

Supplementary Information

Facile One-Pot Synthesis of Ketones from Primary Alcohols Under Mild Condition

Tien Tan Bui,^{a,b} and Hee-Kwon Kim^{*a,b}

^a Department of Nuclear Medicine, Molecular Imaging & Therapeutic Medicine Research Center, Jeonbuk National University Medical School and Hospital, Jeonju, 54907, Republic of Korea

^bResearch Institute of Clinical Medicine of Jeonbuk National University-Biomedical Research Institute of Jeonbuk National University Hospital, Jeonju, 54907, Republic of Korea

* Corresponding author.

Hee-Kwon Kim: Tel: +82 63 250 2768; Fax: +82 63 255 1172.

E-mail address: hkkim717@jbnu.ac.kr (H. Kim).

Table of Contents

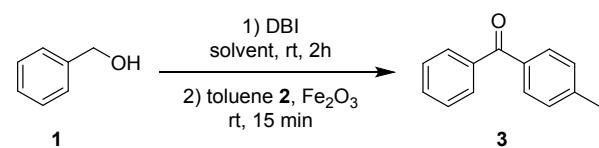
1.General Information	S2
2.Screening of reaction conditions for the preparation of ketones	S3
3.General procedure of the synthesis of ketones	S4
4.General procedure of the synthesis of anhydrides, esters, and amides	S4
5.Characterization of ketones, anhydrides, esters, and amides	S5
6. ^1H and ^{13}C NMR Spectra.....	S16

1.General Information

Commercial chemicals and solvents were used without any purification. Reaction progress was analyzed by thin-layer chromatography (TLC) using silica gel 60 F₂₅₄ pre-coated aluminum plate from Merck and TLC spots were observed under UV light (254nm) exposure. Flash chromatography was carried out using 230–400 mesh silica gel and analytical grade solvents. Stuart SMP10 Melting Point Apparatus was used to record melting points of products. Structure elucidation by NMR (¹H and ¹³C NMR) was performed on Bruker Avance 400 MHz spectrometer. The chemical shifts were reported in δ units (ppm) relative to the residual protonated solvent resonance, the coupling constants (J) quoted in Hz, and multiplicity of signals was abbreviated as follows: singlet (s); doublet (d); doublet of doublet (dd); triplet (t); multiplet (m).

2. Screening of reaction conditions for the preparation of ketones

Table S1. Screening of solvents for the preparation of ketone^a



Entry	Solvent	Yield ^b (%)
1	THF	NR ^c
2	toluene	NR ^c
3	DMF	NR ^c
4	1,4-dioxane	32
5	MeCN	63
6	CH ₂ Cl ₂	94

^a Reaction conditions: compound **1** (1.0 mmol), DBI (2 mmol), toluene **2** (1.5 mmol), Fe₂O₃ (0.1 mmol), solvent (2 mL), 15 min, ^b Isolated yield after purification by flash column chromatography. ^c No reaction.

2. General procedure of the synthesis of ketones (3a-3w)

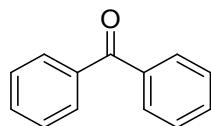
DBI (0.632 g, 2.2 mmol) was added to primary alcohols **1a** (1.00 mmol) in CH₂Cl₂ (2 mL). The reaction mixture was stirred at room temperature for 2 to 4 hours. When the formation of acyl bromide was complete (monitored by TLC), aromatic compound **2a** and nanoparticle α-Fe₂O₃ (0.04 g, 0.5 mmol) were added to the reaction mixture. After stirring at room temperature for 15 minutes, the reaction mixture was quenched with water, and extracted with CH₂Cl₂ (3 x 10 mL). The combined organic layers were dried over sodium sulfate and subsequently concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel using 5% ethyl acetate in hexane as eluent to afford the desired product **3a** (0.171 g, 95%).

3. General procedure of the synthesis of anhydrides, ester, and amides (7a-7i)

DBI (0.632 g, 2.2 mmol) was added to primary alcohols **1a** (1.00 mmol) in CH₂Cl₂ (2 mL). The reaction mixture was stirred at room temperature for 2 to 4 hours until generation of the acyl bromide was complete (monitored by TLC). Nucleophile **6** (1 mmol) and Et₃N (0.202 g, 2 mmol) were added dropwise to the reaction mixture at 0 °C. The reaction mixture was stirred at room temperature until complete disappearance of the nucleophile (monitored by TLC). For compounds **7a-7c**, the mixture was concentrated under reduced pressure and purified by flash column chromatography to provide the corresponding anhydride. For compounds **7d-7i**, the reaction mixture was extracted with CH₂Cl₂ (20 mL), and then washed with water (3 x 10 mL). The organic layer was dried over Na₂SO₄ and concentrated under reduced pressure. The crude residue was purified by flash column chromatography to give the corresponding ester or amide product.

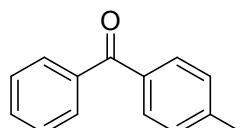
4. Characterization data for compounds

benzophenone (3a):



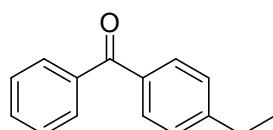
White solid (0.171 g, 95%); m.p. 47 – 49 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.85 – 7.82 (m, 4H), 7.64 – 7.59 (m, 2H), 7.53 – 7.49 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 196.80, 137.59, 132.44 (3C), 130.09 (4C), 128.29 (4C); HRMS (ESI) m/z (M+H)⁺ calcd for C₁₃H₁₁O = 183.0810, found 183.0811.

phenyl(p-tolyl)methanone (3b):



White solid (0.176 g, 90%); m.p. 57 – 59°C; ¹H NMR (400 MHz, CDCl₃) δ 7.81 – 7.79 (m, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.62 – 7.58 (m, 1H), 7.51 – 7.48 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 196.55, 143.26, 137.95, 134.87, 132.18, 130.33 (2C), 129.95 (2C), 128.99 (2C), 128.23 (2C), 21.66; HRMS (ESI) m/z (M+H)⁺ calcd for C₁₄H₁₃O = 197.0966, found 197.0966.

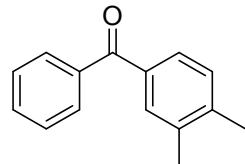
(4-ethylphenyl)(phenyl)methanone (3c):



Colorless oil (0.185 g, 88%); ¹H NMR (400 MHz, CDCl₃) δ 7.83 – 7.80 (m, 2H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.62 – 7.58 (m, 1H), 7.52 – 7.48 (m, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 2.79 (q, *J* = 8.0 Hz, 2H), 1.31 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 196.59, 149.47, 137.95, 135.08, 132.20, 130.45 (2C), 129.99 (2C), 128.23 (2C), 127.83 (2C), 29.01, 15.33; HRMS

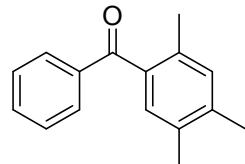
(ESI) m/z (M+H)⁺ calcd for C₁₅H₁₅O = 211.1123, found 211.1122.

(3,4-dimethylphenyl)(phenyl)methanone (3d):



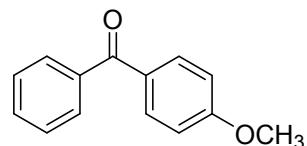
White solid (0.189 g, 90%); m.p. 46 – 48 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.81 – 7.79 (m, 2H), 7.64 (s, 1H), 7.61 – 7.57 (m, 2H), 7.60 – 7.54 (m, 1H), 7.56 – 7.54 (dd, *J* = 1.6 Hz, *J* = 1.6 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 2.37 (s, 3H), 2.35 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 196.73, 141.98, 138.09, 136.76, 135.30, 132.09, 131.19, 129.95 (2C), 129.44, 128.11 (2C), 128.05, 20.04, 19.78; HRMS (ESI) m/z (M+H)⁺ calcd for C₁₅H₁₅O = 211.1123, found 211.1122.

phenyl(2,4,5-trimethylphenyl)methanone (3e):



Colorless oil (0.204 g, 91%); ¹H NMR (400 MHz, CDCl₃) δ 7.84 – 7.80 (m, 2H), 7.61 – 7.57 (m, 1H), 7.49 – 7.45 (m, 2H), 7.12 (s, 1H), 7.08 (s, 1H), 2.31 (s, 3H), 2.30 (s, 3H), 2.25 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 198.73, 139.26, 138.30, 136.01, 134.48, 133.29, 132.78, 132.42, 130.21, 130.09 (2C), 128.35 (2C), 19.70, 19.59, 191.19; HRMS (ESI) m/z (M+H)⁺ calcd for C₁₆H₁₇O = 225.1279, found 225.1278.

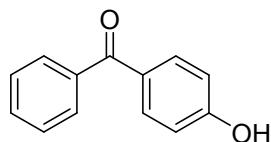
(4-methoxyphenyl)(phenyl)methanone (3f):



White solid (0.163 g, 77%); m.p. 58 – 60 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 8.8

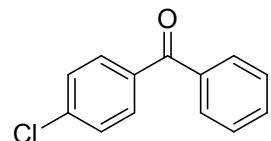
Hz, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.85 – 7.83 (m, 2H), 7.64 – 7.60 (m, 1H), 7.54 – 7.50 (m, 2H), 7.38 (d, J = 8.8 Hz, 1H), 7.04 (d, J = 9.2 Hz, 1H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.65, 164.18, 154.41, 137.59, 134.96, 132.45 (2C), 131.73, 129.99, 128.35, 121.78, 121.35, 113.98, 21.66; HRMS (ESI) m/z ($\text{M}+\text{H})^+$ calcd for $\text{C}_{14}\text{H}_{13}\text{O}_2$ = 213.0916, found 213.0916.

(4-hydroxyphenyl)(phenyl)methanone (3g):



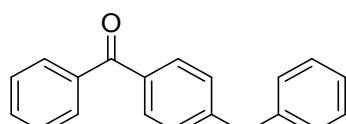
White solid (0.184 g, 95%); m.p. 129 – 131 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, J = 8.8 Hz, 2H), 7.79 – 7.77 (m, 2H), 7.62 – 7.57 (m, 1H), 7.52 – 7.48 (m, 2H), 6.96 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.40, 160.31, 138.09, 133.05 (2C), 132.14, 130.21, 129.84 (2C), 128.27 (2C), 115.30 (2C); HRMS (ESI) m/z ($\text{M}+\text{H})^+$ calcd for $\text{C}_{13}\text{H}_{11}\text{O}_2$ = 199.0759, found 199.0759.

(4-chlorophenyl)(phenyl)methanone (3h):



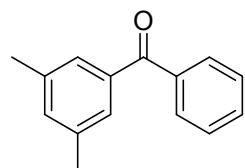
White solid (0.162 g, 75%); M.p. 59 – 61 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.79 – 7.74 (m, 4H), 7.63 – 7.57 (m, 1H), 7.53 – 7.44 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 195.49, 138.91, 137.26, 135.88, 132.65, 131.47 (2C), 129.94 (2C), 128.65 (2C), 128.42 (2C); HRMS (ESI) m/z ($\text{M}+\text{H})^+$ calcd for $\text{C}_{13}\text{H}_{10}\text{ClO}$ = 217.0420, found 217.0421.

(4-benzylphenyl)(phenyl)methanone (3i):



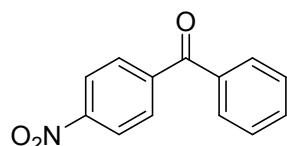
Light yellow oil (0.252 g, 93%). ^1H NMR (400 MHz, CDCl_3) δ 7.82 – 7.79 (m, 2H), 7.78 (d, J = 8.4 Hz, 2H), 7.62 – 7.57 (m, 1H), 7.51 – 7.47 (m, 2H), 7.36 – 7.31 (m, 4H), 7.25 – 7.22 (m, 3H), 4.09 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.44, 146.17, 140.12, 137.81, 135.52, 132.26, 130.49 (2C), 129.98 (2C), 129.01 (2C), 128.83 (2C), 128.65 (2C), 128.23 (2C), 126.43, 41.97; HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{20}\text{H}_{17}\text{O} = 273.1279$, found 273.1279.

(3,5-dimethylphenyl)(phenyl)methanone (3k):



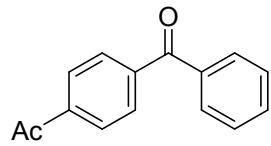
White solid (0.193 g, 92%); m.p. 48 – 50 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.83 – 7.81 (dd, J = 1.2 Hz, J = 1.2 Hz, 2H), 7.60 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 8.0 Hz, 2H), 7.42 (s, 2H), 7.24 (s, 1H), 2.46 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.17, 137.94 (2C), 134.09 (2C), 132.26 (2C), 130.03 (2C), 128.22 (2C), 127.83 (2C), 21.26 (2C); HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{15}\text{H}_{15}\text{O} = 211.1123$, found 211.1122.

(4-nitrophenyl)(phenyl)methanone (3n):



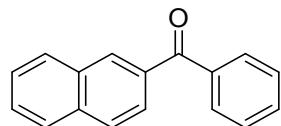
Yellow solid (0.174 g, 77%); m.p. 57 – 59 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.37 (d, J = 8.8 Hz, 2H), 7.97 (d, J = 8.8 Hz, 2H), 7.83 – 7.81 (m, 2H), 7.70 – 7.66 (m, 1H), 7.57 – 7.53 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 194.80, 149.85, 142.90, 136.30, 133.48, 130.71 (2C), 130.11 (2C), 128.70 (2C), 128.55 (2C); HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{13}\text{H}_{10}\text{NO}_3 = 228.0661$, found 228.0664.

1-(4-benzoylphenyl)ethan-1-one (3o):



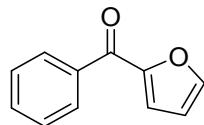
White solid (0.168 g, 75%); m.p. 60 – 62 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.09 (d, J = 8.4 Hz, 2H), 7.89 (d, J = 8.4 Hz, 2H), 7.83 – 7.81 (m, 2H), 7.66 – 7.62 (m, 1H), 7.54 – 7.50 (m, 2H), 2.69 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.53, 195.97, 141.34, 139.57, 136.92, 133.00, 130.11 (2C), 130.05 (2C), 128.49 (2C), 128.18 (2C), 26.91; HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{15}\text{H}_{13}\text{O}_2$ = 225.0916, found 225.0915.

naphthalen-2-yl(phenyl)methanone (3p):



White solid (0.215 g, 93%); m.p. 68 – 70 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, J = 8.0 Hz, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.96 – 7.94 (dd, J = 1.6 Hz, J = 2.0 Hz, 1H), 7.90 – 7.88 (m, 2H), 7.65 – 7.59 (m, 2H), 7.56 – 7.46 (m, 3H), 7.48 (t, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 198.04, 138.33, 136.37, 133.73, 133.24, 131.28, 130.97, 130.43 (2C), 128.47, 128.42 (2C), 127.79, 127.27, 126.48, 125.71, 124.35; HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{17}\text{H}_{13}\text{O}$ = 233.0966, found 233.0967.

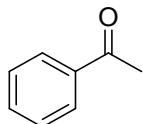
furan-2-yl(phenyl)methanone (3q):



Light yellow oil (0.150 g, 87%); ^1H NMR (400 MHz, CDCl_3) δ 7.99 (d, J = 7.6 Hz, 1H), 7.72 – 7.70 (m, 2H), 7.62 – 7.59 (m, 1H), 7.52 – 7.49 (m, 2H), 7.24 (d, J = 1.2 Hz, 1H), 6.61 – 6.60 (dd, J = 1.6 Hz, J = 1.6 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.57, 152.30, 147.13, 137.27, 132.59, 129.29 (2C), 128.43 (2C), 120.59, 112.23; HRMS (ESI) m/z (M+H) $^+$ calcd for

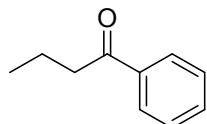
$C_{11}H_9O_2 = 173.0603$, found 173.0604.

acetophenone (3r):



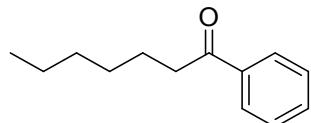
Light yellow oil (0.112 g, 93%); 1H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.97 (dd, $J = 1.2$ Hz, $J = 1.2$ Hz, 2H), 7.58 (t, $J = 7.2$ Hz, 1H), 7.48 (t, $J = 8.0$ Hz, 2H), 2.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.16, 137.14, 133.11, 128.58 (2C), 128.31 (2C), 26.62; HRMS (ESI) m/z (M+H) $^+$ calcd for $C_8H_9O = 121.0653$, found 121.0656.

1-phenylbutan-1-one (3s):



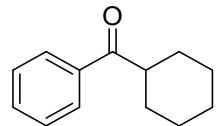
Light yellow oil (0.137 g, 93%); 1H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.97 (m, 2H), 7.59 – 7.55 (m, 1H), 7.50 – 7.46 (m, 2H), 2.97 (t, $J = 7.6$ Hz, 2H), 1.84 – 1.77 (m, 2H), 1.03 (t, $J = 7.6$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.43, 137.13, 132.86, 128.55 (2C), 128.04 (2C), 40.54, 17.79, 13.91; HRMS (ESI) m/z (M+H) $^+$ calcd for $C_{10}H_{13}O = 149.0966$, found 149.0965.

1-phenylheptan-1-one (3t):



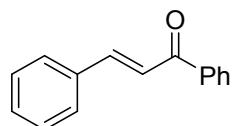
Light yellow oil (0.175 g, 92%); 1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, $J = 8.0$ Hz, 2H), 7.57 (t, $J = 8.0$ Hz, 1H), 7.48 (t, $J = 6.8$ Hz, 2H), 2.98 (t, $J = 7.2$ Hz, 2H), 1.79 – 1.72 (m, 2H), 1.40 – 1.34 (m, 6H), 0.94 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.62, 137.12, 132.85, 128.55 (2C), 128.06 (2C), 38.65, 31.69, 29.07, 24.36, 22.55, 14.06; HRMS (ESI) m/z (M+H) $^+$ calcd for $C_{13}H_{19}O = 191.1436$, found 191.1437.

cyclohexyl(phenyl)methanone (3u):



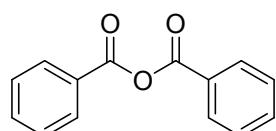
White solid (0.167 g, 89%); m.p. 54 – 56 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.98 – 7.95 (m, 2H), 7.59 – 7.54 (m, 1H), 7.50 (d, J = 8.0 Hz, 2H), 3.32 – 3.25 (m, 1H), 1.93 – 1.85 (m, 4H), 1.81 – 1.75 (m, 1H), 1.57 – 1.50 (m, 2H), 1.48 – 1.36 (m, 2H), 1.34 – 1.25 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 203.90, 136.38, 132.72, 128.58 (2C), 128.26 (2C), 45.65, 29.44 (2C), 26.75, 25.89 (2C); HRMS (ESI) m/z ($\text{M}+\text{H}$) $^+$ calcd for $\text{C}_{13}\text{H}_{17}\text{O}$ = 189.1279, found 189.1280.

(E)-chalcone (3v):



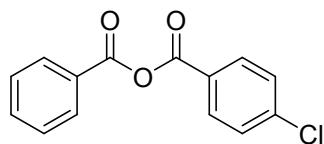
White solid (0.183 g, 88%); m.p. 54 – 56 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.06 – 8.04 (m, 2H), 7.86 (d, J = 15.6 Hz, 1H), 7.68 – 7.65 (m, 2H), 7.63 – 7.59 (m, 1H), 7.58 (d, J = 15.6 Hz, 1H), 7.53 – 7.51 (m, 2H), 7.46 – 7.43 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.57, 144.86, 138.24, 134.91, 132.81, 130.57, 128.98 (2C), 128.65 (2C), 128.53 (2C), 128.47 (2C), 122.13; HRMS (ESI) m/z ($\text{M}+\text{H}$) $^+$ calcd for $\text{C}_{15}\text{H}_{13}\text{O}$ = 209.0966, found 209.0965.

Benzoic anhydride (7a):



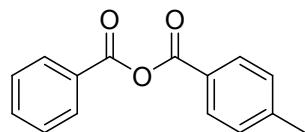
Colorless oil (0.219 g, 97%); ^1H NMR (400 MHz, CDCl_3) δ 8.19 (d, J = 7.6 Hz, 4H), 7.69 – 7.68 (m, 2H), 7.55 (t, J = 8.0 Hz, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.37 (2C), 134.54 (2C), 130.58 (5C), 128.89 (5C); HRMS (ESI) m/z ($\text{M}+\text{Na}$) $^+$ calcd for $\text{C}_{14}\text{H}_{10}\text{O}_3\text{Na}$ = 249.0528, found 249.0527.

Benzoic 4-chlorobenzoic anhydride (7b):



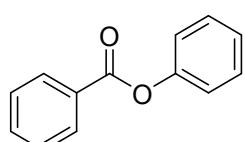
White solid (0.247 g, 95%); m.p. 108 – 110 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.17 (d, $J = 7.2$ Hz, 2H), 8.11 (t, $J = 8.0$ Hz, 2H), 7.71 (t, $J = 7.2$ Hz, 1H), 7.58 (d, $J = 8.0$ Hz, 2H), 7.54 (d, $J = 7.6$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.11, 161.55, 141.44, 134.69, 131.89 (2C), 130.60 (2C), 129.39 (2C), 129.32 (2C), 128.94 (2C); HRMS (ESI) m/z (M+Na) $^+$ calcd for $\text{C}_{14}\text{H}_9\text{ClO}_3\text{Na} = 283.0138$, found 283.0137.

Benzoic 4-methylbenzoic anhydride (7c):



Colorless oil (0.230 g, 96%); ^1H NMR (400 MHz, CDCl_3) δ 8.19 – 8.17 (m, 2H), 8.07 – 8.05 (dd, $J = 2.4$ Hz, $J = 2.4$ Hz, 2H), 7.72 – 7.67 (m, 1H), 7.57 – 7.53 (m, 2H), 7.35 – 7.33 (dd, $J = 2.4$ Hz, $J = 2.4$ Hz, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.56, 162.52, 145.69, 134.54, 130.68 (2C), 130.58 (2C), 129.62 (2C), 128.89 (2C), 126.24, 126.12, 21.85; HRMS (ESI) m/z (M+Na) $^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{O}_3\text{Na} = 263.0684$, found 263.0681.

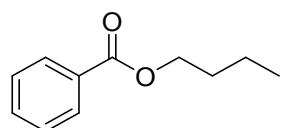
Phenyl benzoate (7d):



White solid (0.178 g, 90%); m.p. 67 – 69 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.25 (d, $J = 1.2$ Hz, 2H), 7.71 (t, $J = 7.2$ Hz, 1H), 7.35 (d, $J = 8.0$ Hz, 2H), 7.25 (d, $J = 8.0$ Hz, 2H), 7.05 (t, $J = 7.2$ Hz, 1H).

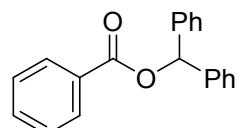
Hz, 1H), 8.23 (d, J = 1.2 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.56 – 7.52 (m, 2H), 7.48 – 7.43 (m, 2H), 7.32 – 7.30 (m, 1H), 7.26 (d, J = 1.2 Hz, 1H), 7.24 (d, J = 1.2 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 165.18, 151.00, 133.58, 130.19 (2C), 129.63, 129.50 (2C), 128.58 (2C), 125.89, 121.72 (2C); HRMS (ESI) m/z (M+Na) $^+$ calcd for $\text{C}_{13}\text{H}_{10}\text{O}_2\text{Na}$ = 221.0578, found 221.0578.

butyl benzoate (7e):



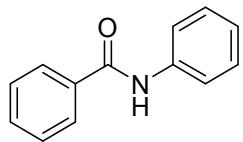
Colorless oil (0.165 g, 93%); ^1H NMR (400 MHz, CDCl_3) δ 8.08 (d, J = 1.2 Hz, 1H), 8.05 (d, J = 1.2 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.48 – 7.44 (m, 2H), 4.35 (t, J = 6.8 Hz, 2H), 1.81 – 1.74 (m, 2H), 1.55 – 1.46 (m, 2H), 1.00 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 166.70, 132.78, 130.56, 129.53 (2C), 128.31 (2C), 64.84, 30.80, 19.30, 13.77; HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{11}\text{H}_{15}\text{O}_2$ = 179.1072, found 179.1075.

Benzydryl benzoate (7f):



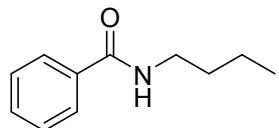
White solid (0.253 g, 88%); m.p. 91 – 93 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.18 (d, J = 1.0 Hz, 1H), 8.16 (d, J = 1.2 Hz, 1H), 7.60 – 7.58 (m, 1H), 7.50 – 7.45 (m, 6H), 7.38 (t, J = 6.8 Hz, 4H), 7.33 – 7.29 (m, 2H), 7.14 (s, 1H); ^{13}C NMR (150 MHz, CDCl_3) δ 165.57, 140.31, 133.15 (2C), 130.27, 129.82 (2C), 128.58 (4C), 128.46 (2C), 127.98 (2C), 127.16 (4C), 77.45; HRMS (ESI) m/z (M+Na) $^+$ calcd for $\text{C}_{20}\text{H}_{16}\text{O}_2\text{Na}$ = 311.1048, found 311.1047.

N-phenylbenzamide (7g):



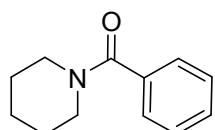
White solid (0.177 g, 90%); m.p. 164 – 166 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, J = 7.2 Hz, 2H), 7.85 (bs, 1H), 7.68 (d, J = 8.0 Hz, 2H), 7.60 – 7.55 (m, 1H), 7.53 – 7.49 (m, 2H), 7.42 – 7.38 (m, 2H), 7.20 – 7.16 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 165.70, 137.93, 135.04, 131.85, 129.12 (2C), 128.81 (2C), 127.01 (2C), 124.59, 120.19 (2C); HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{13}\text{H}_{12}\text{NO} = 198.0919$, found 198.0919.

N-butylbenzamide (7h):



White solid (0.164 g, 93%); m.p. 39 – 40 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.78 – 7.76 (m, 2H), 7.52 – 7.48 (m, 1H), 7.45 – 7.42 (m, 2H), 6.21 (bs, 1H, N-H), 3.50 (q, J = 7.2 Hz, 2H), 1.66 – 1.58 (m, 2H), 1.48 – 1.38 (m, 2H), 0.97 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.56, 134.87, 131.30, 128.54 (2C), 126.83 (2C), 39.83, 31.76, 20.17, 13.79; HRMS (ESI) m/z (M+H) $^+$ calcd for $\text{C}_{11}\text{H}_{16}\text{NO} = 178.1232$, found 178.1232.

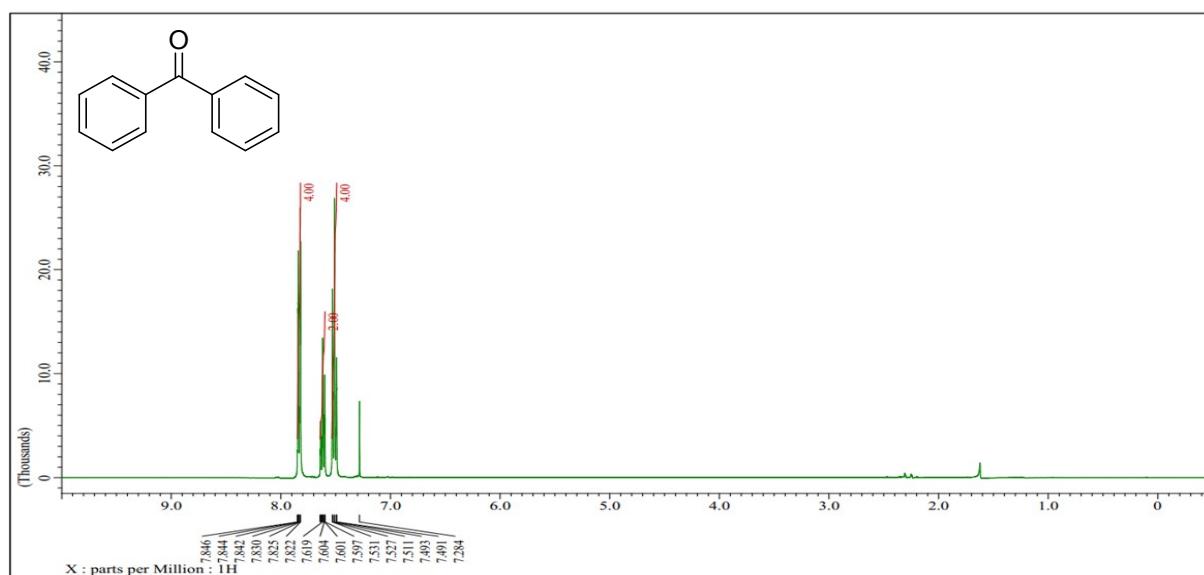
phenyl(piperidin-1-yl)methanone (7i):



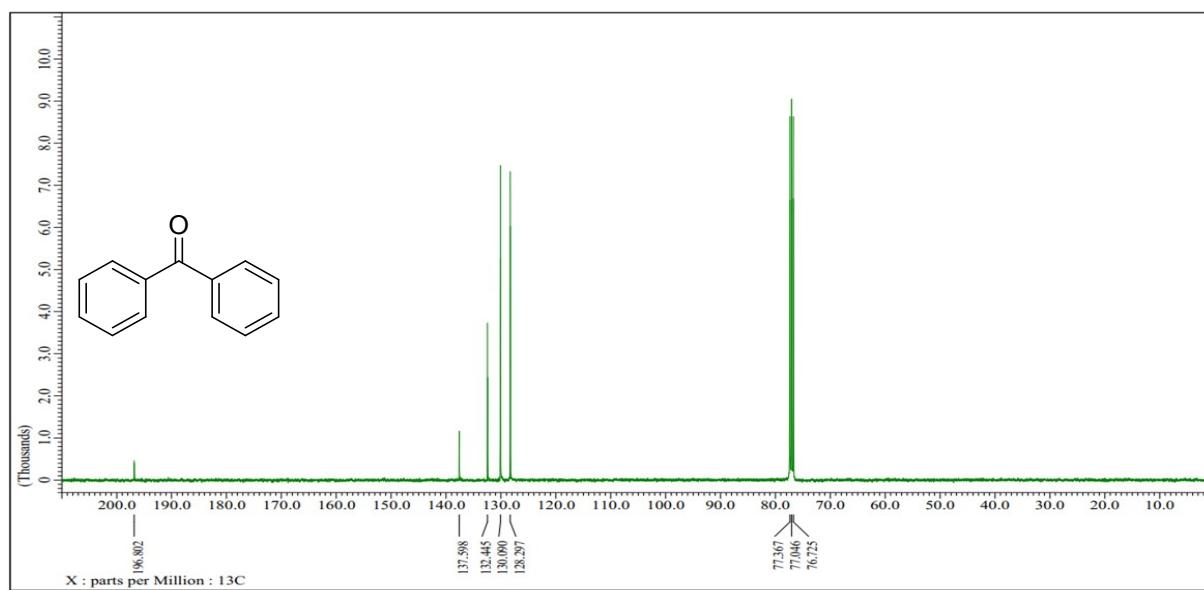
Colorless oil (0.161 g, 85%); ^1H NMR (400 MHz, DMSO-d_6) δ 7.45 – 7.42 (m, 3H), 7.37 – 7.34 (m, 2H), 3.57 (s, 2H), 3.26 (s, 2H), 7.64 – 7.59 (m, 2H), 1.53 (s, 2H), 1.46 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 169.81, 137.30, 129.85, 128.32 (2C), 127.15 (2C), 49.72, 46.34,

26.48, 24.55 (2C); HRMS (ESI) m/z ($M+Na$)⁺ calcd for $C_{12}H_{15}NONa = 212.1051$, found 212.1053.

benzophenone (3a)

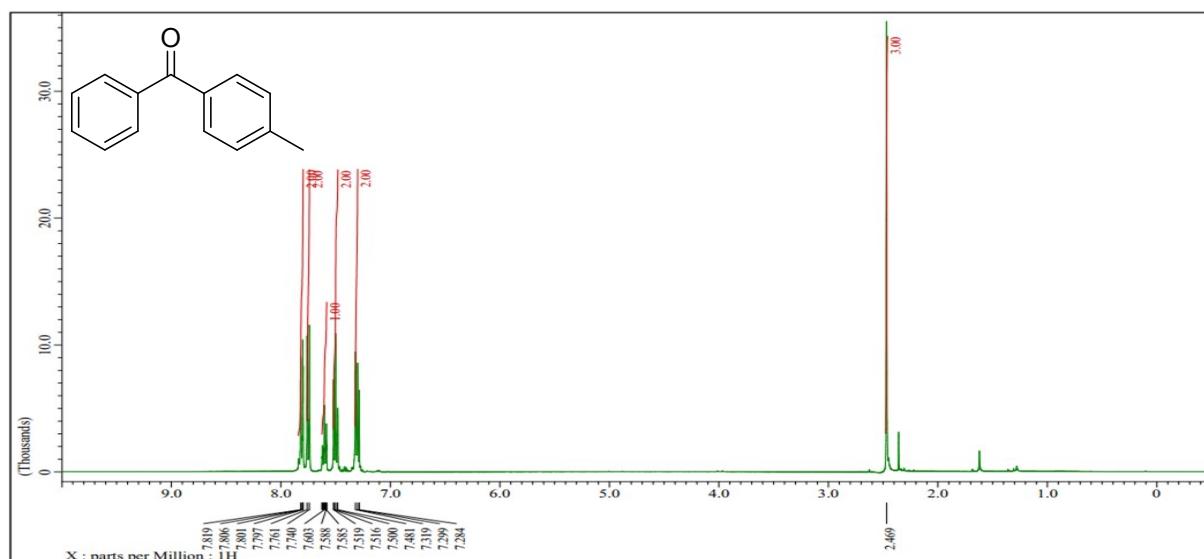


¹H NMR spectrum of benzophenone (3a)

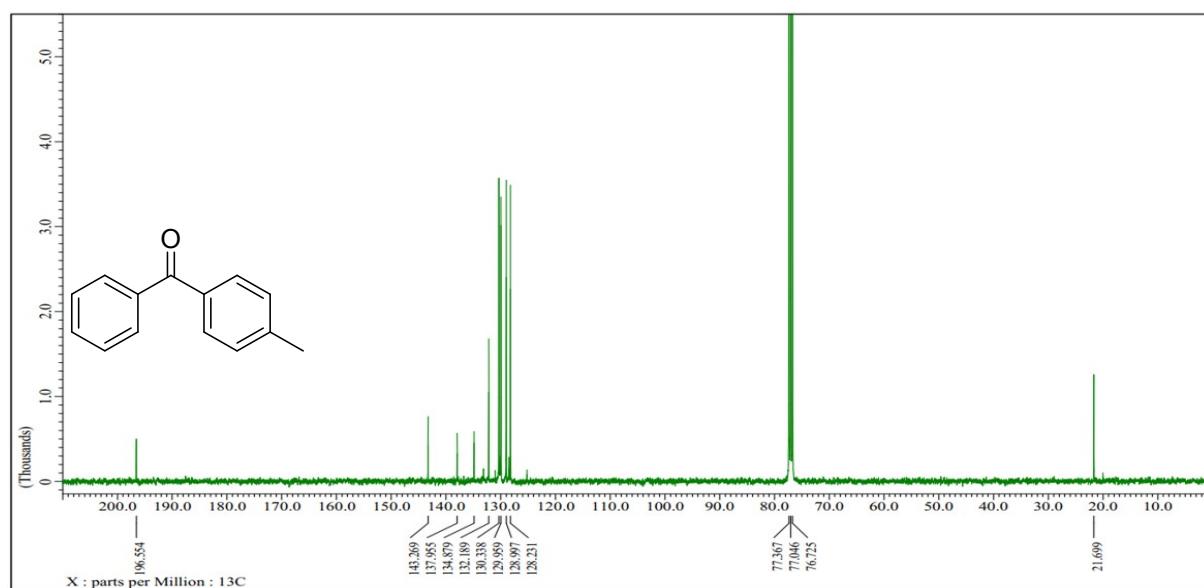


¹³C NMR spectrum of benzophenone (3a)

phenyl(p-tolyl)methanone (3b)

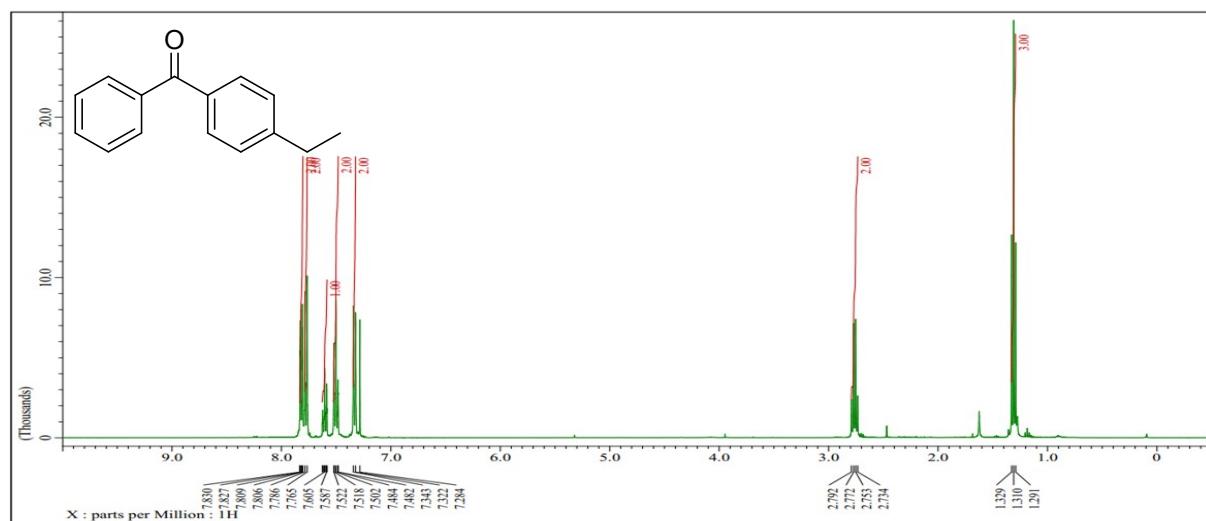


¹H NMR spectrum of phenyl(p-tolyl)methanone (**3b**)

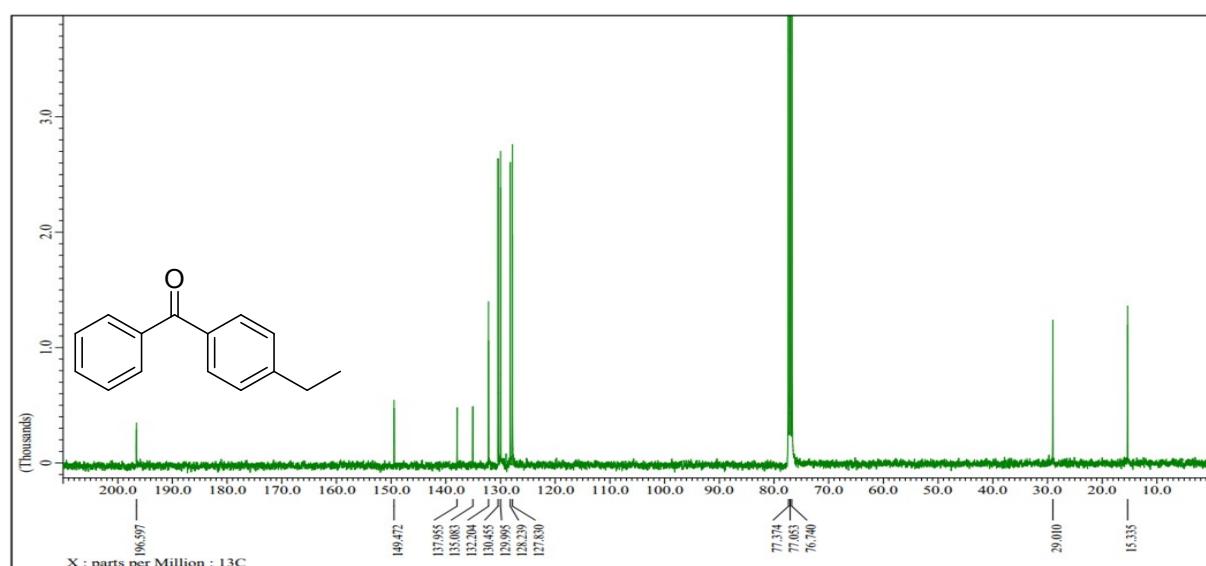


¹³C NMR spectrum of phenyl(p-tolyl)methanone (**3b**)

(4-ethylphenyl)(phenyl)methanone (3c)

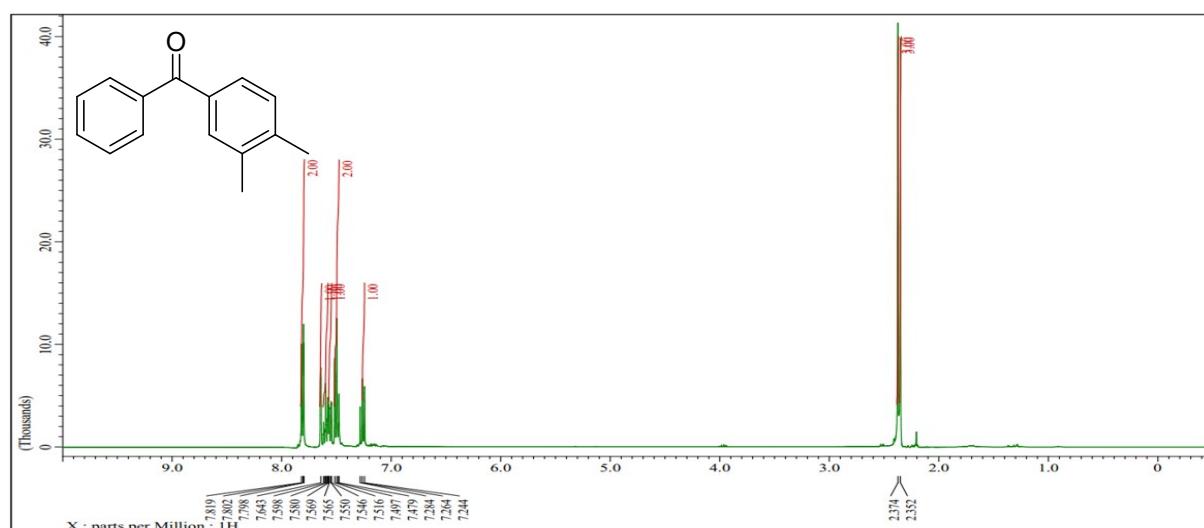


¹H NMR spectrum of (4-ethylphenyl)(phenyl)methanone (**3c**)

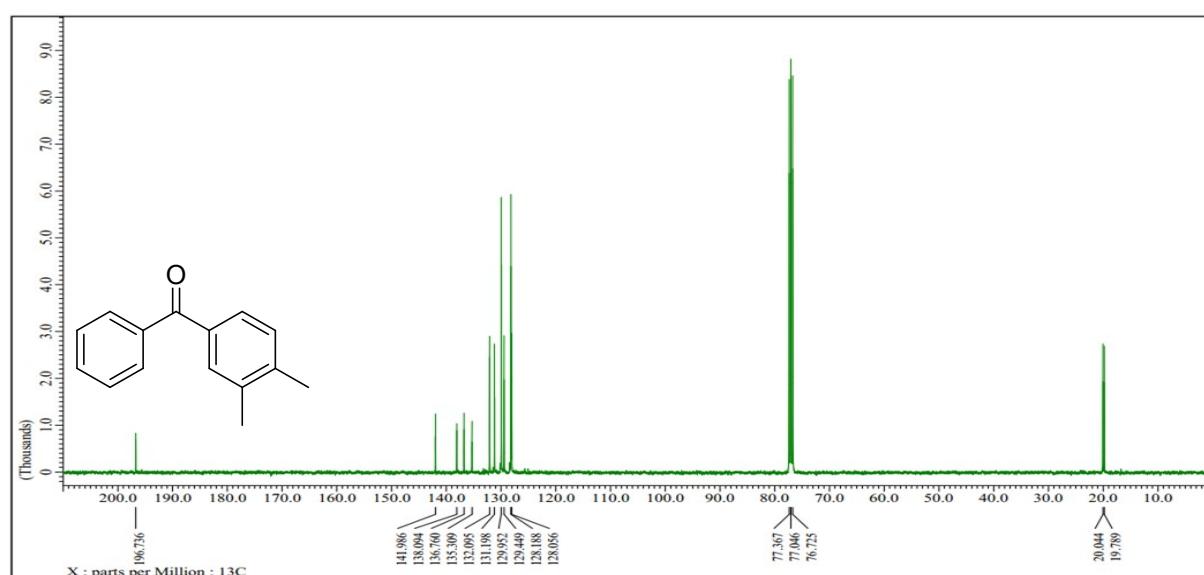


¹³C NMR spectrum of (4-ethylphenyl)(phenyl)methanone (**3c**)

(3,4-dimethylphenyl)(phenyl)methanone (3d)

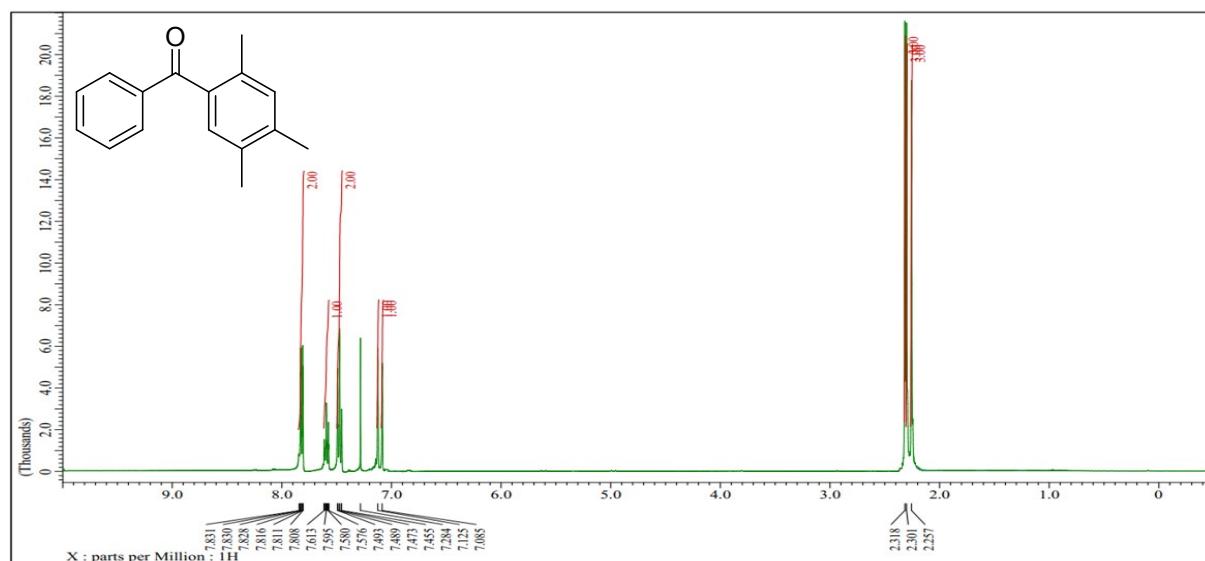


¹H NMR spectrum of (3,4-dimethylphenyl)(phenyl)methanone (**3d**)

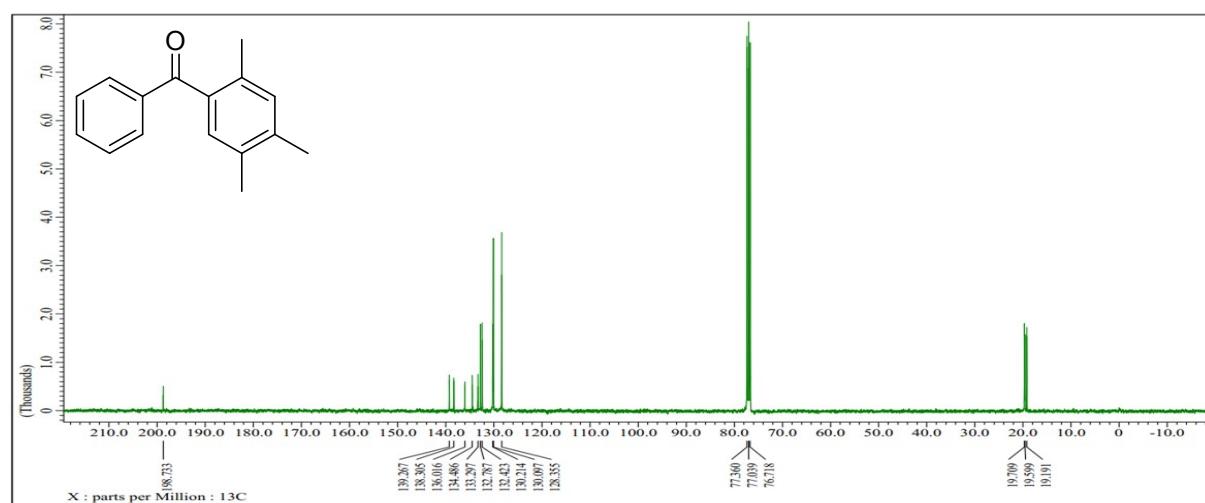


¹³C NMR spectrum of (3,4-dimethylphenyl)(phenyl)methanone (**3d**)

phenyl(2,4,5-trimethylphenyl)methanone (3e)

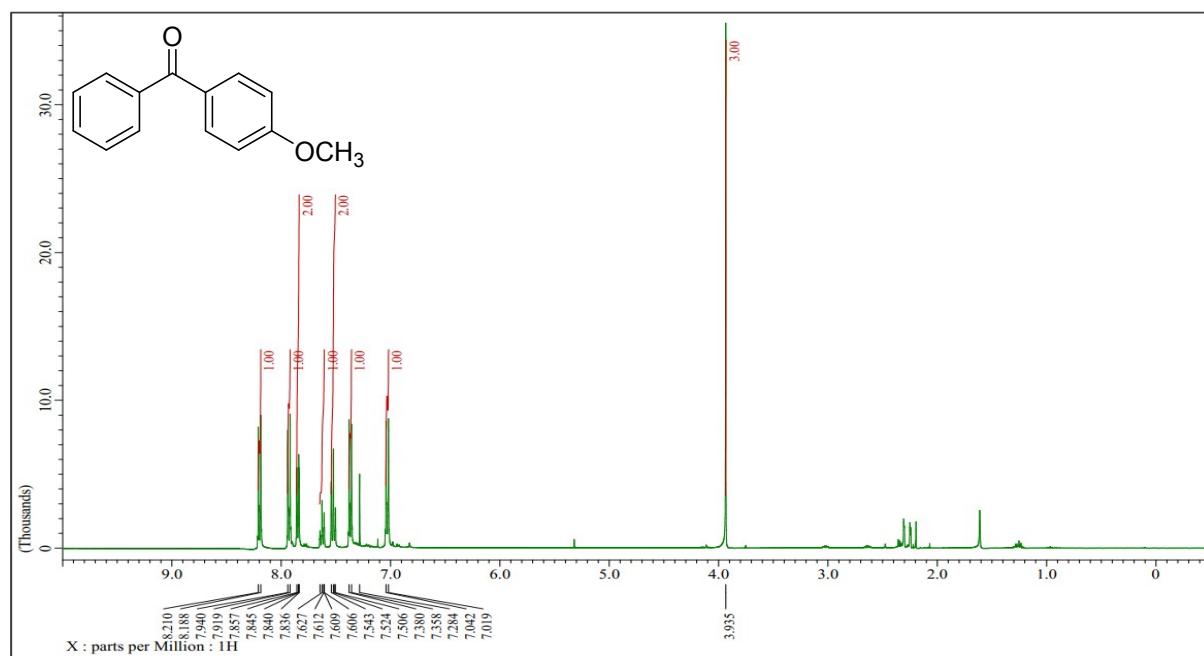


¹H NMR spectrum of phenyl(2,4,5-trimethylphenyl)methanone (3e)

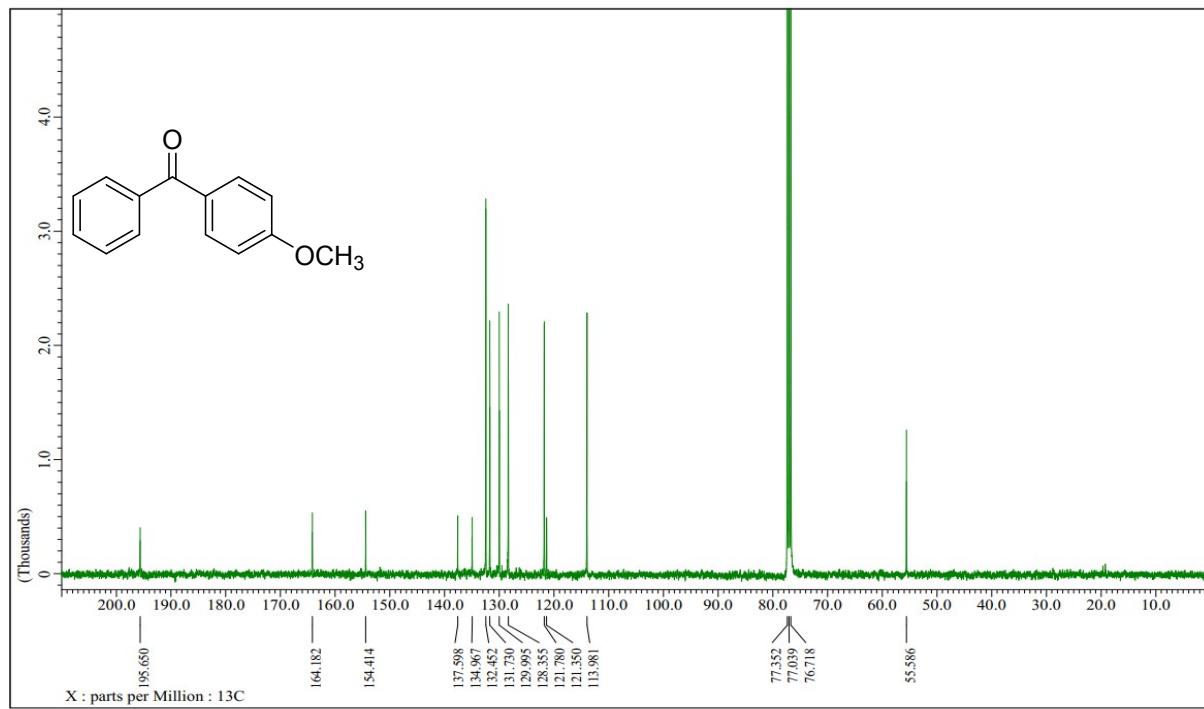


¹³C NMR spectrum of phenyl(2,4,5-trimethylphenyl)methanone (3e)

(4-methoxyphenyl)(phenyl)methanone (3f)

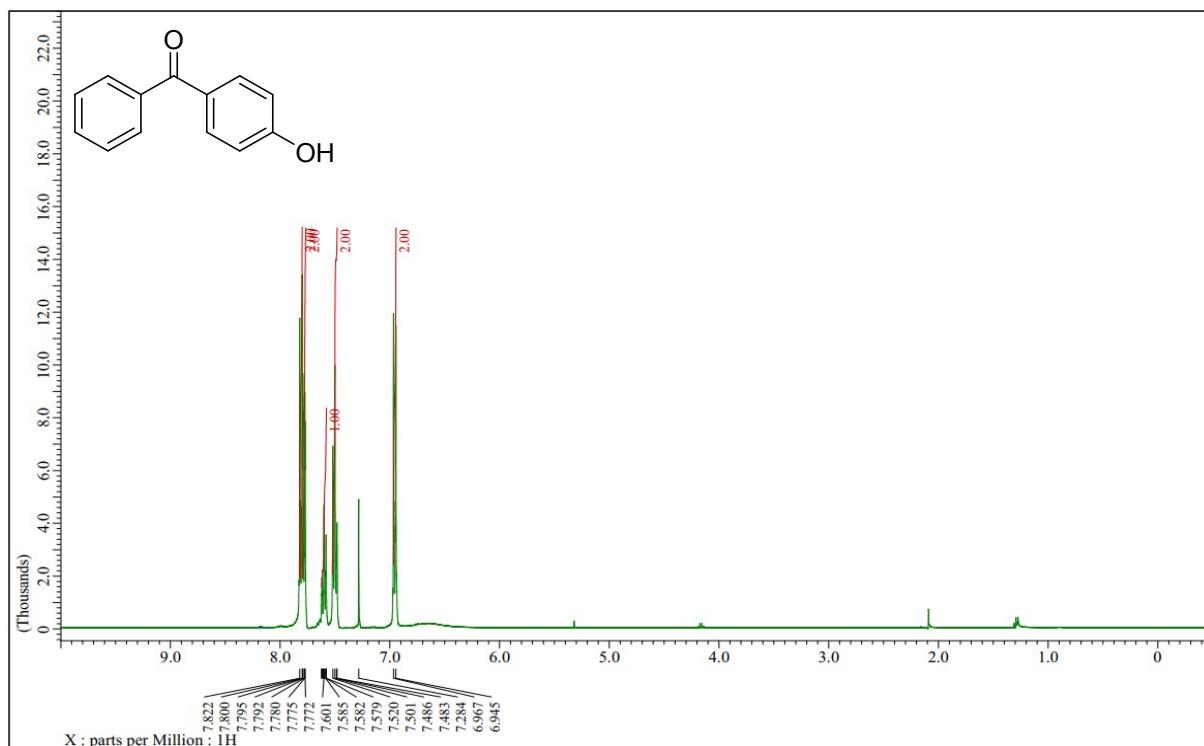


¹H NMR spectrum of (4-methoxyphenyl)(phenyl)methanone **3f**)

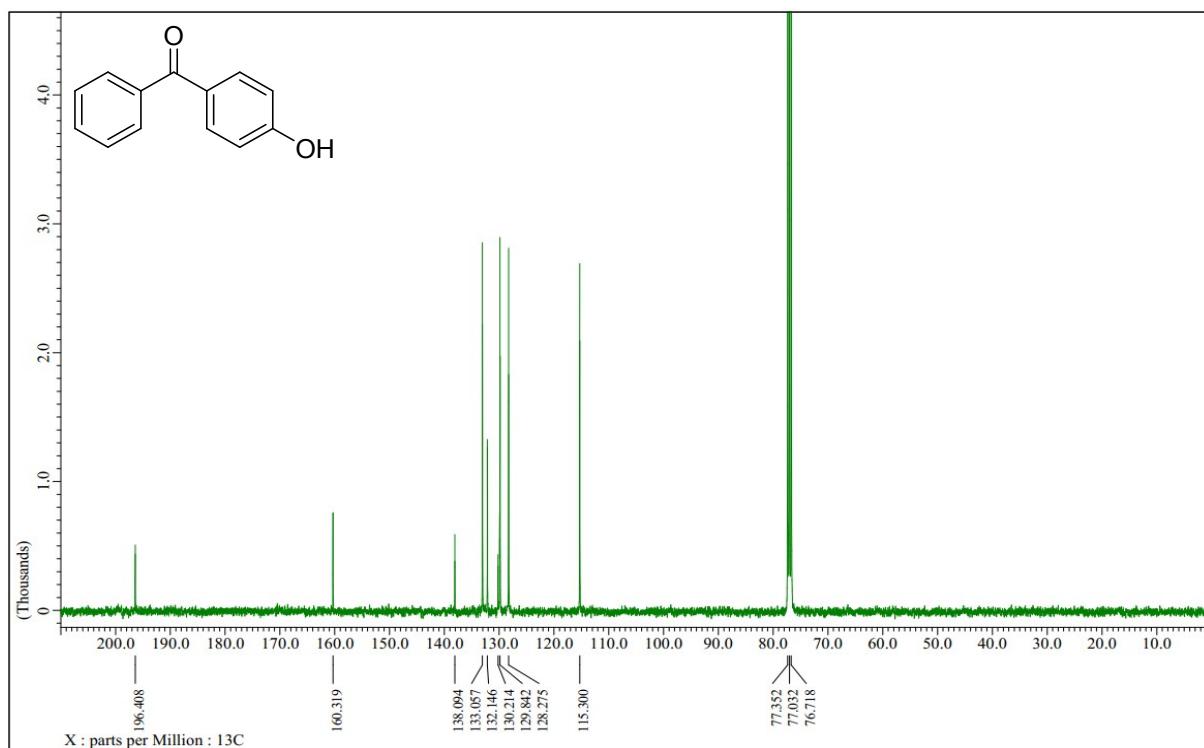


¹³C NMR spectrum of (4-methoxyphenyl)(phenyl)methanone (**3f**)

(4-hydroxyphenyl)(phenyl)methanone (3g)

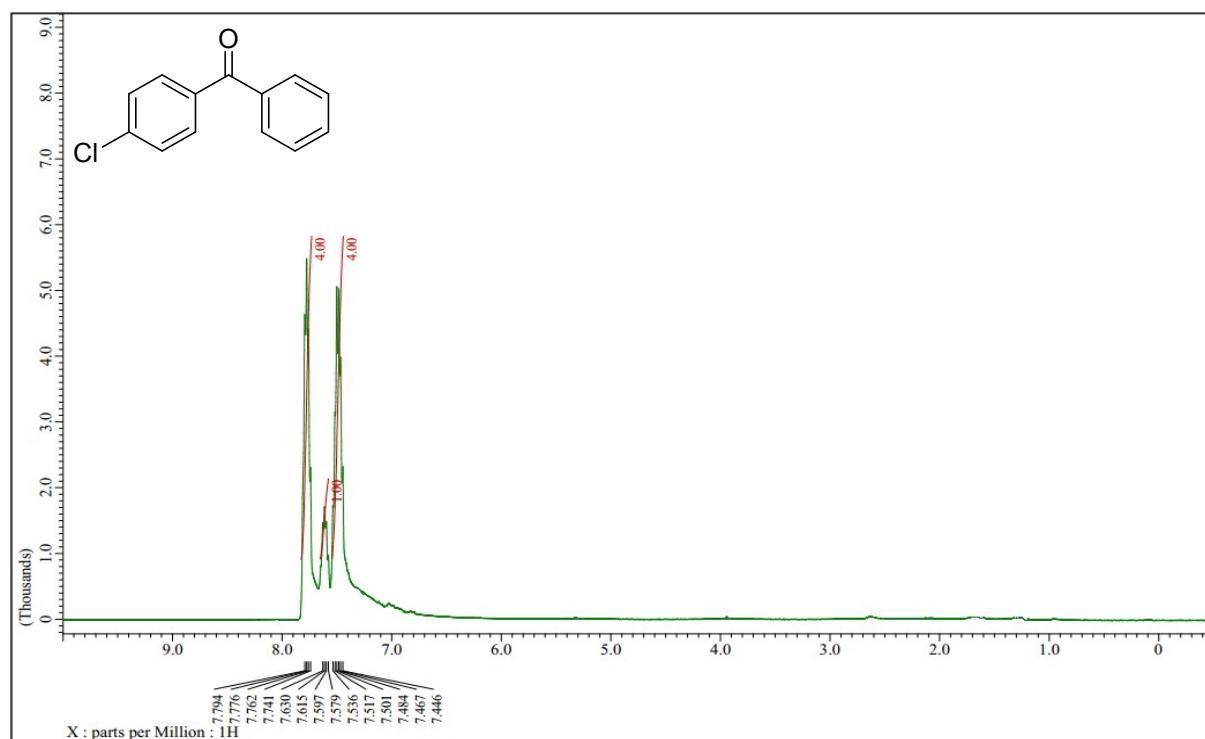


¹H NMR spectrum of (4-hydroxyphenyl)(phenyl)methanone (3g)

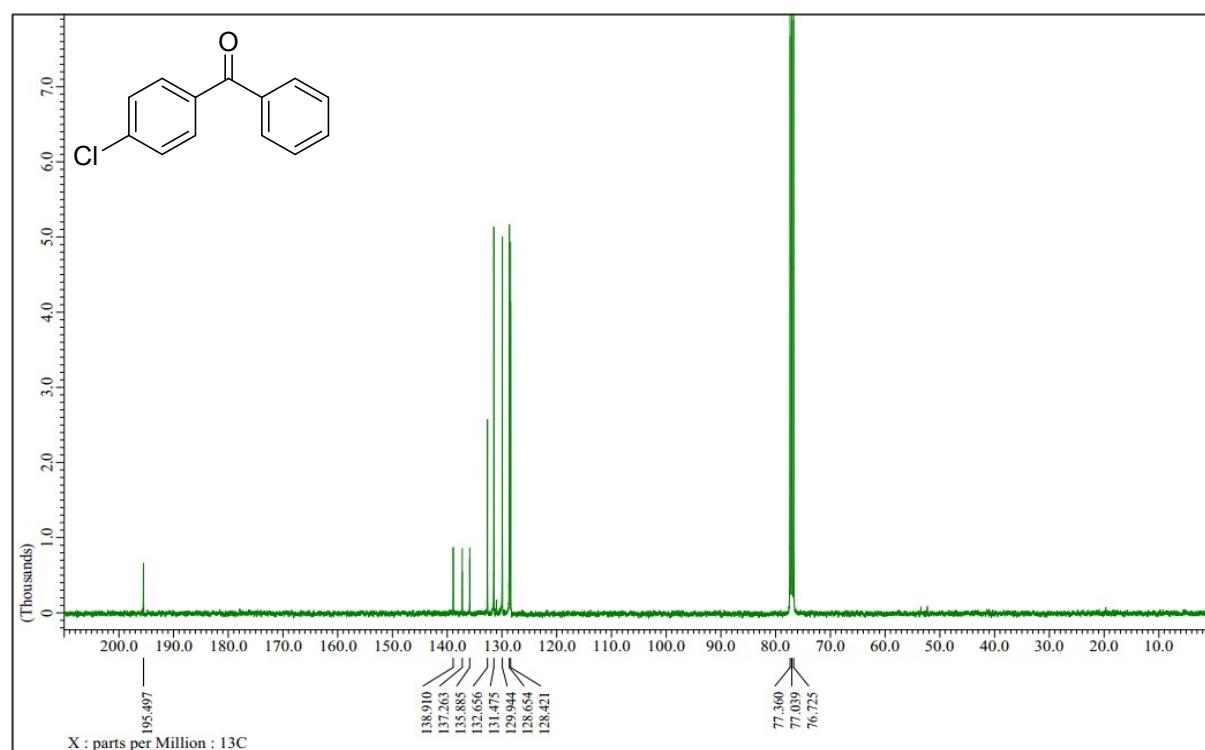


¹³C NMR spectrum of (4-hydroxyphenyl)(phenyl)methanone (3g)

(4-chlorophenyl)(phenyl)methanone (3h**)**

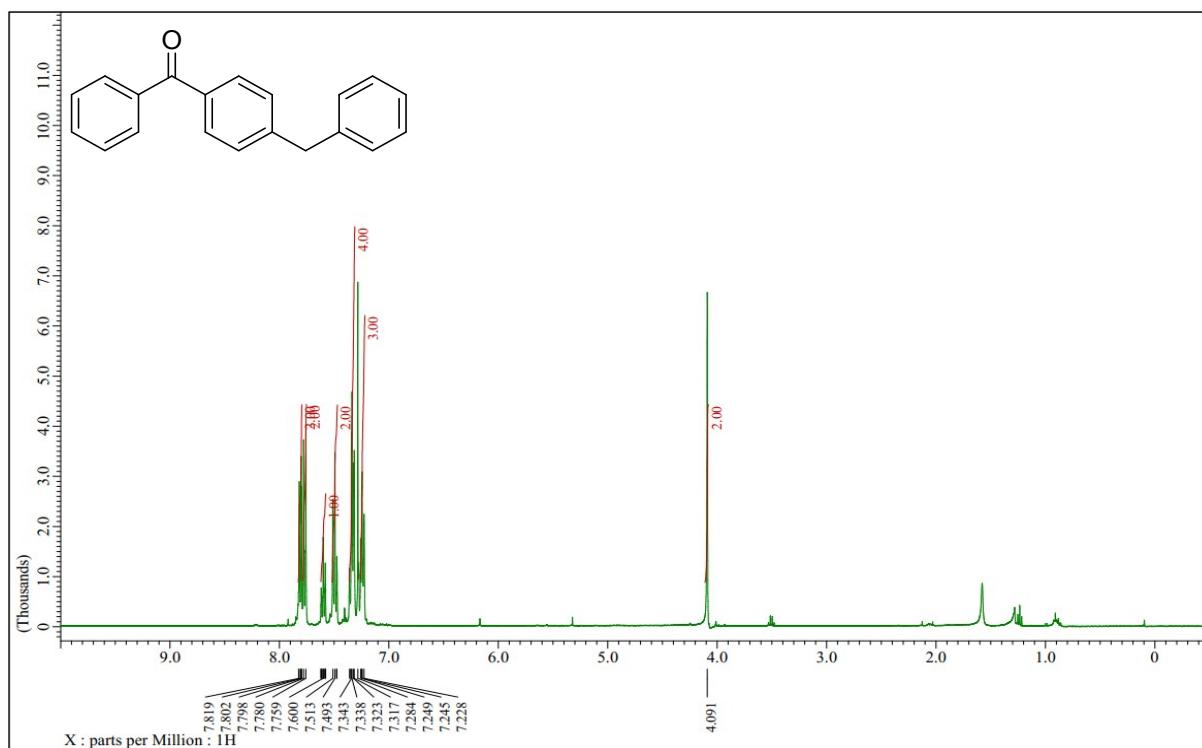


¹H NMR spectrum of (4-chlorophenyl)(phenyl)methanone (**3h**)

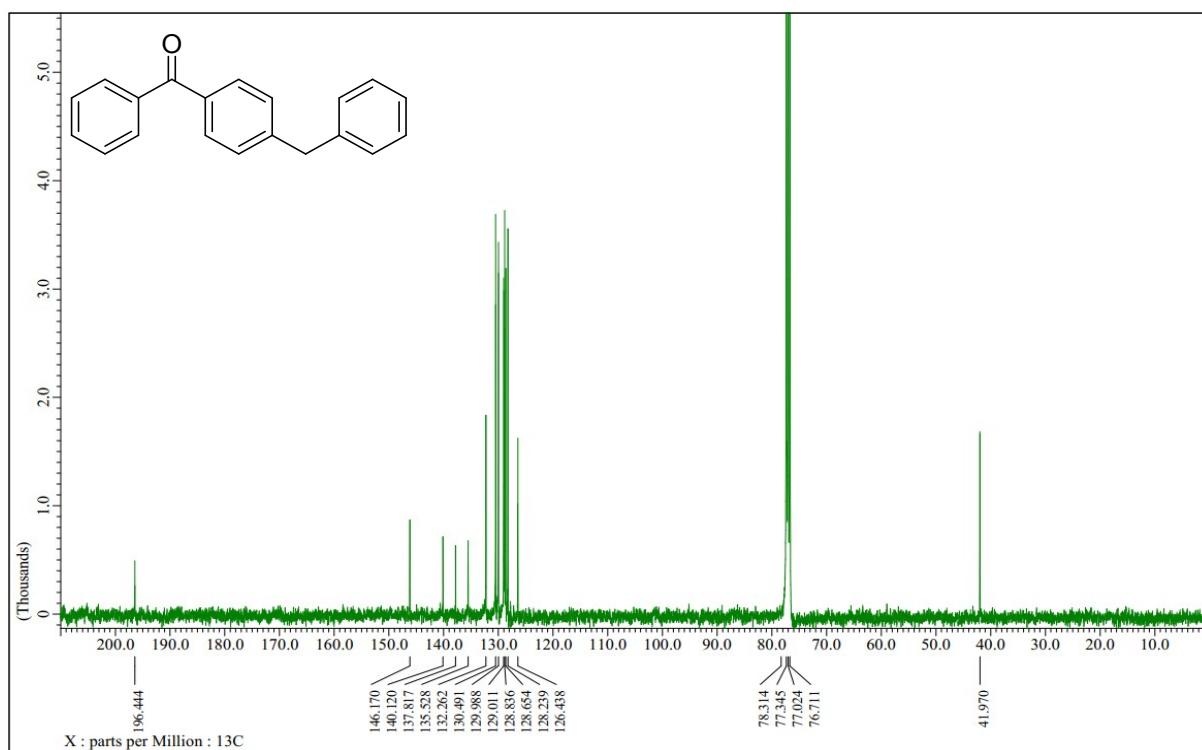


¹³C NMR spectrum of (4-chlorophenyl)(phenyl)methanone (**3h**)

(4-benzylphenyl)(phenyl)methanone (3i**)**

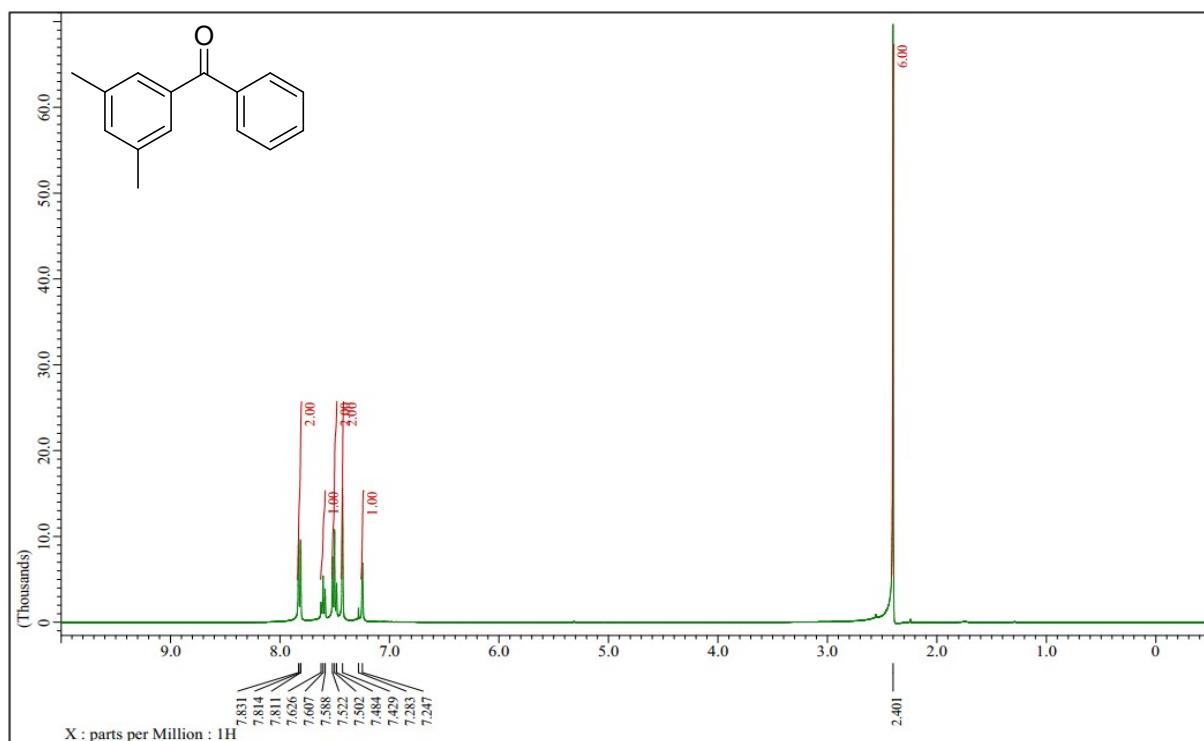


¹H NMR spectrum of (4-benzylphenyl)(phenyl)methanone (**3i**)

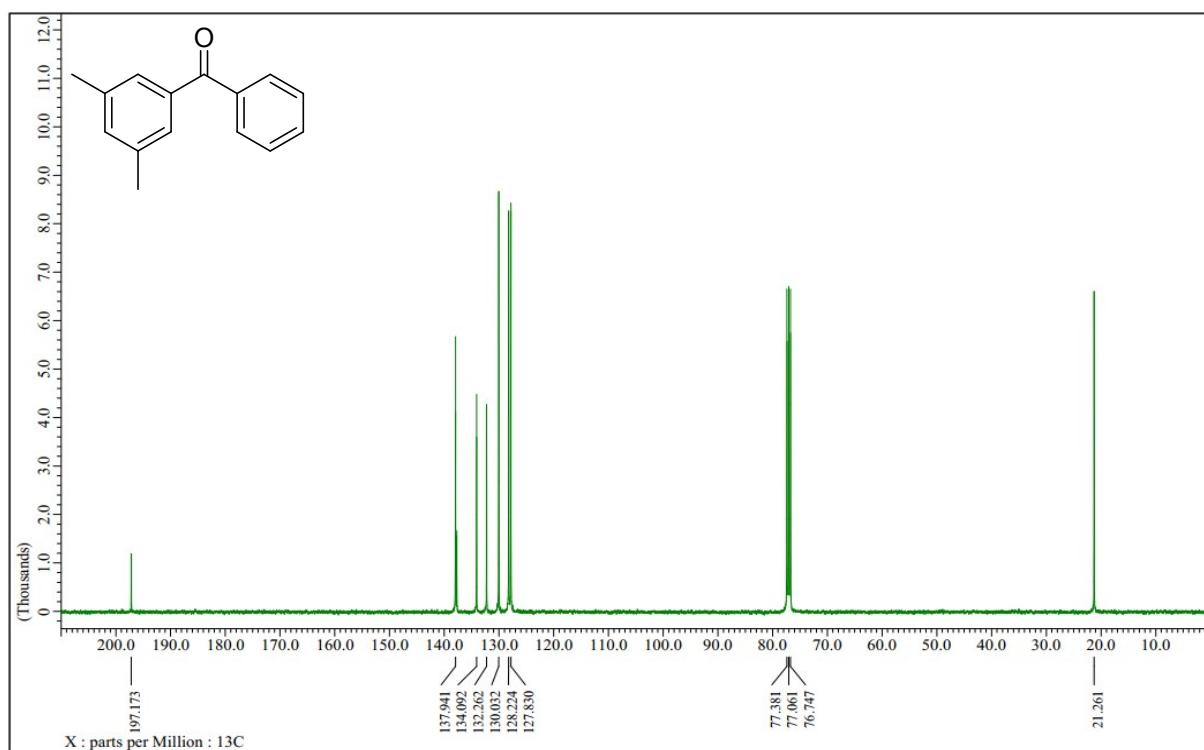


¹³C NMR spectrum of (4-benzylphenyl)(phenyl)methanone (**3i**)

(3,5-dimethylphenyl)(phenyl)methanone (3k)

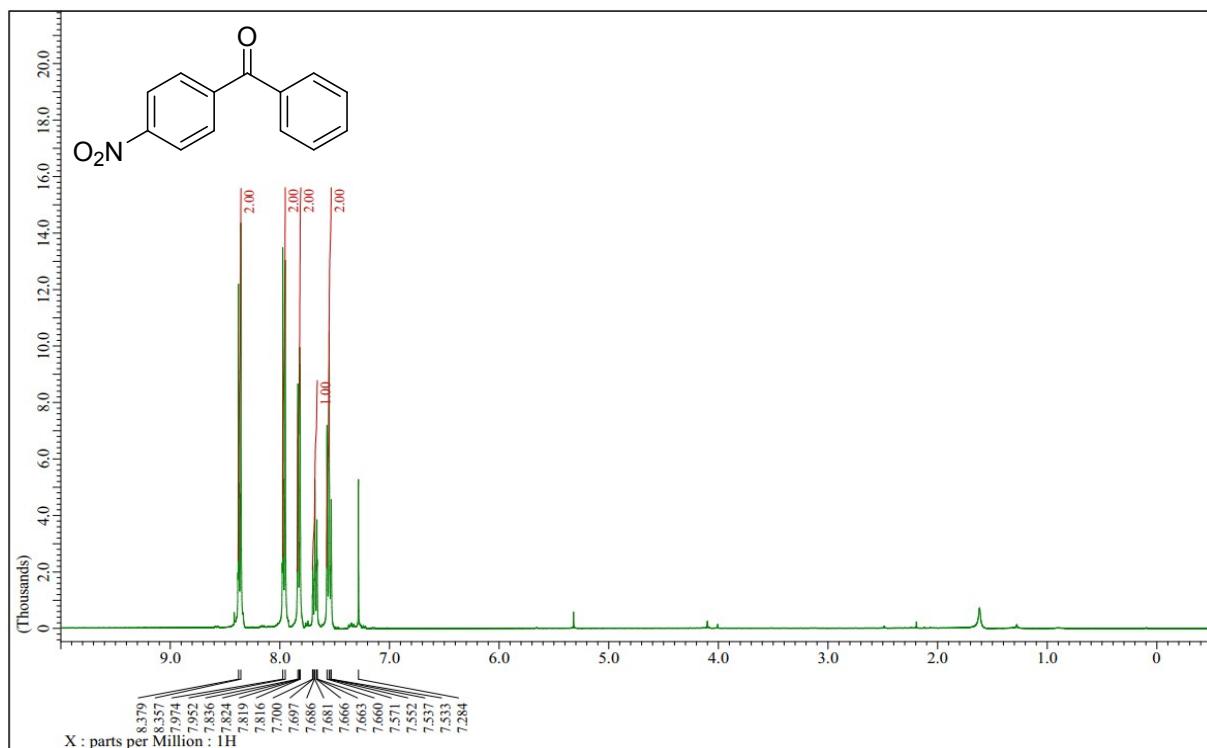


¹H NMR spectrum of (3,5-dimethylphenyl)(phenyl)methanone (**3k**)

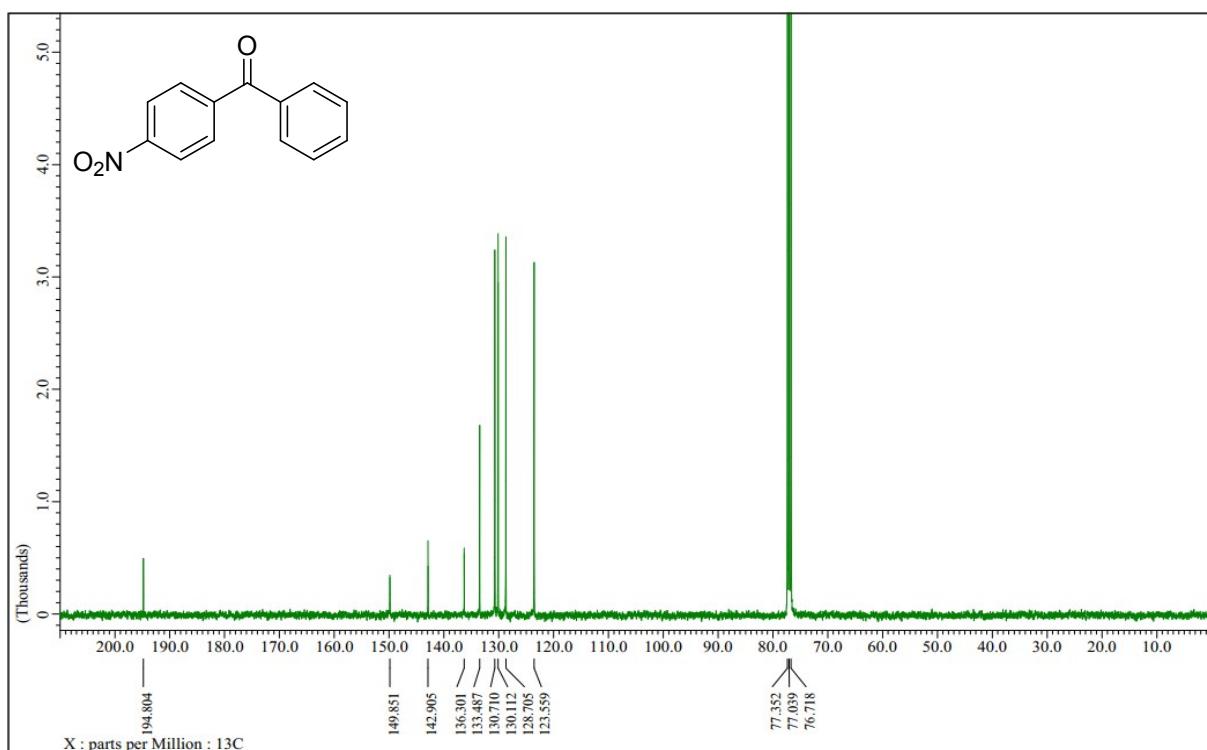


¹³C NMR spectrum of (3,5-dimethylphenyl)(phenyl)methanone (**3k**)

(4-nitrophenyl)(phenyl)methanone (3n**)**

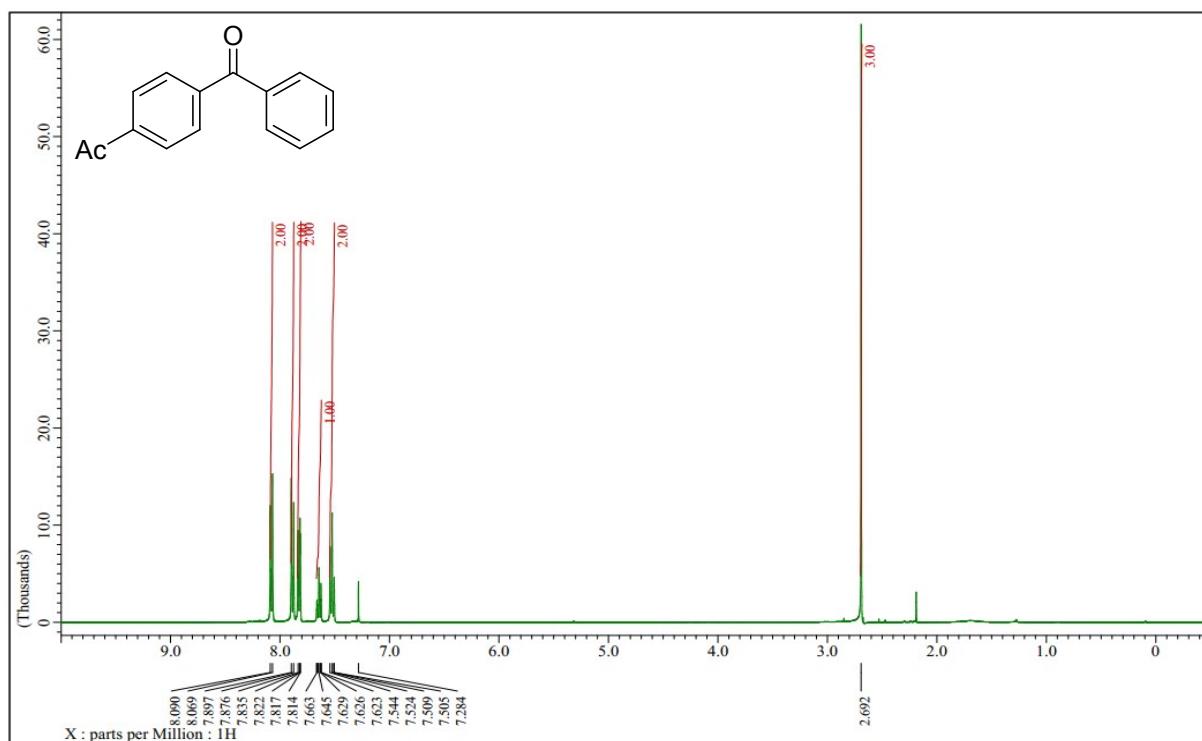


¹H NMR spectrum of (4-nitrophenyl)(phenyl)methanone (**3n**)

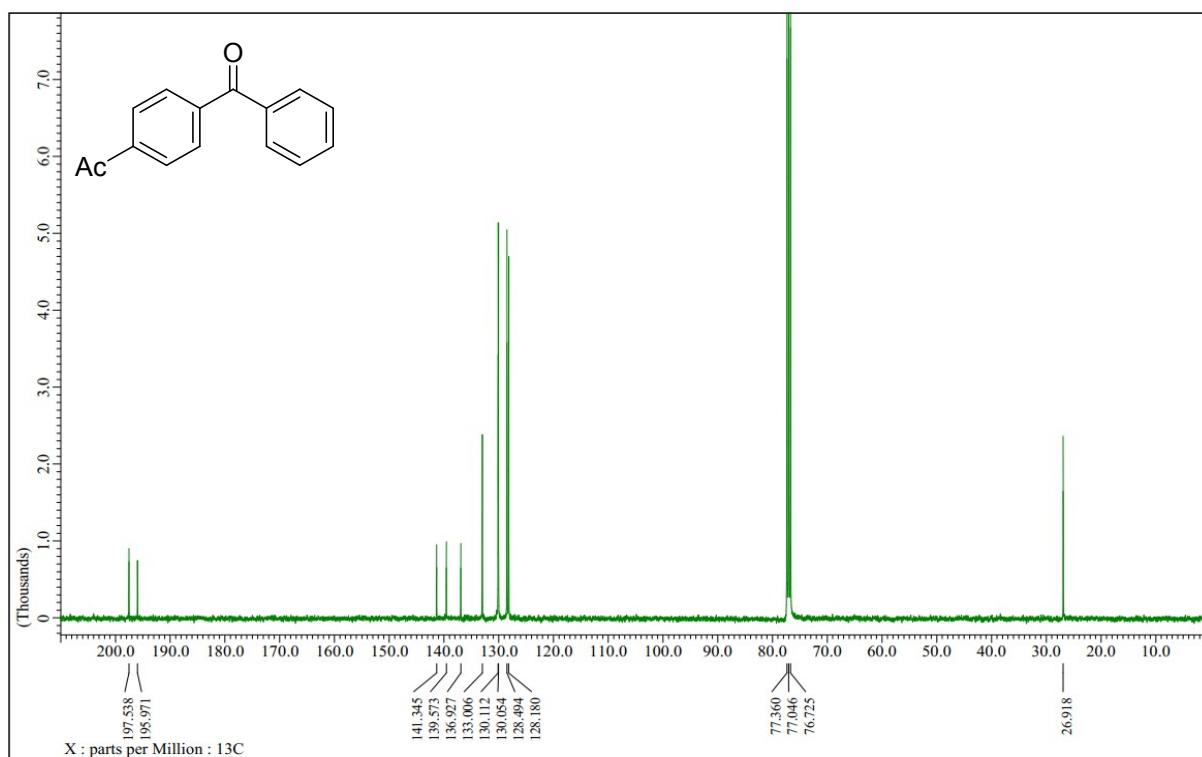


¹³C NMR spectrum of (4-nitrophenyl)(phenyl)methanone (**3n**)

1-(4-benzoylphenyl)ethan-1-one (3o**)**

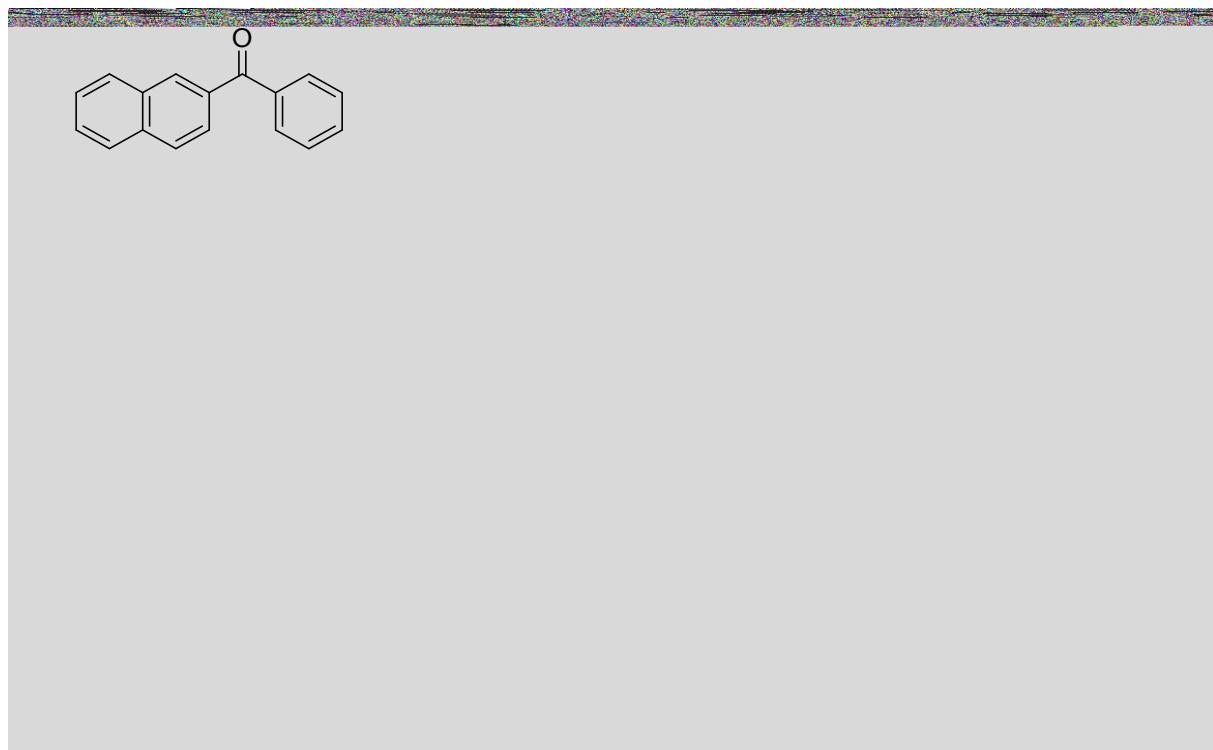


¹H NMR spectrum of 1-(4-benzoylphenyl)ethan-1-one (**3o**)

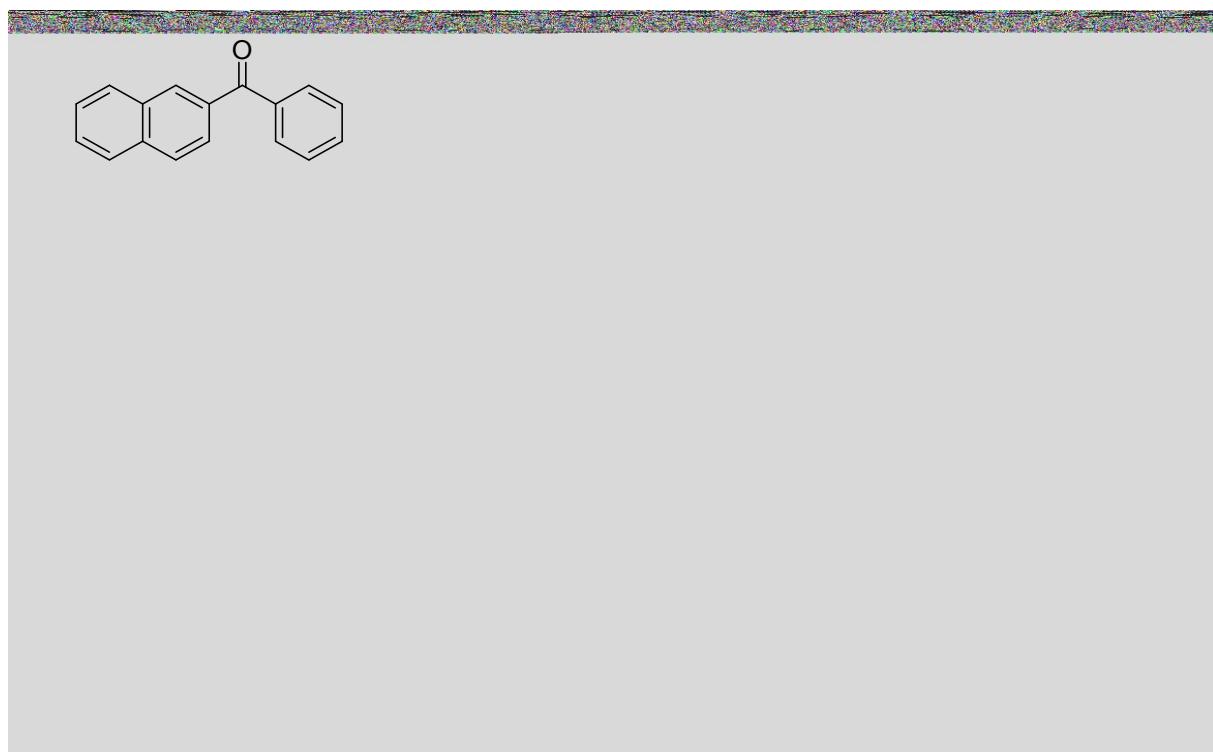


¹³C NMR spectrum of 1-(4-benzoylphenyl)ethan-1-one (**3o**)

naphthalen-2-yl(phenyl)methanone (3p**)**

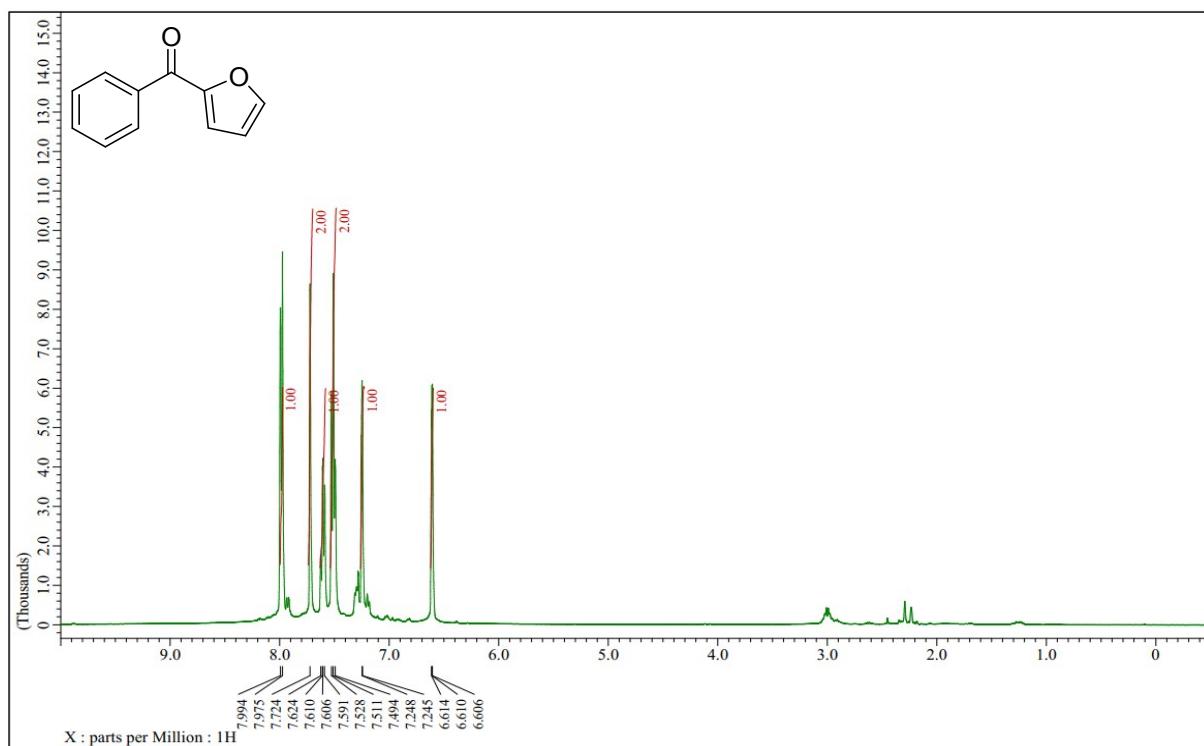


¹H NMR spectrum of naphthalen-2-yl(phenyl)methanone (**3p**)

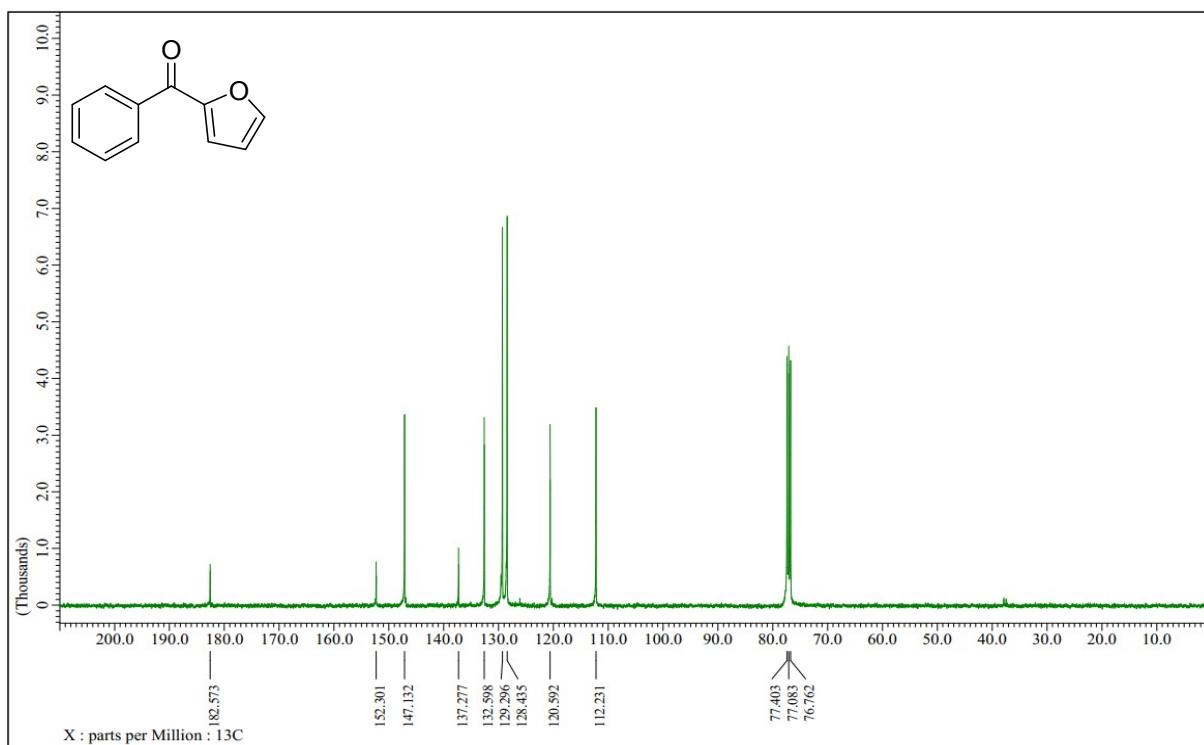


¹³C NMR spectrum of naphthalen-2-yl(phenyl)methanone (**3p**)

furan-2-yl(phenyl)methanone (3q**)**

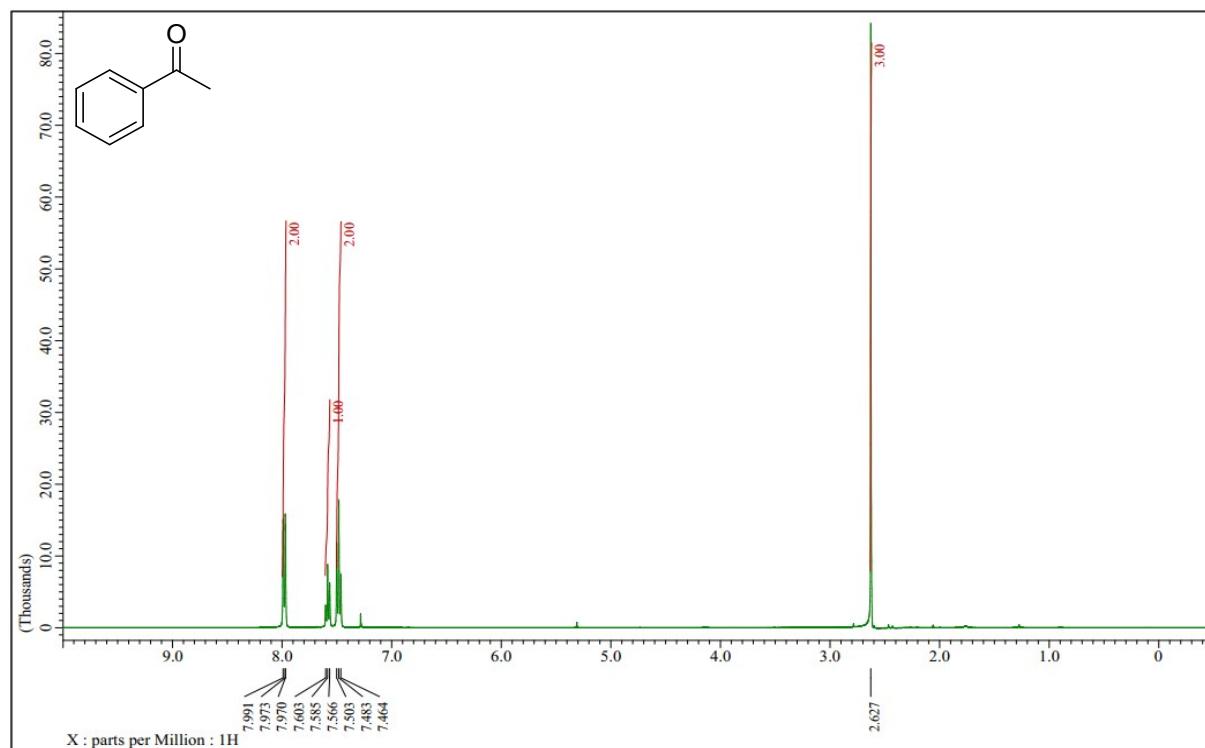


¹H NMR spectrum of furan-2-yl(phenyl)methanone (**3q**)

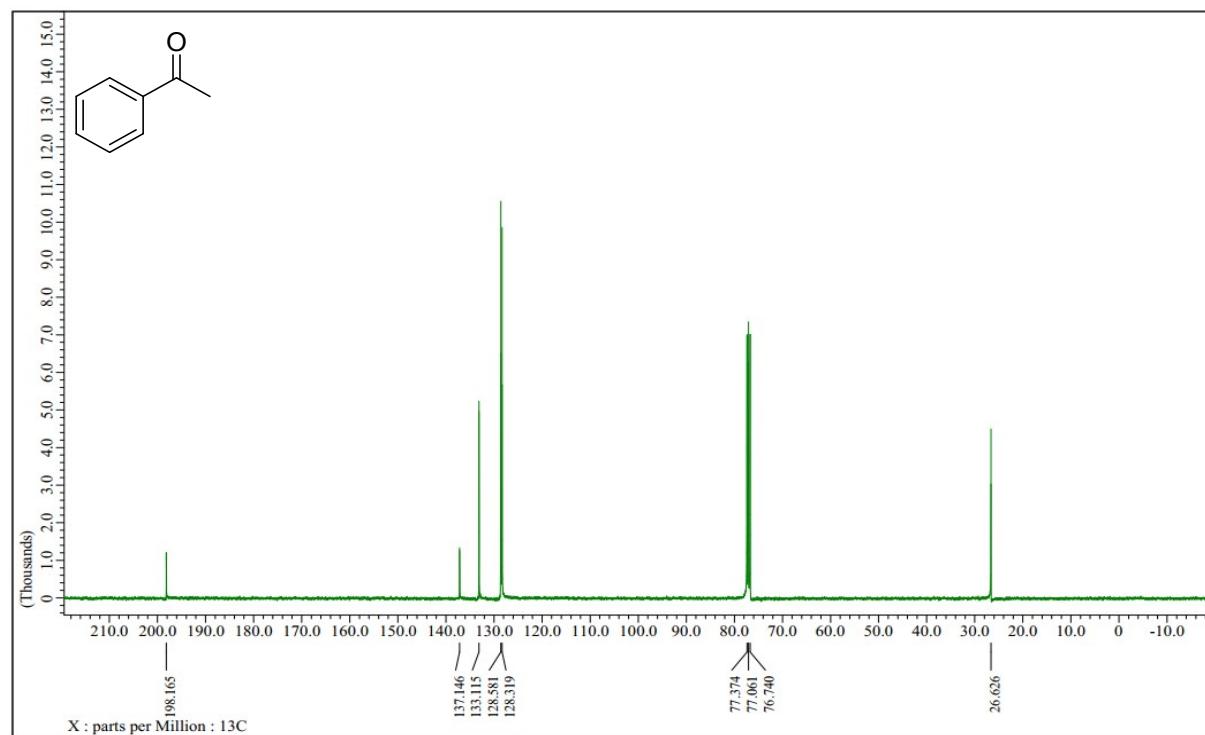


¹³C NMR spectrum of furan-2-yl(phenyl)methanone (**3q**)

acetophenone (3r)

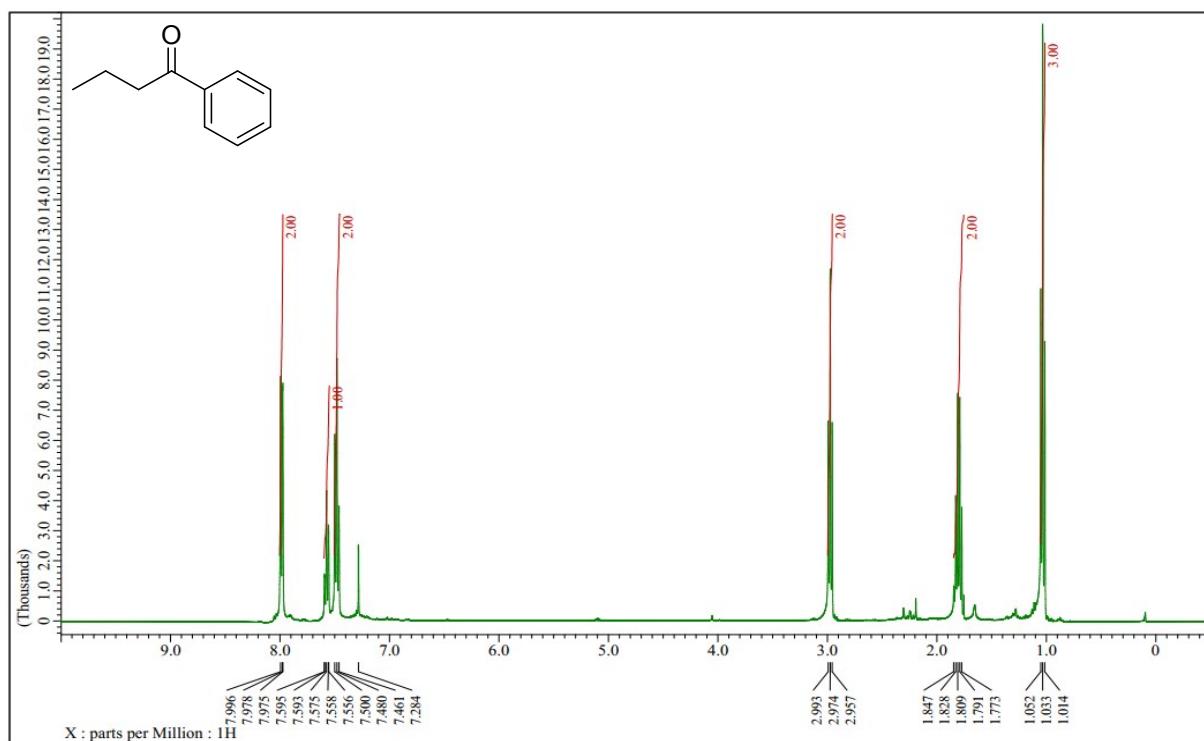


¹H NMR spectrum of acetophenone (3r)

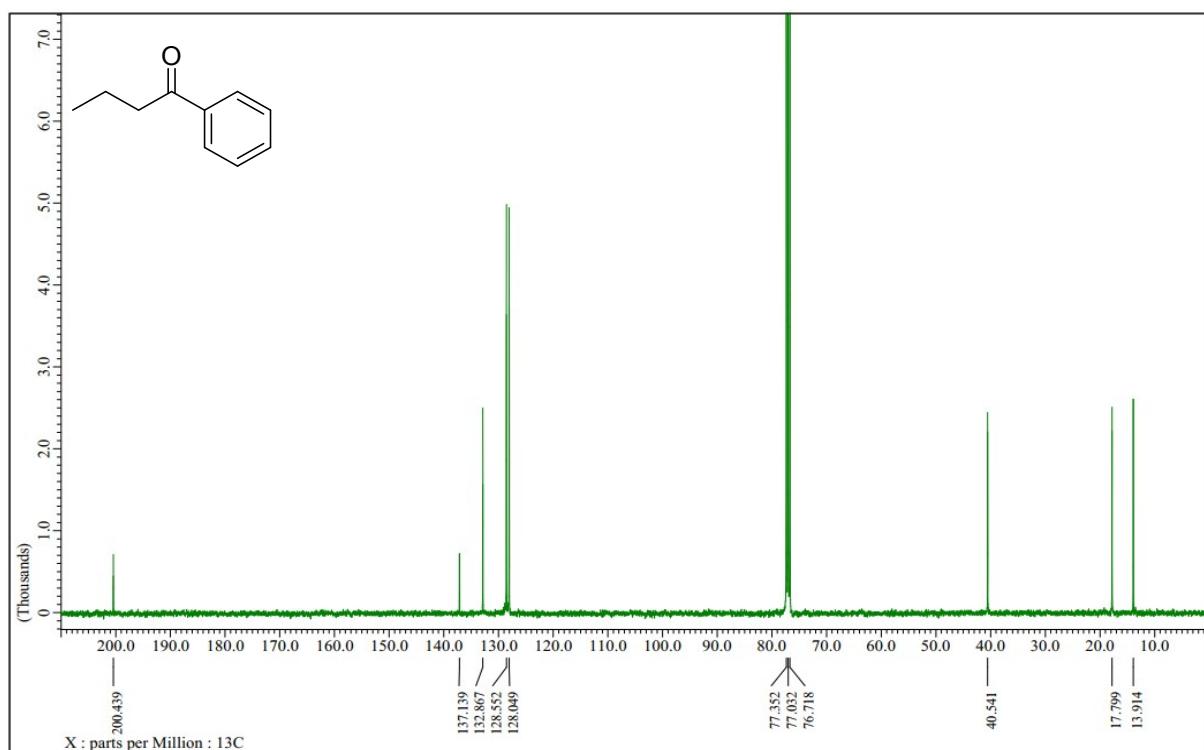


¹³C NMR spectrum of acetophenone (3r)

1-phenylbutan-1-one (3s)

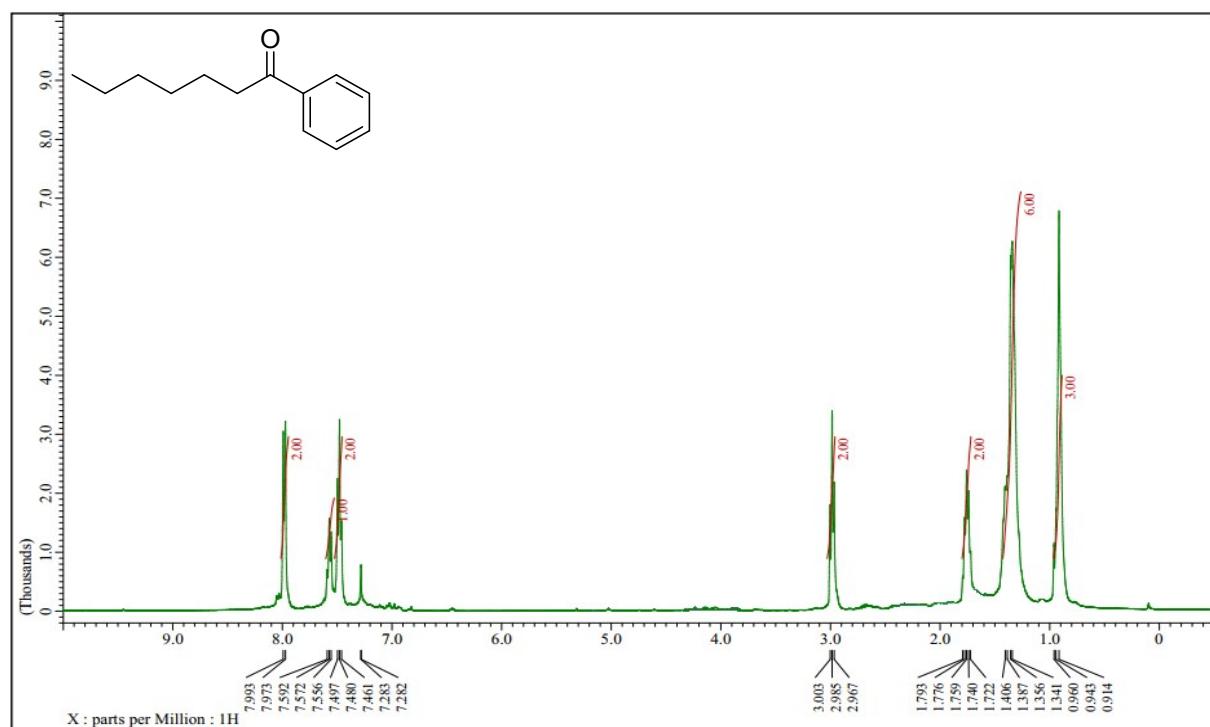


¹H NMR spectrum of 1-phenylbutan-1-one (3s)

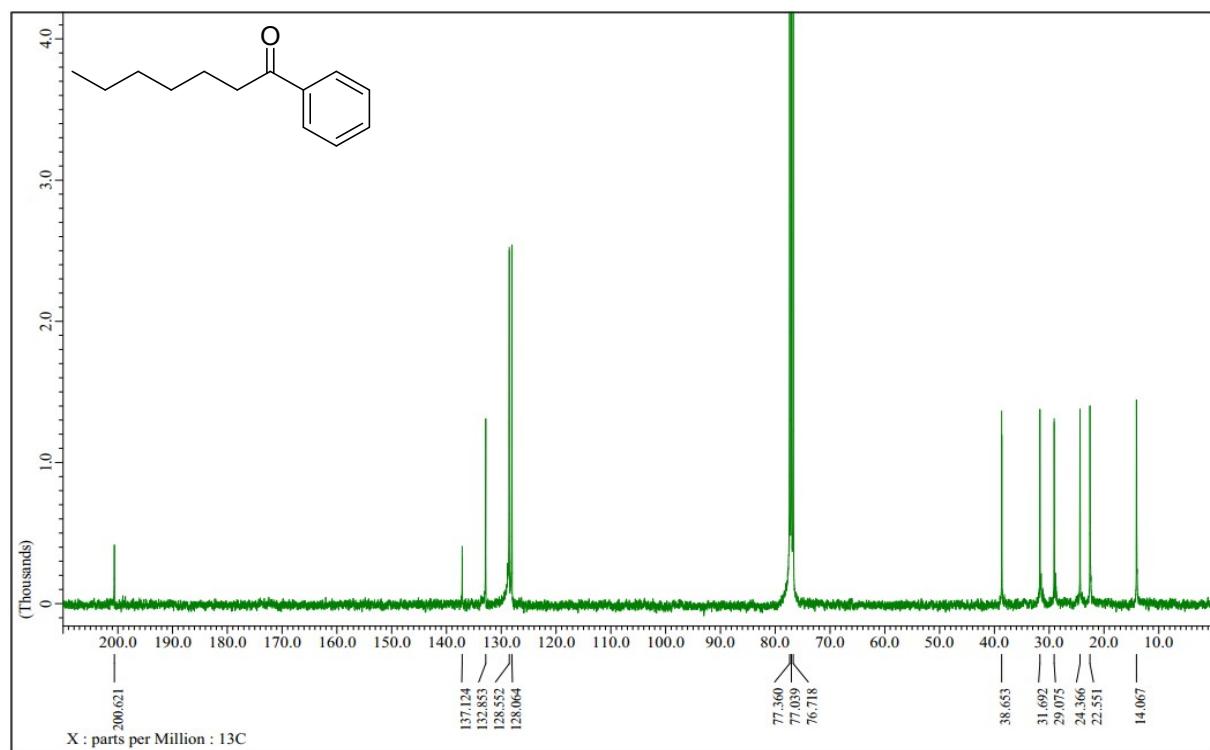


¹³C NMR spectrum of 1-phenylbutan-1-one (3s)

1-phenylheptan-1-one (3u)

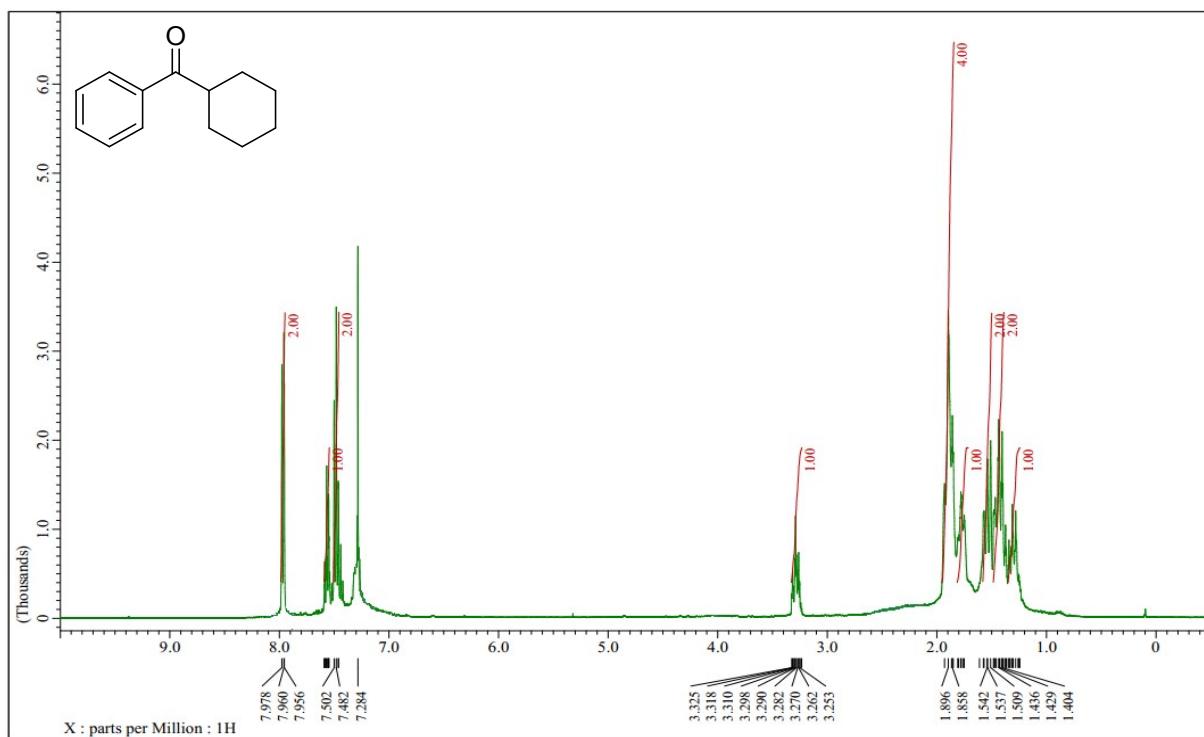


¹H NMR spectrum of 1-phenylheptan-1-one (**3u**)

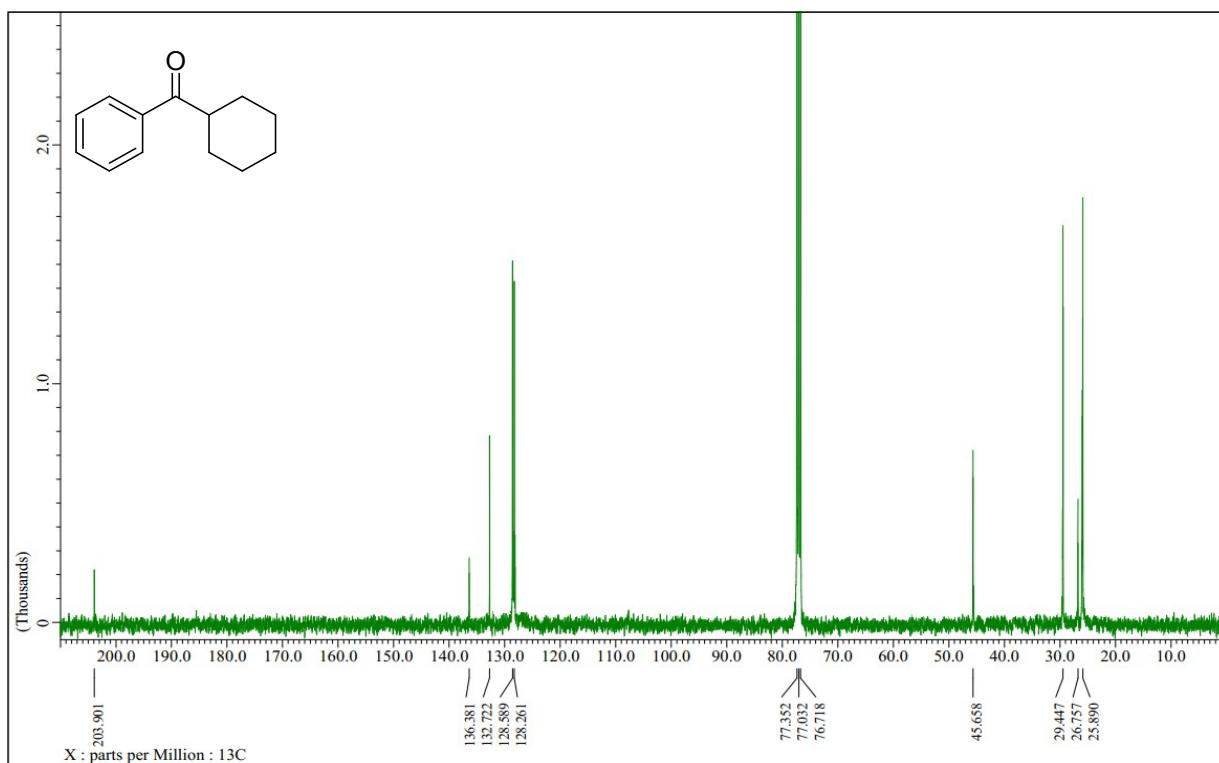


¹³C NMR spectrum of 1-phenylheptan-1-one (**3u**)

cyclohexyl(phenyl)methanone (3v**)**

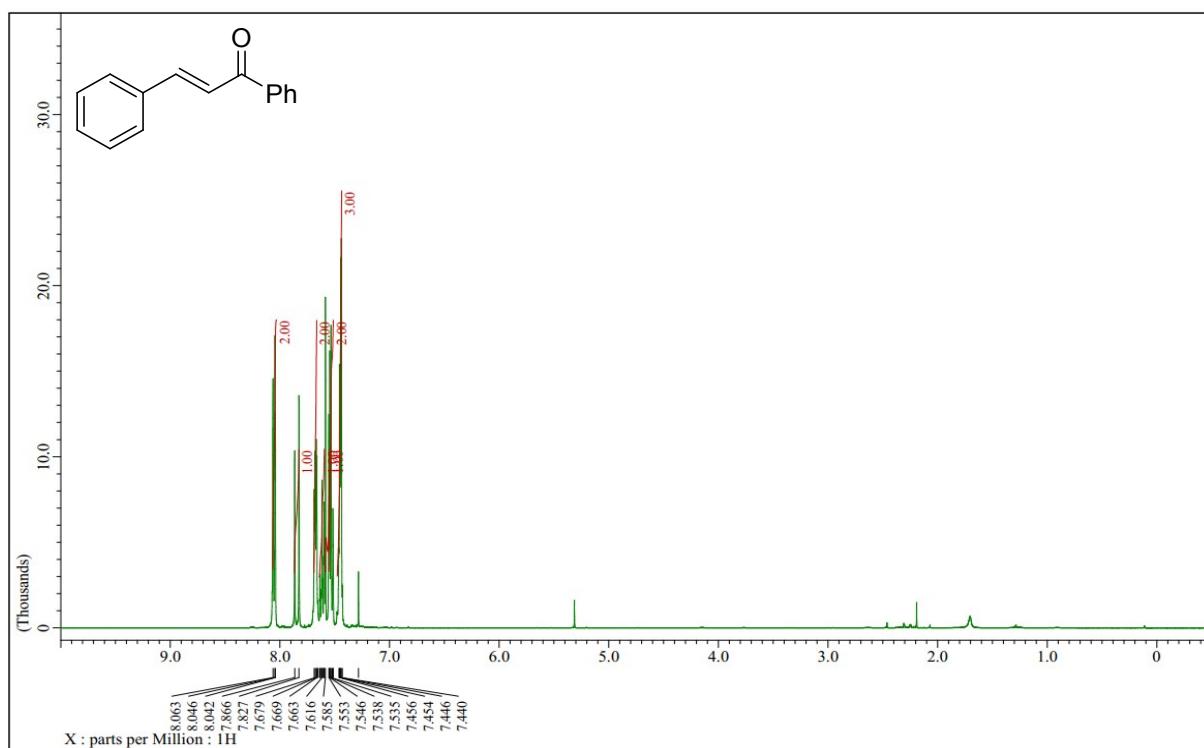


¹H NMR spectrum of cyclohexyl(phenyl)methanone (**3v**)

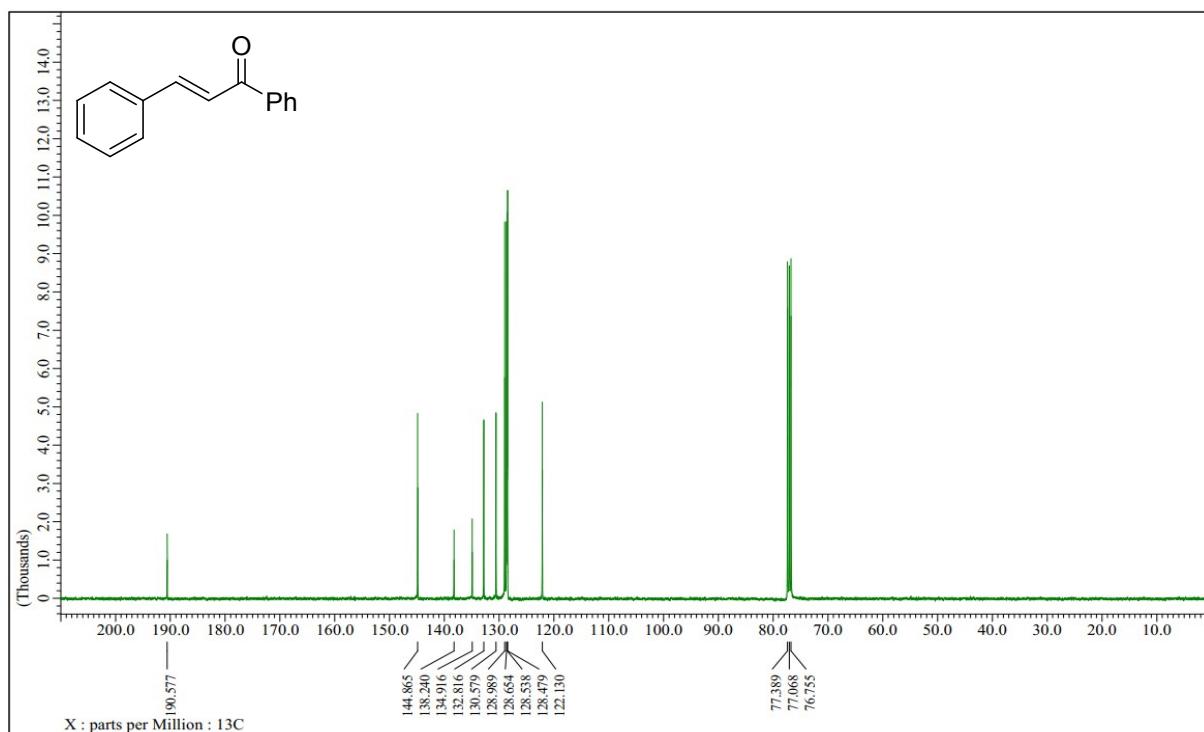


¹³C NMR spectrum of cyclohexyl(phenyl)methanone (**3v**)

(E)-chalcone (3w)

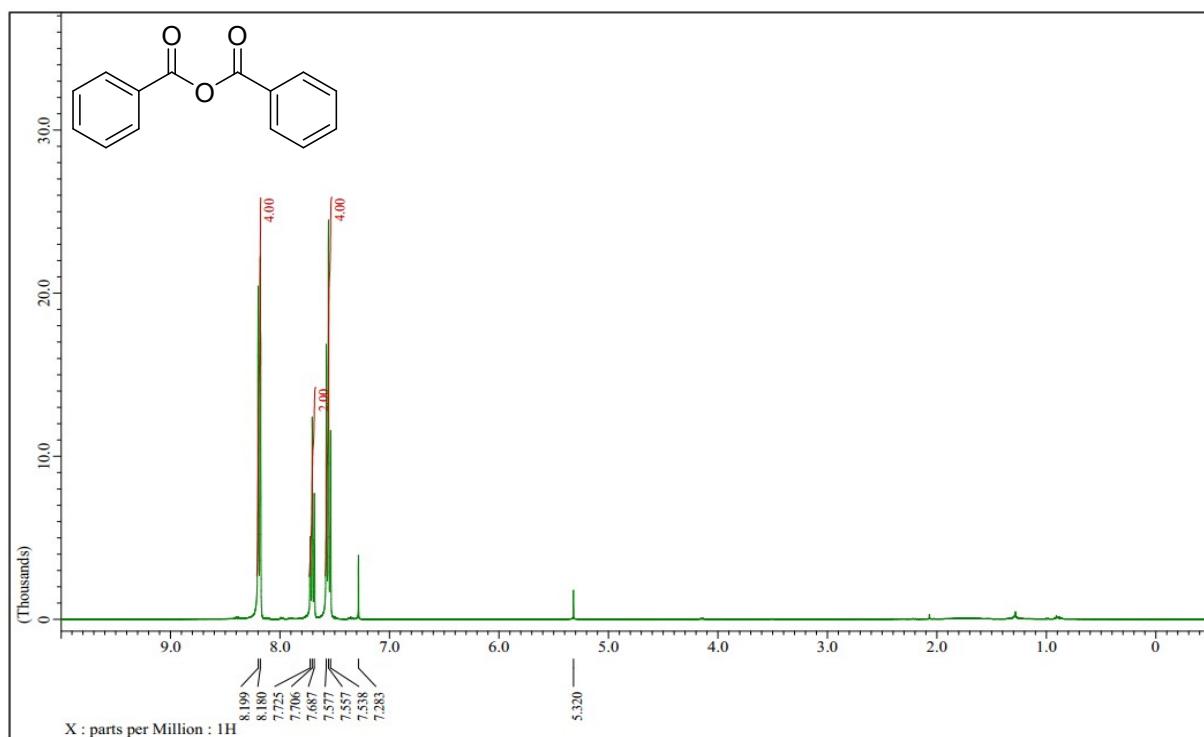


¹H NMR spectrum of (E)-chalcone (3w)

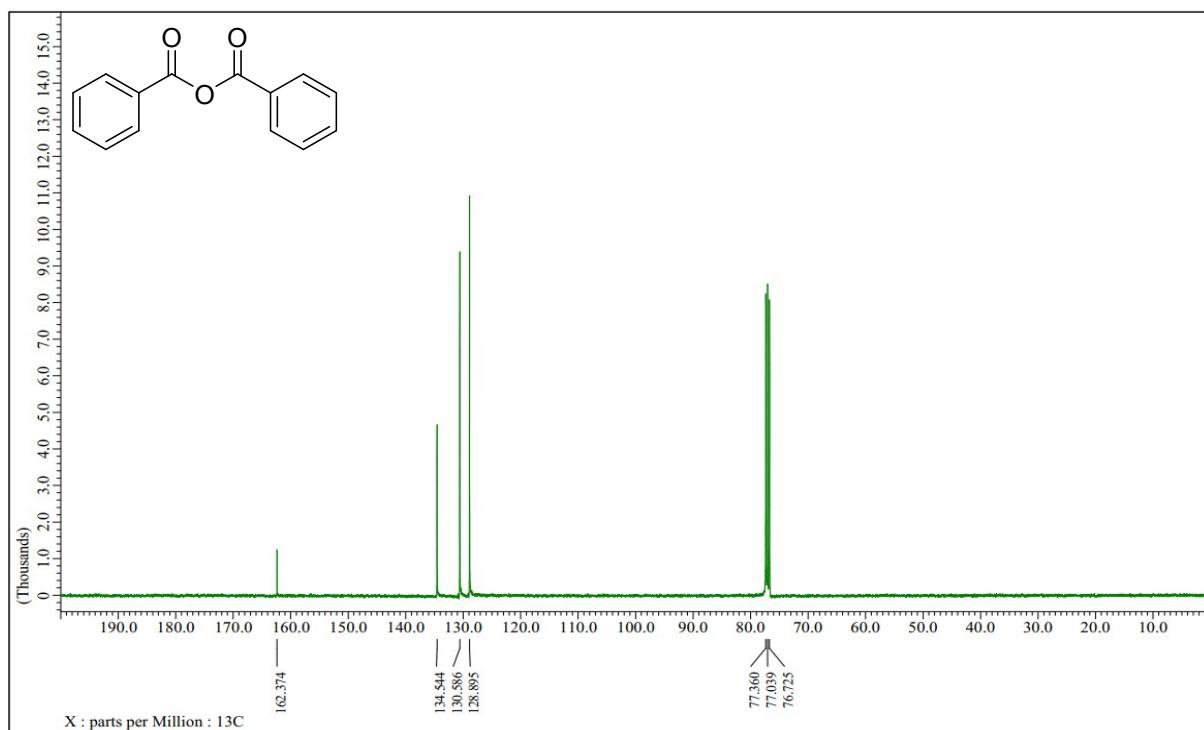


¹³C NMR spectrum of (E)-chalcone (3w)

Benzoic anhydride (7a)

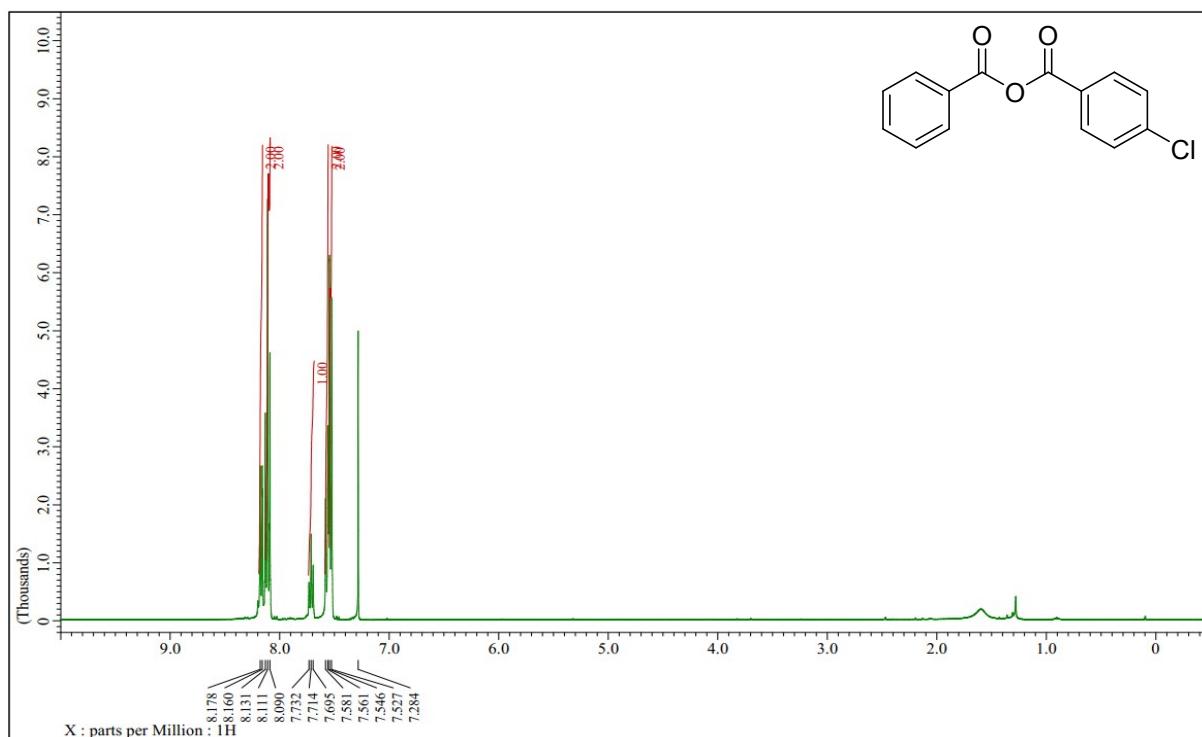


¹H NMR spectrum of benzoic anhydride (7a)

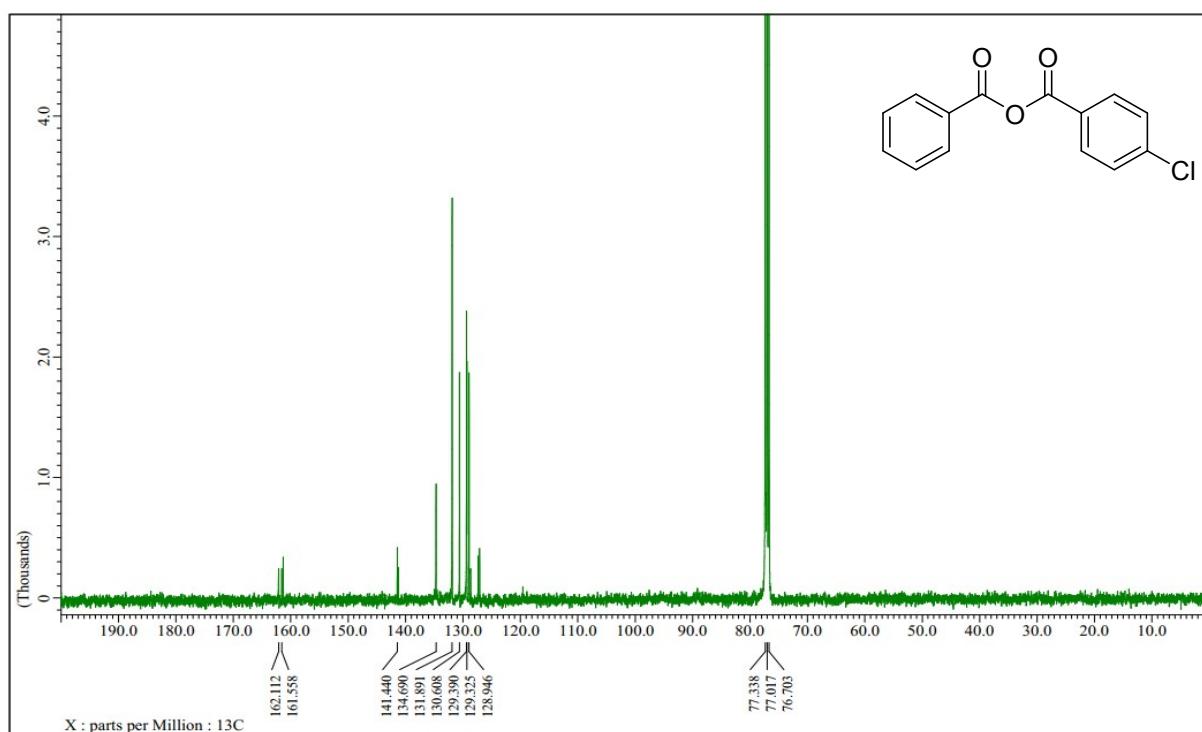


¹³C NMR spectrum of benzoic anhydride (7a)

Benzoic 4-chlorobenzoic anhydride (7b)

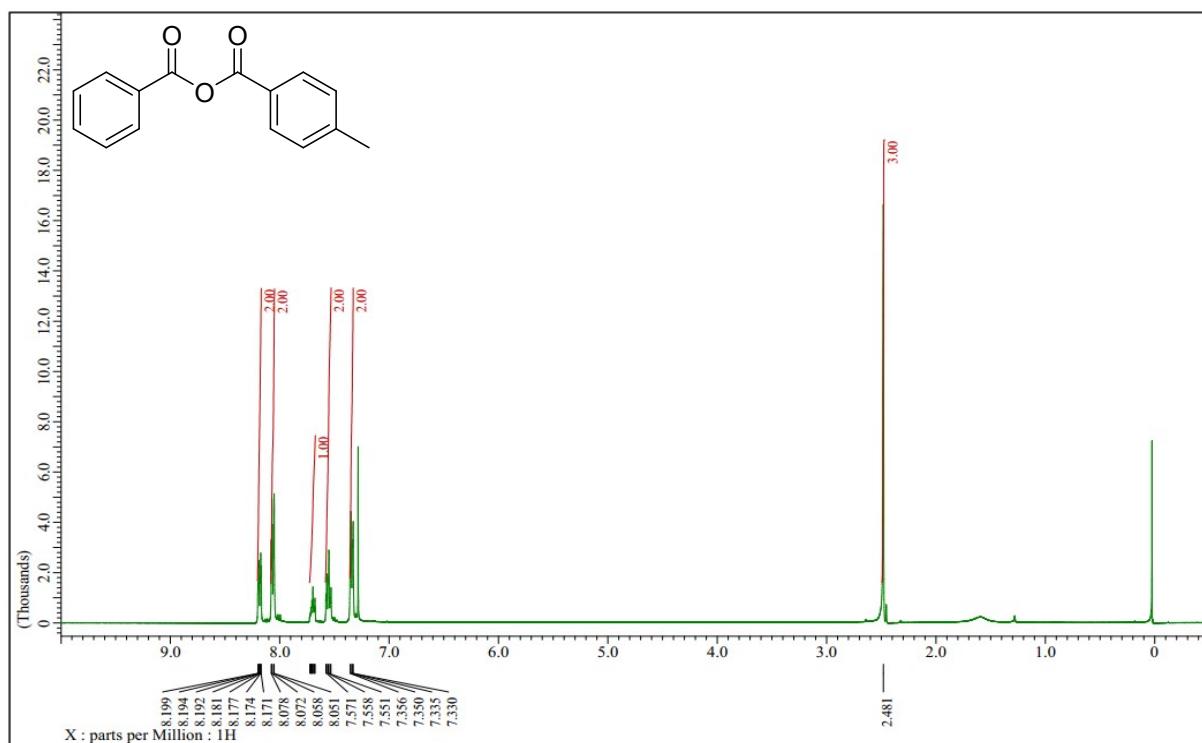


¹H NMR spectrum of benzoic 4-chlorobenzoic anhydride (7b)

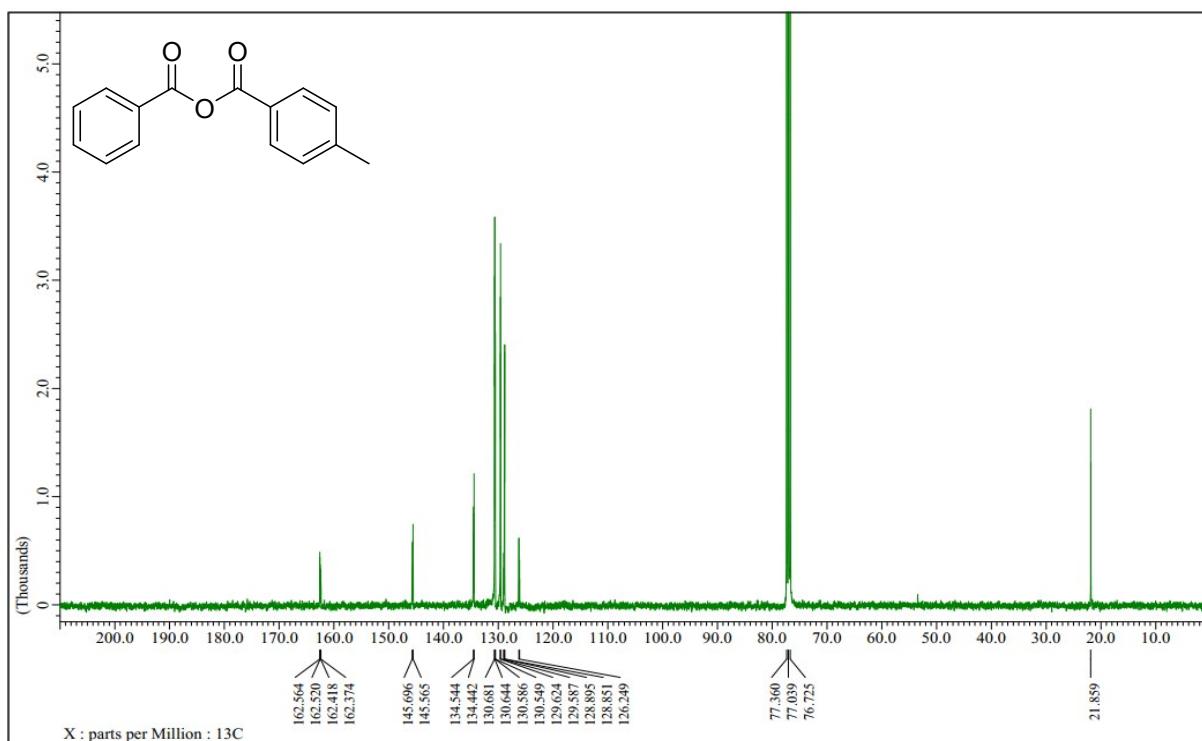


¹³C NMR spectrum of benzoic 4-chlorobenzoic anhydride (7b)

Benzoic 4-methylbenzoic anhydride (7c)

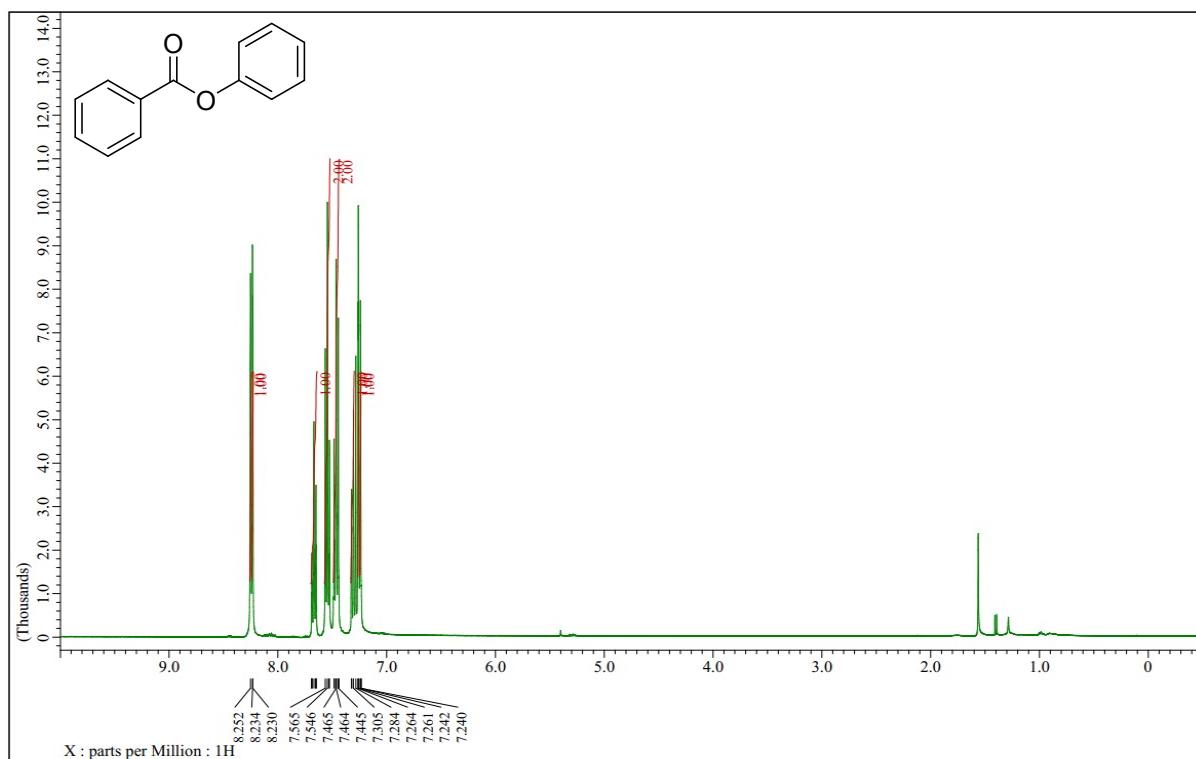


¹H NMR spectrum of benzoic 4-methylbenzoic anhydride (7c)

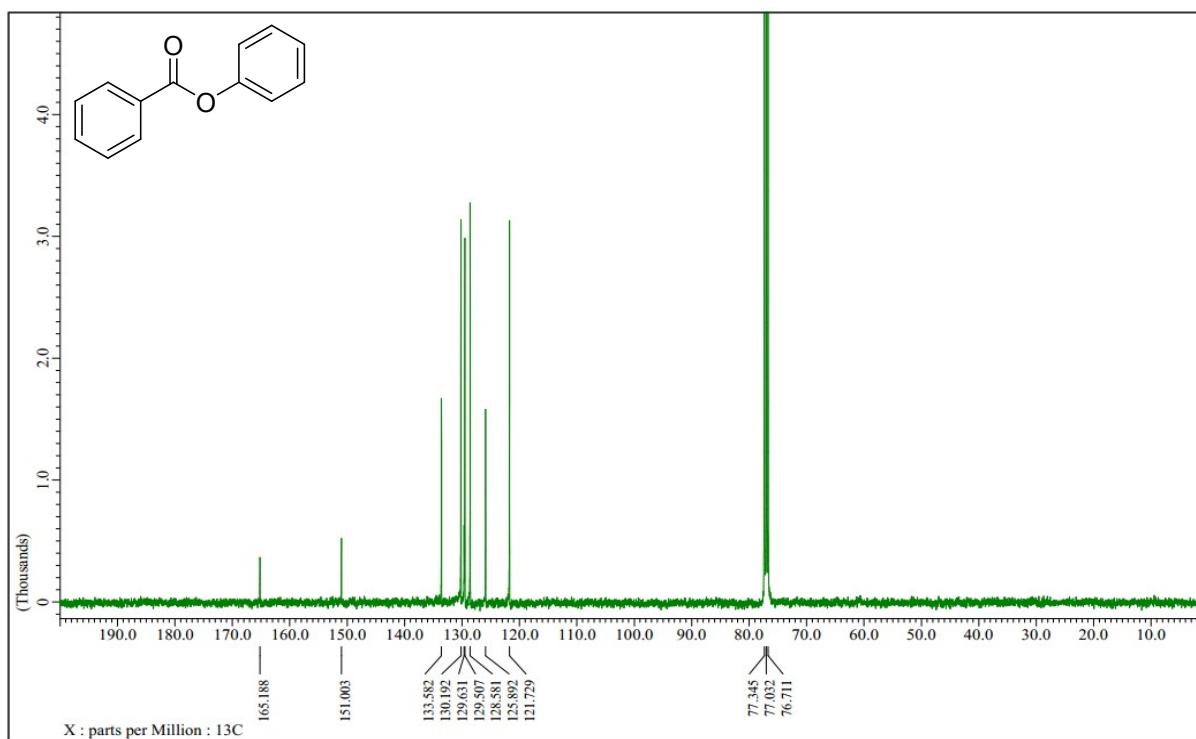


¹³C NMR spectrum of benzoic 4-methylbenzoic anhydride (7c)

Phenyl benzoate (7d)

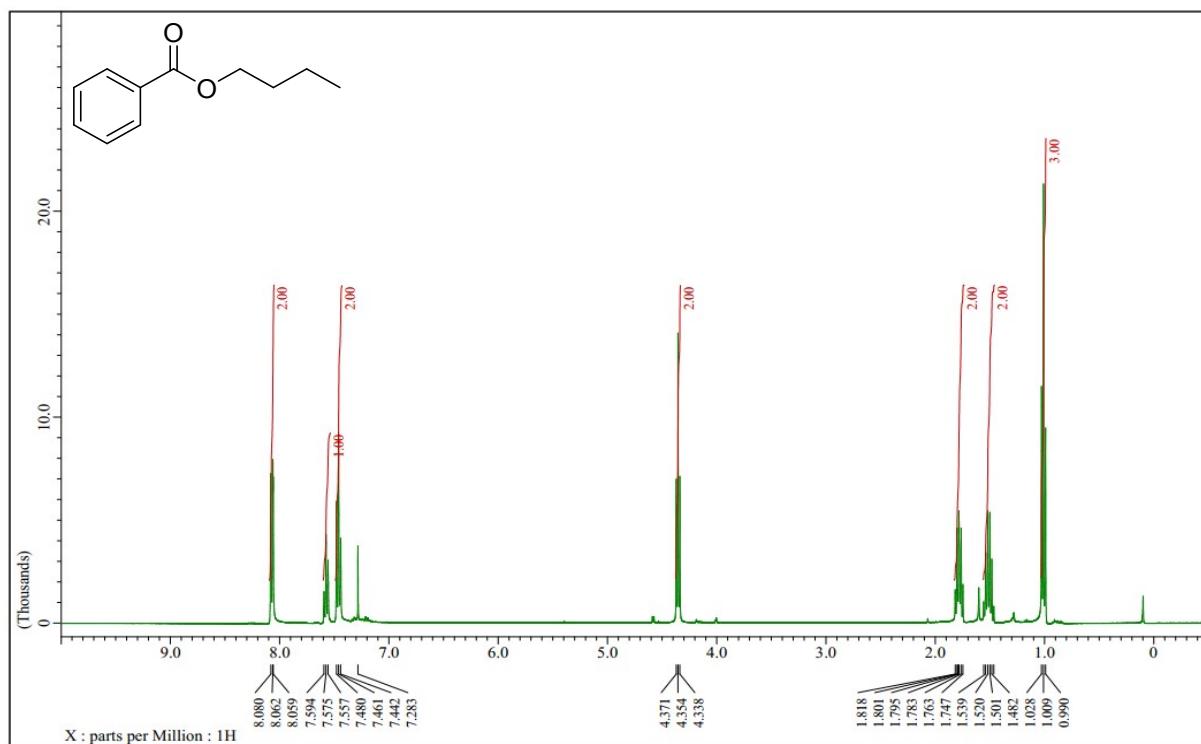


¹H NMR spectrum of phenyl benzoate (**7d**)

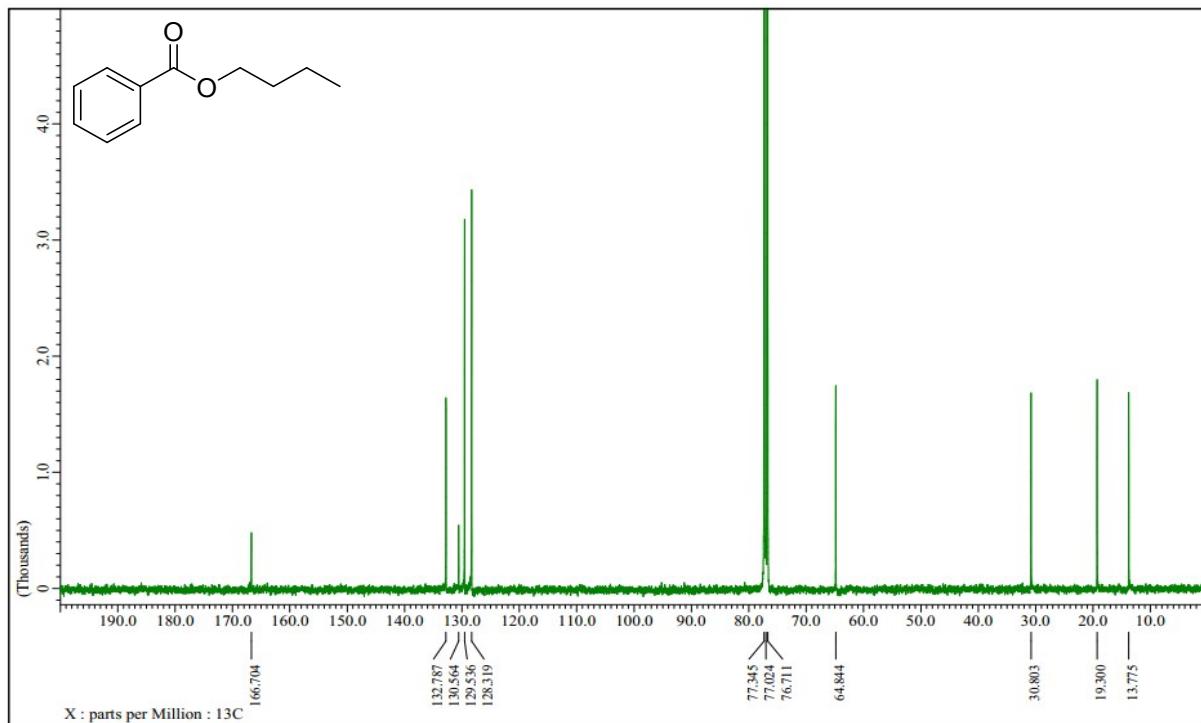


¹³C NMR spectrum of phenyl benzoate (**7d**)

butyl benzoate (7e)

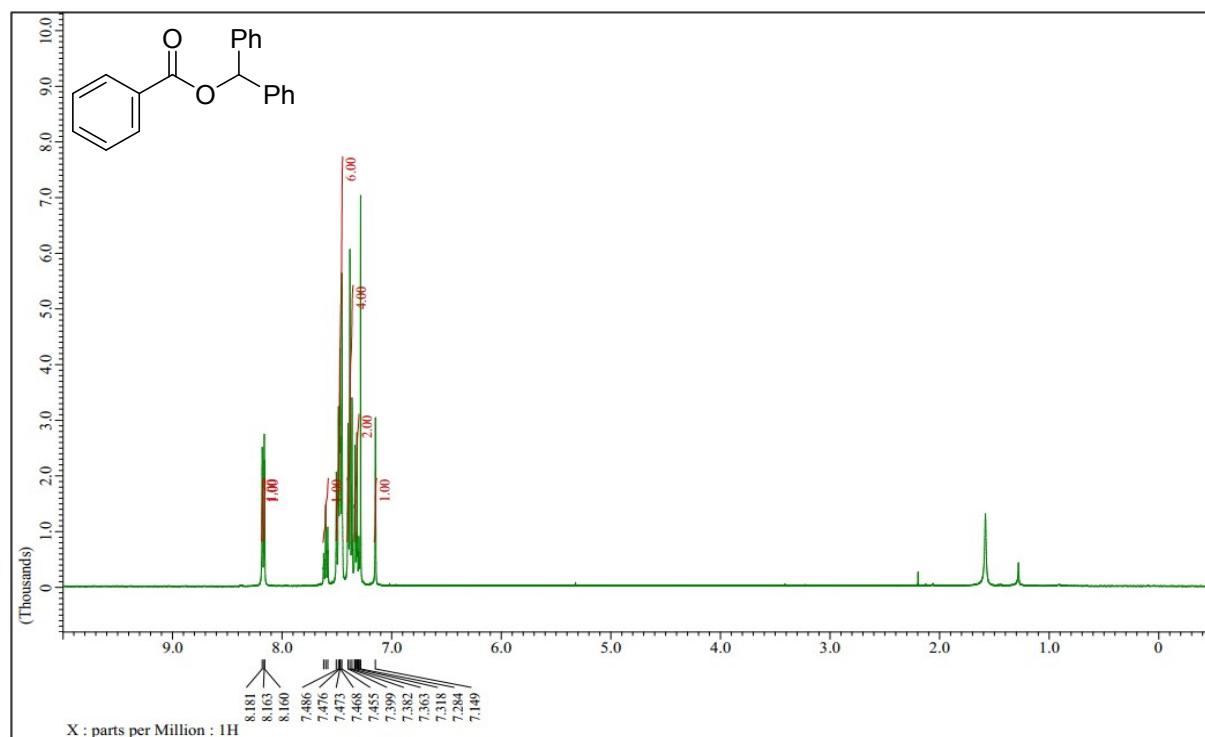


¹H NMR spectrum of butyl benzoate (**7e**)

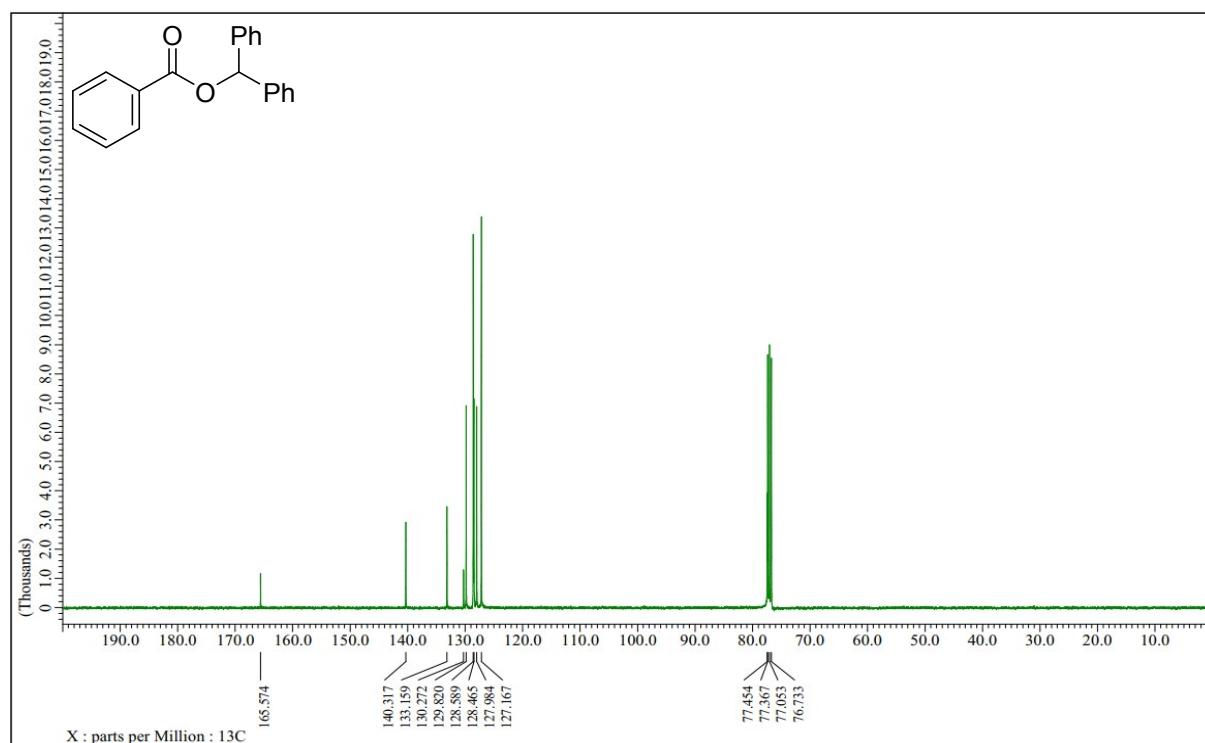


¹³C NMR spectrum of butyl benzoate (**7e**)

Benzylbenzoate (7f)

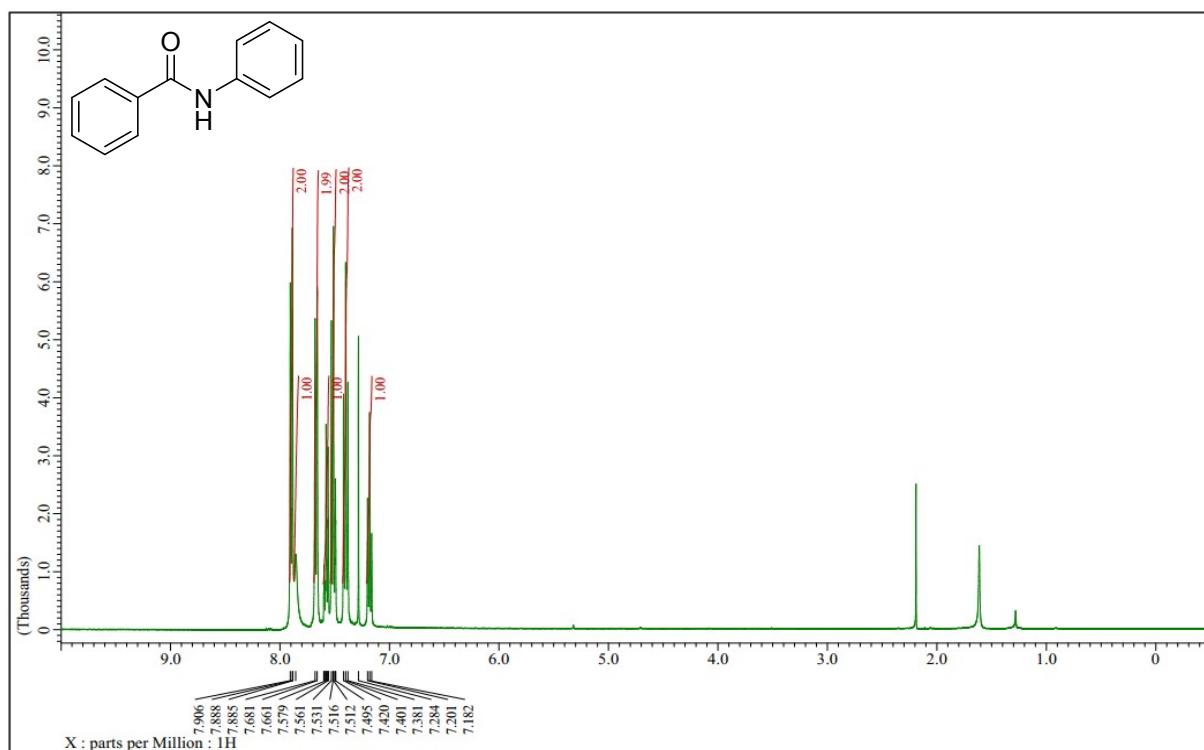


¹H NMR spectrum of benzylbenzoate (7f)

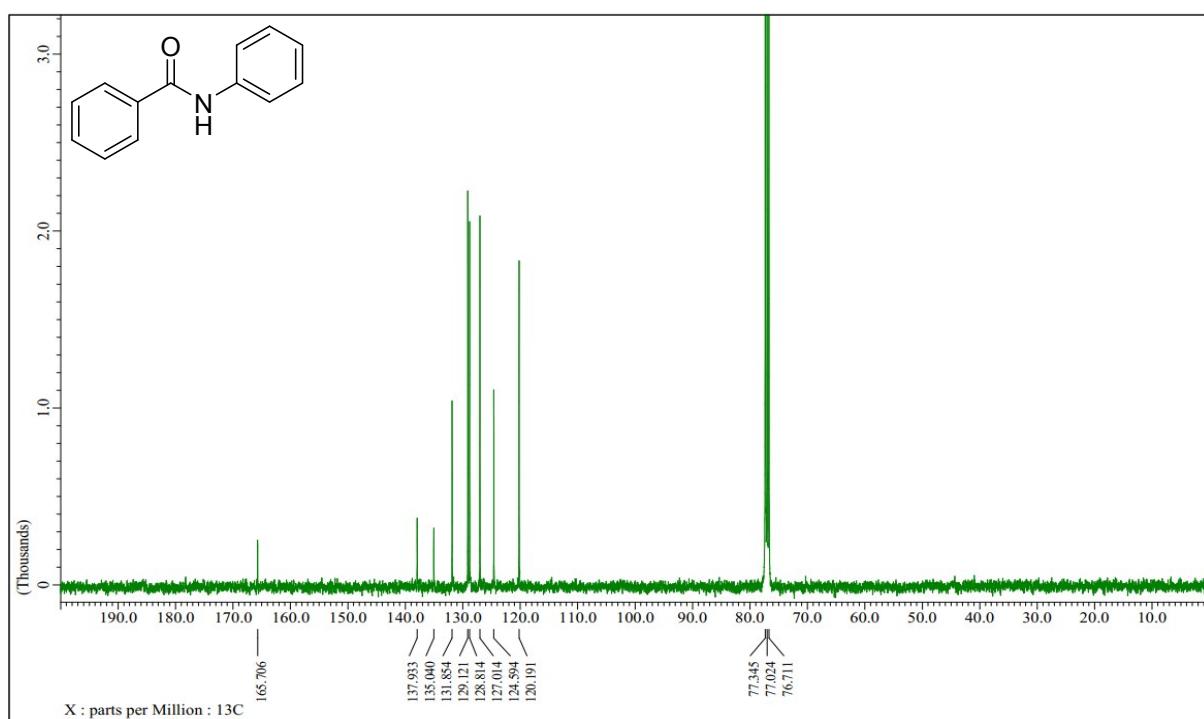


¹³C NMR spectrum of benzylbenzoate (7f)

N-phenylbenzamide (7g)

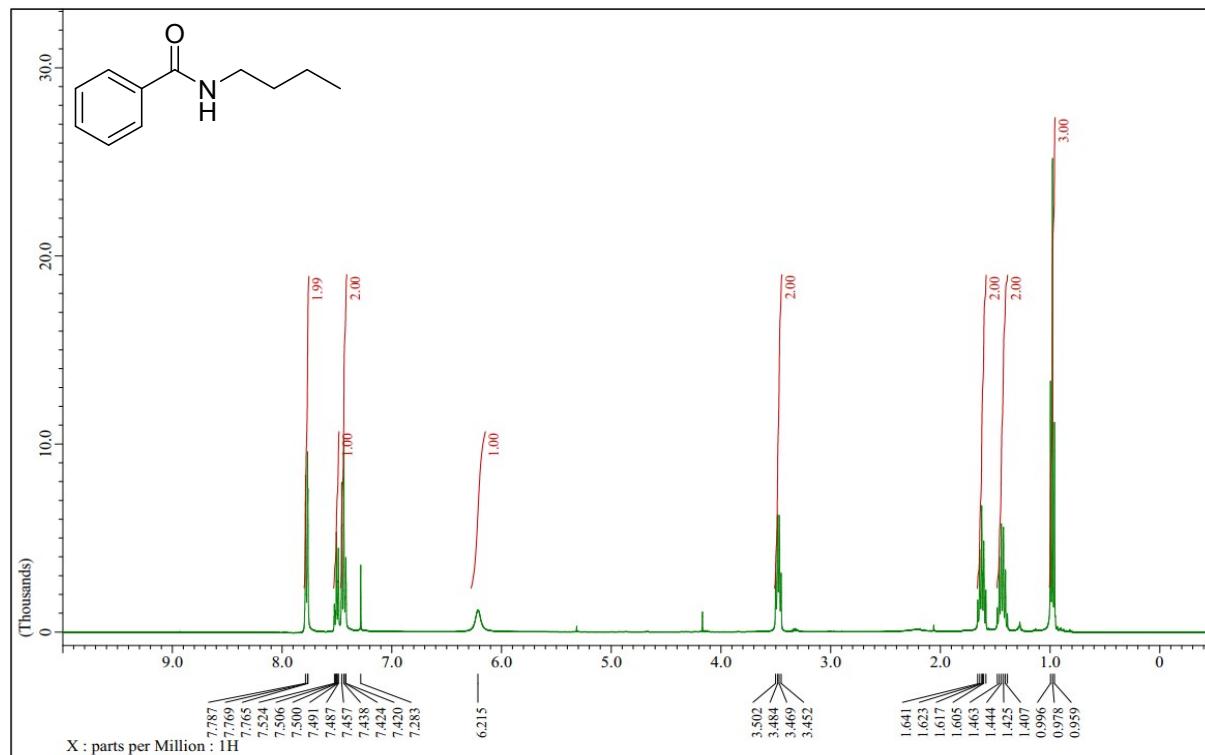


¹H NMR spectrum of *N*-phenylbenzamide (7g)

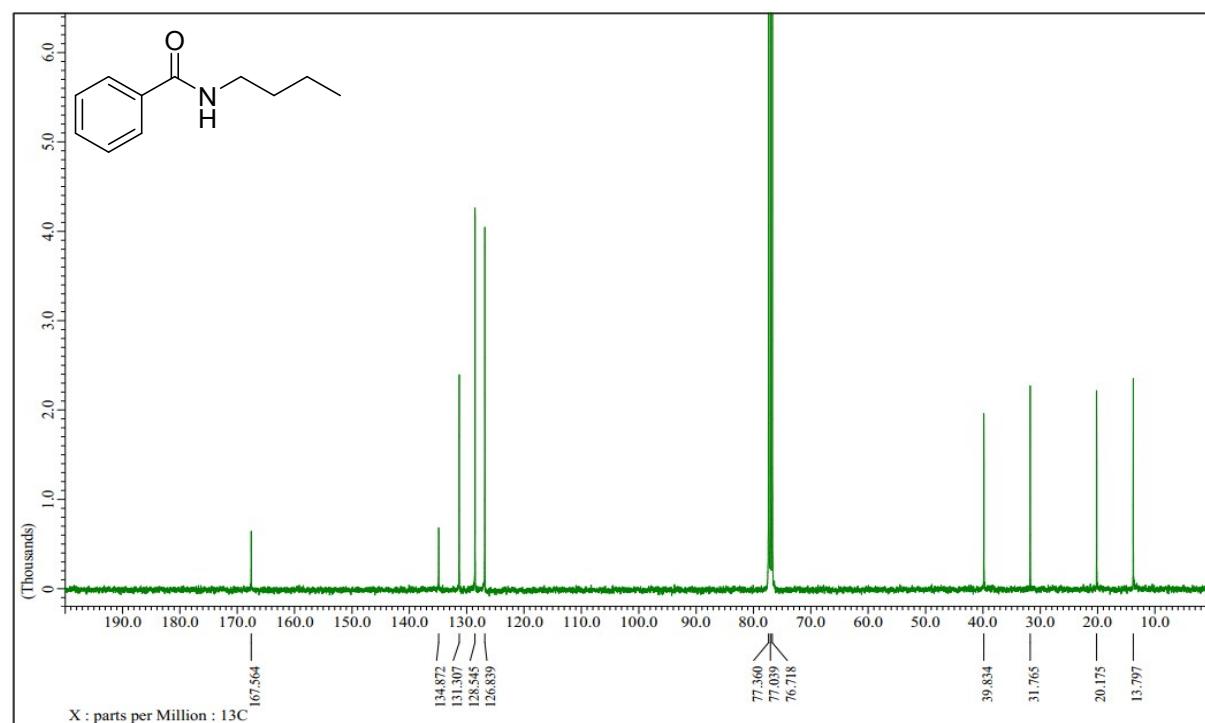


¹³C NMR spectrum of *N*-phenylbenzamide (7g)

N-butylbenzamide (7h)

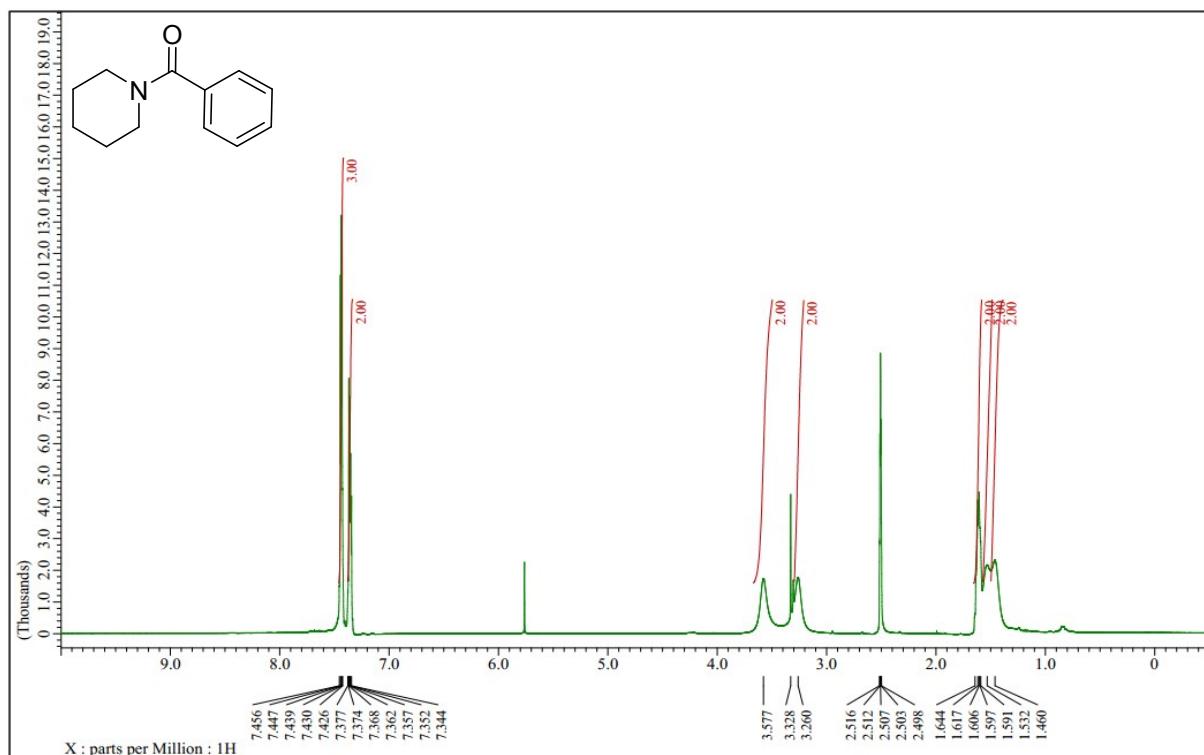


¹H NMR spectrum of *N*-butylbenzamide (**7h**)

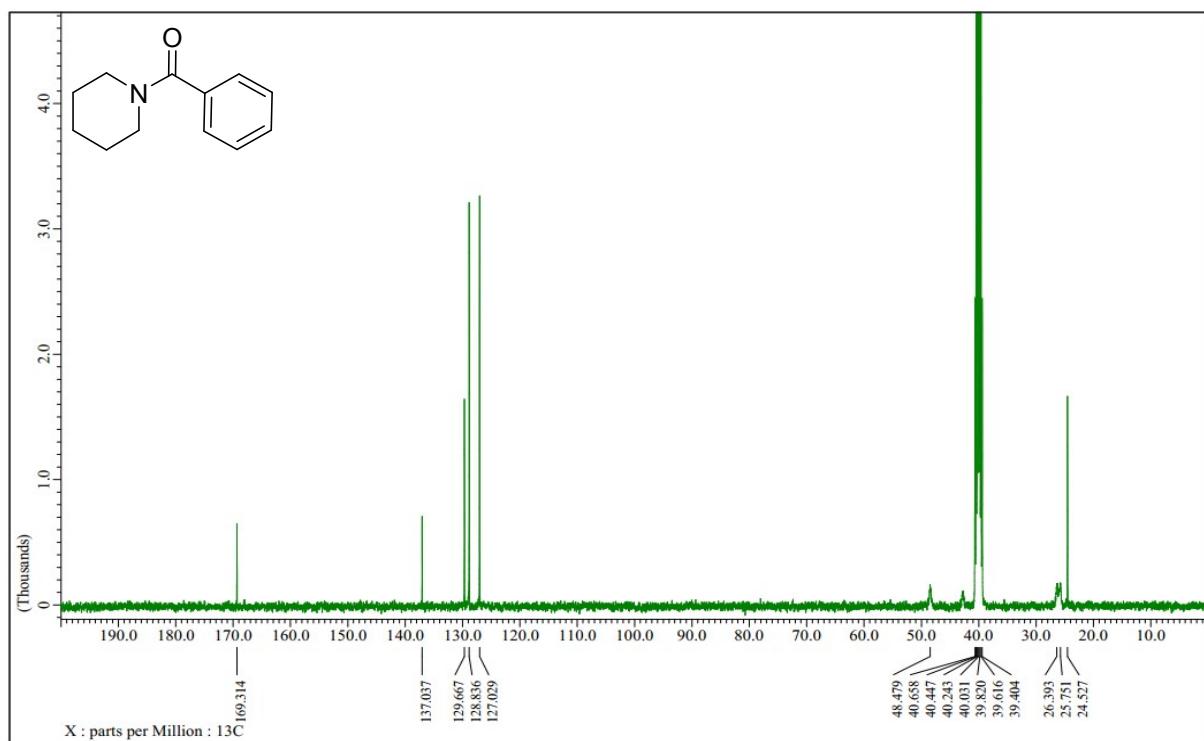


¹³C NMR spectrum of *N*-butylbenzamide (**7h**)

phenyl(piperidin-1-yl)methanone (7i)

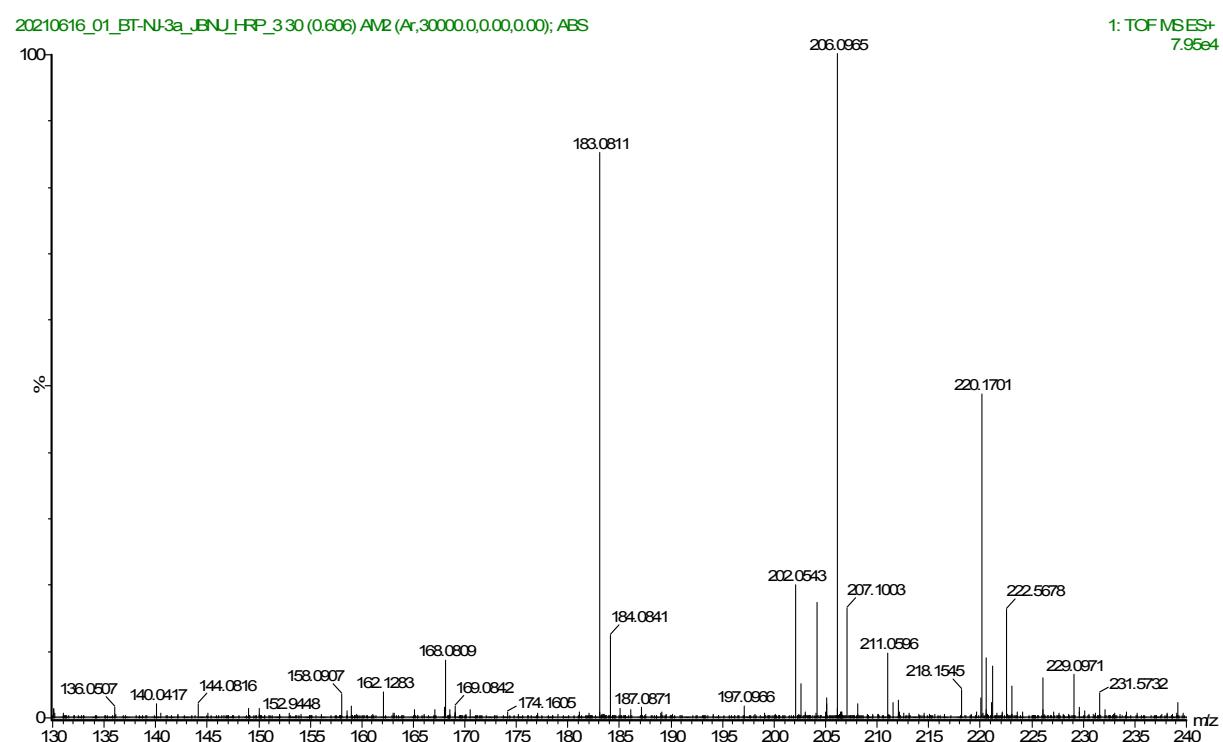


¹H NMR spectrum of phenyl(piperidin-1-yl)methanone (7i)

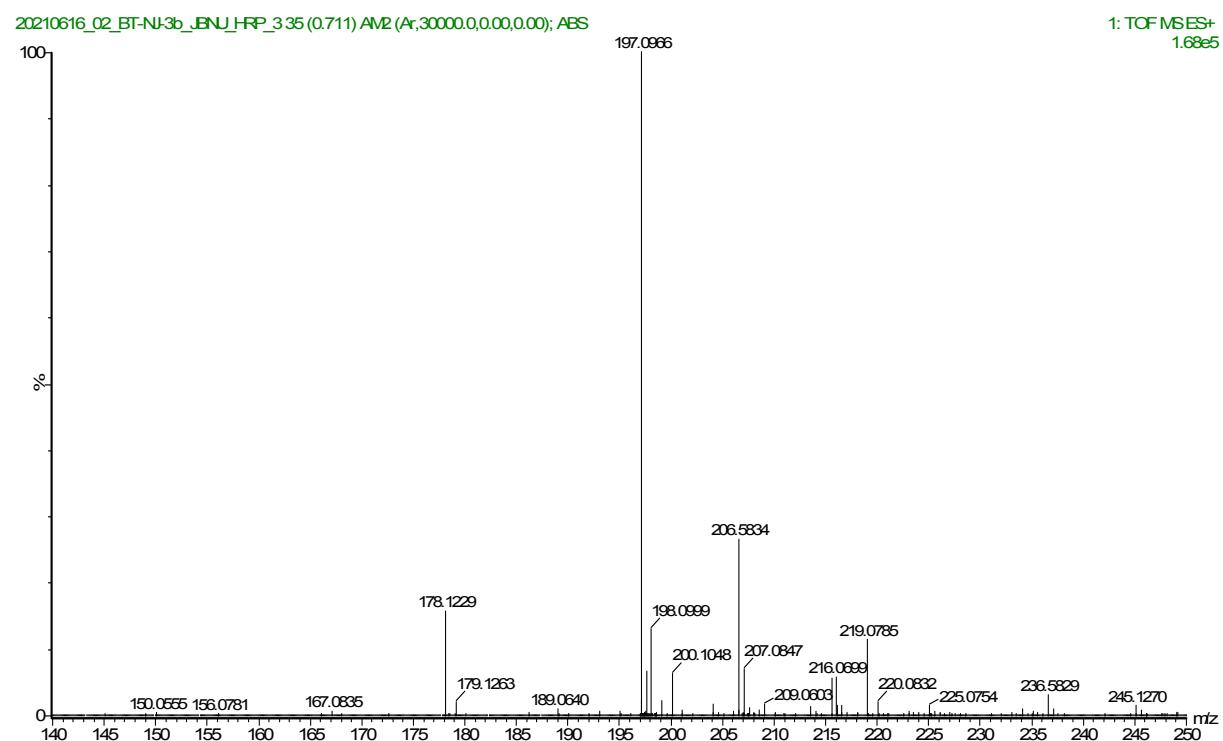


¹³C NMR spectrum of phenyl(piperidin-1-yl)methanone (7i)

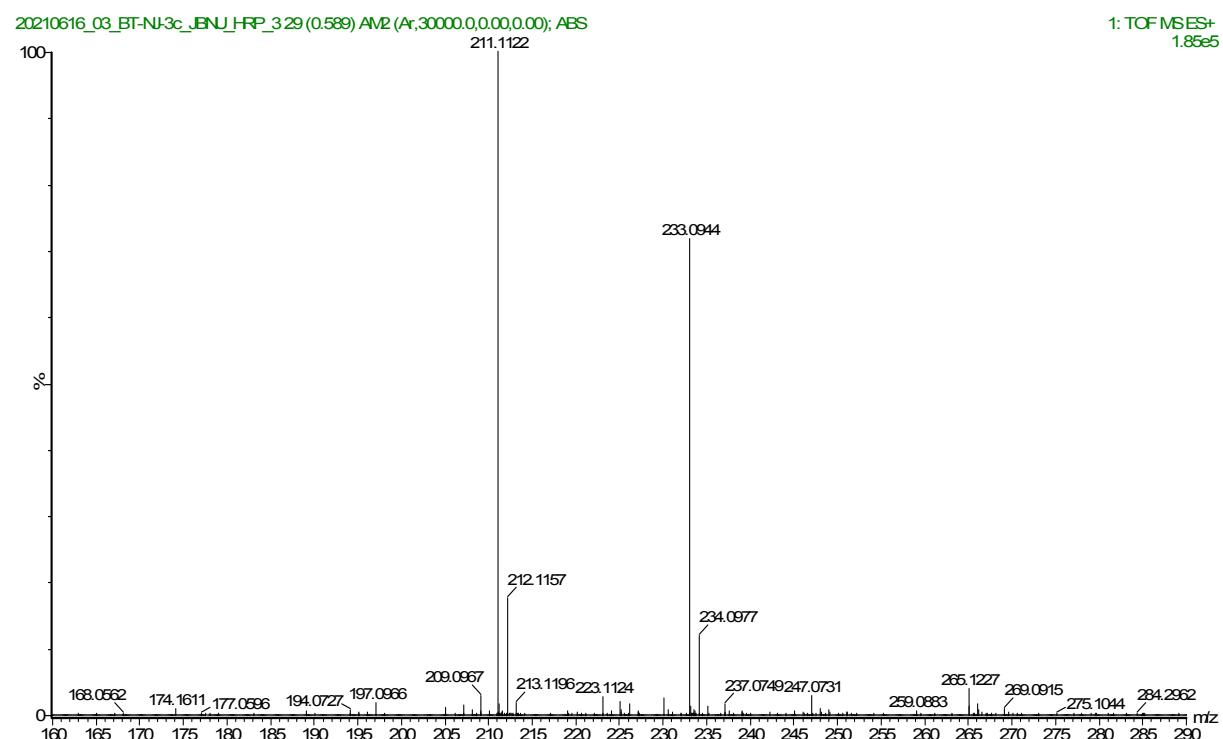
HRMS analysis of benzophenone (3a)



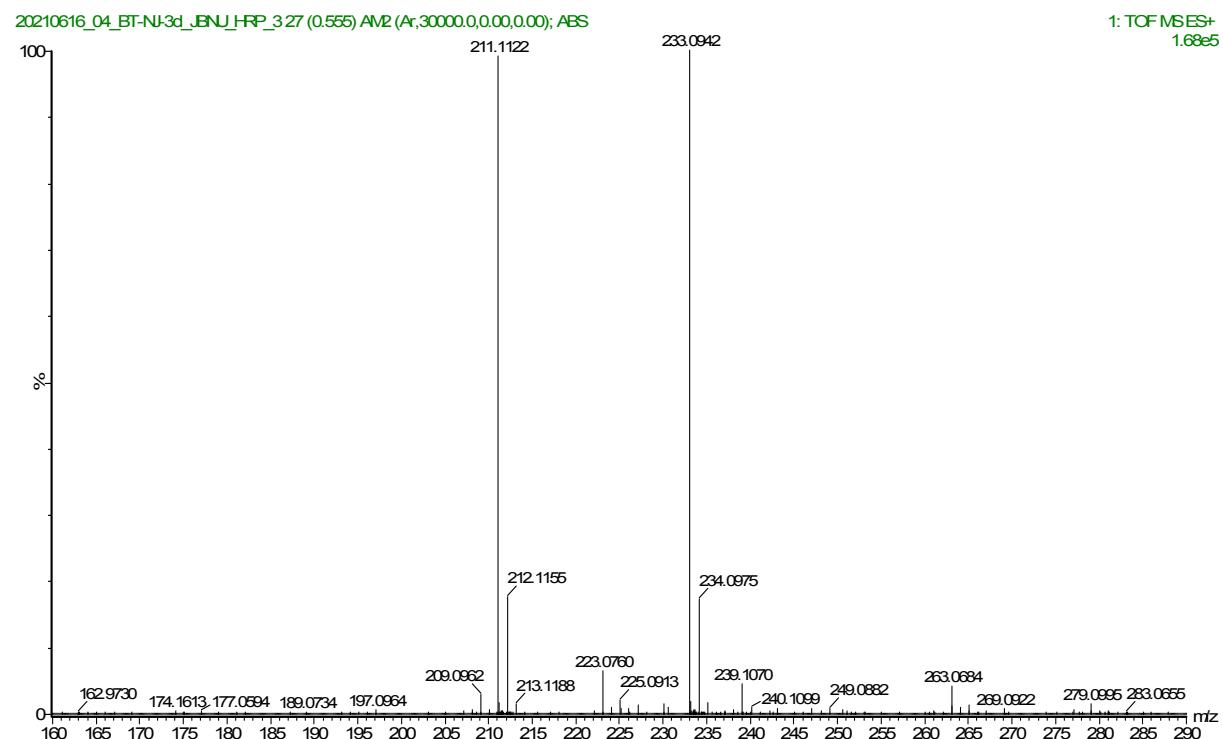
HRMS analysis of phenyl(p-tolyl)methanone (3b)



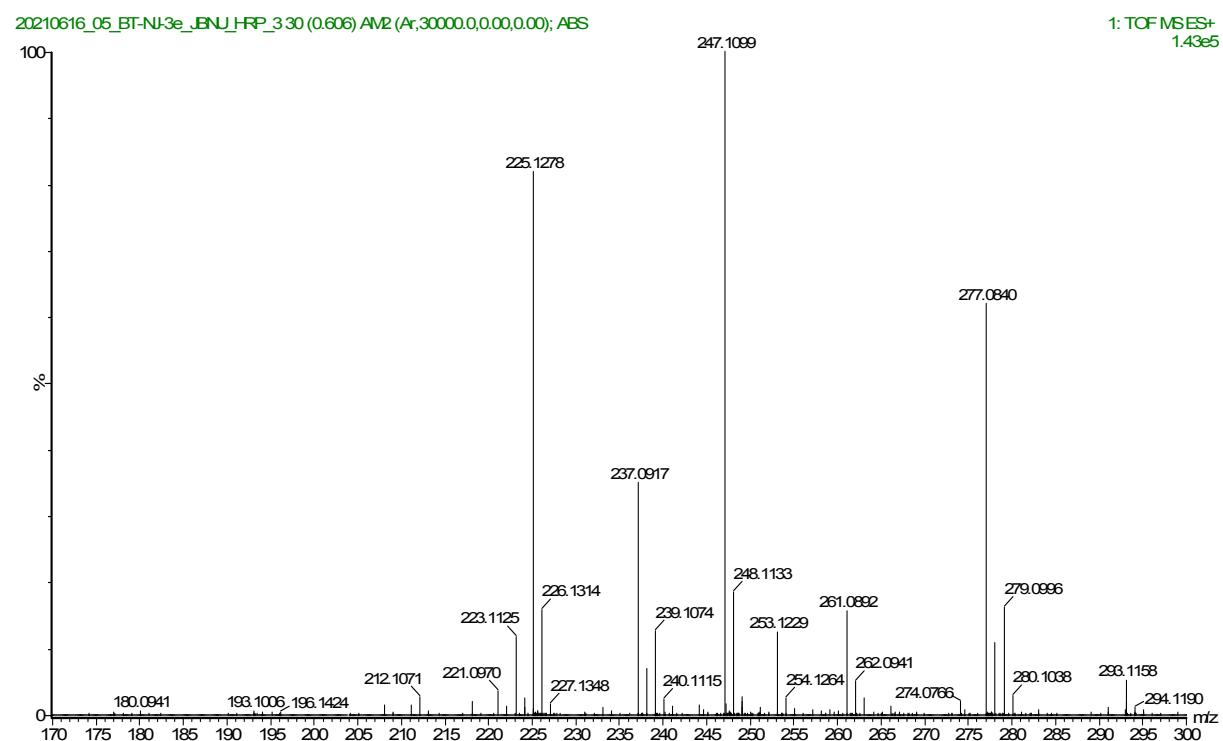
HRMS analysis of (4-ethylphenyl)(phenyl)methanone (3c)



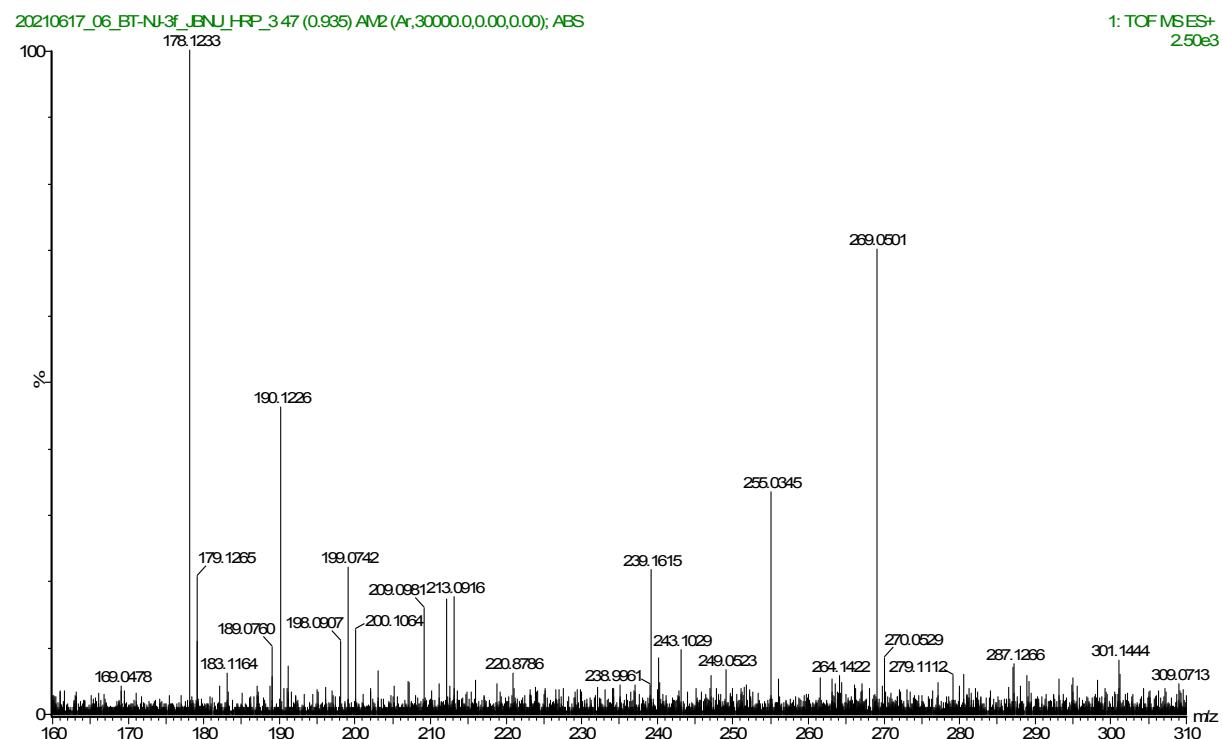
HRMS analysis of (3,4-dimethylphenyl)(phenyl)methanone (3d)



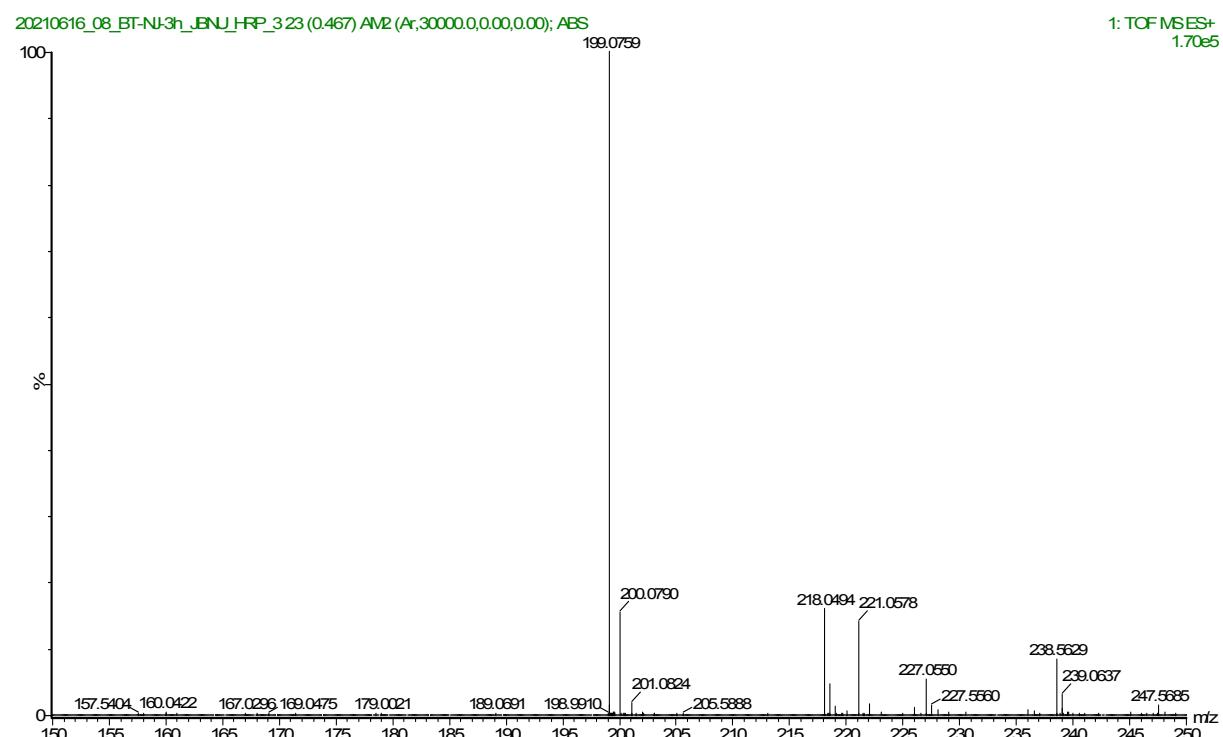
HRMS analysis of phenyl(2,4,5-trimethylphenyl)methanone (3e)



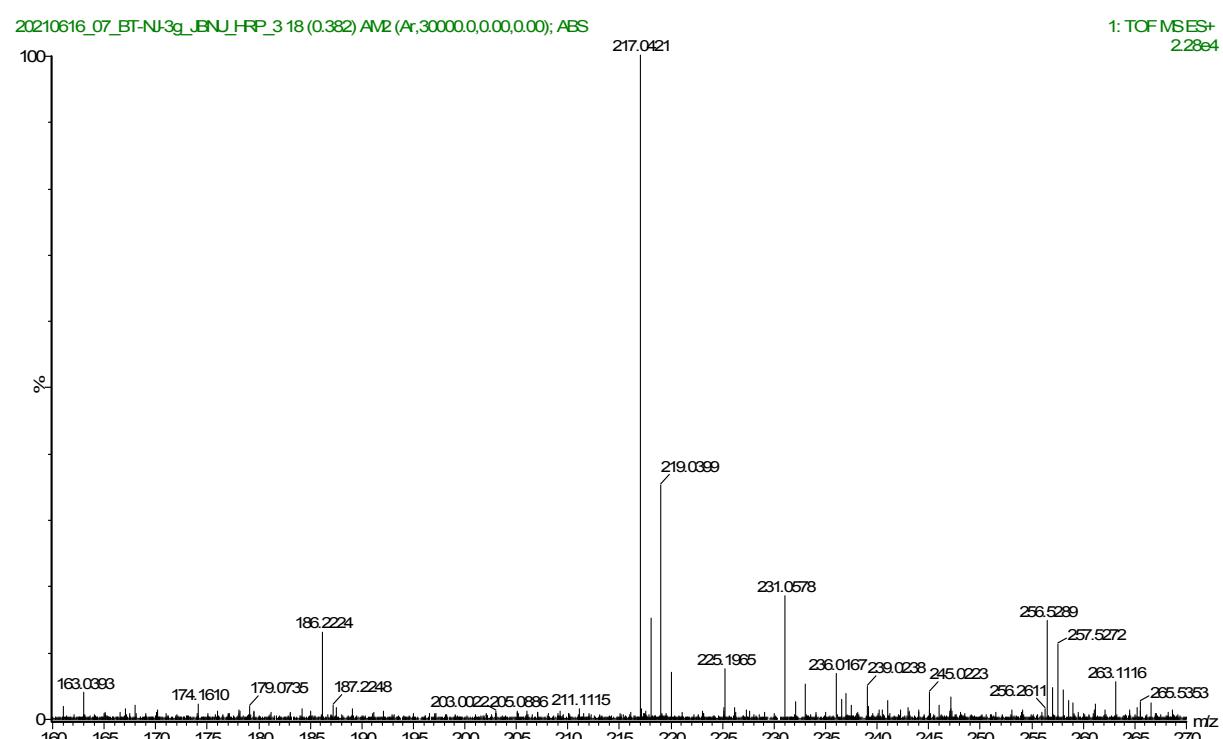
HRMS analysis of (4-methoxyphenyl)(phenyl)methanone (3f)



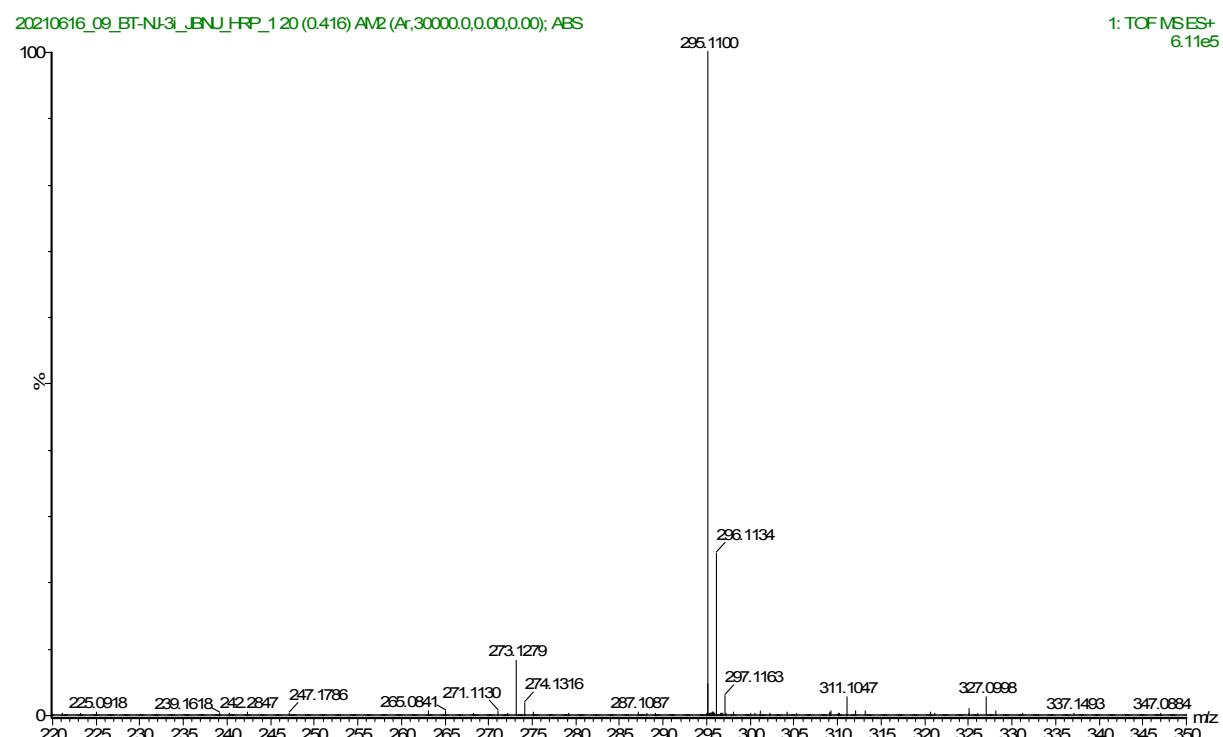
HRMS analysis of (4-hydroxyphenyl)(phenyl)methanone (3g)



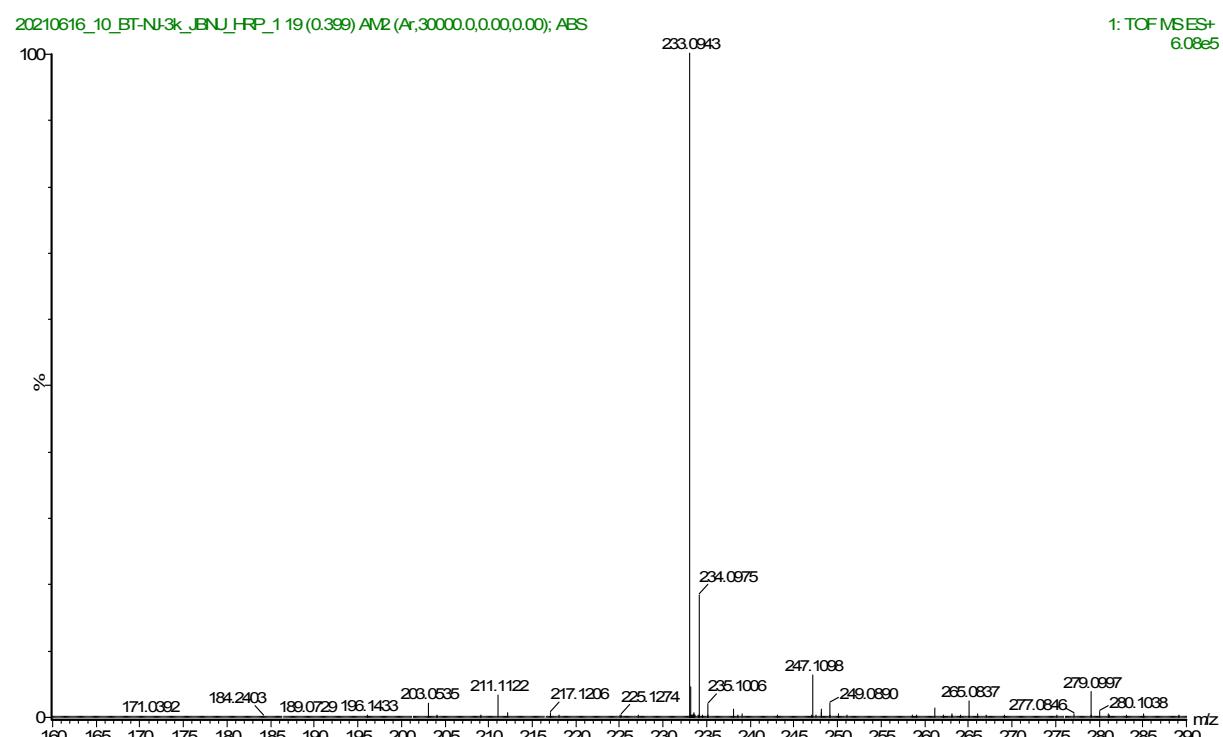
HRMS analysis of (4-chlorophenyl)(phenyl)methanone (3h)



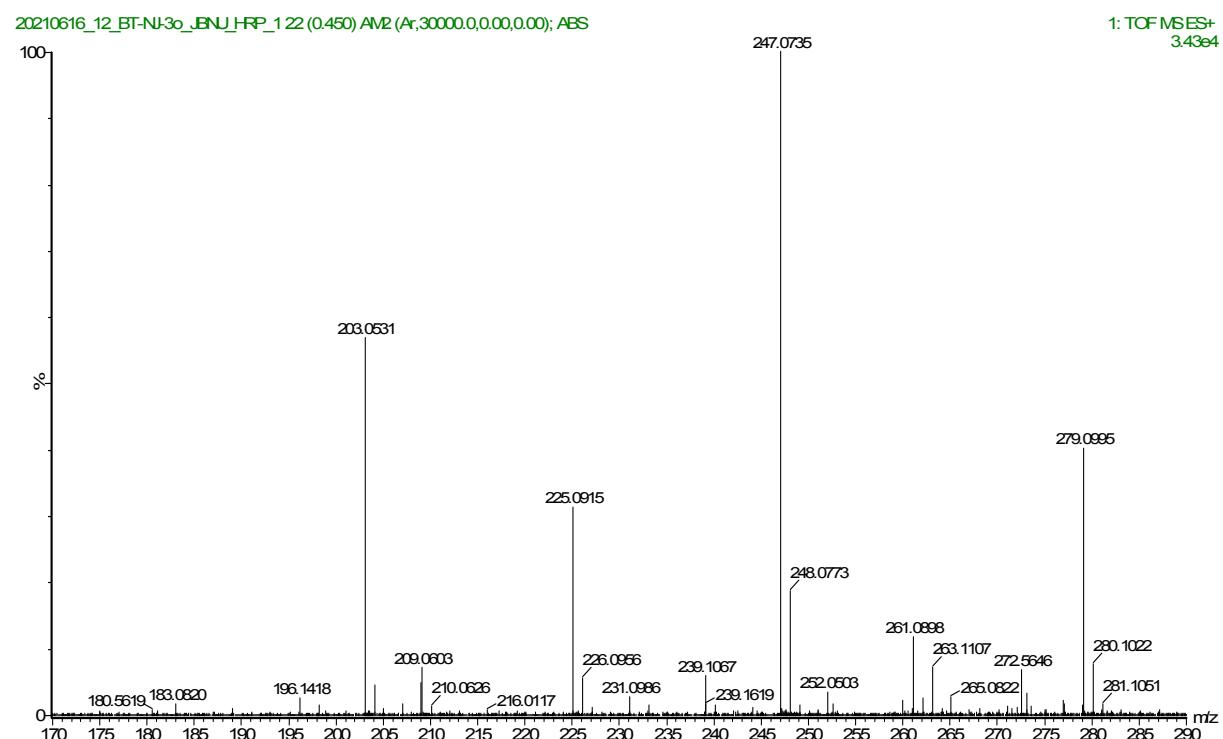
HRMS analysis of (4-benzylphenyl)(phenyl)methanone (3i)



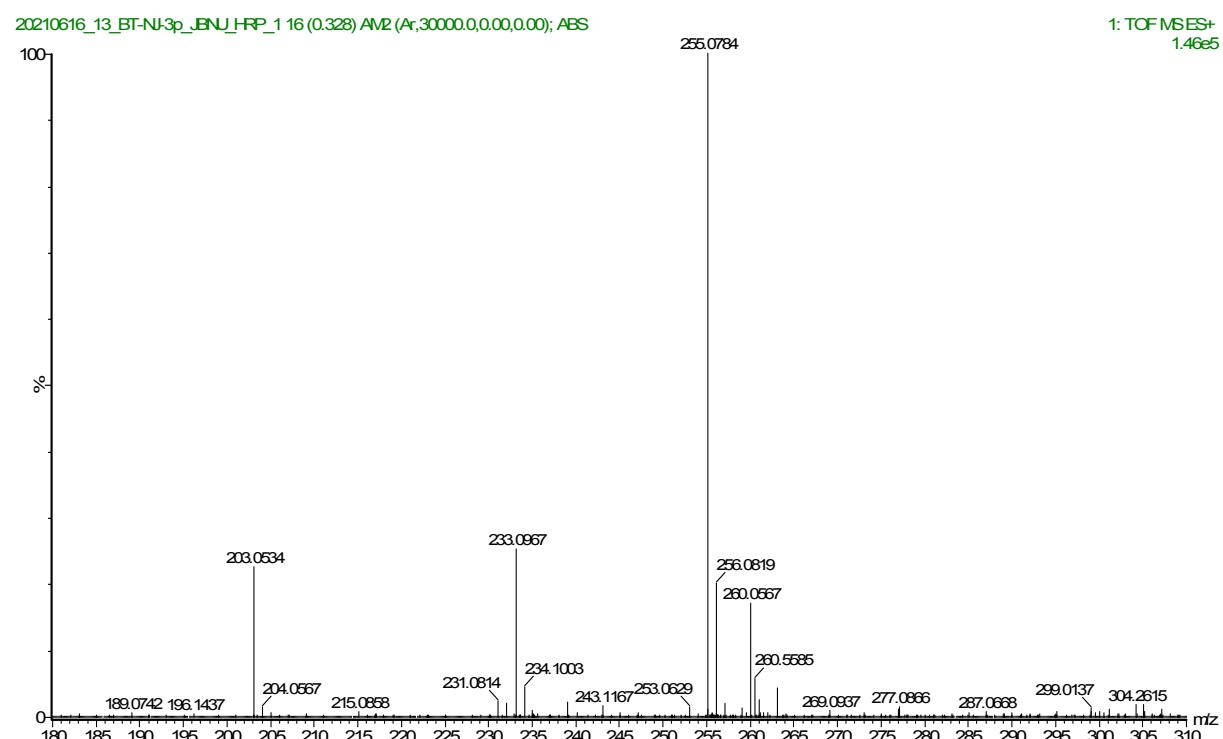
HRMS analysis of (3,5-dimethylphenyl)(phenyl)methanone (3k)



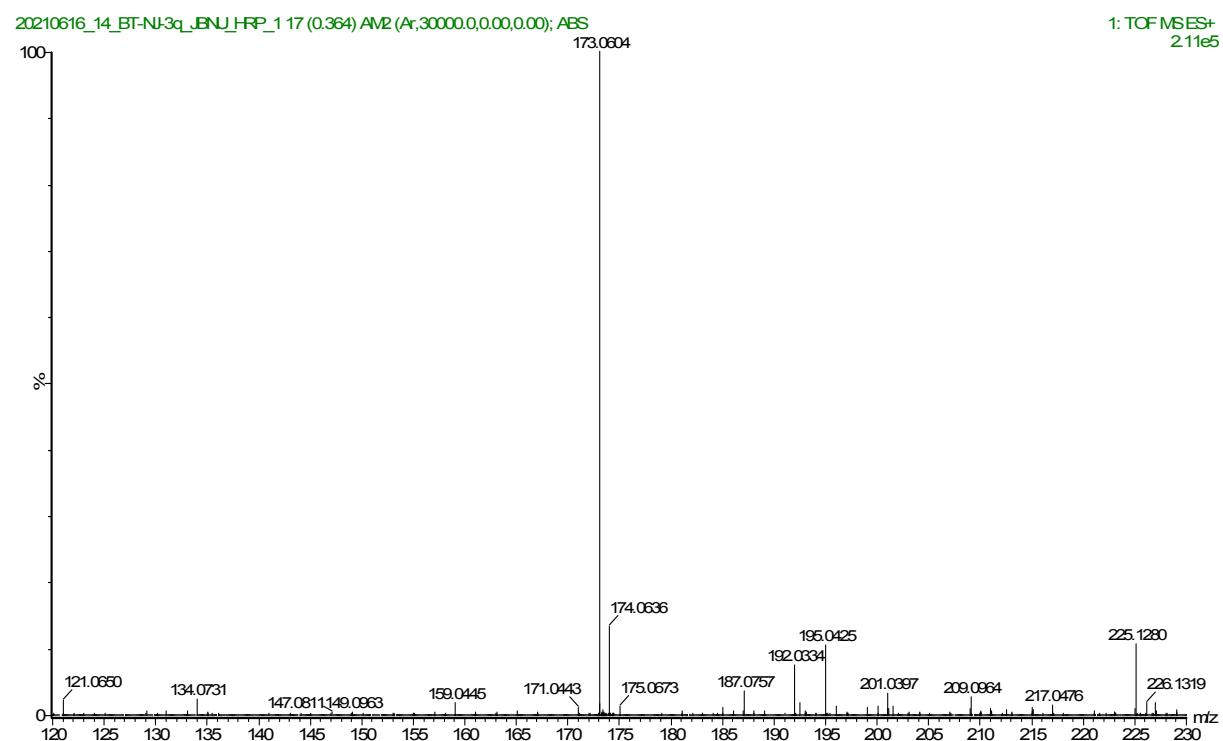
HRMS analysis of 1-(4-benzoylphenyl)ethan-1-one (3o)



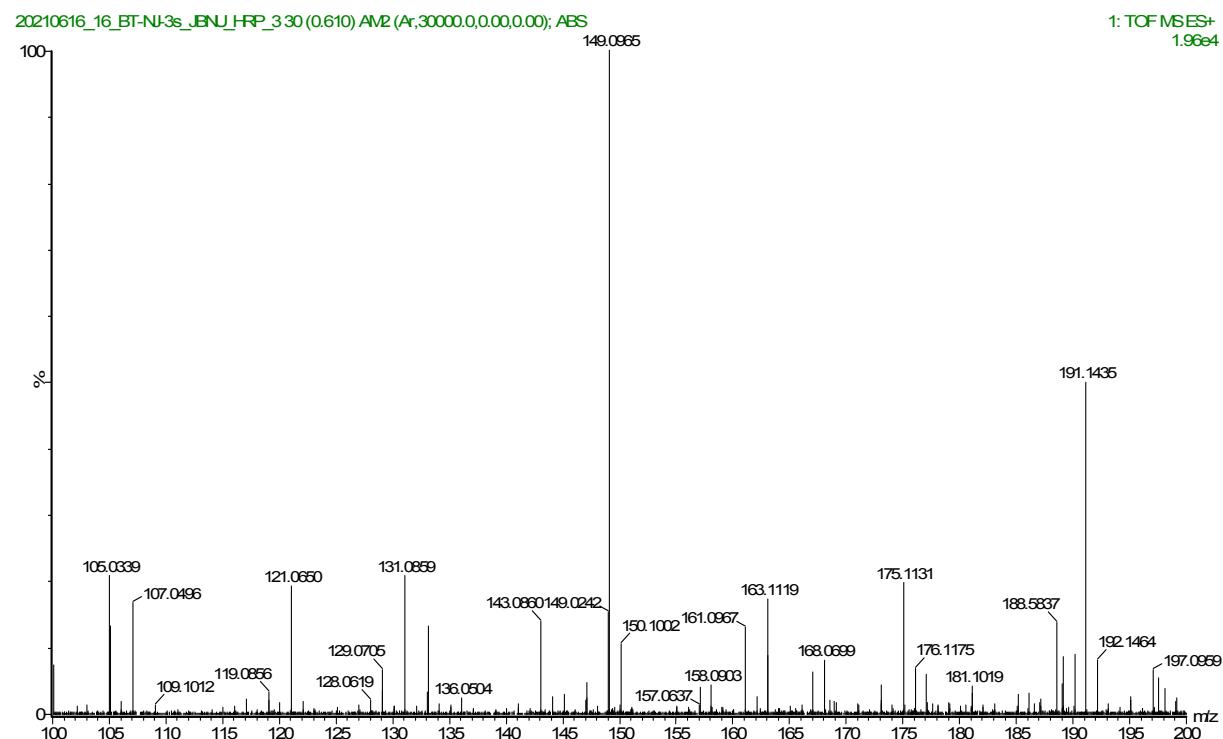
HRMS analysis of naphthalen-2-yl(phenyl)methanone (3p)



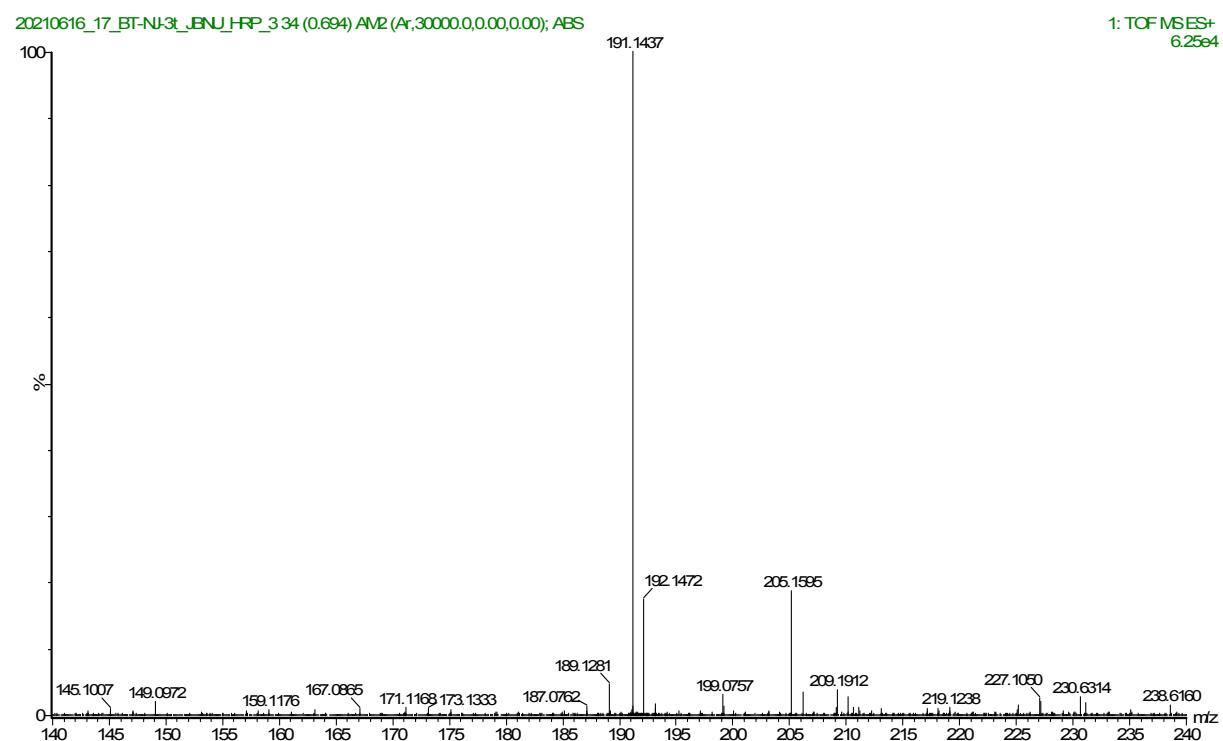
HRMS analysis of furan-2-yl(phenyl)methanone (3q)



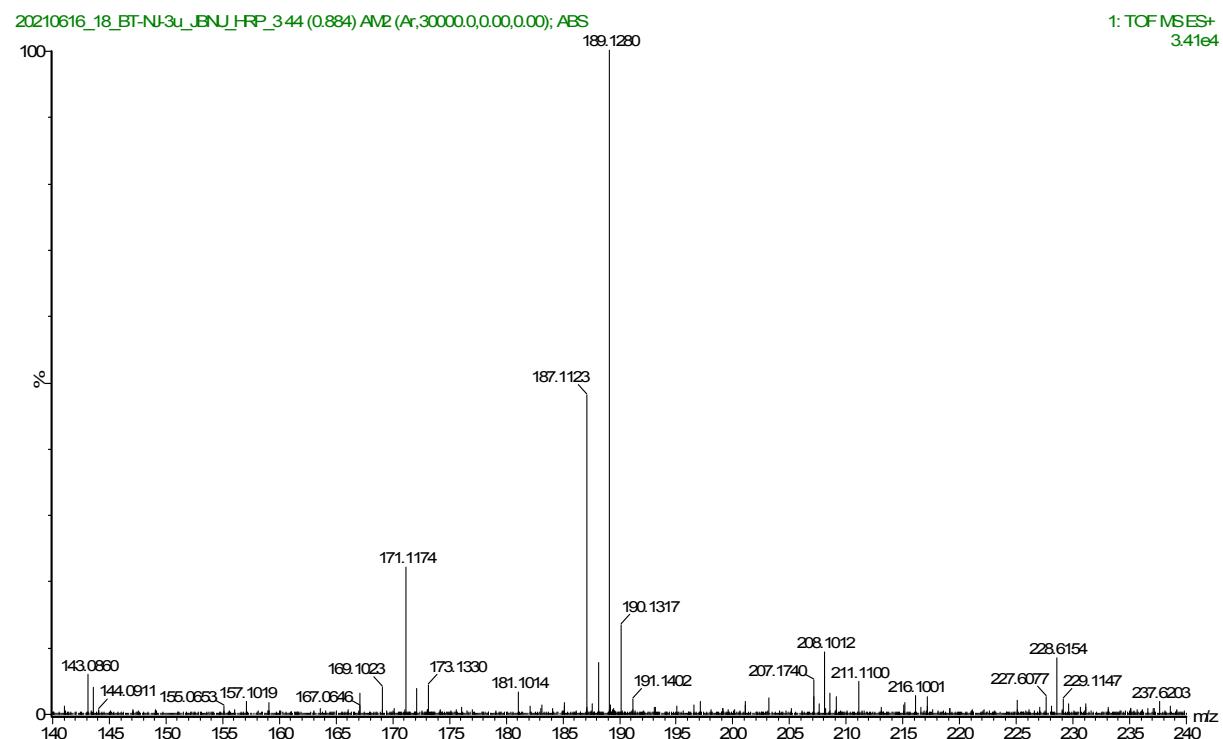
HRMS analysis of 1-phenylbutan-1-one (3s)



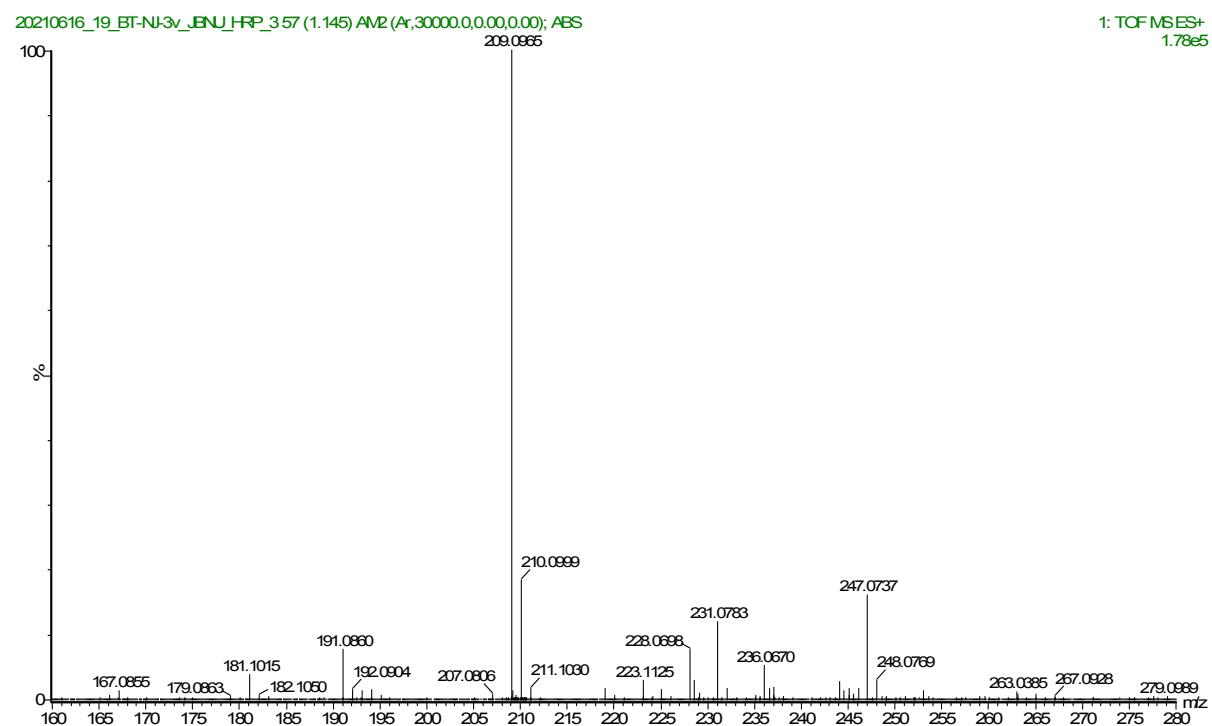
HRMS analysis of 1-phenylheptan-1-one (3t)



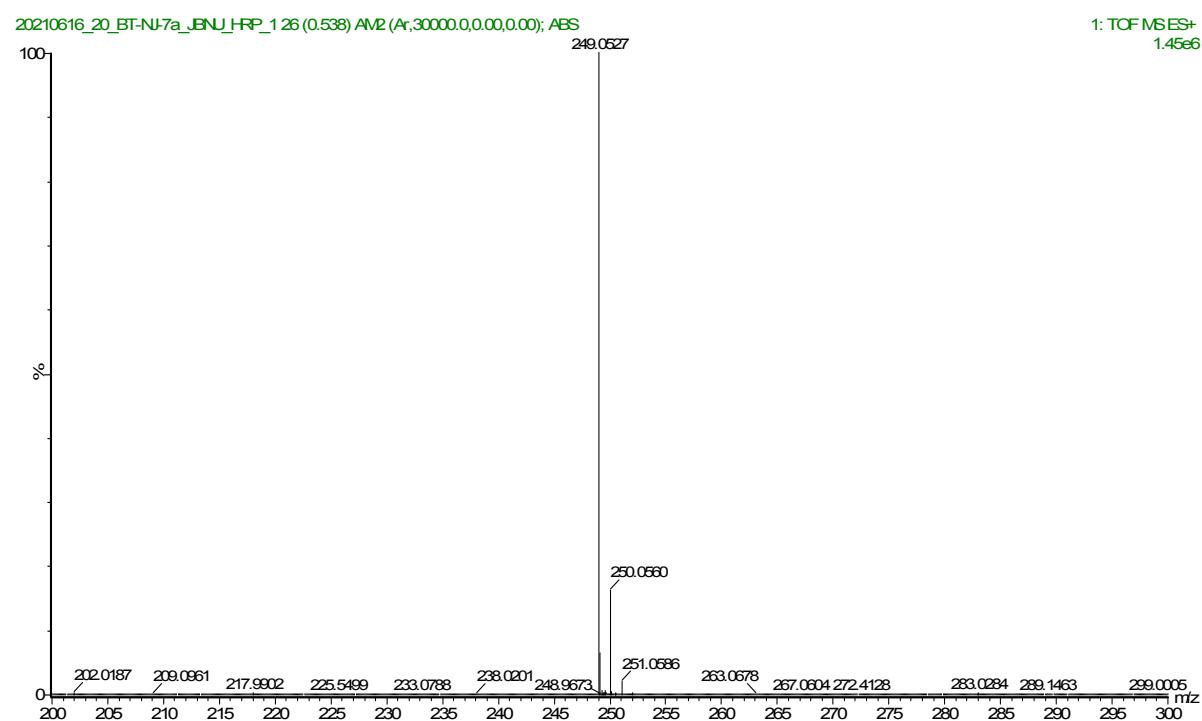
HRMS analysis of cyclohexyl(phenyl)methanone (3u)



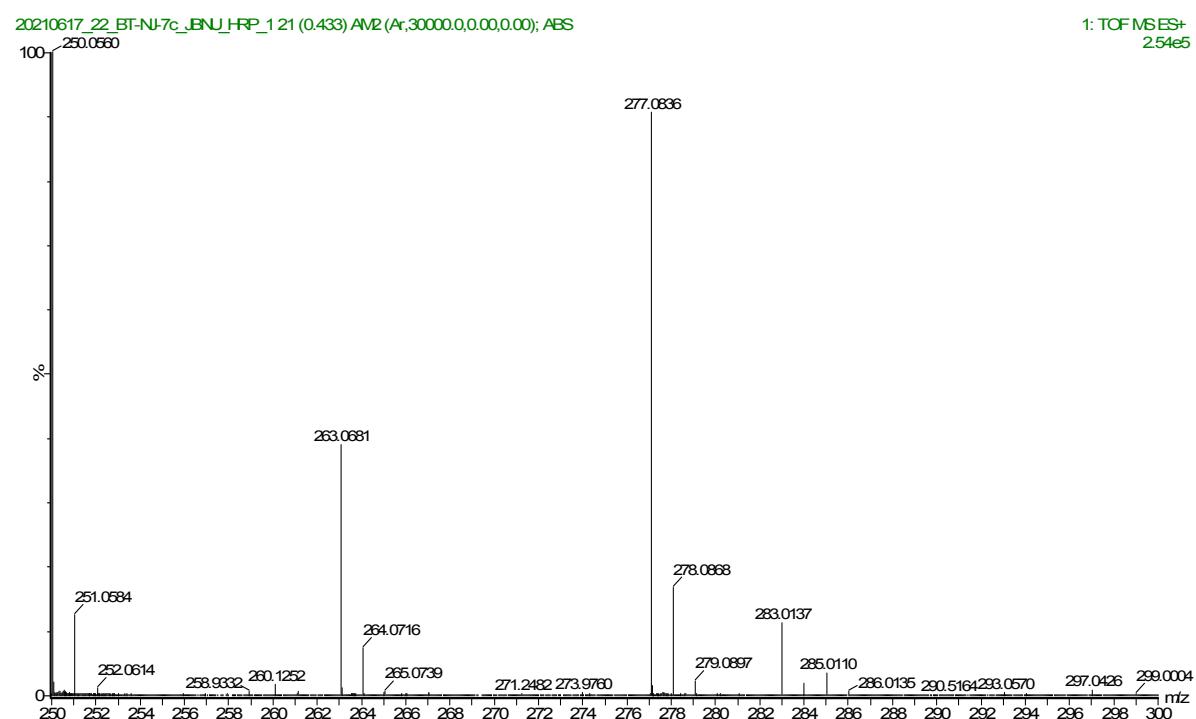
HRMS analysis of (E)-chalcone (3v)



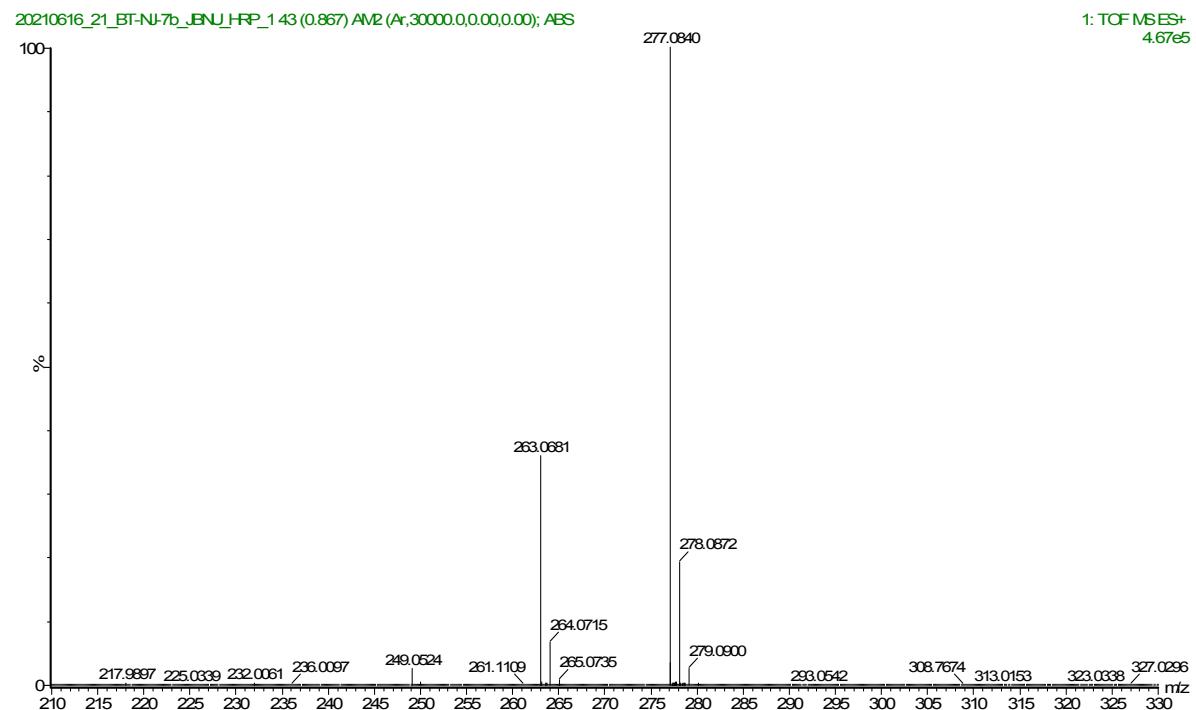
HRMS analysis of Benzoic anhydride (7a)



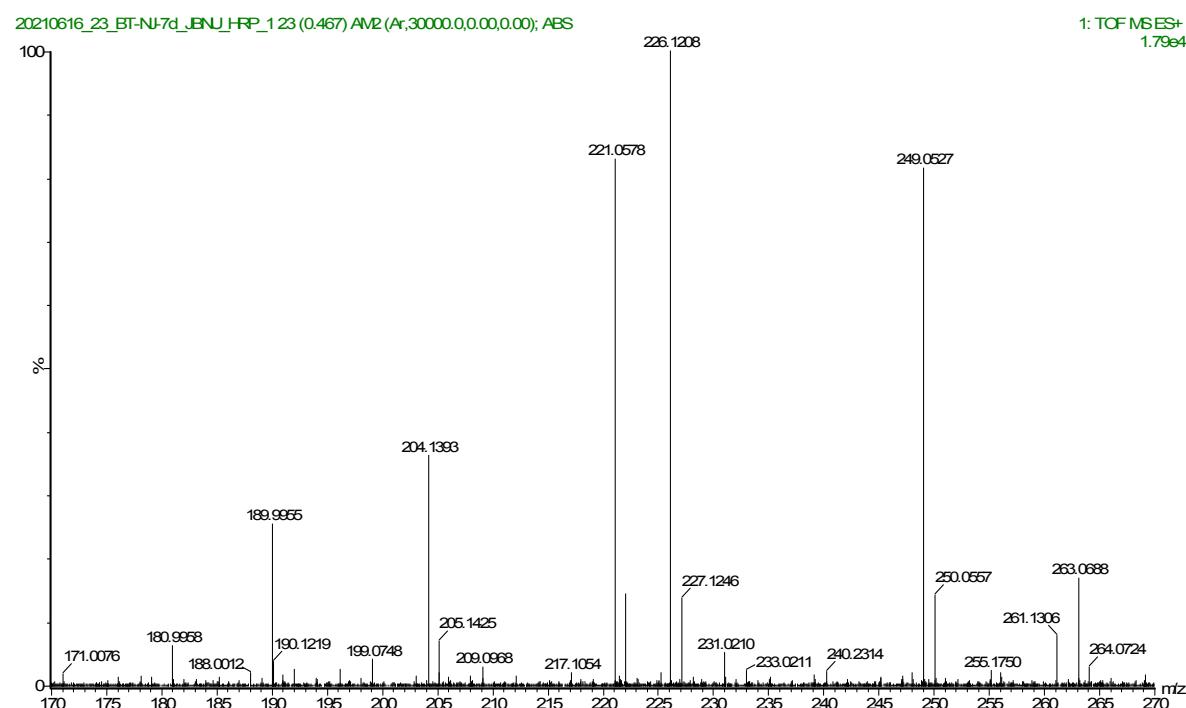
HRMS analysis of Benzoic 4-chlorobenzoic anhydride (7b)



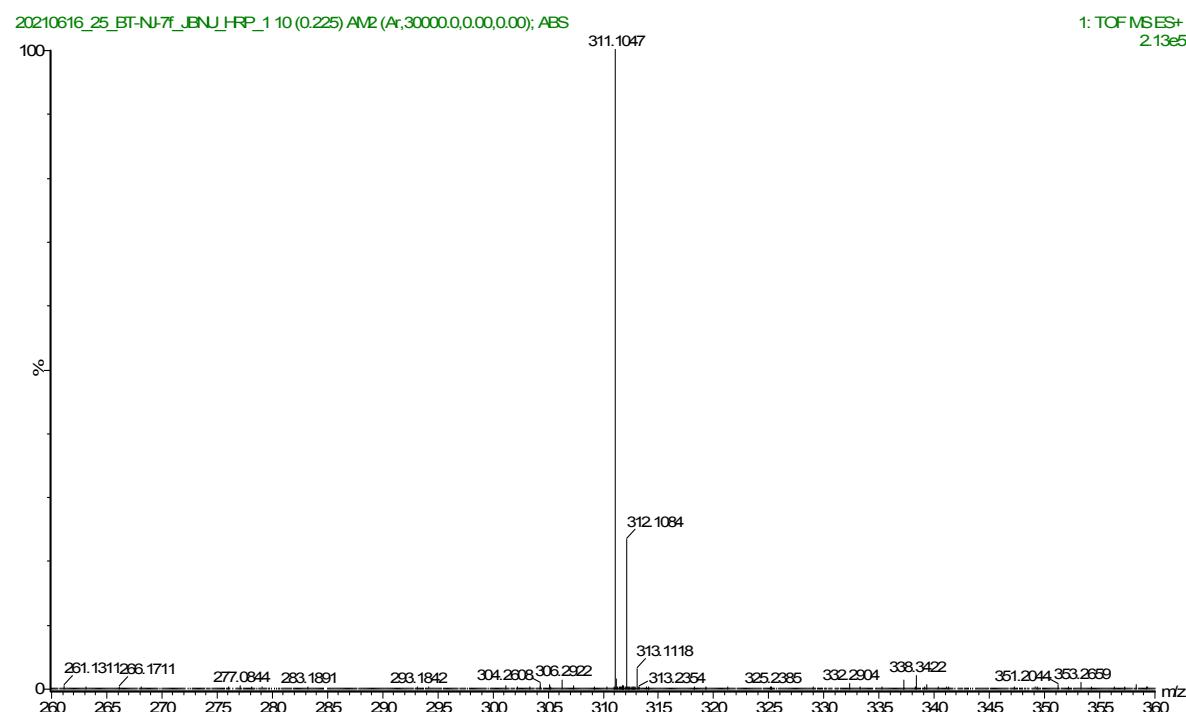
HRMS analysis of Benzoic 4-methylbenzoic anhydride (7c)



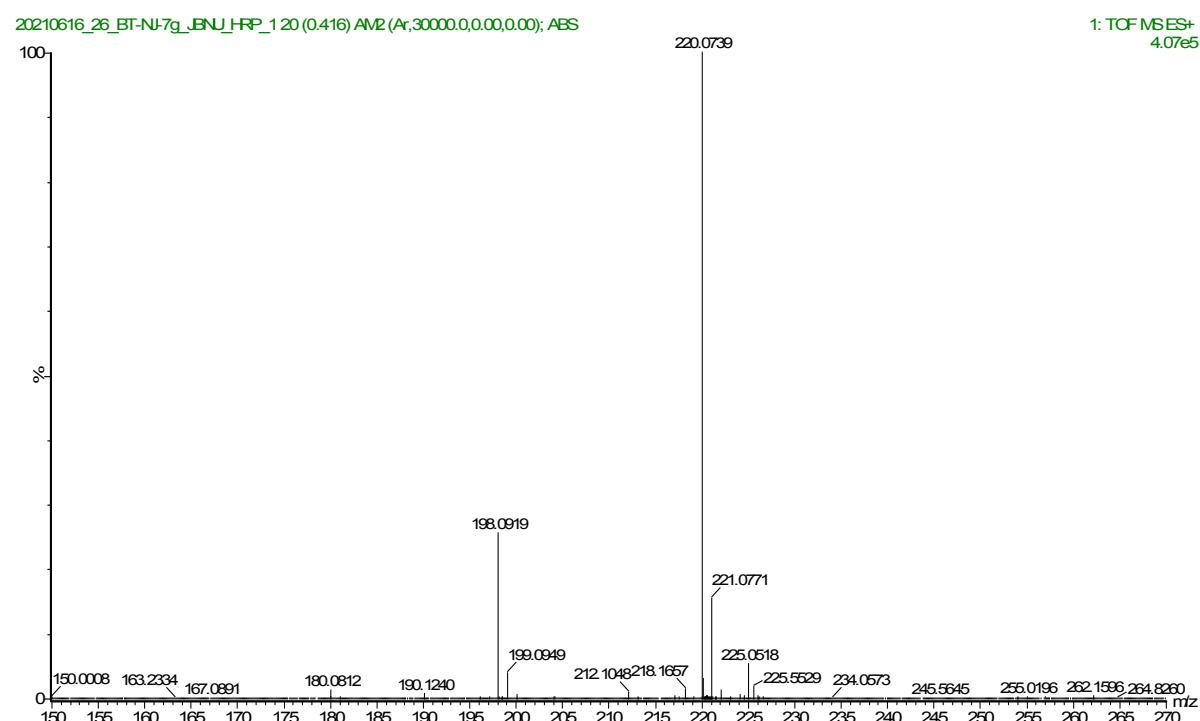
HRMS analysis of Phenyl benzoate (7d)



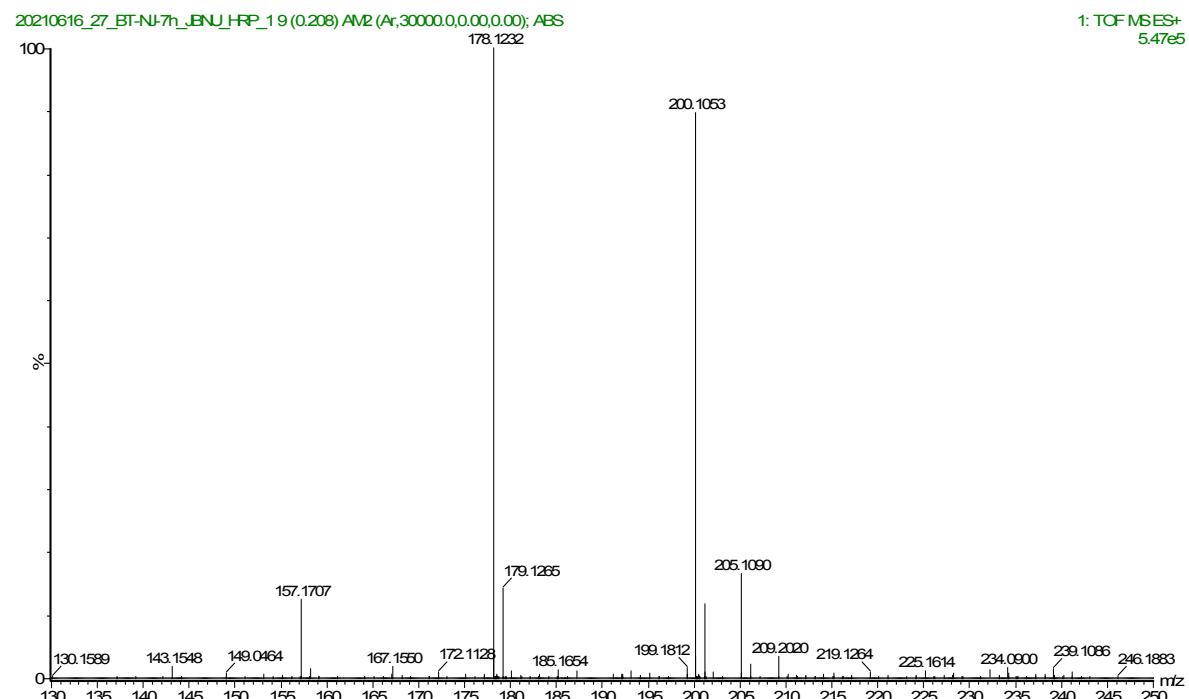
HRMS analysis of Benzydryl benzoate (7f)



HRMS analysis of *N*-phenylbenzamide (7g)



HRMS analysis of *N*-butylbenzamide (7h)



HRMS analysis of phenyl(piperidin-1-yl)methanone (7i)

