

Electronic Supplementary Material (ESI) for RSC Advances.

This journal is © The Royal Society of Chemistry 2023

## Co-catalyzed Arylation of Aldehydes and Aryltrimethylgermanes

Qiang Zhang,\* Xiao Zou, Ningqi Zhang, Bo Liu

Shaanxi Key Laboratory of Catalysis, School of Chemistry and Environmental Science, Shaanxi University of Technology, Han zhong, 723001, P. R. China

E-mail: zhangqiang22@126.com

|   |    |
|---|----|
| 1. Experimental reagents and instruction.....                     | 1  |
| 2. General experimental procedures.....                           | 2  |
| 3. Experimental characterization data for diarylmethanols .....   | 3  |
| 4. Experimental characterization data for benzil derivatives..... | 10 |
| 5. The NMR spectra of diarylmethanols.....                        | 16 |
| 6. The NMR spectra of benzil derivatives .....                    | 33 |

### 1. Experimental reagents and instruction

Chemicals were either purchased or purified by standard techniques without special instructions. The reactions were monitored using analytical thin layer chromatography (TLC, GF-254). Flash chromatography was performed using silica gel (300-400 mesh) with freshly distilled solvents. The boiling range of petroleum ether in this research is 60-90 °C. Arylglyoxals<sup>1</sup> and were prepared according to the reported procedures. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were measured on a Bruker spectrometer, using CDCl<sub>3</sub> as the solvent with tetramethylsilane (TMS) as an internal standard at room temperature. The mass spectra of the starting materials and the intermediates were recorded on a Bruker Avance Mass Spectrometer (maXis, ESI). Chemical shifts are given in  $\delta$  relative to TMS, the coupling constants  $J$  are given in Hz.

[1] a) M. B. Floyd, M. T. Du, P. F. Fabio, L. A. Jacob, B. D. Johnson, *J. Org. Chem.*, **1985**, *50*, 5022–5027; (b) B. Khalili, P. Jajarmi, B. Eftekhari-Sis, M. M. Hashemi, *J. Org. Chem.* **2008**, *73*, 2090–2095.

## 2. General experimental procedures

Aryltrimethylgermanes were synthesized from the corresponding arylbromides and chlorotrimethylgermane according to the literature procedure<sup>2</sup> with a slight modification. Trimethyl(phenyl)germane. To a 500 mL three necked flask were fitted with a magnetic stirrer, a thermometer, and a pressure equalizing dropping funnel. The flask was charged with bromobenzene (15.7 g, 100 mmol), and dry THF (200 mL) under Ar atmosphere. The reaction mixture was cooled to *ca.* –80 °C and *n*-BuLi/hexane (2.5 M, 52 mL, 130 mmol) was added dropwise over 1.5 h. Upon completion of the addition, the reaction mixture was stirred at –80 °C for 3 h, chlorotrimethylgermane (18.4, 120 mmol) was added dropwise and then allowed to warm to room temperature. The resulting mixture was acidified with 2 N HCl (26 mL) and stirred for overnight. After being concentrated to 1/3 volume, the mixture was poured into water, extracted with diethyl ether and washed with water, dried over MgSO<sub>4</sub>, followed by filtration under rotary evaporation, and the residue was purified by column chromatography (silica gel, petroleum ether / ethyl acetate, v/v) to give a colorless liquid (22.3 g, yield 86 %) (17.3 g, yield 89 %). The product<sup>[2c]</sup> was used without further purification in the next step.

### (1) The best reaction condition of the synthesis of diarylmethanols

A 10 mL pressure tubes was charged with CoI<sub>2</sub> (3.9 mg, 2.5 mol %), **tmphen (L8)**, 3.0 mg, 2.5 mol %), K<sub>2</sub>CO<sub>3</sub> (1.0 mmol), aldehyde (0.5 mmol), aryltrimethylgermane(0.65 mmol), and THF (2 mL) into the reaction tube stirred for 10 min at room temperature. Then, the mixture was heated at 65 °C for 12 h. After completion of the reaction, as indicated by TLC, the reaction mixture was extracted with ethyl acetate (3×10 mL), concentrated and purified by flash column on a silica gel (silica gel 200-300 mesh), petroleum ether/ethyl acetate as the eluent, to give the product. The identity and purity of the product was confirmed by <sup>1</sup>H NMR and <sup>13</sup>C NMR spectroscopic analysis.

### (2) The best reaction condition of the synthesis of benzil derivatives

A 10 mL pressure tubes was charged with CoI<sub>2</sub> (3.9 mg, 2.5 mol %), **tmphen (L8)**, 3.0 mg, 2.5 mol %), Cs<sub>2</sub>CO<sub>3</sub> (1.0 mmol), arylglyoxal (0.5 mmol), aryltrimethylgermane(0.65 mmol), and THF (2 mL) into the reaction tube stirred for 10 min at room temperature. Then, the mixture was heated at 65 °C for 12 h. After completion of the reaction, as indicated by TLC, the reaction mixture was

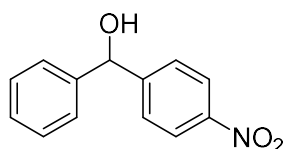
---

[2] a) S. M. Moerlein, *J. Org. Chem.* **1987**, 52, 664–667; b) Z. T. Zhang, J. P. Pitteloud, L. Cabrera, Y. Liang, M. Toribio, S. F. Wnuk, *Org. Lett.* **2010**, 12, 816–819; b) N. Komami, K. Matsuoka, A. N. M. Kojima, T. Yoshino, S. Matsunaga, *Chemistry A European Journal*, **2019**, 24, 1217-1220.

extracted with ethyl acetate (3×10 mL), concentrated and purified by flash column on a silica gel (silica gel 200-300 mesh), petroleum ether/ethyl acetate as the eluent, to give the product. The identity and purity of the product was confirmed by  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectroscopic analysis.

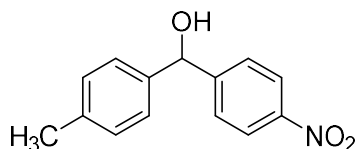
### 3. Experimental characterization data for diarylmethanols

#### 4-nitrophenyl(phenyl)methanol<sup>3</sup> (3a)



(4-nitrophenyl)(phenyl)methanol (**3a**). The product was isolated as a light-yellow solid (105 mg, 92%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 52–53 °C; IR (neat,  $\text{cm}^{-1}$ ): 1350( $\text{NO}_2$ ), 1540( $\text{NO}_2$ ), 3340(OH); The NMR spectra of 4-nitrophenyl(phenyl)methanol are shown as Attached Fig.1 and Attached Fig.2 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz)  $\delta$  2.48 (brs, 1H), 5.91 (s, 1H), 7.30-7.35 (m, 5H), 7.57 (d,  $J = 12.0$  Hz, 2H), 8.18 (d,  $J = 12.0$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz)  $\delta$  123.7, 126.7, 127.0, 127.0, 128.4, 128.9, 142.6, 147.1, 150.6; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{13}\text{H}_{11}\text{NO}_3 + \text{Na}$ ) 252.0637, found 252.0651. ( $\text{C}_{13}\text{H}_{11}\text{NO}_3 + \text{Na}$ ).

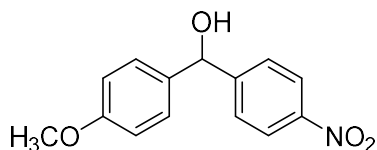
#### (4-nitrophenyl)(4-tolyl)methanol<sup>4</sup> (3b)



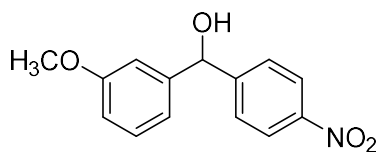
4-nitrophenyl-4-tolylmethanol (**3b**). The product was isolated as a light-yellow solid (114 mg, 94%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 6:1(v/v) as the eluent. mp 98–100 °C; IR (neat  $\text{cm}^{-1}$ ): 1350( $\text{NO}_2$ ), 1540( $\text{NO}_2$ ), 2870( $\text{CH}_3$ ), 2960( $\text{CH}_3$ ), 3341(OH); The NMR spectra of 4-nitrophenyl-4-tolylmethanol are shown as Attached Fig.3 and Attached Fig.4 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.32 (d,  $J = 3.0$  Hz, 1H), 2.36 (s, 3H), 5.90 (d,  $J = 3.0$  Hz, 1H), 7.16-7.26 (m, 4 H), 7.59 (d,  $J = 6.9$  Hz, 2H), 8.19 (d,  $J = 6.9$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  21.0, 75.3, 123.5, 126.6, 126.9, 129.5, 138.2, 139.9, 147.0, 150.9; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{13}\text{NO}_3 + \text{Na}$ ) 266.0793, found 266.0784. ( $\text{C}_{14}\text{H}_{13}\text{NO}_3 + \text{Na}$ ).

[3] C. M. Qin, H. Y. Wu, J. Cheng, J. X. Chen, M. C. Liu, W. W. Zhang, W. K. Su, J. C. Ding, *J. Org. Chem.* **2007**, 72, 4102–667.

<sup>4</sup> S. H. Lin, X. Y. Lu, *J. Org. Chem.* 2007, 72, 9757–9761.

(4-methoxyphenyl)(4-nitrophenyl)methanol<sup>4</sup> (3c)

(4-methoxyphenyl)(4-nitrophenyl)methanol (**3c**). The product was isolated as a light-yellow solid (120 mg, 93%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 6:1(v/v) as the eluent. mp 54–56 °C; IR (neat  $\text{cm}^{-1}$ ): 1350( $\text{NO}_2$ ), 1540( $\text{NO}_2$ ), 2850( $\text{OCH}_3$ ), 2930( $\text{OCH}_3$ ), 3340 (OH); The NMR spectra of (4-methoxyphenyl)(4-nitrophenyl)methanol are shown as Attached Fig.5 and Attached Fig.6 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.74 (brs, 1H), 3.79 (s, 3H), 5.86 (s, 1H), 6.82-6.93(m, 4H), 7.25-7.30 (m, 3H), 7.58 (d,  $J = 8.6$  Hz, 2H), 8.18 (d,  $J = 8.6$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  55.2, 75.3, 112.4, 113.4, 118.9, 127.0, 128.2, 130.9, 144.0, 147.1, 151.0, 159.9; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{13}\text{NO}_4+\text{Na}$ ) 282.0742, found 282.0749. ( $\text{C}_{14}\text{H}_{13}\text{NO}_3+\text{Na}$ ).

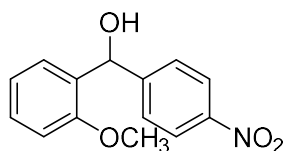
3-methoxyphenyl(4-nitrophenyl)methanol<sup>5</sup> (3d)

(3-methoxyphenyl)(4-nitrophenyl)methanol (**3d**). The product was isolated as an Oil (120 mg, 93%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 8:1(v/v) as the eluent. IR (neat  $\text{cm}^{-1}$ ): 1360( $\text{NO}_2$ ), 1550( $\text{NO}_2$ ), 2851( $\text{OCH}_3$ ), 2932( $\text{OCH}_3$ ), 3342(OH); The NMR spectra of (3-methoxyphenyl)(4-nitrophenyl)methanol are shown as Attached Fig.7 and Attached Fig.8 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.78 (brs, 1H), 3.79 (s, 3H), 5.86 (s, 1H), 6.82 (m, 3H), 7.25-7.30 (m, 1H), 7.57 (d,  $J = 9.0$  Hz, 2H), 8.17 (d,  $J = 9.0$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  55.2, 75.3, 112.3, 113.4, 118.9, 123.6, 127.0, 129.9, 144.3, 147.1, 150.6, 159.9; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{13}\text{NO}_4+\text{Na}$ ) 282.0742, found 282.0753. ( $\text{C}_{14}\text{H}_{13}\text{NO}_3+\text{Na}$ ).

(2-methoxyphenyl)(4-nitrophenyl)methanol<sup>6</sup> (3e)

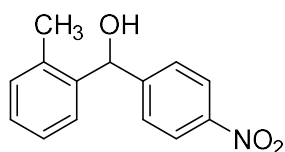
<sup>5</sup> H. M. Zheng, Q. Zhang, J. X. Chen, M. C. Liu, S. H. Cheng, J. C. Ding, H. Y. Wu, W. K. Su, *J. Org. Chem.* **2009**, *74*, 943–945.

<sup>6</sup> H. Zhao, M. Cheng, T. Zhang, M. Z. Cai, *J. Organomet. Chem.* **2015**, *777*, 50–56.



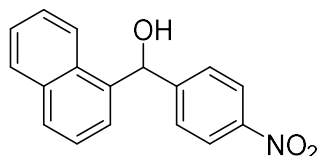
(2-methoxyphenyl)(4-nitrophenyl)methanol (**3e**). The product was isolated as an Oil (118 mg, 91%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 8:1(v/v) as the eluent. IR (neat  $\text{cm}^{-1}$ ): 1355( $\text{NO}_2$ ), 1554( $\text{NO}_2$ ), 2853( $\text{OCH}_3$ ), 2935( $\text{OCH}_3$ ), 3345(OH); The NMR spectra of (2-methoxyphenyl)(4-nitrophenyl)methanol are shown as Attached Fig.9 and Attached Fig.10 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  3.17 (s, 1H), 3.80 (s, 3H), 6.09 (s, 1H), 6.89-6.92 (m, 2H), 7.21-7.32 (m, 2H), 7.55 (d,  $J = 8.8$  Hz, 2H), 8.15 (d,  $J = 8.8$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  55.4, 71.6, 110.9, 121.1, 123.4, 127.1, 127.8, 128.2, 129.0, 129.5, 130.6, 150.8; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{13}\text{NO}_4+\text{Na}$ ) 282.0742, found 282.0746. ( $\text{C}_{14}\text{H}_{13}\text{NO}_3+\text{Na}$ ).

(4-nitrophenyl)(o-tolyl)methanol<sup>7</sup> (**3f**)



(4-nitrophenyl)(o-tolyl)methanol (**3f**). The product was isolated as an Oil (25.4 mg, 92%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. IR (neat  $\text{cm}^{-1}$ ): 1355( $\text{NO}_2$ ), 1554( $\text{NO}_2$ ), 2870( $\text{CH}_3$ ), 2960( $\text{CH}_3$ ), 3345(OH); The NMR spectra of (4-nitrophenyl)(o-tolyl)methanol are shown as Attached Fig.11 and Attached Fig.12 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.30 (s, 3H), 2.45 (s, 1H), 6.07 (s, 1H), 7.15-7.25 (m, 3H), 7.30-7.33 (m, 1H), 7.50 (d,  $J = 8.8$  Hz, 2H), 8.16 (d,  $J = 8.8$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  19.4, 72.7, 123.6, 126.5, 127.0, 127.5, 128.3, 131.0, 135.6, 140.4, 147.1, 150.2; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{13}\text{NO}_3+\text{Na}$ ) 266.0793, found 266.0797. ( $\text{C}_{14}\text{H}_{13}\text{NO}_3+\text{Na}$ ).

naphthalen-1-yl(4-nitrophenyl)methanol<sup>[5]</sup> (**3g**)

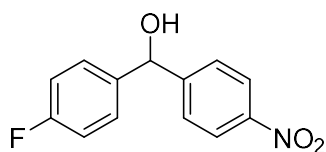


naphthalen-1-yl(4-nitrophenyl)methanol (**3g**). The product was isolated as a light-yellow solid (129 mg, 93%) after column chromatography purification using a solution of petroleum ether and ethyl

<sup>7</sup> T. Zou, S. S. Pi, J. H. Li, *Org. Lett.* **2009**, *11*, 453–456.

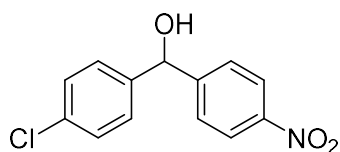
acetate 5:1(v/v) as the eluent. mp 51–52 °C; IR (neat  $\text{cm}^{-1}$ ): 1380( $\text{NO}_2$ ), 1564( $\text{NO}_2$ ), 3345(OH); The NMR spectra of naphthalen-1-yl(4-nitrophenyl)methanol are shown as Attached Fig.13 and Attached Fig.14 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.79 (brs, 1H), 6.55 (s, 1H), 7.47-7.51 (m, 4H), 7.58 (d,  $J = 8.9$  Hz, 2H), 7.85-7.91 (m, 2H), 8.01-8.04 (m, 1H), 8.15 (d,  $J = 8.9$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  73.4, 123.6, 123.7, 125.3, 125.6, 126.0, 126.6, 127.5, 129.0, 129.4, 130.5, 134.2, 137.8, 147.3, 150.3; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{17}\text{H}_{13}\text{NO}_3 + \text{Na}$ ) 302.0793, found 302.0799. ( $\text{C}_{17}\text{H}_{13}\text{NO}_3 + \text{Na}$ ).

(4-fluorophenyl)(4-nitrophenyl)methanol<sup>[5]</sup> (3h)



(4-fluorophenyl)(4-nitrophenyl)methanol (**3h**). The product was isolated as a light-yellow solid (117 mg, 95%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 74–76 °C; IR (neat  $\text{cm}^{-1}$ ): 1384( $\text{NO}_2$ ), 1562( $\text{NO}_2$ ), 3350(OH); The NMR spectra of (4-fluorophenyl)(4-nitrophenyl)methanol are shown as Attached Fig.15 and Attached Fig.16 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.40 (s, 1H), 5.93 (s, 1H), 7.04-7.09 (m, 2H), 7.32-7.36 (m, 2H), 7.57 (d,  $J = 6.9$  Hz, 2H), 8.21 (d,  $J = 6.9$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  74.8, 115.8 (d,  $J\text{-}C_F = 21.5$  Hz), 123.7, 127.0, 128.5 (d,  $J\text{-}C_F = 8.2$  Hz), 138.5, 147.3, 150.5, 162.5 (d,  $J\text{-}C_F = 246.2$  Hz); HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{13}\text{H}_{10}\text{FNO}_3 + \text{Na}$ ) 270.0542, found 270.0549. ( $\text{C}_{13}\text{H}_{10}\text{FNO}_3 + \text{Na}$ ).\_

(4-chlorophenyl)(4-nitrophenyl)methanol<sup>8</sup> (3i)

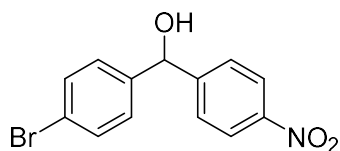


(4-chlorophenyl)(4-nitrophenyl)methanol (**3i**). The product was isolated as a light-yellow solid (121 mg, 92%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 8:1(v/v) as the eluent. mp 132–134 °C; IR (neat  $\text{cm}^{-1}$ ): 1386( $\text{NO}_2$ ), 1566( $\text{NO}_2$ ), 3348(OH); The NMR spectra of (4-chlorophenyl)(4-nitrophenyl)methanol are shown as Attached Fig.17 and Attached Fig.18 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.43 (d,  $J =$

<sup>8</sup> K. Li, N. F. Hu, R. S. Luo, W. C. Yuan, W. J. Tang. *J. Org. Chem.* **2013**, 78, 6350–6355.

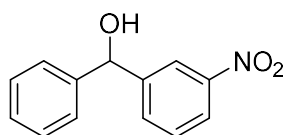
3.5 Hz, 1H), 5.90 (d,  $J = 3.5$  Hz, 1H), 7.27-7.35 (m, 4H), 7.55 (d,  $J = 8.9$  Hz, 2H), 8.19 (d,  $J = 8.9$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  74.6, 123.6, 126.8, 127.8, 127.8, 128.9, 134.0, 140.9, 150.0; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{13}\text{H}_{10}\text{ClNO}_3 + \text{Na}$ ) 286.0247, found 286.0254. ( $\text{C}_{13}\text{H}_{10}\text{ClNO}_3 + \text{Na}$ ).

(4-bromophenyl)(4-nitrophenyl)methanol<sup>9</sup> (3j)



(4-bromophenyl)(4-nitrophenyl)methanol (**3j**). The product was isolated as a light-yellow solid (140 mg, 91%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 6:1(v/v) as the eluent. mp 160–162 °C; IR (neat  $\text{cm}^{-1}$ ): 1378( $\text{NO}_2$ ), 1561( $\text{NO}_2$ ), 3353(OH); The NMR spectra of (4-bromophenyl)(4-nitrophenyl)methanol are shown as Attached Fig.19 and Attached Fig.20 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.43 (d,  $J = 3.3$  Hz, 1H), 5.89 (d,  $J = 3.3$  Hz, 1H), 7.23 (d,  $J = 6.7$  Hz, 2H), 7.48-7.56 (m, 4H), 8.20 (d,  $J = 6.8$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  74.5, 122.0, 123.5, 126.7, 128.0, 131.7, 141.3, 147.1, 149.8; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{13}\text{H}_{10}\text{BrNO}_3 + \text{Na}$ ) 329.9742, found 329.9747. ( $\text{C}_{13}\text{H}_{10}\text{BrNO}_3 + \text{Na}$ ).

3-nitrophenyl-phenylmethanol<sup>10</sup> (3k)

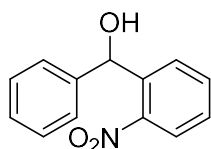


(3-nitrophenyl)(phenyl)methanol (**3k**). The product was isolated as a light-yellow solid (97 mg, 85%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 68–70 °C; IR (neat  $\text{cm}^{-1}$ ): 1379( $\text{NO}_2$ ), 1562( $\text{NO}_2$ ), 3351(OH); The NMR spectra of (3-nitrophenyl)(phenyl)methanol are shown as Attached Fig.21 and Attached Fig.22 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.75 (s, H), 5.91 (s, 1H), 7.33-7.38 (m, 5H), 7.49 (t,  $J = 7.9$  Hz, 1H), 7.71(d,  $J = 7.9$  Hz, 1H), 8.11 (d,  $J = 7.9$  Hz, 1H), 8.29 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz)  $\delta$  75.3, 121.3, 122.4, 126.6, 128.3, 128.9, 129.3, 132.4, 142.8, 145.8, 148.3; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{13}\text{H}_{11}\text{NO}_3 + \text{Na}$ ) 252.0637, found 252.0644 ( $\text{C}_{13}\text{H}_{11}\text{NO}_3 + \text{Na}$ ).

2-nitrophenyl-phenylmethanol<sup>10</sup> (3l)

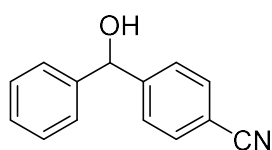
<sup>9</sup> R. G. La, A. Coluccia, V. Famigliini, S. Pelliccia, L. Monti, D. Vullo, E. Nuti, V. Alterio, G. De Simone, S. M. Monti, P. W. Pan, S. Parkkila, C. T. Supuran, A. Rossello, R. Silvestri, *J. Med. Chem.* **2015**, *58*, 8564–8572;

<sup>10</sup> S. J. Chang, S. L. Zhou, H. M. Gau, *RSC Advances*, **2015**, *5*, 9368–9373.



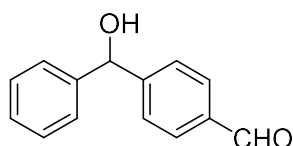
(2-nitrophenyl)(phenyl)methanol(**3j**). The product was isolated as a light-yellow solid (87 mg, 76%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 58–59 °C; IR (neat  $\text{cm}^{-1}$ ): 1373( $\text{NO}_2$ ), 1558( $\text{NO}_2$ ), 3348(OH); The NMR spectra of (2-nitrophenyl)(phenyl)methanol are shown as Attached Fig.23 and Attached Fig.24 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  3.04 (s, 1H), 6.40 (s, 1H), 7.29–7.33 (m, 5H), 7.45 (t,  $J = 7.5$  Hz, 1H), 7.63 (t,  $J = 8.1$  Hz, 1H), 7.74 (d,  $J = 7.5$  Hz, 1H), 7.91 (d,  $J = 8.1$  Hz, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  71.4, 124.7, 126.9, 128.0, 128.5, 128.5, 129.4, 133.4, 138.5, 141.5, 148.3; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{13}\text{H}_{11}\text{NO}_3+\text{Na}$ ) 252.0637, found 252.0645 ( $\text{C}_{13}\text{H}_{11}\text{NO}_3+\text{Na}$ ).

#### 4-cyanophenyl-phenylmethanol<sup>11</sup> (3m)



4-(hydroxy(phenyl)methyl)benzonitrile (**3m**). The product was isolated as a light-yellow solid (91 mg, 87%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 6:1(v/v) as the eluent. mp 68–70 °C; IR (neat  $\text{cm}^{-1}$ ): 2221(CN), 3348(OH); The NMR spectra of 4-(hydroxy(phenyl)methyl)benzonitrile are shown as Attached Fig.25 and Attached Fig.26 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.31 (d,  $J = 3.0$  Hz, 1H), 5.87 (d,  $J = 3.0$  Hz, 1H), 7.33–7.34 (m, 5H), 7.52 (d,  $J = 8.6$  Hz, 2H), 7.63 (d,  $J = 8.6$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  75.6, 118.8, 126.6, 126.7, 127.0, 127.0, 128.3, 128.9, 132.2, 142.8; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{11}\text{NO}+\text{Na}$ ) 232.0738, found 232.0734 ( $\text{C}_{14}\text{H}_{11}\text{NO}+\text{Na}$ ).

#### 4-formylphenyl-phenylmethanol<sup>11</sup> (3n)



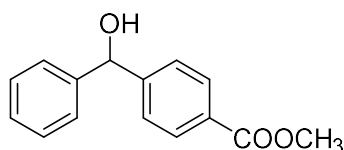
4-formylphenyl-phenylmethanol(**3n**). The product was isolated as a light-yellow solid (98 mg, 93%)

<sup>11</sup> a) Y. Hayashi, N. Yamamura, T. Kusakawa, T. Harada, *Chem. Eur. J.*, **2016**, 22, 12095–12105; b) J. Karthikeyan, M. Jeganmohan, C. H Cheng, *Chem. Eur. J.* **2010**, 16, 8989–8992.



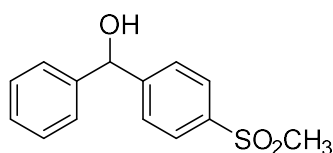
after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 76–78 °C; IR (neat  $\text{cm}^{-1}$ ): 1710(CHO), 2720(CHO), 2749(CHO), 3348(OH); The NMR spectra of 4-formylphenyl-phenylmethanol are shown as Attached Fig.27 and Attached Fig.28 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.88 (brs, 1H), 5.88 (s, 1H), 7.27-7.36 (m, 5H), 7.56 (d,  $J = 8.0$  Hz, 2H), 7.83 (d,  $J = 8.0$  Hz, 2H), 9.94 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  75.8, 126.7, 126.9, 128.0, 128.7, 129.9, 135.5, 143.1, 150.5, 192.1; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{12}\text{O}_2 + \text{Na}$ ) 235.0735, found 235.0742 ( $\text{C}_{14}\text{H}_{12}\text{O}_2 + \text{Na}$ ).

methyl 4-(hydroxy(phenyl)methyl)benzoate<sup>12</sup> (3o)



methyl 4-(hydroxy(phenyl)methyl)benzoate(**3o**). The product was isolated as a light-yellow solid (66 mg, 55%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 61–62 °C; IR (neat  $\text{cm}^{-1}$ ): 1730(COO), 3351(OH); The NMR spectra of methyl 4-(hydroxy(phenyl)methyl)benzoate are shown as Attached Fig.29 and Attached Fig.30 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.59 (brs, 1H), 3.89 (s, 3H), 5.86 (s, 1H), 7.19-7.35 (m, 5H), 7.45 (d,  $J = 8.3$  Hz, 2H), 7.99 (d,  $J = 8.3$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  52.1, 75.9, 126.3, 126.6, 127.9, 128.7, 129.2, 129.8, 143.3, 148.7, 166.9; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{15}\text{H}_{14}\text{O}_3 + \text{Na}$ ) 265.0841, found 265.0847 ( $\text{C}_{15}\text{H}_{14}\text{O}_3 + \text{Na}$ ).

(4-(methylsulfonyl)phenyl)(phenyl)methanol<sup>5</sup> (3p)



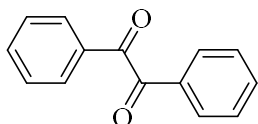
(4-(methylsulfonyl)phenyl)(phenyl)methanol(**3p**). The product was isolated as a light-yellow solid (119 mg, 91%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 125–126 °C; IR (neat  $\text{cm}^{-1}$ ): 1560( $\text{SO}_2$ ), 3351(OH); The NMR spectra of (4-(methylsulfonyl)phenyl)(phenyl)methanol are shown as Attached Fig.31 and Attached Fig.32 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.42 (s, 1H), 3.03 (s, 3H), 5.91 (d,  $J = 2.5$  Hz, 1H), 7.33-7.37 (m, 5H), 7.61 (d,  $J = 8.1$  Hz, 2H), 7.90 (d,  $J = 8.1$

<sup>12</sup> T. Yamamoto, T. Furusawa, A. Zhumagazin, T. Yamakawa, Y. Oe, T. Ohta, *Tetrahedron*, **2015**, 71, 19–26.

Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  44.5, 75.6, 126.7, 127.2, 127.5, 127.5, 128.2, 128.8, 142.9, 150.0; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{14}\text{O}_3\text{S}+\text{Na}$ ) 285.0561, found 285.0567 ( $\text{C}_{14}\text{H}_{14}\text{O}_3\text{S}+\text{Na}$ ).

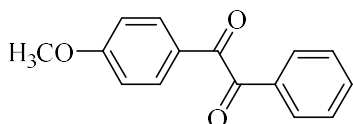
#### 4. Experimental characterization data for benzil derivatives

##### Benzyl<sup>13</sup> (4a)



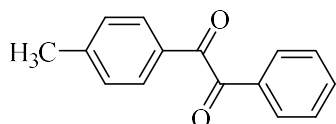
Benzyl(4a). The product was isolated as a light-yellow solid (99 mg, 95%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 94–95 °C; IR (neat  $\text{cm}^{-1}$ ): 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of benzyl are shown as Attached Fig.33 and Attached Fig.34 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.48-7.54 (m, 4H), 7.62-7.68 (m, 2H), 7.95-8.00 (m, 4H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  128.9, 129.5, 132.2, 134.7, 194.5; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_{10}\text{O}_2+\text{H}$ ) 211.2400, found 211.2410 ( $\text{C}_{15}\text{H}_{12}\text{O}_3+\text{H}$ ).

##### 1-(4-methoxyphenyl)-2-phenylethane-1, 2-dione<sup>14</sup>(4b)



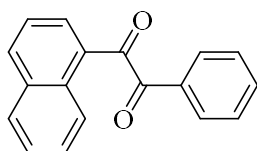
1-(4-methoxyphenyl)-2-phenylethane-1,2-dione(4b). The product was isolated as a light-yellow solid (113 mg, 94%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 62–63 °C; IR (neat  $\text{cm}^{-1}$ ): 2830( $\text{OCH}_3$ ), 2812( $\text{OCH}_3$ ), 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1-(4-methoxyphenyl)-2-phenylethane-1,2-dione are shown as Attached Fig.35 and Attached Fig.36 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  3.89 (s, 3H), 6.94-6.99 (m, 2H), 7.46-7.64 (m, 3H), 7.91-7.99 (m, 8.4 Hz, 4H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  55.6, 114.4, 126.0, 128.9, 129.8, 133.2, 134.6, 140.0, 165.0, 193.1, 194.8; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{15}\text{H}_{12}\text{O}_3+\text{H}$ ) 241.0865, found 241.0873 ( $\text{C}_{15}\text{H}_{12}\text{O}_3+\text{H}$ ).

##### 1-phenyl-2-*p*-tolylethane-1, 2-dione<sup>14</sup> (4c)



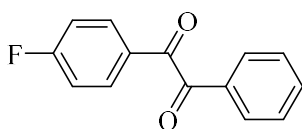
1-phenyl-2-(p-tolyl)ethane-1,2-dione(**4c**). The product was isolated as a light-yellow solid (104 mg, 93%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 99–101 °C; IR (neat  $\text{cm}^{-1}$ ): 2958( $\text{CH}_3$ ), 2861( $\text{CH}_3$ ), 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1-phenyl-2-(p-tolyl)ethane-1,2-dione are shown as Attached Fig.37 and Attached Fig.38 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.43 (s, 3H), 7.28-7.31 (m, 2H), 7.46-7.52 (m, 2H), 7.61-7.64 (m, 1H), 7.85-7.88 (m, 2H), 7.94-7.98 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  21.9, 128.9, 129.7, 129.8, 129.9, 130.0, 130.6, 134.8, 146.2, 194.2, 194.7; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{15}\text{H}_{12}\text{O}_2+\text{H}$ ) 225.0916, found 225.0922 ( $\text{C}_{15}\text{H}_{12}\text{O}_2+\text{H}$ ).

#### 1-(naphthalen-1-yl)-2-phenylethane-1,2-dione<sup>14</sup> (**4d**)



1-(naphthalen-1-yl)-2-phenylethane-1,2-dione(**4d**). The product was isolated as a light-yellow solid (119 mg, 92%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 101–103 °C; IR (neat  $\text{cm}^{-1}$ ): 1688(-CO-CO-), 1622(-CO-CO-); The NMR spectra of 1-(naphthalen-1-yl)-2-phenylethane- 1,2-dione are shown as Attached Fig.39 and Attached Fig.40 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.49-7.67 (m, 6H), 7.90-8.05 (m, 5H), 9.30-9.46 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  124.5, 126.0, 127.2, 128.6, 129.0, 129.5, 131.0, 133.4, 134.1, 134.8, 135.1, 136.0, 194.6, 197.2; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{18}\text{H}_{12}\text{O}_2+\text{H}$ ) 261.0916, found 261.0923 ( $\text{C}_{18}\text{H}_{12}\text{O}_2+\text{H}$ ).

#### 1-(4-fluorophenyl)-2-phenylethane-1, 2-dione<sup>15</sup> (**4e**)



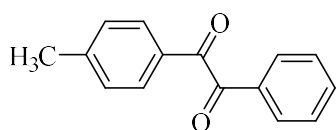
1-(4-fluorophenyl)-2-phenylethane-1,2-dione(**4e**). The product was isolated as a light-yellow solid (104 mg, 91%) after column chromatography purification using a solution of petroleum ether and

15 E. Anders, T. Clark, T. Gassner, *Chem. Ber.* **1986**, *119*, 1350–1360.

13 R. Ramajayam, R. Giridhar, M. R. Yadav, *Chem. Heterocycl. Compd.* **2006**, *42*, 901–906.

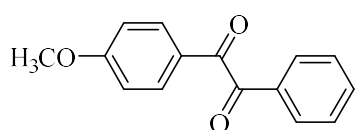
ethyl acetate 10:1(v/v) as the eluent. mp 62–64 °C; IR (neat  $\text{cm}^{-1}$ ): 1688(-CO-CO-), 1622(-CO-CO-); The NMR spectra of 1-(4-fluorophenyl)-2-phenylethane-1,2-dione are shown as Attached Fig.41 and Attached Fig.42 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.15-7.26 (m, 2H), 7.50-7.54 (m, 2H), 7.55-7.68 (m, 1H), 7.95-8.05 (m, 4H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  116.2, 116.5, 129.0, 129.5, 129.6, 129.9, 132.6, 132.7, 132.9, 134.9, 165.0, 168.5, 192.6, 194.0; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_9\text{FO}_2+\text{H}$ ) 229.0665, found 229.0669 ( $\text{C}_{14}\text{H}_9\text{FO}_2+\text{H}$ ).

1-phenyl-2-*p*-tolylethane-1, 2-dione<sup>14</sup> (4f)

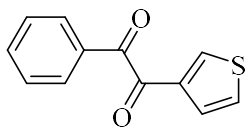


1-phenyl-2-(*p*-tolyl)ethane-1,2-dione(4f). The product was isolated as a light-yellow solid (104 mg, 93%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 99–101 °C; IR (neat  $\text{cm}^{-1}$ ): 2958( $\text{CH}_3$ ), 2861( $\text{CH}_3$ ), 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1-phenyl-2-(*p*-tolyl)ethane-1,2-dione are shown as Attached Fig.43 and Attached Fig.44 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.43 (s, 3H), 7.28-7.31 (m, 2H), 7.46-7.52 (m, 2H), 7.61-7.64 (m, 1H), 7.85-7.88 (m, 2H), 7.94-7.98 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  21.9, 128.9, 129.7, 129.8, 129.9, 130.0, 130.6, 134.8, 146.2, 194.2, 194.7; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{15}\text{H}_{12}\text{O}_2+\text{H}$ ) 225.0916, found 225.0922 ( $\text{C}_{15}\text{H}_{12}\text{O}_2+\text{H}$ ).

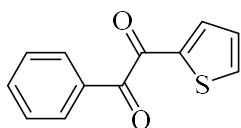
1-(4-methoxyphenyl)-2-phenylethane-1, 2-dione<sup>14</sup>(4g)



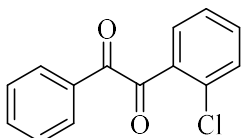
1-(4-methoxyphenyl)-2-phenylethane-1,2-dione(4b). The product was isolated as a light-yellow solid (113 mg, 94%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 15:1(v/v) as the eluent. mp 62–63 °C; IR (neat  $\text{cm}^{-1}$ ): 2830( $\text{OCH}_3$ ), 2812( $\text{OCH}_3$ ), 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1-(4-methoxyphenyl)-2-phenylethane-1,2-dione are shown as Attached Fig.45 and Attached Fig.46 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  3.89 (s, 3H), 6.94-6.99 (m, 2H), 7.46-7.64 (m, 3H), 7.91-7.99 (m, 8.4 Hz, 4H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  55.6, 114.4, 126.0, 128.9, 129.8, 133.2, 134.6, 140.0, 165.0, 193.1, 194.8; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{15}\text{H}_{12}\text{O}_3+\text{H}$ ) 241.0865, found 241.0873 ( $\text{C}_{15}\text{H}_{12}\text{O}_3+\text{H}$ ).

1-phenyl-2-(thiophen-3-yl) ethane-1, 2-dione<sup>16</sup>(4h)

1-phenyl-2-(thiophen-3-yl) ethane-1, 2-dione(**4h**). The product was isolated as a light-yellow solid (72 mg, 67%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 15:1(v/v) as the eluent. mp 81–82 °C; IR (neat  $\text{cm}^{-1}$ ): 3011(thiophene), 1620(-CO-CO-); The NMR spectra of 1-phenyl-2-(thiophen-3-yl) ethane-1, 2-dione are shown as Attached Fig.47 and Attached Fig.48 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.39-7.54 (m, 3H), 7.63-7.70 (m, 2H), 7.99-8.02 (m, 2H), 8.21(s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  120.0, 129.3, 129.8, 131.1, 131.2, 132.7, 135.0, 141.5, 193.0, 193.8; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{12}\text{H}_8\text{O}_2\text{S}+\text{H}$ ) 217.0323, found 217.0328 ( $\text{C}_{12}\text{H}_8\text{O}_2\text{S}+\text{H}$ ).

1-phenyl-2-(thiophen-2-yl) ethane-1, 2-dione<sup>17</sup>(4i)

1-phenyl-2-(thiophen-2-yl) ethane-1, 2-dione(**4i**). The product was isolated as a light-yellow solid (25.4 mg, 59%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 61–62 °C; IR (neat  $\text{cm}^{-1}$ ): 3010(thiophene), 1682(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1-phenyl-2-(thiophen-2-yl) ethane-1,2-dione are shown as Attached Fig.49 and Attached Fig.50 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.19-7.23 (m, 1H), 7.50-7.68 (m, 2H), 7.69-7.86 (m, 3H), 8.07 (d,  $J = 7.9$ , 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  128.7, 128.9, 130.2, 132.6, 134.8, 136.6, 136.8, 139.9, 185.5, 192.0; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{12}\text{H}_8\text{O}_2\text{S}+\text{H}$ ) 217.0323, found 217.0331 ( $\text{C}_{12}\text{H}_8\text{O}_2\text{S}+\text{H}$ ).

1-(2-chlorophenyl)-2-phenylethane-1,2-dione<sup>17</sup>(4j)

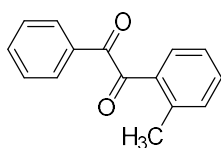
1-(2-chlorophenyl)-2-phenylethane-1,2-dione (**4j**). The product was isolated as a light-yellow solid

17 C. J. Walsh, B. K. Mandal, *J. Org. Chem.* **1999**, *64*, 6102–6105.

18 S. Newman, G. B. Iahlei, *J. Org. Chem.* **1958**, *23*, 666–669.

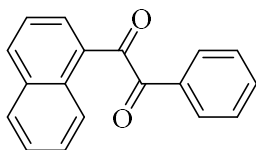
(95 mg, 78%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 8:1(v/v) as the eluent. mp 47–49 °C; IR (neat  $\text{cm}^{-1}$ ): 1685(-CO-CO-), 1622(-CO-CO-); The NMR spectra of 1-(2-chlorophenyl)-2-phenylethane-1,2-dione are shown as Attached Fig.51 and Attached Fig.52 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.41-7.57 (m, 5H), 7.64-7.67 (m, 1H), 7.89-7.94 (m, 1H), 8.02-8.05 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  127.4, 128.9, 130.2, 130.5, 132.1, 132.4, 133.8, 134.0, 134.5, 134.6, 192.1, 193.7; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{14}\text{H}_9\text{ClO}_2+\text{H}$ ) 245.0369, found 245.0374 ( $\text{C}_{14}\text{H}_9\text{ClO}_2+\text{H}$ ).

#### 1-phenyl-2-o-tolyethane-1,2-dione<sup>18</sup>(4k)



1-phenyl-2-o-tolyethane-1,2-dione(**4k**). The product was isolated as a light-yellow solid (97 mg, 87%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 5:1(v/v) as the eluent. mp 57–59 °C; IR (neat  $\text{cm}^{-1}$ ): 2960( $\text{CH}_3$ ), 2869( $\text{CH}_3$ ), 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1-phenyl-2-o-tolyethane-1,2-dione are shown as Attached Fig.53 and Attached Fig.54 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.72 (s, 3H), 7.27-7.40 (m, 2H), 7.48-7.55 (m, 3H), 7.64-7.70 (m, 2H), 7.97-7.80 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  21.9, 126.0, 127.9, 129.0, 129.9, 131.8, 132.6, 133.1, 133.8, 134.7, 141.3, 194.8, 196.8; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{15}\text{H}_{12}\text{O}_2+\text{H}$ ) 225.0916, found 225.0921 ( $\text{C}_{15}\text{H}_{12}\text{O}_2+\text{H}$ ).

#### 1-(naphthalen-1-yl)-2-phenylethane-1,2-dione<sup>19</sup> (4l)



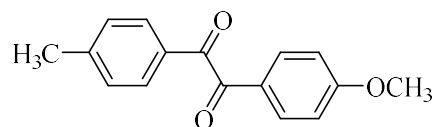
1-(naphthalen-1-yl)-2-phenylethane-1,2-dione(**4l**). The product was isolated as a light-yellow solid (118 mg, 91%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 101–102 °C; IR (neat):1680(-CO-CO-), 1620(-CO-CO-)  $\text{cm}^{-1}$ ; The NMR spectra of 1-(naphthalen-1-yl)-2-phenylethane-1,2-dione are shown as Attached Fig.55 and Attached Fig.56 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$

19 J. Tatsugi, Y. Izawa, *J. Chem. Res. S.* **1988**, 356–357.

15 E. Anders, T. Clark, T. Gassner, *Chem. Ber.* **1986**, 119, 1350–1360.

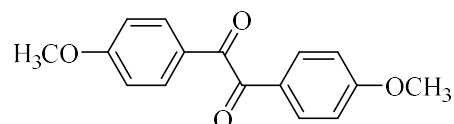
7.49-7.67 (m, 6H), 7.90-8.05 (m, 5H), 9.30-9.46 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  124.5, 126.0, 127.2, 128.6, 129.0, 129.5, 131.0, 133.4, 134.1, 134.8, 135.1, 136.0, 194.6, 197.2; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{18}\text{H}_{12}\text{O}_2+\text{H}$ ) 261.0916, found 261.0923 ( $\text{C}_{18}\text{H}_{12}\text{O}_2+\text{H}$ ).

1-(4-methoxyphenyl)-2-p-tolyloethane-1,2-dione<sup>20</sup>(4m)



1-(4-methoxyphenyl)-2-p-tolyloethane-1,2-dione(**4l**). The product was isolated as a light-yellow solid (117 mg, 92%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 97–98 °C; IR (neat): 2950( $\text{CH}_3$ ), 2860( $\text{OCH}_3$ ), 2812( $\text{OCH}_3$ ), 1680(-CO-CO-), 1620(-CO-CO-) $\text{cm}^{-1}$ ; The NMR spectra of 1-(4-methoxyphenyl)-2-p-tolyloethane-1,2-dione are shown as Attached Fig.57 and Attached Fig.58 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.43 (s, 3H), 3.88 (s, 3H), 6.97 (d,  $J = 8.9$ , 2H), 7.30 (d,  $J = 7.9$ , 2H), 7.87 (d,  $J = 8.2$ , 2H), 7.94 (d,  $J = 8.2$ , 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  127.4, 128.9, 130.2, 130.5, 132.1, 132.4, 133.8, 134.0, 134.5, 134.6, 192.1, 193.7; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{16}\text{H}_{14}\text{O}_3+\text{H}$ ) 255.1021, found 255.1028 ( $\text{C}_{16}\text{H}_{14}\text{O}_3+\text{H}$ ).

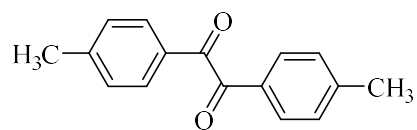
1,2-bis(4-methoxyphenyl)ethane-1,2-dione<sup>21</sup>(4n)



1,2-bis(4-methoxyphenyl)ethane-1,2-dione (**4l**). The product was isolated as a light-yellow solid (127 mg, 94%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 130–132 °C; IR (neat): 2860( $\text{OCH}_3$ ), 2812( $\text{OCH}_3$ ), 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1,2-bis(4-methoxyphenyl)ethane-1,2-dione are shown as Attached Fig.59 and Attached Fig.60 in supplementary material, respectively.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  3.87 (s, 6H), 6.96 (dd,  $J_1 = 8.9$  Hz,  $J_2 = 1.95$  Hz, 4H), 7.94 (dd,  $J_1 = 8.9$  Hz,  $J_2 = 1.98$  Hz, 4H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  55.5, 114.2, 126.2, 132.4, 164.7, 193.4; HRMS (ESI)  $m/z$  calcd for ( $\text{C}_{16}\text{H}_{14}\text{O}_4+\text{H}$ ) 271.0970, found 271.0968 ( $\text{C}_{16}\text{H}_{14}\text{O}_4+\text{H}$ ).

20 U. Wille, J. Andropof, *Aust. J. Chem.* **2007**, *60*, 420–428.

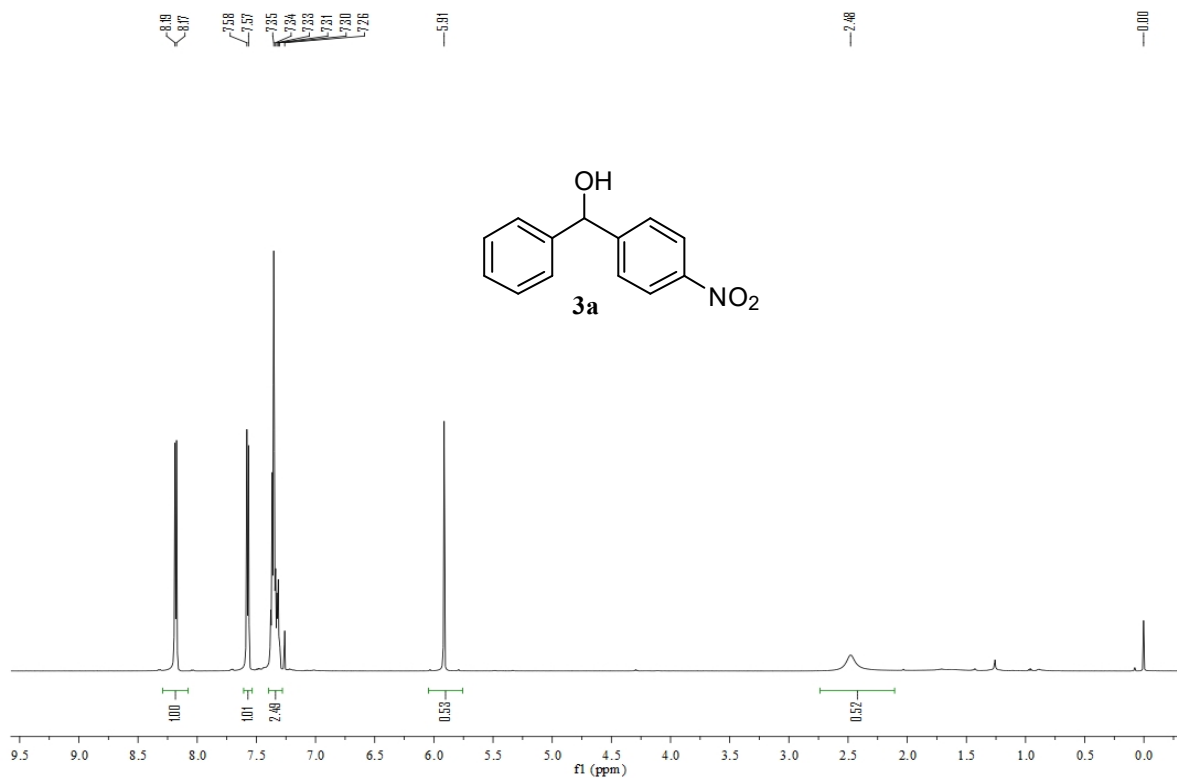
21 J. K. Joseph, S. L. Jain, B. Sain, *Eur. J. Org. Chem.* **2006**, 590–594.

1,2-dip-tolyethane-1,2-dione<sup>20</sup>(40)

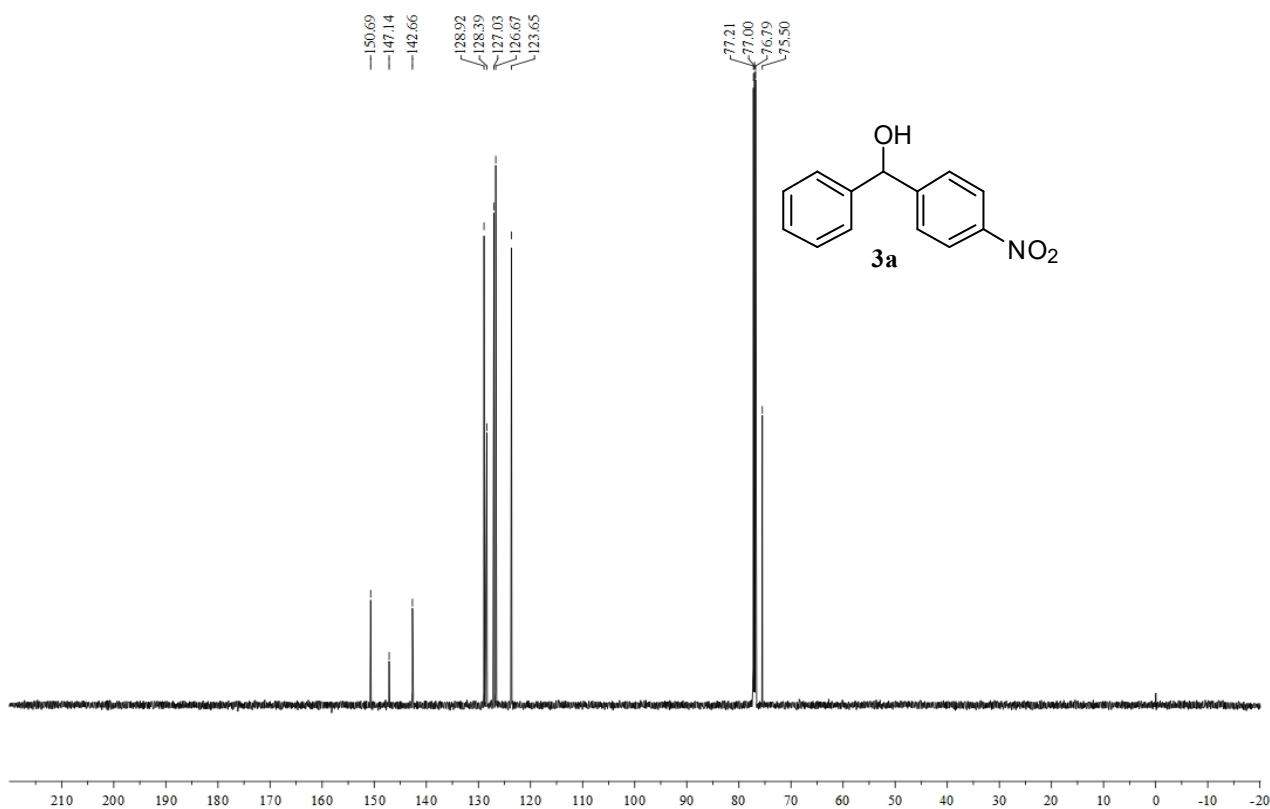
1,2-dip-tolyethane-1,2-dione(**41**). The product was isolated as a light-yellow solid (118 mg, 93%) after column chromatography purification using a solution of petroleum ether and ethyl acetate 10:1(v/v) as the eluent. mp 106–107 °C; IR (neat): 2960(CH<sub>3</sub>), 2869(CH<sub>3</sub>), 1680(-CO-CO-), 1620(-CO-CO-); The NMR spectra of 1,2-dip-tolyethane-1,2-dione are shown as Attached Fig.61 and Attached Fig.62 in supplementary material, respectively. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 2.42 (s, 6H), 7.29 (dd, *J*<sub>1</sub> = 8.46 Hz, *J*<sub>2</sub> = 0.5 Hz, 4H), 7.86 (dd, *J*<sub>1</sub> = 6.54 Hz, *J*<sub>2</sub> = 1.7 Hz, 4H), 8.02-8.05 (m, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 21.8, 129.6, 129.9, 130.6, 146.0, 194.4; HRMS (ESI) m/z calcd for (C<sub>16</sub>H<sub>14</sub>O<sub>2</sub>+H) 239.1072, found 255. 239.1076 (C<sub>16</sub>H<sub>14</sub>O<sub>2</sub>+H).



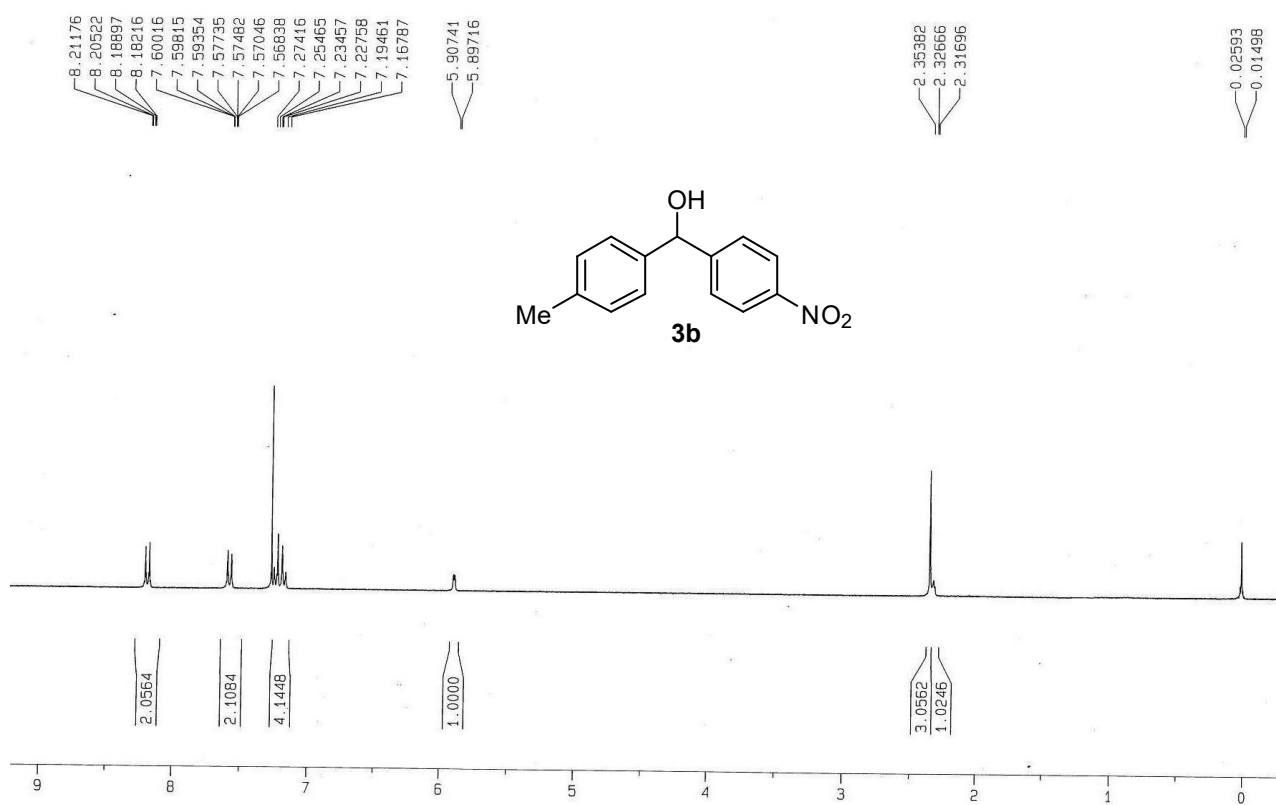
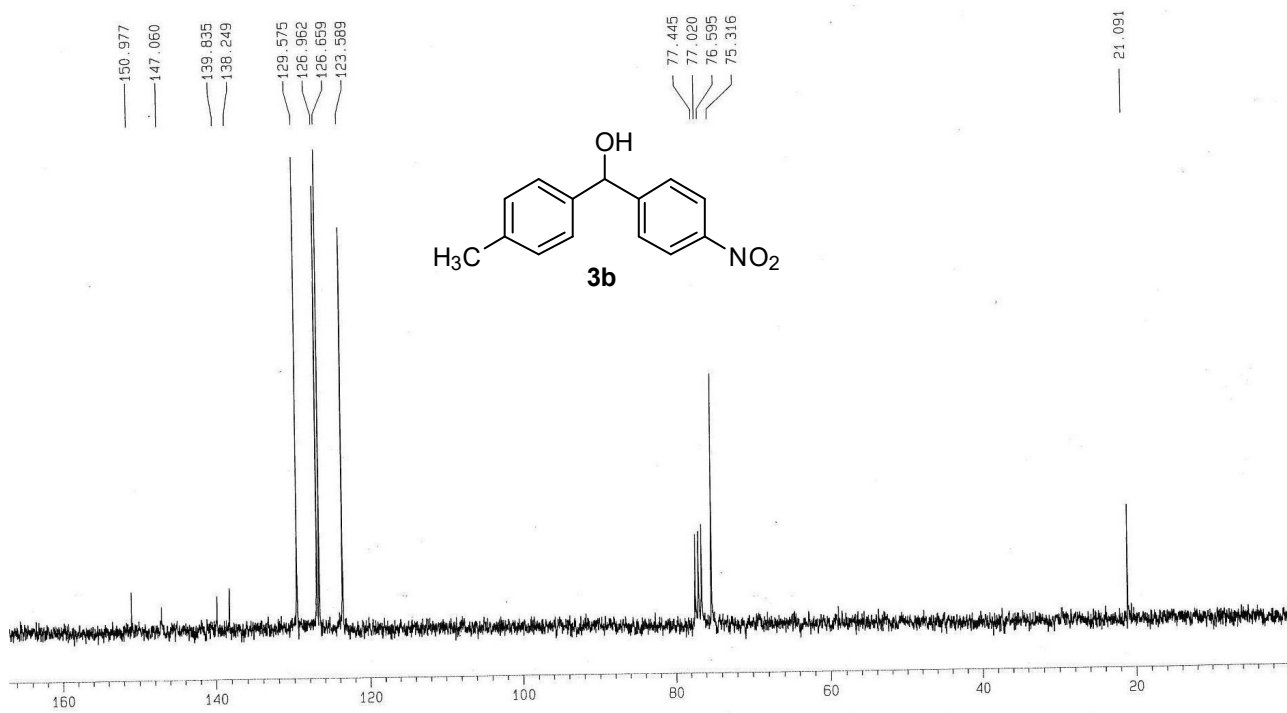
## 5. The NMR spectra of diarylmethanols

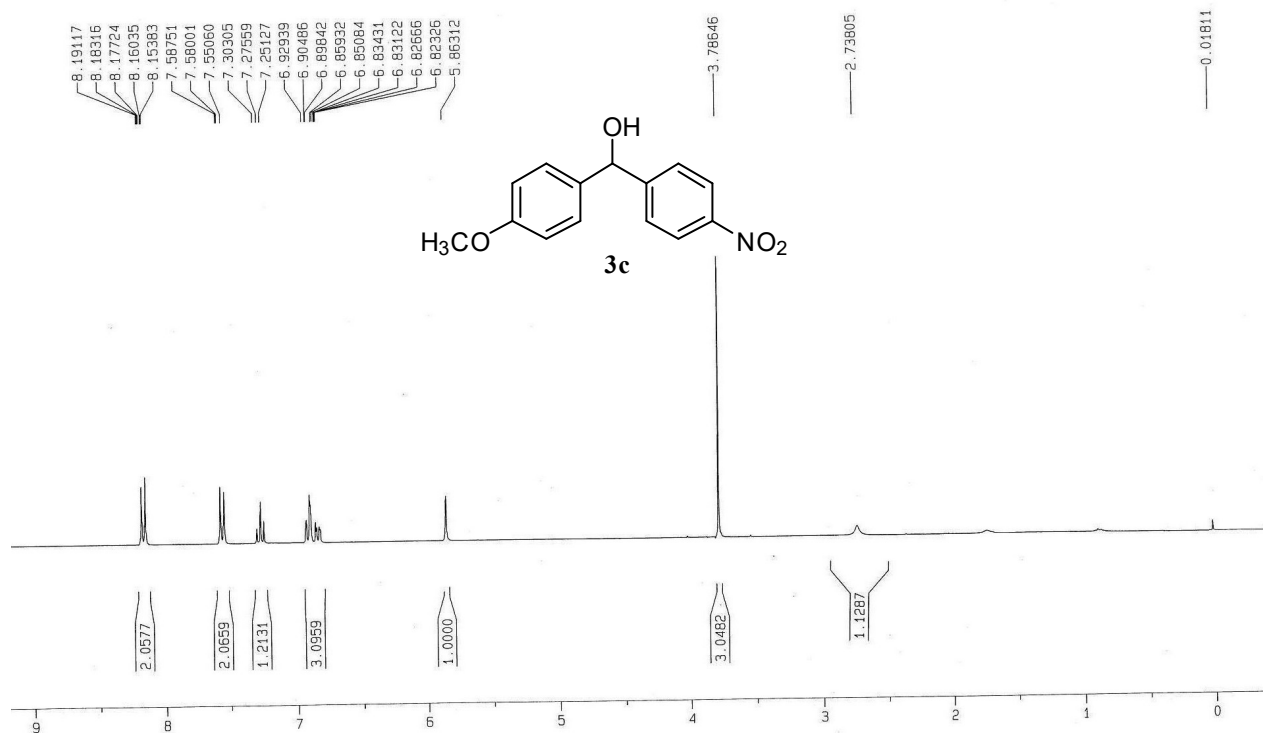


Attached Fig.1 <sup>1</sup>H NMR spectrum of (4-nitrophenyl)(phenyl)methanol recorded in CDCl<sub>3</sub>

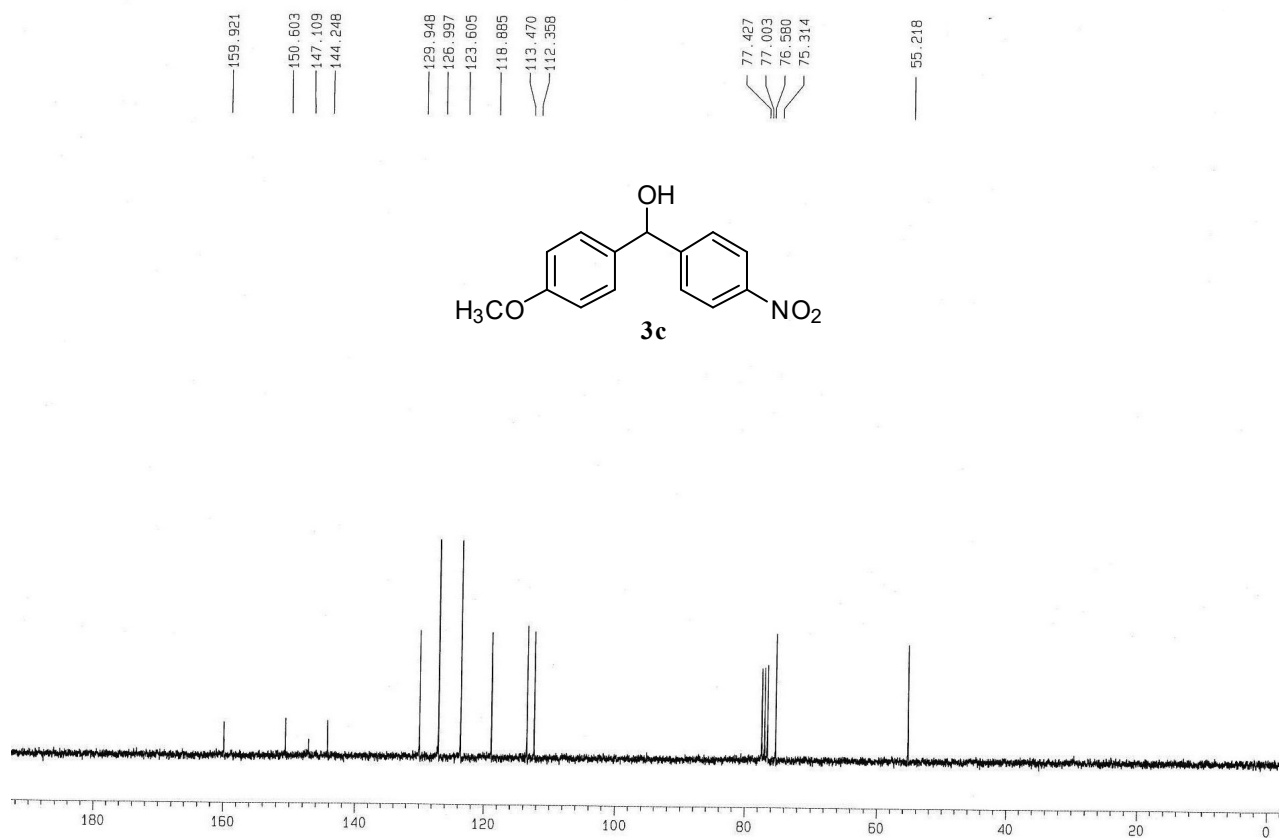


Attached Fig.2 <sup>13</sup>C NMR spectrum of (4-nitrophenyl)(phenyl)methanol recorded in CDCl<sub>3</sub>

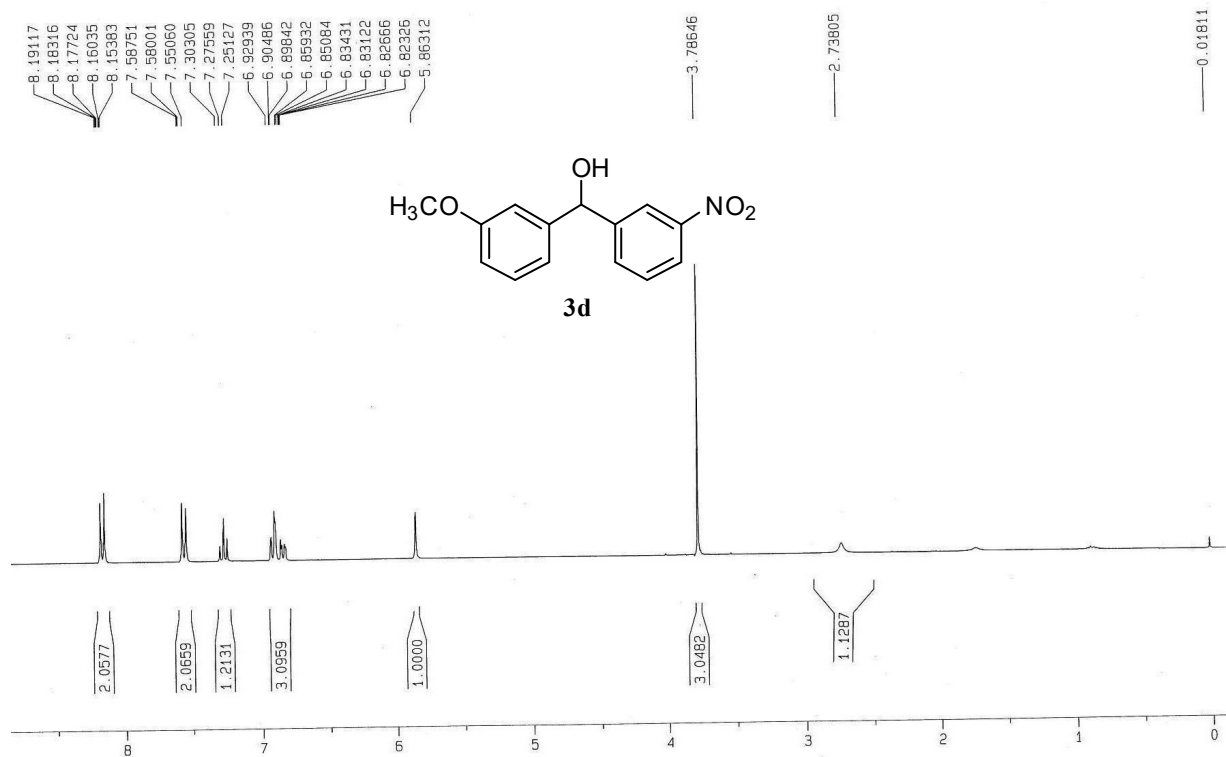
Attached Fig.3 <sup>1</sup>H NMR spectrum of (4-nitrophenyl)(*p*-tolyl)methanol recorded in CDCl<sub>3</sub>Attached Fig.4 <sup>13</sup>C NMR spectrum of (4-nitrophenyl)(*p*-tolyl)methanol recorded in CDCl<sub>3</sub>



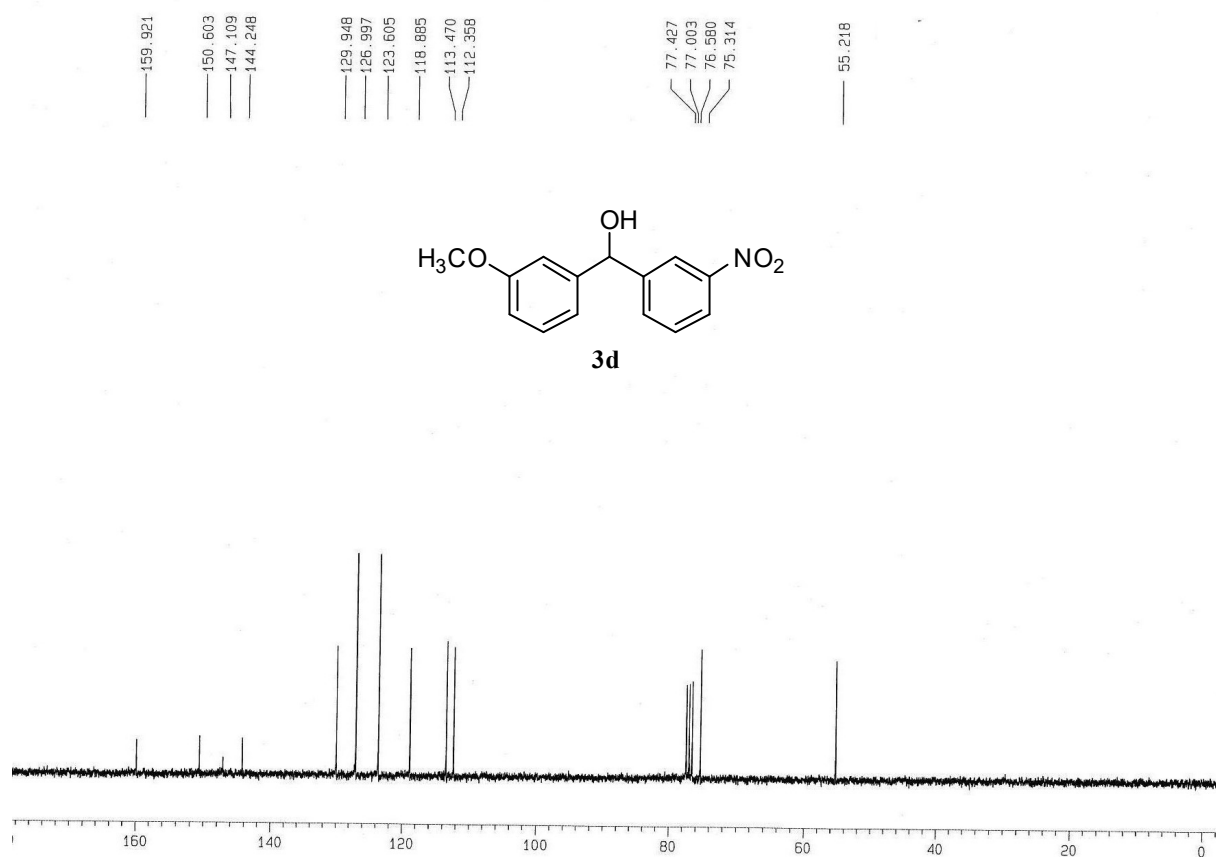
Attached Fig.5 <sup>1</sup>H NMR spectrum of (4-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



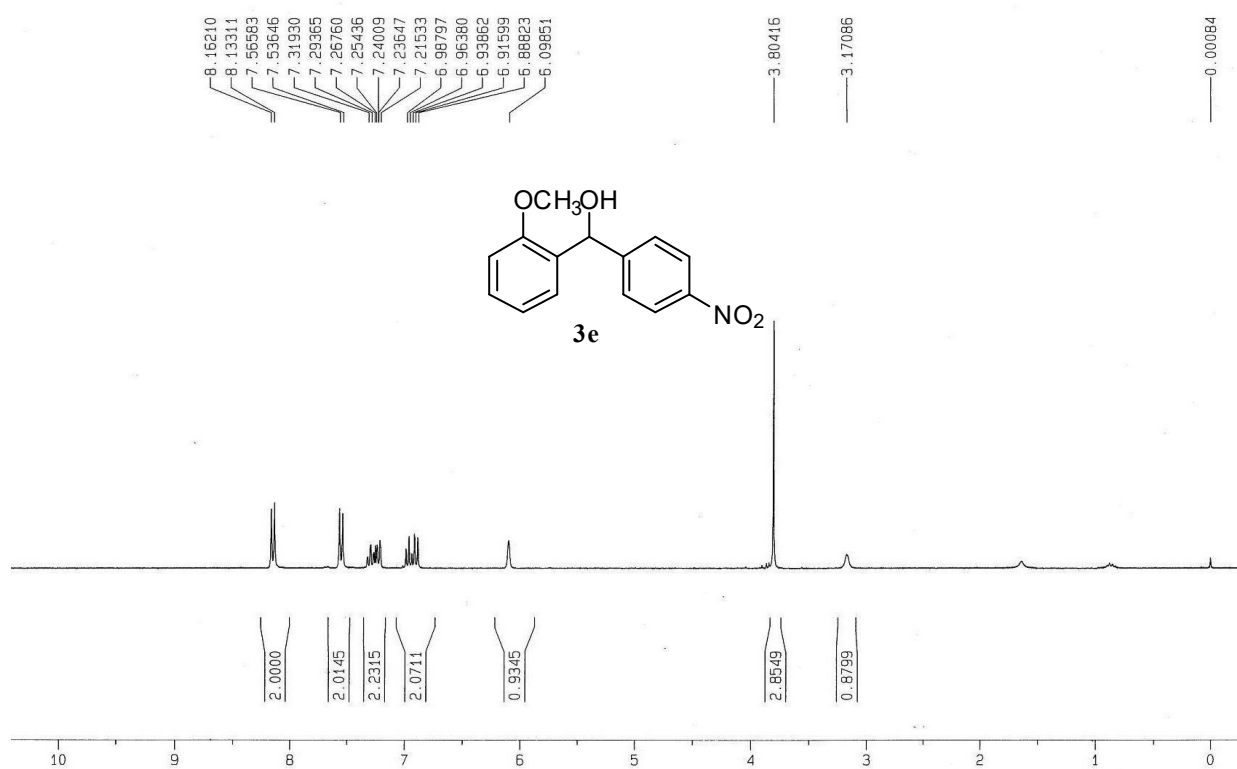
Attached Fig.6 <sup>13</sup>C NMR spectrum of (4-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



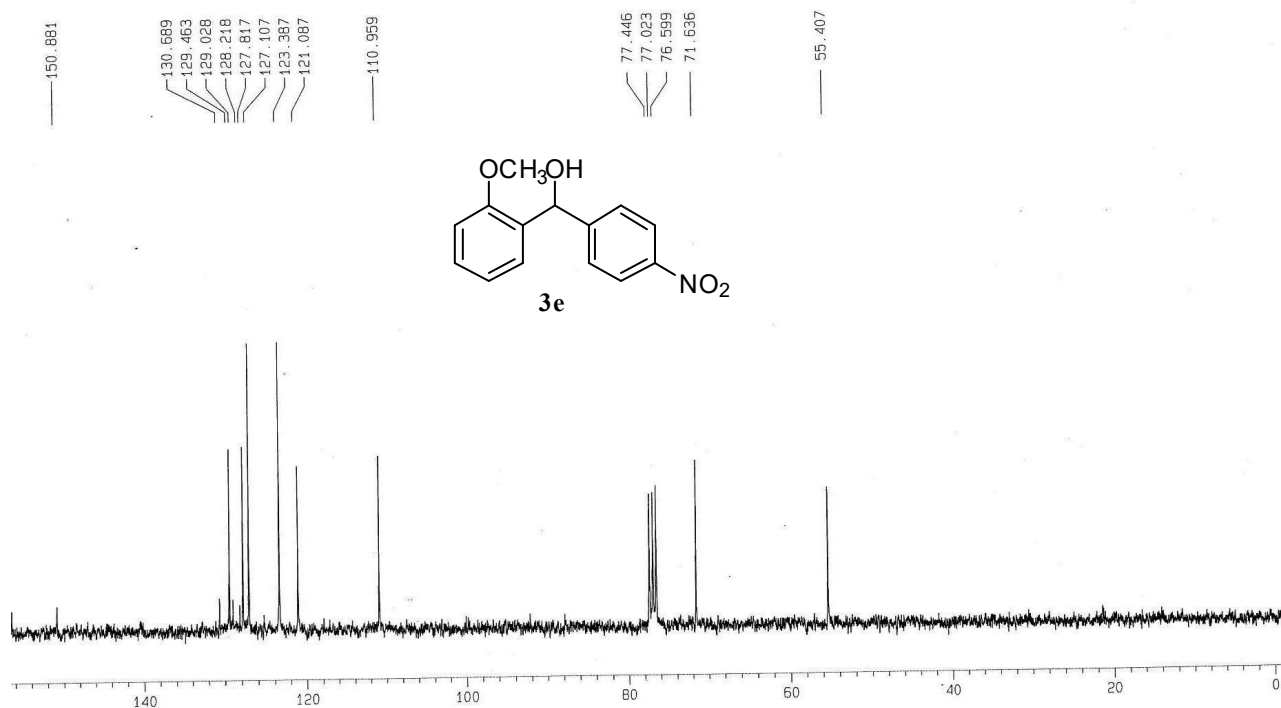
Attached Fig.7 <sup>1</sup>H NMR spectrum of (3-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



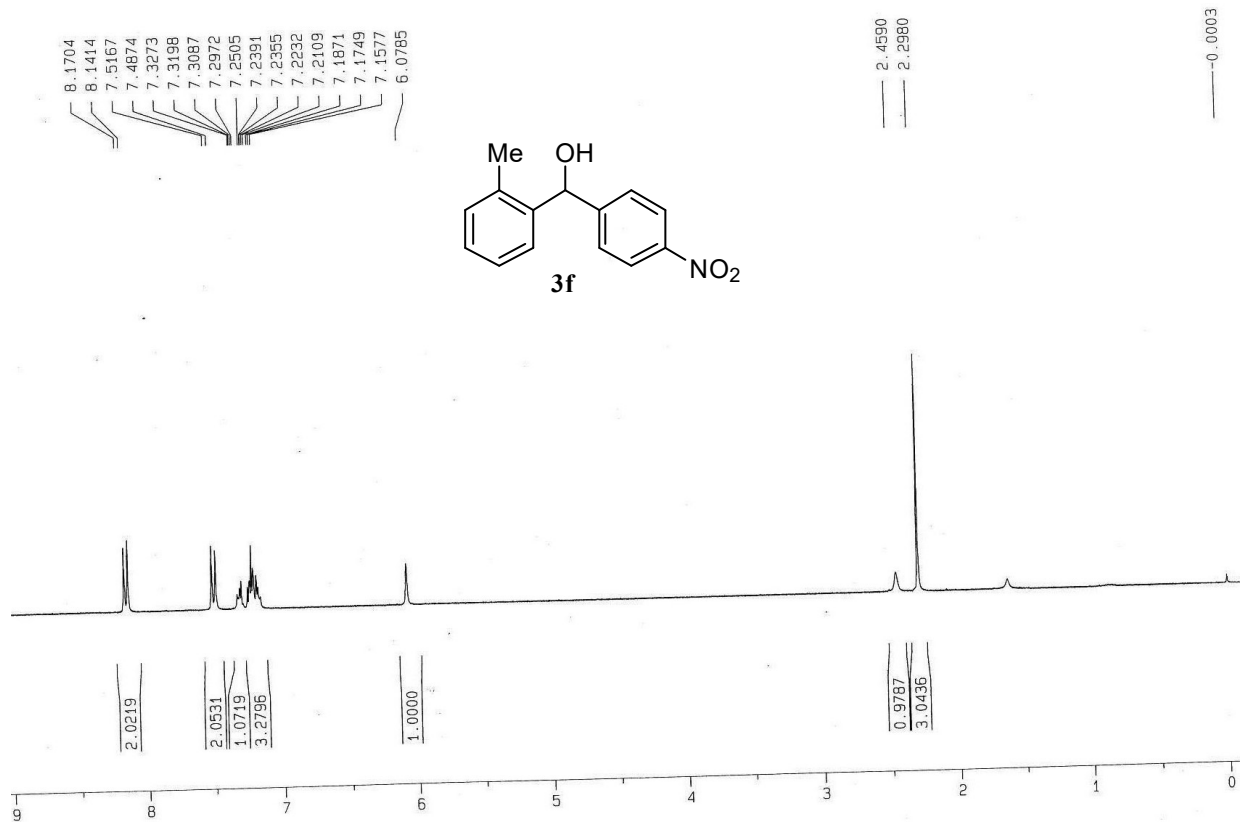
Attached Fig.8 <sup>13</sup>C NMR spectrum of (3-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



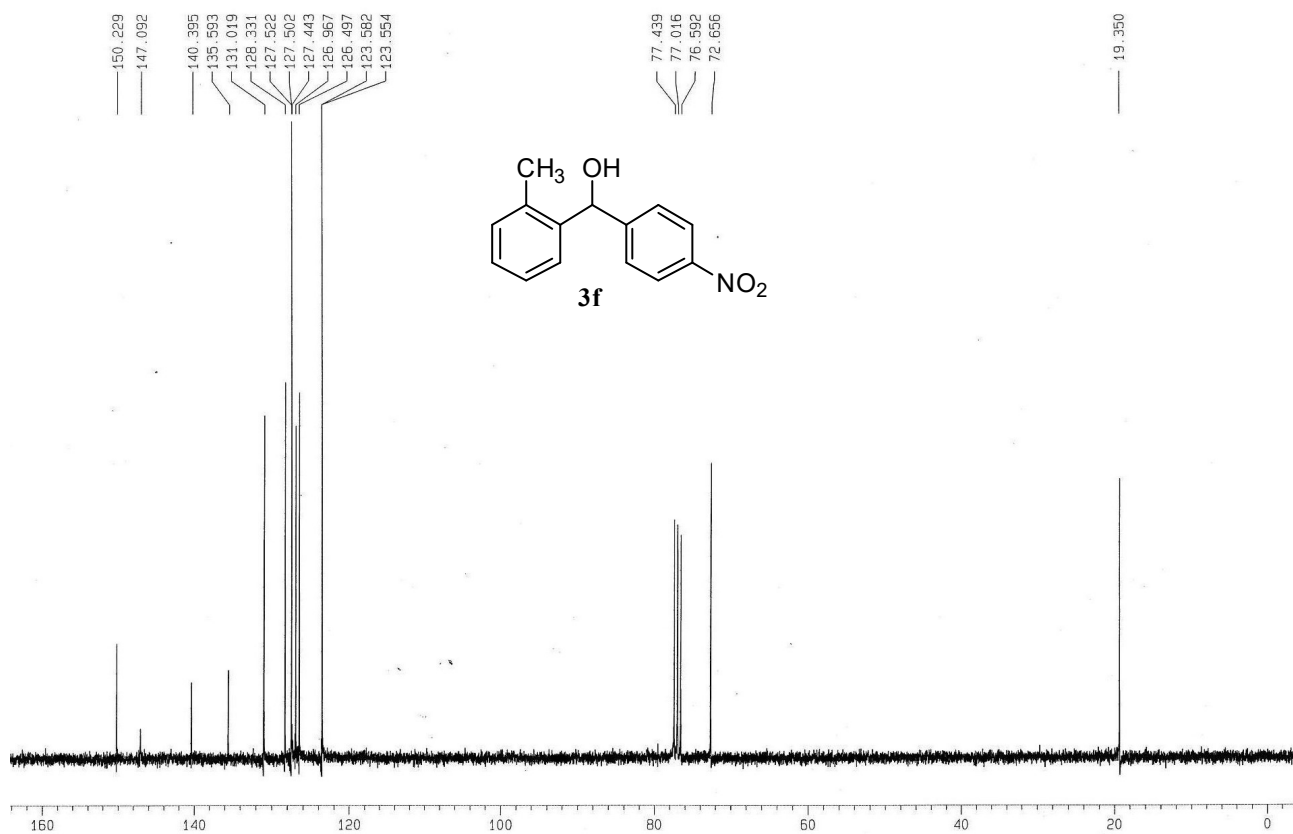
Attached Fig.9 <sup>1</sup>H NMR spectrum of (2-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



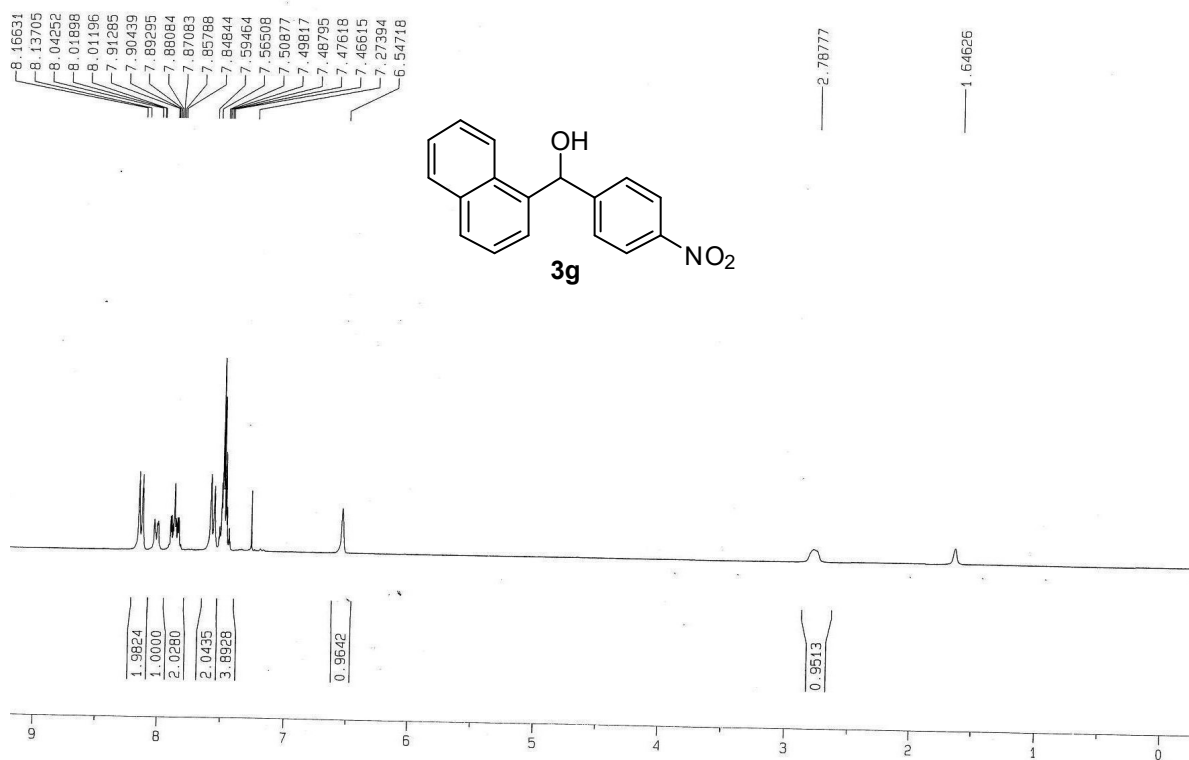
Attached Fig.10 <sup>13</sup>C NMR spectrum of (2-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



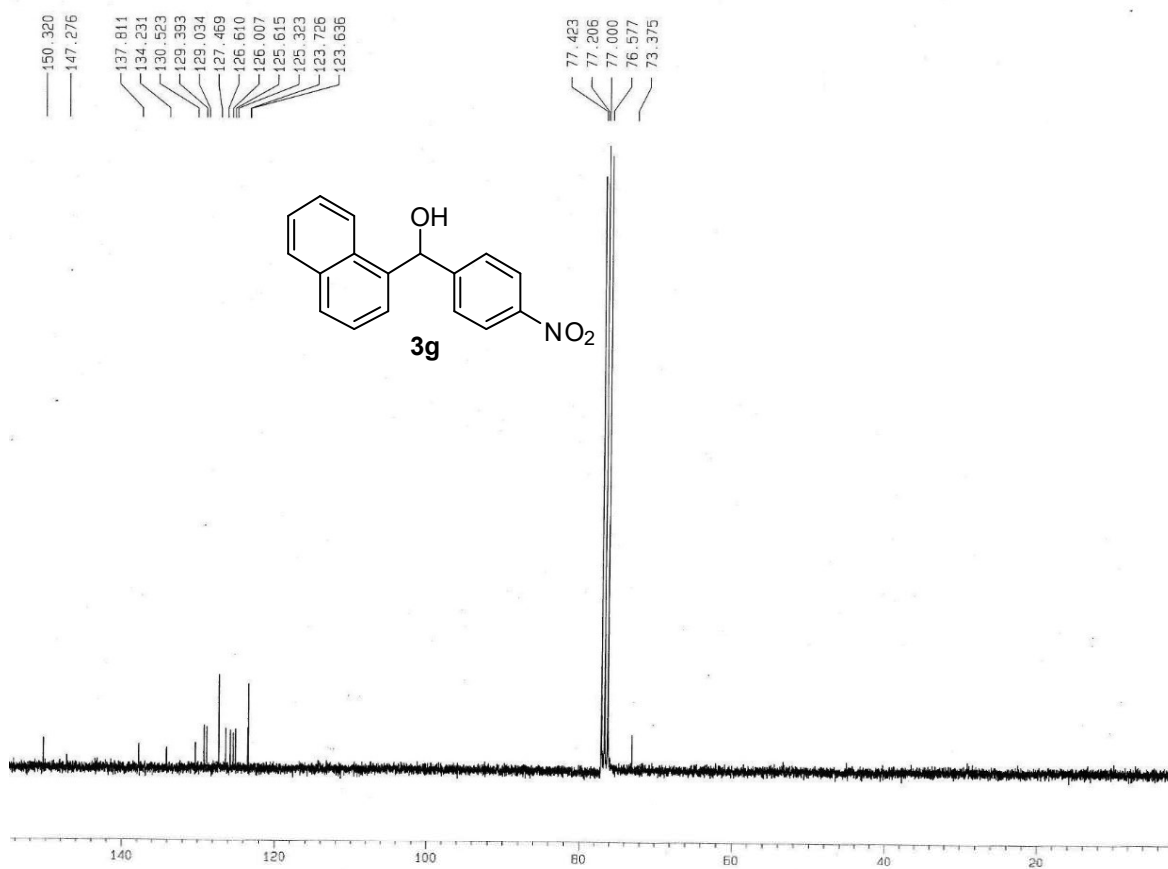
Attached Fig.11 <sup>1</sup>H NMR spectrum of (2-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



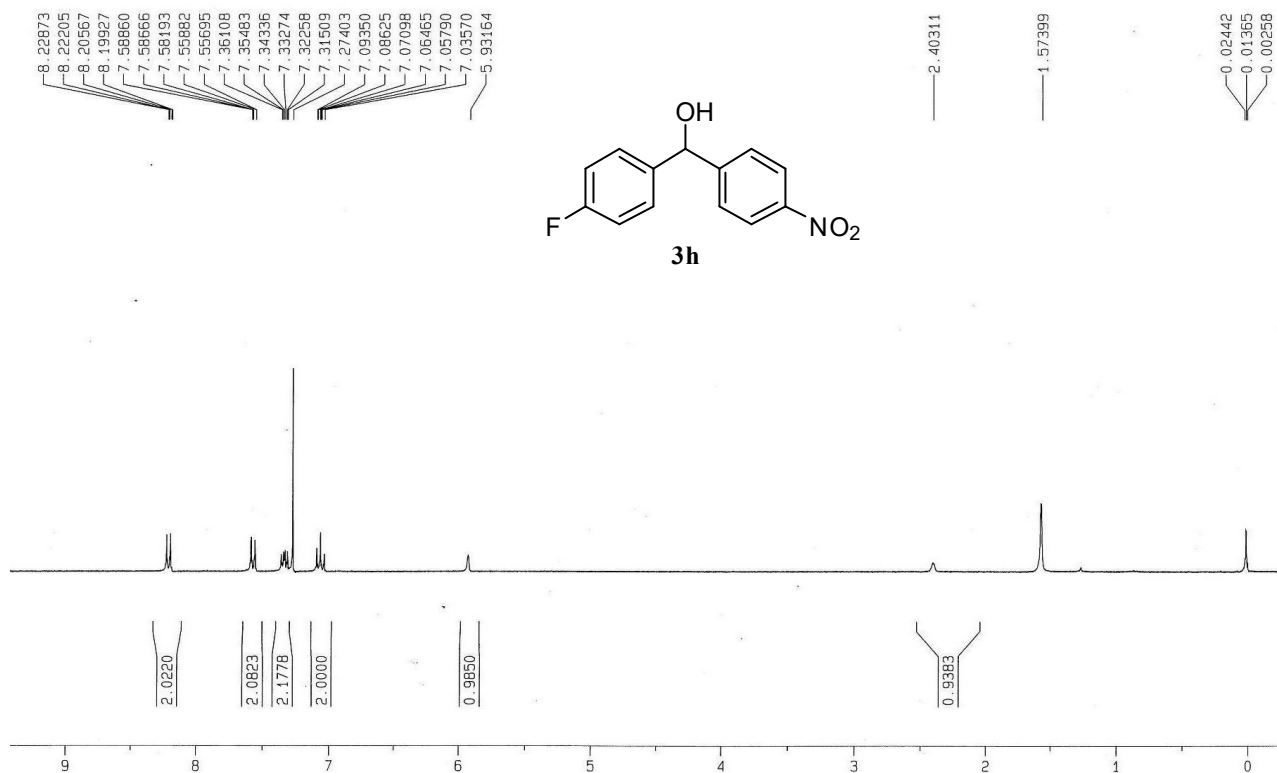
Attached Fig.12 <sup>13</sup>C NMR spectrum of (2-methoxyphenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



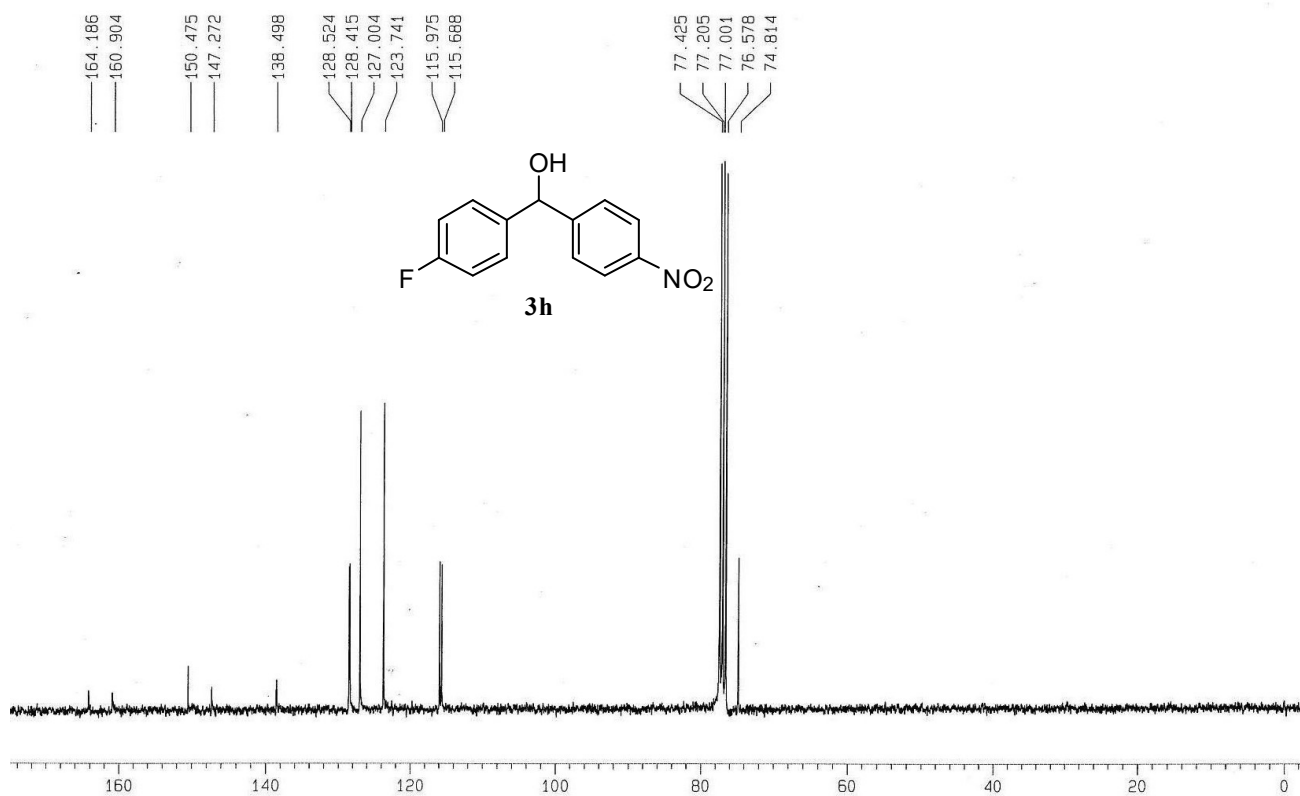
Attached Fig.13 <sup>1</sup>H NMR spectrum of naphthalen-1-yl(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



Attached Fig.14 <sup>13</sup>C NMR spectrum of naphthalen-1-yl(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>

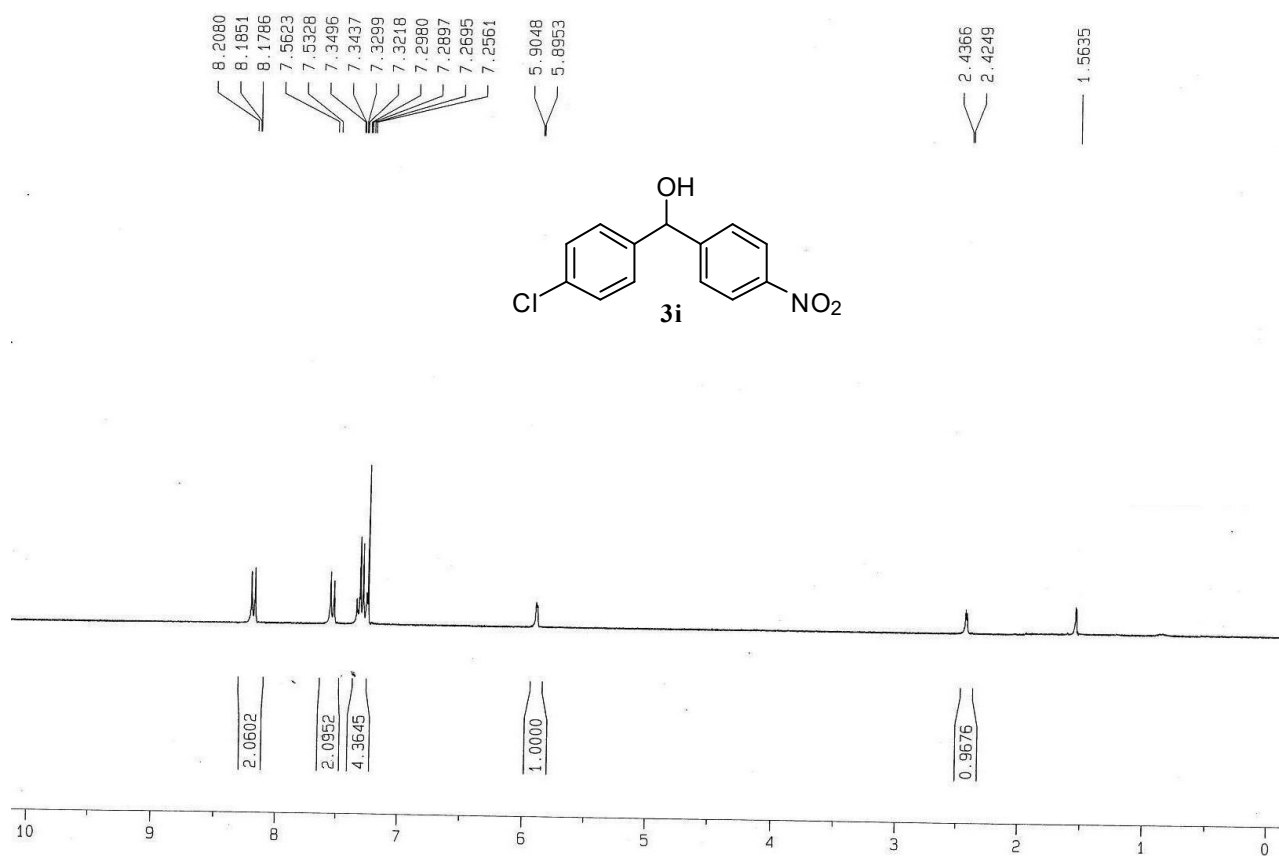


Attached Fig.15 <sup>1</sup>H NMR spectrum of (4-fluorophenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>

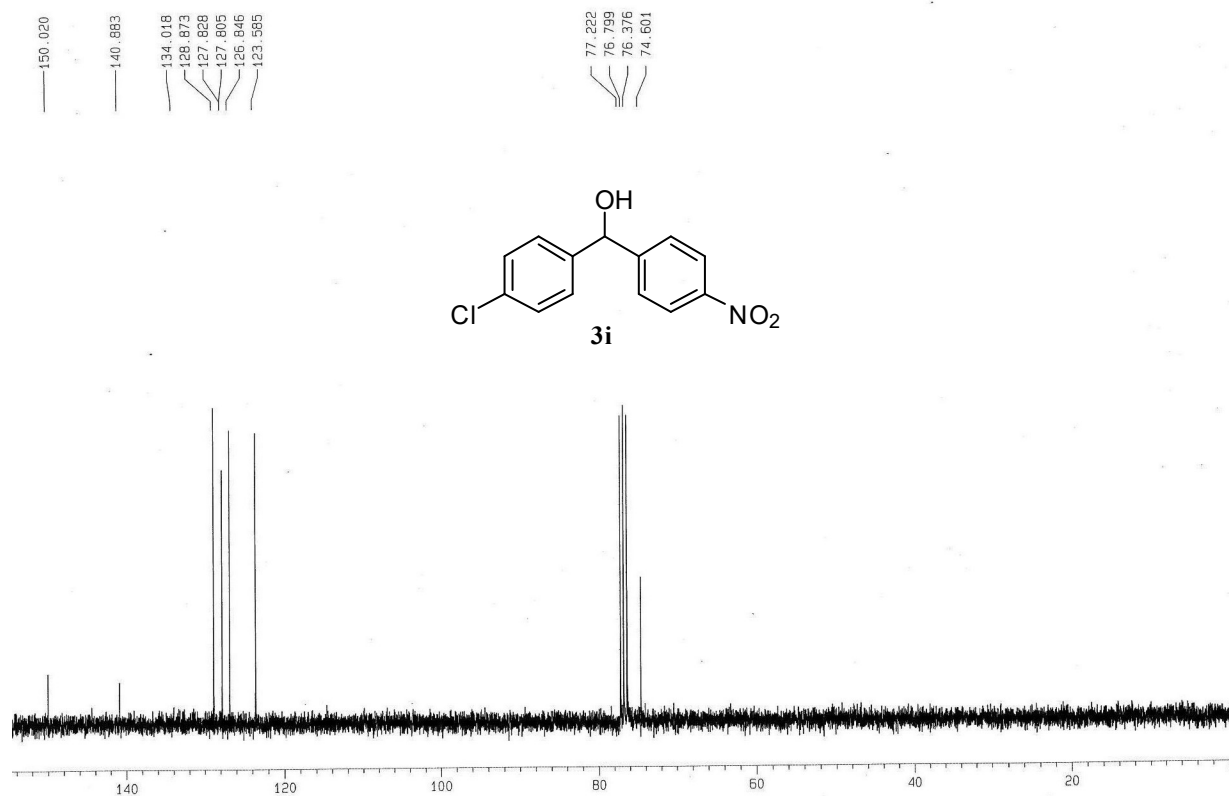


Attached Fig.16 <sup>13</sup>C NMR spectrum of (4-fluorophenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>

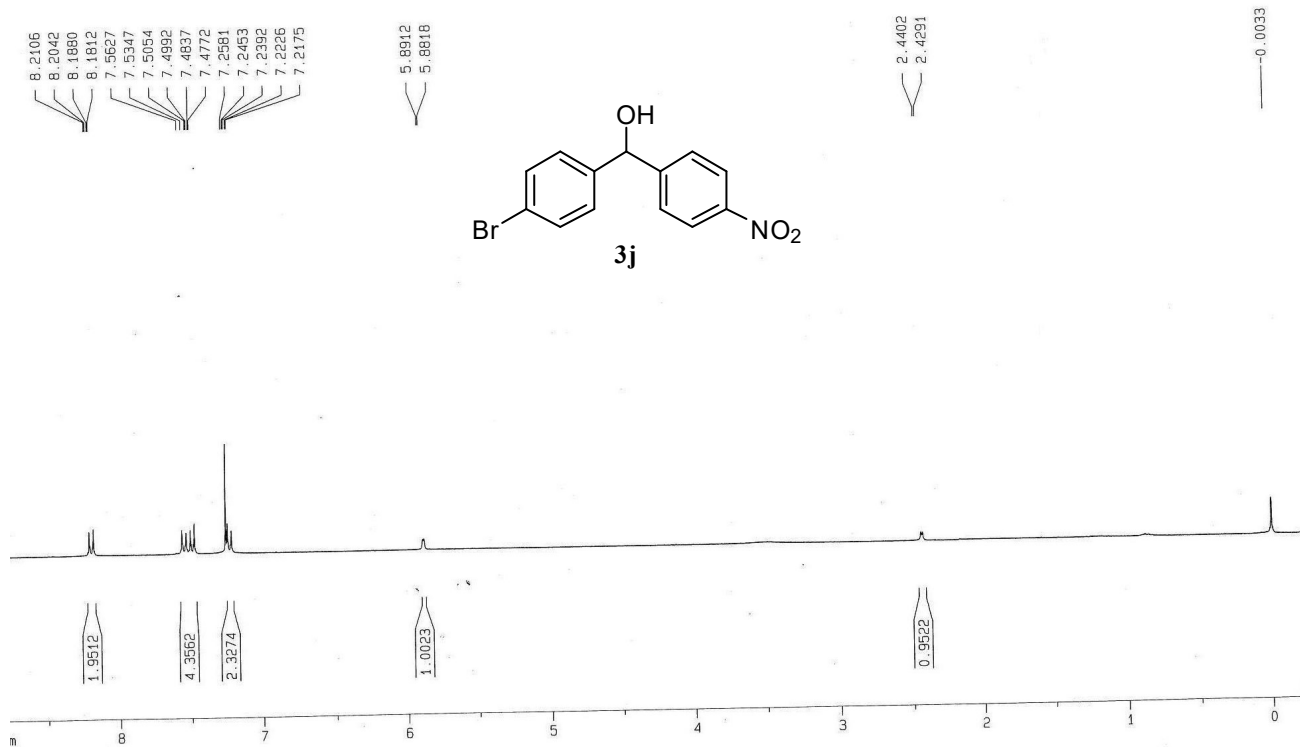




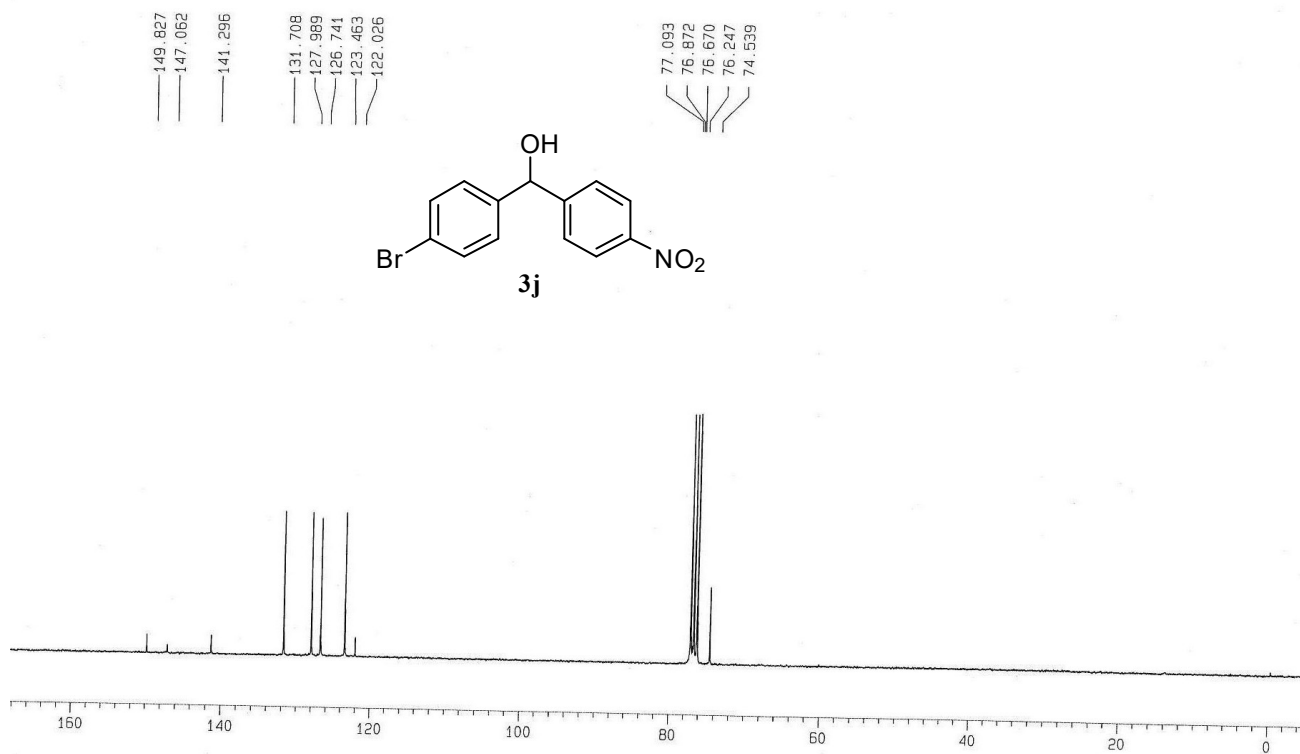
Attached Fig.17 <sup>1</sup>H NMR spectrum of (4-chlorophenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



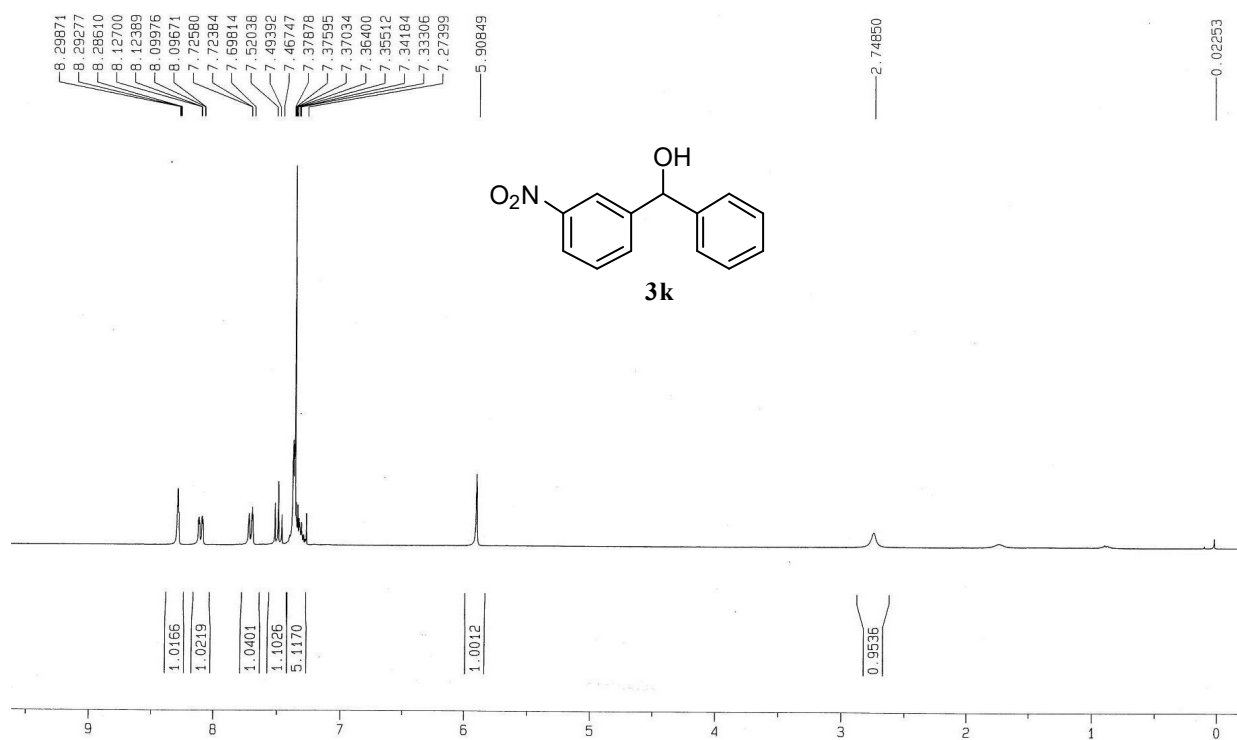
Attached Fig.18 <sup>13</sup>C NMR spectrum of (4-chlorophenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



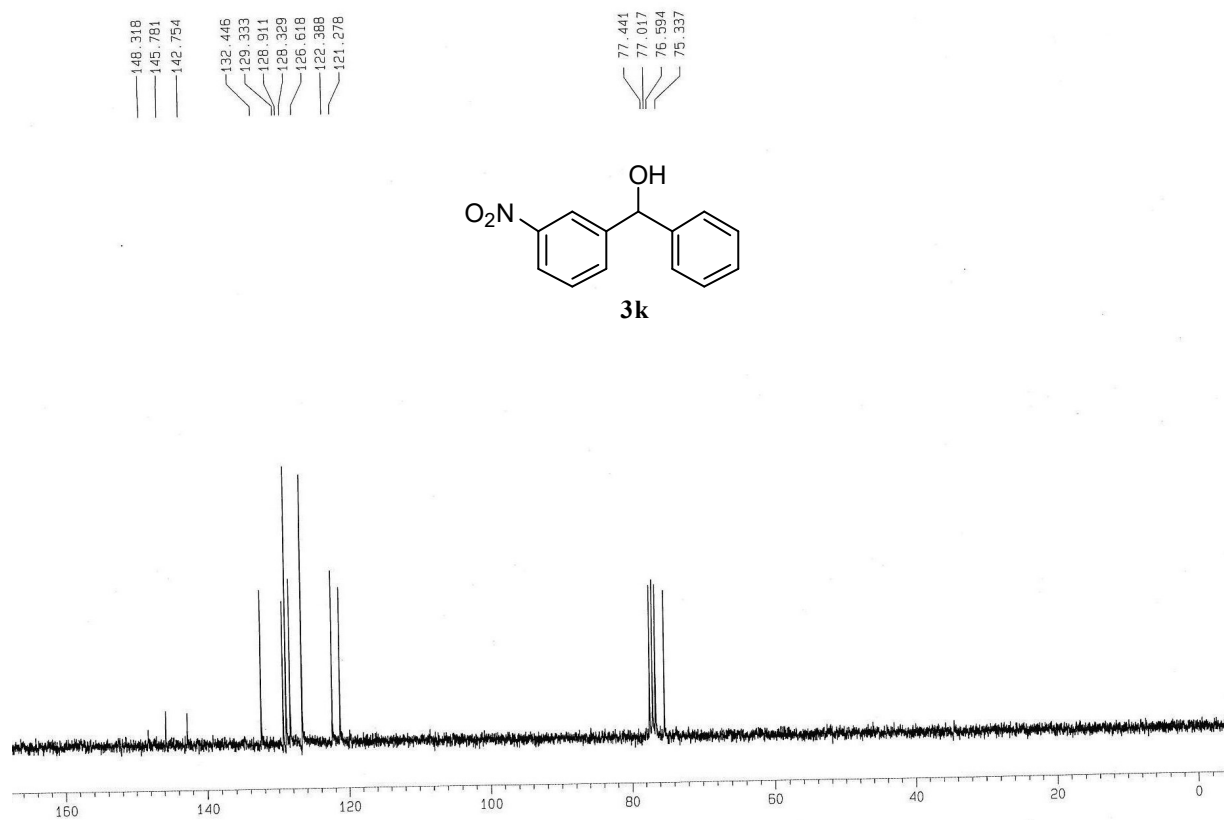
Attached Fig.19 <sup>1</sup>H NMR spectrum of (4-bromophenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



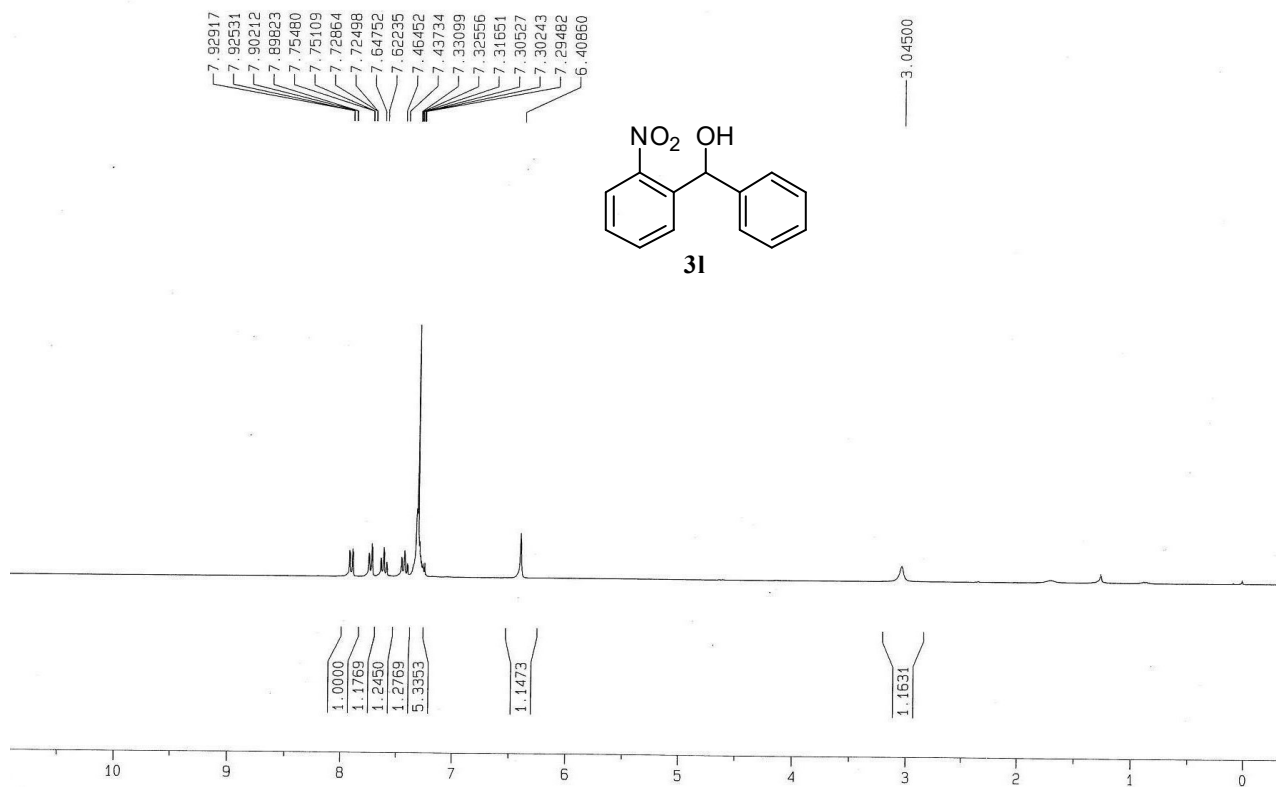
Attached Fig.20 <sup>13</sup>C NMR spectrum of (4-bromophenyl)(4-nitrophenyl)methanol recorded in CDCl<sub>3</sub>



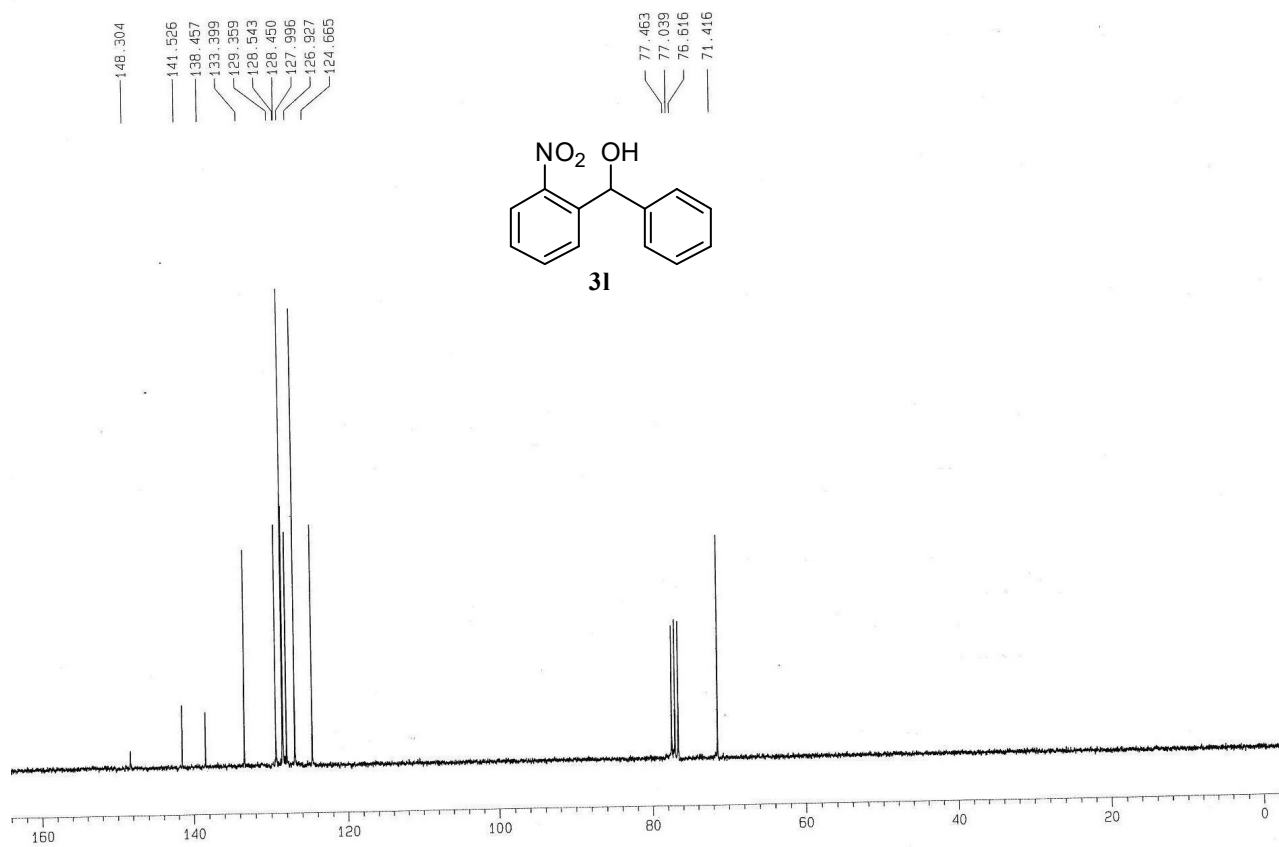
Attached Fig.21 <sup>1</sup>H NMR spectrum of (3-nitrophenyl)(phenyl)methanol recorded in CDCl<sub>3</sub>



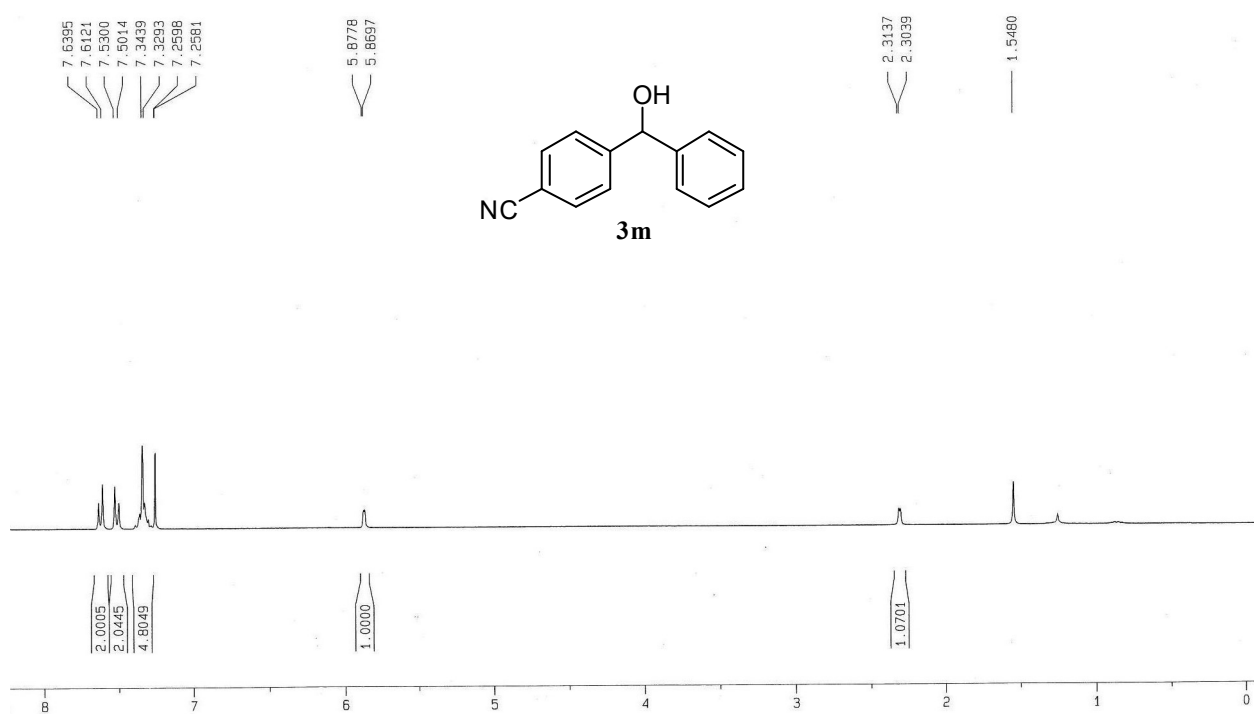
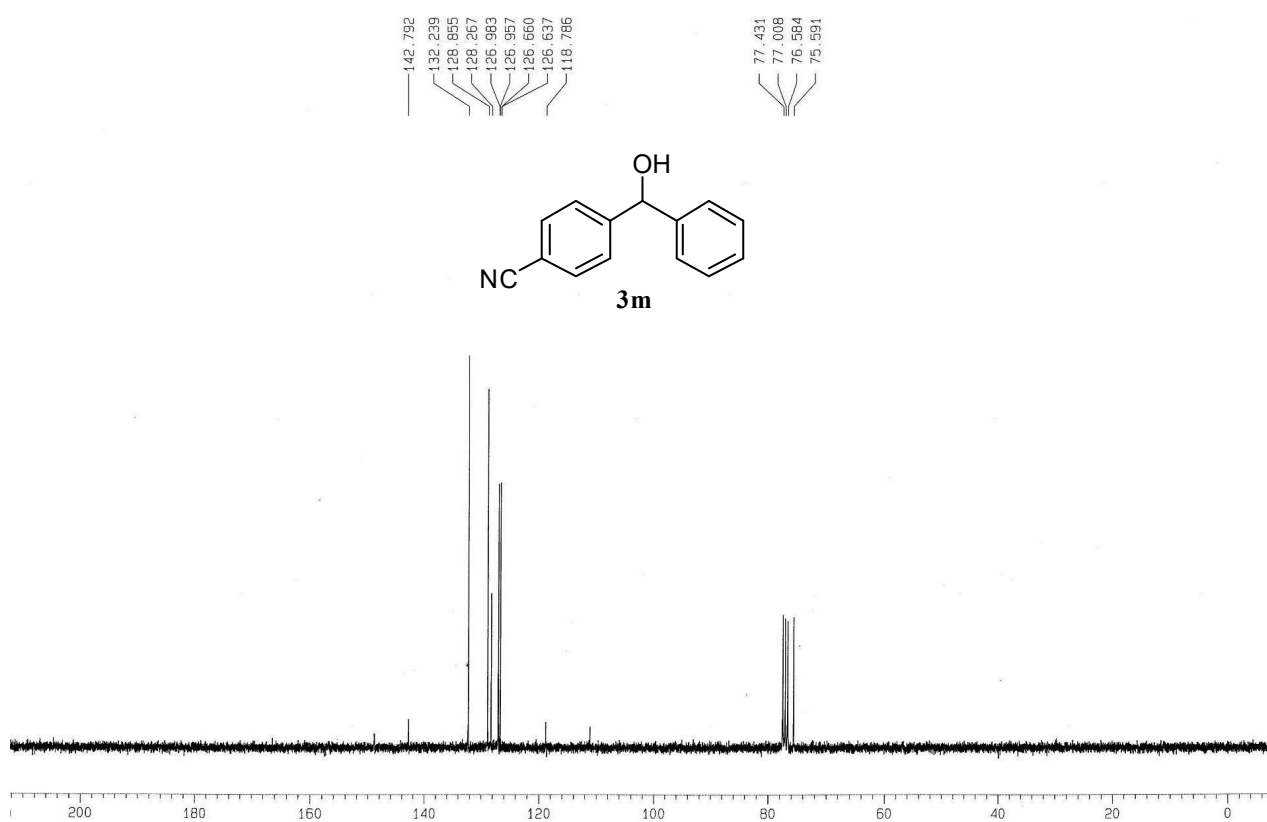
Attached Fig.22 <sup>13</sup>C NMR spectrum of (3-nitrophenyl)(phenyl)methanol recorded in CDCl<sub>3</sub>

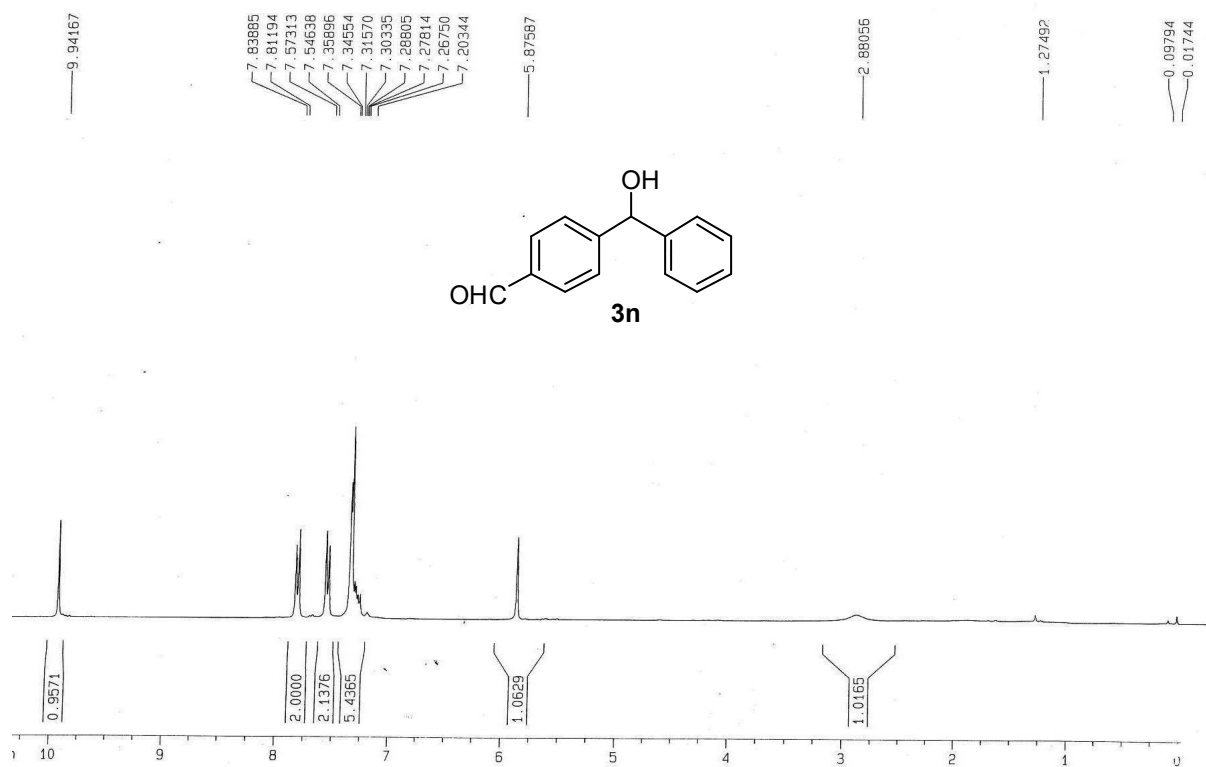
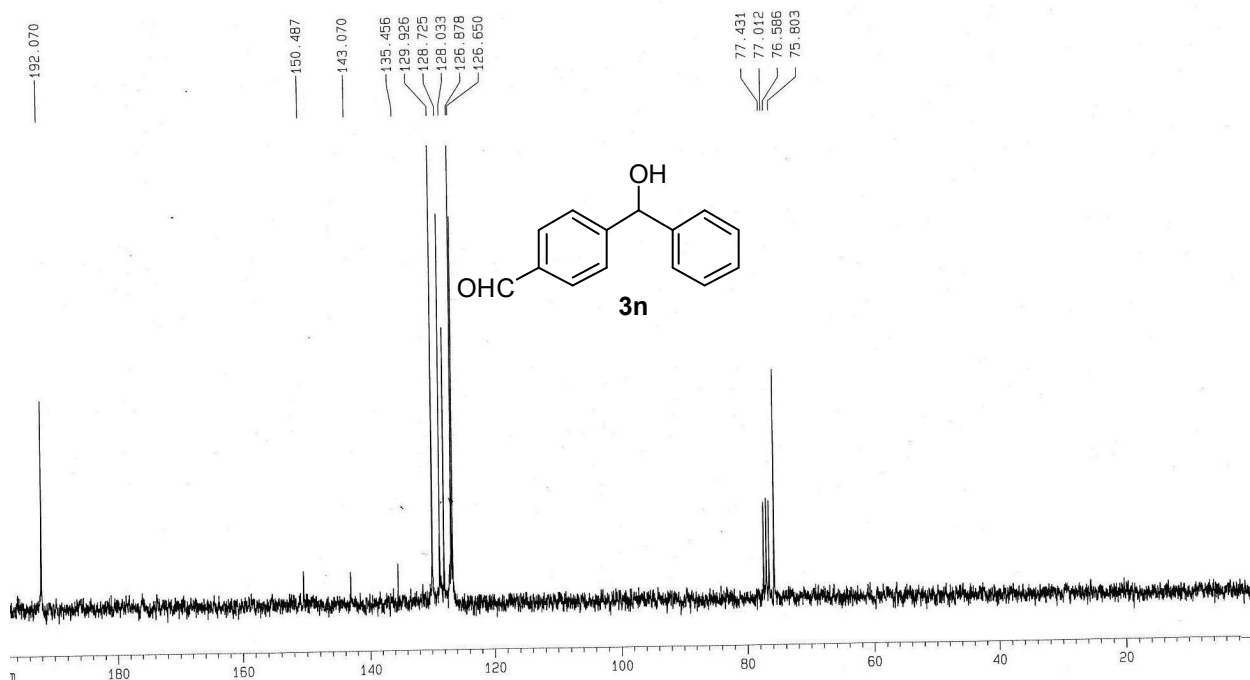


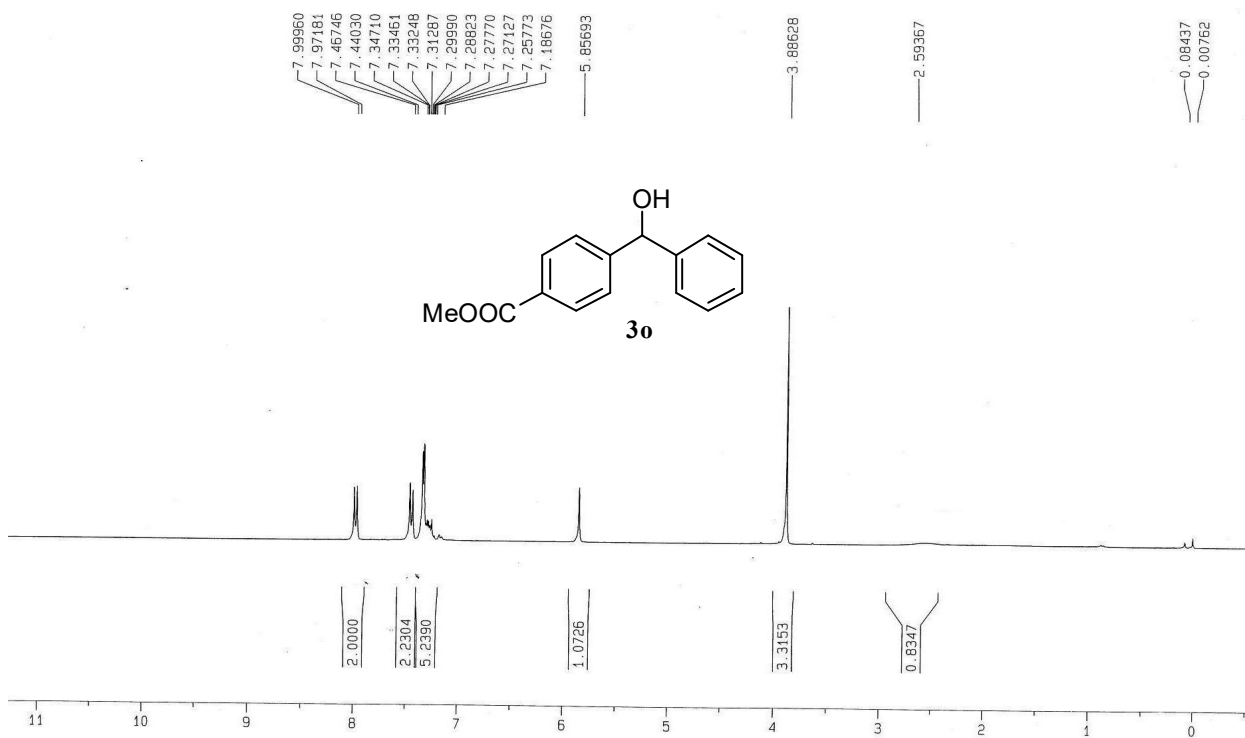
Attached Fig.23 <sup>1</sup>H NMR spectrum of (2-nitrophenyl)(phenyl)methanol recorded in CDCl<sub>3</sub>



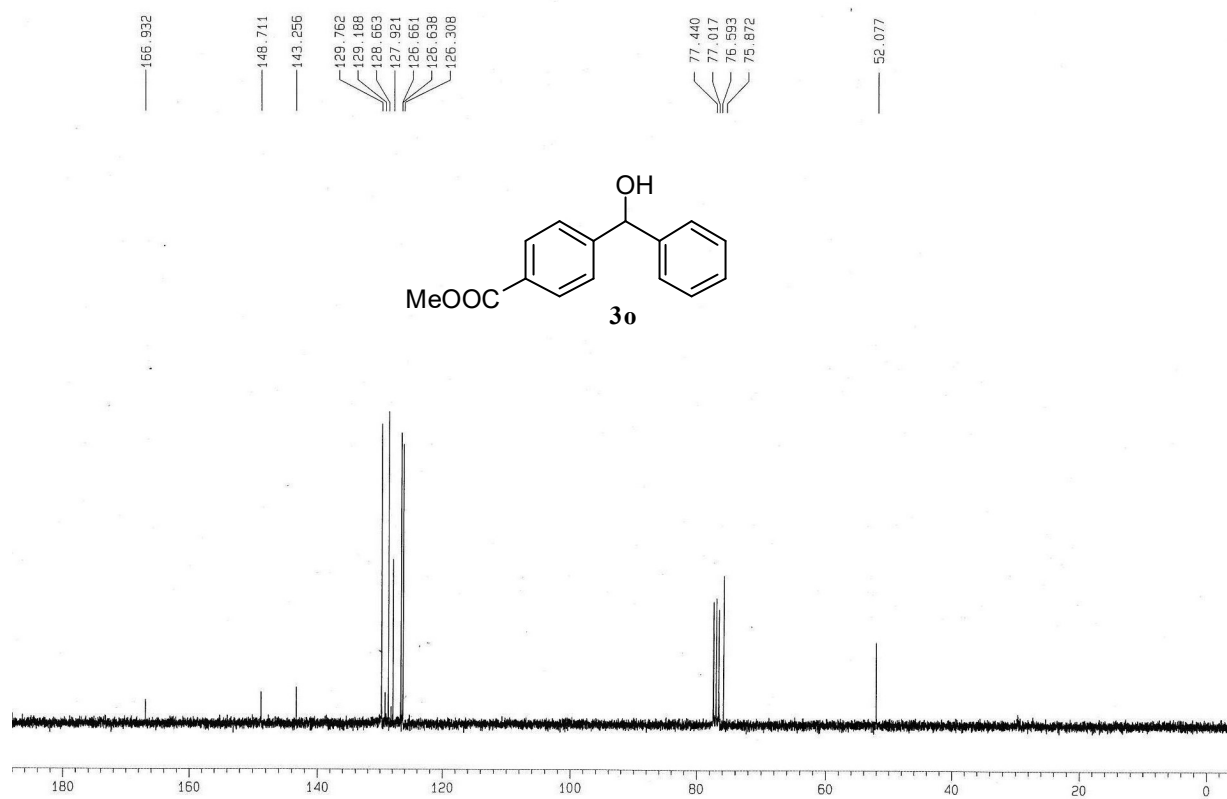
Attached Fig.24 <sup>13</sup>C NMR spectrum of (2-nitrophenyl)(phenyl)methanol recorded in CDCl<sub>3</sub>

Attached Fig.25 <sup>1</sup>H NMR spectrum of 4-(hydroxy(phenyl)methyl)benzonitrile recorded in CDCl<sub>3</sub>Attached Fig.26 <sup>13</sup>C NMR spectrum of 4-(hydroxy(phenyl)methyl)benzonitrile recorded in CDCl<sub>3</sub>

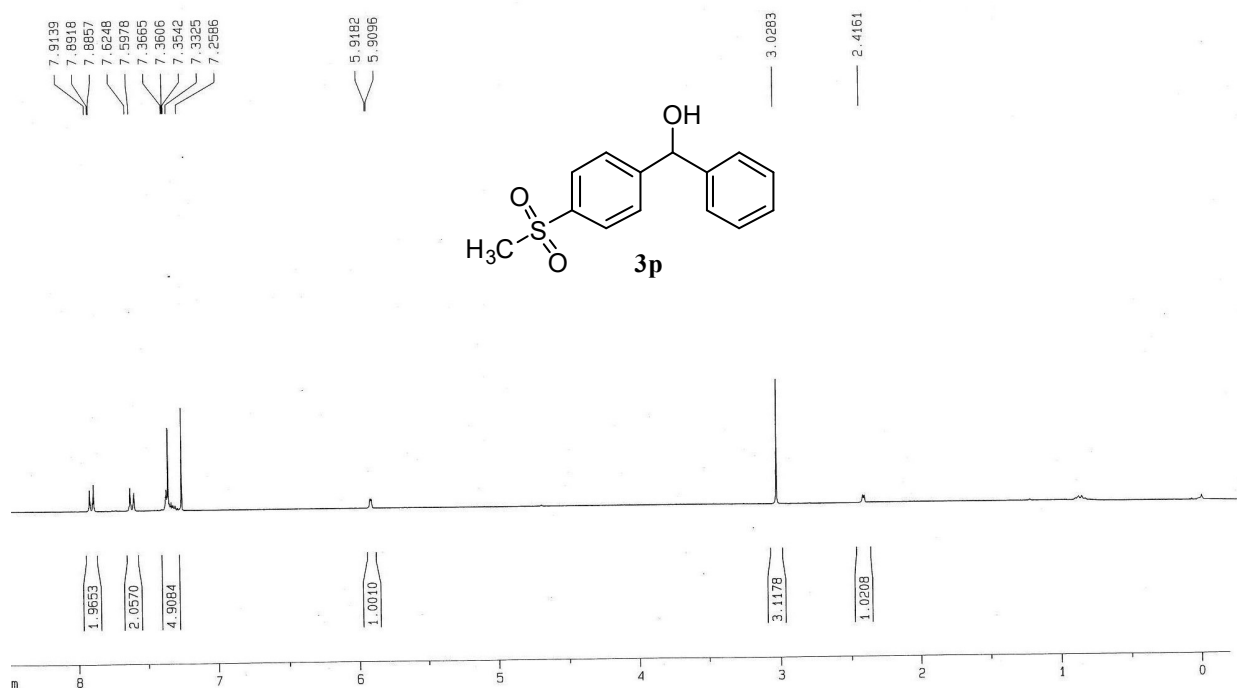
Attached Fig.27 <sup>1</sup>H NMR spectrum of 4-(hydroxy(phenyl)methyl)benzamide recorded in CDCl<sub>3</sub>Attached Fig.28 <sup>13</sup>C NMR spectrum of 4-(hydroxy(phenyl)methyl)benzamide recorded in CDCl<sub>3</sub>



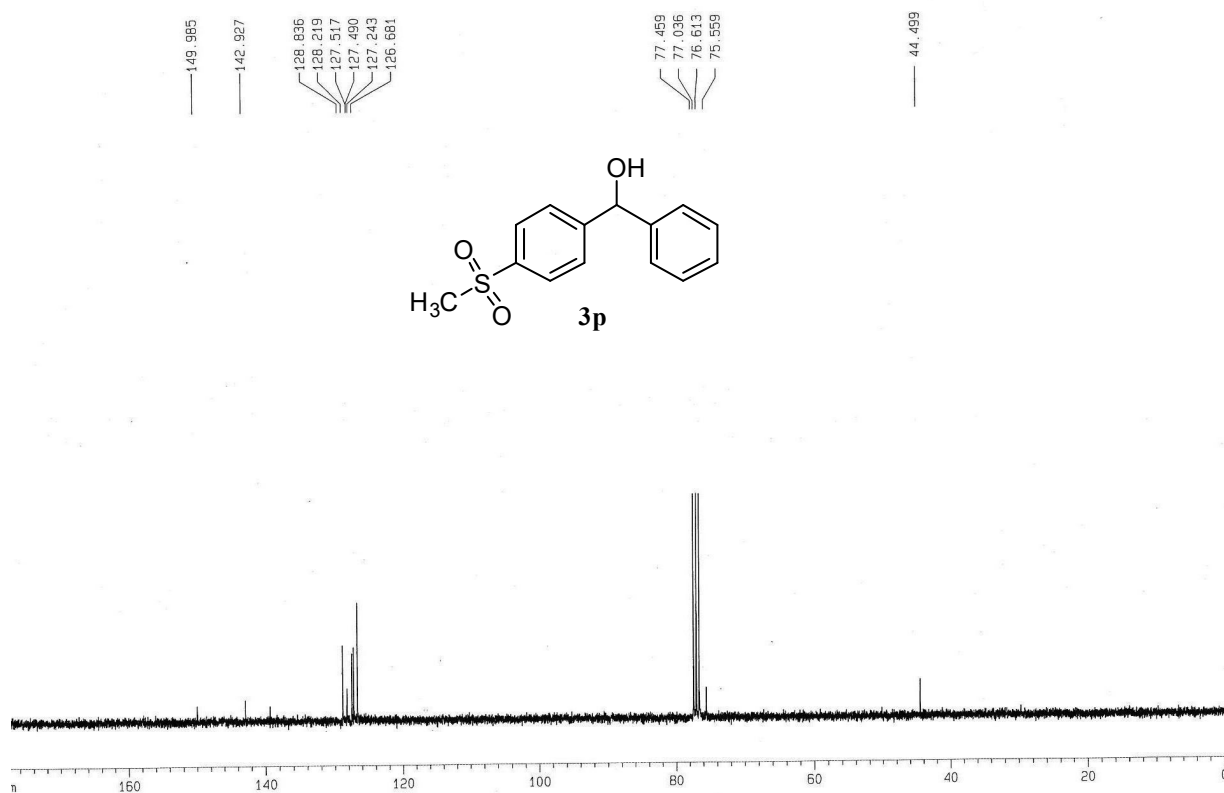
Attached Fig.29 <sup>1</sup>H NMR spectrum of 4-(hydroxy(phenyl)methyl)benzonitrile recorded in CDCl<sub>3</sub>



Attached Fig.30 <sup>13</sup>C NMR spectrum of 4-(hydroxy(phenyl)methyl)benzonitrile recorded in CDCl<sub>3</sub>



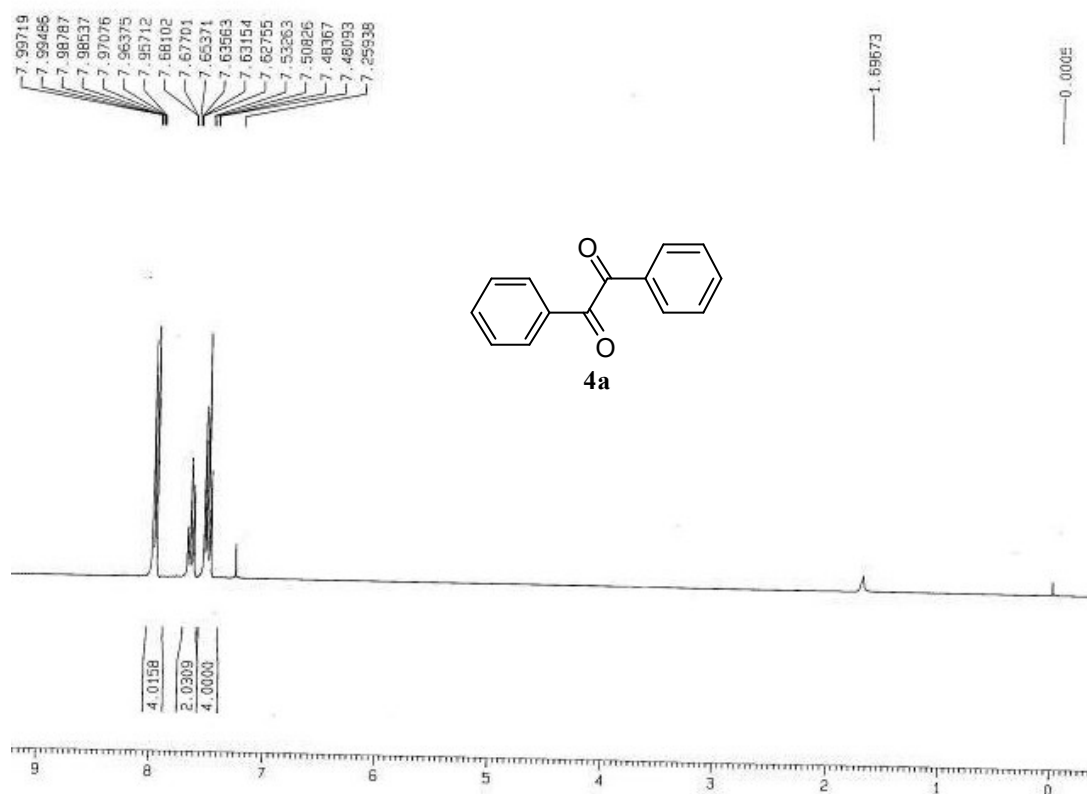
Attached Fig.31 <sup>1</sup>H NMR spectrum of 4-(hydroxy(phenyl)methyl)benzenitrile recorded in CDCl<sub>3</sub>



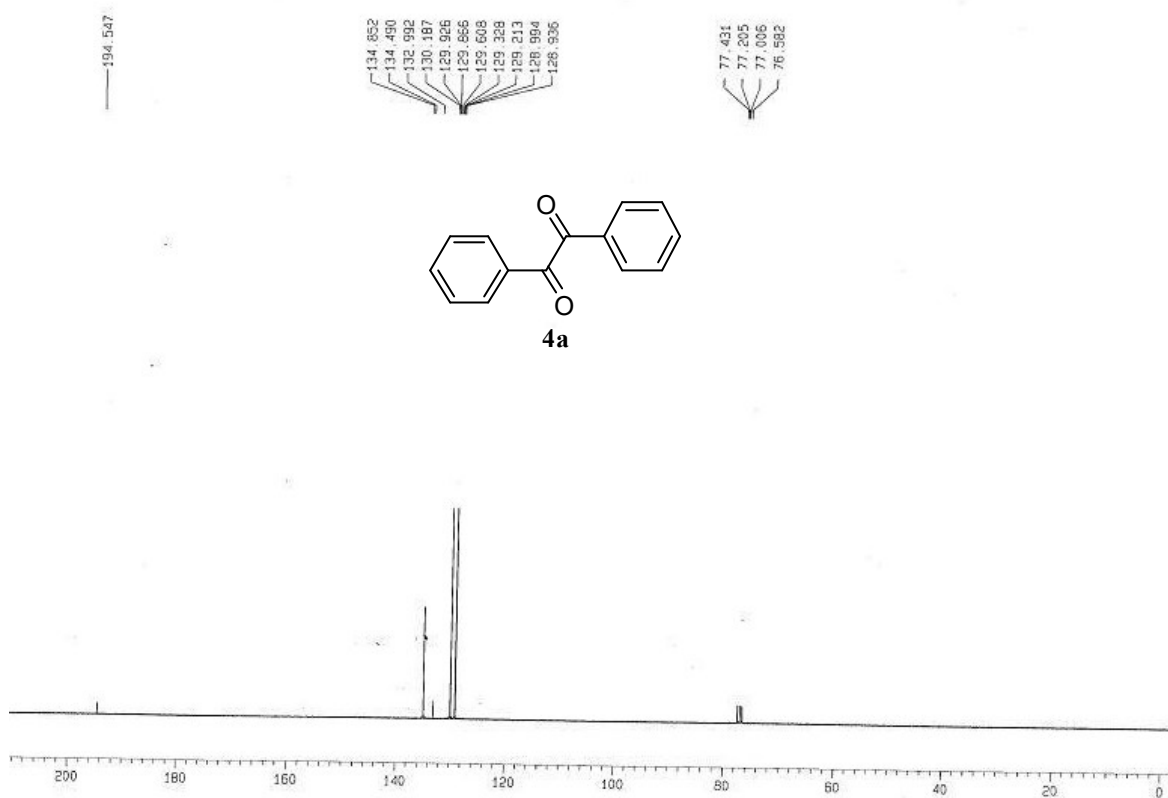
Attached Fig.32 <sup>13</sup>C NMR spectrum of 4-(hydroxy(phenyl)methyl)benzenitrile recorded in CDCl<sub>3</sub>



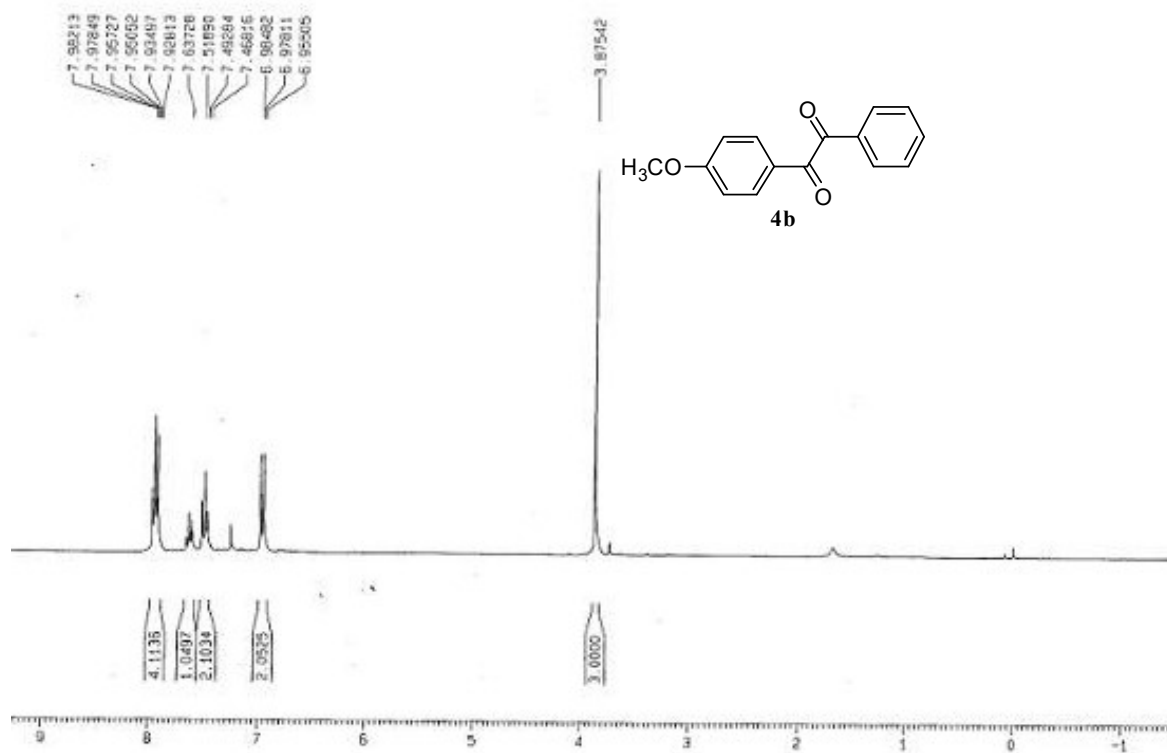
## 6. The NMR spectra of benzil derivatives



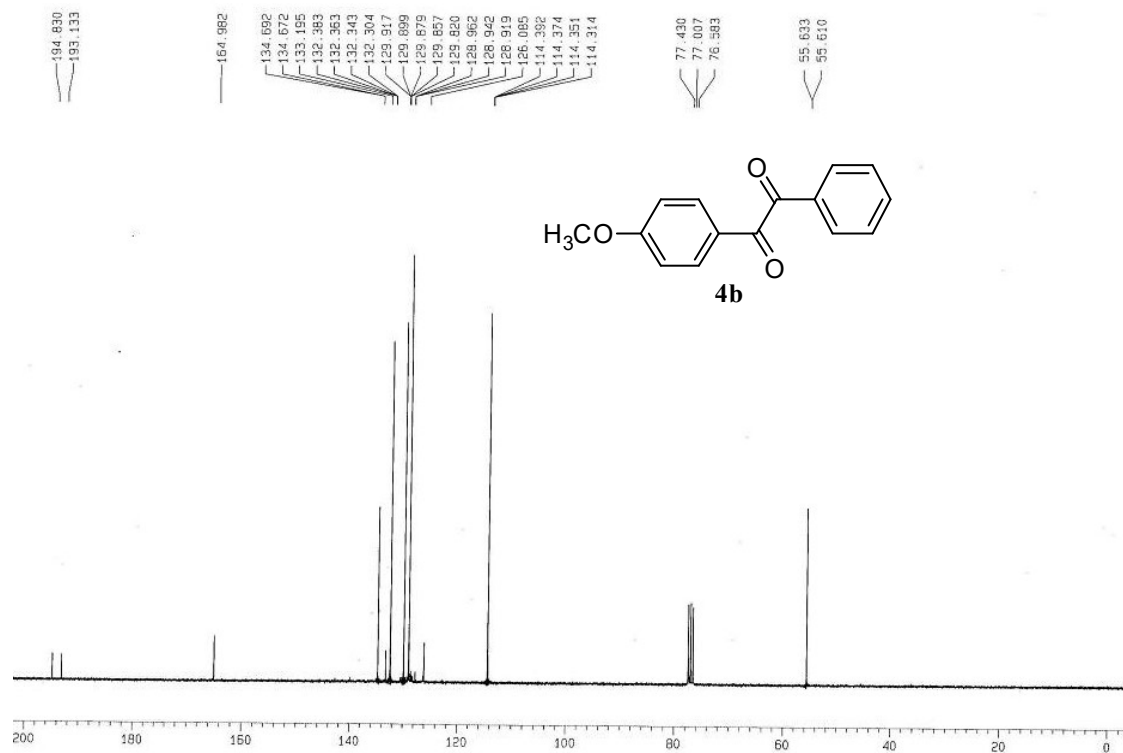
Attached Fig.33 <sup>1</sup>H NMR spectrum of benzil recorded in CDCl<sub>3</sub>



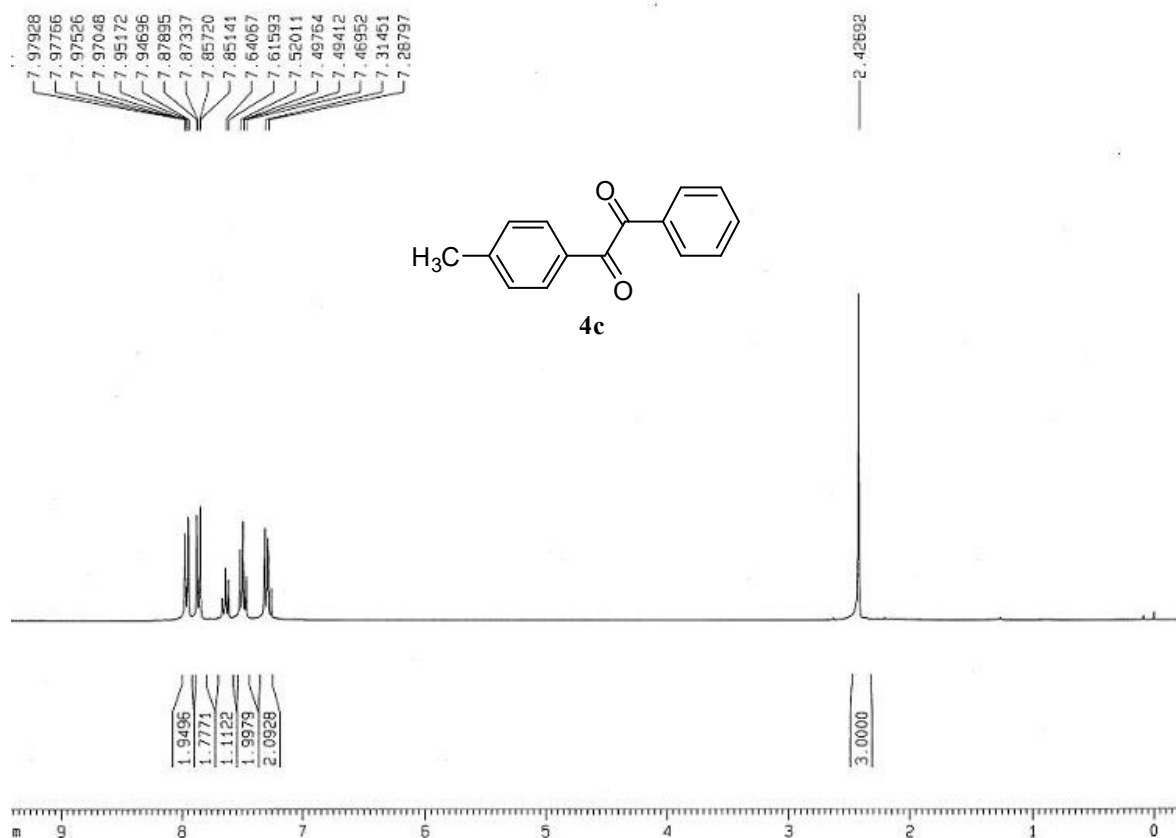
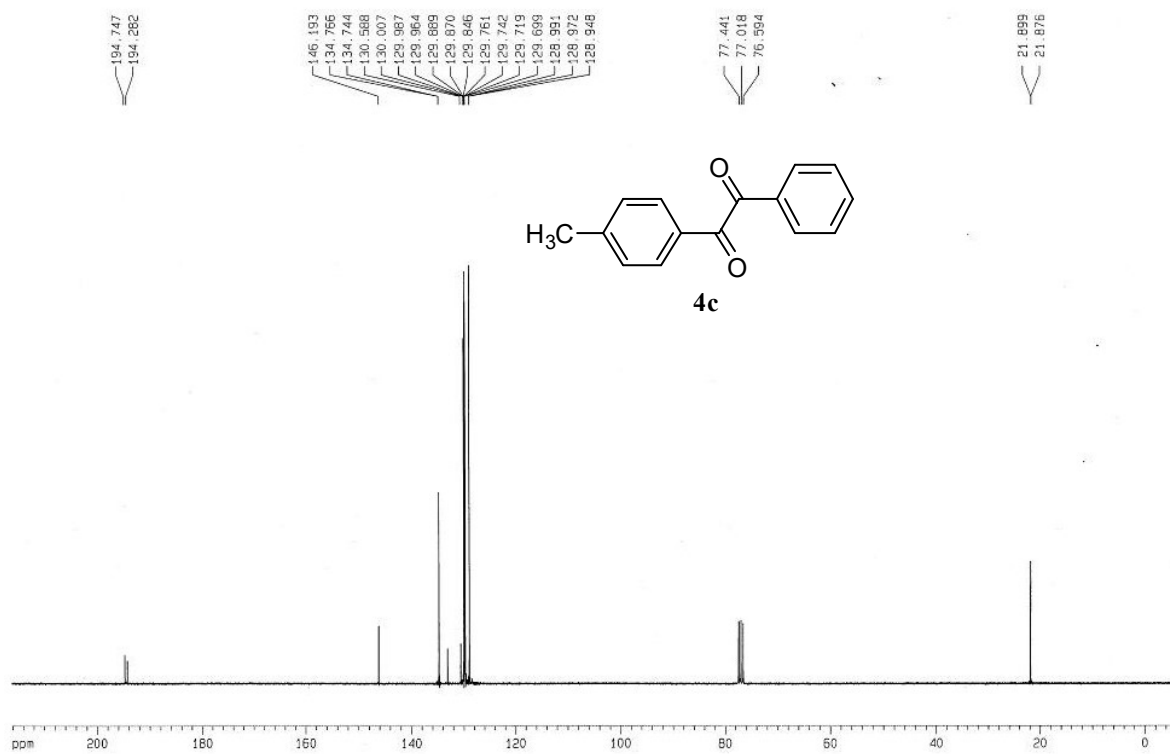
Attached Fig. 34 <sup>13</sup>C NMR spectrum of benzil recorded in CDCl<sub>3</sub>

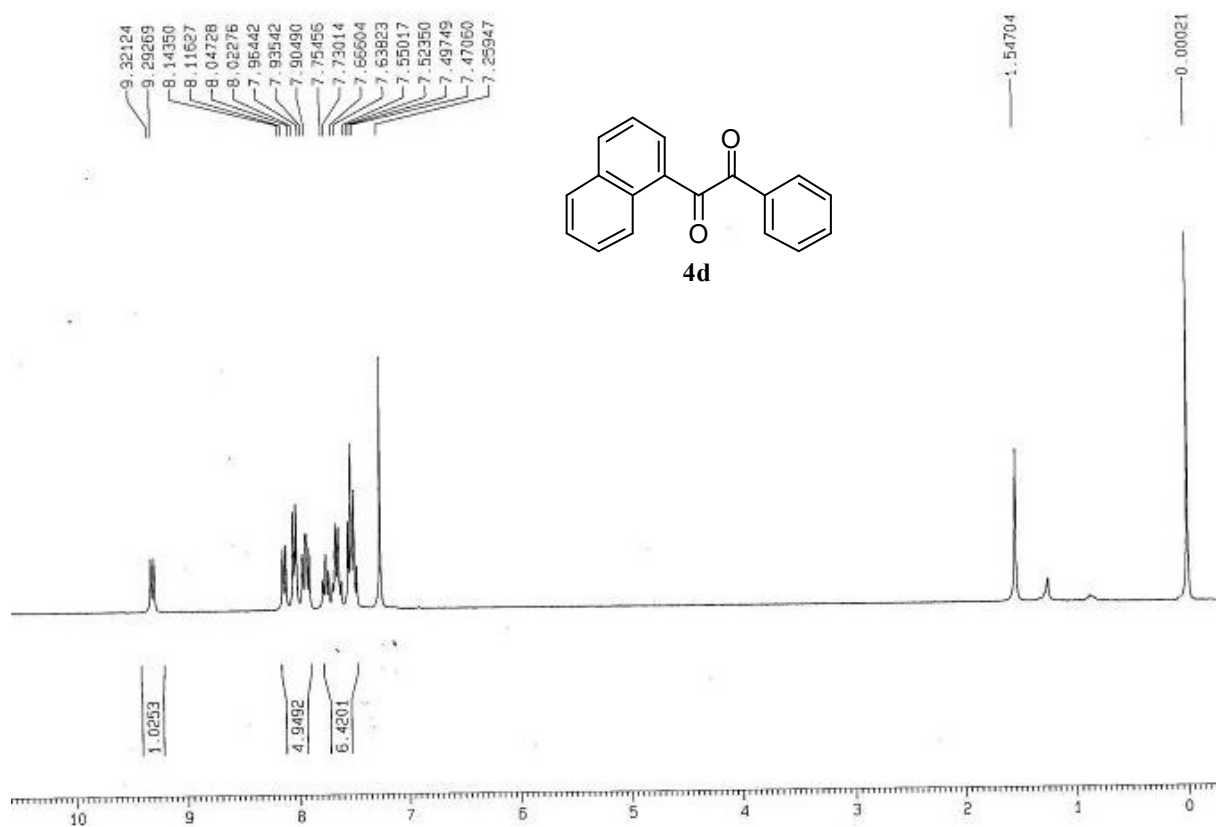


Attached Fig.35 <sup>1</sup>H NMR spectrum of 1-(4-methoxyphenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

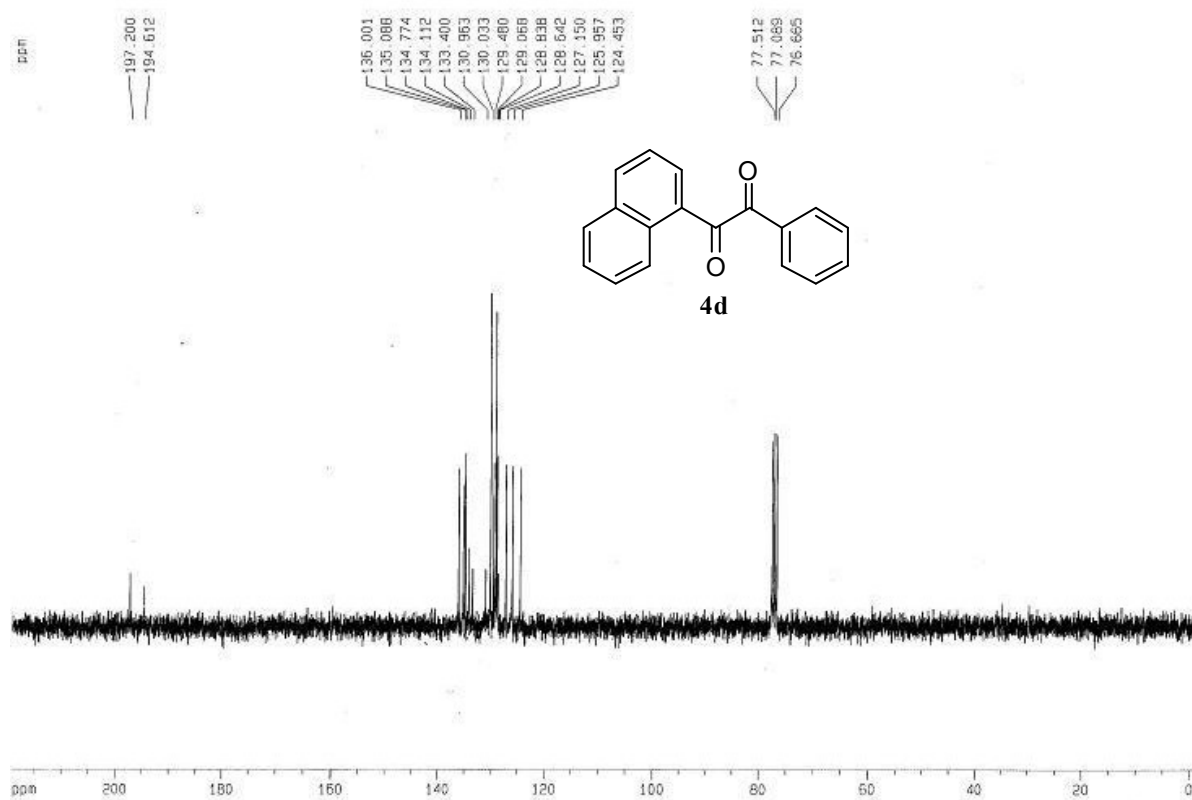


Attached Fig.36 <sup>13</sup>C NMR spectrum of 1-(4-methoxyphenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

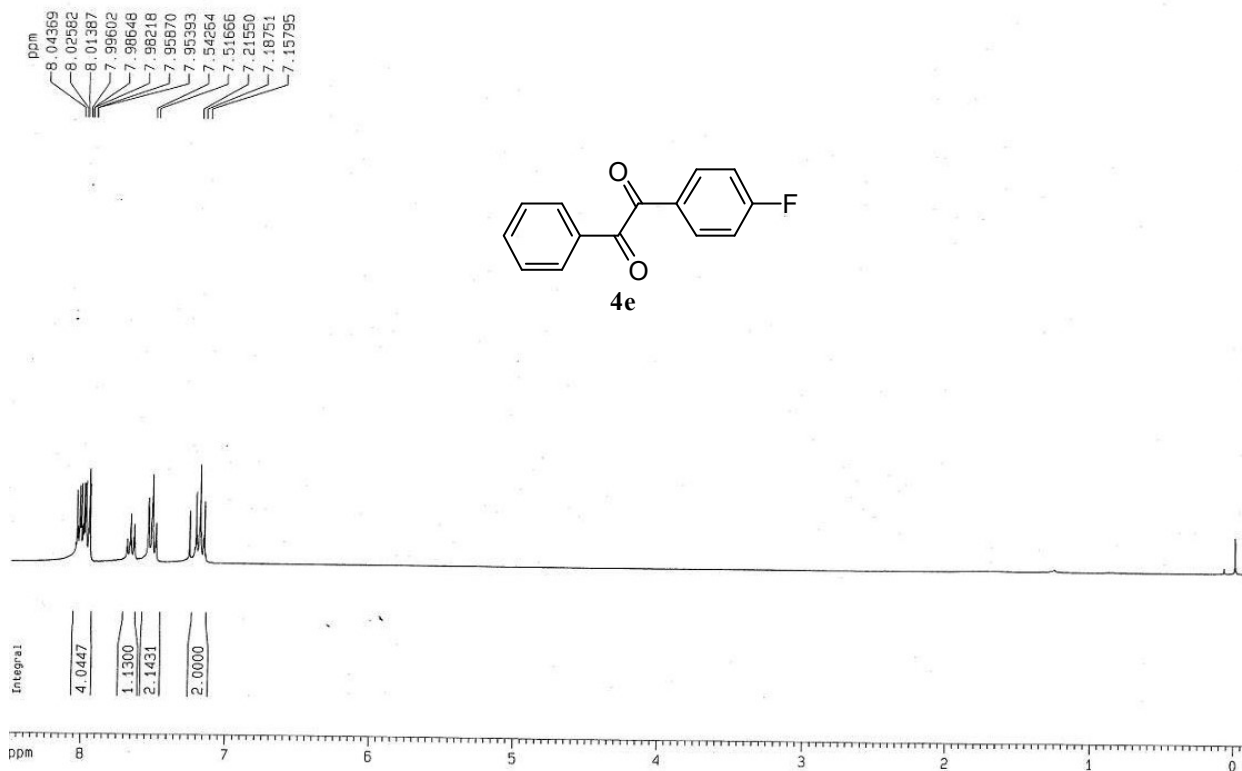
Attached Fig.37 <sup>1</sup>H NMR spectrum of 1-phenyl-2-(p-tolyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>Attached Fig.38 <sup>13</sup>C NMR spectrum of 1-(4-fluorophenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>



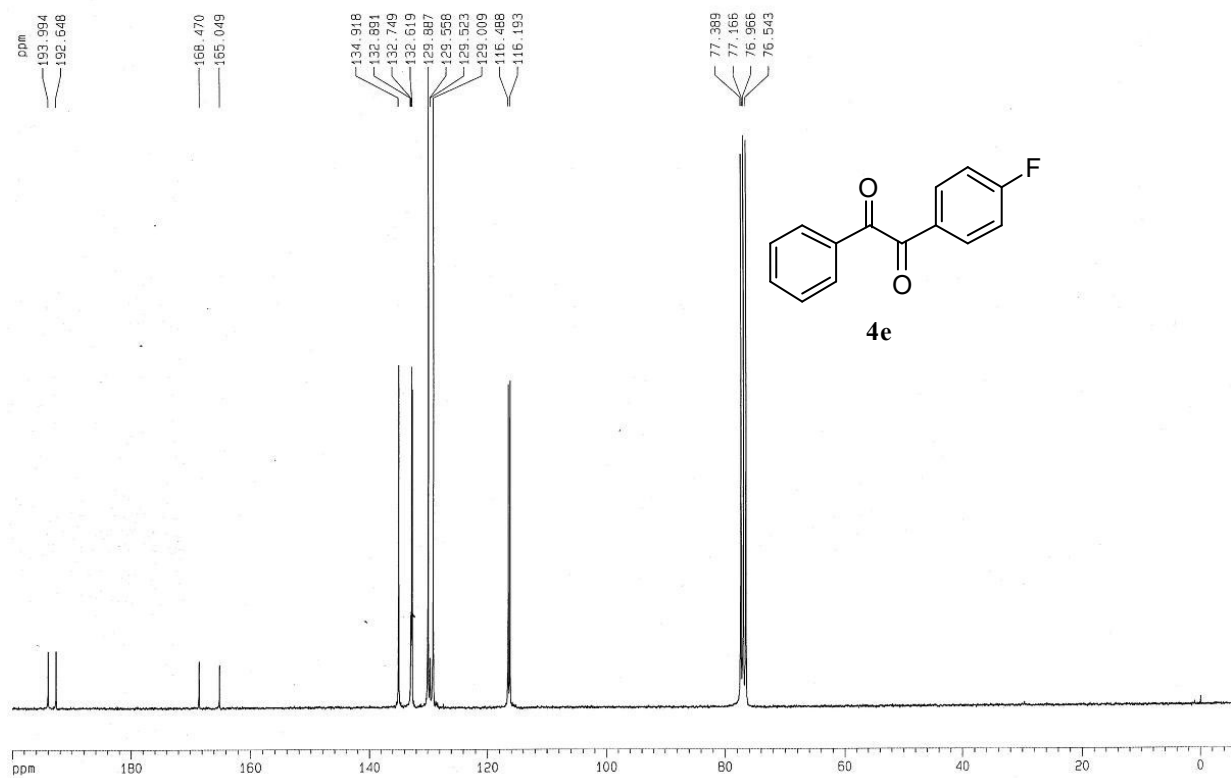
Attached Fig.39 <sup>1</sup>H NMR spectrum of 1-(naphthalen-1-yl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>



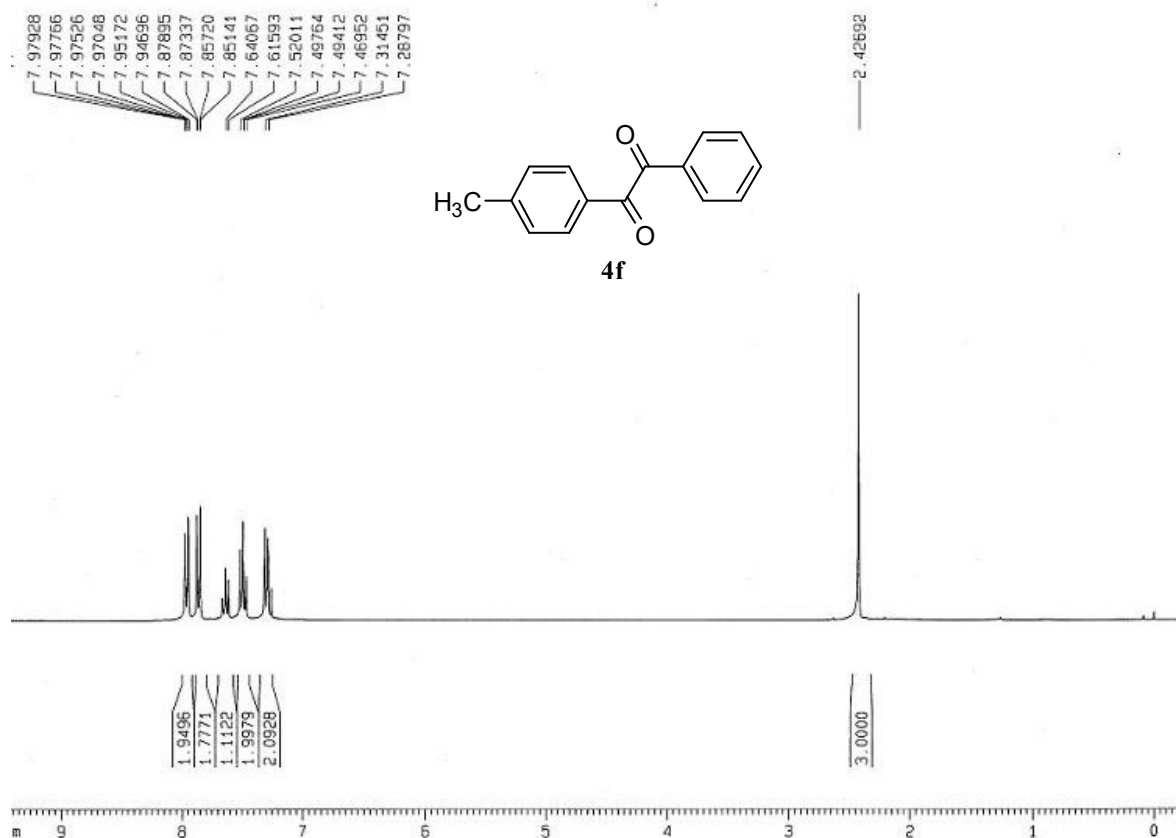
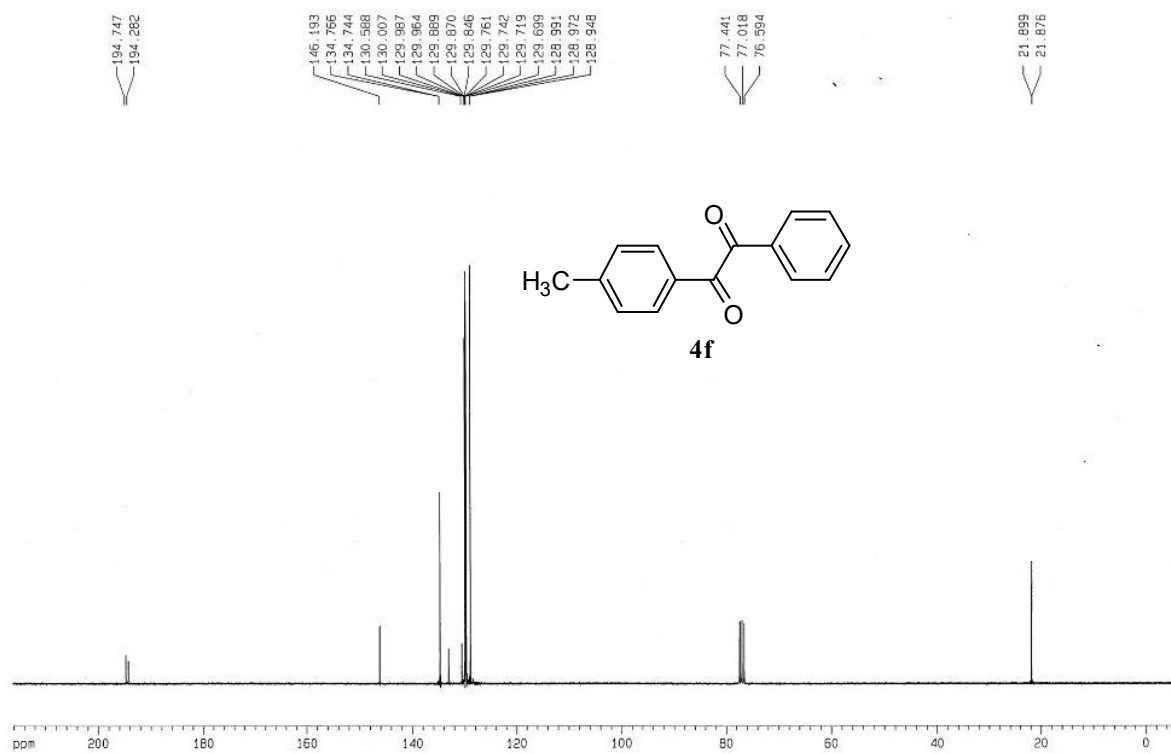
Attached Fig.40 <sup>13</sup>C NMR spectrum of 1-(naphthalen-1-yl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

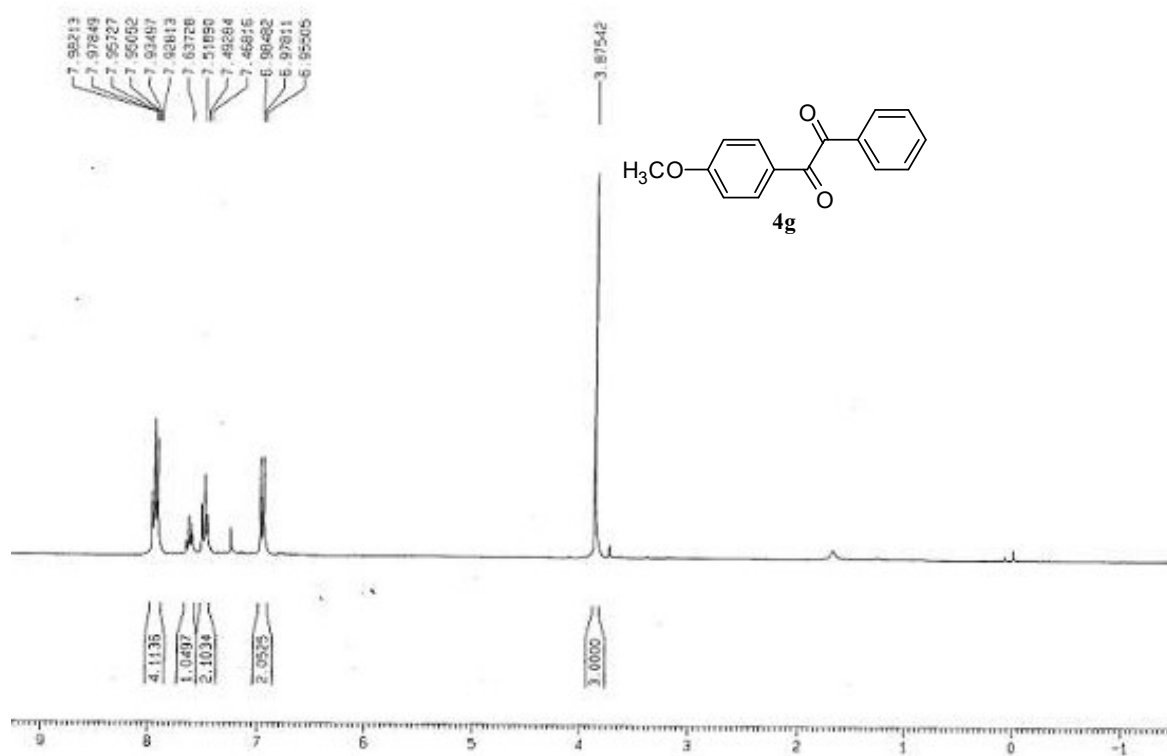


Attached Fig.41 <sup>1</sup>H NMR spectrum of 1-(4-fluorophenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

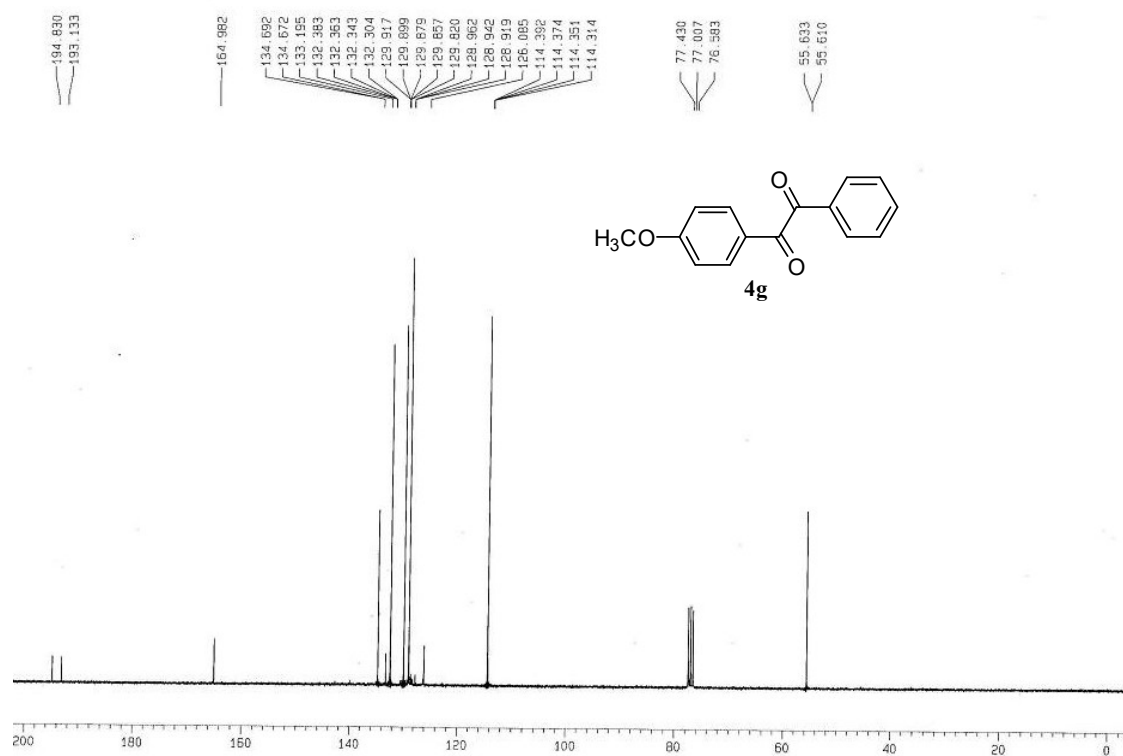


Attached Fig.42 <sup>13</sup>C NMR spectrum of 1-(4-fluorophenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

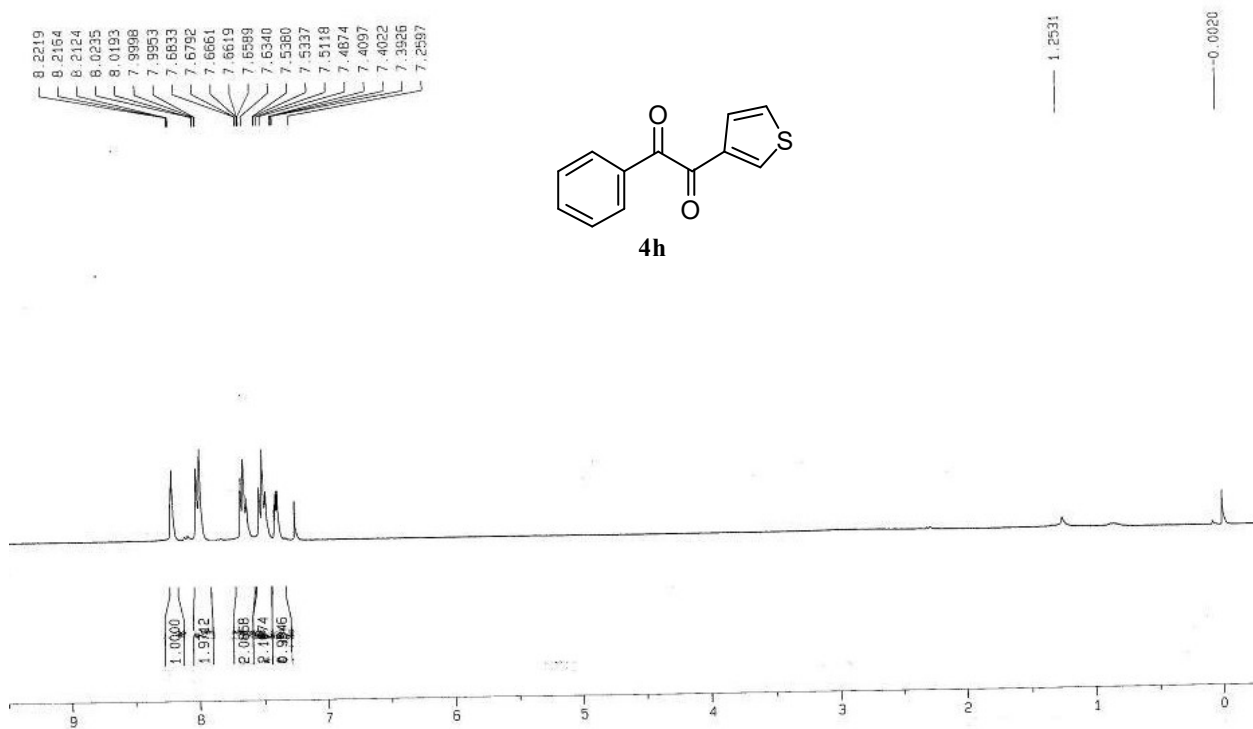
Attached Fig.43 <sup>1</sup>H NMR spectrum of 1-phenyl-2-(p-tolyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>Attached Fig.44 <sup>13</sup>C NMR spectrum of 1-(4-fluorophenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>



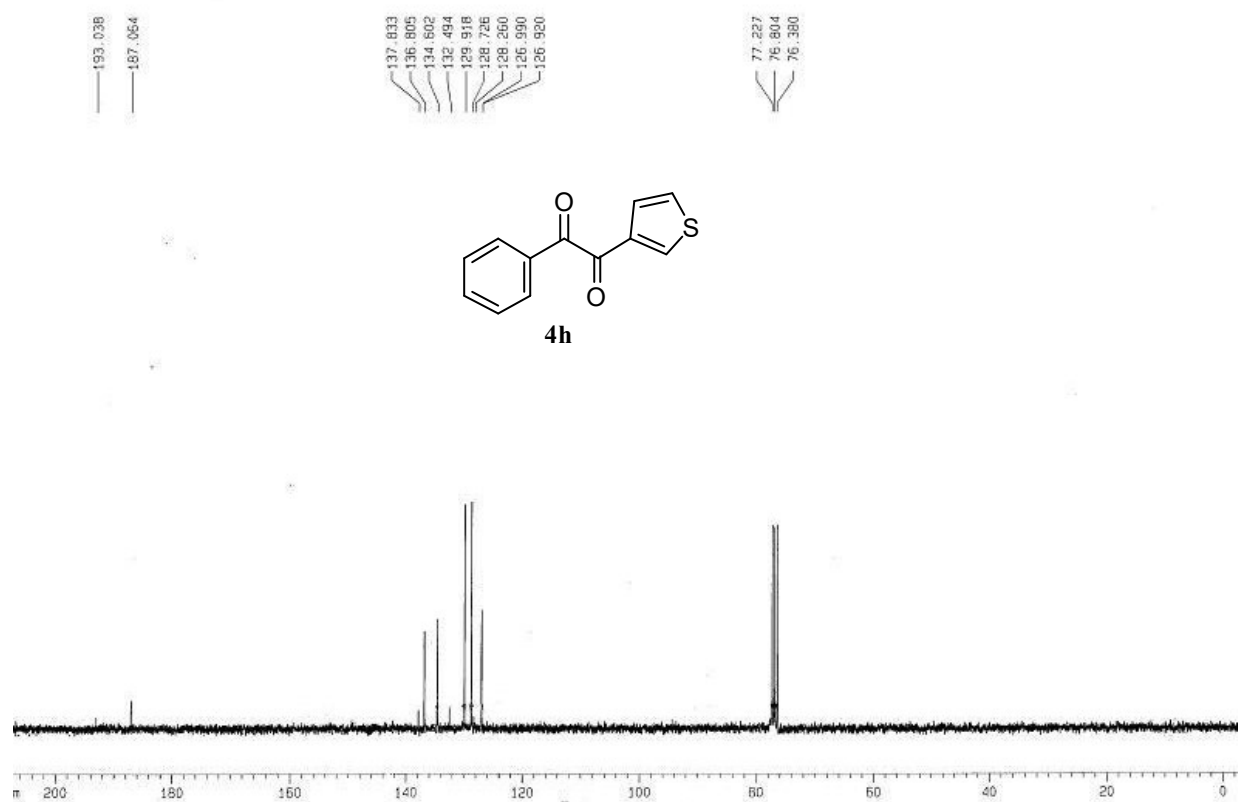
Attached Fig.45 <sup>1</sup>H NMR spectrum of 1-(4-methoxyphenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>



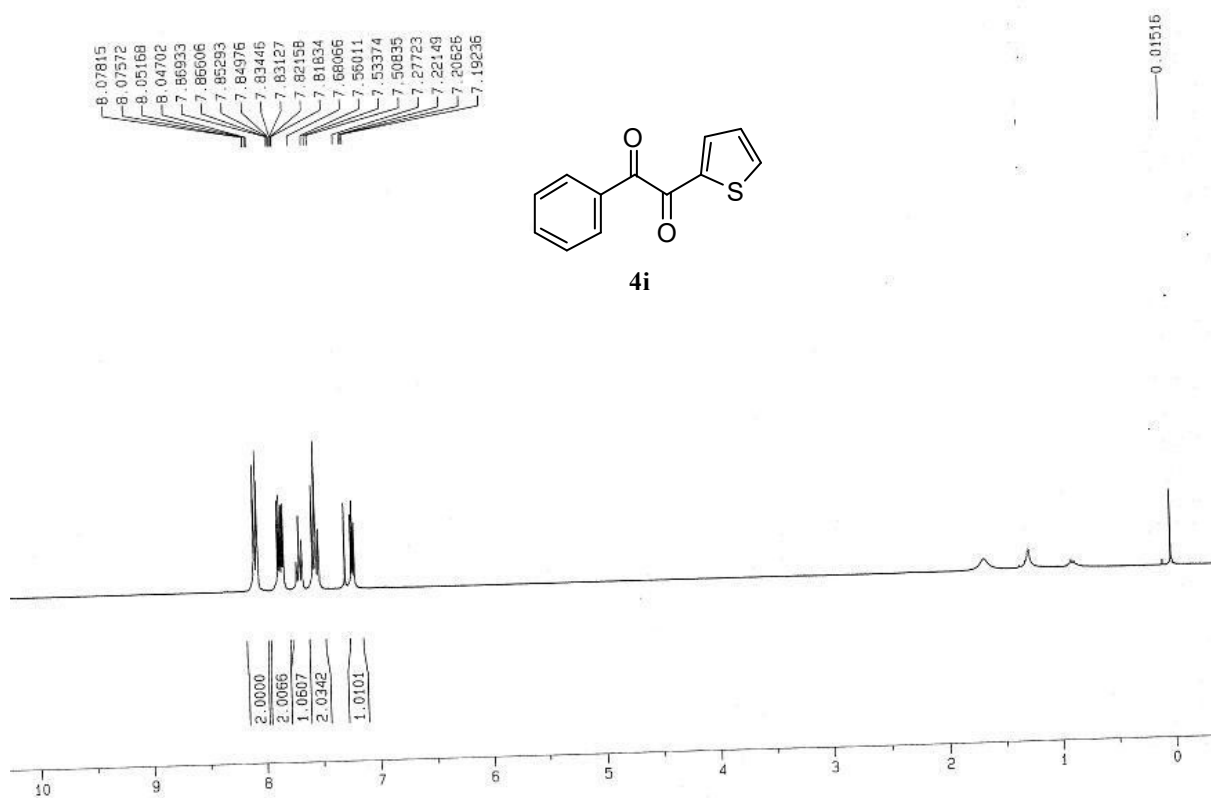
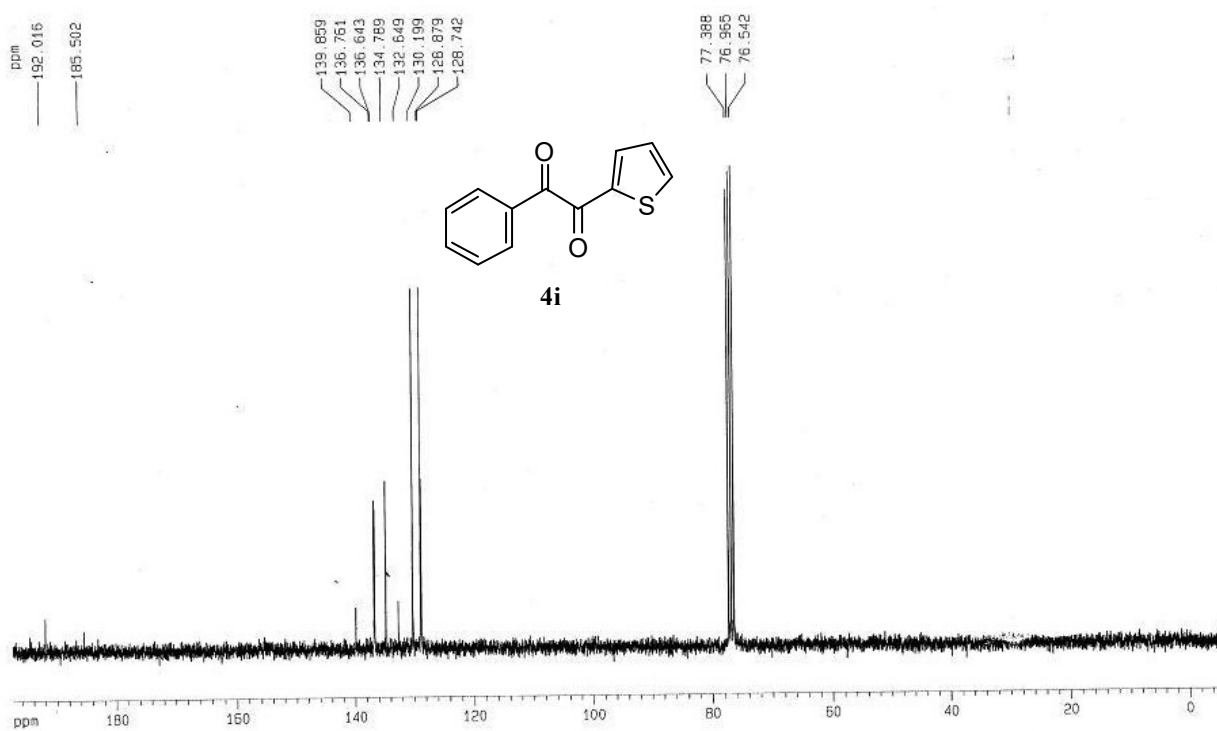
Attached Fig.46 <sup>13</sup>C NMR spectrum of 1-(4-methoxyphenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

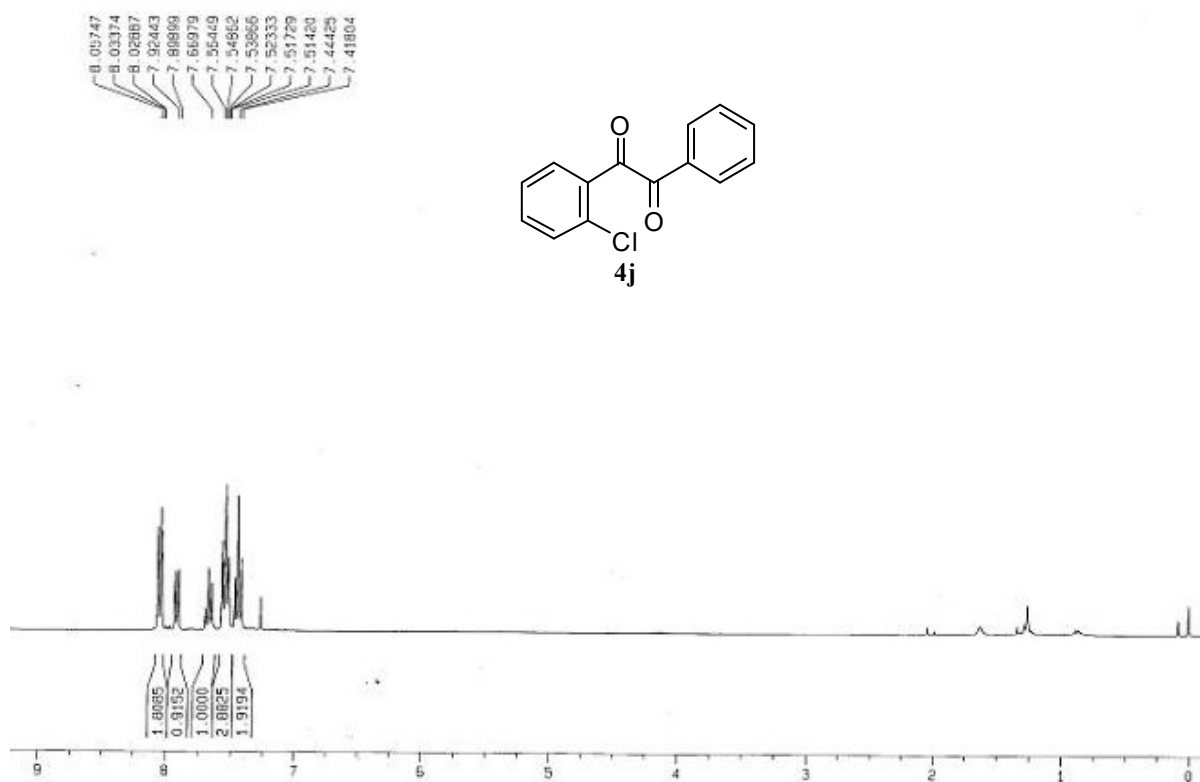


Attached Fig.47 <sup>1</sup>H NMR spectrum of 1-phenyl-2-(thiophen-3-yl)ethane-1,2-dione recorded in CDCl<sub>3</sub>

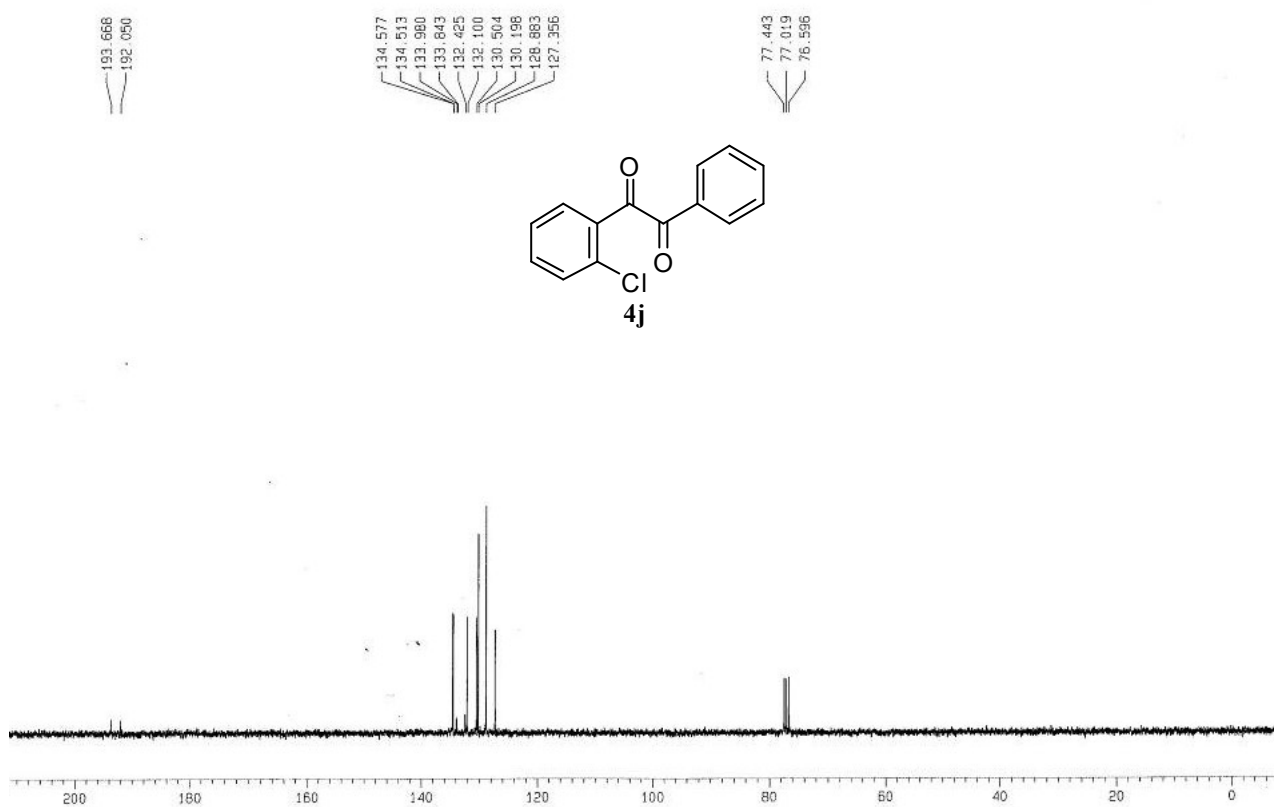




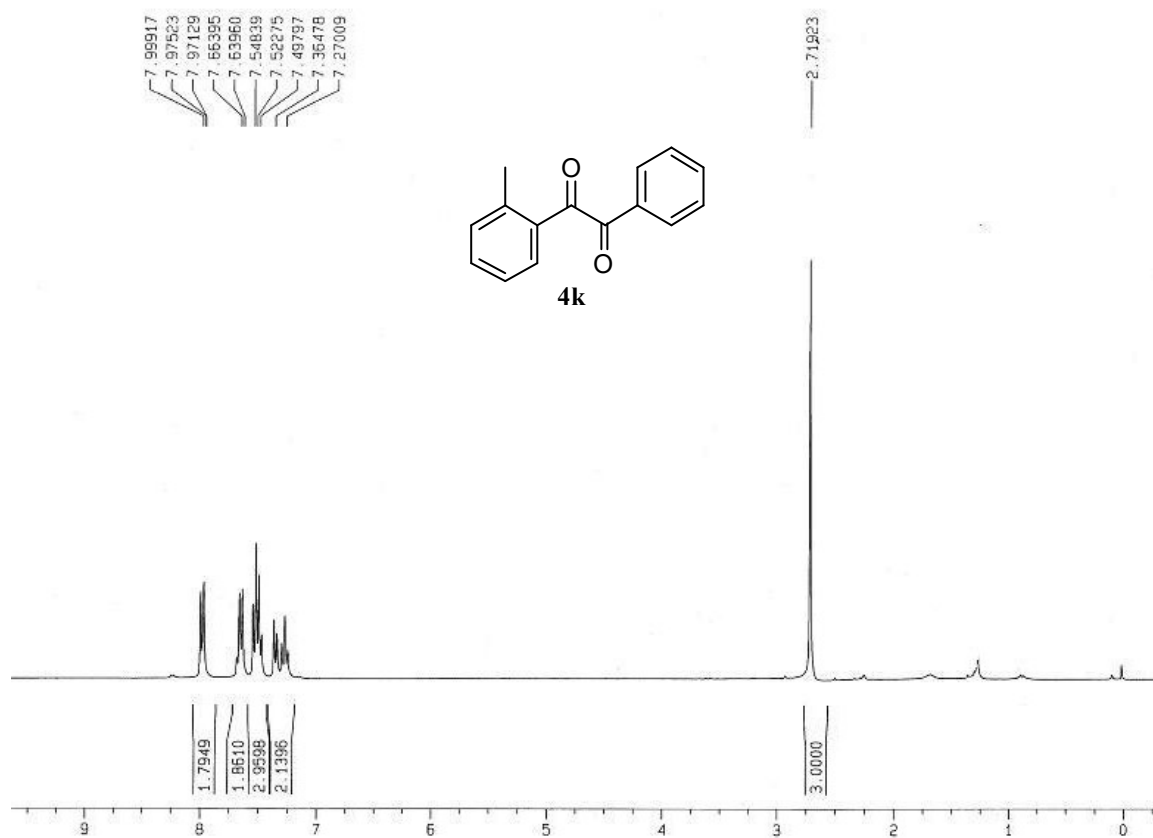
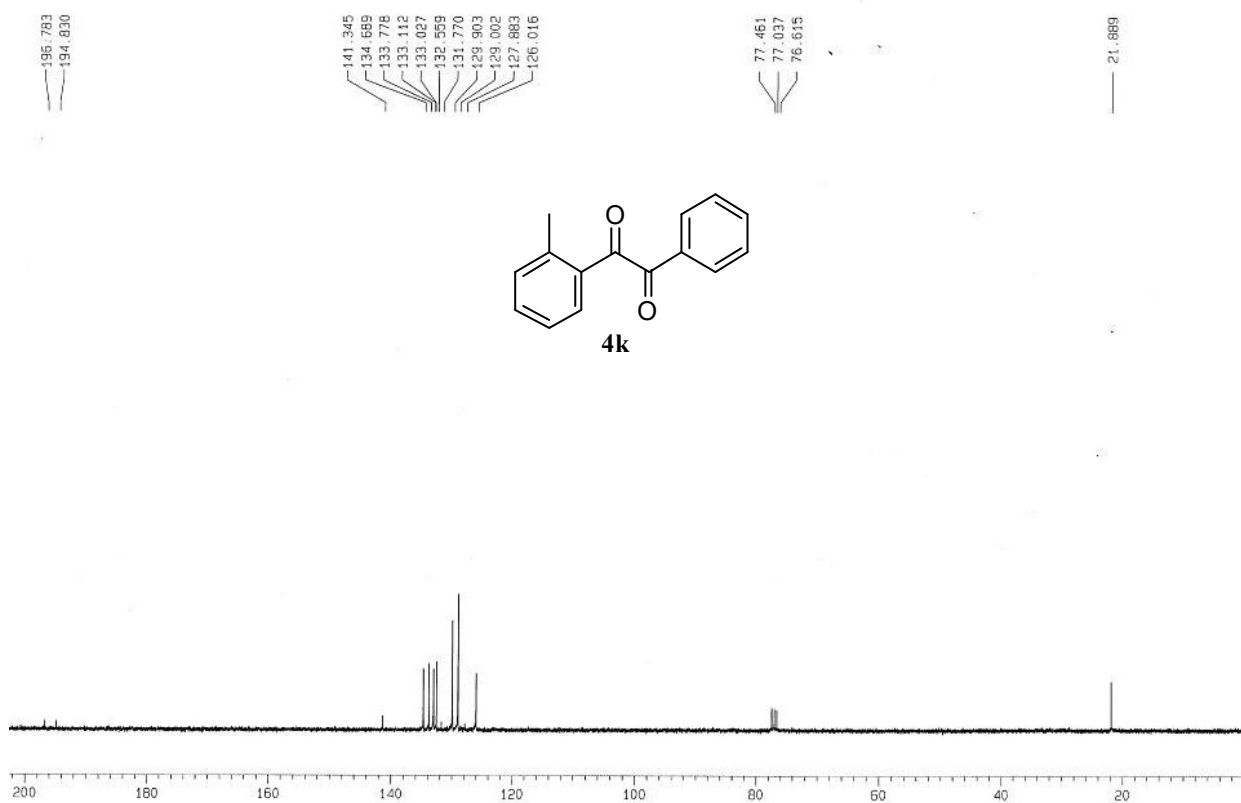
**Attached Fig.48**  $^{13}\text{C}$  NMR spectrum of 1-phenyl-2-(thiophen-3-yl)ethane-1,2-dione recorded in  $\text{CDCl}_3$ **Attached Fig.49**  $^1\text{H}$  NMR spectrum of 1-phenyl-2-(thiophen-2-yl)ethane-1,2-dione recorded in  $\text{CDCl}_3$ **Attached Fig.50**  $^{13}\text{C}$  NMR spectrum of 1-phenyl-2-(thiophen-2-yl)ethane-1,2-dione recorded in  $\text{CDCl}_3$

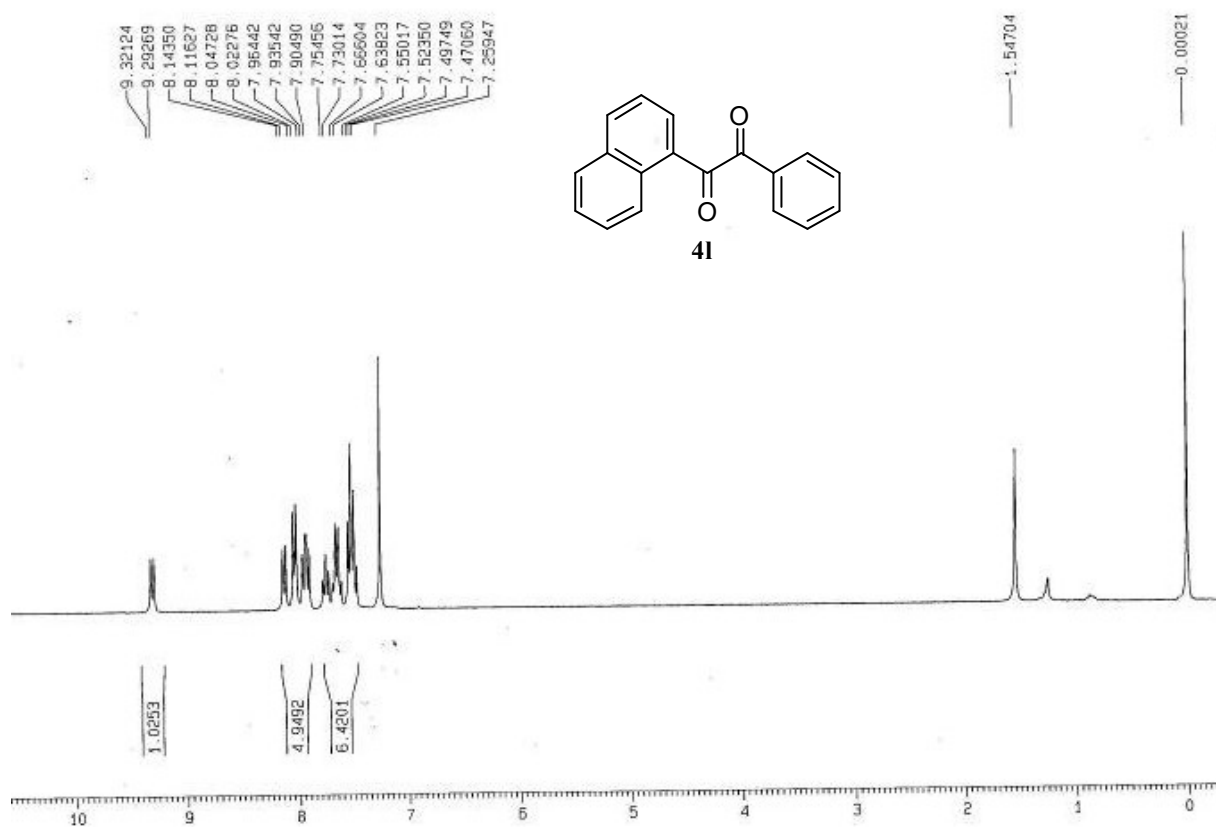


Attached Fig.51 <sup>1</sup>H NMR spectrum of 1-(2-chlorophenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

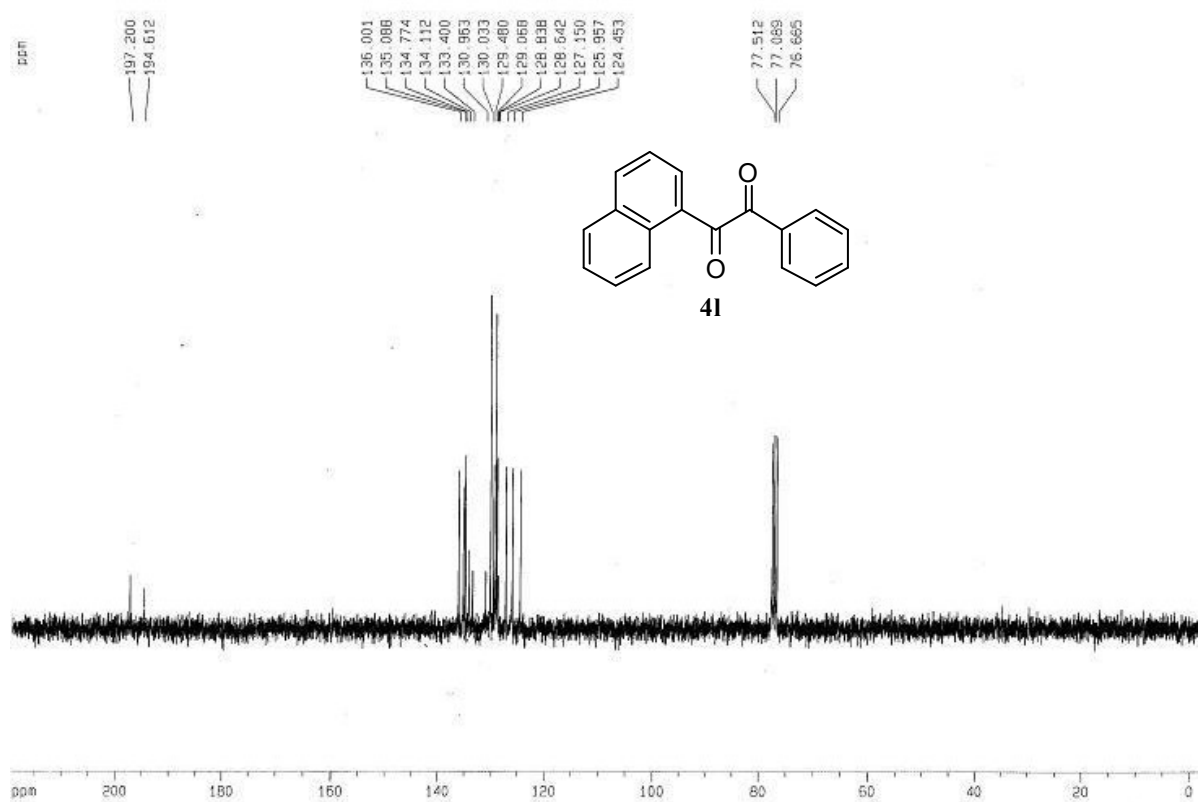


Attached Fig.52 <sup>13</sup>C NMR spectrum of 1-(2-chlorophenyl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

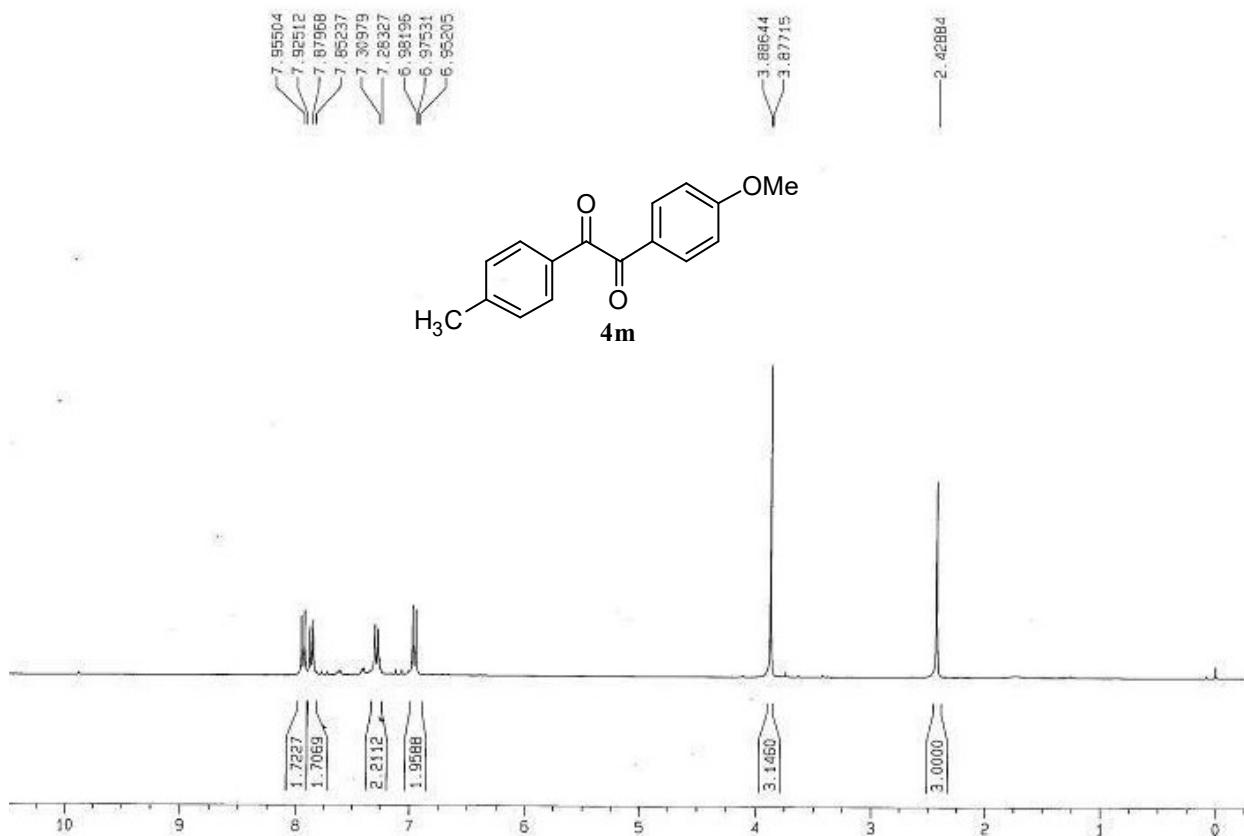
Attached Fig.53 <sup>1</sup>H NMR spectrum of 1-phenyl-2-(*o*-tolyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>Attached Fig.54 <sup>13</sup>C NMR spectrum of 1-phenyl-2-(*o*-tolyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>



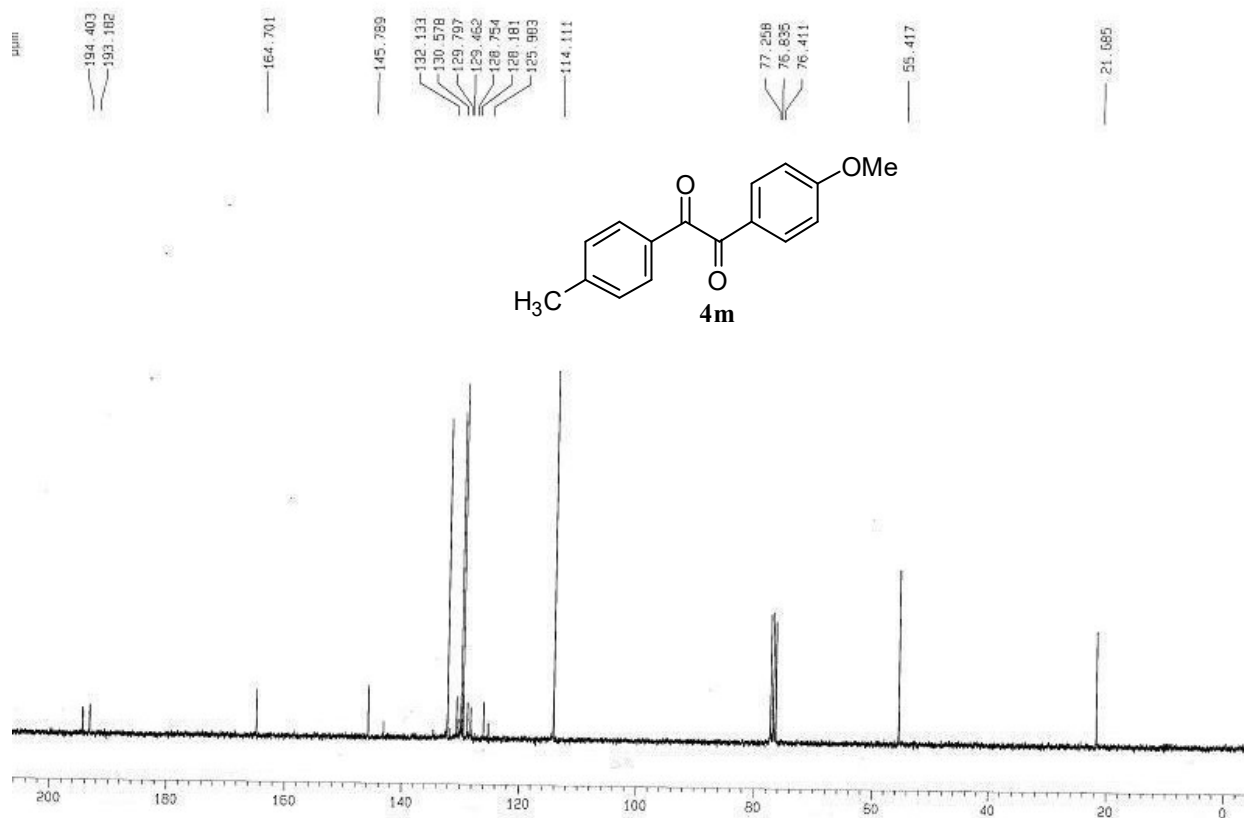
Attached Fig.55 <sup>1</sup>H NMR spectrum of 1-(naphthalen-1-yl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>



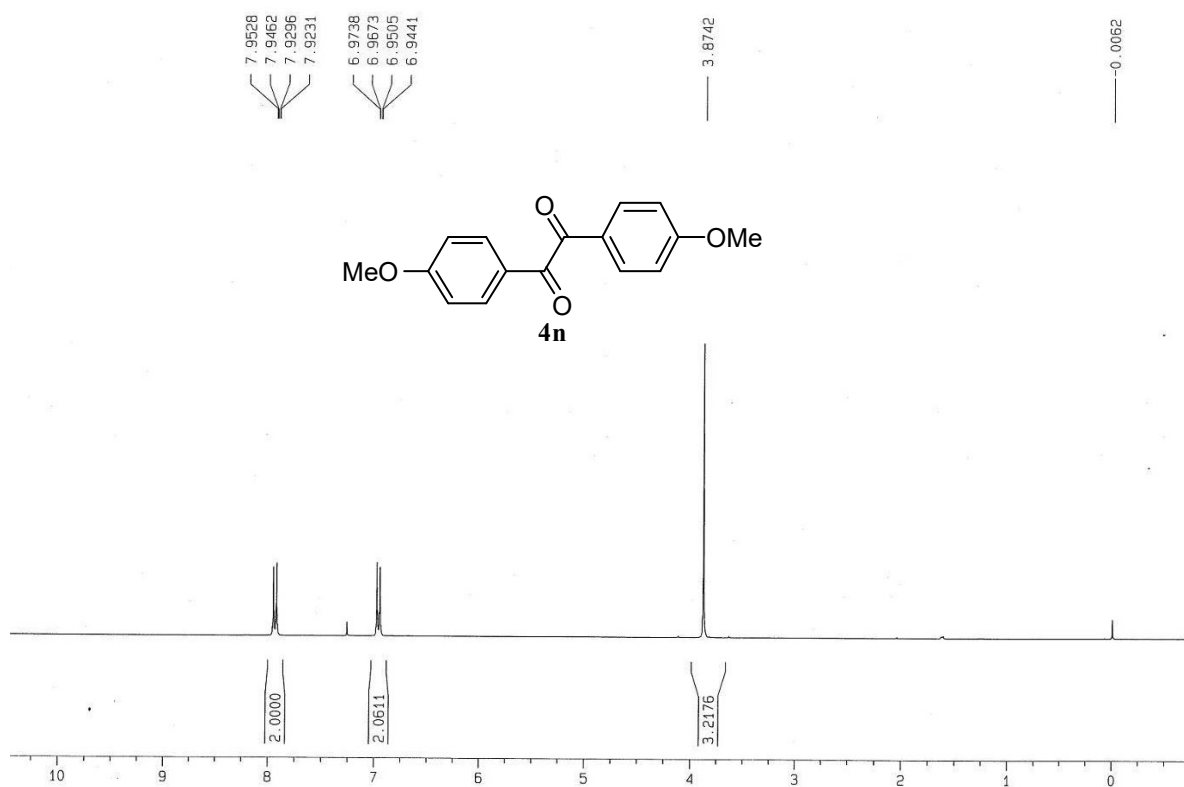
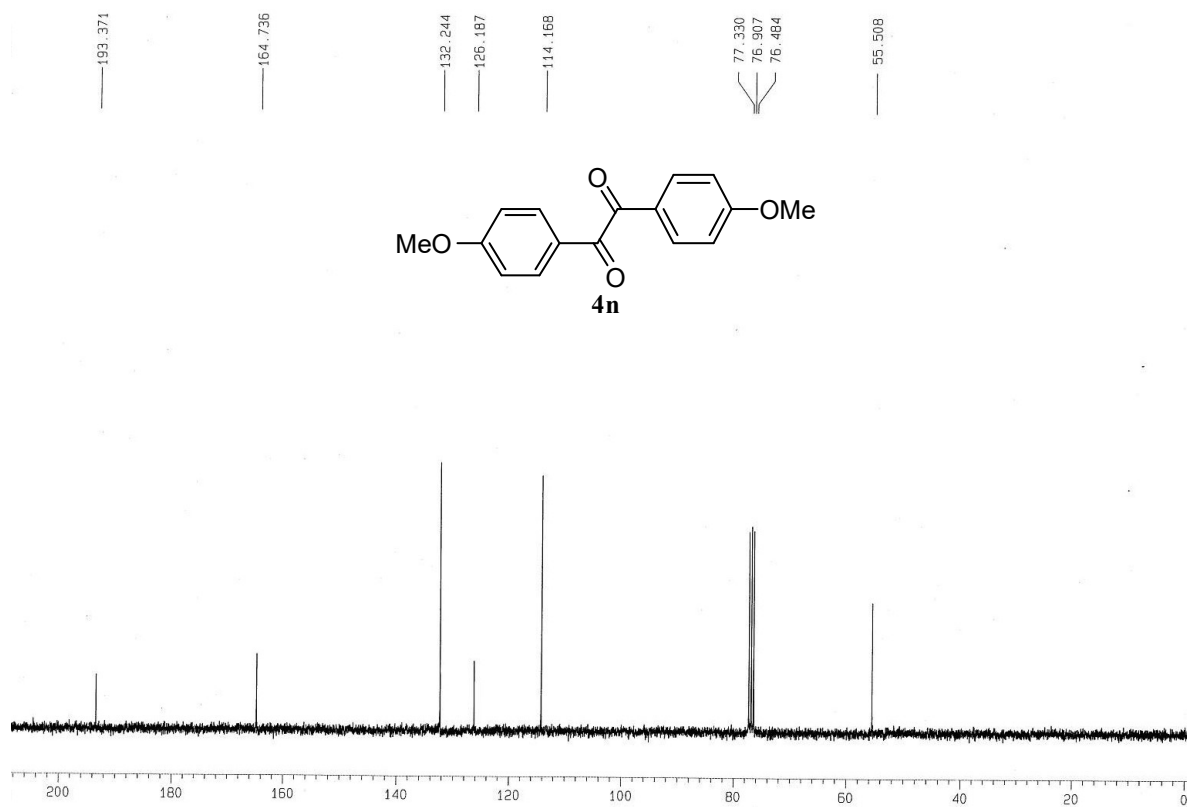
Attached Fig.56 <sup>13</sup>C NMR spectrum of 1-(naphthalen-1-yl)-2-phenylethane-1,2-dione recorded in CDCl<sub>3</sub>

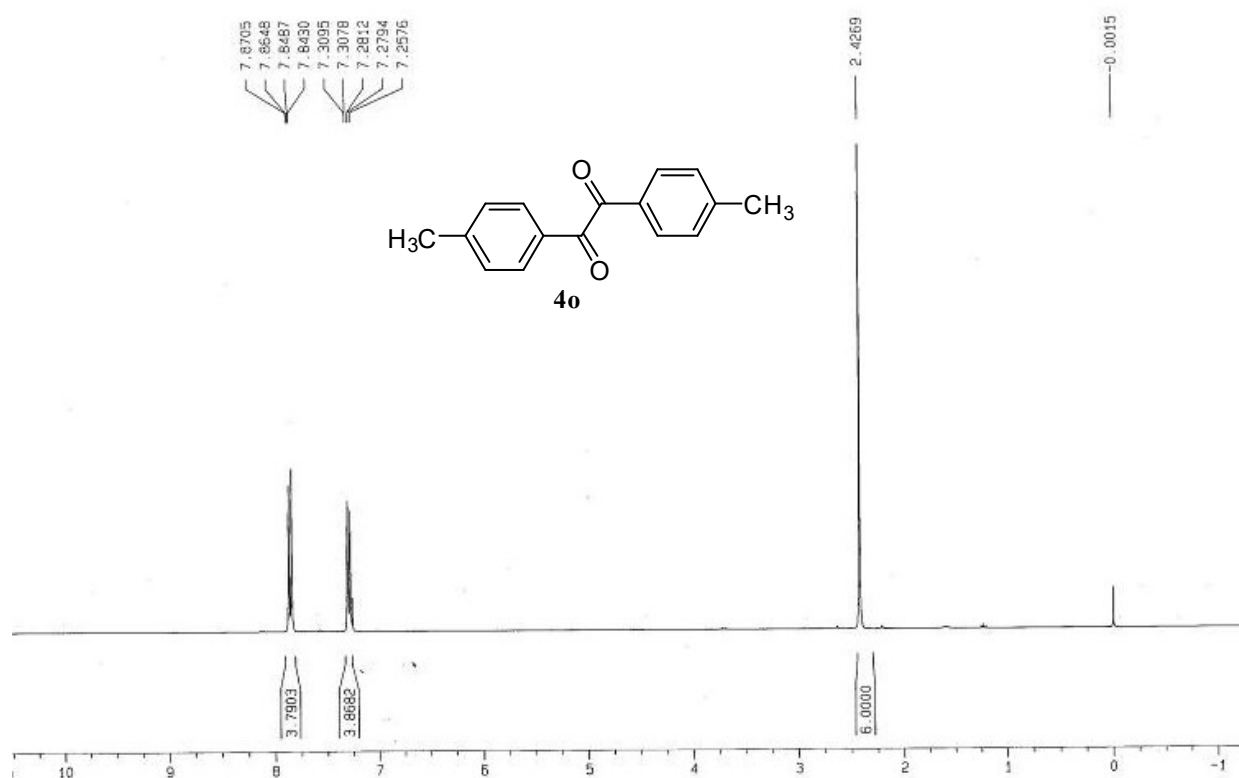
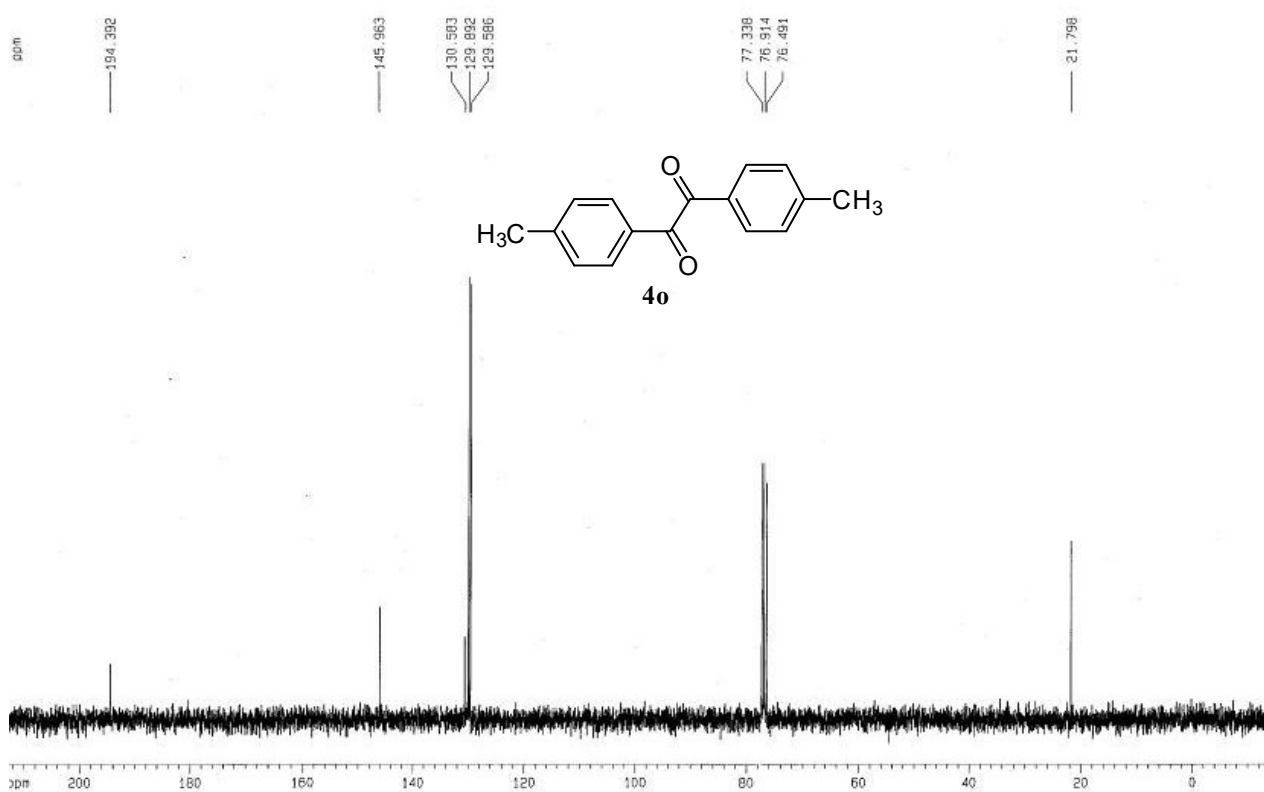


Attached Fig.57 <sup>1</sup>H NMR spectrum of 1-(4-methoxyphenyl)-2-(p-tolyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>



Attached Fig.58 <sup>13</sup>C NMR spectrum of 1-(4-methoxyphenyl)-2-(p-tolyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>

Attached Fig.59 <sup>1</sup>H NMR spectrum of 1,2-bis(4-methoxyphenyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>Attached Fig.60 <sup>13</sup>C NMR spectrum of 1,2-bis(4-methoxyphenyl)ethane-1,2-dione recorded in CDCl<sub>3</sub>

Attached Fig.61 <sup>1</sup>H NMR spectrum of 1,2-di-p-tolyethane-1,2-dione recorded in CDCl<sub>3</sub>Attached Fig.62 <sup>13</sup>C NMR spectrum of 1,2-di-p-tolyethane-1,2-dione recorded in CDCl<sub>3</sub>