Supporting Information

SeO2 in water: a mild and efficient promoter for deprotection of acetyl, methoxymethyl and tetrahydropyranyl ethers and sequel oxidation of methyl/methylene carbons of alpha carbonyl carbon

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1. General methods

Organic solvents were dried by standard method, the reagents (chemicals) were purchased from commercial sources, and used without further purification. All reactions were monitored by TLC using precoated silica gel aluminum plates. Visualization of TLC plates was accomplished with an UV lamp. Column chromatography was performed using silica gel 60–120 mesh size (RANKEM Limited) with EtOAc–hexanes as eluent. Melting points were recorded on Perfit apparatus and are uncorrected. All products were characterized by NMR, IR and MS spectra. ^{1}H and ^{13}C NMR spectra were recorded in deuterated chloroform ($CDCl_3$) on a 500 MHz and 125 MHz spectrometer (Bruker), respectively. Chemical shifts were reported in parts per million (ppm, δ) downfield from

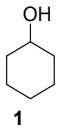
tetramethylsilane. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), and broad (br).

2. **Experimental Section**

General procedure for deprotection of acetyl esters, tetrahydropyranyl and methoxymethyl ethers of alcohol and phenol: SeO_2 (1 mmol) was added to a stirred solution of Esters and ethers (1 mmol) in a water (1ml) and 3-4 drops of dioxane, suspension obtained, applied heating to 80°C. After TLC monitoring, the resulting reaction mixture was poured in cold water and extracted with EtOAc. The organic layer was washed with brine, dried with anhyd.Na_2SO_4, and concentrated in *vacuo* to give the corresponding product which was purified by silica gel column chromatography with hexane- EtOAc eluent to obtain the products **1 to 11** (table 3) in excellent yield 85-95% and 30-40% for deacetylation, detetrahydropyranylation and demethoxymethylation respectively.

General procedure for deprotection of acetyl esters, tetrahydropyranyl ethers and methoxymethyl ethers of alcohols and phenols and sequel oxidation of alpha carbonyl carbon: SeO_2 (3 mmol) was added to a stirred solution of Esters and ethers (1 mmol) in a water (1ml) and 3 to 4 drops of dioxane, suspension obtained, applied heating to 80°C, gave products **12 to 21** (table 4) in excellent yield 85-95% and 30-40% for deacetylation, detetrahydropyranylation and demethoxymethylation followed by sequel oxidation of alpha carbonyl carbon respectively.

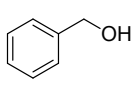
3. Characterization data for selected synthesized compounds.



1

Cyclohexanol (1): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 3.75 (s,1H), 3.08-3.04 (m, 1H), 2.32 (t, *J* = 6 Hz, 1H), 1.64-1.61 (m, 4H), 1.51 (t, *J* = 6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 69.148, 36.270, 25.144, 23.100; GC-MS (m/z): 100 [$M^{+\cdot}$, $C_6H_{12}O$].

Phenylmethanol (2): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.46-7.41 (m,2H), 7.37 (d, *J* = 8 Hz, 1H), 7.15 (d, *J* = 7.5 Hz, 2H) 4.79 (s, 1H), ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 142.62, 131.54, 130.71, 129.62, 69.13; GC-MS (m/z): 108 [$M^{+\cdot}$, C_7H_8O].



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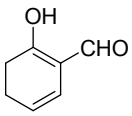
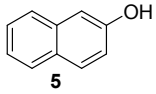


4

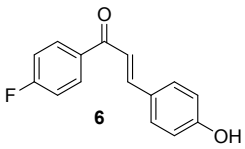
2-Hydroxybenzaldehyde (4): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 11.01 (s, 1H), 9.88 (t, *J* = 4.5 Hz, 1H)), 7.52 (dd, *J* = 8.5 Hz, 2H), 6.98 (t, *J* = 10 Hz, 2H), ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 194.36, 162.15, 136.27, 131.54, 122.37, 122.13, 117.69; GC-MS (m/z): 124 [$M]^{+\cdot}$ for $C_7H_8O_2$].

2-Naphthol (5): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.76 (t, *J* = 8 Hz, 2H)), 7.68 (d, *J* = 10 Hz, 1H),7.44 (d, *J* = 9 Hz, 1H), 7.34 (d, *J* = 9 Hz, 1H),7.10-7.15 (m, 2H), 5.02 (s, *1H*), ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 153.36, 134.65, 129.98, 129.03, 127.87, 126.65, 126.46, 123.75, 117.80, 109.58; GC-MS (m/z): 144 [$M]^{+\cdot}$ for $C_{10}H_8O$].



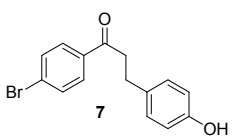
5

(E)-1-(4-fluorophenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one (6): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 8.02(d, *J* = 8.5 Hz, 2H), 7.74 (d, *J* = 15.5 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 16 Hz, 1H), 7.39 (t, *J* = 8.5 Hz, 2H), 6.98 (d, *J* = 8.5 Hz, 2H), 6.24 (s, 1H, br, D_2O exchangeable). ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 187.50, 164.68, 162.67, 141.94, 132.02, 131.52, 131.45, 129.53, 122.46, 116.42, 116.25. IR ν_{max} (KBr, cm^{-1}): 3415 (OH str), 2931, 2873 (aromatic C-H str), 1681 (C=O str), 1597 (aromatic, C=C str), 1263, 1081, 860, 737. GC-MS (m/z): 242 [$M^{+\cdot}$, $C_{15}H_{11}FO_2$].



6

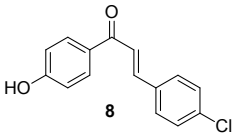
1-(4-bromophenyl)-3-(4-hydroxyphenyl)propan-1-one (7): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 8.02 (d, *J* = 7.5 Hz, 2H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H) , 7.39 (d, *J* = 8.5 Hz, 2H), 5.45 (s, 1H), 2.80 (t, *J* = 6.5 Hz, 2H), 2.73 (t, *J* = 6.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 199.12, 157.13, 136.27, 133.63, 131.54, 130.78,



7

129.62, 129.30, 115.19, 45.81, 30.17; IR ν_{max} (KBr, cm^{-1}): 3425 (OH str), 2928, 2885 (aromatic C-H str), 1705 (C=O str), 1599 (aromatic, C=C str), 1265, 1079, 862, 725; GC-MS (m/z): 304, 306 [$M^{+\cdot}$, $C_{15}H_{13}BrO_2$].

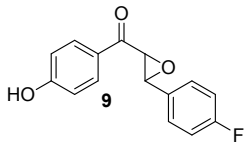
(E)-3-(4-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (8): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm



8

7.87 (d, *J* = 8.5 Hz, 2H), 7.54 (dd, *J* = 8.5, 5 Hz, 2H), 7.05 (d, *J* = 8.5 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H), 6.42 (s, 1H, br, D_2O exchangeable); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 187.20, 162.37, 141.64, 131.72, 131.22, 131.15, 129.23, 122.16, 116.12, 115.95; IR ν_{max} (KBr, cm^{-1}): 3411 (OH str), 2930, 2881 (aromatic C-H str), 1688 (C=O str), 1594 (aromatic, C=C str), 1270, 1089, 868, 729. GC-MS (m/z): 258 [$M^{+\cdot}$, $C_{15}H_{11}ClO_2$].

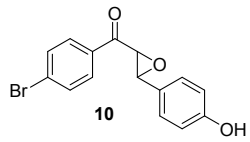
(3-(4-fluorophenyl)oxiran-2-yl)(4-hydroxyphenyl)methanone (9): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm



9

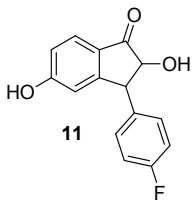
8.02(d, *J* = 8.5 Hz, 2H), 7.73 (dd, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 8.5 Hz, 2H) , 7.52 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.5 Hz, 2H), 5.62 (s, 1H), 4.22 (d, *J* = 2.0 Hz, 1H), 4.17 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 197.32, 156.54, 138.65, 130.97, 130.68, 129.97, 129.68, 128.68, 127.96, 126.67, 116.65, 71.12, 59.35; IR ν_{max} (KBr, cm^{-1}): 3421 (OH str), 2937, 2879 (aromatic C-H str), 1686 (C=O str), 1596 (aromatic, C=C str), 1267, 1088, 867, 733; GC-MS (m/z): 258 [$M^{+\cdot}$, $C_{15}H_{11}FO_3$].

(4-bromophenyl)(3-(4-hydroxyphenyl)oxiran-2-yl)methanone (10): ^{1}H NMR ($CDCl_3$, 500 MHz) δ



10

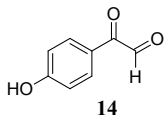
ppm 8.01(d, *J* = 9.0 Hz, 2H), 7.75 (d, *J* = 8.0Hz, 1H), 7.63 (dd, *J* = 8.5, 5 Hz, 2H), 7.45 (d, *J* = 9.5 Hz, 1H) , 7.13 (d, *J* = 9.0 Hz, 2H), 5.40 (s, 1H), 4.39 (d, *J* = 2.5 Hz, 1H), 4.28 (d, *J* = 2.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 198.01, 159.07, 133.01, 130.92, 129.62, 129.29, 128.66, 128.07, 117.13, 73.13, 60.17; IR ν_{max} (KBr, cm^{-1}): 3411 (OH str), 2933, 2879 (aromatic C-H str), 1689 (C=O str), 1595 (aromatic, C=C str), 1275, 1079, 869, 725; GC-MS (m/z): 318, 320 [$M^{+\cdot}$, C15H11BrO_3].



11

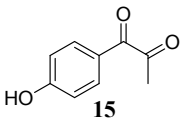
3-(4-fluorophenyl)-2,5-dihydroxy-2,3-dihydroinden-1-one (14): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.87 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.06 (d, *J* = 9 Hz, 2H),6.95 (d, *J* = 9 Hz, 2H), 6.4 (s, 1H) 5.29 (t, *J* = 7 Hz, 1H), 5.22 (d, *J* = 1.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 195.55, 161.83, 137.36, 131.82, 131.42, 129.79, 125.99, 123.01, 116.23, 75.01, 63.53. IR ν_{max} (KBr, cm^{-1}): 3405 (OH str), 2922, 2875 (aromatic C-H str), 1688 (C=O str), 1595 (aromatic, C=C str), 1266, 1089, 858, 731. GC-MS (m/z): 258 [$M^{+\cdot}$,$C_{15}H_{11}FO_3$].

2-(4-hydroxyphenyl)-2-oxoacetaldehyde (14): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 9.50(s, 1H), 7.88-7.86 (m, 2H), 6.89-6.87 (m, 2H), 5.58 (s, 1H, br, D_2O exchangeable); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 190.69, 187.73, 163.98, 132.91, 130.67, 116.55; GC-MS (m/z): 150 $[M]^{+\cdot}$ for $C_8H_6O_3$].



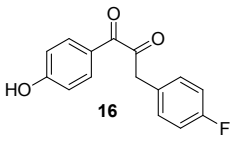
14

1-(4-hydroxyphenyl)propane-1,2-dione (15): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.93-7.90 (m, 2H), 6.92-6.89 (m, 2H), 6.55 (s, 1H), 2.18 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 197.85, 192.83, 164.85, 131.44, 124.80, 117.22, 23.05; GC-MS (m/z): 164 [$M^{+\cdot}$, $C_9H_8O_3$].



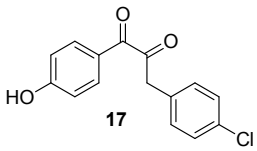
15

3-(4-fluorophenyl)-1-(4-hydroxyphenyl)propane-1,2-dione (16): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.73(d, *J* = 9.0 Hz, 1H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.53 (d, *J* = 9.0 Hz, 1H), 7.38 (d, *J* = 8.5 Hz, 2H) , 6.98 (d, *J* = 8.5 Hz, 2H), 5.19 (s, 1H), 3.99 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 197.12, 191.10, 166.42, 163.17, 131.54, 130.71, 129.62, 129.30, 122.38, 117.19, 116.11, 50.89;; IR ν_{max} (KBr, cm^{-1}): 3415 (OH str), 2935, 2879 (aromatic C-H str), 1705, 1715 (C=O str), 1593 (aromatic, C=C str), 1268, 1087, 865, 731; GC-MS (m/z): 258 [$M^{+\cdot}$, C15H11FO_3].



16

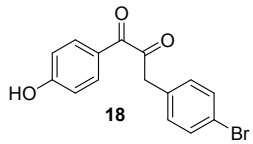
3-(4-chlorophenyl)-1-(4-hydroxyphenyl)propane-1,2-dione(17): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 8.02 (d, *J* = 8.5 Hz, 2H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.50 (d,



17

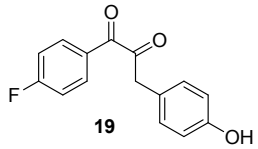
J = 8.0 Hz, 1H) , 7.38 (d, *J* = 8.5 Hz, 2H), 5.45 (s, 1H), 3.79 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 197.41, 190.12, 157.13, 140.10, 133.63, 131.54, 130.78, 129.62, 129.30, 116.19, 50.81; IR ν_{max} (KBr, cm^{-1}): 3407 (OH str), 2933, 2875 (aromatic C-H str), 1689 (C=O str), 1594 (aromatic, C=C str), 1270, 1090, 870, 729; GC-MS (m/z): 274 [$M^{+\cdot}$, $C_{15}H_{11}ClO_3$].

3-(4-bromophenyl)-1-(4-hydroxyphenyl)propane-1,2-dione(18): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.86 (d, *J* = 8.5 Hz, 2H), 7.54-7.52 (m, 2H), 7.05 (d, *J* = 9.0 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H), 6.42 (s, 1H), 3.85 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 196.62, 191.12, 157.29, 133.01, 130.92, 129.87, 129.29, 128.66, 128.07, 116.93, 51.77; IR ν_{max} (KBr, cm^{-1}): 3425 (OH str), 2928, 2885 (aromatic C-H str), 1687 (C=O str), 1599 (aromatic, C=C str), 1265, 1079, 862, 725; GC-MS (m/z): 318, 320 [$M^{+\cdot}$, $C_{15}H_{11}BrO_3$].



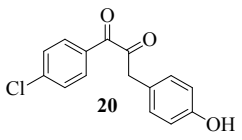
18

1-(4-fluorophenyl)-3-(4-hydroxyphenyl)propane-1,2-dione (19): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 78.03-7.99 (m, 2H), 7.58 (d, *J* = 7.5 Hz, 2H), 7.53-7.50 (m, 3H), 7.33 (t, *J* = 8.5 Hz, 1H) , 7.13 (d, *J* = 8.5 Hz, 2H), 5.31 (s, 1H), 2.79 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 197.65, 190.05, 168.52, 156.60, 130.68, 129.97, 128.68, 127.78, 116.66, 115.32, 51.12; IR ν_{max} (KBr, cm^{-1}): 3417 (OH str), 2935, 2871 (aromatic C-H str), 1679 (C=O str), 1581 (aromatic, C=C str), 1267, 1088, 867, 741; GC-MS (m/z): 258 [$M^{+\cdot}$, $C_{15}H_{11}FO_3$].



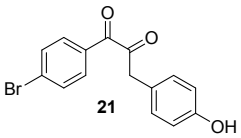
19

1-(4-chlorophenyl)-3-(4-hydroxyphenyl)propane-1,2-dione (20): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.97-7.94 (m, 3H), 7.55-7.43 (m, 3H), 7.47 (t, *J* = 9.0 Hz, 1H) , 6.98 (dd, *J* = 8.5, 2.0 Hz, 1H), 5.31 (s, 1H), 2.73 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 197.27, 191.55, 157.77, 131.68, 130.49, 130.05, 129.65, 128.97, 128.65, 127.66, 117.54, 48.52; IR ν_{max} (KBr, cm^{-1}): 3401 (OH str), 2931, 28851 (aromatic C-H str), 1688 (C=O str), 1594 (aromatic, C=C str), 1275, 1091, 867, 729; GC-MS (m/z): 274 [$M^{+\cdot}$, $C_{15}H_{11}ClO_3$].



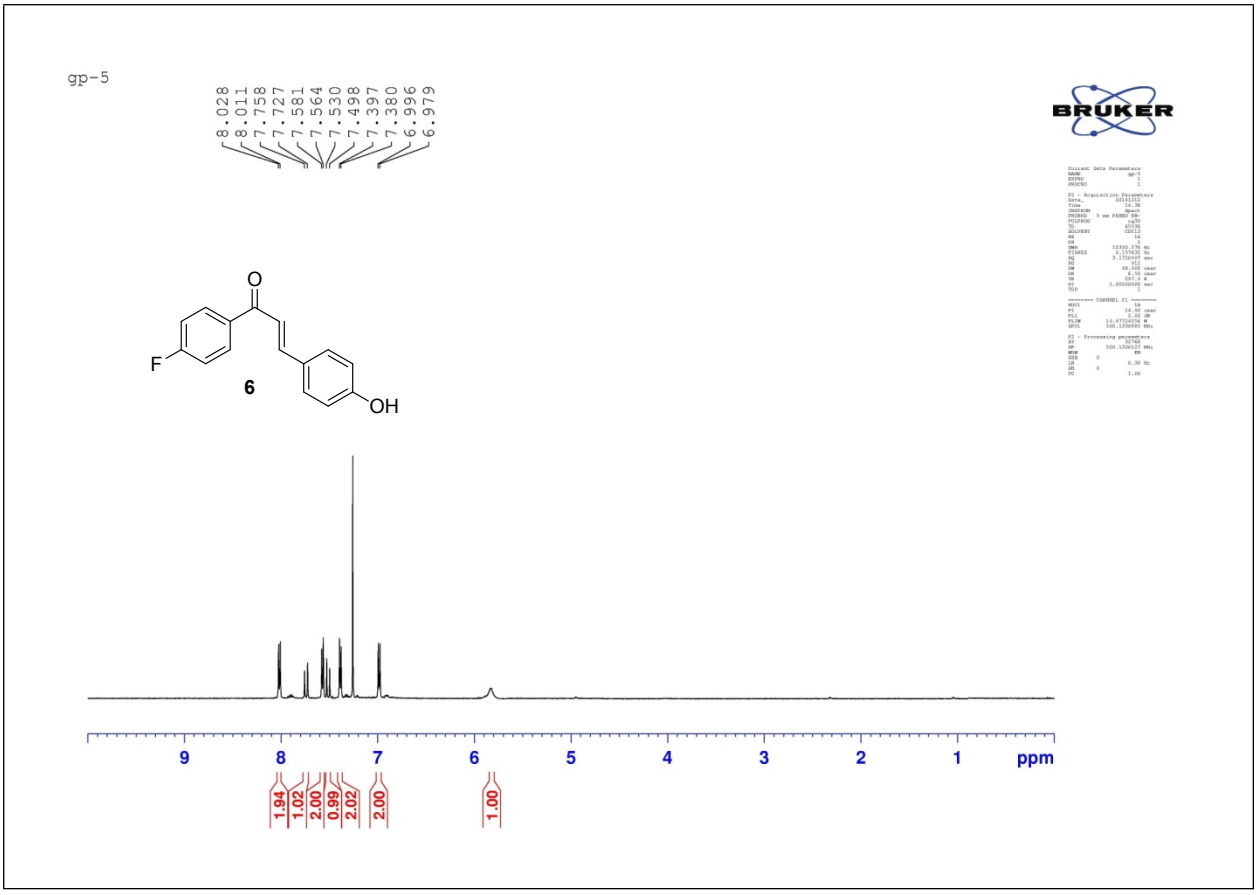
20

1-(4-bromophenyl)-3-(4-hydroxyphenyl)propane-1,2-dione (21): ^{1}H NMR ($CDCl_3$, 500 MHz) δ ppm 7.88-7.79 (m, 3H), 7.57 (d, *J* = 7.5 Hz, 1H), 7.64-7.59 (m, 3H), 7.33 (t, *J* = 8.5 Hz, 1H) , 6.94 (d, *J* = 8.5 Hz, 3H), 5.34 (s, 1H), 2.71 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ ppm 196.68, 190.25, 157.05, 141.35, 131.77, 130.65, 130.49, 129.65, 128.97, 116.56, 49.85; IR ν_{max} (KBr, cm^{-1}): 3405 (OH str), 2930, 2871 (aromatic C-H str), 1675 (C=O str), 1591 (aromatic, C=C str), 1259, 1071, 865, 733;GC-MS (m/z): 318, 320 [$M^{+\cdot}$, $C_{15}H_{11}BrO_3$].



21

4. ^{1}H NMR and ^{13}C NMR Spectra for selected synthesized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BRUKER
O
F
OH
6
9
8
7
6
5
4
3
2
1
ppm
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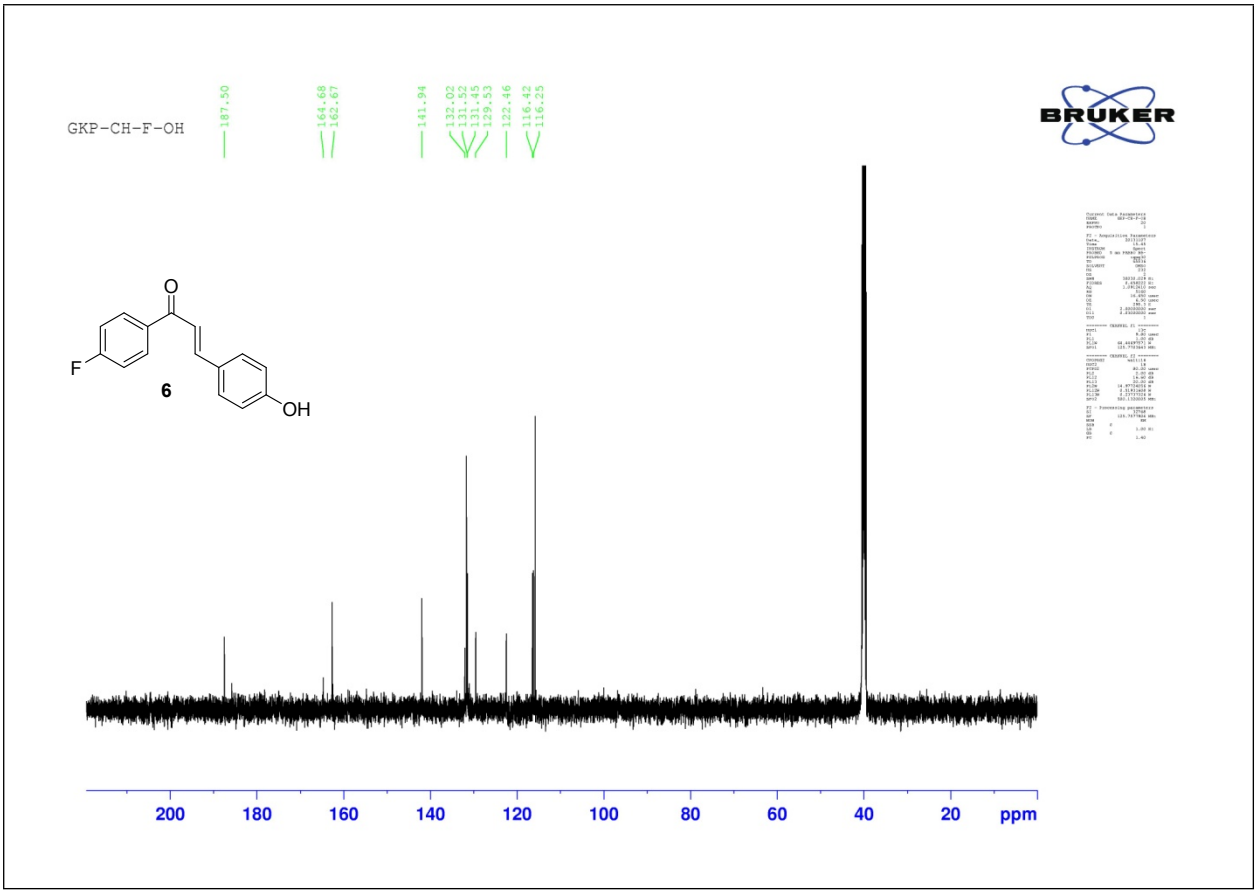
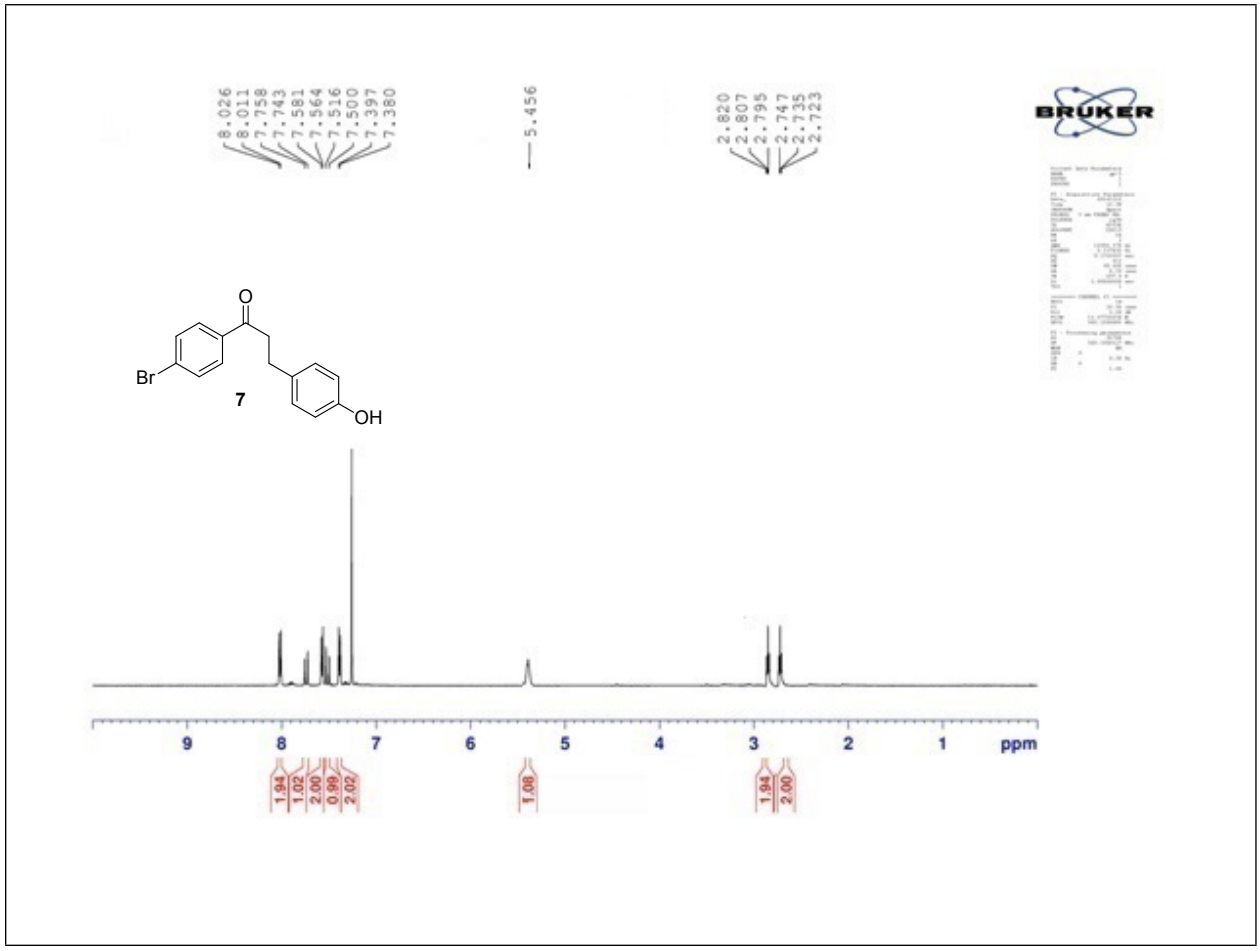
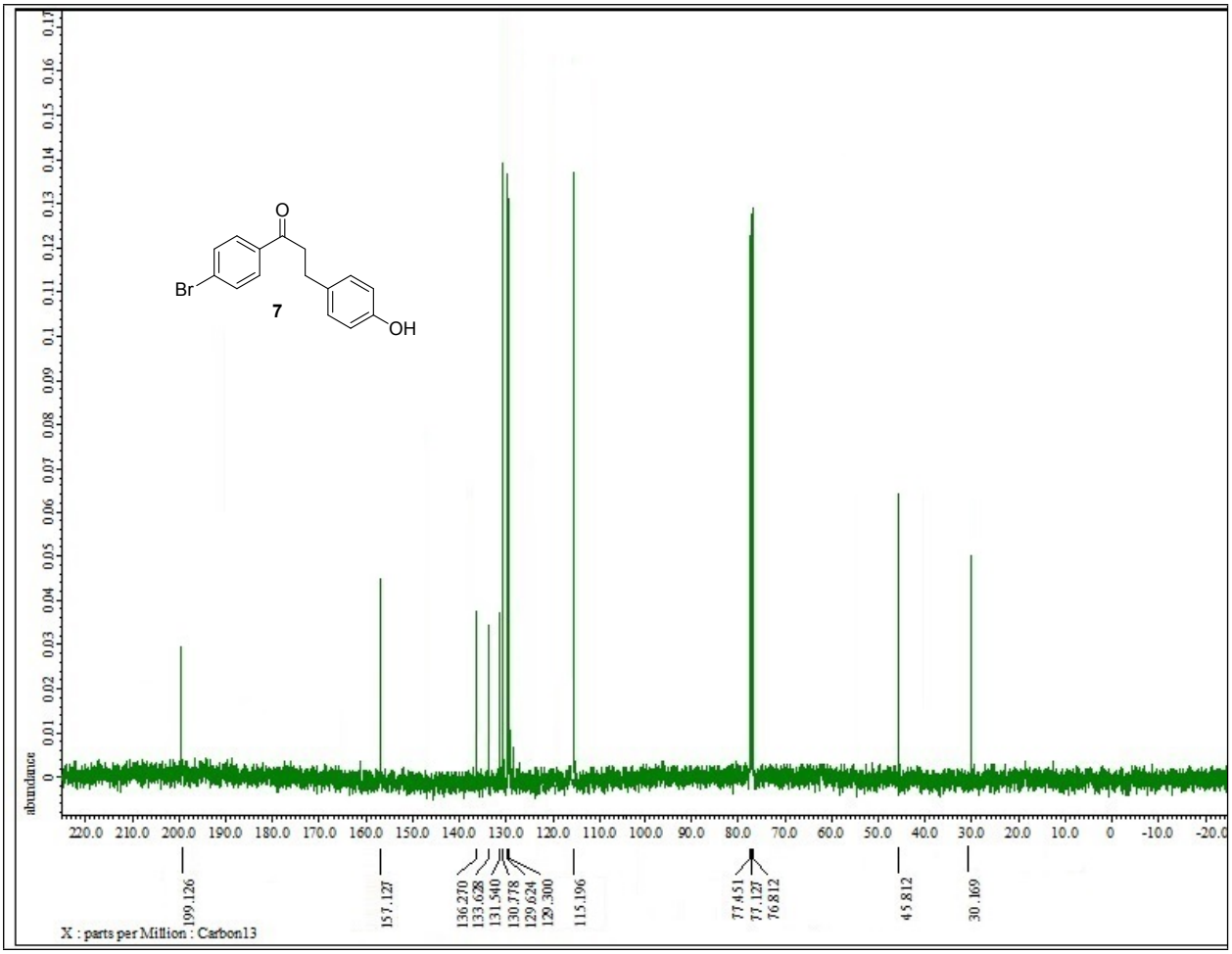
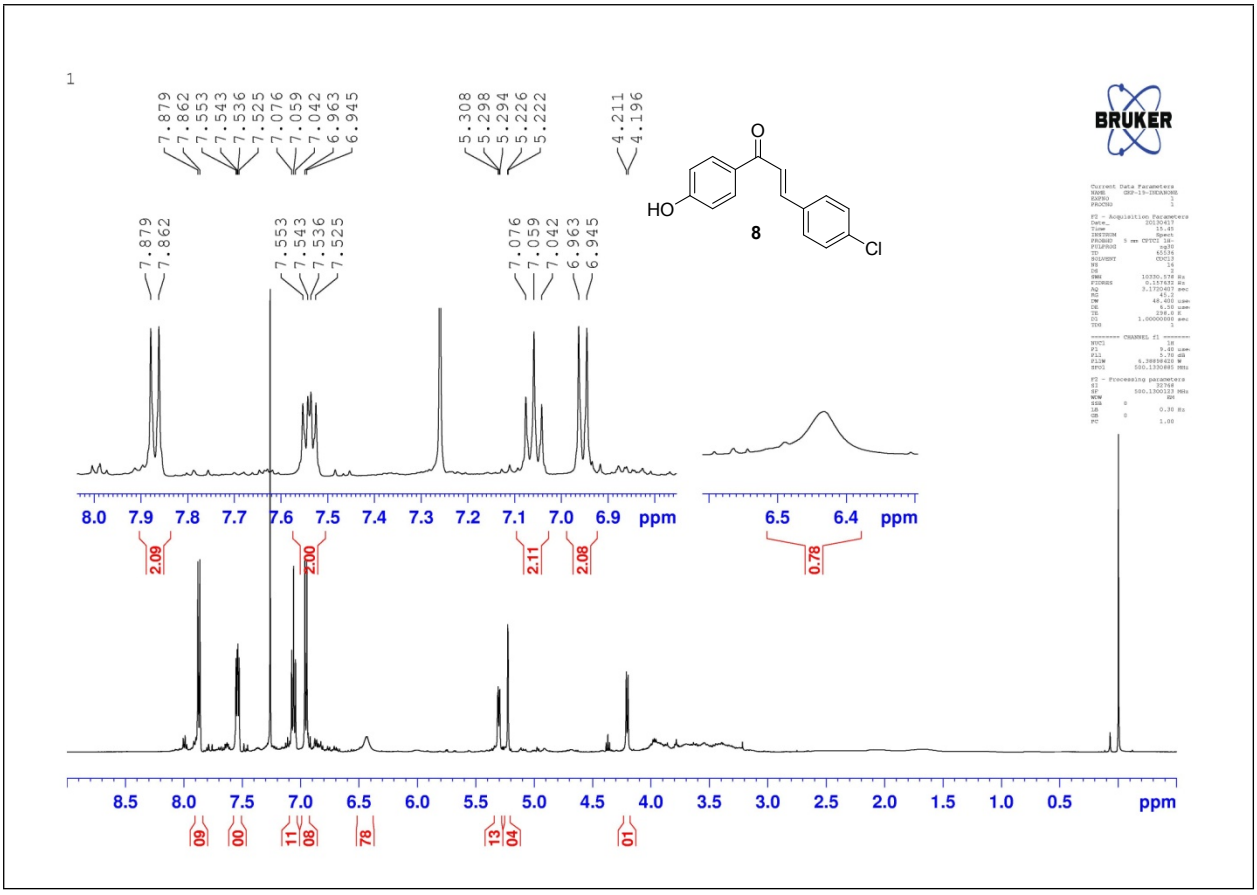
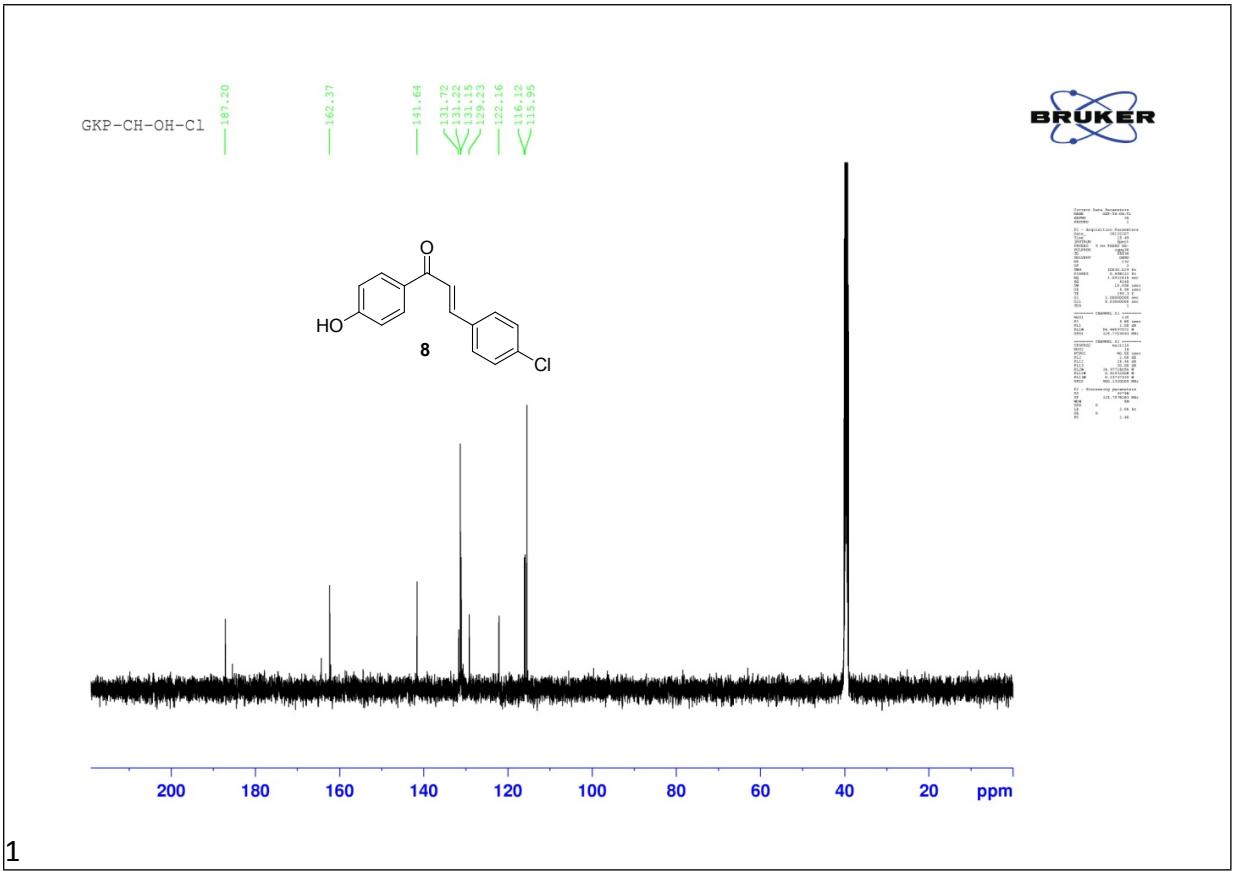
1.02
2.00
0.99
2.02
2.00
1.00


GKP-CH-F-OH
187.50
164.68
162.67
141.94
132.02
131.52
131.45
129.53
122.46
116.42
116.25
BRUKER
O
F
OH
6
200
180
160
140
120
100
80
60
40
20
ppm

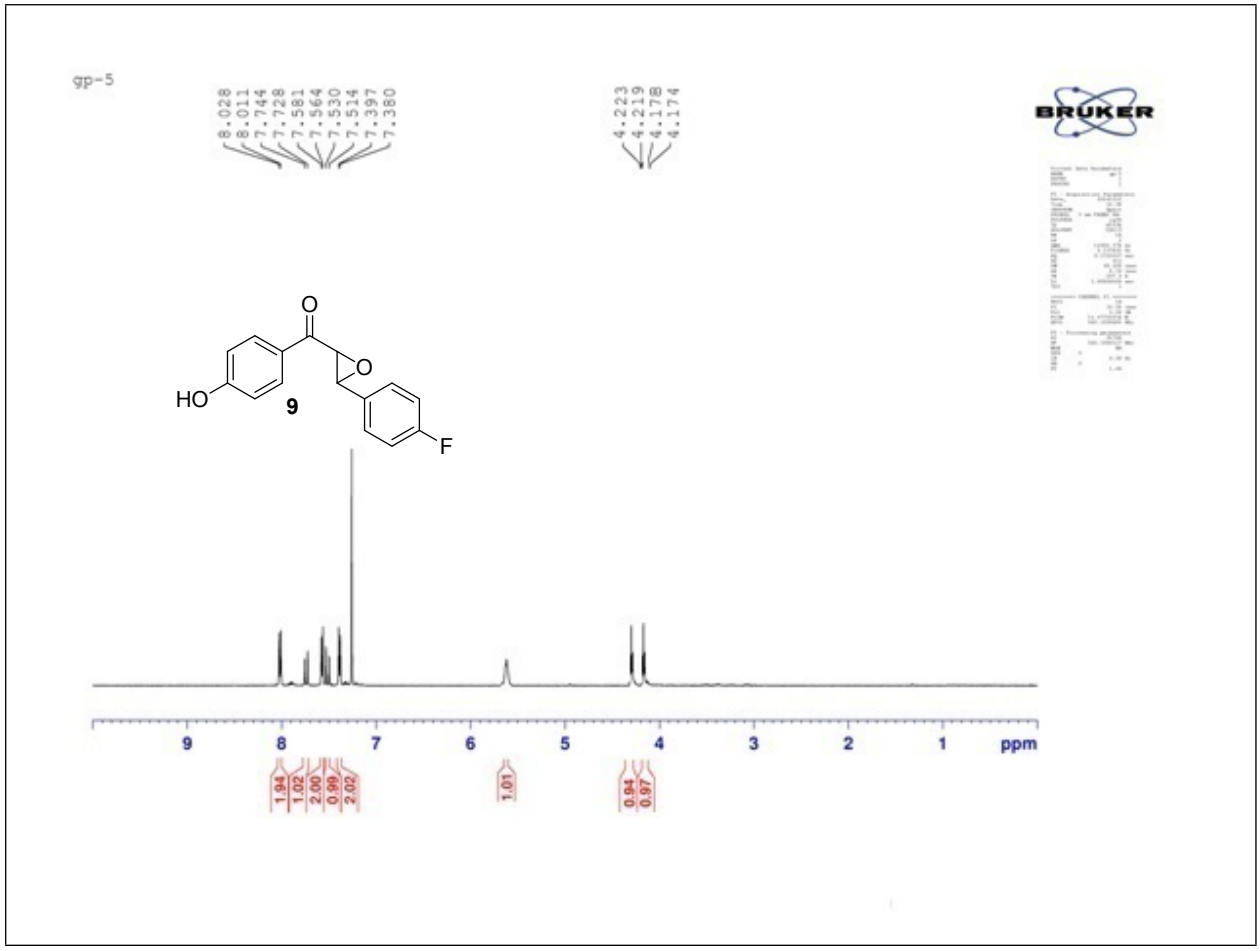

8.026
8.011
7.758
7.743
7.581
7.564
7.516
7.500
7.397
7.380
5.456
2.820
2.807
2.795
2.747
2.735
2.723
BRUKER
O
Br
OH
7
9
8
7
6
5
4
3
2
1
ppm
1.94
1.02
2.00
0.99
2.02
1.06
1.94
2.00

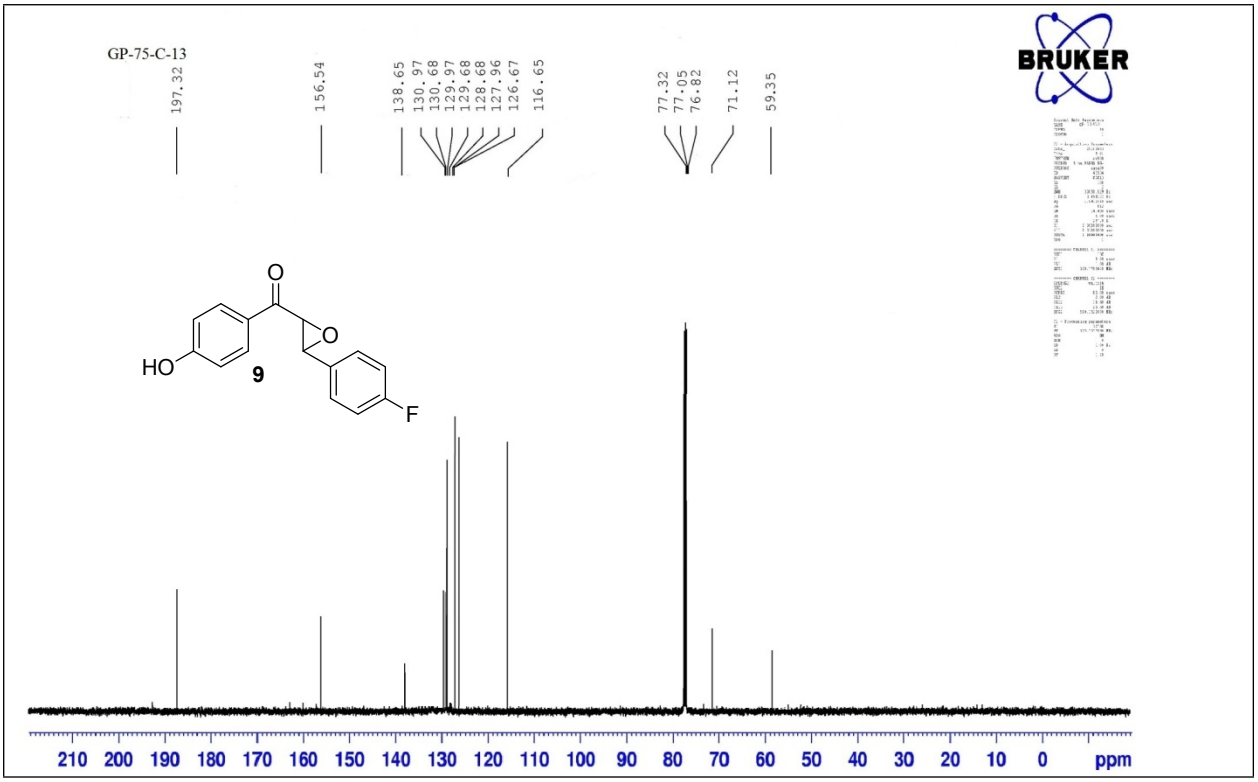

O
Br
7
OH
abundance
X : parts per Million : Carbon13
199.126
157.127
136.270
133.628
131.540
130.778
129.624
129.300
115.196
77.451
77.127
76.812
45.812
30.169

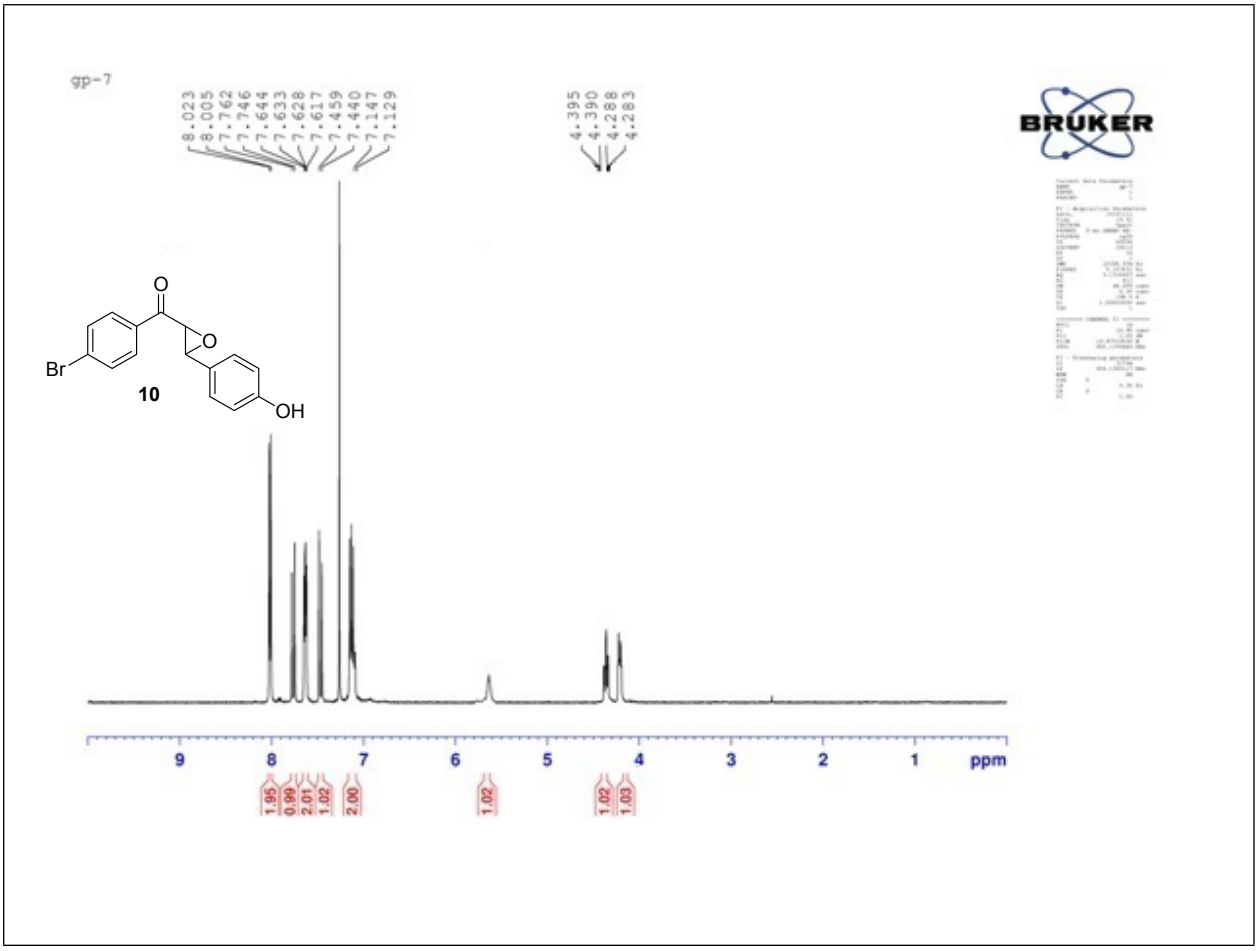

1
7.879
7.862
7.553
7.543
7.536
7.525
7.076
7.059
7.042
6.963
6.945
5.308
5.298
5.294
5.226
5.222
4.211
4.196
HO
O
Cl
8
BRUKER
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
6.5 6.4 ppm
2.09
2.00
2.11
2.08
0.78
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
09
00
11
08
78
13
04
01

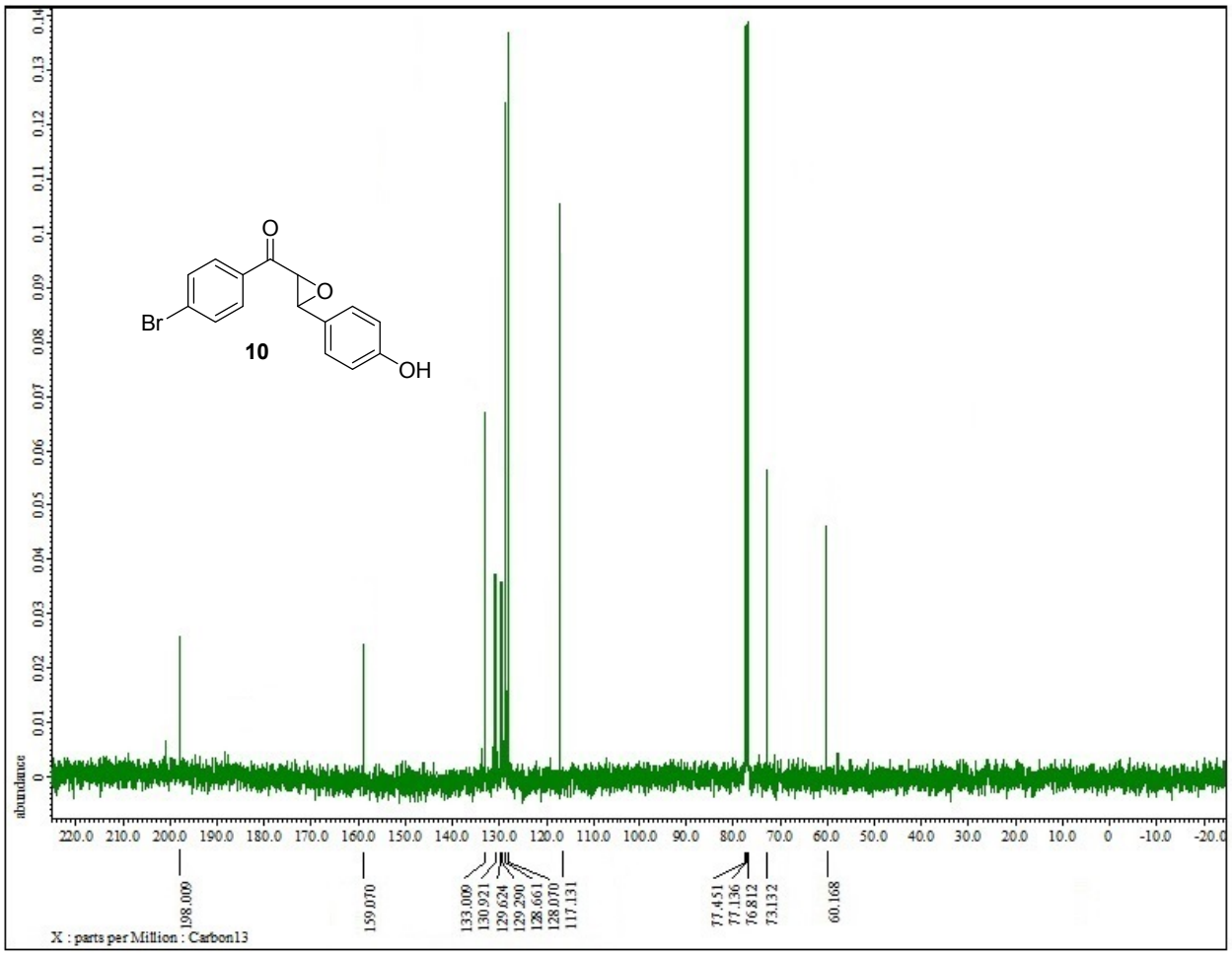

GKP-CH-OH-Cl
187.20
162.37
141.64
131.72
131.22
131.15
129.23
122.16
116.12
115.95
BRUKER
O
HO
Cl
8
200
180
160
140
120
100
80
60
40
20
ppm

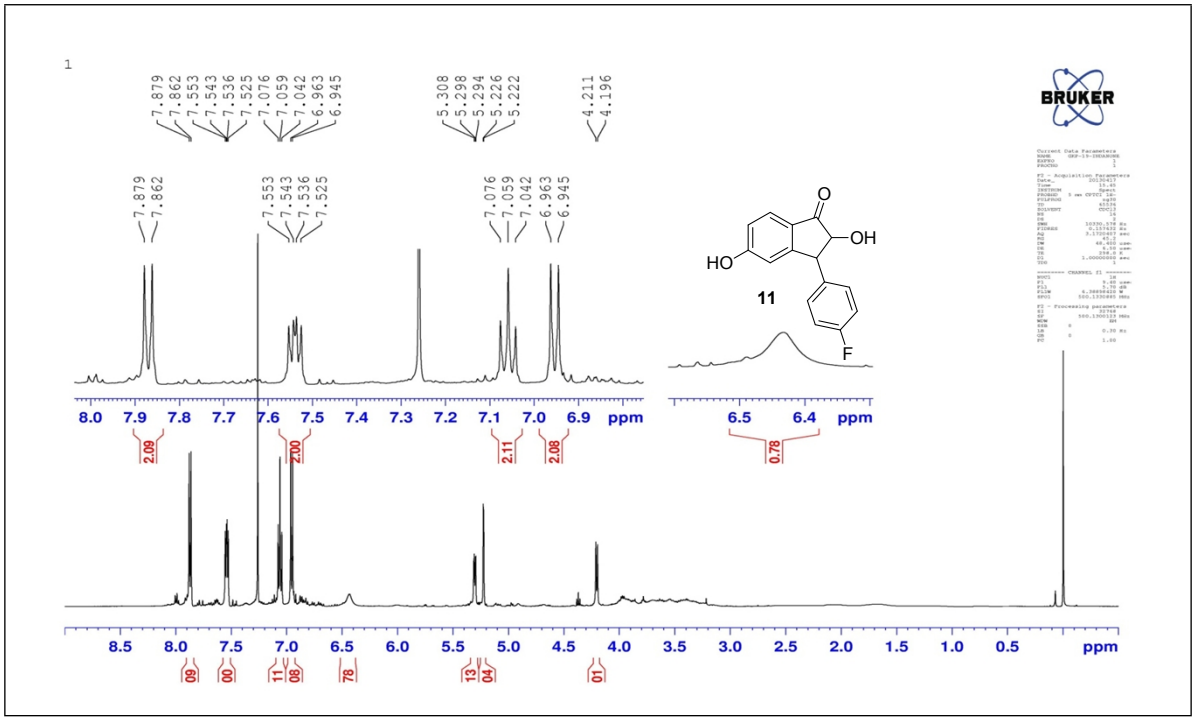
1

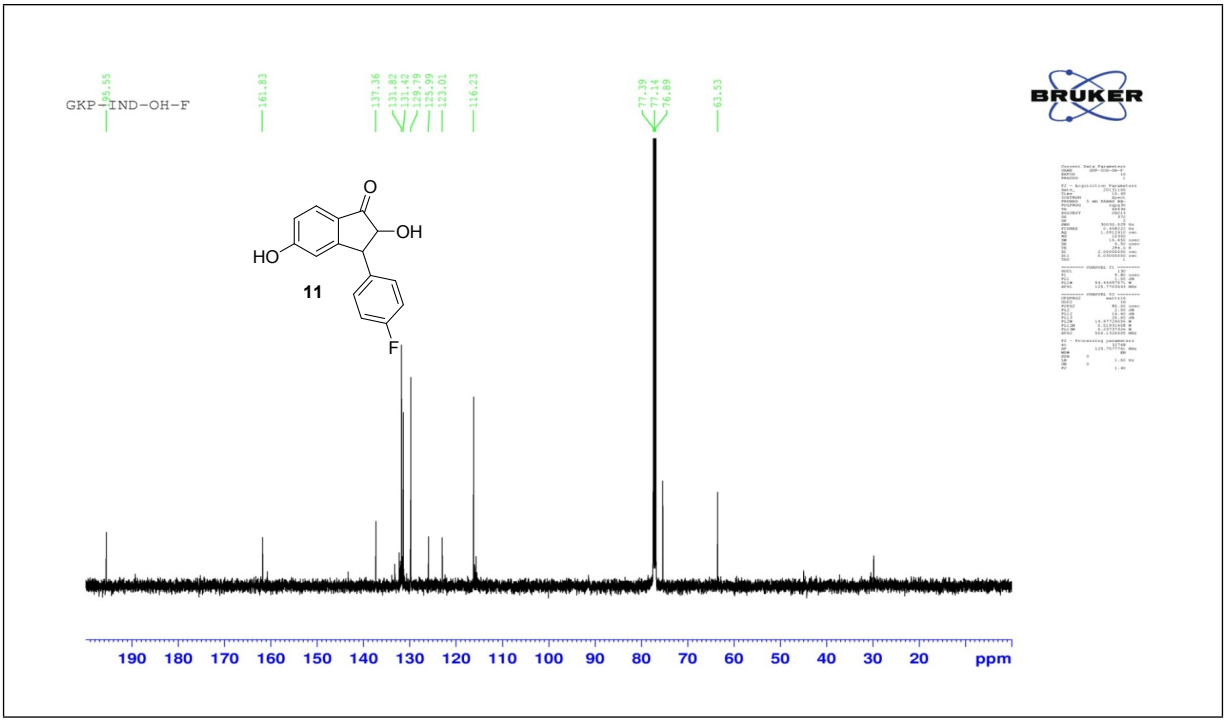

gp-5
8.028
8.011
7.744
7.728
7.581
7.564
7.530
7.514
7.397
7.380
4.223
4.219
4.178
4.174
BRUKER
O
HO
O
F
9
9
8
7
6
5
4
3
2
1
ppm
1.94
1.02
2.00
0.99
2.02
1.01
0.04
0.97

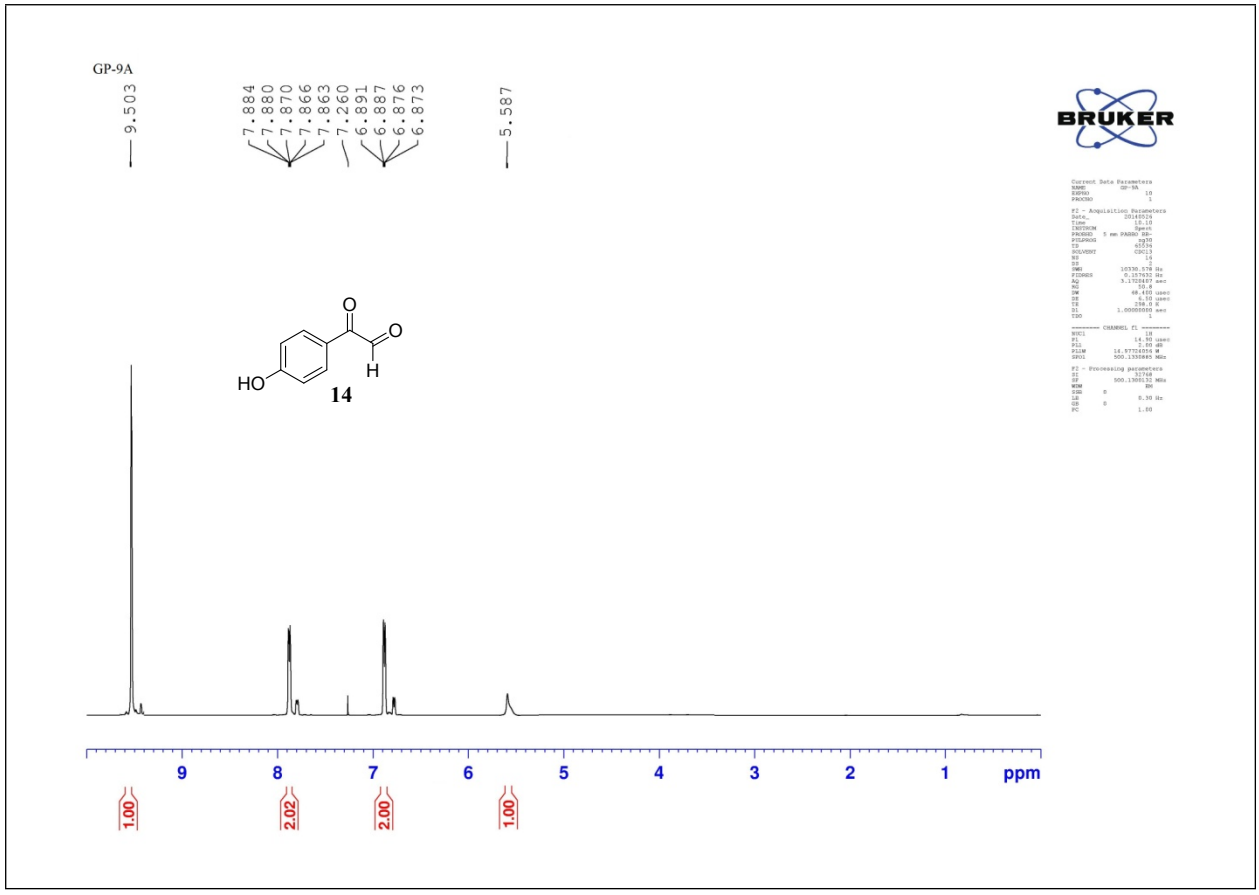

GP-75-C-13
197.32
156.54
138.65
130.97
130.68
129.97
129.68
128.68
127.96
126.67
116.65
77.32
77.05
76.82
71.12
59.35
BRUKER
O
O
HO
9
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

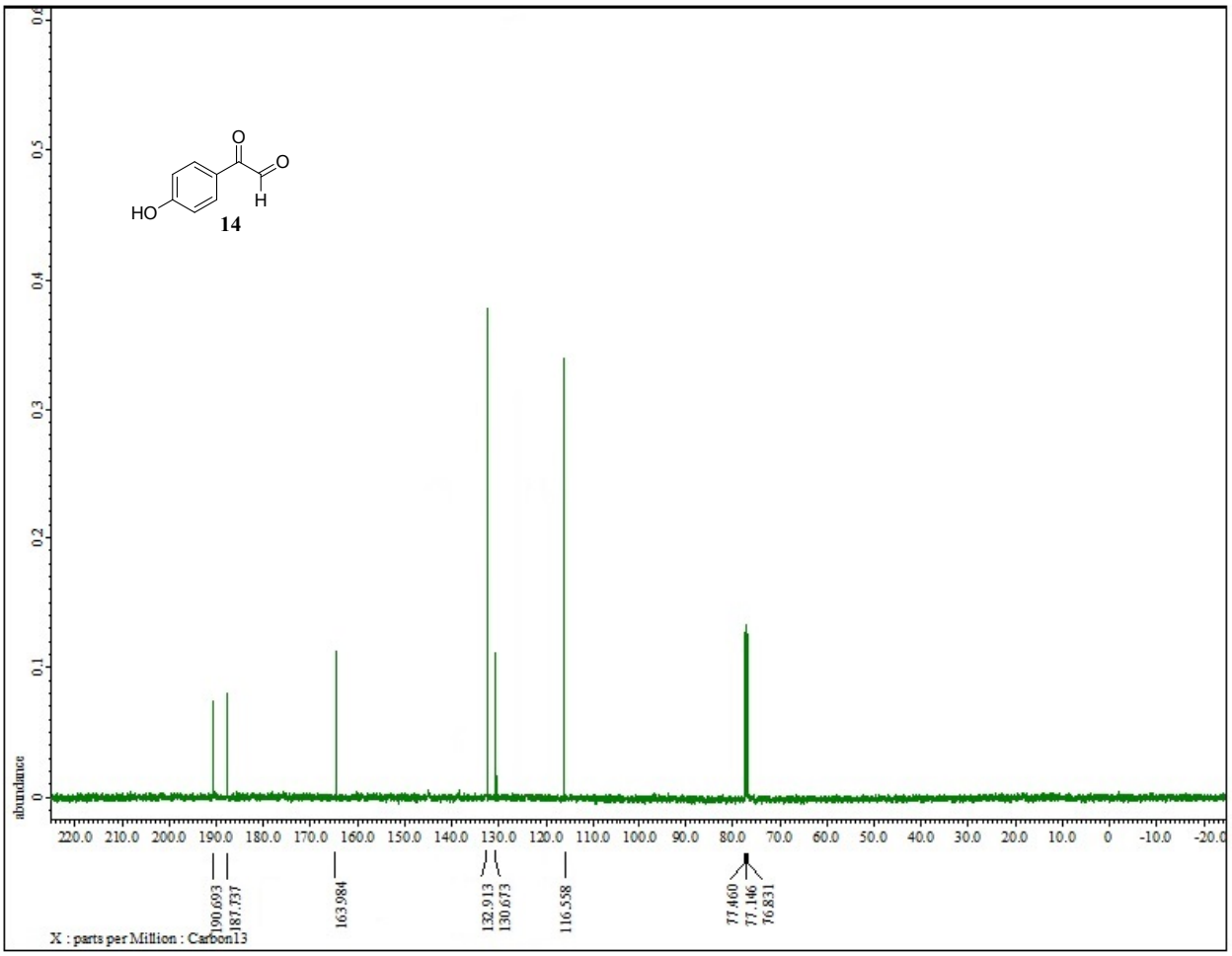

gp-7
8.023
8.005
7.762
7.746
7.644
7.633
7.628
7.617
7.459
7.440
7.147
7.129
4.395
4.390
4.288
4.283
BRUKER
O
O
Br
OH
10
9
8
7
6
5
4
3
2
1
ppm
1.95
0.99
2.01
1.02
2.00
1.02
1.02
1.03

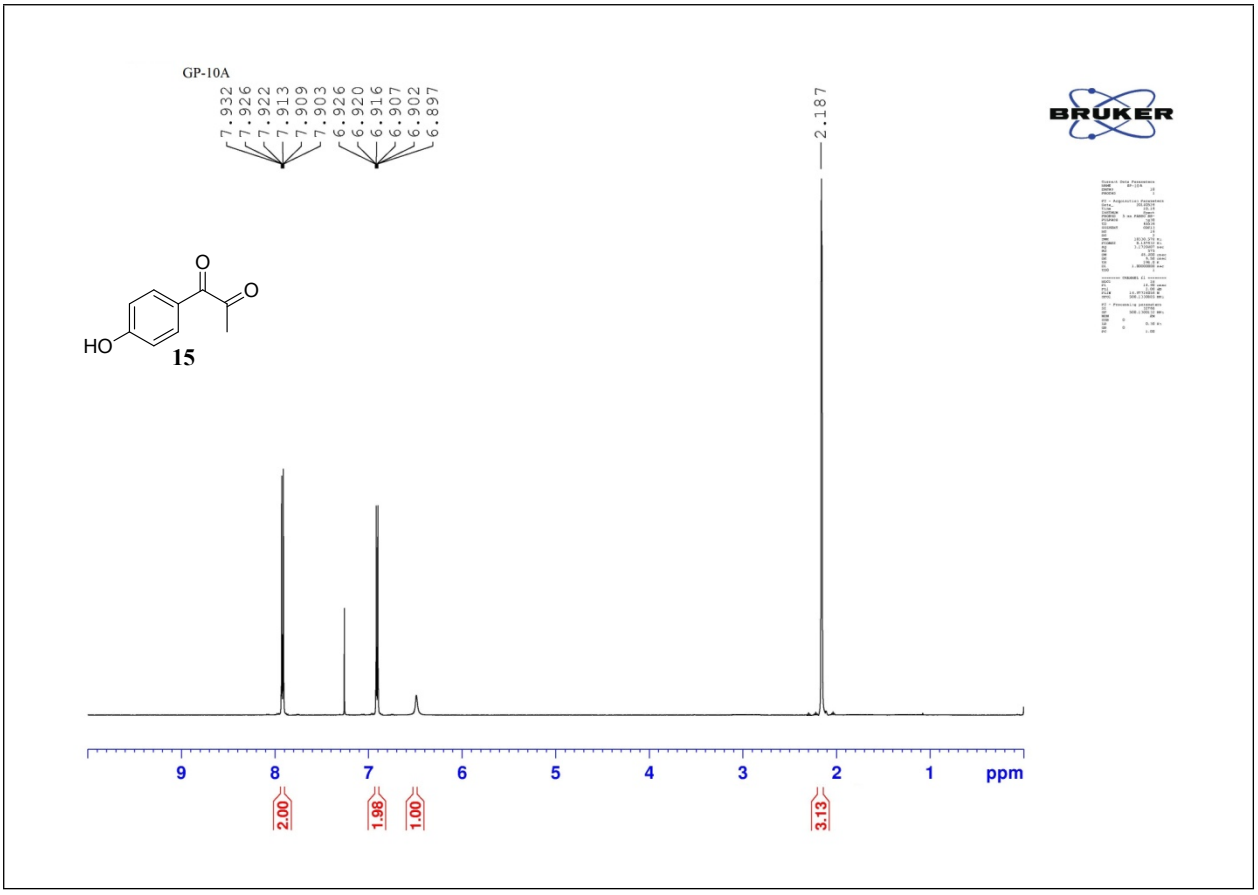

O
O
Br
OH
10
abundance
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
198.009
159.070
133.009
130.921
129.624
129.290
128.661
128.070
117.131
77.451
77.136
76.812
73.132
60.168
X : parts per Million : Carbon13

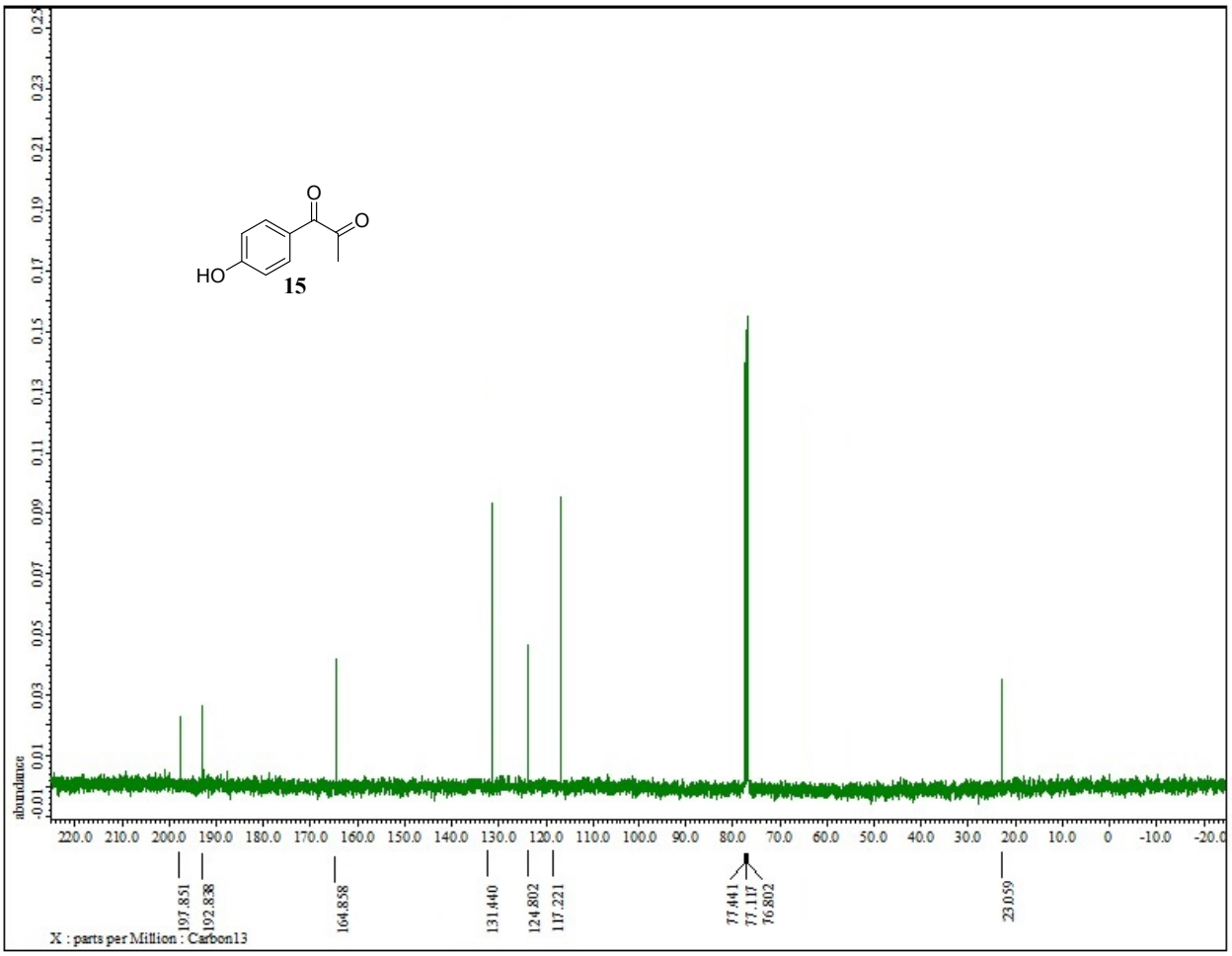

1
7.879
7.862
7.553
7.543
7.536
7.525
7.076
7.059
7.042
6.963
6.945
5.308
5.298
5.294
5.226
5.222
4.211
4.196
BRUKER
O
OH
HO
11
F
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
6.5 6.4 ppm
2.09
2.00
2.11
2.08
0.78
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
09
00
11
08
78
13
04
01

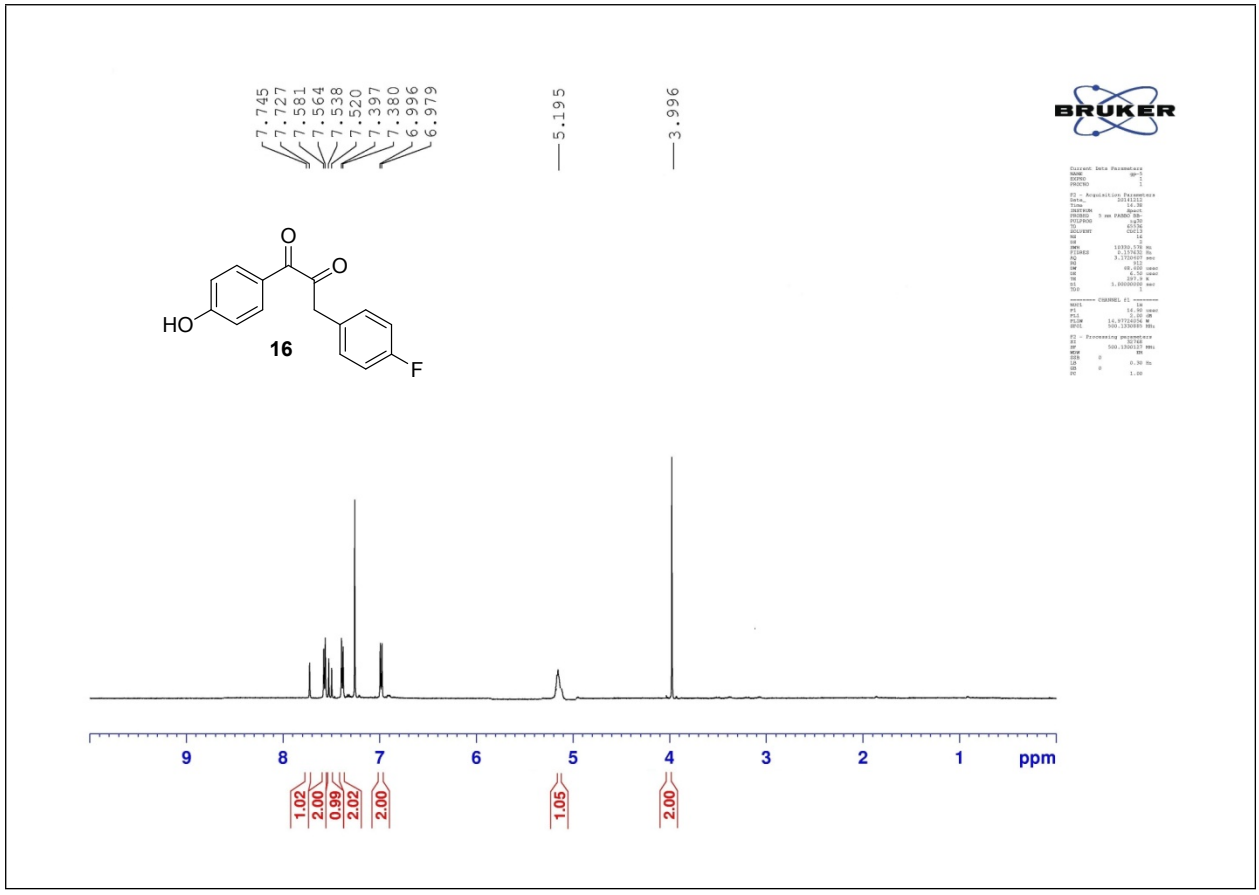

GKP-IND-OH-F
195.55
161.83
137.36
131.82
131.42
129.79
125.99
123.01
116.23
77.39
77.14
76.89
63.53
BRUKER
O
OH
HO
11
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

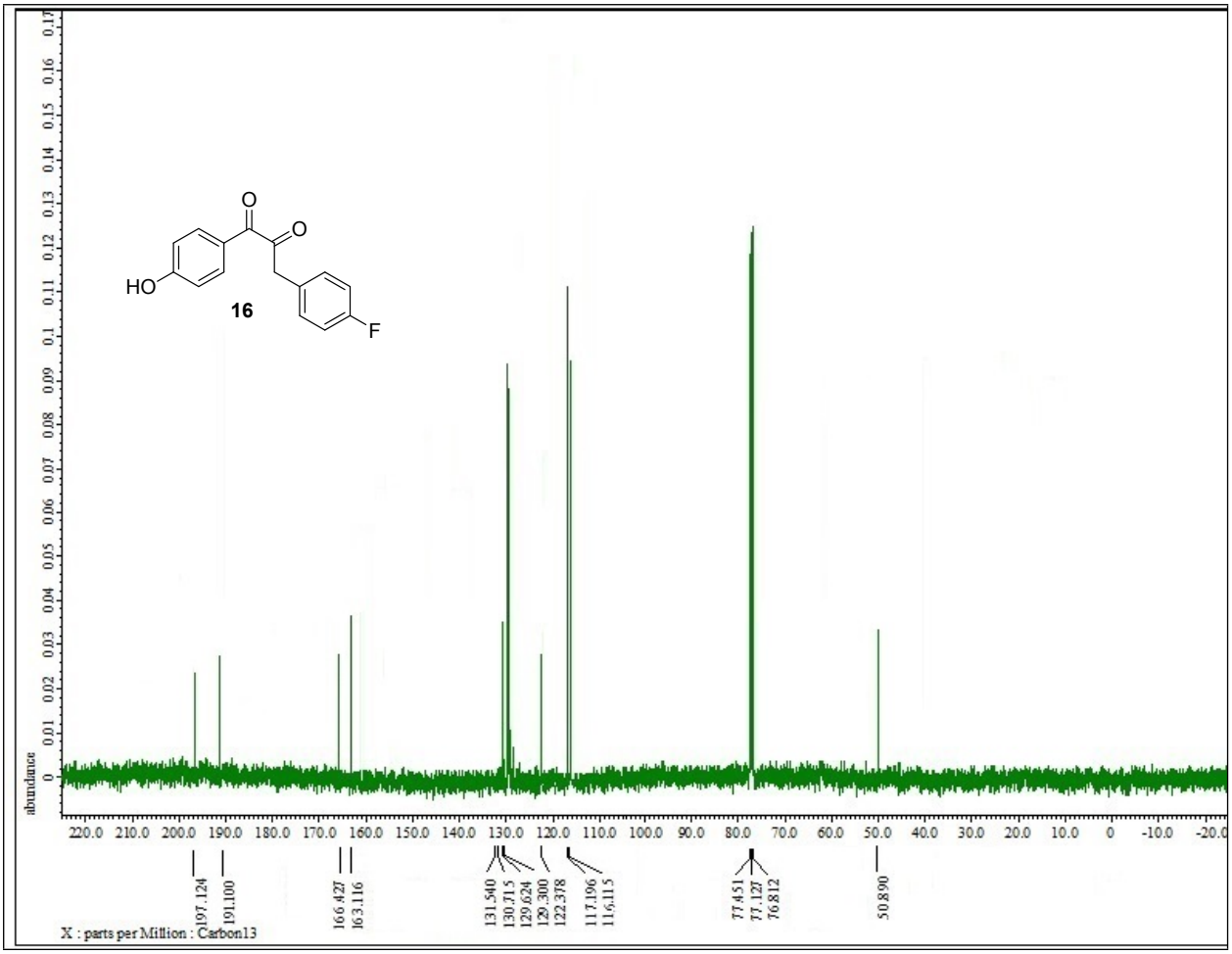

GP-9A
9.503
7.884
7.880
7.870
7.866
7.863
7.260
6.891
6.887
6.876
6.873
5.587
BRUKER
HO
O
O
H
14
9
8
7
6
5
4
3
2
1
ppm
1.00
2.02
2.00
1.00

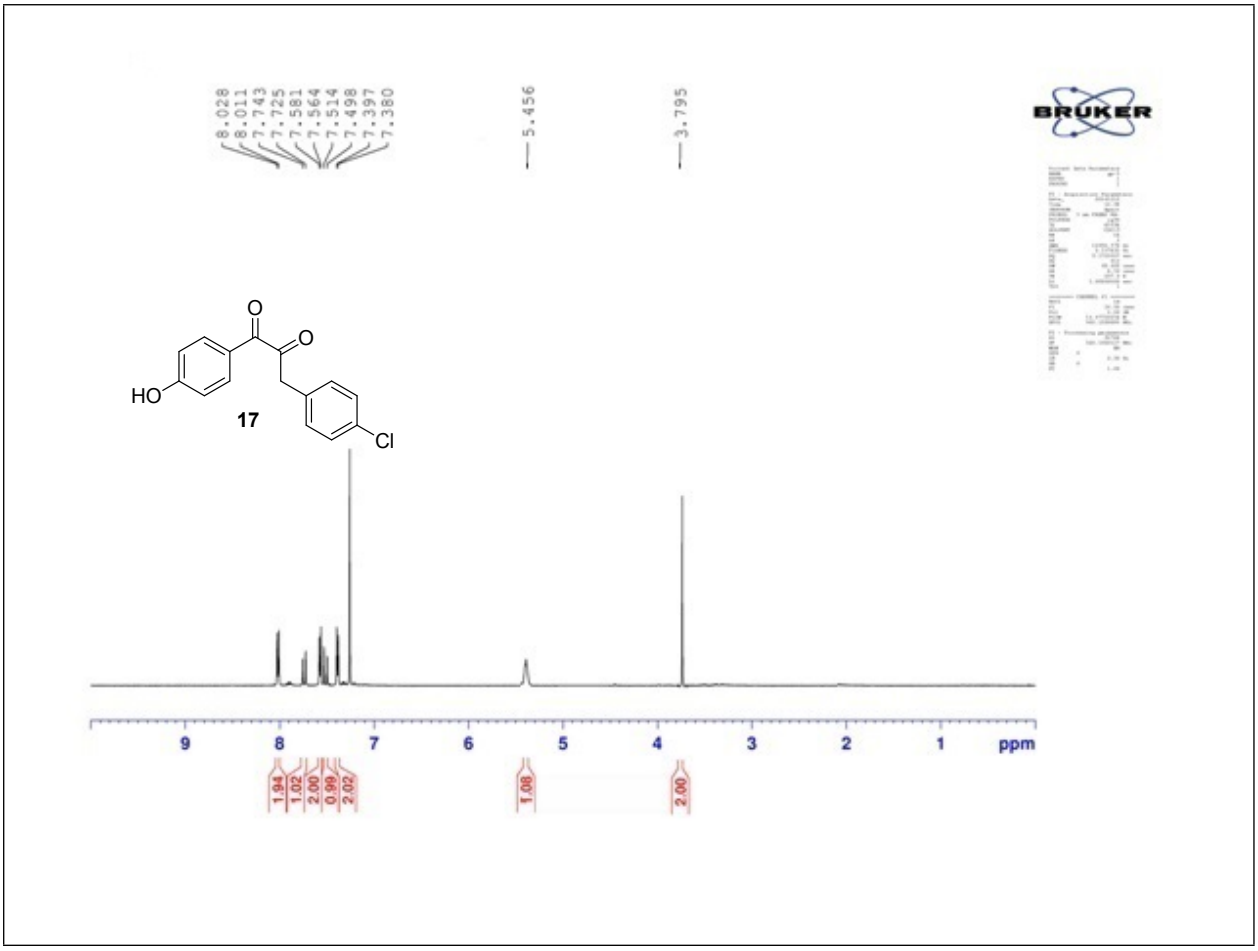

O
O
H
HO
14
abundance
0.6
0.5
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
190.693
187.737
163.984
132.913
130.673
116.558
77.460
77.146
76.831
X : parts per Million : Carbon13

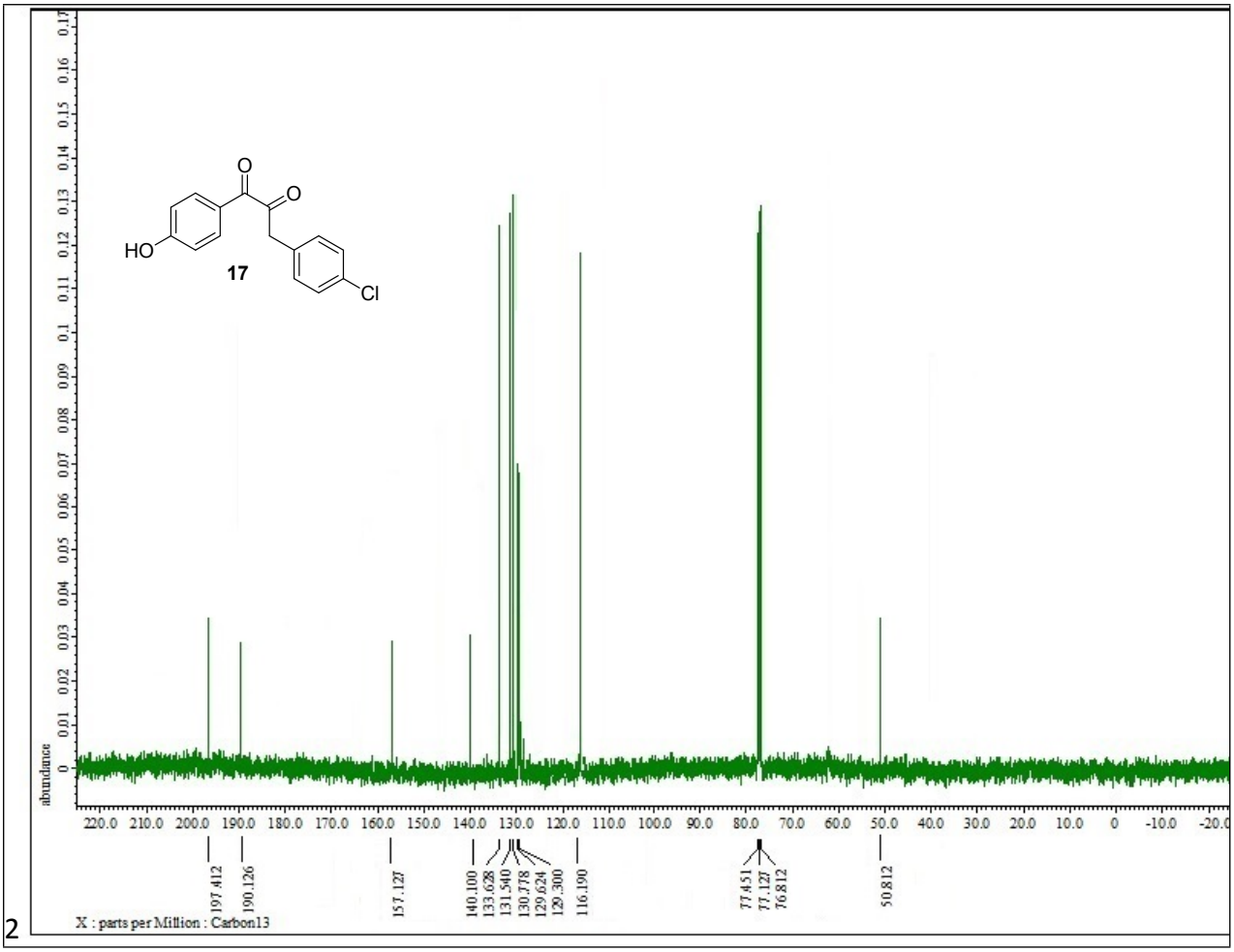

GP-10A
7.932
7.926
7.922
7.913
7.909
7.903
6.926
6.920
6.916
6.907
6.902
6.897
2.187
BRUKER
O
O
HO
15
9
8
7
6
5
4
3
2
1
ppm
2.00
1.98
1.00
3.13


O
O
HO
15
abundance
197.851
192.838
164.858
131.440
124.802
117.221
77.441
77.117
76.802
23.059
X : parts per Million : Carbon13

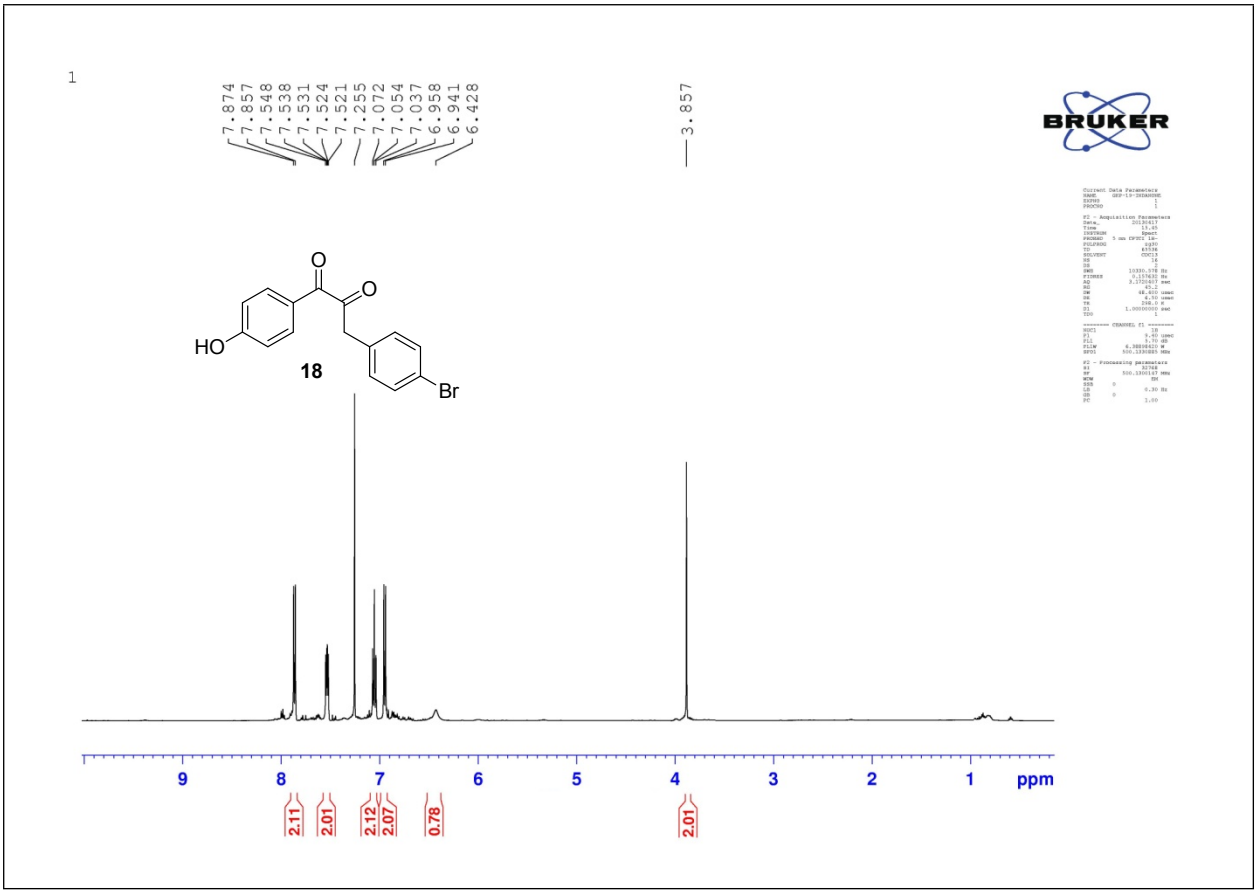

7.745
7.727
7.581
7.564
7.538
7.520
7.397
7.380
6.996
6.979
5.195
3.996
BRUKER
HO
O
O
F
16
9
8
7
6
5
4
3
2
1
ppm
1.02
2.00
0.99
2.02
2.00
1.05
2.00

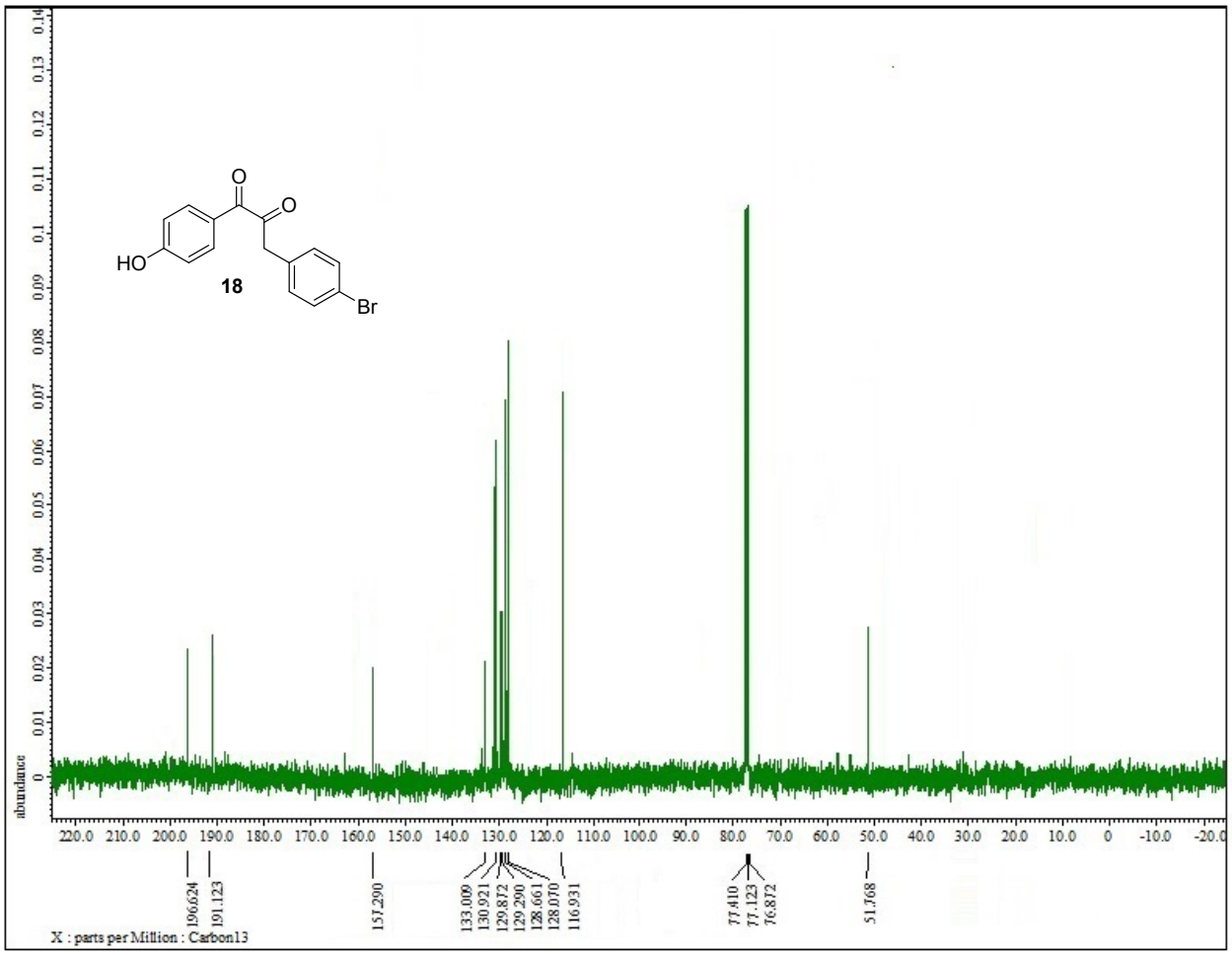

O
O
HO
F
16
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
197.124
191.100
166.427
163.116
131.540
130.715
129.624
129.300
122.378
117.196
116.115
77.451
77.127
76.812
50.890
X : parts per Million : Carbon13

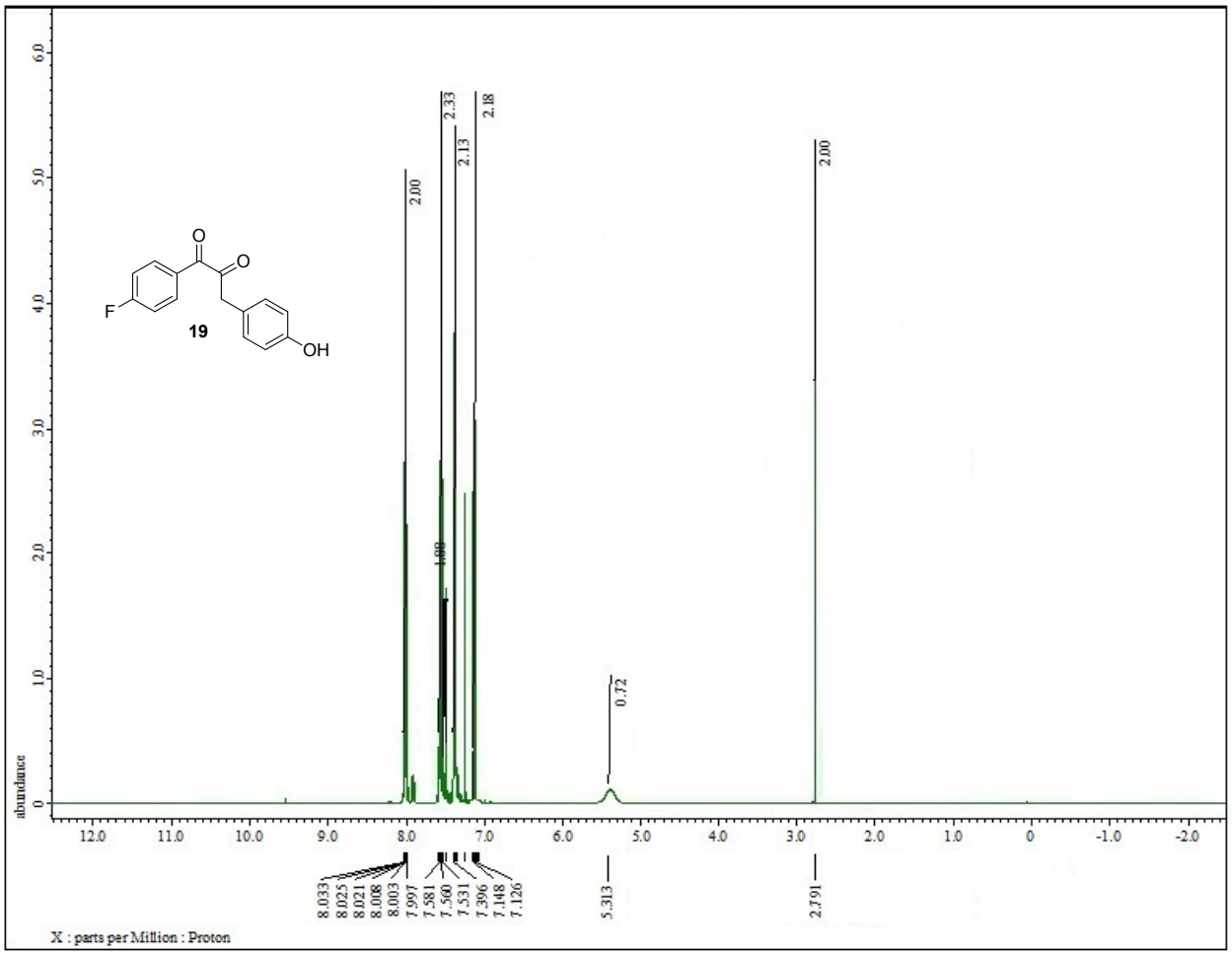

8.028
8.011
7.743
7.725
7.581
7.564
7.514
7.498
7.397
7.380
5.456
3.795
BRUKER
O
O
HO
Cl
17
9
8
7
6
5
4
3
2
1
ppm
1.94
1.02
2.00
0.99
2.02
1.06
2.00

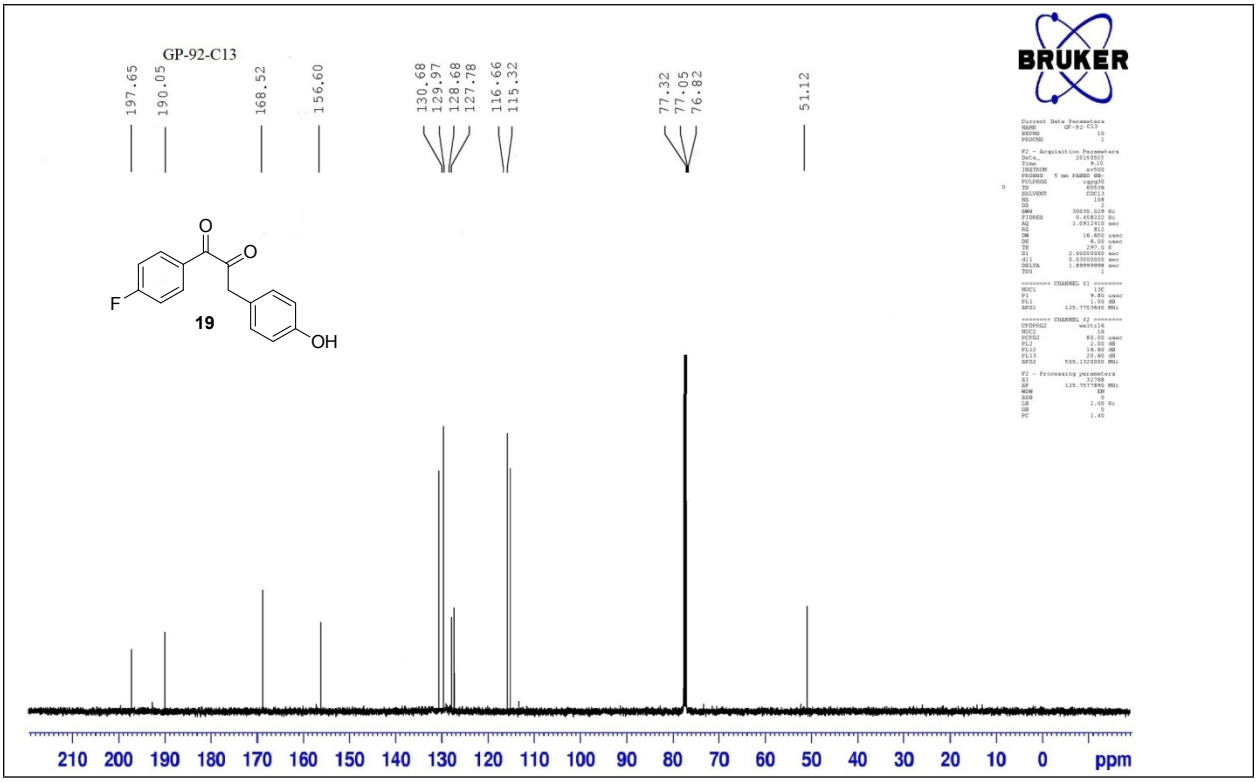

O
O
HO
17
Cl
abundance
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
197.412
190.126
157.127
140.100
133.628
131.540
130.778
129.624
129.300
116.190
77.451
77.127
76.812
50.812
X : parts per Million : Carbon13

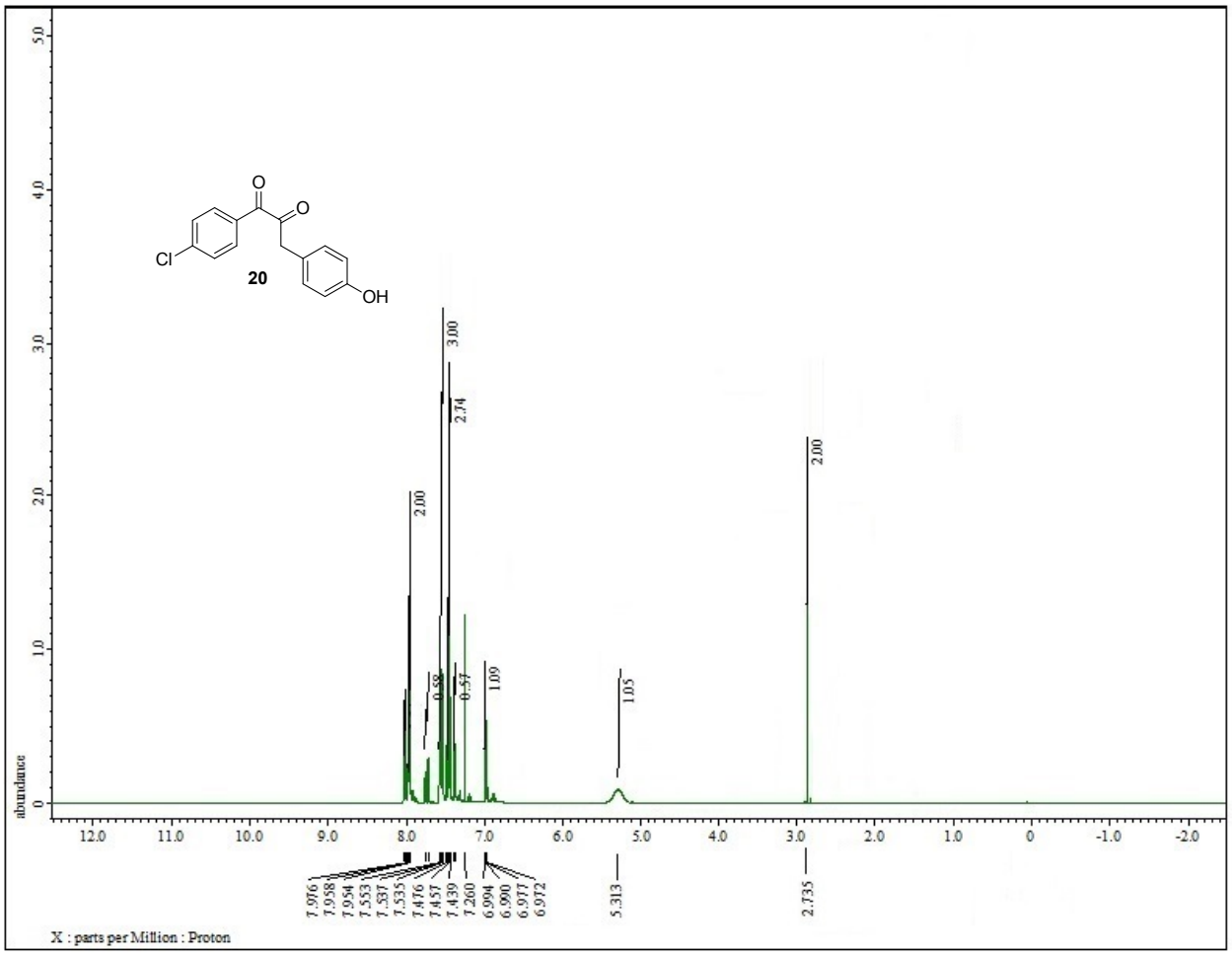
2

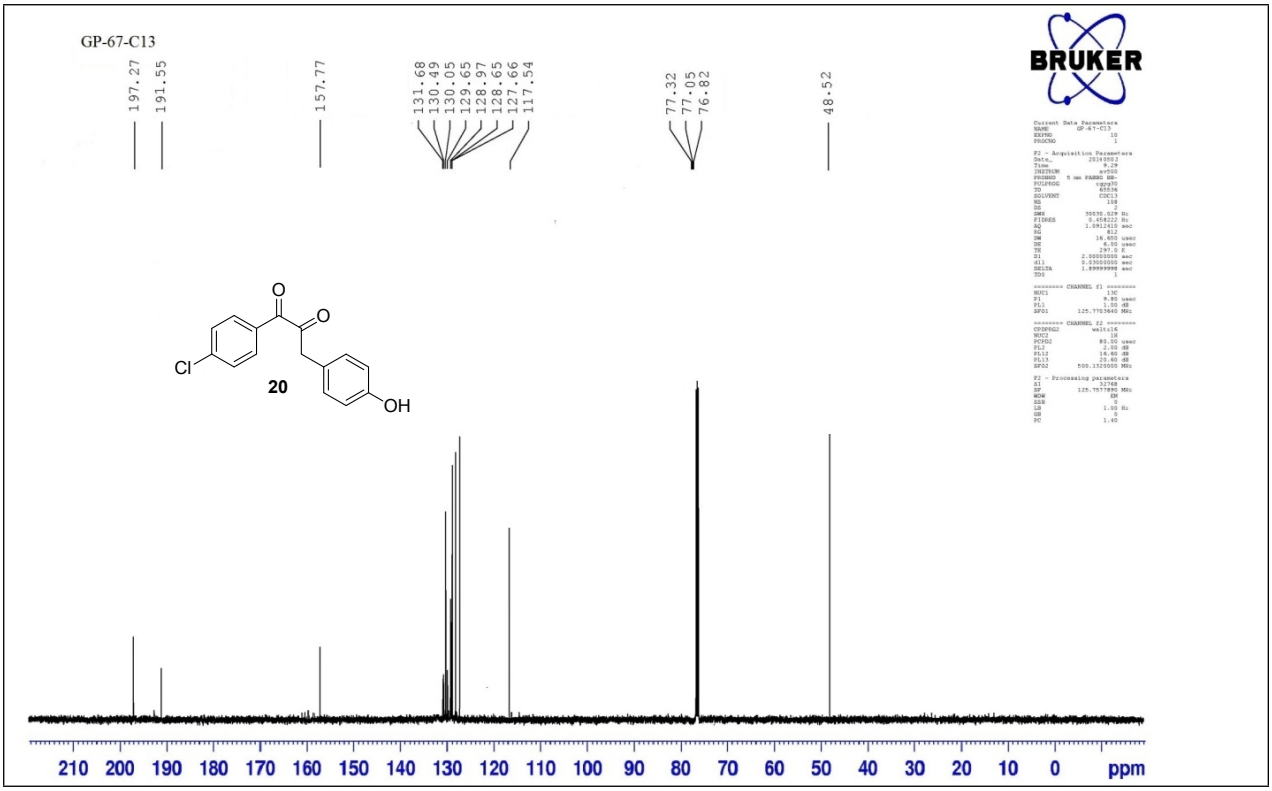

1
7.874
7.857
7.548
7.538
7.531
7.524
7.521
7.255
7.072
7.054
7.037
6.958
6.941
6.428
3.857
BRUKER
HO
O
O
Br
18
9
8
7
6
5
4
3
2
1
ppm
2.11
2.01
2.12
2.07
0.78
2.01

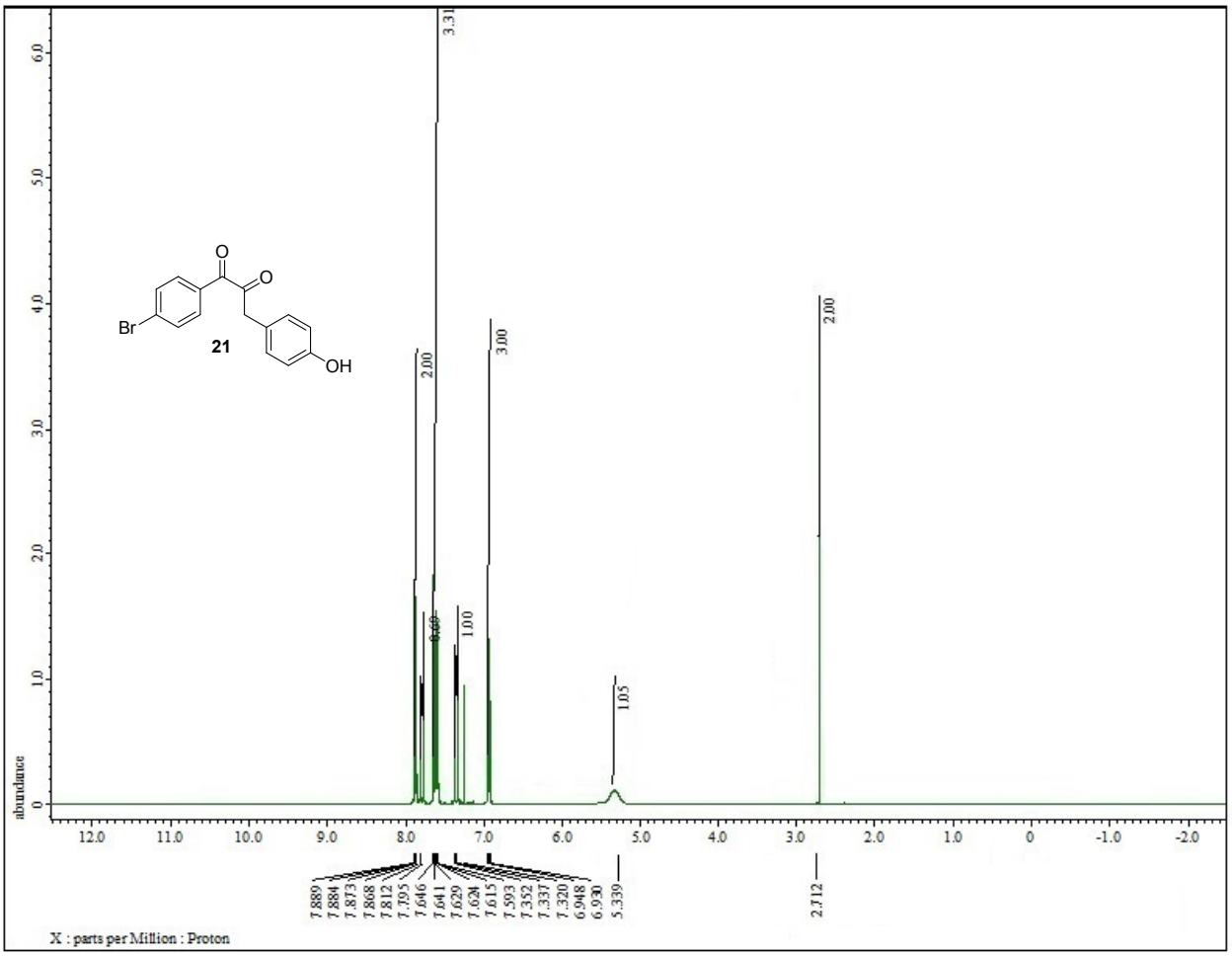

O
O
HO
18
Br
abundance
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
196.624
191.123
157.290
133.009
130.921
129.872
129.290
128.661
128.070
116.931
77.410
77.123
76.872
51.768
X : parts per Million : Carbon13

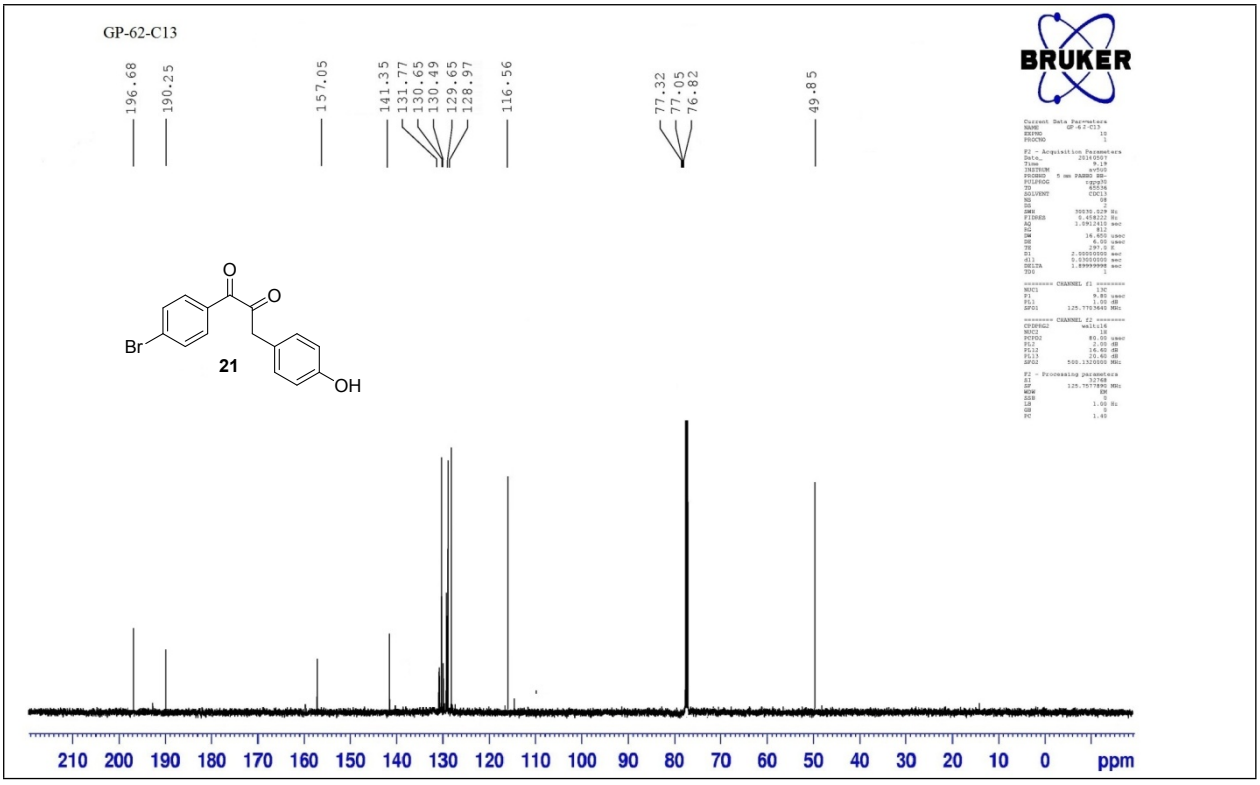

19
F
O
O
OH
abundance
2.00
2.33
2.13
2.18
1.00
0.72
2.00
8.033
8.025
8.021
8.008
8.003
7.997
7.581
7.560
7.531
7.396
7.148
7.126
5.313
2.791
X : parts per Million : Proton


GP-92-C13
197.65
190.05
168.52
156.60
130.68
129.97
128.68
127.78
116.66
115.32
77.32
77.05
76.82
51.12
O
O
F
19
OH
BRUKER
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
Cl
OH
20
abundance
X : parts per Million : Proton
2.00
3.00
2.74
2.00
0.58
0.57
1.09
1.05
7.976
7.958
7.954
7.553
7.537
7.535
7.476
7.457
7.439
7.260
6.994
6.990
6.977
6.972
5.313
2.735


GP-67-C13
197.27
191.55
157.77
131.68
130.49
130.05
129.65
128.97
128.65
127.66
117.54
77.32
77.05
76.82
48.52
BRUKER
O
O
Cl
OH
20
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
Br
21
OH
3.31
2.00
6.66
1.00
3.00
1.05
2.00
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.889
7.884
7.873
7.868
7.812
7.795
7.646
7.641
7.629
7.624
7.615
7.593
7.352
7.337
7.320
6.948
6.930
5.339
2.712
X : parts per Million : Proton


GP-62-C13
196.68
190.25
157.05
141.35
131.77
130.65
130.49
129.65
128.97
116.56
77.32
77.05
76.82
49.85
BRUKER
Br
O
O
OH
21
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm