Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

1. Supplementary data.

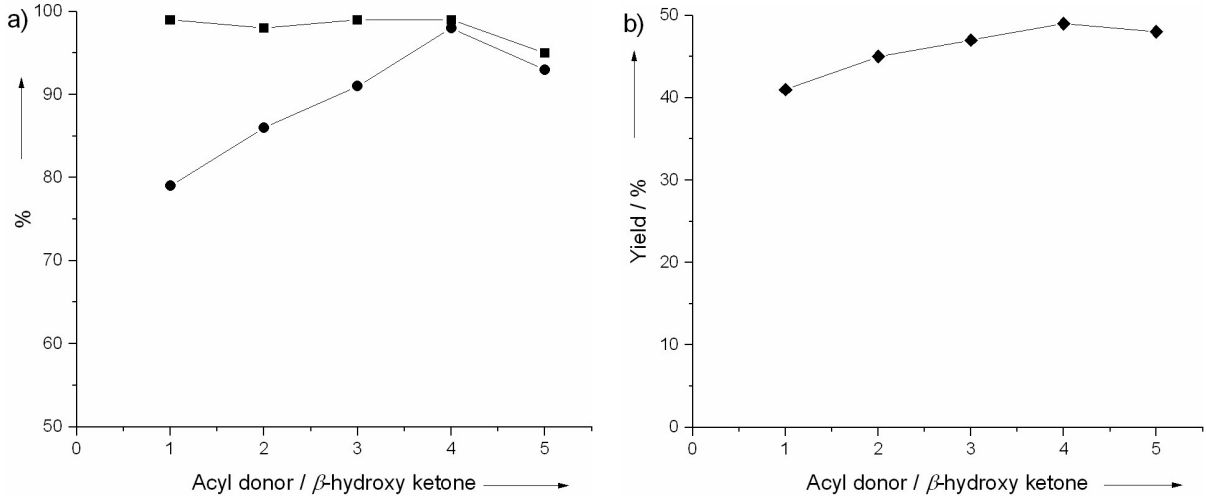


Figure S1. The influence of molar ratio of acyl donor (isopropenyl acetate) on CAL-B catalysed kinetic resolution of β-hydroxy ketone (**3a)**. ee of **3a'** (●), ee of **4a** (■), yield of **4a** (◆). Reaction condition: 0.4 mmol racemic **3a**, 40 mg CAL-B, 2 ml diisopropyl ether, 37°C, 3 d.

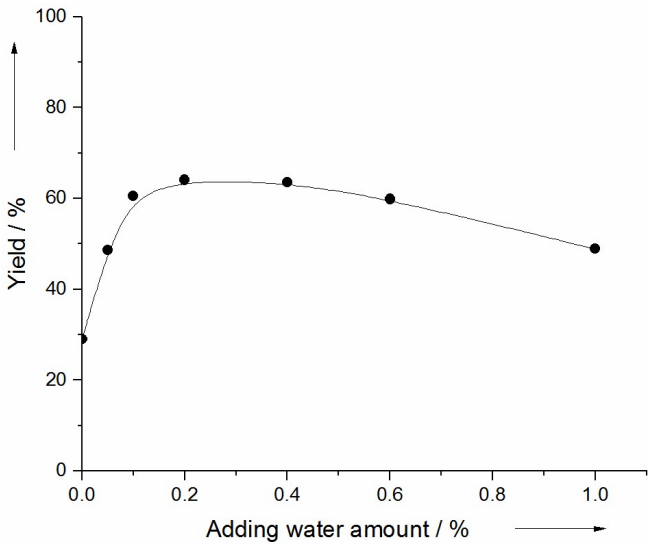


Figure S2. The influence of adding water amount on the CAL-B catalyzed decarboxylative aldol reaction. Reaction condition: 0.4 mmol 4-nitrobenzaldehyde, 0.8 mmol ethyl acetoacetate, 40 mg CAL-B, 2 mL diisopropyl ether, 37^{o}C, 3 d.

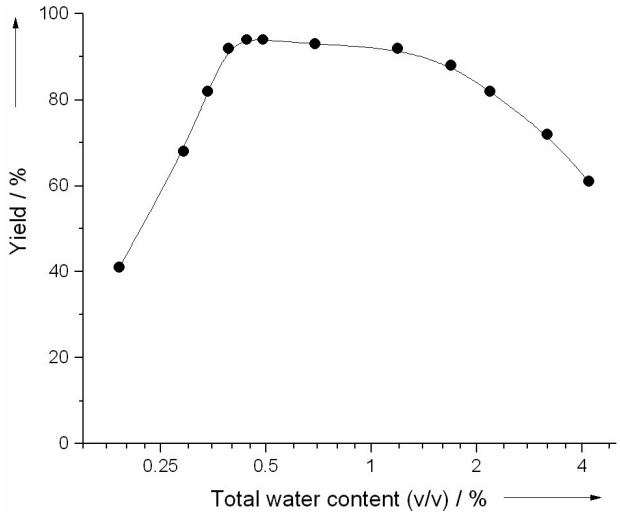


Figure S3. The influence of total water content (v/v) on MML catalysed decarboxylative aldol reaction. Reaction condition: 0.4 mmol 4-nitrobenzaldehyde, 0.8 mmol ethyl acetoacetate, 40 mg MML, 2 mL diisopropyl ether, 37^{o}C, 3 d.

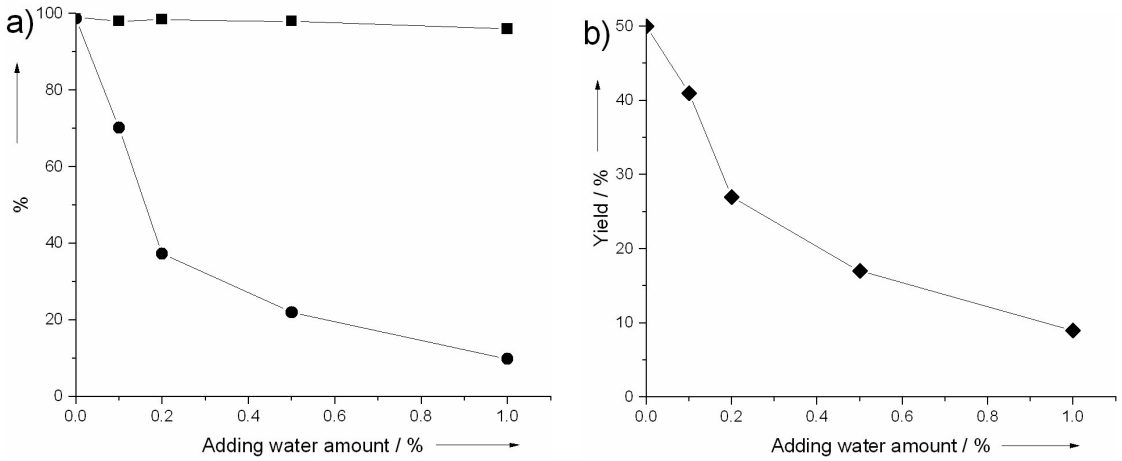


Figure S4. The influence of the adding water amount on CAL-B catalyzed kinetic resolution of *β*-hydroxy ketone (**3a)**. ee of **3a'** (●), ee of **4a** (■), yield of **4a** (◆). Reaction condition: 0.4 mmol racemic *β*-hydroxy ketone , 1.6 mmol isopropenyl acetate, 40 mg CAL-B, 2 ml diisopropyl ether, 37°C, 3 d.

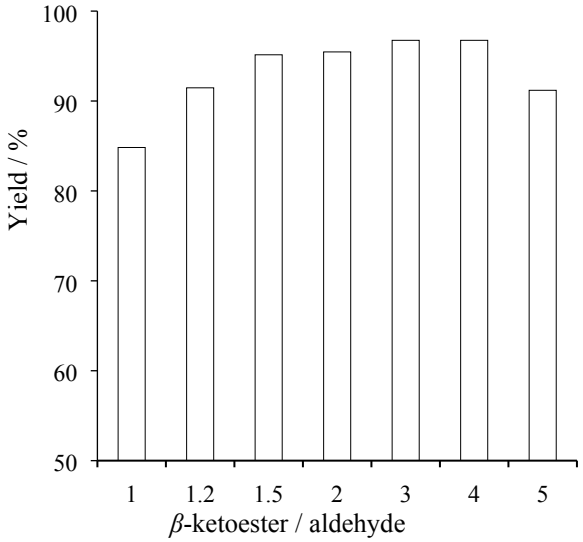


Figure S5. The influence of molar ratio of *β*-ketoester (ethyl acetoacetate) on the MML catalyzed decarboxylative aldol reaction. Reaction condition: 0.4 mmol 4-nitrobenzaldehyde, 40 mg CAL-B, 2 mL diisopropyl ether, 37°C, 3 d.

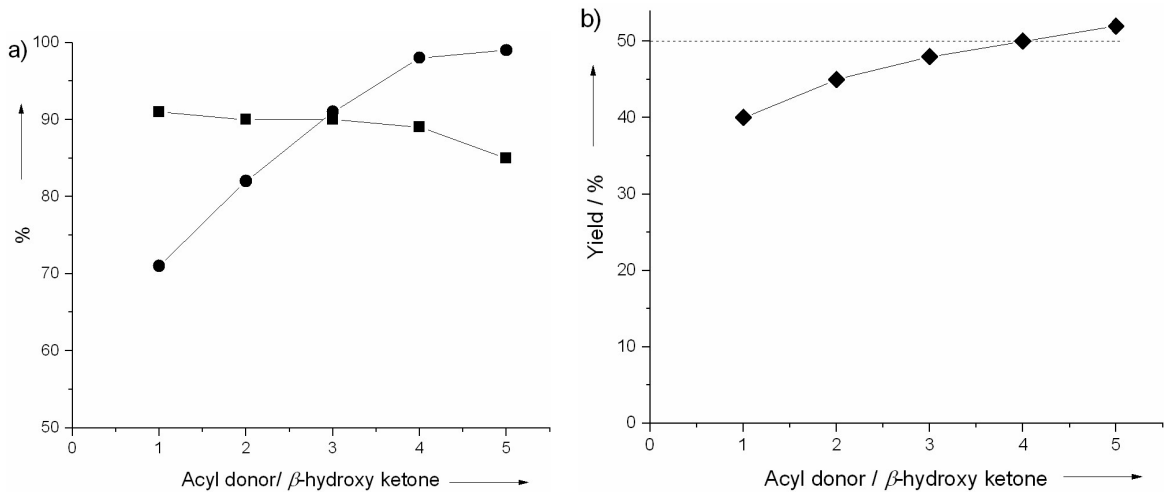


Figure S6. The influence of molar ratio of acyl donor (isopropenyl acetate) on kinetic resolution of *β*-hydroxy ketone (**3g)**. ee of **3g'** (●), ee of **4g** (■), yield of **4g** (◆). Reaction condition: 0.4 mmol racemic**3g**, 40 mg CAL-A, 2 ml toluene, 37°C, 2 d.

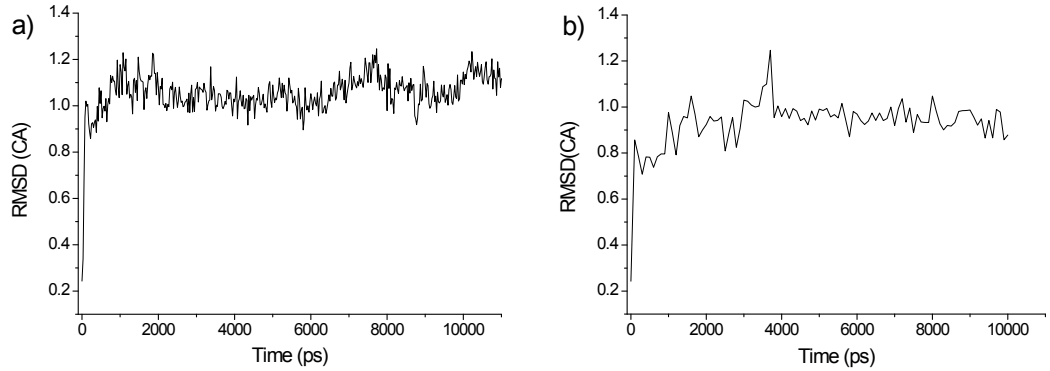
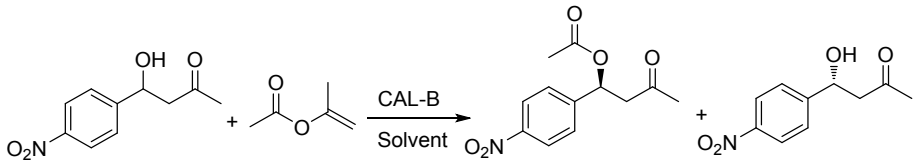


Figure S7. RMSD of CA backbone of CAL-B covalently bound by (*R*)-**4a** (a) and (*S*)-**4a** (b), respectively, during the MD simulation process (10ns).

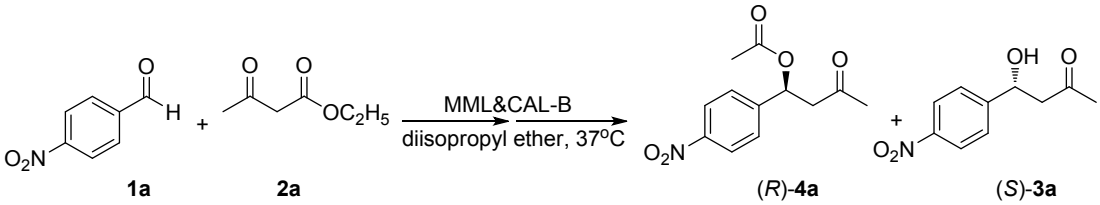
Table S1. CAL-B catalysed kinetic resolution of β-hydroxy ketone (**3a**) in different solvents.[a]



Entry	Solvent	ee of **3a'** / %[b]	Yield of **3a'** / %[b]	ee of **4a** / %[b]	Yield of **4a** / %[b]
1	diisopropyl ether	99	50	99	49
2	TBME	86	53	99	45
3	toluene	46	68	99	30
4	isooctane	26	79	99	20
5	acetone	12	88	96	8
6	THF	8	92	-	5
7	isopropenyl acetate	5	95	-	4
8	acetonitrile	<1	99	-	n.d.[c]
9	DMF	<1	99	-	n.d.[c]
10	DMSO	<1	99	-	n.d.[c]

[a] Reaction conditions: 0.4 mmol racemic β-hydroxy ketone **3a**, 40 mg CAL-B, 2 mmol isopropenyl acetate, 2 ml solvent, 37°C, 72 h; [b] Determined by chiral HPLC analysis using AD-H column; [c] n.d. means not detected.

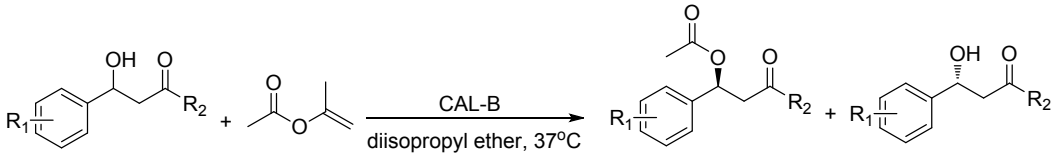
Table S2. The influence of water content on MML&CAL-B catalyzed one pot cascade [a]



Entry	Adding water amount / %	Total water content / %	ee of **3a** / %[b]	Yield of **3a** / %[b]	ee of **4a** / %[b]	Yield of **4a** / %[b]
1	0.00	0.19	93	33	99	30
2	0.10	0.29	97	41	98	40
3	0.20	0.39	98	48	99	47
4	0.30	0.49	72	58	98	37
5	0.40	0.59	38	70	98	22

[a] Reaction conditions: 0.4 mmol aldehyde, 0.6 mmol *β*-ketoester, 40 mg CAL-B, 40 mg MML, 2 mL diisopropyl ether, 37°C, 3 d; after completion of decarboxylative aldol reaction, adding 1.6 mmol isopropenyl acetate into the reaction mixture, 3 d; [b] Determined by chiral HPLC analysis.

Table S3. CAL-B catalyzed kinetic resolution of *β*-hydroxy ketones[a]

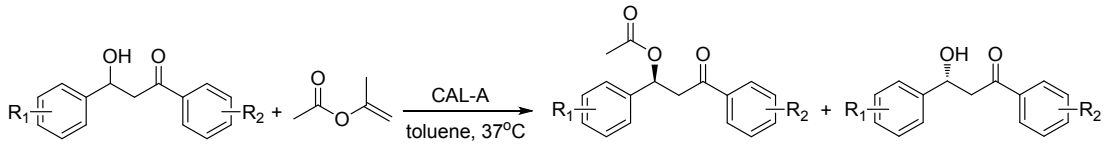


(*R,S*)-**3** (*R*)-**4** (*S*)-**3'**

Entry	R_1	R_2	Time / d	ee of **3**' / %[b]	Yield of **3**' / %[b]	ee of **4** / %[b]	Yield of **4** / %[b]
1	*p*-NO_2	CH_3	3	99	50	99	49
2	*m*-NO_2	CH_3	3	99	50	98	43
3	*p*-CF_3	CH_3	3	98	50	99	48
4	*p*-CN	CH_3	3	94	51	95	45
5	*p*-NO_2	*n*-C_3H_7	7	90	54	98	42
6	*p*-NO_2	*c*-C_3H_5	3	98	49	96	48

[a] Reaction conditions: 0.4 mmol racemic *β*-hydroxy ketone, 40 mg CAL-B, 1.6 mmol isopropenyl acetate, 2 mL diisopropyl ether, 37°C; [b] Determined by chiral HPLC analysis.

Table S4. CAL-A catalyzed kinetic resolution of 1,3-biphenyl *β*-hydroxy ketones[a]



(*R,S*)-**3** (*R*)-**4** (*S*)-**3'**

Entry	R_1	R_2	Time / d	ee of **3**' / %[b]	Yield of **3**' / %[b]	ee of **4** / %[b]	Yield of **4** / %[b]
1	*p*-NO_2	H	2	99	46	90	52
2	*p*-CF_3	H	2	99	48	95	50
3	*p*-CF_3	*p*-Cl	2	99	47	92	52
4	*p*-CF_3	*p*-CH_3	2	99	48	94	51
5	*p*-CF_3	*p*-OCH_3	2	99	48	94	50
6	*p*-CF_3	*m*-OCH_3	7	98	51	89	47

[a] Reaction conditions: 0.4 mmol racemic *β*-hydroxy ketone, 40 mg CAL-A, 1.6 mmol isopropenyl acetate, 2 mL toluene, 37°C; [b] Determined by chiral HPLC analysis.

2. Synthesis of compounds

2.1 Synthesis of racemic β-hydroxy ketones

Aldehyde (10 mmol) and β-ketoester (15 mmol) was dissolved into diisopropyl ether (50 mL) in a 250 mL Erlenmeyer flask. 100 μL H_2O was added into the reaction mixture, which was then shaken at 200 rpm under 37°C for 0.5 h. After that, MML (1.0 g) was added into the reaction mixture. The decarboxylative aldol reaction was carried out at 200 rpm under 37°C for 3 d. The reaction mixture was then concentrated and subjected to a silicon column chromatography for purification. The eluent was hexane:ethyl acetate = 3:1.

2.2 Synthesis of racemic acylated β-hydroxy ketone derivatives

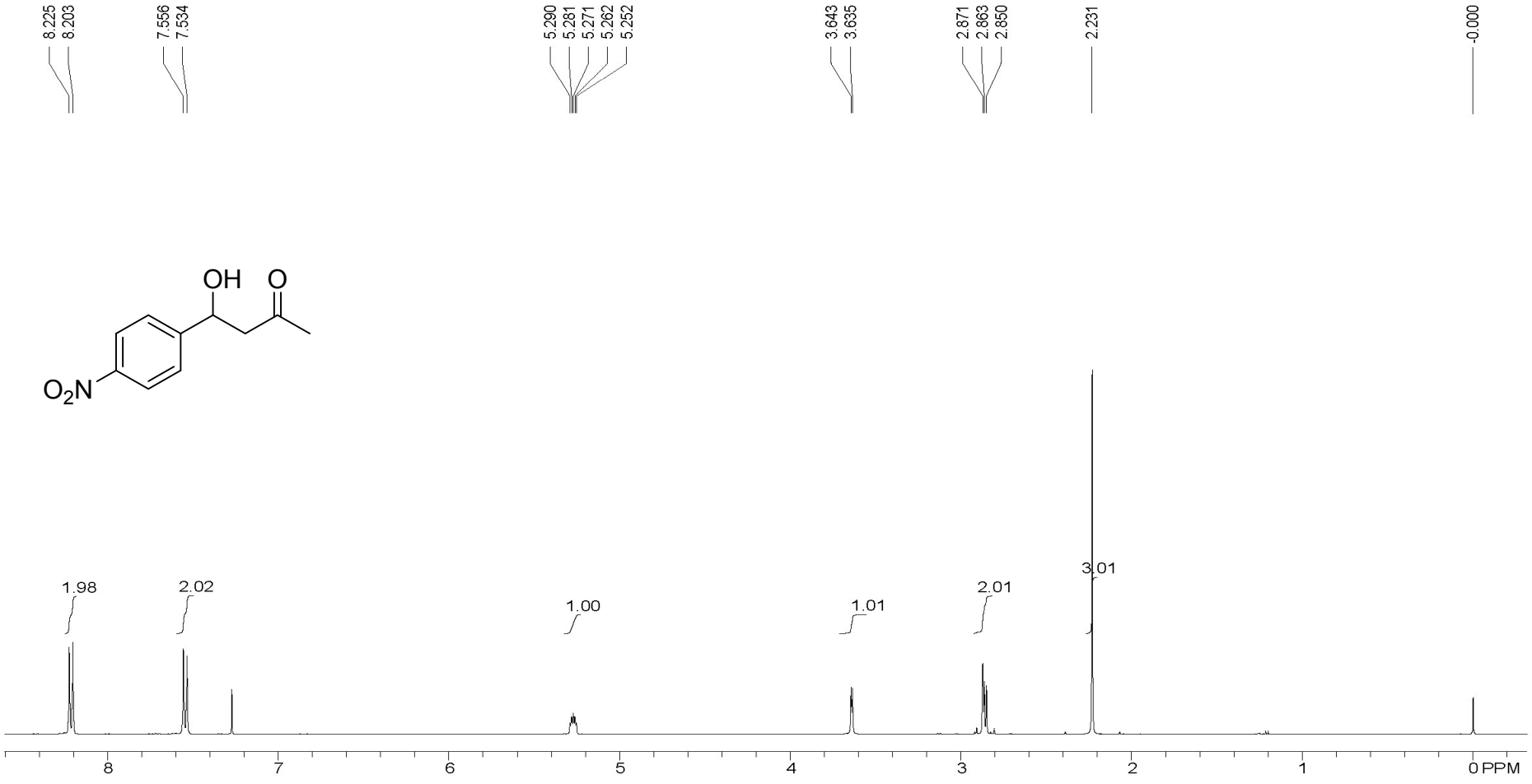
Racemic β-hydroxy ketone (0.5 mmol) and acetyl chloride (1.0 mmol) were dissolved in dichloromethane (5 mL) in a round-bottomed flask. The mixture was stirred magnetically and cooled to 0°C by an ice-water bath. Then pyridine (0.6 mmol) was added dropwise under stirring. The mixture was then heated to 25°C and reacted for 1-2 h. After that, the organic phase was washed with 2 M HCl, saturated $NaHCO_3$ and water sequentially and then dried over anhydrous magnesium sulfate. After filtration, the dichloromethane was evaporated in vacuum. The product was obtained in quantitative yield without further purification.

2.3 Synthesis of aromatic β-ketoesters

To a dried three-necked flask equipped with a dropping funnel, a condenser, and a magnetic stirrer was added NaH (280 mmol), diethyl carbonate (200 mmol), and toluene (100 mL). The mixture was heated to reflux. A solution of aromatic ketone (100 mmol) in toluene (50 mL) was added dropwise from the dropping funnel over 1-2 h. After the addition, the mixture was heated to reflux until the evolution of hydrogen ceased (15-20 min). After the reaction was cooled to room temperature, glacial acetic acid (30 mL) was added dropwise and a heavy, pasty solid was formed. Ice-water was added until the solid was dissolved completely. The toluene layer was separated, and the water layer was extracted with EtOAc (3×100 mL). The combined organic solution was washed with water (100 mL) and brine (100 mL), then dried over Na_2SO_4. After evaporation of the solvent, the mixture was subjected to a silicon chromatography. The eluent was hexane:ethyl acetate = 20 : 1 ~ 10 : 1.

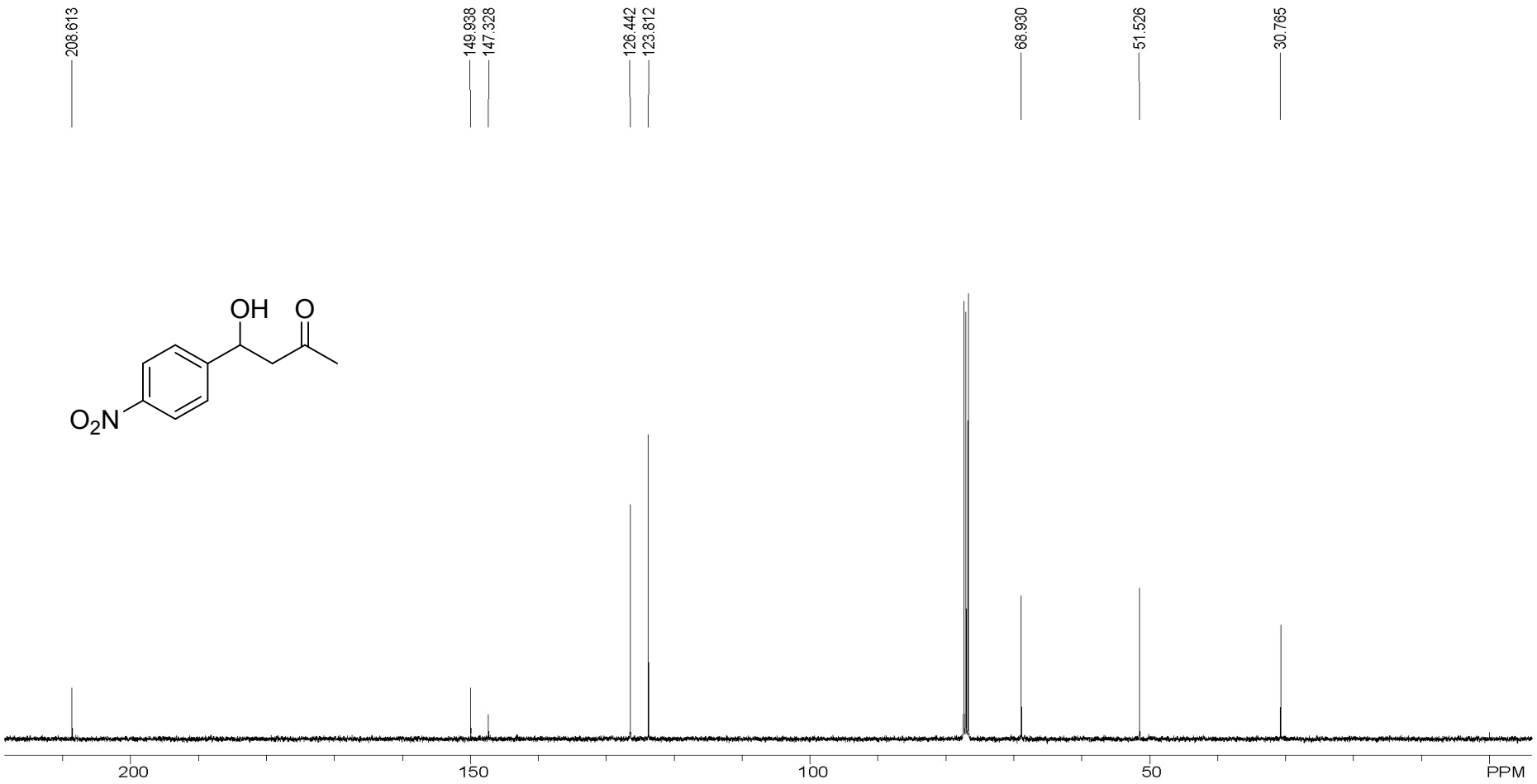
3. NMR spectra of β-hydroxy ketones

4-hydroxy-4-(4-nitrophenyl)butan-2-one (3a)



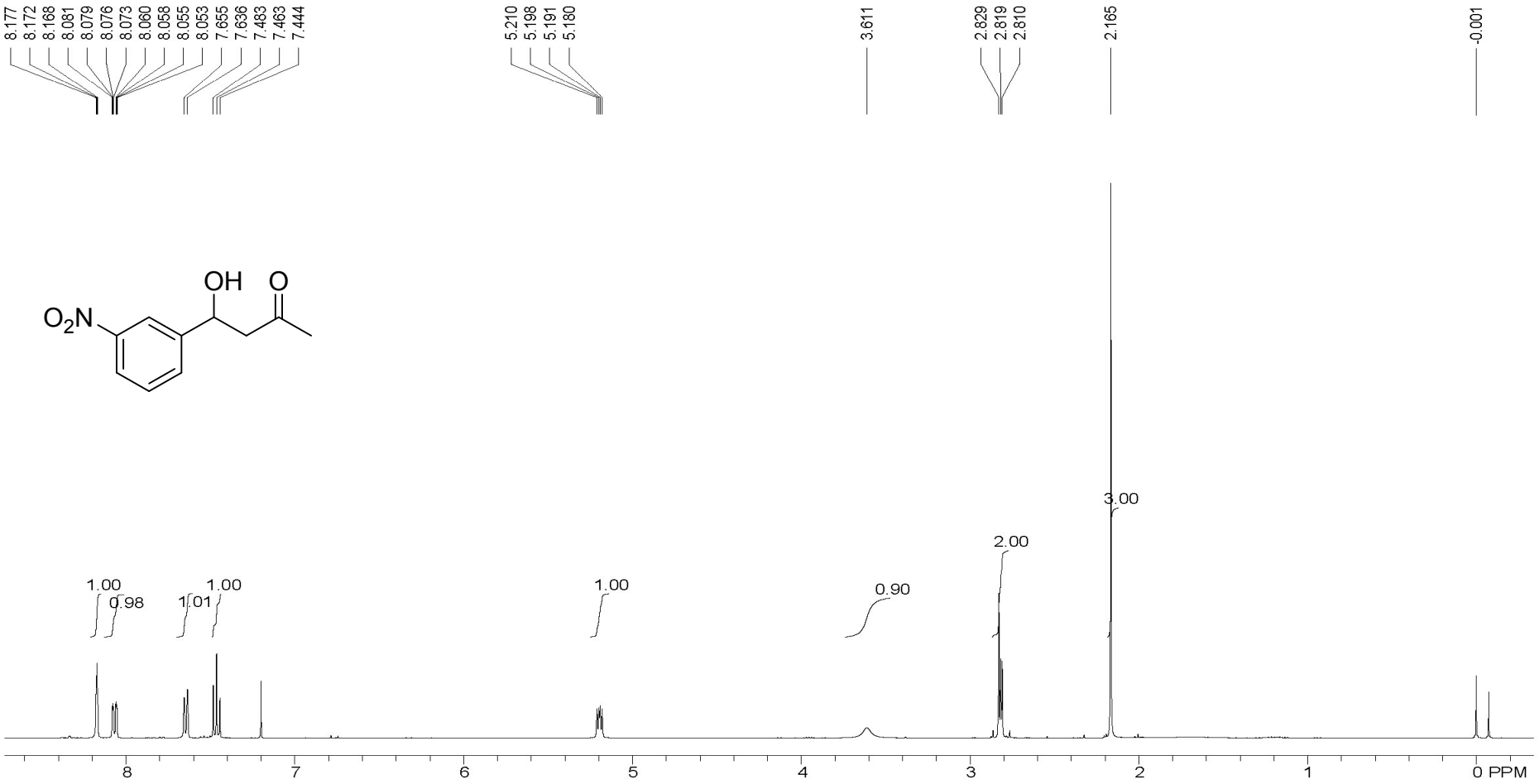
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.22-7.53 (m, 4H), 5.28 (m, 1H), 3.64 (d, *J* = 3.2 Hz, 1H), 2.87-2.85 (m, 2H), 2.23 (s, 3H) ppm.

4-hydroxy-4-(4-nitrophenyl)butan-2-one (3a)



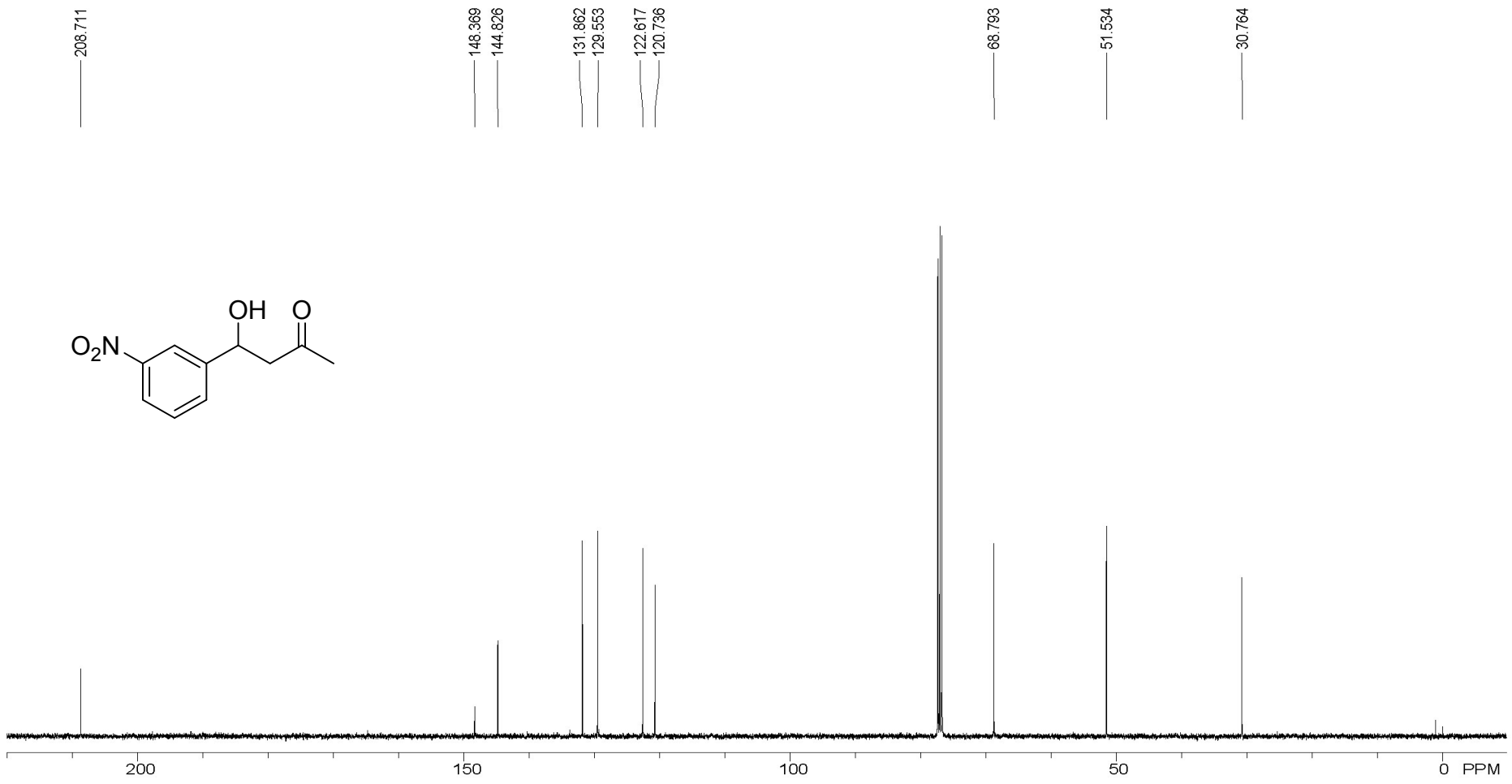
^{13}C NMR (400 MHz, $CDCl_3$) δ = 208.6, 149.9, 147.3, 126.4, 123.8, 68.9, 51.5, 30.8 ppm.

4-hydroxy-4-(3-nitrophenyl)butan-2-one (3b)



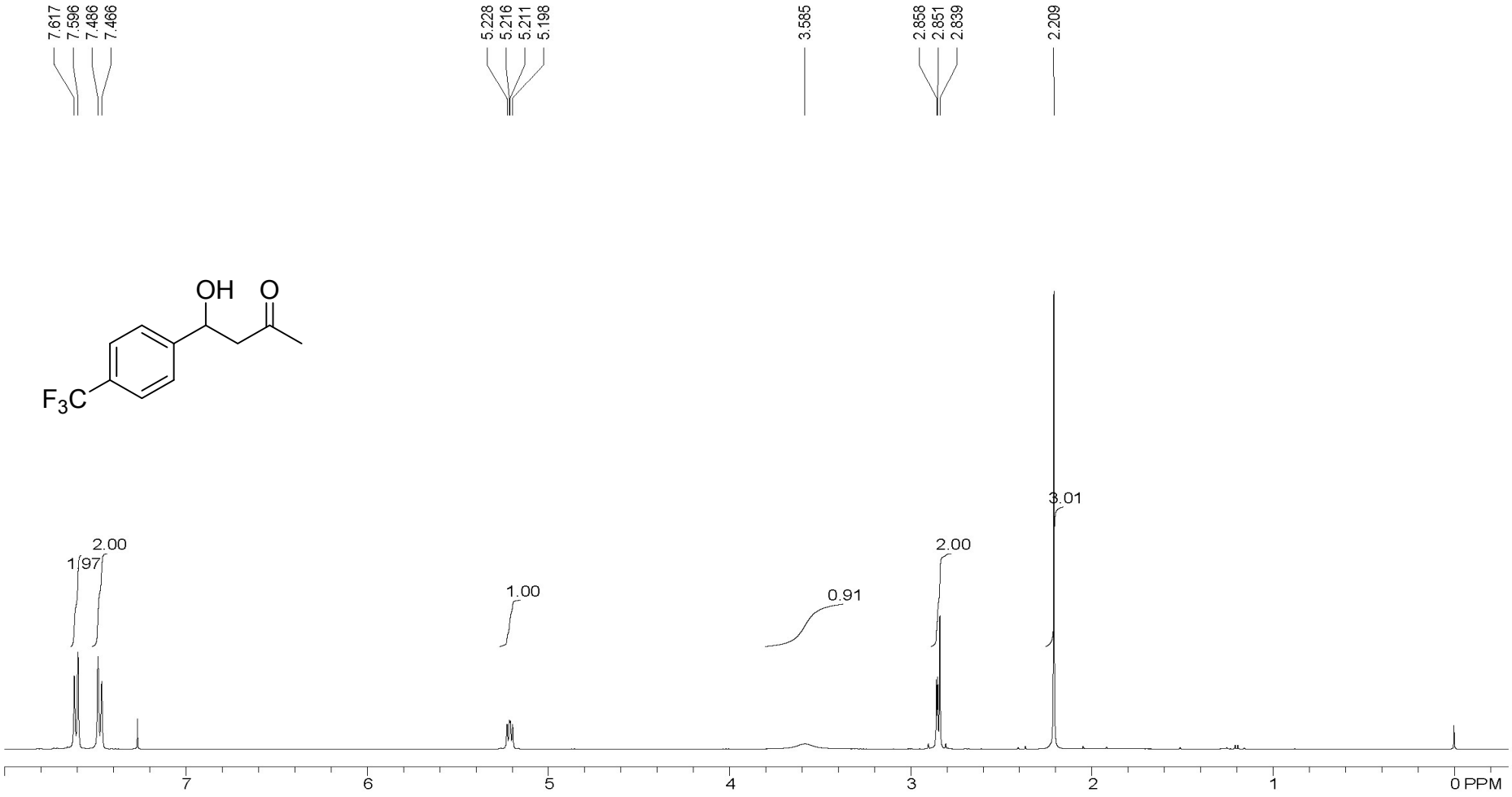
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.17-7.44 (m, 4H), 5.19 (dd, *J* = 4.8 Hz, *J* = 7.5 Hz, 1H), 3.61 (br, 1H), 2.83-2.81 (m, 2H), 2.17 (s, 3H) ppm.

4-hydroxy-4-(3-nitrophenyl)butan-2-one (3b)



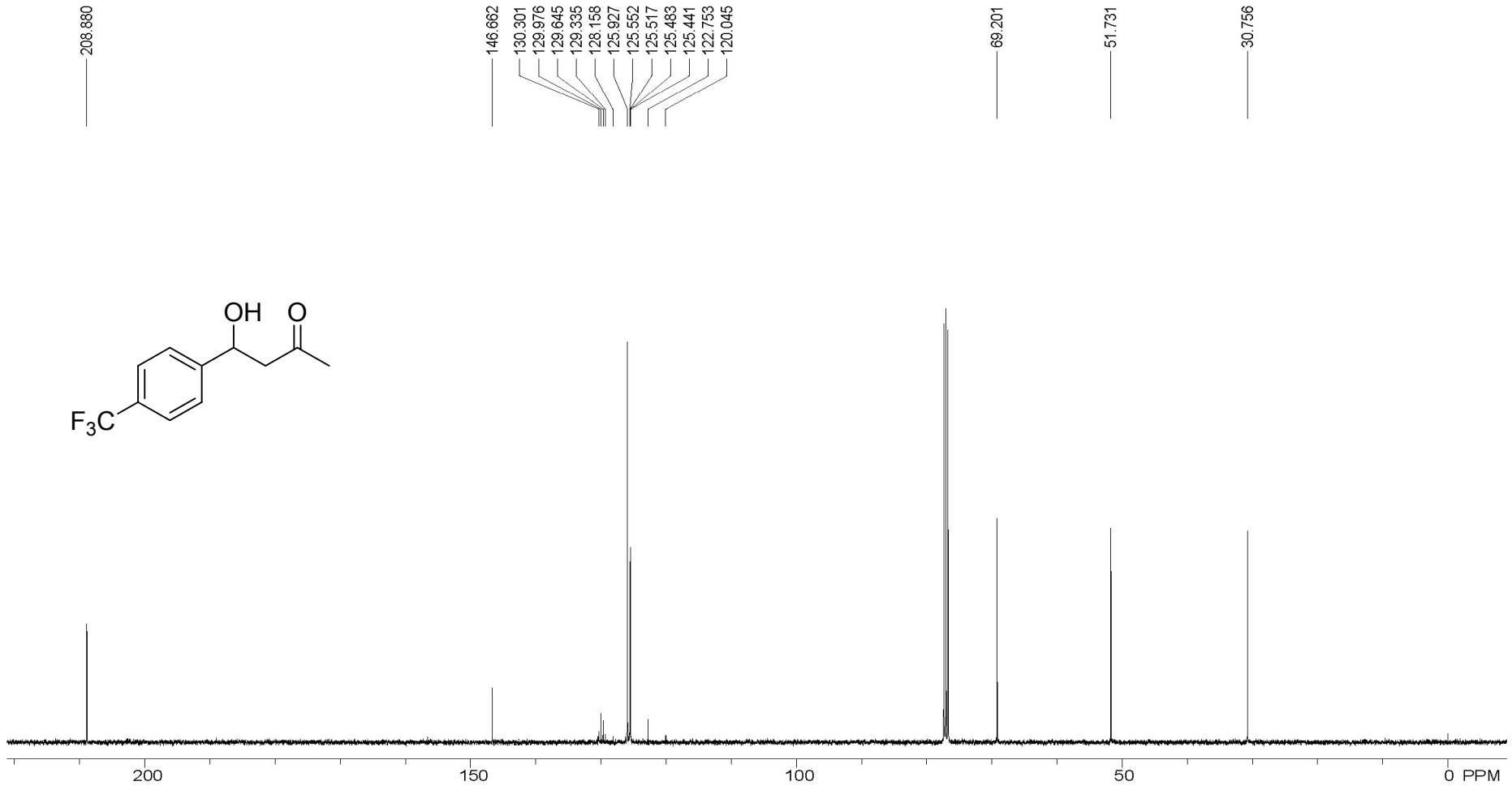
^{13}C NMR (400 MHz, $CDCl_3$) δ = 208.7, 148.4, 144.8, 131.9, 129.6, 122.6, 120.7, 68.8, 51.5, 30.8 ppm.

4-hydroxy-4-[4-(trifluoromethyl)phenyl]butan-2-one (3c)



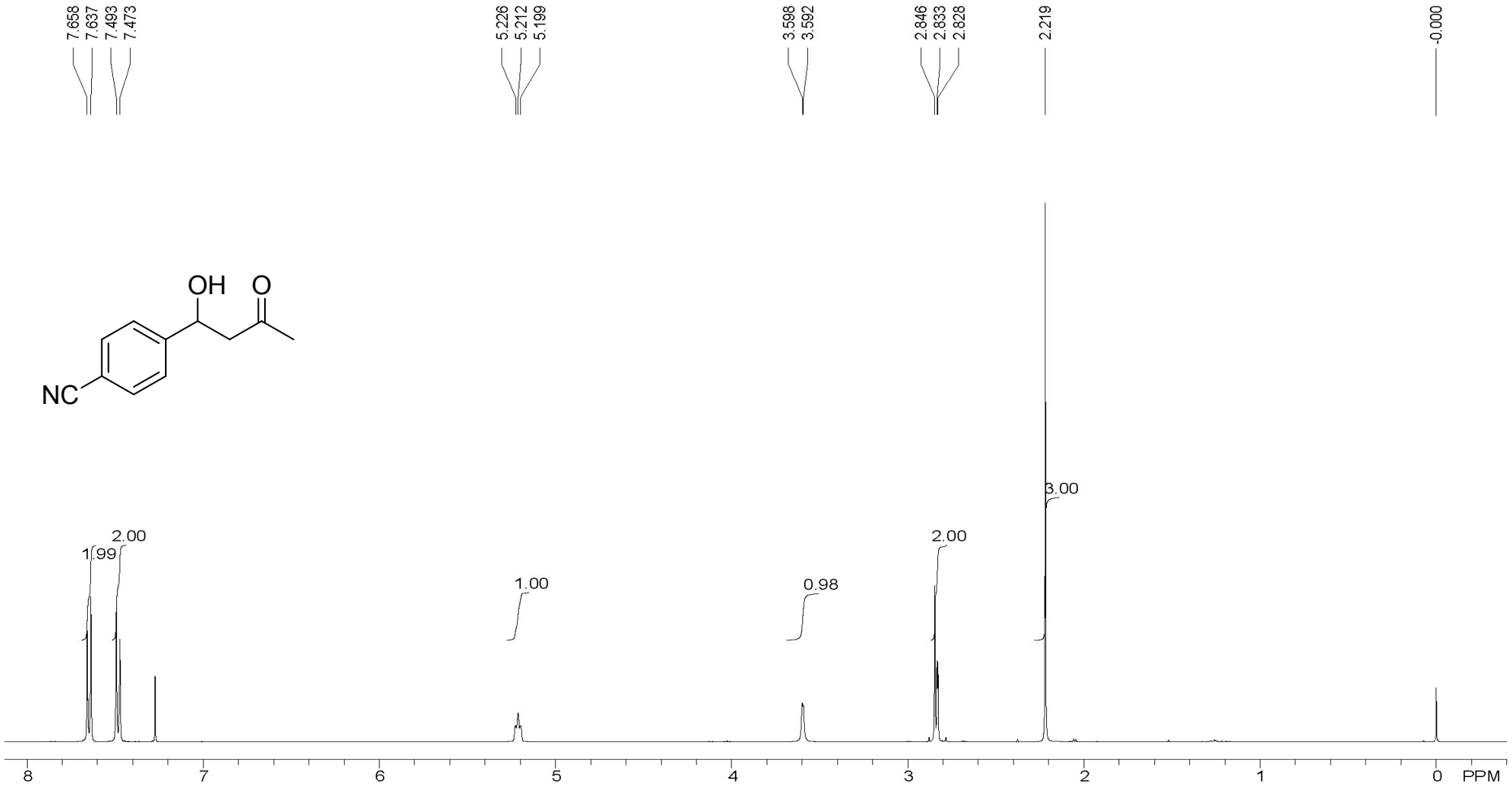
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.62-7.47 (m, 4H), 5.21 (dd, *J* = 5.1 Hz, *J* = 7.1 Hz, 1H), 3.59 (br, 1H), 2.86-2.84 (m, 2H), 2.21 (s, 3H) ppm.

4-hydroxy-4-[4-(trifluoromethyl)phenyl]butan-2-one (3c)



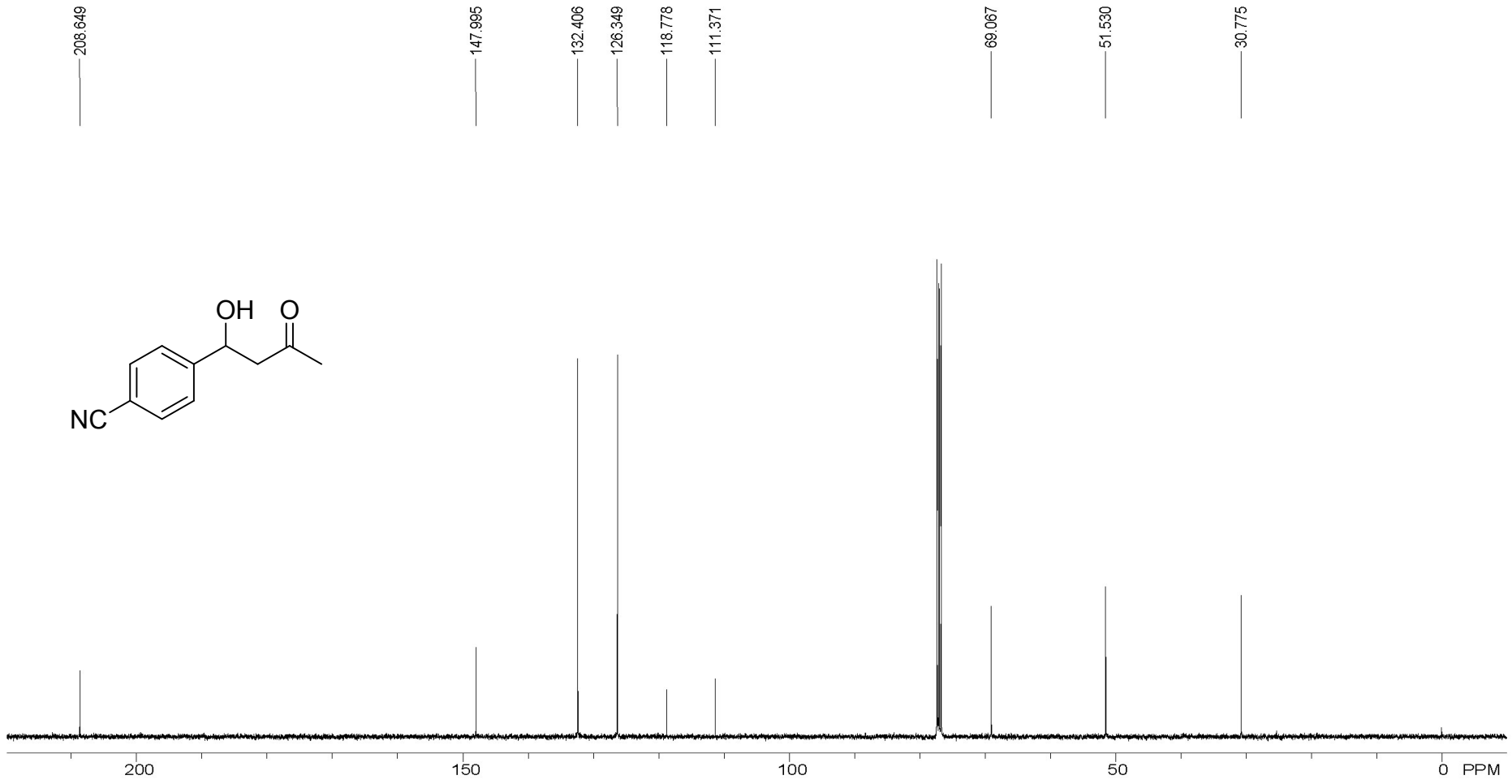
^{13}C NMR (400 MHz, $CDCl_3$) δ = 208.9, 146.7, 129.8 (q, *J* = 32.4 Hz), 125.9, 125.5 (q, *J* = 3.73 Hz), 124.1 (q, *J* = 272.2 Hz), 69.2, 51.7, 30.8 ppm.

4-(4-cyanophenyl)-4-hydroxybutan-2-one (3d)



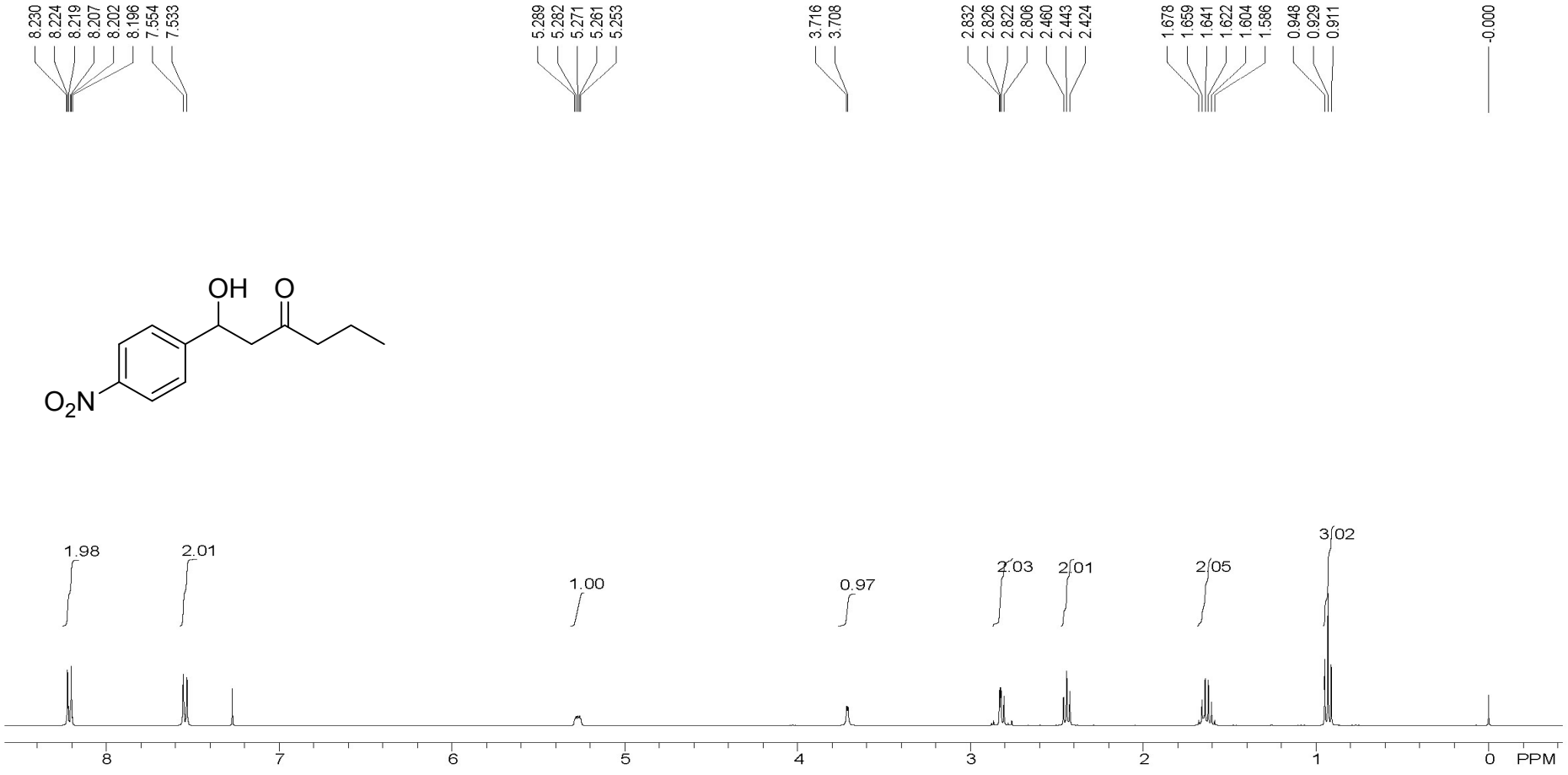
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.66-7.47 (m, 4H), 5.21 (t, *J* = 5.3 Hz, 1H), 3.60 (d, *J* = 2.5 Hz, 1H), 2.85-2.83 (m, 2H), 2.22 (s, 3H) ppm.

4-(4-cyanophenyl)-4-hydroxybutan-2-one (3d)



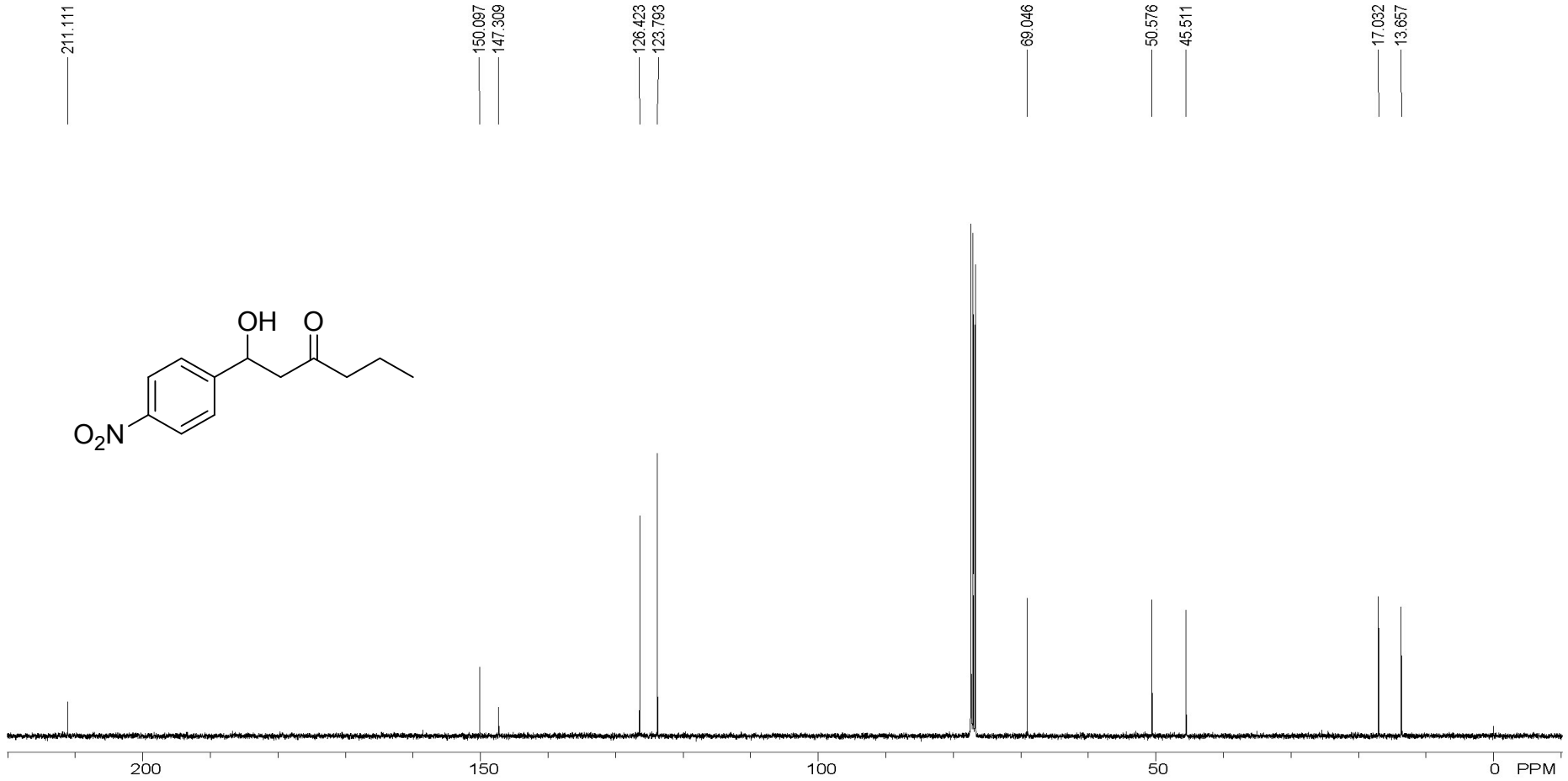
^{13}C NMR (400 MHz, $CDCl_3$) δ = 208.6, 148.0, 132.4, 126.3, 118.8, 111.4, 69.1, 51.5, 30.8 ppm.

1-hydroxy-1-(4-nitrophenyl)hexan-3-one (3e)



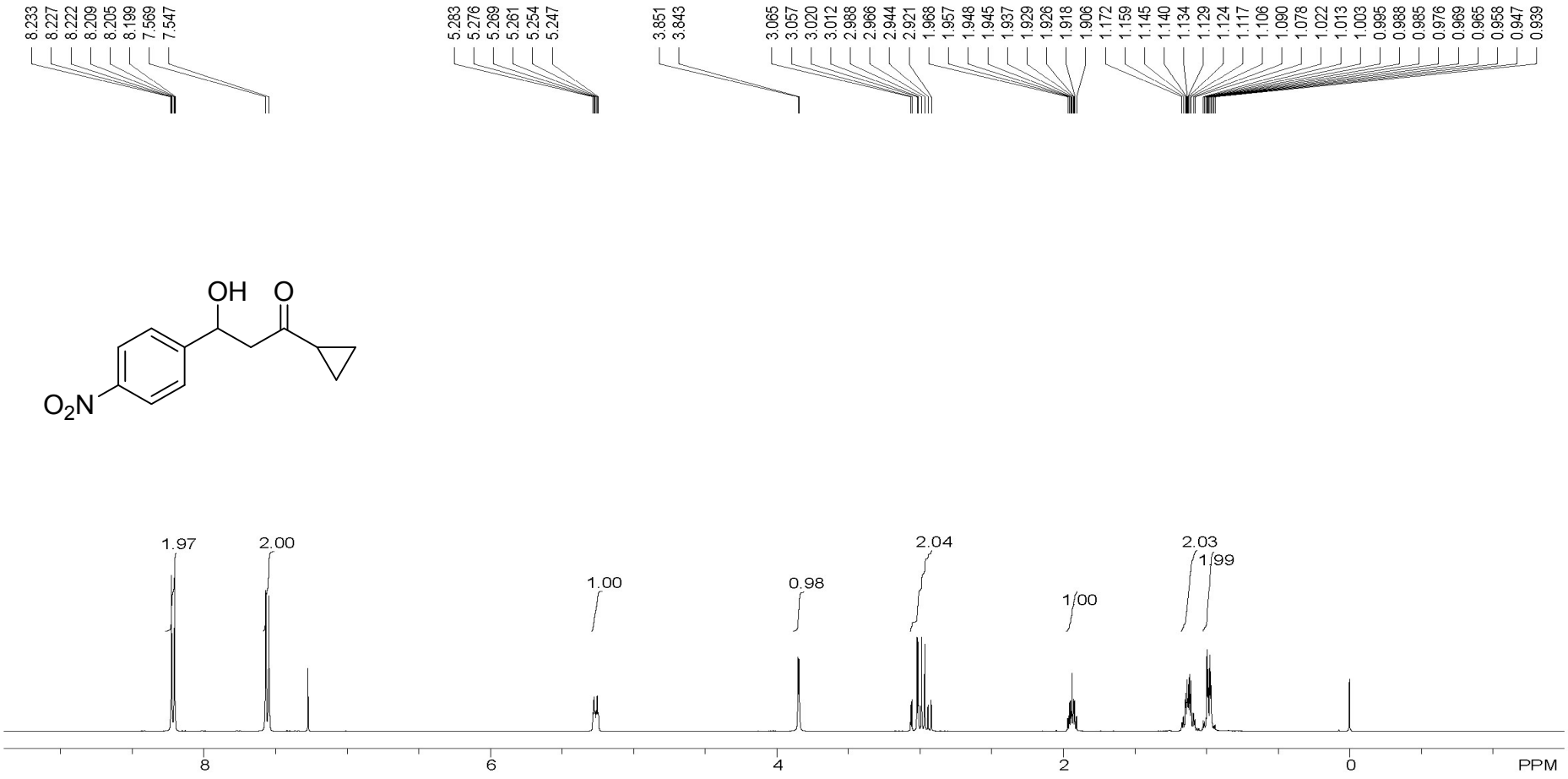
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.23-7.53 (m, 4H), 5.27 (m, 1H), 3.71 (d, *J* = 3.0 Hz, 1H), 2.83-2.81 (m, 2H), 2.44 (t, *J* = 7.3 Hz, 2H), 1.63 (m, *J* = 7.4 Hz, 2H), 0.93(t, *J* = 7.4 Hz, 3H) ppm.

1-hydroxy-1-(4-nitrophenyl)hexan-3-one (3e)



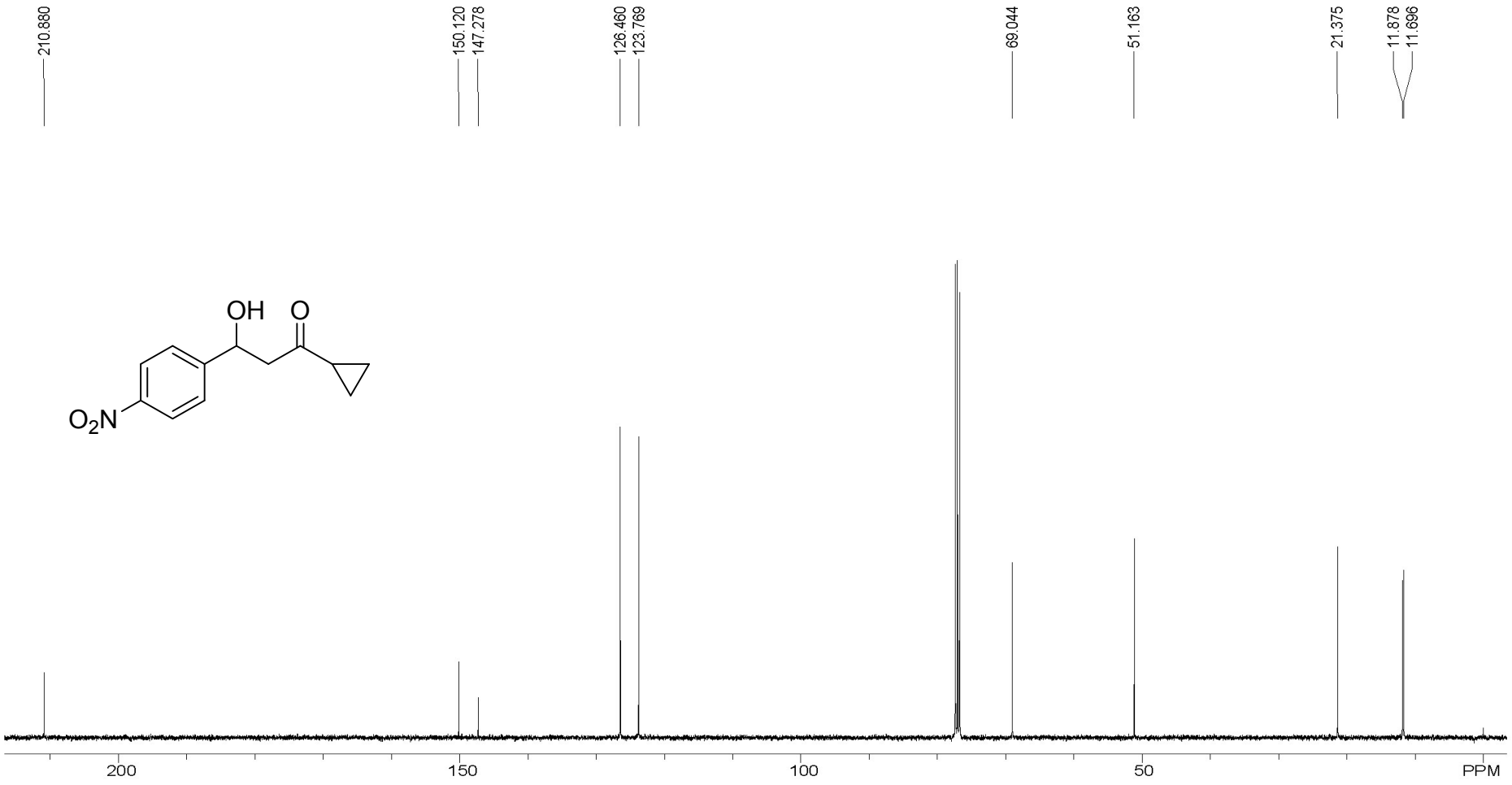
^{13}C NMR (400 MHz, $CDCl_3$) δ = 211.1, 150.1, 147.3, 126.4, 123.8, 69.0, 50.6, 45.5, 17.0, 13.7 ppm.

1-cyclopropyl-3-hydroxy-3-(4-nitrophenyl)propan-1-one (3f)



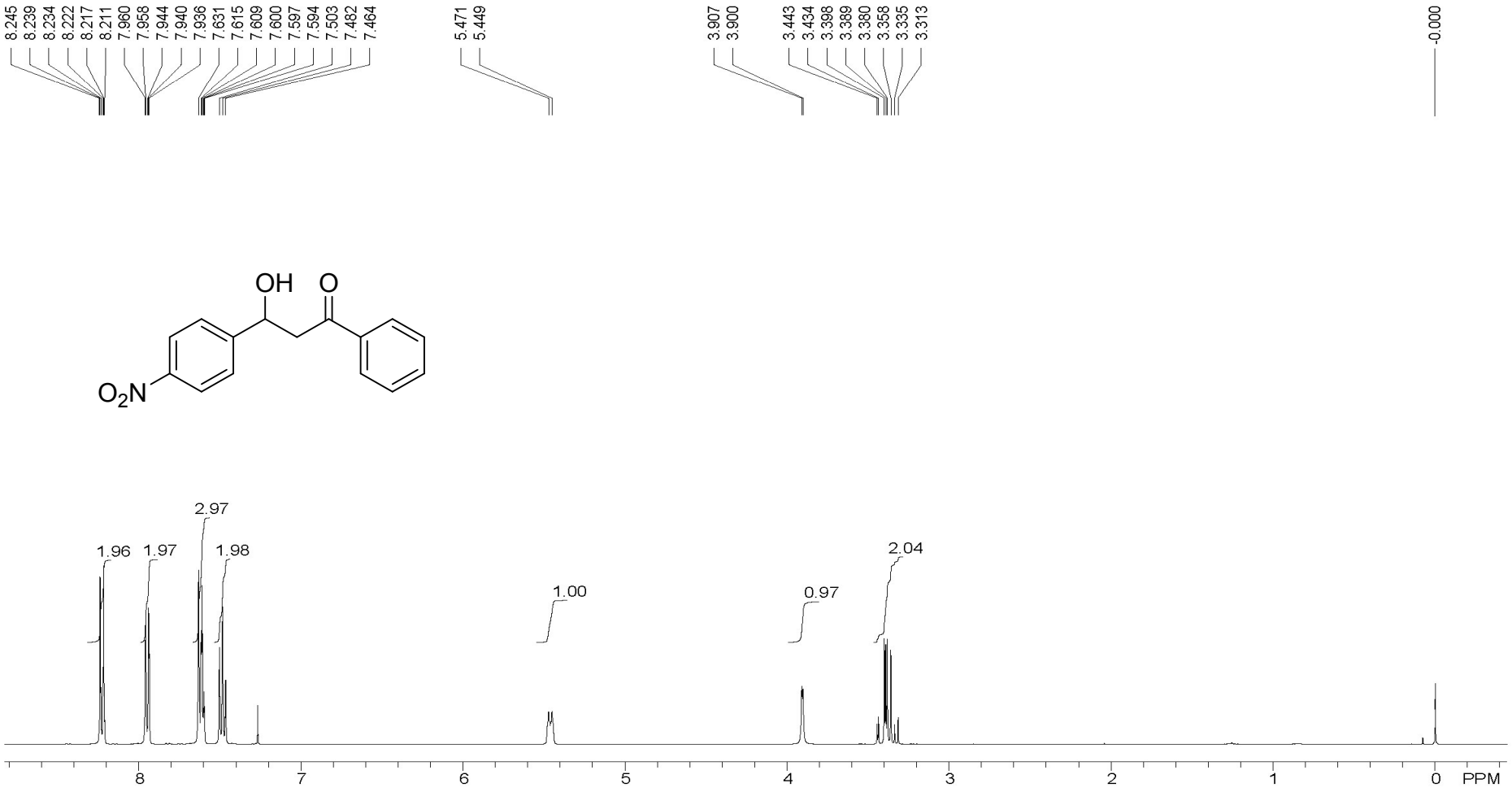
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.23-7.55 (m, 4H), 5.27 (dt, *J* = 3.0 Hz, *J* = 8.9 Hz, 1H), 3.85 (d, *J* = 3.0 Hz, 1H), 3.07-2.92 (m, 2H), 1.97-1.91 (m, 1H), 1.17-1.08 (m, 2H), 1.02-0.94 (m, 2H) ppm.

1-cyclopropyl-3-hydroxy-3-(4-nitrophenyl)propan-1-one (3f)



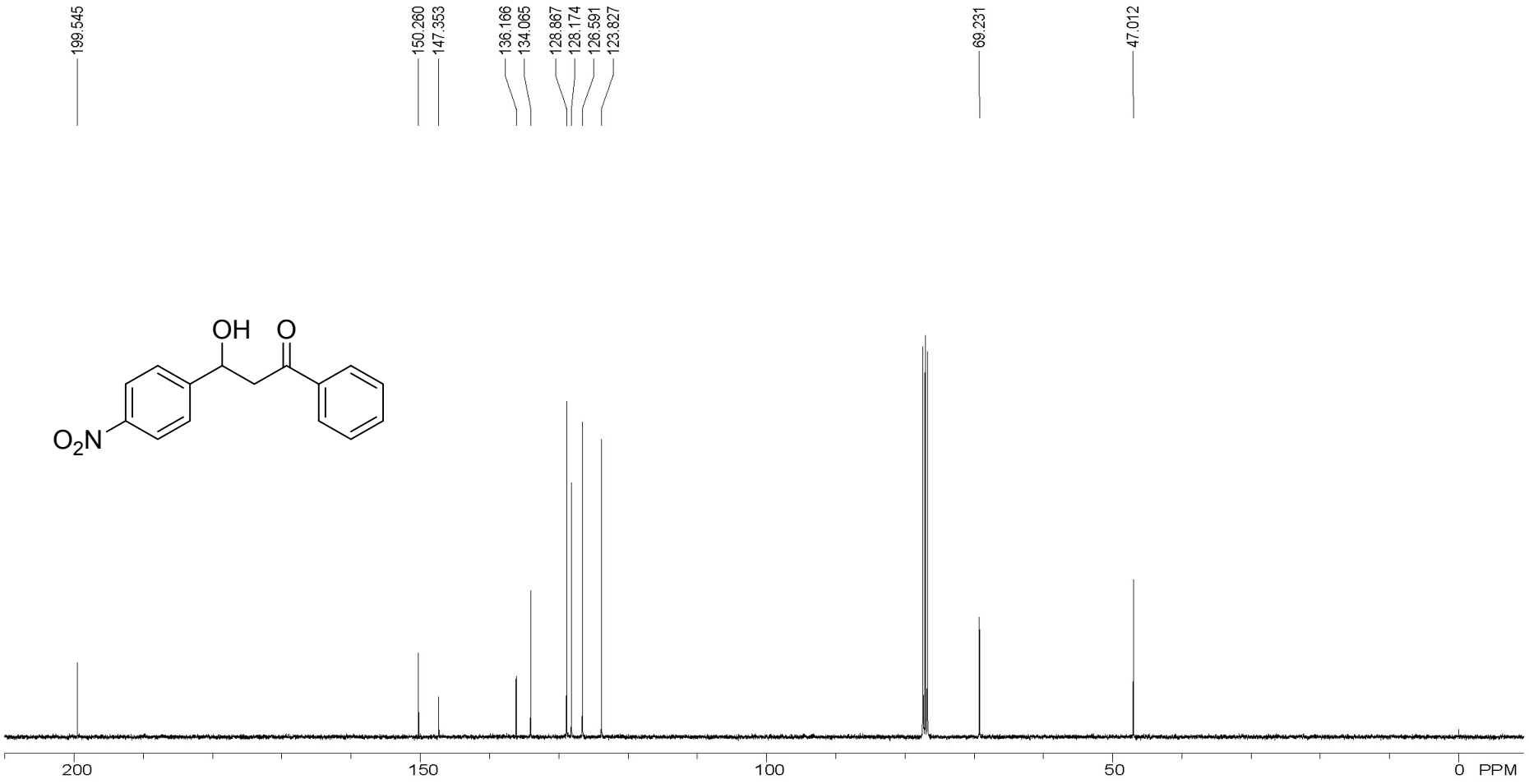
^{13}C NMR (400 MHz, $CDCl_3$) δ = 210.9, 150.1, 147.3, 126.5, 123.8, 69.0, 51.2, 21.4, 11.9, 11.7 ppm.

3-hydroxy-3-(4-nitrophenyl)-1-phenylpropan-1-one (3g)



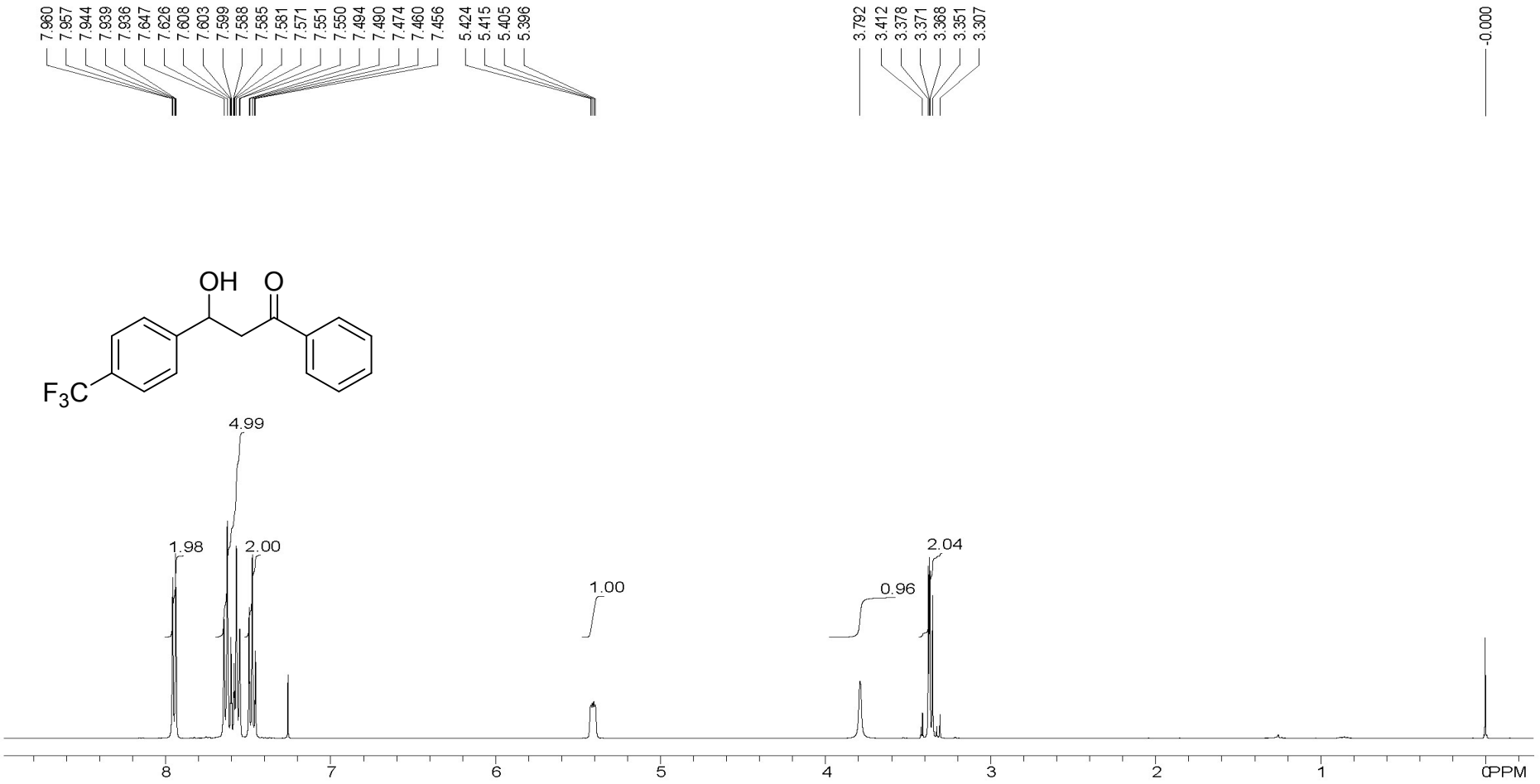
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.25-7.46 (m, 9H), 5.46 (d, *J* = 8.6 Hz, 1H), 3.90 (d, *J* = 2.9 Hz, 1H), 3.44-3.31 (m, 2H) ppm.

3-hydroxy-3-(4-nitrophenyl)-1-phenylpropan-1-one (3g)



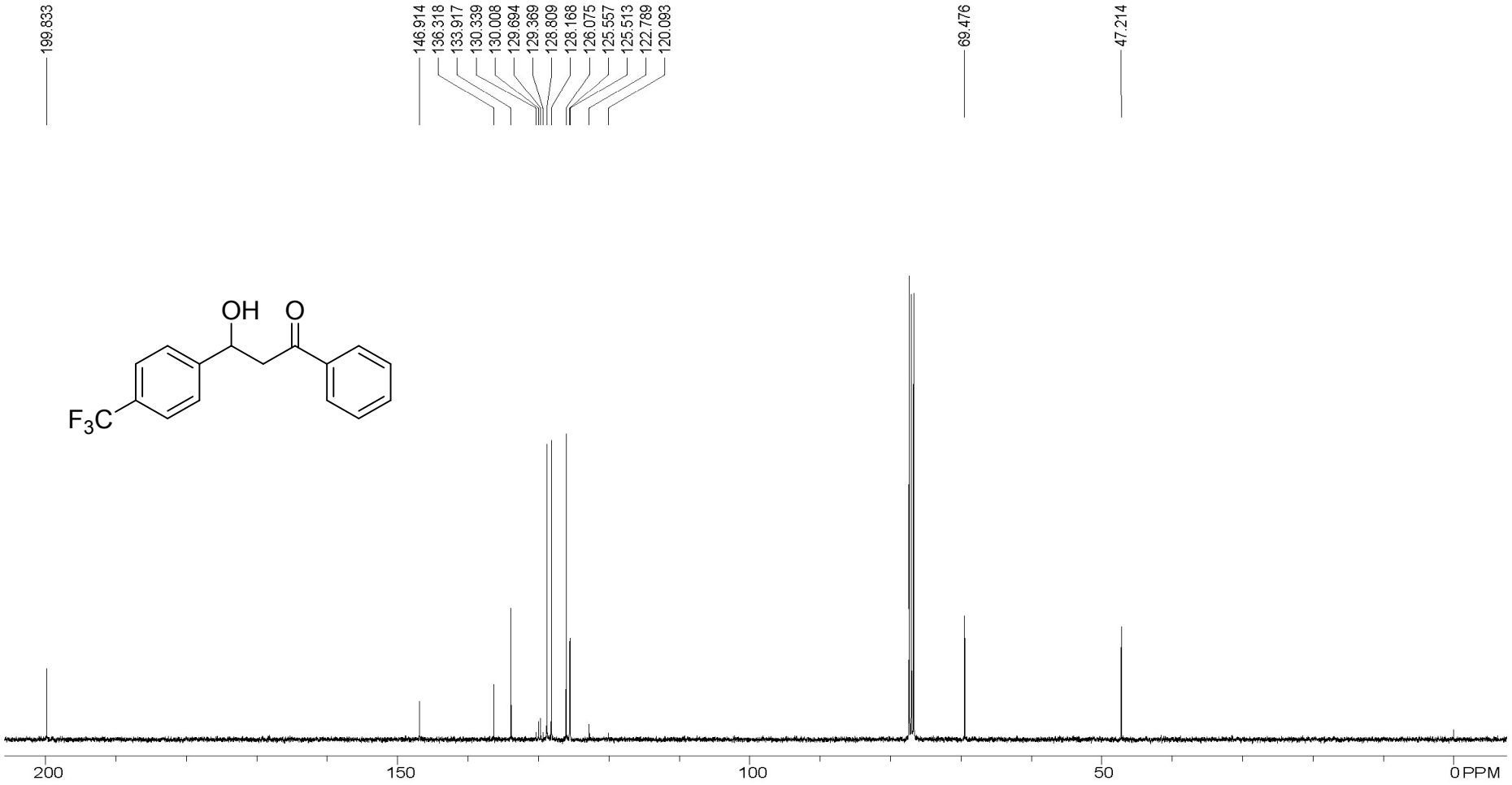
^{13}C NMR (400 MHz, $CDCl_3$) δ = 199.5, 150.3, 147.4, 136.2, 134.1, 128.9, 128.2, 126.6, 123.8, 69.2, 47.0 ppm.

3-hydroxy-1-phenyl-3-[4-(trifluoromethyl)phenyl]propan-1-one (3h)



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.96-7.46 (m, 9H), 5.41 (dd, *J* = 3.6 Hz, *J* = 7.6 Hz, 1H), 3.80(br, 1H), 3.42-3.31 (m, 2H) ppm.

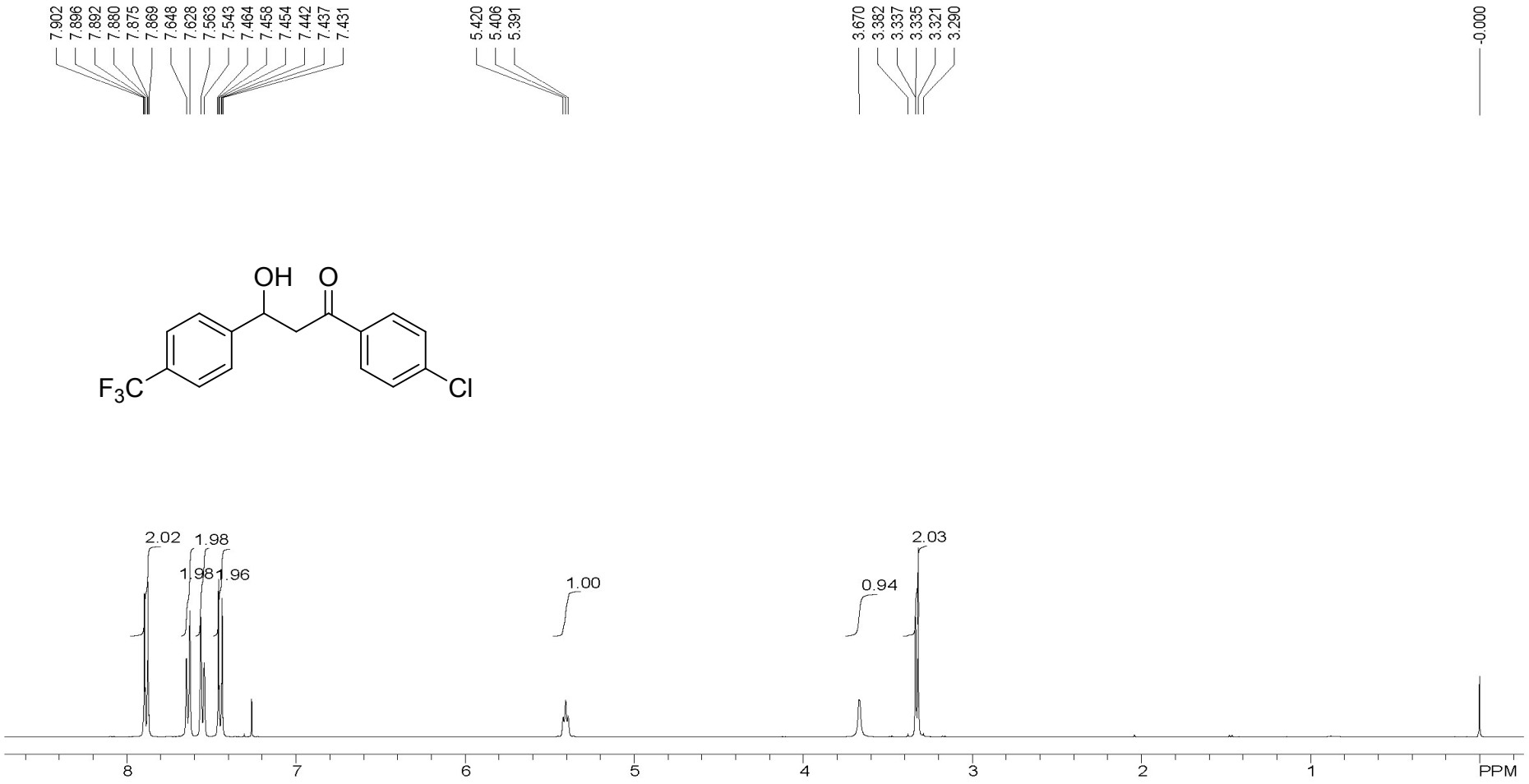
3-hydroxy-1-phenyl-3-[4-(trifluoromethyl)phenyl]propan-1-one (3h)



^{13}C NMR (400 MHz, $CDCl_3$) δ = 199.8, 146.9, 136.3, 133.9, 129.9 (q, *J* = 32.5 Hz), 128.8, 128.2, 126.1, 125.5 (q, *J* = 3.9 Hz), 121.4 (q, *J* = 271.3 Hz), 69.5, 47.2

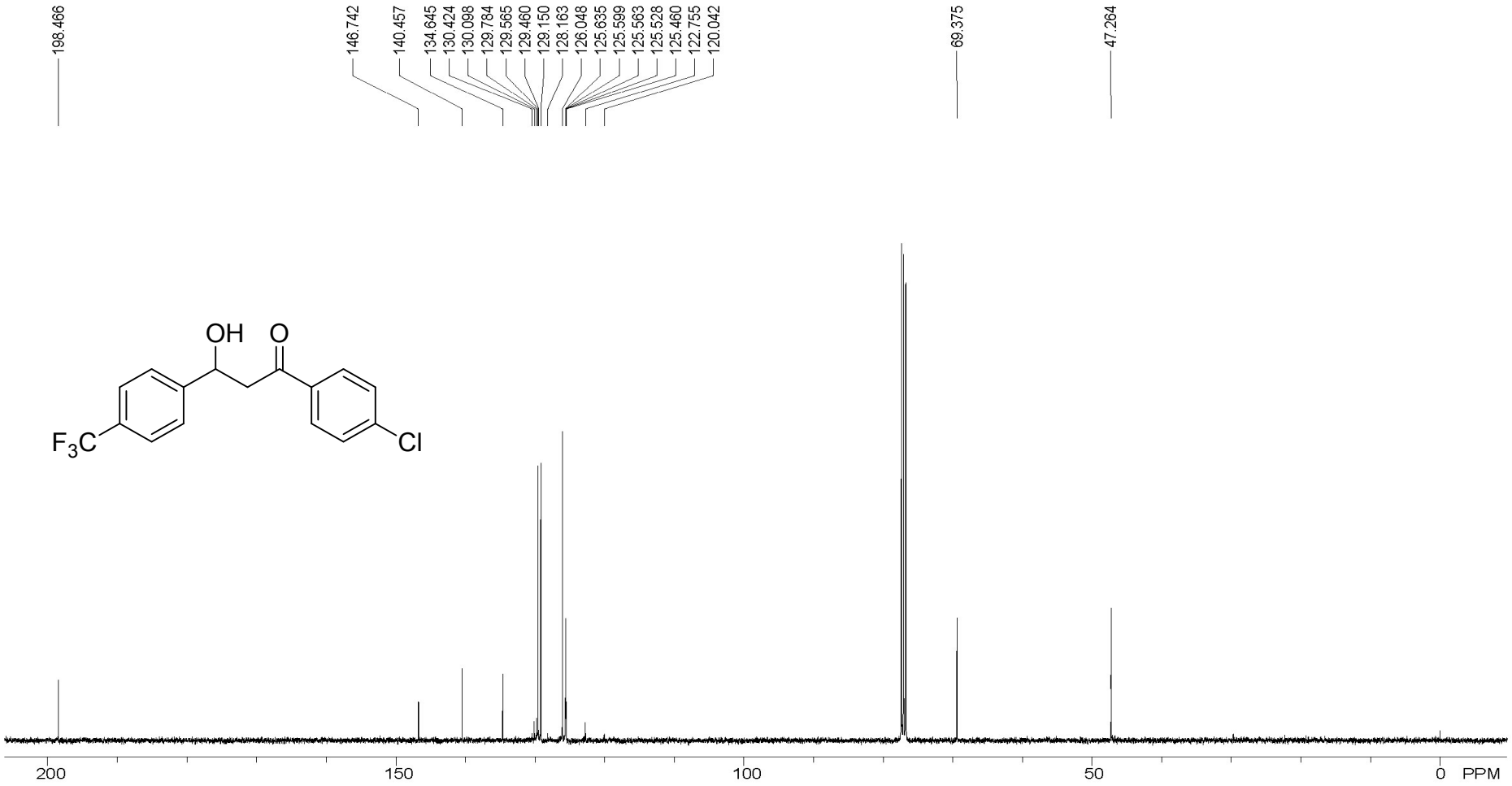
ppm.

1-(4-chlorophenyl)-3-hydroxy-3-[4-(trifluoromethyl)phenyl]propan-1-one (3i)



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.90-7.43 (m, 8H), 5.41 (t, *J* = 5.8 Hz, 1H), 3.67 (br, 1H), 3.38-3.29 (m, 2H) ppm.

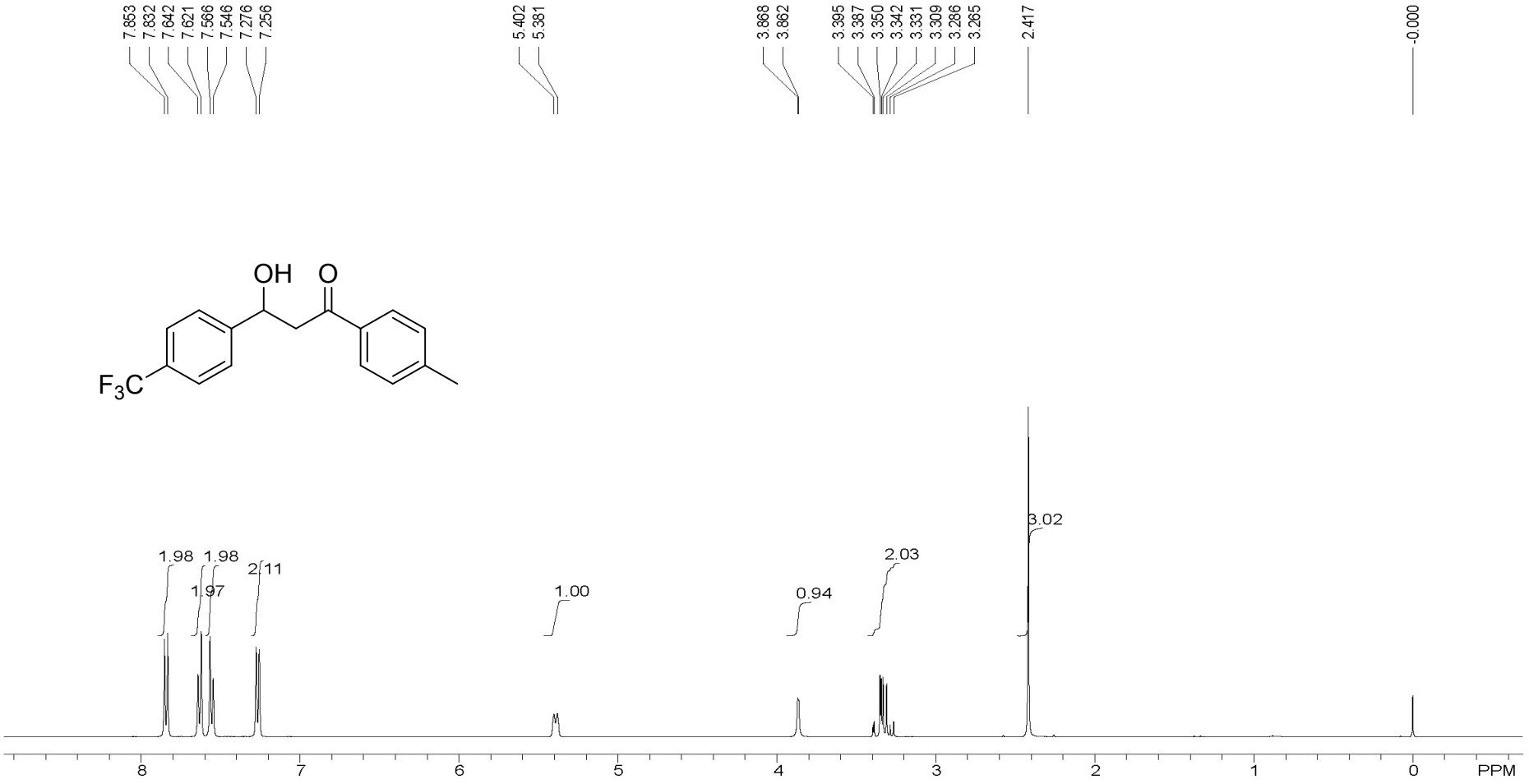
1-(4-chlorophenyl)-3-hydroxy-3-[4-(trifluoromethyl)phenyl]propan-1-one (3i)



^{13}C NMR (400 MHz, $CDCl_3$) δ = 198.5, 146.7, 140.5, 134.6, 129.9 (q, *J* = 32.1 Hz), 129.6, 129.2, 126.0, 125.6 (q, *J* = 3.6 Hz), 124.1 (q, *J* = 272.4 Hz), 69.4, 47.3

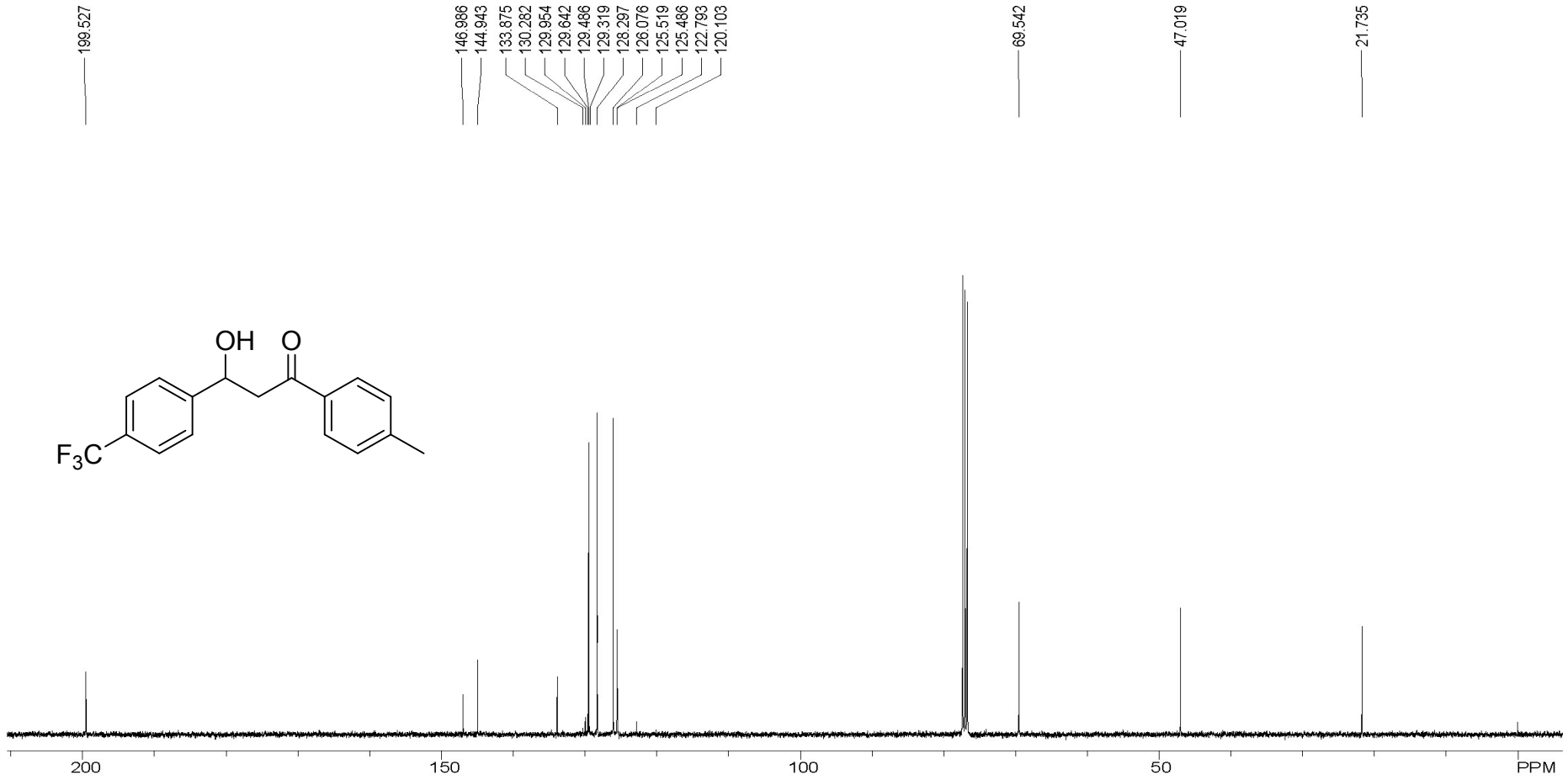
ppm.

3-hydroxy-1-(4-methylphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3j)



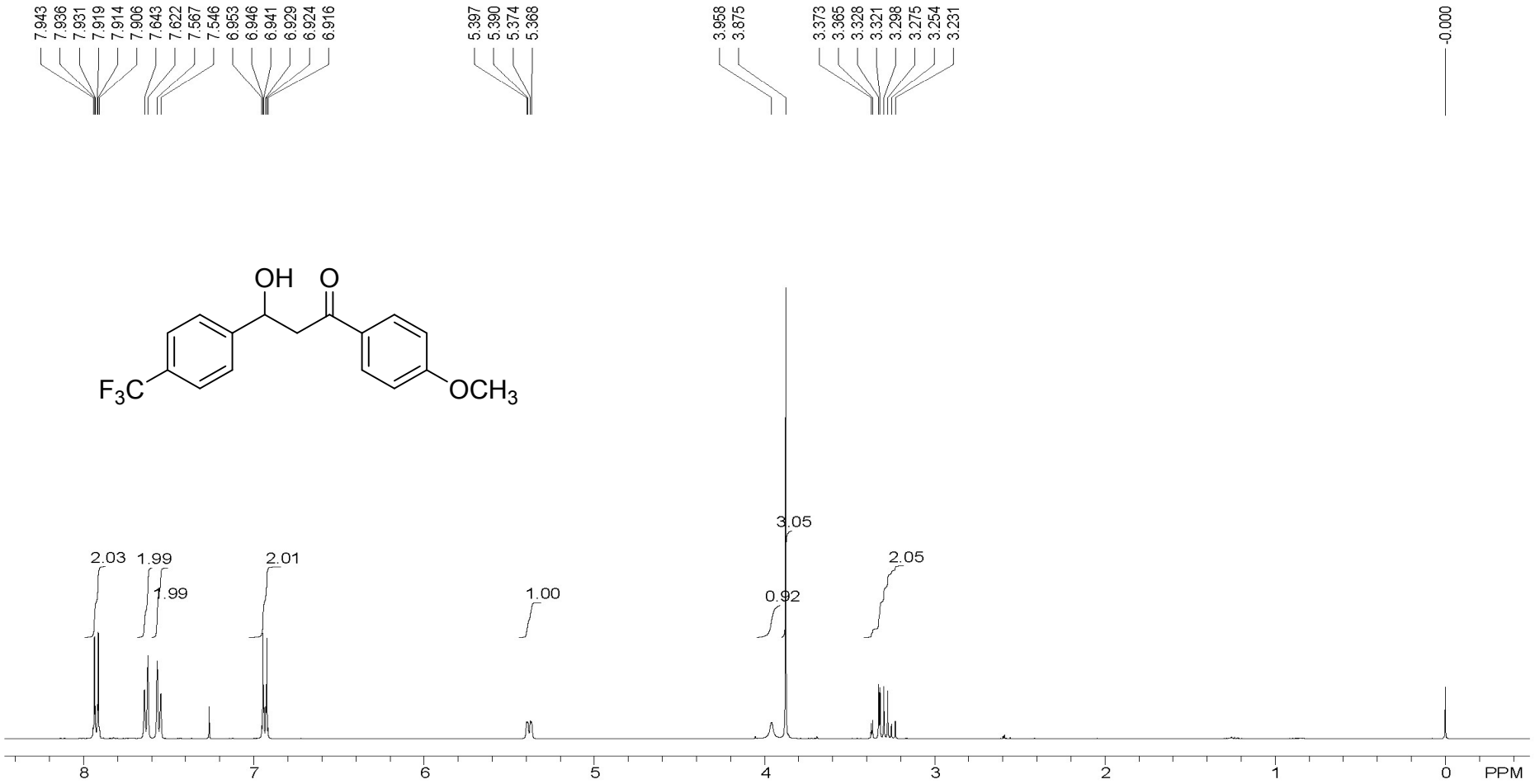
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85-7.26 (m, 8H), 5.39 (d, *J* = 8.6 Hz, 1H), 3.87 (d, *J* = 2.3 Hz, 1H), 3.35-3.31 (m, 2H), 2.42 (s, 3H) ppm.

3-hydroxy-1-(4-methylphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3j)



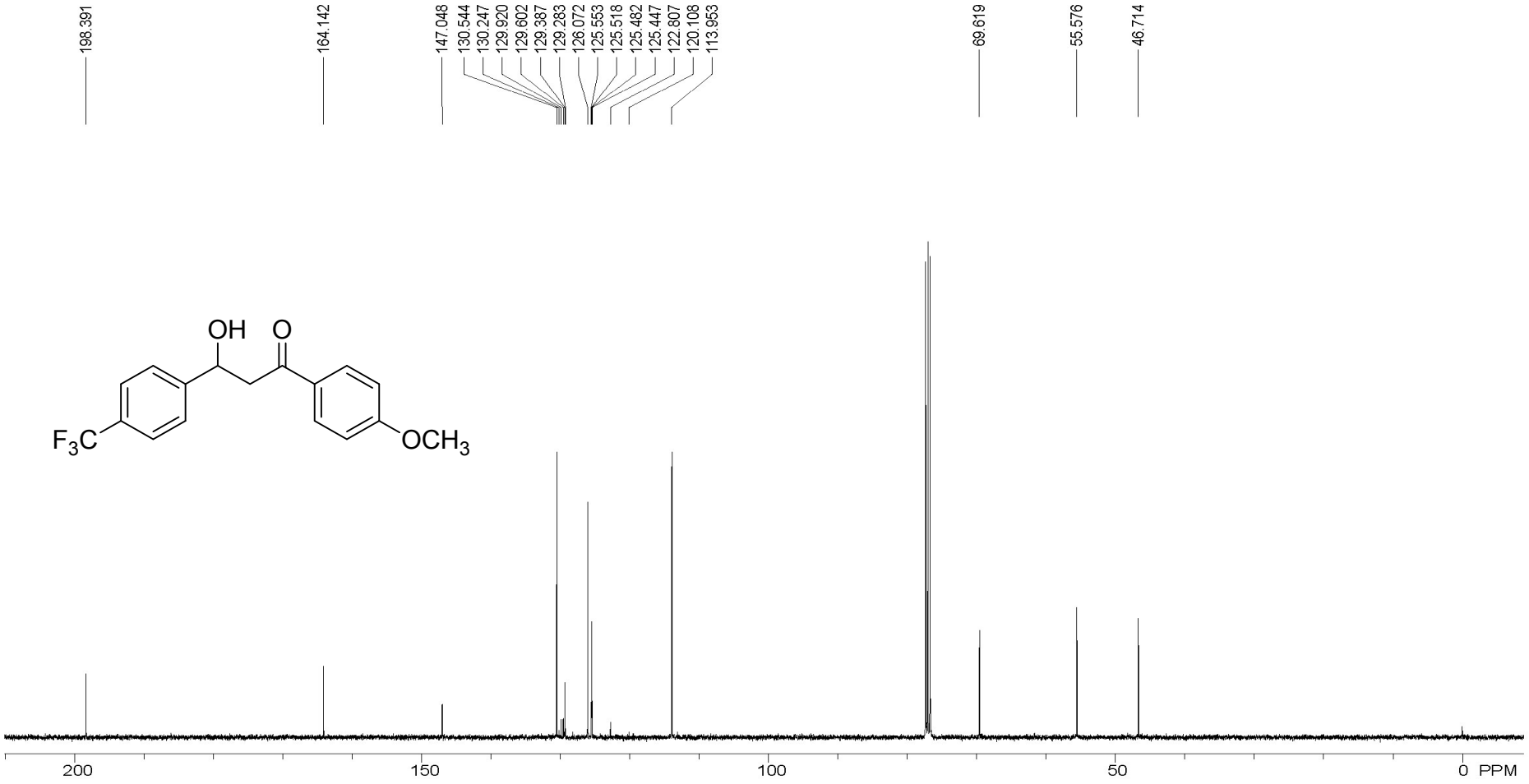
^{13}C NMR (400 MHz, $CDCl_3$) δ = 199.5, 147.0, 144.9, 133.9, 129.8 (q, *J* = 32.3 Hz), 129.5, 128.3, 126.1, 125.5 (q, *J* = 3.8 Hz), 121.4 (q, *J* = 270.7 Hz), 69.5, 47.0, 21.7 ppm.

3-hydroxy-1-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3k)



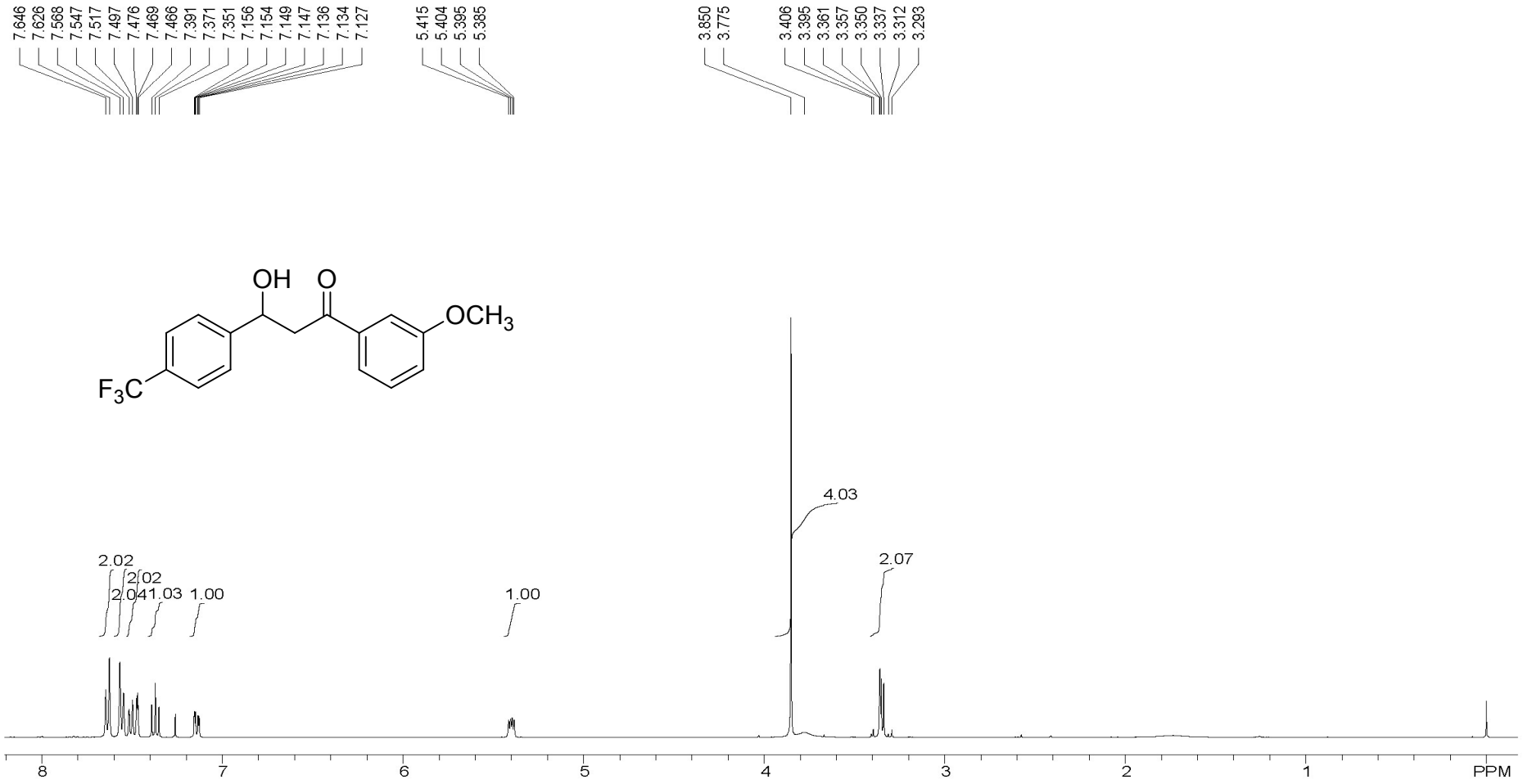
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.94-6.92 (m, 8H), 5.38 (dd, *J* = 2.5 Hz, *J* = 9.0 Hz, 1H), 3.96 (br, 1H), 3.88 (s, 3H), 3.37-3.23 (m, 2H) ppm.

3-hydroxy-1-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3k)



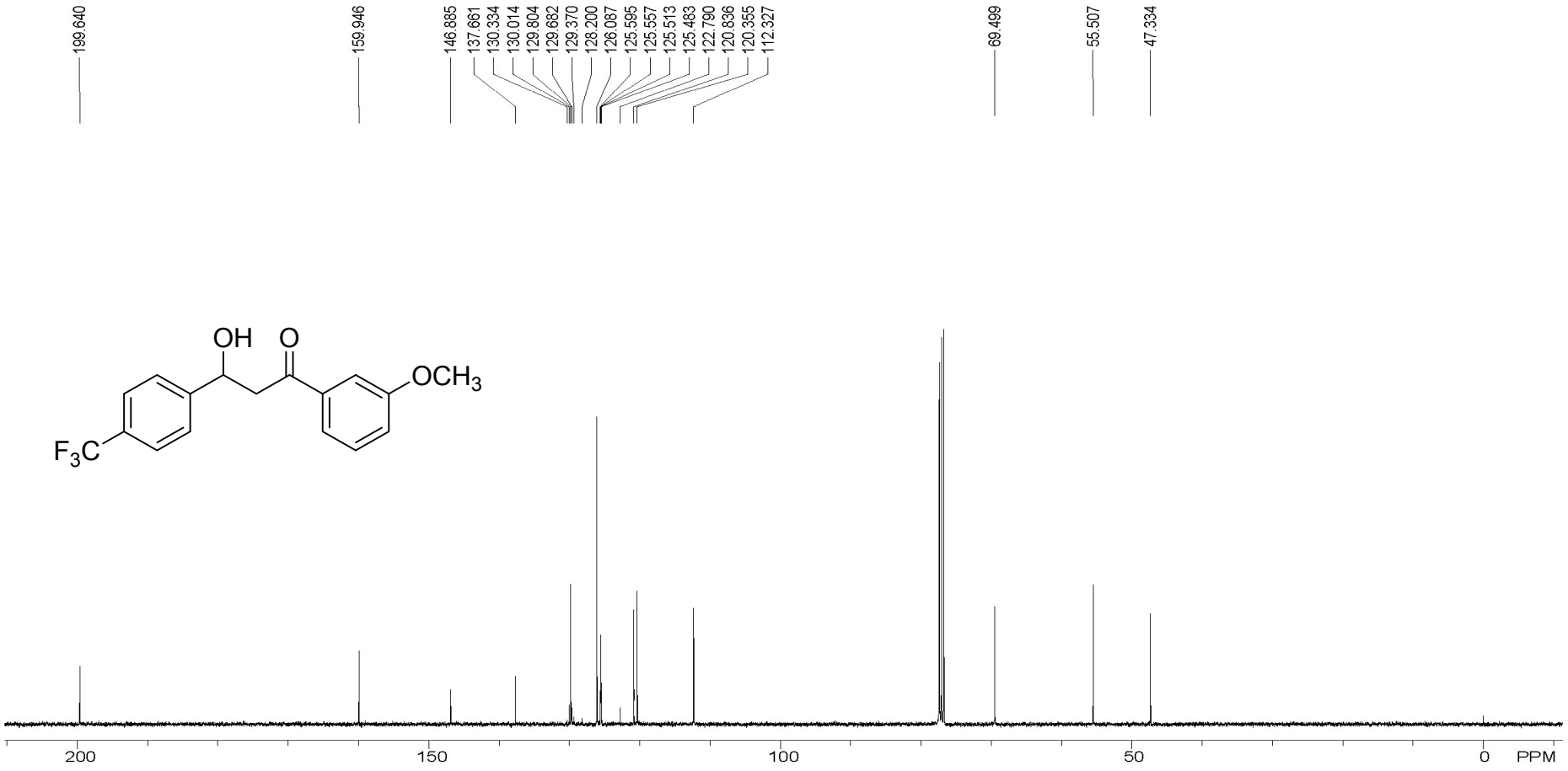
^{13}C NMR (400 MHz, $CDCl_3$) δ = 198.4, 164.1, 147.0, 130.5, 129.8 (q, *J* = 32.3 Hz), 129.4, 126.1, 125.5 (q, *J* = 3.6 Hz), 121.5 (q, *J* = 271.6 Hz), 69.6, 55.6, 46.7 ppm.

3-hydroxy-1-(3-methoxyphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3l)



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.65-7.13 (m, 8H), 5.40 (dd, *J* = 4.1 Hz, *J* = 7.8 Hz, 1H), 3.85 (s, 3H), 3.78 (br, 1H), 3.41-3.29 (m, 2H) ppm.

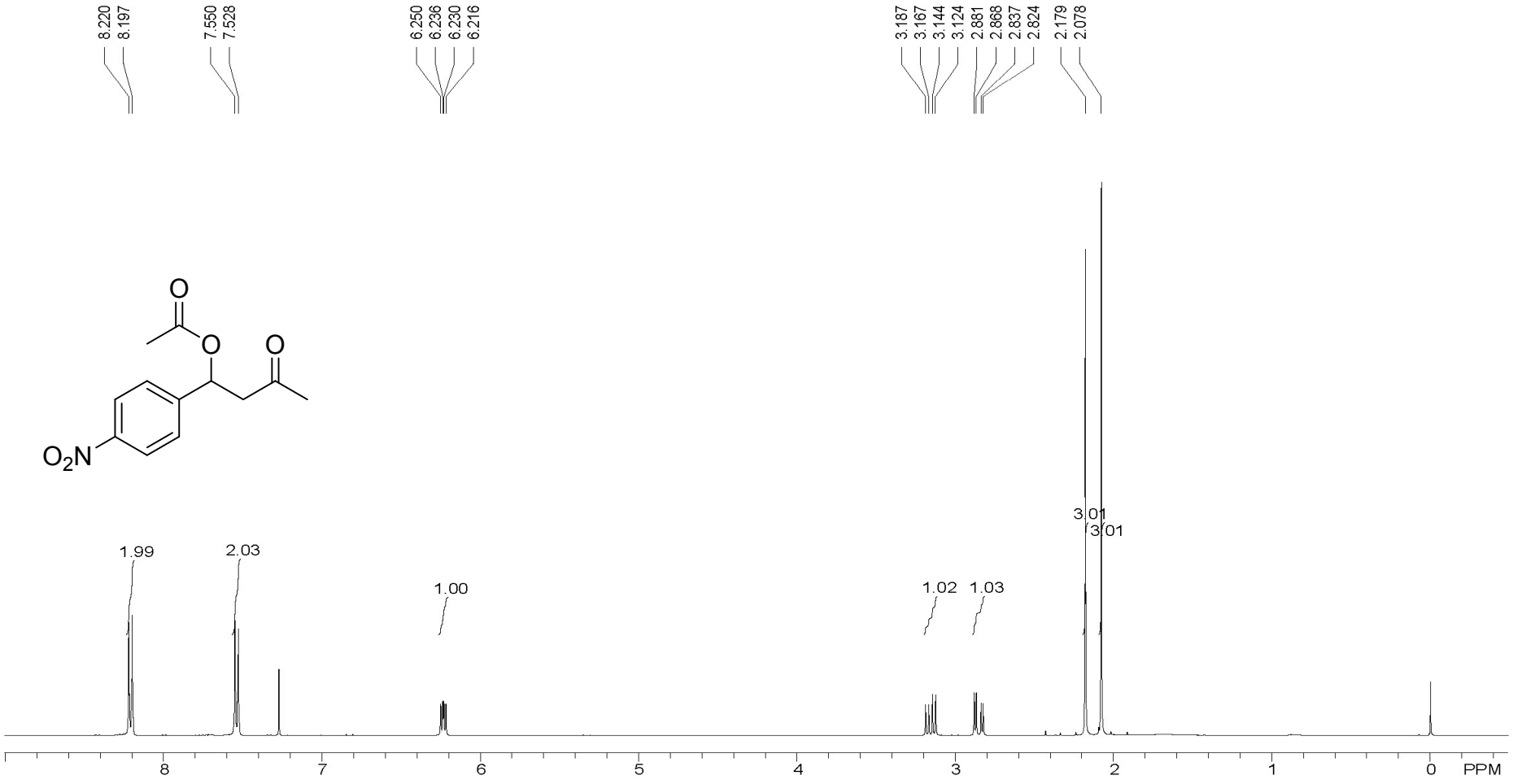
3-hydroxy-1-(3-methoxyphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3l)



^{13}C NMR (400 MHz, $CDCl_3$) δ = 199.6, 159.9, 146.9, 137.7, 129.9, 129.8 (q, *J* = 32.3 Hz), 126.1, 125.5 (q, *J* = 3.7 Hz), 121.5 (q, *J* = 272.1 Hz), 120.8, 120.4, 112.3, 69.5, 55.5, 47.3 ppm.

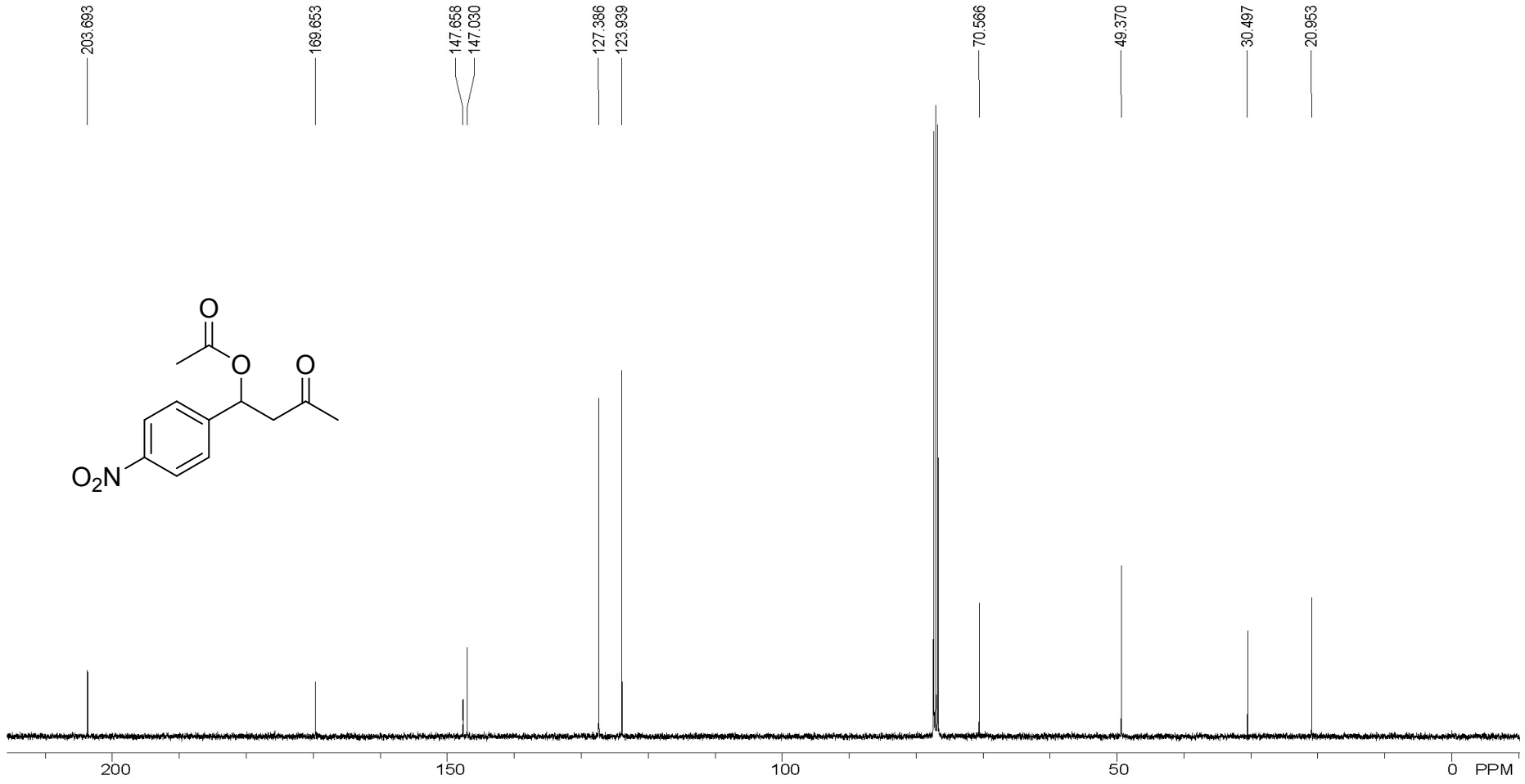
4. NMR spectra of acylated β-hydroxy ketone derivatives

1-(4-nitrophenyl)-3-oxobutyl acetate (4a)



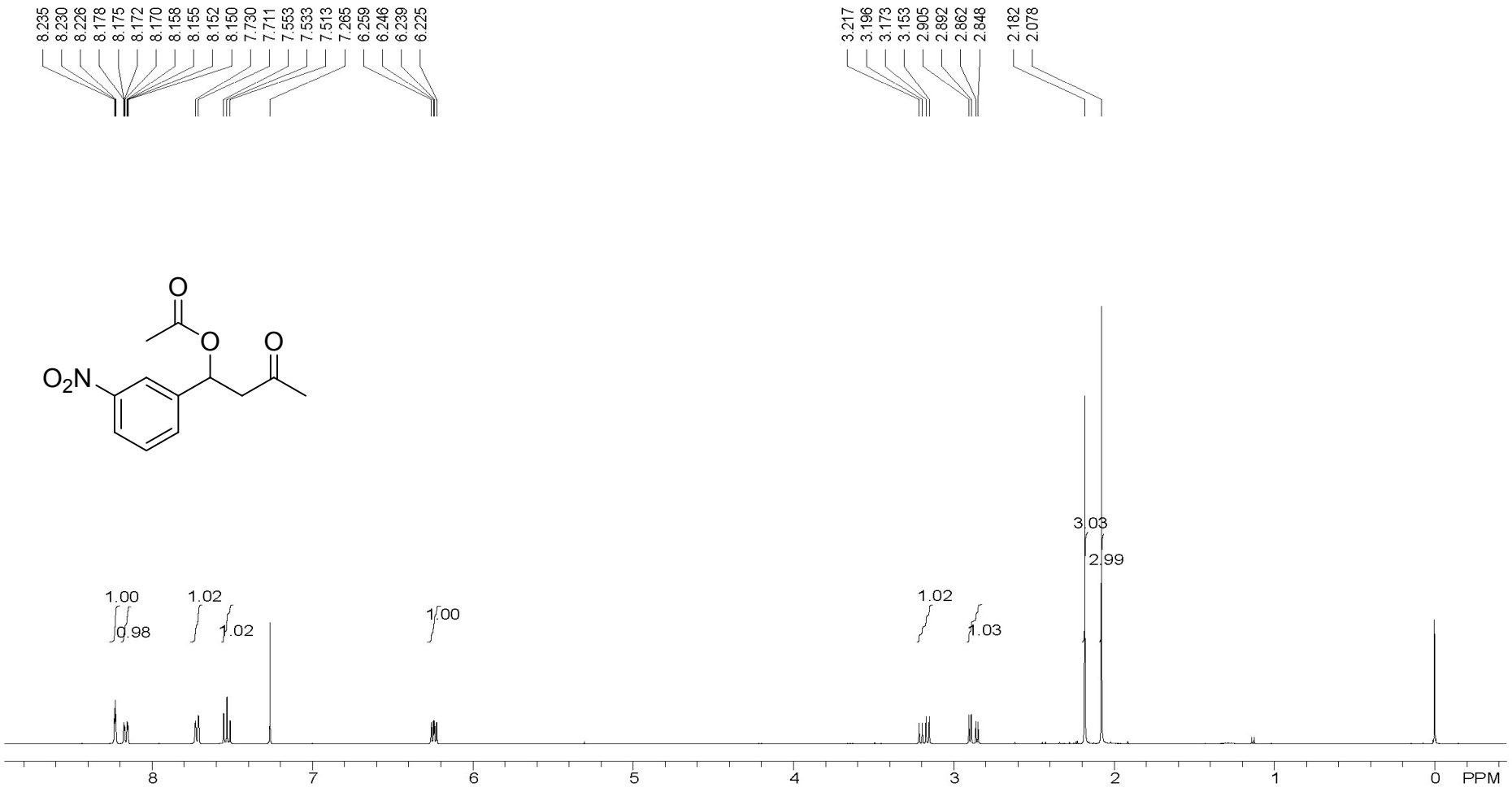
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.22-7.53 (m, 4H), 6.23 (dd, *J* = 5.4 Hz, *J* = 8.1 Hz, 1H), 3.19-2.82 (m, 2H), 2.18 (s, 3H), 2.08 (s, 3H) ppm.

1-(4-nitrophenyl)-3-oxobutyl acetate (4a)



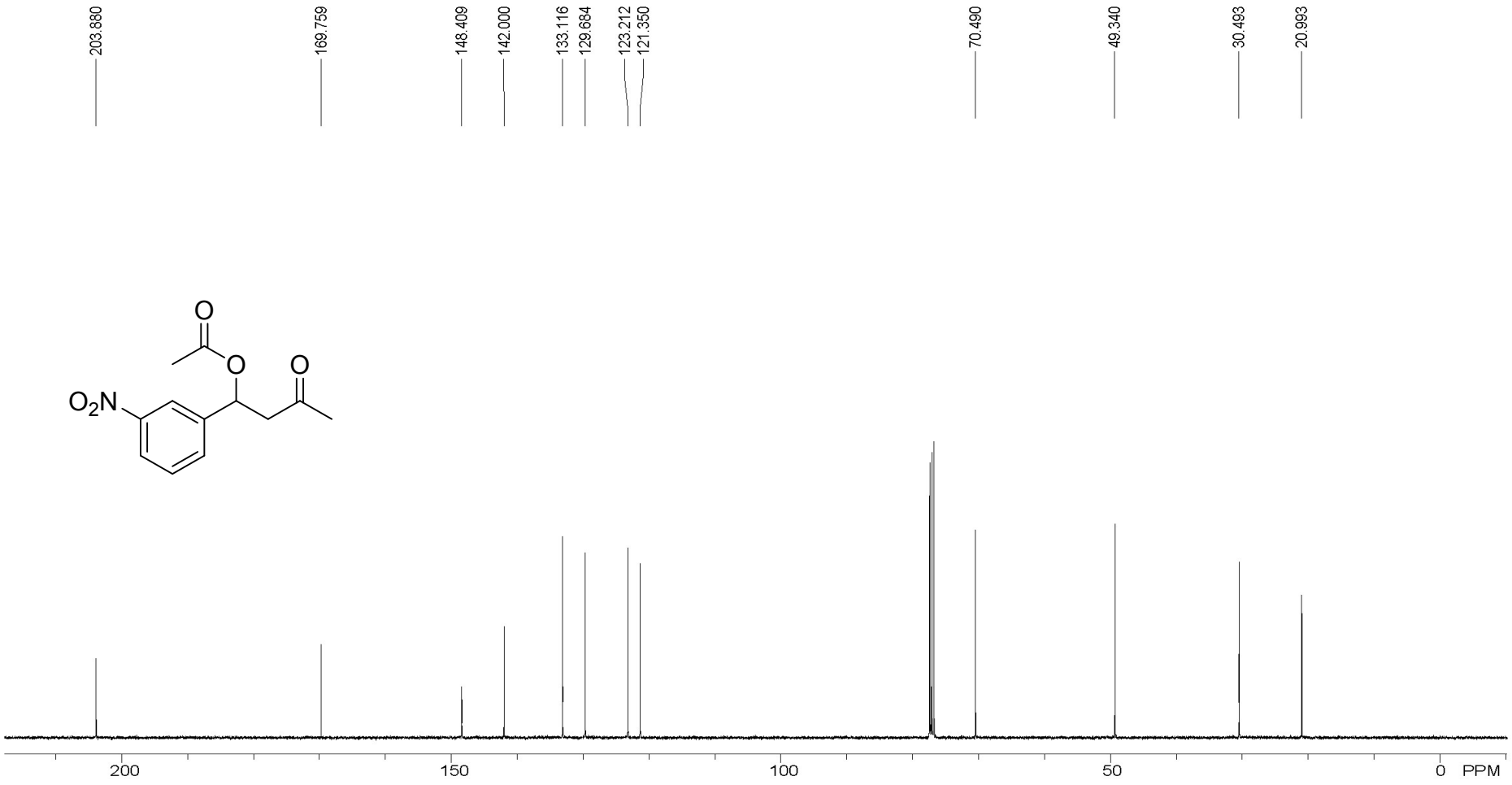
^{13}C NMR (400 MHz, $CDCl_3$) δ = 203.7, 169.7, 147.7, 147.0, 127.4, 123.9, 70.6, 49.4, 30.5, 21.0 ppm.

1-(3-nitrophenyl)-3-oxobutyl acetate (4b)



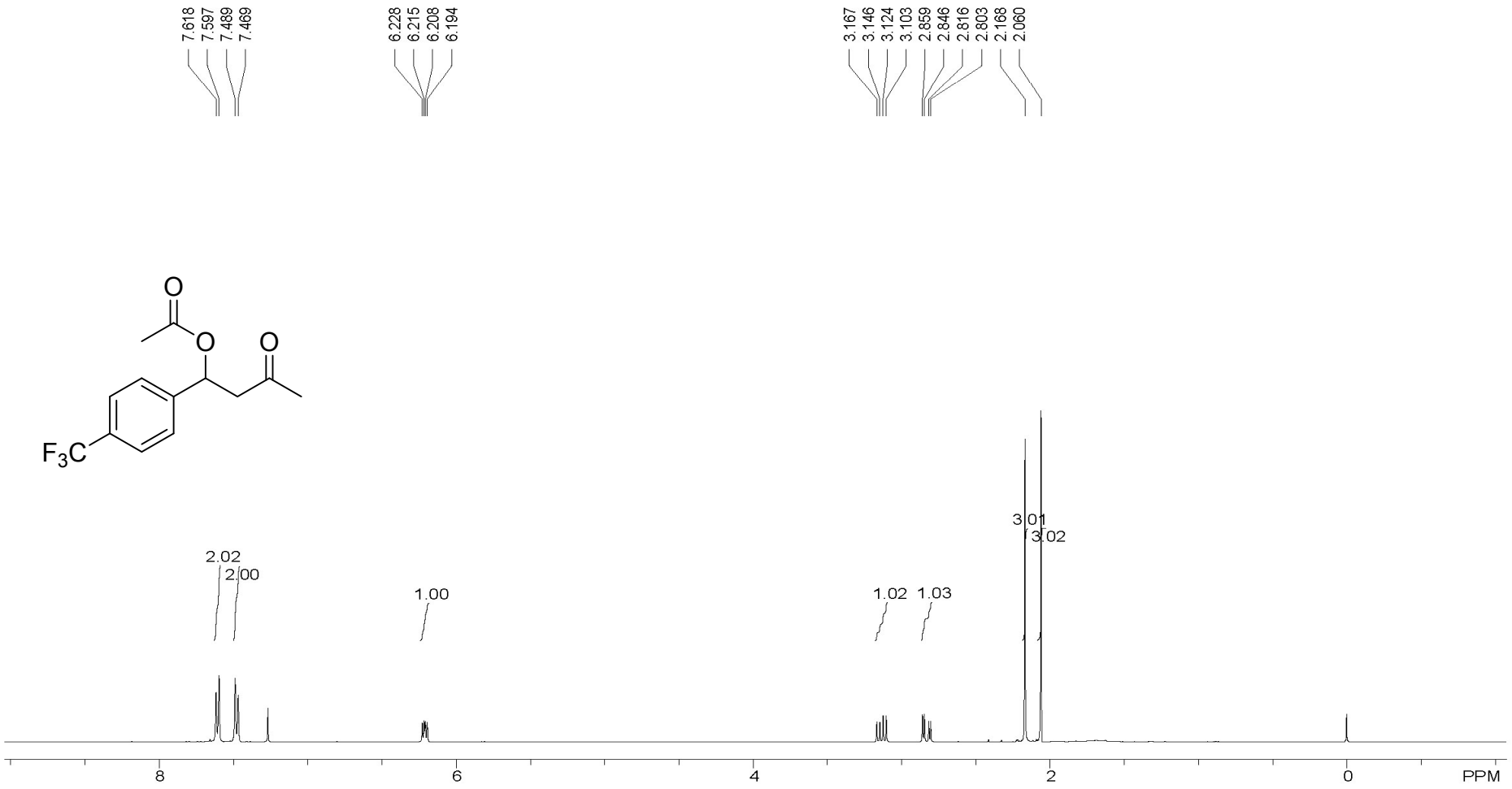
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.24-7.51 (m, 4H), 6.24 (dd, *J* = 5.5 Hz, *J* = 8.0 Hz, 1H), 3.22-2.85 (m, 2H), 2.18 (s, 3H), 2.08 (s, 3H) ppm.

1-(3-nitrophenyl)-3-oxobutyl acetate (4b)



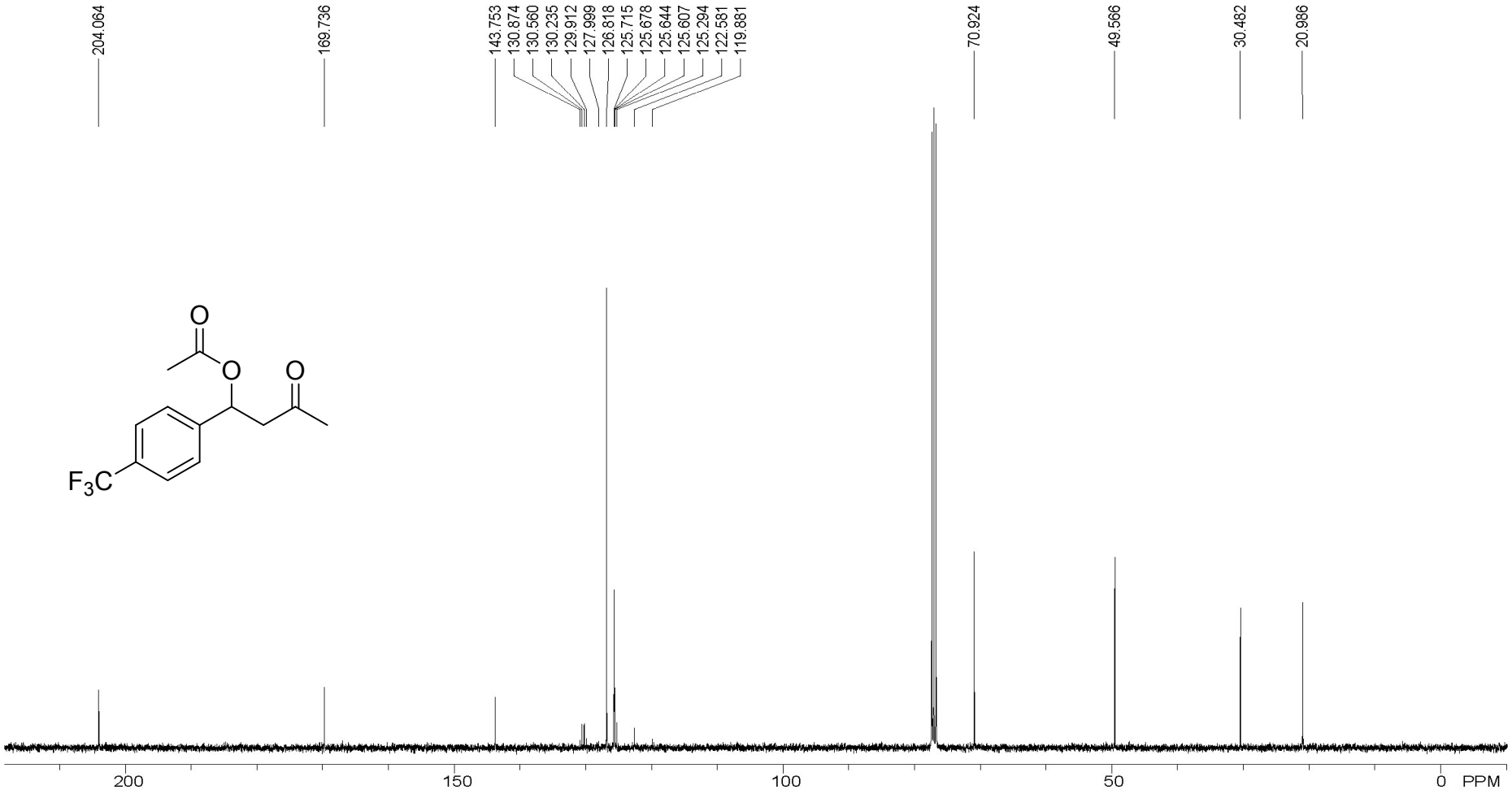
^{13}C NMR (400 MHz, $CDCl_3$) δ = 203.9, 169.8, 148.4, 142.0, 133.1, 129.7, 123.2, 121.4, 70.5, 49.3, 30.5, 21.0 ppm.

3-oxo-1-[4-(trifluoromethyl)phenyl]butyl acetate (4c)



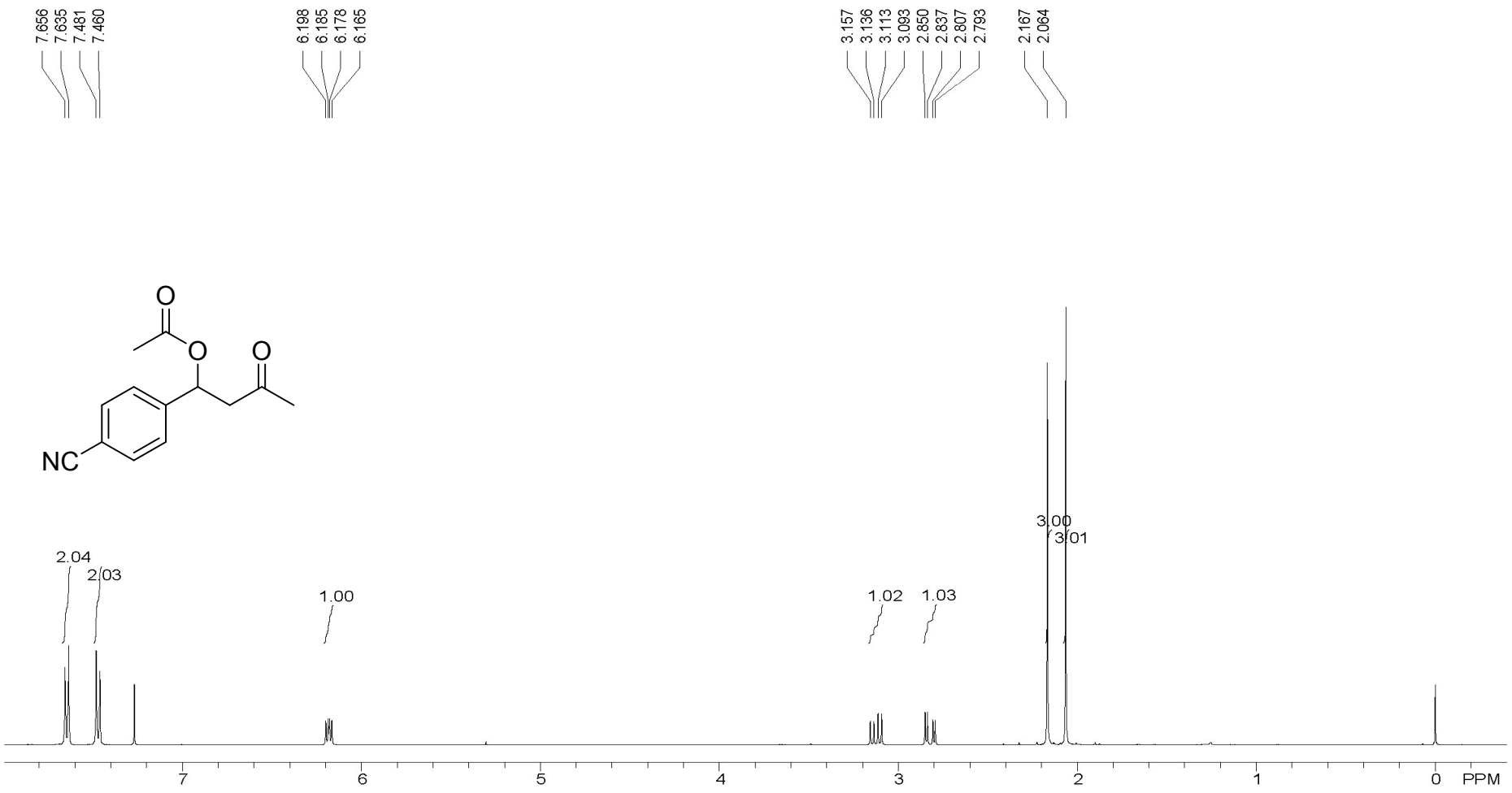
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.62-7.47 (m, 4H), 6.21 (dd, *J* = 5.2 Hz, *J* = 8.4 Hz, 1H), 3.17-2.80 (m, 2H), 2.17 (s, 3H), 2.06 (s, 3H) ppm.

3-oxo-1-[4-(trifluoromethyl)phenyl]butyl acetate (4c)



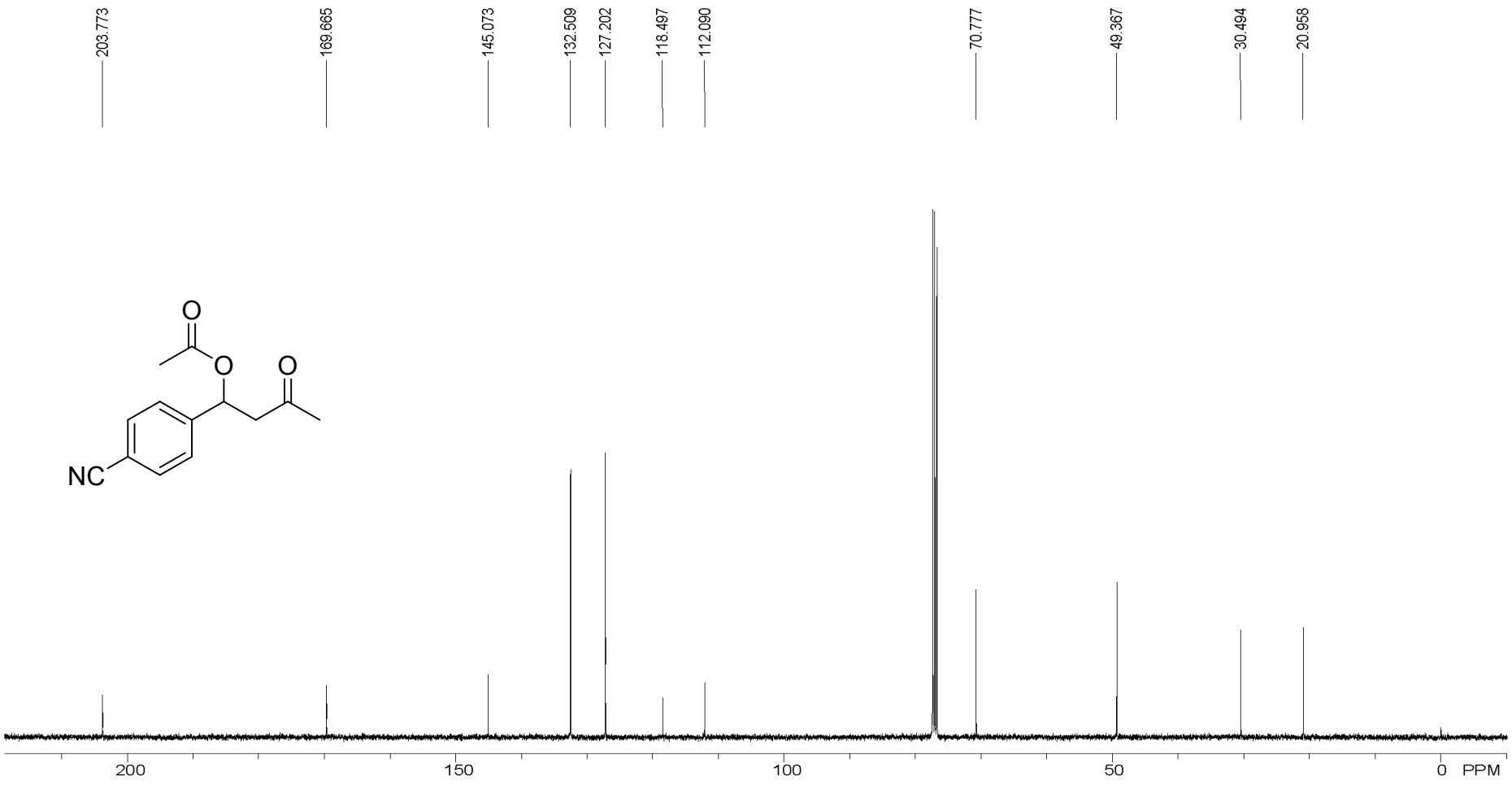
^{13}C NMR (400 MHz, $CDCl_3$) δ = 204.1, 169.7, 143.8, 120.4 (q, *J* = 32.3 Hz), 126.8, 125.7 (q, *J* = 3.63 Hz), 123.9 (q, *J* = 272.3 Hz), 70.9, 49.6, 30.5, 21.0 ppm.

1-(4-cyanophenyl)-3-oxobutyl acetate (4d)



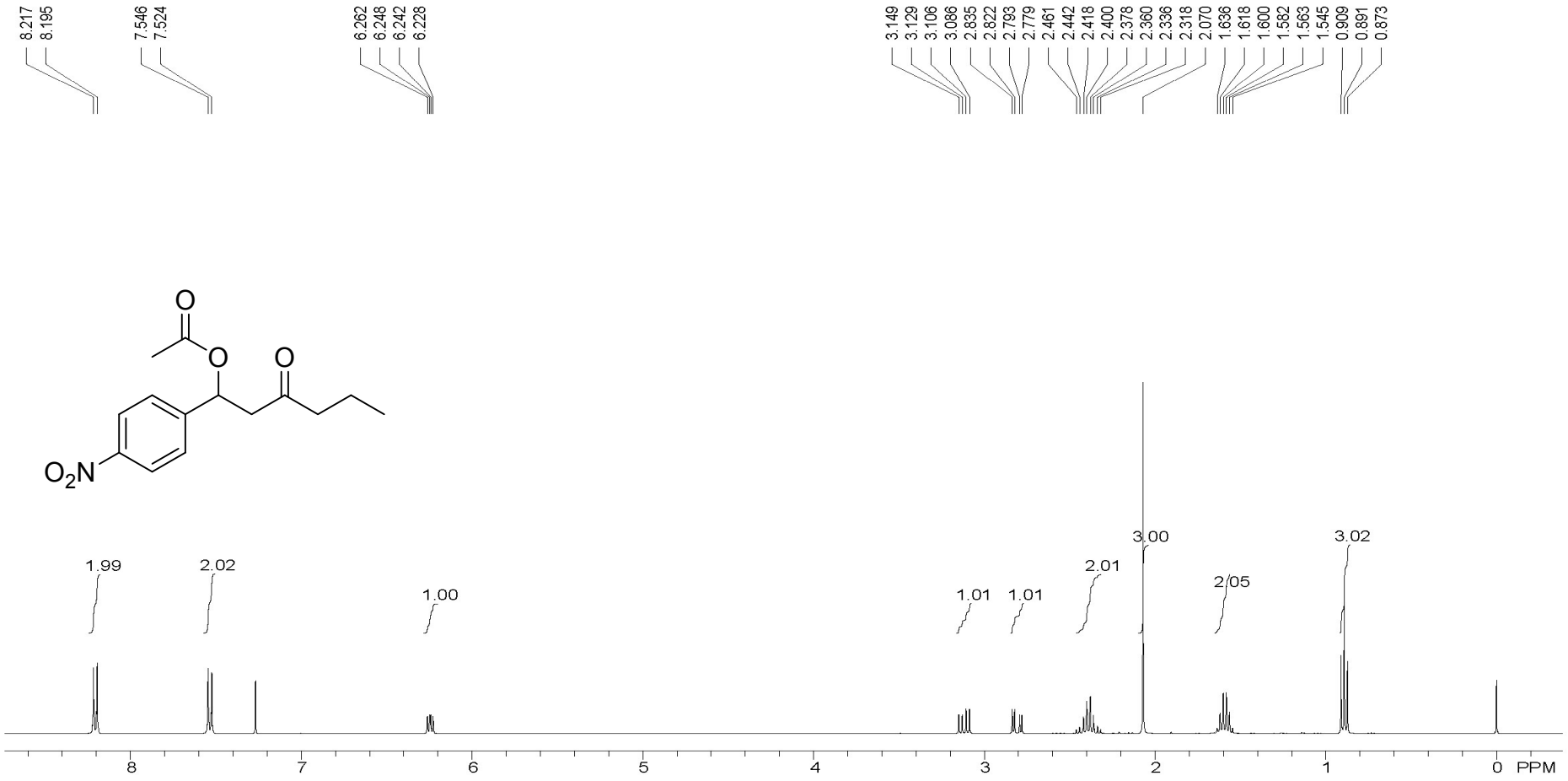
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.66-7.46 (m, 4H), 6.18 (dd, *J* = 5.3 Hz, *J* = 8.1 Hz, 1H), 3.16-2.79 (m, 2H), 2.17 (s, 3H), 2.06 (s, 3H) ppm.

1-(4-cyanophenyl)-3-oxobutyl acetate (4d)



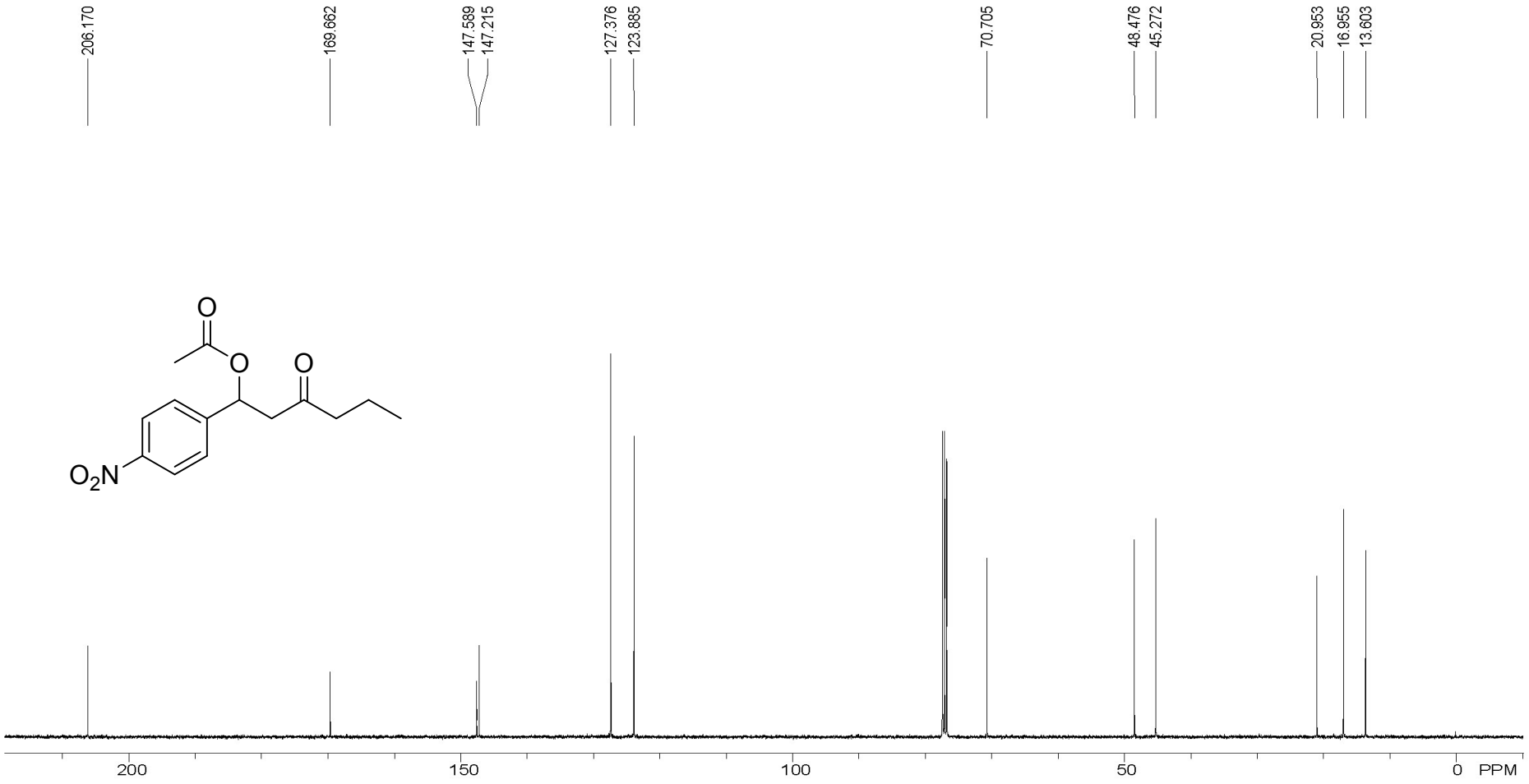
^{13}C NMR (400 MHz, $CDCl_3$) δ = 203.8, 169.7, 145.1, 132.5, 127.2, 118.5, 112.1, 70.8, 49.4, 30.5, 21.0 ppm.

1-(4-nitrophenyl)-3-oxohexyl acetate (4e)



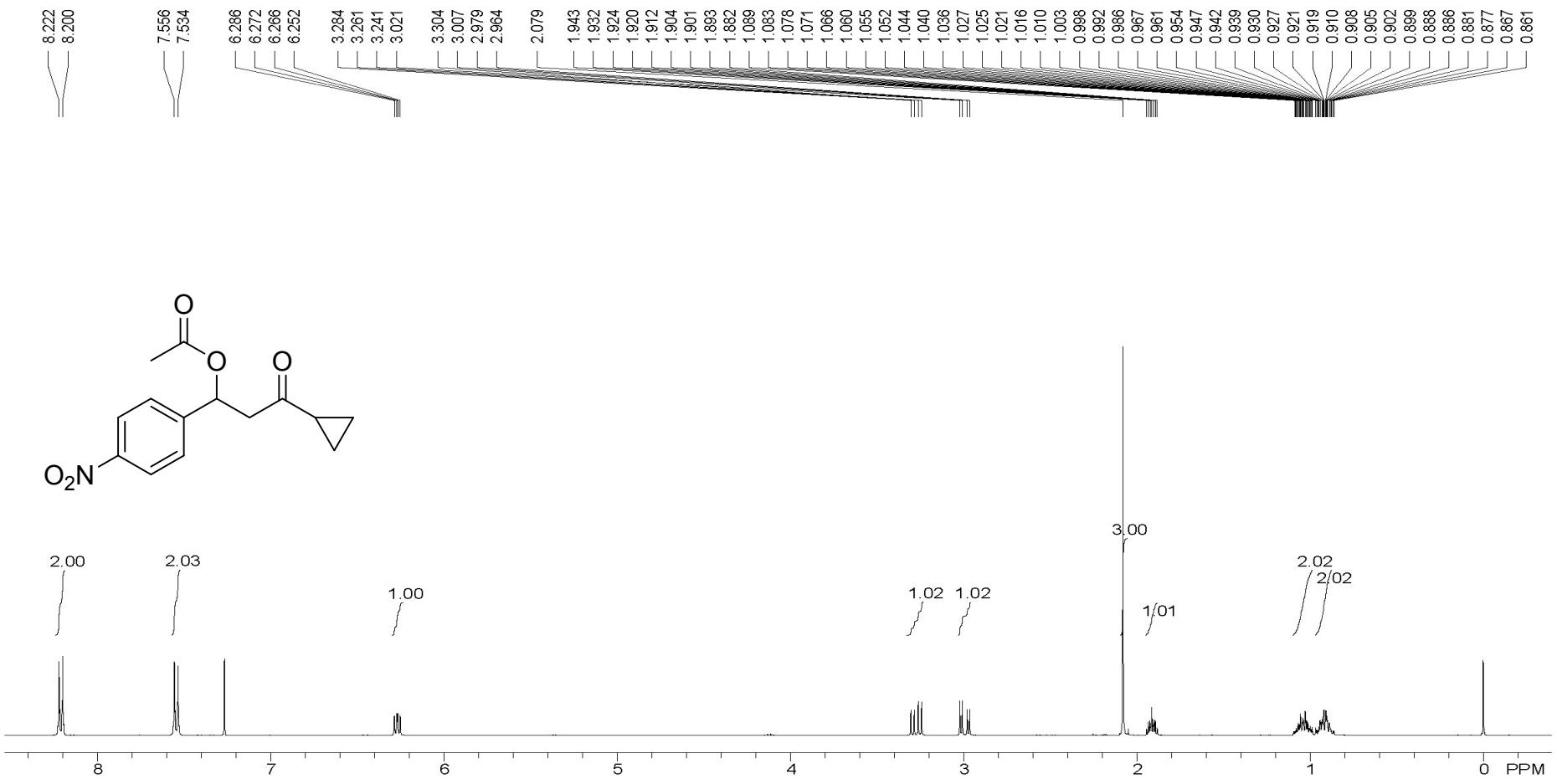
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.22-7.52 (m, 4H), 6.25 (dd, *J* = 5.5 Hz, *J* = 8.1 Hz,1H) , 3.15-2.78 (m, 2H), 2.46-2.32 (m, 2H), 2.07 (s, 3H), 1.59 (m, *J* = 7.3 Hz, 2H), 0.89 (t, *J* = 7.4 Hz, 3H) ppm.

1-(4-nitrophenyl)-3-oxohexyl acetate (4e)



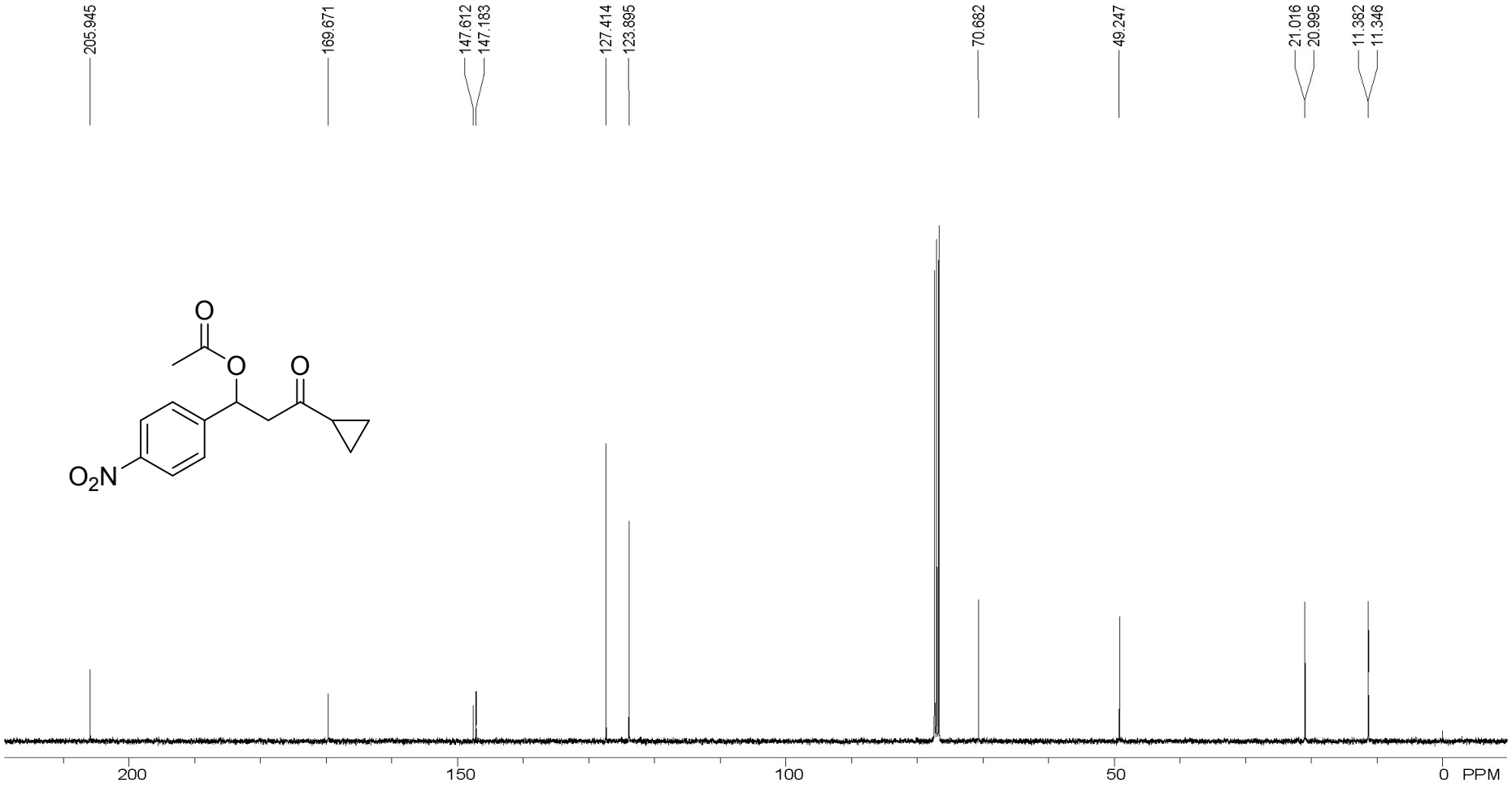
^{13}C NMR (400 MHz, $CDCl_3$) δ = 206.2, 169.7, 147.6, 147.2, 127.4, 123.9, 70.7, 48.5, 45.3, 21.0, 17.0, 13.6 ppm.

3-cyclopropyl-1-(4-nitrophenyl)-3-oxopropyl acetate (4f)



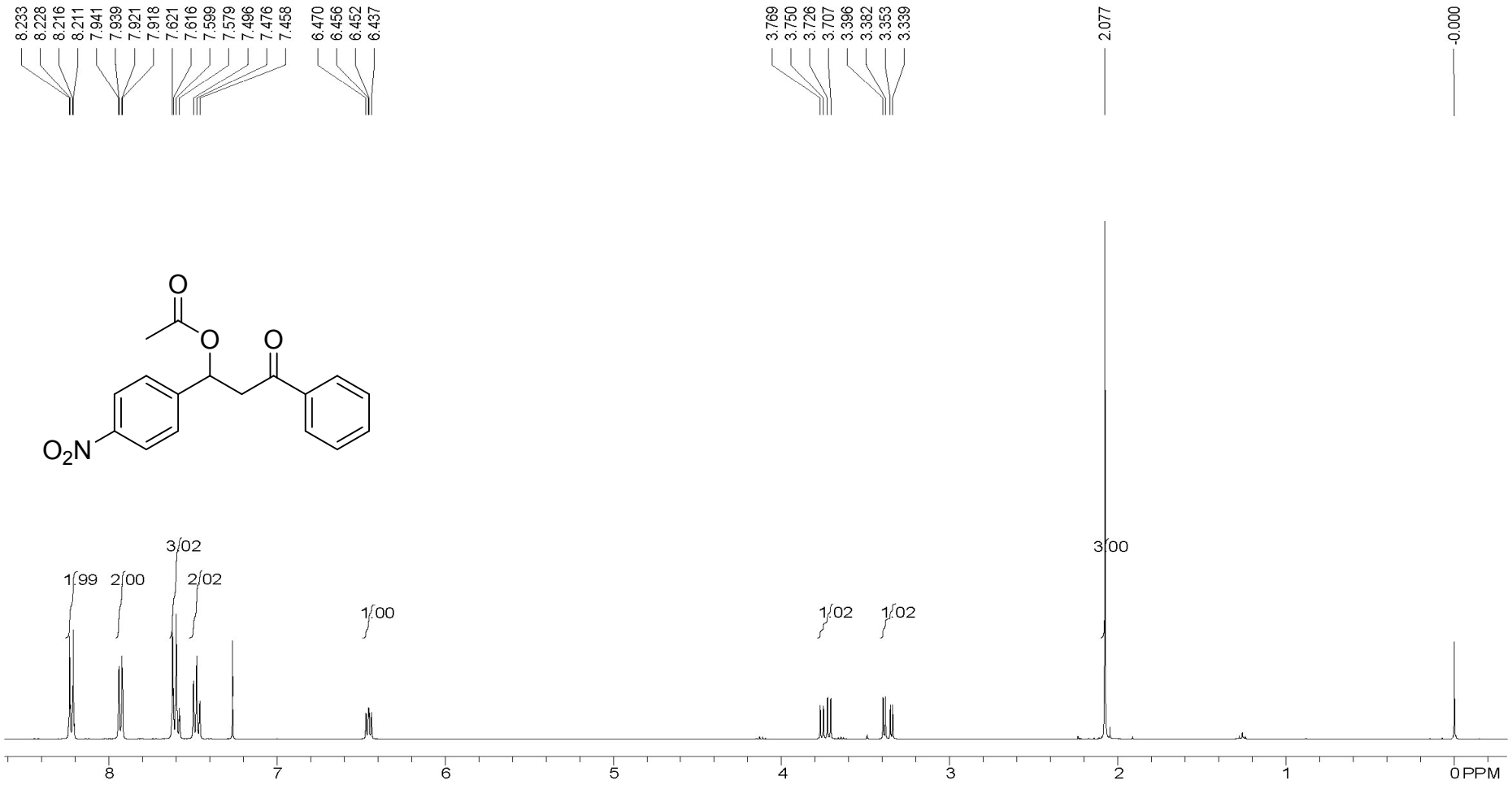
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.22-7.53 (m, 4H), 6.27 (dd, *J* = 5.6 Hz, *J* = 7.8 Hz, 1H), 3.28-2.96 (m, 2H), 2.08 (s, 3H), 1.94-1.88 (m, 1H), 1.09-0.99 (m, 2H), 0.97-0.86 (m, 2H) ppm.

3-cyclopropyl-1-(4-nitrophenyl)-3-oxopropyl acetate (4f)



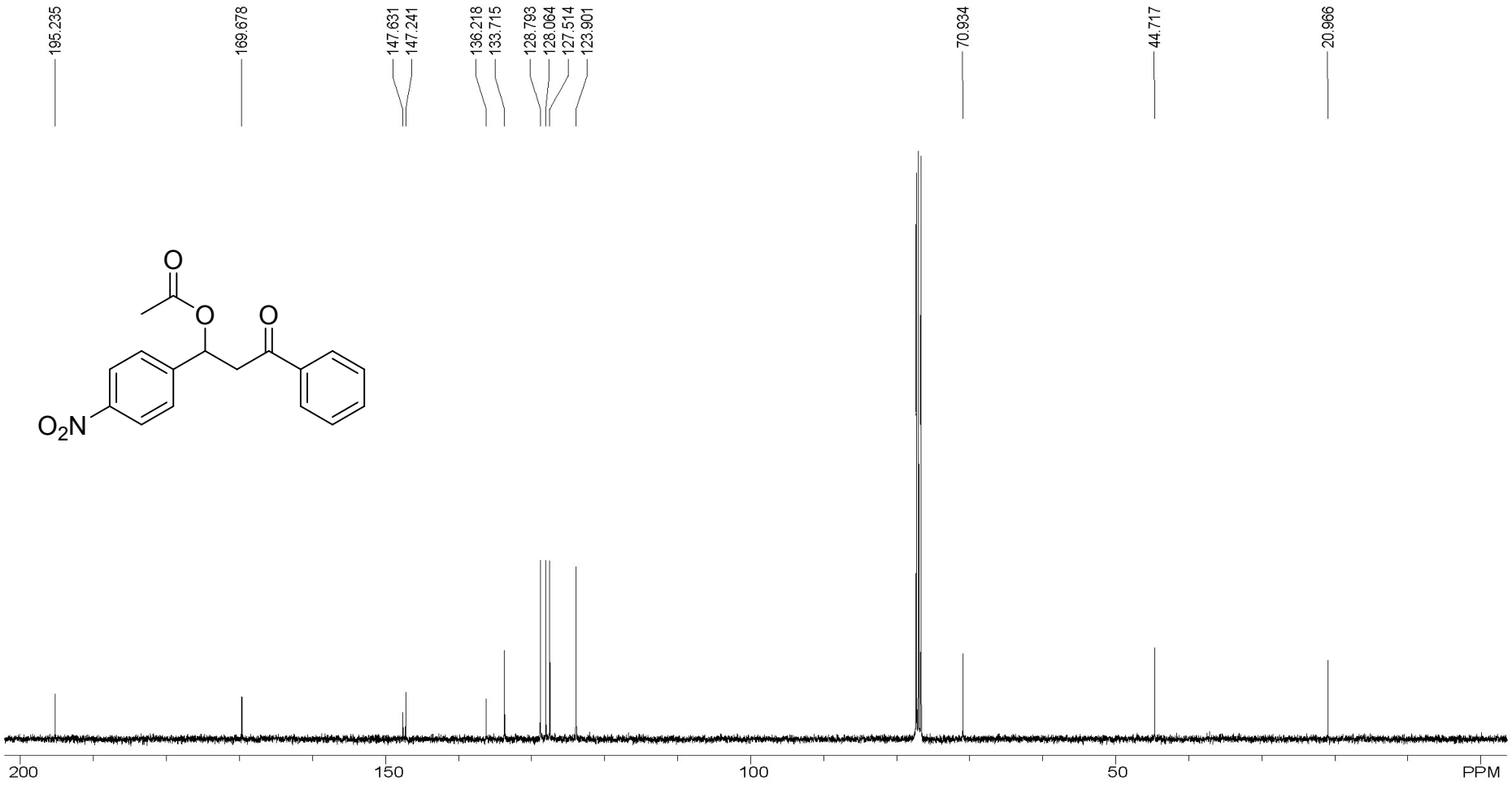
^{13}C NMR (400 MHz, $CDCl_3$) δ = 205.9, 169.7, 147.6, 147.2, 127.4, 123.9, 70.7, 49.2, 21.02, 21.00, 11.4, 11.3 ppm.

1-(4-nitrophenyl)-3-oxo-3-phenylpropyl acetate (4g)



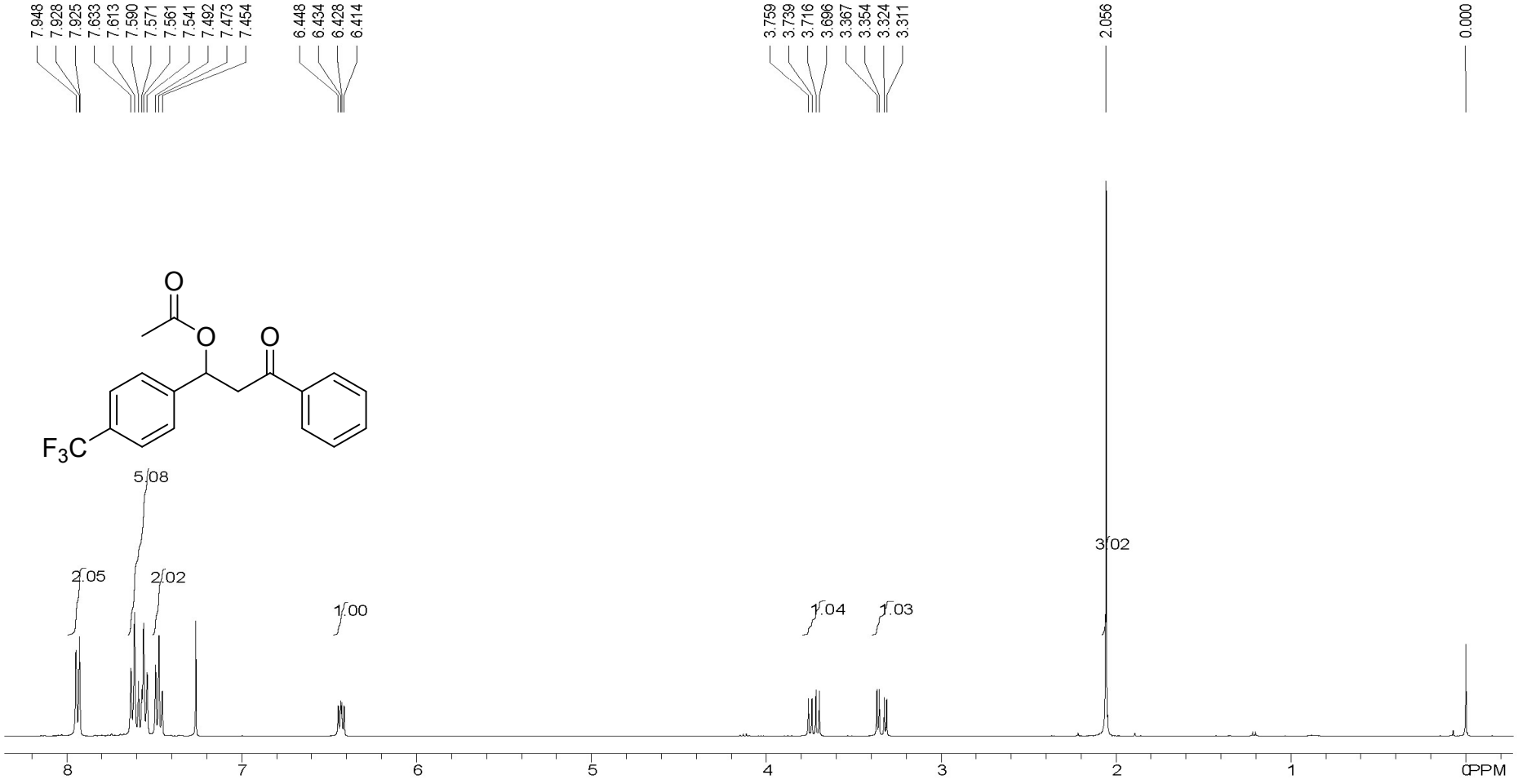
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.23-7.46 (m, 9H), 6.45 (dd, *J* = 5.7 Hz, *J* = 7.5 Hz, 1H), 3.77-3.34 (m, 2H), 2.08 (s, 3H) ppm.

1-(4-nitrophenyl)-3-oxo-3-phenylpropyl acetate (4g)



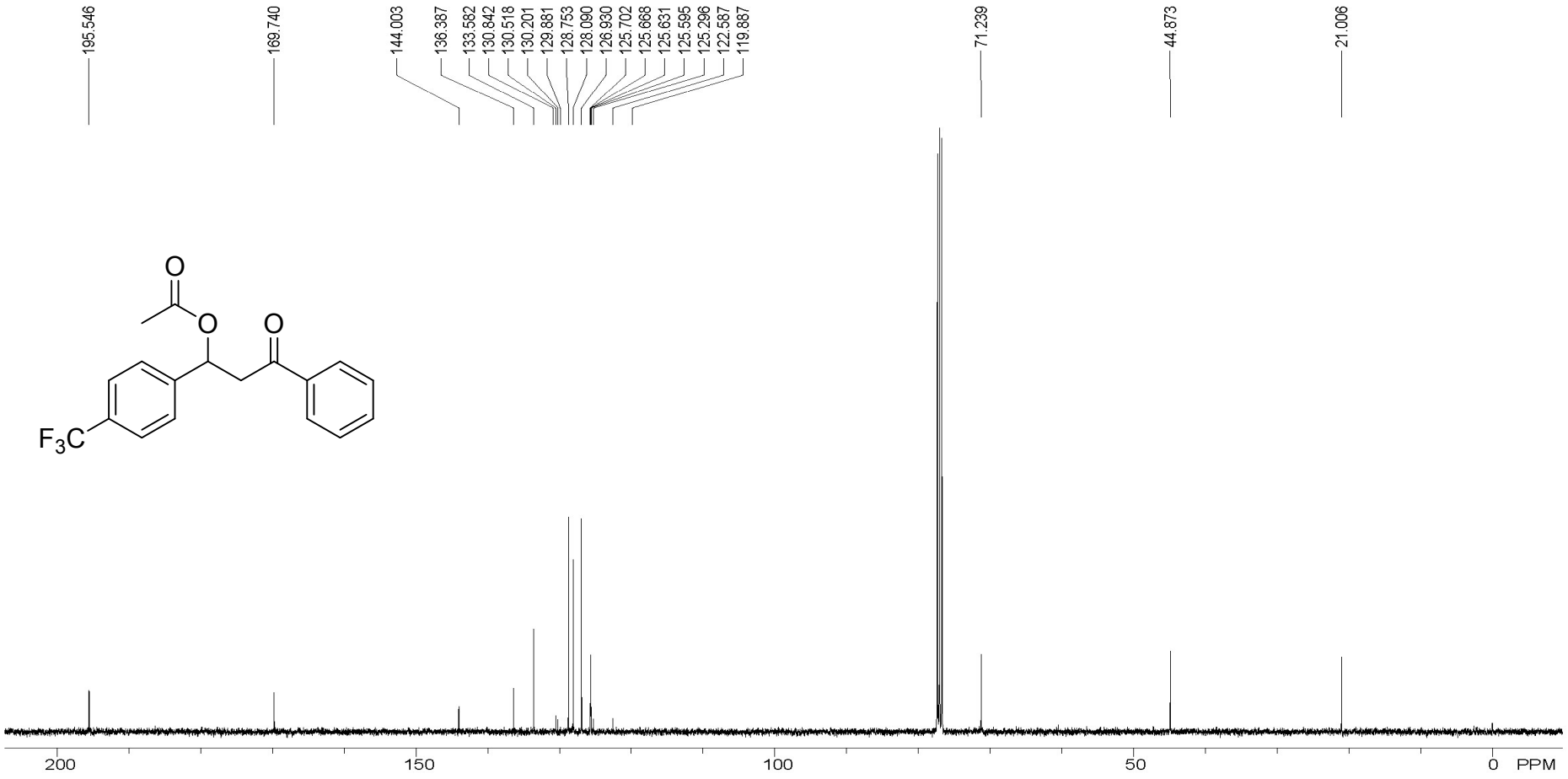
^{13}C NMR (400 MHz, $CDCl_3$) δ = 195.2, 169.7, 147.6, 147.2, 136.2, 133.7, 128.8, 128.1, 127.5, 123.9, 70.9, 44.7, 21.0 ppm.

3-oxo-3-phenyl-1-[4-(trifluoromethyl)phenyl]propyl acetate (4h)



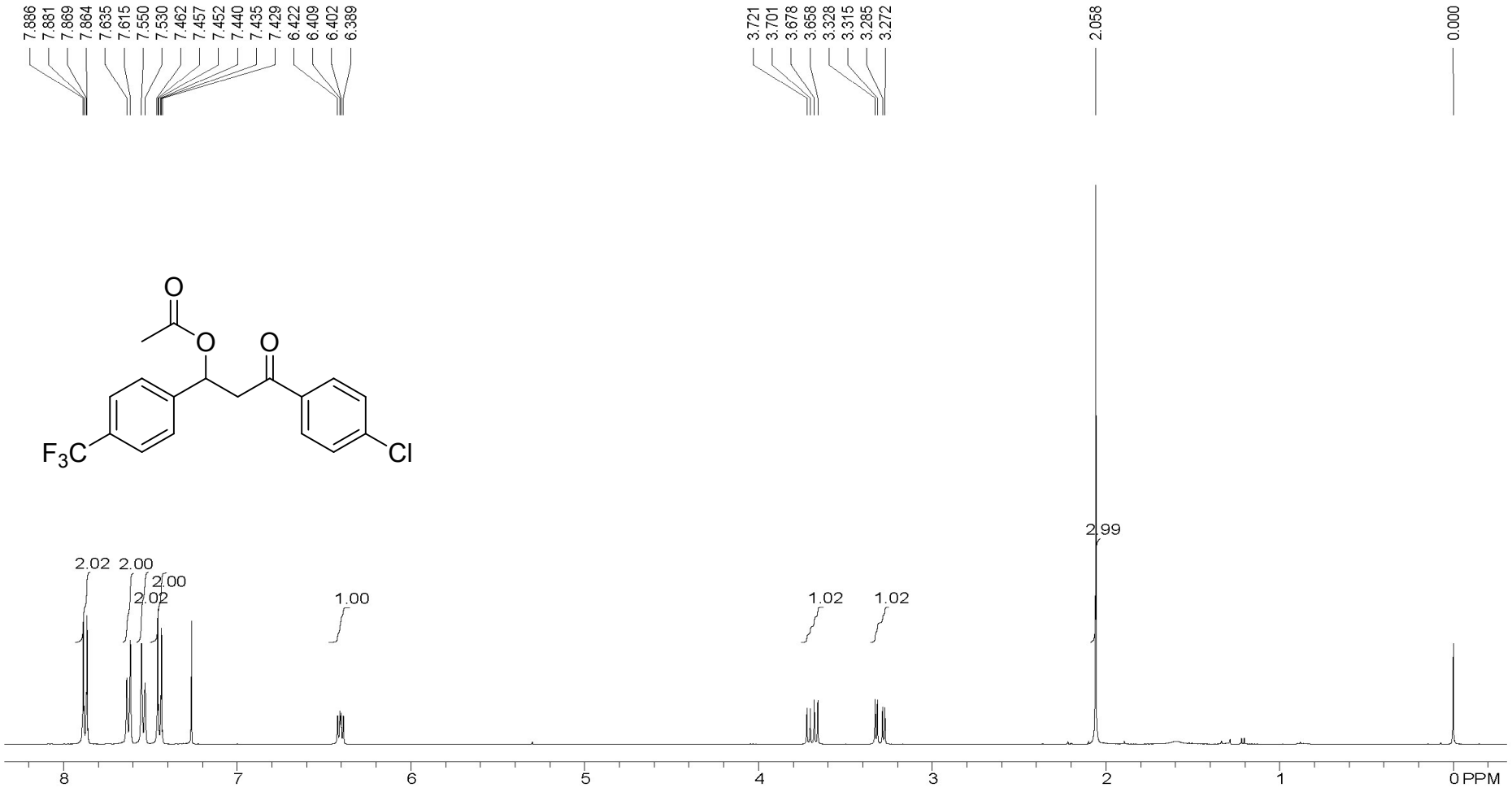
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.95-7.45 (m, 9H), 6.43 (dd, *J* = 5.4 Hz, *J* = 8.0 Hz, 1H), 3.76-3.31 (m, 2H), 2.06 (s, 3H) ppm.

3-oxo-3-phenyl-1-[4-(trifluoromethyl)phenyl]propyl acetate (4h)



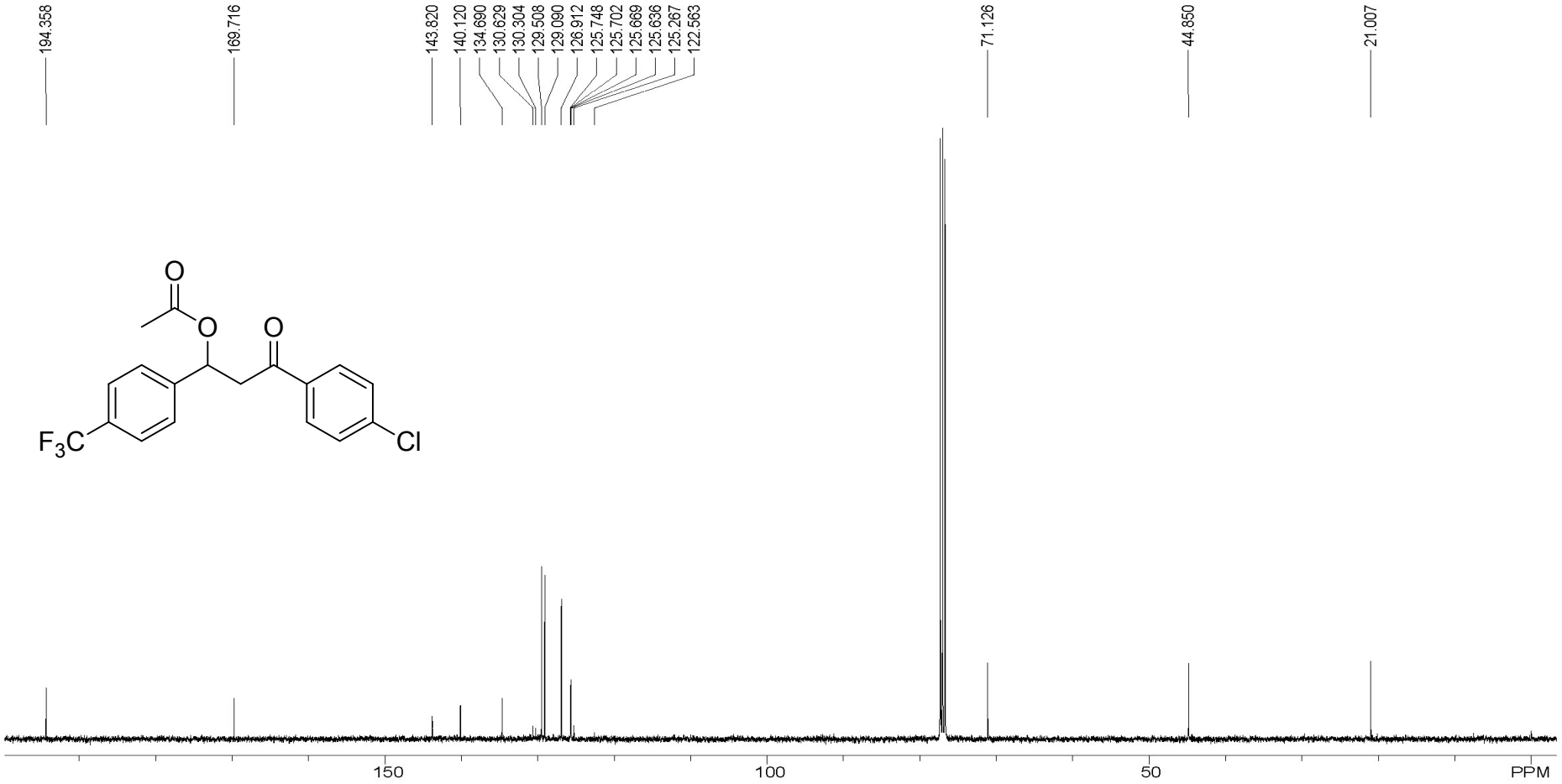
^{13}C NMR (400 MHz, $CDCl_3$) δ = 195.5, 169.7, 144.0, 136.4, 133.6, 130.4 (q, *J* = 31.9 Hz), 128.8, 128.1, 126.9, 125.6 (q, *J* = 3.6 Hz), 123.9 (q, *J* = 272.5 Hz), 71.2, 44.9, 21.0 ppm.

3-(4-chlorophenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4i)



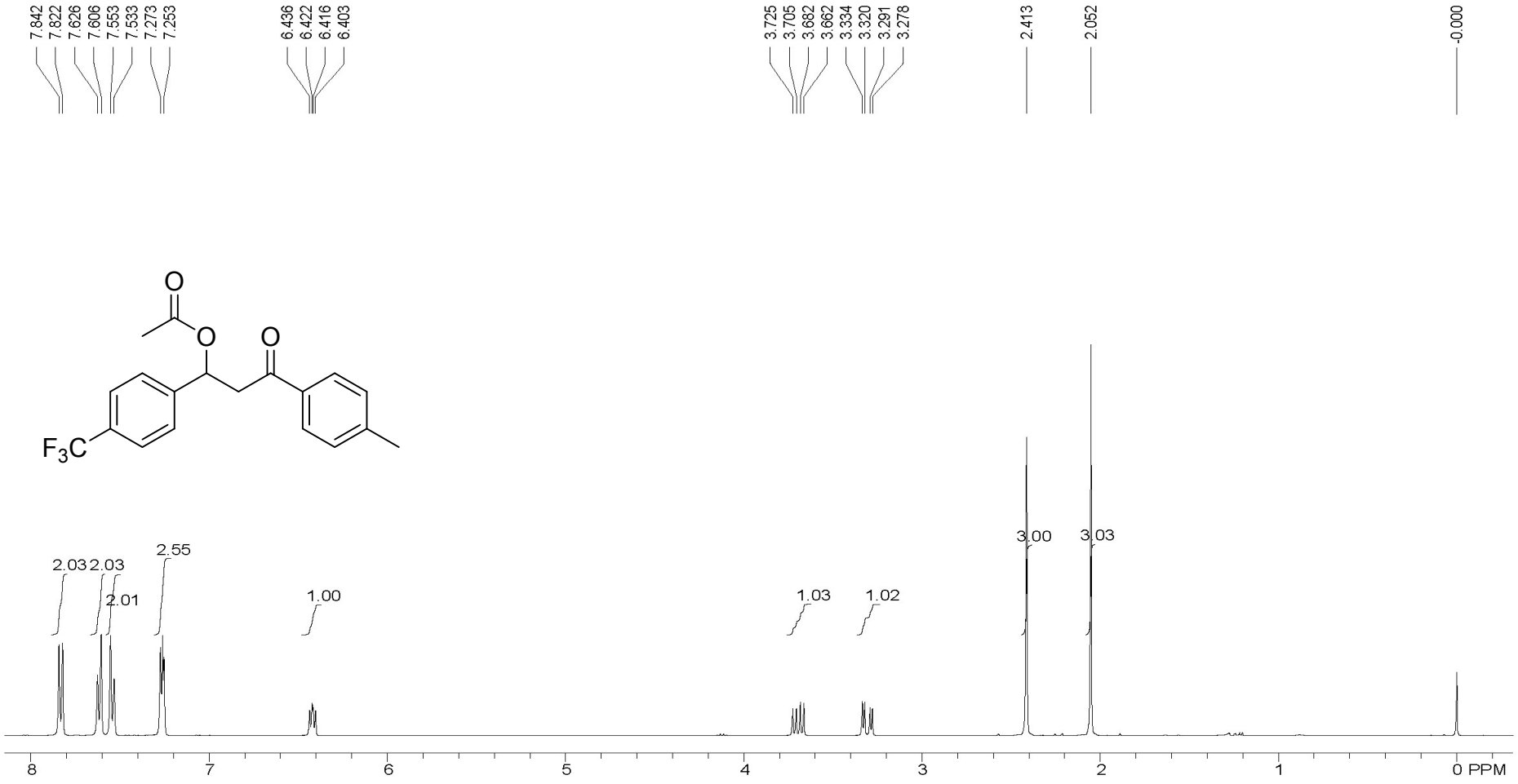
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.89-7.43 (m, 8H), 6.41 (dd, *J* = 5.1 Hz, *J* = 7.9 Hz, 1H), 3.72-3.27 (m, 2H), 2.06 (s, 3H) ppm.

3-(4-chlorophenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4i)



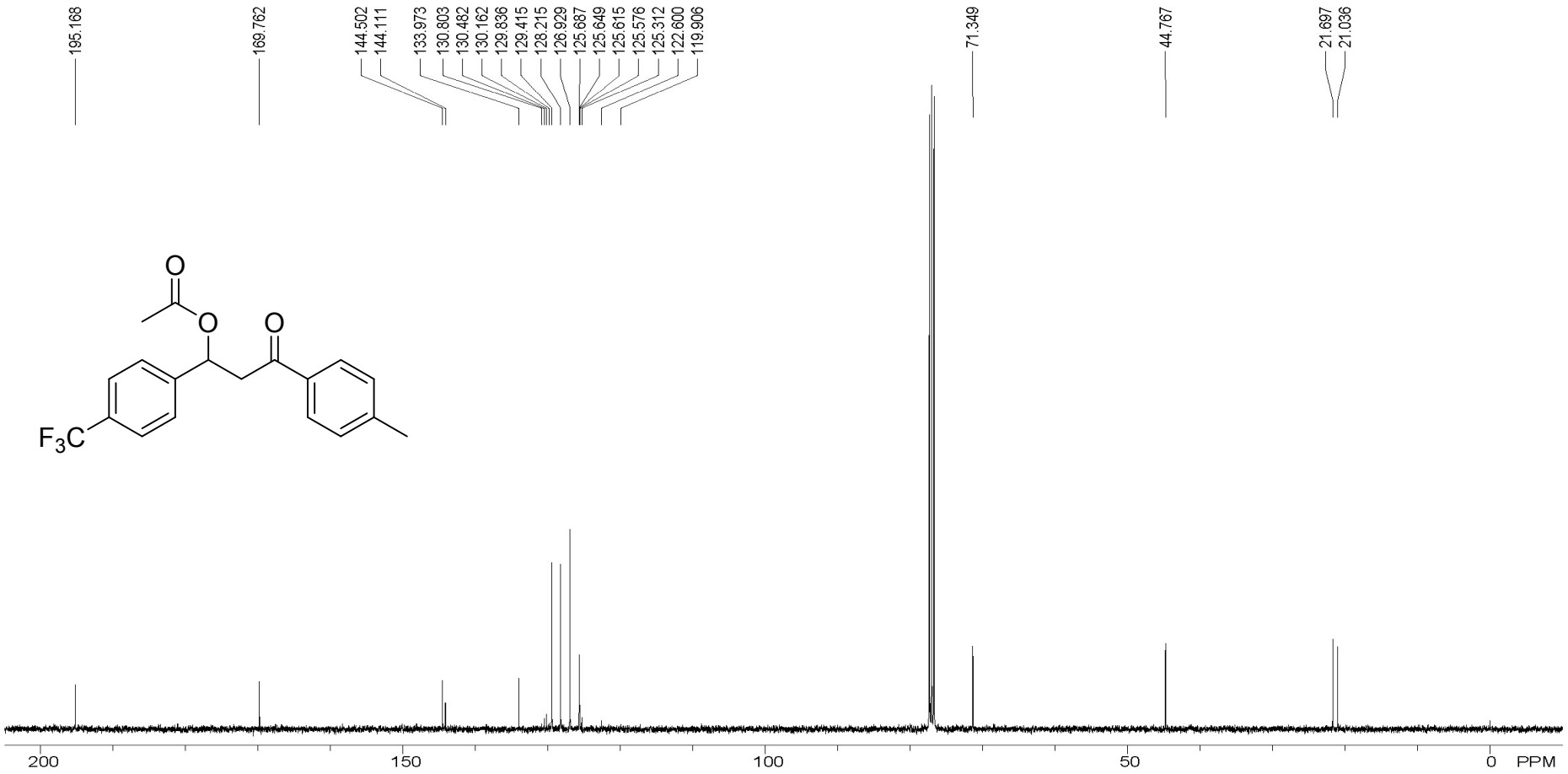
^{13}C NMR (400 MHz, $CDCl_3$) δ = 194.4, 169.7, 143.8, 140.1, 134.7, 130.4 (q, *J* = 32.7 Hz), 129.5, 129.1, 126.9, 125.7 (q, *J* = 3.8 Hz), 123.9 (q, *J* = 272.1 Hz), 71.1, 44.9, 21.0 ppm.

3-(4-methylphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4j)



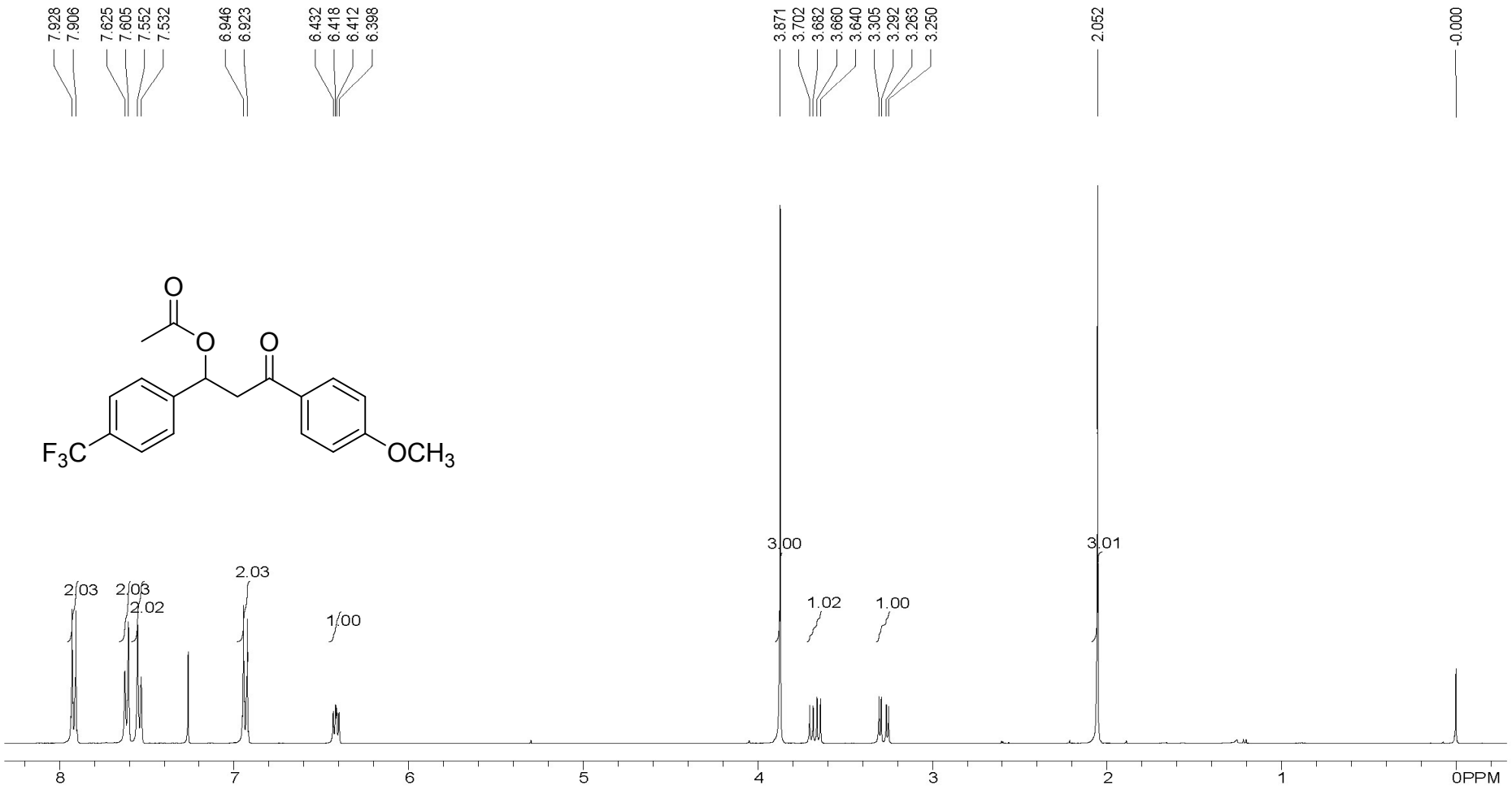
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.84-7.25 (m, 8H), 6.42 (dd, *J* = 5.4 Hz, *J* = 7.8 Hz, 1H), 3.73-3.28 (m, 2H), 2.41 (s, 3H), 2.05 (s, 3H) ppm.

3-(4-methylphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4j)



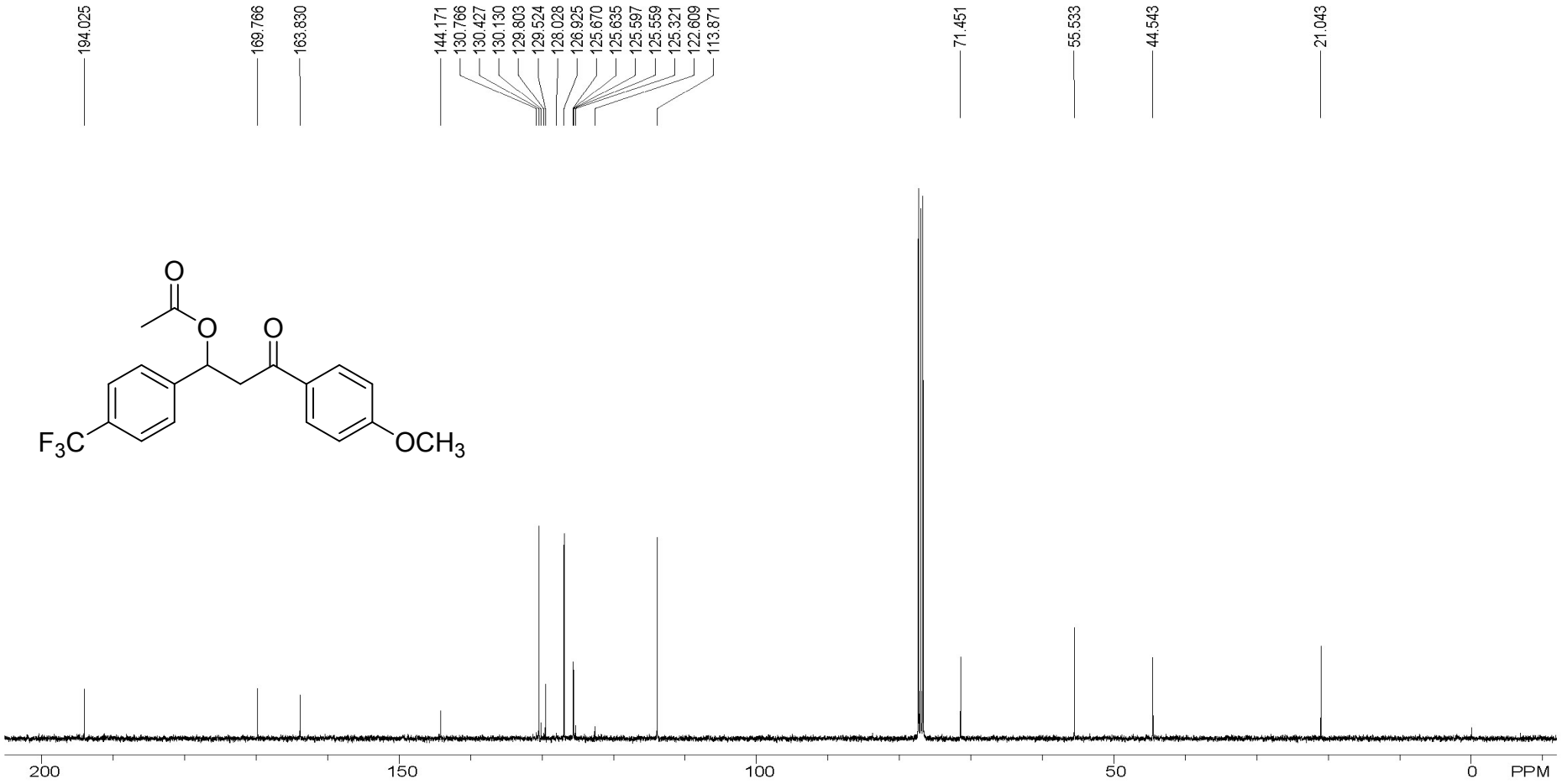
^{13}C NMR (400 MHz, $CDCl_3$) δ = 195.2, 169.8, 144.5, 144.1, 134.0, 130.3 (q, *J* = 32.2 Hz), 129.4, 128.2, 126.9, 125.6 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 272.9 Hz), 71.3, 44.8, 21.7, 21.0 ppm.

3-(4-methoxyphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4k)



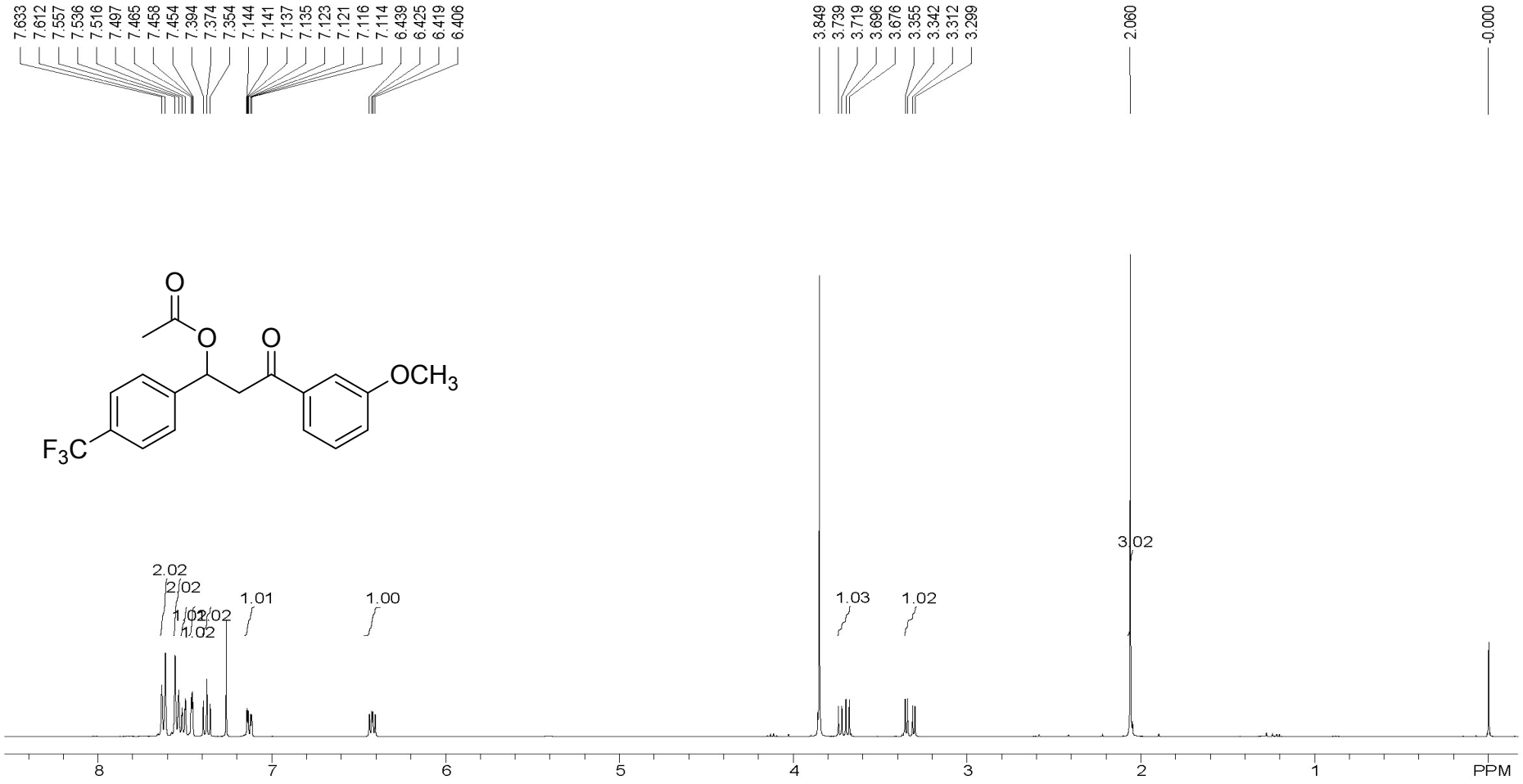
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.93-6.92 (m, 8H), 6.42 (dd, *J* = 5.4 Hz, *J* = 7.8 Hz, 1H), 3.87 (s, 3H), 3.70-3.25 (m, 2H), 2.41 (s, 3H), 2.05 (s, 3H) ppm.

3-(4-methoxyphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4k)



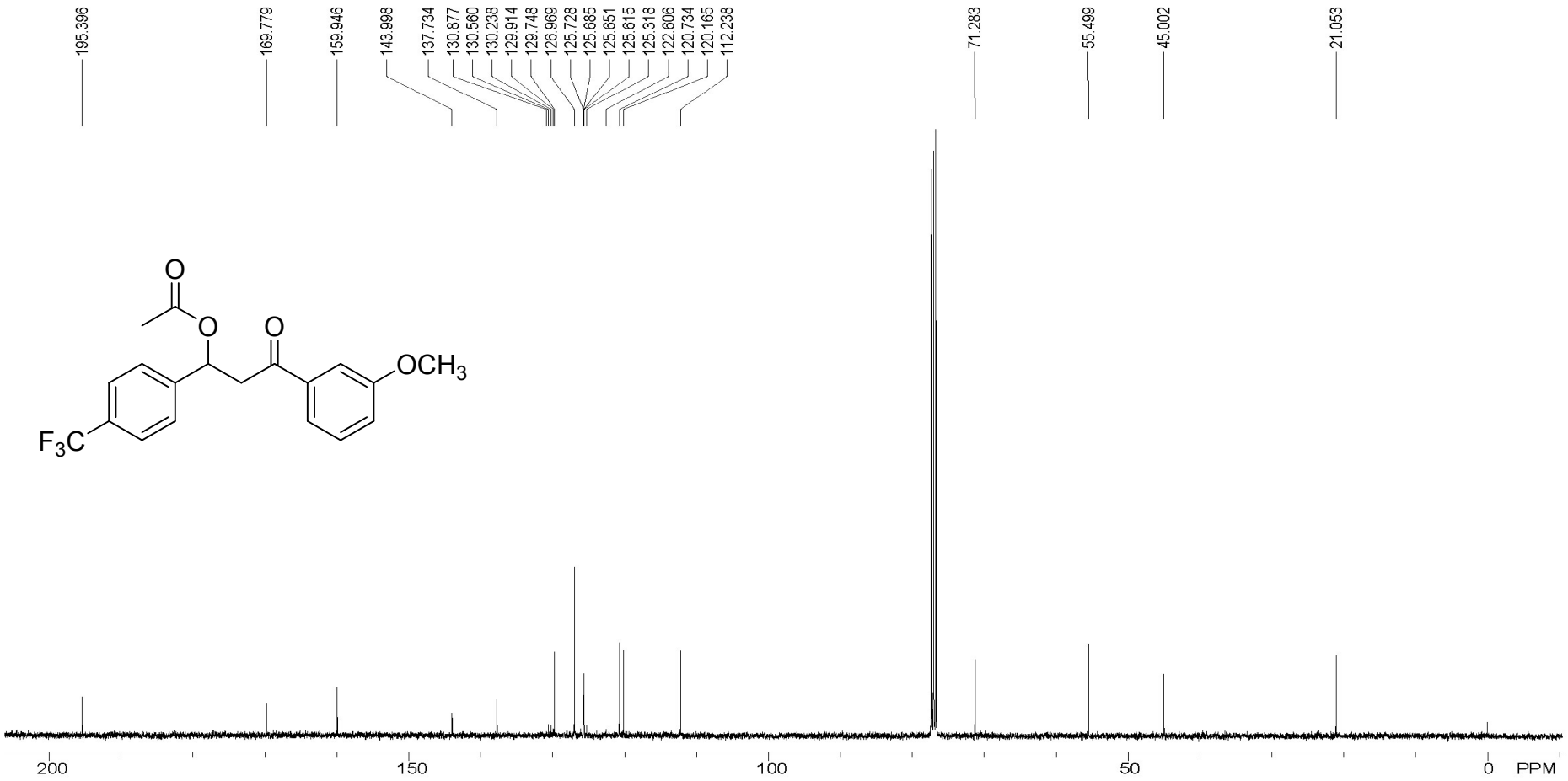
^{13}C NMR (400 MHz, $CDCl_3$) δ = 194.0, 169.8, 163.8, 144.2, 130.4, 130.3 (q, *J* = 32.3 Hz), 129.5, 126.9, 125.6 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 272.8 Hz), 113.9, 71.5, 55.5, 44.5, 21.0 ppm.

3-(3-methoxyphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl)propy] acetate (4l)



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.63-7.11 (m, 8H), 6.42 (dd, *J* = 5.4 Hz, *J* = 7.8 Hz, 1H), 3.85 (s, 3H), 3.74-3.30 (m, 2H), 2.41 (s, 3H), 2.06 (s, 3H) ppm.

3-(3-methoxyphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl)propy] acetate (4l)



^{13}C NMR (400 MHz, $CDCl_3$) δ = 195.4, 169.8, 159.9, 144.0, 137.7, 130.4 (q, *J* = 32.3 Hz), 129.7, 127.0, 125.7 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 273.0 Hz), 120.7, 120.2 112.2, 71.3, 55.5, 45.0, 21.1 ppm.

5. Chiral LC conditions

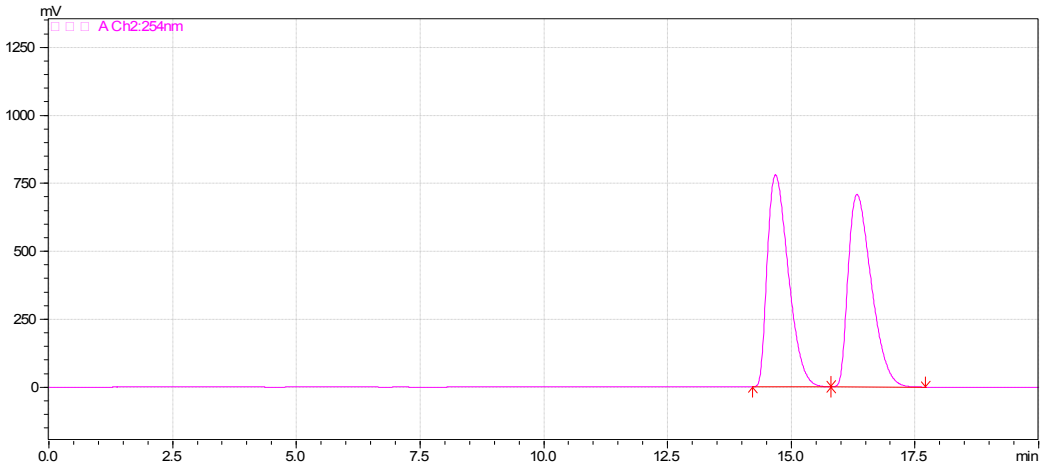
4-hydroxy-4-(4-nitrophenyl)butan-2-one (3a)

& 1-(4-nitrophenyl)-3-oxobutyl acetate (4a)

LC condition of 3a:

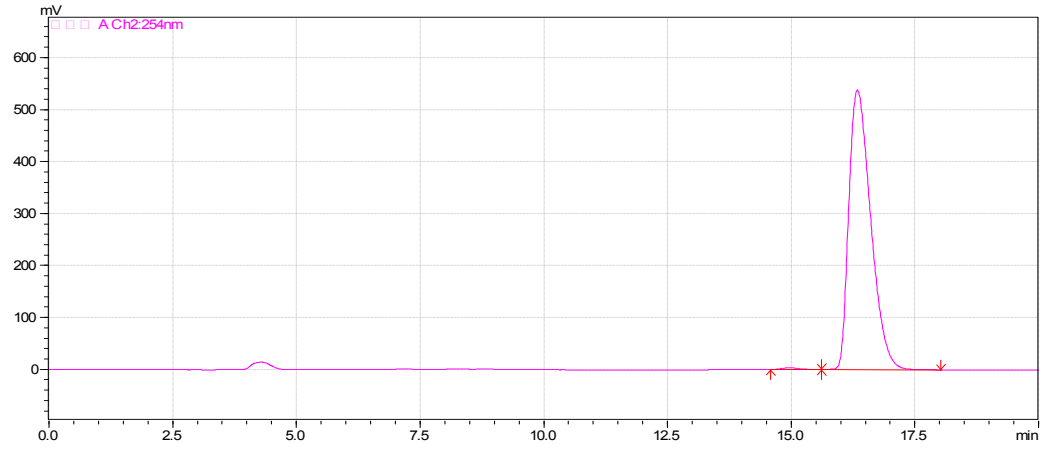
Column: OJ-H;
Eluent: Hexane/Isopropanol = 80/20, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**3a**: 16.4 min; (*R*)-**3a**: 14.7 min

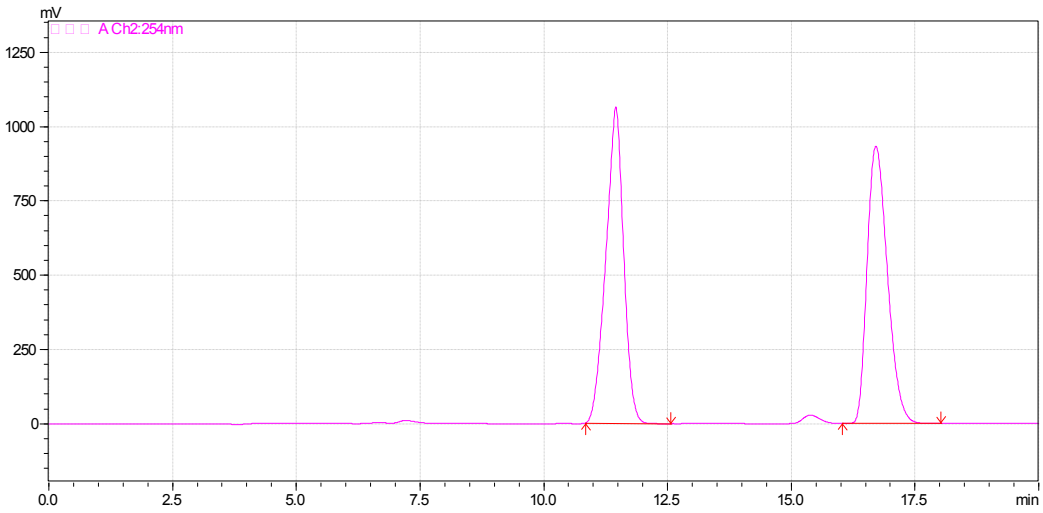
Spectrum of reaction sample



LC condition of 4a:

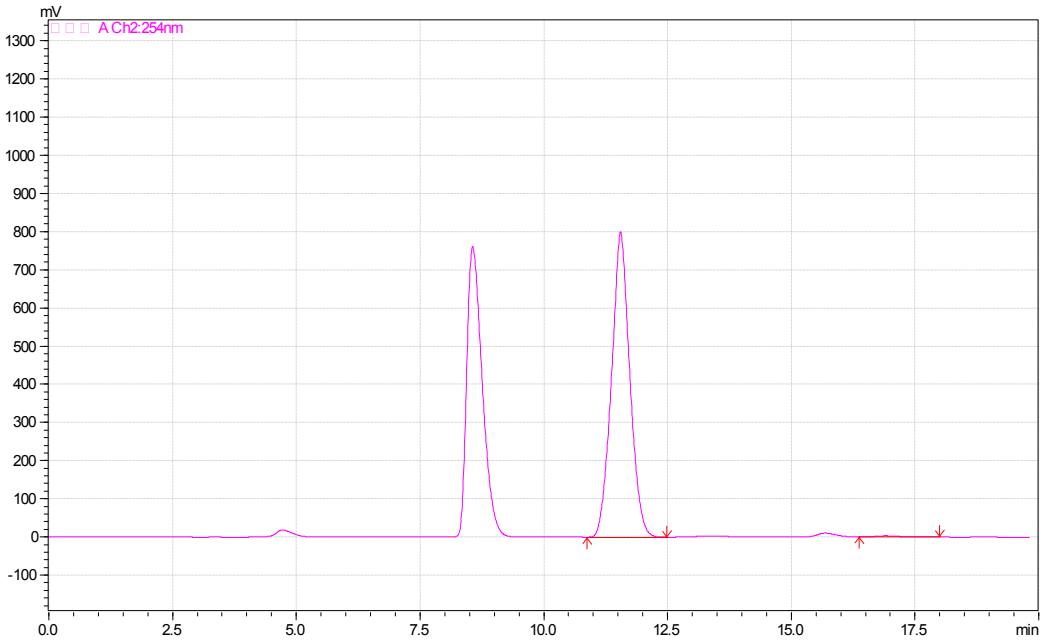
Column: AD-H;
Eluent: Hexane/Isopropanol = 70/30, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**4a**: 16.7 min; (*R*)-**4a**: 11.5 min

Spectrum of reaction sample



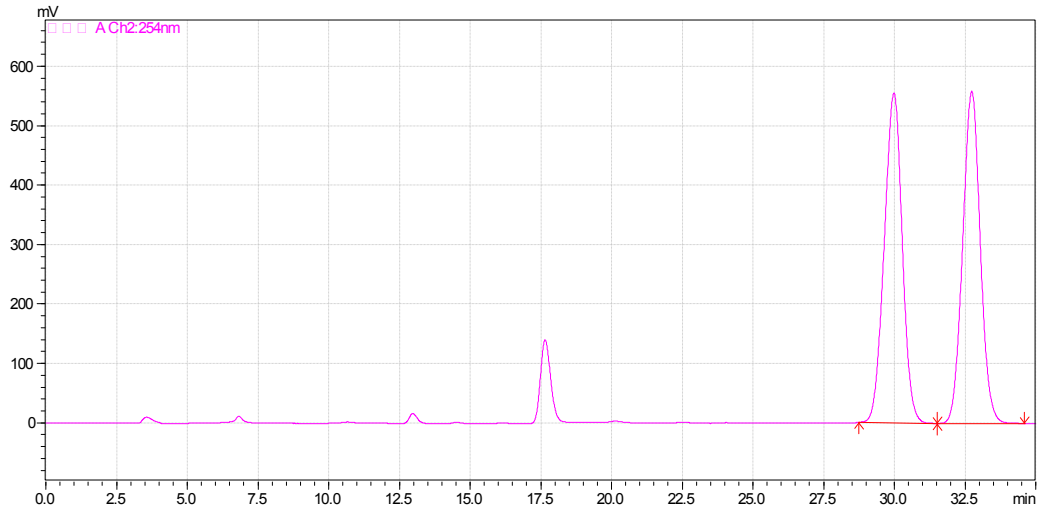
4-hydroxy-4-(3-nitrophenyl)butan-2-one (3b)

& 1-(3-nitrophenyl)-3-oxobutyl acetate (4b)

LC condition of 3b:

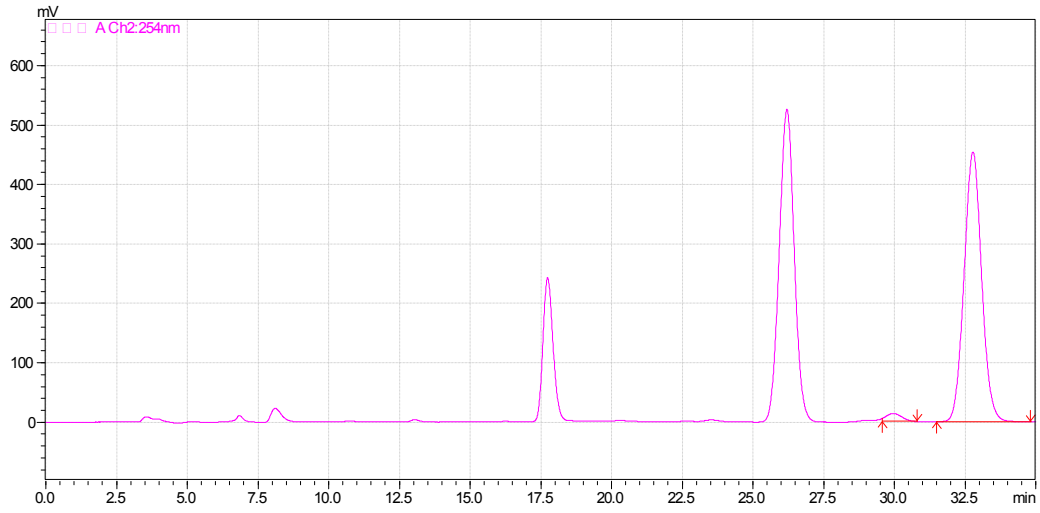
Column: AD-H;
Eluent: Hexane/Isopropanol = 95/5, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**3b**: 32.8 min; (*R*)-**3b**: 30.0 min

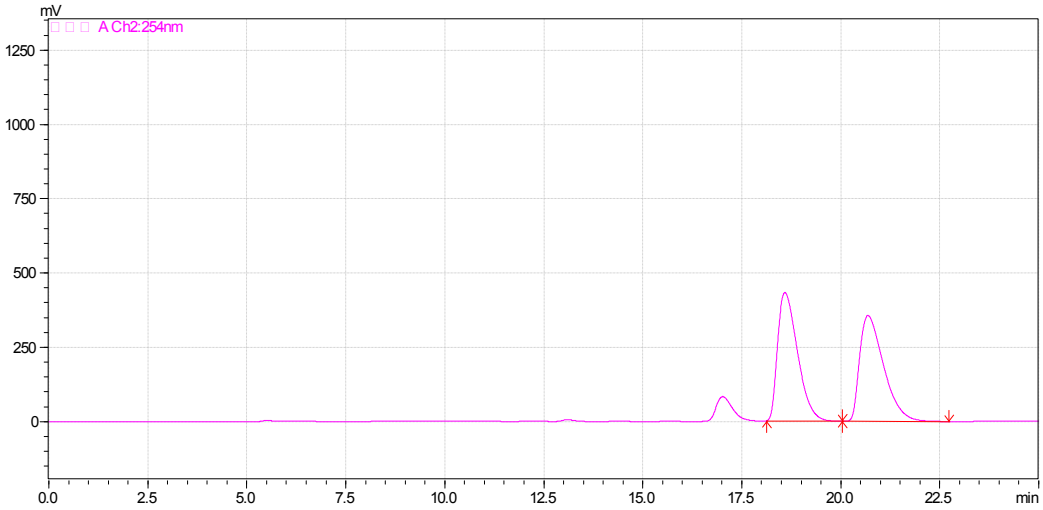
Spectrum of reaction sample



LC condition of 4b:

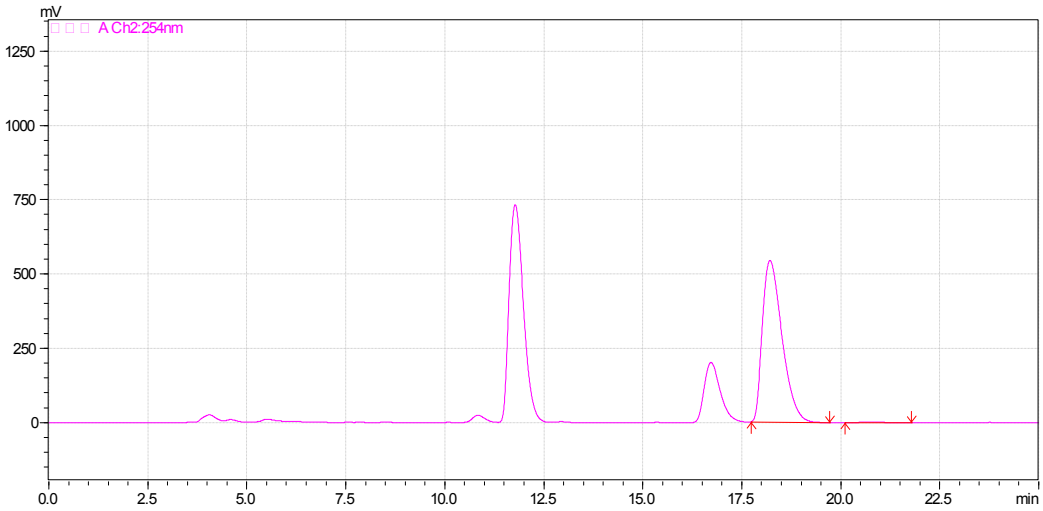
Column: OJ-H;
Eluent: Hexane/Isopropanol = 70/30, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**4b**: 20.8 min; (*R*)-**4b**: 18.6 min

Spectrum of reaction sample



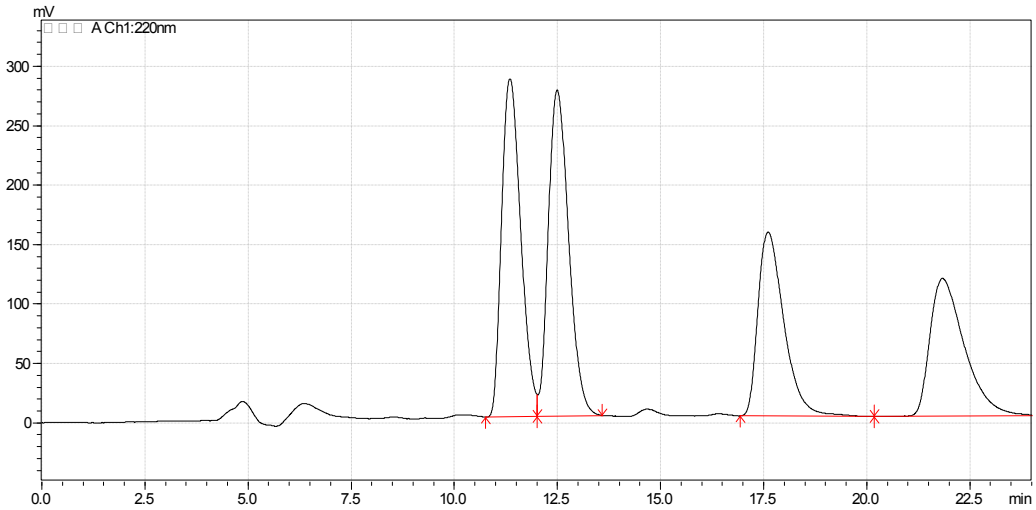
4-hydroxy-4-[4-(trifluoromethyl)phenyl]butan-2-one (3c)

& 3-oxo-1-[4-(trifluoromethyl)phenyl]butyl acetate (4c)

LC condition of 3c & 4c:

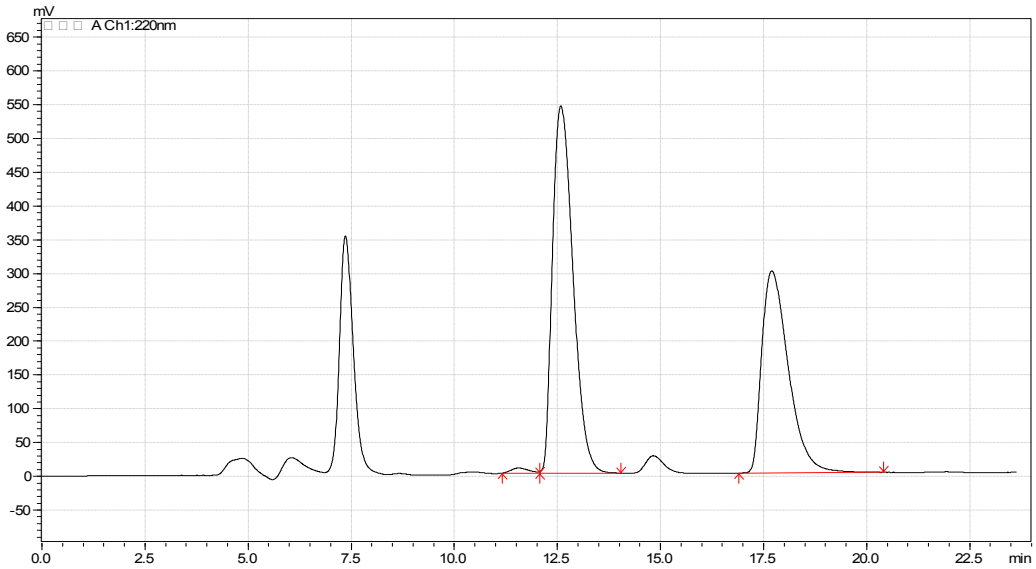
Column: OJ-H;
Eluent: Hexane/Isopropanol = 85/15, 0.8 ml min^{-1};
UV detector: 220 nm
Column temperatrue: 0°C

Spectrum of racemic standard



Retention time: (*S*)-**3c**: 17.8 min; (*R*)-**3c**: 21.9 min;
(*S*)-**4c**: 11.4 min; (*R*)-**4c**: 12.6 min

Spectrum of reaction sample



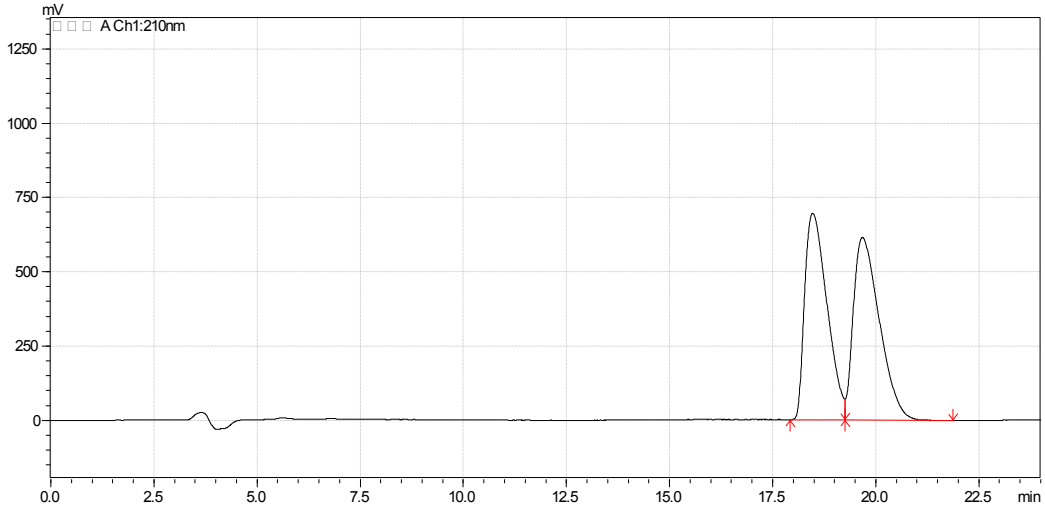
4-(4-cyanophenyl)-4-hydroxybutan-2-one (3d)

& 1-(4-cyanophenyl)-3-oxobutyl acetate (4d)

LC condition of 3d:

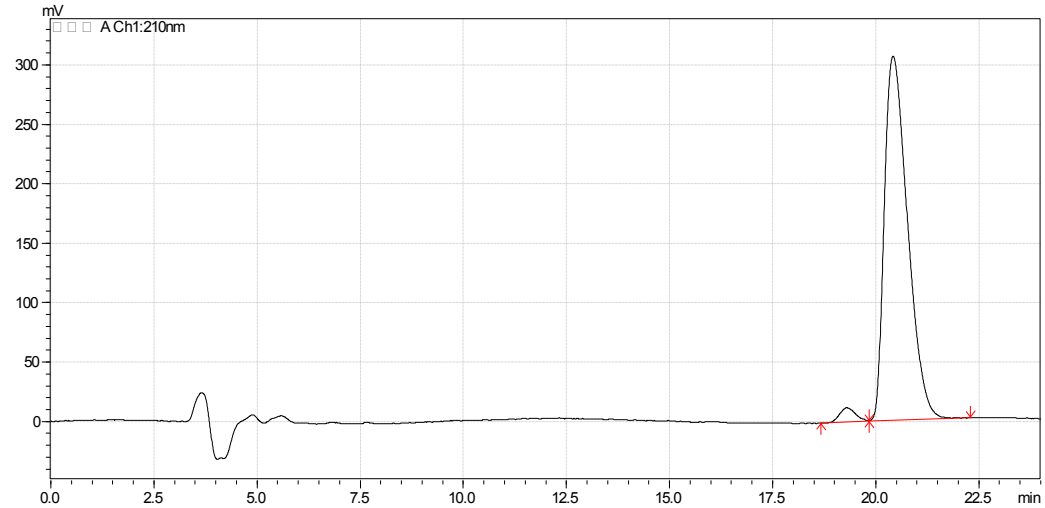
Column: OJ-H;
Eluent: Hexane/Isopropanol = 85/15, 1.0 ml min^{-1};
UV detector: 210 nm

Spectrum of racemic standard



Retention time: (*S*)-**3d**: 19.8 min; (*R*)-**3d**: 18.5 min

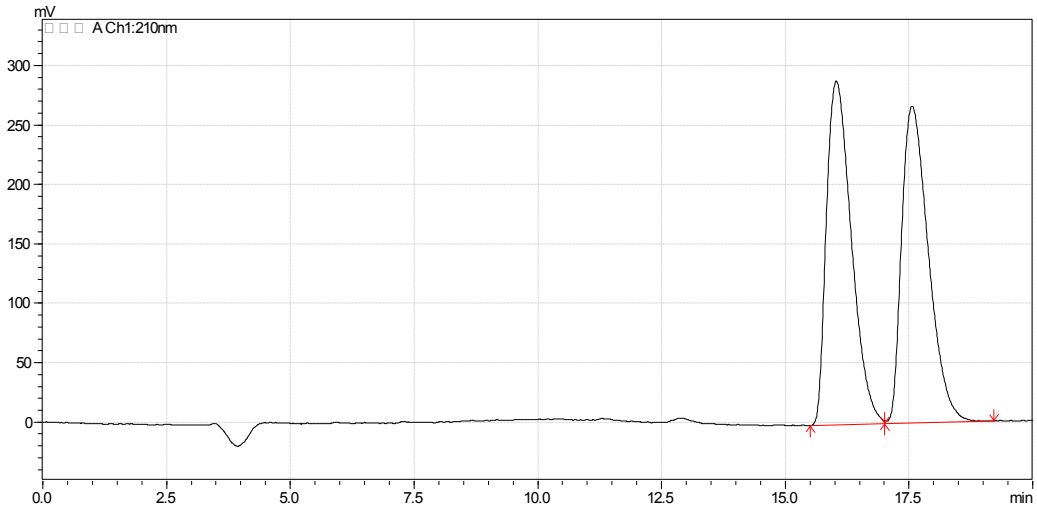
Spectrum of reaction sample



LC condition of 4d:

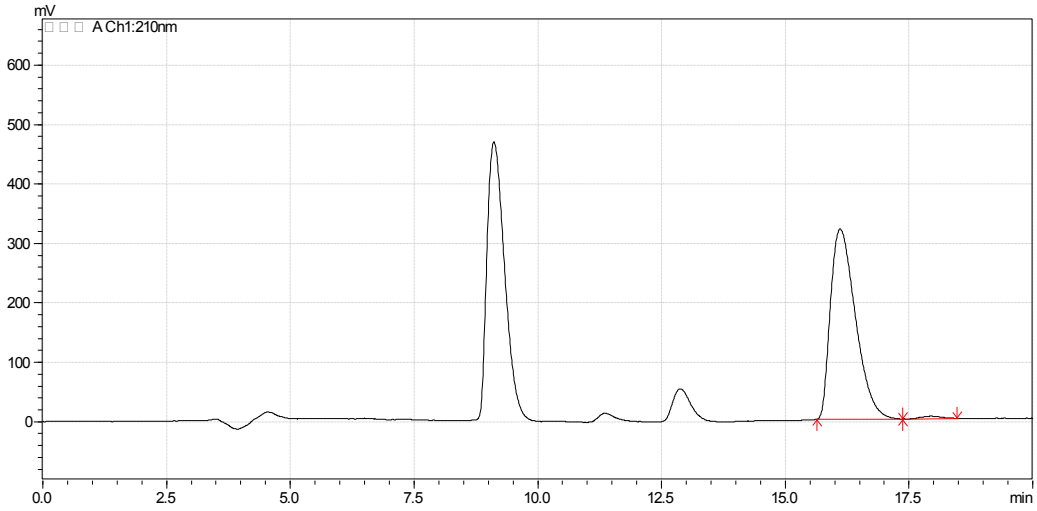
Column: OJ-H;
Eluent: Hexane/Isopropanol = 70/30, 1.0 ml min^{-1};
UV detector: 210 nm

Spectrum of racemic standard



Retention time: (*S*)-**4d**: 17.6 min; (*R*)-**4d**: 16.2 min

Spectrum of reaction sample



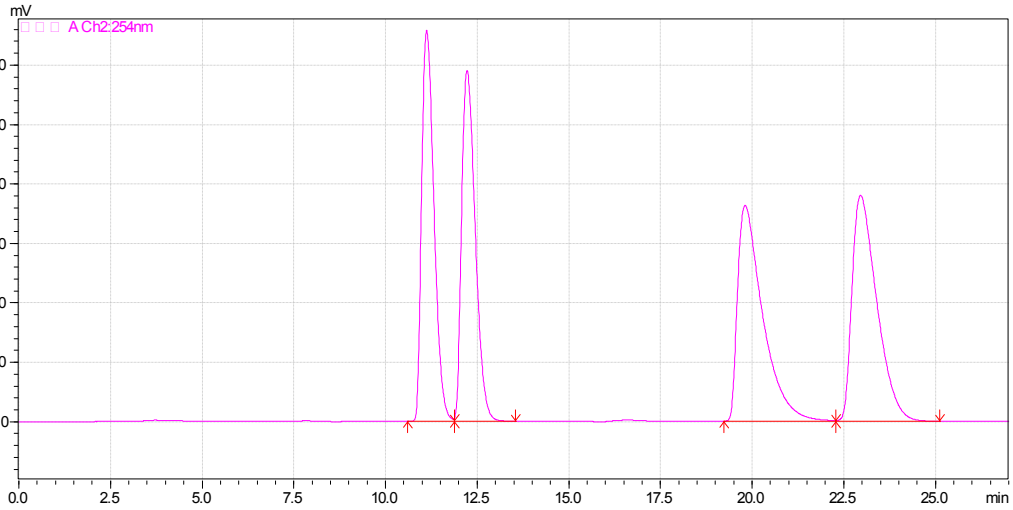
1-hydroxy-1-(4-nitrophenyl)hexan-3-one (3e)

& 1-(4-nitrophenyl)-3-oxohexyl acetate (4e)

LC condition of 3e & 4e:

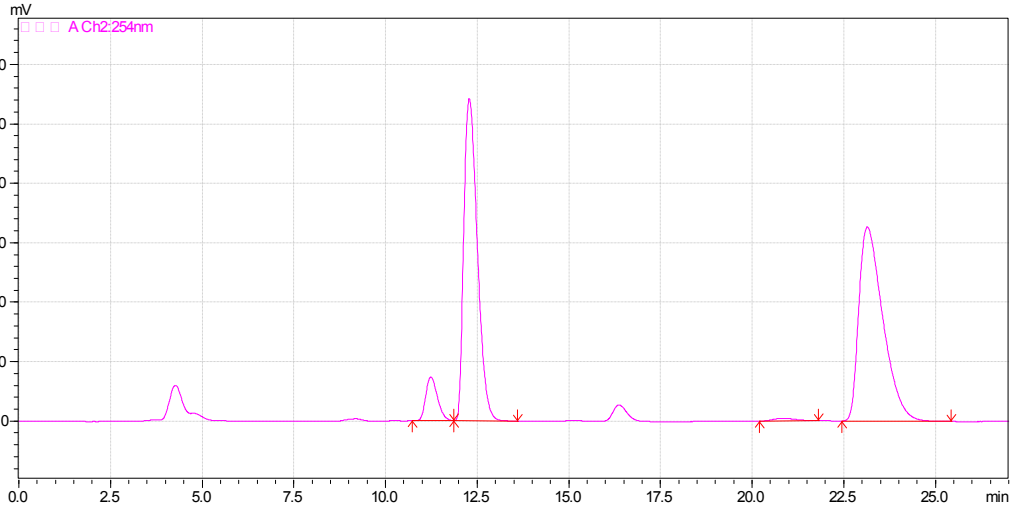
Column: OJ-H;
Eluent: Hexane/Isopropanol = 80/20, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**3e**: 12.3 min; (*R*)-**3e**: 11.1 min;
(*S*)-**4e**: 19.8 min; (*R*)-**4e**: 23.0 min

Spectrum of reaction sample



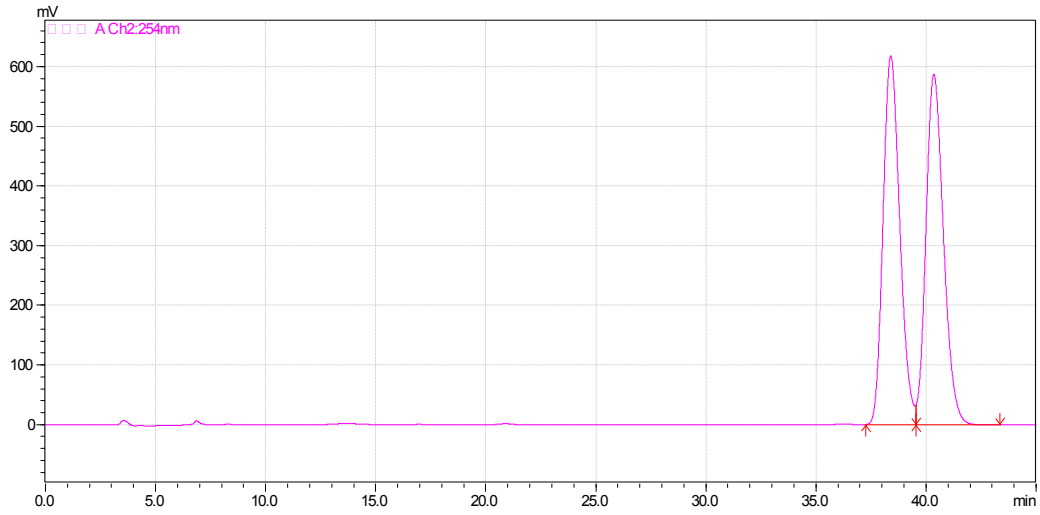
1-cyclopropyl-3-hydroxy-3-(4-nitrophenyl)propan-1-one (3f)

& 3-cyclopropyl-1-(4-nitrophenyl)-3-oxopropyl acetate (4f)

LC condition of 3f:

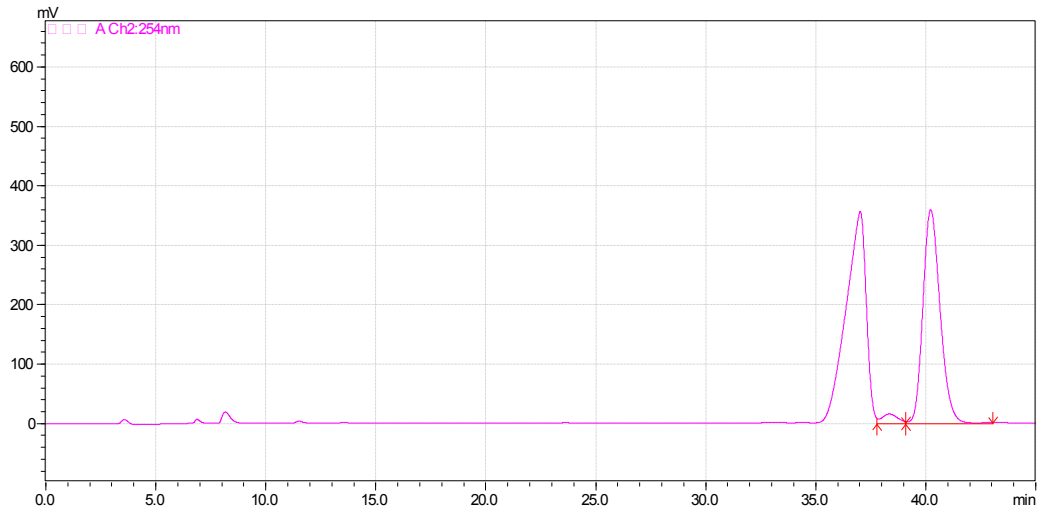
Column: AD-H;
Eluent: Hexane/Isopropanol = 95/5, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**3f**: 40.4 min; (*R*)-**3f**: 38.4 min

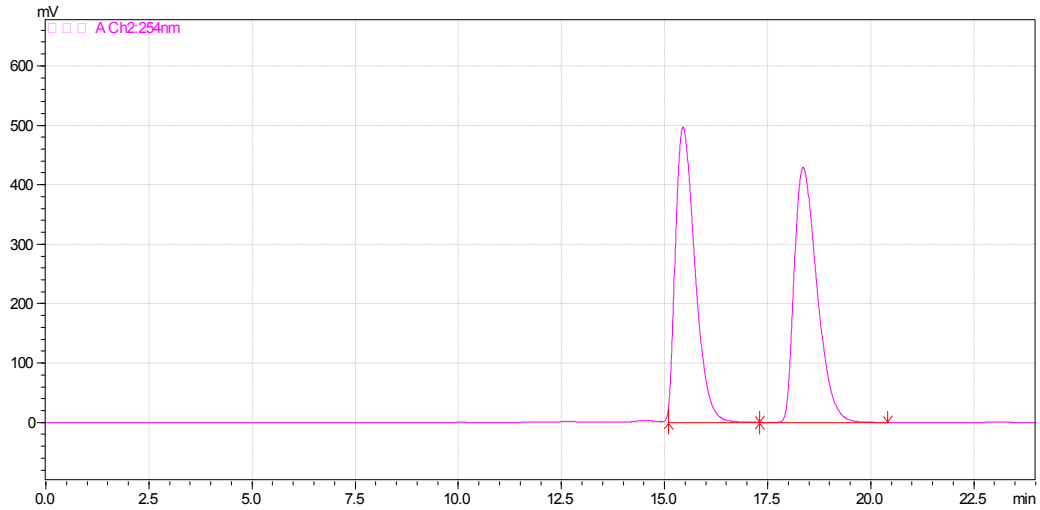
Spectrum of reaction sample



LC condition of 4f:

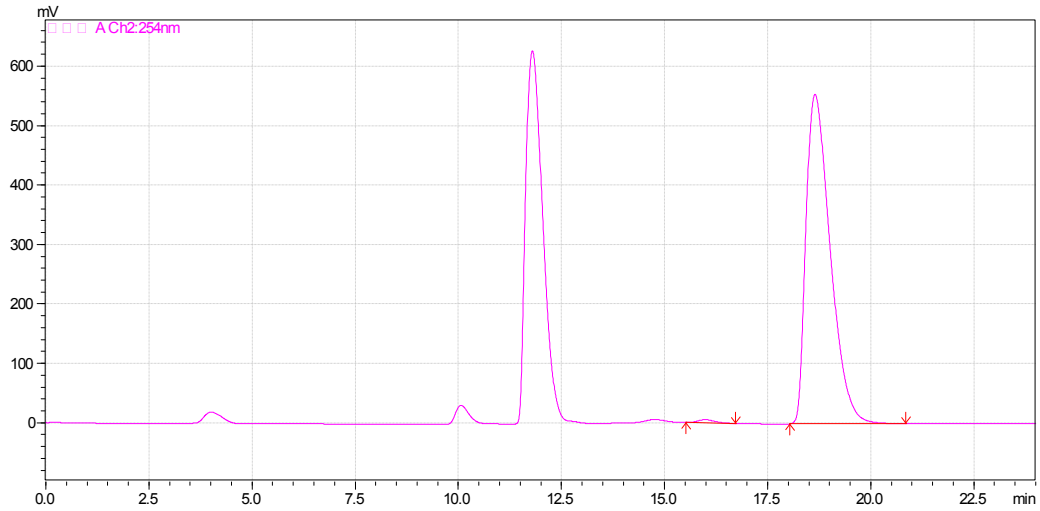
Column: OJ-H;
Eluent: Hexane/Isopropanol = 70/30, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**4f**: 15.5 min; (*R*)-**4f**: 18.7 min

Spectrum of reaction sample



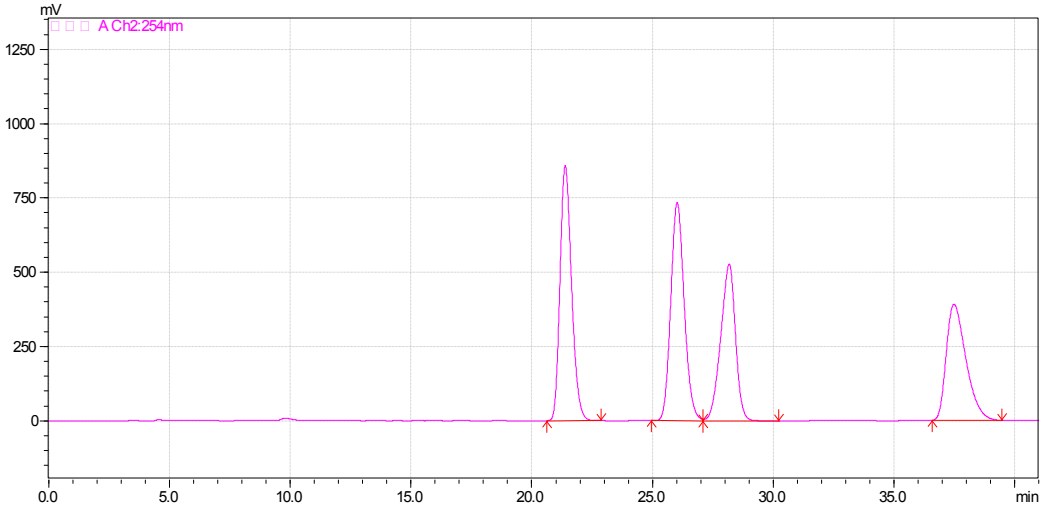
3-hydroxy-3-(4-nitrophenyl)-1-phenylpropan-1-one (3g)

& 1-(4-nitrophenyl)-3-oxo-3-phenylpropyl acetate (4g)

LC condition of 3g & 4g:

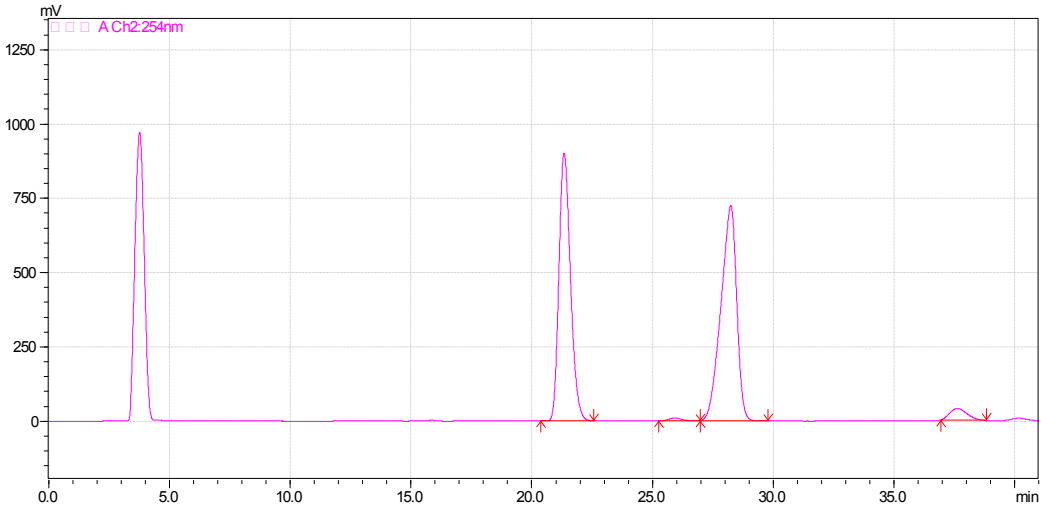
Column: AD-H;
Eluent: Hexane/Isopropanol = 85/15, 1.0 ml min^{-1};
UV detector: 254 nm

Spectrum of racemic standard



Retention time: (*S*)-**3g**: 21.4 min; (*R*)-**3g**: 26.0 min;
(*S*)-**4g**: 37.6 min; (*R*)-**4g**: 28.2 min

Spectrum of reaction sample



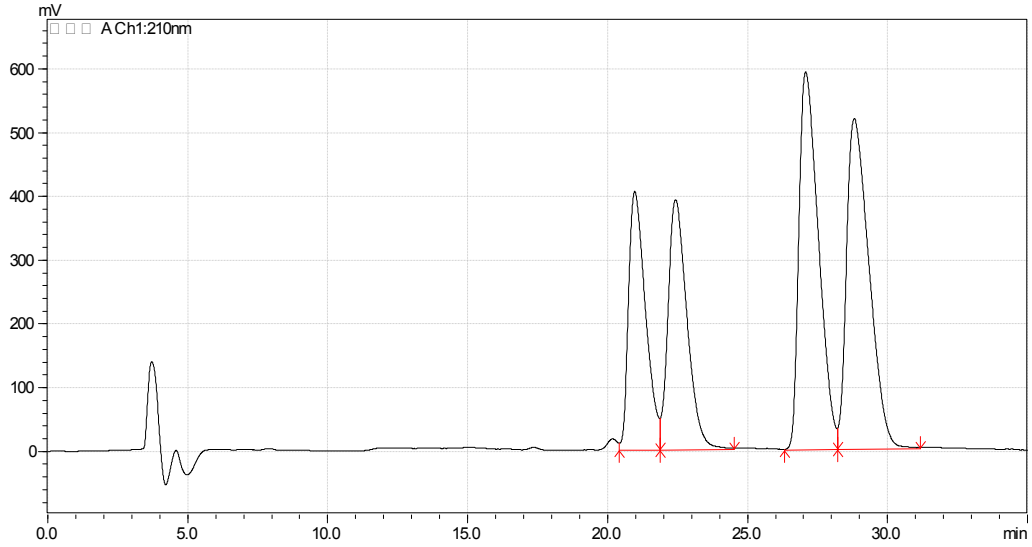
3-hydroxy-1-phenyl-3-[4-(trifluoromethyl)phenyl]propan-1-one (3h)

& 3-oxo-3-phenyl-1-[4-(trifluoromethyl)phenyl]propyl acetate (4h)

LC condition of 3h & 4h:

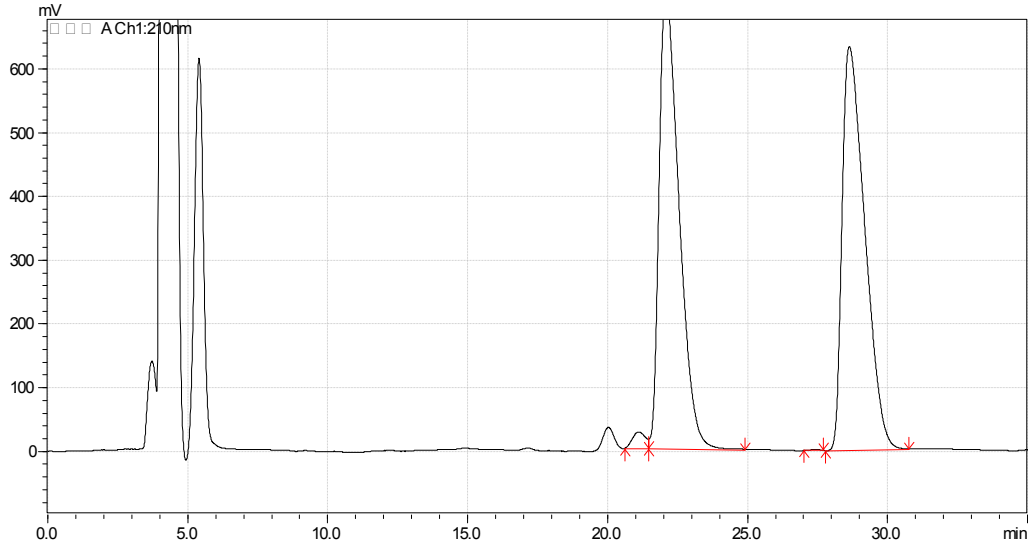
Column: OJ-H;
Eluent: Hexane/Isopropanol = 95/5, 1.0 ml min^{-1};
UV detector: 210 nm

Spectrum of racemic standard



Retention time: (*S*)-**3h**: 28.7 min; (*R*)-**3h**: 27.1 min;
(*S*)-**4h**: 21.0 min; (*R*)-**4h**: 22.2 min

Spectrum of reaction sample



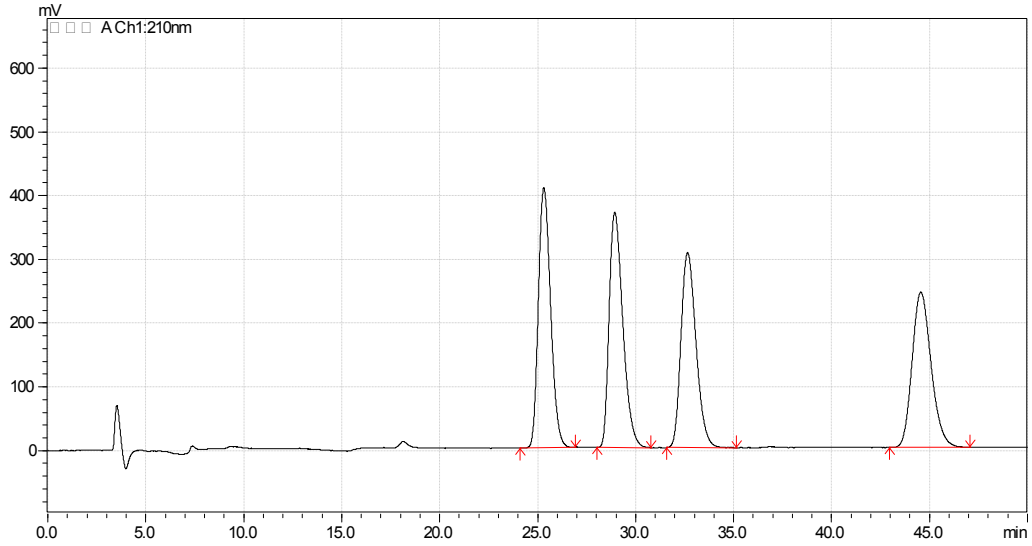
1-(4-chlorophenyl)-3-hydroxy-3-[4-(trifluoromethyl)phenyl]propan-1-one (3i)

& 3-(4-chlorophenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4i)

LC condition of 3i & 4i:

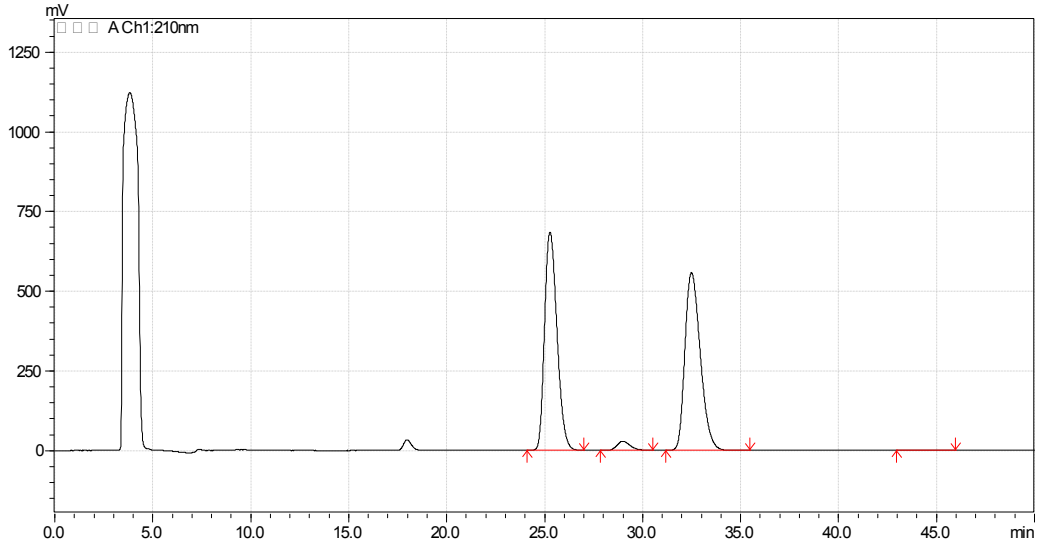
Column: AD-H;
Eluent: Hexane/Isopropanol = 95/5, 1.0 ml min^{-1};
UV detector: 210 nm

Spectrum of racemic standard



Retention time: (*S*)-**3i**: 32.5 min; (*R*)-**3i**: 44.6 min;
(*S*)-**4i**: 29.0 min; (*R*)-**4i**: 25.3 min

Spectrum of reaction sample



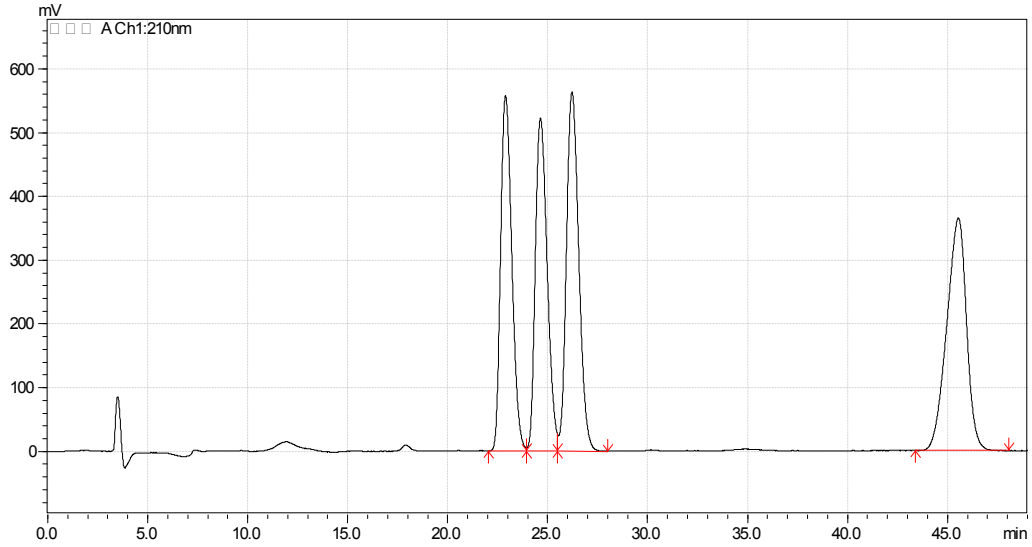
3-hydroxy-1-(4-methylphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3j)

& 3-(4-methylphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4j)

LC condition of 3j & 4j:

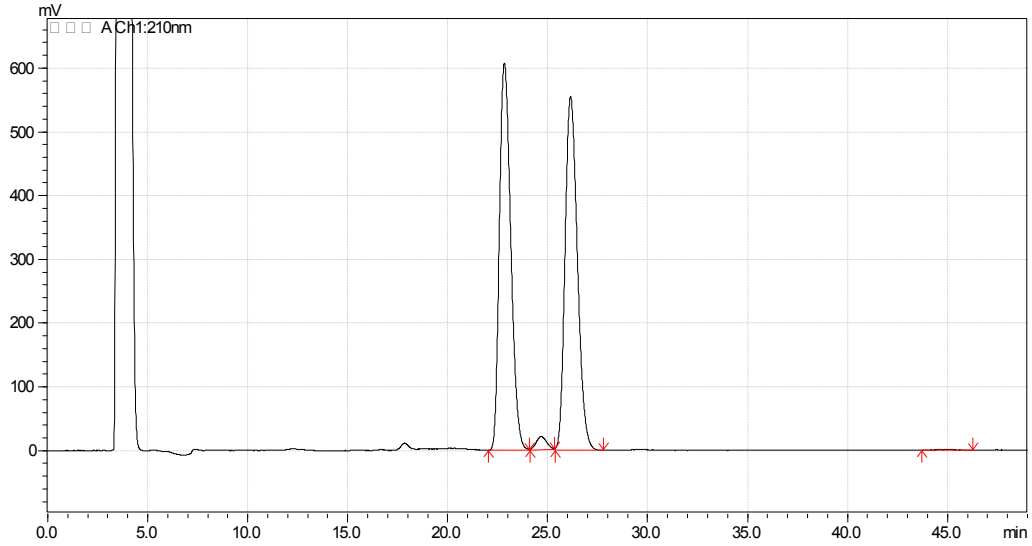
Column: AD-H;
Eluent: Hexane/Isopropanol = 96/4, 1.0 ml min^{-1};
UV detector: 210 nm

Spectrum of racemic standard



Retention time: (*S*)-**3j**: 26.3 min; (*R*)-**3j**: 45.6 min;
(*S*)-**4j**: 24.7 min; (*R*)-**4j**: 22.9 min

Spectrum of reaction sample



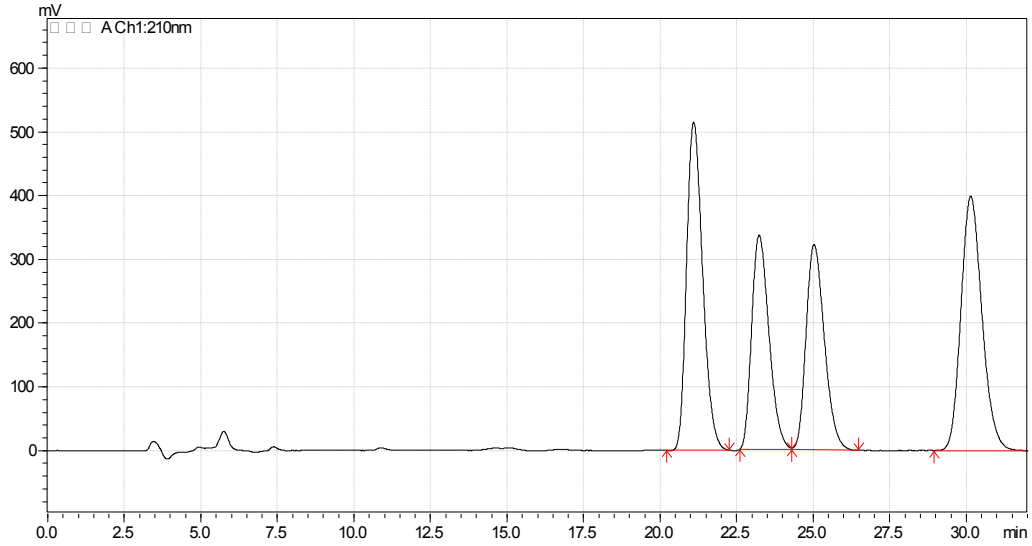
3-hydroxy-1-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3k)

& 3-(4-methoxyphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl acetate (4k)

LC condition of 3k & 4k:

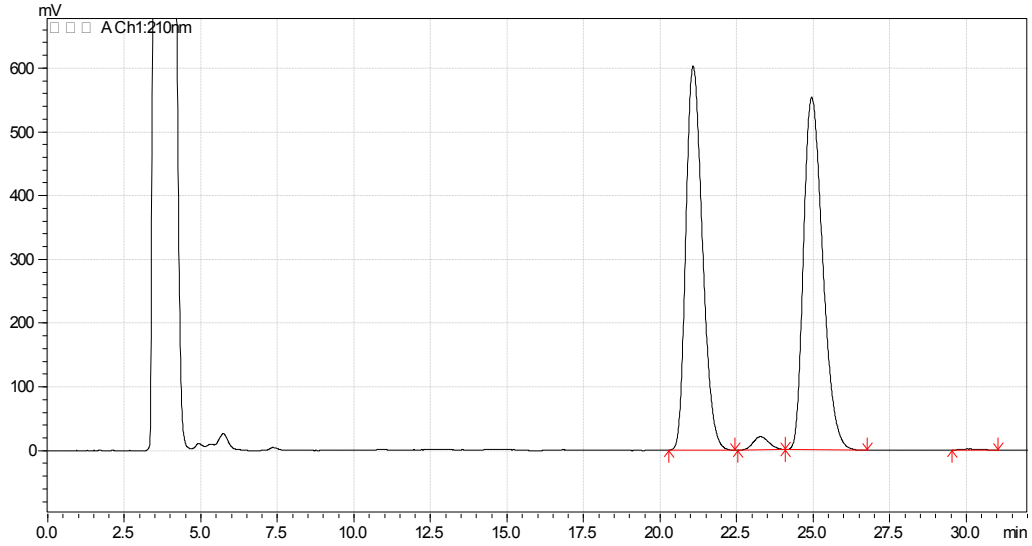
Column: AD-H;
Eluent: Hexane/Isopropanol = 90/10, 1.0 ml min^{-1};
UV detector: 210 nm

Spectrum of racemic standard



Retention time: (*S*)-**3k**: 21.1 min; (*R*)-**3k**: 30.2 min;
(*S*)-**4k**: 23.2 min; (*R*)-**4k**: 25.0 min

Spectrum of reaction sample



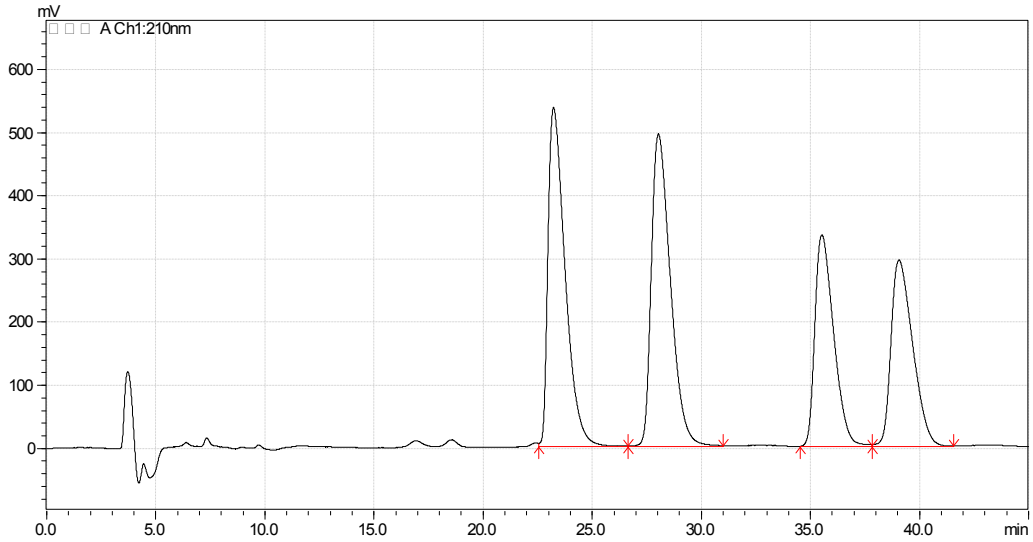
3-hydroxy-1-(3-methoxyphenyl)-3-[4-(trifluoromethyl)phenyl]propan-1-one (3l)

& 3-(3-methoxyphenyl)-3-oxo-1-[4-(trifluoromethyl)phenyl)propy] acetate (4l)

LC condition of 3l & 4l:

Column: OJ-H;
Eluent: Hexane/Isopropanol = 94/6, 1.0 ml min^{-1};
UV detector: 210 nm

Spectrum of racemic standard



Retention time: (*S*)-**3l**: 35.6 min; (*R*)-**3l**: 39.1 min;
(*S*)-**4l**: 23.3 min; (*R*)-**4l**: 28.1 min

Spectrum of reaction sample