Supplementary data

Magnesium-based multifunctional metal-organic framework: Synthesis, thermally induced structural variation, selective gas adsorption, photoluminescence and heterogeneous catalytic study

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Table S1

Intermolecular contacts for compounds **1** (Å, °)

D-H···A	d(D-H)	d(H-A)	d(D···A)	∠DHA	Symmetry transform
O4-H1...O5	0.81(3)	2.04(3)	2.824(15)	165(2)	2-x, y, 3/2-z
O4-H2...O5	0.81(3)	1.993)	2.794(15)	176(2)	x, -y, -1/2+z
O3-H3...O7	0.87(2)	1.82(2)	2.674(14)	168(2)	-
O3-H4...O5	0.83(2)	1.91(2)	2.725(15)	169(2)	3/2-x, 1/2+y, 3/2-z
O7-H5...O6	0.90(3)	1.82(3)	2.693(15)	164(2)	-1/2+x, -1/2+y, z
N5-H6...O6	0.91(2)	1.98(2)	2.814(15)	152(18)	-

Table S2

Solvent effect in aldol condensation of *p*-nitrobenzaldehyde with acetone catalyzed by compound **1**[i]

Solvent	product	Isolated yield (wt %)	Selectivity (wt %)
THF	*β*-aldol product	62	100
THF-water (9:1)	*β*-aldol product	75	100
THF-water (7:1)	*β*-aldol product	79	100
THF-water (5:1)	*β*-aldol product	81	100
THF-water (3:1)	*β*-aldol product	82	100
THF-water (1:1)	*β*-aldol product	72	100
Water	*β*-aldol product	29	100

[i]Reaction conditions: *p*-nitrobenzaldehyde (2 mmol), acetone (4 mmol), tetrahydrofuran (3 ml), water (1 ml) and catalysts (5 mg); temperature = 5-10 °C. Yields were isolated after 6 h of reaction.

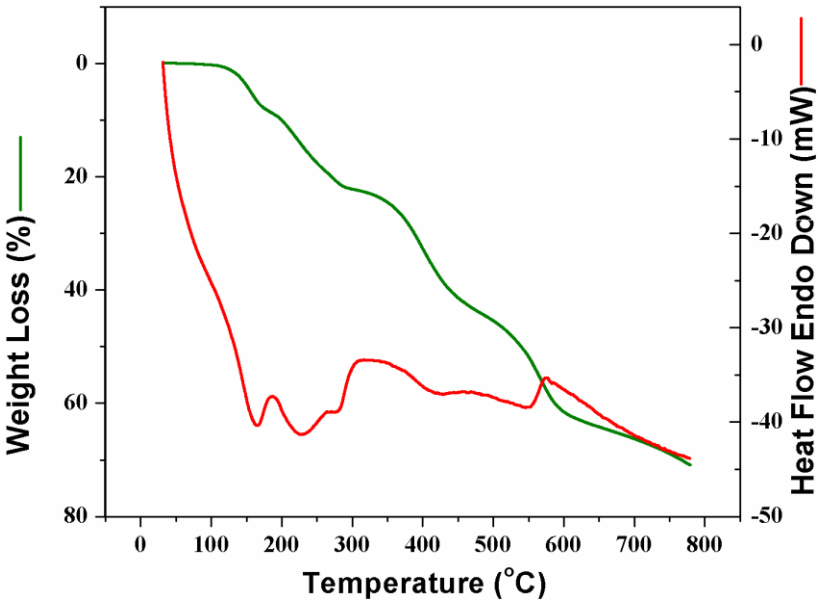


Fig. S1. TGA and DTA curve of compound **1.**

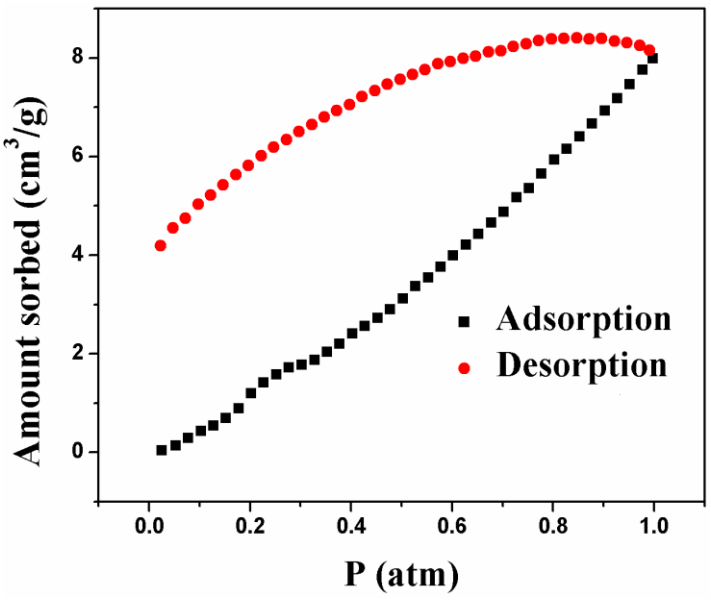


Fig. S2. CO_2 adsorption-desorption isotherm of compound **1** at 298 K.

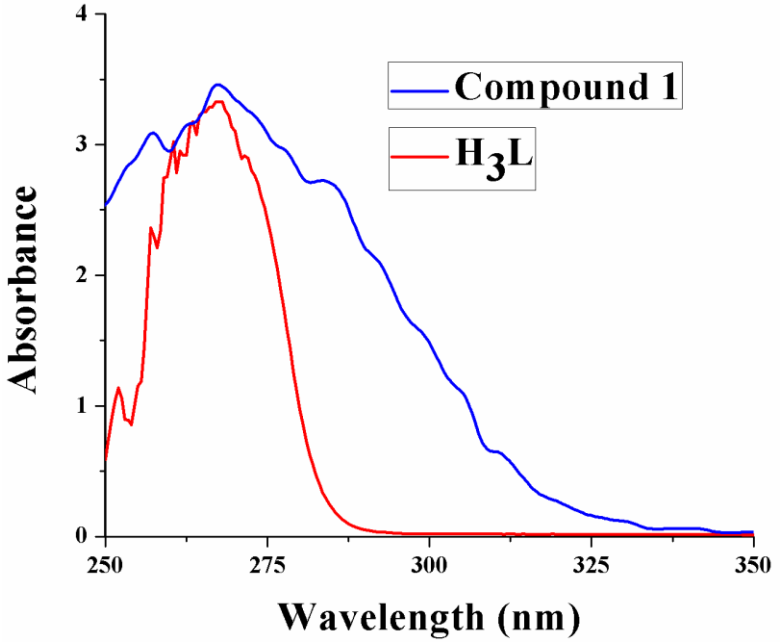


Fig. S3. Solid state UV-VIS spectra of ligand and compound **1**

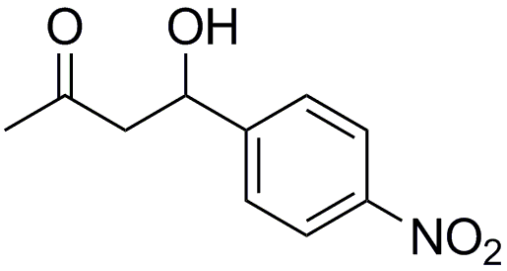
General Information

All chemicals were purchased from Aldrich and were used as received except benzaldehyde. All solvents used were analytical grade and were used as received from Merck India Pvt. Ltd. Liquid aldehydes were distilled before use. Benzaldehyde was kept over NaA molecular sieves to trap possible traces of benzoic acid. All reactions were carried out in air, without any special precautions. Column chromatography was performed over silica gel (mesh 60-120) and hexane/ethyl acetate combination was used as the eluent. ^{1}H NMR spectra were recorded at ambient temperature in $CDCl_3$ with tetramethylsilane as internal standard. The chemical shifts (δ) and coupling constants (*J*) were expressed in ppm and Hz, respectively on Bruker Avance 300 instrument.

Elemental analysis of the products was performed by using Perkin-Elmer 240C elemental analyzer.

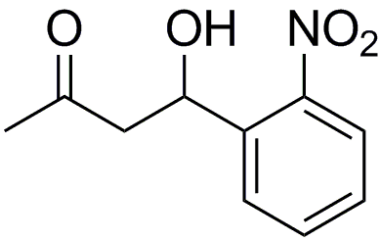
Characterization of Products

4-hydroxy-4-(4-nitrophenyl)-butan-2-one (Table 3, entry 1):



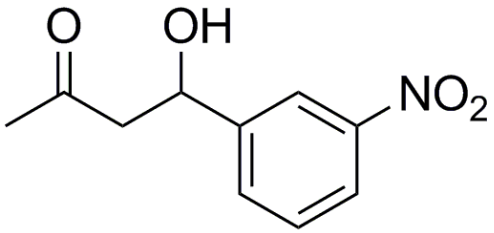
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.07 (d, *J* = 8.8 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 5.20 (m, 1H), 3.57 (br s, 1H), 2.81 (m, 2H), 2.15 (s, 3H); Anal. Calcd. for $C_{10}H_{11}NO_4$: C, 57.41%; H, 5.30%; N, 6.69%. Found: C, 57.6%; H, 5.4%; N, 6.6%.

4-hydroxy-4-(2-nitrophenyl)-butan-2-one (Table 3, entry 2):



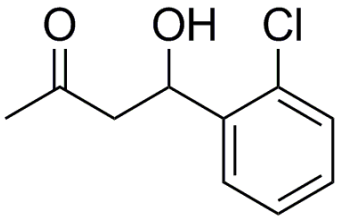
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.75 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 10.0 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.9 Hz, 1H), 5.52 (m, 1H), 3.93 (br s, 1H), 2.86 (d, *J* = 17.2 Hz, 1H), 2.63 (dd, *J* = 17.2, 9.3 Hz, 1H), 2.06 (s, 3H); Anal. Calcd. for $C_{10}H_{11}NO_4$: C, 57.41%; H, 5.30%; N, 6.69%. Found: C, 57.4%; H, 5.3%; N, 6.6%.

4-hydroxy-4-(3-nitrophenyl)-butan-2-one (table 3, entry 3):



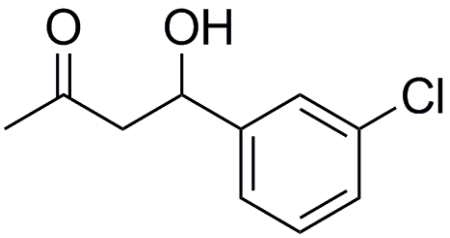
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.12 (s, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.61 (d, *J* = 8.0Hz, 1H), 7.41 (t, *J* = 7.9 Hz, 1H), 5.17 (m, 1H), 3.69 (br s, 1H), 2.81 (m, 2H), 2.13 (s, 3H); Anal. Calcd. for $C_{10}H_{11}NO_4$: C, 57.41%; H, 5.30%; N, 6.69%. Found: C, 57.4%; H, 5.3%; N, 6.7%.

4-hydroxy-4-(2-chlorophenyl)-butan-2-one (Table 3, entry 4):



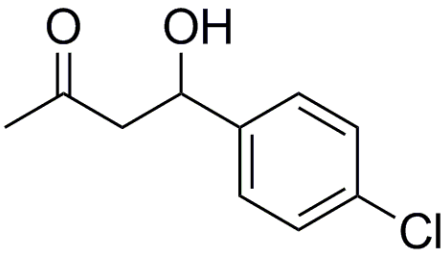
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.62 (d, *J* = 7.2 Hz, 1H), 7.34-7.19 (m, 3H), 5.51 (d, *J* = 9.7 Hz, 1H), 3.53 (br s, 1H), 3.03-2.97 (dd, *J* = 17.8 Hz, 2 Hz, 1H), 2.72-2.63 (dd, *J* = 17.8 Hz, 9.7 Hz, 1H), 2.22 (s, 3H); Anal. Calcd. for $C_{10}H_{11}ClO_2$: C, 60.46%; H, 5.58%. Found: C, 60.5%; H, 5.6%.

4-hydroxy-4-(3-chlorophenyl)-butan-2-one (Table 3, entry 5):



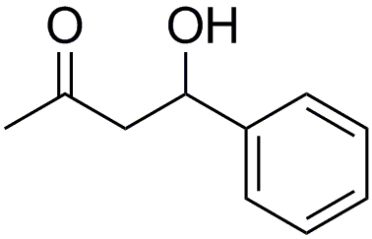
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.35 (s, 1H), 7.29-7.18 (m, 3H), 5.12-5.08 (m, 1H), 3.49 (s, 1H), 2.89-2.79 (m, 2H), 2.18 (s, 3H); Anal. Calcd. for $C_{10}H_{11}ClO_2$: C, 60.46%; H, 5.58%. Found: C, 60.4%; H, 5.6%.

4-hydroxy-4-(4-chlorophenyl)-butan-2-one (Table 3, entry 6):



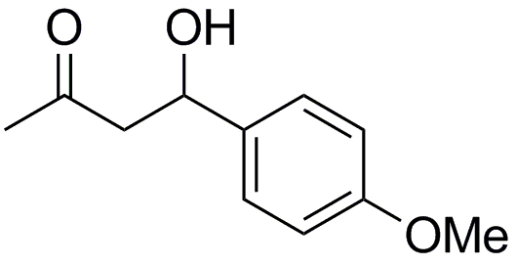
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.45 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.3 Hz, 2H), 5.10-5.07 (m, 1H), 3.47 (d, *J* = 3.1 Hz, 1H), 2.82-2.78 (m, 2H), 2.17 (s, 3H); Anal. Calcd. for $C_{10}H_{11}ClO_2$: C, 60.46%; H, 5.58%. Found: C, 60.4%; H, 5.5%.

4-hydroxy-4-phenylbutan-2-one (Table 3, entry 7):



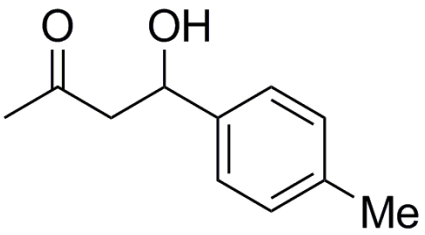
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.3 (m, 5H), 5.16 (m, 1H), 3.25 (br s, 1H), 2.88 (m, 2H), 2.15 (s, 3H); Anal. Calcd. for $C_{10}H_{12}O_2$: C, 73.15%; H, 7.27%. Found: C, 73.2%; H, 7.2%.

4-hydroxy-4-(4-methoxyphenyl)-butan-2-one (Table 3,entry 8):



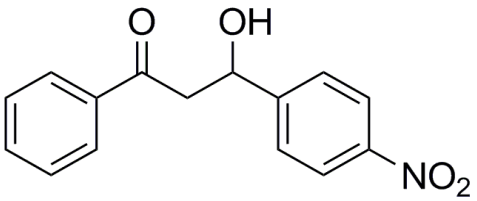
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.2 (d, *J* = 8.8 Hz, 2H), 6.9 (d, *J* = 8.8 Hz, 2H), 4.9 (d, *J* = 8.2 Hz, 1H), 4.05 (br s, 1H), 3.8 (s, 3H), 2.75 (m, 2H), 2.15 (s, 3H); Anal. Calcd. for $C_{11}H_{14}O_3$: C, 68.02%; H, 7.27%. Found: C, 68.0%; H, 7.2%.

4-hydroxy-4-(4-methylphenyl)-butan-2-one (Table 3, entry 9):



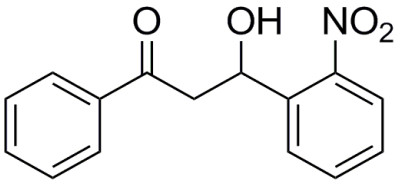
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.25 (d, *J* = 8.3 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 5.12 (d, *J* = 8.9 Hz, 1H), 3.21 (d, *J* = 3.1 Hz, 1H), 2.87-2.81 (m, 2H), 2.34 (s, 3H), 2.22 (s, 3H); Anal. Calcd. for $C_{11}H_{14}O_3$: C, 74.13%; H, 7.92%. Found: C, 74.0%; H, 7.9%.

3-hydroxy-3-(4-nitrophenyl)-1-phenylpropane-1-one (Table 3, entry 10):



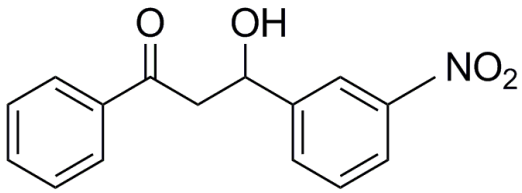
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.24 (d, *J* = 8.8 Hz, 2H), 7.95 (d, *J* = 8.1 Hz, 2H), 7.64-7.59 (m, 3H), 7.5-7.45 (m,2H), 5.46 (d,8.6 Hz, 1H), 3.84 (d, 3.1 Hz, 1H), 3.39-3.37 (m, 2H); Anal. Calcd. for $C_{15}H_{13}NO_4$: C, 66.41%; H, 4.83%; N, 5.16%. Found: C, 66.4%; H, 4.8%; N, 5.2%.

3-hydroxy-3-(2-nitrophenyl)-1-phenylpropane-1-one (Table 3, entry 11):



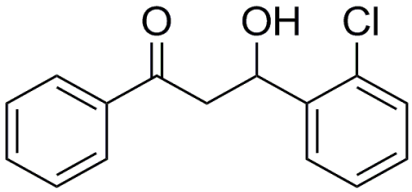
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.00-7.96 (m, 4H), 7.7 (t, *J* = 7.6 Hz, 1H), 7.6 (t, *J* = 7.4Hz, 1H), 7.5-7.45 (m,3H), 5.86 (d, *J* = 9.3 Hz, 1H), 4 (d, *J* = 3 Hz, 1H), 3.77-3.71 (dd, *J* = 18.6 Hz, 2.1 Hz, 1H), 3.25-3.16 (dd, *J* = 17.7 Hz, 9.3 Hz, 1H); Anal. Calcd. for $C_{15}H_{13}NO_4$: C, 66.41%; H, 4.83%; N, 5.16%. Found: C, 66.4%; H, 4.8%; N, 5.1%.

3-hydroxy-3-(3-nitrophenyl)-1-phenylpropane-1-one (Table 3, entry 12):



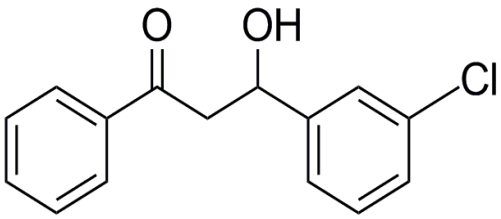
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.32 (s, 1H), 8.16 (d, *J* = 9.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.79 (d, *J* = 8.3 Hz, 1H), 7.64-7.58 (m,2H), 7.53-7.46 (m, 2H), 5.48-5.43 (m, 1H), 3.88-3.87 (m, 1H), 3.42-3.38 (m, 2H); Anal. Calcd. for $C_{15}H_{13}NO_4$: C, 66.41%; H, 4.83%; N, 5.16%. Found: C, 66.3%; H, 4.8%; N, 5.1%.

3-hydroxy-3-(2-chlorophenyl)-1-phenylpropane-1-one (Table 3, entry 13):



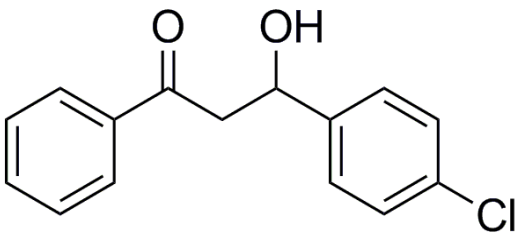
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.97 (d, *J* = 7.6 Hz, 2H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.58 (d, *J* = 7.5Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.37-7.24 (m,3H), 5.69 (d, *J* = 9.1 Hz, 1H), 3.83 (d, *J* = 3 Hz, 1H), 3.61-3.54 (dd, *J* = 17.7 Hz, 2.1 Hz, 1H), 3.19-3.10 (dd, *J* = 17.8 Hz, 9.6 Hz, 1H); Anal. Calcd. for $C_{15}H_{13}ClO_2$: C, 69.10%; H, 5.03%. Found: C, 69.0%; H, 5.0%.

3-hydroxy-3-(3-chlorophenyl)-1-phenylpropane-1-one (Table 3, entry 14):



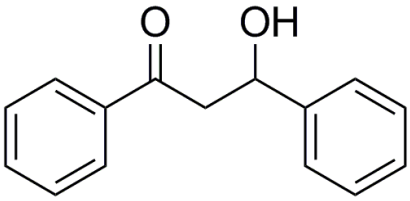
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.98-7.24 (m, 9H), 5.35-5.26 (m, 1H), 3.71 (d, *J* = 3 Hz, 1H), 3.48-3.43 (m, 2H); Anal. Calcd. for $C_{15}H_{13}ClO_2$: C, 69.10%; H, 5.03%. Found: C, 69.1%; H, 5.0%.

3-hydroxy-3-(4-chlorophenyl)-1-phenylpropane-1-one (Table 3, entry 15):



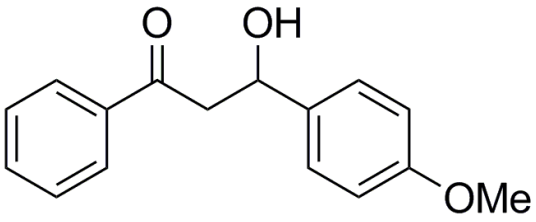
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.96-7.35 (m, 9H), 5.39 (d, *J* = 9.2 Hz, 1H), 3.65 (d, *J* = 3 Hz, 1H), 3.50-3.19 (m, 2H); Anal. Calcd. for $C_{15}H_{13}ClO_2$: C, 69.10%; H, 5.03%. Found: C, 69.0%; H, 5.0%.

3-hydroxy-1,3-biphenylpropane-1-one (Table 3, entry 16):



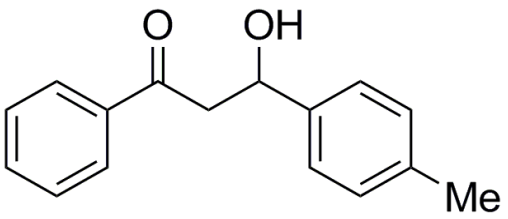
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.92 (d, *J* = 7.4 Hz, 2H), 7.55-7.27 (m, 8H), 5.30-5.26 (m, 1H), 3.67 (s, 1H), 3.42-3.29 (m, 2H); Anal. Calcd. for $C_{15}H_{14}O_2$: C, 79.62%; H, 6.24%. Found: C, 79.5%; H, 6.2%.

3-hydroxy-3-(4-methoxyphenyl)-1-phenylpropane-1-one (Table 3, entry 17):



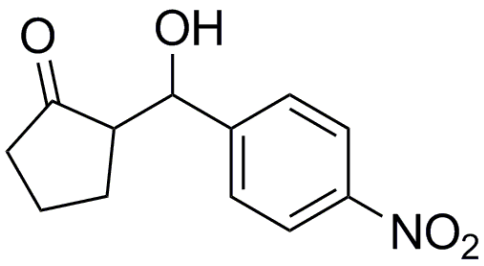
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.92 (d, *J* = 7.4 Hz, 2H), 7.43-7.24 (m, 5H), 6.92-6.88 (m, 2H), 5.32-5.28 (m, 1H), 3.80 (s, 3H), 3.5 (br s, 1H), 3.37-3.34 (m, 2H); Anal. Calcd. for $C_{16}H_{16}O_3$: C, 74.98%; H, 6.29%. Found: C, 74.9%; H, 6.2%.

3-hydroxy-3-(4-tolyl)-1-phenylpropane-1-one (Table 3, entry 18):



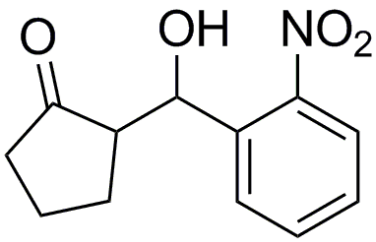
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.96-7.93 (m, 2H), 7.52-7.18 (m, 7H), 5.31-5.28 (m, 1H), 3.52 (s, 1H), 3.37-3.30 (m, 2H), 2.38 (s, 3H); Anal. Calcd. for $C_{16}H_{16}O_2$: C, 79.97%; H, 6.71%. Found: C, 79.9%; H, 6.6%.

2-(hydroxy-(4-nitrophenyl)-methyl)-cyclopentanone (Table 3, entry 19):



^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.24 (d, *J* = 8.8 Hz, 2H), 7.55-7.5 (m, 2H), 4.86 (d, *J* = 9.2 Hz, 1H), 3.84 (d, *J* = 3.1 Hz, 1H), 2.51-1.69 (m, 7H); Anal. Calcd. for $C_{12}H_{13}NO_4$: C, 61.27%; H, 5.57%; N, 5.95%. Found: C, 61.3%; H, 5.6%; N, 5.9%.

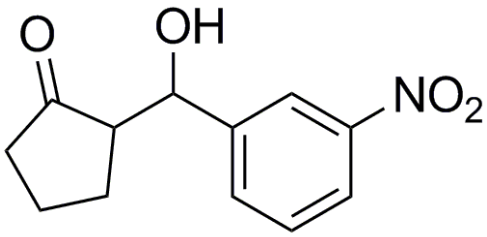
2-(hydroxy-(2-nitrophenyl)-methyl)-cyclopentanone (Table 3, entry 20):



^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.02 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.64-7.59 (m, 1H), 7.5-7.45 (m, 1H), 5.46 (d, *J* = 8.6 Hz, 1H), 4 (d, *J* = 2.9 Hz, 1H), 2.64-

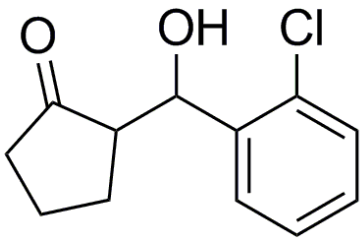
1.61 (m, 7H); Anal. Calcd. for $C_{12}H_{13}NO_4$: C, 61.27%; H, 5.57%; N, 5.95%. Found: C, 61.2%; H, 5.5%; N, 5.9%.

2-(hydroxy-(3-nitrophenyl)-methyl)-cyclopentanone (Table 3, entry 21)



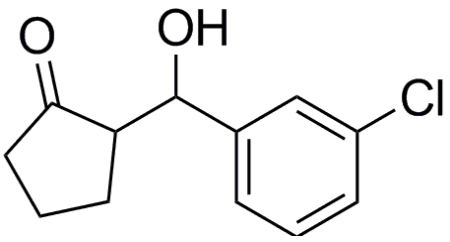
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.23 (s, 1H), 8.18-8.11 (m, 1H), 7.71-7.66 (m, 1H), 7.56-7.5 (m, 1H), 4.84-4.79 (m, 1H), 3.63 (d, *J* = 4.9 Hz, 1H), 2.50-1.71 (m, 7H); Anal. Calcd. for $C_{12}H_{13}NO_4$: C, 61.27%; H, 5.57%; N, 5.95%. Found: C, 61.2%; H, 5.6%; N, 5.9%.

2-(hydroxy-(2-chlorophenyl)-methyl)-cyclopentanone (Table 3, entry 22):



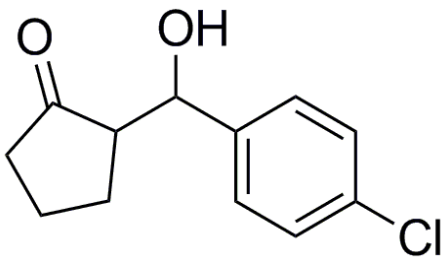
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.59 (d, *J* = 1.7 Hz, 1H), 7.56-7.18 (m, 3H), 5.3 (d, *J* = 9.3 Hz, 1H), 4.53 (d, *J* = 1.2 Hz, 1H), 2.47-1.7 (m, 7H); Anal. Calcd. for $C_{12}H_{13}ClO_2$: C, 64.15%; H, 5.83%. Found: C, 64.1%; H, 5.8%.

2-(hydroxy-(3-chlorophenyl)-methyl)-cyclopentanone (Table 3, entry 23):



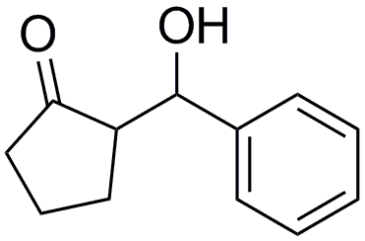
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.56 (s, 1H), 7.4-7.24 (m, 3H), 4.69 (d, *J* = 9.2 Hz, 1H), 4.66 (s, 1H), 2.45-1.7 (m, 7H); Anal. Calcd. for $C_{12}H_{13}ClO_2$: C, 64.15%; H, 5.83%. Found: C, 64.1%; H, 5.8%.

2-(hydroxy-(4-chlorophenyl)-methyl)-cyclopentanone (Table 3, entry 24):



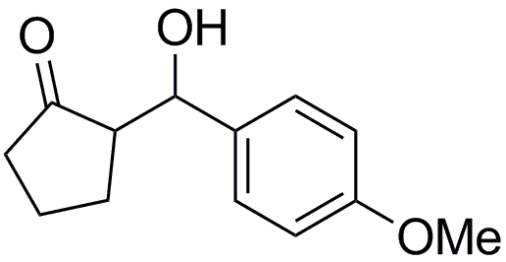
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.44 (d, *J* = 8.5 Hz, 2H), 7.19 (d, *J* = 8.3 Hz, 2H), 5.23 (br, s, 1H), 4.67-4.59 (m, 1H), 2.79 (d, *J* = 4.5 Hz, 1H), 2.4-1.68 (m, 6H); Anal. Calcd. for $C_{12}H_{13}ClO_2$: C, 64.15%; H, 5.83%. Found: C, 64.1%; H, 5.8%.

2-(hydroxy-phenyl-methyl)-cyclopentanone (Table 3, entry 25):



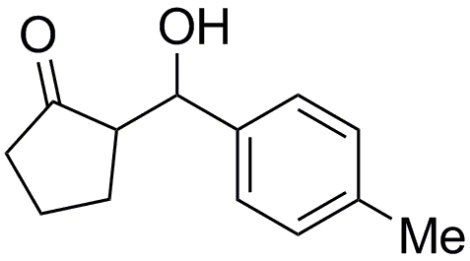
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.37-7.25 (m, 5H), 4.72 (d, *J* = 9.2 Hz, 1H), 3.5 (s, 1H), 2.62-1.72 (m, 7H); Anal. Calcd. for $C_{12}H_{13}O_2$: C, 75.76%; H, 7.42%. Found: C, 75.7%; H, 7.4%.

2-(hydroxy-(4-methoxyphenyl)-methyl)-cyclopentanone (Table 3, entry 26):



^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.22 (d, *J* = 8.8 Hz, 2H), 6.9 (d, *J* = 8.8 Hz, 2H), 5.23 (d, *J* = 5.2 Hz, 1H), 4.5 (br s, 1H), 3.8 (s, 3H), 2.9-1.6 (m, 7H); Anal. Calcd. for $C_{13}H_{16}O_3$: C, 70.89%; H, 7.32%. Found: C, 70.9%; H, 7.3%.

2-(hydroxy-(4-methylphenyl)-methyl)-cyclopentanone (Table 3, entry 27):



^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm): 7.26-7.14 (m, 4H), 4.67 (d, *J* = 9.2 Hz, 1H), 4.49 (s, 1H), 2.46-1.68 (m, 10H); Anal. Calcd. for $C_{13}H_{16}O_2$: C, 76.44%; H, 7.90%. Found: C, 76.5%; H, 7.9%.

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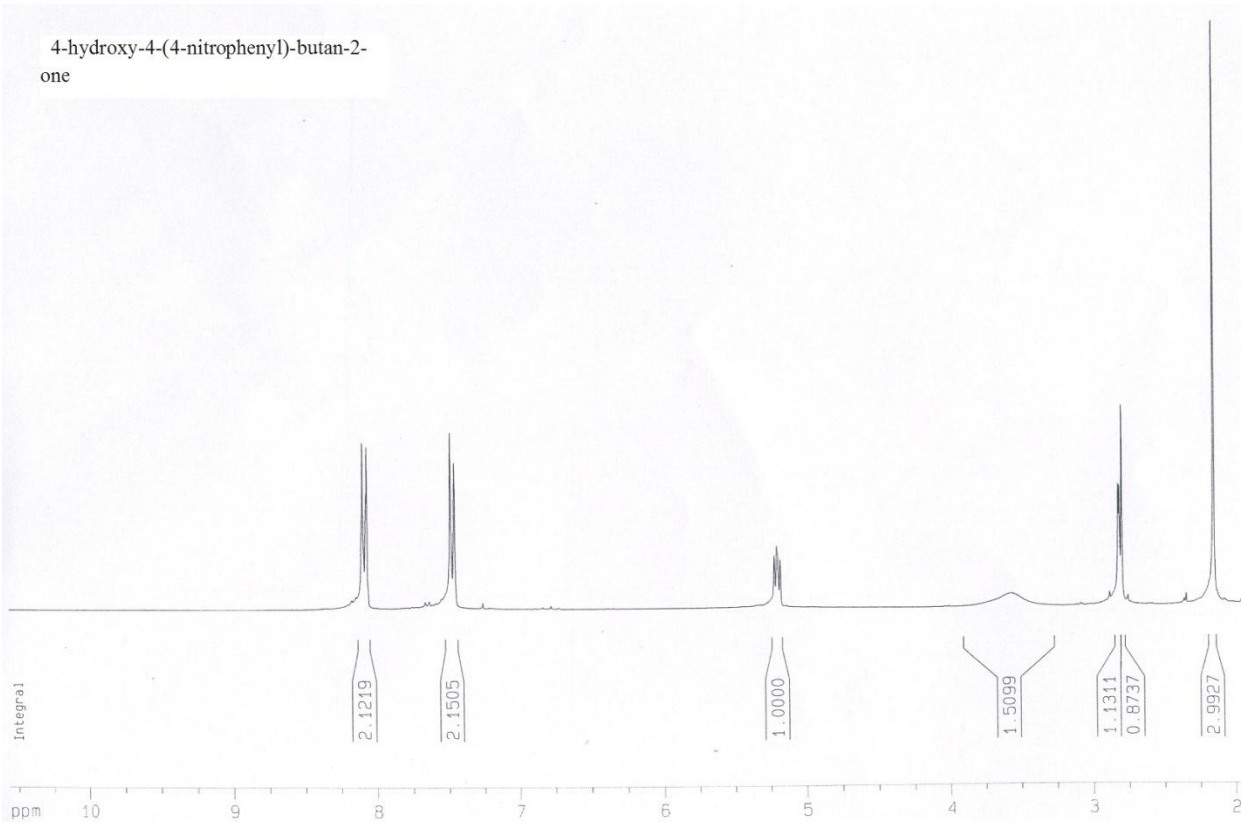
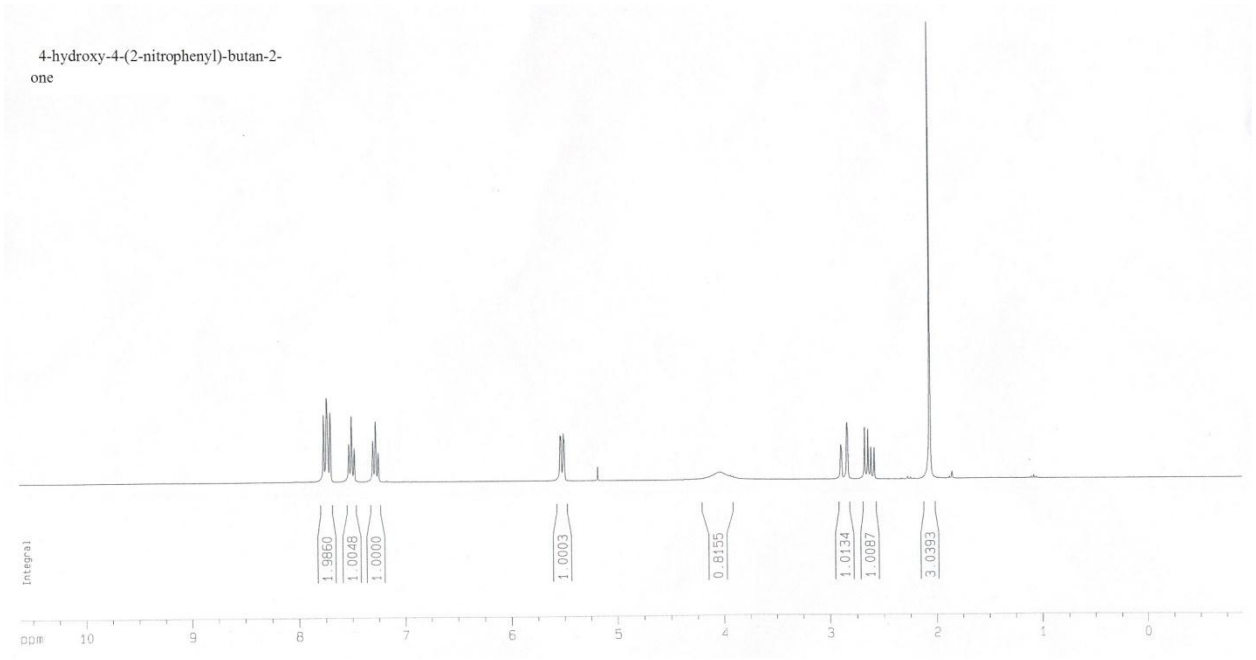
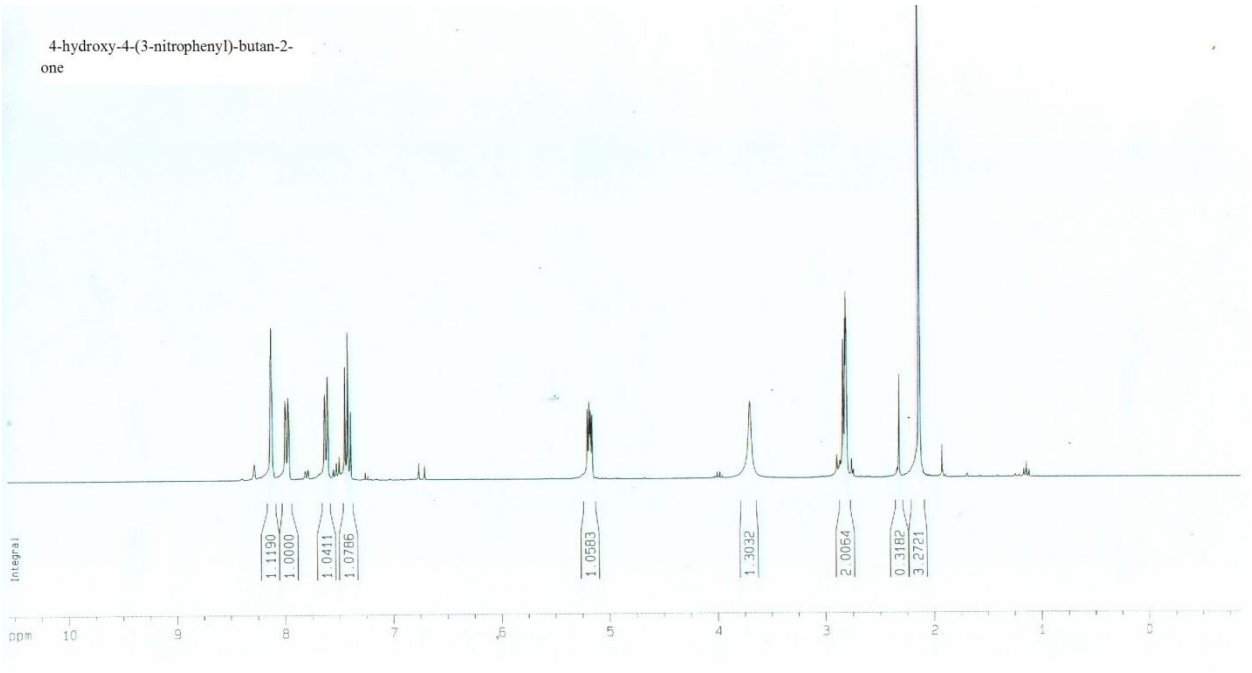
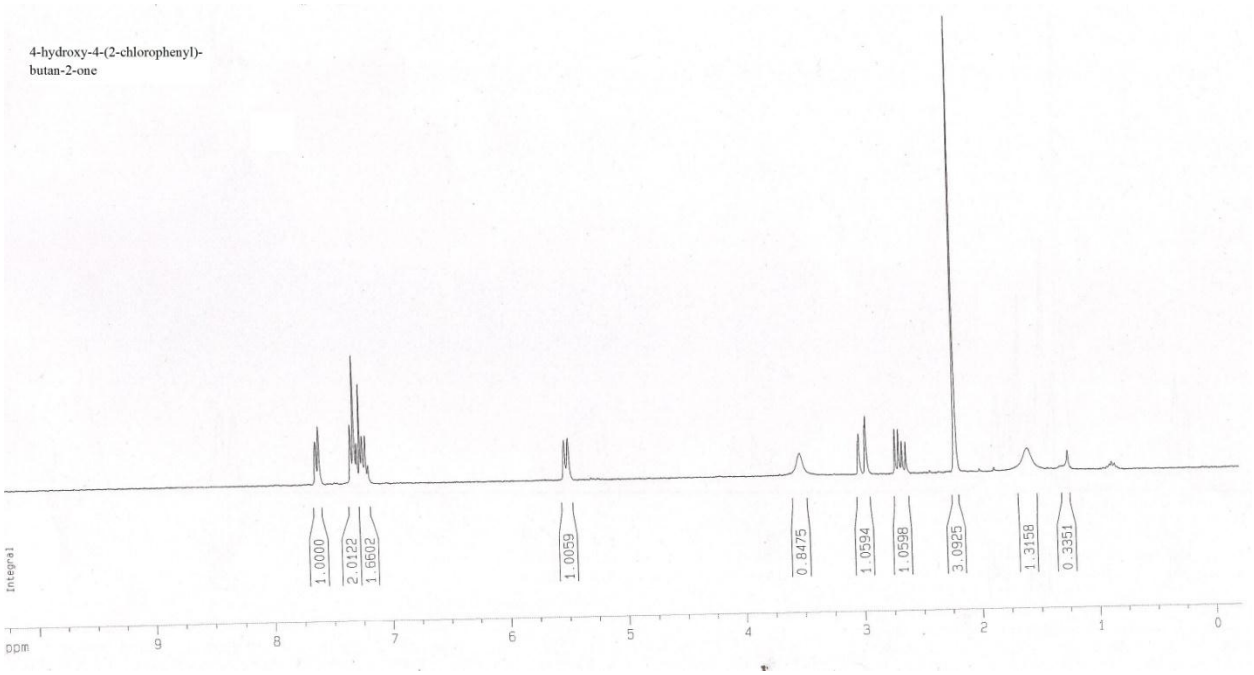
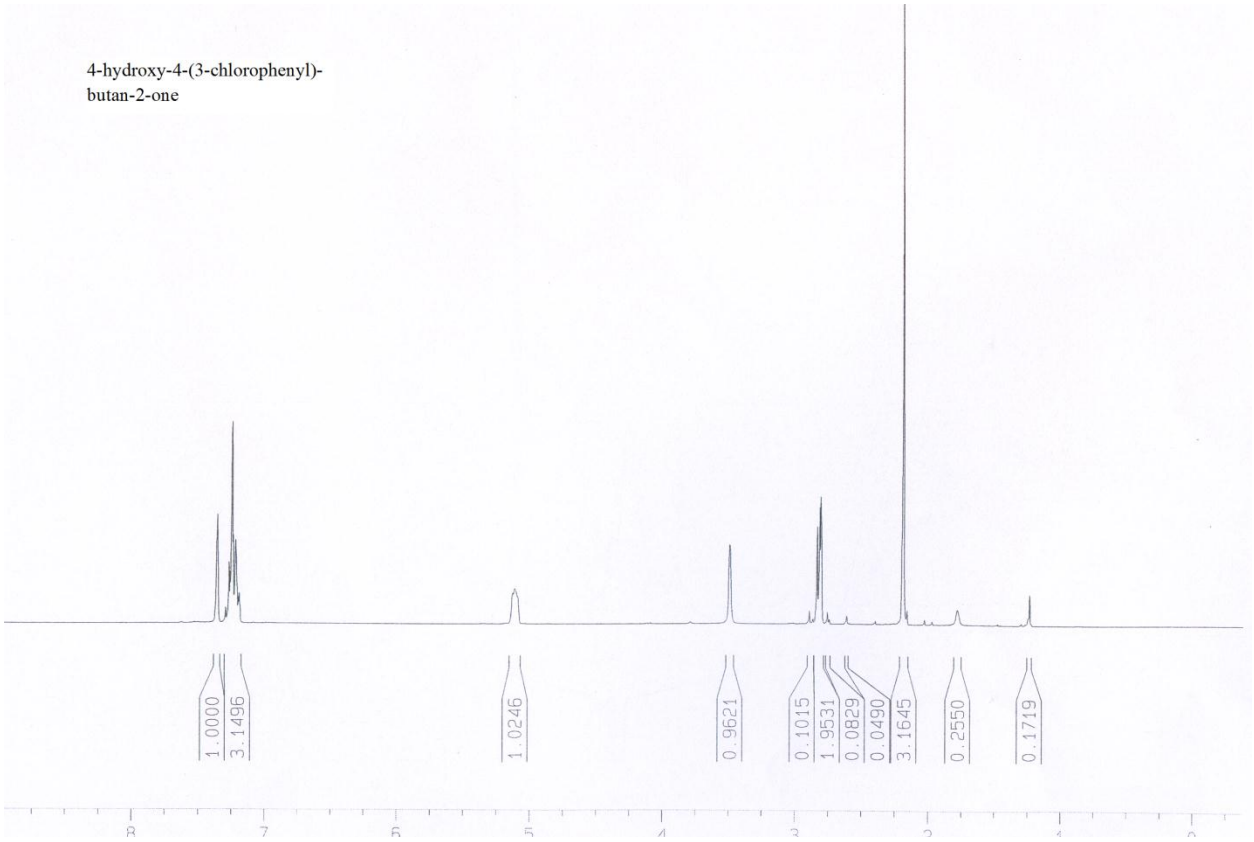
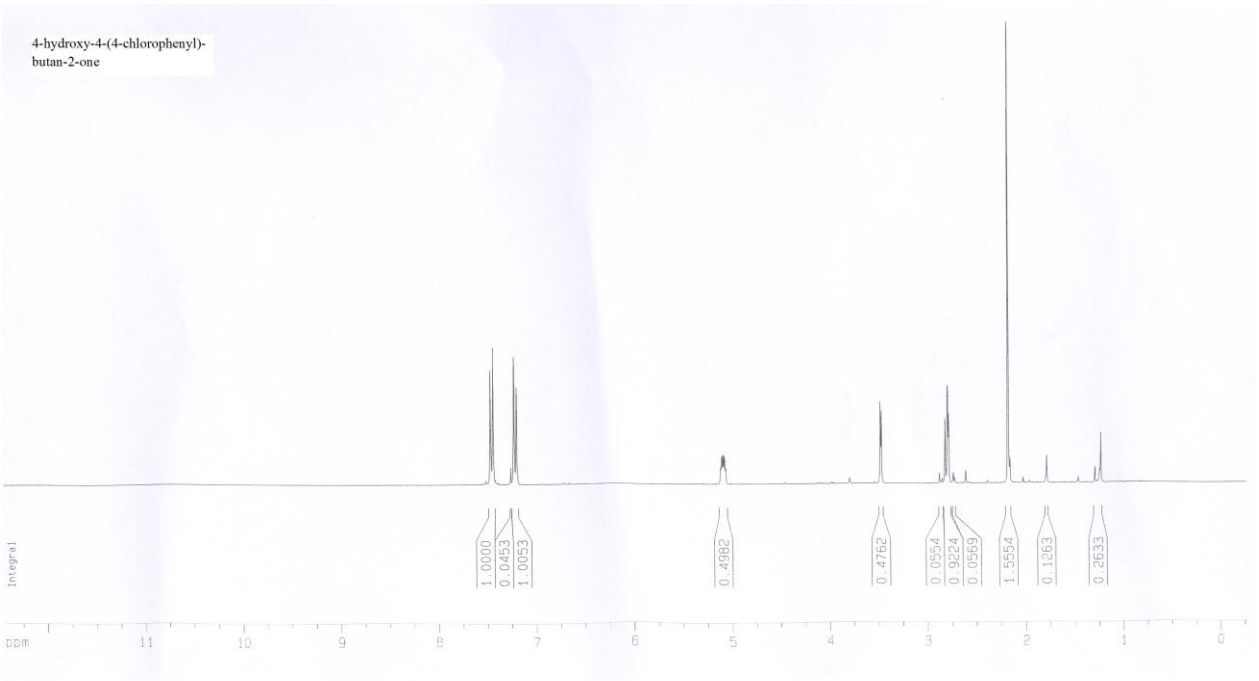

4-hydroxy-4-(4-nitrophenyl)-butan-2-one
Integral
2.1219
2.1505
1.0000
1.5099
1.1311
0.8737
2.9927
ppm
10
9
8
7
6
5
4
3
2

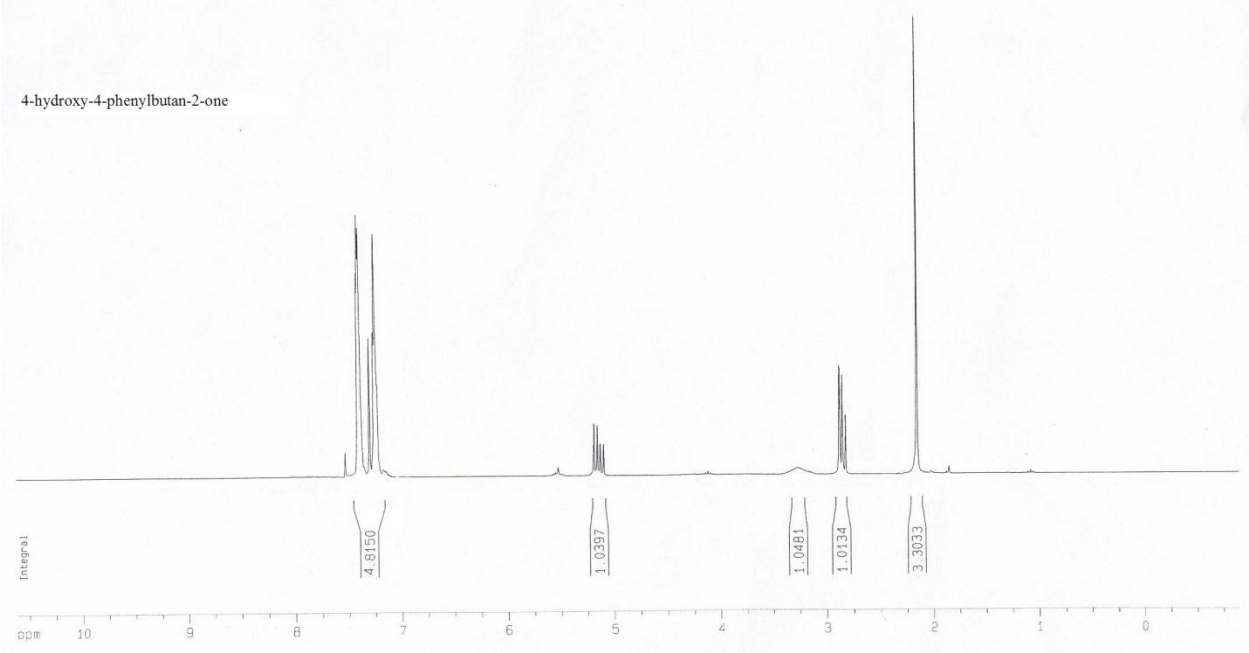

4-hydroxy-4-(2-nitrophenyl)-butan-2-one
Integral
1.9860
1.0048
1.0000
1.0003
0.8155
1.0134
1.0087
3.0393
ppm
10
9
8
7
6
5
4
3
2
1
0

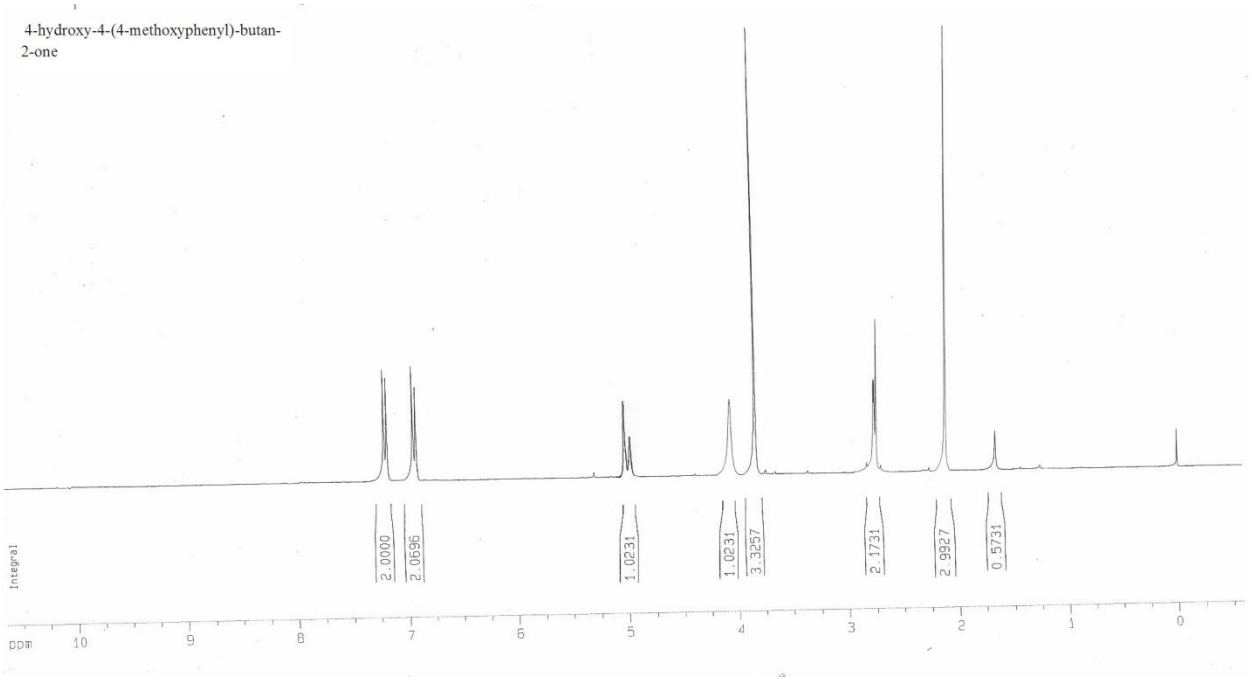

4-hydroxy-4-(3-nitrophenyl)-butan-2-one
Integral
1.1190
1.0000
1.0411
1.0786
1.0583
1.3032
2.0064
0.3182
3.2721
ppm
10
9
8
7
6
5
4
3
2
1
0

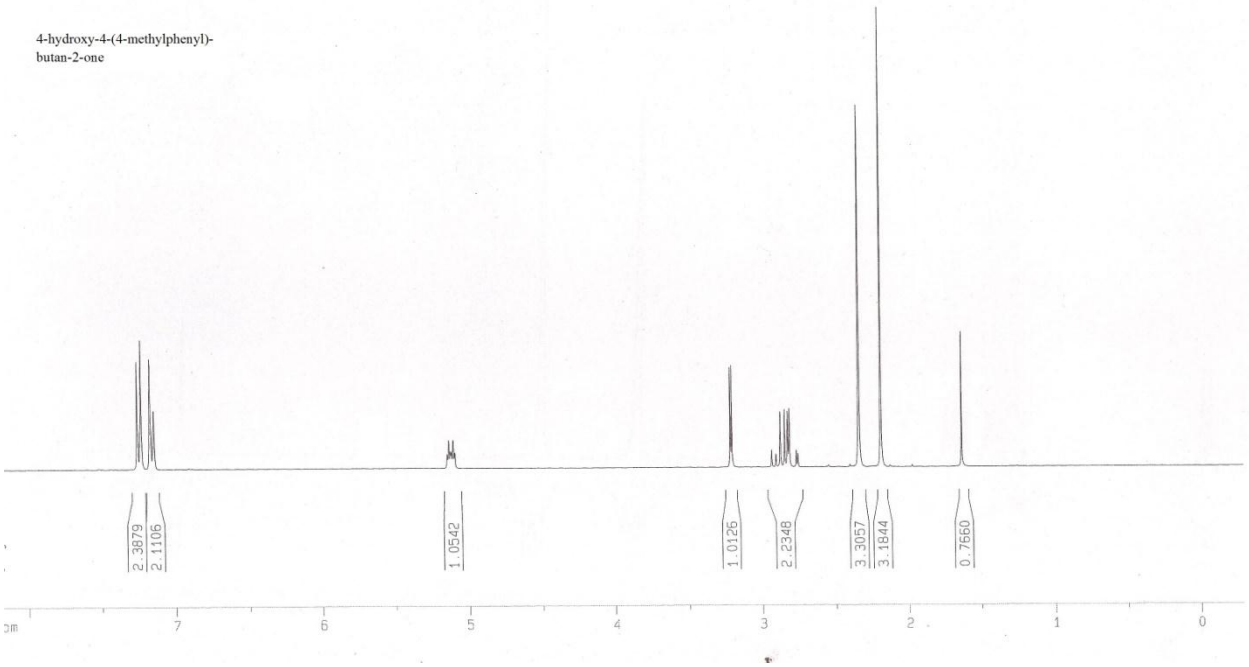

4-hydroxy-4-(2-chlorophenyl)-
butan-2-one
Integral
1.0000
2.0122
1.6602
1.0059
0.8475
1.0594
1.0598
3.0925
1.3158
0.3351
ppm
9
8
7
6
5
4
3
2
1
0

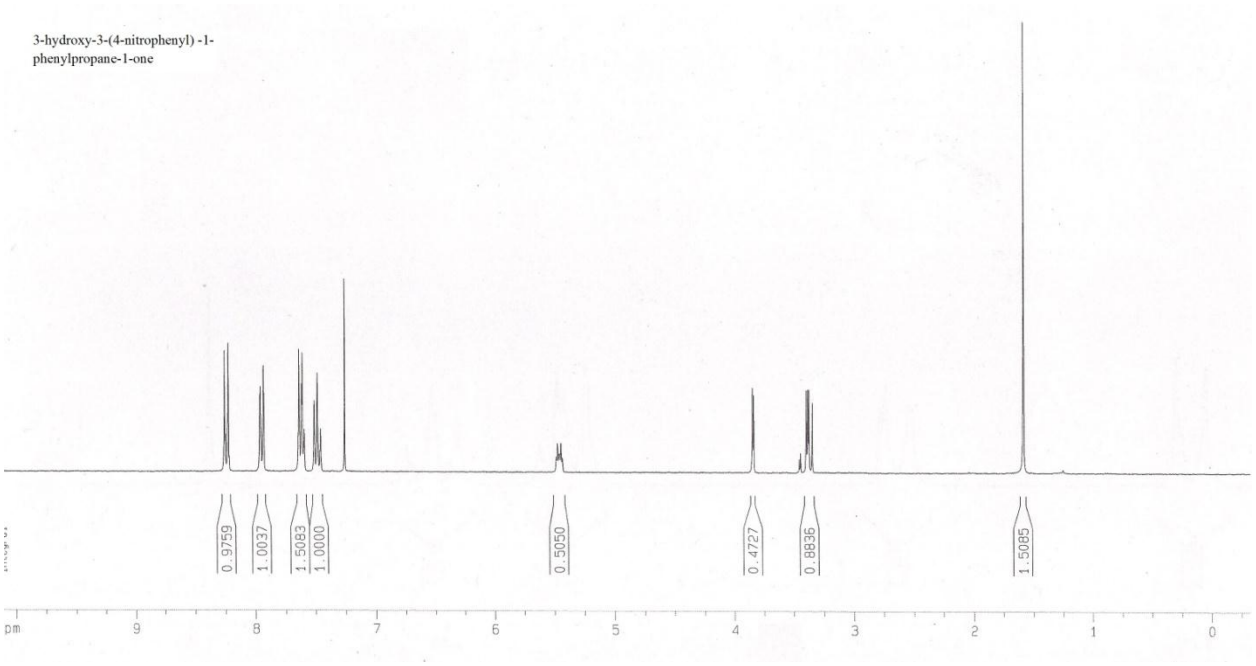

4-hydroxy-4-(3-chlorophenyl)-
butan-2-one
1.0000
3.1496
1.0246
0.9621
0.1015
1.9531
0.0829
0.0490
3.1645
0.2550
0.1719

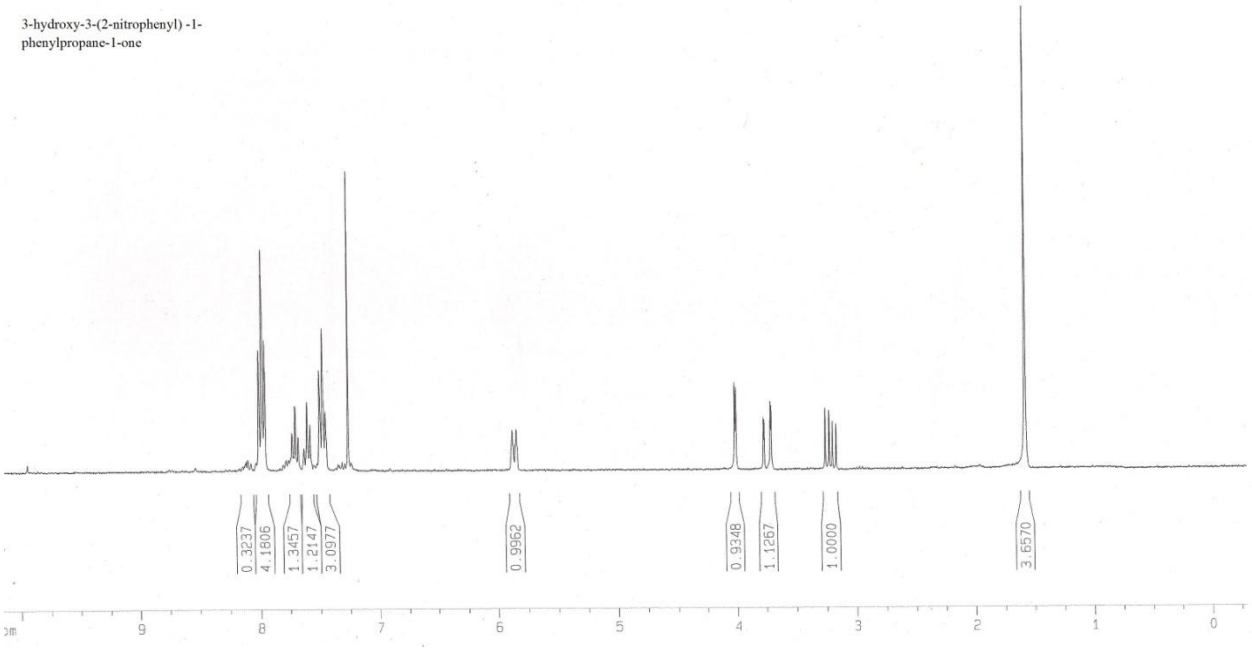

4-hydroxy-4-(4-chlorophenyl)-
butan-2-one
Integral
1.0000
0.0453
1.0053
0.4982
0.4762
0.0554
0.9824
0.0569
1.5554
0.1263
0.2633
ppm
11
10
9
8
7
6
5
4
3
2
1
0

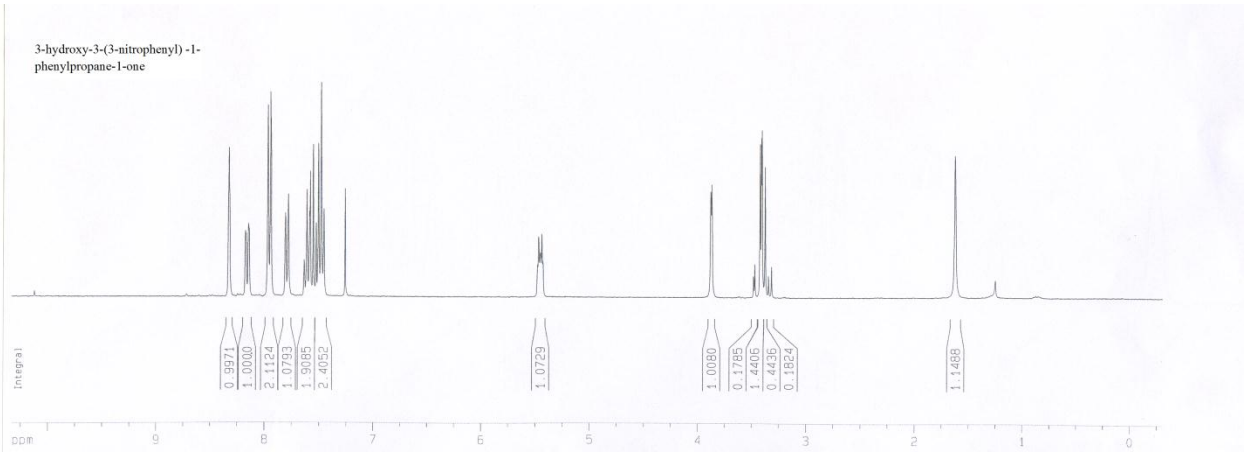

4-hydroxy-4-phenylbutan-2-one
Integral
4.8150
1.0397
1.0481
1.0134
3.3033
ppm
10
9
8
7
6
5
4
3
2
1
0

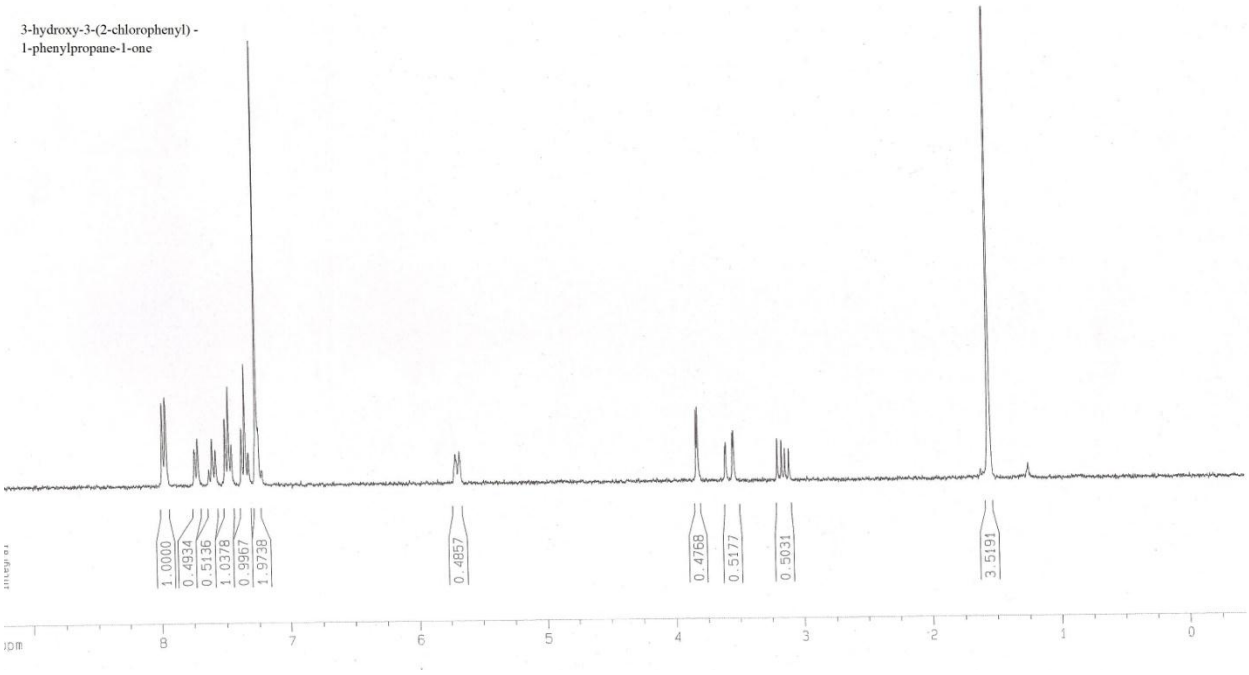

4-hydroxy-4-(4-methoxyphenyl)-butan-2-one
Integral
2.0000
2.0696
1.0231
1.0231
3.3257
2.1731
2.9827
0.5731
ppm
10
9
8
7
6
5
4
3
2
1
0


4-hydroxy-4-(4-methylphenyl)-
butan-2-one
2.3879
2.1106
1.0542
1.0126
2.2348
3.3057
3.1844
0.7660
7
6
5
4
3
2
1
0

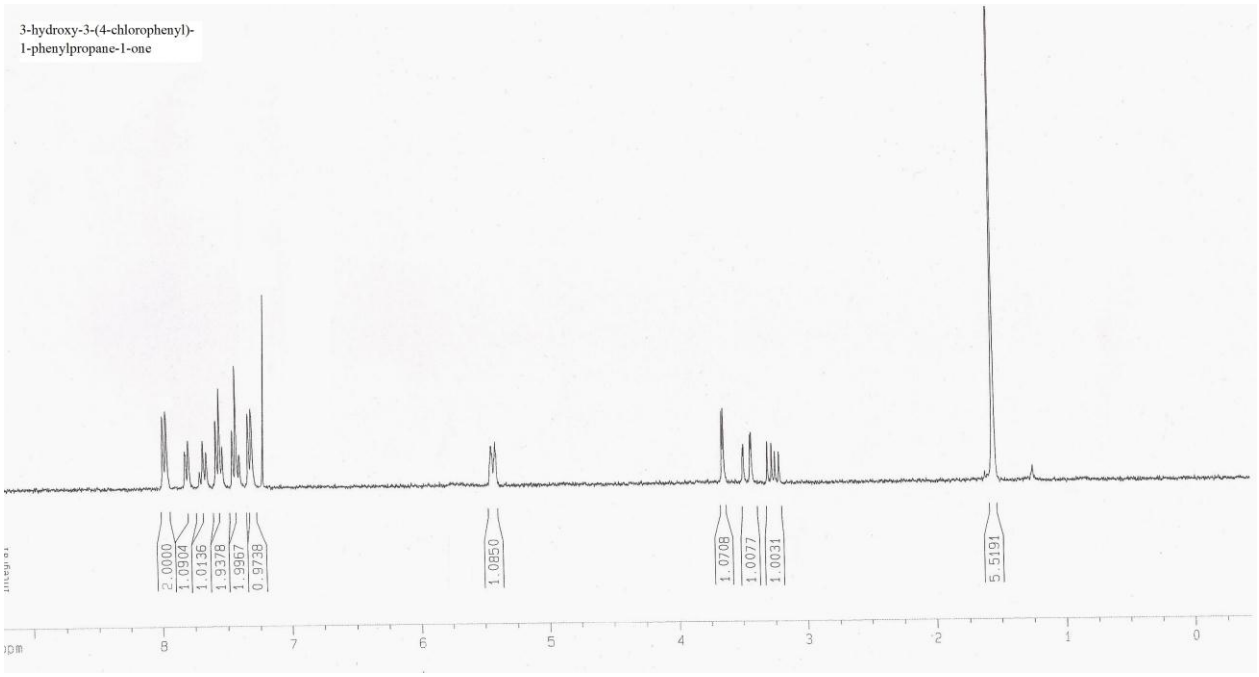

3-hydroxy-3-(4-nitrophenyl) -1-
phenylpropane-1-one
0.9759
1.0037
1.5083
1.0000
0.5050
0.4727
0.8836
1.5085
pm
9
8
7
6
5
4
3
2
1
0

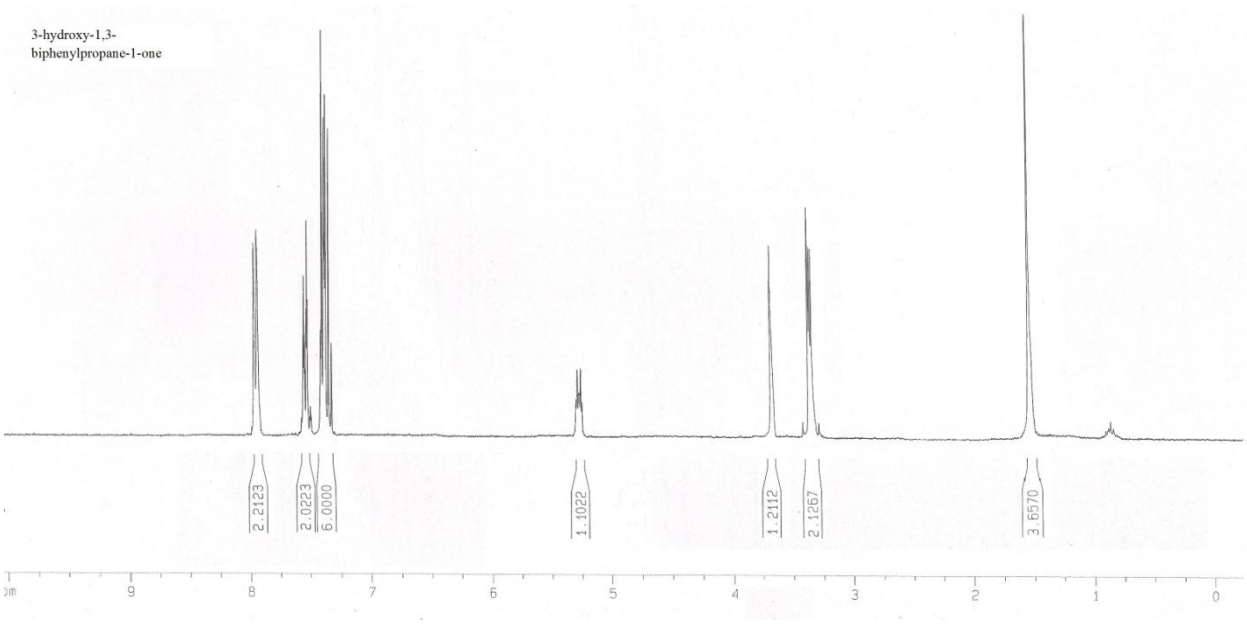

3-hydroxy-3-(2-nitrophenyl) -1-
phenylpropane-1-one
0.3237
4.1806
1.3457
1.2147
3.0977
0.9962
0.9348
1.1267
1.0000
3.6570
9
8
7
6
5
4
3
2
1
0

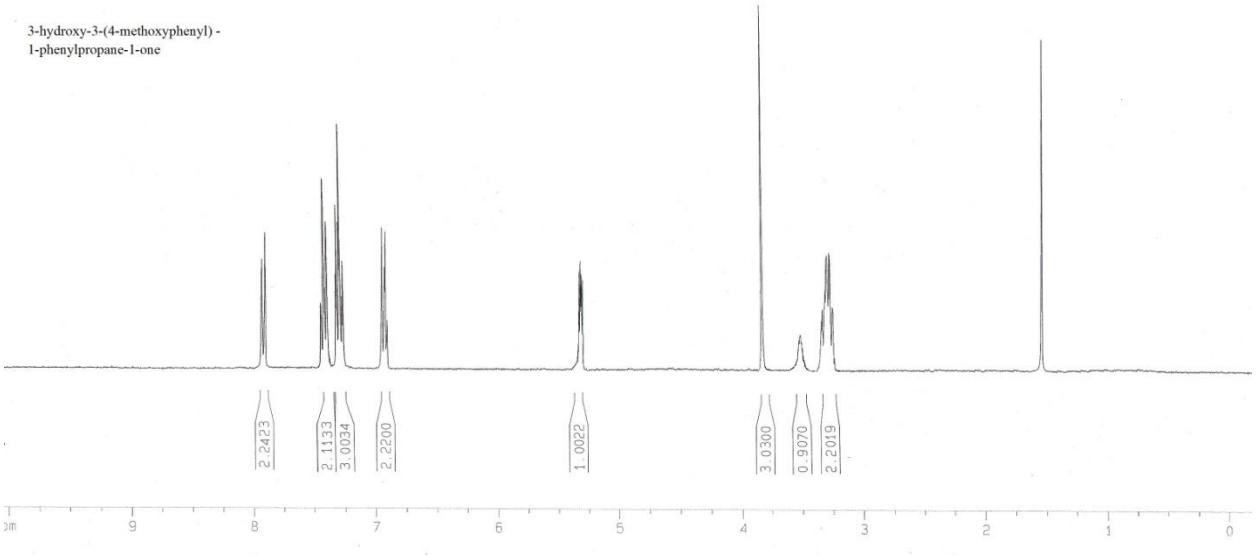

3-hydroxy-3-(3-nitrophenyl) -1-
phenylpropane-1-one
Integral
0.9971
1.0000
2.1124
1.0793
1.9085
2.4052
1.0729
1.0080
0.1785
1.4406
0.4436
0.1824
1.1488
ppm
9
8
7
6
5
4
3
2
1
0

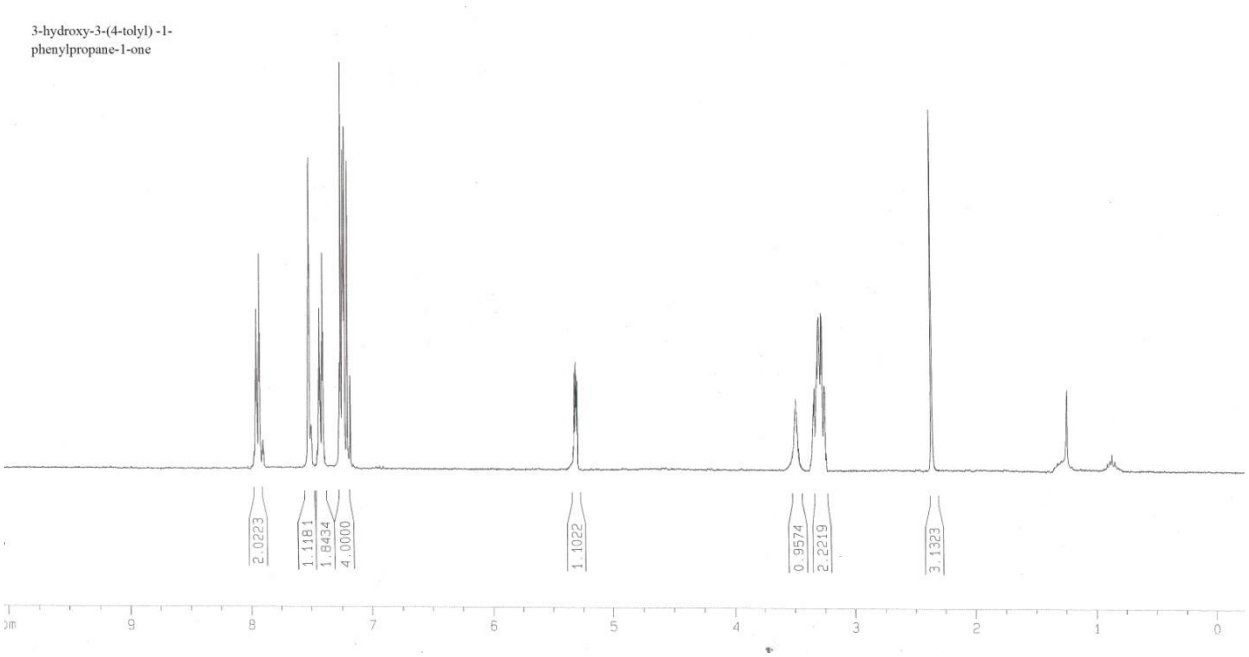

3-hydroxy-3-(2-chlorophenyl) -
1-phenylpropane-1-one
1.0000
0.4934
0.5136
1.0378
0.9967
1.9738
0.4857
0.4768
0.5177
0.5031
3.5191
ppm
8
7
6
5
4
3
2
1
0

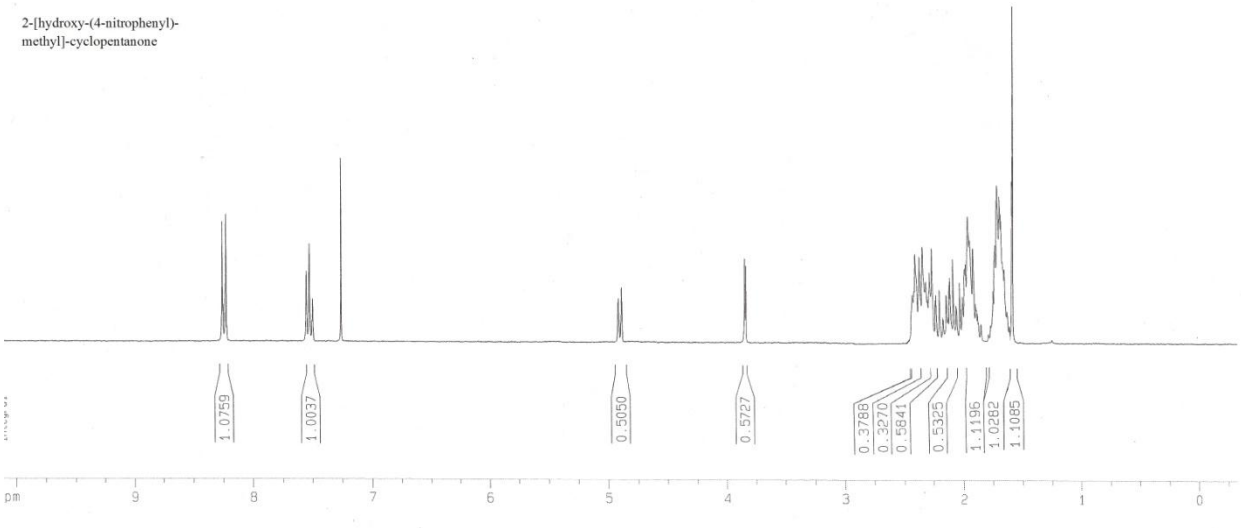

3-hydroxy-3-(3-chlorophenyl) -
1-phenylpropane-1-one
1.9967
1.0378
2.0000
1.0272
2.0227
1.9030
1.0807
1.4768
3.2191
0.0031
8
7
6
5
4
3
2
1
0

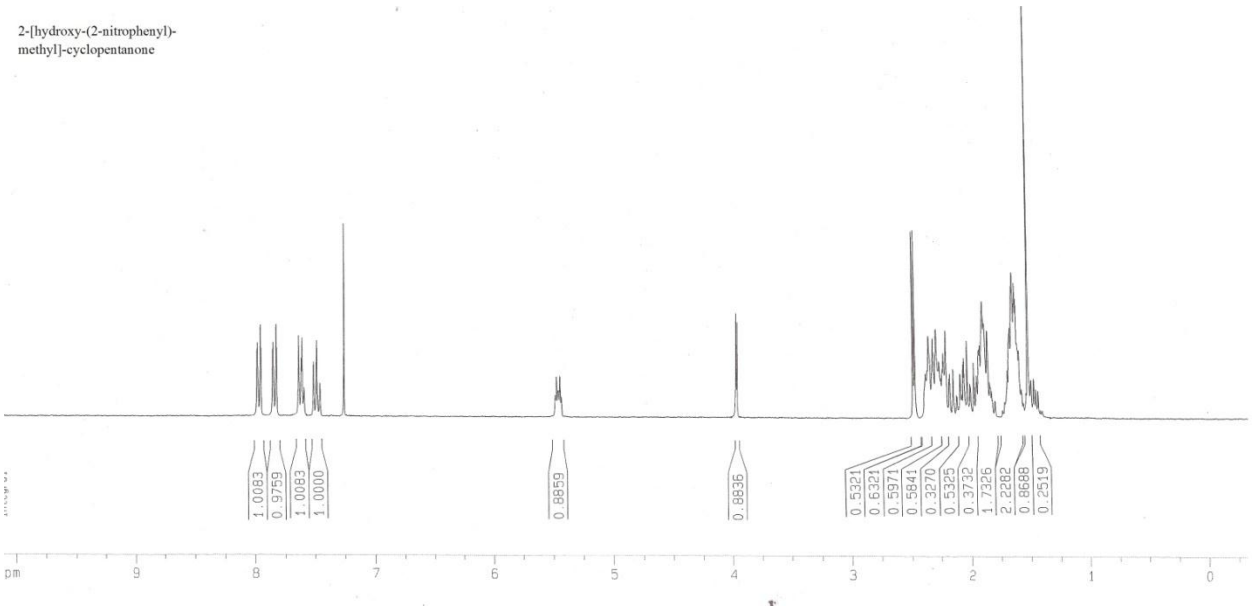

3-hydroxy-3-(4-chlorophenyl)-
1-phenylpropane-1-one
2.0000
1.0904
1.0136
1.9378
1.9967
0.9738
1.0850
1.0708
1.0077
1.0031
5.5191
8
7
6
5
4
3
2
1
0

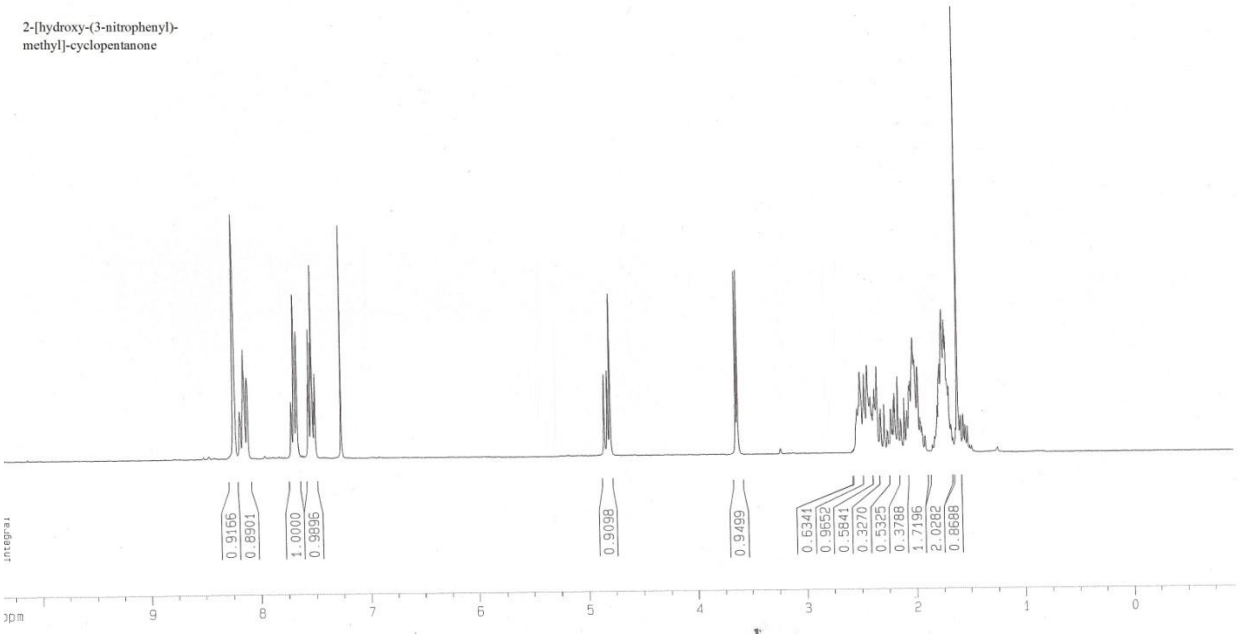

3-hydroxy-1,3-
biphenylpropane-1-one
2.2123
2.0223
6.0000
1.1022
1.2112
2.1267
3.6570
9
8
7
6
5
4
3
2
1
0

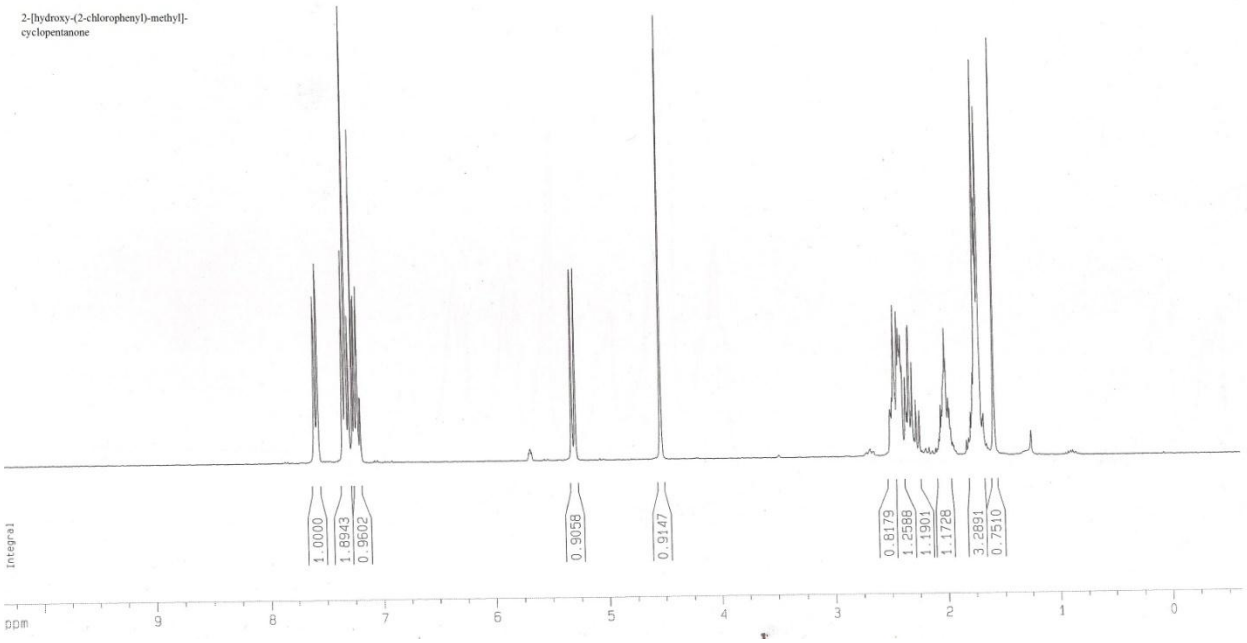

3-hydroxy-3-(4-methoxyphenyl) -
1-phenylpropane-1-one
2.2423
2.1133
3.0034
2.2200
1.0022
3.0300
0.9070
2.2019
9
8
7
6
5
4
3
2
1
0

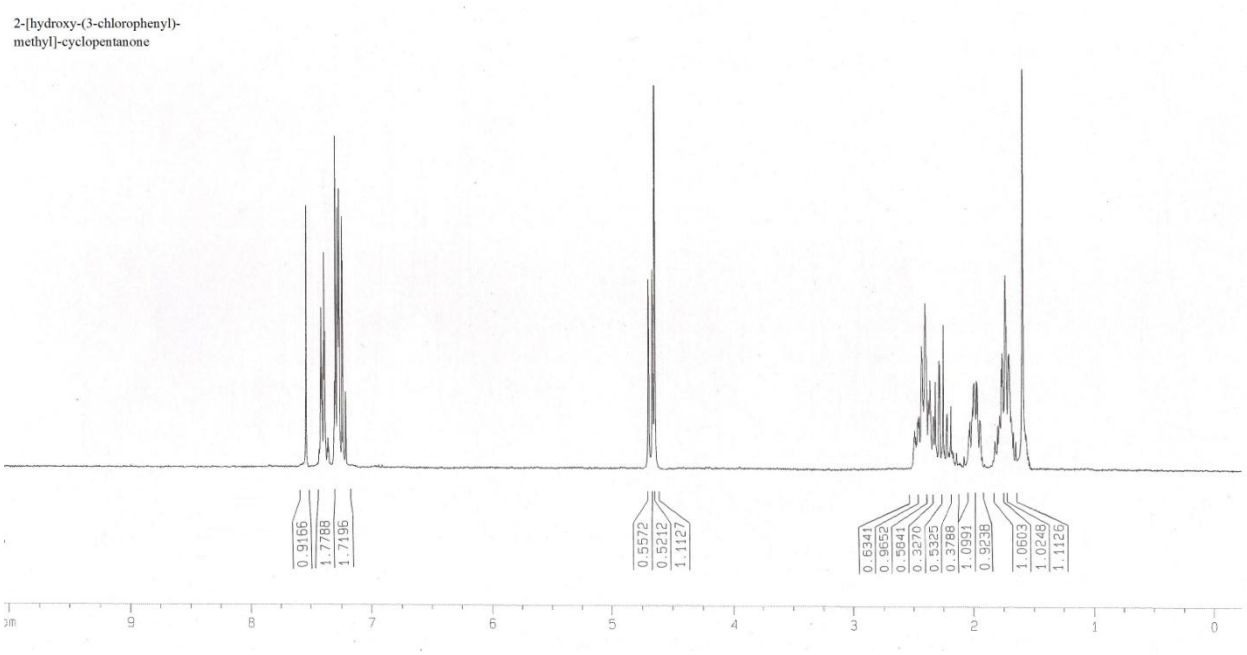

3-hydroxy-3-(4-tolyl) -1-
phenylpropane-1-one
2.0223
1.1181
1.8434
4.0000
1.1022
0.9574
2.2219
3.1323
9
8
7
6
5
4
3
2
1
0

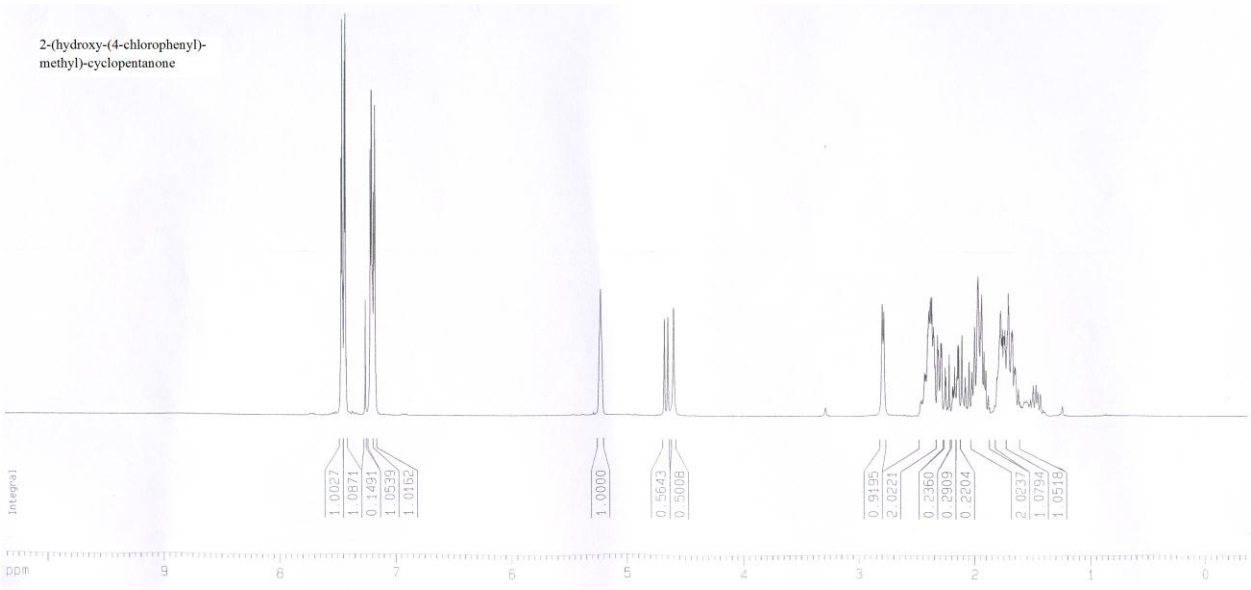

2-[hydroxy-(4-nitrophenyl)-
methyl]-cyclopentanone
1.0759
1.0037
0.5050
0.5727
0.3788
0.3270
0.5841
0.5325
1.1196
1.0282
1.1085
pm
9
8
7
6
5
4
3
2
1
0

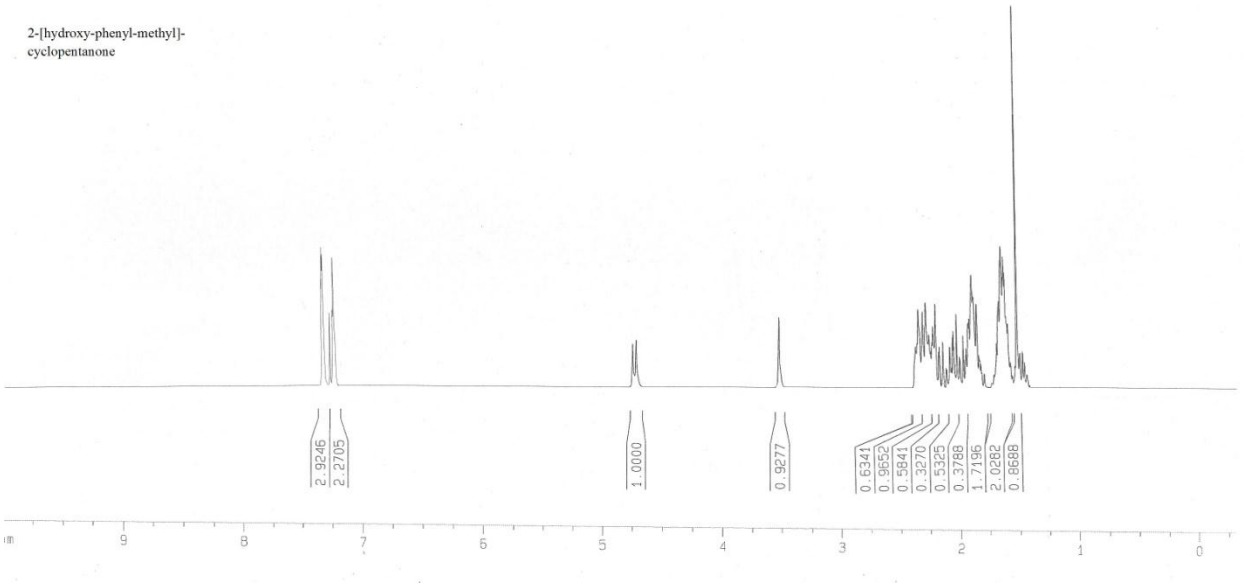

2-[hydroxy-(2-nitrophenyl)-
methyl]-cyclopentanone
1.0083
0.9759
1.0083
1.0000
0.8859
0.8836
0.5321
0.6321
0.5971
0.5841
0.3270
0.5325
0.3732
1.7326
2.2282
0.8688
0.2519
pm
9
8
7
6
5
4
3
2
1
0

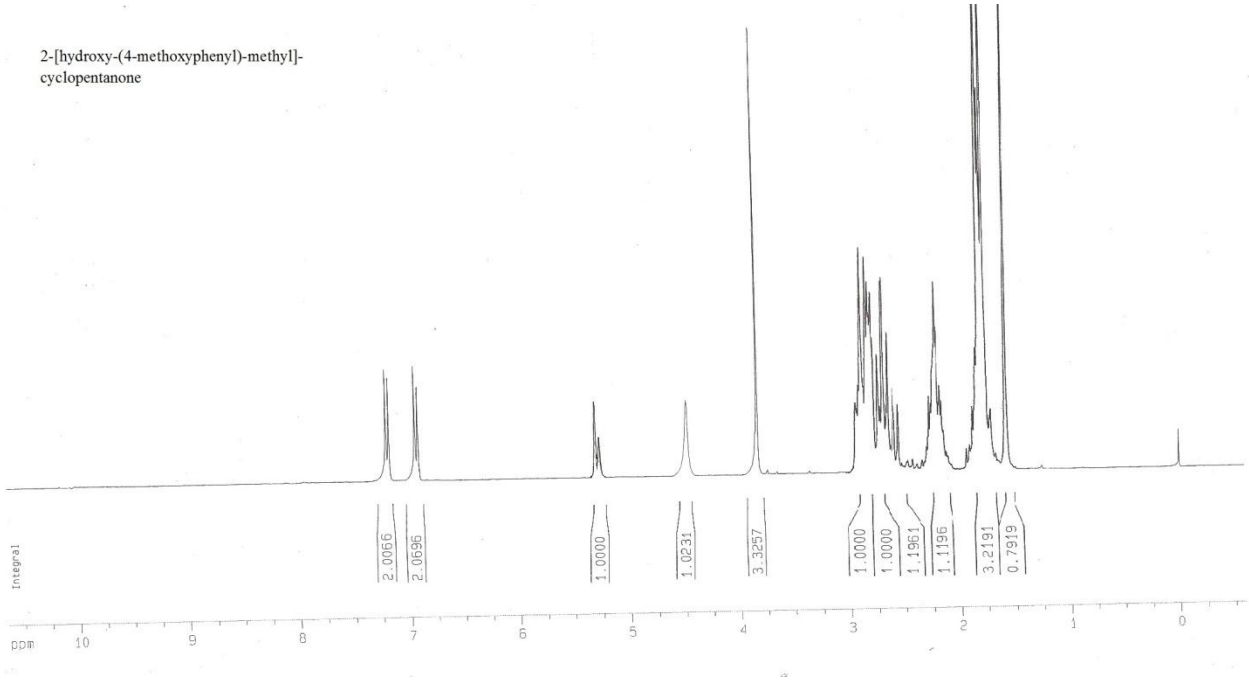

2-[hydroxy-(3-nitrophenyl)-
methyl]-cyclopentanone
0.9166
0.8901
1.0000
0.9896
0.9098
0.9499
0.6341
0.9652
0.5841
0.3270
0.5325
0.3788
1.7196
2.0282
0.8688
ppm
9
8
7
6
5
4
3
2
1
0

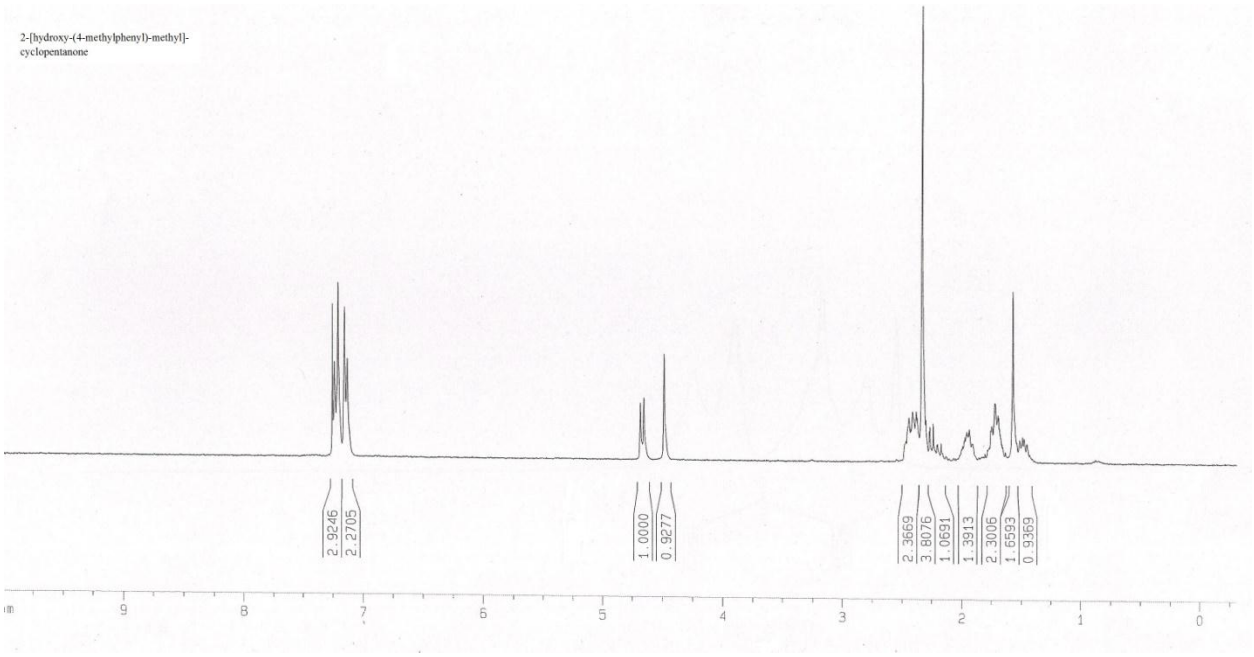

2-[hydroxy-(2-chlorophenyl)-methyl]-
cyclopentanone
integral
1.0000
1.8943
0.9602
0.9058
0.9147
0.8179
1.2588
1.1901
1.1728
3.2891
0.7510
ppm
9
8
7
6
5
4
3
2
1
0


2-[hydroxy-(3-chlorophenyl)-
methyl]-cyclopentanone
0.9166
1.7788
1.7196
0.5572
0.5212
1.1127
0.6341
0.9652
0.5641
0.3270
0.5325
0.3788
1.0991
0.9238
1.0603
1.0248
1.1126
9
8
7
6
5
4
3
2
1
0


2-(hydroxy-(4-chlorophenyl)-
methyl)-cyclopentanone
Integral
1.0027
1.0871
0.1491
1.0539
1.0162
1.0000
0.5643
0.5008
0.9195
2.0221
0.2360
0.2909
0.2204
2.0237
1.0794
1.0518
ppm
9
8
7
6
5
4
3
2
1
0


2-[hydroxy-phenyl-methyl]-
cyclopentanone
2.9246
2.2705
1.0000
0.9277
0.6341
0.9652
0.5841
0.3270
0.5325
0.3788
1.7196
2.0282
0.8688
9
8
7
6
5
4
3
2
1
0


2-[hydroxy-(4-methoxyphenyl)-methyl]-
cyclopentanone
Integral
2.0066
2.0696
1.0000
1.0231
3.3257
1.0000
1.0000
1.1961
1.1196
3.2191
0.7919
ppm
10
9
8
7
6
5
4
3
2
1
0


2-[hydroxy-(4-methylphenyl)-methyl]-
cyclopentanone
2.9246
2.2705
1.0000
0.9277
2.3669
3.8076
1.0691
1.3913
2.3006
1.6593
0.9369
9
8
7
6
5
4
3
2
1
0