.3 Hz) ppm;

HRMS *m/z* (ESI) calcd for $C_{16}H_{13}FNaO_3$ $(M + Na)^+$, 295.0741, found 295.0743.

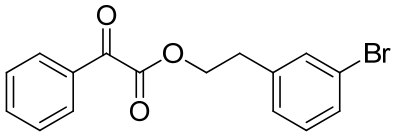
33) 

2-Bromophenethyl 2-oxo-2-phenylacetate (3ak):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(2-bromophenyl)ethanol **2k** (160.8 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 99.3 mg (75%) of **3ak**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.94-7.89 (m, 2H), 7.67-7.62 (m, 1H), 7.57 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.50-7.44 (m, 2H), 7.30-7.21 (m, 2H), 7.12 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 4.64 (t, *J* = 6.8 Hz, 2H), 3.24 (t, *J* = 6.8 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.0, 163.5, 136.3, 134.9, 133.0, 132.3, 131.3, 130.0, 128.8, 128.7, 127.6, 124.6, 64.8, 35.1 ppm;

HRMS *m/z* (ESI) calcd for $C_{16}H_{13}BrNaO_3$ $(M + Na)^+$, 354.9940, found 354.9946.

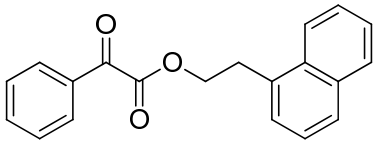
34) 

3-Bromophenethyl 2-oxo-2-phenylacetate (3al):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(3-bromophenyl)ethanol **2l** (160.8 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 90.4 mg (68%) of **3al**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ =7.90-7.83 (m, 2H), 7.68-7.61 (m, 1H), 7.52-7.45 (m, 2H), 7.42-7.36 (m, 2H), 7.22-7.16 (m, 2H), 4.60 (t, *J* = 6.8 Hz, 2H), 3.06 (t, *J* = 6.8 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.1, 163.6, 139.3, 134.9, 132.23, 132.00, 130.2, 130.02, 129.96, 128.9, 127.6, 122.6, 65.9, 34.5 ppm;

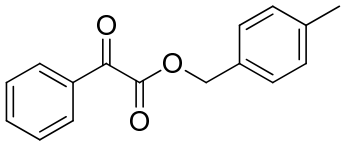
HRMS *m/z* (ESI) calcd for $C_{16}H_{13}BrNaO_3$ $(M + Na)^+$, 354.9940, found 354.9945.

35) 

2-(Naphthalen-1-yl)ethyl 2-oxo-2-phenylacetate (3am):[6]

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-(naphthalen-1-yl)ethanol **2am** (137.8 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 13 h, afforded 81.4 mg (67%) of **3am**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.10 (d, *J* = 8.8 Hz, 1H), 7.91-7.85 (m, 3H), 7.80-7.75 (m, 1H), 7.65-7.58 (m, 1H), 7.56-7.36 (m, 6H), 4.72 (t, *J* = 7.4 Hz, 2H), 3.56 (t, *J* = 7.4 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.1, 163.6, 134.8, 133.9, 132.7, 132.3, 131.9, 130.0, 128.9, 128.8, 127.7, 127.3, 126.4, 125.8, 125.5, 123.3, 65.9, 32.0 ppm.

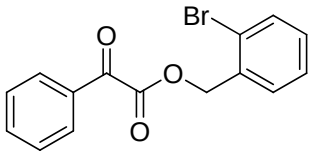
36) 

4-Methylbenzyl 2-oxo-2-phenylacetate (3an):[6]

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), *p*-tolylmethanol **2n** (97.8 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL)

under O_2 (balloon) at 110 ^oC for 14 h, afforded 73.8 mg (73%) of **3an**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.98-7.93 (m, 2H), 7.68-7.60 (m, 1H), 7.52-7.45 (m, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 5.37 (s, 2H), 2.36 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.1, 163.7, 138.8, 134.9, 132.4, 131.5, 130.0, 129.4, 128.9, 128.8, 67.8, 21.2 ppm.

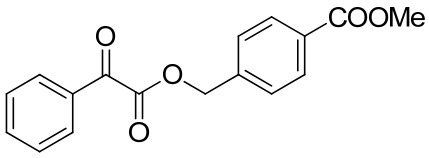
37) 

2-Bromobenzyl 2-oxo-2-phenylacetate (3ao):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), (2-bromophenyl)methanol **2o** (149.6 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 10 h, afforded 73.8 mg (58%) of **3ao**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.04-8.00 (m, 2H), 7.69-7.62 (m, 1H), 7.60 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.53-7.48 (m, 3H), 7.34 (td, J_1 = 7.4 Hz, J_2 = 1.2 Hz, 1H), 7.34 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 5.50 (s, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.9, 163.4, 135.0, 133.9, 133.0, 132.3, 130.3, 130.1, 128.9, 127.7, 123.6, 67.1 ppm;

HRMS *m/z* (ESI) calcd for $C_{15}H_{11}BrNaO_3$ $(M + Na)^+$, 340.9784, found 340.9790.

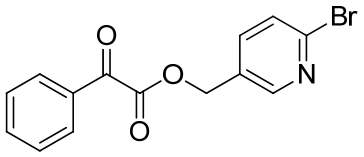
38) 

Methyl 4-((2-oxo-2-phenylacetoxy)methyl)benzoate (3ap):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), methyl 4-(hydroxymethyl)benzoate **2p** (74.8 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 15 h, afforded 74.8 mg (63%) of **3ap**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.06 (d, *J* = 8.0 Hz, 2H), 8.00-7.95 (m, 2H), 7.69-7.62 (m, 1H), 7.54-7.46 (m, 4H), 5.46 (s, 2H), 3.92 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.7, 166.5, 163.3, 139.4, 135.0, 132.2, 130.4, 130.0, 129.9, 128.9, 128.0, 66.8, 52.1 ppm;

HRMS *m/z* (ESI) calcd for $C_{17}H_{14}NaO_5$ $(M + Na)^+$, 321.0733, found 321.0737.

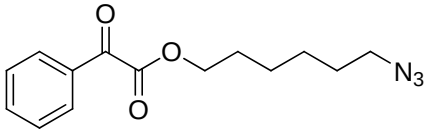
39) 

(6-Bromopyridin-3-yl)methyl 2-oxo-2-phenylacetate (3aq):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), (6-bromopyridin-3-yl)methanol **2q** (94.0 mg, 0.48 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 24 h, afforded 58.3 mg (46%) of **3aq**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.47 (d, *J* = 2.4 Hz, 1H), 8.00-7.94 (m, 2H), 7.70-7.64 (m, 2H), 7.56-7.48 (m, 3H), 5.38 (s, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.2, 163.0, 150.2, 142.6, 138.8, 135.2, 132.1, 130.0, 129.6, 129.0, 128.2, 64.1 ppm;

HRMS *m/z* (ESI) calcd for $C_{14}H_{11}BrNO_3$ $(M + H)^+$, 319.9917, found 319.9923.

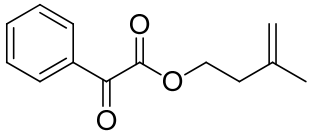
40) 

6-Azidohexyl 2-oxo-2-phenylacetate (3ar):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 6-azidohexan-1-ol **2r** (114.6 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 16 h, afforded 62.0 mg (56%) of **3ar**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.03-7.98 (m, 2H), 7.70-7.64 (m, 1H), 7.55-7.48 (m, 2H), 4.39 (t, *J* = 6.6 Hz, 2H), 3.27 (t, *J* = 7.0 Hz, 2H), 1.85-1.74 (m, 2H), 1.67-1.56 (m, 2H), 1.50-1.40 (m, 4H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.3, 163.9, 134.9, 132.4, 129.9, 128.8, 66.0, 51.2, 28.6, 28.2, 26.2, 25.3 ppm;

HRMS *m/z* (ESI) calcd for $C_{14}H_{17}N_3NaO_3$ $(M + Na)^+$, 298.1162, found 298.1164.

41) 

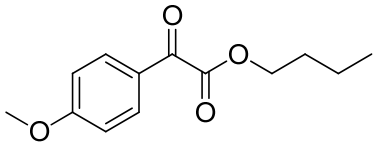
3-Methylbut-3-en-1-yl 2-oxo-2-phenylacetate (3as):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 3-methylbut-3-en-1-ol **2s** (68.9 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL)

under O_2 (balloon) at 110 ^oC for 13 h, afforded 48.9 mg (56%) of **3as**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.00 (d, *J* = 7.2 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 4.87 (s, 1H), 4.80 (s, 1H), 4.52 (t, *J* = 7.0 Hz, 2H), 2.50 (t, *J* = 7.0 Hz, 2H), 1.81 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.3, 163.8, 140.9, 134.9, 132.4, 130.1, 128.9, 113.0, 64.3, 36.5, 22.4 ppm;

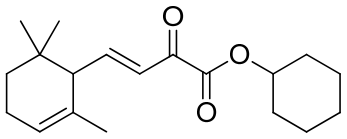
HRMS *m/z* (ESI) calcd for $C_{13}H_{14}NaO_3$ $(M + Na)^+$, 241.0835, found 241.0836.

42) 

Butyl 2-(4-methoxyphenyl)-2-oxoacetate (4a):[7]

The reaction of 1-(4-methoxyphenyl)ethanone **1a** (60.1 mg, 0.40 mmol), butan-1-ol (59.4 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 14 h, afforded 53.6 mg (57%) of **4a**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.02-7.96 (m, 2H), 7.00-6.95 (m, 2H), 4.38 (t, *J* = 6.8 Hz, 2H), 3.89 (s, 3H), 1.81-1.70 (m, 2H), 1.51-1.40 (m, 2H), 0.97 (d, *J* = 7.4 Hz, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.9, 165.0, 164.3, 132.5, 125.5, 114.2, 65.9, 55.6, 30.4, 19.0, 13.6 ppm.

43) 

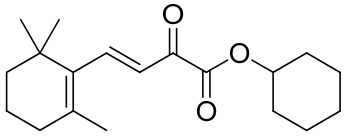
(*E*)-Cyclohexyl 2-oxo-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-enoate (4b):

The reaction of (*E*)-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-one **[α-Ionone]** (76.9 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 16 h, afforded 77.0 mg (63%) of **4b**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 6.97 (dd, J_1 = 16.0 Hz, J_1 = 10.0 Hz, 1H), 6.55 (d, *J* = 15.6 Hz, 1H), 5.53 (s, 1H), 4.99-4.90 (m, 1H), 2.38 (d, *J* = 9.6 Hz, 1H), 2.10-2.02 (m, 2H), 1,98-1.90 (m, 2H), 1.82-1.73 (m, 2H), 1.62-1.20 (m, 11H), 0.94 (s, 3H), 0.86 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.0, 162.2, 155.6, 131.2, 126.4, 123.2, 75.2, 54.8, 32.8, 31.3, 31.1, 27.7, 26.8, 25.1,

23.6, 23.0, 22.8 ppm;

HRMS *m/z* (ESI) calcd for $C_{19}H_{28}NaO_3$ $(M + Na)^+$, 327.1931, found 327.1936.

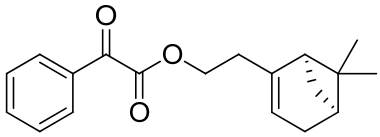
44) 

(*E*)-Cyclohexyl 2-oxo-4-(2,6,6-trimethylcyclohex-1-en-1-yl)but-3-enoate (4c):

The reaction of (*E*)-4-(2,6,6-trimethylcyclohex-1-en-1-yl)but-3-en-2-one **[β-Ionone]** (76.9 mg, 0.40 mmol), cyclohexanol **2a** (80.1 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 16 h, afforded 63.7 mg (52%) of **4a**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.64 (d, *J* = 16.4 Hz, 1H), 7.69 (d, *J* = 16.4 Hz, 1H), 5.00-4.91 (m, 1H), 2.13 (t, *J* = 5.8 Hz, 2H), 1.97-1.91 (m, 2H), 1.85 (s, 3H), 1.82-1.74 (m, 2H), 1.66-1.20 (m, 10H), 1.12 (s, 6H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 184.3, 162.5, 148.1, 141.5, 136.6, 124.5, 75.1, 40.0, 34.3, 34.1, 31.3, 28.7, 25.2, 23.6, 21.9, 18.7 ppm;

HRMS *m/z* (ESI) calcd for $C_{19}H_{28}NaO_3$ $(M + Na)^+$, 327.1931, found 327.1935.

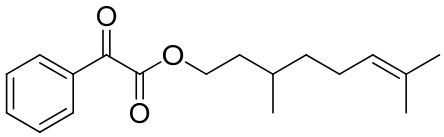
45) 

2-((1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethyl 2-oxo-2-phenylacetate (4d):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-((1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethanol **[(-)-Nopol]** (133.0 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 12 h, afforded 90.7 mg (76%) of **4d**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.03-7.98 (m, 2H), 7.69-7.63 (m, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 5.38-5.35 (m, 1H), 4.47-4.33 (m, 2H), 2.45 (td, J_1 = 7.0 Hz, J_1 = 1.2 Hz, 2H), 2.41-2.35 (m, 1H), 2.32-2.15 (m, 2H), 2.12-2.06 (m, 2H), 1.28 (s, 3H), 1.16 (d, *J* = 8.4 Hz, 1H), 0.83 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.4, 163.9, 143.3, 134.8, 132.4, 130.0, 128.8, 119.5, 64.4, 45.6, 40.6, 38.0, 35.7, 31.6, 31.3, 26.2, 21.1 ppm;

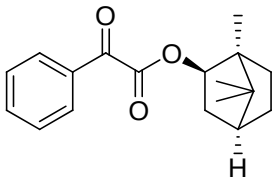
HRMS *m/z* (ESI) calcd for $C_{19}H_{22}NaO_3$ $(M + Na)^+$, 321.1461, found 321.1465.

46) 

3,7-Dimethyloct-6-en-1-yl 2-oxo-2-phenylacetate (4e):[8]

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 3,7-dimethyloct-6-en-1-ol **[β-citronellol]** (125.0 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 13 h, afforded 87.3 mg (76%) of **4e**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.03-7.98 (m, 2H), 7.70-7.63 (m, 1H), 7.52 (t, *J* = 7.8 Hz, 2H), 5.12-5.05 (m, 1H), 4.47-4.38 (m, 2H), 2.26-1.81 (m, 2H), 1.80-1.78 (m, 1H), 1.67 (s, 3H), 1.65-1.55 (m, 5H), 1.44-1.32 (m, 1H), 1.28-1.16 (m, 1H), 0.96 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.5, 164.0, 134.9, 132.5, 131.5, 130.0, 128.9, 124.3, 64.8, 36.9, 35.2, 29.4, 25.7, 25.3, 19.3, 17.6 ppm;

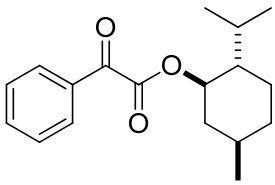
47) 

(1*S*,2*R*,4*S*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 2-oxo-2-phenylacetate (4f):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), (1*S*,2*R*,4*S*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol **[(-)-Borneol]** (123.4 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 14 h, afforded 50.6 mg (44%) of **4f**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.02-7.96 (m, 2H), 7.70-7.64 (m, 1H), 7.53 (t, *J* = 7.8 Hz, 2H), 5.26-5.20 (m, 1H), 2.55-2.45 (m, 1H), 2.00-1.90 (m, 1H), 1.80-1.73 (m, 2H), 1.40-1.24 (m, 2H), 1.20 (dd, J_1 = 7.0 Hz, J_2 = 3.6 Hz, 1H), 0.97 (s, 3H), 0.93 (s, 3H), 0.91 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.8, 164.6, 134.8, 132.6, 129.9, 128.9, 82.6, 49.1, 48.1, 44.9, 36.5, 27.9, 27.0, 19.7, 18.8, 13.6 ppm;

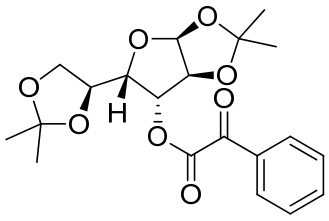
HRMS *m/z* (ESI) calcd for $C_{18}H_{22}NaO_3$ $(M + Na)^+$, 309.1461, found 321.1463.

48) 

2-Isopropyl-5-methylcyclohexyl 2-oxo-2-phenylacetate (4g):[9]

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), 2-isopropyl-5-methylcyclohexanol **[menthol]** (125.0 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 17 h, afforded 84.6 mg (73%) of **4g**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.02-7.96 (m, 2H), 7.69-7.63 (m, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 5.01 (td, J_1 = 11.0 Hz, J_2 = 4.8 Hz, 1H), 2.22-2.14 (m, 1H), 2.02-1.90 (m, 1H), 1.78-1.70 (m, 2H), 1.64-1.48 (m, 2H), 1.32-1.04 (m, 3H), 0.96 (d, *J* = 6.8 Hz, 3H), 0.91 (d, *J* = 6.8 Hz, 3H), 0.85 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.9, 164.0, 134.9, 132.6, 130.0, 129.0, 77.4, 46.9, 40.7, 34.1, 31.6, 26.2, 23.4, 22.0, 20.7, 16.2 ppm.

59) 

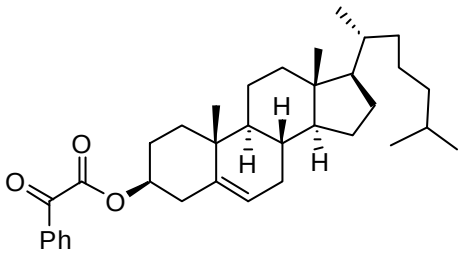
(3a*S*,5*S*,6*R*,6a*S*)-5-((*S*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl 2-oxo-2-phenylacetate (4h):

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), (3a*S*,5*R*,6*R*,6a*S*)-5-((*S*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-ol **[diacetone-*D*-glucose]** (208.2 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 15 h, afforded 72.8 mg (46%) of **4h**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.05 (d, *J* = 7.3 Hz, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 2H), 5.94 (d, *J* = 3.6, 1H), 5.66 (d, *J* = 3.2 Hz, 1H), 4.66 (d, *J* = 3.6 Hz, 1H), 4.27 (dd, J_1 = 8.4 Hz, J_2 = 3.2 Hz, 1H), 4.22-4.14 (m, 1H), 4.12-4.08 (m, 1H), 4.02 (dd, J_1 = 8.8 Hz, J_2 = 3.6 Hz, 1H), 1.56 (s, 3H), 1.47 (s, 3H), 1.34 (s, 6H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 185.7, 162.5, 135.2, 132.2, 130.1, 128.9, 112.6, 109.5, 105.3, 83.2, 80.1, 77.2, 72.3, 67.6, 26.9, 26.7, 26.2, 25.2

ppm;

HRMS *m/z* (ESI) calcd for $C_{20}H_{25}O_8$ $(M + H)^+$, 393.1544, found 393.1549.



60)

(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11, 12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 2-oxo-2-phenylacetate (4i):[10]

The reaction of acetophenone **1a** (48.1 mg, 0.40 mmol), **cholesterol** (309.3 mg, 0.80 mmol), CuBr (5.7 mg, 0.040 mmol), and TEMP (11.3 mg, 0.080 mmol) in $PhCH_3$ (2.00 mL) under O_2 (balloon) at 110 ^oC for 17 h, afforded 137.9 mg (66%) of **4i**.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.03-7.97 (m, 2H), 7.69-7.63 (m, 1H), 7.52 (t, *J* = 7.8 Hz, 2H), 5.45 (d, *J* = 4.4 Hz, 1H), 4.98-4.88 (m, 1H), 2.50 (d, *J* = 8.0 Hz, 2H), 2.06-1.72 (m, 6H), 1.65-1.43 (m, 6H), 1.38-1.08 (m, 11H), 1.06-0.94 (m, 3H), 1.04 (s, 3H), 0.92 (d, *J* = 6.8 Hz, 3H), 0.870 (d, *J* = 6.4 Hz, 3H), 0.866 (d, *J* = 6.4 Hz, 3H), 0.69 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ = 186.7, 163.5, 139.0, 134.8, 132.5, 130.0, 128.9, 123.4, 76.6, 56.7, 56.1, 50.0, 42.3, 39.7, 39.5, 37.9, 36.9, 36.6, 36.2, 35.8, 31.9, 31.8, 28.2, 28.0, 27.6, 24.3, 23.8, 22.8, 22.5, 21.0, 19.3, 18.7, 11.8 ppm.

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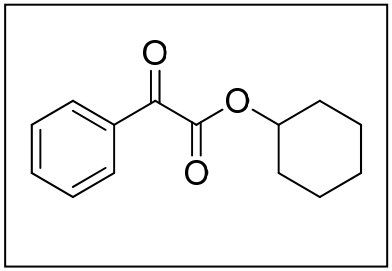
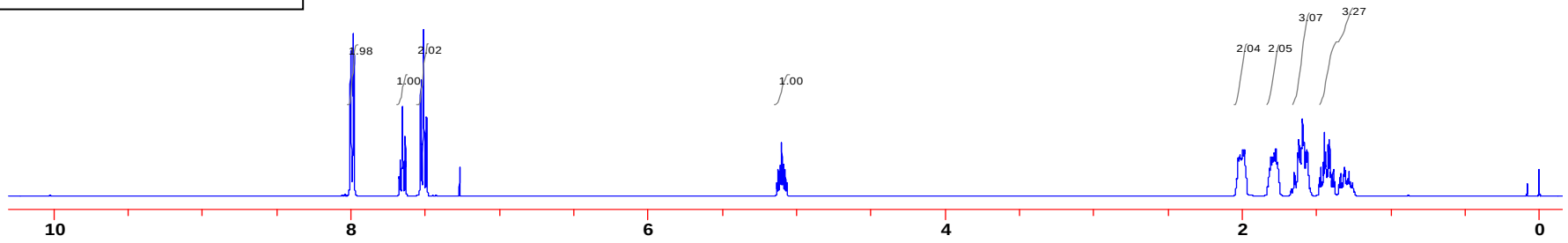
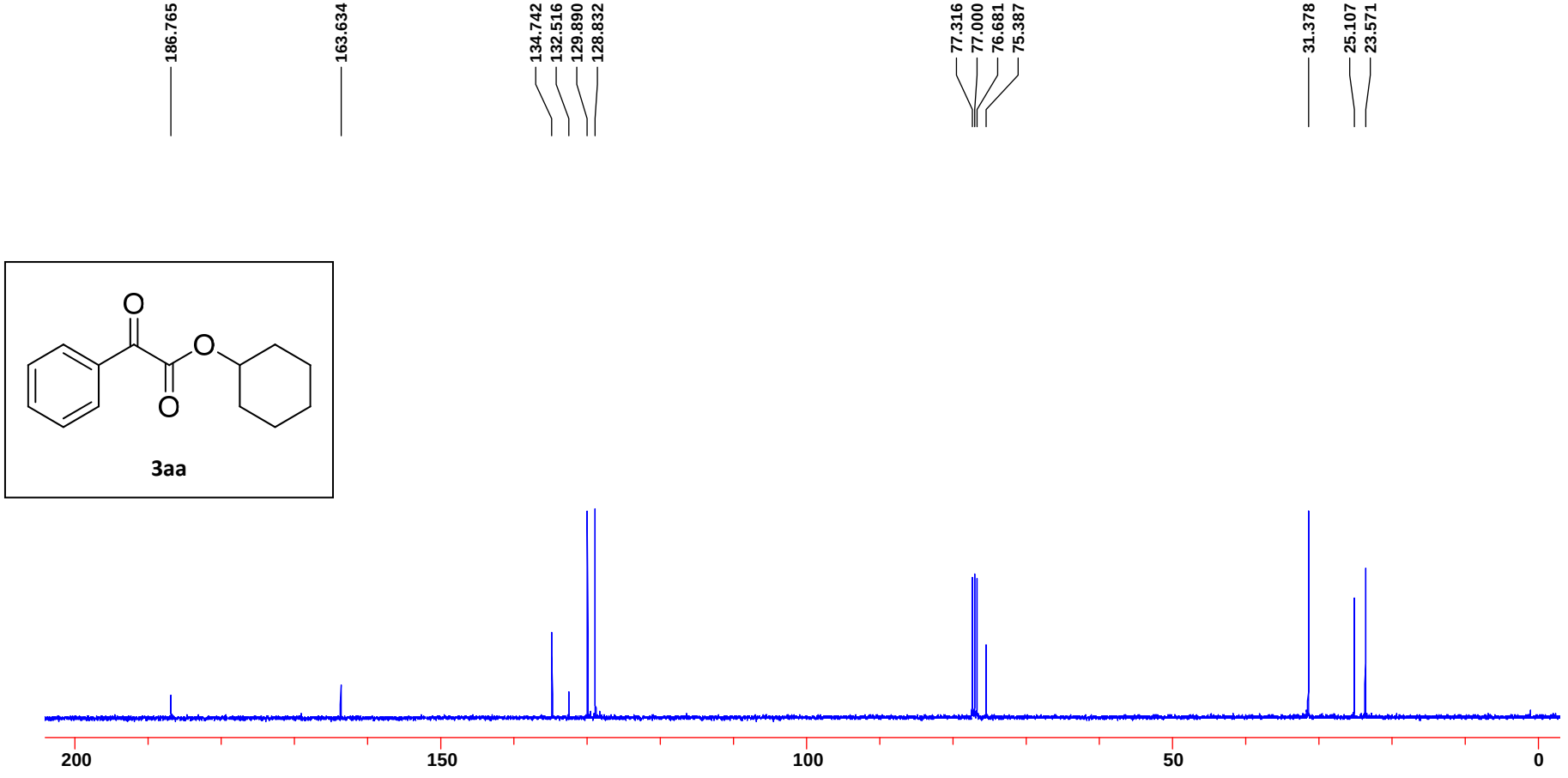
^{1}H NMR and ^{13}C NMR Spectra of Products



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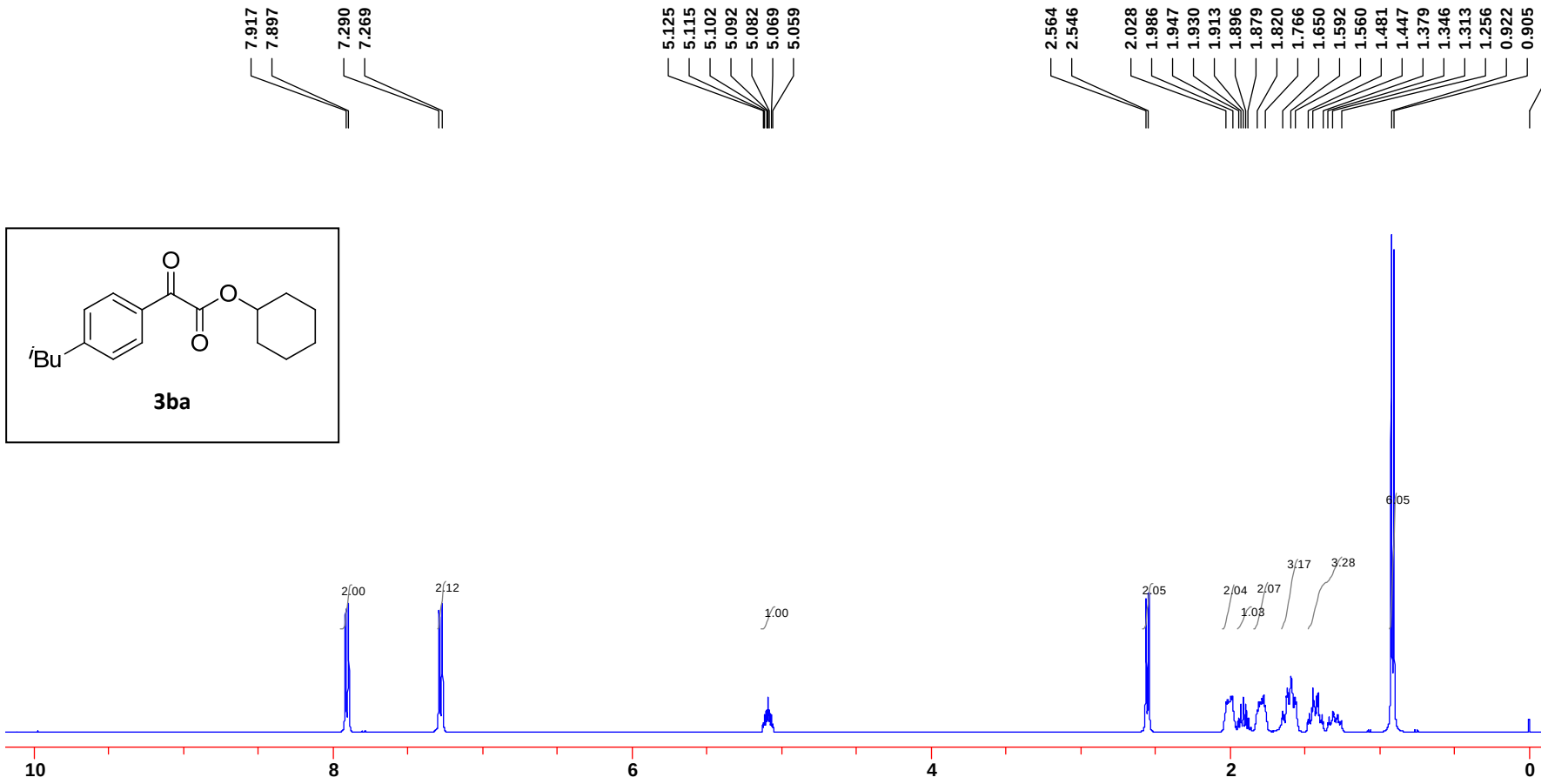
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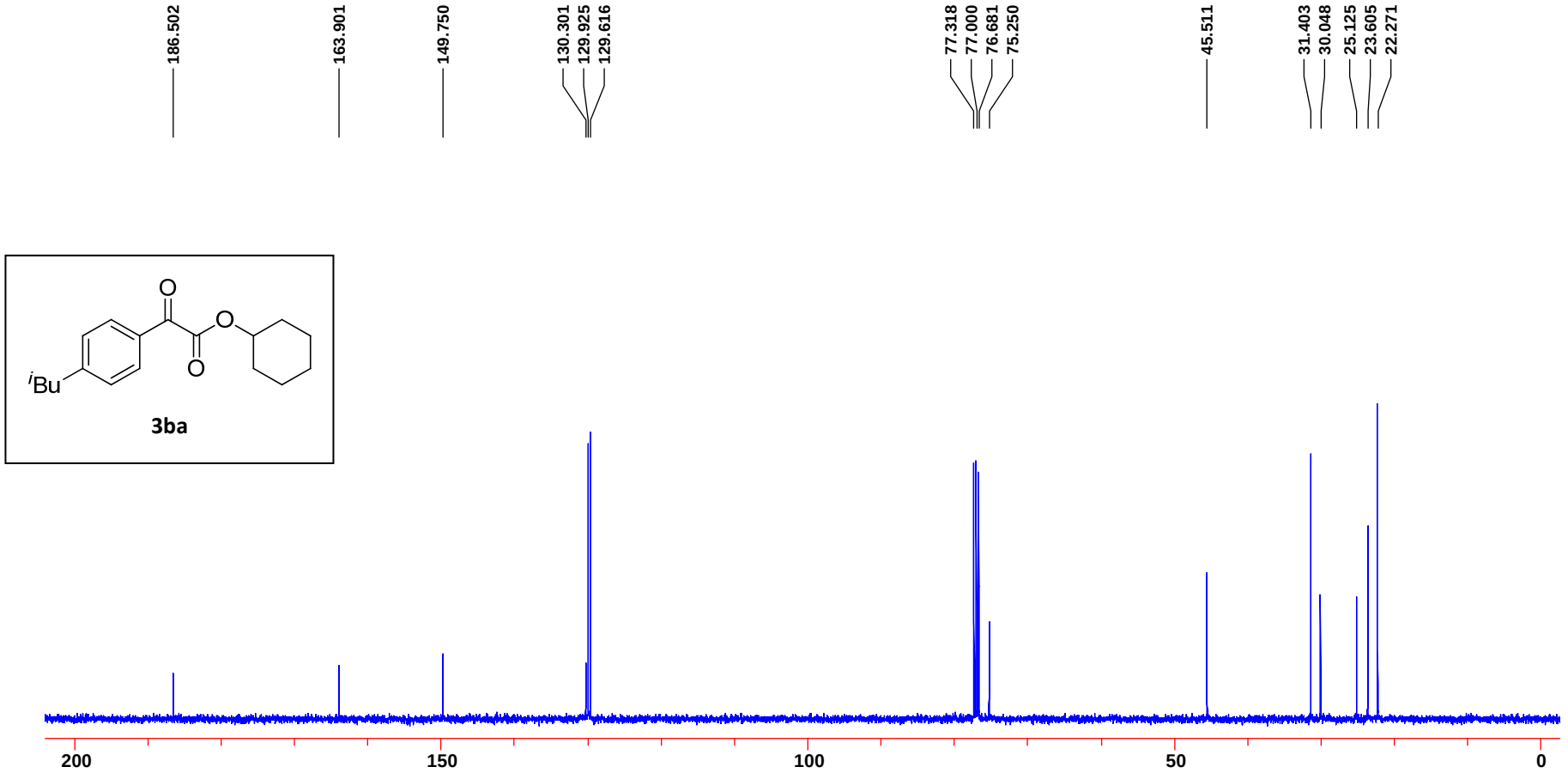
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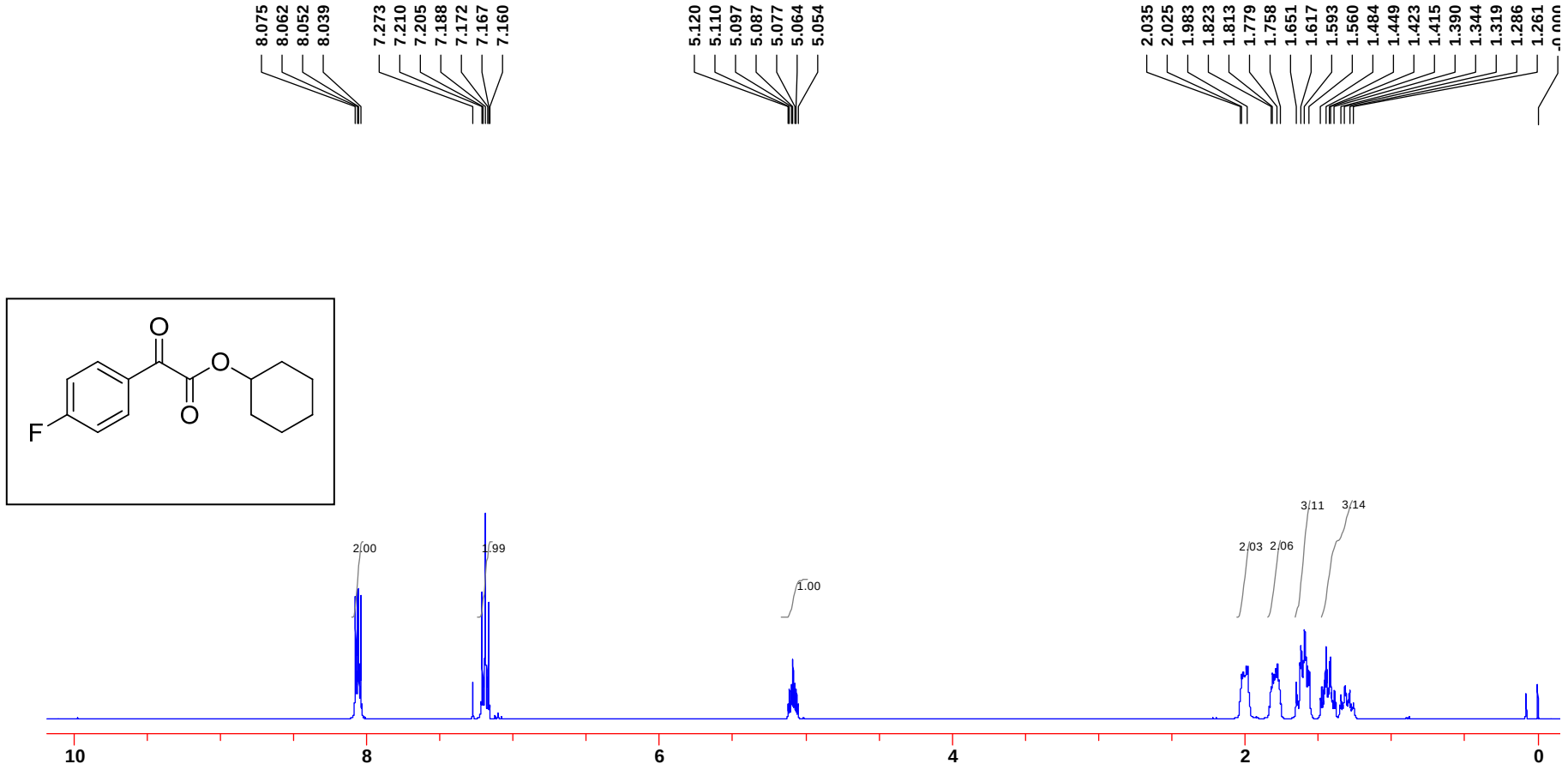
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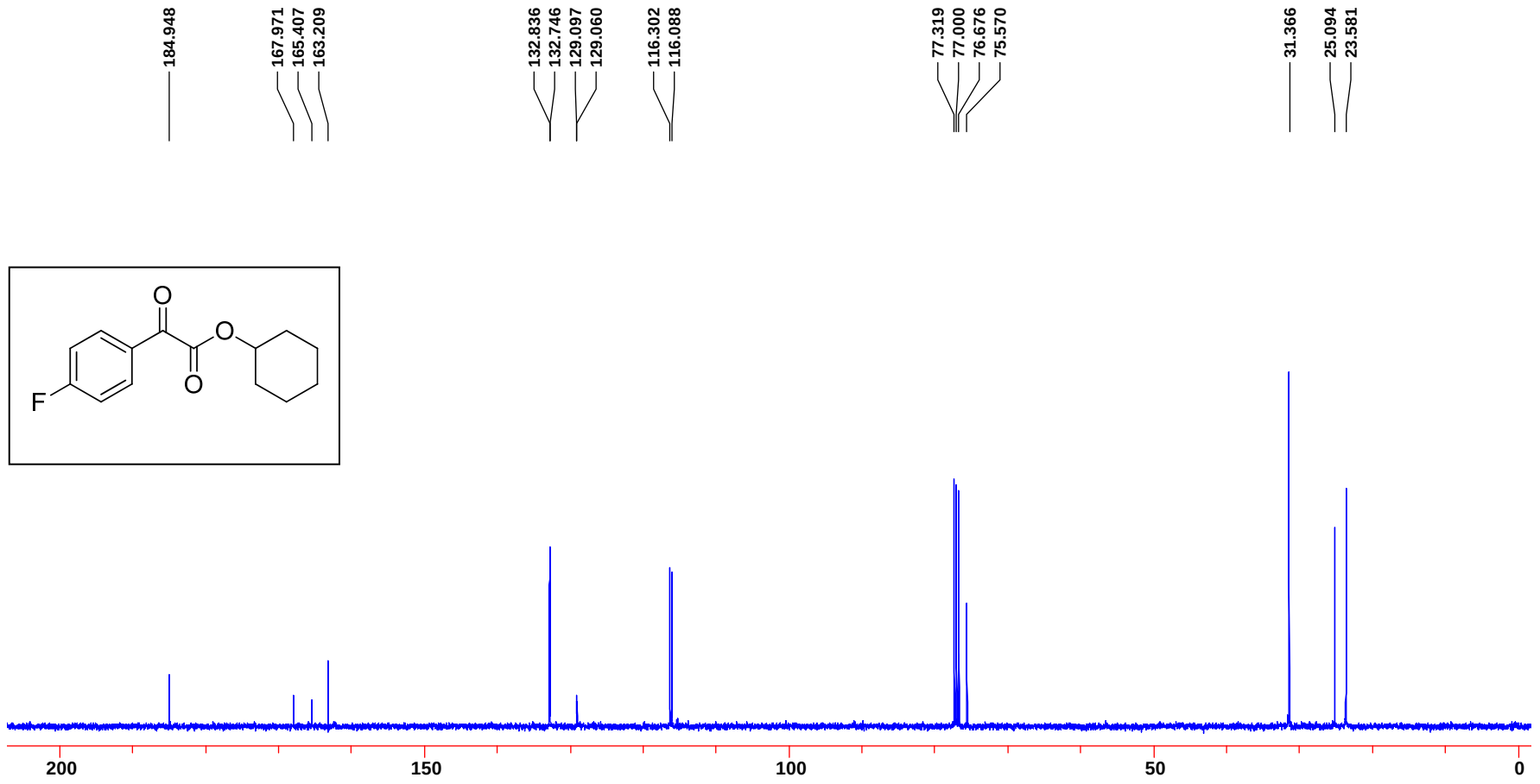
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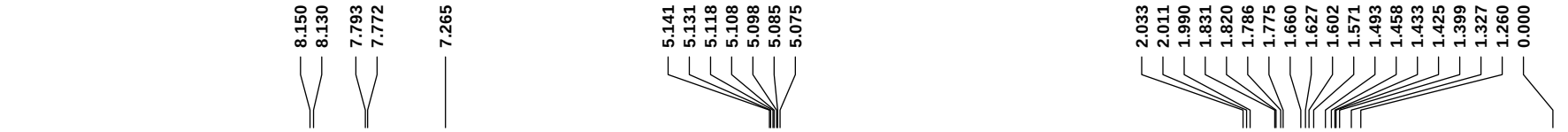
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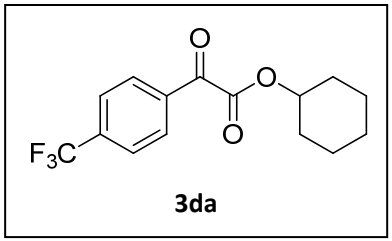
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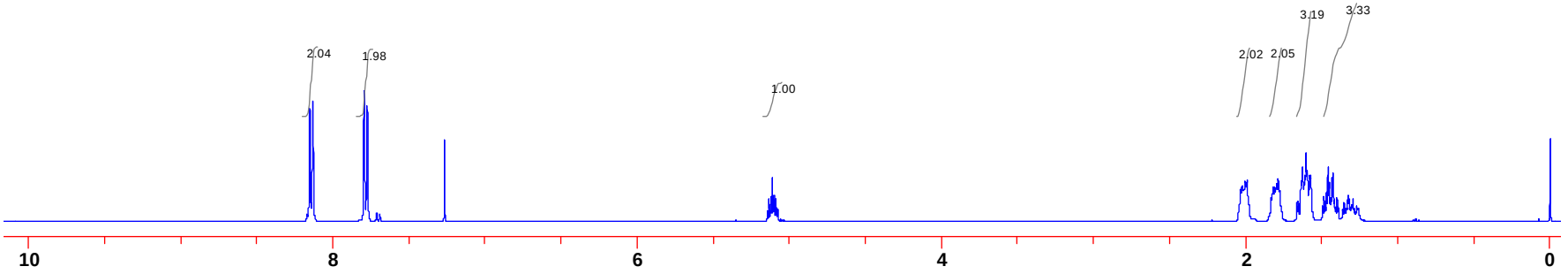
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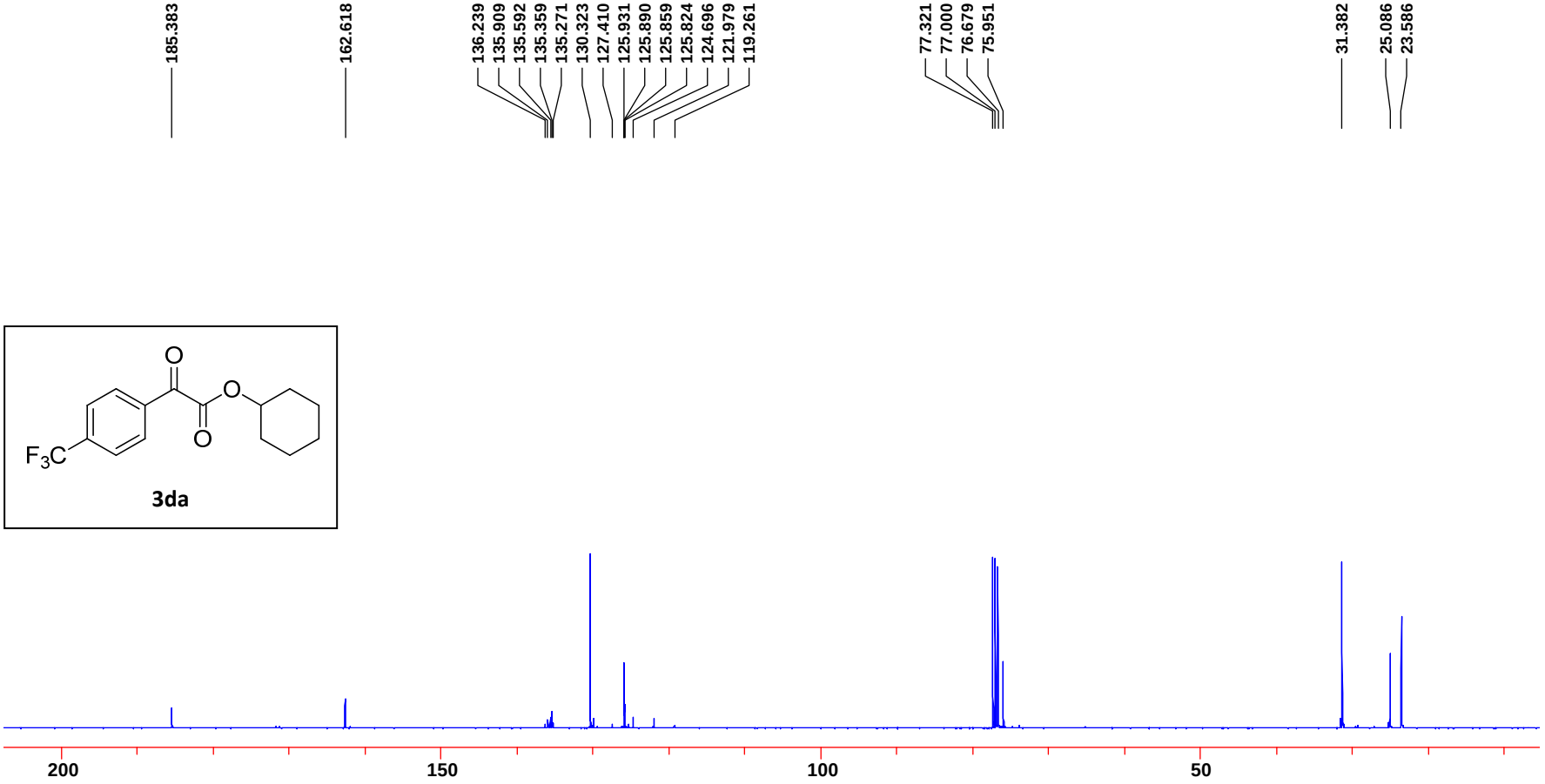
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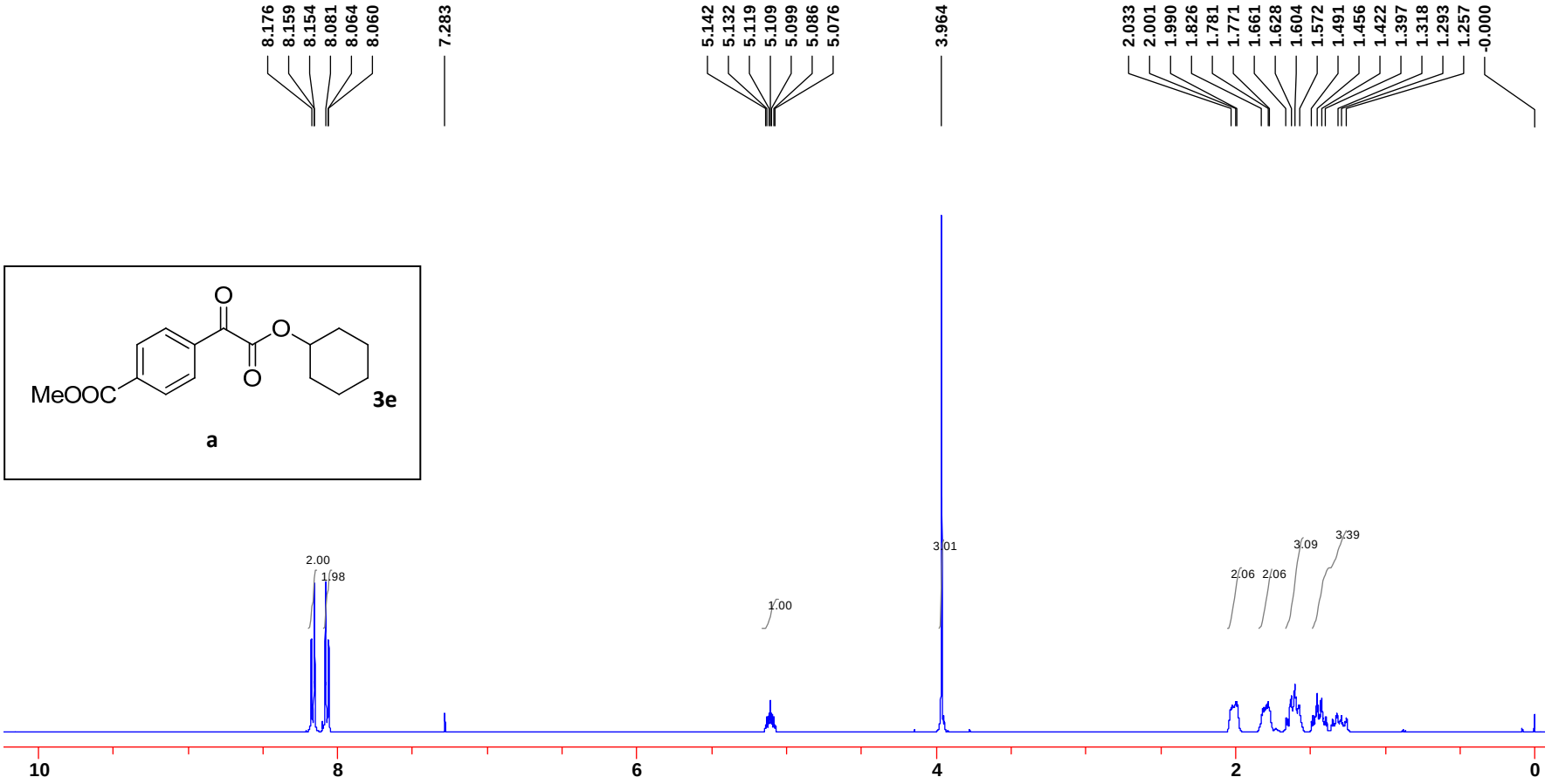
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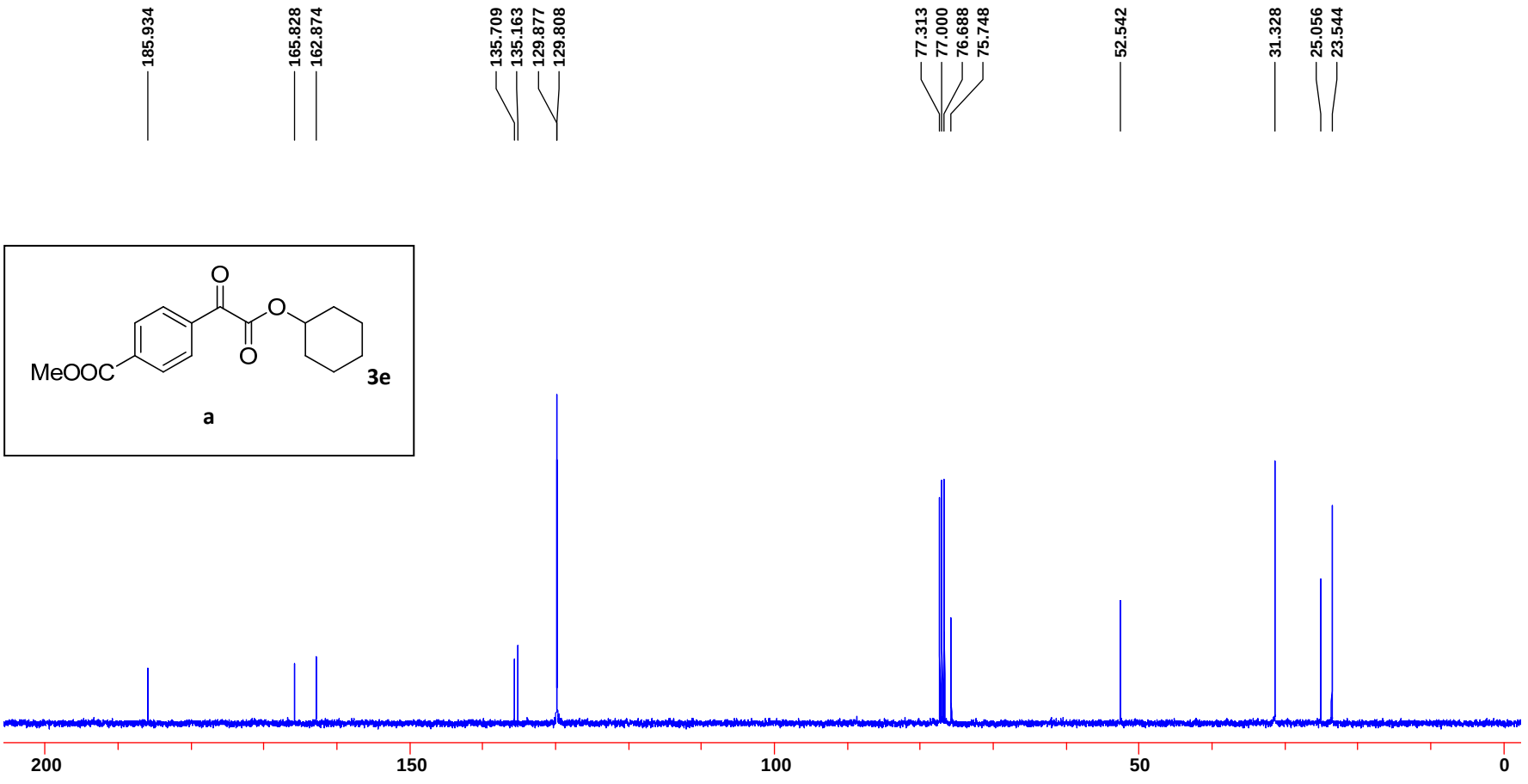
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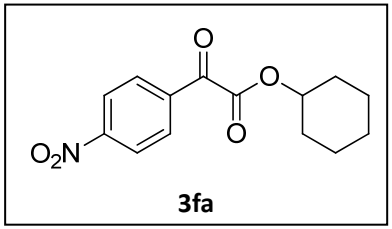
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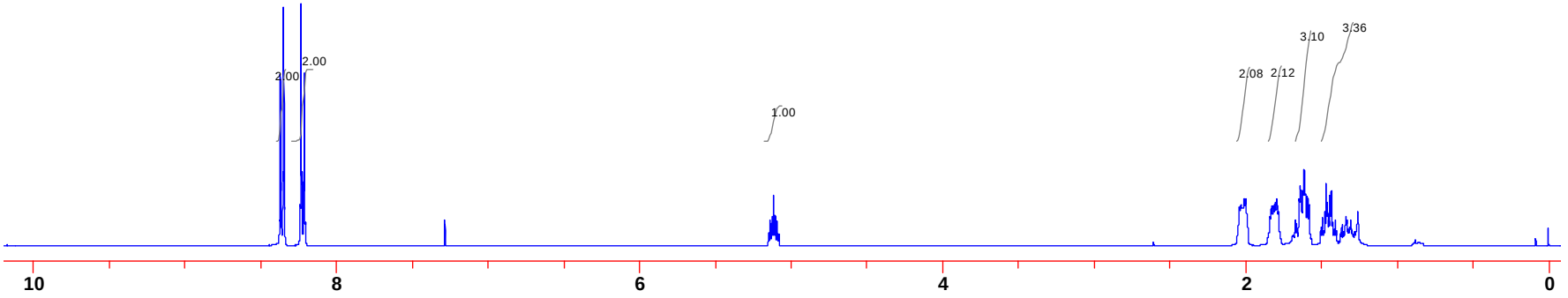
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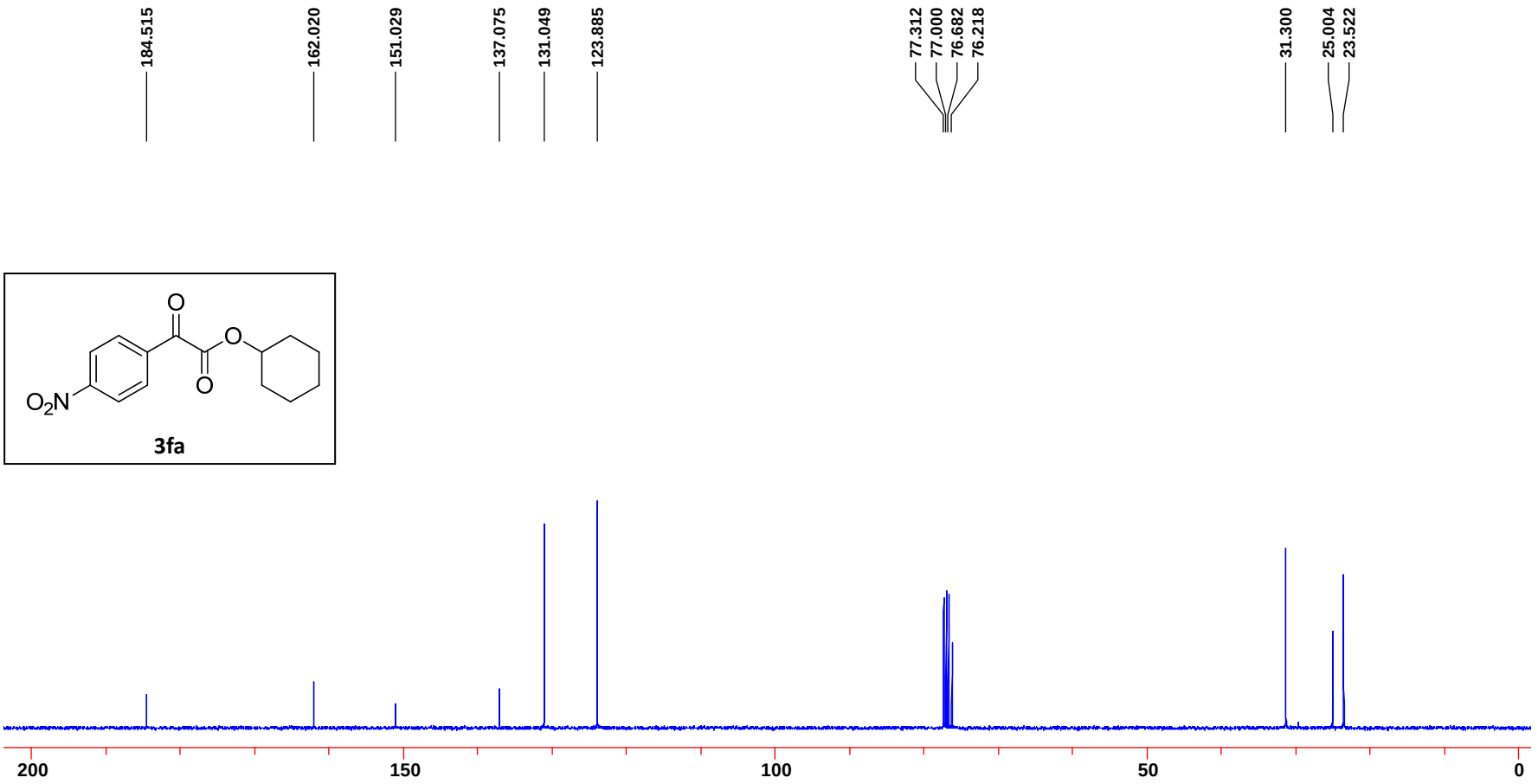
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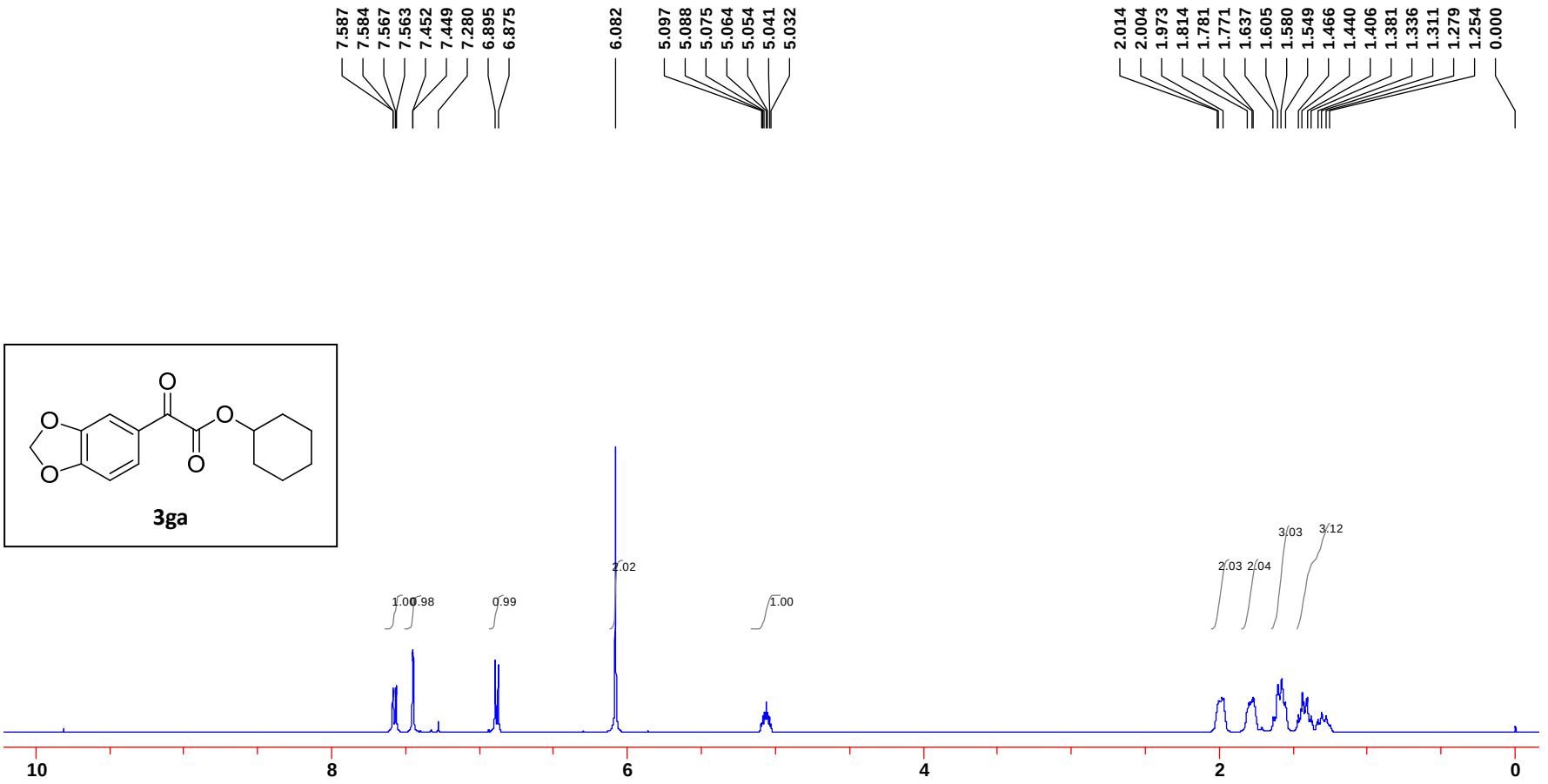
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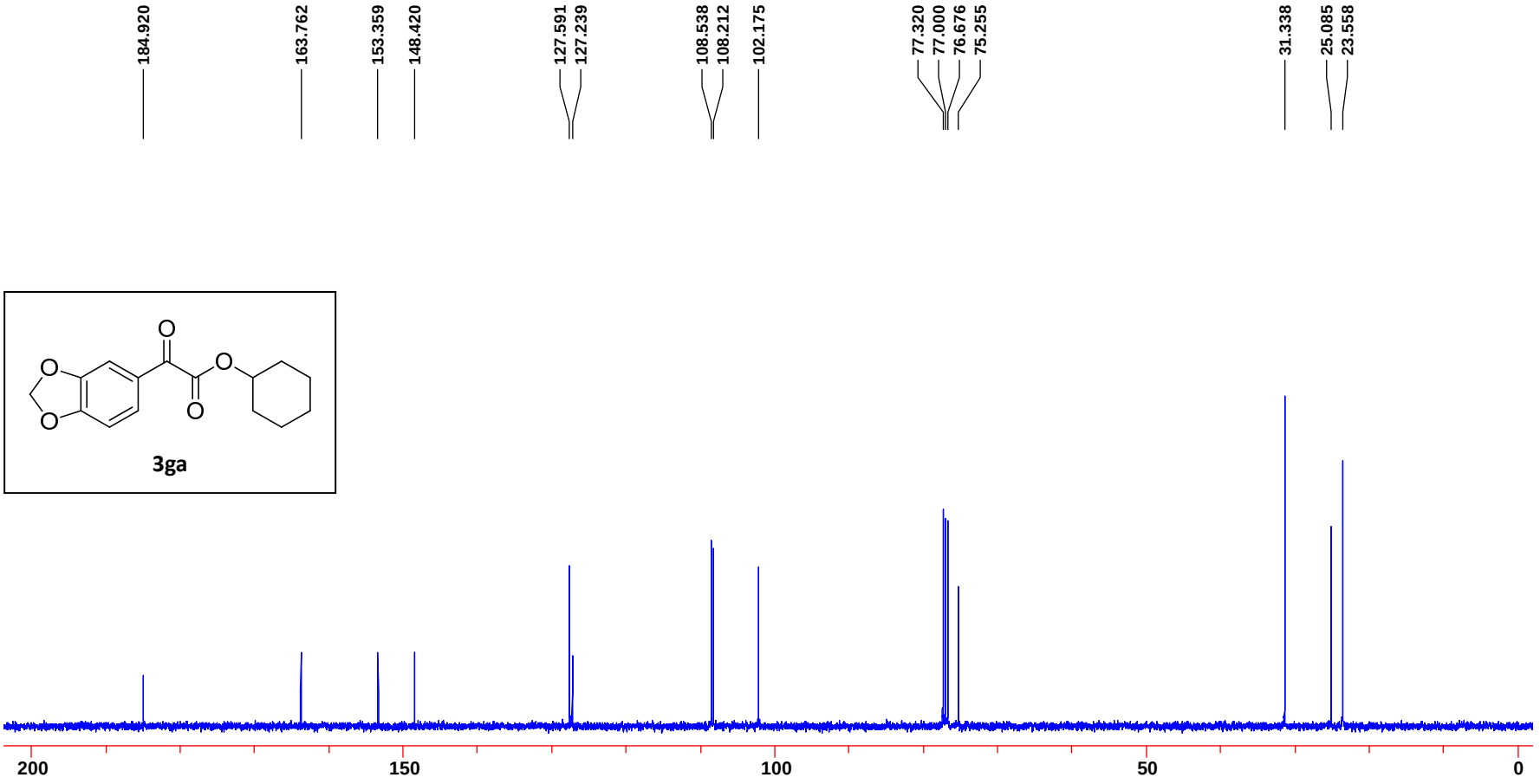
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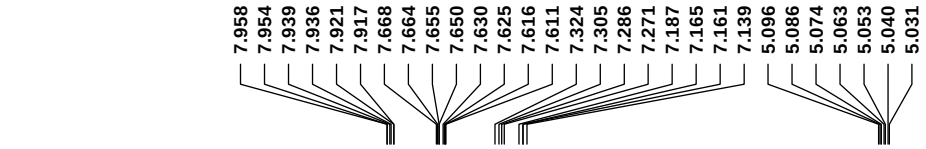
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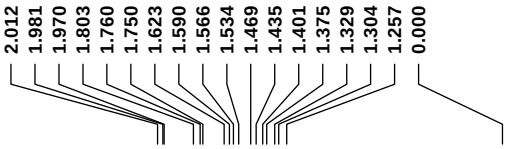
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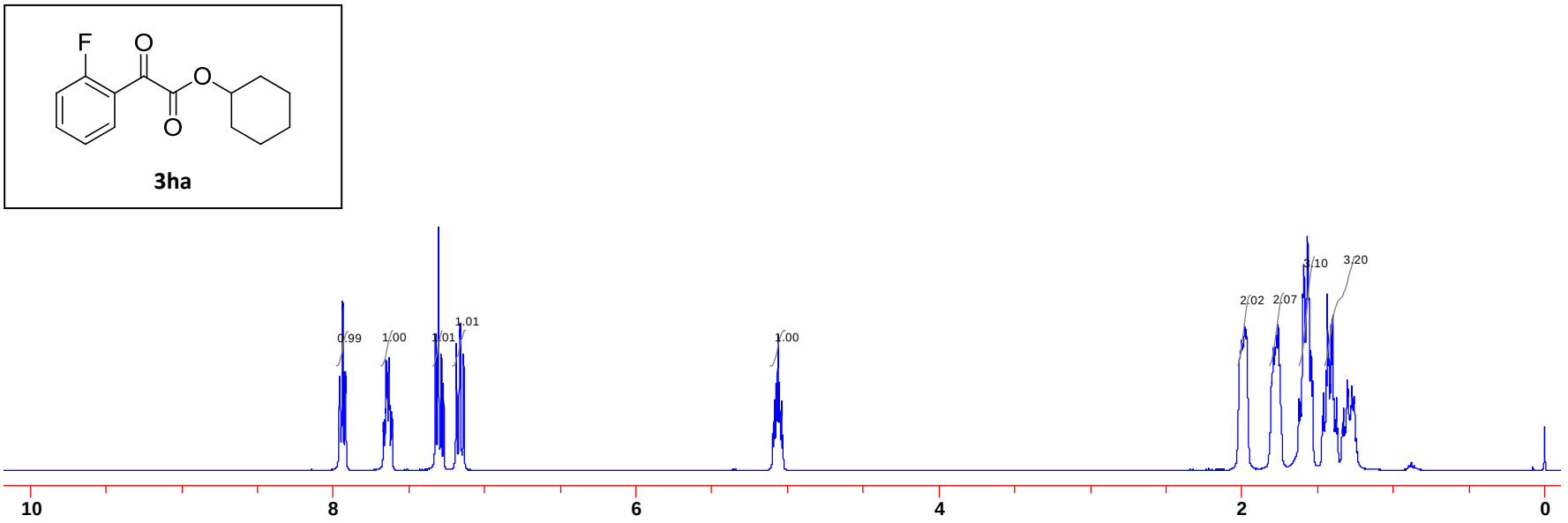
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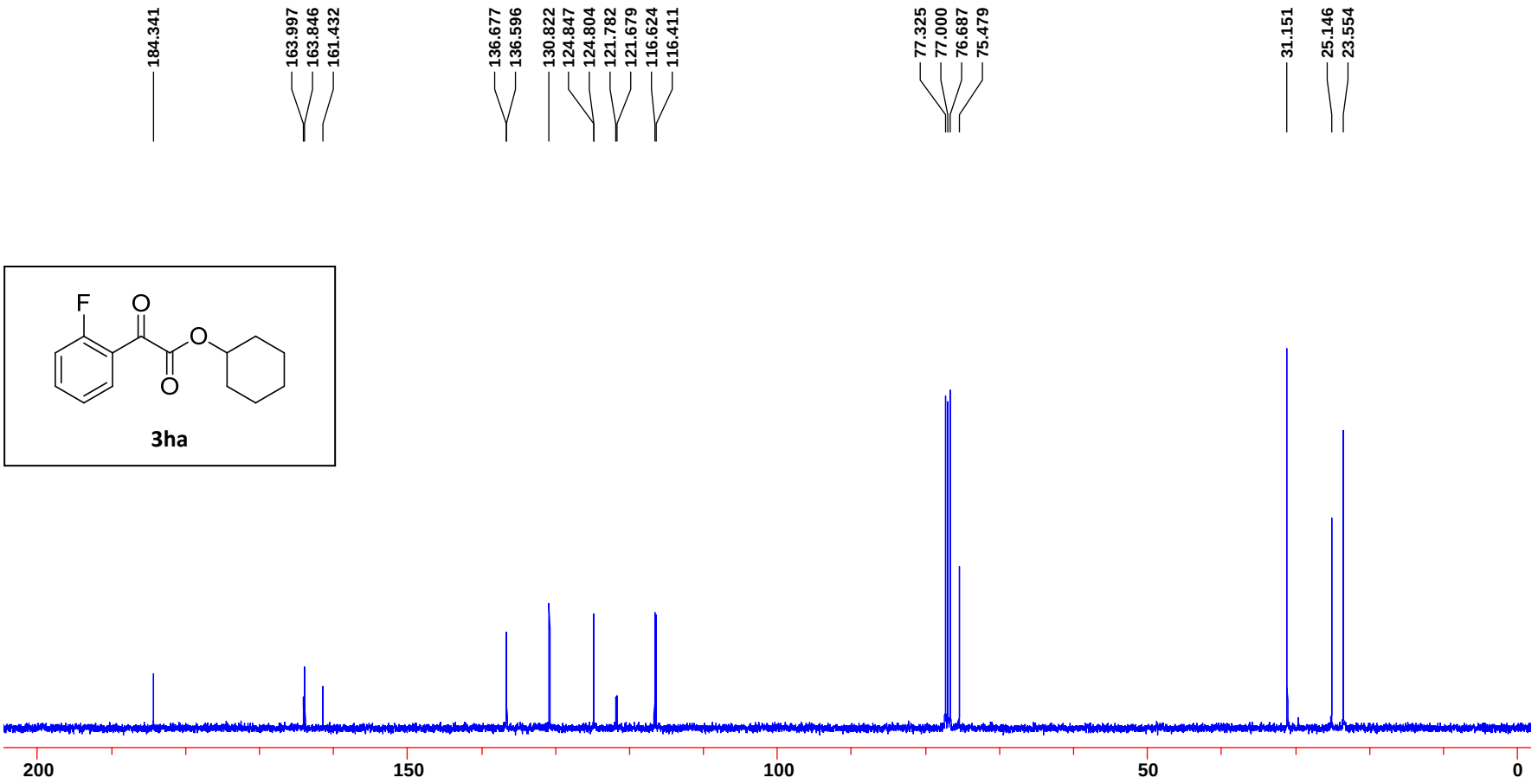
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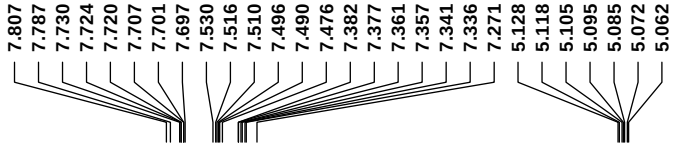
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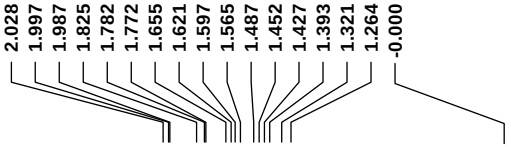
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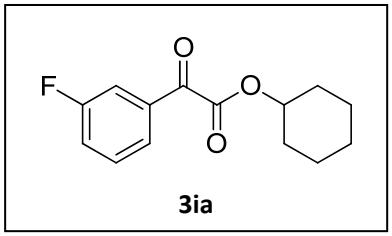
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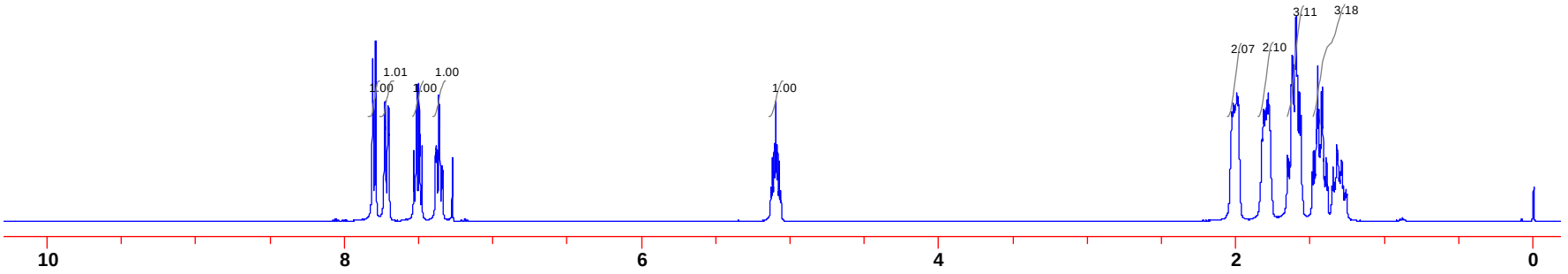
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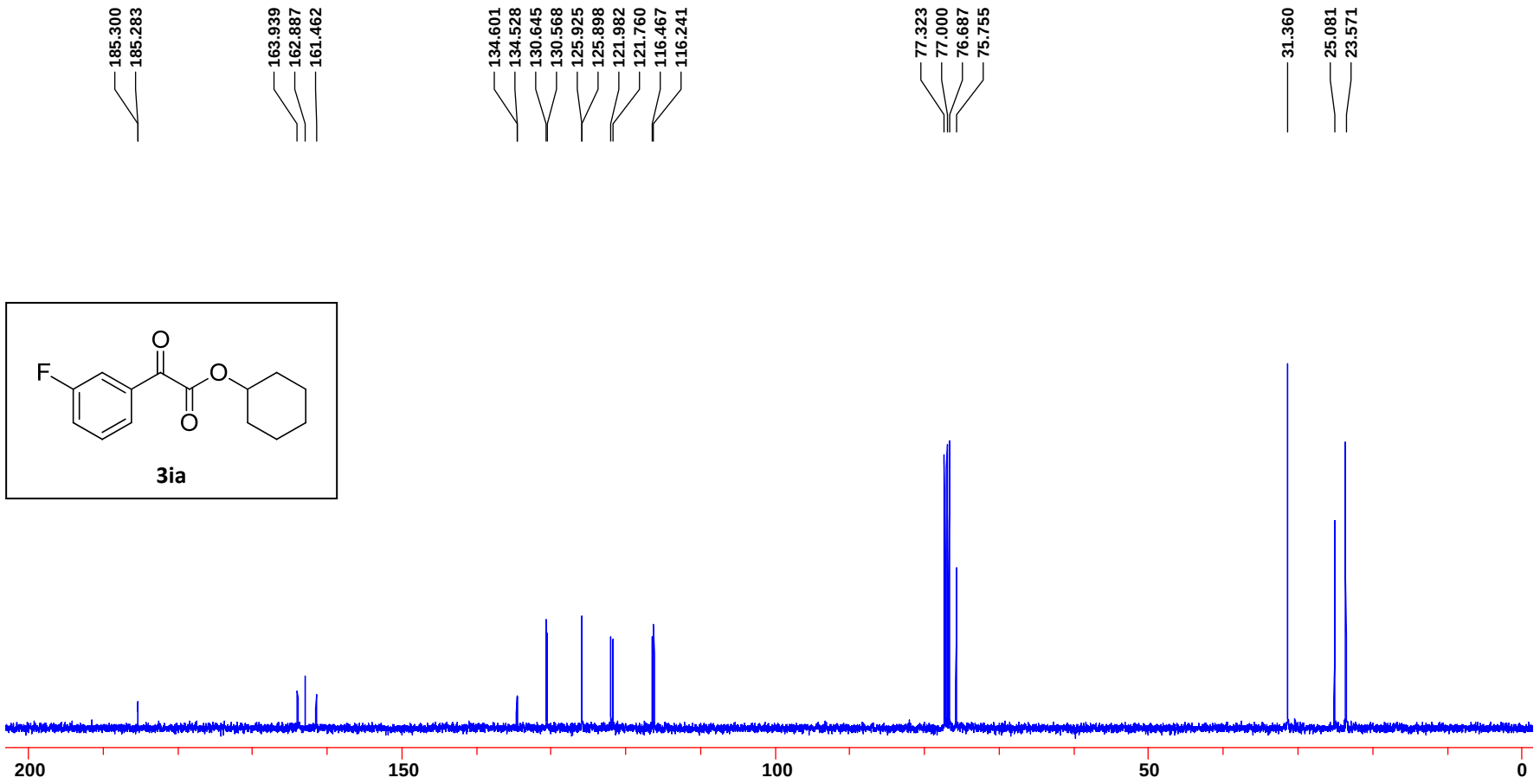
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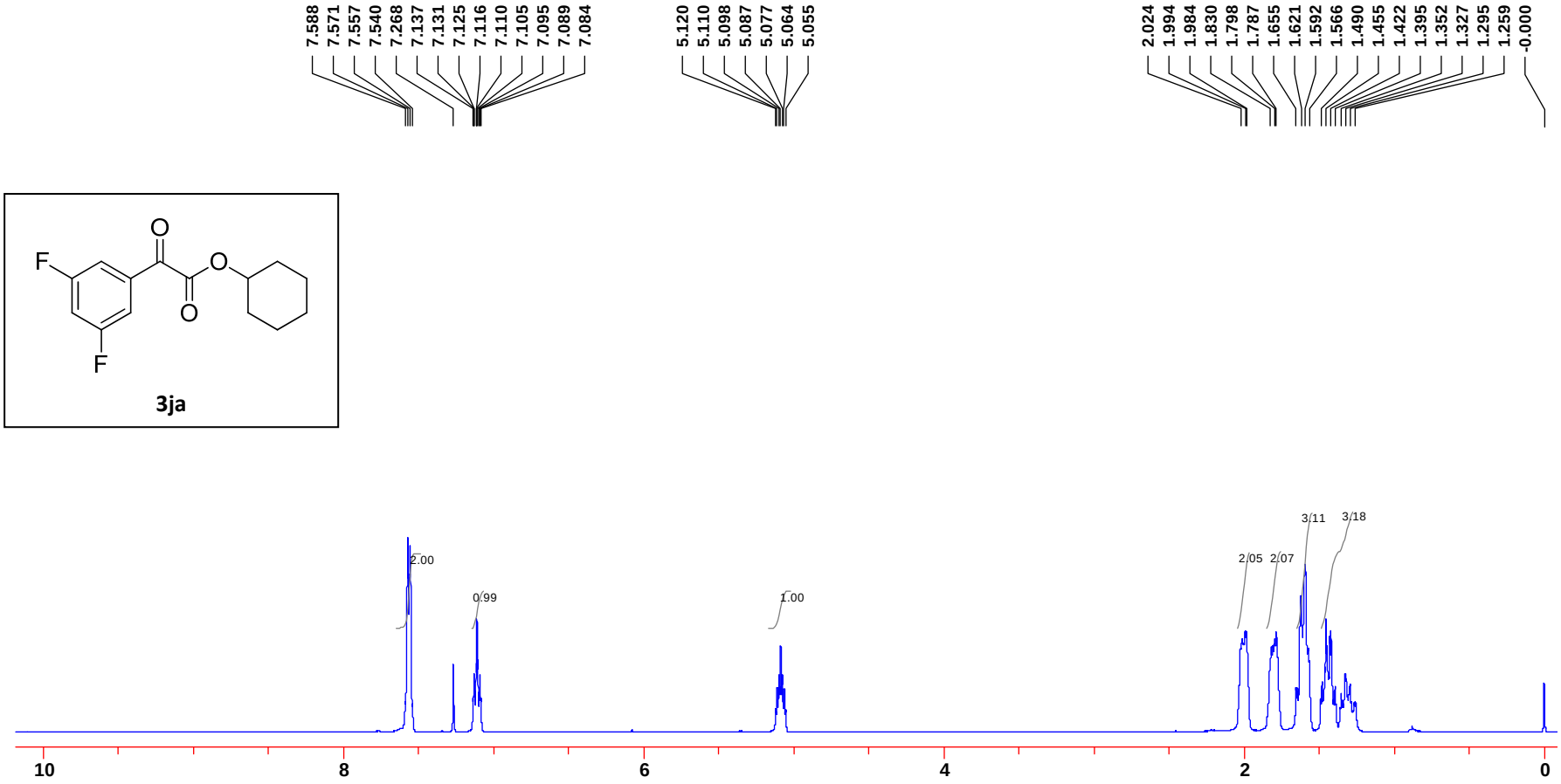
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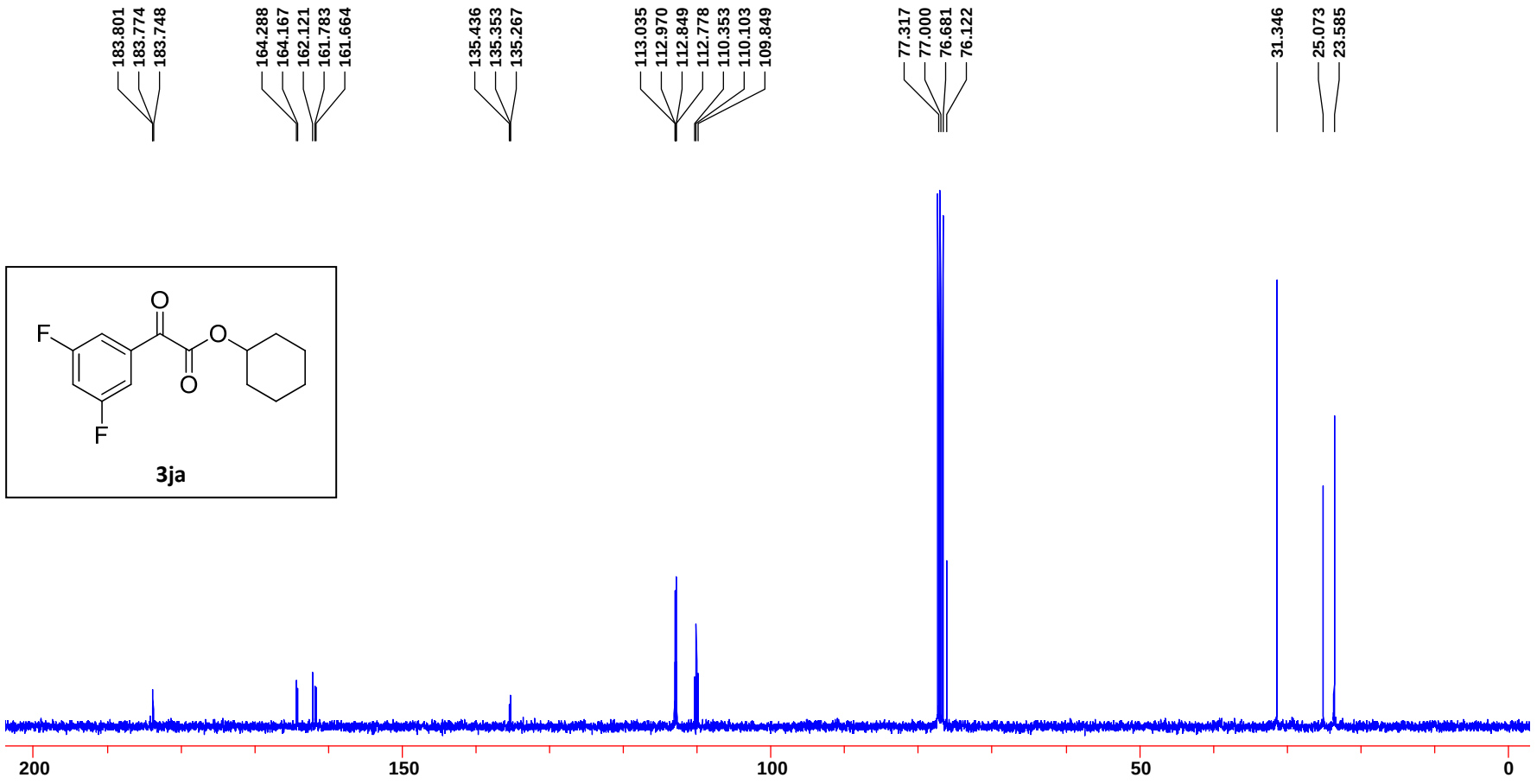
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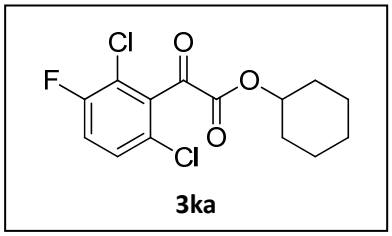
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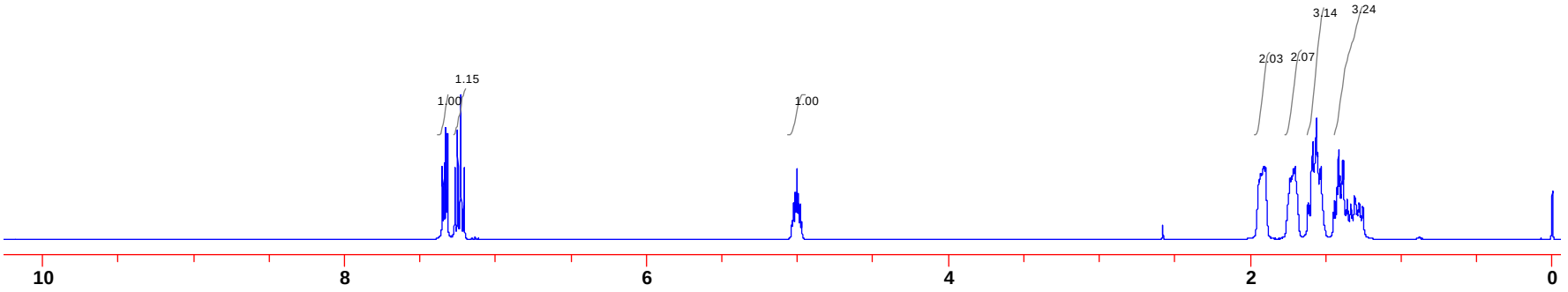
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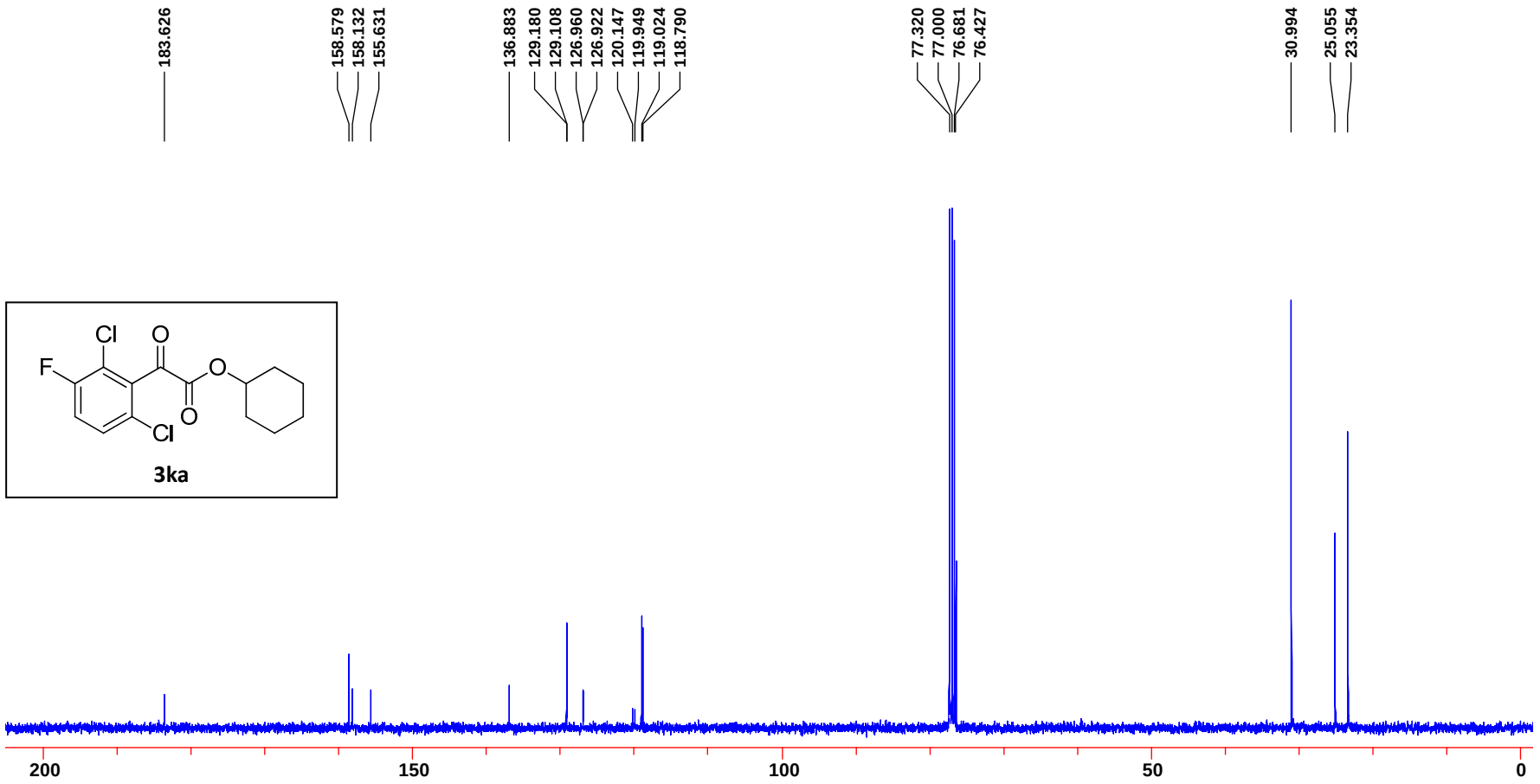
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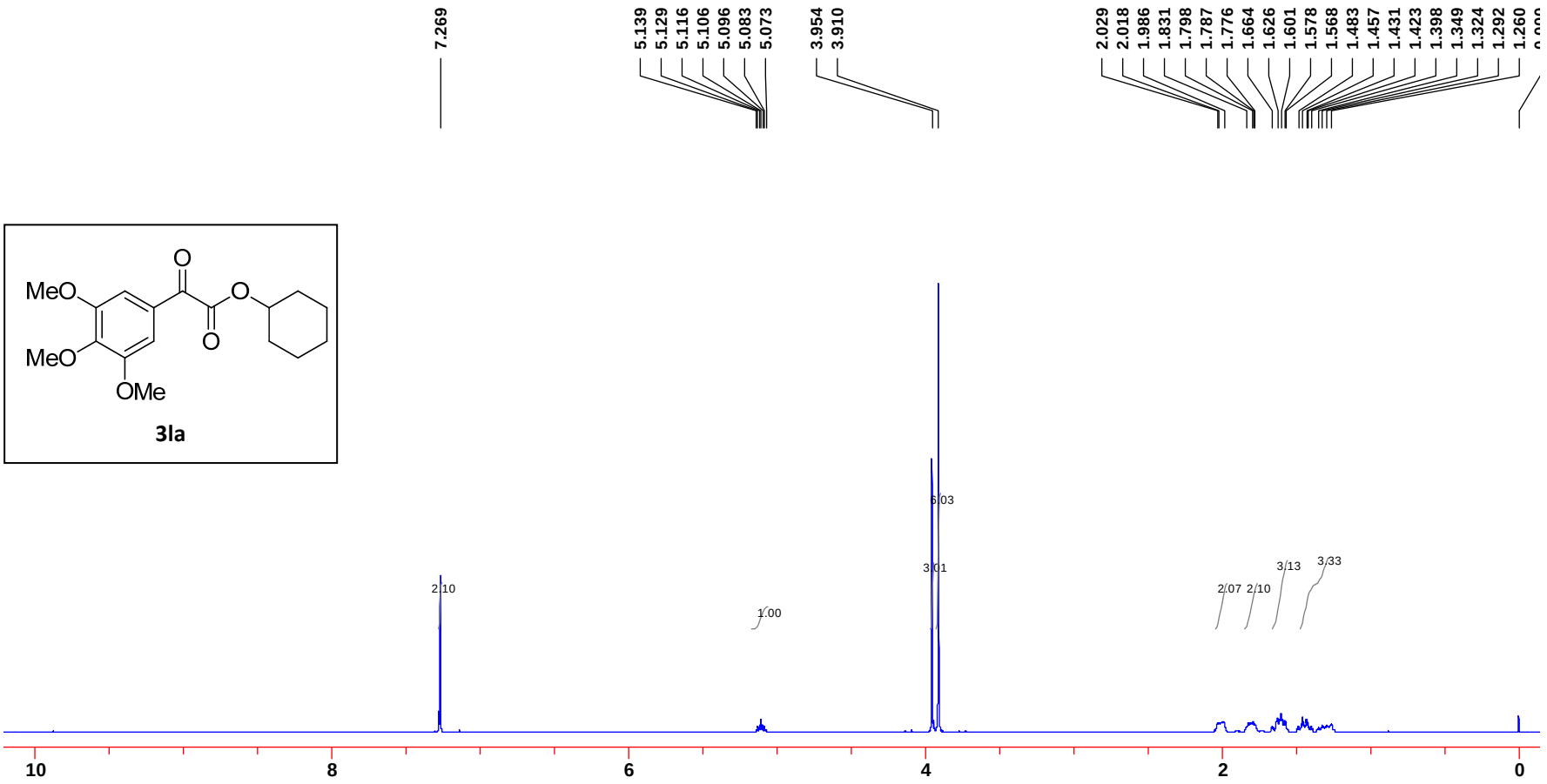
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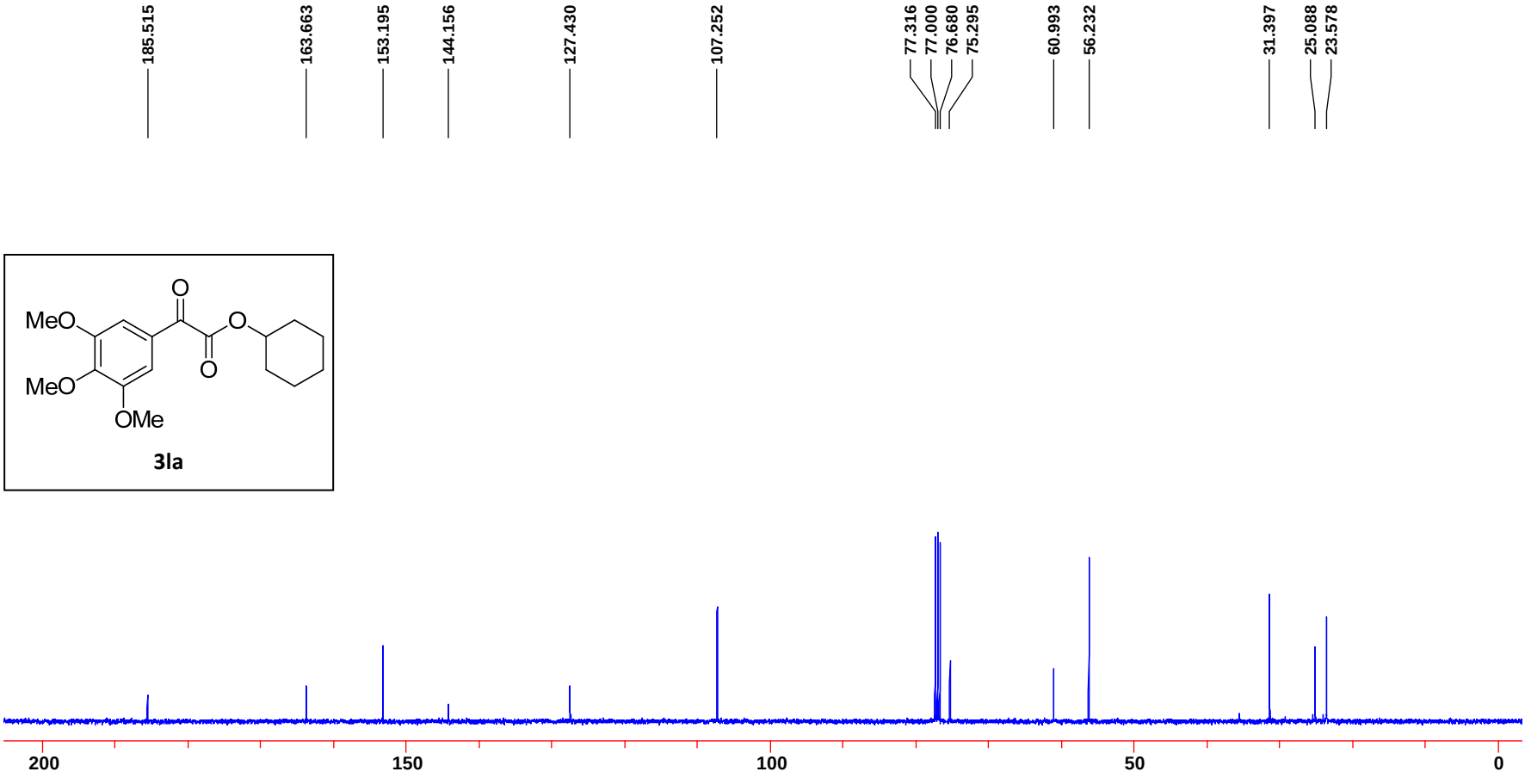
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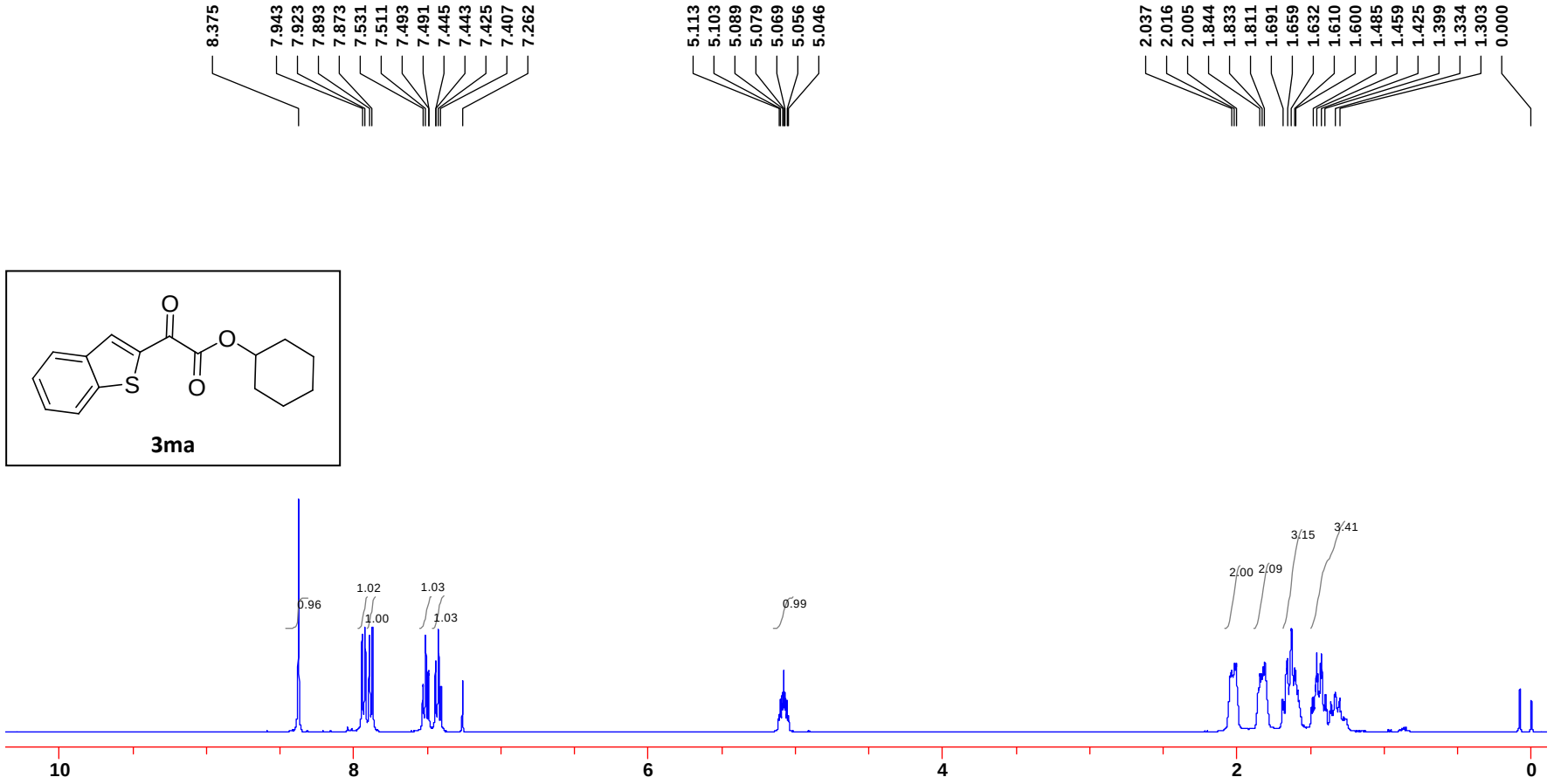
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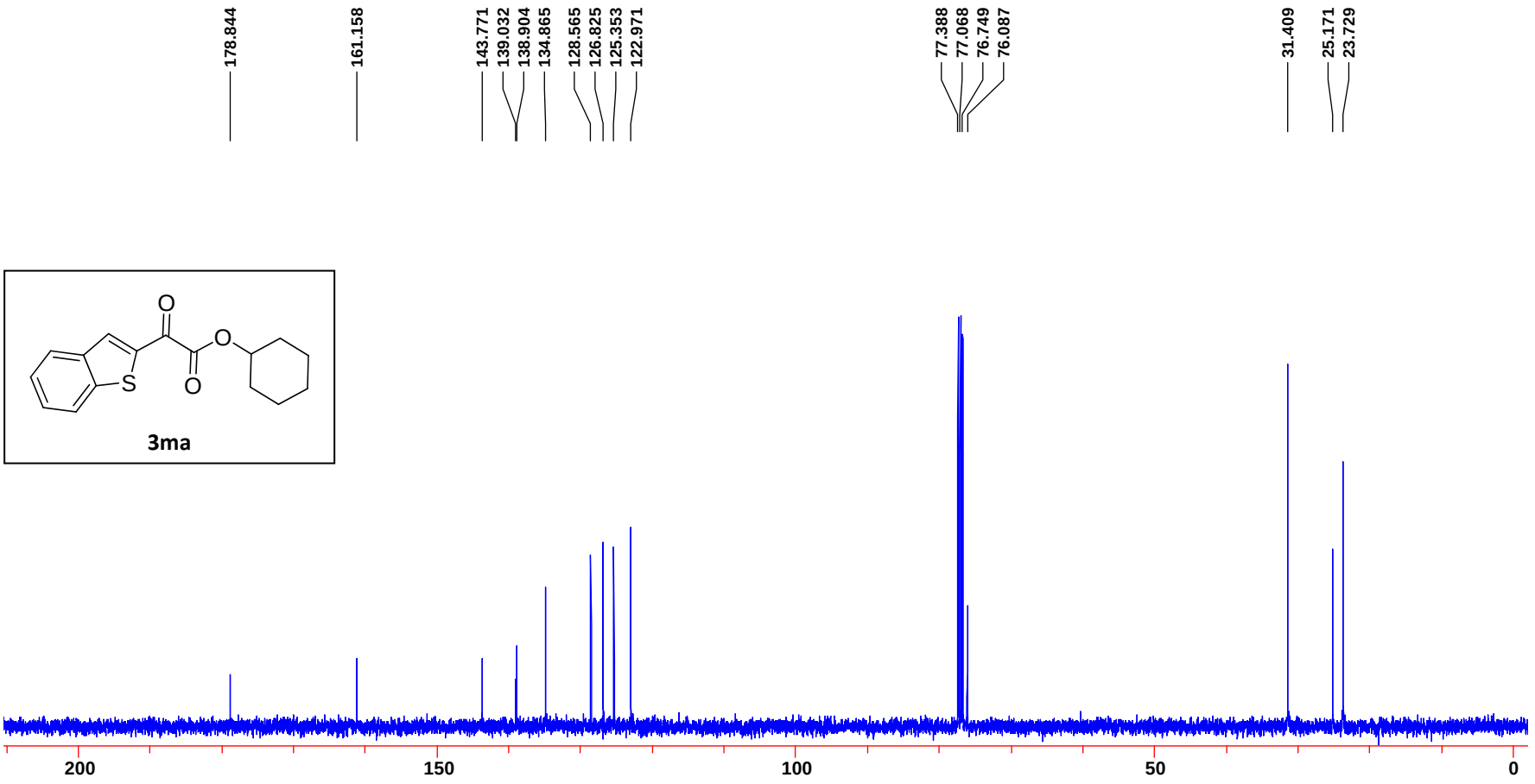
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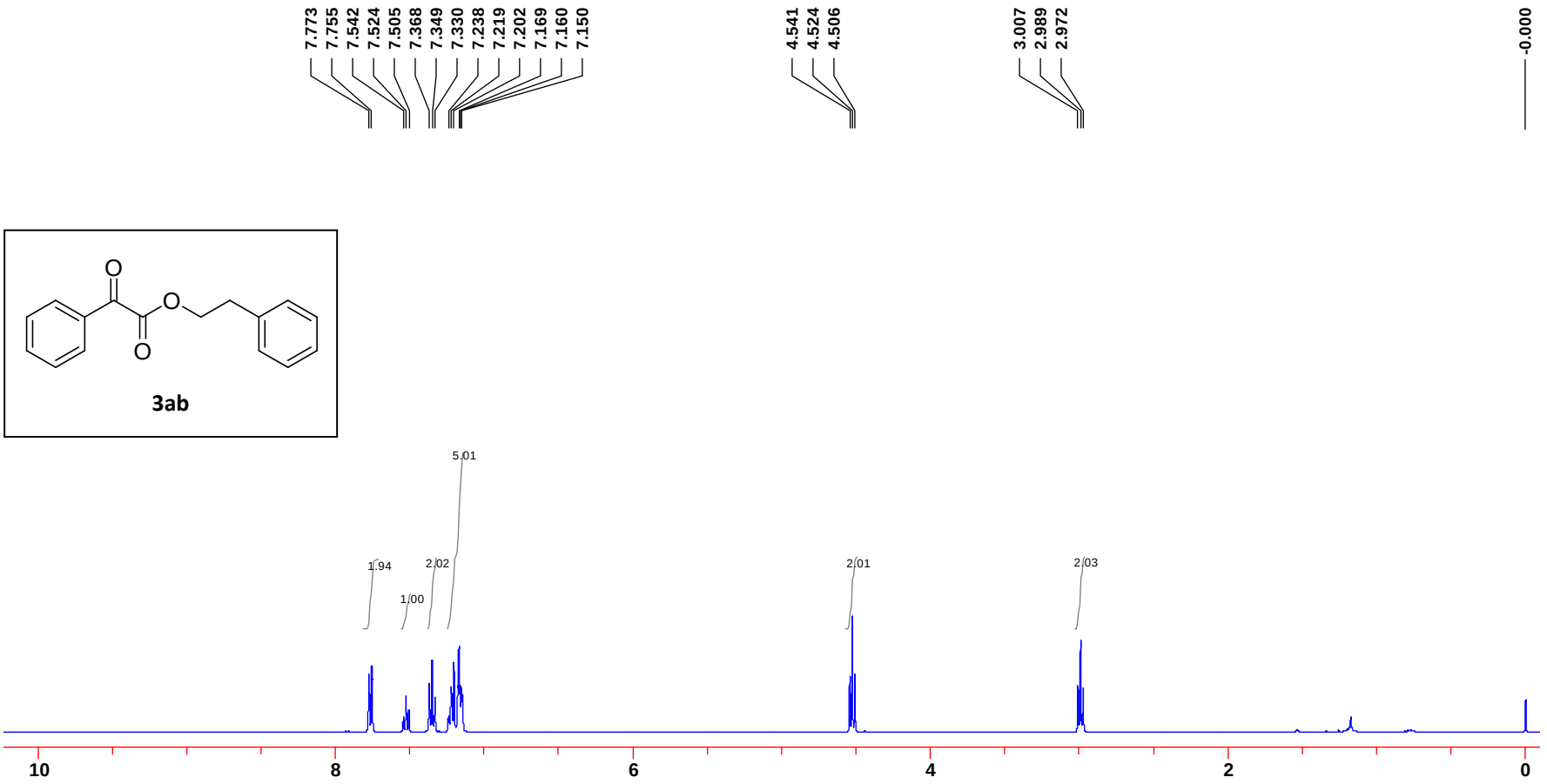
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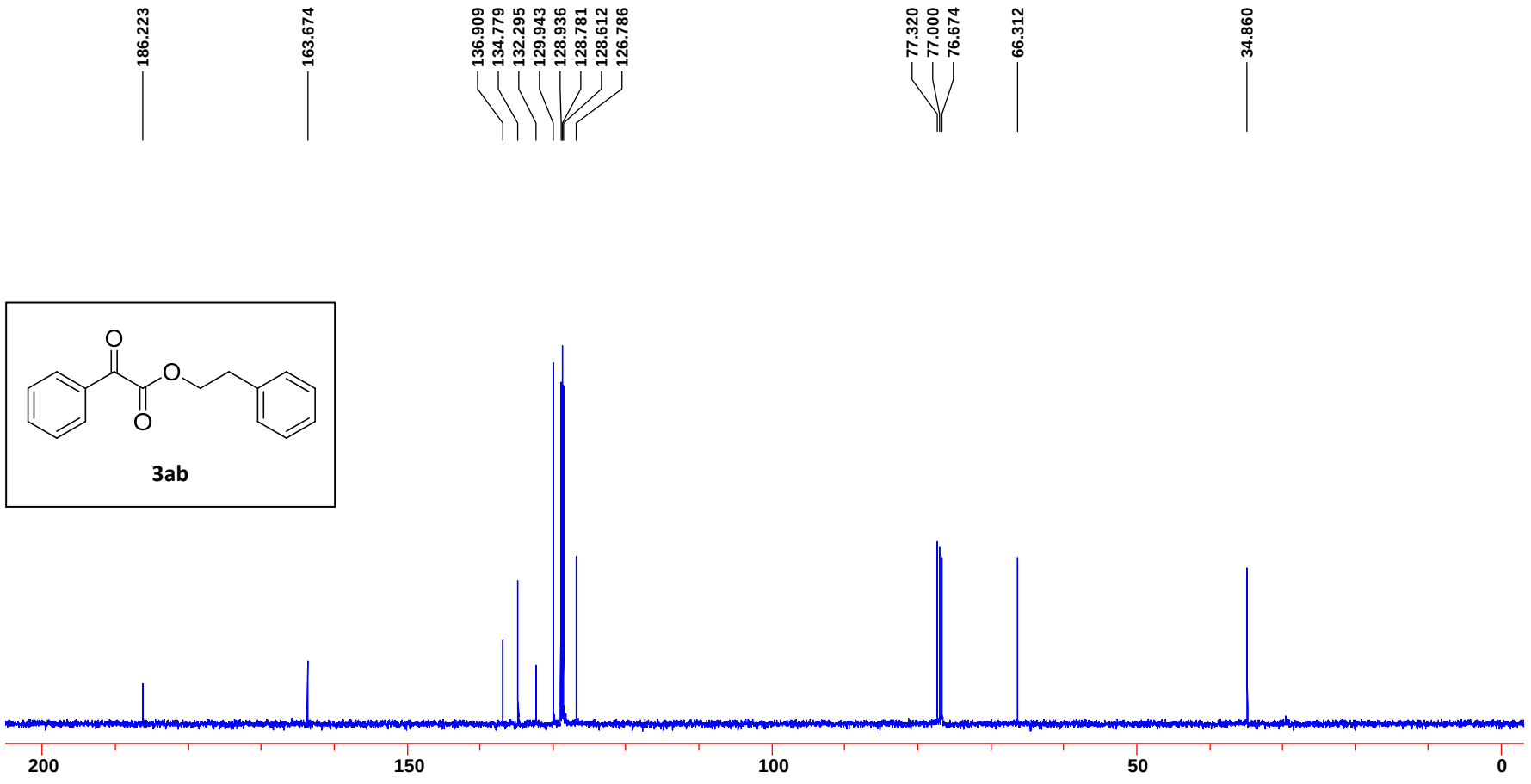
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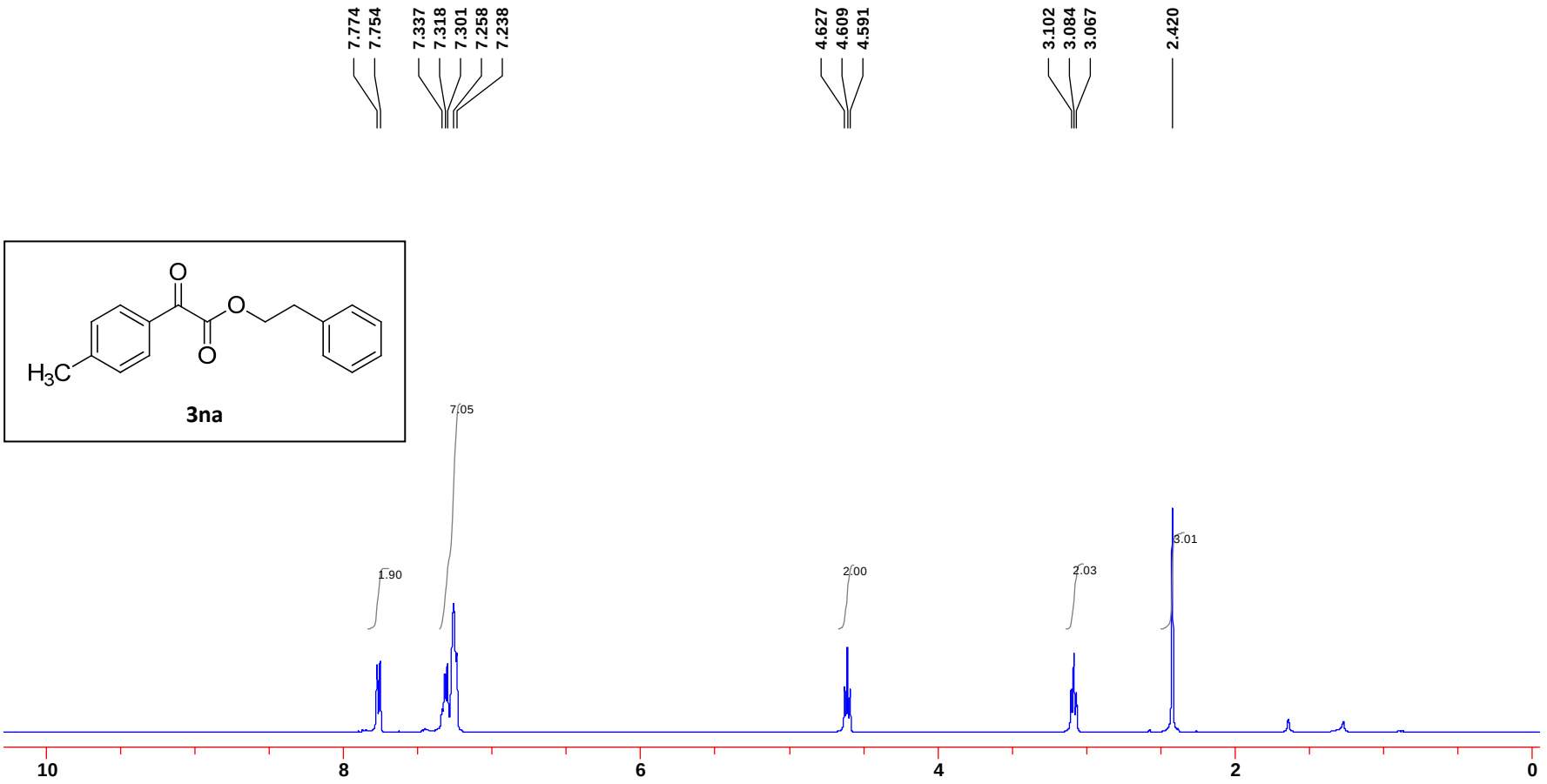
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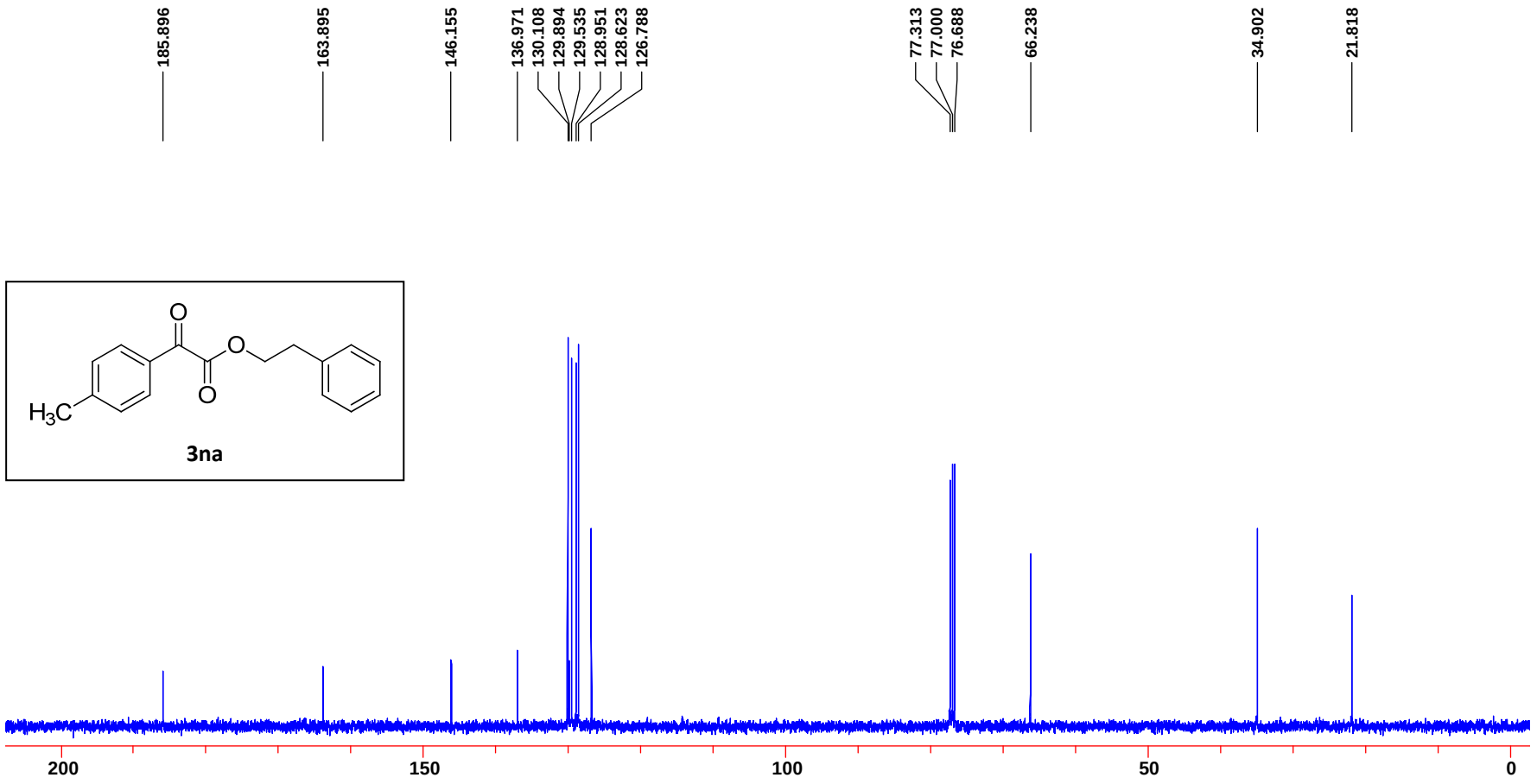
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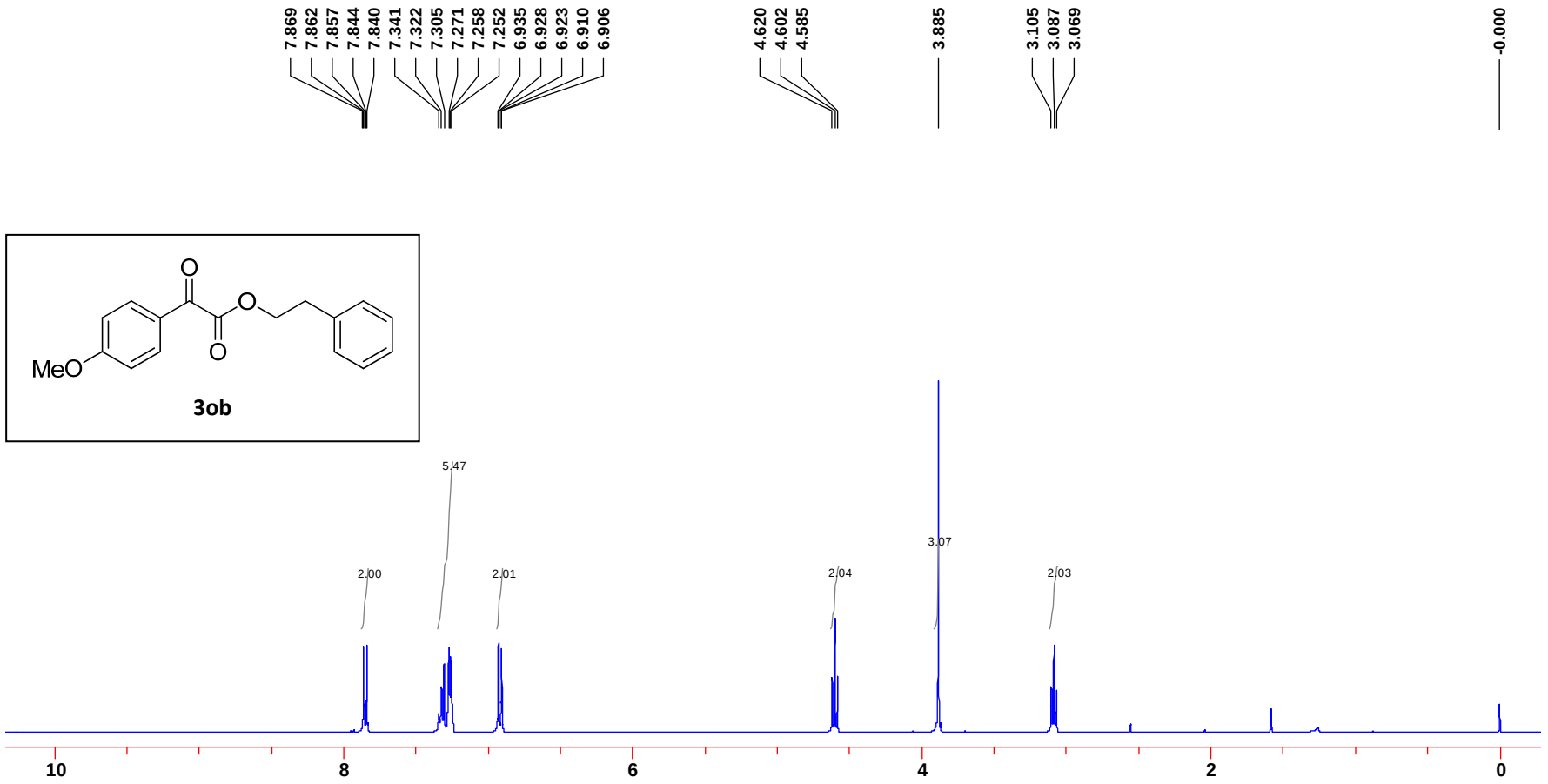
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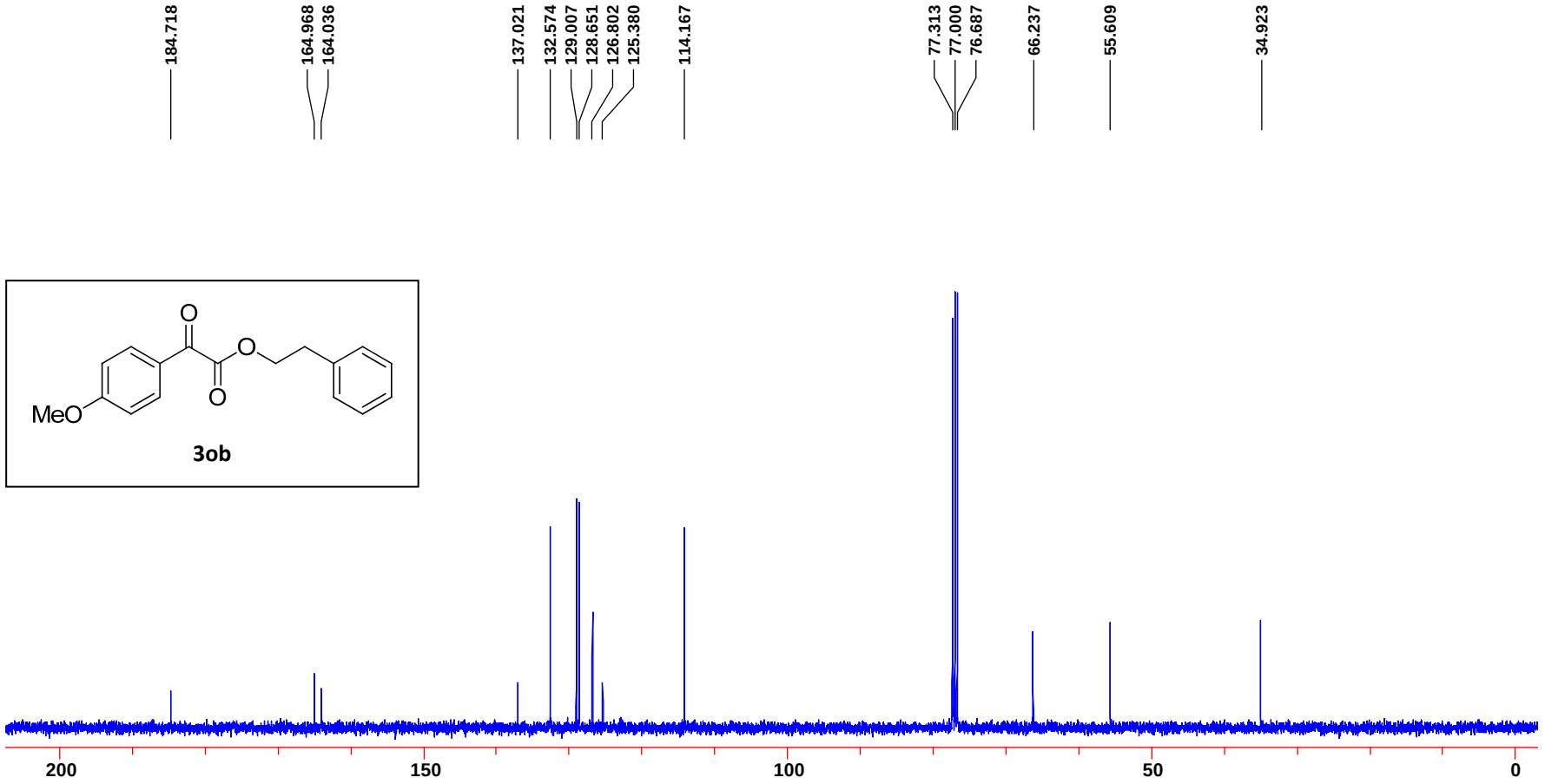
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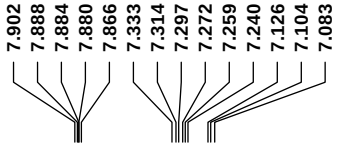
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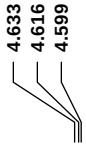
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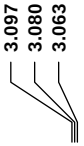
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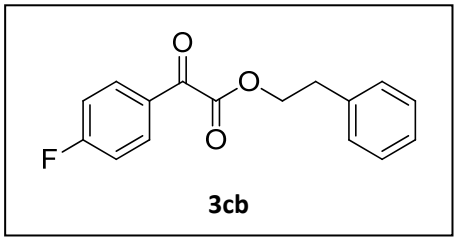
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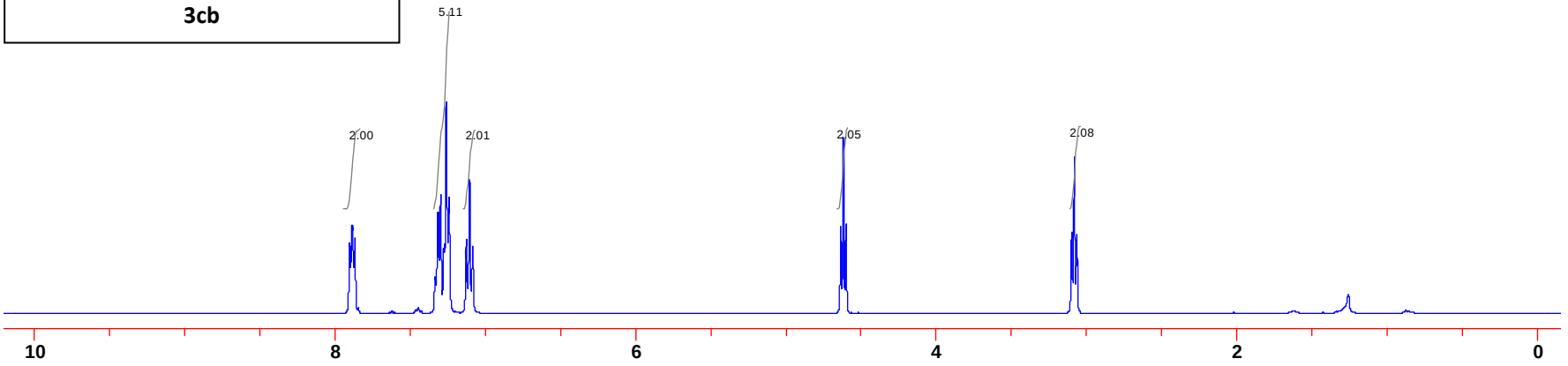
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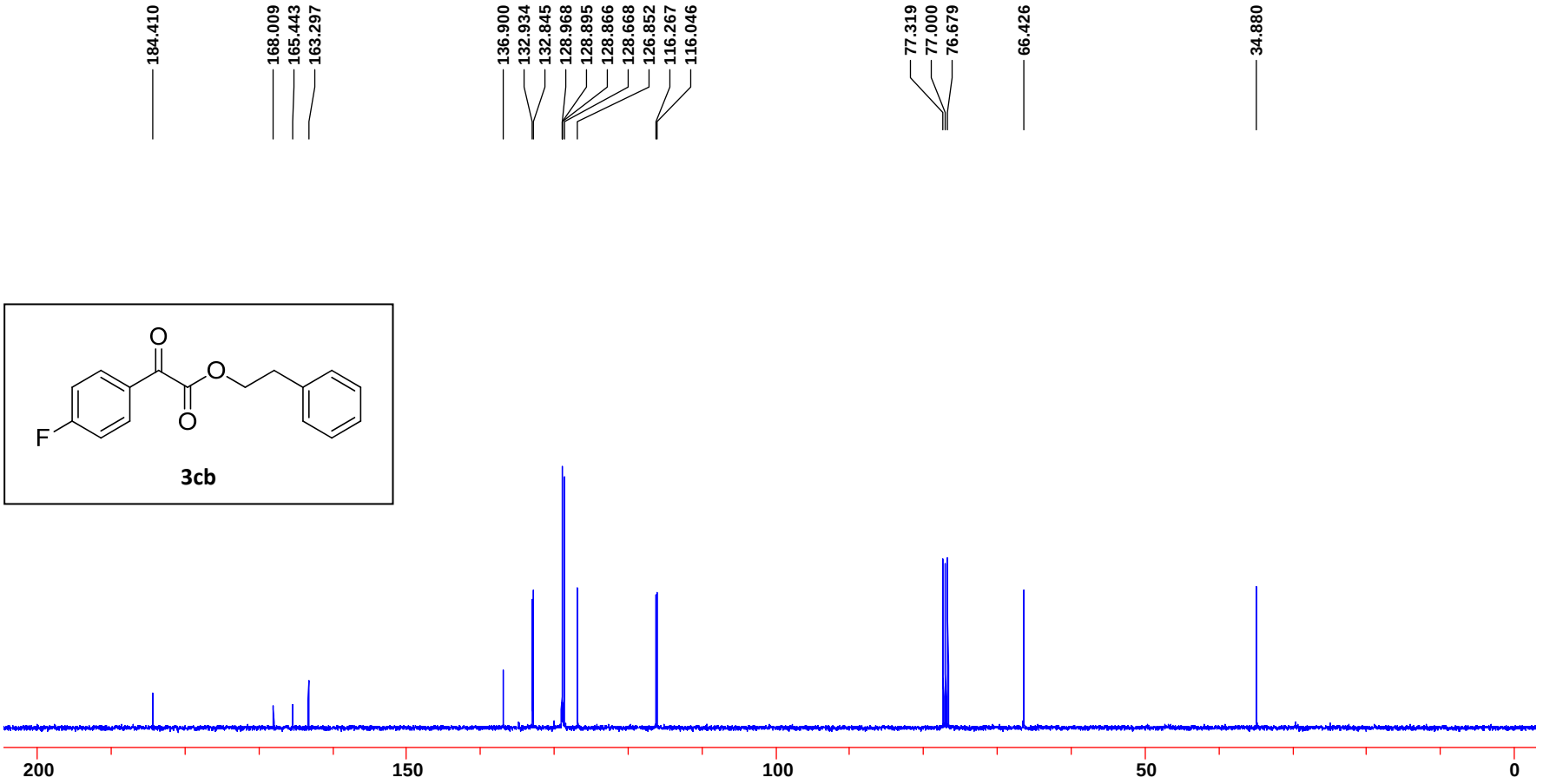
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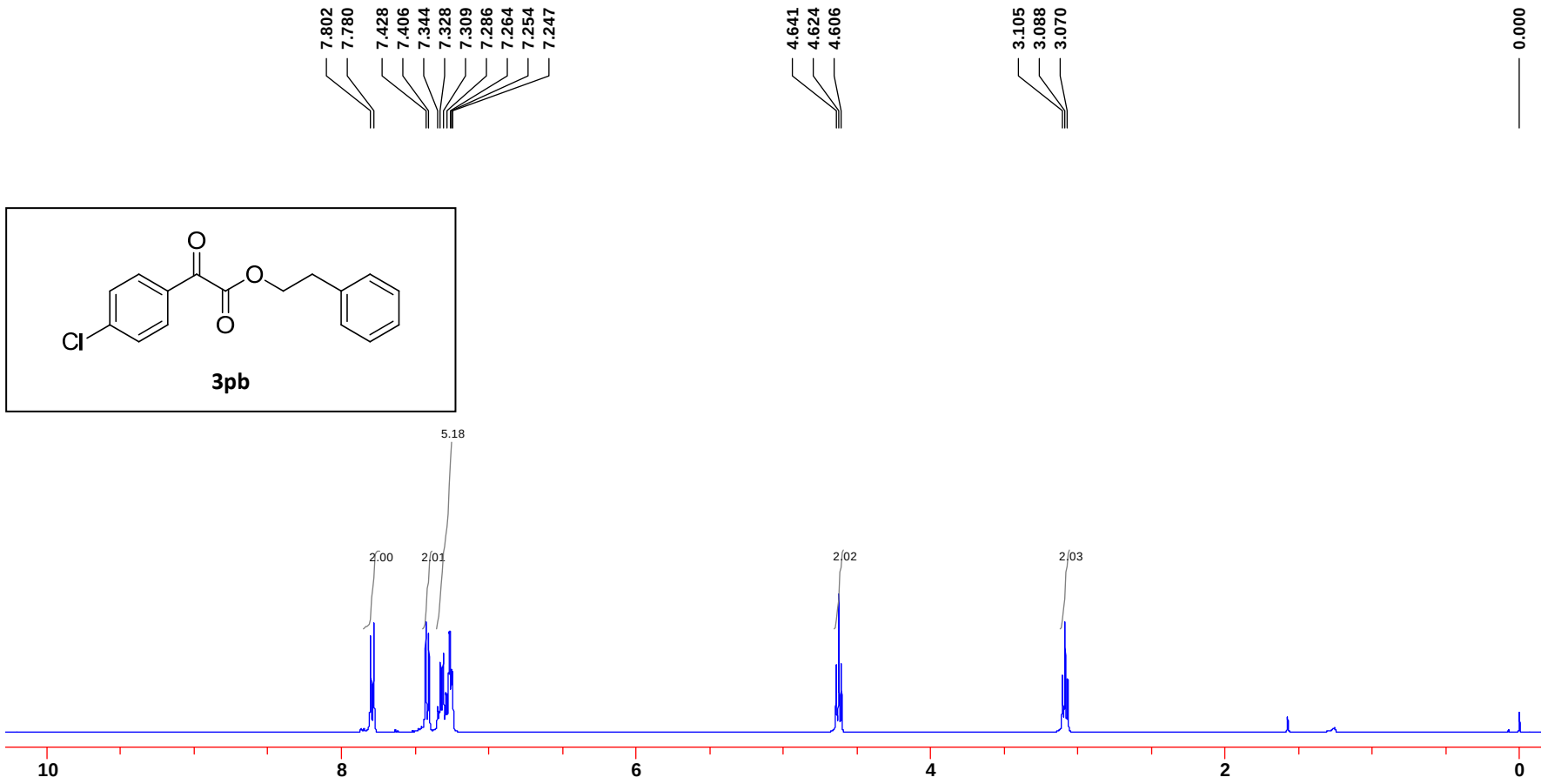
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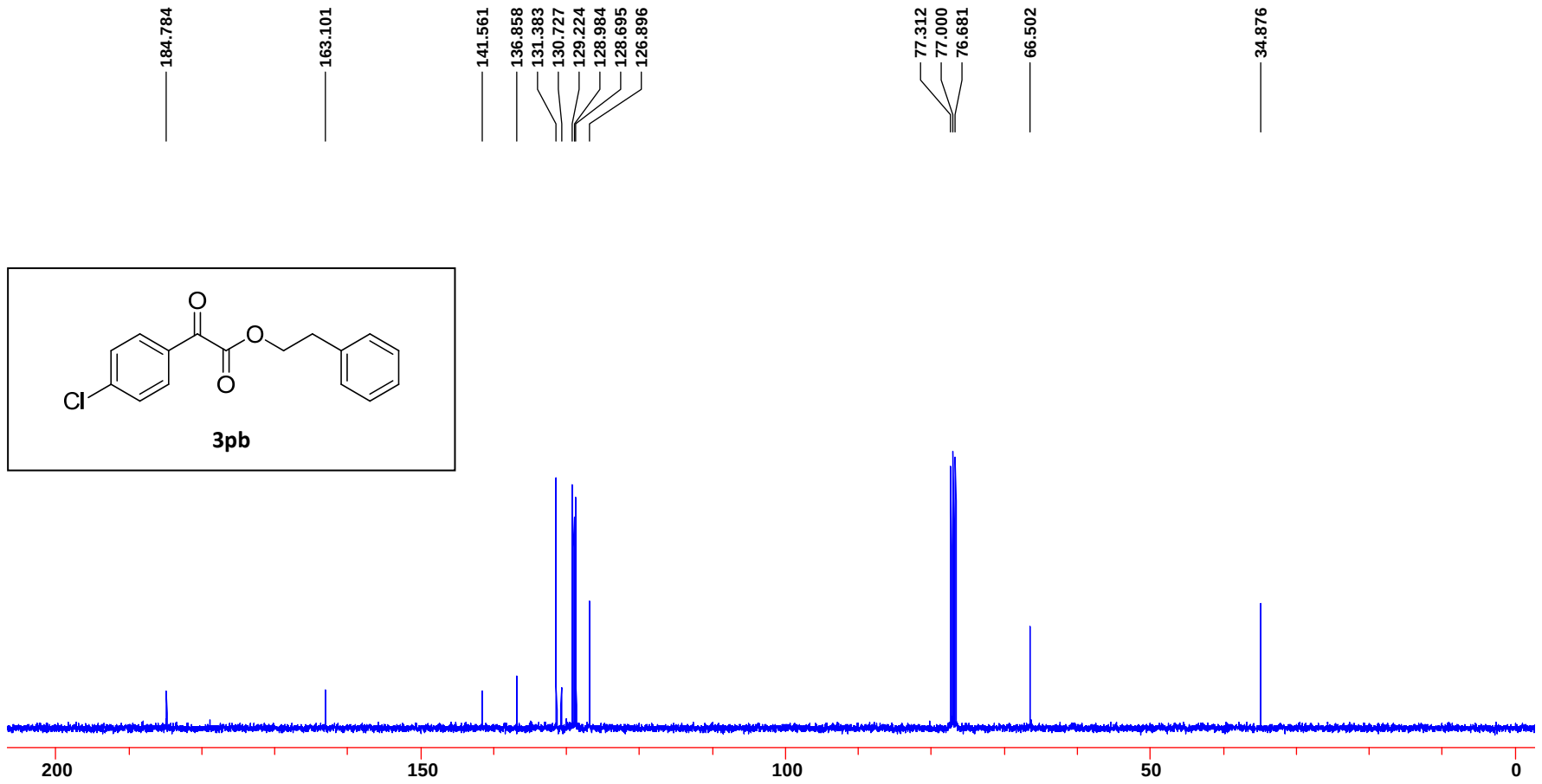
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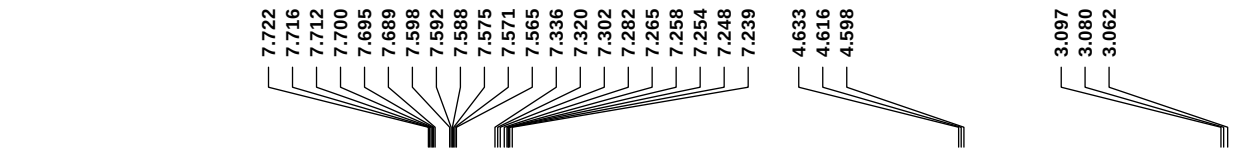
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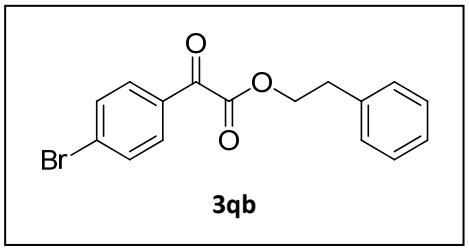
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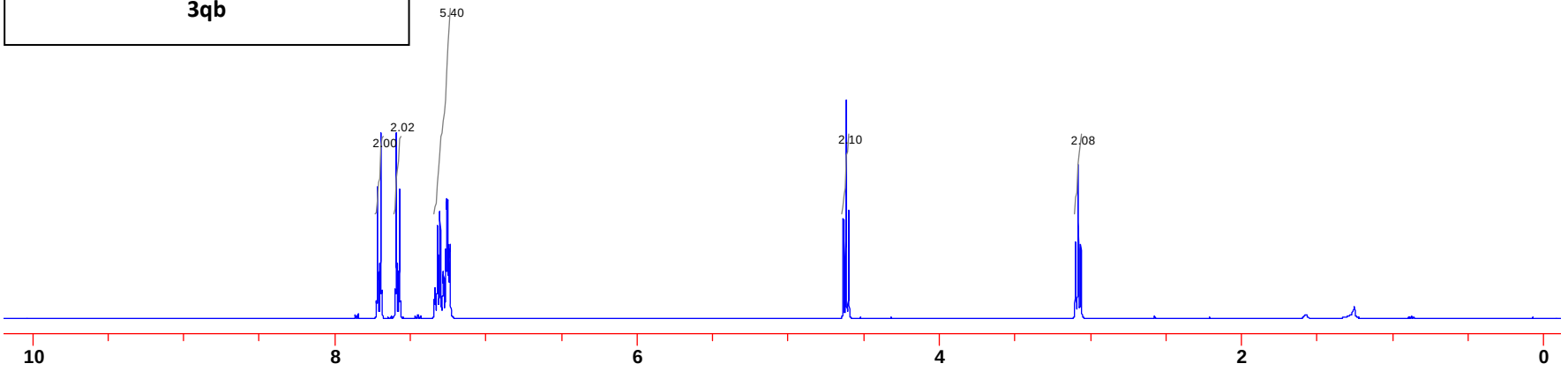
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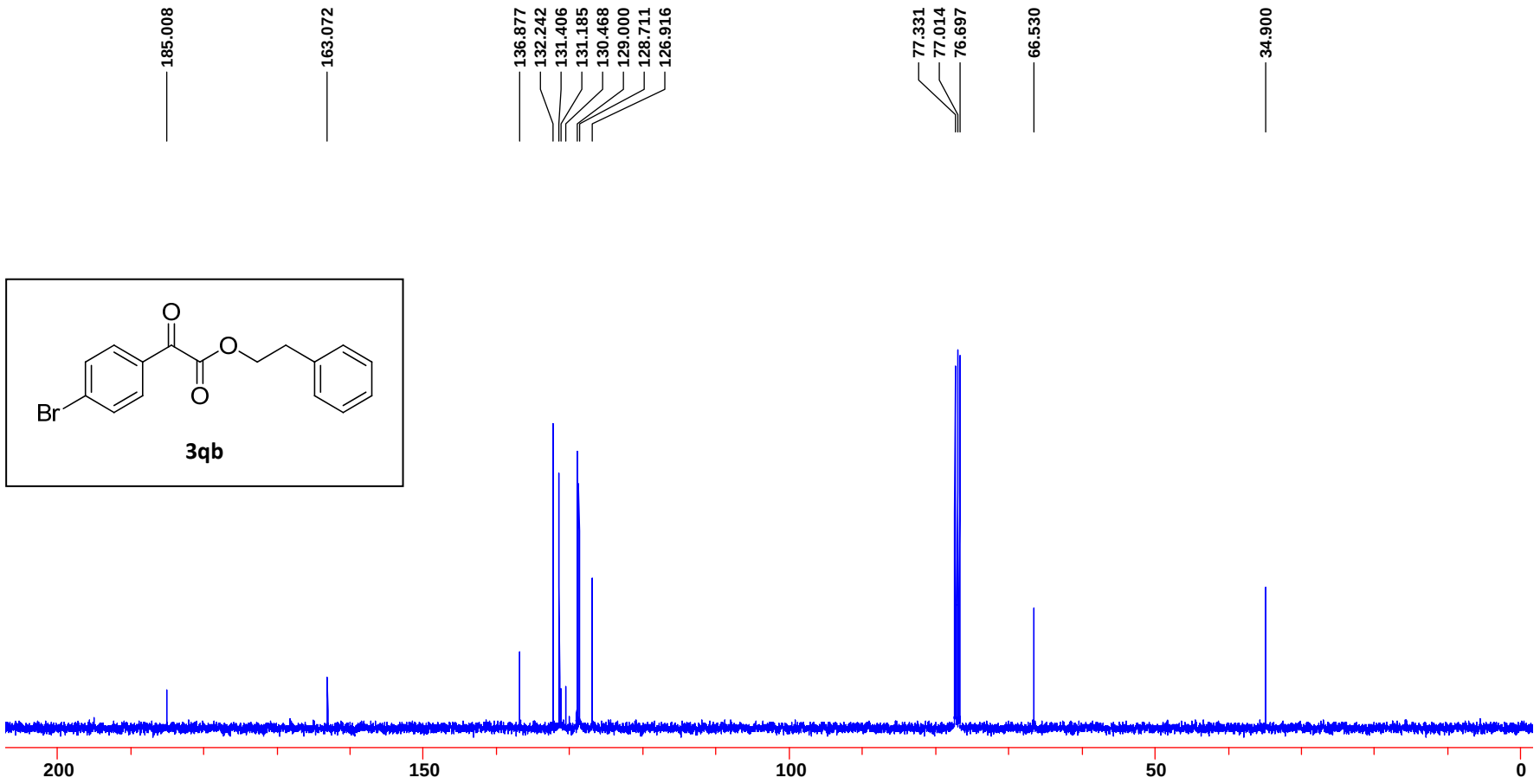
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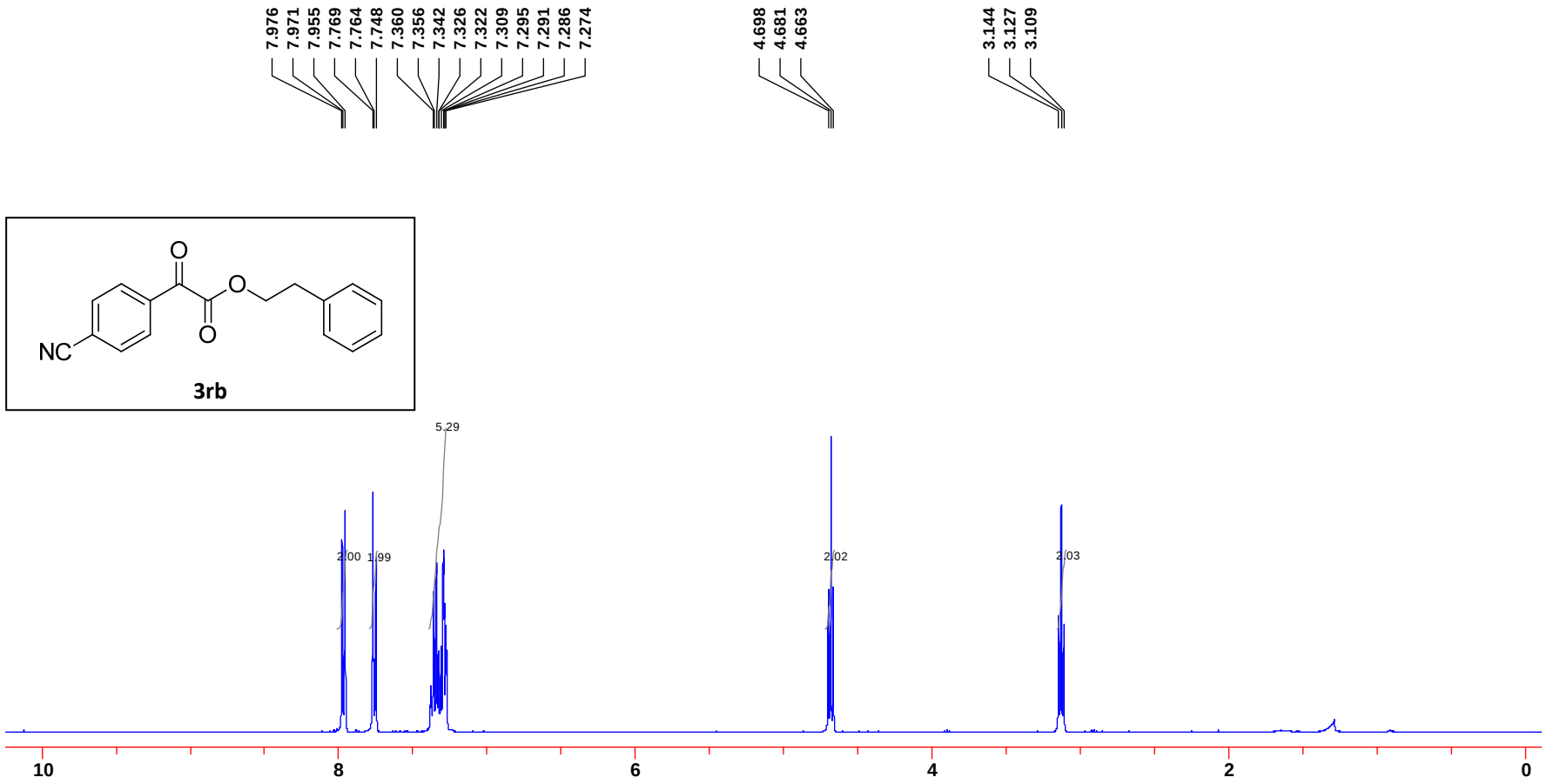
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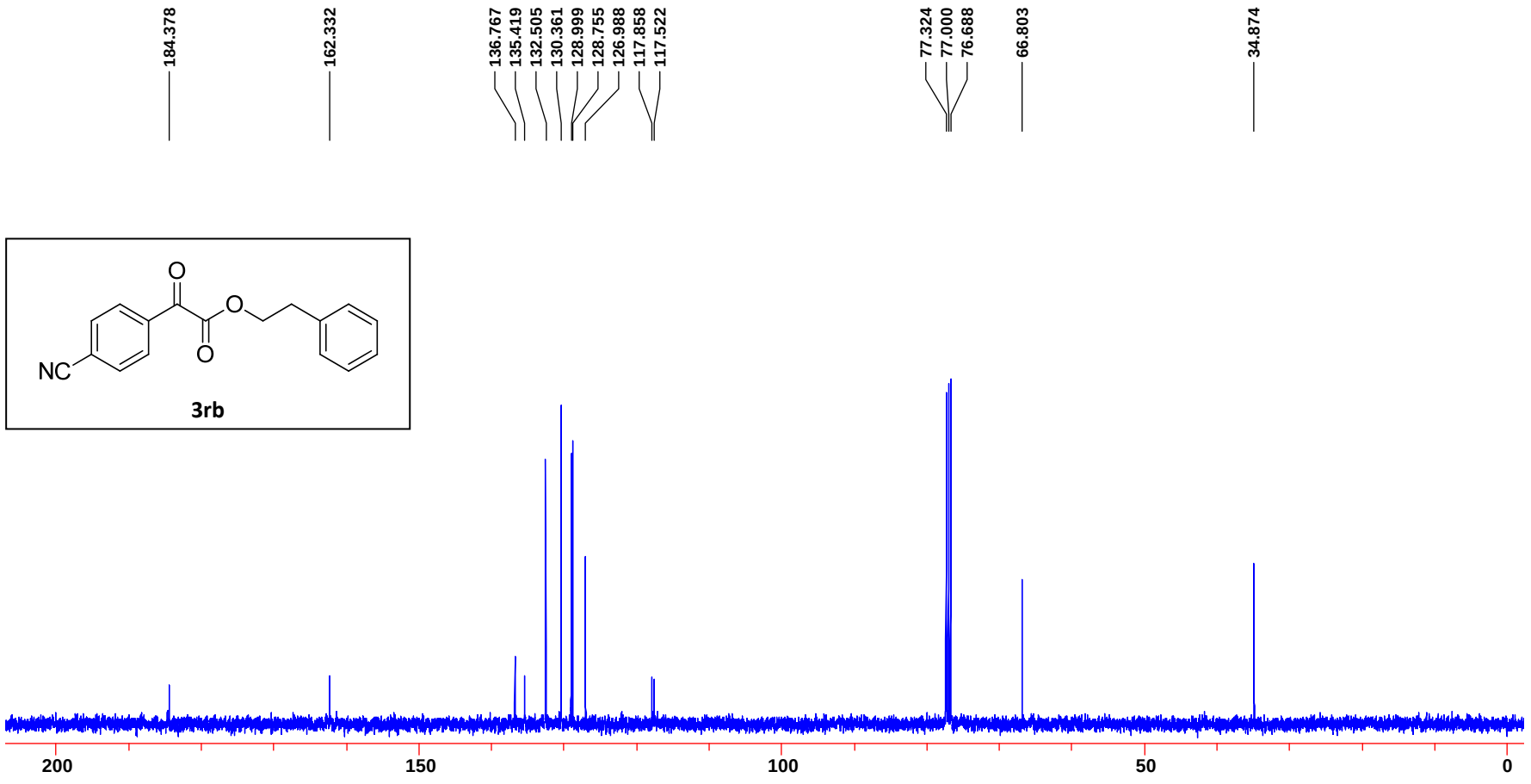
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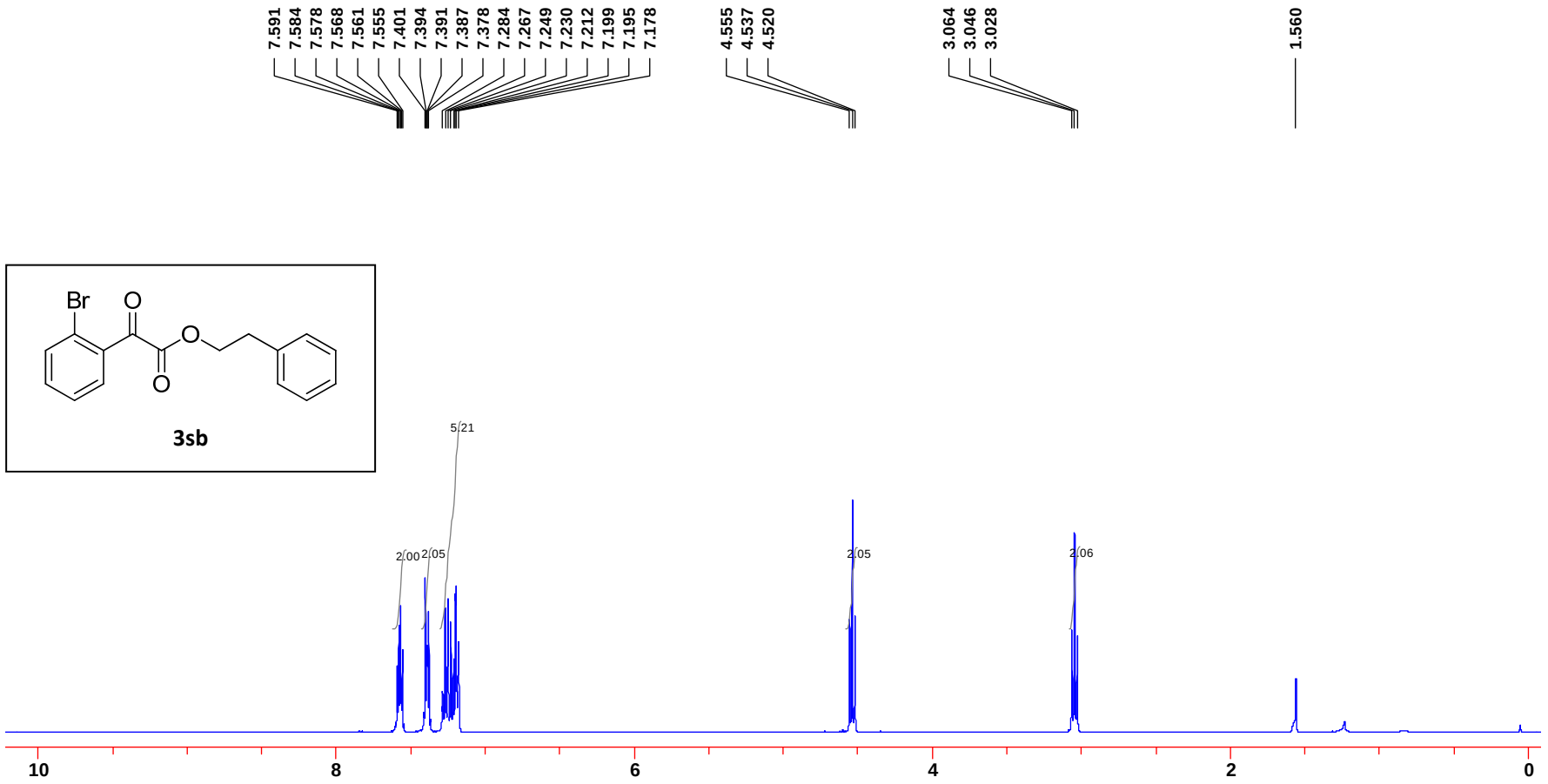
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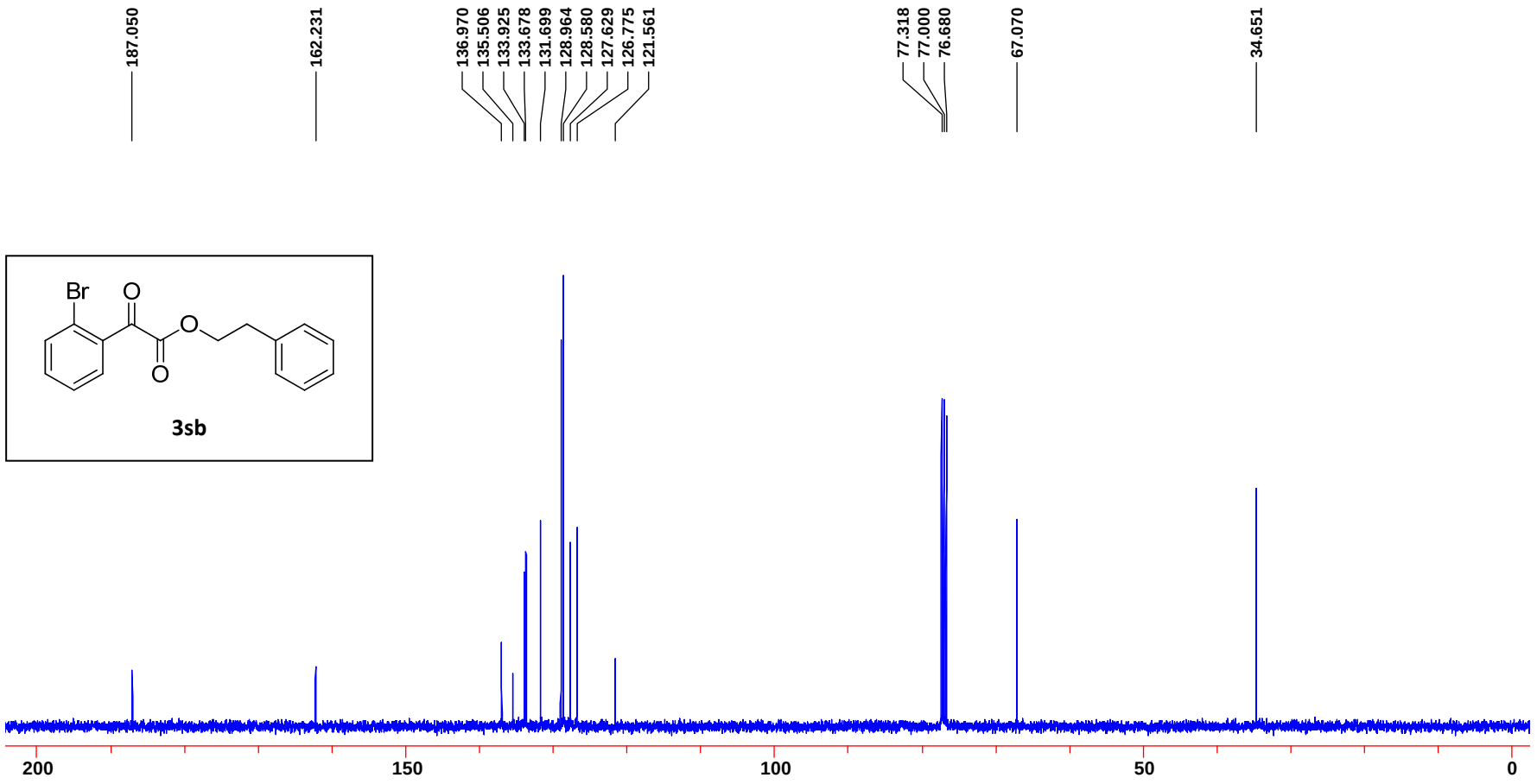
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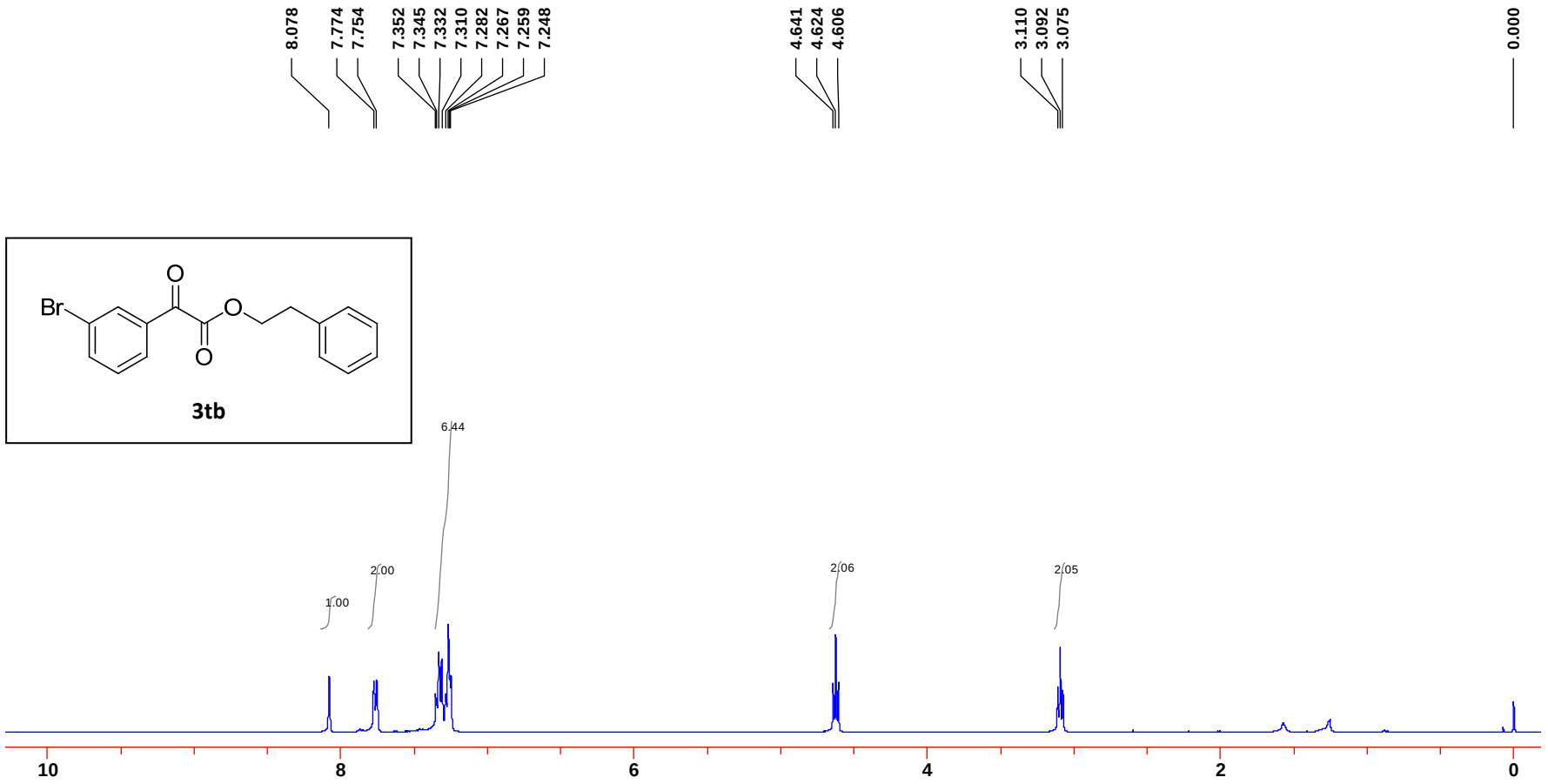
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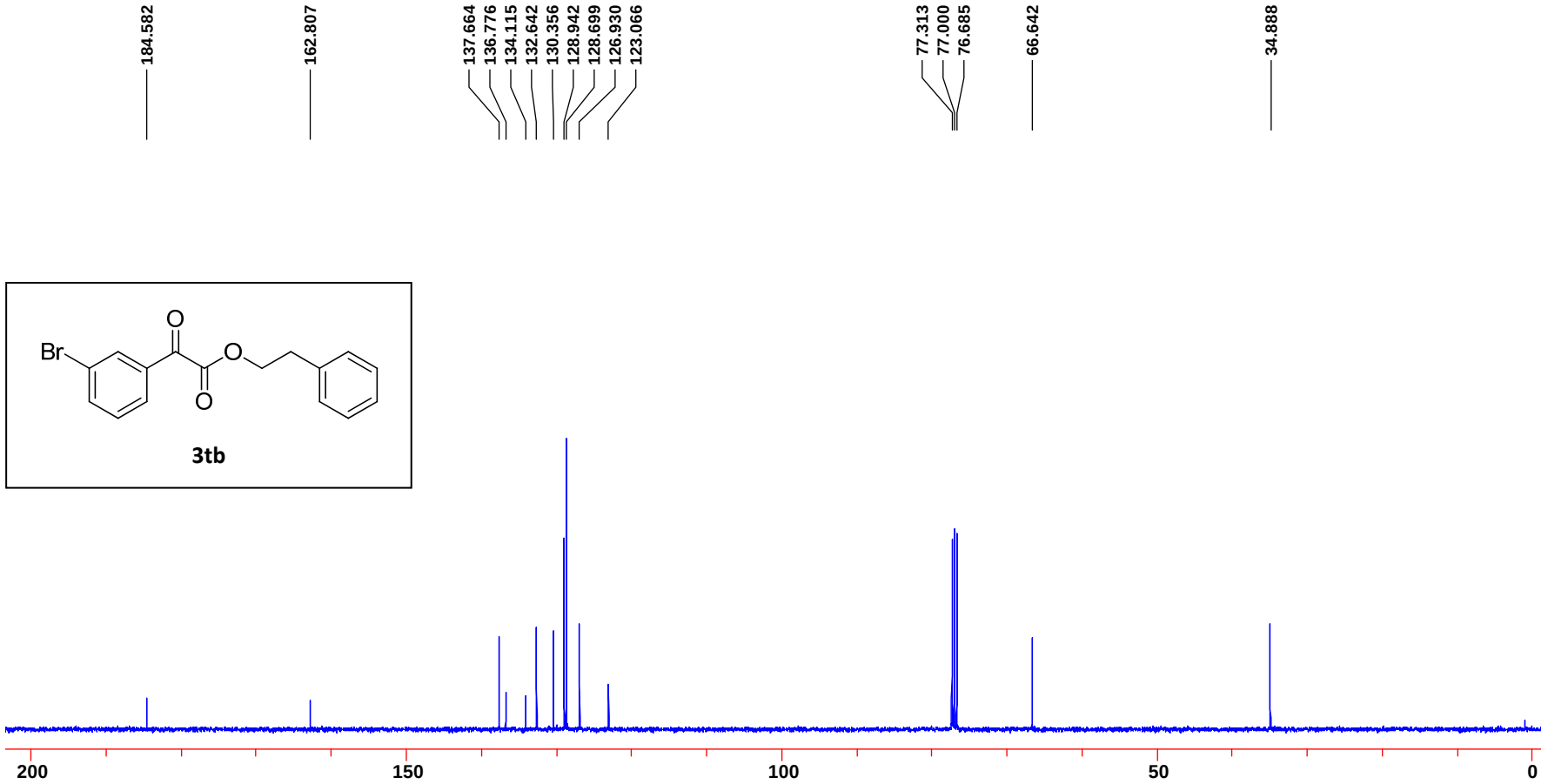
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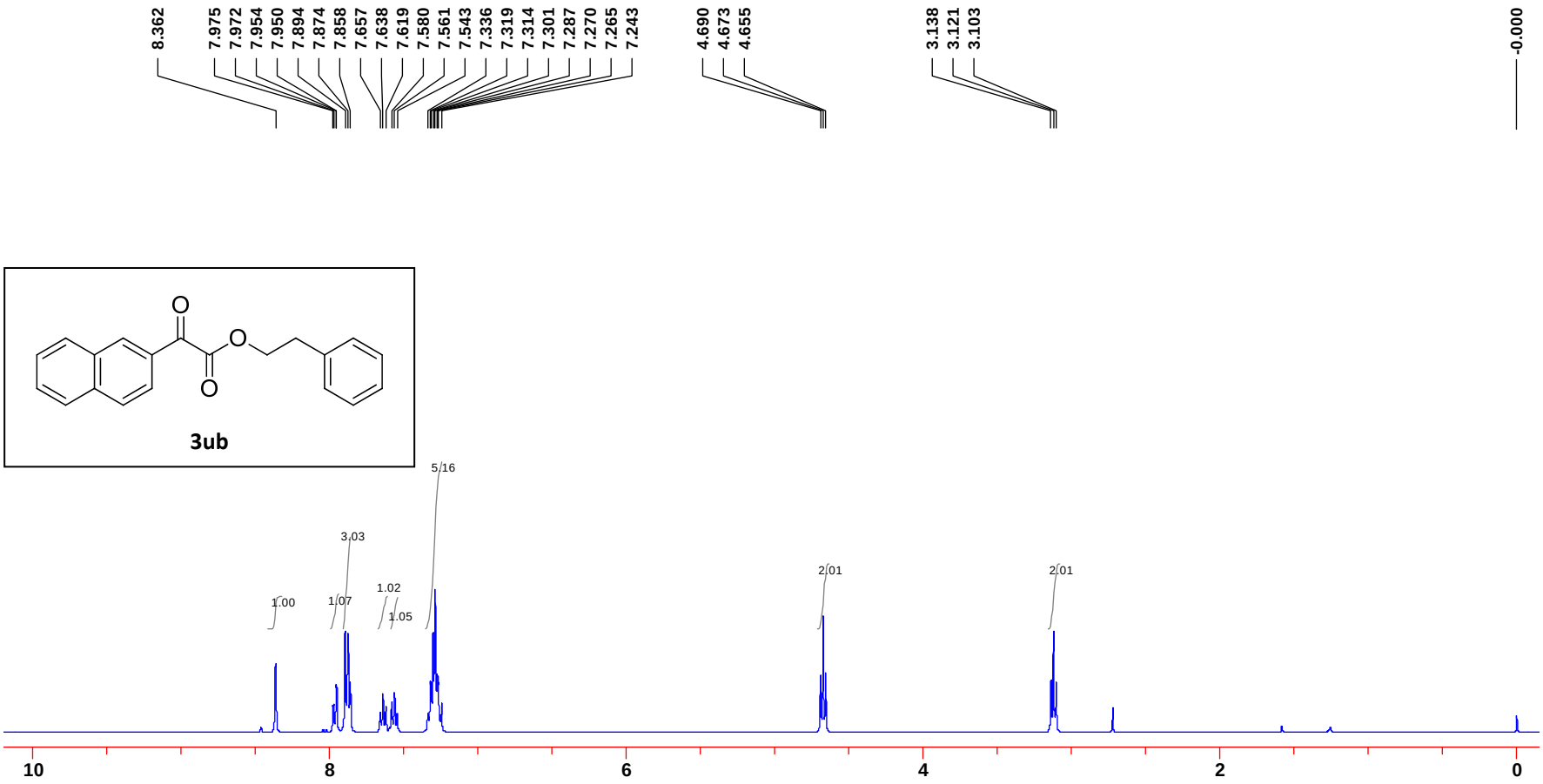
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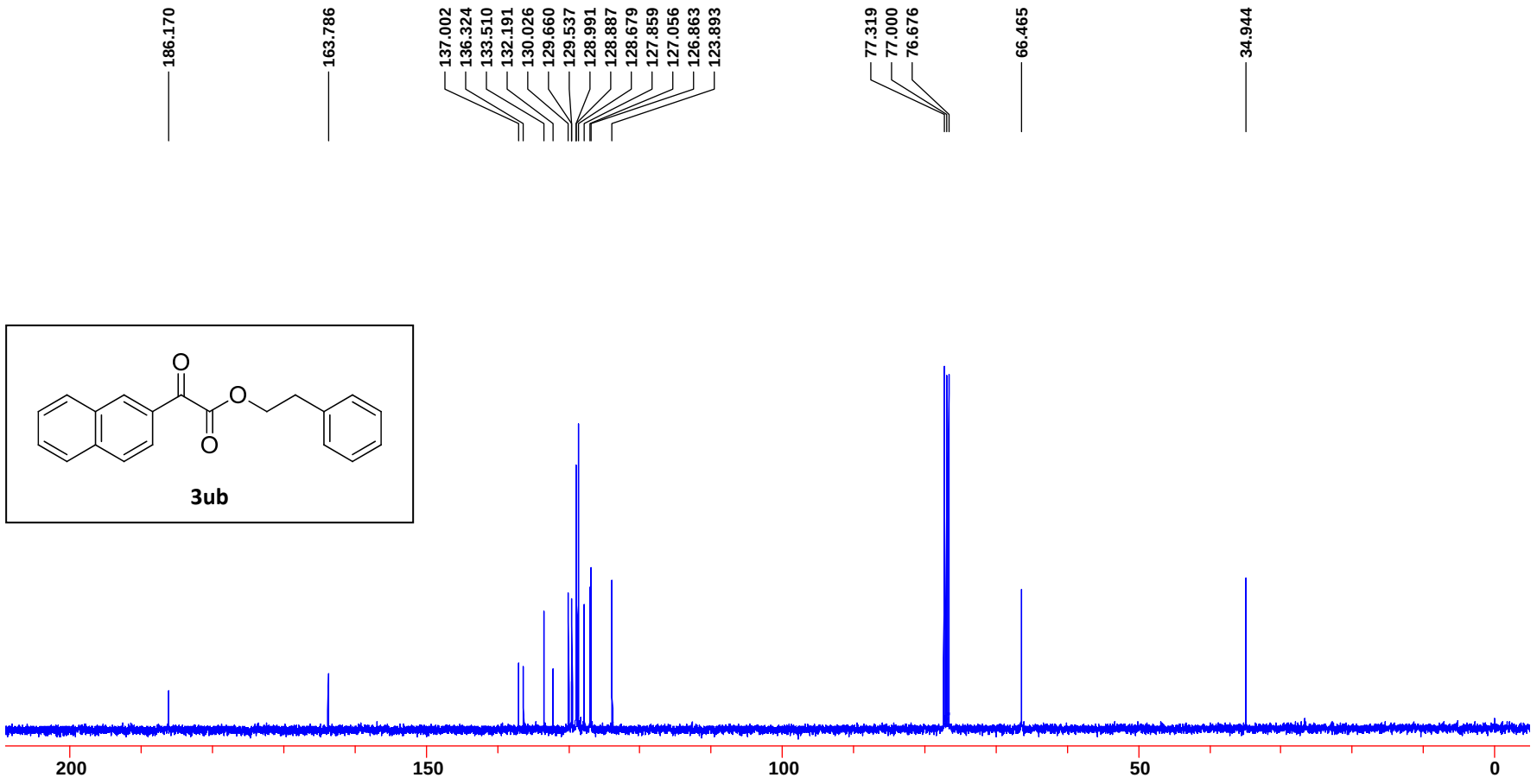
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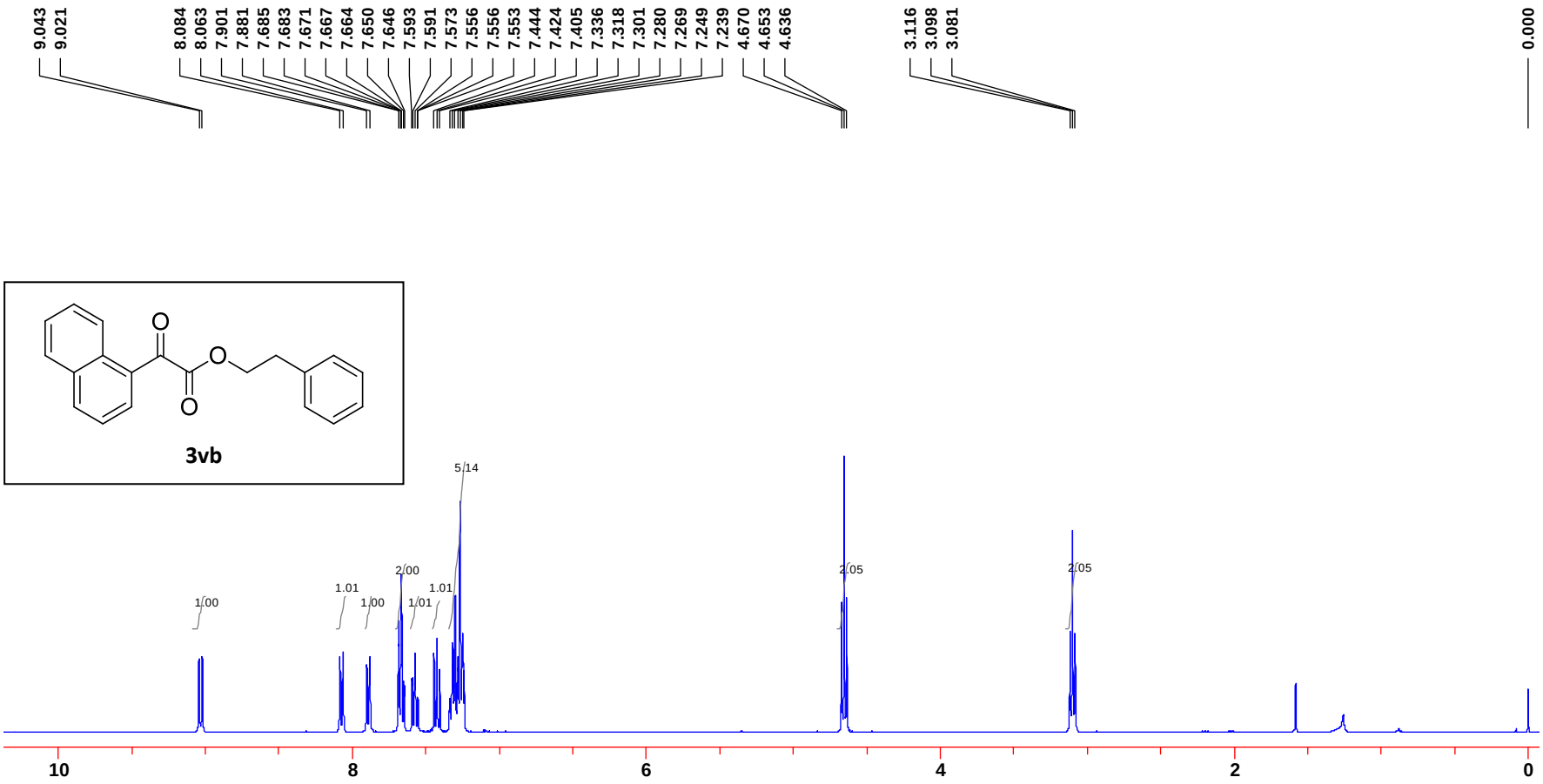
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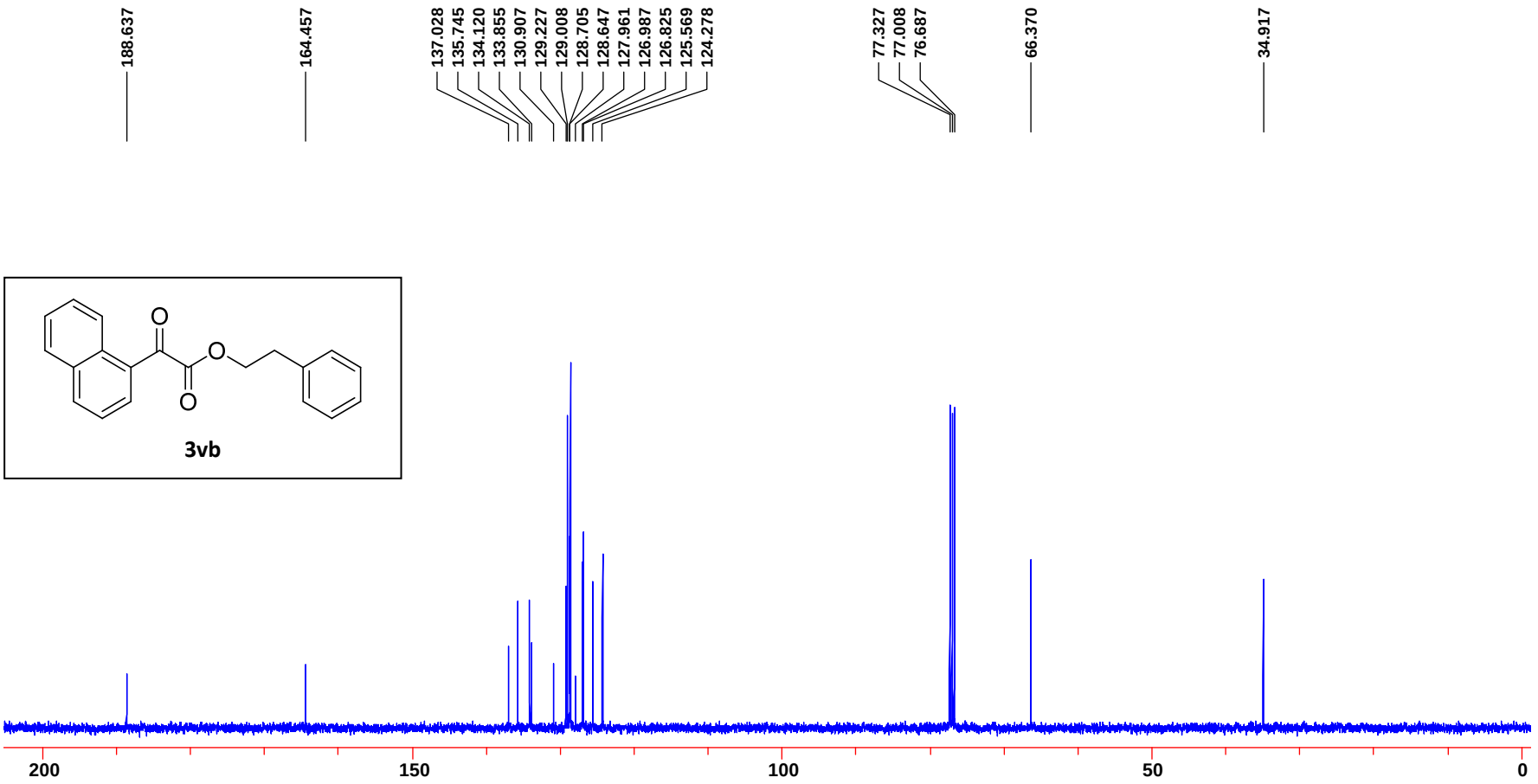
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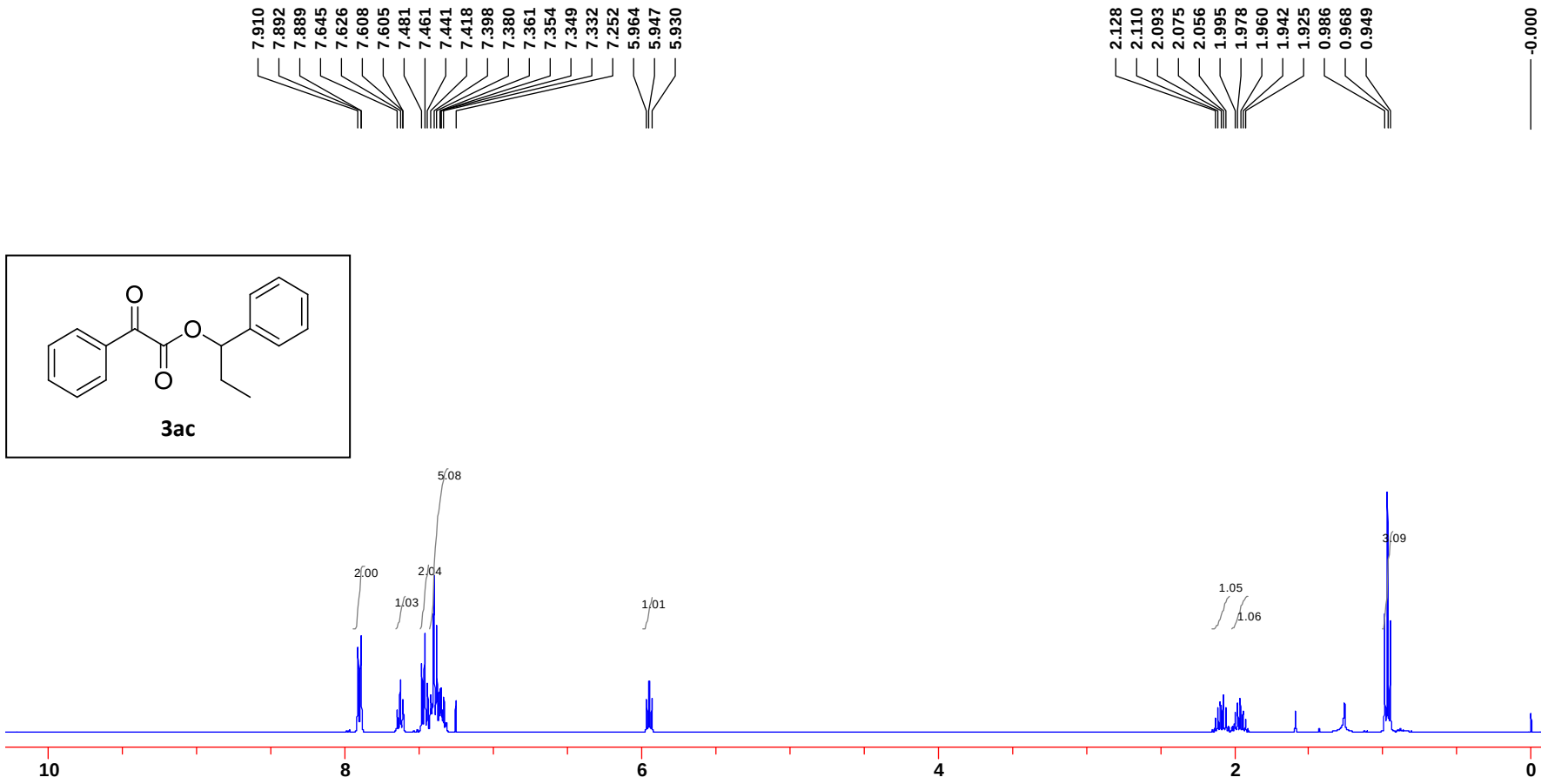
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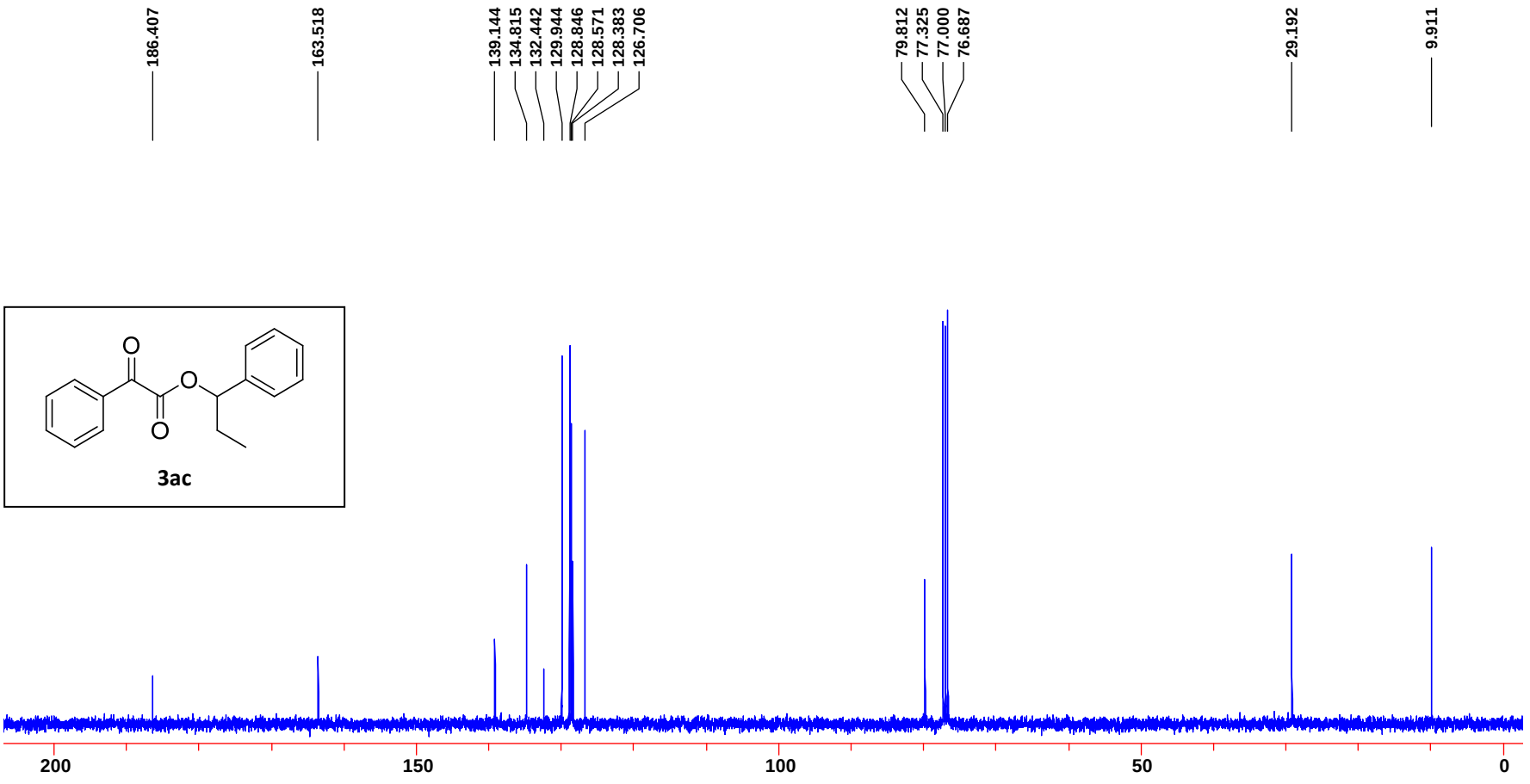
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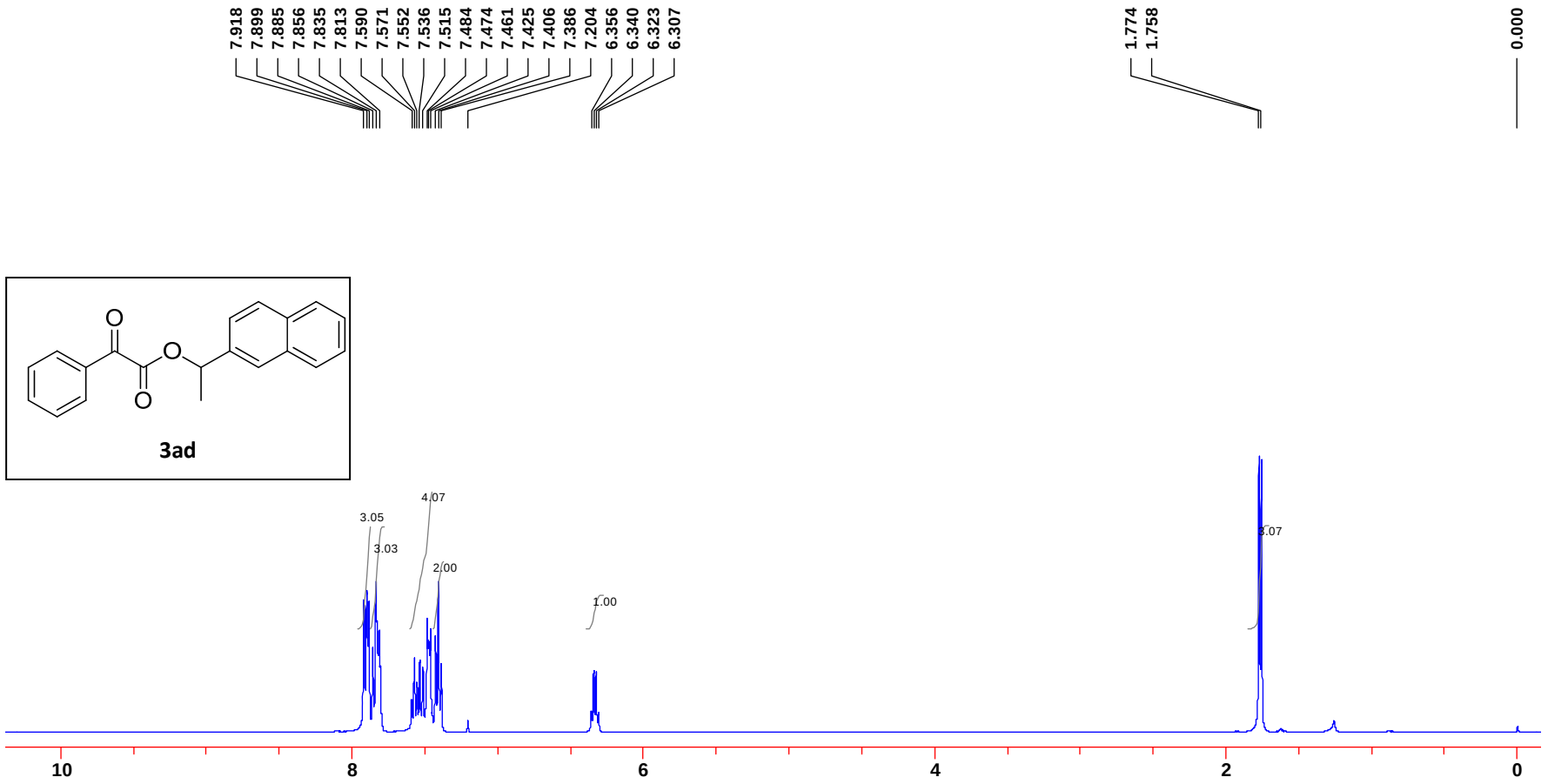
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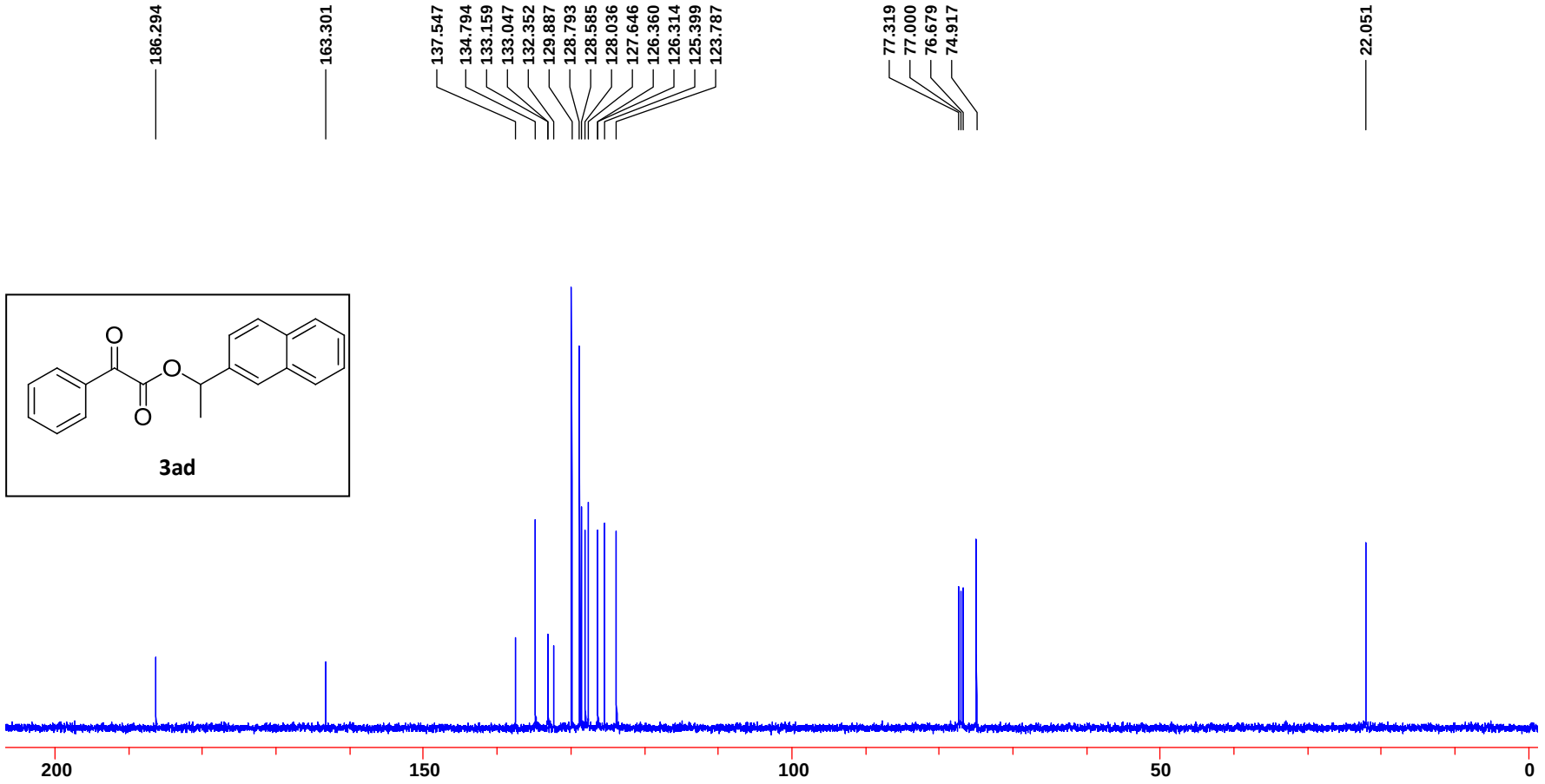
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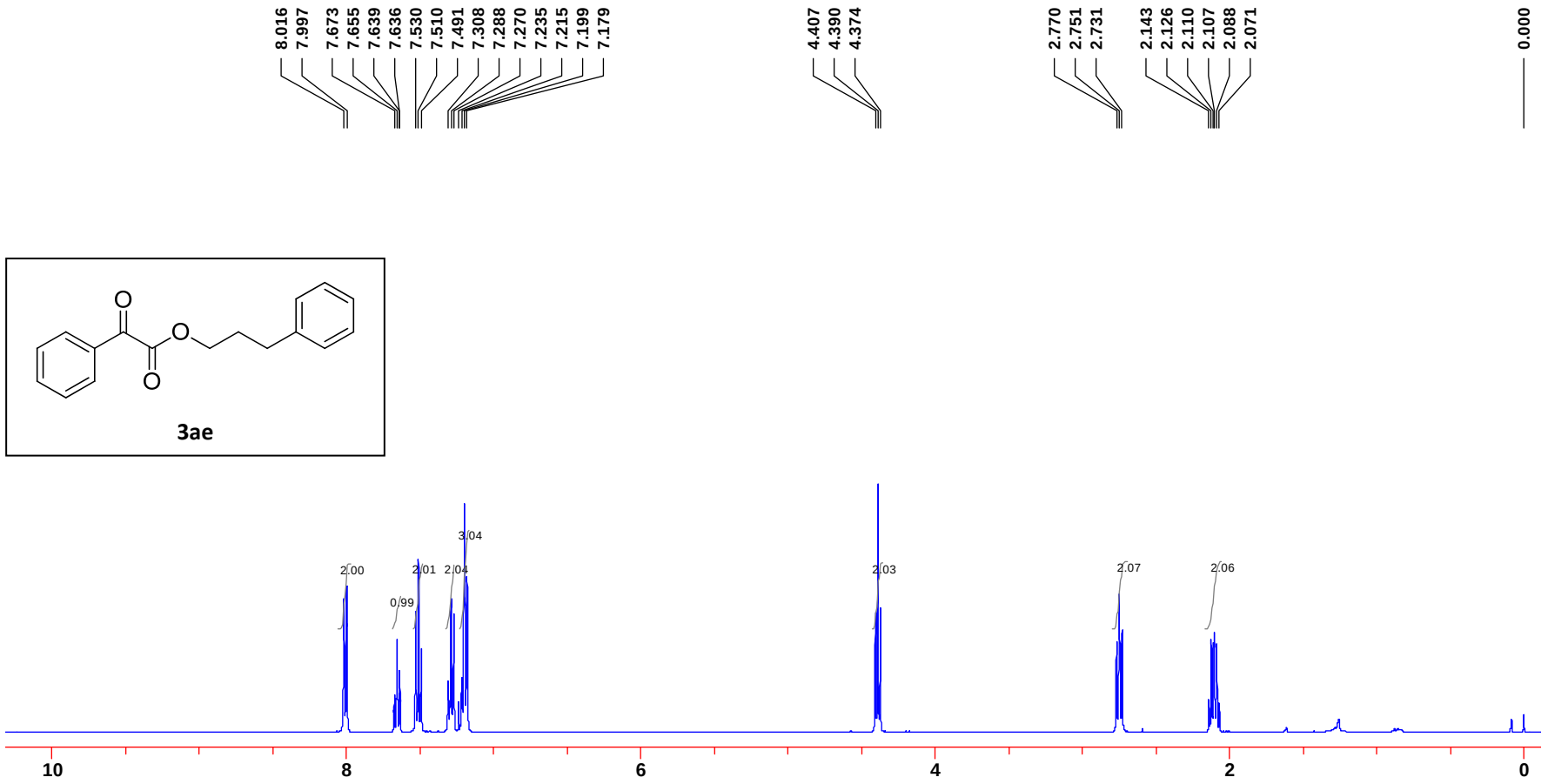
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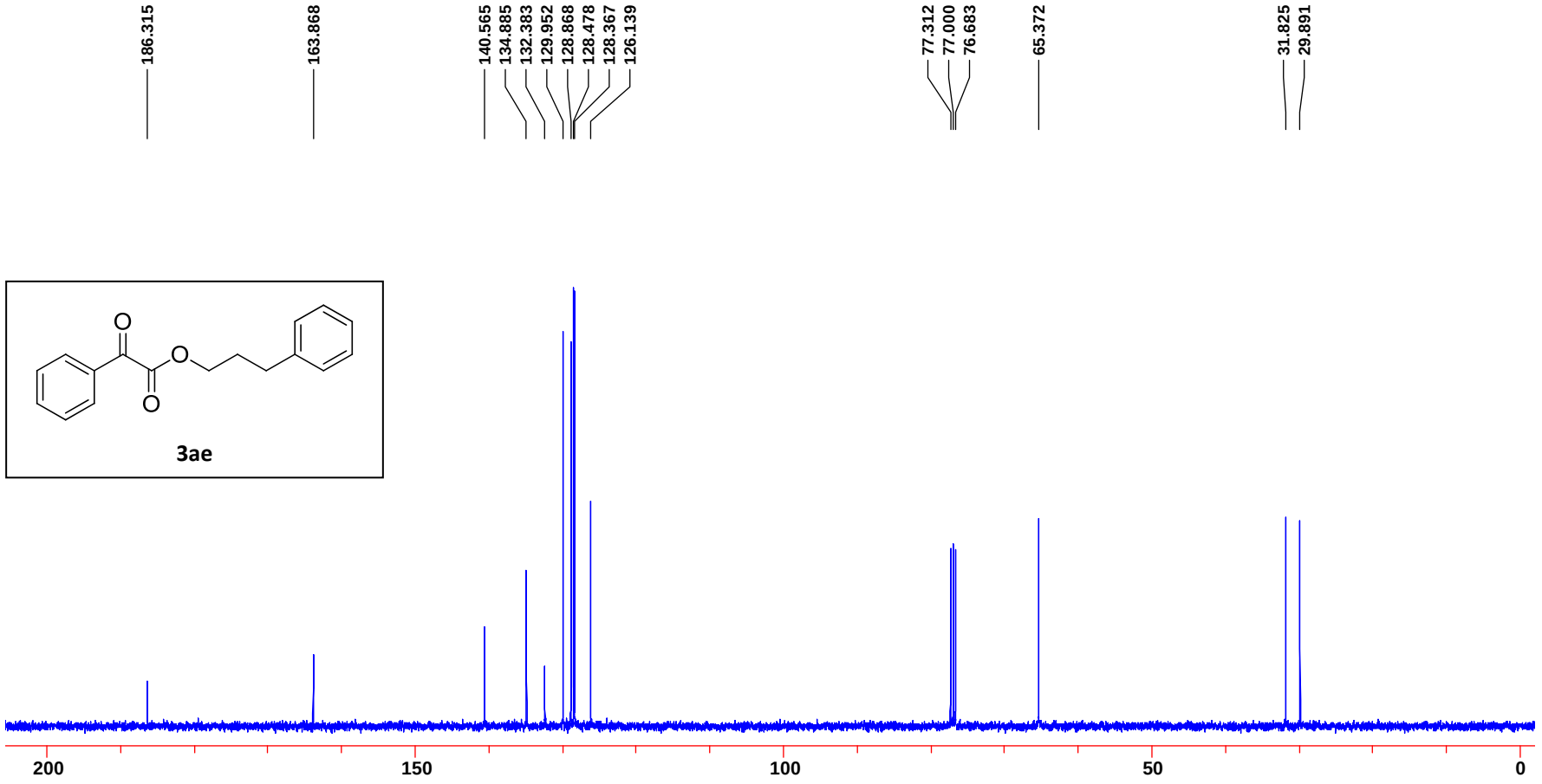
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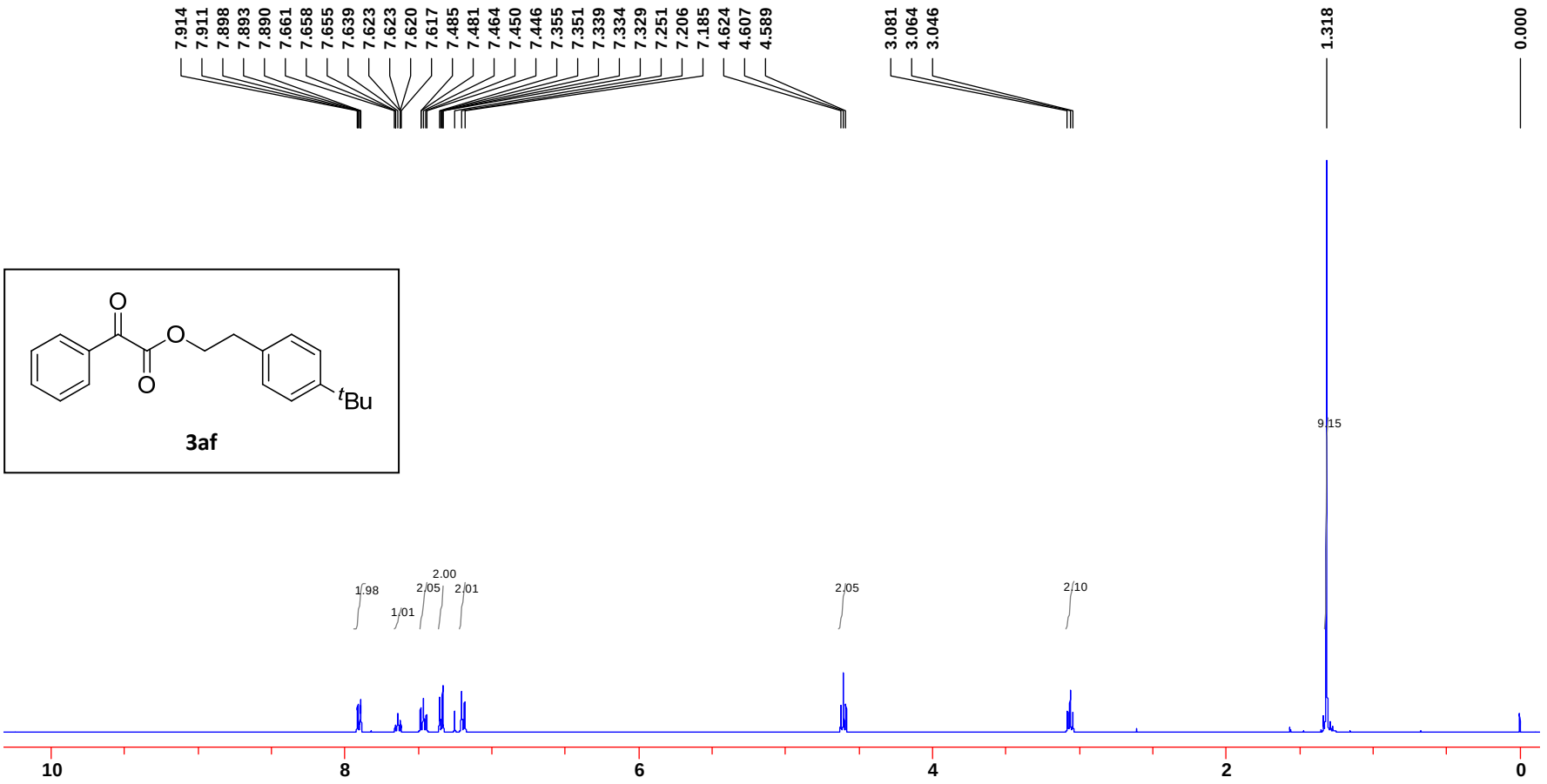
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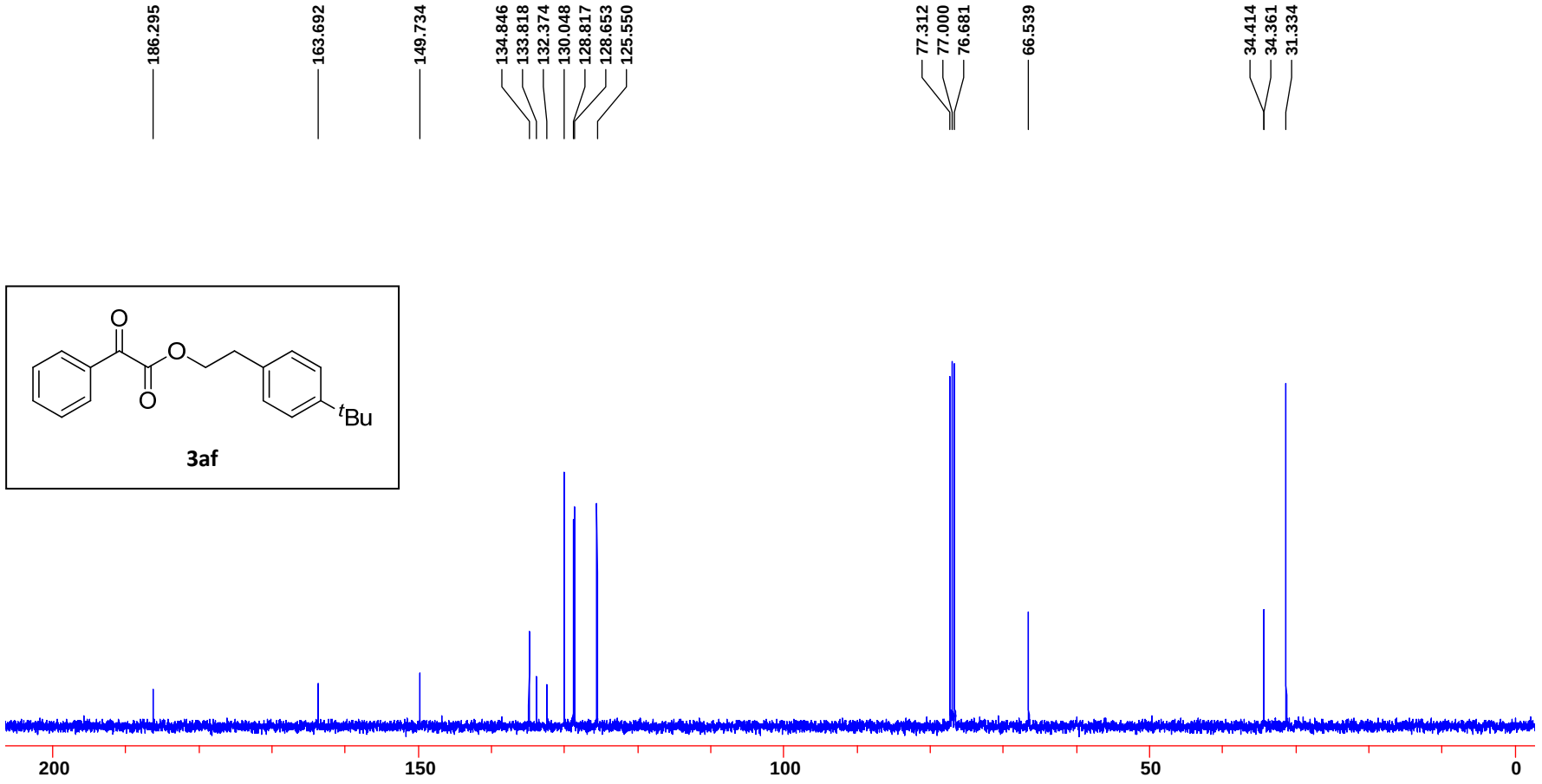
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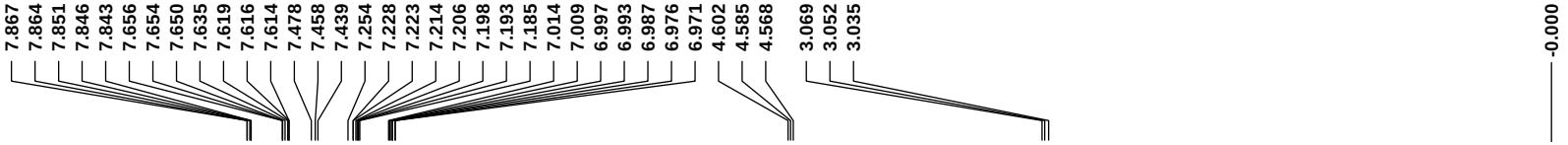
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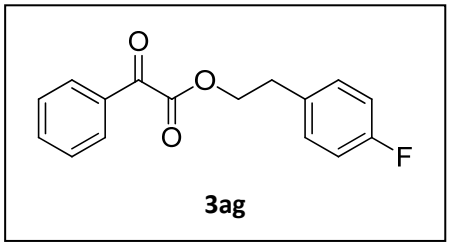
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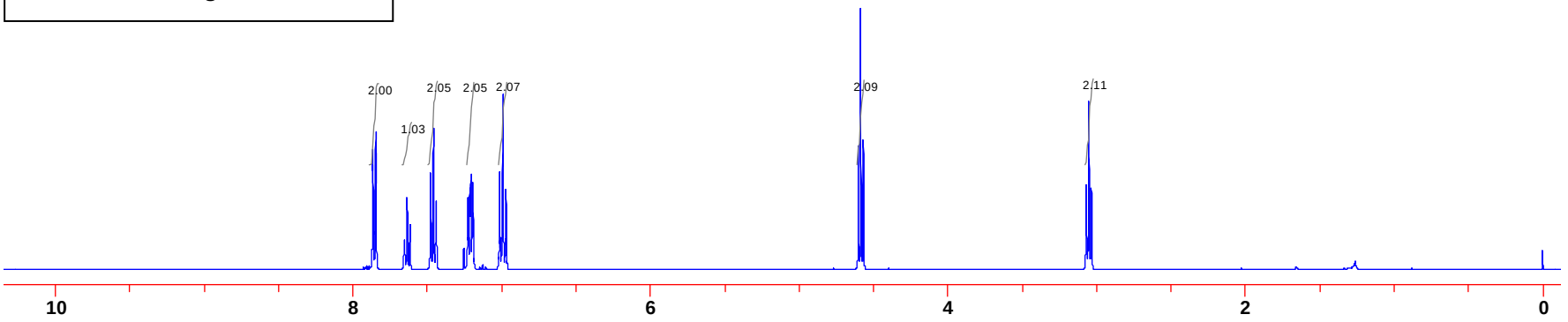
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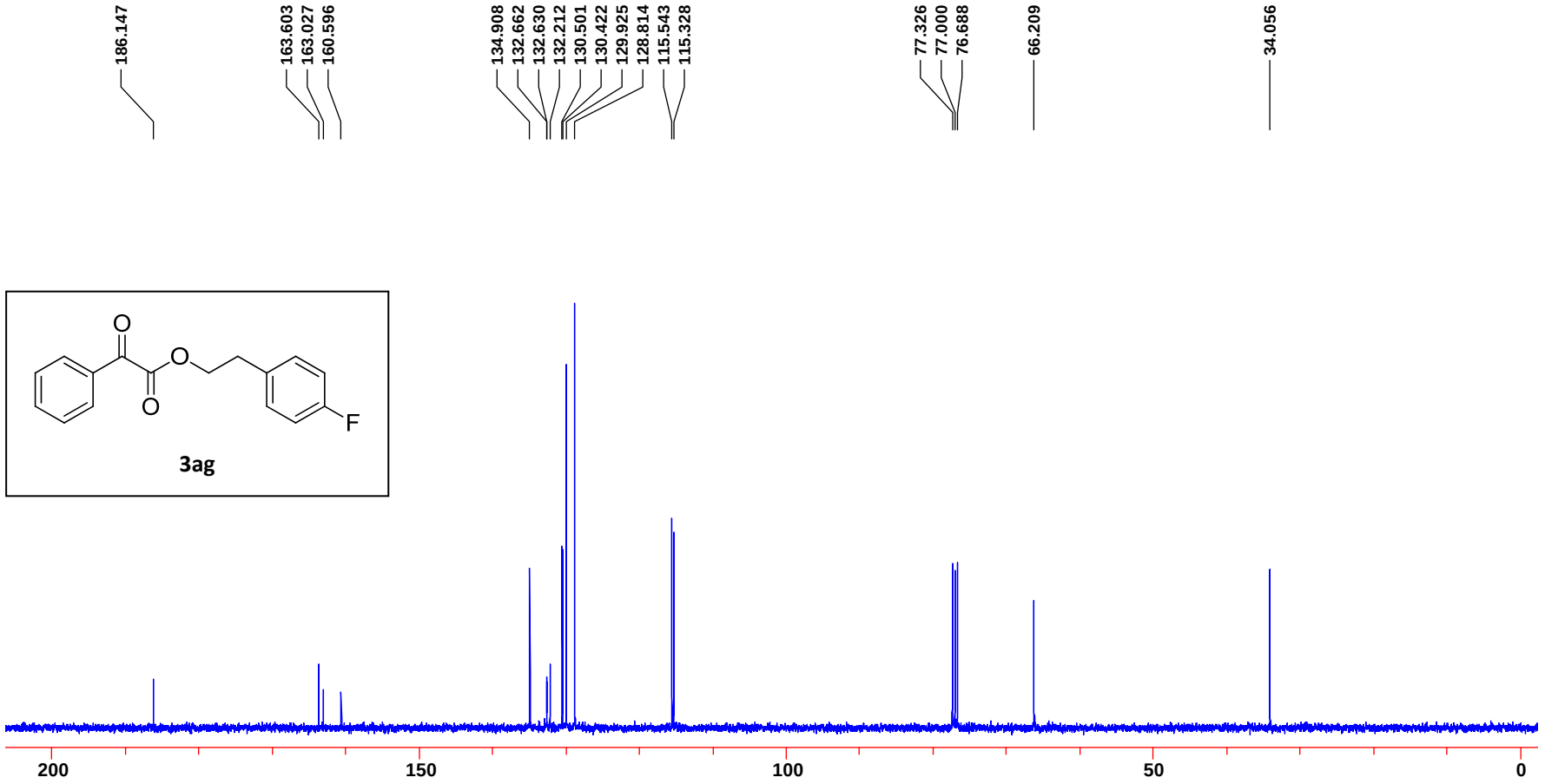
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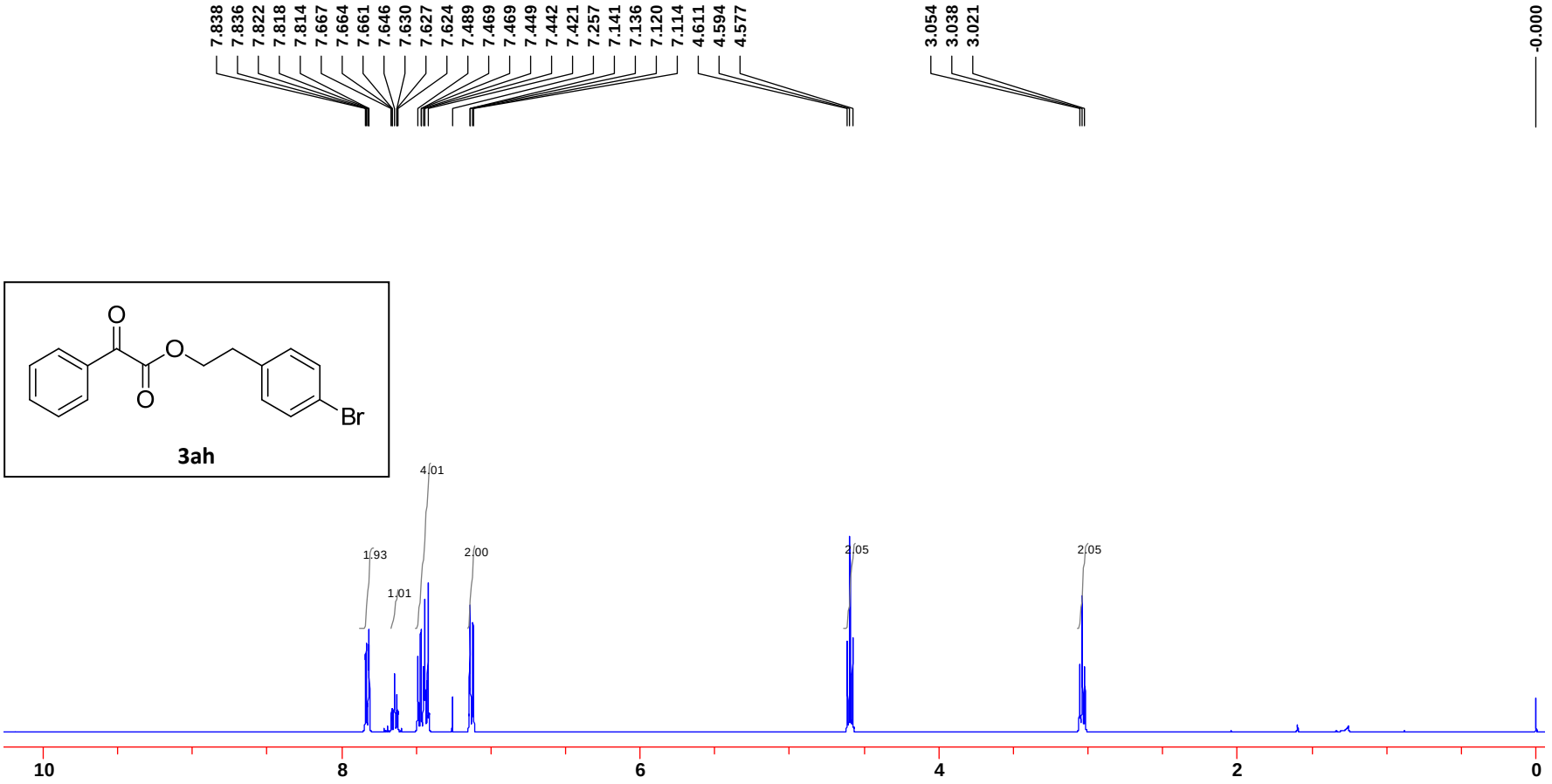
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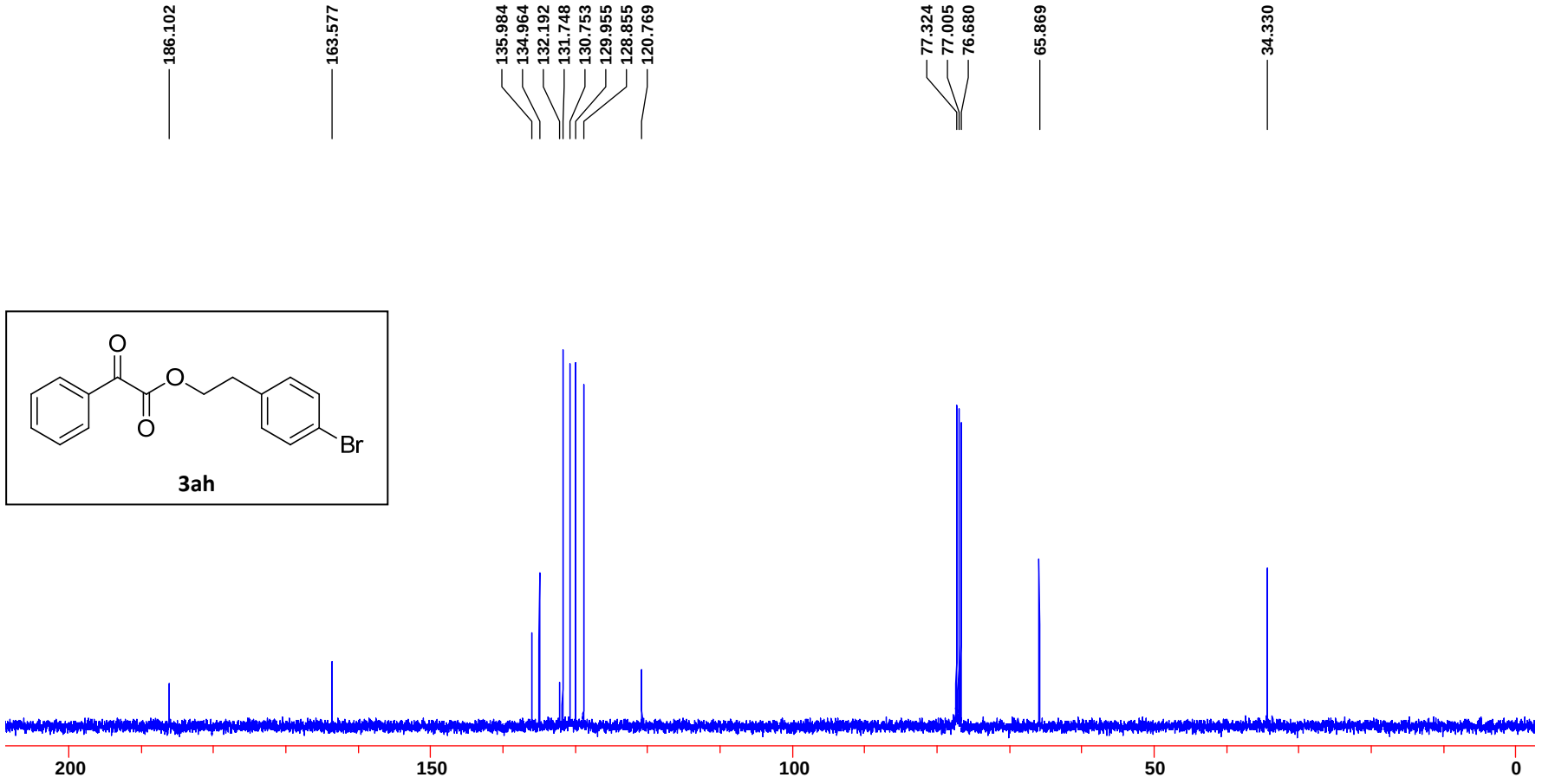
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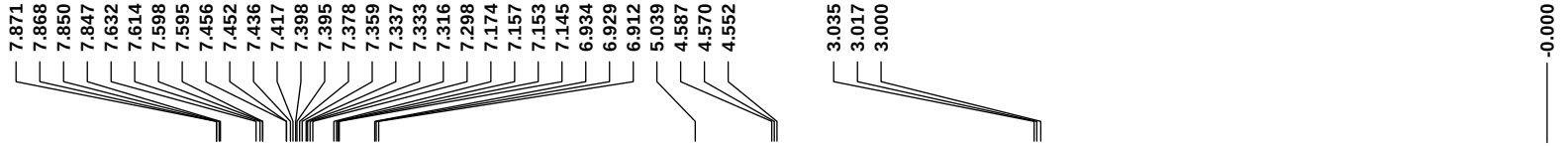
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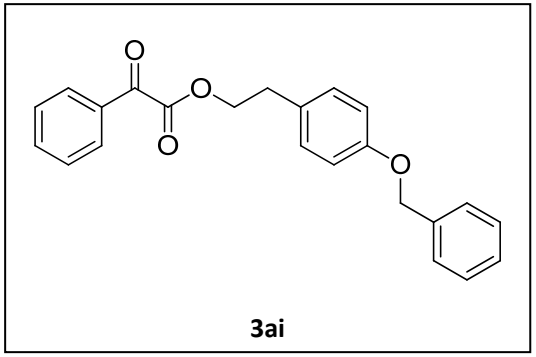
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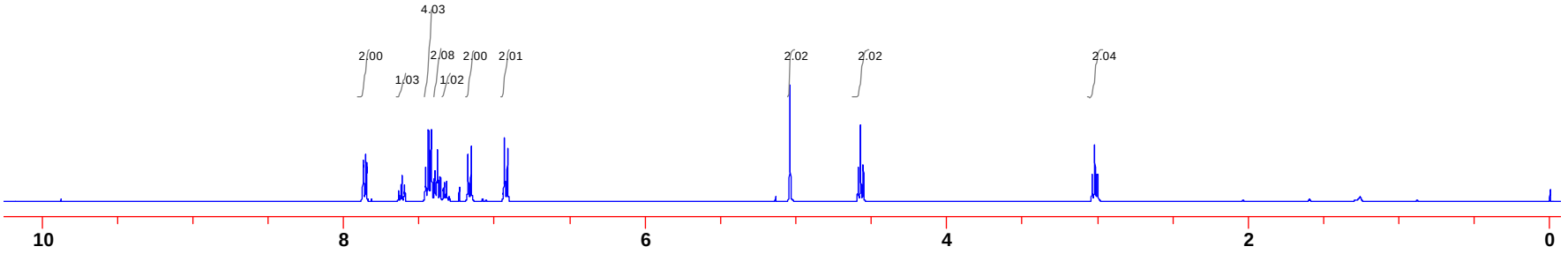
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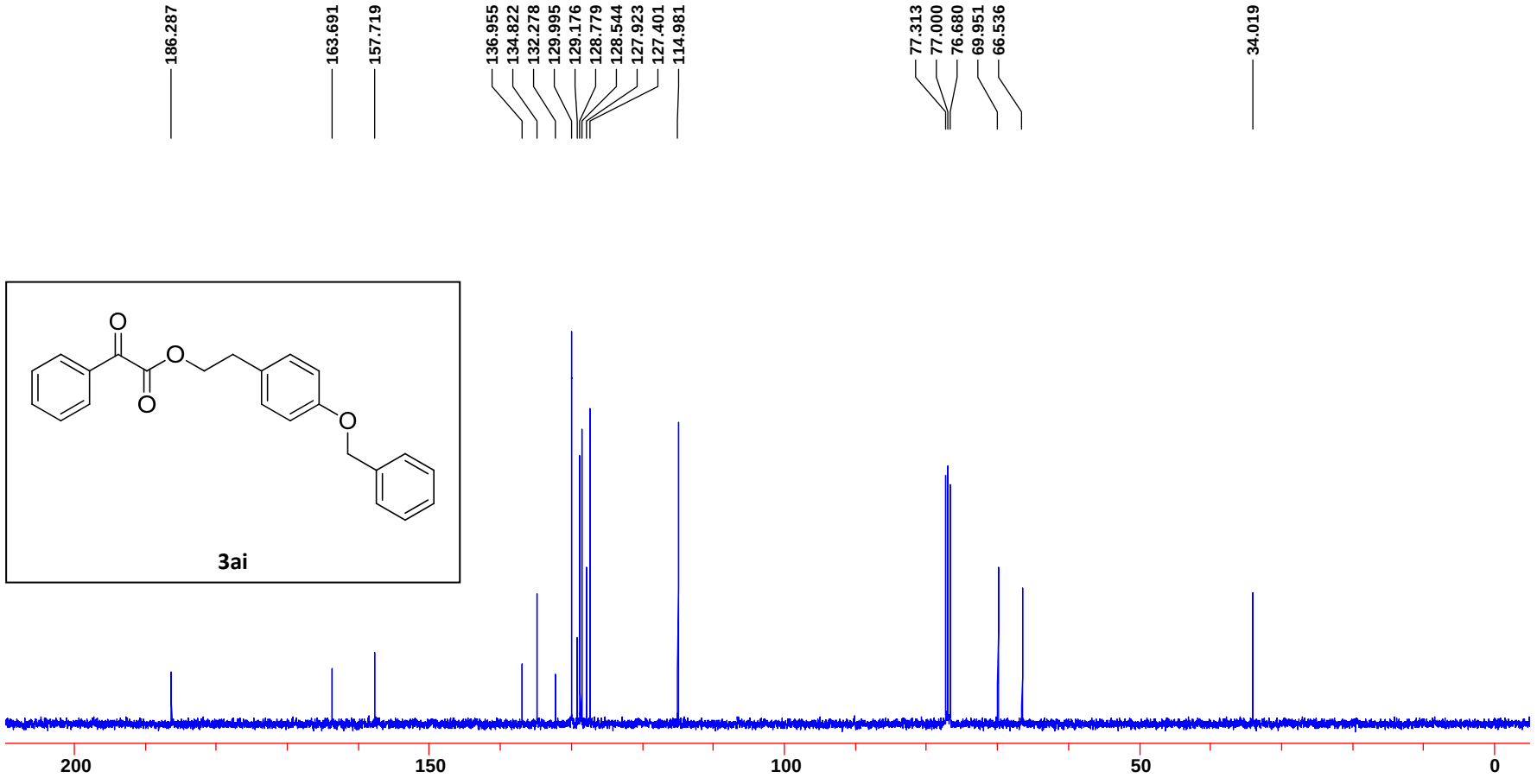
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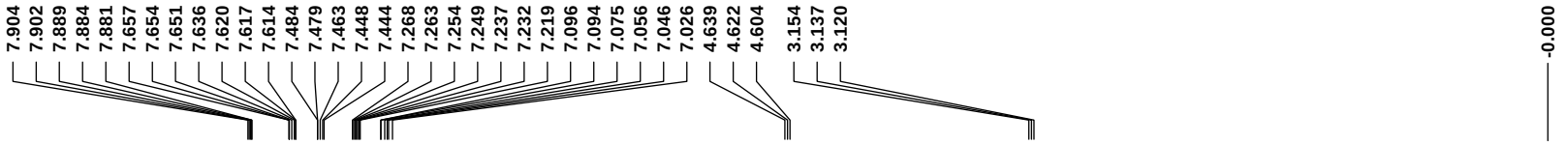
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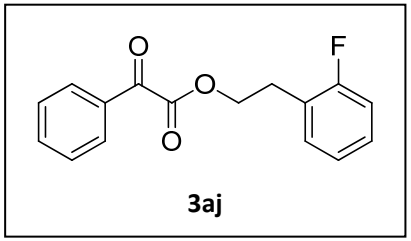
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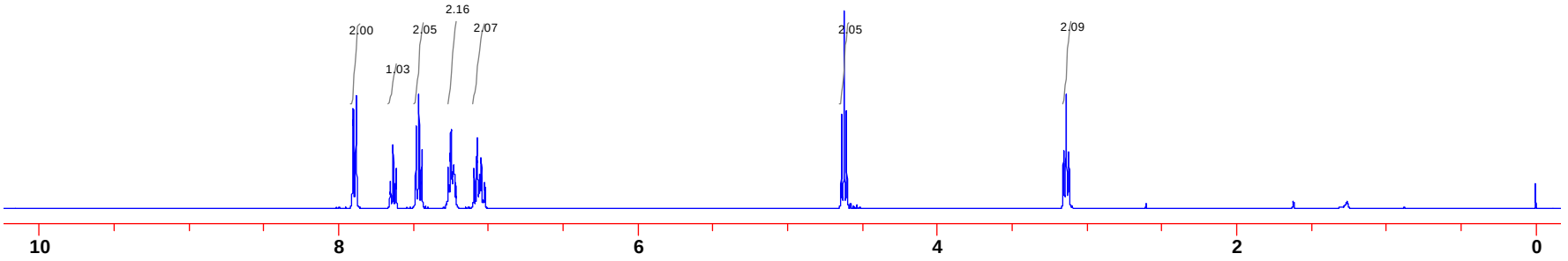
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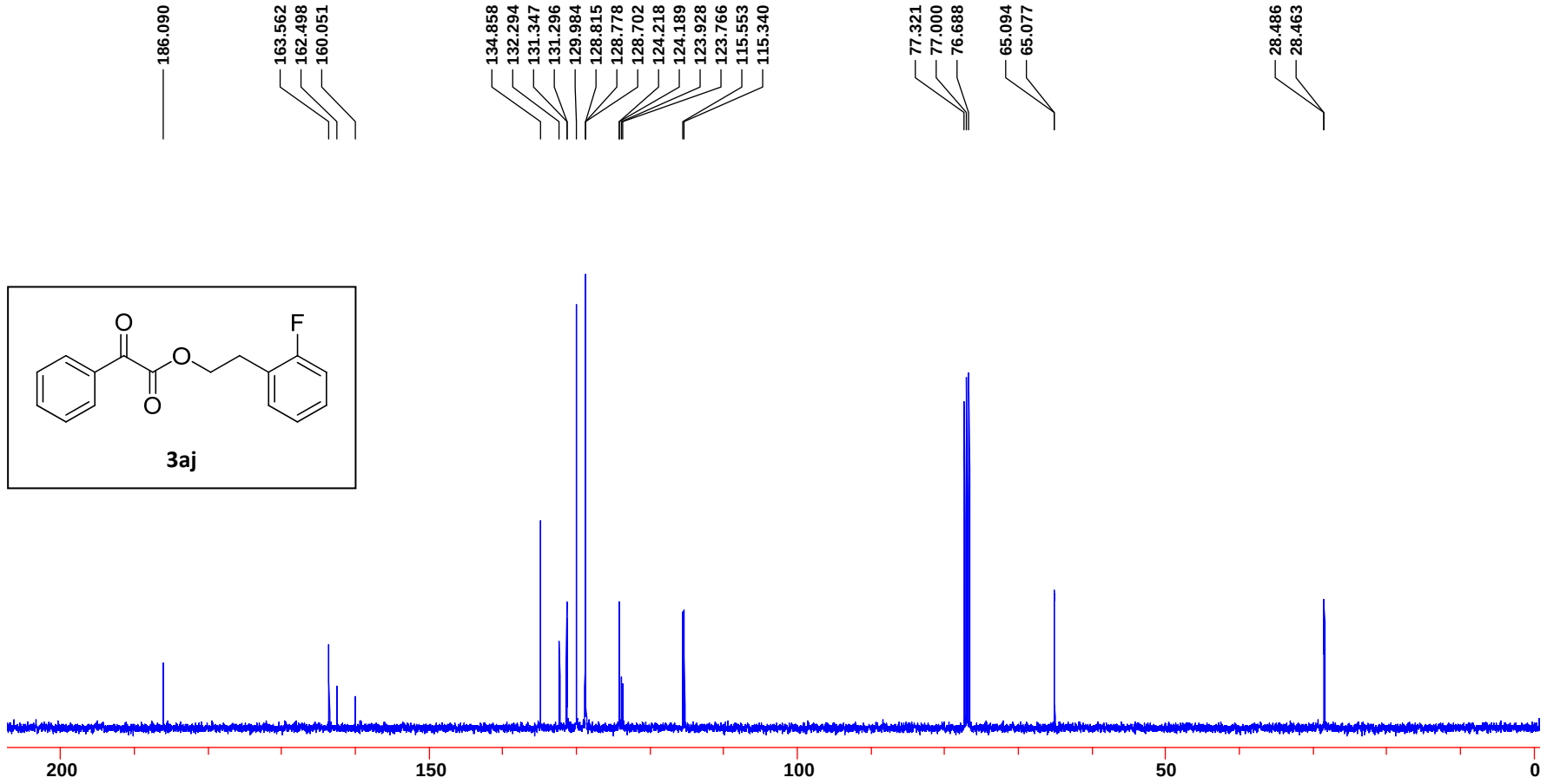
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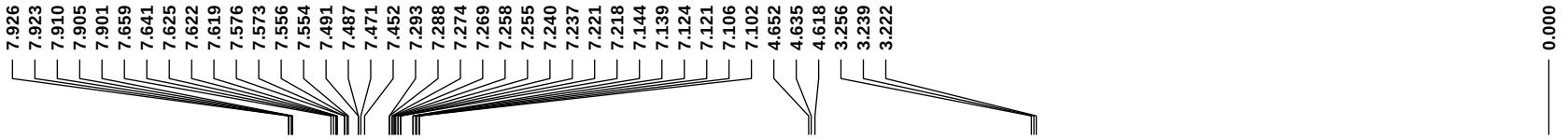
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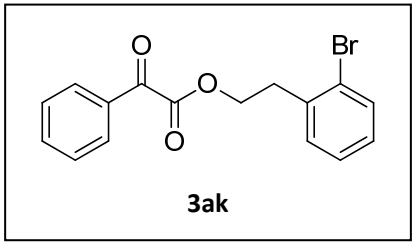
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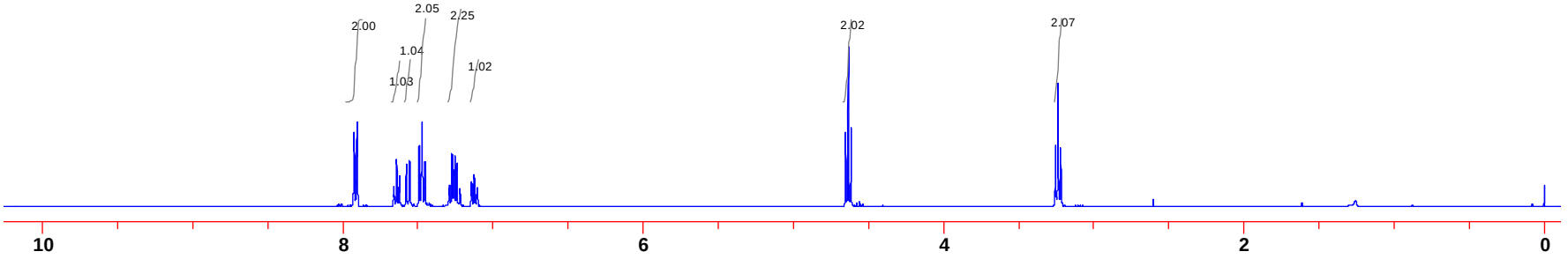
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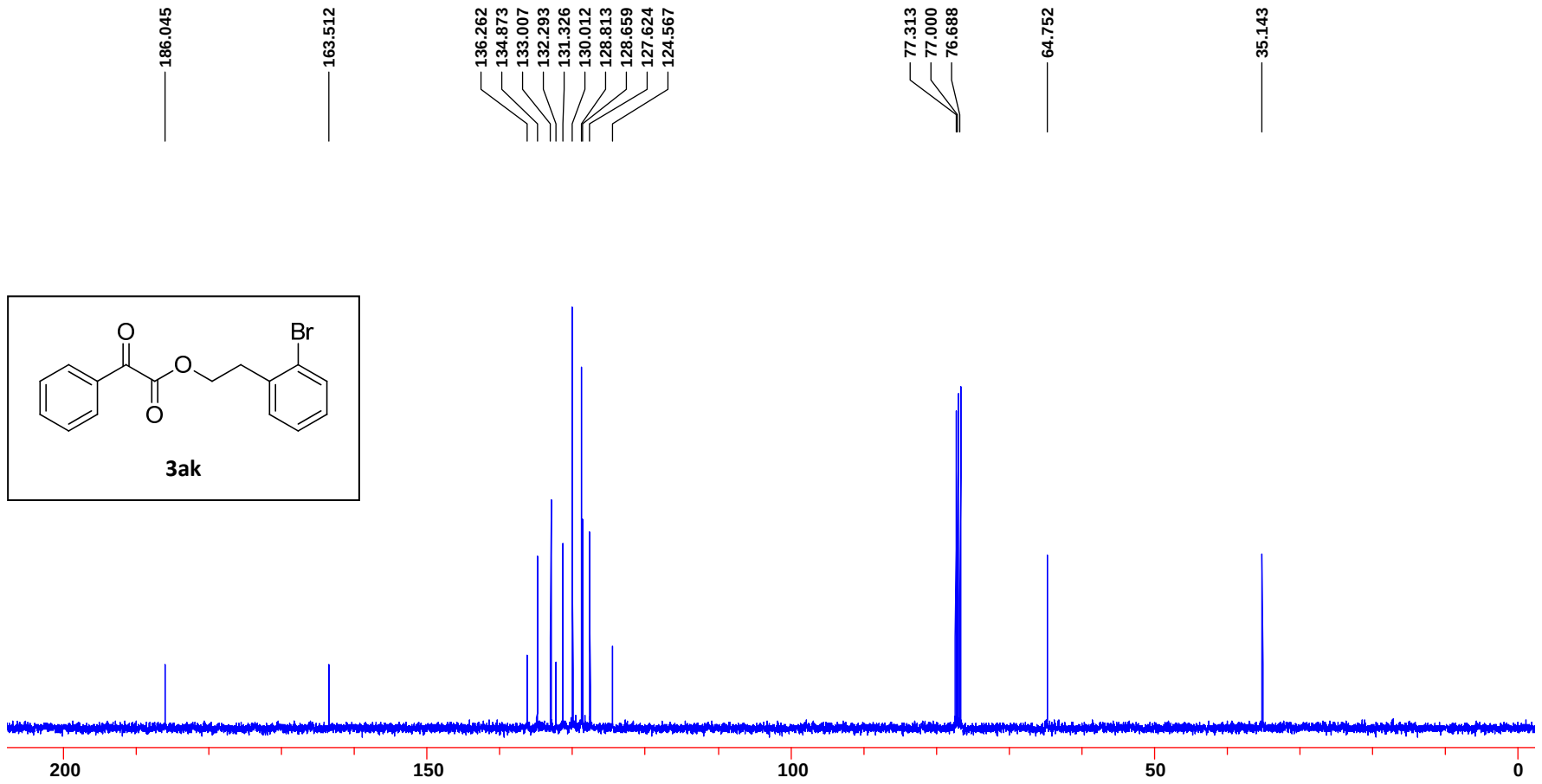
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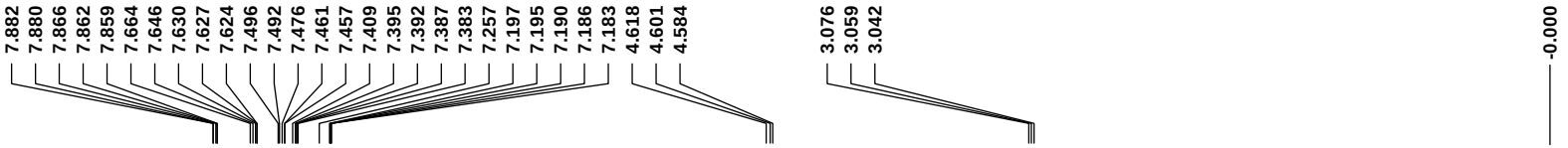
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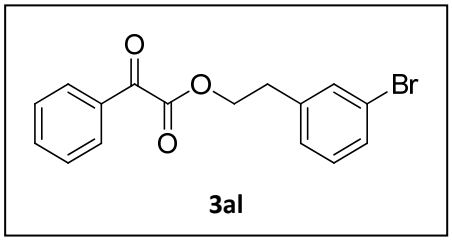
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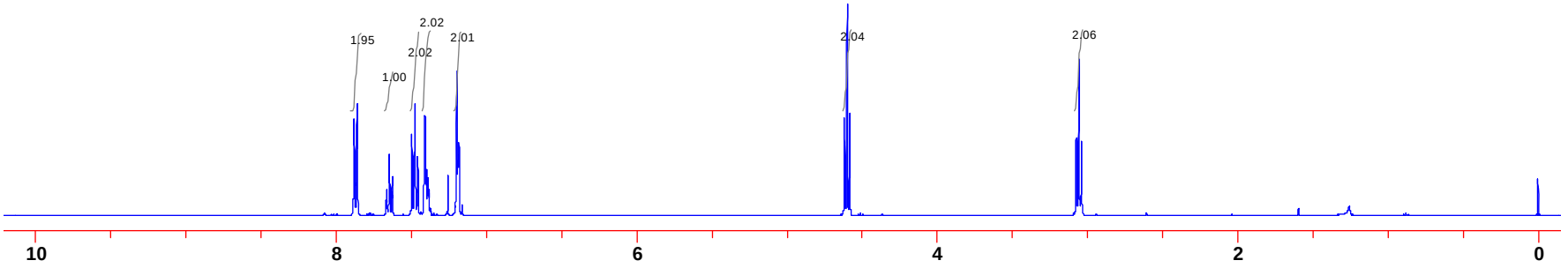
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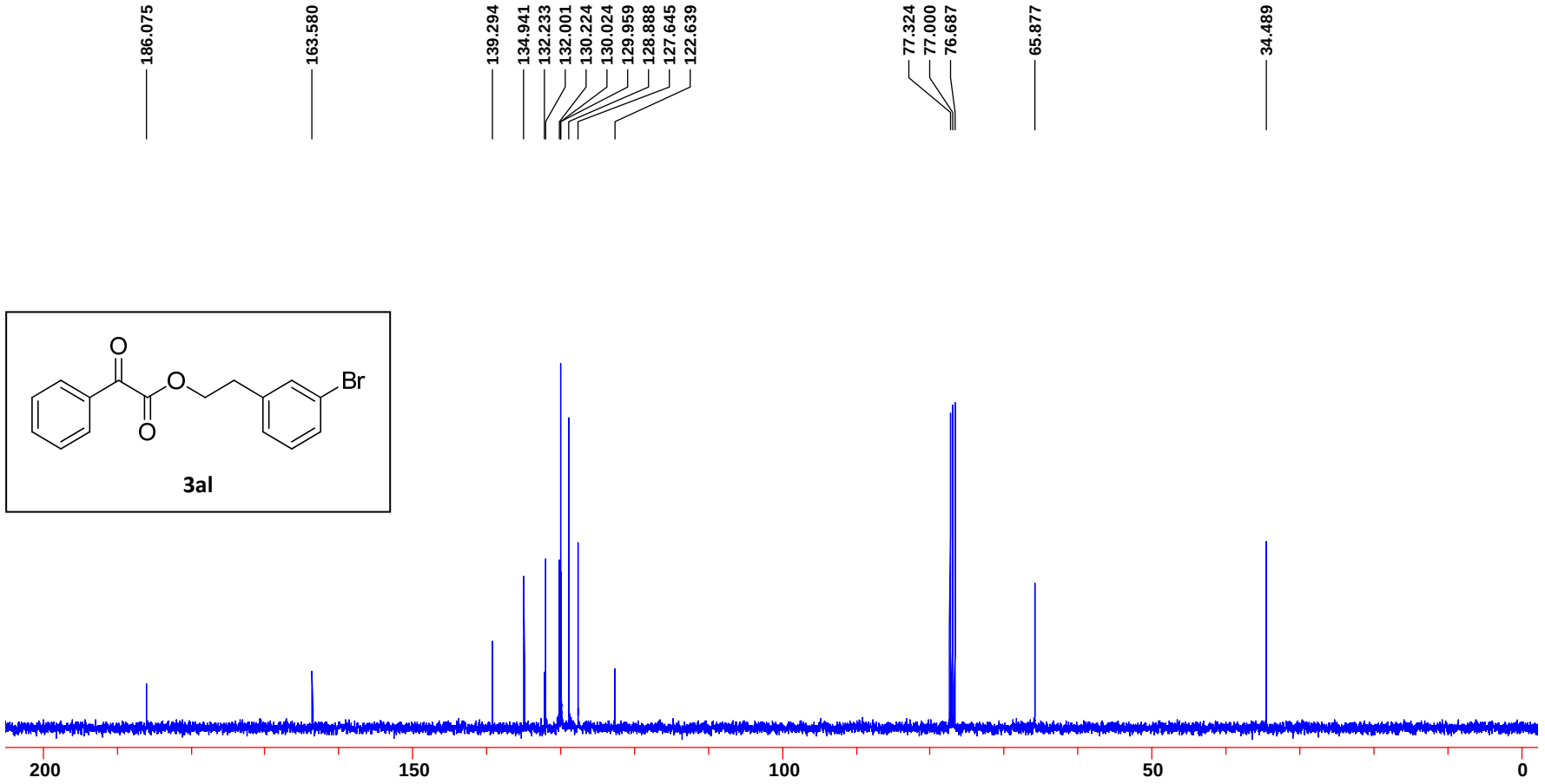
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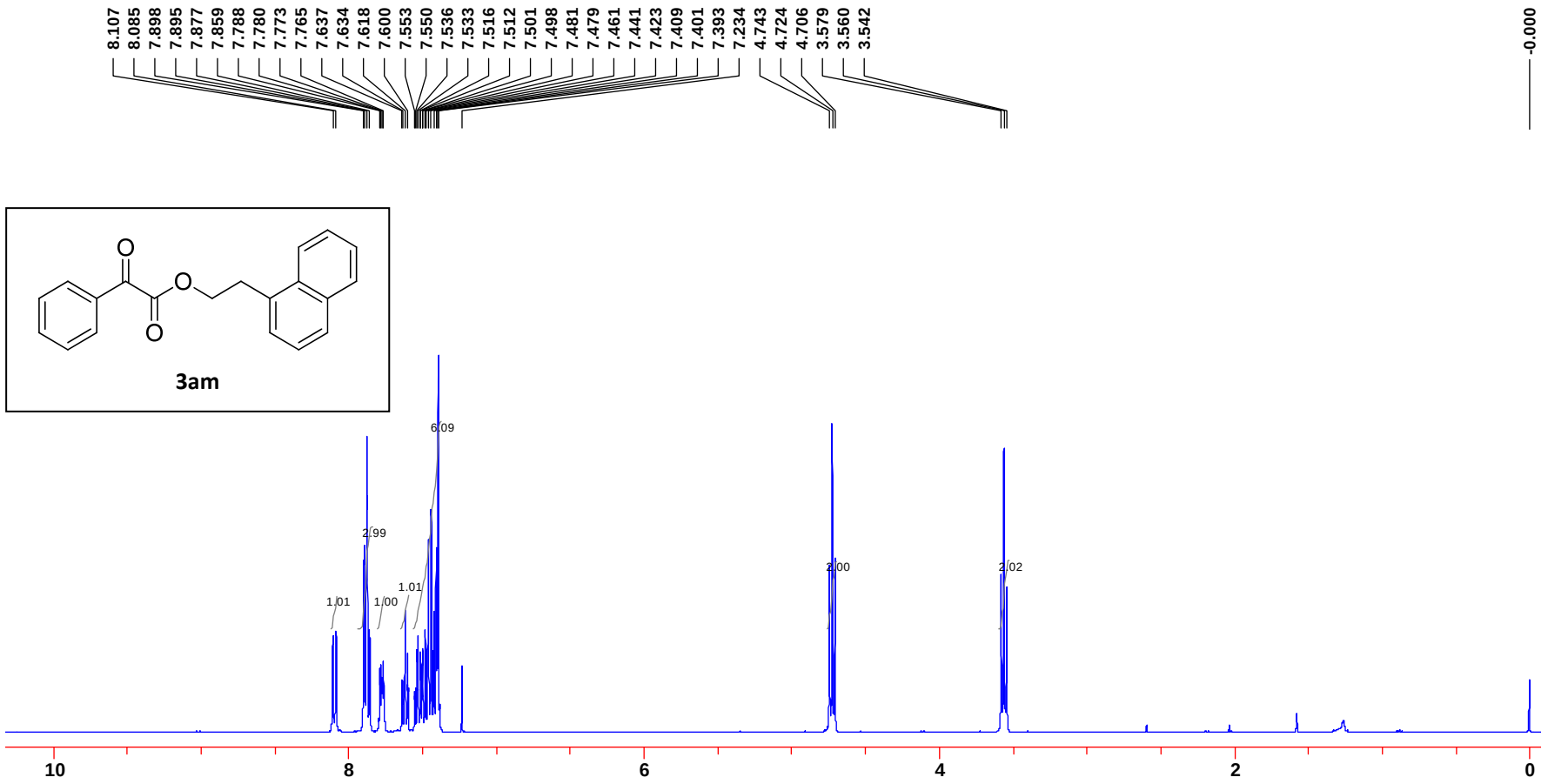
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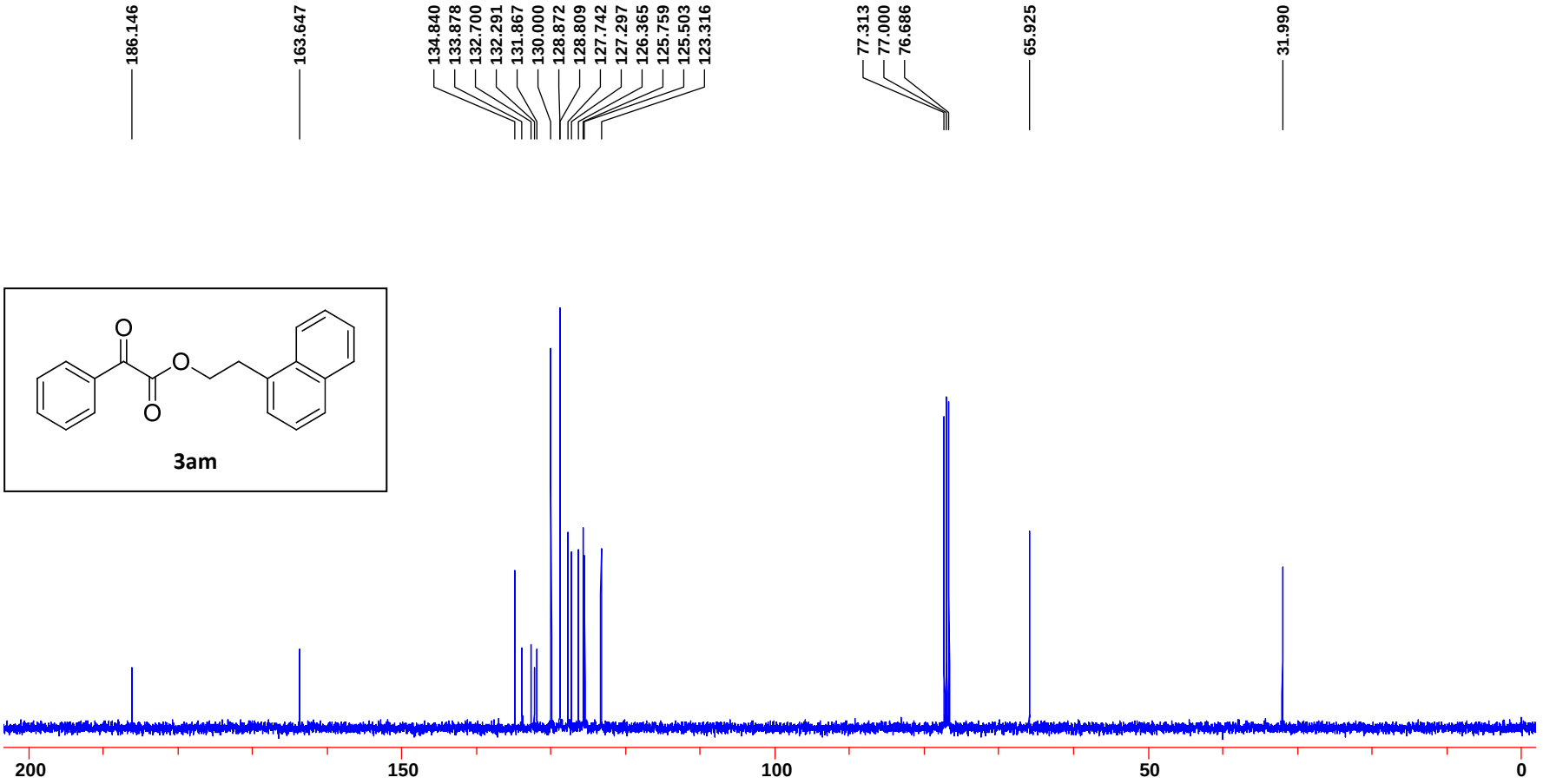
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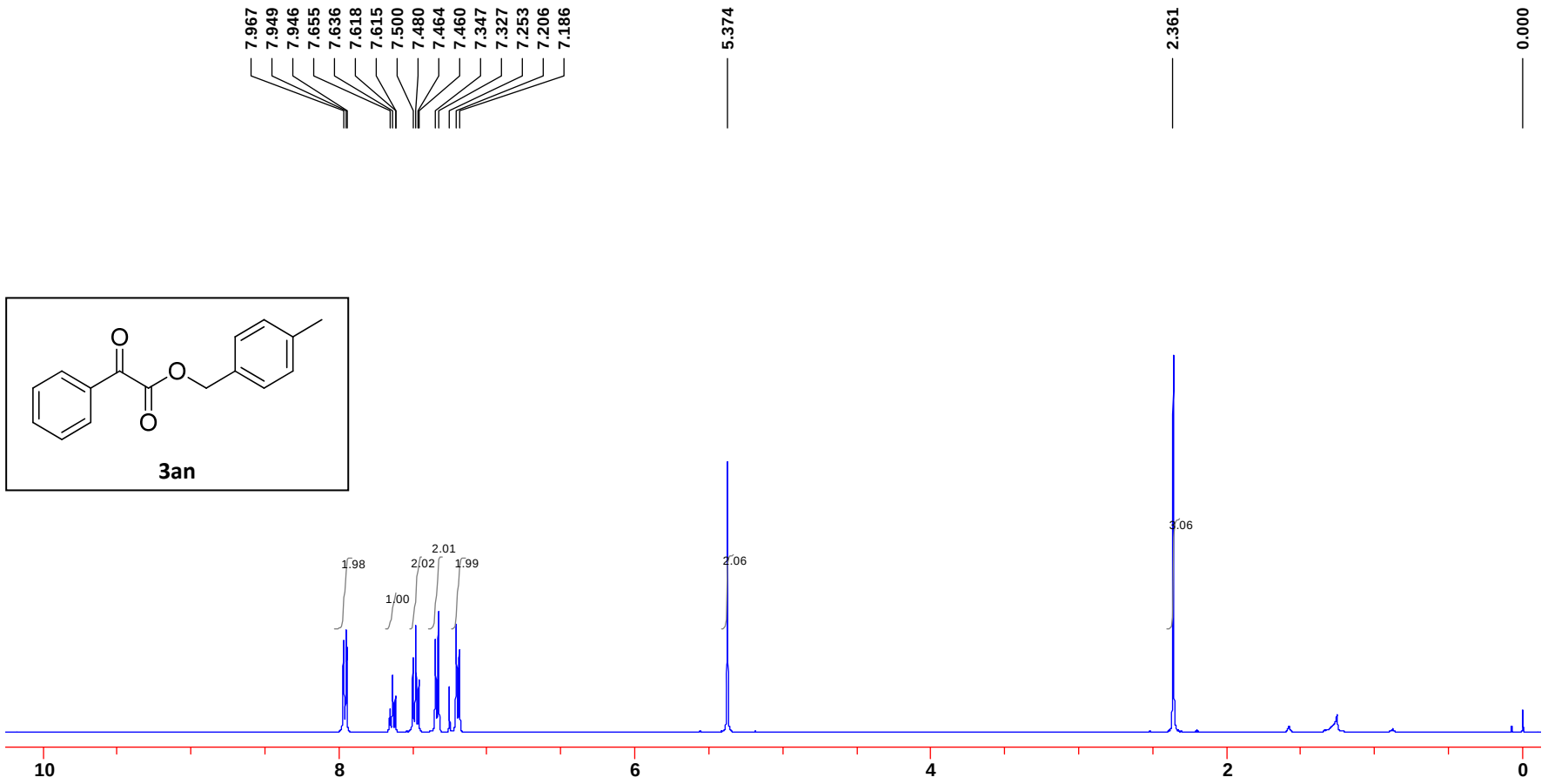
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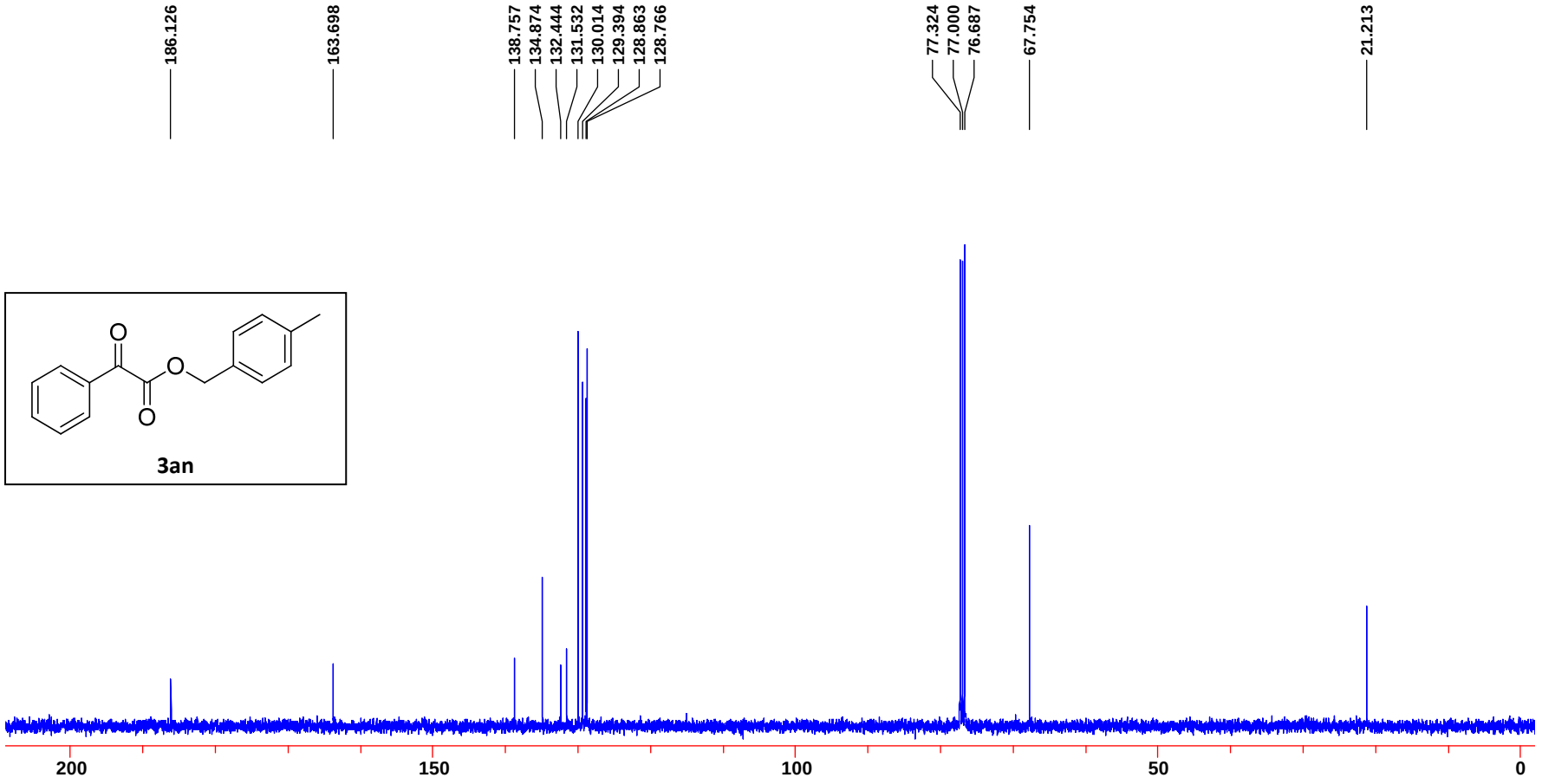
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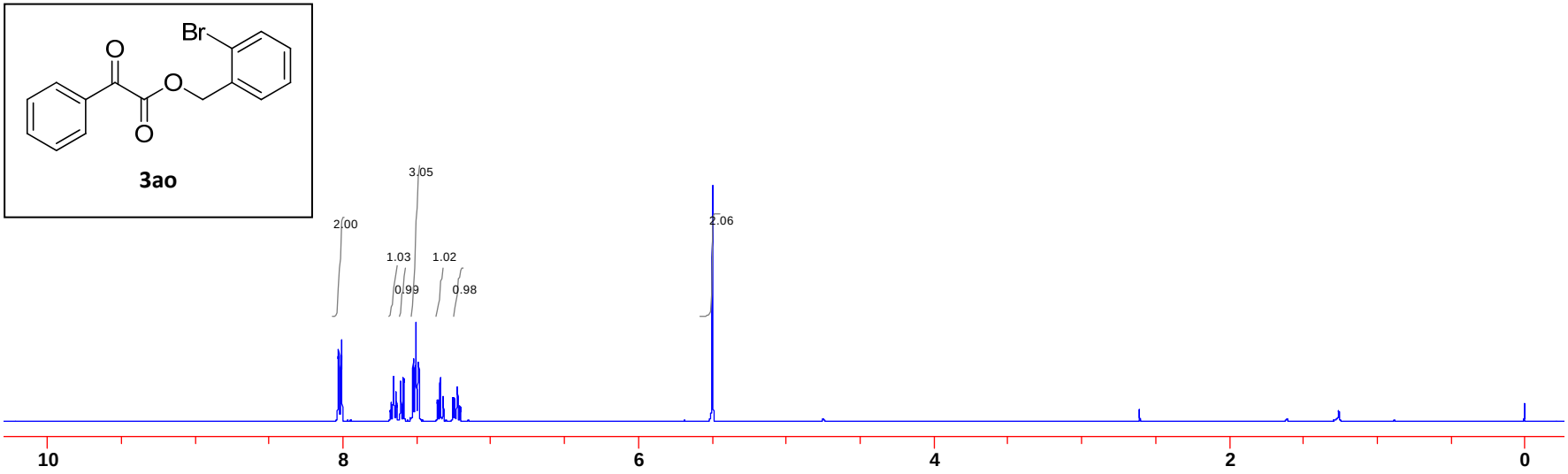
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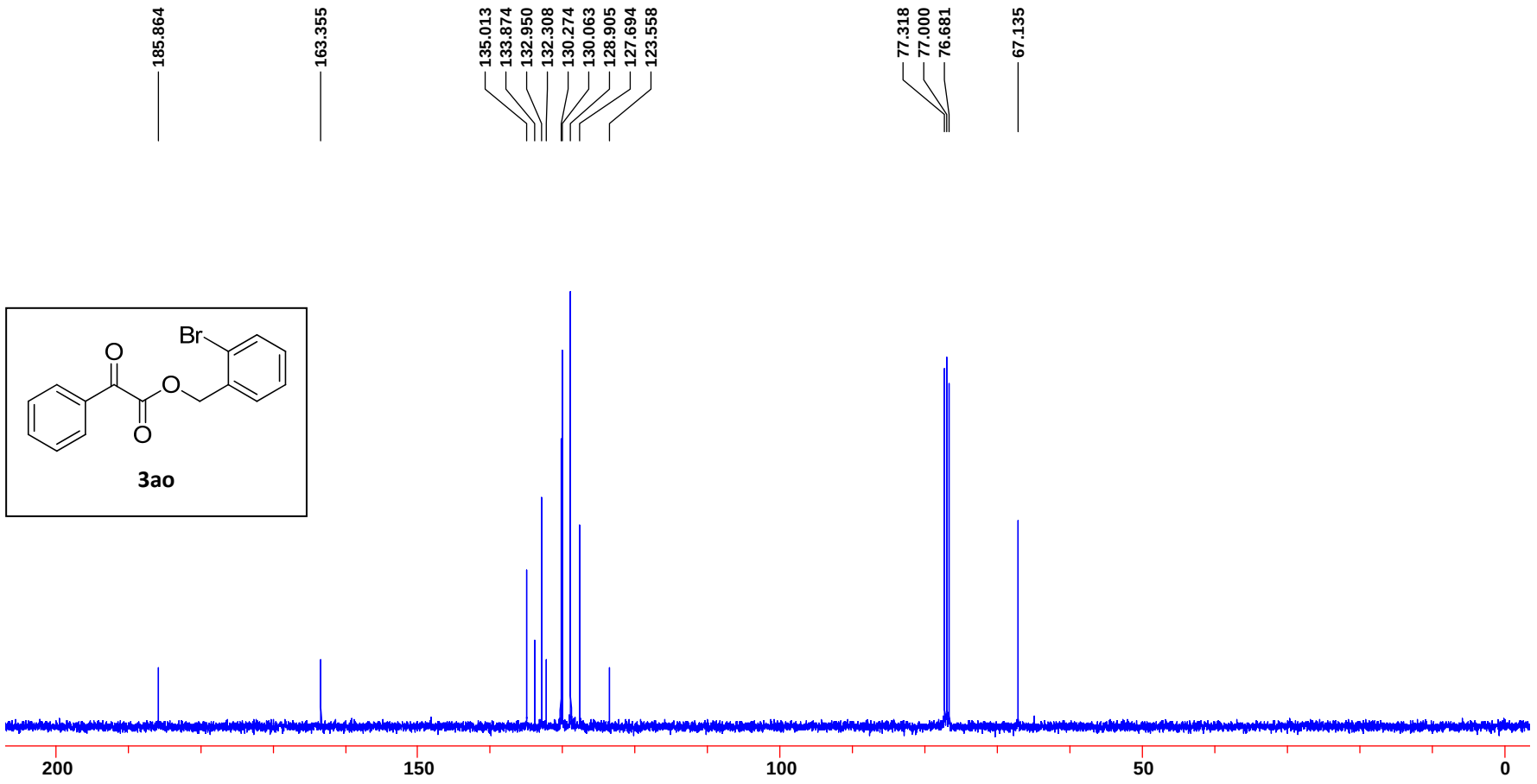
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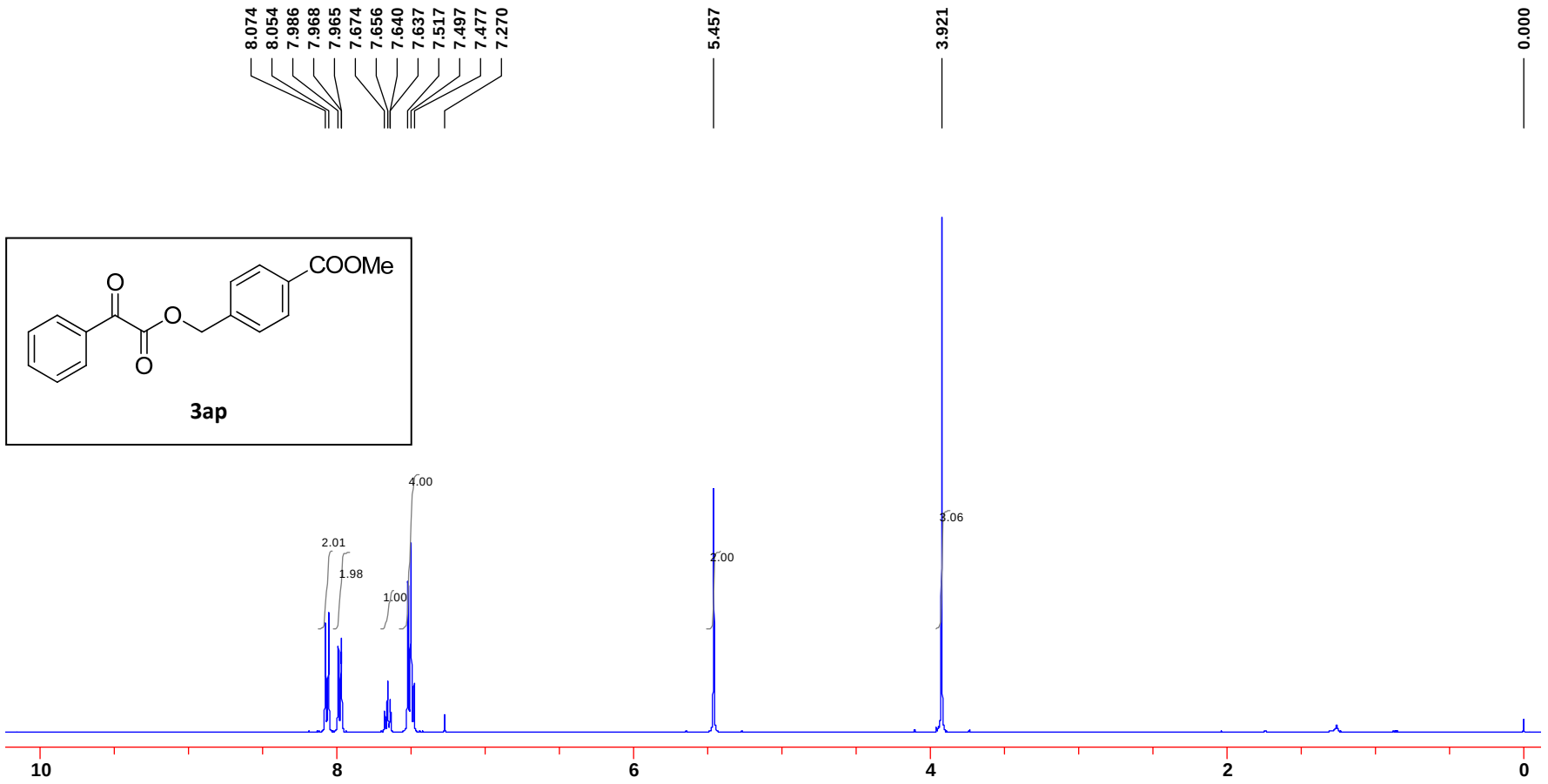
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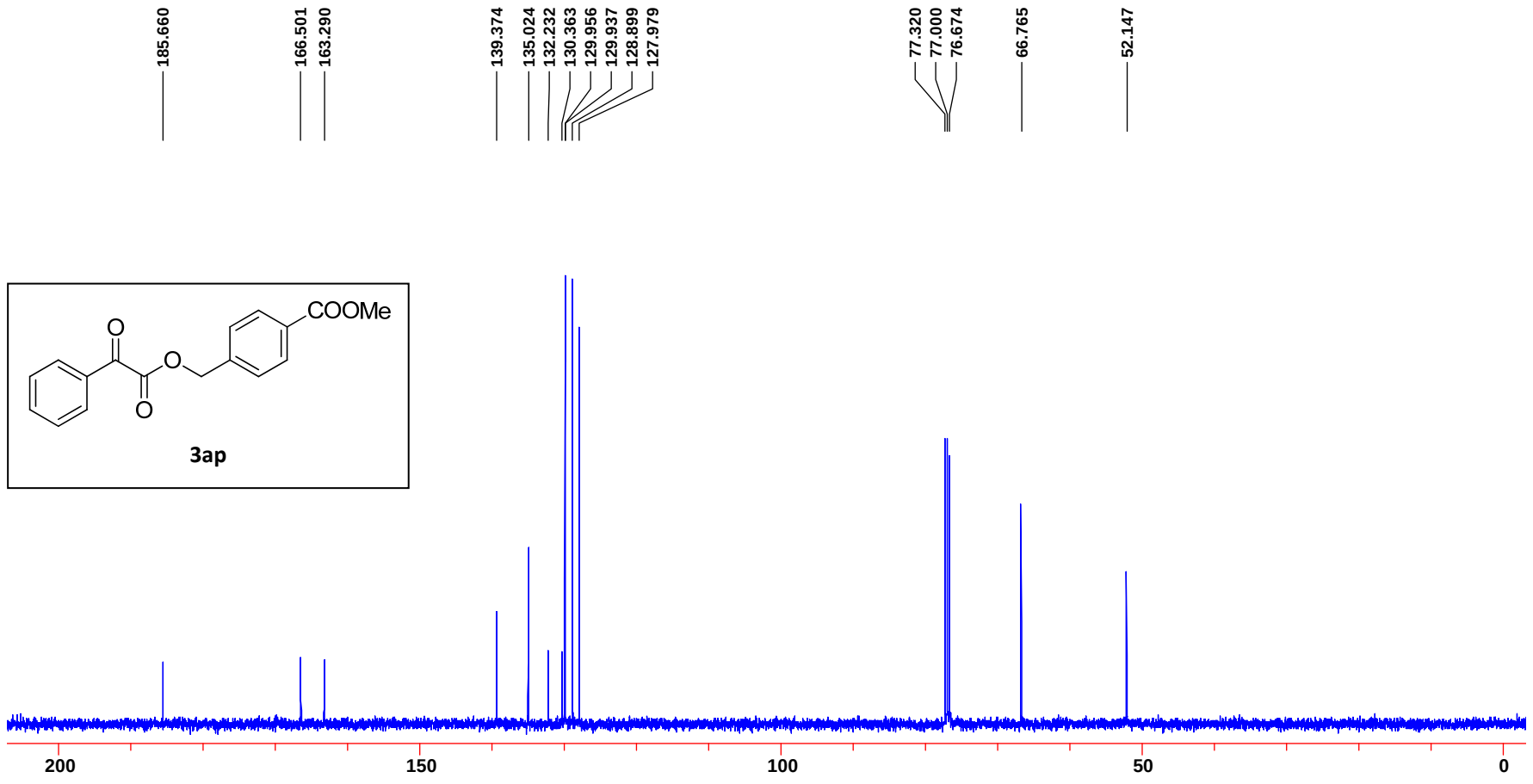
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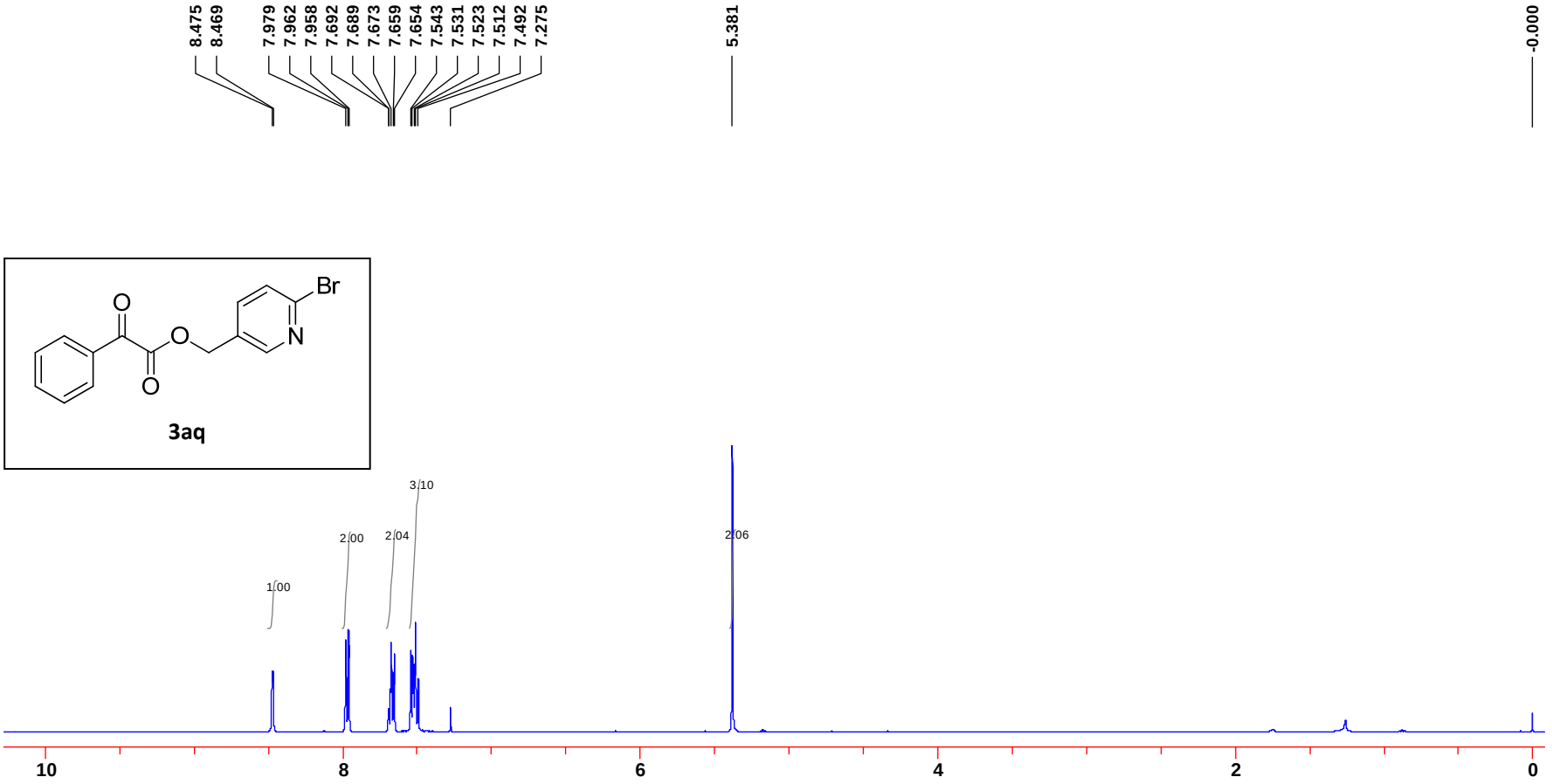
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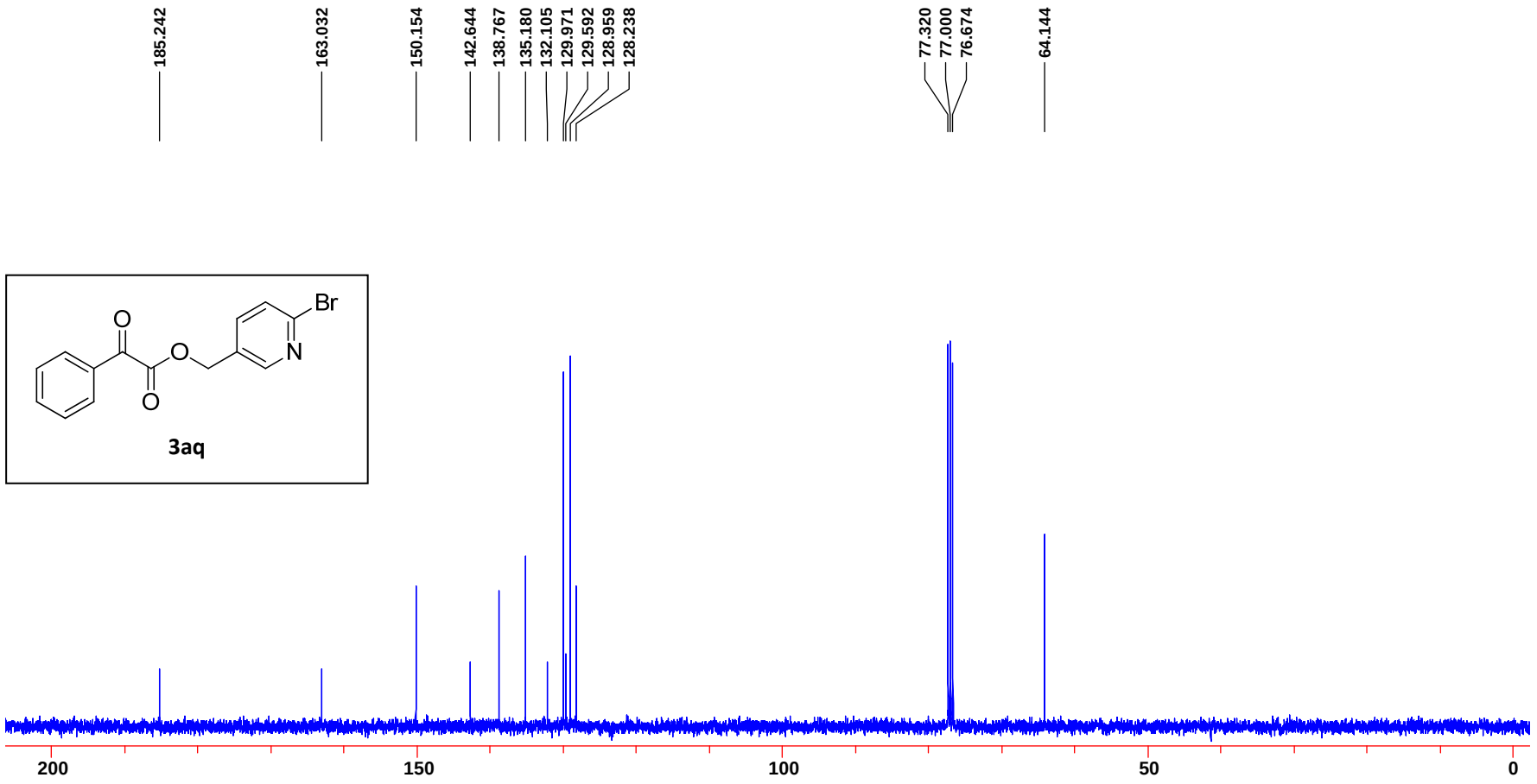
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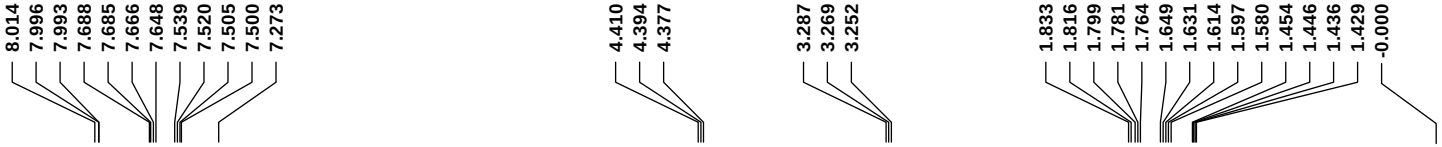
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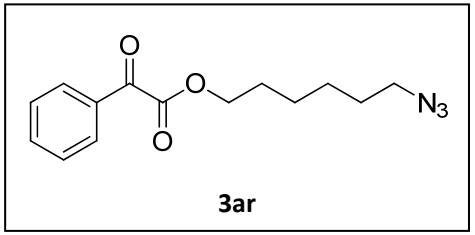
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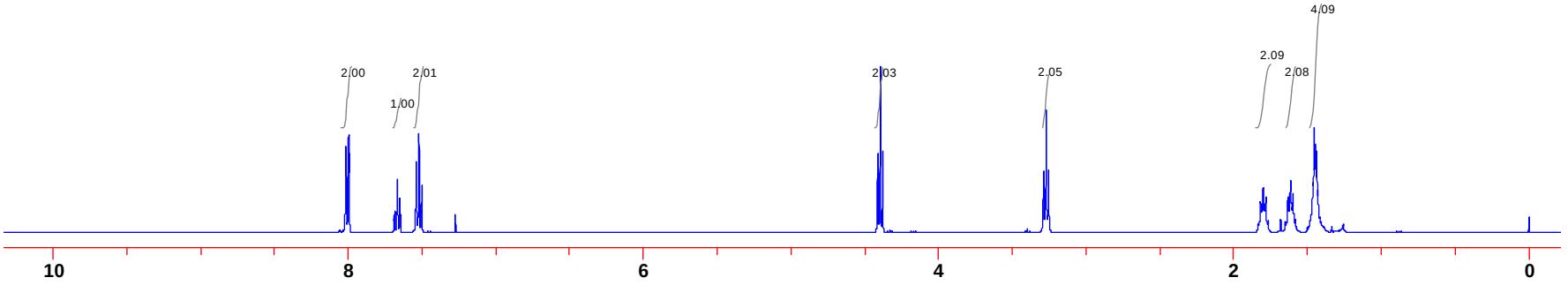
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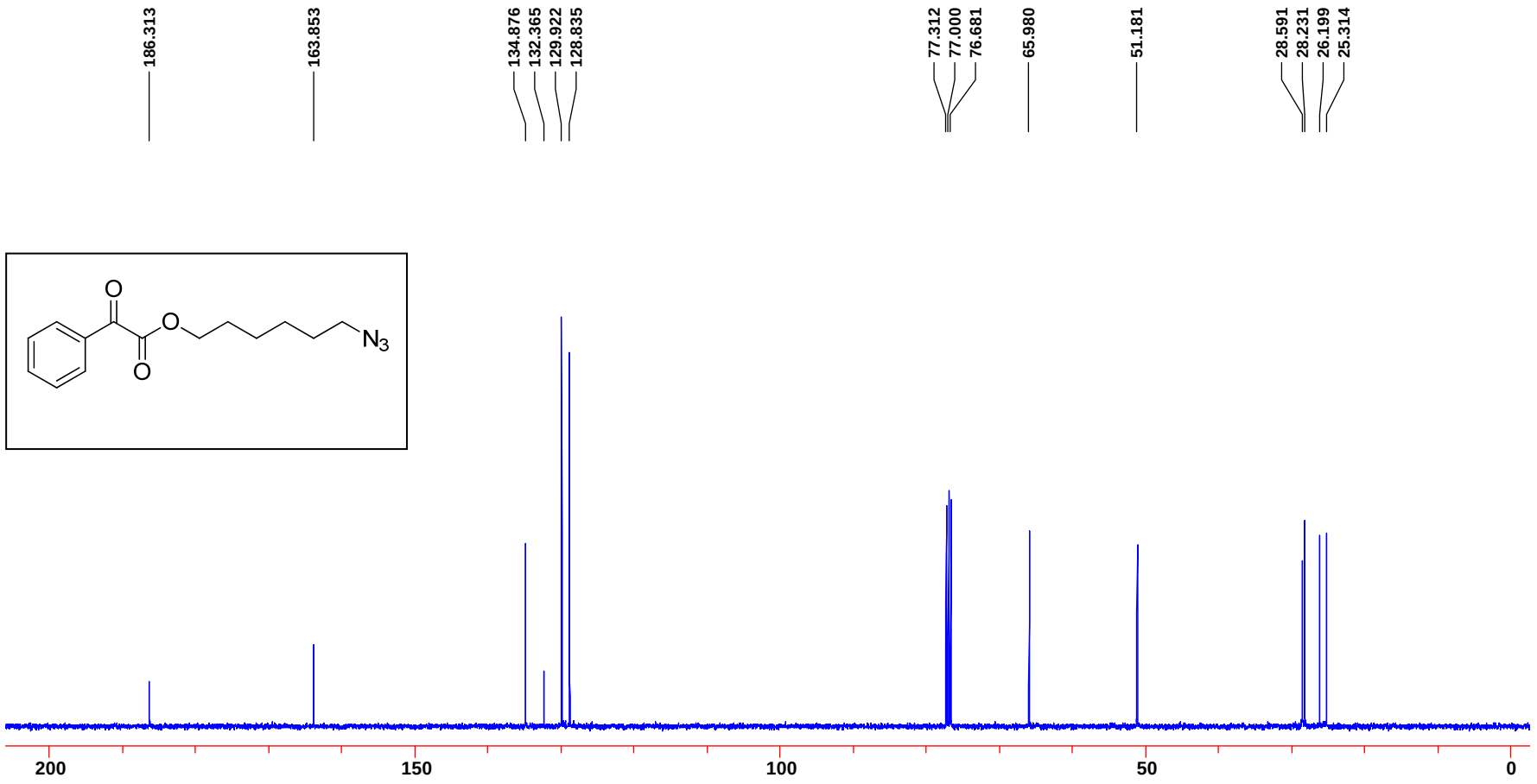
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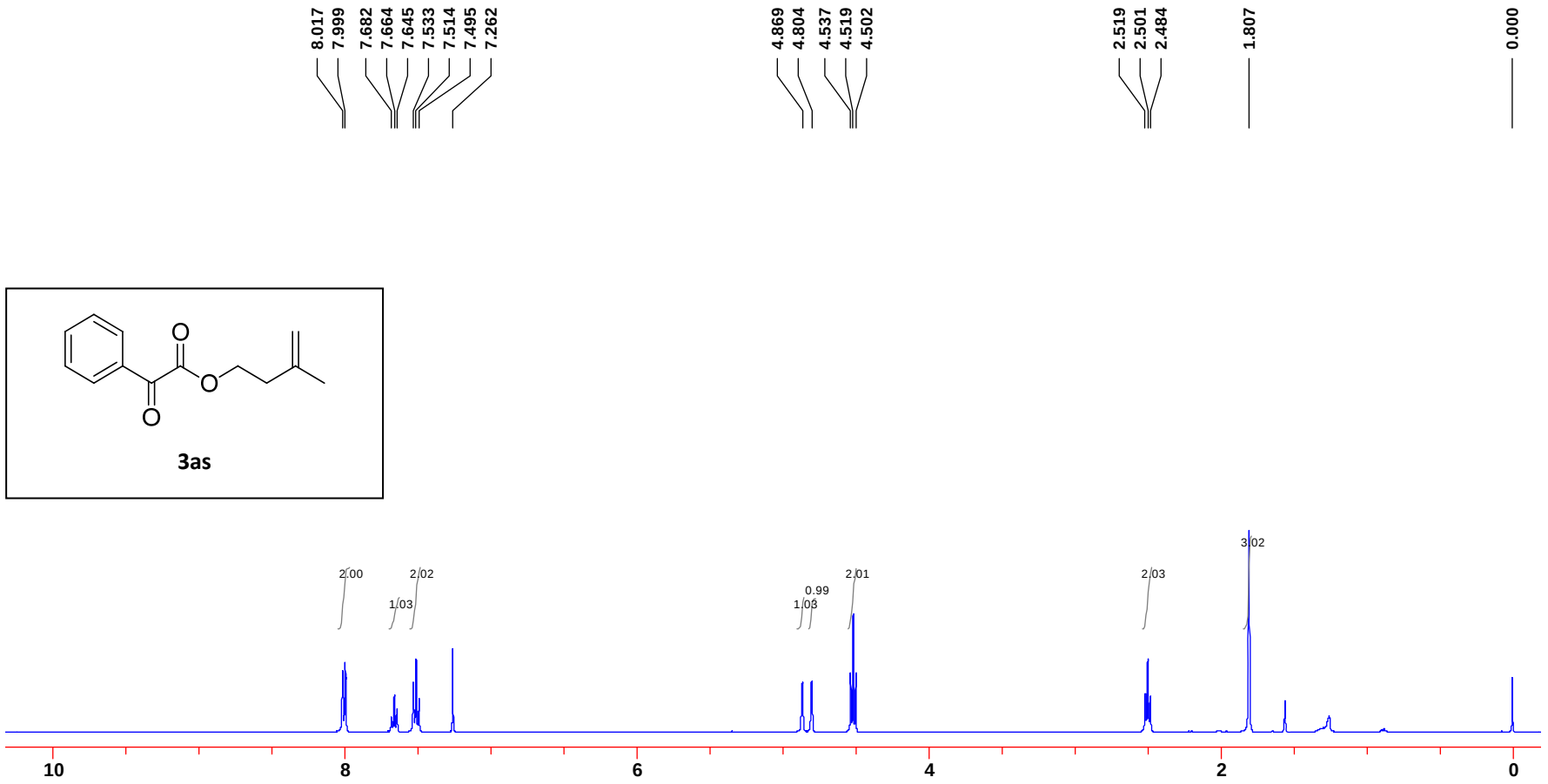
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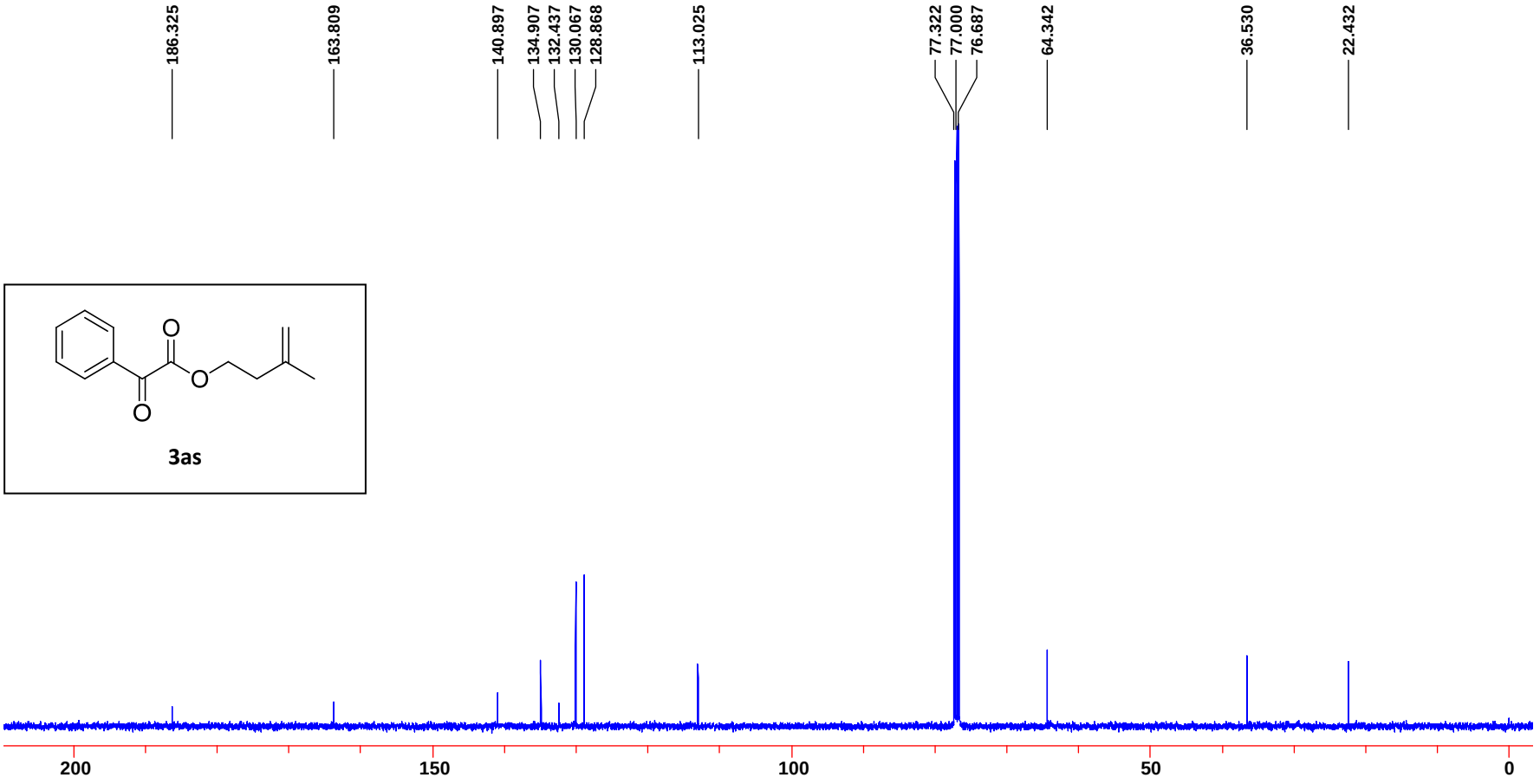
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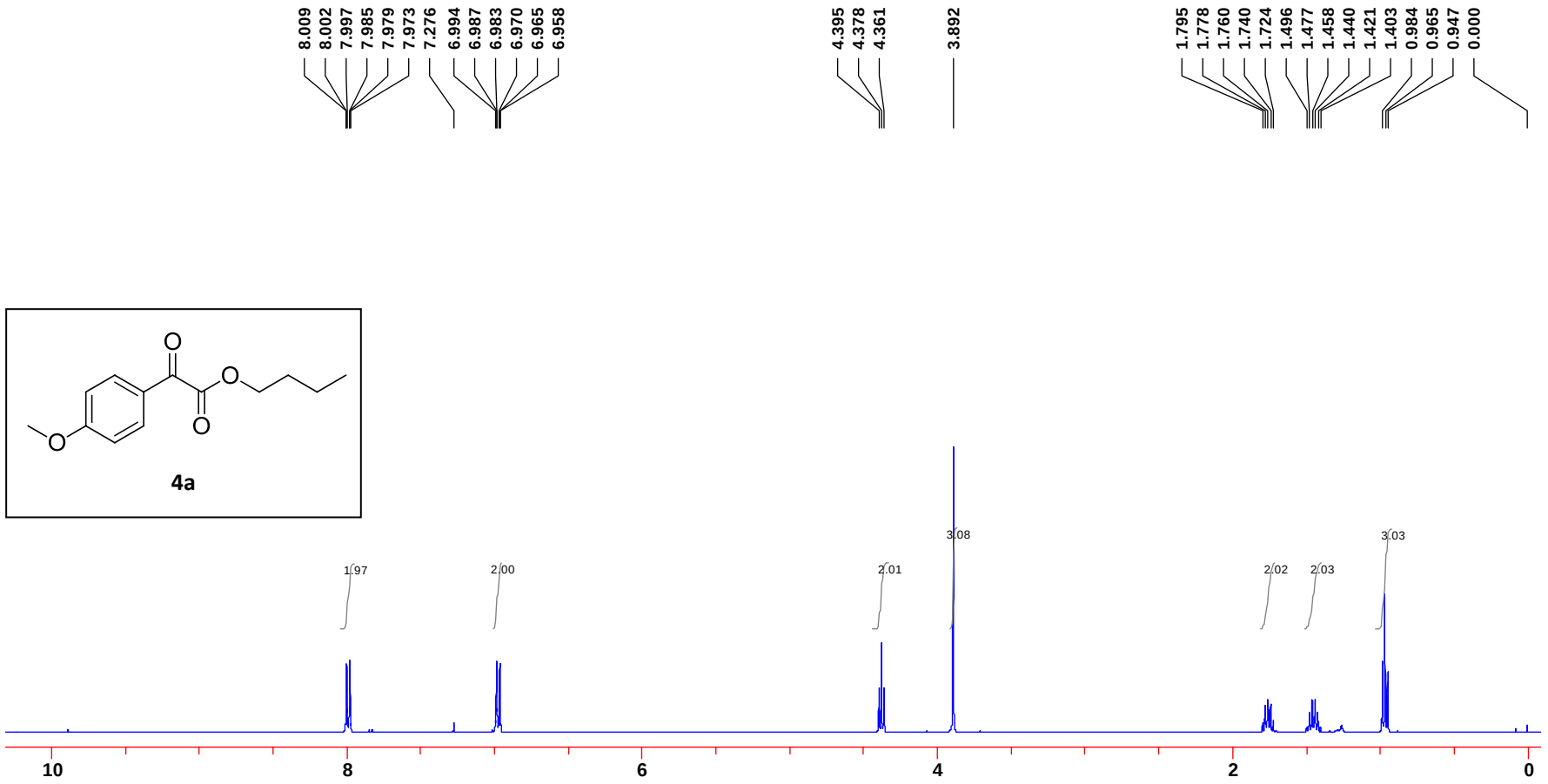
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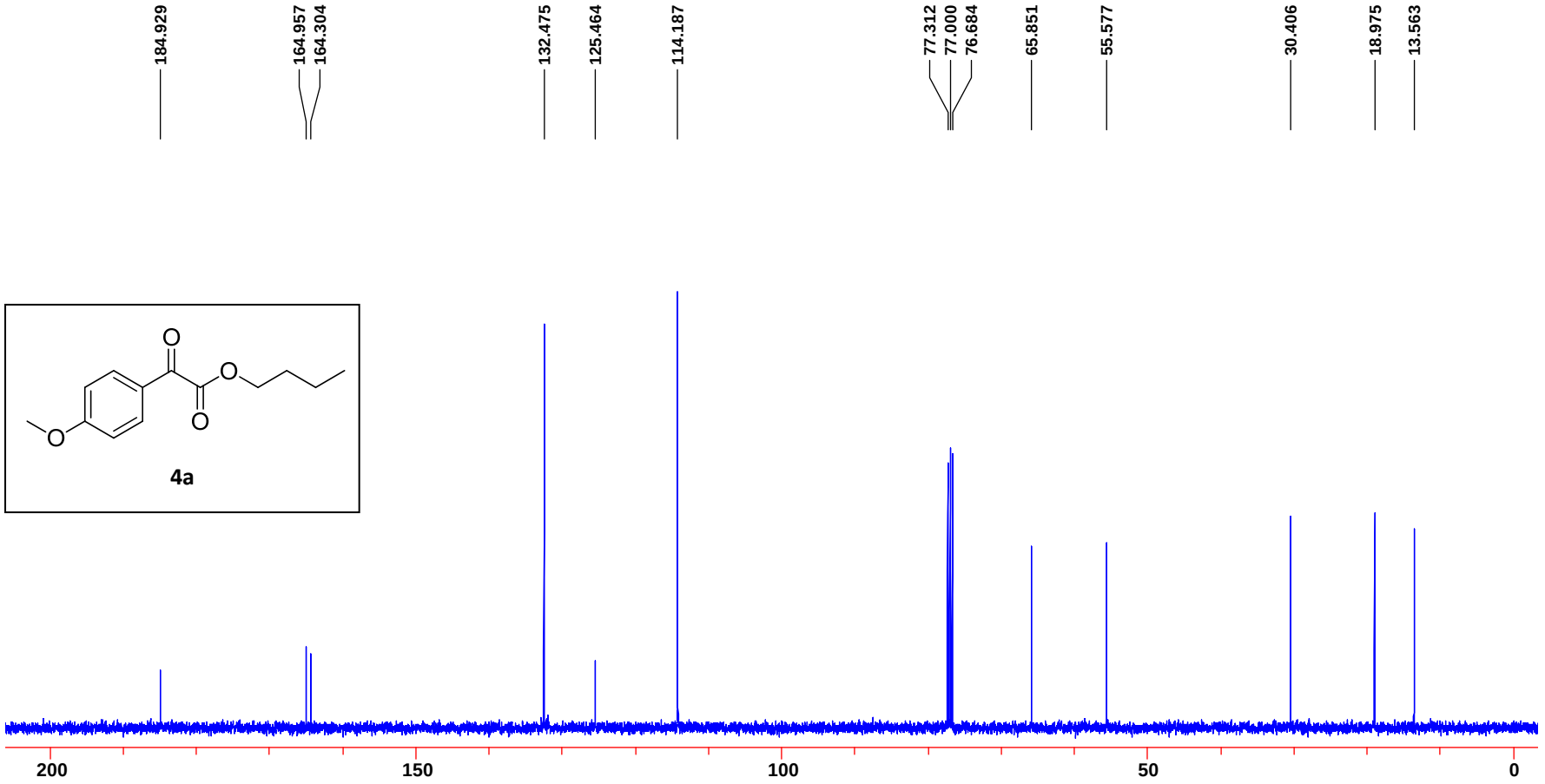
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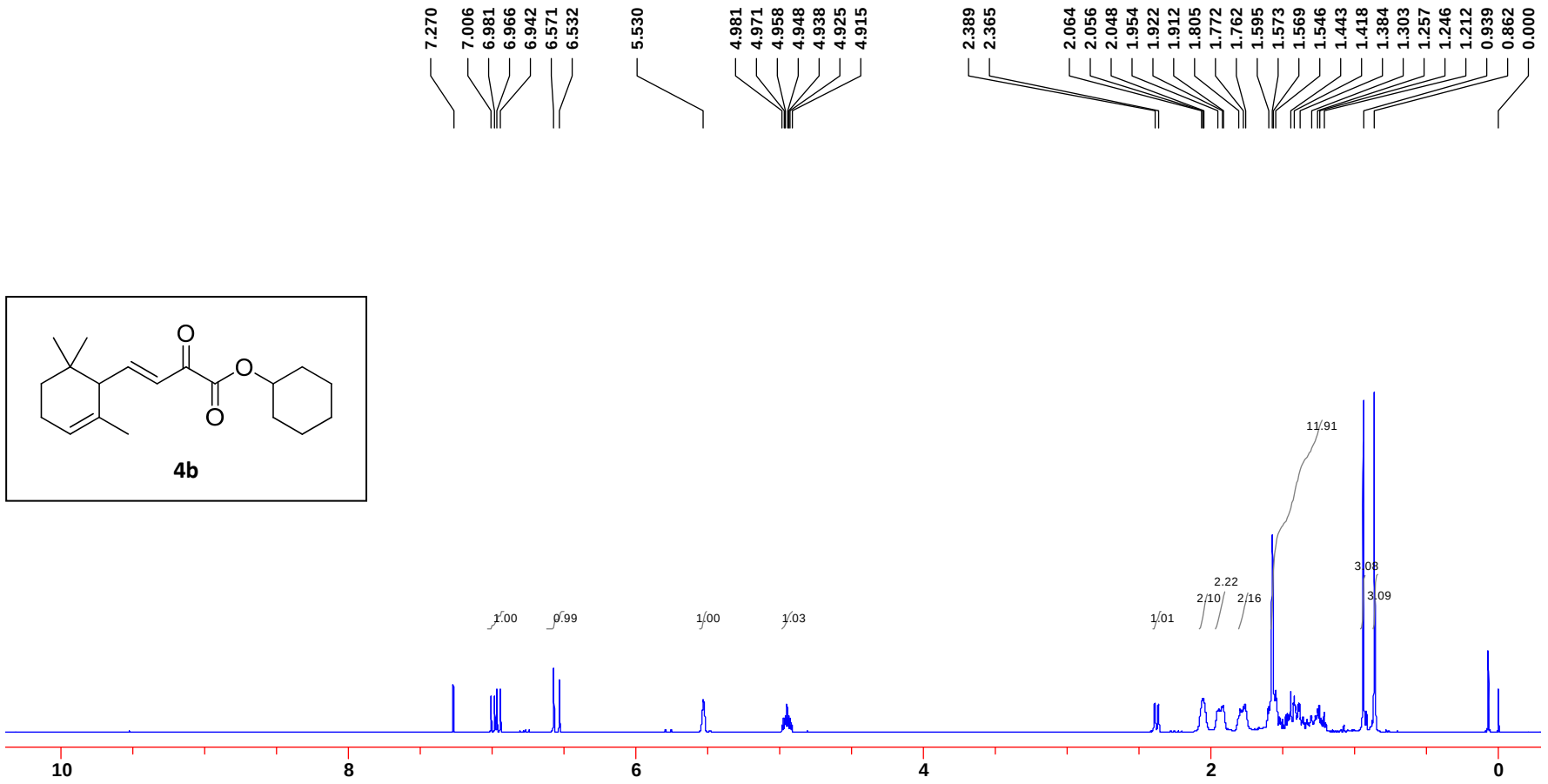
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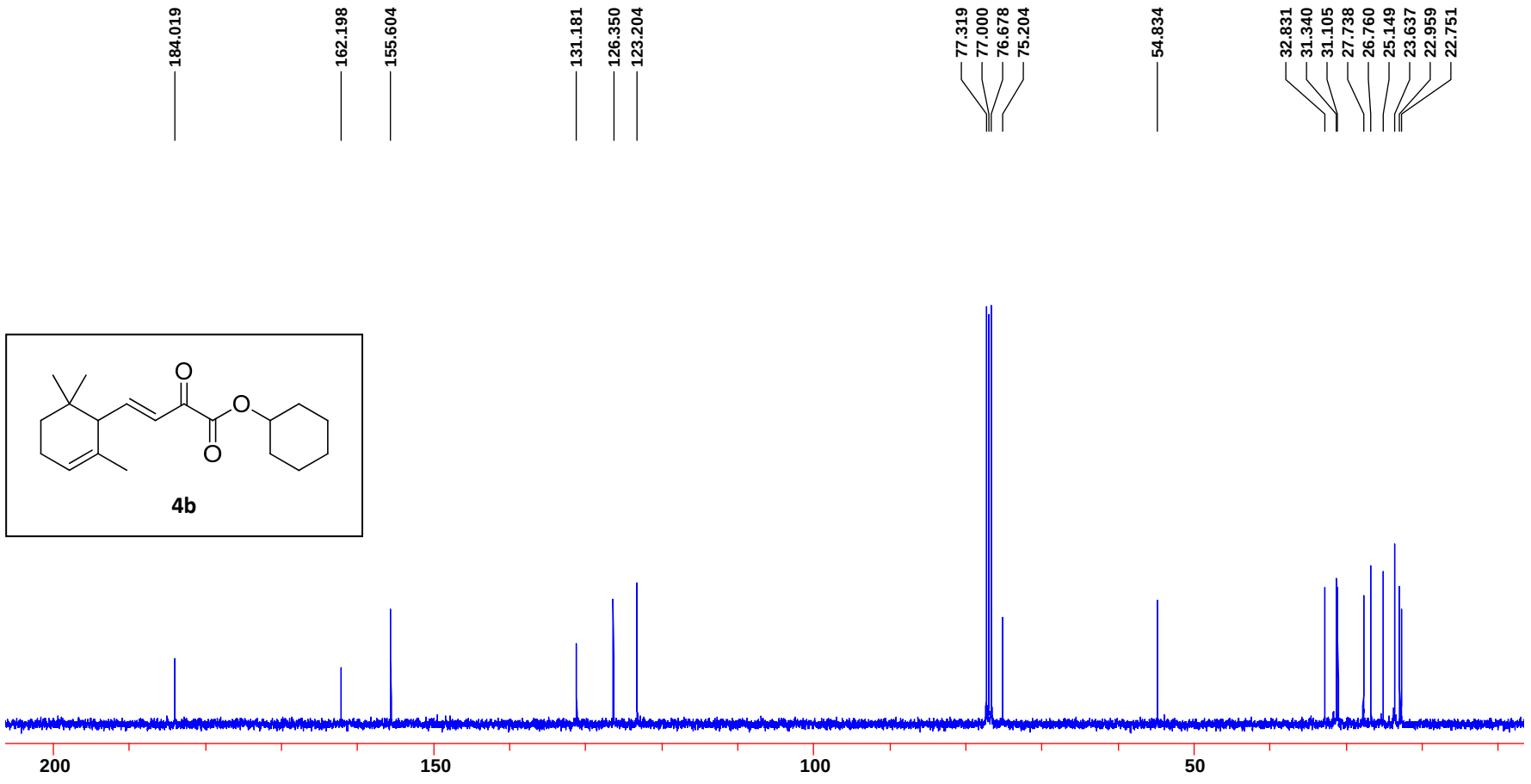
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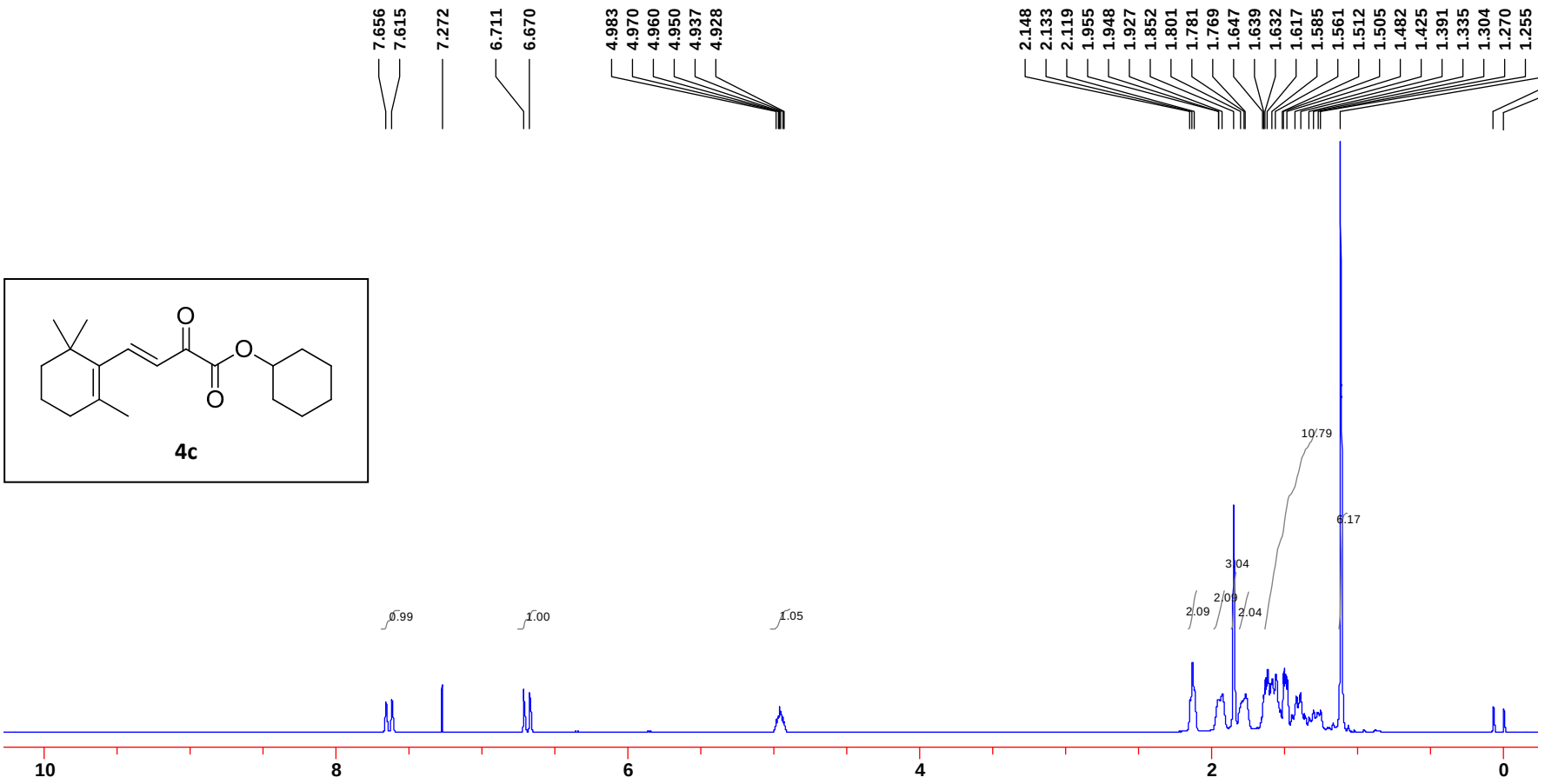
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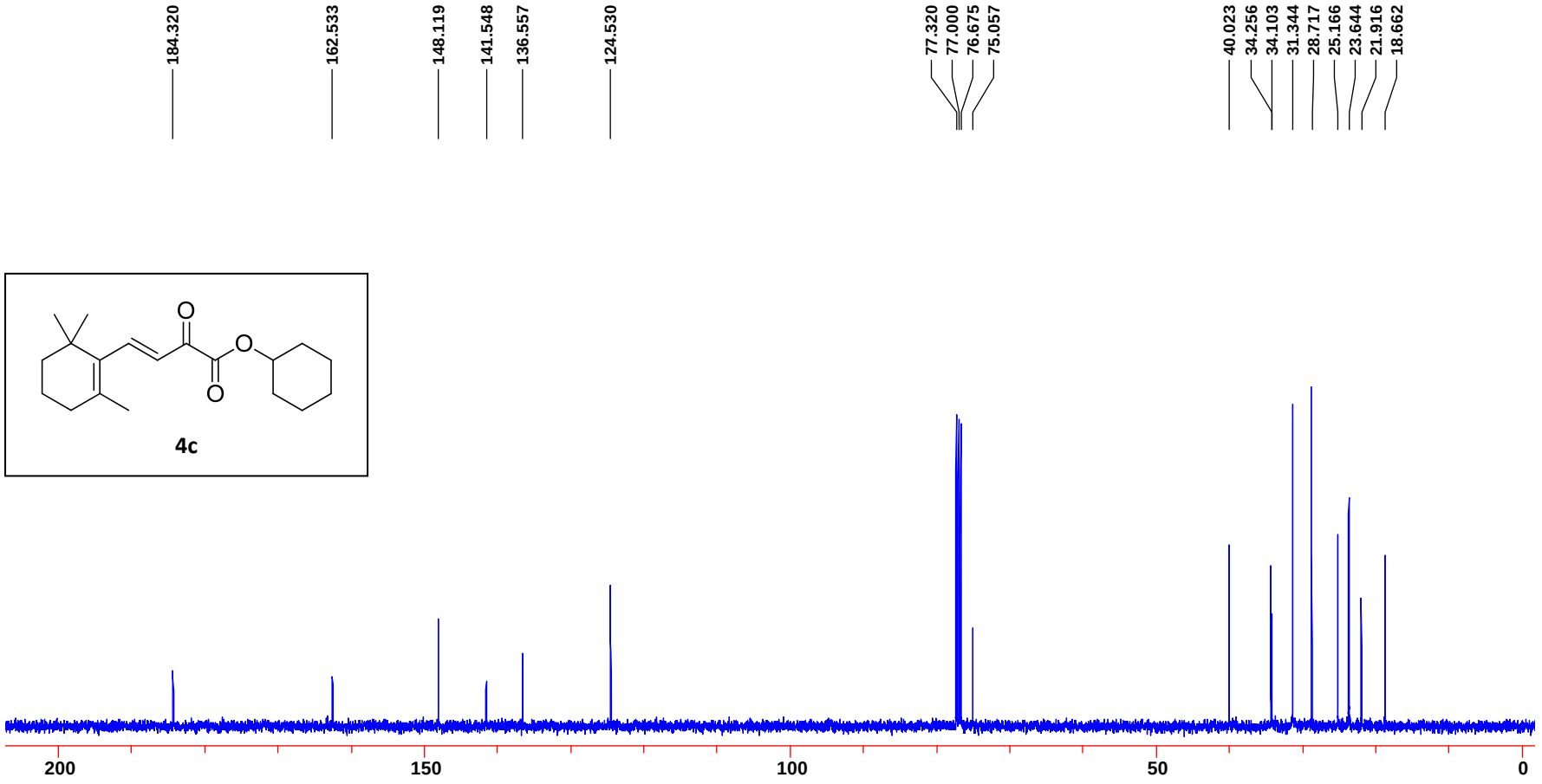
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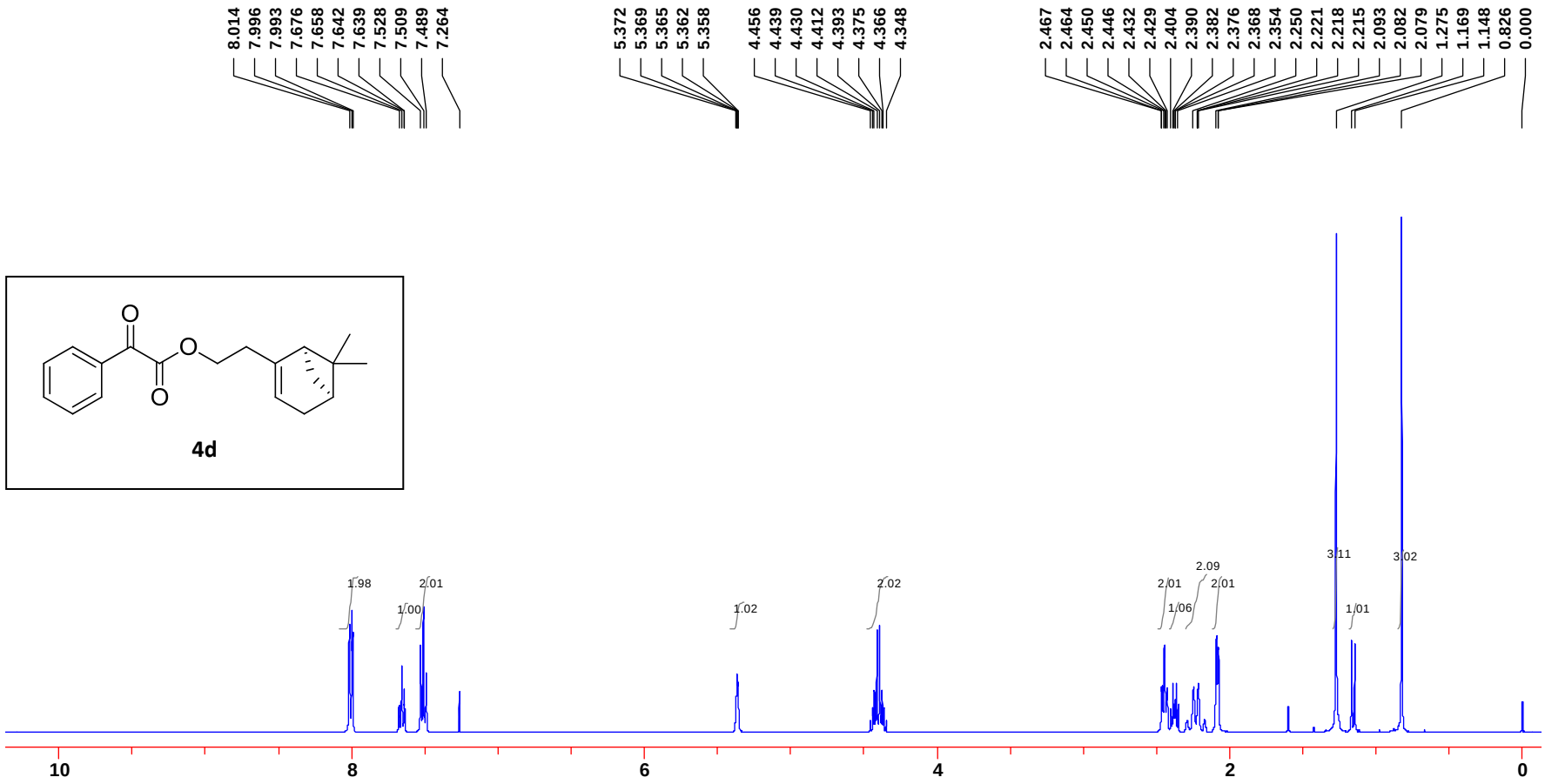
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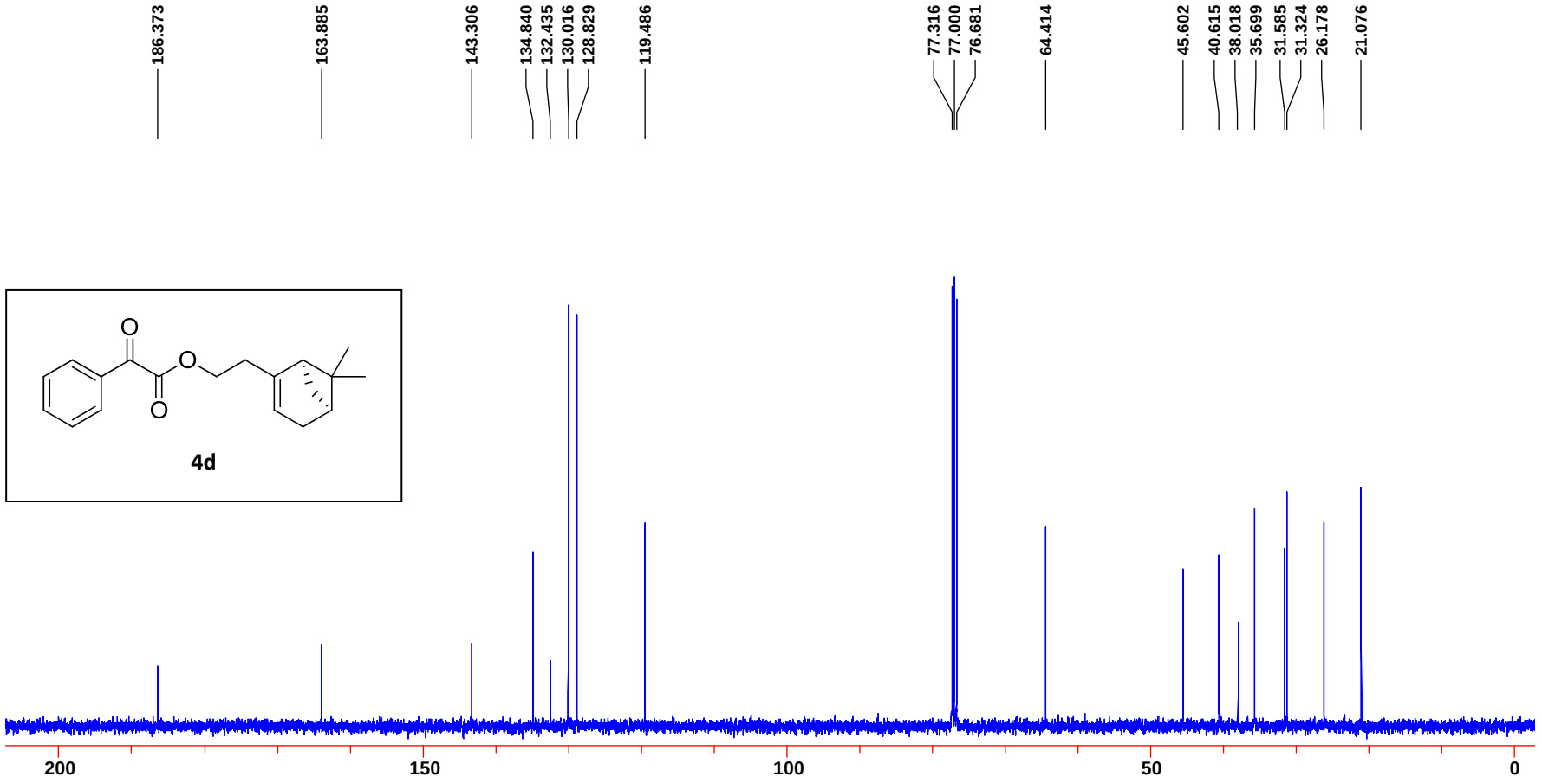
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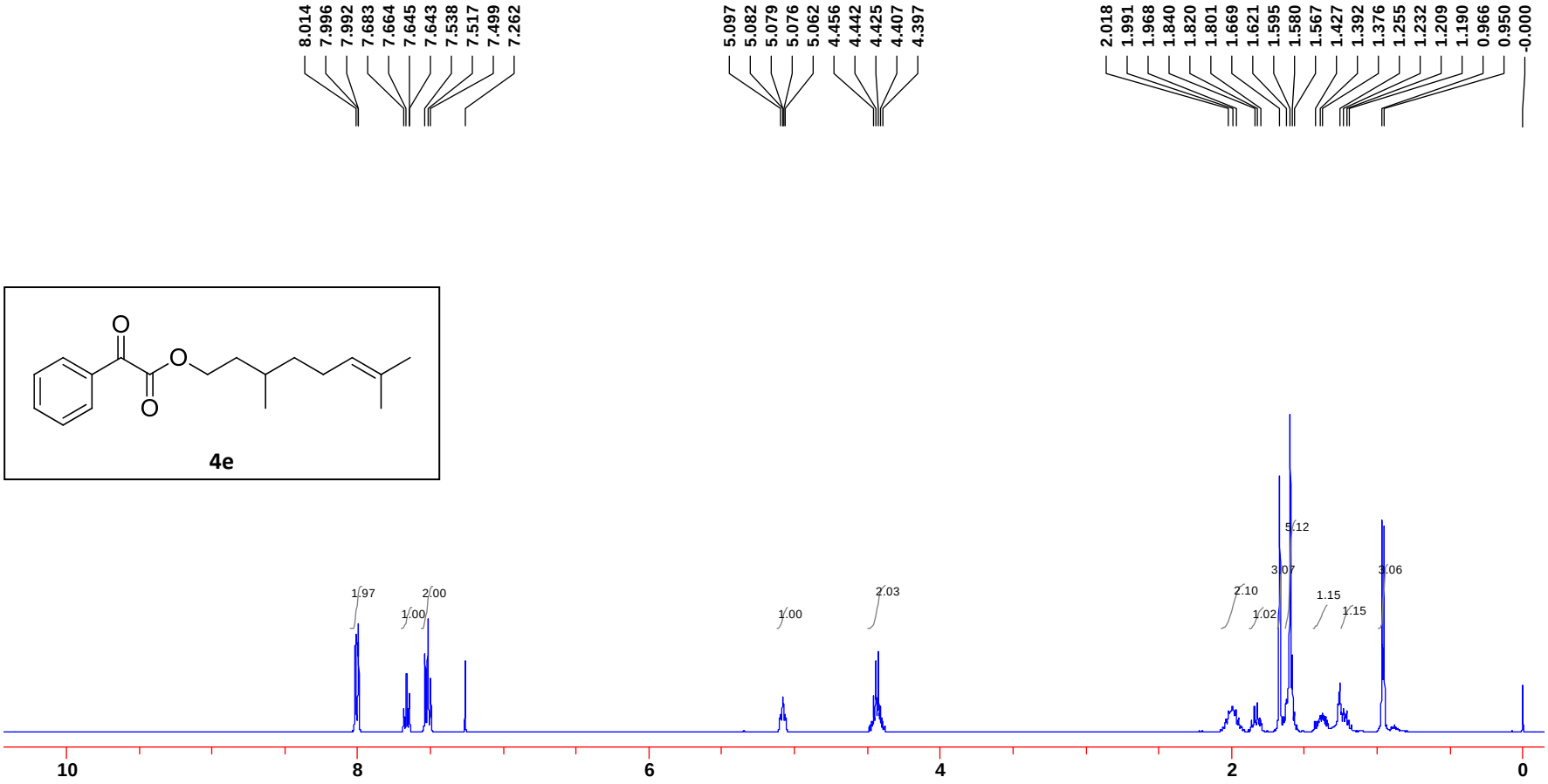
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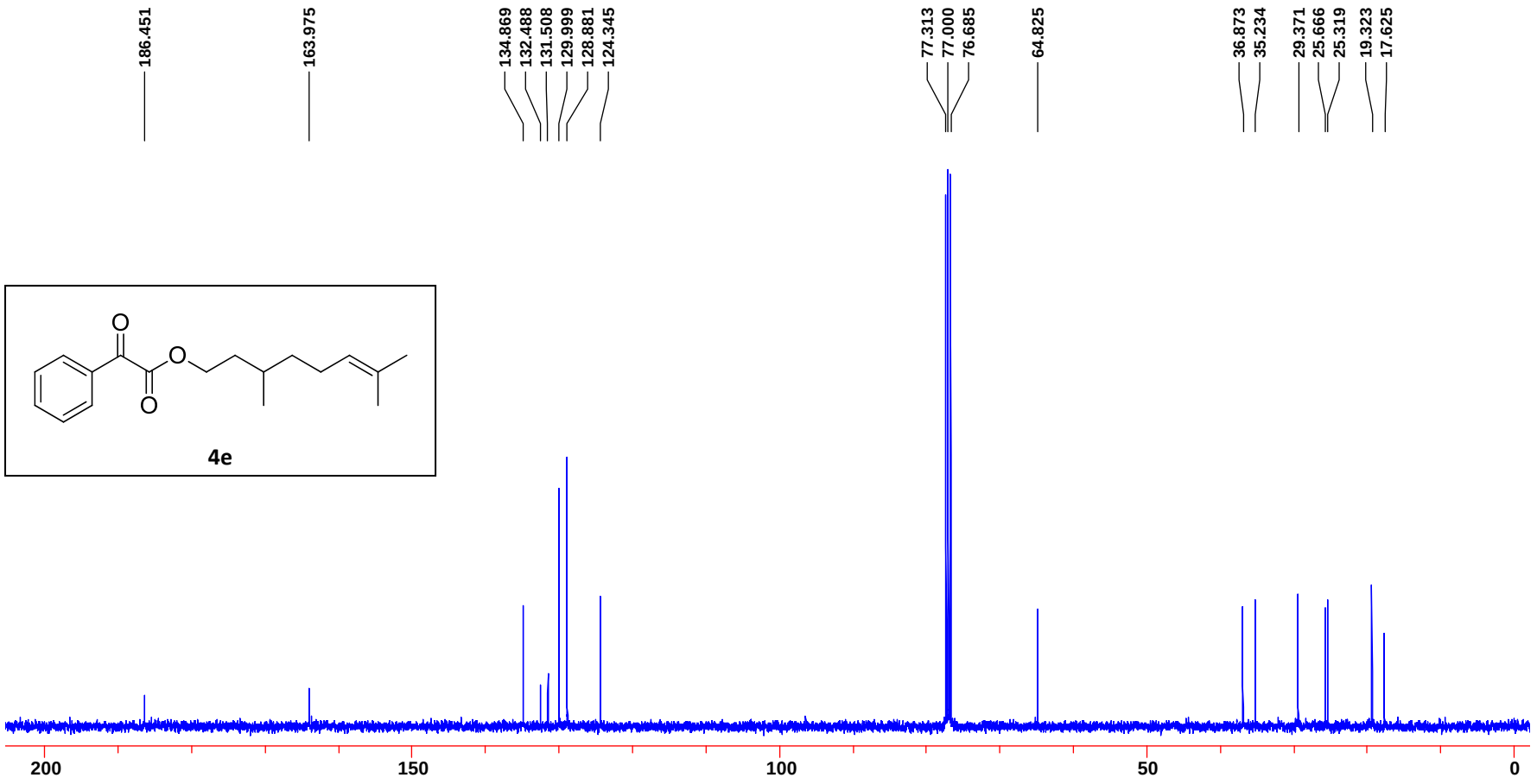
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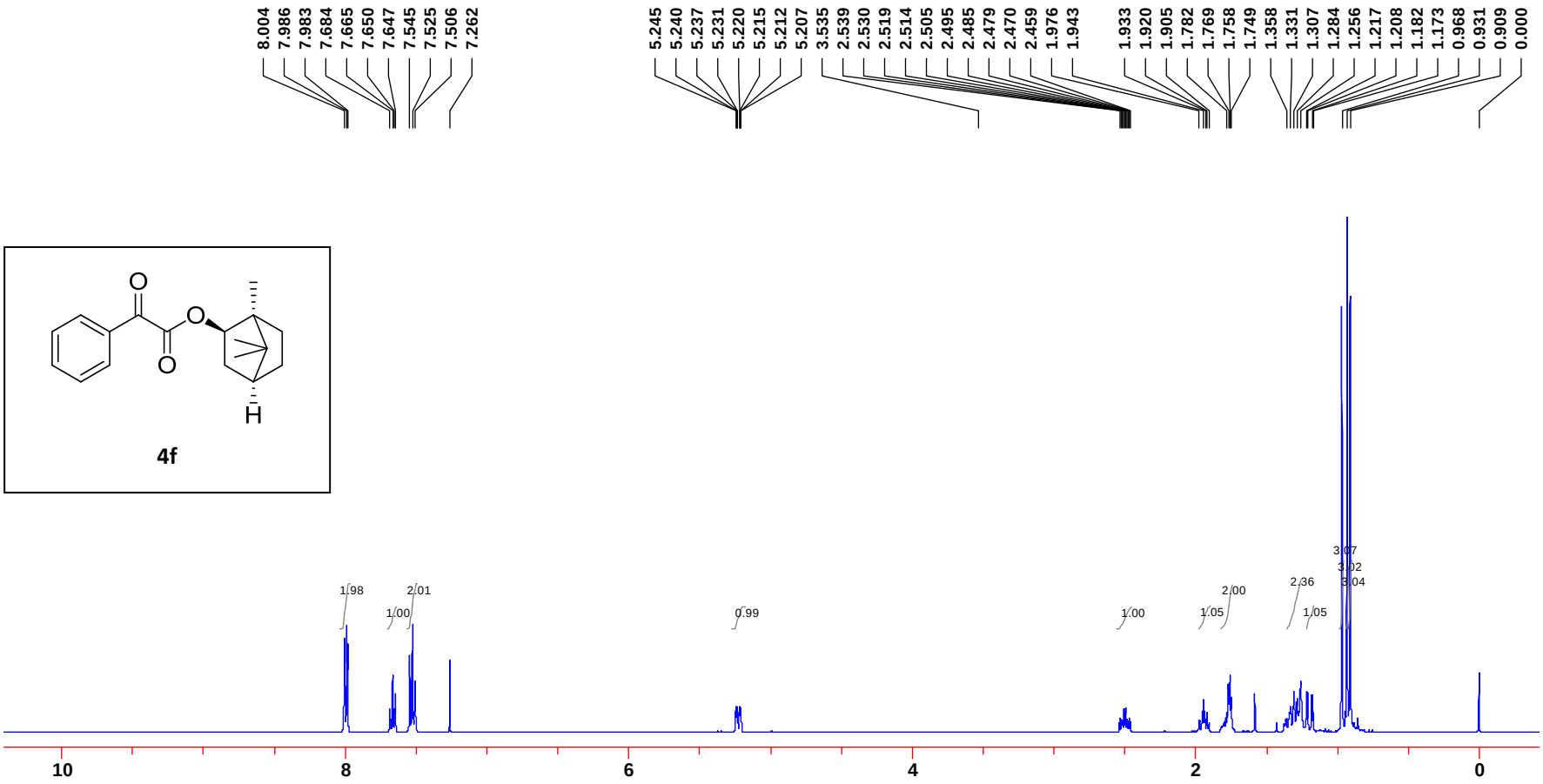
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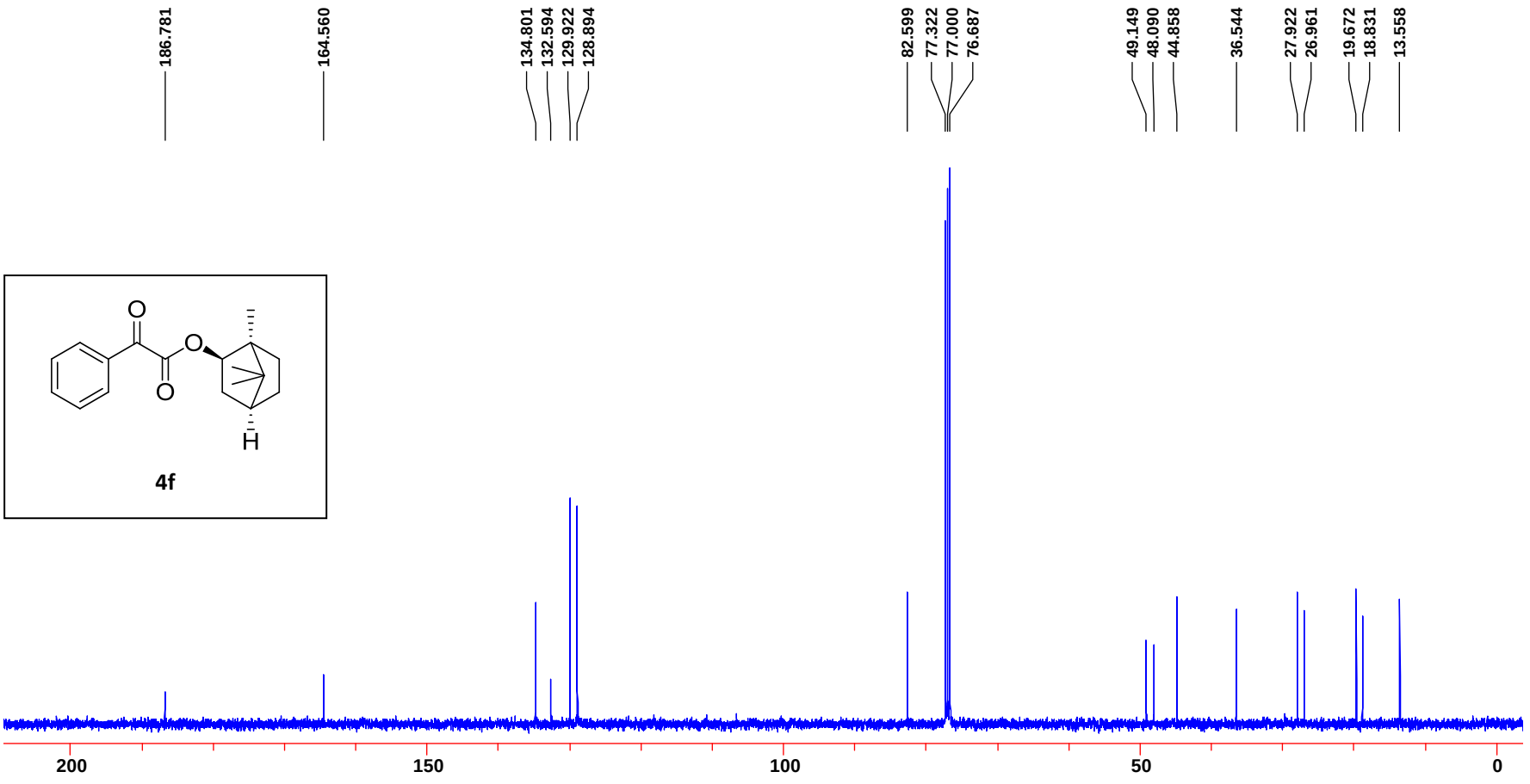
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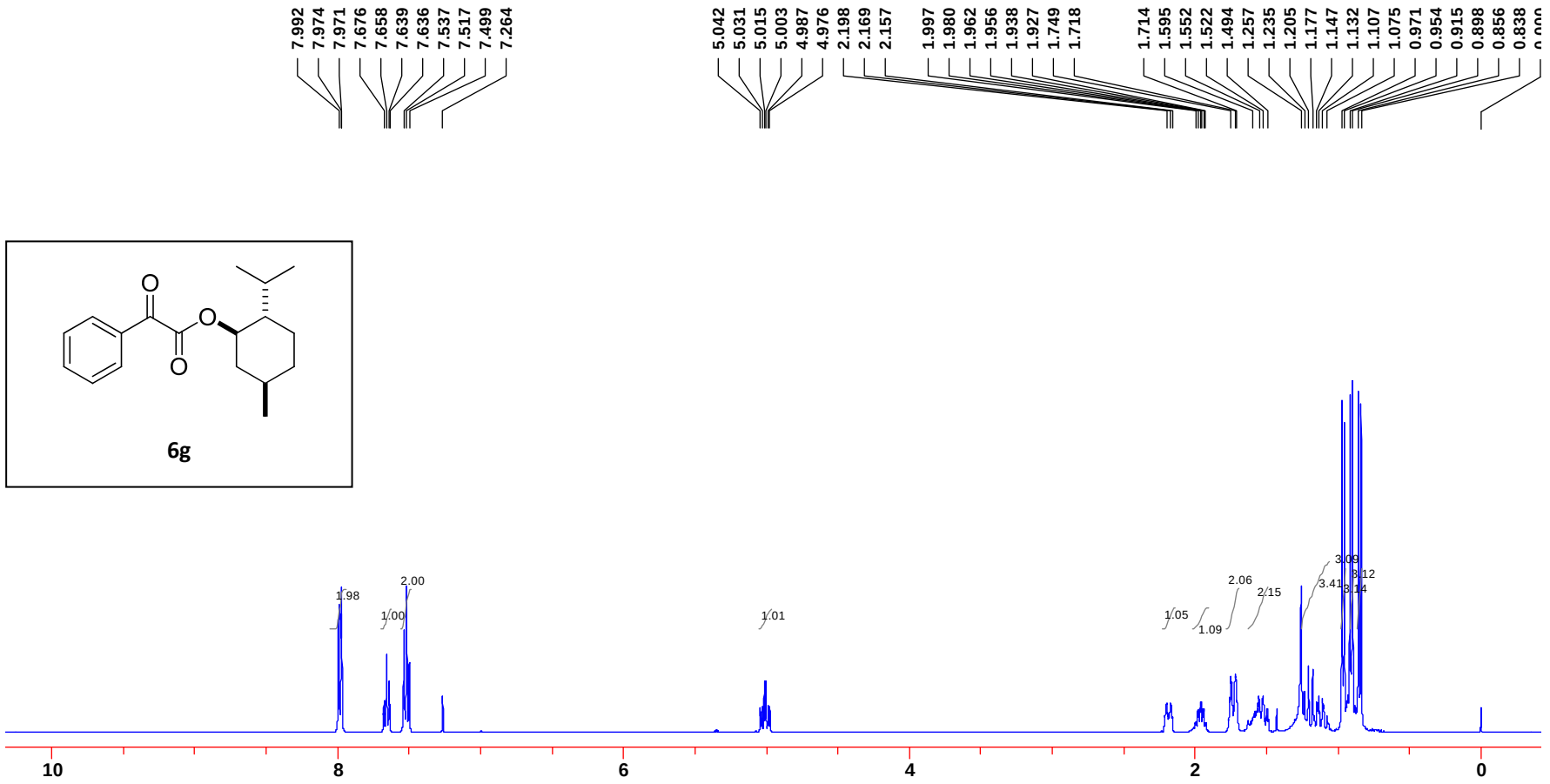
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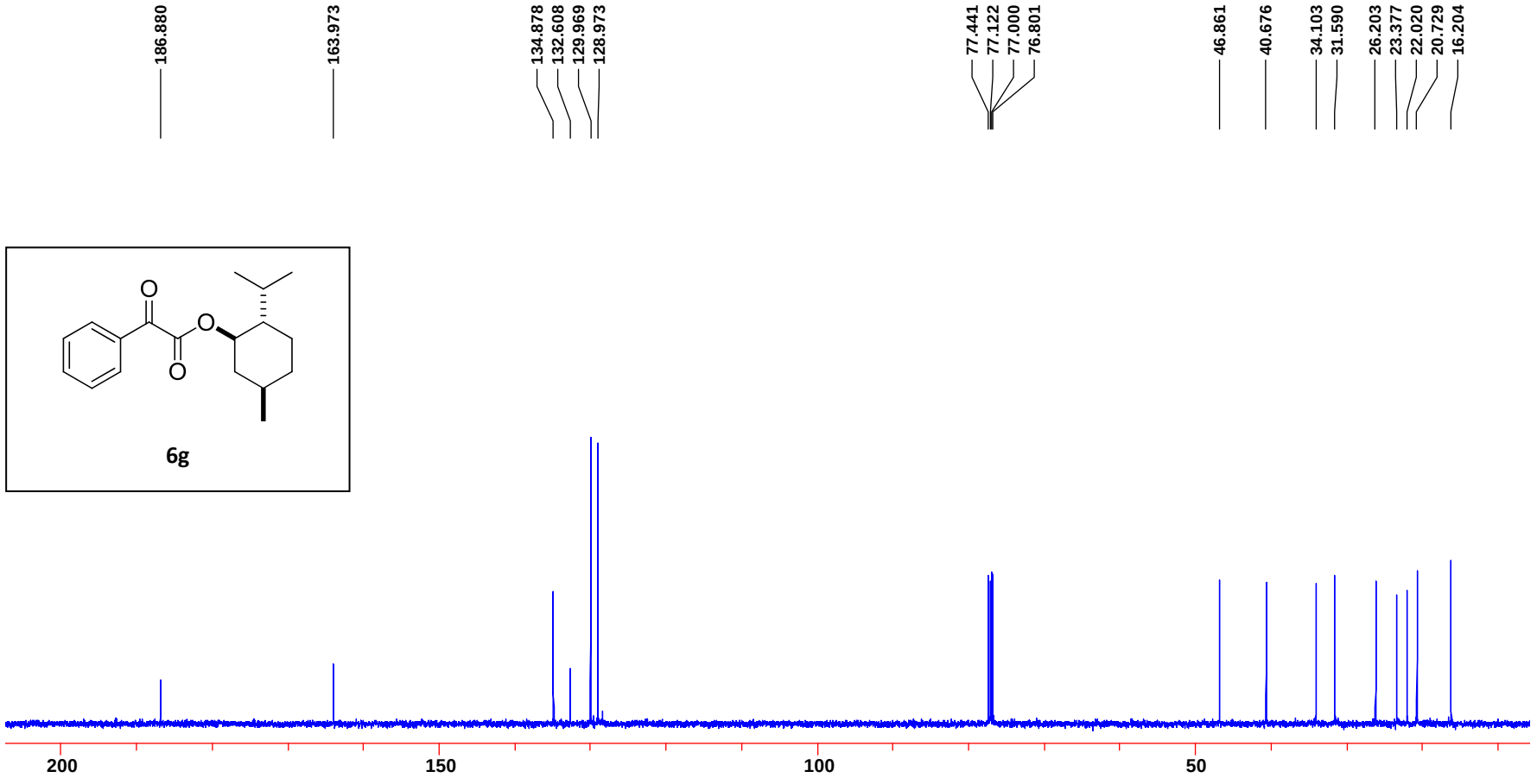
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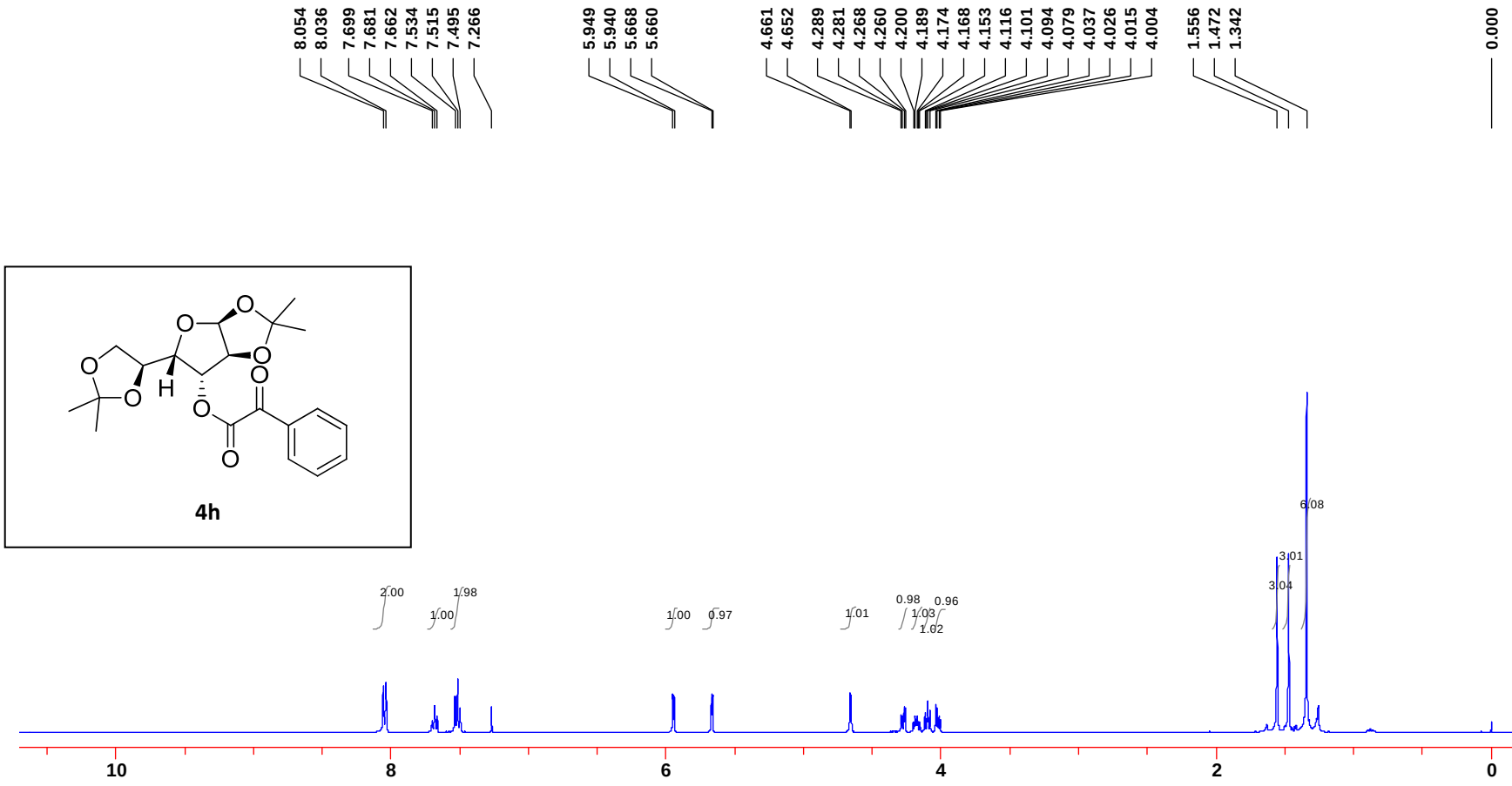
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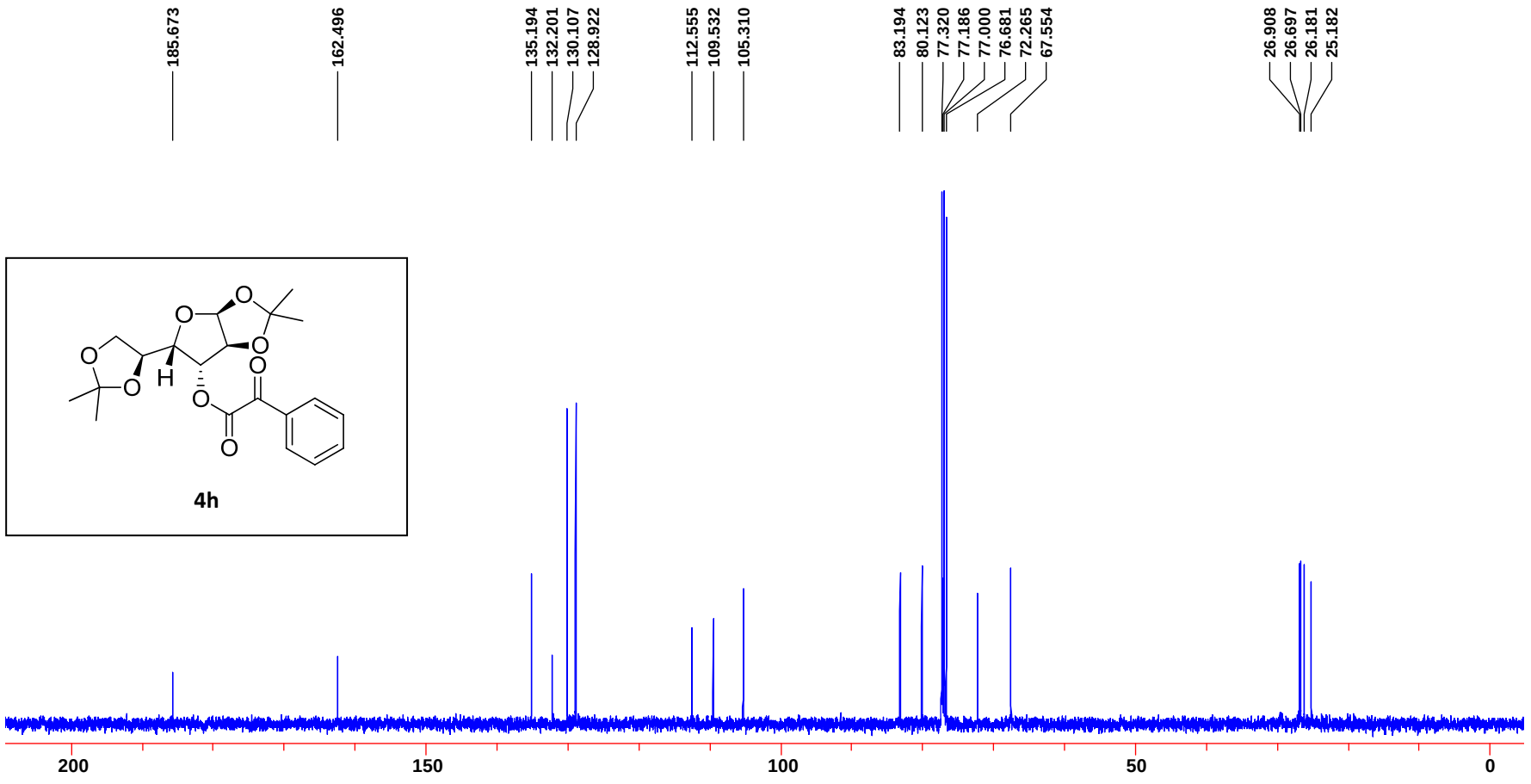
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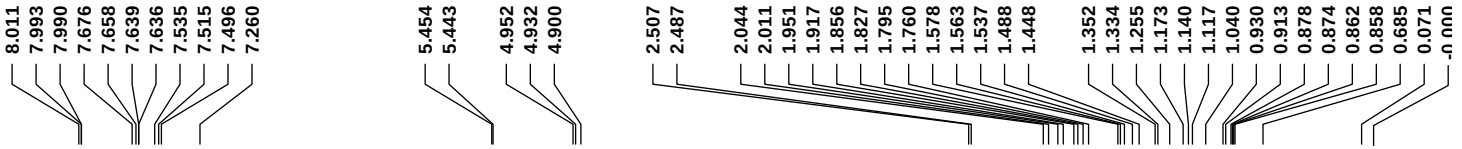
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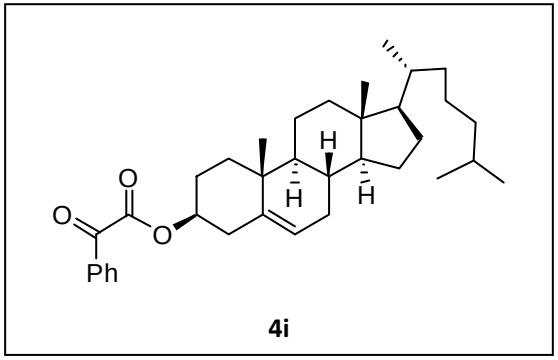
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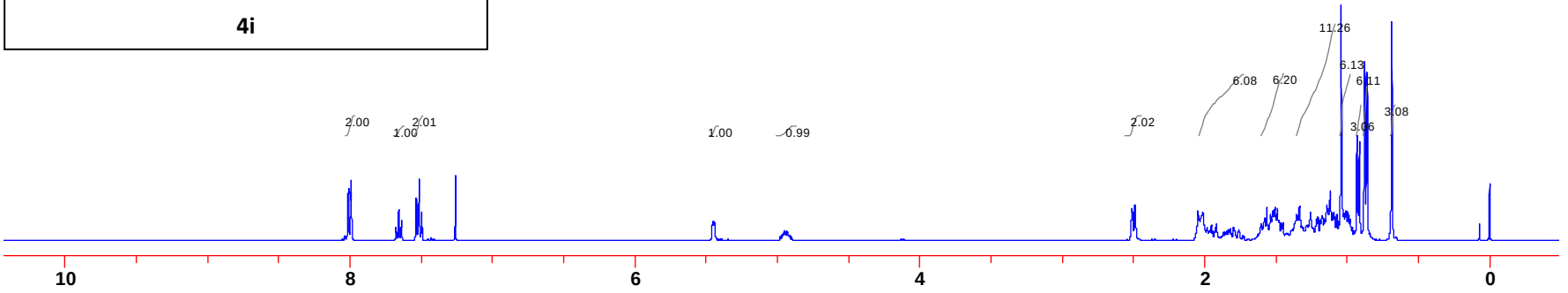
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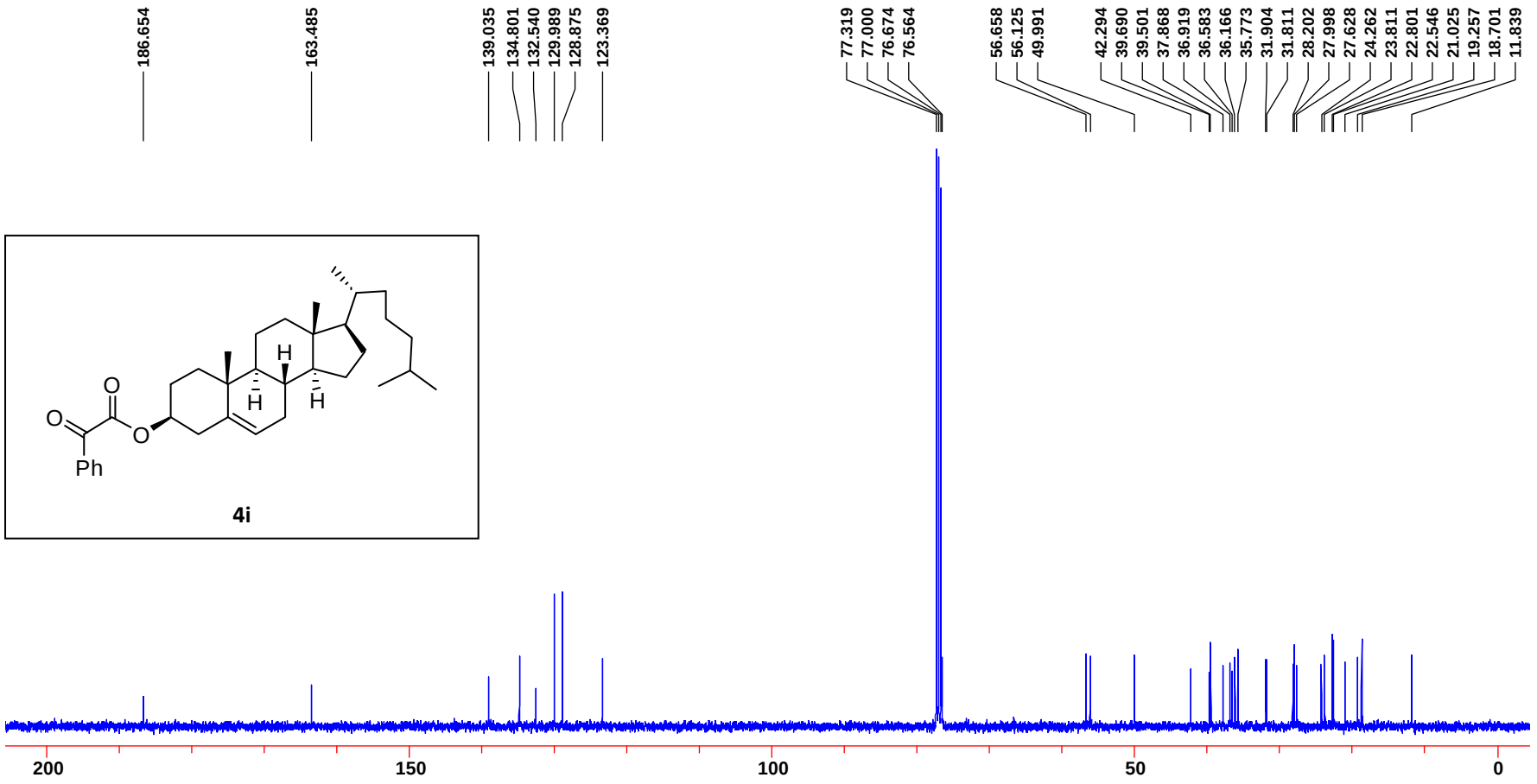
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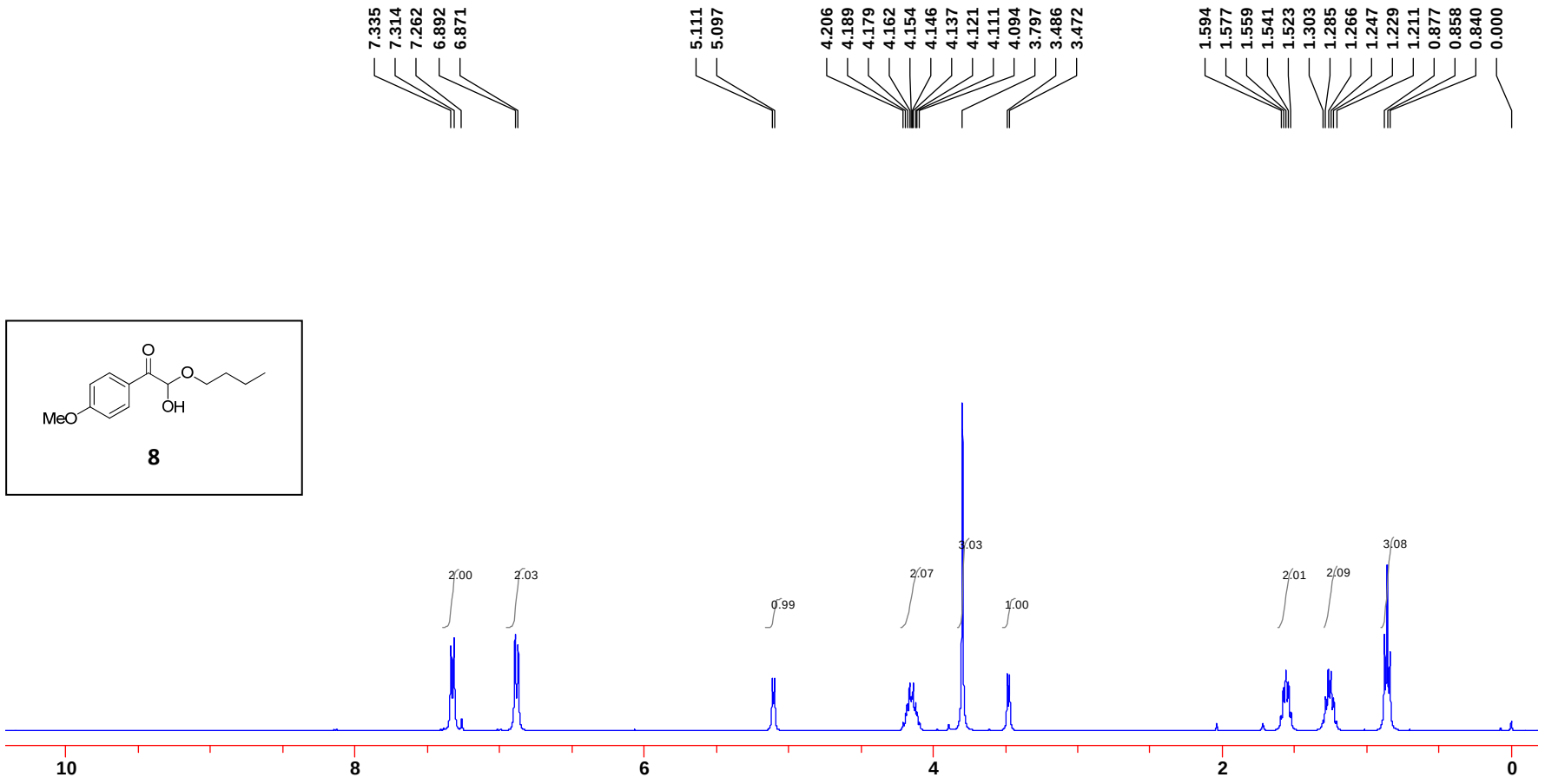
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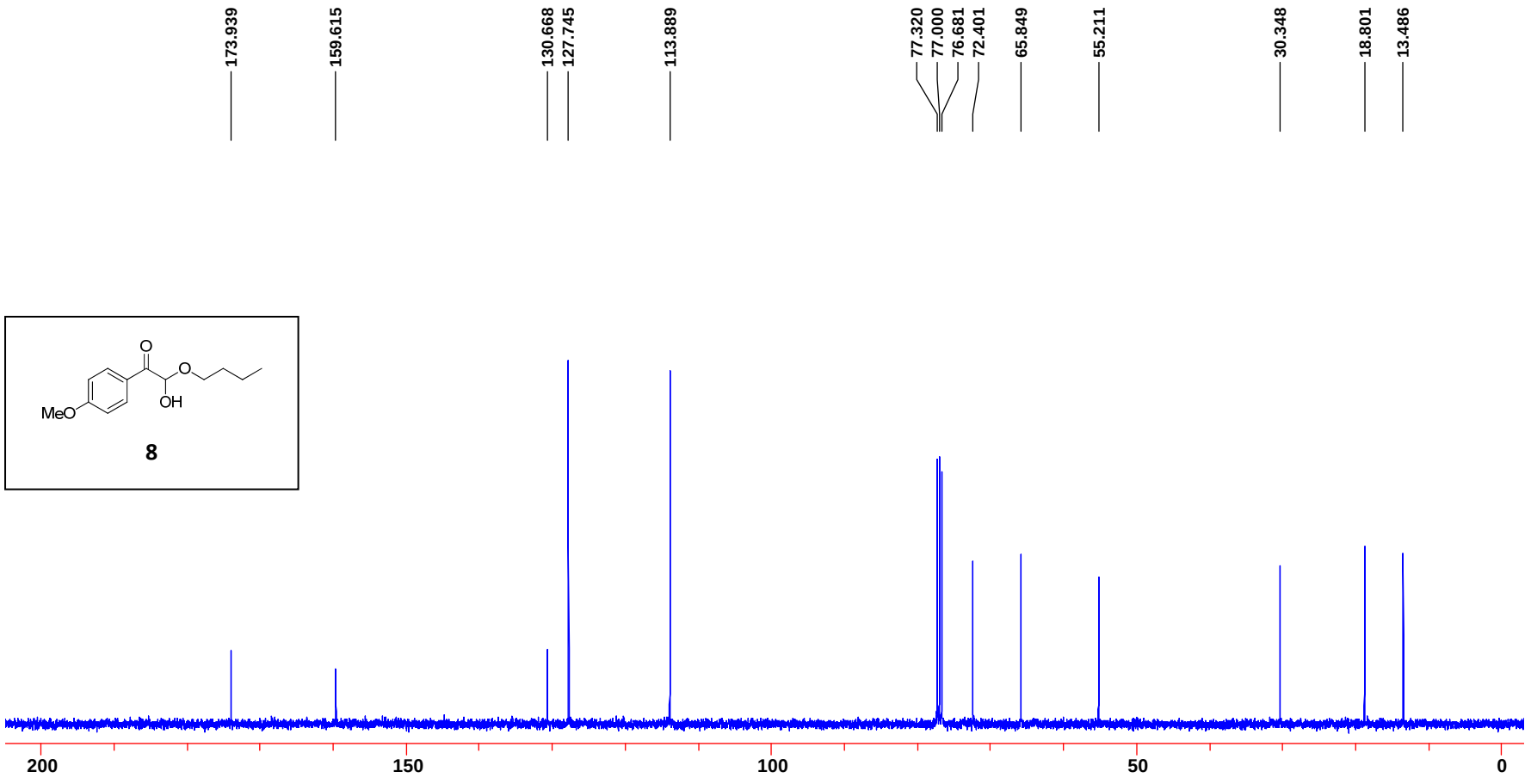
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