

## Supporting Informations

# Easy access to benzylic esters directly from alkyl benzenes under metal-free conditions

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### General information:

All the reagents were commercial grade and used without purification. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F<sub>254</sub> (0.25mm). NMR spectra were recorded in CDCl<sub>3</sub> with tetramethylsilane as the internal standard for <sup>1</sup>H NMR (400 MHz) CDCl<sub>3</sub> solvent as the internal standard for <sup>13</sup>C NMR (75 MHz and 100 MHz). HRMS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat.

**General procedure for the synthesis of benzyl benzoate (aa):** A mixture of Bu<sub>4</sub>NI (36.9 mg, 10 mol %) and toluene (**a**) (1 mL) were taken in an oven dried round bottom flask fitted with a condenser. To this mixture an aqueous solution of TBHP (70% in H<sub>2</sub>O) (857 μL, 6 equiv.) was added and the reaction mixture was heated at 80 °C for 6 h. During this period formation of benzyl benzoate (**aa**) was observed as judged from TLC. The reaction mixture

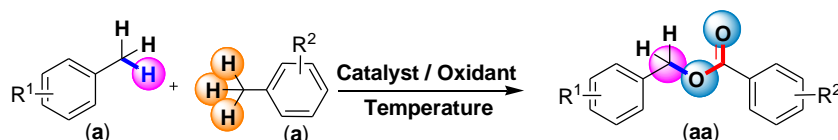
was cooled to room temperature and admixed with ethyl acetate (20 mL). The ethyl acetate layer was washed successively with a 5% solution of sodium bicarbonate (2 x 5mL) and a 5% solution of sodium thiosulphate (2 x 5 mL). The ethyl acetate layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and the solvent was evaporated under reduced pressure. The crude product was purified over a column of silica gel and eluted with (98: 2, hexane / ethyl acetate) to afford benzyl benzoate (**aa**) (201 mg, 95% yield).

**General procedure for the synthesis of 1-phenylethyl benzoate (ak):** A mixture of Bu<sub>4</sub>NI (36.9 mg, 10 mol %), toluene (**a**) (0.5 mL) and ethylbenzene (**k**) (0.5 mL) were taken in an oven dried round bottom flask fitted with a condenser. To this mixture an aqueous solution of TBHP (70% in H<sub>2</sub>O) (857 μL, 6 equiv.) was added and the reaction mixture was heated at 80 °C for 6 h. During this period formation of 1-phenylethyl benzoate (**ak**) was observed as judged from TLC. The reaction mixture was cooled to room temperature and admixed with ethyl acetate (20 mL). The ethyl acetate layer was washed successively with a 5% solution of sodium bicarbonate (2 x 5mL) and a 5% solution of sodium thiosulphate (2 x 5 mL). The ethyl acetate layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and the solvent was evaporated under reduced pressure. The crude product was purified over a column of silica gel and eluted with (98: 2, hexane / ethyl acetate) to afford 1-phenylethyl benzoate (**ak**) (198 mg, 95% yield).

**General procedure for the synthesis of 2-phenylpropan-2-yl benzoate (al):** A mixture of Bu<sub>4</sub>NI (36.9 mg, 10 mol %), toluene (**a**) (0.5 mL) and isopropylbenzene (**l**) (0.5 mL) were taken in an oven dried round bottom flask fitted with a condenser. To this mixture an aqueous solution of TBHP (70% in H<sub>2</sub>O) (857 μL, 6 equiv.) was added and the reaction mixture was heated at 80 °C for 6 h. During this period formation of 1-phenylethyl benzoate (**al**) was observed as judged from TLC. The reaction mixture was cooled to room temperature and admixed with ethyl acetate (20 mL). The ethyl acetate layer was washed successively with a 5% solution of sodium bicarbonate (2 x 5mL) and a 5% solution of sodium thiosulphate (2 x

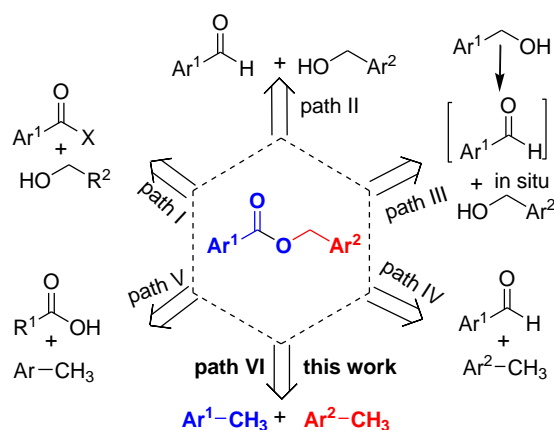
5 mL). The ethyl acetate layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and the solvent was evaporated under reduced pressure. The crude product was purified over a column of silica gel and eluted with (98: 2, hexane / ethyl acetate) to afford 2-phenylpropan-2-yl benzoate (**al**) (180 mg, 75% yield).

**Table S1.** Screening of Reaction Conditions.<sup>a</sup>

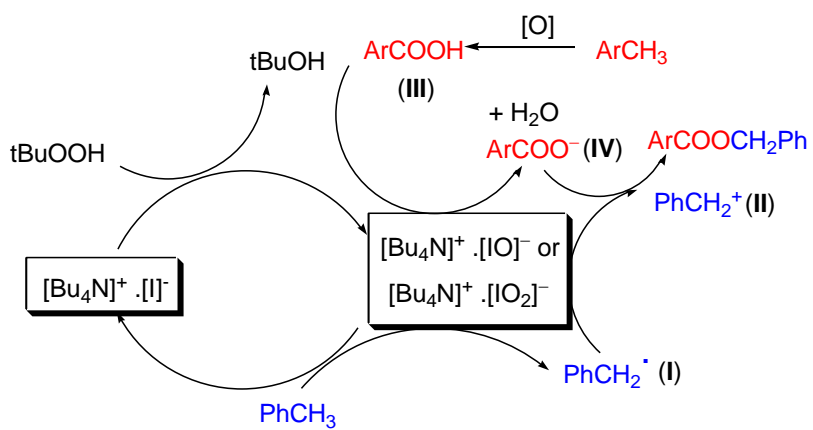


Entry	Catalyst (mol%)	Oxidant (Equiv.)	Temp (°C)	Yield % <sup>b</sup>
1.	Cu(OAc) <sub>2</sub> ·2 H <sub>2</sub> O (10)	TBHP in decane (4)	100	3
2.	Bu <sub>4</sub> NI (10)	TBHP in decane (4)	25	30
3.	Bu <sub>4</sub> NI (10)	TBHP in decane (6)	80	90
<b>4.</b>	<b>Bu<sub>4</sub>NI (10)</b>	<b>Aq. TBHP (6)</b>	<b>80</b>	<b>95</b>
5.	Bu <sub>4</sub> NI (10)	Aq. TBHP (6)	100	95
6.	Bu <sub>4</sub> NI (20)	Aq. TBHP (6)	80	95
7.	Bu <sub>4</sub> NI (5)	Aq. TBHP (6)	80	60
8.	Bu <sub>4</sub> NI (10)	Aq. TBHP (5)	80	50
9.	Bu <sub>4</sub> NI (10)	Aq. H <sub>2</sub> O <sub>2</sub> (6)	80	00
10.	Bu <sub>4</sub> NI (10)	DDQ (6)	80	00
11.	Bu <sub>4</sub> NI (10)	PhI(OAc) <sub>2</sub> (6)	80	00
12.	Bu <sub>4</sub> NBr (10)	Aq. TBHP (6)	80	00
13.	KI (10)	Aq. TBHP (6)	80	00
14.	I <sub>2</sub> (10)	Aq. TBHP (6)	80	00
15.	nil	Aq. TBHP (6)	80	00
16.	Bu <sub>4</sub> NI (10)	nil	80	00

<sup>a</sup>Toluene (1mL), Reaction time: 6 h, <sup>b</sup> Isolated yield.



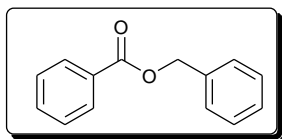
**Scheme S1.** Various routes to benzylic esters.



**Scheme S2.** Proposed mechanism of the oxidative esterification.

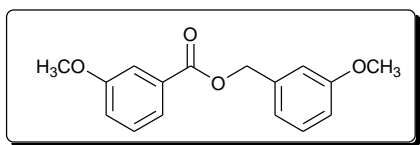
## Spectral Data

### Benzyl benzoate (aa):



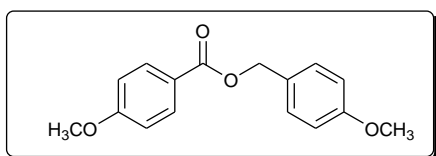
Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 5.36 (s, 2H), 7.33–7.45 (m, 7H), 7.54 (t, 1H,  $J = 7.6$  Hz), 8.08 (d, 2H,  $J = 8.4$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 66.7, 128.2, 128.3, 128.4, 128.6, 129.7, 130.2, 133.0, 136.1, 166.4; IR (KBr): 3066, 3033, 2923, 1718, 1451, 1314, 1271, 1109, 1070, 1026, 711  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{14}\text{H}_{12}\text{O}_2$ : C 79.22, H 5.70; found C 79.20, H 5.78.

### 3-Methoxybenzyl 3-methoxybenzoate (bb):



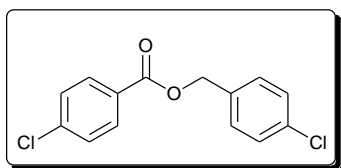
Yellowish liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.81 (s, 3H), 3.83 (s, 3H), 5.33 (s, 2H), 6.88 (d, 1H,  $J = 8.4$  Hz), 6.98 (s, 1H), 7.02 (d, 1H,  $J = 7.6$  Hz), 7.08–7.11 (m, 1H), 7.28–7.35 (m, 2H), 7.60 (s, 1H), 7.68 (d, 1H,  $J = 7.6$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 55.4, 55.6, 66.8, 113.8, 114.4, 119.6, 120.5, 122.3, 129.6, 129.8, 131.6, 137.7, 159.8, 159.9, 166.4; IR (KBr): 2938, 2837, 1717, 1602, 1587, 1489, 1456, 1275, 1225, 1104, 1043, 756  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_4$ : C 70.57, H 5.92; found C 70.62, H 5.84.

### 4-Methoxybenzyl 4-methoxybenzoate (cc):



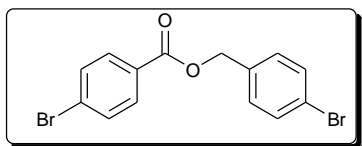
Yellowish liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.79 (s, 3H), 3.82 (s, 3H), 5.25 (s, 2H), 6.87–6.90 (m, 4H), 7.36 (d, 2H,  $J = 8.4$  Hz), 7.99 (d, 2H,  $J = 8.8$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 55.4, 55.5, 66.3, 113.7, 114.1, 122.8, 128.6, 130.1, 131.8, 159.7, 163.5, 166.4; IR (KBr): 3002, 2957, 2837, 1707, 1606, 1513, 1255, 1166, 1097, 1029, 823, 769  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_4$  ( $\text{MH}^+$ ) 273.1121; found 273.1115.

#### 4-Chlorobenzyl 4-chlorobenzoate (dd):



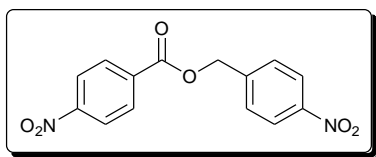
White solid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 5.31 (s, 2H), 7.37–7.42 (m, 6H), 7.99 (d, 2H,  $J = 8.8$  Hz);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 66.1, 128.3, 128.8, 128.9, 129.7, 131.0, 131.1, 134.3, 139.6, 165.4; IR (KBr): 3049, 2927, 2852, 1715, 1592, 1488, 1400, 1307, 1274, 1172, 1123, 1091, 1014, 848, 810, 756  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{14}\text{H}_{10}\text{Cl}_2\text{O}_2$  ( $\text{MH}^+$ ) 281.0131; found 281.0124.

#### 4-Bromobenzyl 4-bromobenzoate (ee):



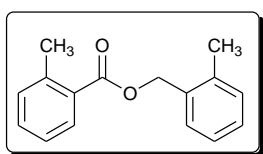
White solid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 5.30 (s, 2H), 7.31 (d, 2H,  $J = 8$  Hz), 7.52 (d, 2H,  $J = 8.4$  Hz), 7.58 (d, 2H,  $J = 8.4$  Hz), 7.91 (d, 2H,  $J = 8.4$  Hz);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 66.2, 122.5, 128.4, 128.8, 130.0, 131.3, 131.9, 134.8, 165.6; IR (KBr): 2928, 2852, 1713, 1588, 1483, 1397, 1271, 1172, 1121, 1105, 1067, 1011, 803, 754  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{14}\text{H}_{10}\text{Br}_2\text{O}_2$  ( $\text{MH}^+$ ) 368.9120; found 368.9123.

#### 4-Nitrobenzyl 4-nitrobenzoate (ff):



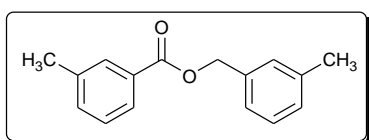
Yellowish gum;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 5.48 (s, 2H), 7.60 (d, 2H,  $J = 8.8$  Hz), 8.22–8.30 (m, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 68.6, 123.2, 124.4, 128.6, 130.9, 137.5, 146.5, 148.8, 166.7; IR (KBr): 2962, 2923, 2849, 1727, 1645, 1604, 1517, 1347, 1274, 1104, 735, 717  $\text{cm}^{-1}$ ; Anal. Calcd. for  $\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}_6$ : C 55.63, H 3.33, N 9.27; found C 55.69, H 3.36, N 9.17.

#### 2-Methylbenzyl 2-methylbenzoate (gg):



Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.40 (s, 3H), 2.60 (s, 3H), 5.34 (s, 2H), 7.18–7.24 (m, 5H), 7.34–7.42 (m, 2H), 7.93 (d, 1H,  $J = 8.4$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 18.9, 21.7, 64.8, 125.7, 126.0, 128.4, 129.2, 129.4, 130.3, 130.6, 131.7, 131.9, 134.1, 136.8, 140.3, 167.0; IR (KBr): 3066, 3022, 2929, 1717, 1605, 1457, 1290, 1250, 1141, 1075, 738  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$  ( $\text{MH}^+$ ) 241.1223; found 241.1219.

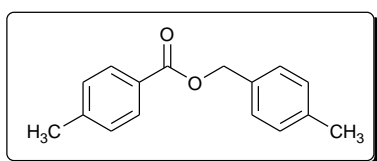
#### 3-Methylbenzyl 3-methylbenzoate (hh):



Yellowish liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.37(s, 3H), 2.38 (s, 3H), 5.31 (s, 2H), 7.14 (d, 1H,  $J = 6.4$  Hz), 7.23–7.34 (m, 5H), 7.88 (d, 2H,  $J = 7.2$  Hz);  $^{13}\text{C}$  NMR (100

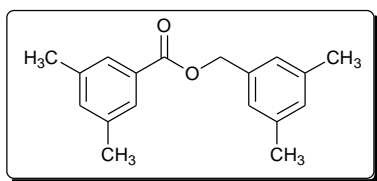
MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 21.2, 21.4, 66.7, 125.3, 126.9, 128.3, 128.5, 129.0, 130.1, 130.2, 133.7, 136.1, 138.1, 138.2, 166.5; IR (KBr): 3027, 2922, 1721, 1610, 1455, 1372, 1276, 1197, 1106, 1081, 781, 746  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$ : C 79.97, H 6.71; found C 79.82, H 6.94.

#### 4-Methylbenzyl 4-methylbenzoate (ii):



Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.32 (s, 3H), 2.35 (s, 3H), 5.28 (s, 2H), 7.16 (t, 4H,  $J = 8.4$  Hz), 7.31 (d, 2H,  $J = 8$  Hz), 7.94 (d, 2H,  $J = 8.4$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 20.9, 21.4, 66.2, 127.5, 128.2, 128.9, 129.1, 129.6, 133.2, 137.7, 143.4, 166.2; IR (KBr): 2923, 2857, 1718, 1613, 1451, 1372, 1271, 1177, 1103, 1018, 807, 754  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$ : C 79.97, H 6.71; found C 79.82, H 6.84.

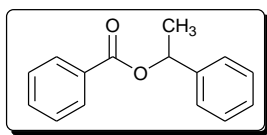
#### 3,5-Dimethylbenzyl 3,5-dimethylbenzoate (jj):



Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.32 (s, 6H), 2.32 (s, 6H), 5.26 (s, 2H), 6.95 (s, 1H), 7.04 (s, 2H), 7.15 (s, 1H), 7.69 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 21.2, 21.3, 66.8, 126.2, 127.5, 129.9, 130.2, 134.7, 136.1, 138.0, 138.2, 166.8; IR (KBr): 3011, 2920, 2863, 1717, 1609, 1456, 1382, 1310, 1209, 1163, 1115, 846, 768  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{18}\text{H}_{20}\text{O}_2$  ( $\text{MH}^+$ ) 269.1536; found 269.1534.

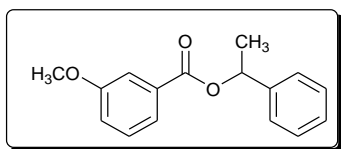


### 1-Phenylethyl benzoate (ak):



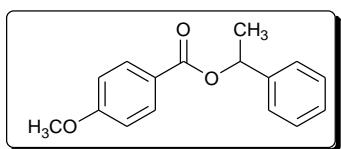
Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.70 (d, 3H,  $J = 6.4$  Hz), 6.18 (q, 1H,  $J = 6.4$  Hz), 7.30–7.49 (m, 7H), 7.56 (t, 1H,  $J = 7.6$  Hz), 8.13 (d, 2H,  $J = 8$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 22.3, 72.8, 126.0, 127.8, 128.3, 128.5, 129.5, 130.5, 132.8, 141.8, 165.6; IR (KBr): 3060, 2981, 1717, 1495, 1451, 1315, 1270, 1176, 1109, 1069, 1026, 761, 712, 698  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{15}\text{H}_{14}\text{O}_2$ : C 79.62, H 6.24; found C 79.69, H 6.17.

### 1-Phenylethyl 3-methoxybenzoate (bk):



Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.68 (d, 3H,  $J = 6.8$  Hz), 3.79 (s, 3H), 6.15 (q, 1H,  $J = 6.4$  Hz), 7.41–7.46 (m, 5H), 7.52–7.56 (m, 2H), 7.94 (d, 2H,  $J = 7.2$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 22.2, 55.4, 75.0, 113.8, 120.5, 126.4, 128.5, 129.0, 129.9, 130.1, 135.0, 140.5, 163.5, 166.6; IR (KBr): 2929, 2846, 1717, 1635, 1587, 1266, 1199, 757, 699  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_3$ : C 74.98, H 6.29; found C 74.92, H 6.35.

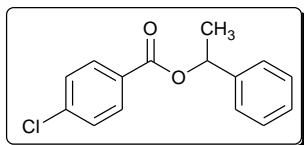
### 1-Phenylethyl 4-methoxybenzoate (ck):



Yellowish liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.65 (d, 3H,  $J = 6.4$  Hz), 3.82 (s, 3H), 6.11 (q, 1H,  $J = 6.4$  Hz), 6.90 (d, 2H,  $J = 7.2$  Hz), 7.28 (t, 1H,  $J = 7.6$  Hz), 7.35 (t, 2H,  $J$

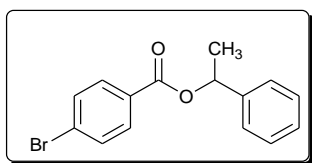
= 7.6 Hz), 7.43 (d, 2H,  $J = 8$  Hz), 8.04 (d, 2H,  $J = 9.2$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 22.6, 55.6, 72.7, 113.7, 123.1, 126.2, 127.9, 128.7, 131.8, 142.2, 163.5, 165.7; IR (KBr): 3063, 3032, 2979, 2934, 2839, 1713, 1606, 1510, 1454, 1258, 1167, 1100, 1029, 847, 769, 698  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_3$ : C 74.98, H 6.29; found C 75.06, H 6.33.

#### 1-Phenylethyl 4-chlorobenzoate (dk):



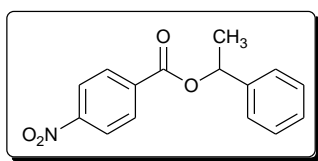
Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.67 (d, 3H,  $J = 6.4$  Hz), 6.12 (q, 1H,  $J = 6.8$  Hz), 7.30–7.44 (m, 7H), 8.00 (d, 2H,  $J = 8.8$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 22.3, 73.2, 126.0, 128.0, 128.5, 128.6, 129.0, 131.0, 139.3, 141.5, 164.8; IR (KBr): 3038, 2981, 2929, 1718, 1594, 1452, 1269, 1103, 1063, 850, 759, 698  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{15}\text{H}_{13}\text{ClO}_2$  ( $\text{MH}^+$ ) 261.0677; found 261.0685.

#### 1-Phenylethyl 4-bromobenzoate (ek):



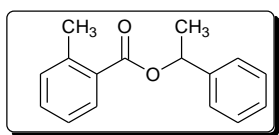
Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.66 (d, 3H,  $J = 6.4$  Hz), 6.11 (q, 1H,  $J = 6.4$  Hz), 7.29–7.43 (m, 6H), 7.56 (d, 2H,  $J = 8.8$  Hz), 7.92 (d, 1H,  $J = 8.8$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 22.2, 73.2, 126.0, 126.6, 127.9, 128.5, 129.4, 131.1, 131.6, 141.5, 164.8; IR (KBr): 3034, 2980, 2931, 1719, 1590, 1269, 1102, 1065, 1012, 848, 756, 698  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{15}\text{H}_{13}\text{BrO}_2$ : C 59.04, H 4.29; found C 59.11, H 4.33.

### 1-Phenylethyl 4-nitrobenzoate (fk):



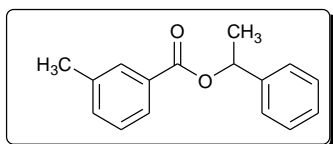
Yellowish liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.71 (d, 3H,  $J = 6.4$  Hz), 6.16 (q, 1H,  $J = 6.8$  Hz), 7.32–7.46 (m, 5H), 8.21–8.27 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 21.8, 73.8, 123.1, 125.8, 127.9, 128.4, 130.3, 135.5, 140.9, 150.1, 163.4; IR (KBr): 3035, 2984, 2934, 1724, 1689, 1607, 1527, 1452, 1351, 1271, 1199, 1103, 1061, 874, 762, 720, 699  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_4$ : C 66.41, H 4.83, N 5.16; found C 66.46, H 4.79, N 5.12.

### 1-Phenylethyl 2-methylbenzoate (gk):



Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.66 (d, 3H,  $J = 6.8$  Hz), 2.58 (s, 3H), 6.11 (q, 1H,  $J = 6.4$  Hz), 7.18–7.36 (m, 6H), 7.43 (d, 2H,  $J = 7.6$  Hz), 7.96 (d, 1H,  $J = 7.6$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 21.7, 22.3, 72.6, 125.6, 126.0, 127.8, 128.5, 129.9, 130.5, 131.6, 131.8, 140.1, 141.8, 166.5; IR (KBr): 3066, 3033, 2980, 2929, 1717, 1456, 1290, 1254, 1143, 1077, 1029, 738, 698  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$  ( $\text{MH}^+$ ) 241.1223; found 241.1216.

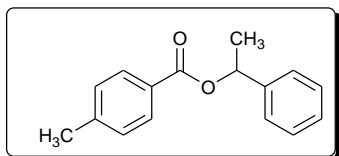
### 1-Phenylethyl 3-methylbenzoate (hk):



Yellowish liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.71 (d, 3H,  $J = 6.4$  Hz), 2.61 (s, 3H), 6.17 (q, 1H,  $J = 6.8$  Hz), 7.33–7.49 (m, 7H), 7.91 (d, 1H,  $J = 8.4$  Hz), 7.96 (d, 1H,  $J =$

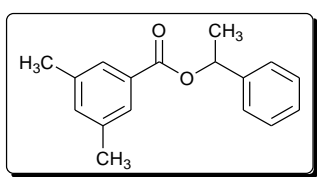
7.6 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 20.5, 22.3, 75.0, 126.4, 126.8, 128.5, 128.9, 129.0, 130.1, 132.7, 133.3, 135.0, 140.5, 163.5; IR (KBr): 2984, 2931, 1738, 1693, 1597, 1452, 1199, 1176, 1059, 983, 761, 699  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$  ( $\text{MH}^+$ ) 241.1223; found 241.1221.

### 1-Phenylethyl 4-methylbenzoate (ik):



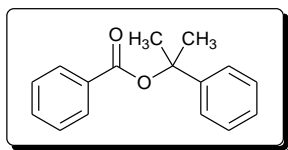
Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.64 (d, 3H,  $J = 6.8$  Hz), 2.58 (s, 3H), 6.11 (q, 1H,  $J = 6.4$  Hz), 7.17–7.35 (m, 6H), 7.43 (d, 2H,  $J = 8$  Hz), 7.96 (d, 1H,  $J = 7.6$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 21.7, 22.3, 72.6, 125.6, 126.0, 127.8, 128.5, 130.5, 131.6, 140.1, 141.8, 166.5; IR (KBr): 3066, 3027, 2979, 2923, 1717, 1455, 1255, 1077, 1029, 738, 698  $\text{cm}^{-1}$ ; HRMS (ESI): calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$  Anal. calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$ : C 79.97, H 6.71; found C 79.85, H 6.67.

### 1-Phenylethyl 3,5-dimethylbenzoate (jk):



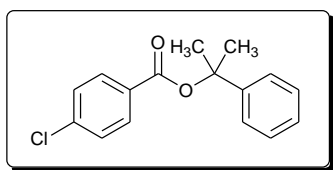
Yellowish liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.68 (d, 3H,  $J = 6.4$  Hz), 2.58 (s, 6H), 6.15 (q, 1H,  $J = 6.8$  Hz), 7.31–7.46 (m, 6H), 7.94 (d, 2H,  $J = 7.2$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 21.3, 22.2, 75.0, 126.4, 128.4, 129.0, 130.0, 133.2, 134.9, 137.2, 140.4, 163.4; IR (KBr): 2923, 2852, 1734, 1635, 1449, 1198, 1177, 979, 760, 744, 698  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{17}\text{H}_{18}\text{O}_2$ : C 80.28, H 7.13; found C 80.37, H 7.09.

### 2-Phenylpropan-2-yl benzoate (al):



Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.91 (s, 6H), 7.24 (t, 2H,  $J = 7.2$  Hz), 7.29–7.34 (m, 2H), 7.39–7.54 (m, 5H), 8.05 (d, 1H,  $J = 7.2$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 28.5, 81.9, 124.0, 126.5, 128.1, 128.8, 129.3, 131.3, 132.4, 145.6, 164.8; IR (KBr): 2981, 2929, 1721, 1450, 1365, 1314, 1281, 1145, 1098, 1070, 1027, 763, 712, 698  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{16}\text{H}_{16}\text{O}_2$ : C 79.97, H 6.71; found C 80.03, H 6.77.

### 2-Phenylpropan-2-yl 4-chlorobenzoate (dl):

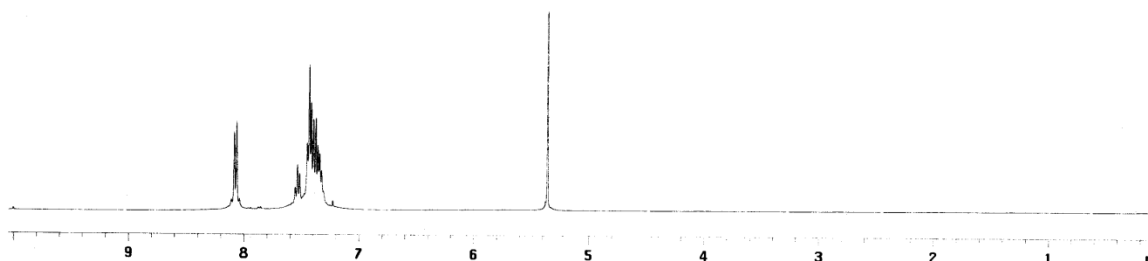


Colourless liquid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.89 (s, 6H), 7.22–7.42 (m, 7H), 7.96 (d, 2H,  $J = 6.8$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 28.5, 82.4, 124.1, 127.0, 128.2, 128.4, 129.8, 130.8, 138.9, 145.4, 164.0; IR (KBr): 2981, 2931, 1725, 1595, 1449, 1365, 1277, 1145, 1116, 1098, 1015, 853, 761, 698  $\text{cm}^{-1}$ ; Anal. calcd. for  $\text{C}_{16}\text{H}_{15}\text{ClO}_2$ : C 69.95, H 5.50; found C 69.87, H 5.54.

## Spectra

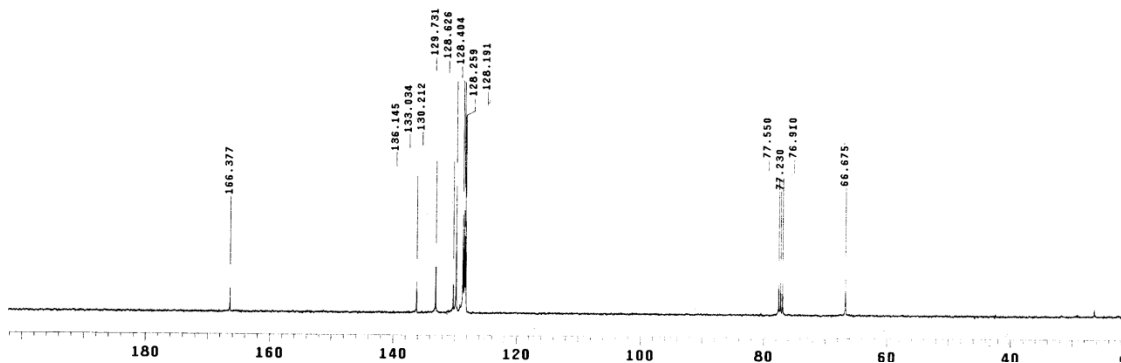
### Benzyl benzoate (aa): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

```
SAMPLE          SPECIAL
date Aug 28 2012 temp not used
solvent CDC13   gain  not used
file           exp  not used
ACQUISITION    hst   0.008
sw 10110.0     pv90 19.700
at 1.996       alfa 20.000
np 39952
fb not used    il     n
bs 4           in     n
d1 1.000       dp     y
nt 32         hs     nn
ct 32
TRANSMITTER    lb     0.10
tn H1         fn     65536
sfrq 399.853  DISPLAY
tof 362.8     sp     -54.4
tpwr 57       wp     4071.3
pw 9.850     rfl    2617.4
DECOUPLER      rfp    0
dn C13       rp     132.1
dof 0        lp     -137.7
dm nnn
dmm c        wc     250
dpr 50       sc     0
dwt 15900    vs     43
nm cdc ph    th     20
```

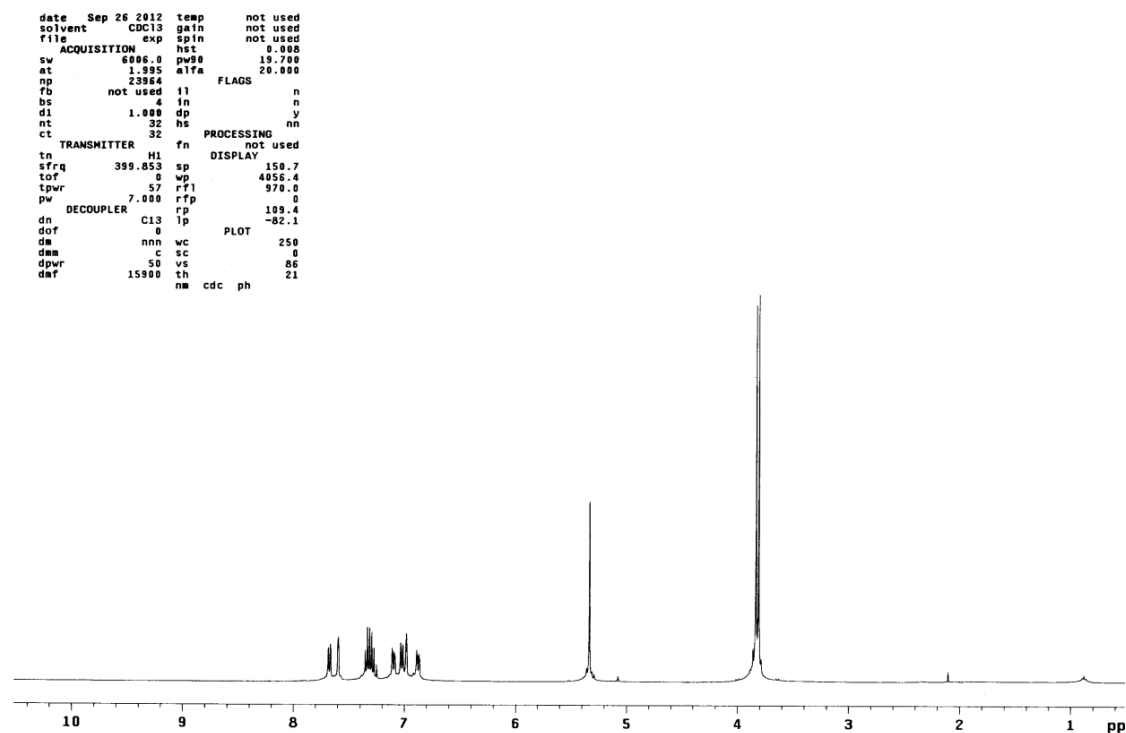


### Benzyl benzoate (aa): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

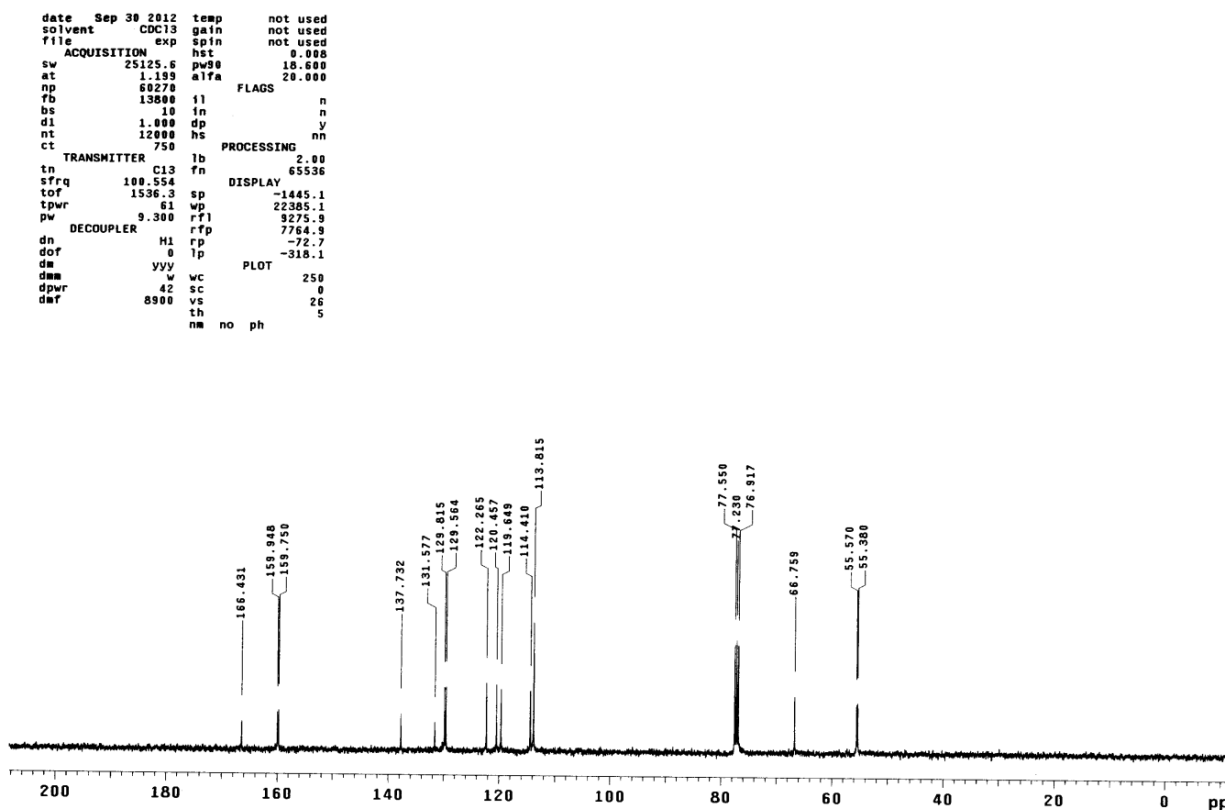
```
SAMPLE          SPECIAL
date Sep 1 2012 temp not used
solvent CDC13   gain  not used
file           exp  not used
ACQUISITION    hst   0.008
sw 25125.6     pv90 18.600
at 1.199       alfa 20.000
np 60270
fb 13600      il     n
bs 32         in     n
d1 1.000       dp     y
nt 12000      hs     nn
ct 928
TRANSMITTER    lb     2.00
tn C13       fn     65536
sfrq 100.554  DISPLAY
tof 1536.3    sp     1705.7
tpwr 61       wp     18620.9
pw 9.300     rfl    9294.3
DECOUPLER      rfp    7764.9
dn H1         rp     -59.1
dof 0        lp     -332.0
dm vvy
dmm w        wc     250
dpr 42       sc     0
dwt 8900     vs     20
nm no ph    th     3
```



### 3-Methoxybenzyl 3-methoxybenzoate (bb): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

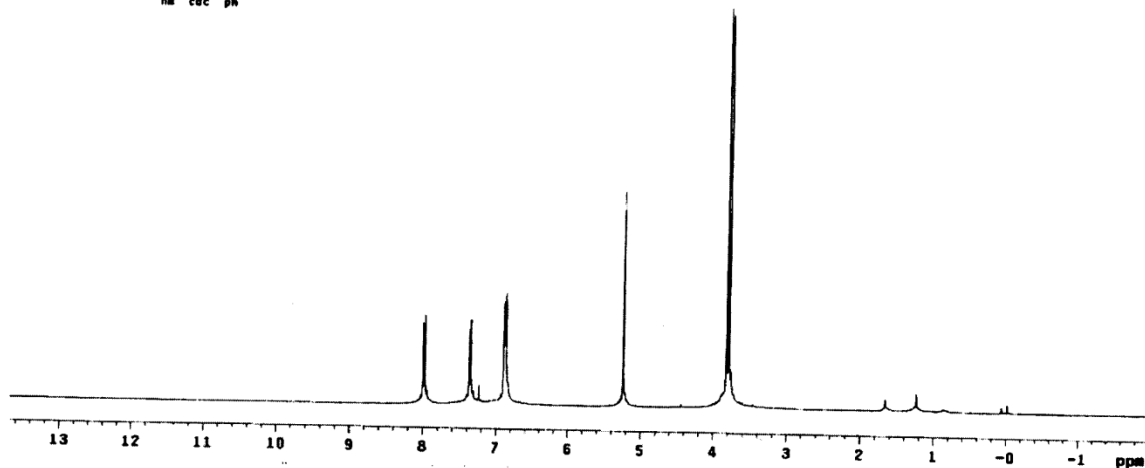


### 3-Methoxybenzyl 3-methoxybenzoate (bb): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



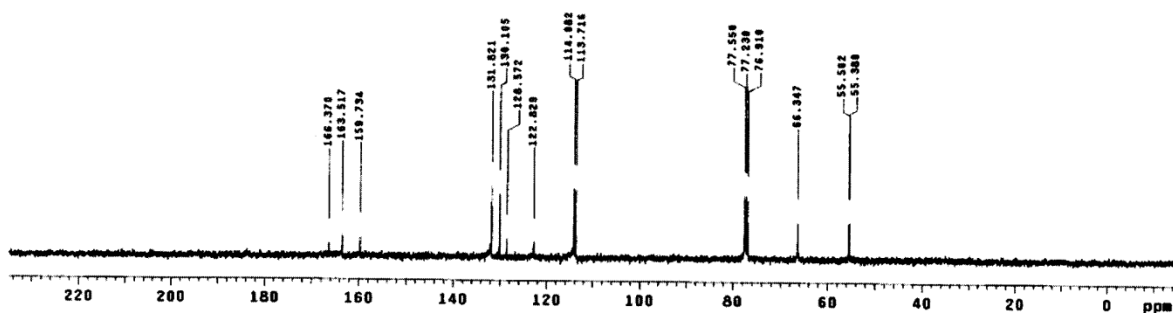
### 4-Methoxybenzyl 4-methoxybenzoate (cc): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

```
SAMPLE          SPECIAL
date OCT  8 2012 temp      not used
solvent CDCl3 gain      not used
file      exp      spin    not used
ACQUISITION hsc      0.000
sw 2500.0 pwr0     10.700
at 1.000 n1fa     20.000
np 25520          FLAGS
fb not used i1      n
bs 6             in      n
d1 1.000         dp      y
at 32           hs      nn
ct              PROCESSING
TRANSMITTER 1b      0.10
tn          M1      fn      65536
sfreq 300.053      DISPLAY
tof 302.0         sp      -804.0
tpwr 57          wp      6300.0
pw 9.050         rfl     3000.0
DECOUPLER C13      rfp     2000.0
dn          0      rp      99.5
dof         0      lp      -80.5
dm          nnn    PLGT
dmc         c      wc      250
dpr         50     sc      0
dcr        15000    ve     00
det         th     th     10
nm          cdc   ph
```



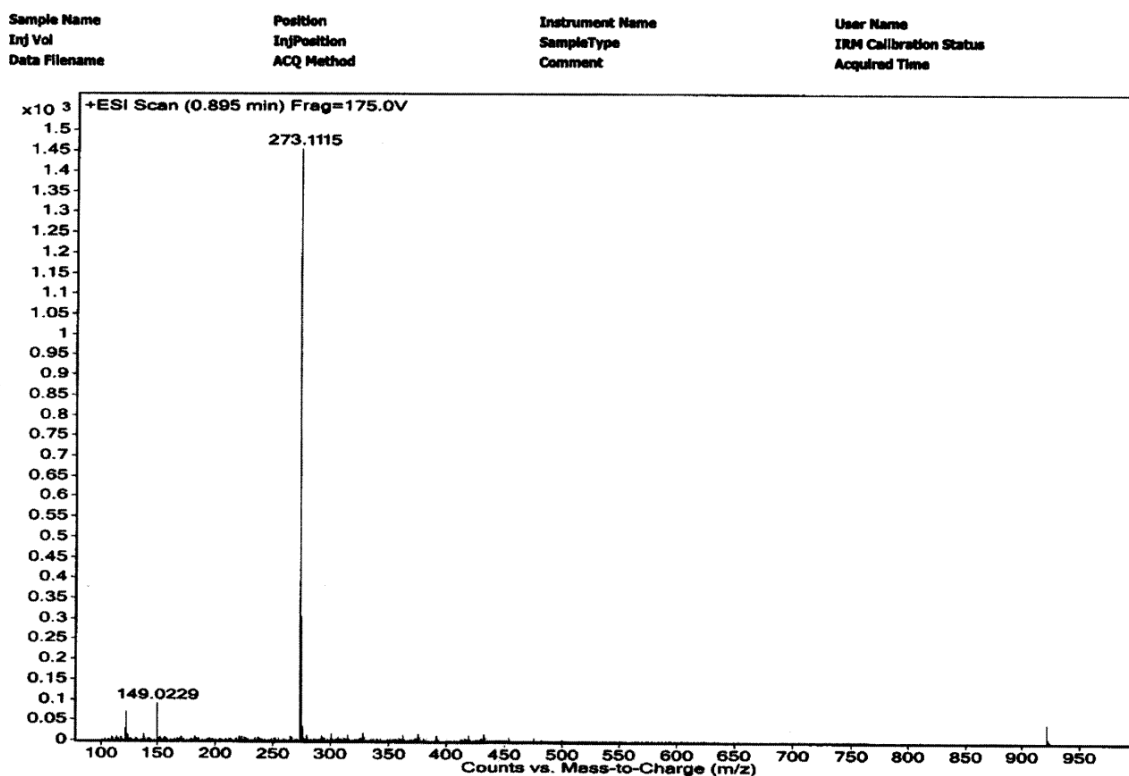
### 4-Methoxybenzyl 4-methoxybenzoate (cc): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

```
SAMPLE          SPECIAL
date OCT  8 2012 temp      not used
solvent CDCl3 gain      not used
file      exp      spin    not used
ACQUISITION hsc      0.000
sw 25125.0 pwr0     10.000
at 1.100 n1fa     20.000
np 90270          FLAGS
fb 13000          i1      n
bs 32            in      n
d1 1.000         dp      y
at 2000          hs      nn
ct 400           PROCESSING
TRANSMITTER C13      1b      2.00
tn          M1      fn      65536
sfreq 100.626      DISPLAY
tof 1536.3         sp      -1514.1
tpwr 61           wp      25125.0
pw 8.300         rfl     9270.0
DECOUPLER H1      rfp     7764.0
dn          0      rp      -80.0
dof         0      lp      -271.4
dm          vvv    PLGT
dmc         w      wc      250
dpr         42     sc      0
dcr        8000    ve     15
det         th     th     3
nm          no   ph
```



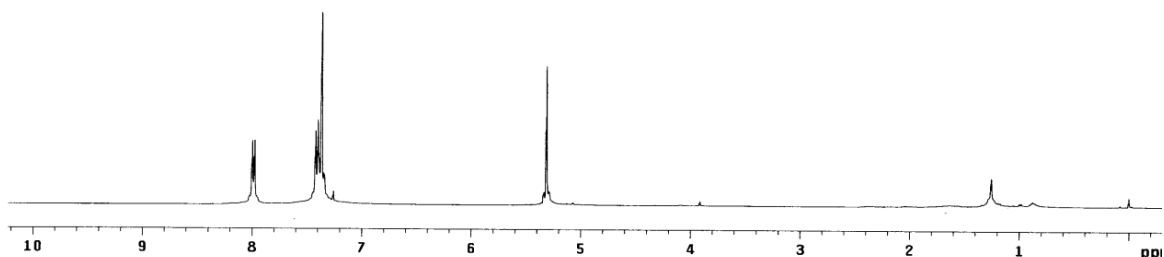


### 4-Methoxybenzyl 4-methoxybenzoate (cc): HRMS

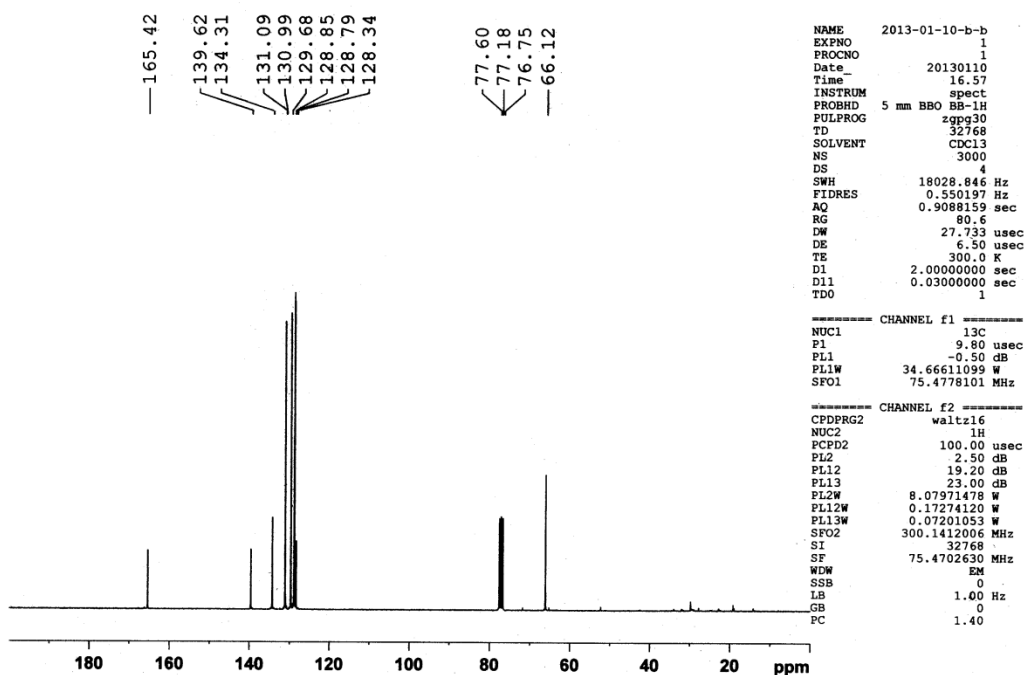


### 4-Chlorobenzyl 4-chlorobenzoate (dd): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

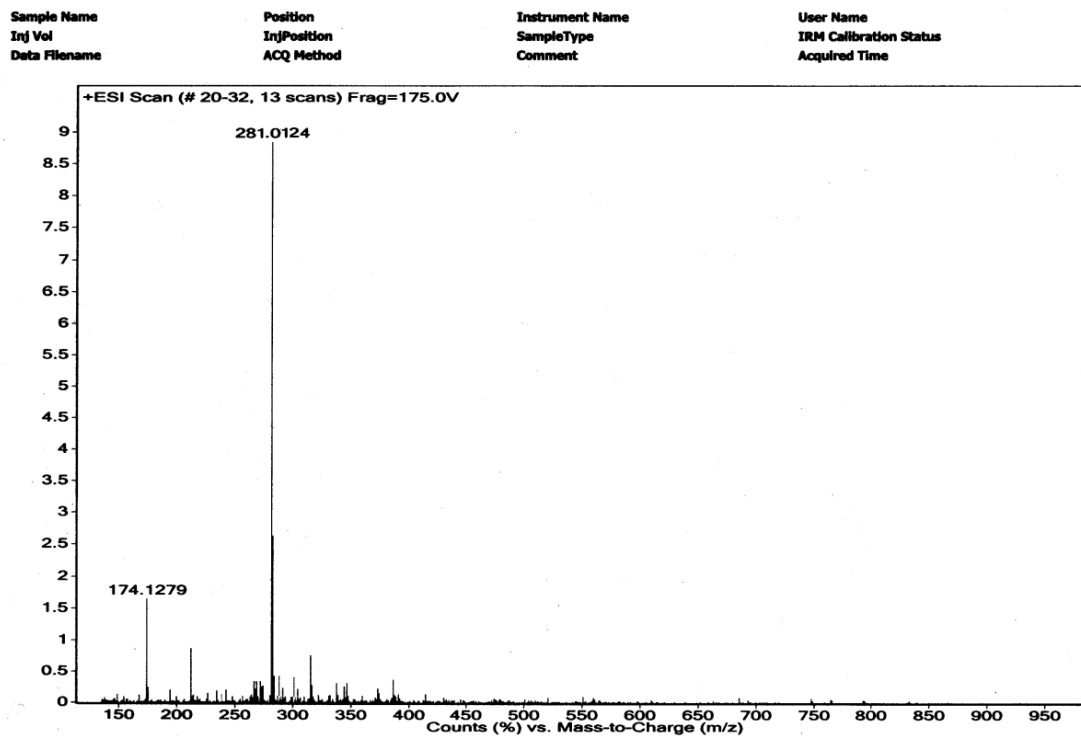
```
SAMPLE          SPECIAL
date Dec 21 2012 temp not used
solvent CDCl3 gain not used
file exp sp1n not used
ACQUISITION exp hst 0.008
sw 6389.8 pw90 19.700
at 1.398 a1fa 20.000
np 25528 FLAGS
fb not used l1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY -166.9
tof 382.0 sp 4257.0
tpwr 57 wp 796.6
pw 9.850 rfl 0
DECOUPLER C13 rfp 81.3
dn 0 lp -58.0
dm nnn c PLOT 250
dwm c wc 0
dpwr 50 sc 0
daf 15900 vs 41
nm cdc ph 12
```



### 4-Chlorobenzyl 4-chlorobenzoate (dd): <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

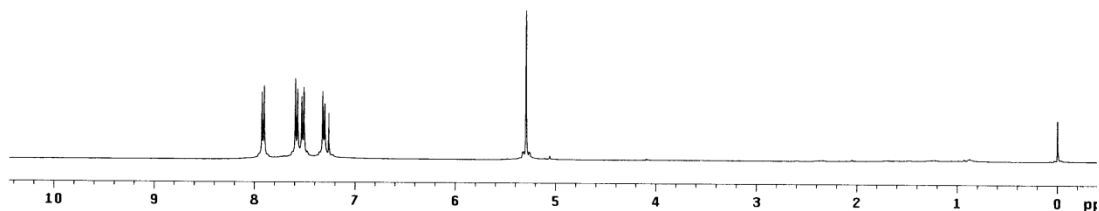


### 4-Chlorobenzyl 4-chlorobenzoate (dd): HRMS

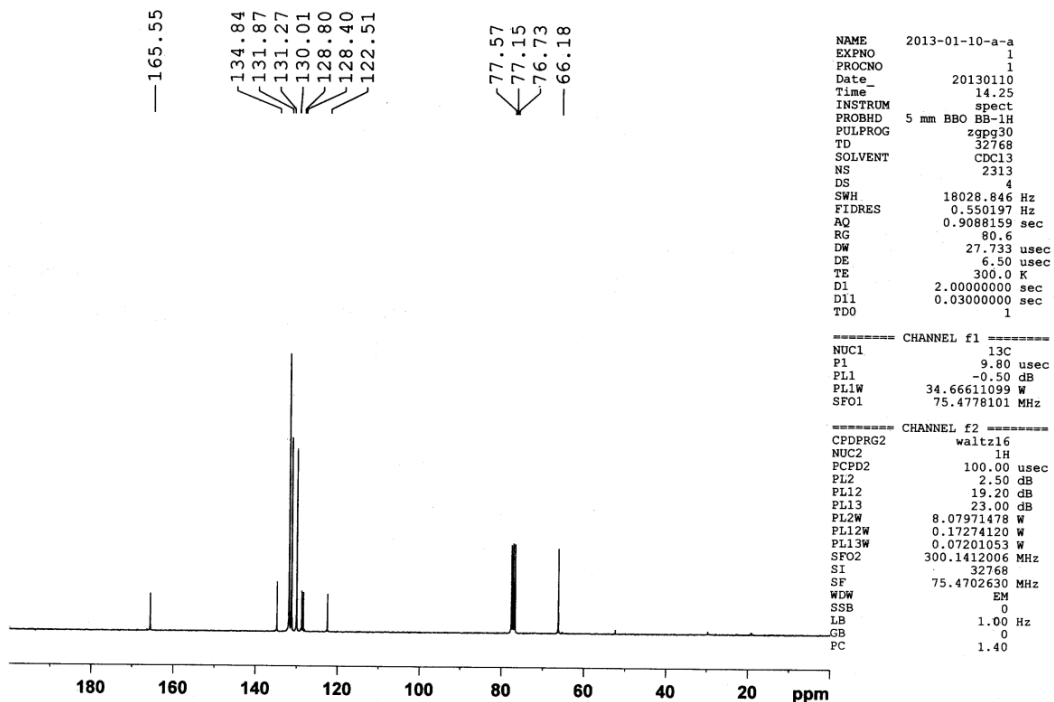


### 4-Bromobenzyl 4-bromobenzoate (ee): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

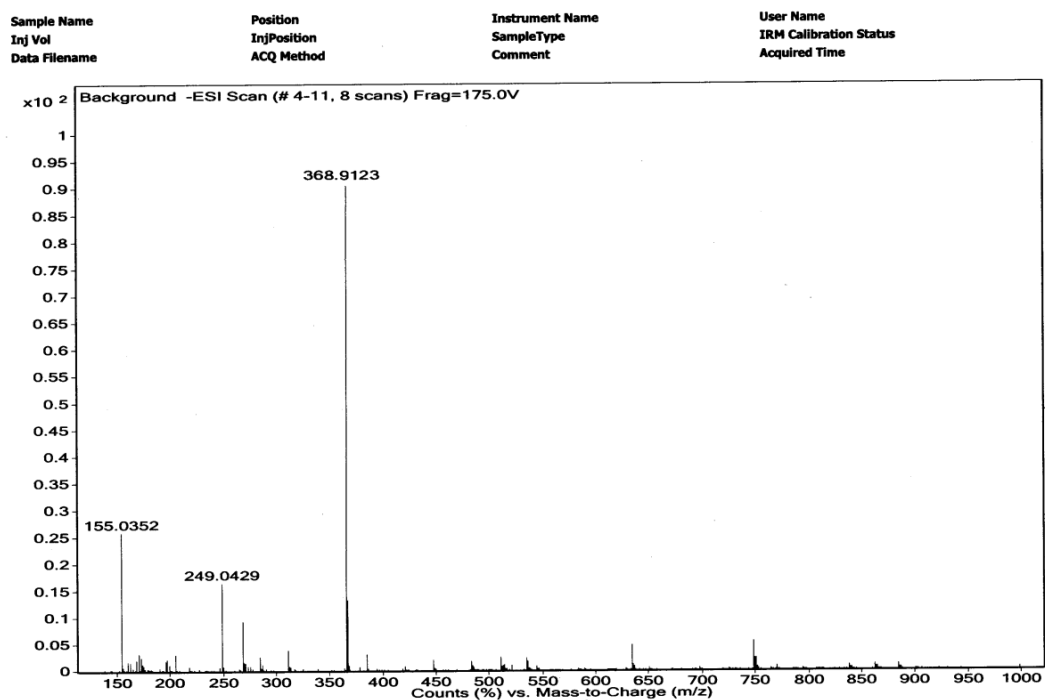
```
SAMPLE          SPECIAL
date    Dec 21 2012  temp    not used
solvent  CDCl3      gain    not used
file     exp       spin    not used
ACQUISITION  hst     0.008
sw       6369.8    pw90    19.700
at       1.838    aifa    20.000
np       25528
fb       not used  il      n
bs       4        in      n
d1       1.000    dp      y
nt       32      hs      nn
ct       32      PROCESSING
tn       H1      lb      0.10
sfrq    399.853  Fn      65536
tof     362.8   sp      -231.3
tpwr    57      wp      4400.1
pw      9.850  rf1     793.7
DECOUPLER C13      rfp     0
dn       0      rp      90.3
dof      0      lp     -73.3
dm       nnn    c      PLOT
dwa      c      wc     250
dpwr     50    vs     0
dnt     15900  th     34
          nm    cdc ph 17
```



### 4-Bromobenzyl 4-bromobenzoate (ee): <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

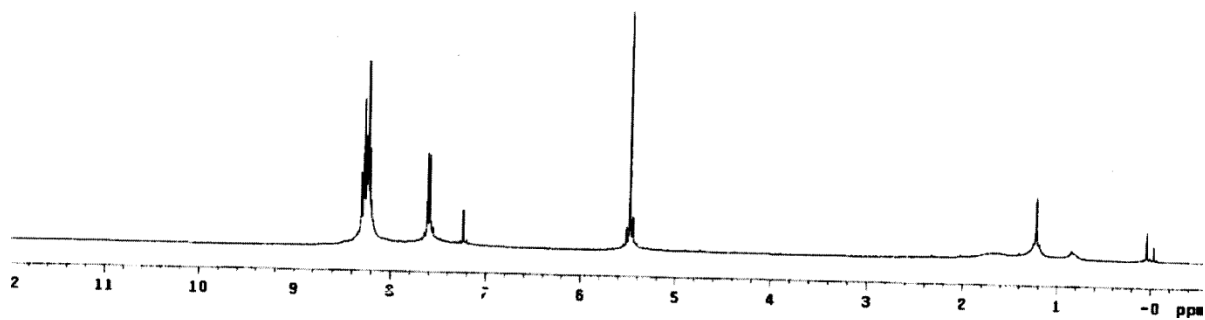


### 4-Bromobenzyl 4-bromobenzoate (ee): HRMS



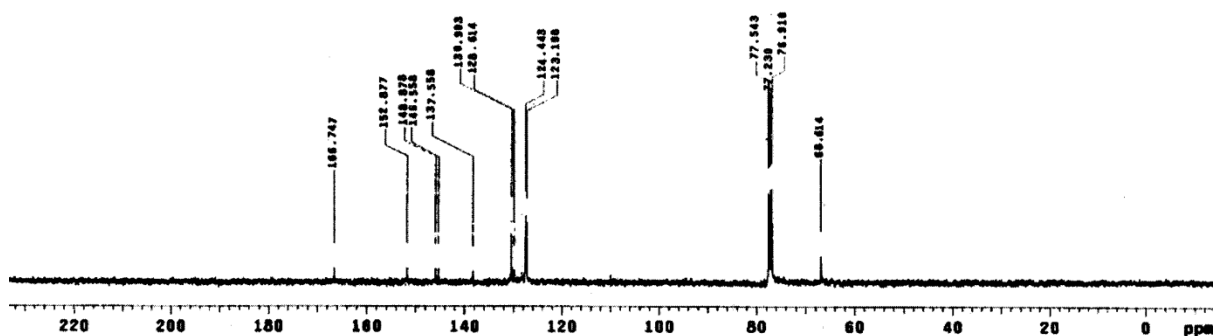
### 4-Nitrobenzyl 4-nitrobenzoate (ff): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

```
expt s2pu1
SAMPLE
date Oct 29 2012 temp SPECIAL
solvent CDCl3 gain not used
rf1e exp spin not used
ACQUISITION hst 8.000
sw 6384.0 pps 13.700
at 1.300 n17a 20.000
np 25526
fb not used 11
bs 4 in n
dl 1.000 dp y
nt 32 hs nn
ct TRANSMITTER 32 PROCESSING 8.10
tn M1 fn 65536
sfrq 399.853 DISPLAY -250.5
tof 382.0 sp 5121.0
tpwr 57 wp 3899.1
pw 9.850 r17 2894.9
DECOUPLER C13 rf 185.3
dn 0 1p -101.1
dm nnh C PLOT
dms C VC 250
dpr 50 sc 0
daf 15000 vs 40
th 6
nm cdc ph 6
```



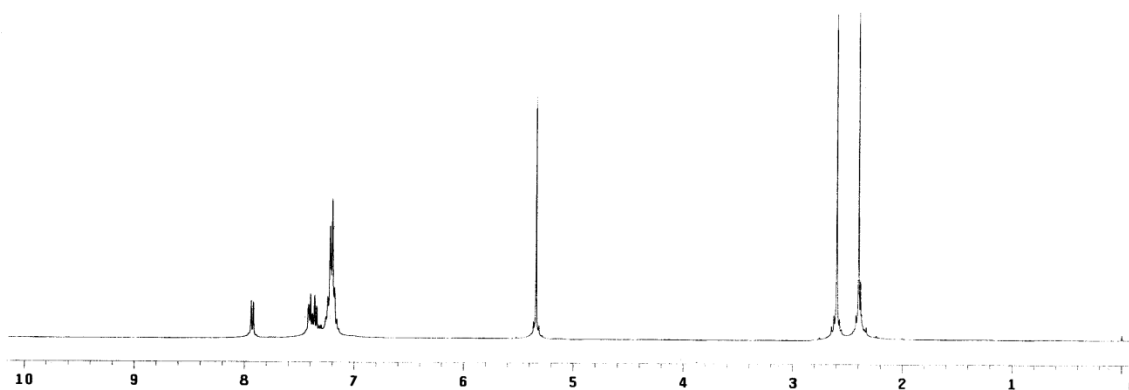
### 4-Nitrobenzyl 4-nitrobenzoate (ff): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

```
exp1 s2pu1
SAMPLE
date OCT 28 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 25125.0 pws 19.000
at 1.100 a1fa 20.000
np 68270 FLAGE
fb 13000 f1 n
bs 32 f2 n
d1 1.000 dp y
nt 5000 ns nn
ct 1472 PROCESSING 2.00
TRANSMITTER lb fn 65536
tn C13 f1
sfrq 100.554 DISPLAY -1511.8
tof 1536.0 sp -25125.8
tpwr 61 wp 8276.7
pw 9.300 rF1 7784.9
DECOUPLER H1 rf -91.7
dn 0 lp -295.0
dm vvy PLOT 250
dwm w vc 0
dpwr 42 sc 0
dof 8000 vs 10
dnt th 2
nm no ph
```

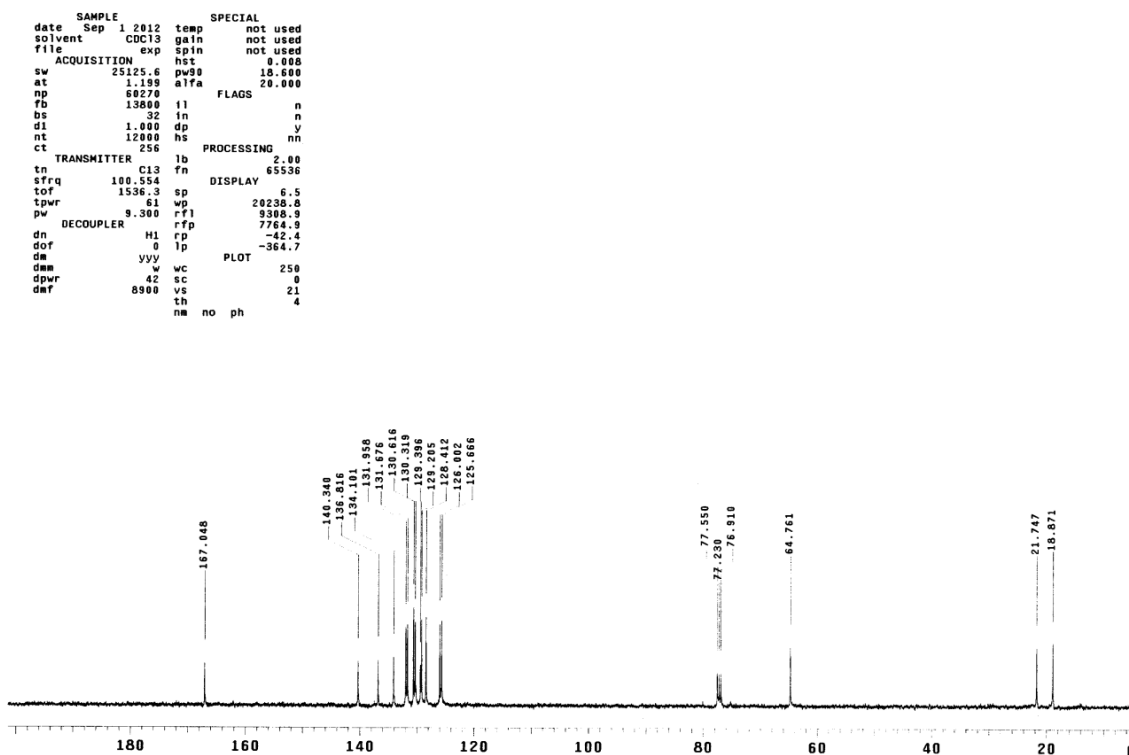


### 2-Methylbenzyl 2-methylbenzoate (gg): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

```
SAMPLE
date Sep 1 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 6389.8 pws 19.700
at 1.998 a1fa 20.000
np 25528 FLAGE
fb not used f1 n
bs 4 f2 n
d1 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING 0.10
TRANSMITTER H1 fn 65536
tn H1 f1
sfrq 399.853 DISPLAY -140.0
tof 362.0 sp 4206.5
tpwr 57 wp 819.6
pw 9.850 rF1 0
DECOUPLER C13 rf 185.0
dn 0 lp -82.0
dm nnn PLOT 250
dwm c wc 0
dpwr 50 sc 0
dof 15900 vs 72
dnt th 11
nm cdc ph
```

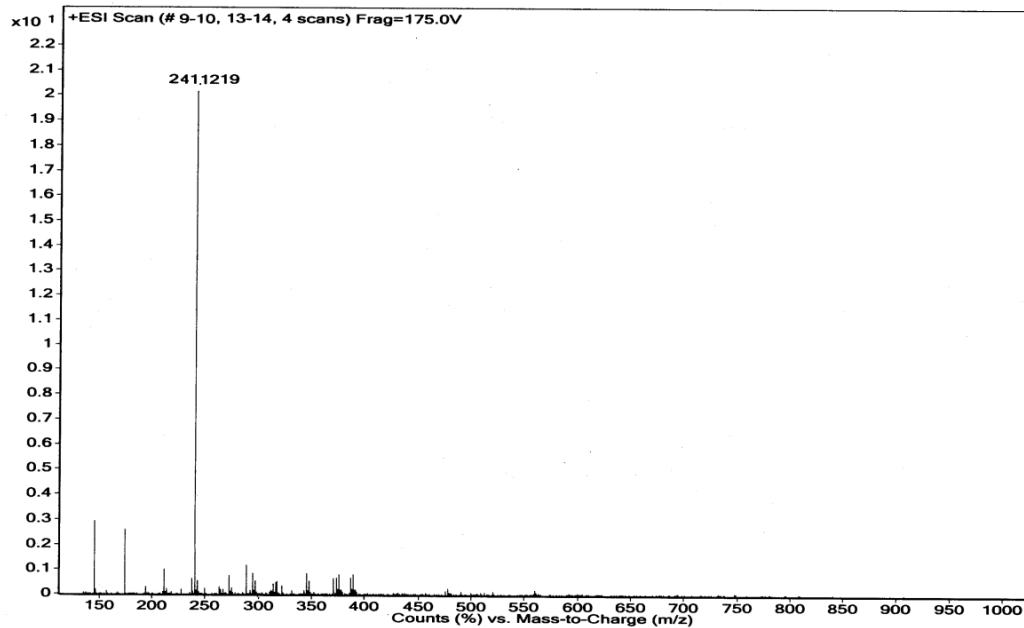


## 2-Methylbenzyl 2-methylbenzoate (gg): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

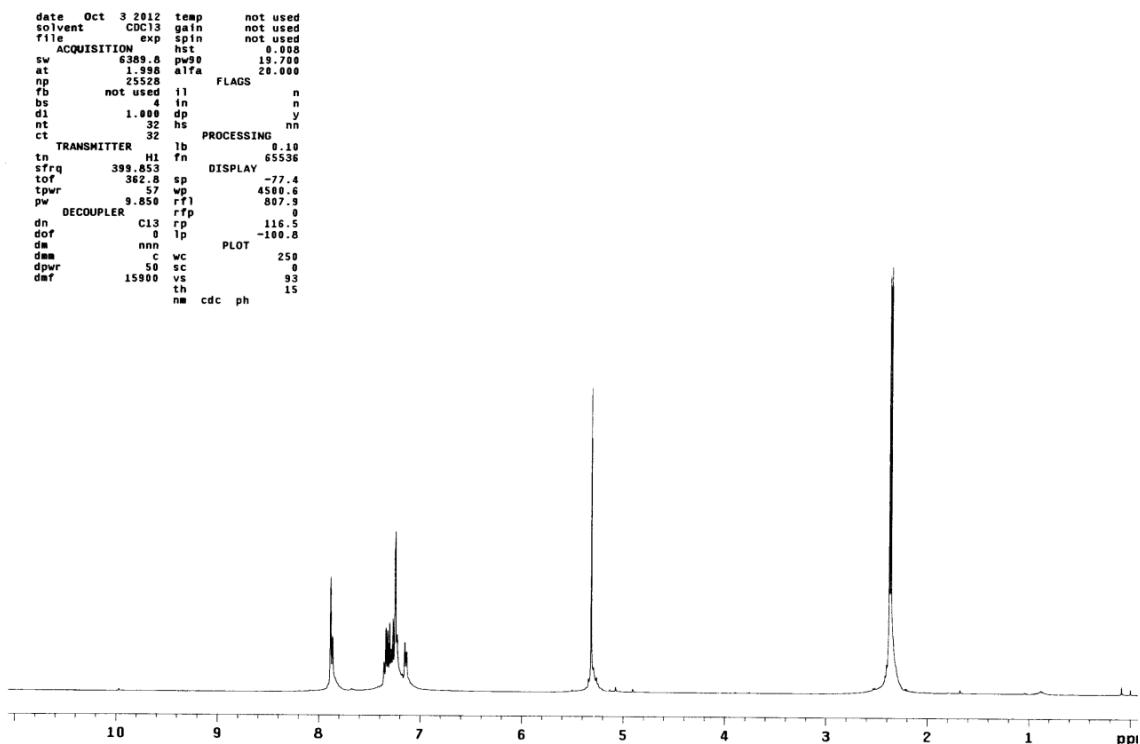


## 2-Methylbenzyl 2-methylbenzoate (gg): HRMS

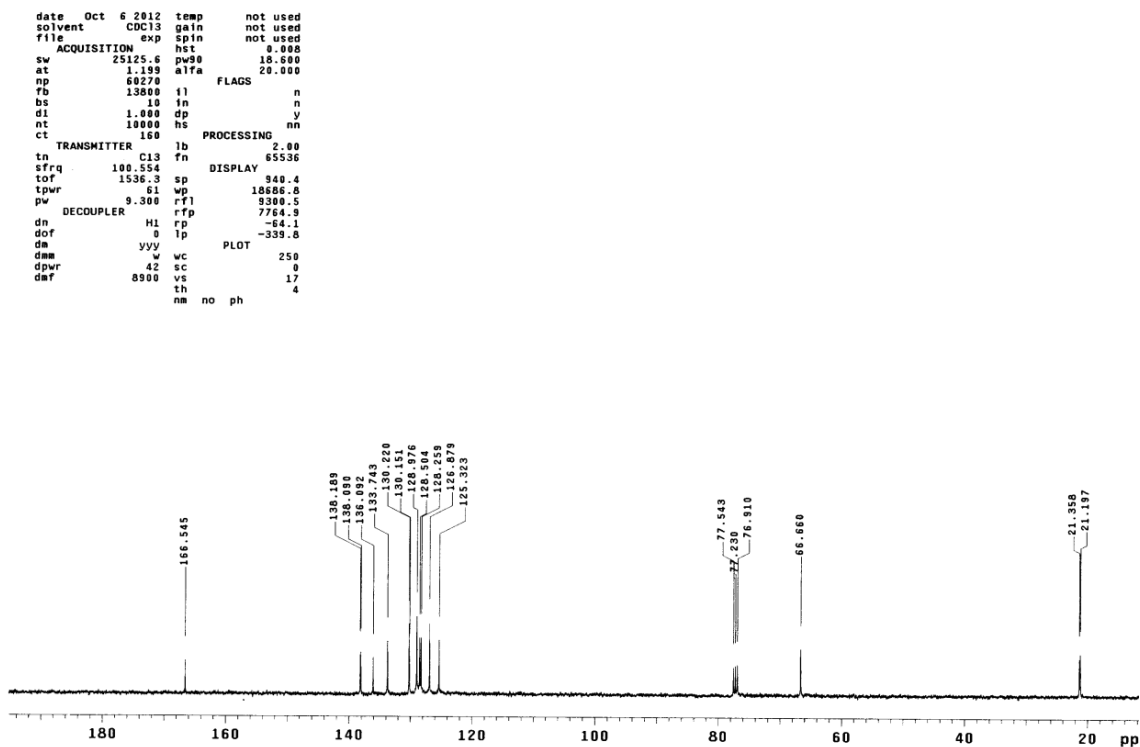
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



### 3-Methylbenzyl 3-methylbenzoate (hh): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

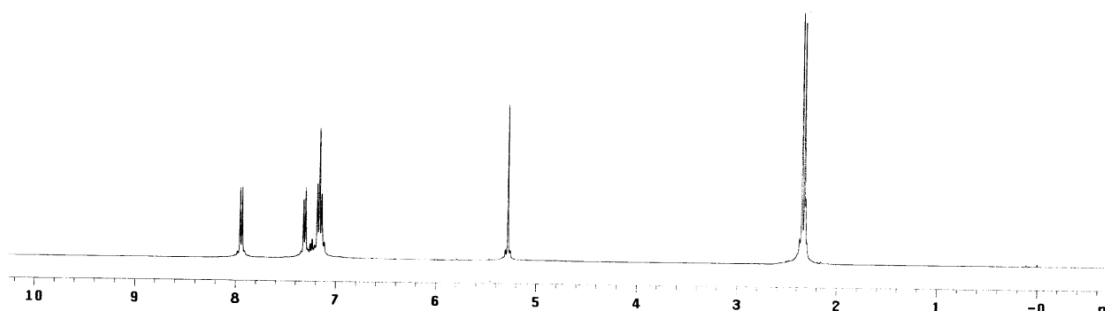


### 3-Methylbenzyl 3-methylbenzoate (hh): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



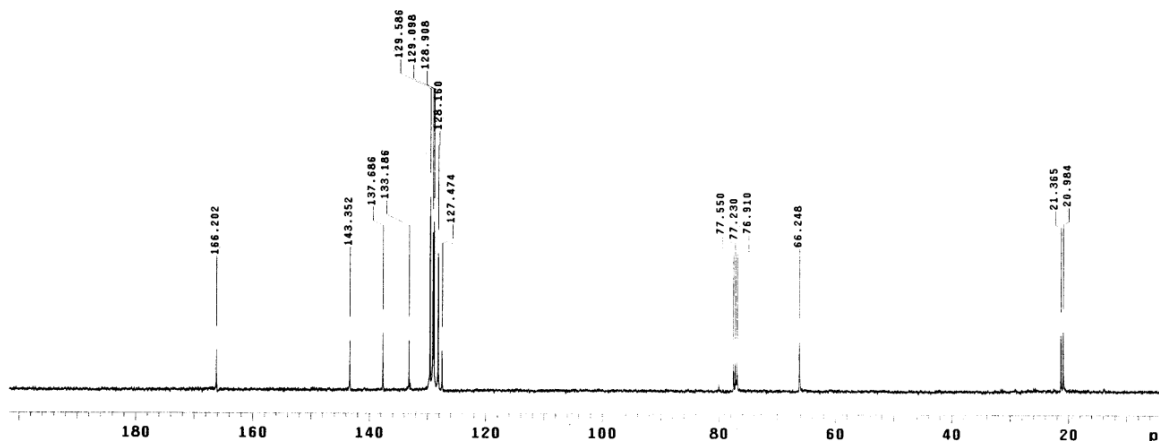
### 4-Methylbenzyl 4-methylbenzoate (ii): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

```
SAMPLE          SPECIAL
date Sep 1 2012 temp not used
solvent CDCl3 gain not used
file          exp spin not used
ACQUISITION   hst not used
sw 6389.8 pw90 19.700
at 1.898 alfa 20.000
np 25528
fb not used i1 FLAGS n
bs 4 in n
dl 1.000 dp y
nt 32 hs nn
ct          PROCESSING 0.10
tn          H1 fn 65536
sfrq 399.853 DISPLAY -374.0
tof 362.8 sp
tpwr 52 wp 4475.2
pw 9.850 rfl 827.4
DECOUPLER C13 rfp 0
dn          rp 122.2
dof 0 lp -99.1
dm          mn PLOT
dwm          wc 250
dpwr 50 sc 0
daf 15900 vs 56
nm          th 20
          cdc ph
```



### 4-Methylbenzyl 4-methylbenzoate (ii): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

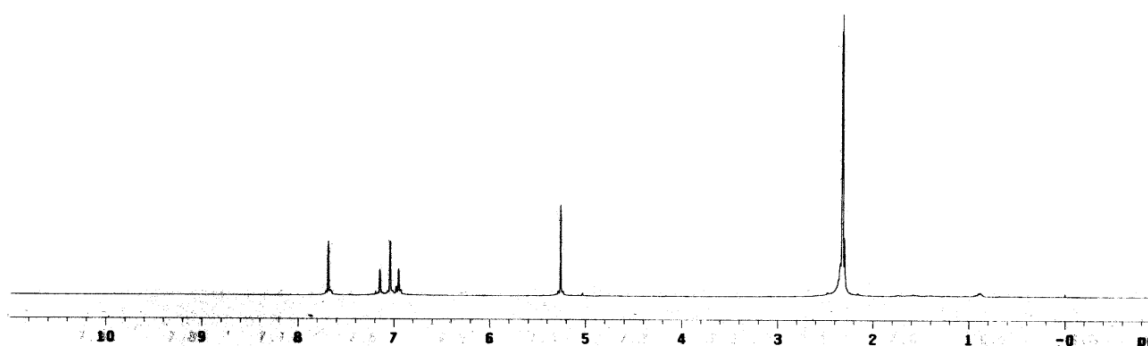
```
SAMPLE          SPECIAL
date Sep 1 2012 temp not used
solvent CDCl3 gain not used
file          exp spin not used
ACQUISITION   hst not used
sw 25125.6 pw90 18.600
at 1.199 alfa 20.000
np 68270
fb 13800 i1 FLAGS n
bs 32 in n
dl 1.000 dp y
nt 12000 hs nn
ct          PROCESSING 2.00
tn          C13 fn 65536
sfrq 100.554 DISPLAY 36.4
tof 1536.3 sp
tpwr 61 wp 20238.8
pw 9.300 rfl 9312.7
DECOUPLER H1 rfp 7764.9
dn          H1 ry -87.0
dof 0 lp -291.6
dm          yvy PLOT
dwm          w wc 250
dpwr 42 sc 0
daf 8900 vs 41
nm          th 4
          no ph
```





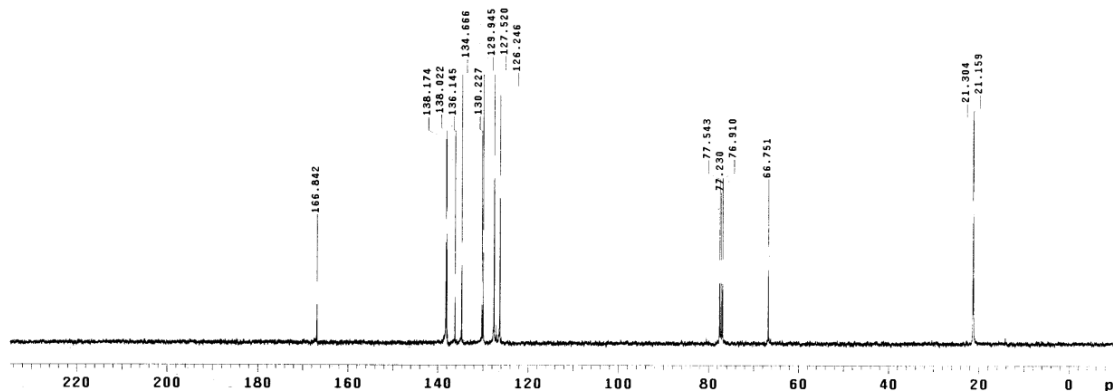
### 3,5-Dimethylbenzyl 3,5-dimethylbenzoate (jj): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

```
SAMPLE          SPECIAL
date Sep 3 2012 temp not used
solvent CDCl3 gain not used
file          exp spin not used
ACQUISITION    hst  0.000
sv  6000.0     pw90 13.700
at  1.595     alpha 20.000
np  23964     FLAGS
fb  not used  11    n
bs  not used  32    n
dl  1.000     dp    y
nt  32       hs    nn
ct
TRANSMITTER    fn  not used
tn  H1       DISPLAY
sfrq 300.053 sp  -441.4
tof  0       wp  6637.7
tpwr 57      rfb  999.5
pw  7.000   rfp  0
DECOUPLER      rp  118.0
dn  C13     1p  -97.2
dof  0
dm  nnh    wc  250
dmm  c     sc  0
dpwr 50    vs  41
def  15000 sh  5
nm  odic  ph
```

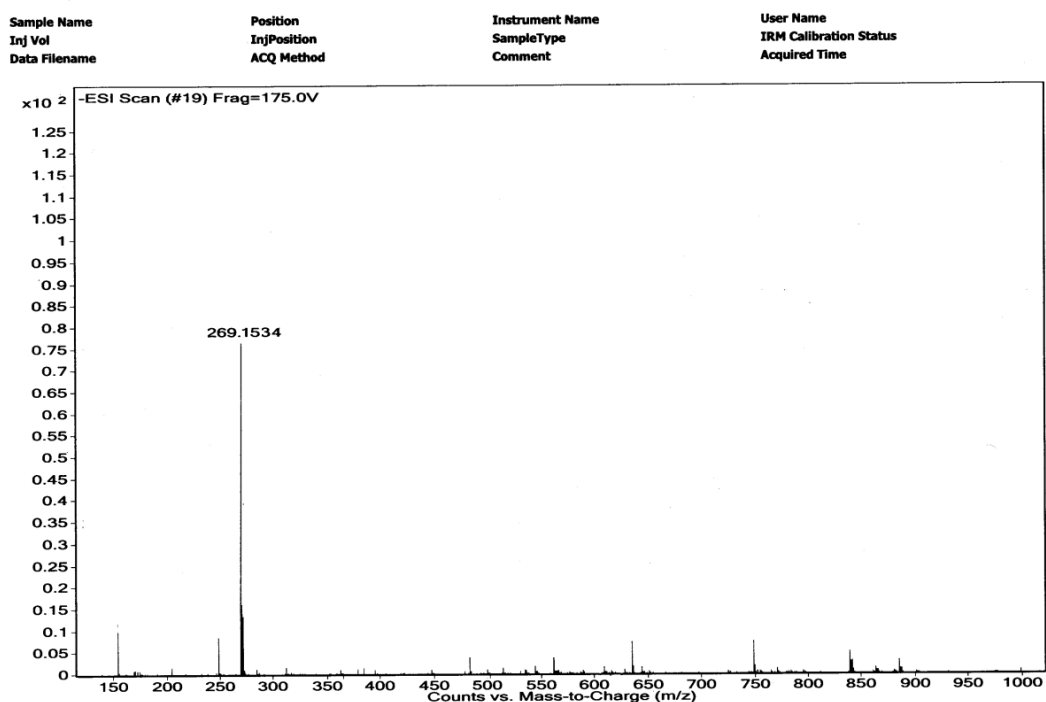


### 3,5-Dimethylbenzyl 3,5-dimethylbenzoate (jj): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

```
SAMPLE          SPECIAL
date Sep 4 2012 temp not used
solvent CDCl3 gain not used
file          exp spin not used
ACQUISITION    hst  0.000
sv  25125.6    pw90 10.000
at  1.199     alpha 20.000
np  60270     FLAGS
fb  13800    11    n
bs  32       1n    n
dl  1.000     dp    y
nt  12000    hs    nn
ct
TRANSMITTER    fb  2.00
tn  C13     tn  65536
sfrq 100.554 sp  -1525.6
tof  1536.3  wp  25125.6
tpwr 61      rfb  9290.5
pw  9.300   rfp  7764.9
DECOUPLER      H1  rp  -71.0
dn  0       1p  -297.7
dof  0
dm  yvy    wc  250
dmm  w     sc  0
dpwr 42    vs  36
def  8900  sh  5
nm  no  ph
```

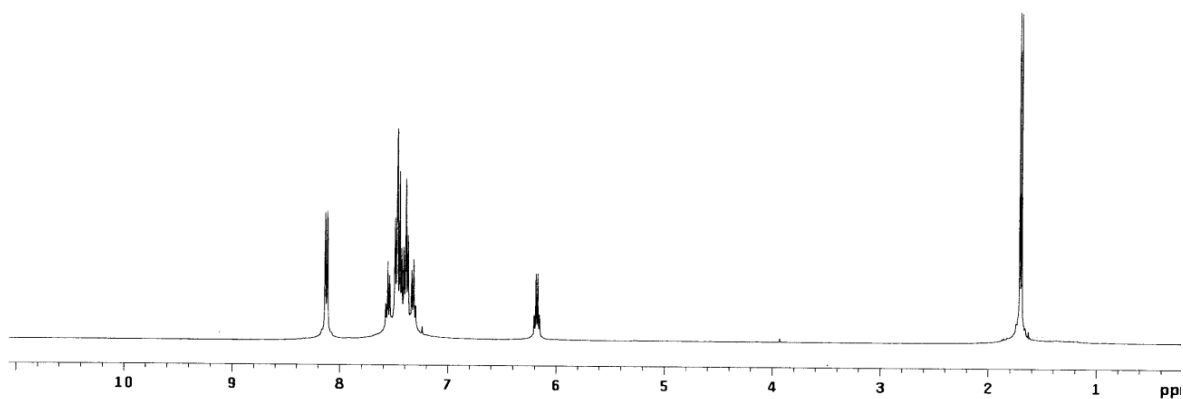


### 3,5-Dimethylbenzyl 3,5-dimethylbenzoate (jj): HRMS

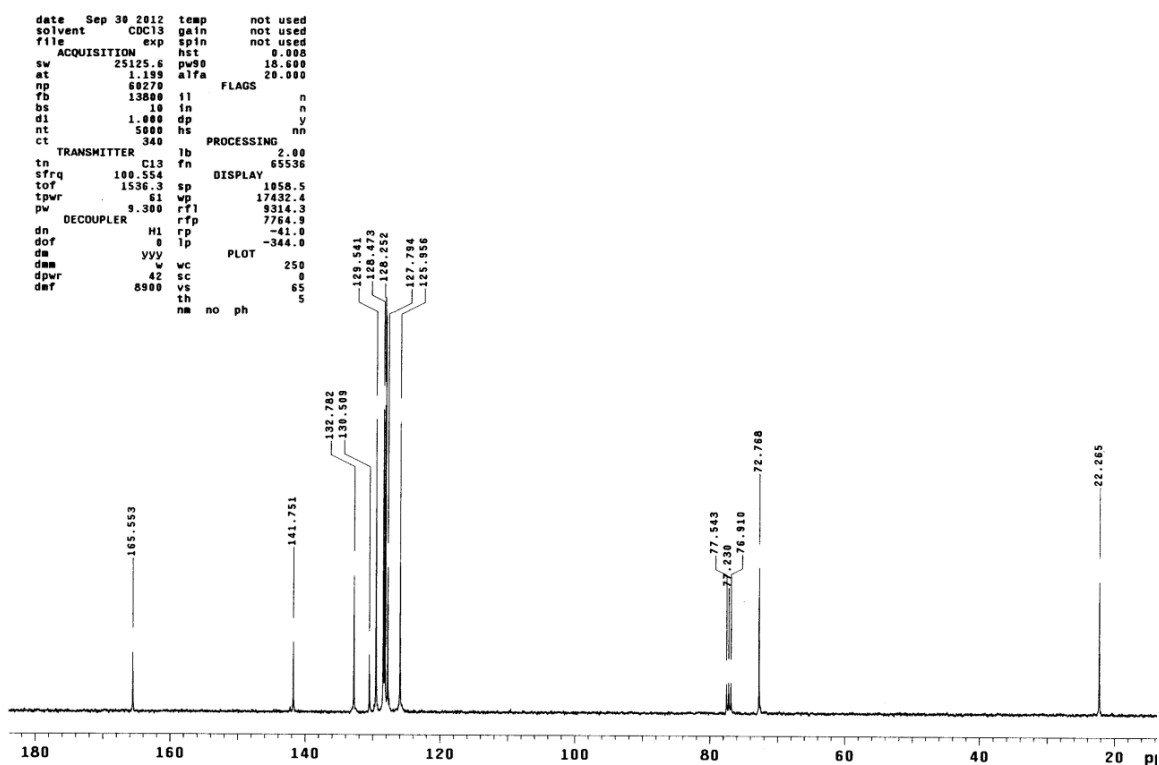


### 1-Phenylethyl benzoate (ak): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

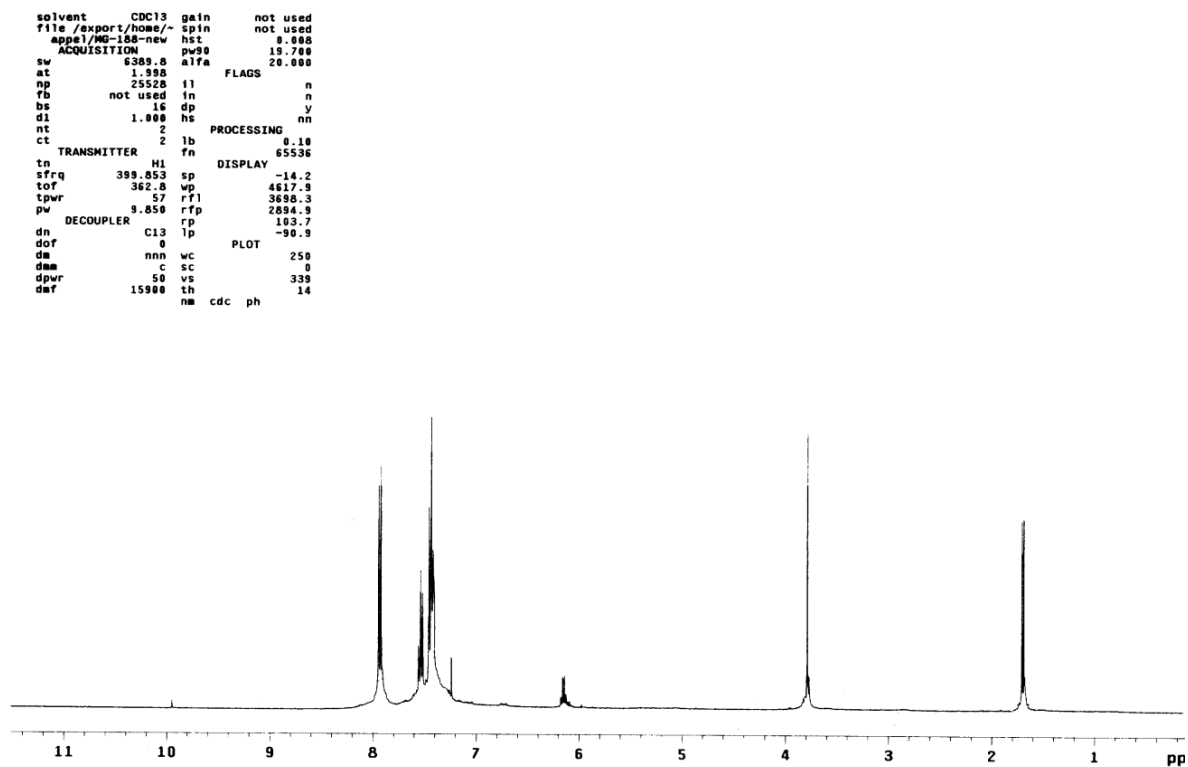
```
date Sep 27 2012 temp not used
solvent CDCl3 gain not used
file ACQUISITION exp spin not used
sw 6006.0 p00 hst 0.008
at 1.895 a1fa 20.000
np 23864 FLAGS
fb not used il n
bs 4 in n
dl 1.000 dp y
nt 32 hs nn
ct PROCESSING
tn H1 fn not used
sfreq 399.853 sp DISPLAY 36.5
tof 0 wp 4387.8
tpwr 57 rfl 3868.4
pv 7.000 rfp 2894.9
DECOUPLER cp 115.5
dn C13 lp -87.4
dof 0 PLOT
dm nns wc 250
dmc c sc 0
dpwr 50 vs 70
daf 15900 th cdc ph 14
```



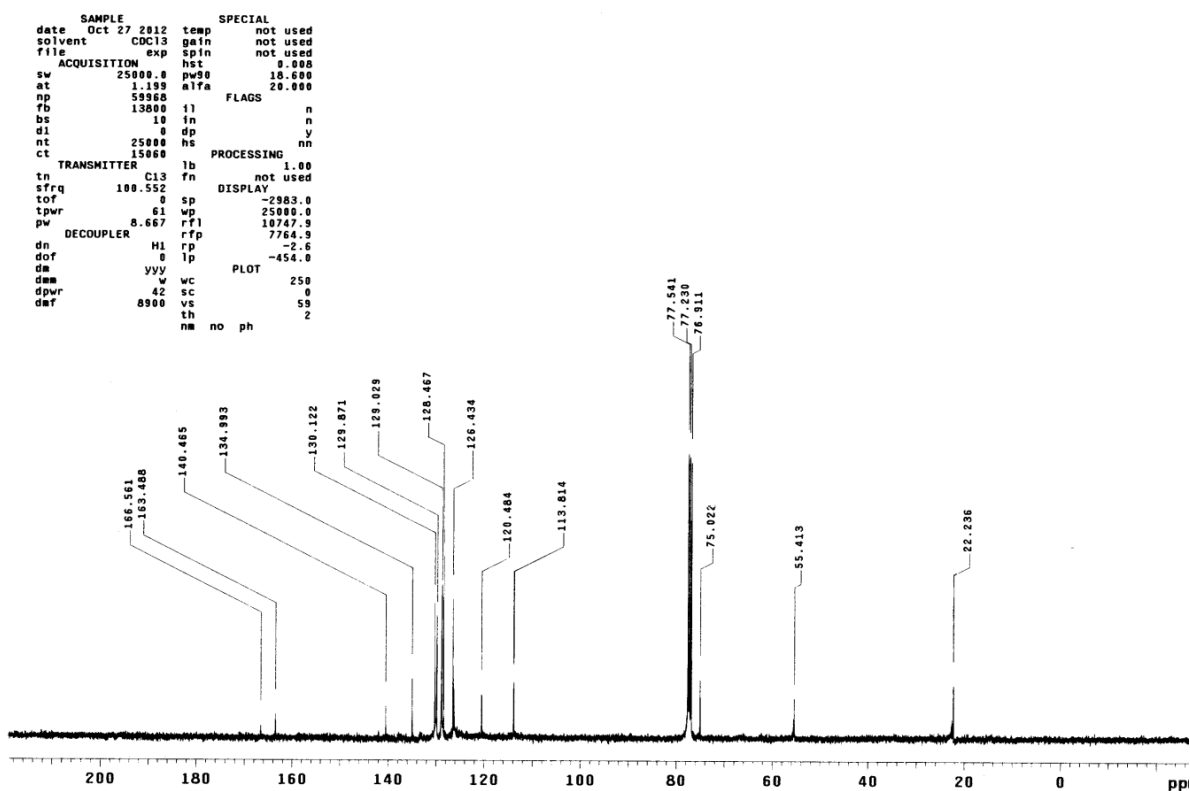
### 1-Phenylethyl benzoate (ak): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)



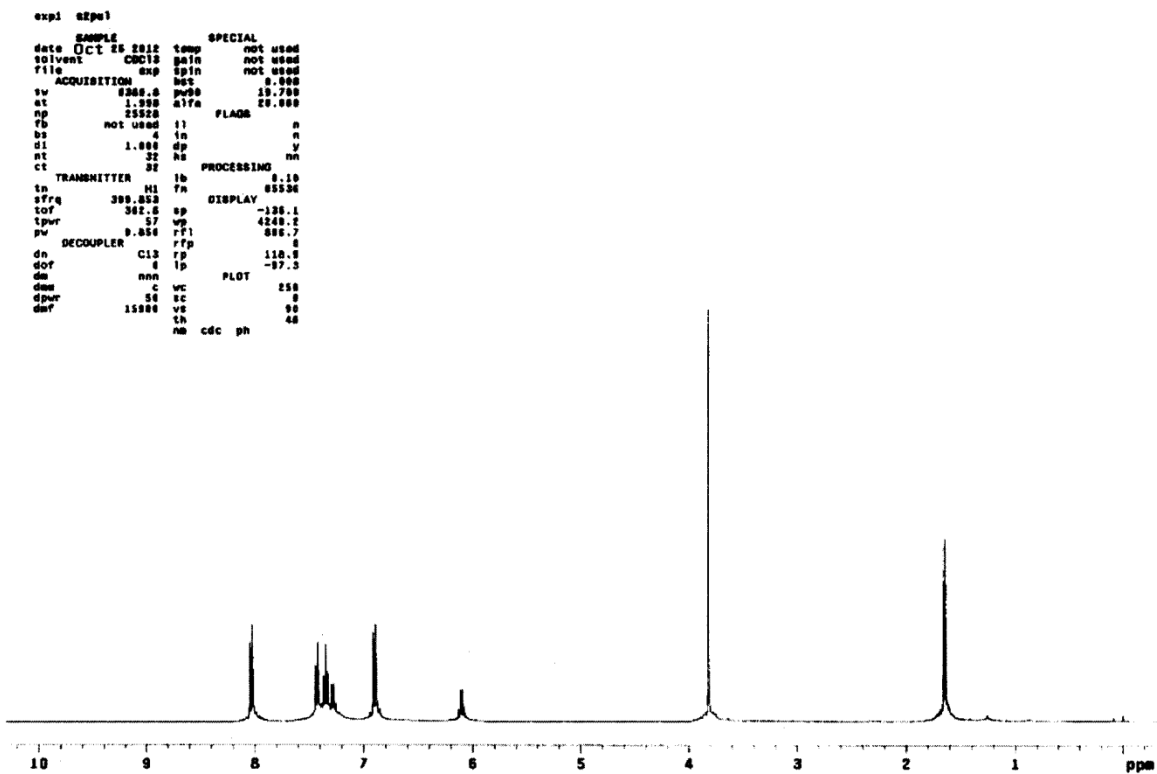
### 1-Phenylethyl 3-methoxybenzoate (bk): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



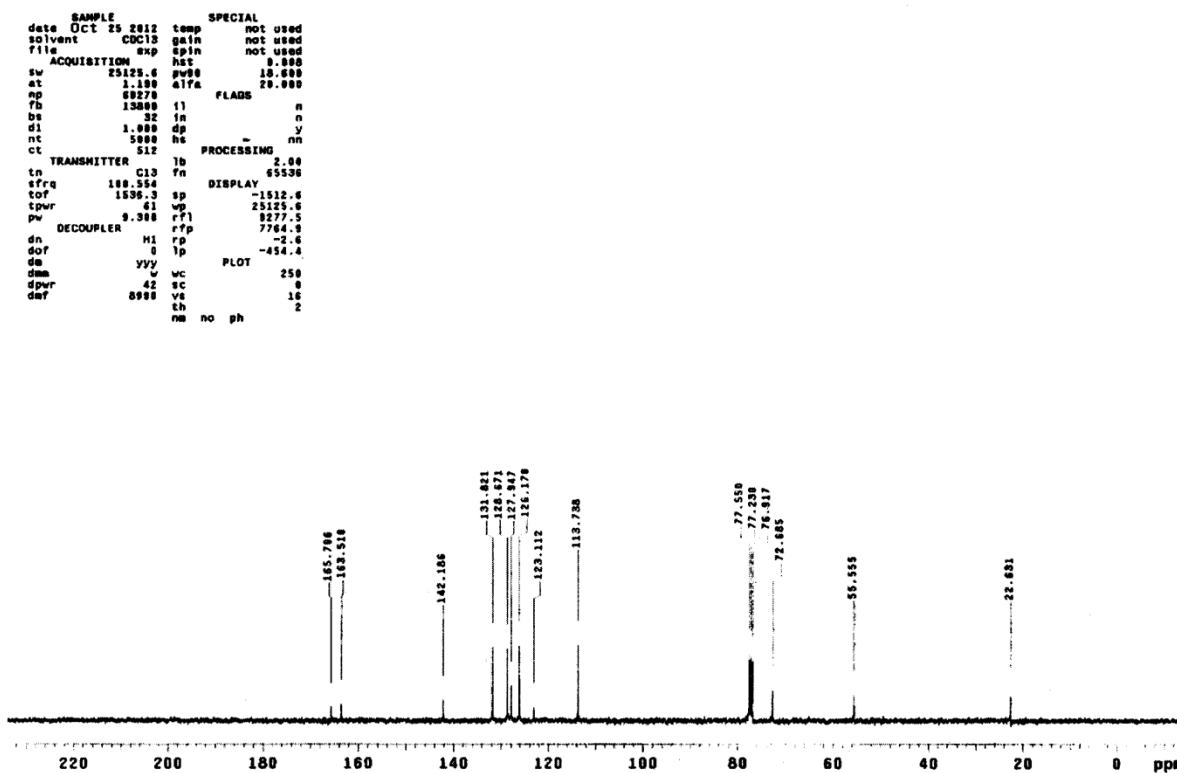
### 1-Phenylethyl 3-methoxybenzoate (bk): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



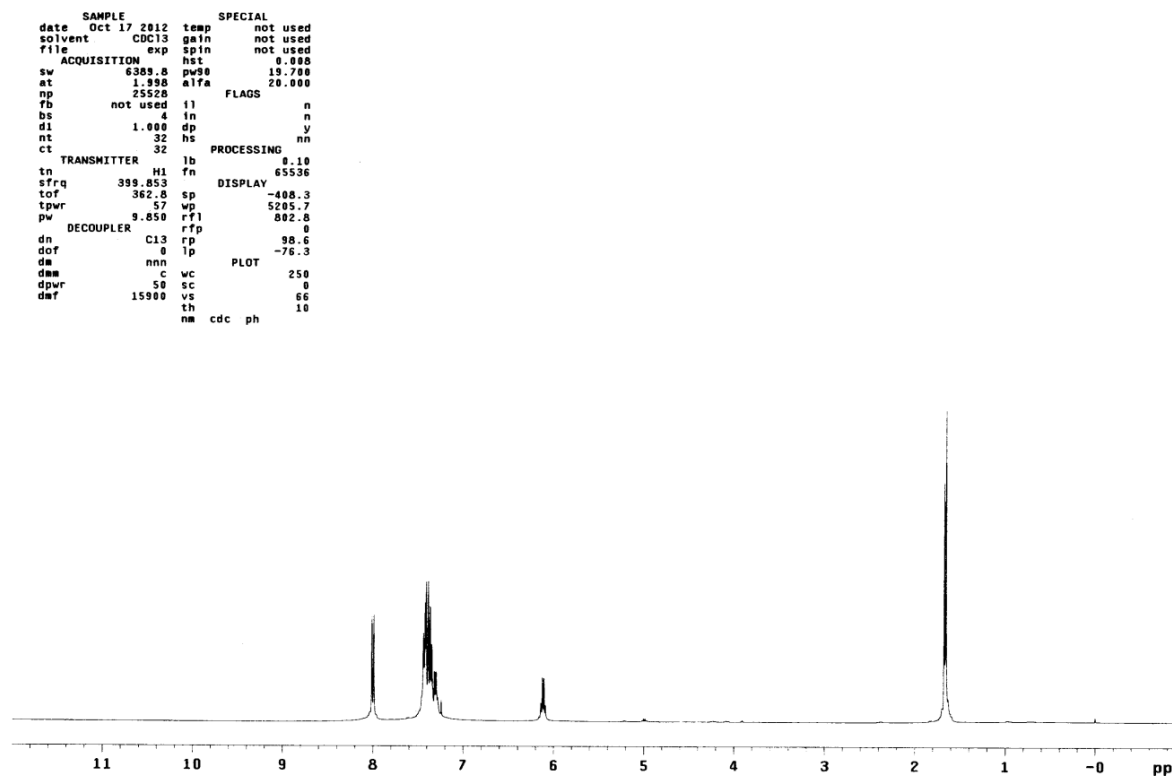
### 1-Phenylethyl 4-methoxybenzoate (ck): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )



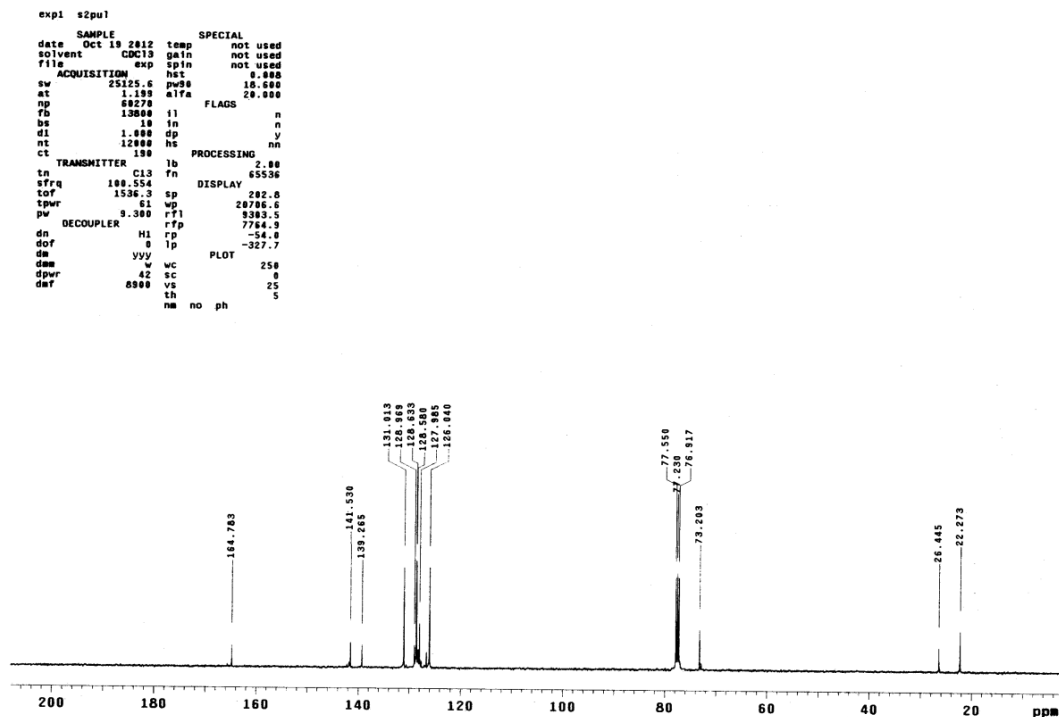
### 1-Phenylethyl 4-methoxybenzoate (ck): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



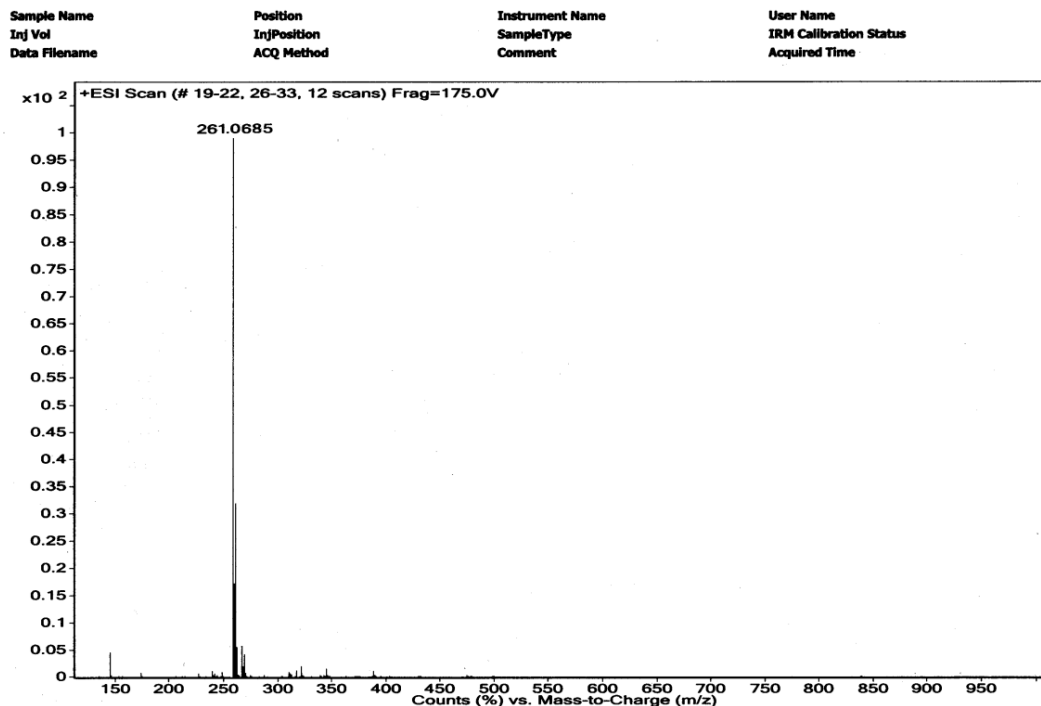
### 1-Phenylethyl 4-chlorobenzoate (dk): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )



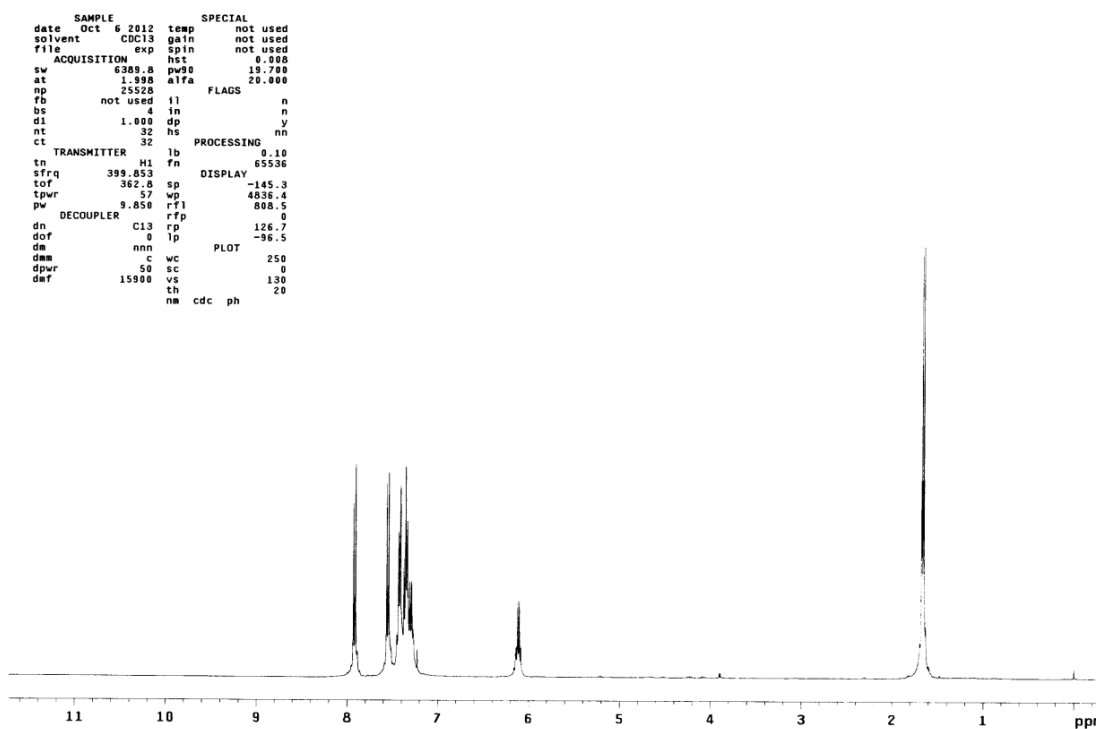
### 1-Phenylethyl 4-chlorobenzoate (dk): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



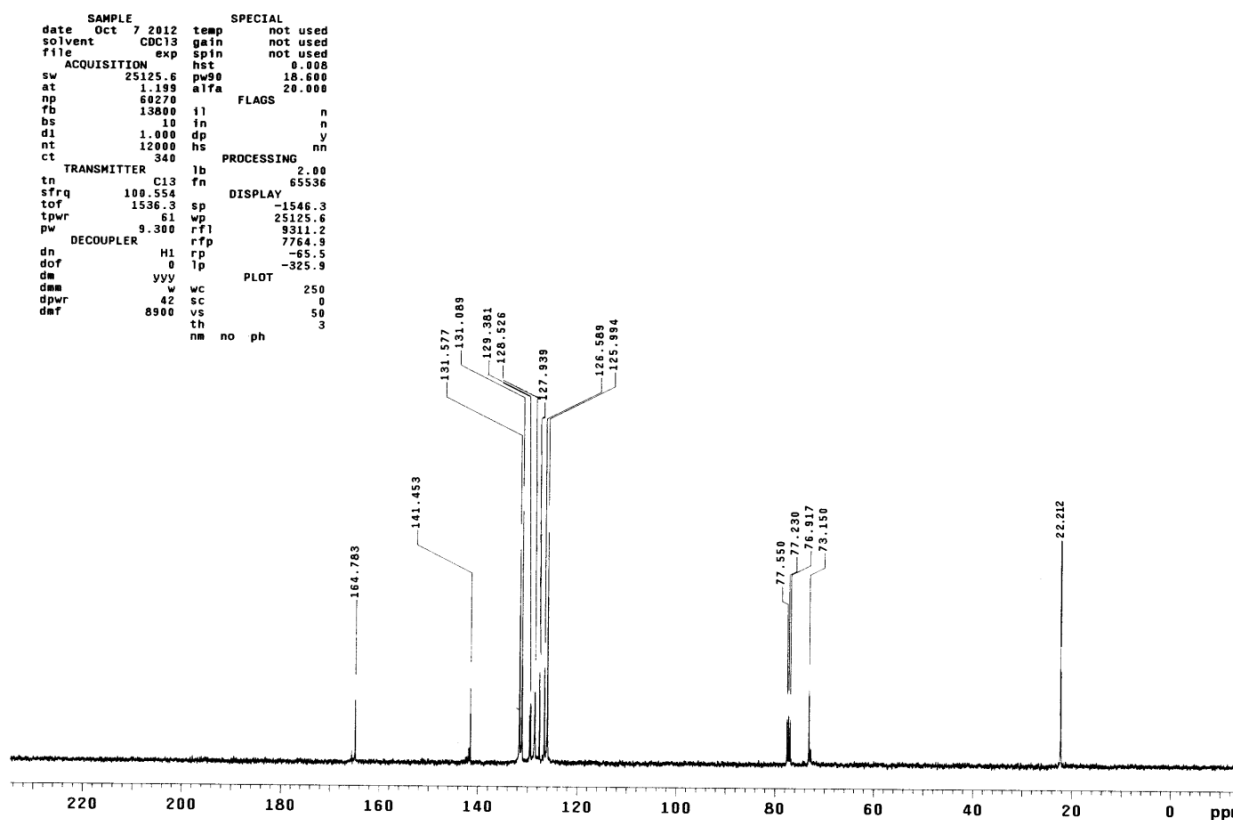
### 1-Phenylethyl 4-chlorobenzoate (dk): HRMS



### 1-Phenylethyl 4-bromobenzoate (ek): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

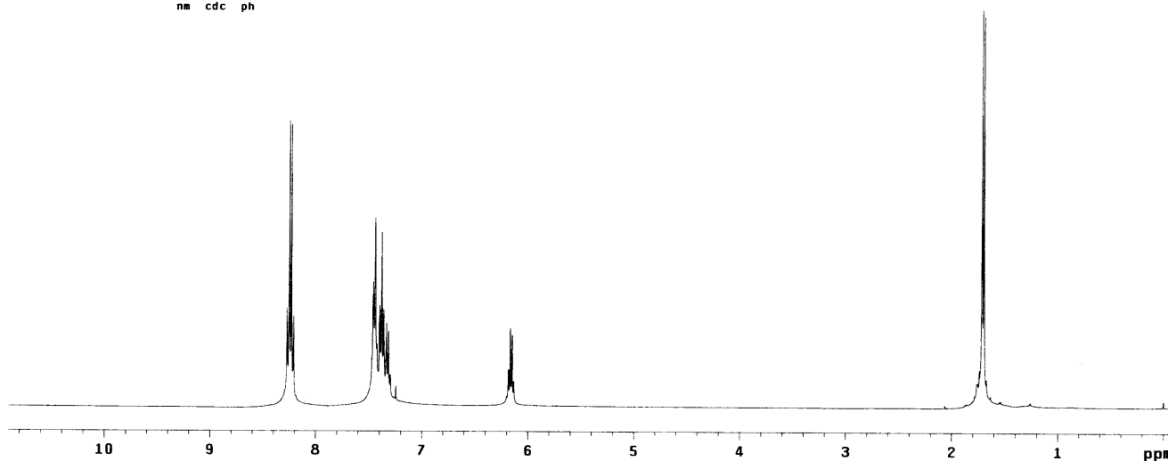


### 1-Phenylethyl 4-bromobenzoate (ek): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



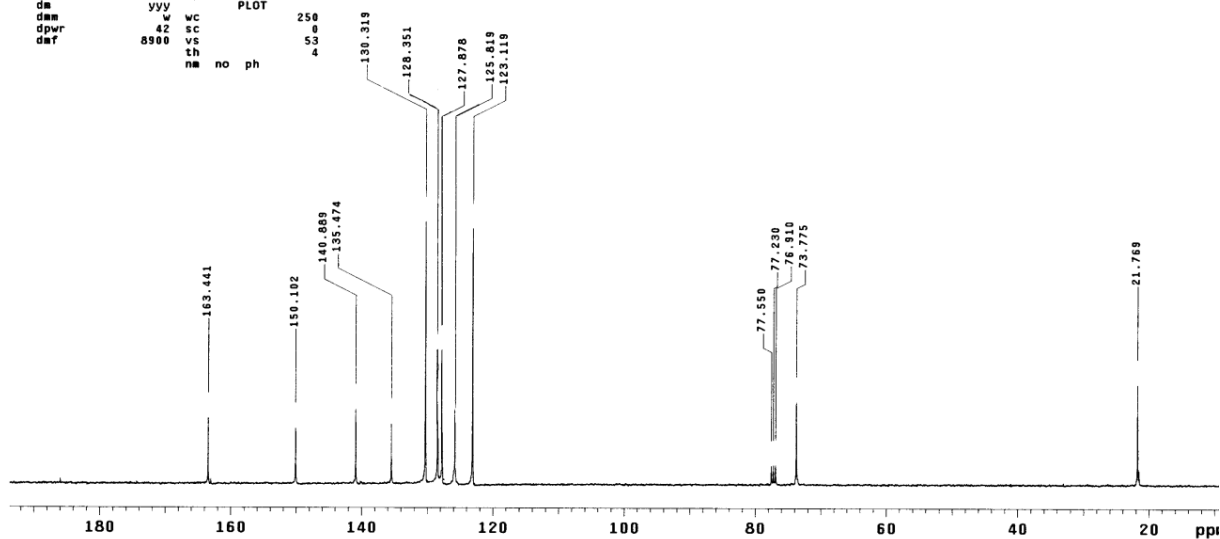
### 1-Phenylethyl 4-nitrobenzoate (fk): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

```
solvent CDCl3 gain not used
file ACQUISITION exp spin not used
sw 6389.8 pw90 19.700
at 1.998 alfa 20.000
np 25528
fb not used f1 FLAGS n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -53.0
tpwr 57 wp 4412.4
pw 9.850 rf1 800.5
DECOUPLER rfp 0
dn C13 rp 114.0
dof 0 lp -89.1
dm nnn PLOT
dmm c wc 250
dpwr 53 sc 0
dfr 15900 vs 85
th 20
nm cdc ph
```



### 1-Phenylethyl 4-nitrobenzoate (fk): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

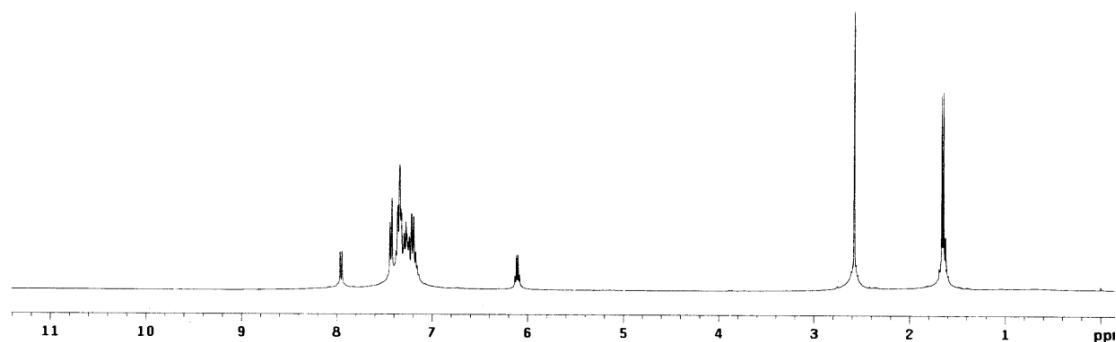
```
SAMPLE SPECIAL
date Oct 6 2012 temp not used
solvent CDCl3 gain not used
file ACQUISITION exp spin not used
sw 25125.6 pw90 18.600
at 1.199 alfa 20.000
np 60270
fb 13800 f1 FLAGS n
bs 10 in n
d1 1.000 dp y
nt 5000 hs nn
ct 230
TRANSMITTER lb 2.80
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp 754.9
tpwr 61 wp 18719.8
pw 9.300 rf1 9321.2
DECOUPLER H1 rfp 7764.9
dn 0 lp -20.2
dof yyy PLOT
dm w wc 250
dmm 42 sc 0
dpwr 8900 vs 53
dfr th 4
nm no ph
```





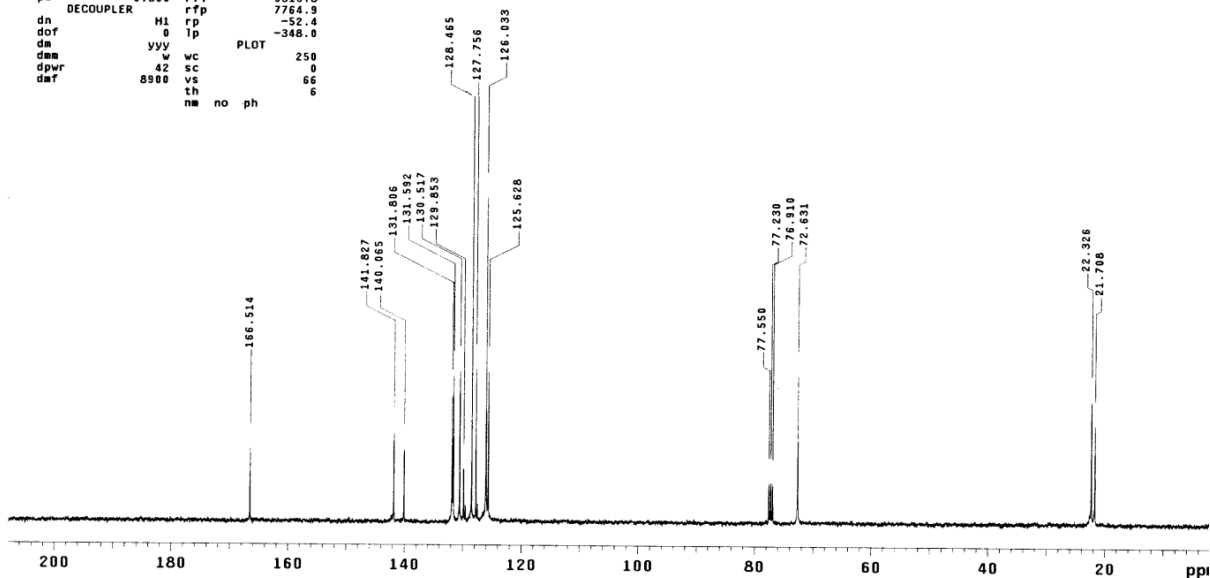
### 1-Phenylethyl 2-methylbenzoate (gk): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

```
SAMPLE          SPECIAL
date Oct 15 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION    hst 0.008
sv 6389.8 pw90 19.700
at 1.198 alfa 20.000
np 25528          FLAGS
fb not used      fl n
bs 4             in n
dl 1.000         dp y
nt 32           hs nn
ct 32           PROCESSING
tn TRANSMITTER  lb 0.10
tr H1          fn 65536
sfrq 399.853   sp DISPLAY
tof 362.8     sp -106.3
tpwr 57      wp 4668.5
pw 9.850    rfl 819.8
DECOUPLER    C13 rp 0
dn 0        rp 101.4
dof 0       lp -89.0
dm nnn      c PLOT
dam 50      wc 250
dpwr 50     sc 0
dnt 15900  vs 112
          th 17
          nm cdc ph
```

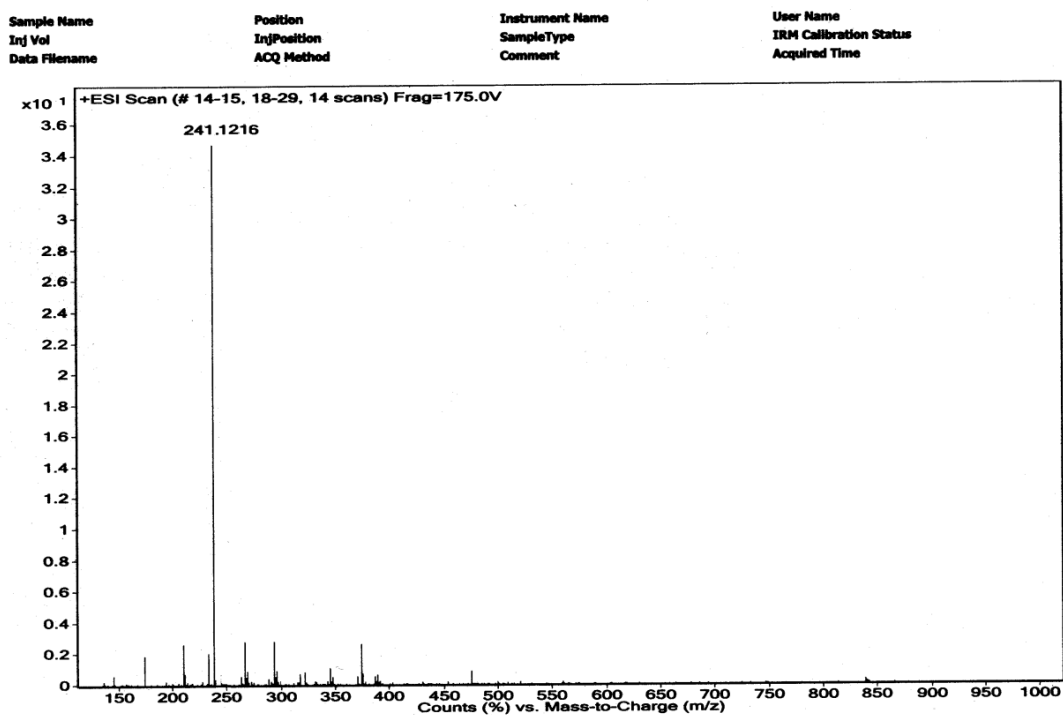


### 1-Phenylethyl 2-methylbenzoate (gk): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

```
SAMPLE          SPECIAL
date Oct 15 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION    hst 0.008
sv 25125.6 pw90 19.800
at 1.199 alfa 20.000
np 60270        FLAGS
fb 13800        fl n
bs 10          in n
dl 1.000       dp y
nt 5000        hs nn
ct 200         PROCESSING
tn TRANSMITTER  lb 2.00
tr C13         fn 65536
sfrq 100.554   sp DISPLAY
tof 1536.3     sp 0.3
tpwr 61       wp 20899.0
pw 9.300     rfl 9315.8
DECOUPLER    H1 rp 7764.9
dn 0         rp -52.4
dof 0        lp -348.0
dm vvv      w PLOT
dam 42      wc 250
dpwr 42     sc 0
dnt 8900   vs 66
          th 6
          nm no ph
```

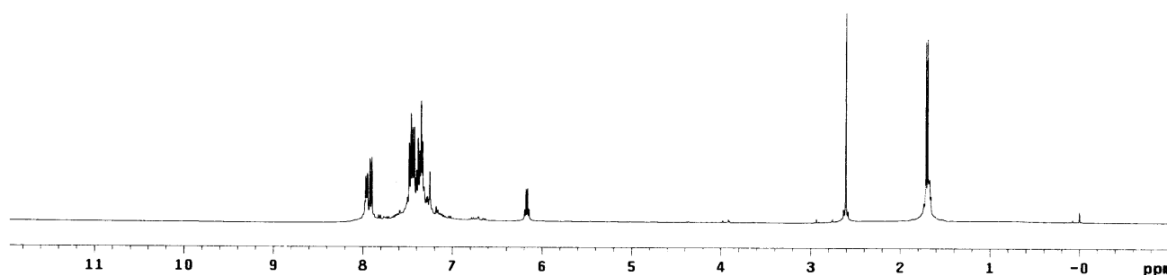


### 1-Phenylethyl 2-methylbenzoate (gk): HRMS



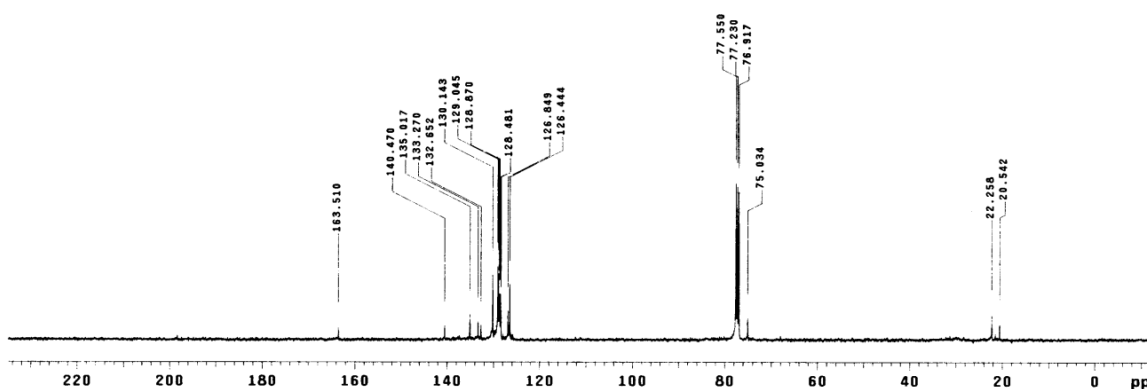
### 1-Phenylethyl 3-methylbenzoate (hk): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

```
SAMPLE          SPECIAL
date Oct 17 2012 temp not used
solvent CDCl3    gain not used
file          exp spin not used
ACQUISITION   hst 0.008
sw 6389.8     pw90 19.700
at 1.998      alfa 20.000
np 25528
fb not used   f1
bs 4          f2
dl 1.000      dp
nt 32         hs
ct
TRANSMITTER    fb 0.10
tn H1         fn 65536
sfrq 399.053  DISPLAY
tof 362.8     sp -436.8
tpwr 57       wp 5214.1
pw 9.850     rf1 797.8
DECOUPLER      rf2 0
dn C13       rp 112.0
dof 0        fd -99.7
da nnn       PLOT
dwa c        wc 250
dpr 50       sc 0
daf 15900    vs 113
                    th 7
                    na cdc ph
```



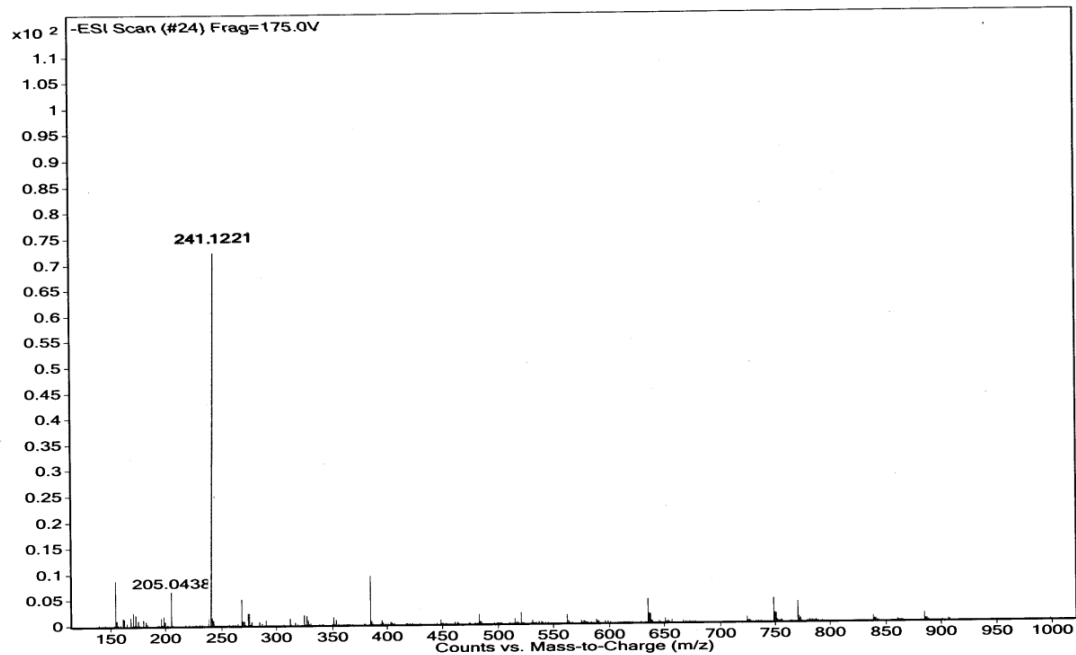
### 1-Phenylethyl 3-methylbenzoate (hk): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

```
date Oct 19 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 25125.6 pps 18.000
at 1.199 a1fa 20.000
np 68270
fb 136000 11 n
bs 10 1n n
d1 1.000 dp y
nt 20000 hs nn
ct 9250
TRANSMITTER 1b PROCESSING 2.00
tn C13 fn DISPLAY 65536
sfrq 100.554
tof 1536.3 sp -1509.5
tpr 61 wp 25125.6
pw 9.300 rfl 8274.4
DECOUPLER rfp 7764.9
dn H1 rp -49.2
dof 0 1p -342.9
dm yyy wc
dmw w wc 250
dwr 42 sc 8
dwt 8900 vs 33
th 2
nm no ph
```

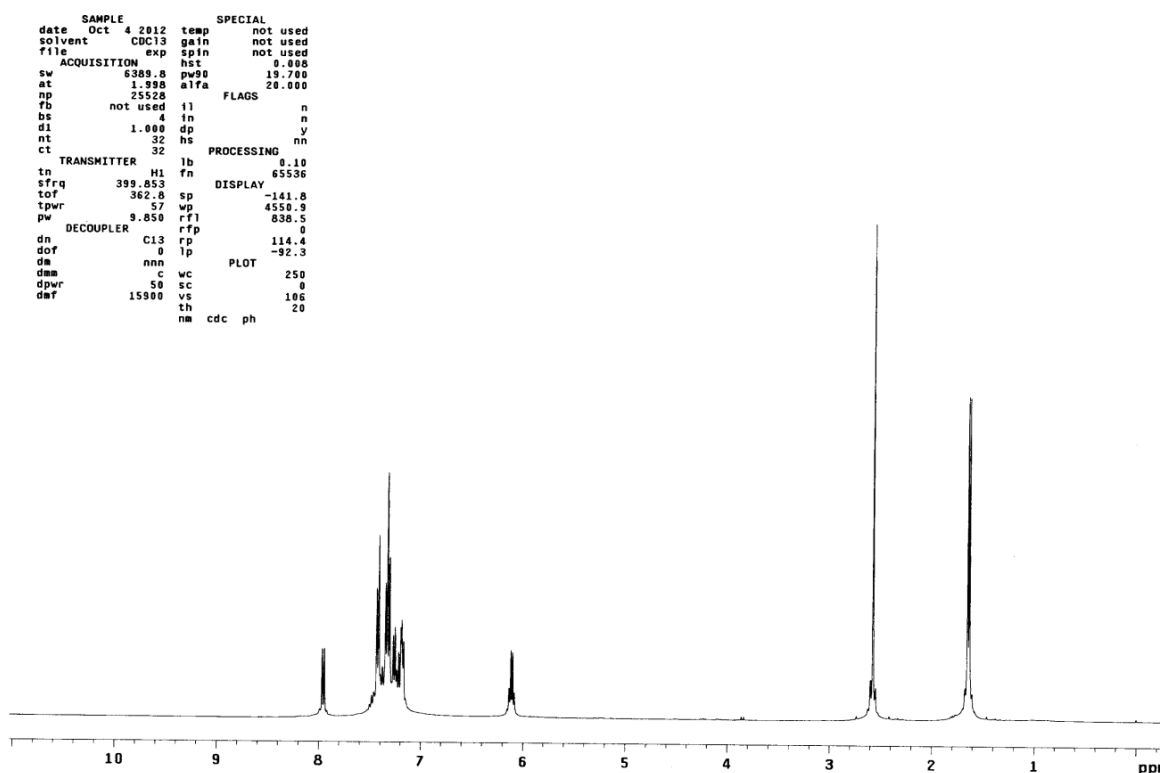


### 1-Phenylethyl 3-methylbenzoate (hk): HRMS

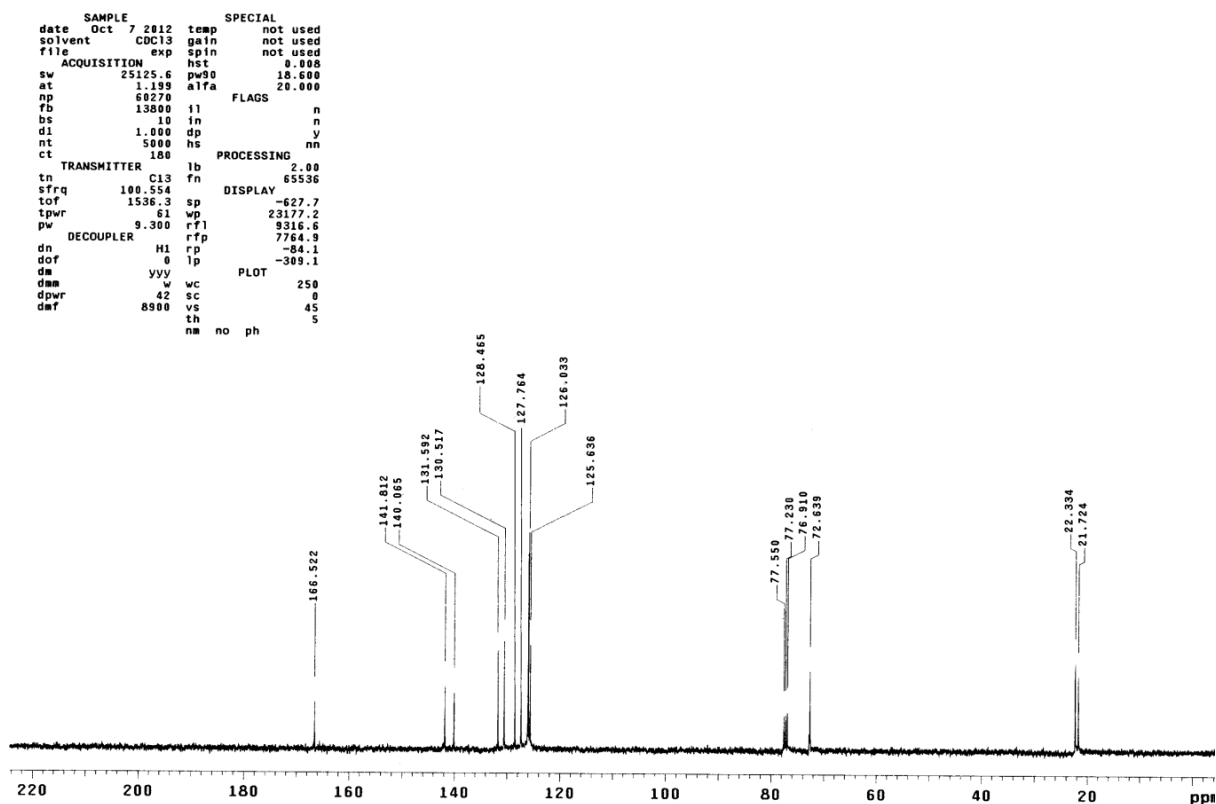
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



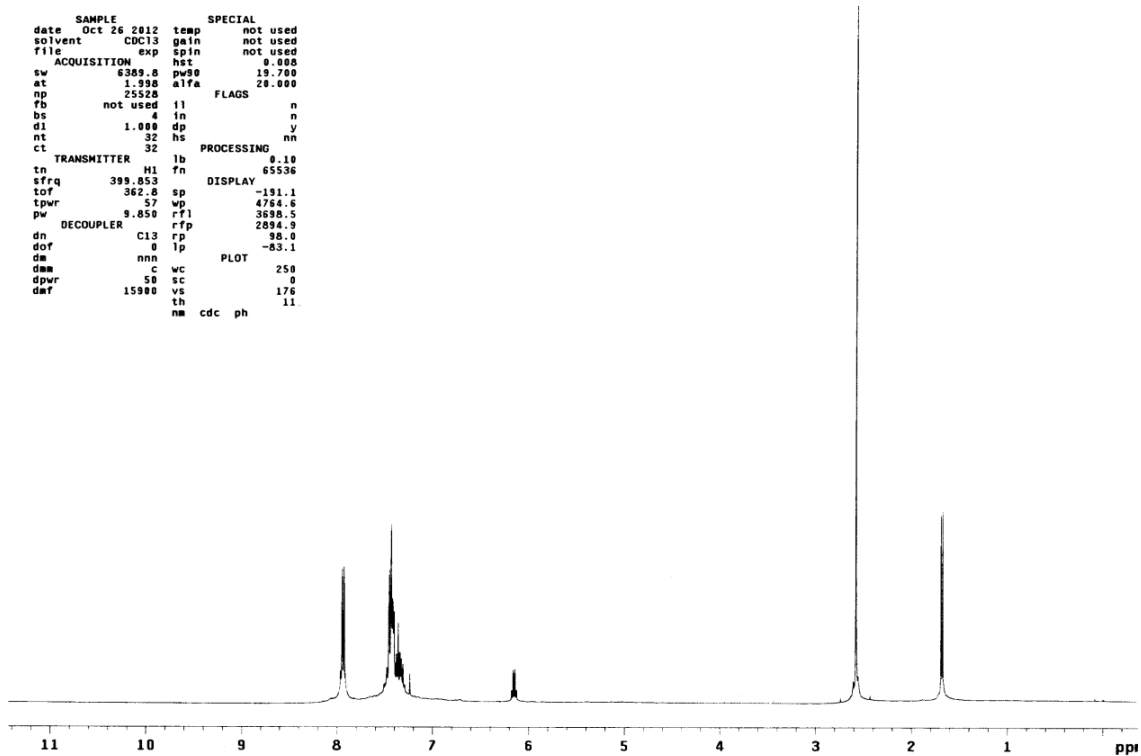
### 1-Phenylethyl 4-methylbenzoate (ik): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



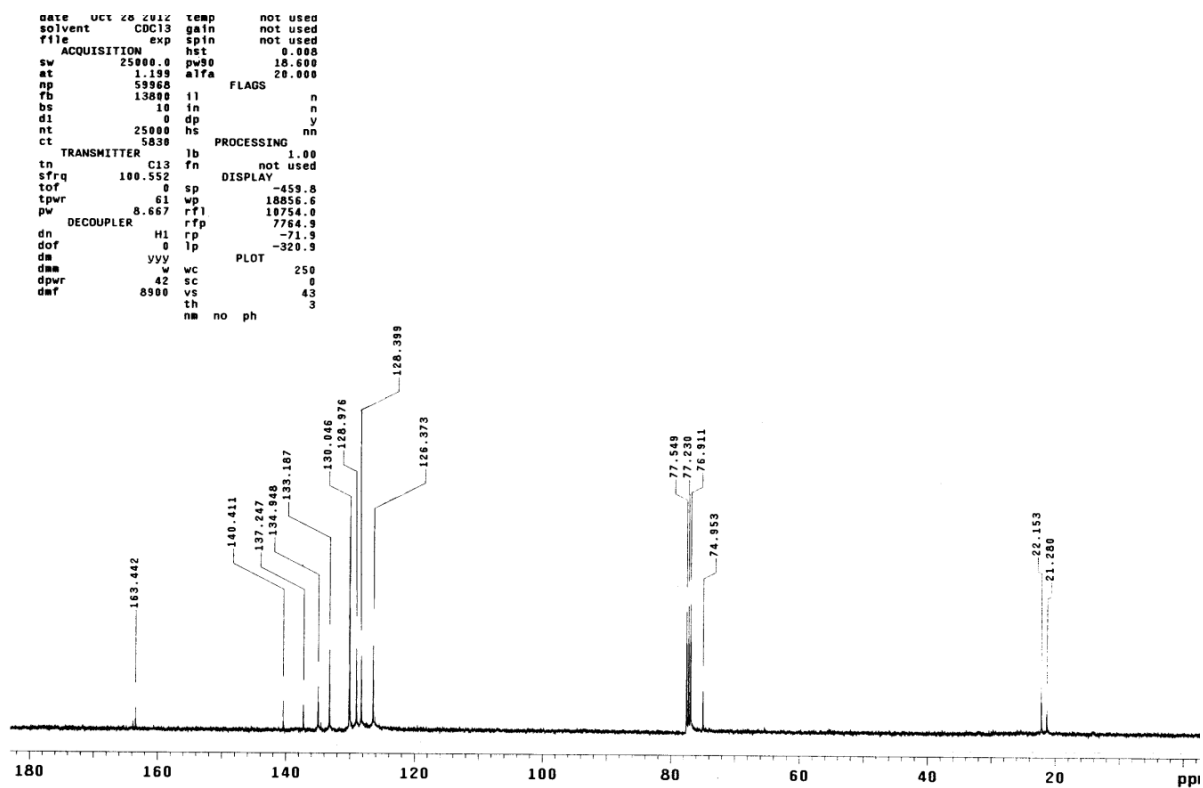
### 1-Phenylethyl 4-methylbenzoate (ik): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)



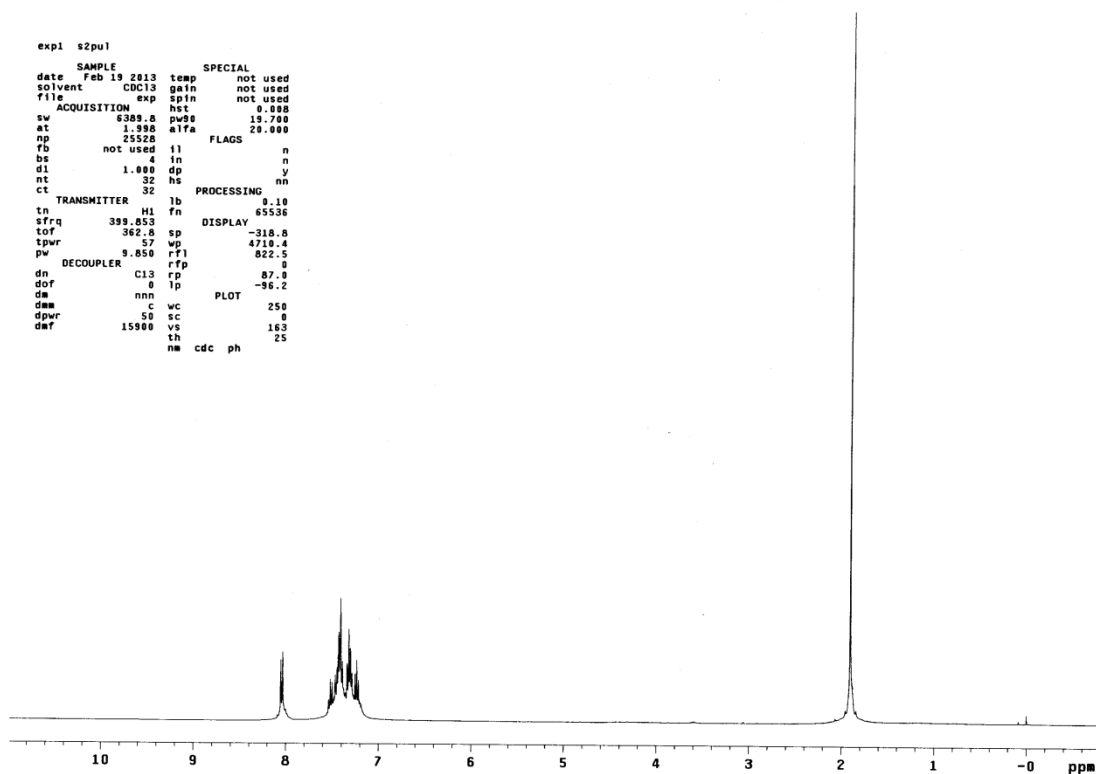
### 1-Phenylethyl 3,5-dimethylbenzoate (jk): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )



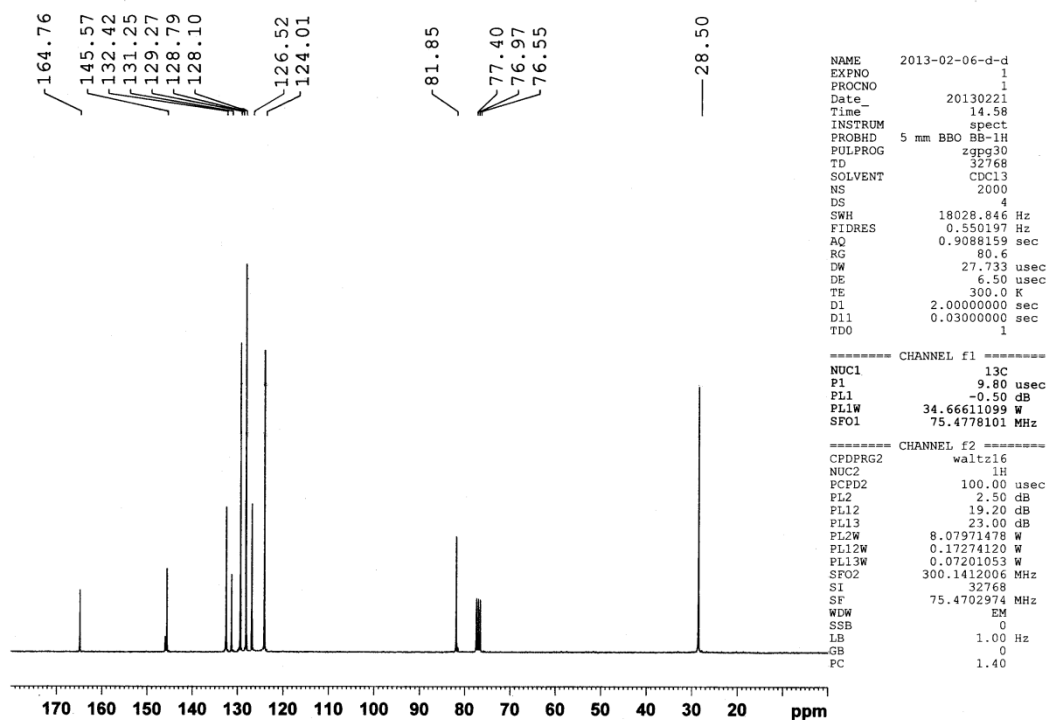
### 1-Phenylethyl 3,5-dimethylbenzoate (jk): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



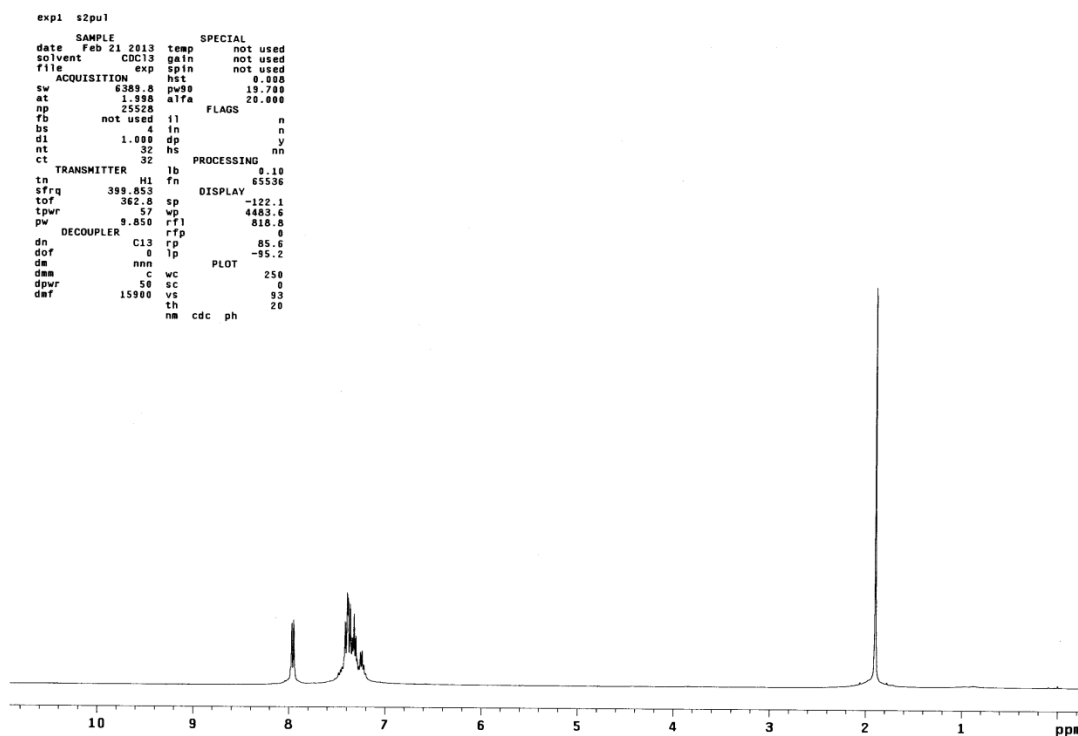
## 2-Phenylpropan-2-yl benzoate (al): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



## 2-Phenylpropan-2-yl benzoate (al): <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



## 2-Phenylpropan-2-yl 4-chlorobenzoate (dl): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



## 2-Phenylpropan-2-yl 4-chlorobenzoate (dl): <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

