

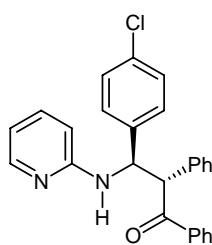
# Supporting Information

## A new mild base-catalyzed Mannich reaction of hetero-arylamines in water: Highly efficient stereoselective synthesis of $\beta$ -aminoketones under microwave heating

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### 3-(4-Chlorophenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4a)



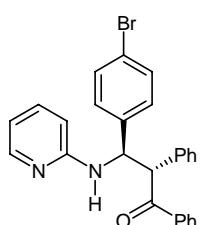
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 7.87-7.83 (m, 3H, ArH, 2H and Py-H, 1H), 7.59 (d, *J* = 8.4 Hz, 2H, ArH), 7.56-7.53 (m, 3H, ArH, 2H and Py-H, 1H), 7.44 (t, *J* = 7.6 Hz, 2H, ArH), 7.29-7.25 (m, 4H, ArH), 7.24-7.15 (m, 2H, Py-H, 1H and ArH, 1H), 6.84 (d, *J* = 9.6 Hz, 1H, NH), 6.39-6.36 (m, 1H, Py-H), 6.33 (d, *J* = 8.4 Hz, 1H, ArH), 5.79 (t, *J* = 10.4 Hz, 1H, NCH), 5.48 (d, *J* = 11.2 Hz, 1H, CH).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.9, 157.6, 147.4, 142.3, 136.7, 136.0, 133.4, 131.2, 129.7, 128.9, 128.5, 128.1, 127.8, 127.2, 112.0, 107.9, 57.5, 55.8.

IR (KBr, *v*, cm<sup>-1</sup>): 3393, 3026, 1662, 1598, 1490, 1148, 1289, 1217, 1091, 815, 700.

HRMS (ESI): m/z calcd for: 413.1416 [M+H]<sup>+</sup>, found: 413.1419.

### 3-(4-Bromophenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4b)



<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 7.87-7.83 (m, 3H, ArH, 2H and Py-H, 1H), 7.58-7.52 (m, 5H, ArH, 4H and Py-H, 1H), 7.45 (d, *J* = 8.0 Hz, 2H, ArH), 7.43-7.40 (m, 2H, ArH), 7.29-7.24 (m, 2H, ArH), 7.22-7.15 (m, 2H, Py-H, 1H and ArH, 1H), 6.83 (d, *J* = 9.6 Hz, 1H, NH), 6.37 (dd, *J*<sub>1</sub> = 5.4 Hz, *J*<sub>2</sub> = 6.6 Hz, 1H, Py-H), 6.33 (d, *J* = 8.4 Hz, 1H, ArH), 5.77 (t, *J* = 10.4 Hz, 1H, NCH), 5.48 (d, *J* = 11.2 Hz, 1H, CH).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.8, 157.6, 147.4, 142.7, 136.7, 136.6, 135.9, 133.5, 130.8, 130.1, 128.9, 128.8, 128.5, 128.1, 127.2, 119.8, 112.0, 108.0, 57.3, 55.8.

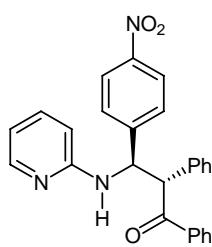
IR (KBr, *v*, cm<sup>-1</sup>): 3388, 3025, 1669, 1598, 1480, 1329, 1289, 1178, 1012, 750, 696.

HRMS (ESI): m/z calcd for: 479.0730 [M+Na]<sup>+</sup>, found: 479.0712.

### 3-(4-Nitrophenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4c)

<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.11 (d, *J* = 8.8 Hz, 2H, ArH), 7.87-7.84 (m, 5H, ArH, 4H and Py-H, 1H), 7.56-7.54 (m, 3H, ArH, 2H and Py-H, 1H), 7.44 (t, *J* = 7.6 Hz, 2H, ArH), 7.29 (t, *J* = 7.6 Hz, 2H, ArH), 7.26-7.17 (m, 2H, Py-H, 1H and ArH, 1H), 6.98 (d, *J* = 9.2 Hz, 1H, NH), 6.41-6.35 (m, 2H, Py-H, 1H and ArH, 1H), 5.93 (t, *J* = 10.4 Hz, 1H, NCH), 5.56 (d, *J* = 11.2 Hz, 1H, CH).

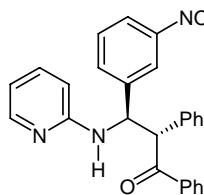
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.6, 157.3, 151.3, 147.4, 146.2, 136.8, 136.3, 135.7, 133.6, 129.2, 128.9, 128.8, 128.6, 128.2, 127.4, 123.1, 112.3, 108.2, 57.2, 56.0.



IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3378, 3025, 1664, 1598, 1520, 1436, 1347, 1281, 1159, 981, 777, 696.

HRMS (ESI): m/z calcd for: 446.1476 [M+H]<sup>+</sup>, found: 446.1464.

### 3-(3-Nitrophenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4d)



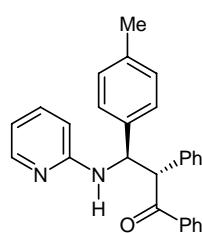
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.52 (s, 1H, ArH), 8.05 (d, *J* = 7.6 Hz, 1H, ArH), 7.96 (dd, *J*<sub>1</sub> = 1.4 Hz, *J*<sub>2</sub> = 8.2 Hz, 1H, ArH), 7.87-7.83 (m, 3H, ArH, 2H and Py-H, 1H), 7.59-7.51 (m, 4H, ArH, 3H and Py-H, 1H), 7.43 (t, *J* = 7.6 Hz, 2H, ArH), 7.29 (t, *J* = 7.6 Hz, 2H, ArH), 7.25-7.13 (m, 3H, ArH, 1H, Py-H, 1H and NH, 1H), 6.40-6.37 (m, 2H, ArH, 1H and Py-H, 1H), 5.91 (t, *J* = 10.4 Hz, 1H, NCH), 5.63 (d, *J* = 10.8 Hz, 1H, CH).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 198.0, 157.4, 147.5, 147.4, 145.8, 136.7, 136.5, 135.9, 135.1, 133.5, 129.3, 128.9, 128.8, 128.5, 128.1, 127.3, 122.5, 121.7, 112.2, 108.3, 57.2, 56.2.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3388, 3063, 1669, 1598, 1530, 1453, 1352, 1291, 767, 697.

HRMS (ESI): m/z calcd for: 446.1476 [M+Na]<sup>+</sup>, found: 446.1489.

### 3-*p*-Tolyl-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4e)

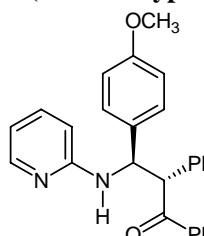


<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 7.86-7.83 (m, 3H, ArH, 2H and Py-H, 1H), 7.56-7.53 (m, 3H, ArH, 2H and Py-H, 1H), 7.45-7.42 (m, 4H, ArH), 7.26 (t, *J* = 7.4 Hz, 2H, ArH), 7.22-7.13 (m, 2H, Py-H, 1H and ArH, 1H), 6.99 (d, *J* = 7.6 Hz, 2H, ArH), 6.73 (d, *J* = 9.2 Hz, 1H, NH), 6.34 (dd, *J*<sub>1</sub> = 5.4 Hz, *J*<sub>2</sub> = 6.6 Hz, 1H, Py-H), 6.30 (d, *J* = 8.4 Hz, 1H, ArH), 5.75 (t, *J* = 10.4 Hz, 1H, NCH), 5.48 (d, *J* = 11.2 Hz, 1H, CH), 2.14 (s, 3H, OCH<sub>3</sub>).

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3385, 1669, 1599, 1514, 1450, 1331, 1287, 771, 745.

HRMS (ESI): m/z calcd for: 393.1962 [M+H]<sup>+</sup>, found: 393.1967.

### 3-(4-Methoxyphenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4f)



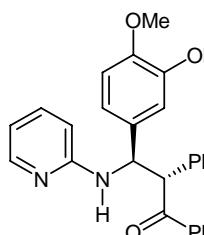
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 7.87-7.83 (m, 3H, ArH, 2H and Py-H, 1H), 7.57-7.53 (m, 3H, ArH, 2H and Py-H, 1H), 7.48 (d, *J* = 8.8 Hz, 2H, ArH), 7.46-7.42 (m, 2H, ArH), 7.28-7.14 (m, 4H, Py-H, 1H and ArH, 3H), 6.76 (d, *J* = 8.8 Hz, 2H, ArH), 6.71 (d, *J* = 10.0 Hz, 1H, NH), 6.35 (dd, *J*<sub>1</sub> = 5.4 Hz, *J*<sub>2</sub> = 6.6 Hz, 1H, Py-H), 6.31 (d, *J* = 8.4 Hz, 1H, ArH), 5.74 (t, *J* = 10.4 Hz, 1H, NCH), 5.47 (d, *J* = 11.2 Hz, 1H, CH), 3.63 (s, 3H, OCH<sub>3</sub>).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 198.0, 157.9, 157.8, 147.4, 137.0, 136.5, 136.2, 135.1, 133.3, 128.8, 128.9, 128.8, 128.4, 128.1, 127.1, 113.2, 111.7, 107.7, 57.8, 55.8, 54.8.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3385, 1667, 1599, 1515, 1450, 1281, 1176, 1031, 761, 695.

HRMS (ESI): m/z calcd for: 409.1911 [M+H]<sup>+</sup>, found: 409.1911.

### 3-(3,4-Dimethoxyphenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4g)



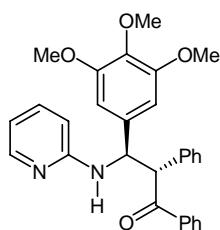
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 7.86 (d, *J* = 8.8 Hz, 3H, ArH, 2H and Py-H, 1H), 7.57-7.54 (m, 3H, ArH, 2H and Py-H, 1H), 7.44 (t, *J* = 7.6 Hz, 2H, ArH), 7.28-7.22 (m, 4H, ArH), 7.15 (t, *J* = 7.4 Hz, Py-H), 7.03 (dd, *J*<sub>1</sub> = 8.2 Hz, *J*<sub>2</sub> = 2.0 Hz, 1H, ArH), 6.74 (d, *J* = 8.0 Hz, 1H, ArH), 6.66 (d, *J* = 9.6 Hz, 1H, NH), 6.36 (dd, *J*<sub>1</sub> = 6.8 Hz, *J*<sub>2</sub> = 5.6 Hz, 1H, Py-H), 6.33 (d, *J* = 8.4 Hz, 1H, ArH), 5.72 (t, *J* = 10.6 Hz, 1H, NCH), 5.51 (d, *J* = 10.8 Hz, 1H, CH), 3.67 (s, 3H, OCH<sub>3</sub>), 3.61 (s, 3H, OCH<sub>3</sub>).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 198.1, 157.8, 148.1, 147.4, 147.3, 137.0, 136.5, 136.3, 135.4, 133.2, 128.8, 128.7, 128.3, 128.0, 127.0, 120.2, 111.7, 111.6, 111.1, 107.6, 57.4, 56.1, 55.4, 55.2.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3388, 1669, 1599, 1487, 1450, 1329, 1289, 1176, 814, 768, 696.

HRMS (ESI): m/z calcd for: 461.1836 [M+Na]<sup>+</sup>, found: 461.1841.

**3-(3,4,5-Trimethoxyphenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4h)**



<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 7.89-7.86 (m, 3H, ArH, 2H and Py-H, 1H), 7.58-7.54 (m, 3H, ArH, 2H and Py-H, 1H), 7.45 (t, *J* = 7.6 Hz, 2H, ArH), 7.16 (t, *J* = 7.2 Hz 1H, Py-H), 6.86 (s, 2H, ArH), 6.70 (d, *J* = 9.6 Hz, 1H, NH), 6.38 (d, *J* = 5.2 Hz, 1H, ArH), 6.36 (dd, *J*<sub>1</sub> = 4.2 Hz, *J*<sub>2</sub> = 5.0 Hz, 1H, Py-H), 5.74 (t, *J* = 10.2 Hz, 1H, NCH), 5.53 (d, *J* = 11.2 Hz, 1H, CH), 3.68 (s, 6H, 2OCH), 3.50 (s, 3H, OCH<sub>3</sub>).

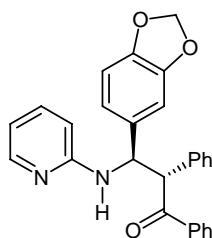
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 198.4, 157.8, 152.3, 147.4, 138.6, 137.0, 136.6, 136.5,

136.2, 133.2, 129.0, 128.7, 128.3, 128.0, 111.8, 107.8, 105.5, 59.8, 57.3, 56.7, 55.9.

IR (KBr, v, cm<sup>-1</sup>): 3382, 2937, 1671, 1595, 1509, 1453, 1324, 1247, 1125, 1008, 705.

HRMS (ESI): m/z calcd for: 469.2122 [M+H]<sup>+</sup>, found: 469.2132.

**3-(Benzo[d][1,3]dioxol-6-yl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4i)**



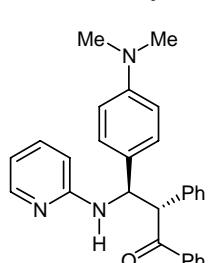
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 7.87-7.85 (m, 3H, ArH, 2H and Py-H, 1H), 7.58-7.52 (m, 3H, ArH, 2H and Py-H, 1H), 7.45 (t, *J* = 7.6 Hz, 2H, ArH), 7.28-7.20 (m, 3H, ArH), 7.17-7.13 (m, 2H, Py-H, 1H and ArH, 1H), 7.00 (dd, *J*<sub>1</sub> = 1.4 Hz, *J*<sub>2</sub> = 8.2 Hz, 1H, ArH), 6.72 (d, *J* = 8.0 Hz, 1H, ArH), 6.67 (d, *J* = 10.0 Hz, 1H, NH), 6.38-6.35 (m, 1H, Py-H), 6.32 (d, *J* = 8.8 Hz, 1H, ArH), 5.87 (d, *J* = 1.2 Hz, 2H, OCH<sub>2</sub>O), 5.71 (t, *J* = 10.4 Hz, 1H, NCH), 5.45 (d, *J* = 10.8 Hz, 1H, CH).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 197.9, 157.7, 147.4, 146.7, 145.7, 137.0, 136.8, 136.6, 136.1, 133.3, 128.8, 128.4, 128.1, 127.1, 121.3, 111.8, 107.9, 107.7, 107.5, 100.6, 57.6, 56.1.

IR (KBr, v, cm<sup>-1</sup>): 3384, 3025, 2968, 1599, 1503, 1487, 1448, 1246, 1040, 930, 749, 696.

HRMS (ESI): m/z calcd for: 423.1704 [M+H]<sup>+</sup>, found: 423.1705.

**3-(4-Dimethylaminophenyl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4j)**



<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 7.85-7.83 (m, 3H, ArH, 2H and Py-H, 1H), 7.56-7.52 (m, 3H, ArH, 2H and Py-H, 1H), 7.44 (t, *J* = 7.6 Hz, 2H, ArH), 7.36 (d, *J* = 8.8 Hz, 2H, ArH), 7.28-7.11 (m, 4H, Py-H, 1H and ArH, 3H), 6.61 (d, *J* = 9.6 Hz, 1H, NH), 6.53 (d, *J* = 8.8 Hz, 2H, ArH), 6.35-6.32 (m, 1H, Py-H), 6.28 (d, *J* = 8.4 Hz, 1H, ArH), 5.66 (t, *J* = 10.4 Hz, 1H, NCH), 5.46 (d, *J* = 10.8 Hz, 1H, CH), 2.76 (s, 6H, NCH<sub>3</sub>).

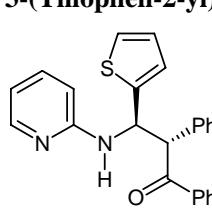
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 197.6, 161.7, 148.6, 147.4, 138.2, 137.2, 136.5, 136.3, 133.2, 131.0, 129.7, 128.8, 128.4, 128.3, 128.1, 127.0, 126.5, 121.0, 119.0, 112.7, 111.8,

111.6, 111.5, 107.6, 57.8, 55.8, 44.7.

IR (KBr, v, cm<sup>-1</sup>): 3379, 3024, 1668, 1599, 1525, 1449, 1331, 1273, 1168, 809, 772, 695.

HRMS (ESI): m/z calcd for: 422.2227 [M+H]<sup>+</sup>, found: 422.2226

**3-(Thiophen-2-yl)-1,2-diphenyl-3-(pyridin-2-ylamino)propan-1-one (4k)**



<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 7.96-7.92 (m, 3H, ArH, 2H and Py-H, 1H), 7.59 (t, *J* = 7.2 Hz, 1H, Py-H), 7.50-7.47 (m, 4H, ArH), 7.25-7.21 (m, 4H, ArH), 7.13 (t, *J* = 7.2 Hz, 1H, Py-H), 7.02 (d, *J* = 3.2 Hz, 1H, thiophen-2-yl-H), 6.82 (dd, *J*<sub>1</sub> = 3.6 Hz, *J*<sub>2</sub> = 5.2 Hz, 2H, thiophen-2-yl-H), 6.40 (dd, *J*<sub>1</sub> = 5.4 Hz, *J*<sub>2</sub> = 6.6 Hz, 1H, Py-H), 6.31 (d, *J* = 8.4 Hz, 1H, NH), 6.25 (t, *J* = 10.4 Hz, 1H, NCH), 5.52 (d, *J* = 11.2 Hz, 1H, CH).

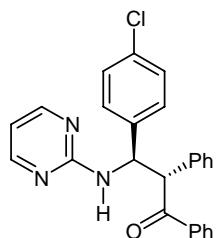
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 197.8, 157.5, 147.3, 147.0, 136.6, 136.4, 136.0, 133.5, 128.9, 128.8, 128.4,

128.2, 127.2, 126.3, 124.7, 124.1, 112.0, 108.3, 58.0, 51.2.

IR (KBr, v, cm<sup>-1</sup>): 3371, 1671, 1598, 1514, 1451, 1330, 1287, 1157, 772, 698.

HRMS (ESI): m/z calcd for: 407.1189 [M+Na]<sup>+</sup>, found: 407.1171.

### **3-(4-Chlorophenyl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4l)**

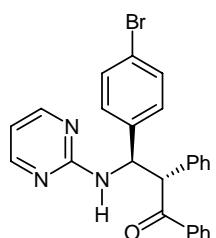


<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 8.15 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.83-7.81 (m, 2H, ArH), 7.61-7.53 (m, 6H, ArH, 5H and NH, 1H), 7.45 (t, *J* = 7.6 Hz, 2H, ArH), 7.30-7.25 (m, 4H, ArH), 7.16 (t, *J* = 7.4 Hz, 1H, Pyrimidine-H), 6.46 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.86 (t, *J* = 10.6 Hz, 1H, NCH), 5.56 (d, *J* = 11.2 Hz, 1H, CH).  
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 197.7, 161.3, 157.7, 141.8, 136.4, 135.9, 133.5, 131.3, 129.7, 128.9, 128.8, 128.5, 128.0, 127.9, 127.3, 110.3, 56.8, 55.9.

IR (KBr, v, cm<sup>-1</sup>): 3399, 3025, 1666, 1586, 1519, 1450, 1539, 1219, 1089, 798, 696.

HRMS (ESI): m/z calcd for: 436.1188 [M+Na]<sup>+</sup>, found: 436.1189.

### **3-(4-Bromophenyl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4m)**

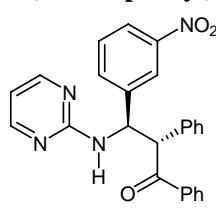


<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 8.15 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.83 (d, *J* = 7.6 Hz, 2H, ArH), 7.61-7.53 (m, 6H, ArH, 5H and NH, 1H), 7.47-7.42 (m, 4H, ArH), 7.27 (t, *J* = 7.6 Hz, 2H, ArH), 7.17 (t, *J* = 7.4 Hz, 1H, Pyrimidine-H), 6.47 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.83 (t, *J* = 10.4 Hz, 1H, NCH), 5.58 (d, *J* = 11.2 Hz, 1H, CH).  
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 197.7, 161.3, 157.7, 142.3, 136.4, 135.9, 133.5, 130.8, 130.1, 128.9, 128.8, 128.5, 128.0, 127.3, 119.9, 110.3, 56.7, 56.0.

IR (KBr, v, cm<sup>-1</sup>): 3389, 3026, 1670, 1585, 1519, 1449, 1359, 1287, 1218, 1072, 1012, 799, 696.

HRMS (ESI): m/z calcd for: 480.0682 [M+Na]<sup>+</sup>, found: 480.0688

### **3-(3-Nitrophenyl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4n)**

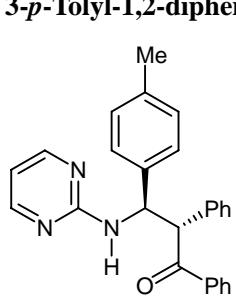


<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 8.56 (s, 1H, ArH), 8.17 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 8.02 (d, *J* = 7.6 Hz, 1H, ArH), 7.99 (dd, *J*<sub>1</sub> = 2.0, *J*<sub>2</sub> = 8.0 Hz, 1H, ArH), 7.83 (d, *J* = 7.2 Hz, 2H, ArH), 7.71 (d, *J* = 9.6 Hz, 1H, NH), 7.58-7.53 (m, 4H, ArH, 3H and Pyrimidine-H, 1H), 7.44 (t, *J* = 7.8 Hz, 2H, ArH), 7.30 (t, *J* = 7.6 Hz, 2H, ArH), 7.19 (t, *J* = 7.2 Hz, 1H, Pyrimidine-H), 6.49 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.95 (t, *J* = 10.6 Hz, 1H, NCH), 5.66 (d, *J* = 11.2 Hz, 1H, CH).  
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 197.6, 161.2, 157.9, 157.8, 147.6, 145.1, 136.2, 135.7, 135.1, 133.7, 129.5, 128.9, 128.8, 128.7, 128.1, 127.5, 122.3, 122.0, 110.7, 56.8, 56.2.

IR (KBr, v, cm<sup>-1</sup>): 3384, 3025, 1672, 1586, 1455, 1412, 1353, 1200, 1030, 984, 696.

HRMS (ESI): m/z calcd for: 425.1609 [M+H]<sup>+</sup>, found: 425.1618.

### **3-p-Tolyl-1,2-diphenyl-3-(pyrimidin-2-ylamino)-propan-1-one (4o)**

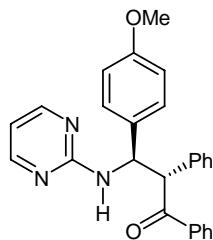


<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>) δ: 8.14 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.83 (d, *J* = 7.2 Hz, 2H, ArH), 7.57-7.43 (m, 8H, ArH, 7H and NH, 1H), 7.26 (t, *J* = 7.6 Hz, 2H, ArH), 7.15 (t, *J* = 7.4 Hz, 1H, Pyrimidine-H), 7.01 (d, *J* = 8.0 Hz, 2H, ArH), 6.43 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.86 (t, *J* = 10.4 Hz, 1H, NCH), 5.57 (d, *J* = 11.2 Hz, 1H, CH), 2.15 (s, 3H, CH<sub>3</sub>).  
<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>) δ: 197.8, 161.5, 157.7, 139.9, 136.8, 136.1, 135.8, 133.4, 128.9, 128.8, 128.5, 128.4, 128.0, 127.7, 110.1, 56.9, 56.1, 20.6.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3387, 3025, 1673, 1587, 1524, 1453, 1409, 1631, 1271, 1121, 1069, 985, 800, 695.

HRMS (ESI): m/z calcd for: 394.1914 [M+H]<sup>+</sup>, found: 394.1911.

### 3-(4-Methoxyphenyl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4p)



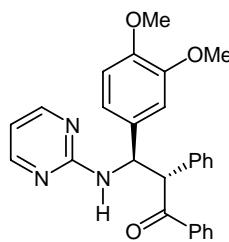
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.20 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.82 (d, *J* = 7.6 Hz, 2H, ArH), 7.57-7.43 (m, 8H, ArH, 7H and NH, 1H), 7.26 (t, *J* = 7.6 Hz, 2H, ArH), 7.15 (t, *J* = 7.6 Hz, 1H, Pyrimidine-H), 6.77 (d, *J* = 8.4 Hz, 2H, ArH), 6.43 (t, *J* = 4.6 Hz, 1H, Pyrimidine-H), 5.85 (t, *J* = 10.6 Hz, 1H, NCH), 5.51 (d, *J* = 11.2 Hz, 1H, CH), 3.63 (s, 3H, OCH<sub>3</sub>).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.9, 161.4, 157.9, 157.7, 136.8, 136.1, 134.9, 133.4, 128.9, 128.8, 128.4, 128.0, 127.2, 113.3, 110.1, 57.1, 55.8, 54.8.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3387, 2952, 1673, 1585, 1515, 1454, 1360, 1247, 1177, 1032, 801, 696.

HRMS (ESI): m/z calcd for: 432.1683 [M+Na]<sup>+</sup>, found: 432.1678.

### 3-(3,4-Dimethoxyphenyl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4q)



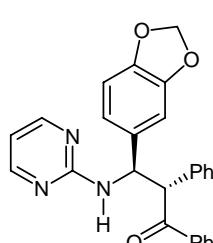
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.15 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.85 (d, *J* = 7.6 Hz, 2H, ArH), 7.58-7.42 (m, 6H, ArH, 5H and NH, 1H), 7.28-7.24 (m, 3H, ArH), 7.17-7.13 (m, 1H, Pyrimidine-H), 7.02 (d, *J* = 8.0 Hz, 1H, ArH), 6.76 (d, *J* = 8.4 Hz, 1H, ArH), 6.44 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.86 (t, *J* = 10.4 Hz, 1H, NCH), 5.59 (d, *J* = 11.2 Hz, 1H, CH), 3.68 (s, 3H, OCH<sub>3</sub>), 3.62 (s, 3H, OCH<sub>3</sub>).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.9, 161.4, 157.7, 157.6, 146.8, 145.8, 136.7, 136.6, 136.1,

696.

HRMS (ESI): m/z calcd for: 462.1789 [M+Na]<sup>+</sup>, found: 462.1794.

### 3-(Benzo[d][1,3]dioxol-6-yl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4r)



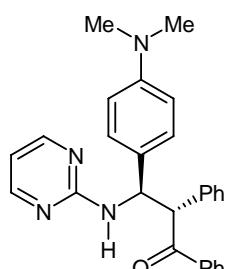
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.15 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.85-7.83 (m, 2H, ArH), 7.58-7.51 (m, 3H, ArH), 7.46 (t, *J* = 7.6 Hz, 2H, ArH), 7.40 (d, *J* = 10.0 Hz, 1H, NH), 7.25 (t, *J* = 7.6 Hz, 2H, ArH), 7.18 (d, *J* = 1.6 Hz, 1H, ArH), 7.15 (t, *J* = 7.4 Hz, 1H, Pyrimidine-H), 7.01 (dd, *J*<sub>1</sub> = 1.6, *J*<sub>2</sub> = 8.0 Hz, 1H, ArH), 6.73 (d, *J* = 8.0 Hz, 1H, ArH), 6.45 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.87 (d, *J* = 4.0 Hz, 2H, CH<sub>2</sub>), 5.83 (t, *J* = 10.8 Hz, 1H, NCH), 5.52 (d, *J* = 11.6 Hz, 1H, CH).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.8, 161.4, 157.7, 146.8, 145.8, 136.7, 136.6, 136.1, 133.4, 128.8, 128.4, 128.0, 127.1, 121.3, 110.2, 107.9, 107.6, 100.6, 57.0, 56.1.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3386, 3024, 1671, 1589, 1532, 1488, 1366, 1244, 1104, 1040, 923, 797, 696.

HRMS (ESI): m/z calcd for: 424.1656 [M+H]<sup>+</sup>, found: 424.1661.

### 3-(4-Dimethylaminophenyl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4s)



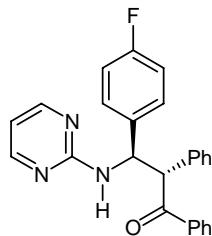
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.13 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.84 (t, *J* = 7.6 Hz, 2H, ArH), 7.57-7.52 (m, 3H, ArH), 7.45 (t, *J* = 7.6 Hz, 2H, ArH), 7.40-7.37 (m, 3H, ArH, 2H and NH, 1H), 7.24 (t, *J* = 7.6 Hz, 2H, ArH), 7.15-7.11 (m, 1H, Pyrimidine-H), 6.55 (d, *J* = 8.8 Hz, 2H, ArH), 6.41 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.81 (t, *J* = 10.8 Hz, 1H, NCH), 5.55 (d, *J* = 11.2 Hz, 1H, CH), 2.76 (s, 6H, NCH<sub>3</sub>).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.9, 161.5, 157.6, 149.2, 137.0, 136.2, 133.3, 130.4, 128.9, 128.8, 128.4, 128.3, 128.0, 127.0, 111.8, 109.9, 62.8, 57.1, 56.7.

IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3383, 3025, 1673, 1585, 1525, 1454, 1358, 1216, 1067, 801, 695.

HRMS (ESI): m/z calcd for: 423.2180 [M+H]<sup>+</sup>, found: 423.2182.

**3-(4-Fluorophenyl)-1,2-diphenyl-3-(pyrimidin-2-ylamino)propan-1-one (4t)**



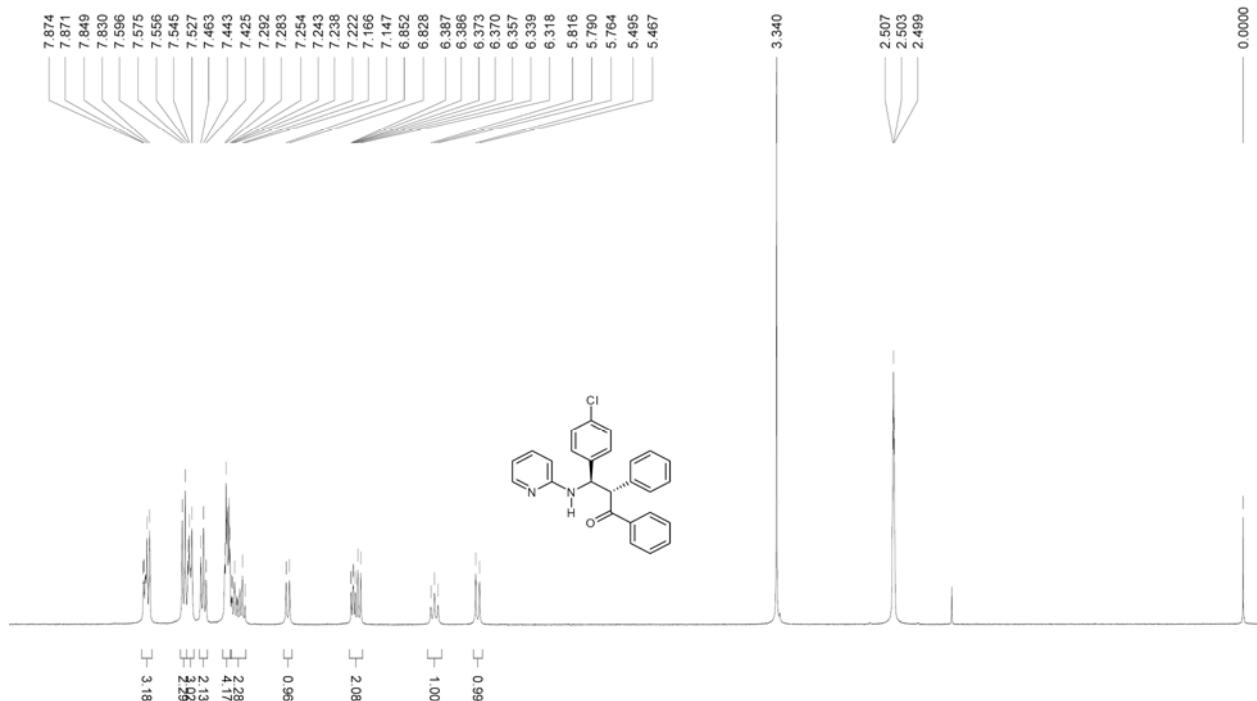
<sup>1</sup>H NMR (400MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.15 (brs, 2H, ArH, 1H and Pyrimidine-H, 1H), 7.82 (d, *J* = 7.2 Hz, 2H, ArH), 7.61 (dd, *J*<sub>1</sub> = 5.6, *J*<sub>2</sub> = 8.8 Hz, 2H, ArH), 7.57-7.53 (m, 4H, ArH, 3H and NH, 1H), 7.44 (t, *J* = 7.8 Hz, 2H, ArH), 7.27 (t, *J* = 7.4 Hz, 2H, ArH), 7.05 (t, *J* = 9.0 Hz, 2H, ArH), 6.46 (t, *J* = 4.8 Hz, 1H, Pyrimidine-H), 5.88 (t, *J* = 10.4 Hz, 1H, NCH), 5.56 (d, *J* = 11.2 Hz, 1H, CH).

<sup>13</sup>C NMR (100MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 197.9, 162.2, 161.4, 159.7, 157.7, 157.6, 139.1, 139.0, 136.6, 136.0, 133.5, 129.8, 129.7, 128.9, 128.8, 128.5, 128.0, 127.3, 114.8, 114.6, 110.3, 57.1, 55.8.

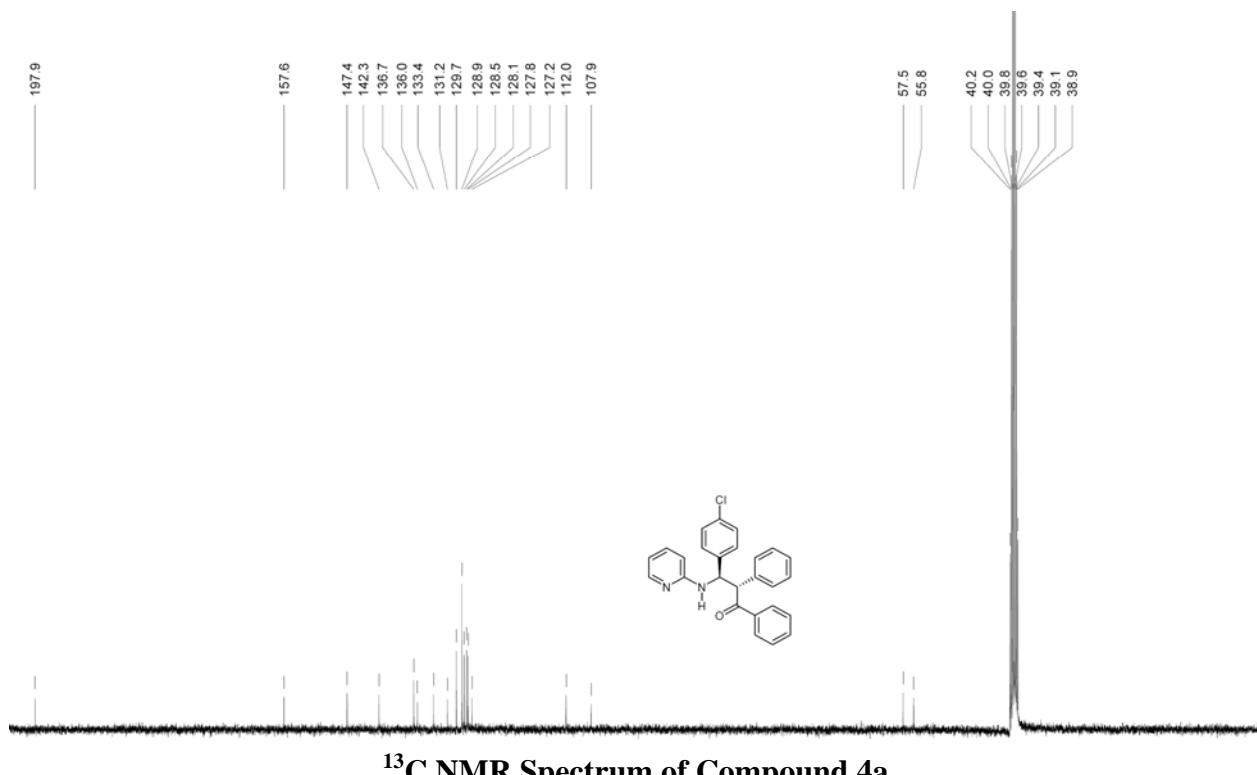
IR (KBr,  $\nu$ , cm<sup>-1</sup>): 3390, 3035, 1666, 1584, 1523, 1451, 1362, 1274, 1158, 1119, 985, 799, 695.

HRMS (ESI): m/z calcd for: 420.1483 [M+H]<sup>+</sup>, found: 420.1500

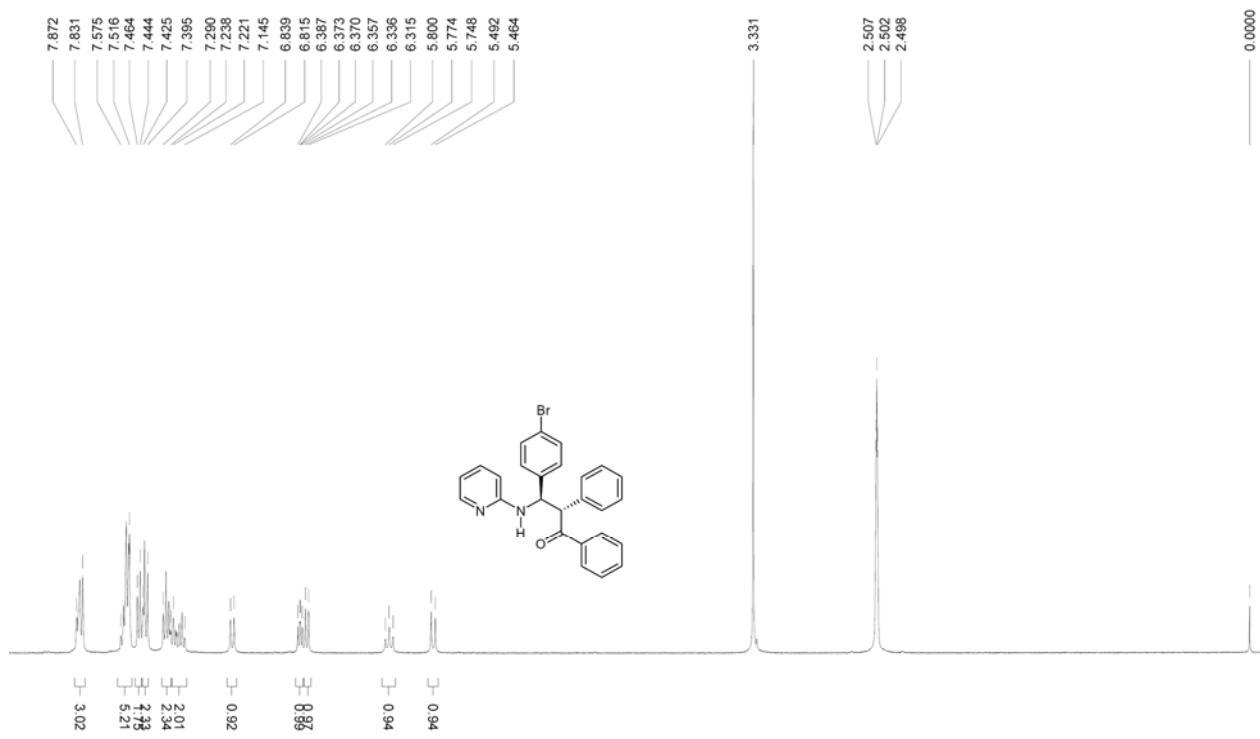
## Copies of spectra for compounds 4



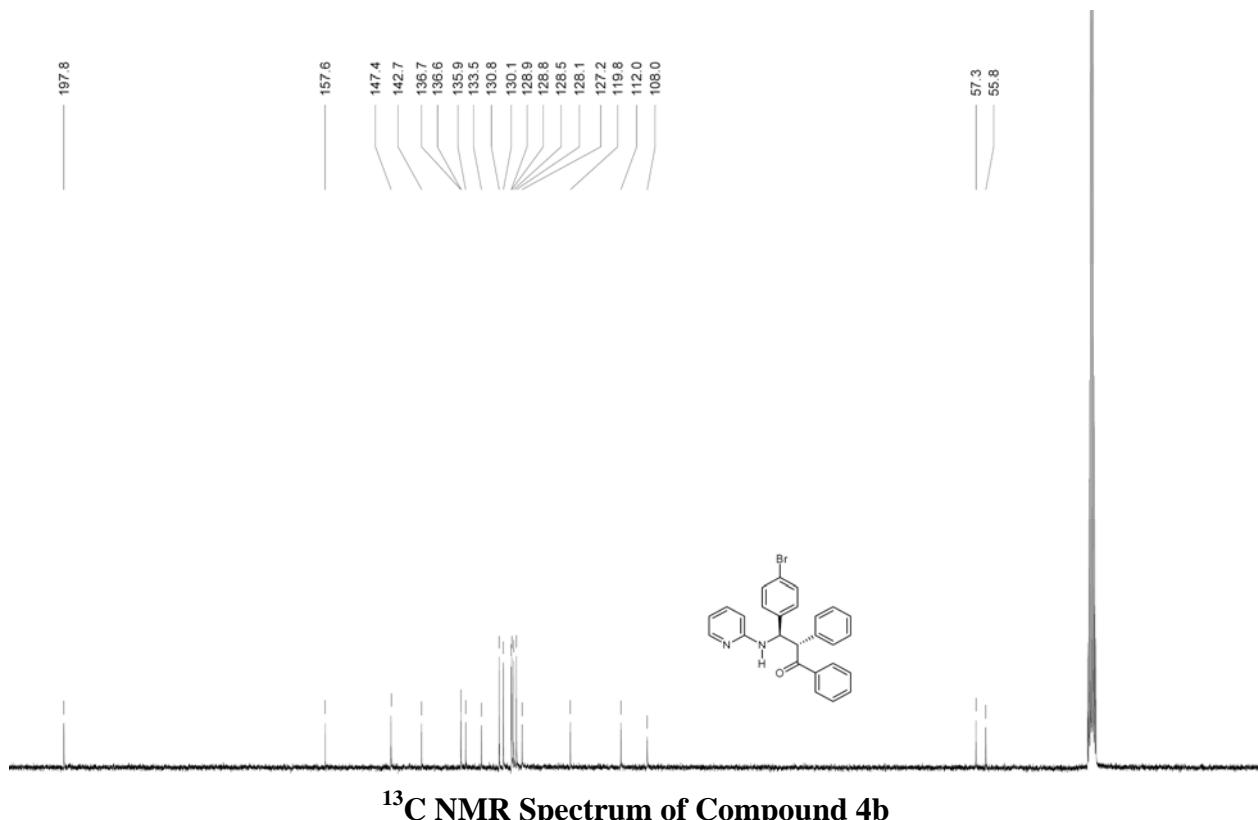
<sup>1</sup>H NMR Spectrum of Compound 4a



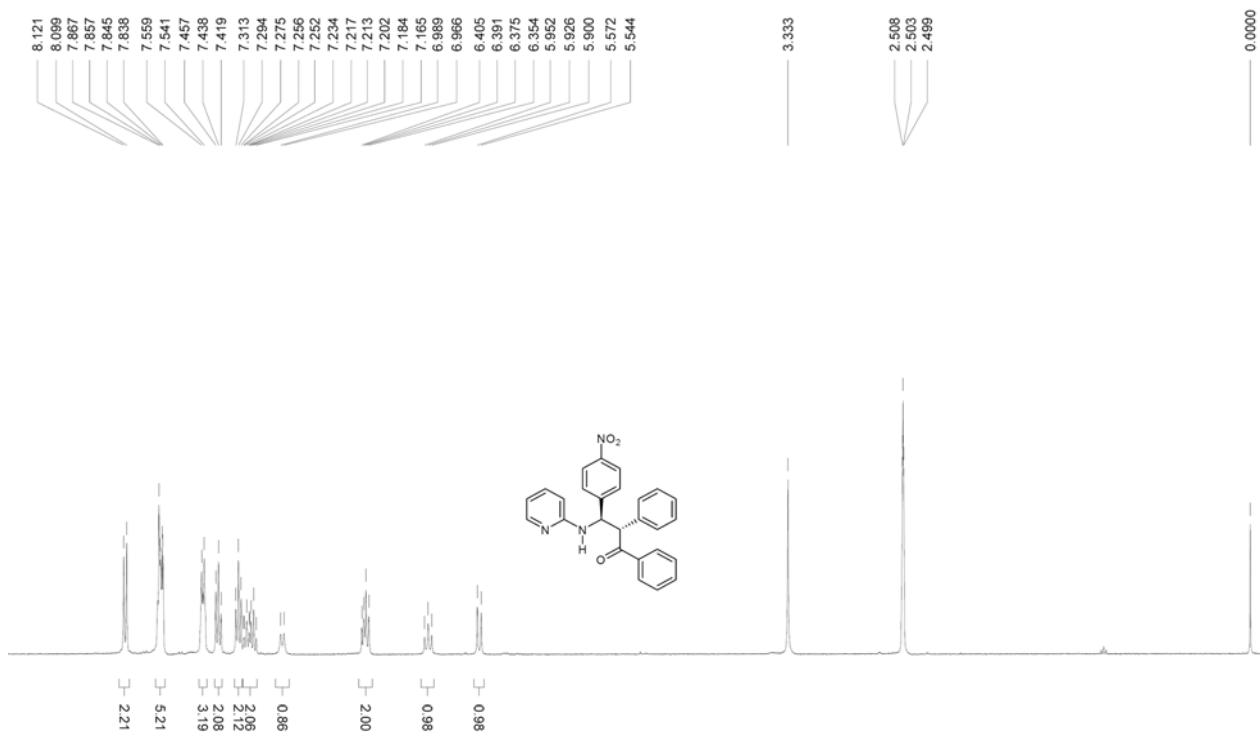
<sup>13</sup>C NMR Spectrum of Compound 4a



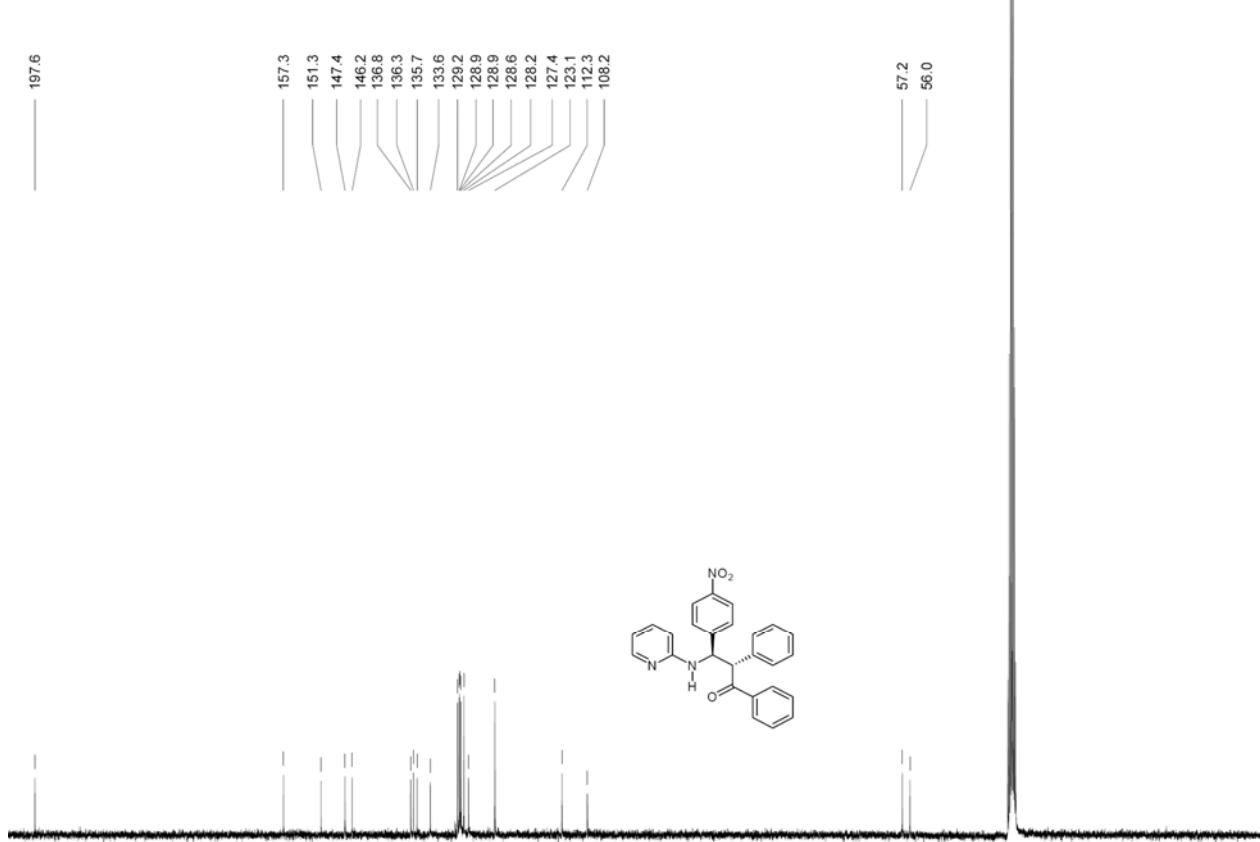
<sup>1</sup>H NMR Spectrum of Compound 4b



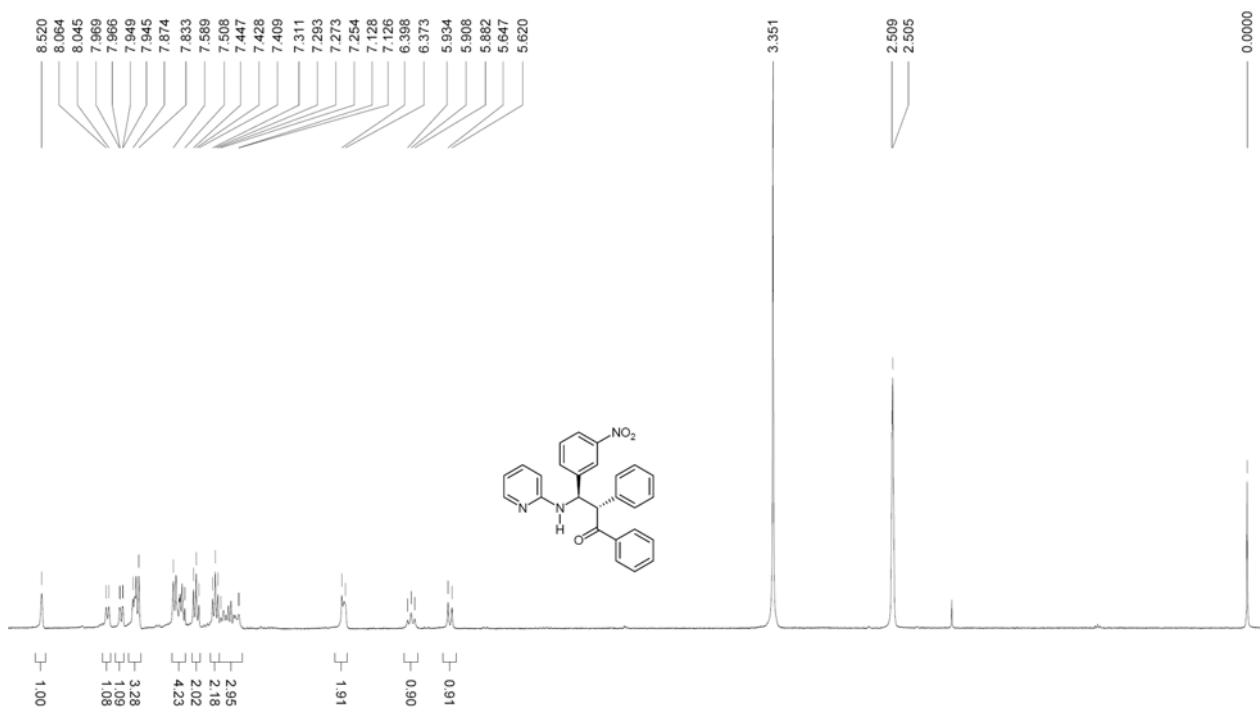
<sup>13</sup>C NMR Spectrum of Compound 4b



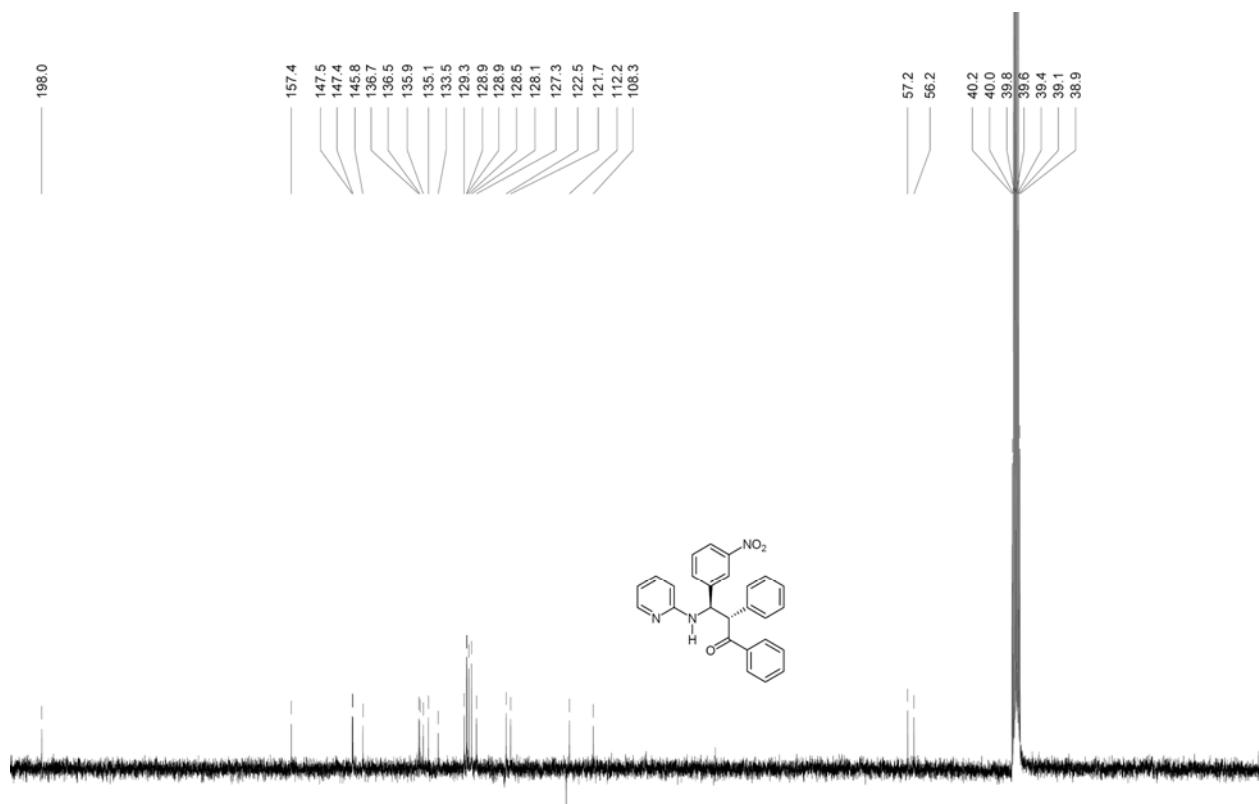
<sup>1</sup>H NMR Spectrum of Compound 4c



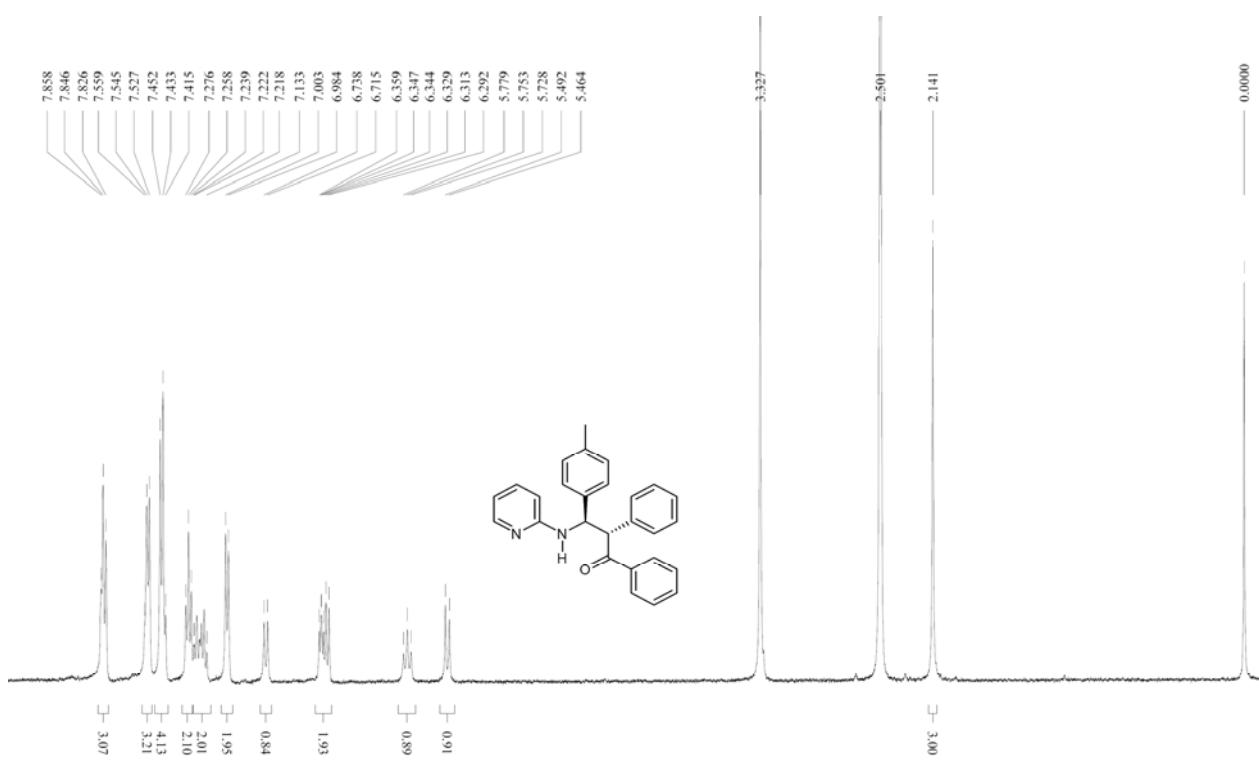
<sup>13</sup>C NMR Spectrum of Compound 4c



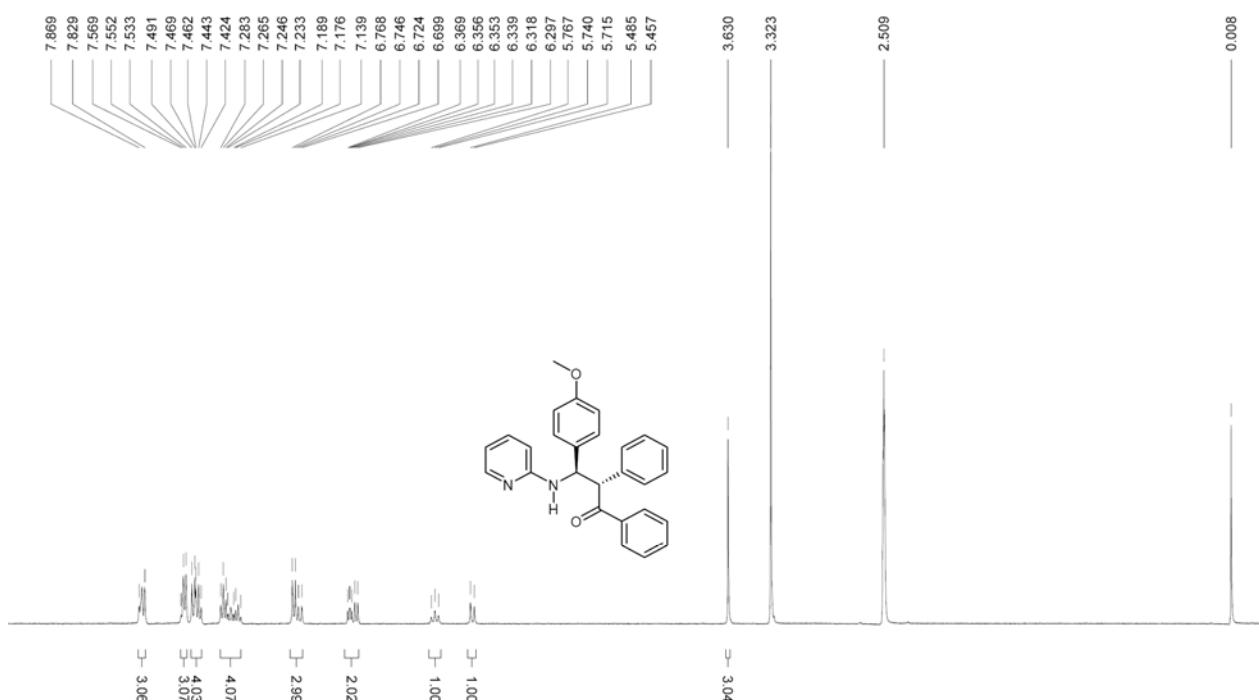
<sup>1</sup>H NMR Spectrum of Compound 4d



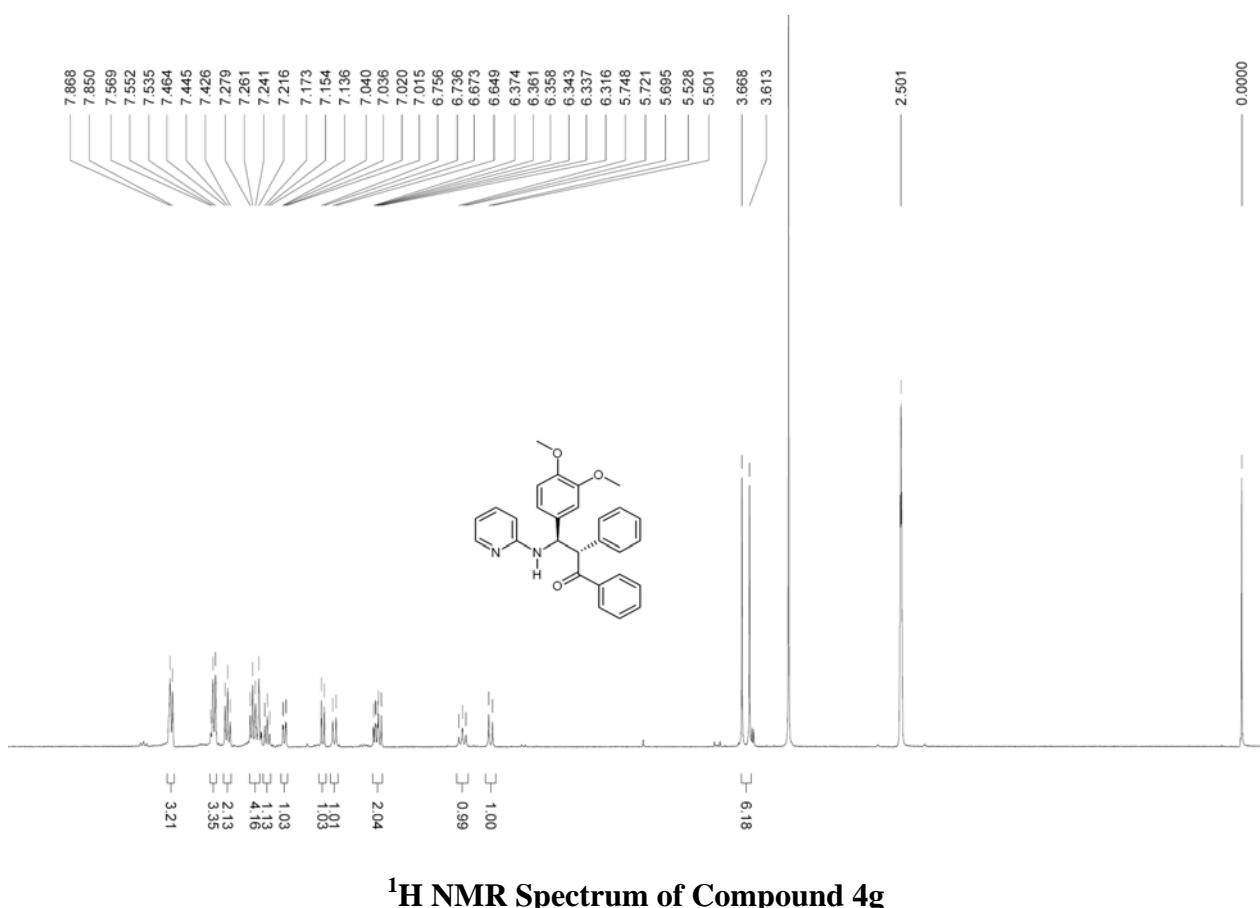
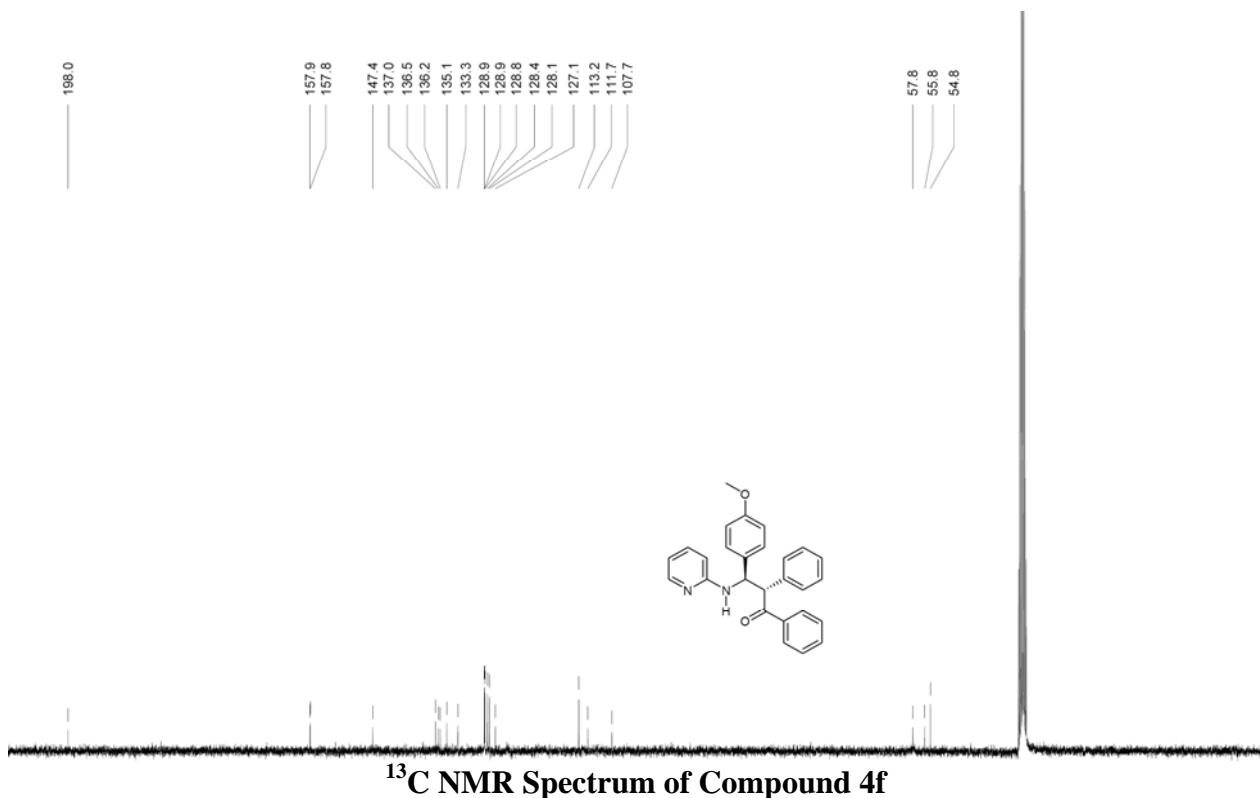
<sup>13</sup>C NMR Spectrum of Compound 4d

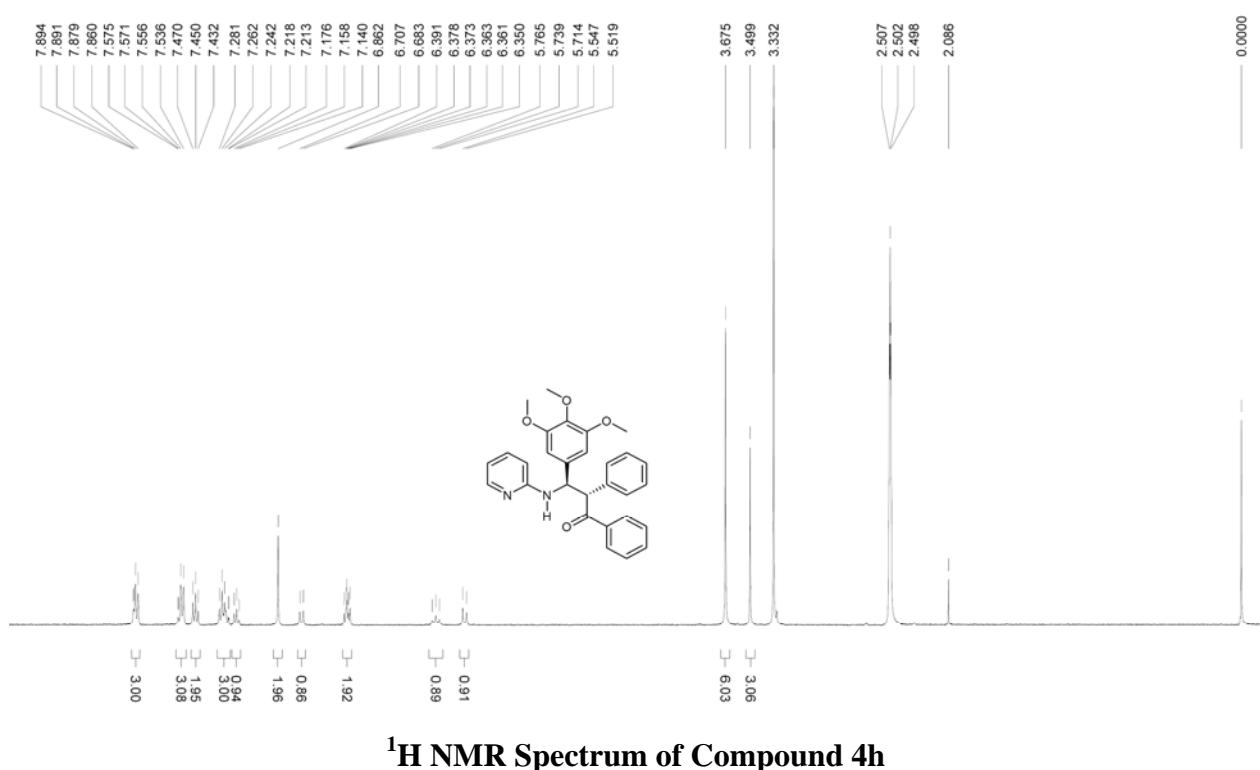
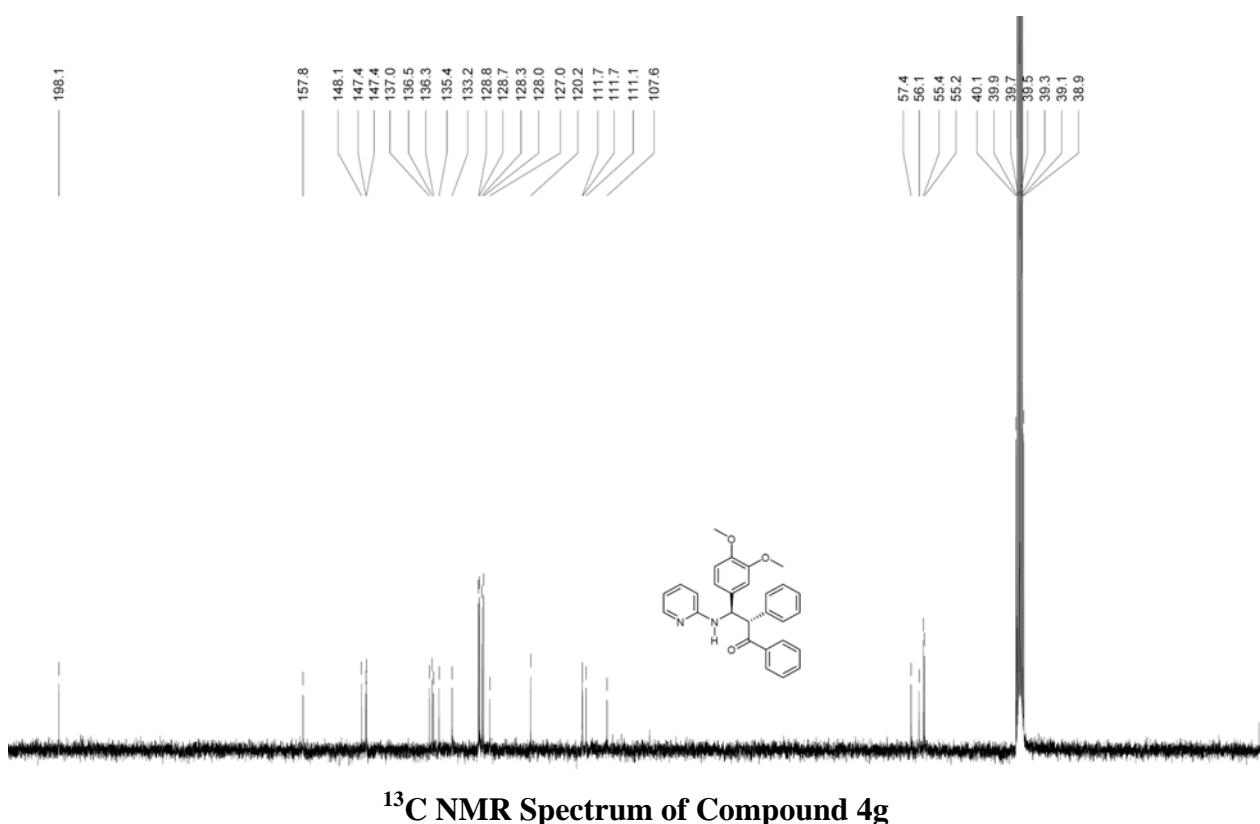


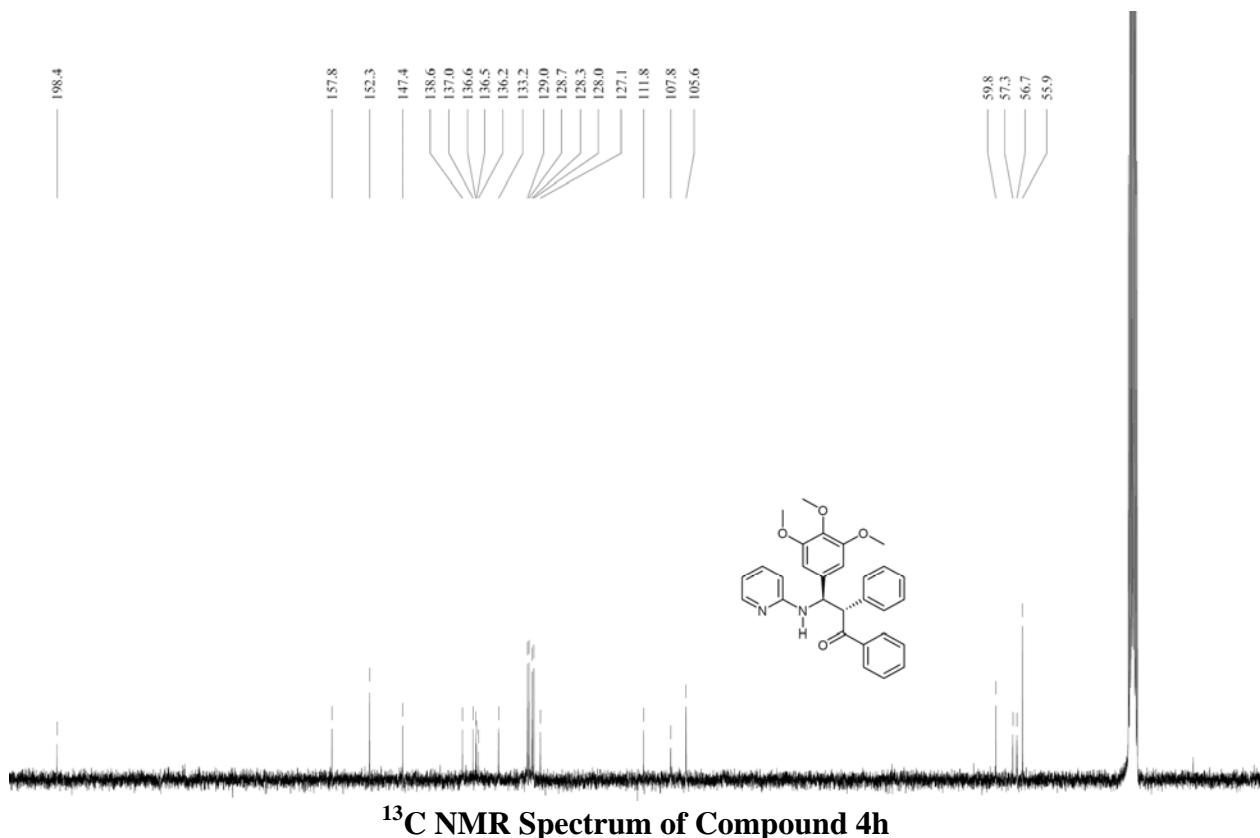
<sup>1</sup>H NMR Spectrum of Compound 4e



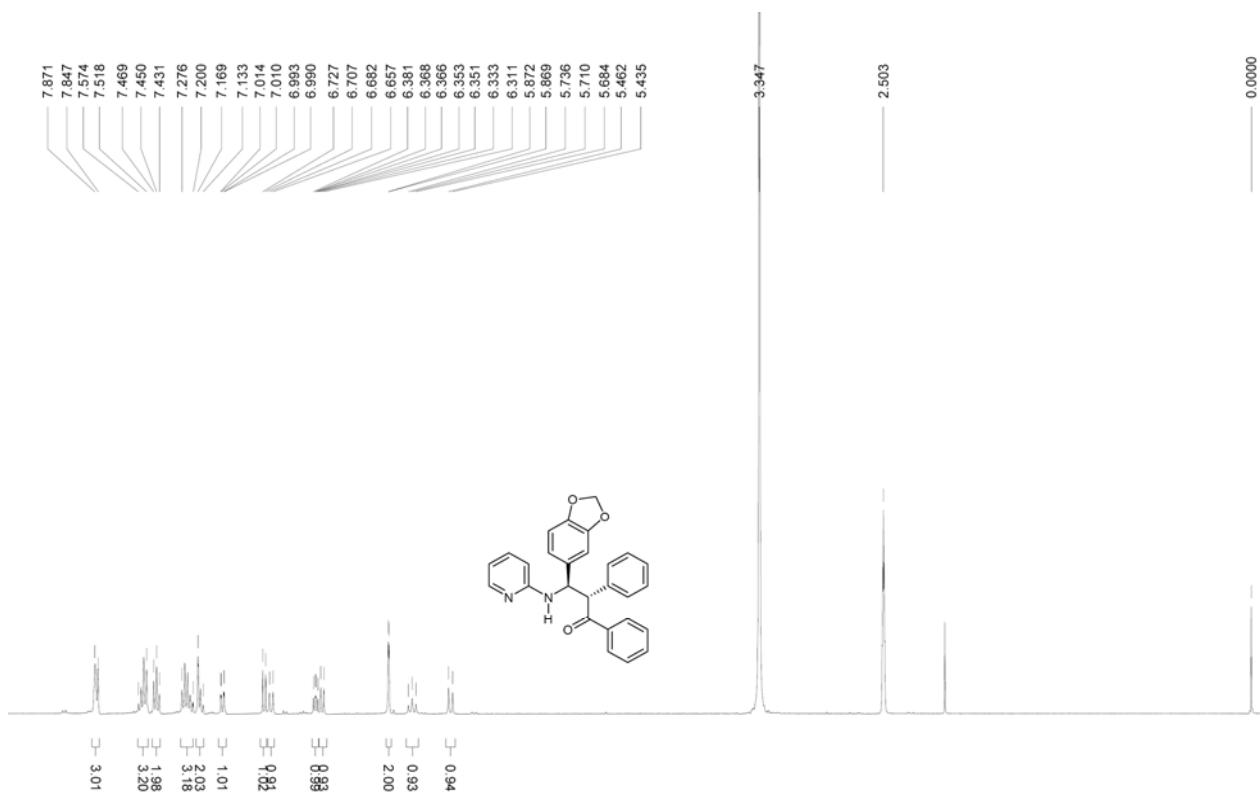
<sup>1</sup>H NMR Spectrum of Compound 4f



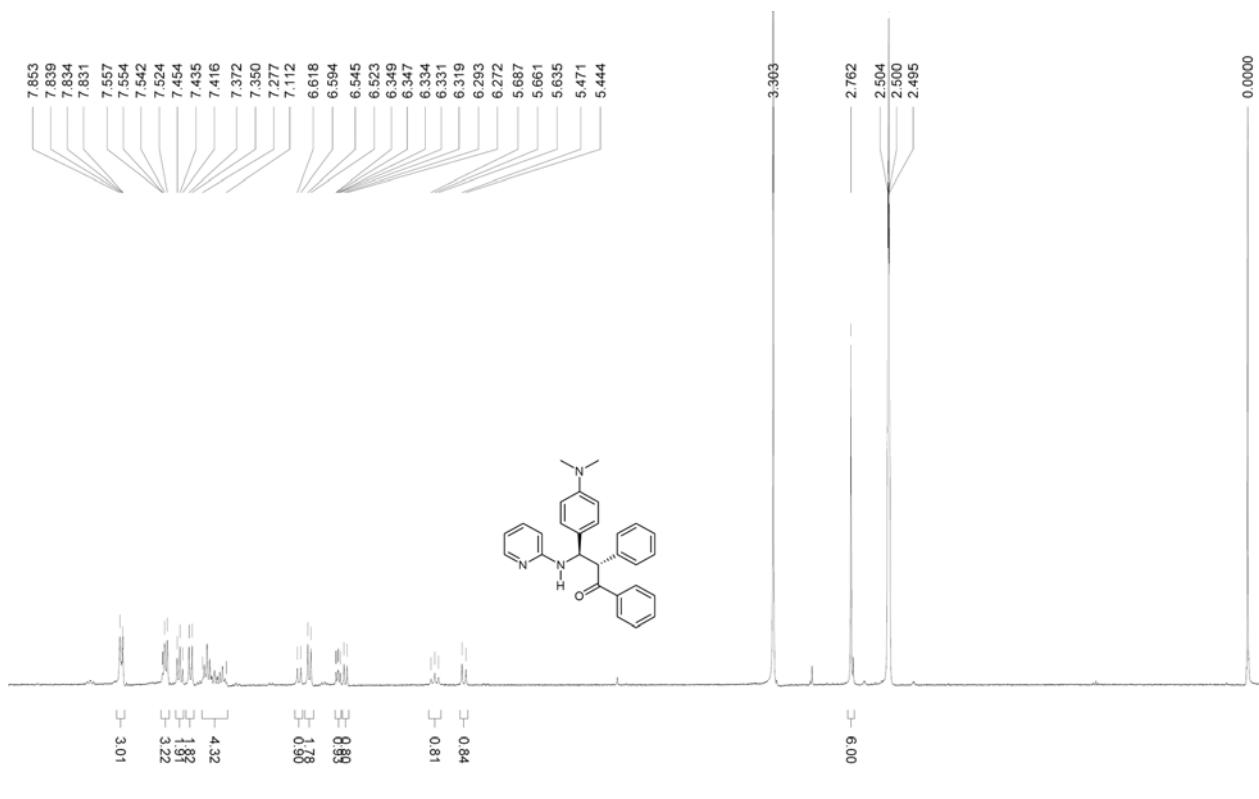




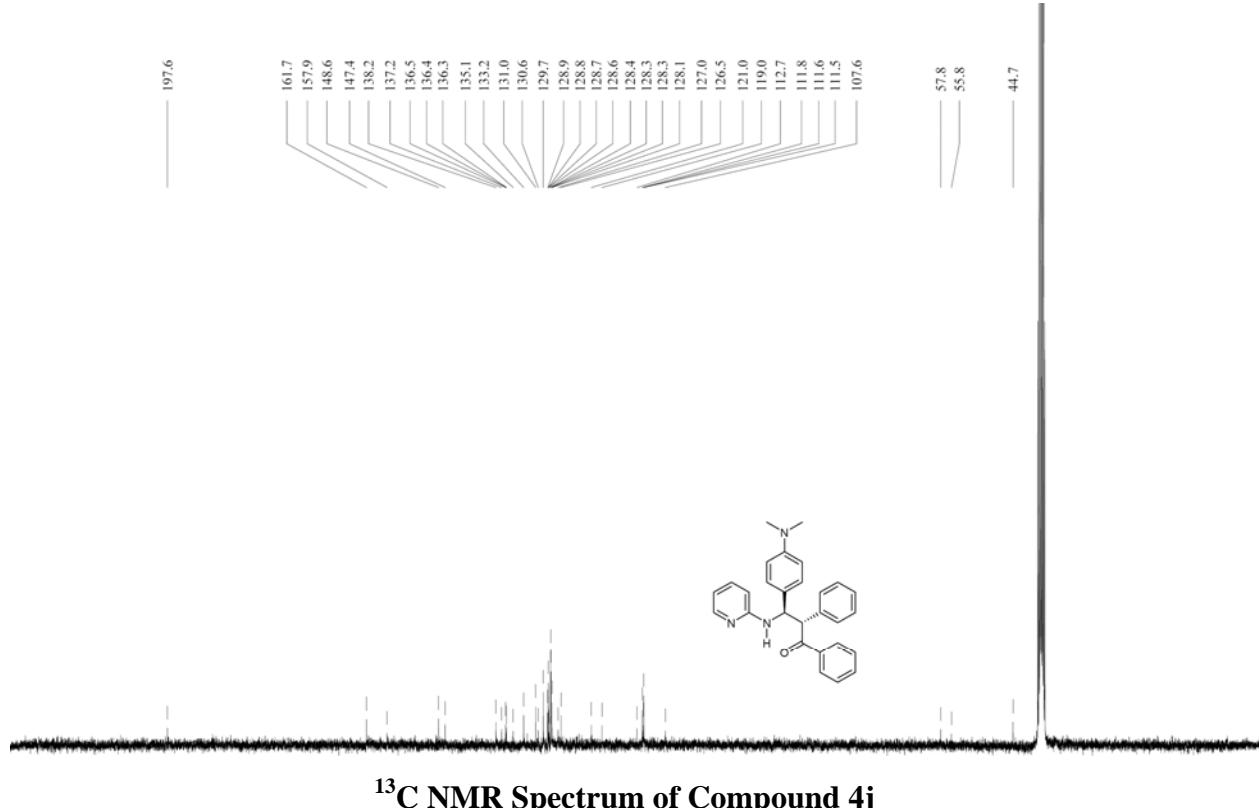
<sup>13</sup>C NMR Spectrum of Compound 4h



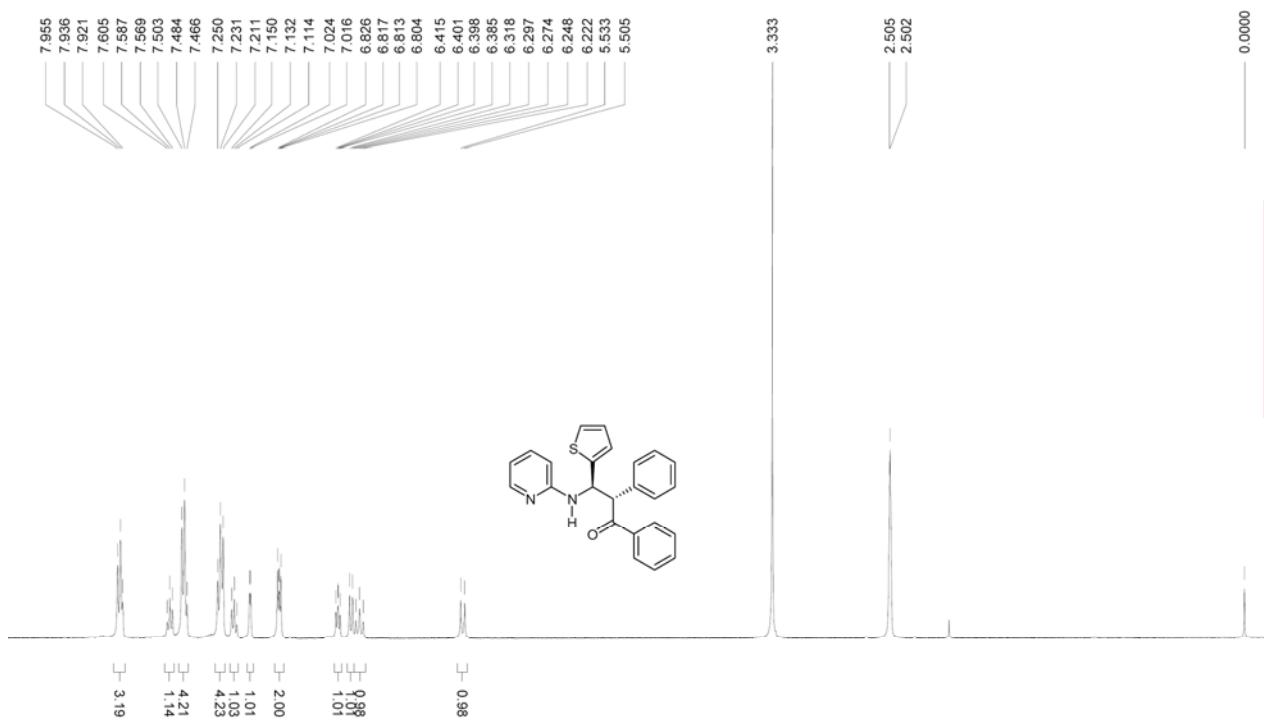
<sup>1</sup>H NMR Spectrum of Compound 4i



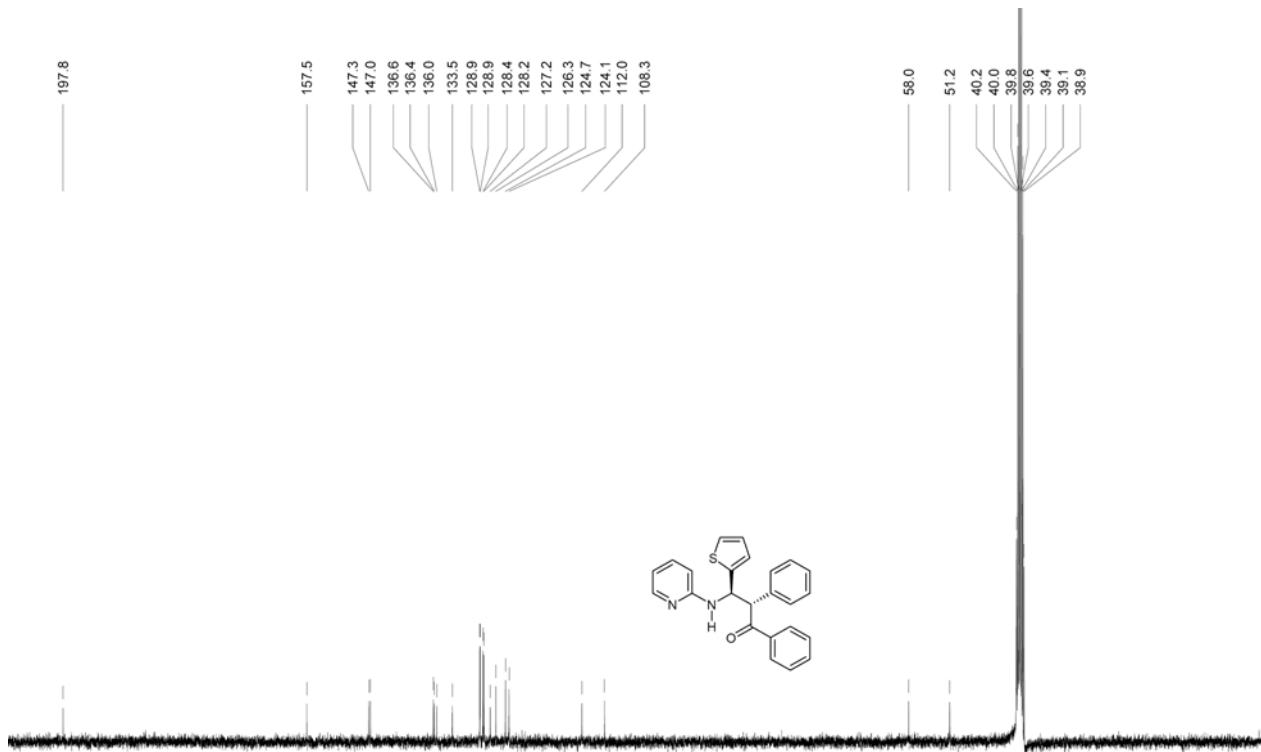
<sup>1</sup>H NMR Spectrum of Compound 4j



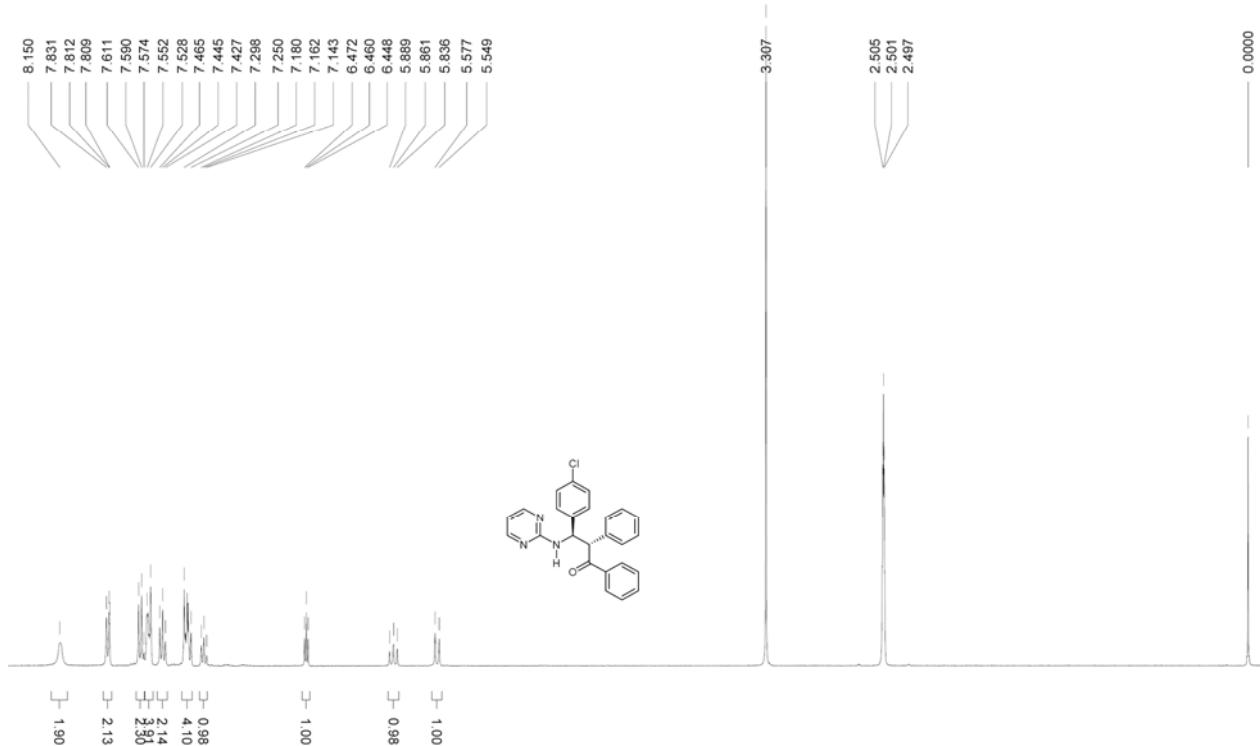
<sup>13</sup>C NMR Spectrum of Compound 4j



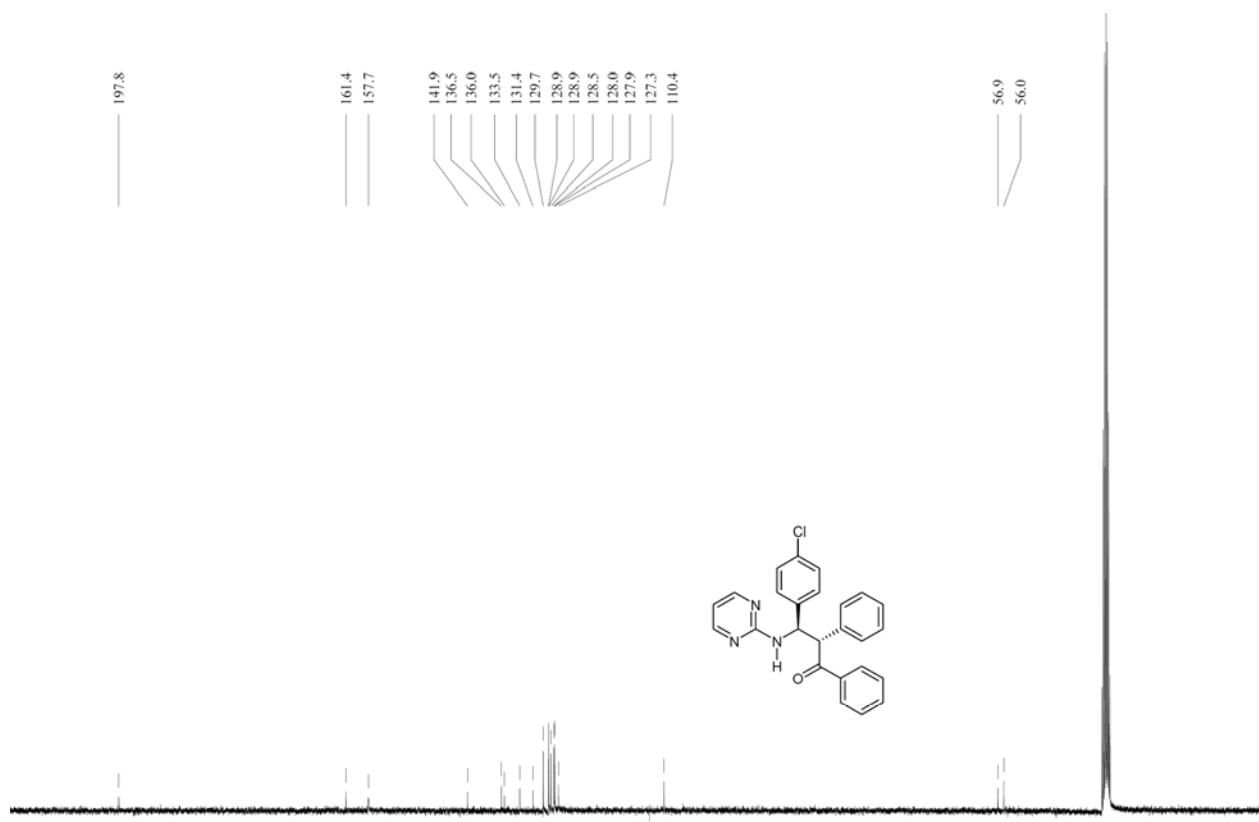
<sup>1</sup>H NMR Spectrum of Compound 4k



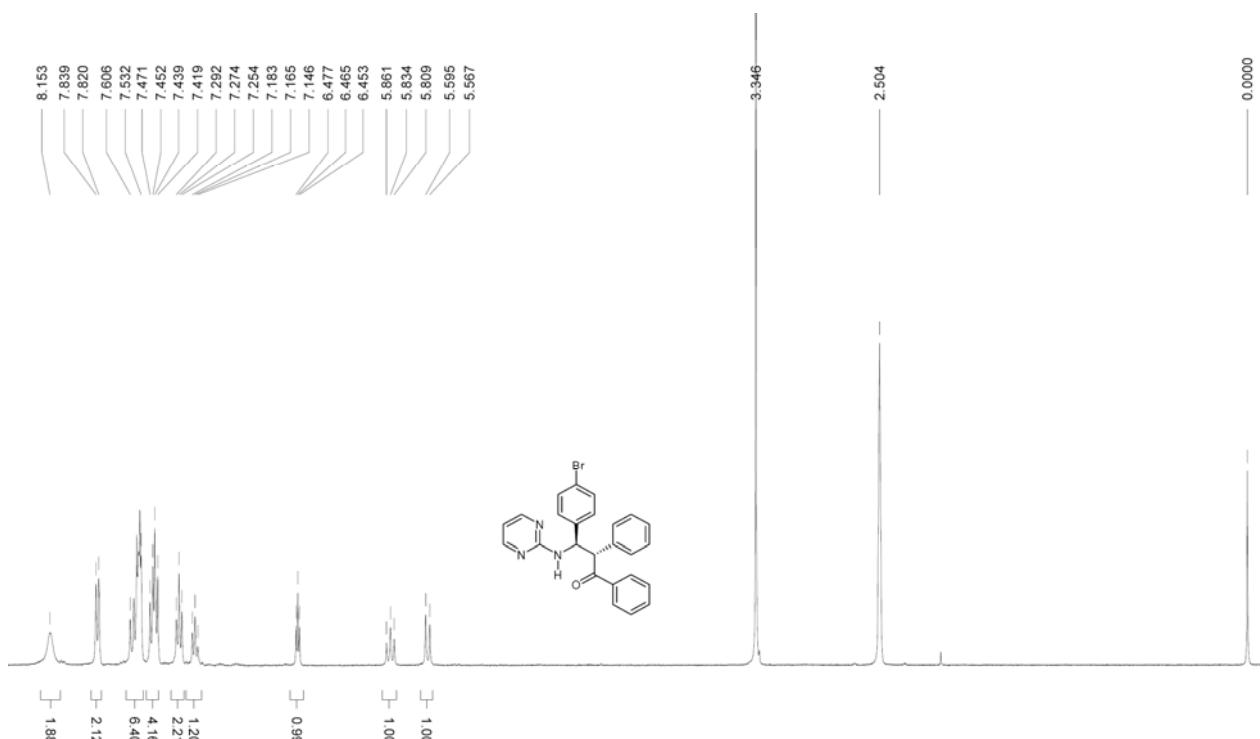
<sup>13</sup>C NMR Spectrum of Compound 4k



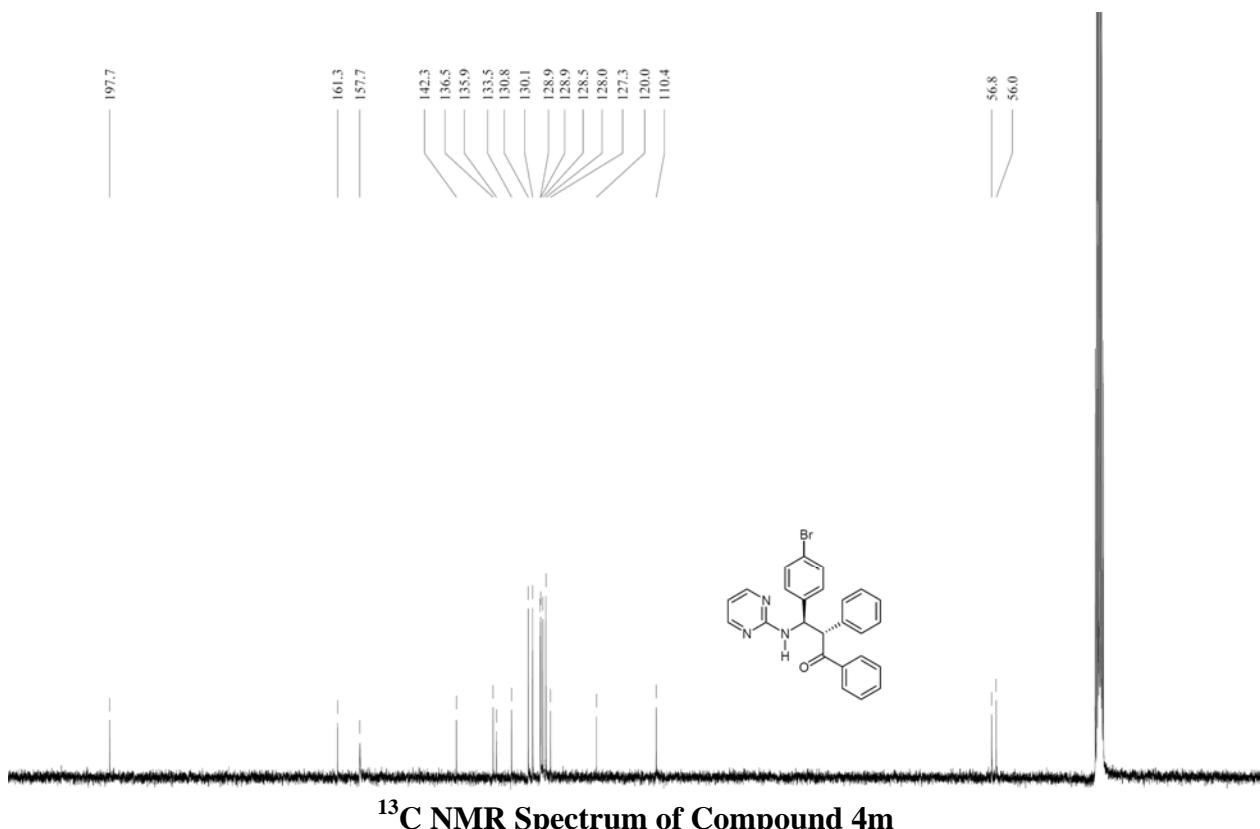
<sup>1</sup>H NMR Spectrum of Compound 4l



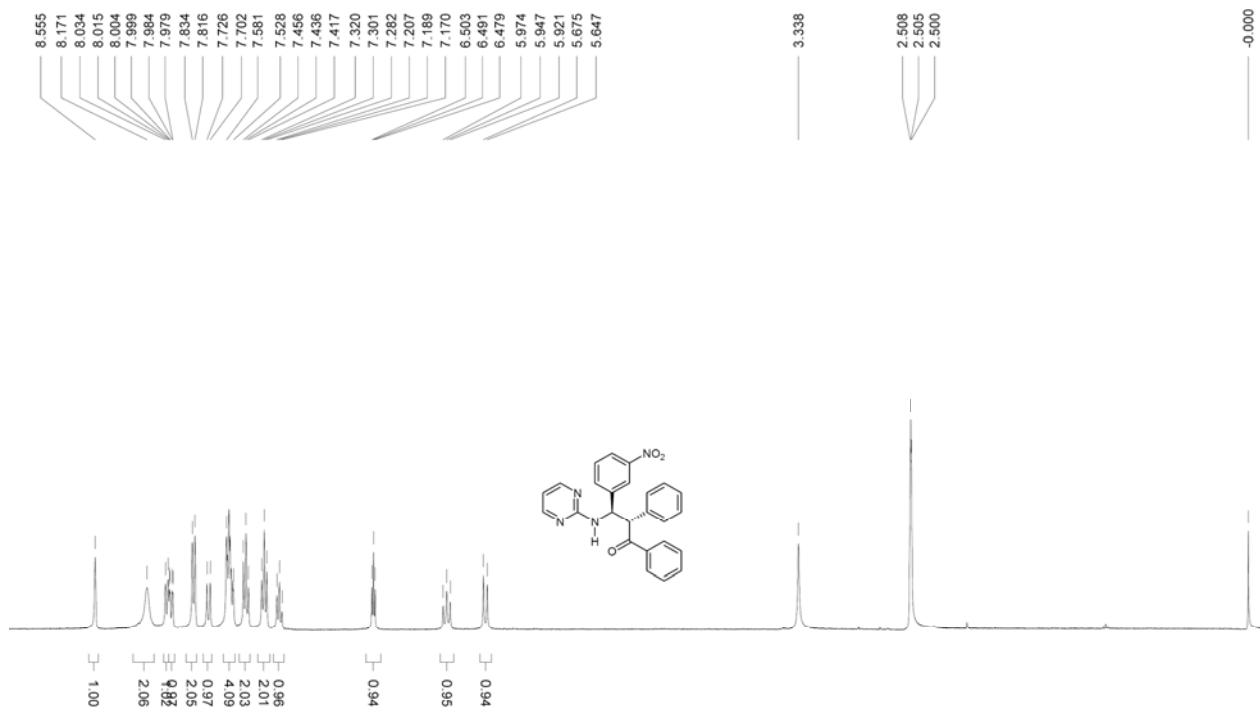
<sup>13</sup>C NMR Spectrum of Compound 4l



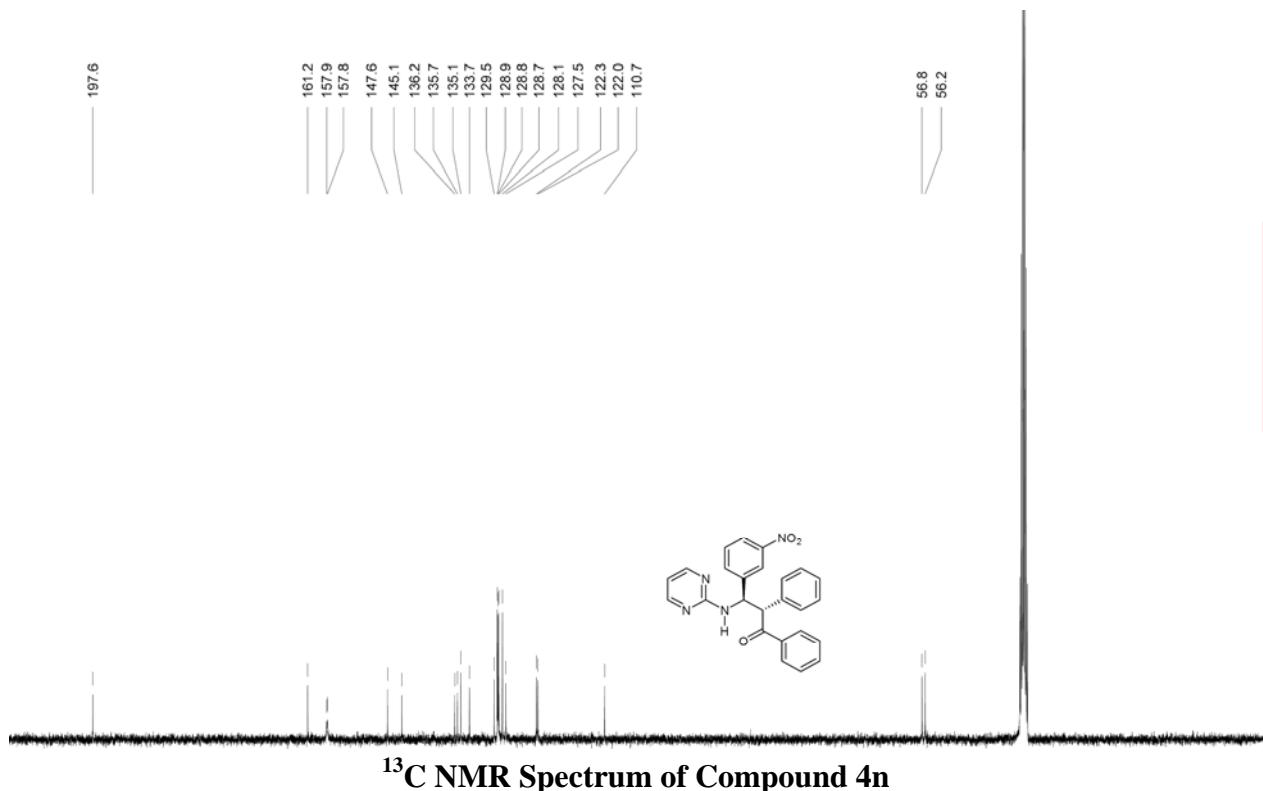
<sup>1</sup>H NMR Spectrum of Compound 4m



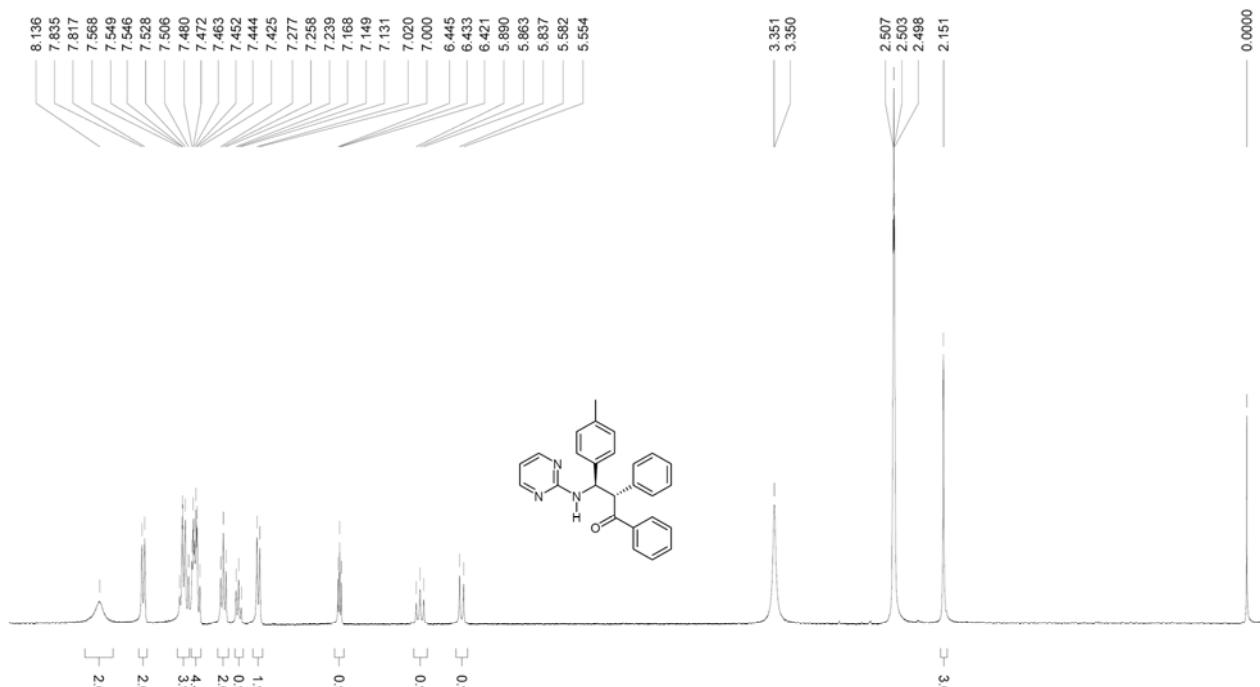
<sup>13</sup>C NMR Spectrum of Compound 4m



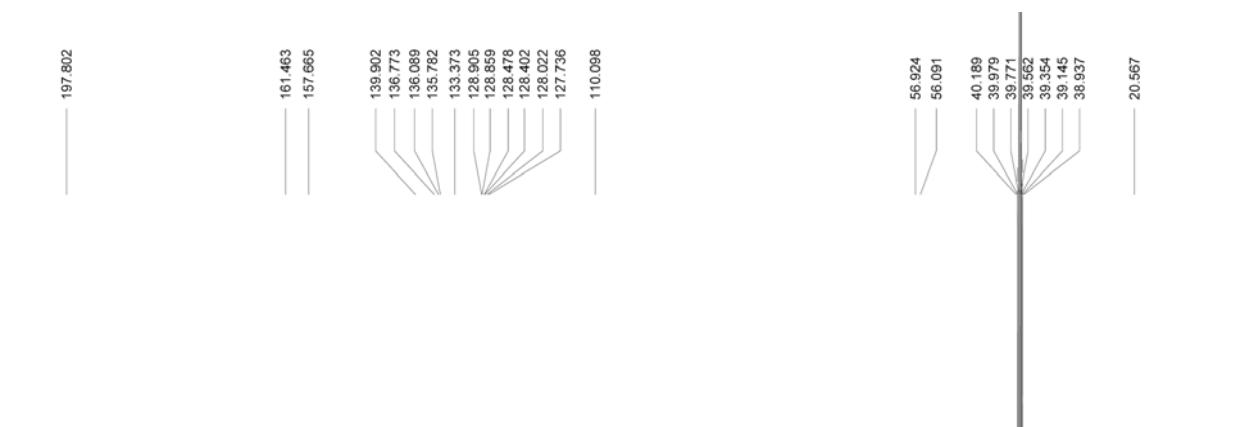
<sup>1</sup>H NMR Spectrum of Compound 4n



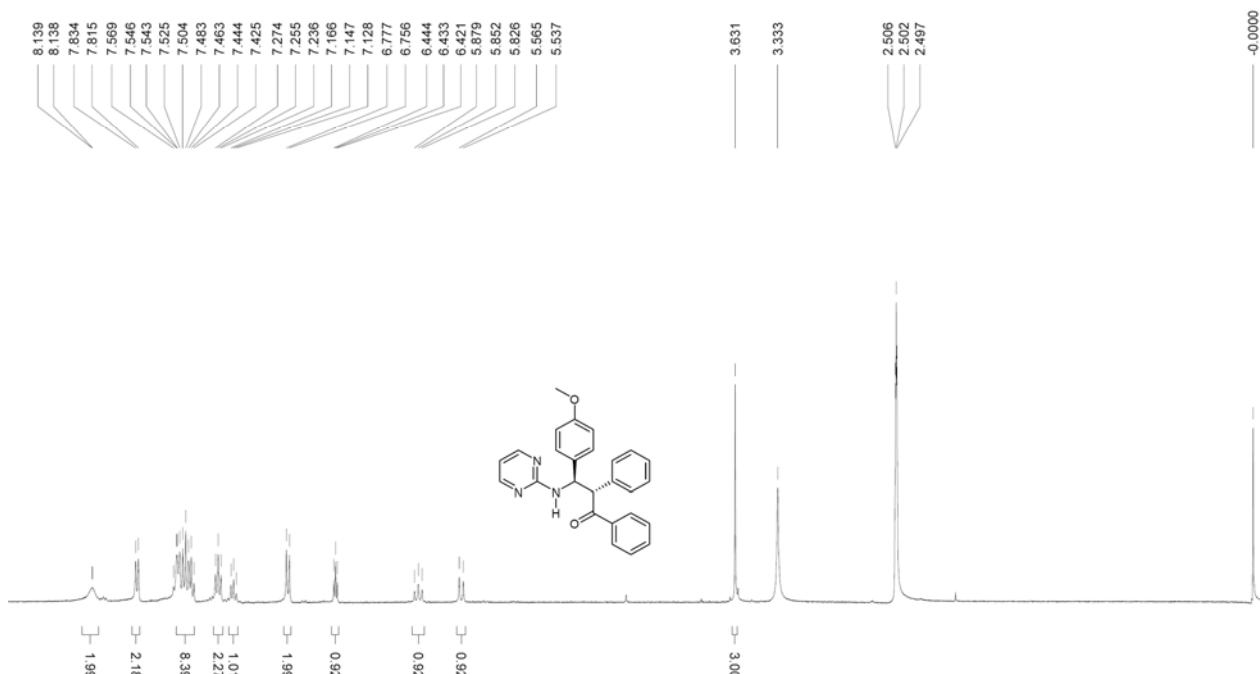
<sup>13</sup>C NMR Spectrum of Compound 4n



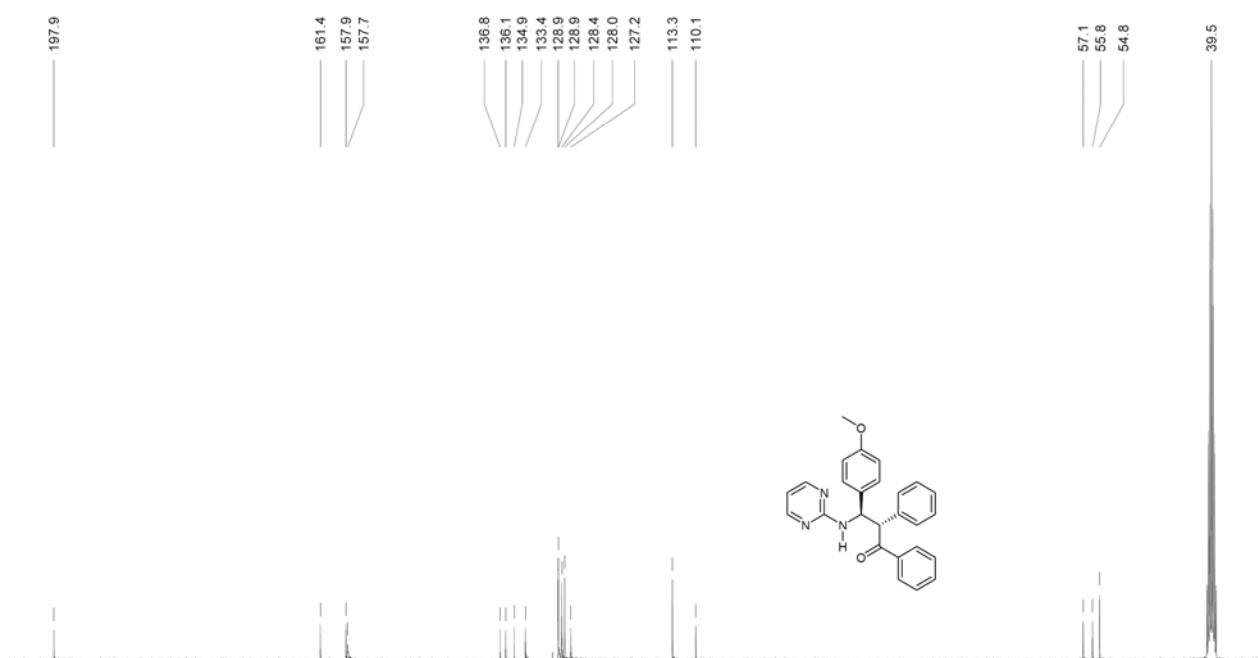
<sup>1</sup>H NMR Spectrum of Compound 4o



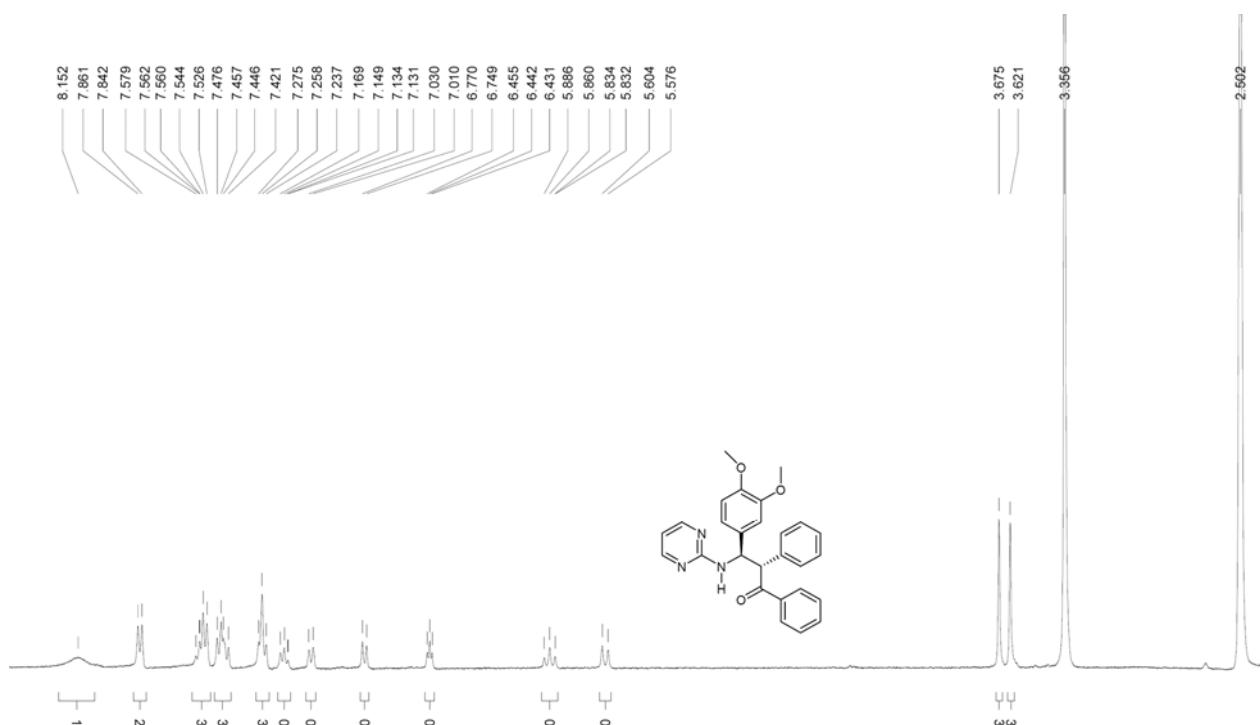
<sup>13</sup>C NMR Spectrum of Compound 4o



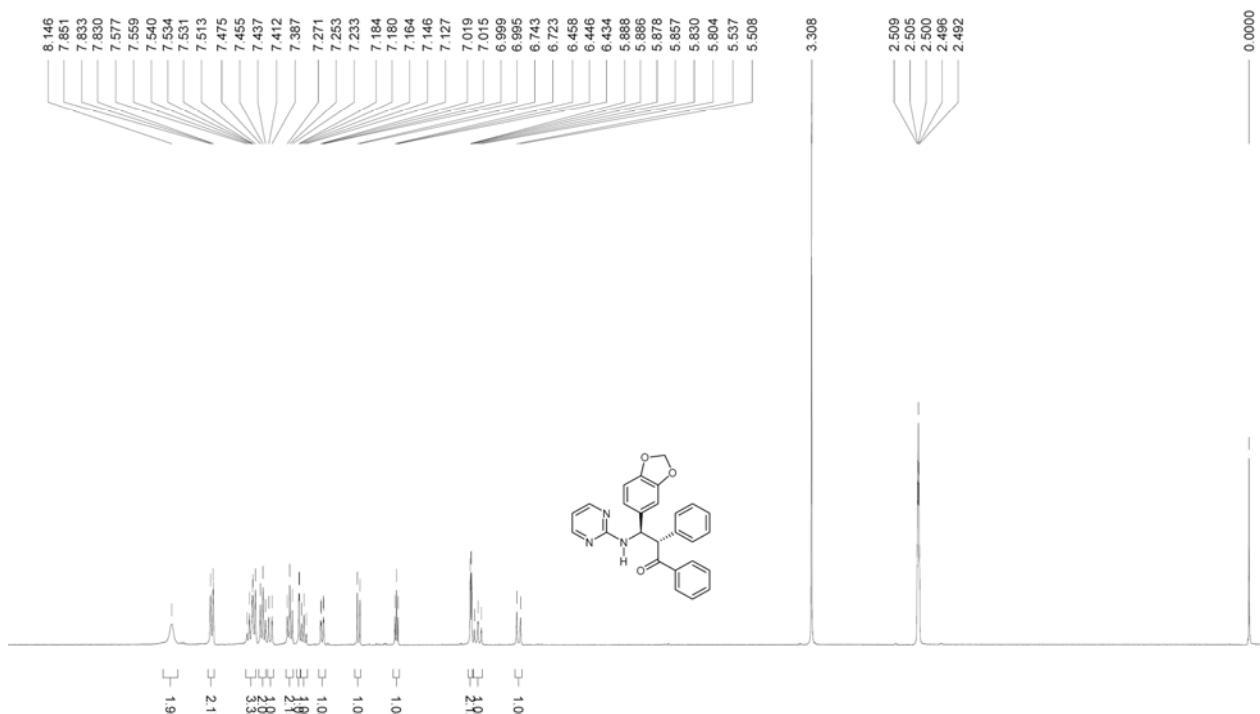
<sup>1</sup>H NMR Spectrum of Compound 4p



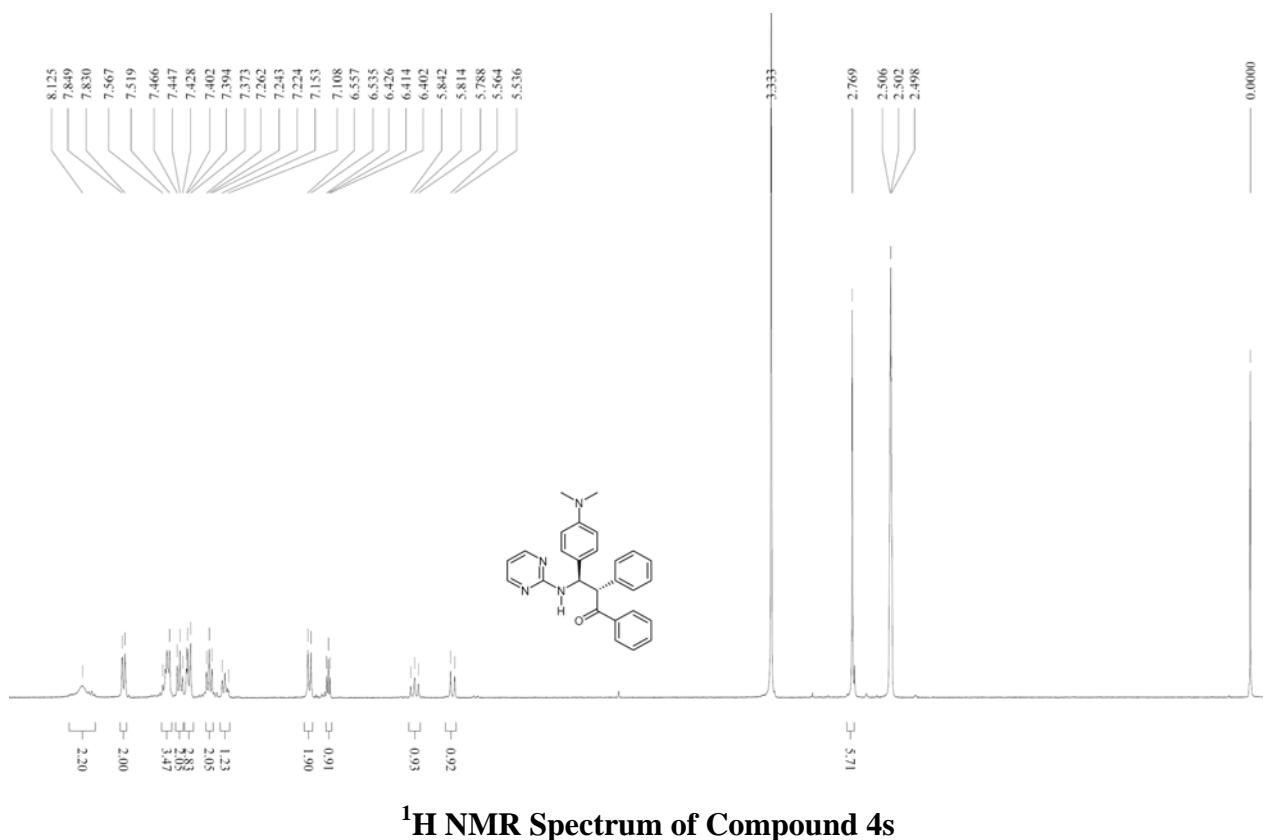
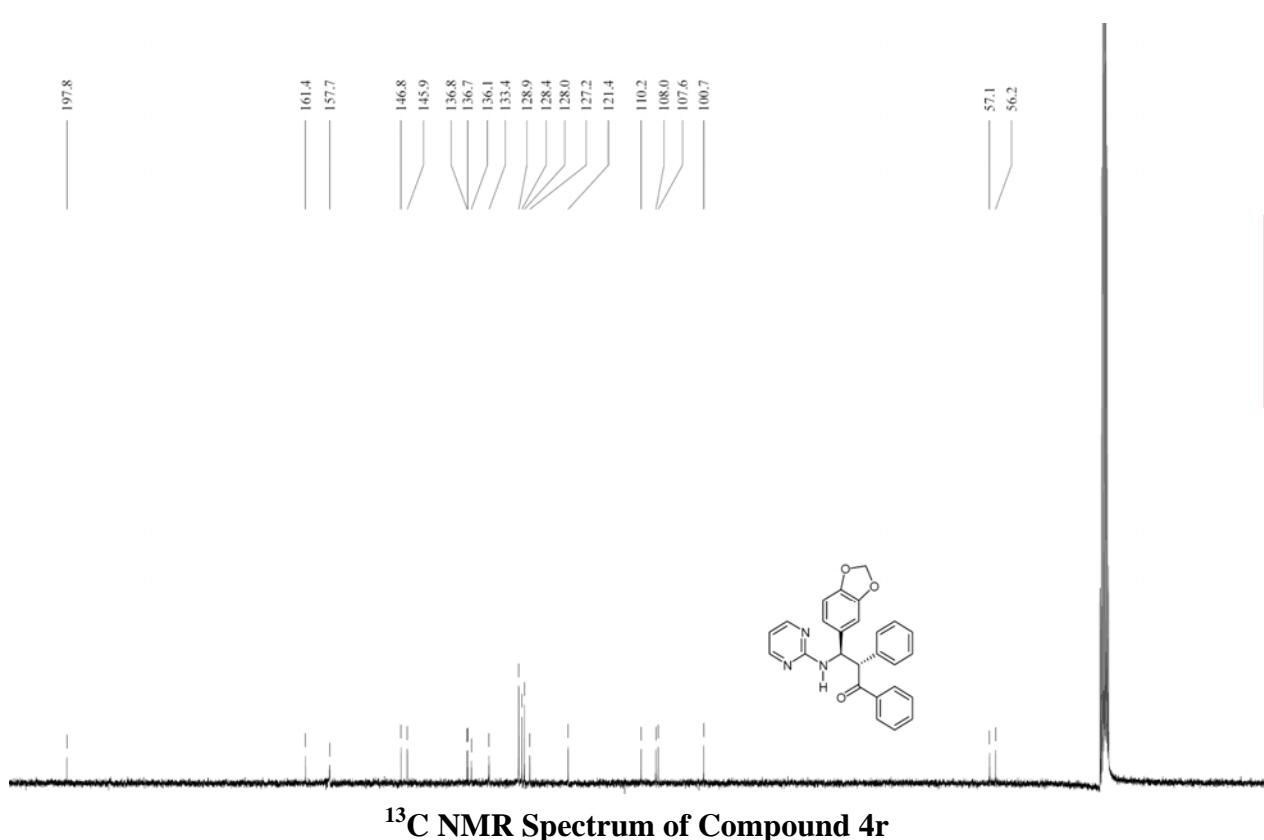
<sup>13</sup>C NMR Spectrum of Compound 4p

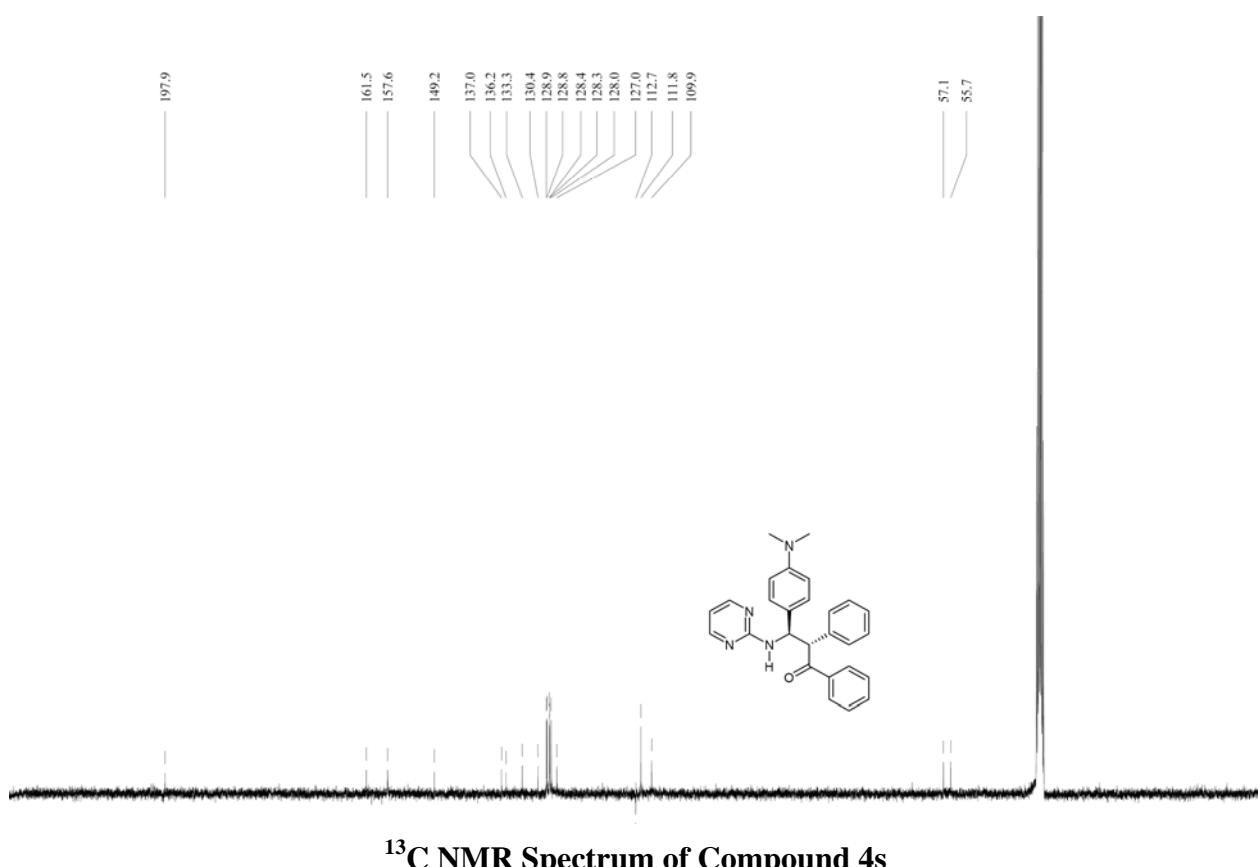


<sup>1</sup>H NMR Spectrum of Compound 4q

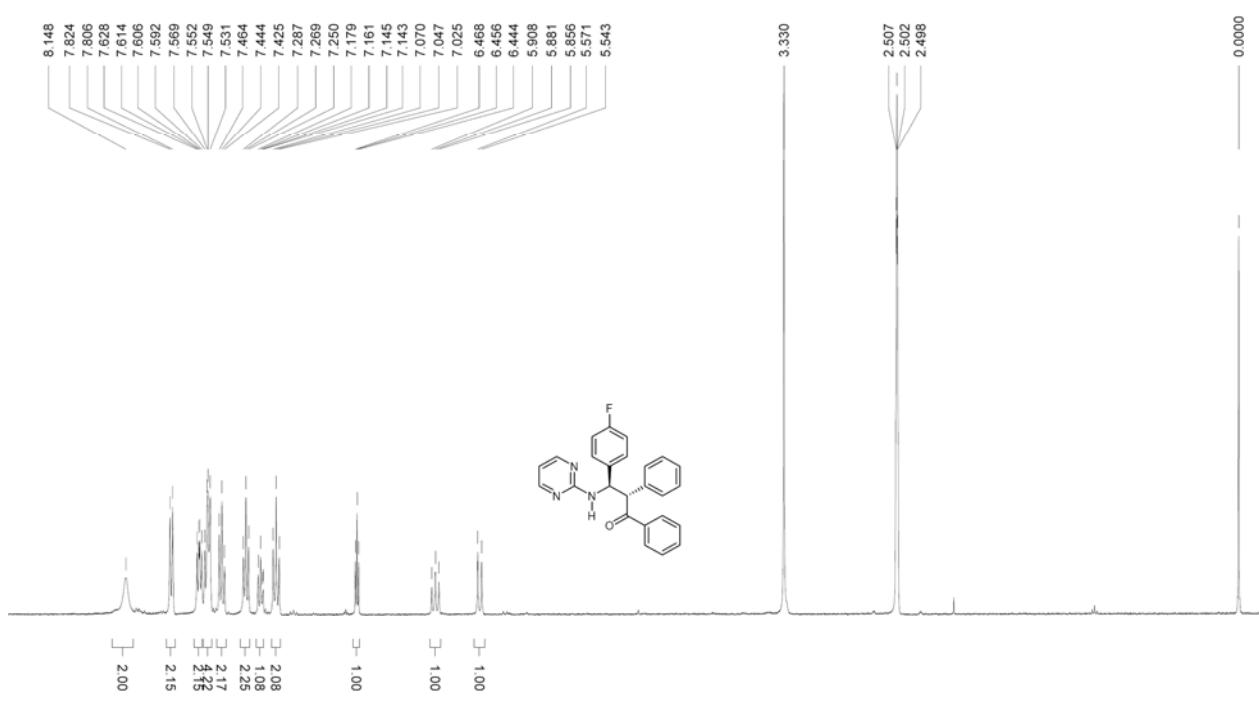


<sup>1</sup>H NMR Spectrum of Compound 4r

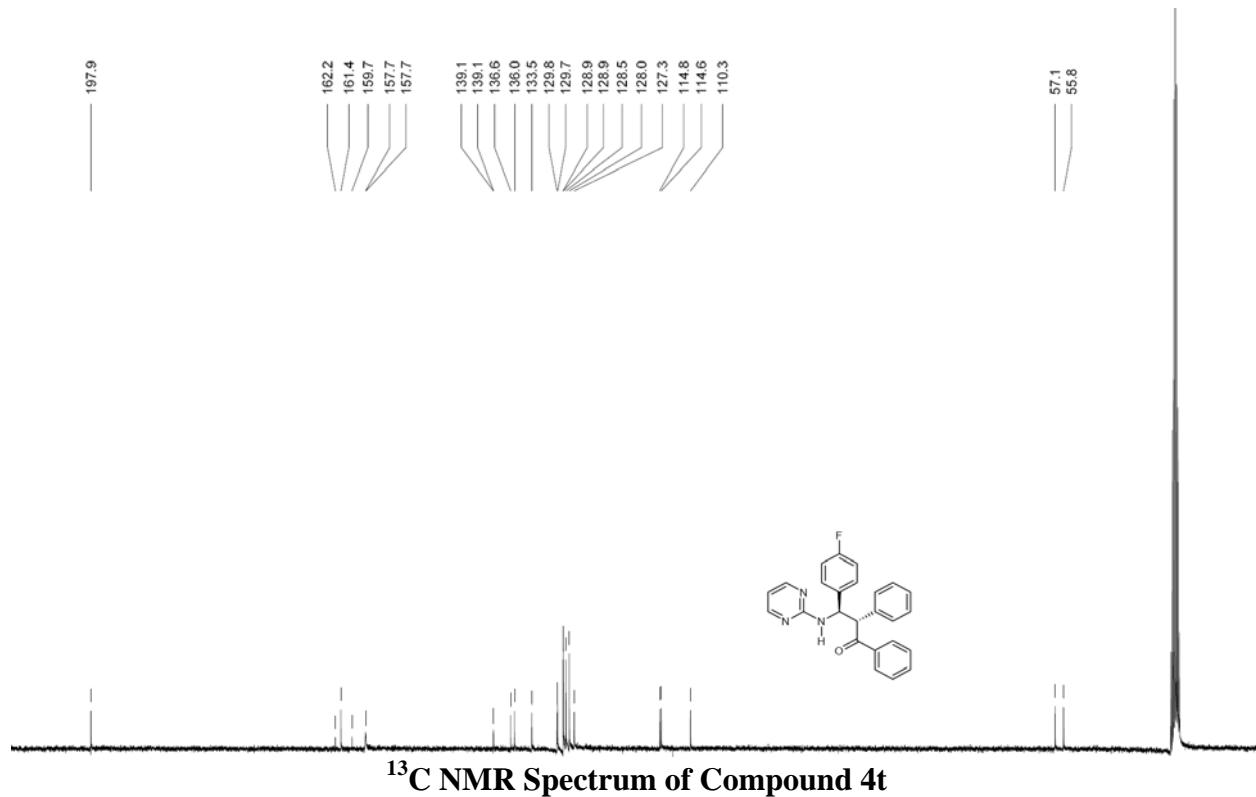




<sup>13</sup>C NMR Spectrum of Compound 4s



<sup>1</sup>H NMR Spectrum of Compound 4t



<sup>13</sup>C NMR Spectrum of Compound 4t