Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Selective hydroxylation of aryl iodides to produce phenols under mild conditions using a supported copper catalyst

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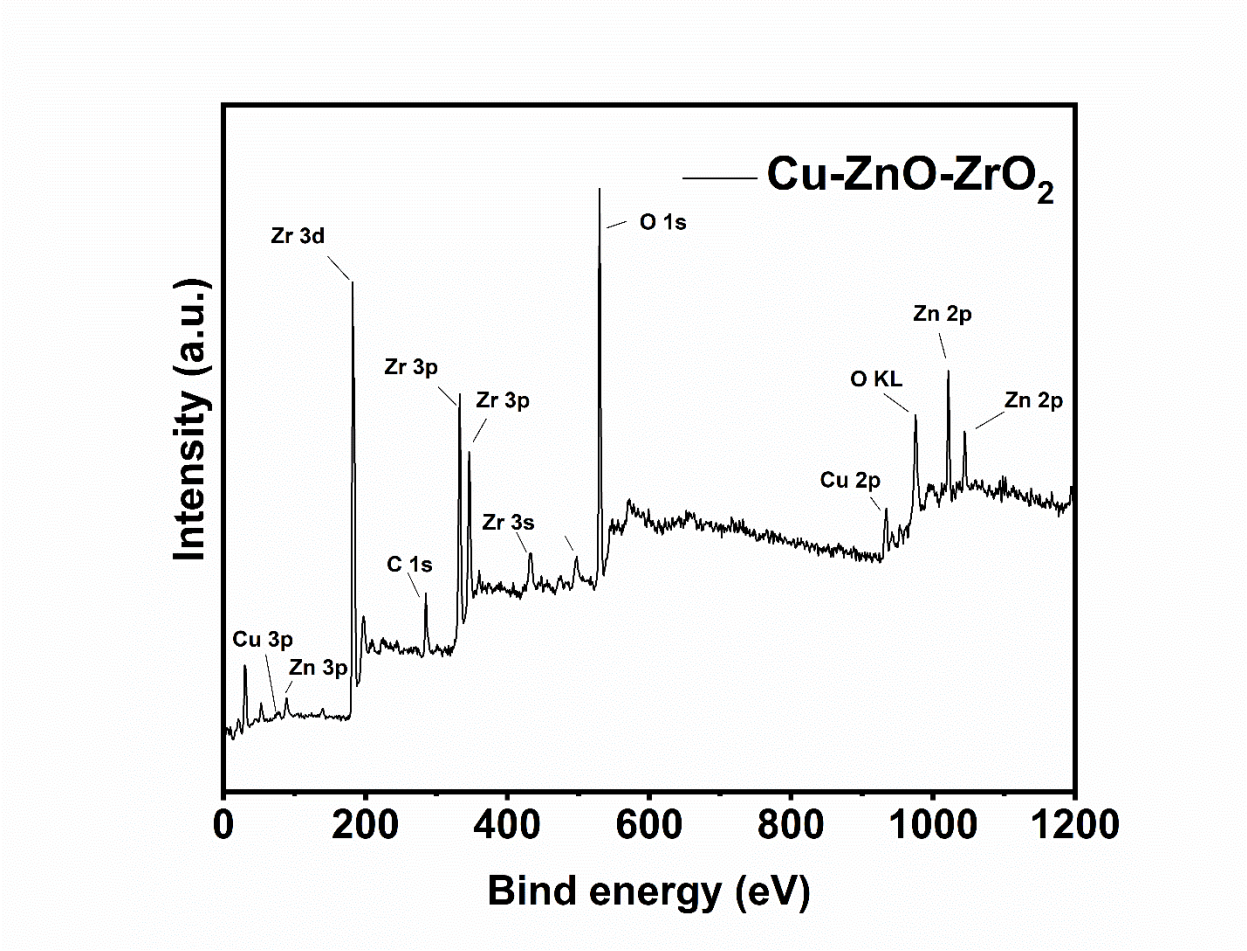


Figure S1. The full XPS spectrum of the catalyst Cu-ZnO-ZrO_2.

Figure S1 shows the full XPS spectrum of the catalyst Cu-ZnO-ZrO_2. As indicated in Figure S1, the main elements on the surface of the sample are Cu, Zn, Zr and O. The photoelectron peaks of these elements appear at binding energies of 932.5 eV (Cu 2p), 1021.5 eV (Zn 2p), 182.1 eV (Zr 3d) and 532.0 eV (O 1s), respectively.

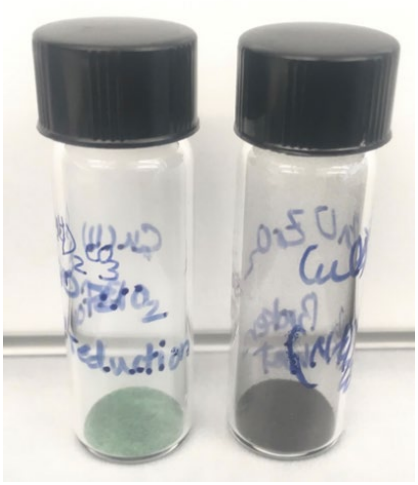


Figure S2. Color change of Cu-ZnO-ZrO_2, before (left) and after the reduction (right).

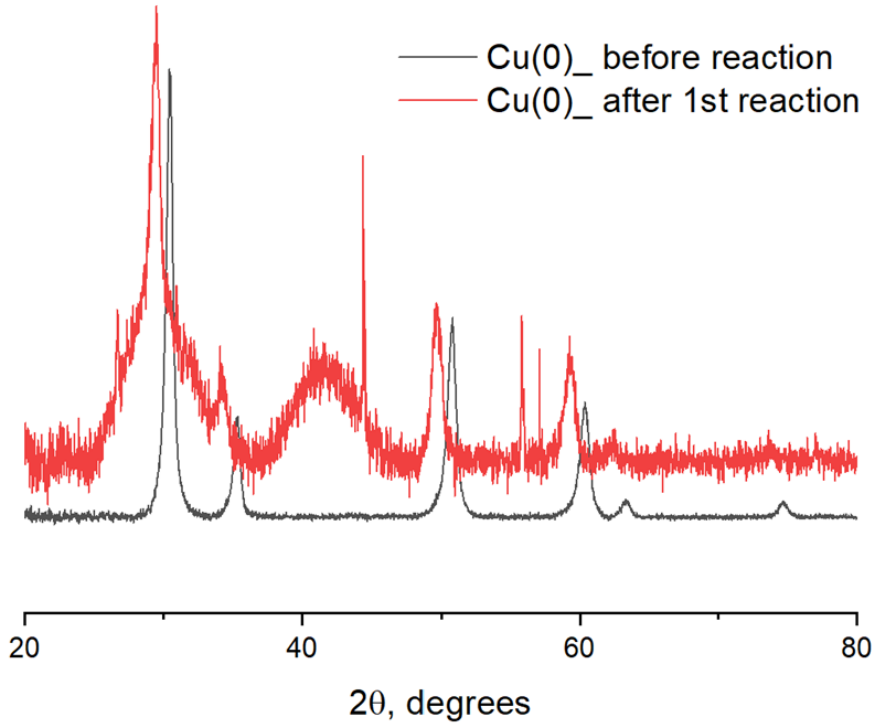


Figure S3. XRD patterns of the catalyst before and after the reaction.

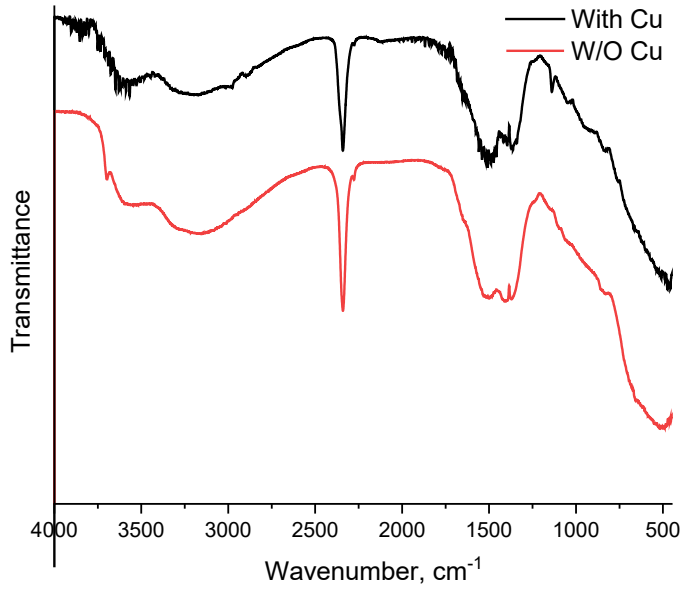


Figure S4. FTIR spectra of the support and catalyst.

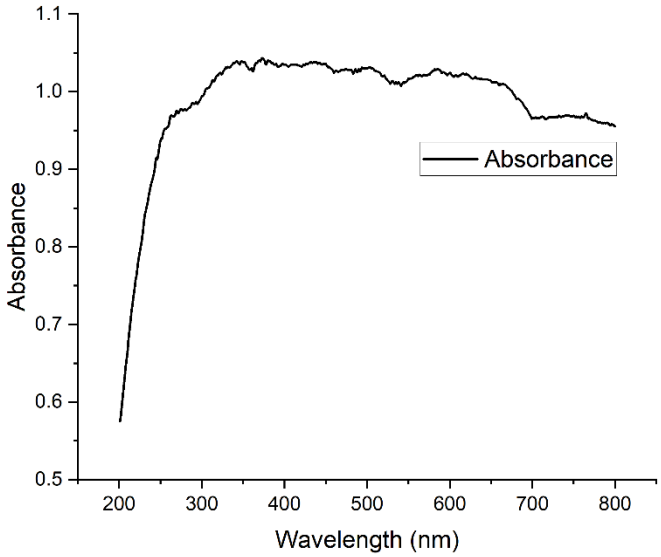


Figure S5. The UV-Vis absorption spectrum of the Cu-ZnO-ZrO_2.

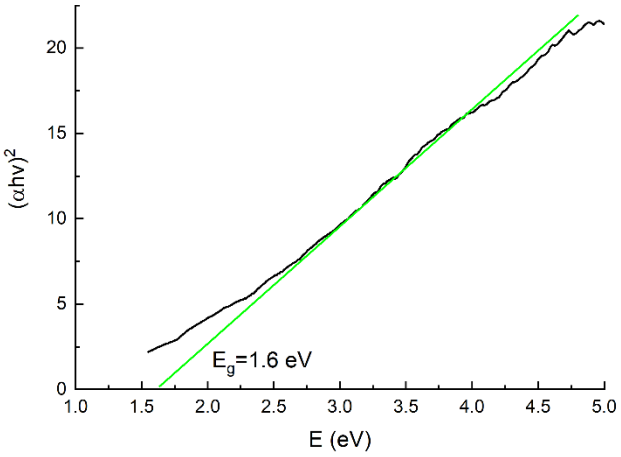


Figure S6. The Tauc plot showing the optical band gap of the Cu-ZnO-ZrO_2.

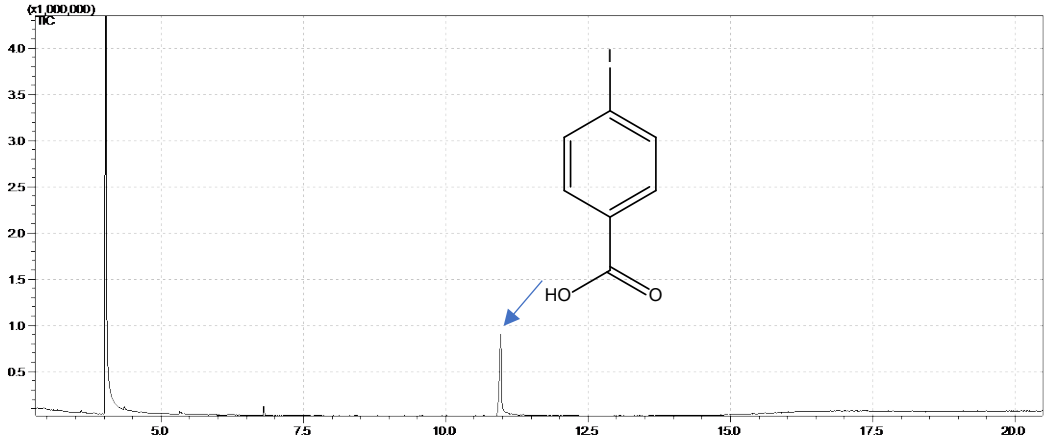


Figure S7. The GC-MS result of the reaction mixture started with 4-carboxylate-iodobenzene.

Surface Area	
Single point surface area at p/p° = 0.249559231:	72.8141 m²/g
BET Surface Area:	77.4631 m²/g
Langmuir Surface Area:	156.6951 m²/g
t-Plot Micropore Area:	7.0749 m²/g
t-Plot external surface area:	70.3881 m²/g
BJH Adsorption cumulative surface area of pores between 1.7000 nm and 300.0000 nm width:	94.6425 m²/g
BJH Desorption cumulative surface area of pores between 1.7000 nm and 300.0000 nm width:	109.5493 m²/g

Figure S8. Surface area data for the catalyst.

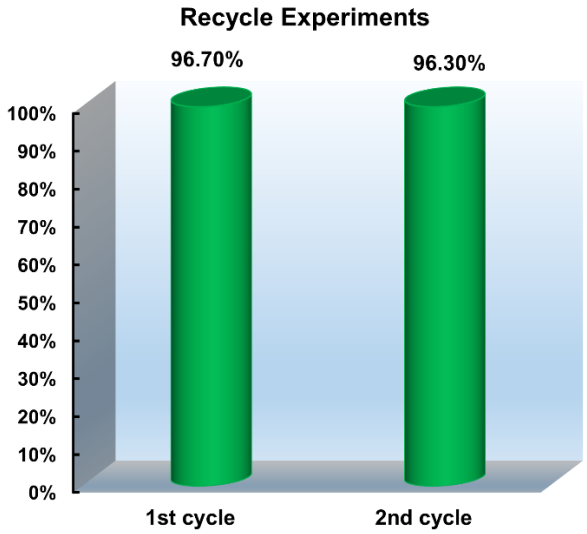
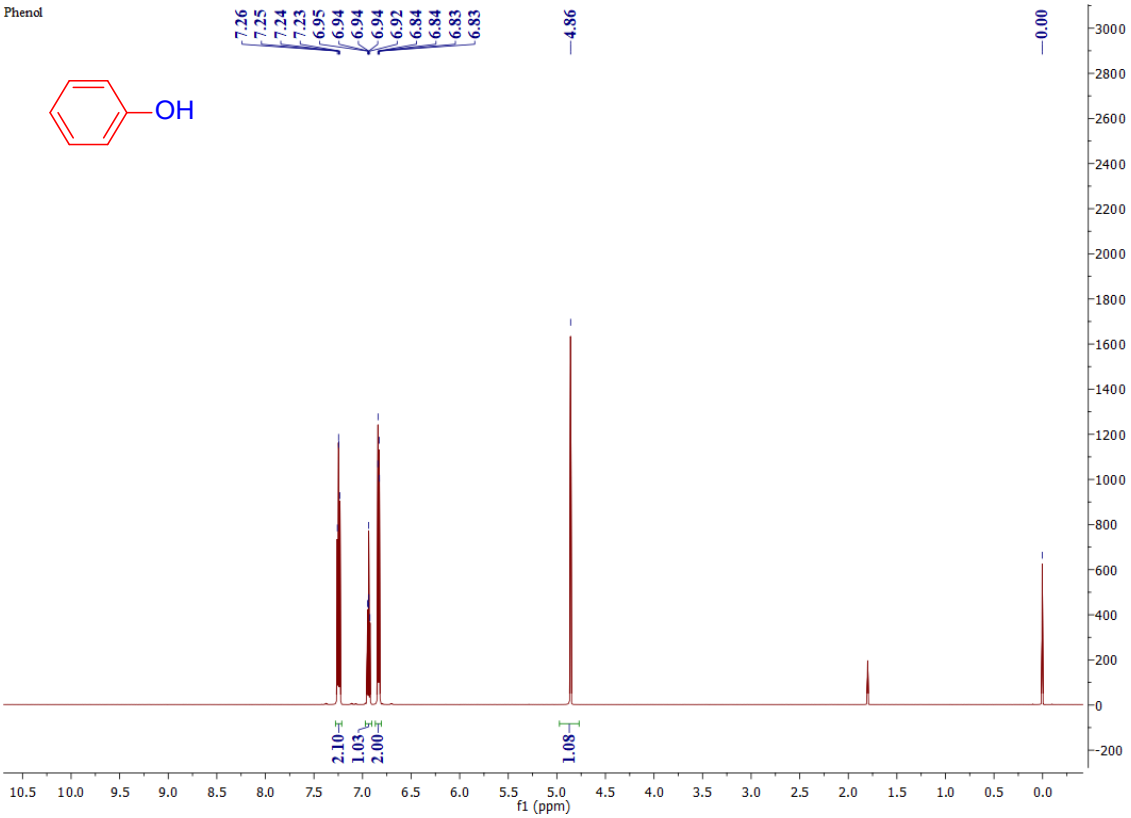
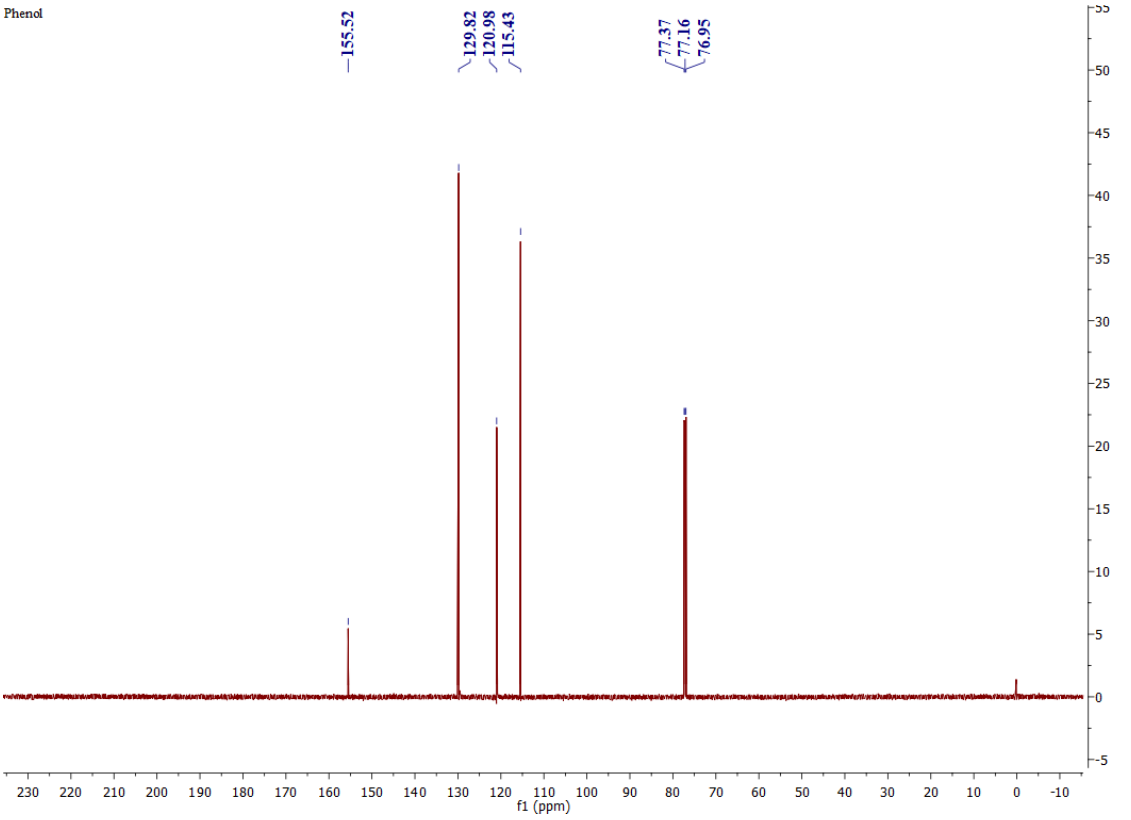
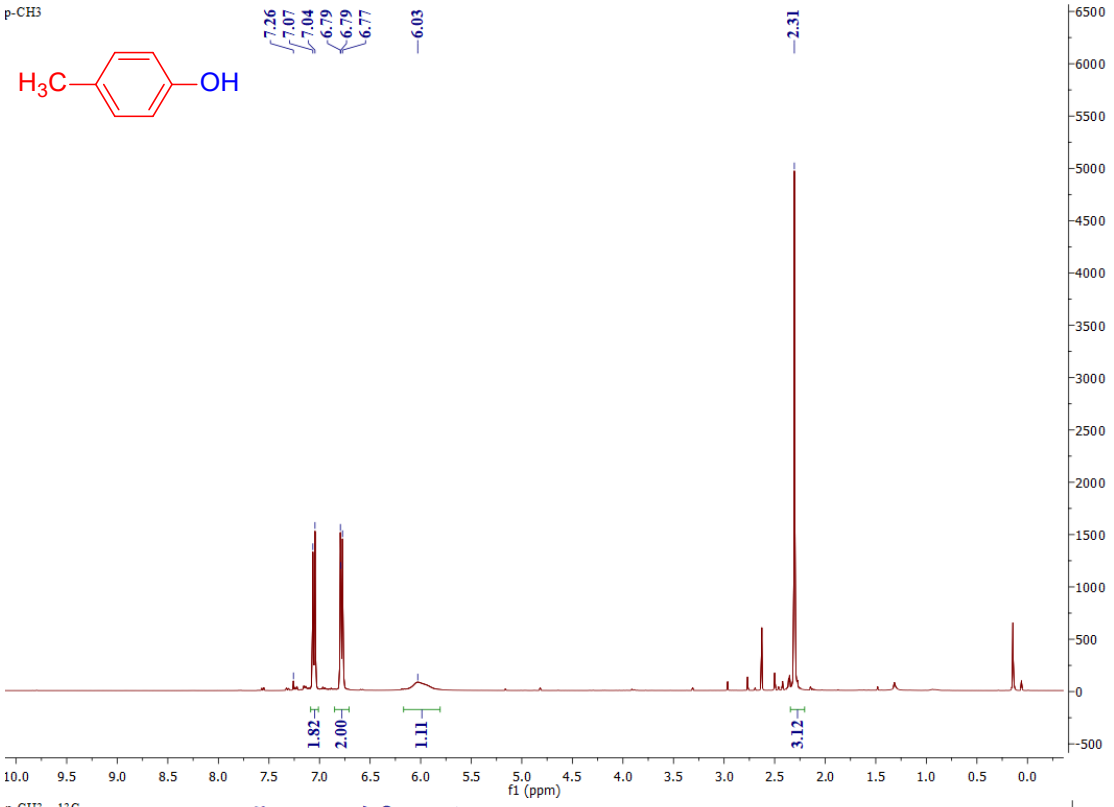


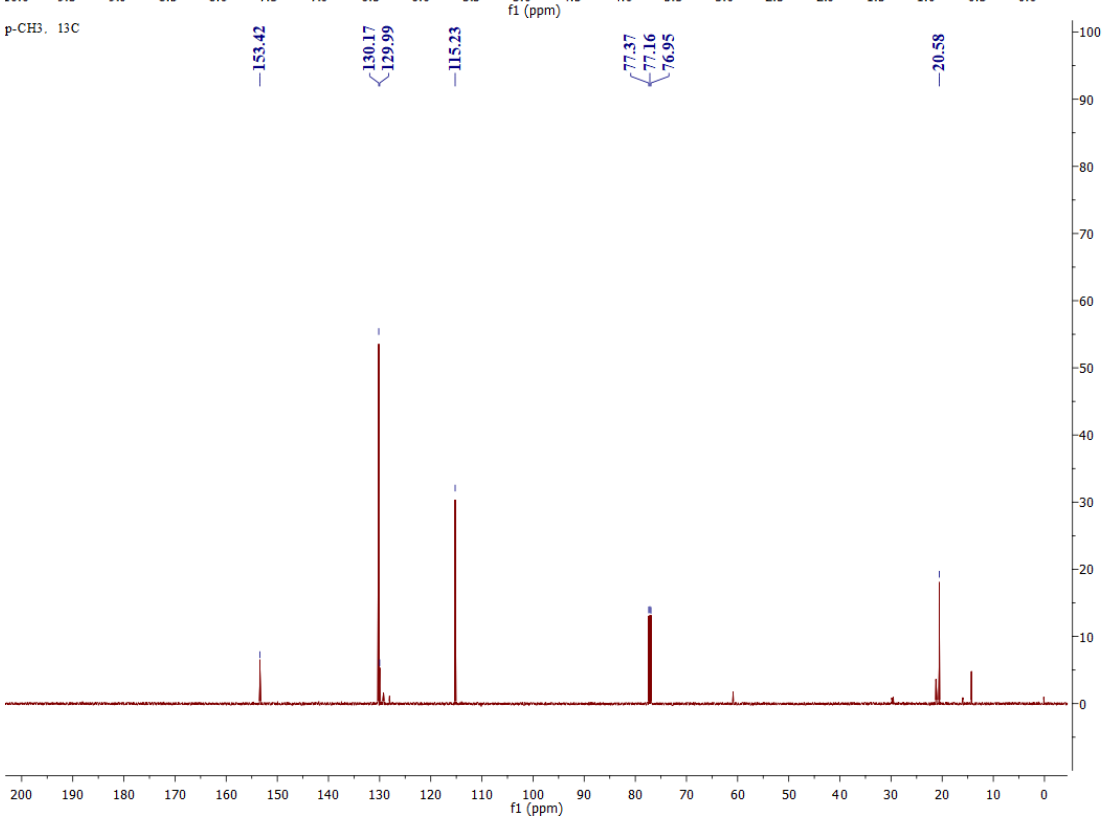
Figure S9. The recycling of the catalyst.

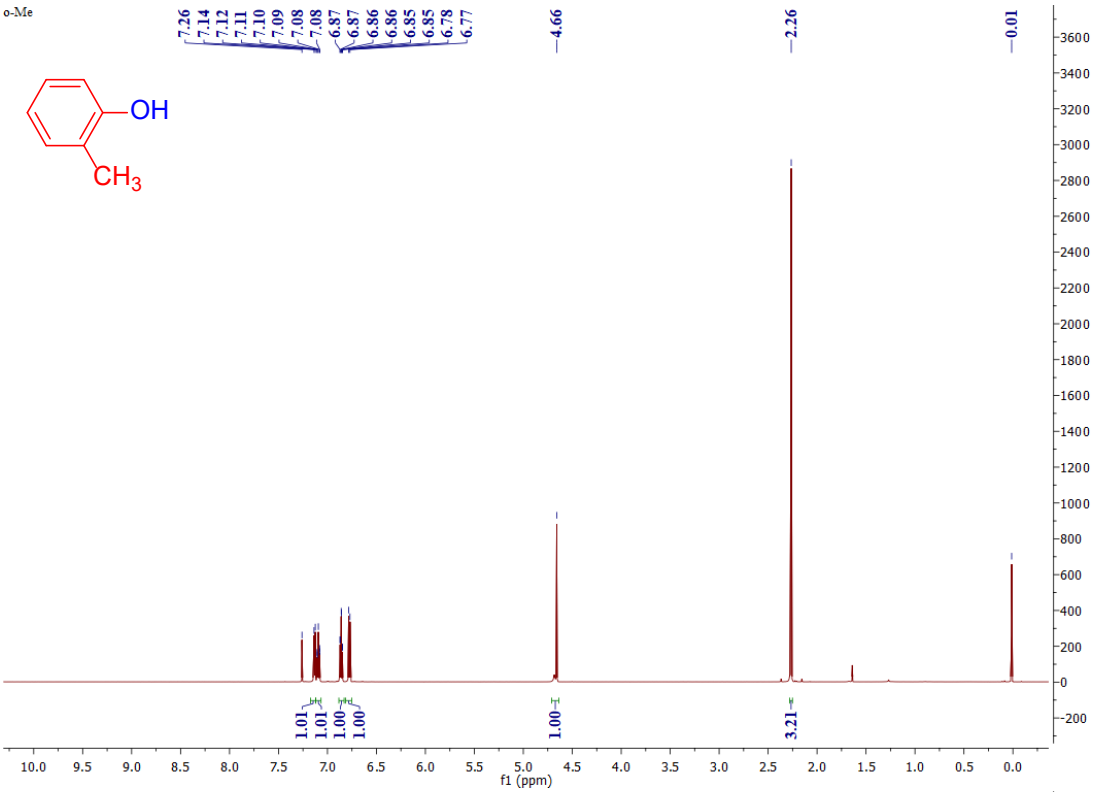
IV. Copies of ^{1}H NMR and ^{13}C NMR Spectra

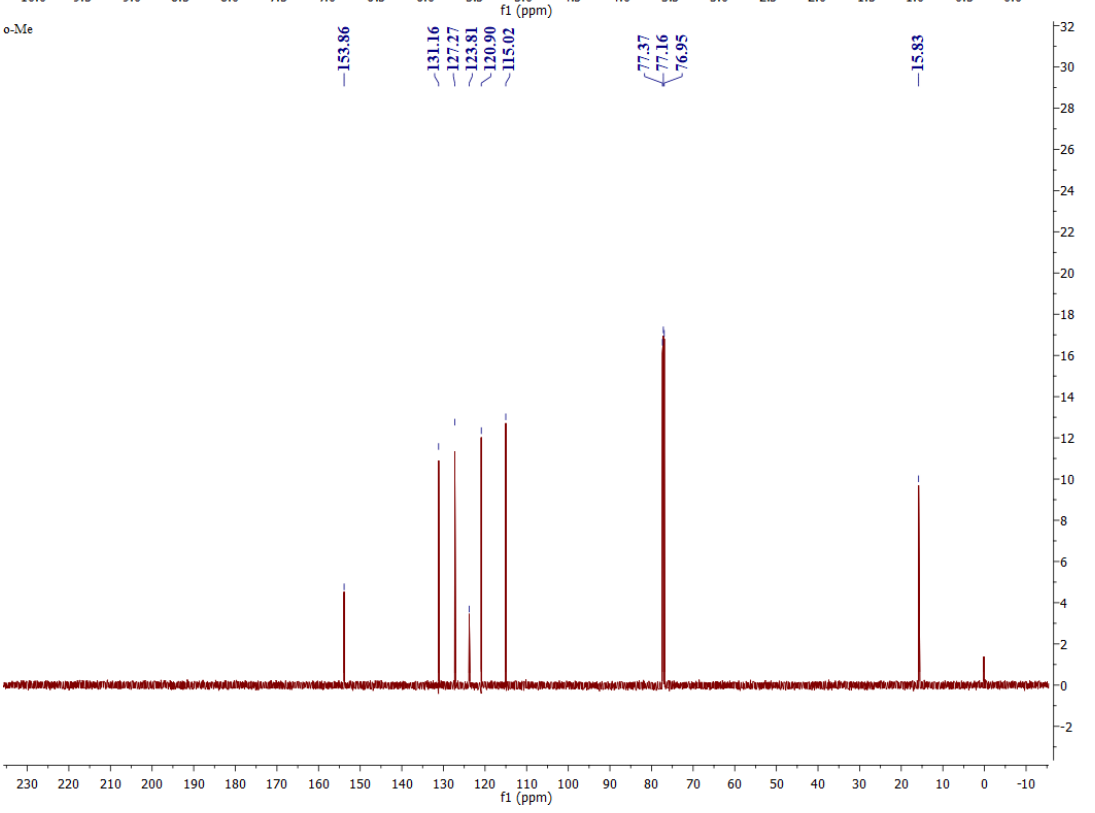


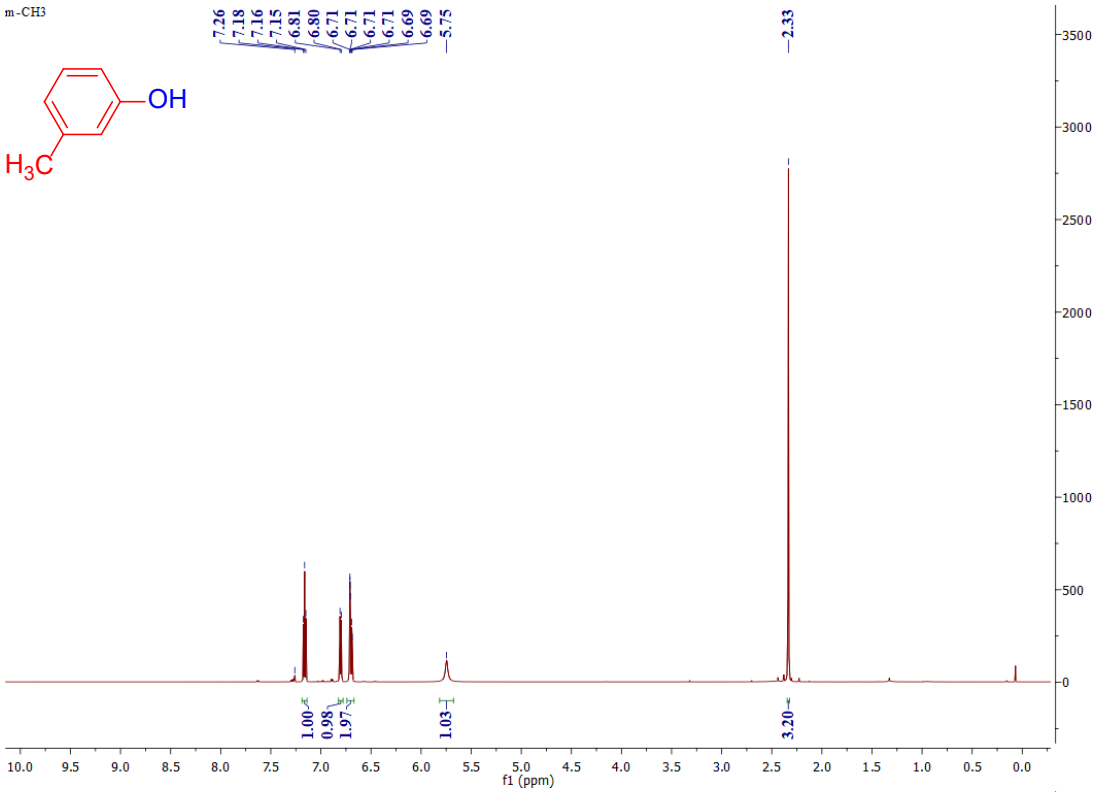


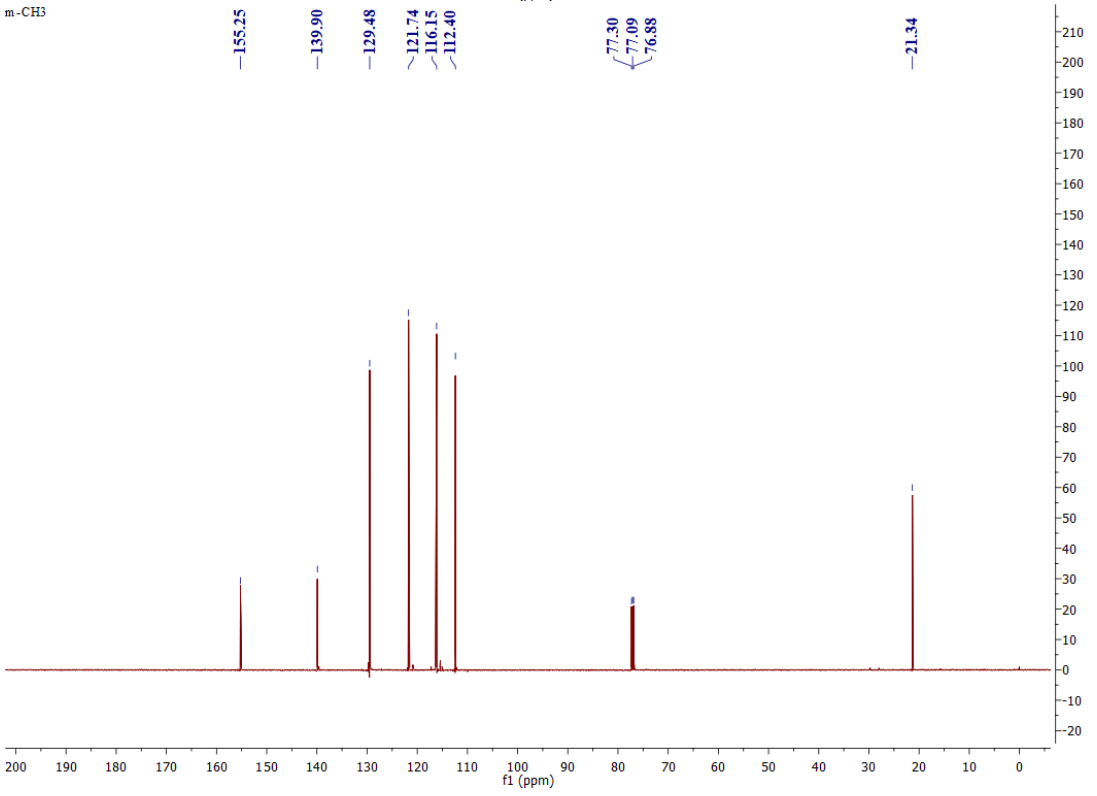

p-CH3
H3C
OH
7.26
7.07
7.04
6.79
6.79
6.77
6.03
2.31
1.82
2.00
1.11
3.12
f1 (ppm)

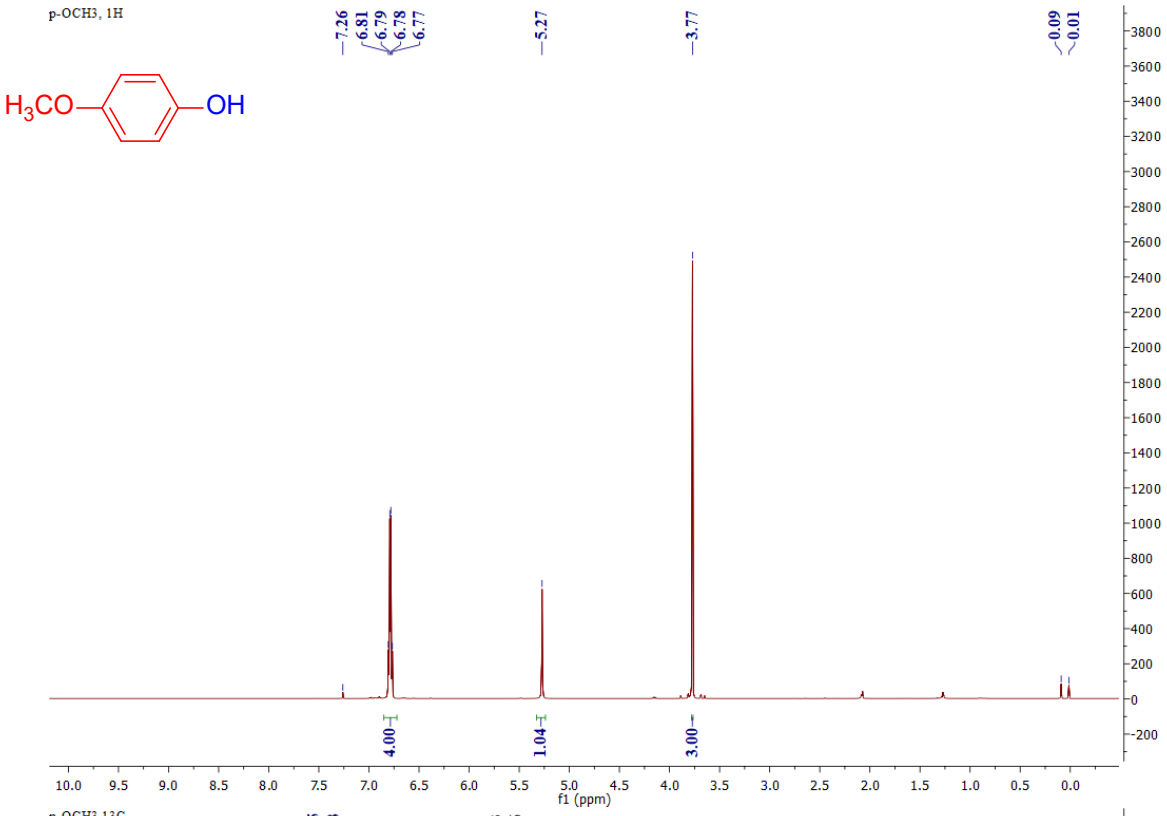

p-CH3, 13C
153.42
130.17
129.99
115.23
77.37
77.16
76.95
20.58
f1 (ppm)

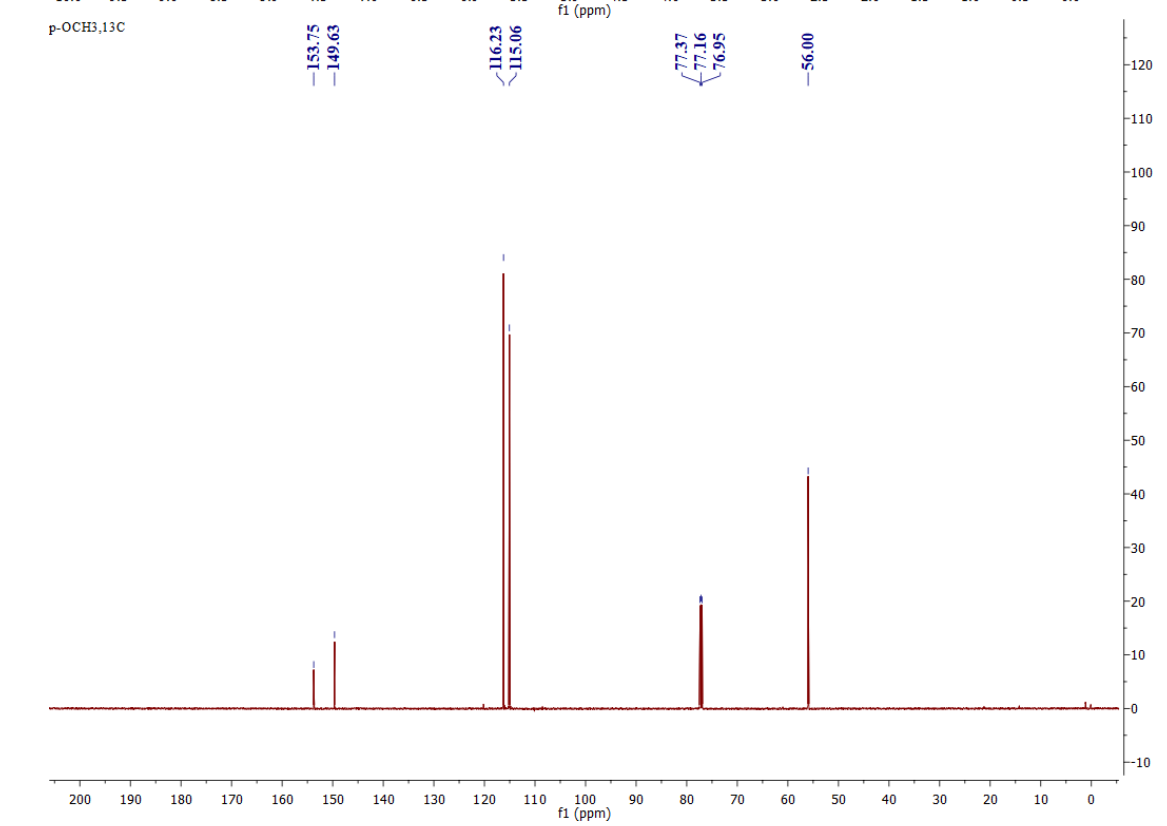

o-Me
OH
CH3
7.26
7.14
7.12
7.11
7.10
7.09
7.08
7.08
6.87
6.87
6.86
6.86
6.85
6.85
6.78
6.77
4.66
2.26
0.01
1.01
1.01
1.00
1.00
1.00
3.21
f1 (ppm)

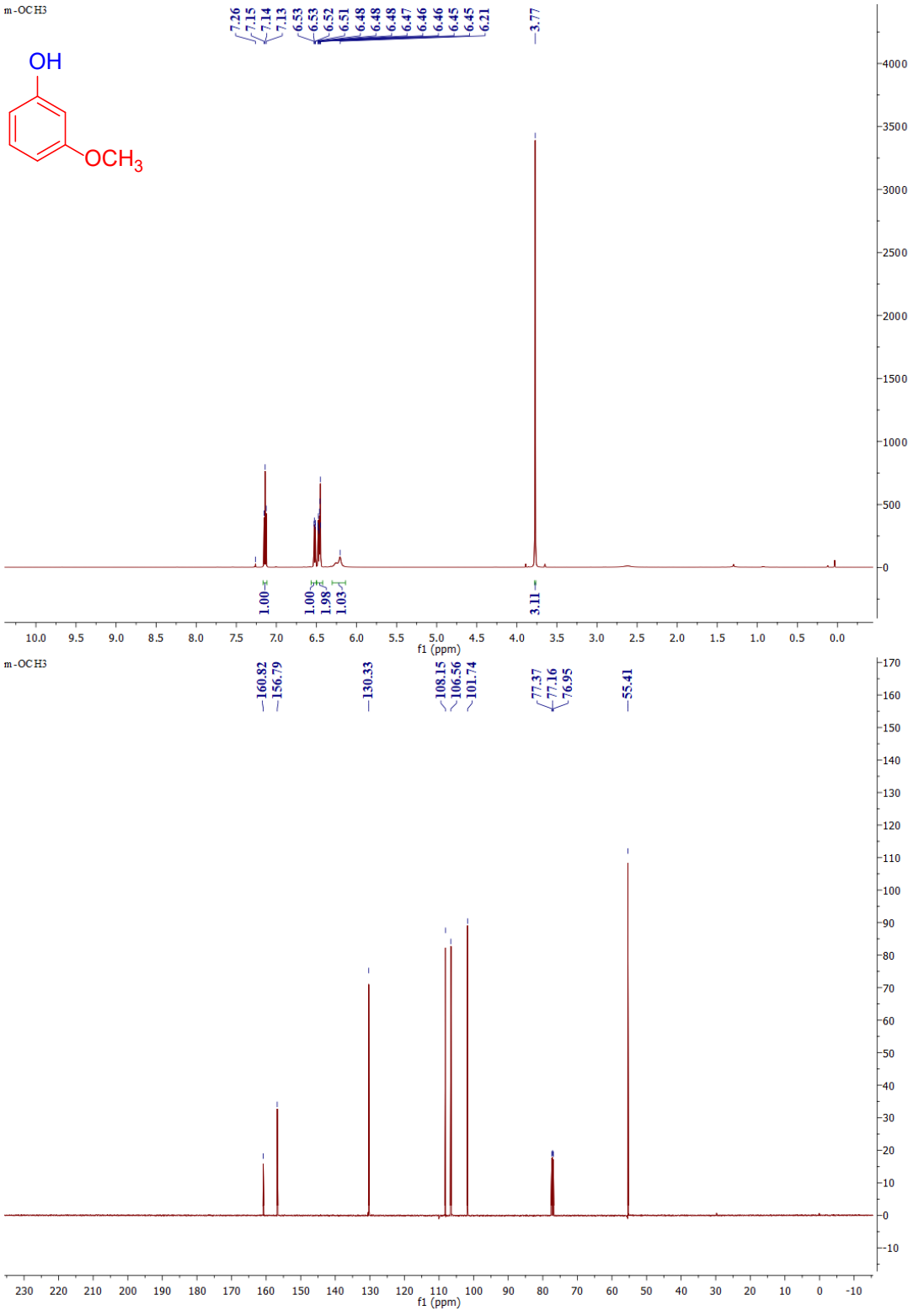

o-Me
153.86
131.16
127.27
123.81
120.90
115.02
77.37
77.16
76.95
15.83
f1 (ppm)

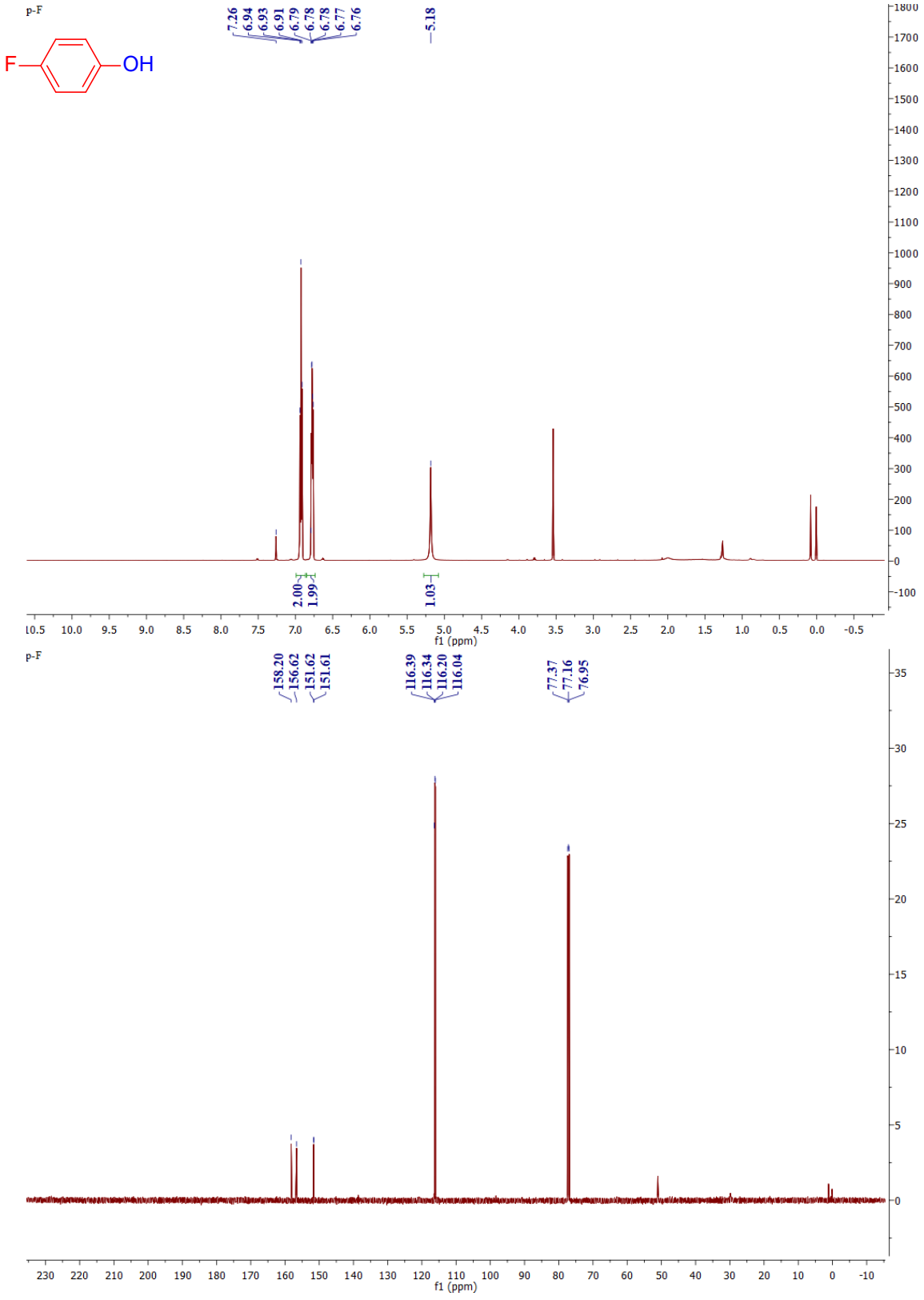

m-CH3
OH
H3C
7.26
7.18
7.16
7.15
6.81
6.80
6.71
6.71
6.71
6.71
6.69
6.69
5.75
2.33
1.00
0.98
1.97
1.03
3.20
f1 (ppm)

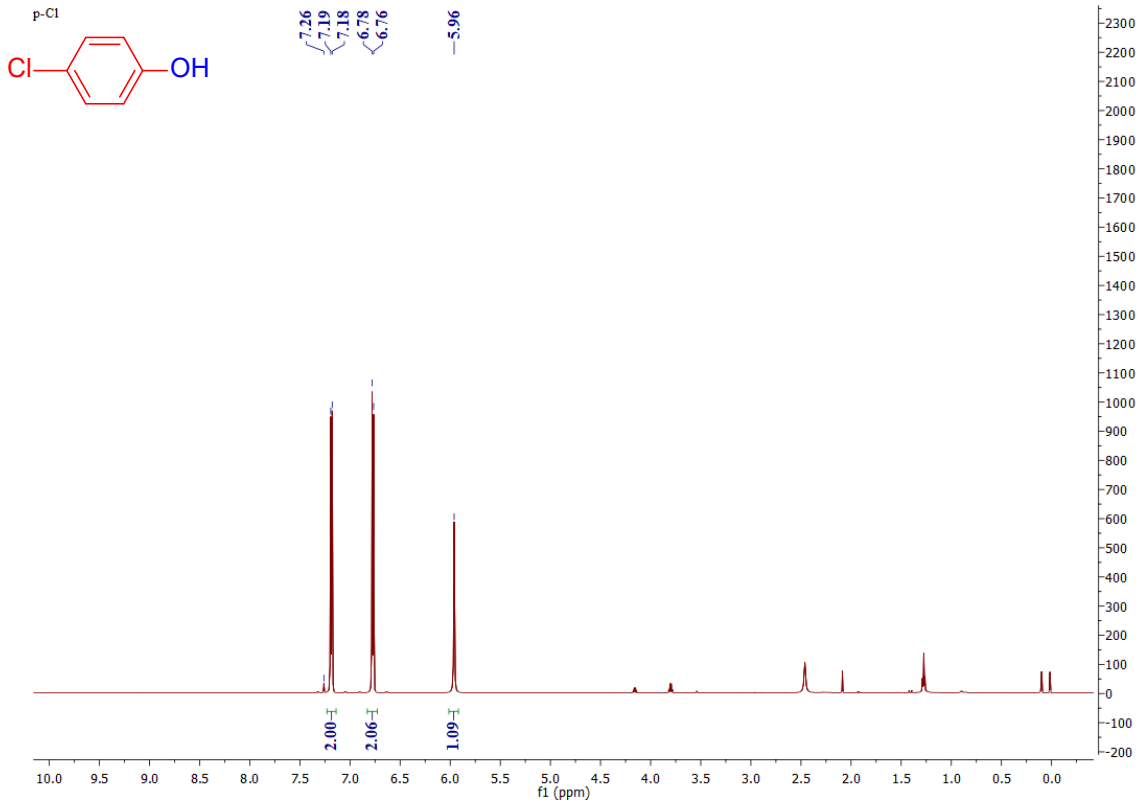

m-CH3
155.25
139.90
129.48
121.74
116.15
112.40
77.30
77.09
76.88
21.34
f1 (ppm)

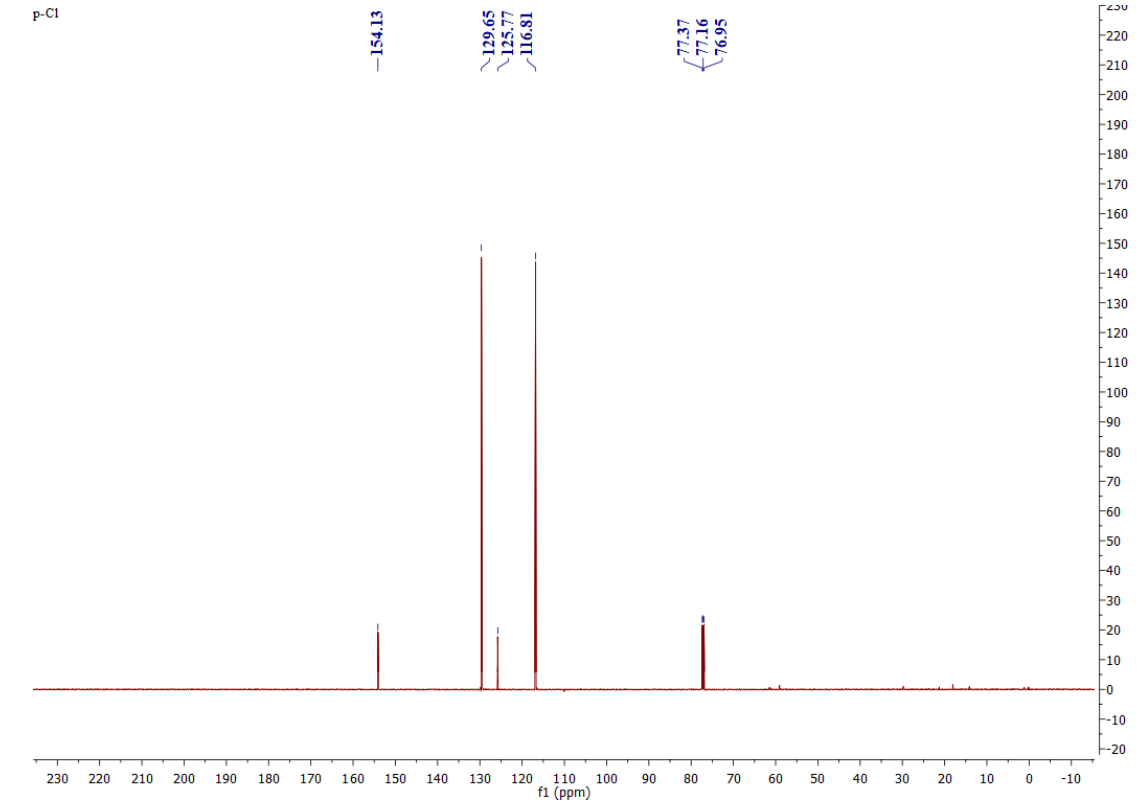

p-OCH3, 1H
H3CO
OH
7.26
6.81
6.79
6.78
6.77
5.27
3.77
0.09
0.01
4.00
1.04
3.00
f1 (ppm)

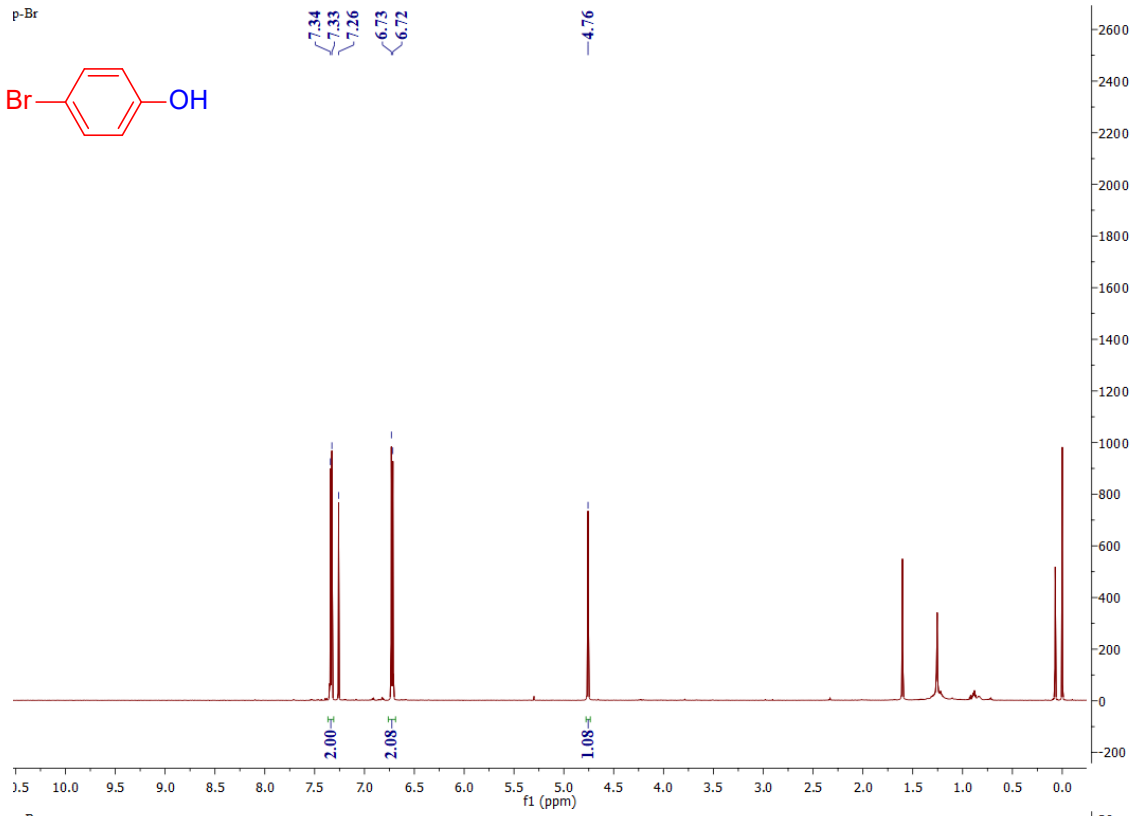

p-OCH3,13C
153.75
149.63
116.23
115.06
77.37
77.16
76.95
56.00
f1 (ppm)

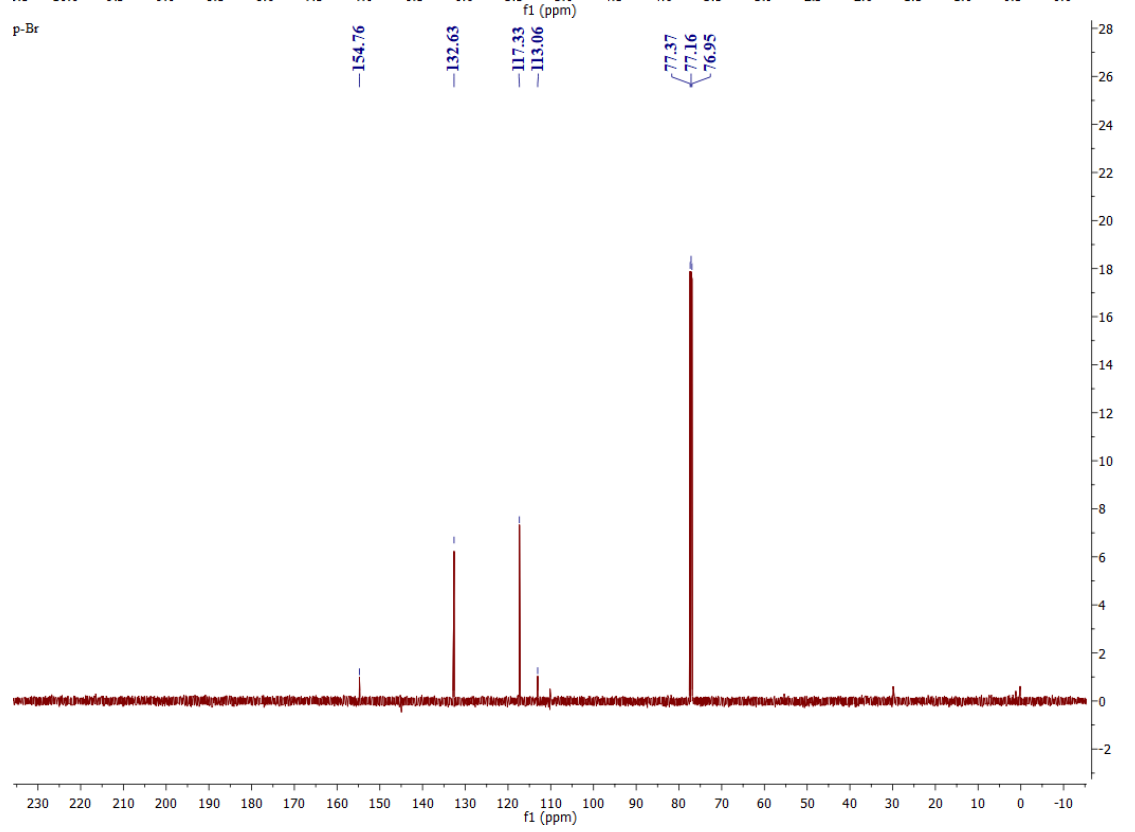

m-OCH3
OH
OCH3
7.26
7.15
7.14
7.13
6.53
6.53
6.52
6.51
6.48
6.48
6.48
6.47
6.46
6.46
6.45
6.45
6.21
3.77
1.00
1.00
1.98
1.03
3.11
f1 (ppm)
m-OCH3
160.82
156.79
130.33
108.15
106.56
101.74
77.37
77.16
76.95
55.41
f1 (ppm)

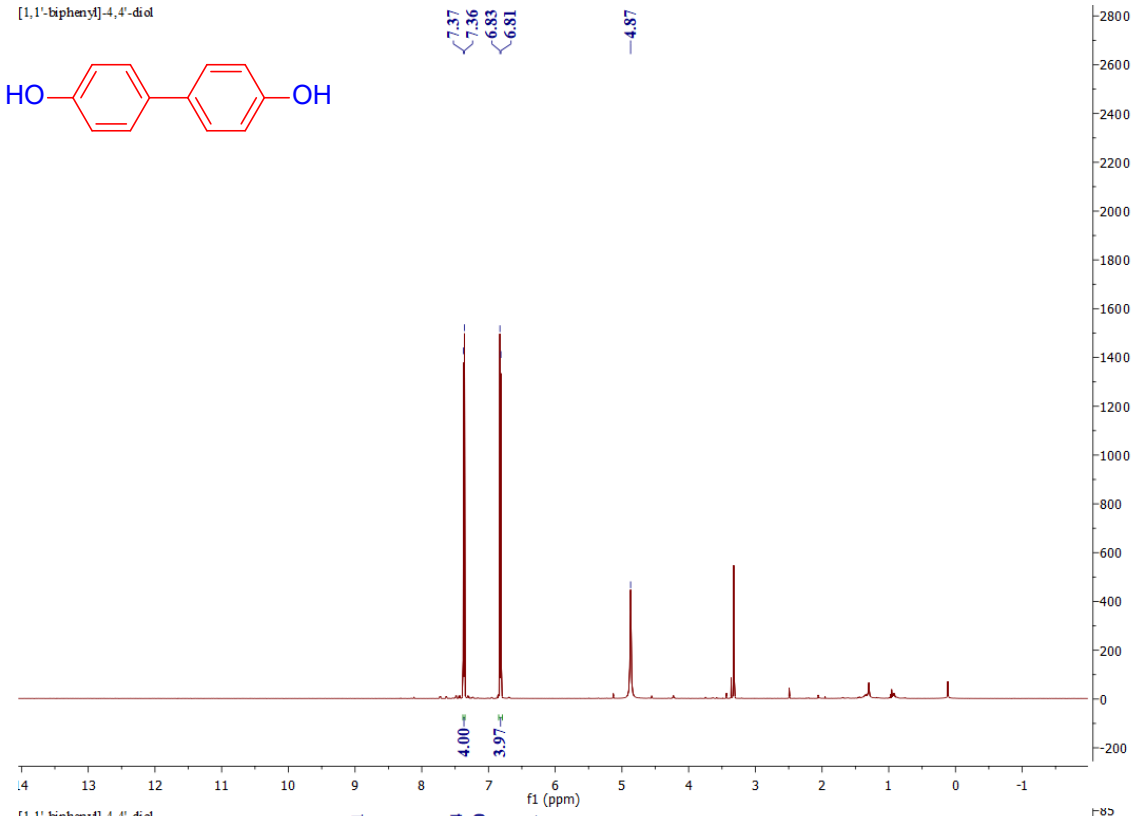

p-F
F
OH
7.26
6.94
6.93
6.91
6.79
6.78
6.78
6.77
6.76
5.18
2.00
1.99
1.03
f1 (ppm)
p-F
158.20
156.62
151.62
151.61
116.39
116.34
116.20
116.04
77.37
77.16
76.95
f1 (ppm)

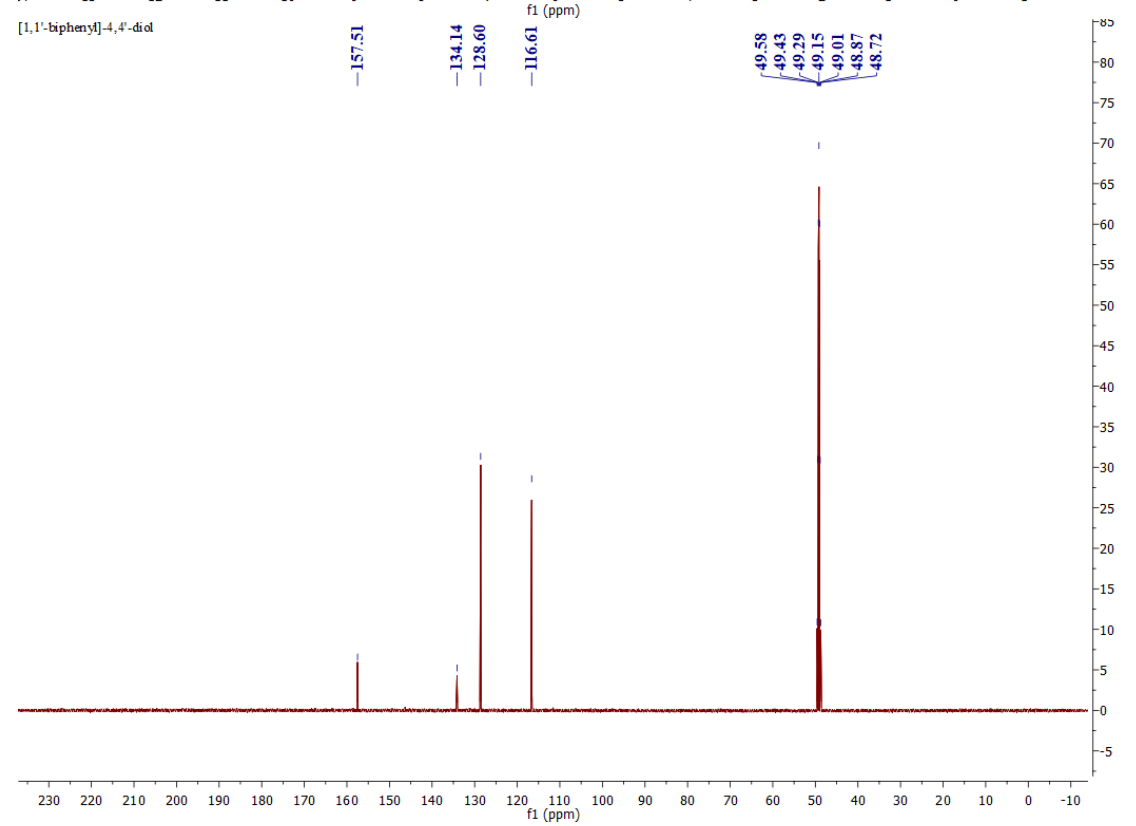

p-Cl
Cl
OH
7.26
7.19
7.18
6.78
6.76
5.96
2.00
2.06
1.09
f1 (ppm)

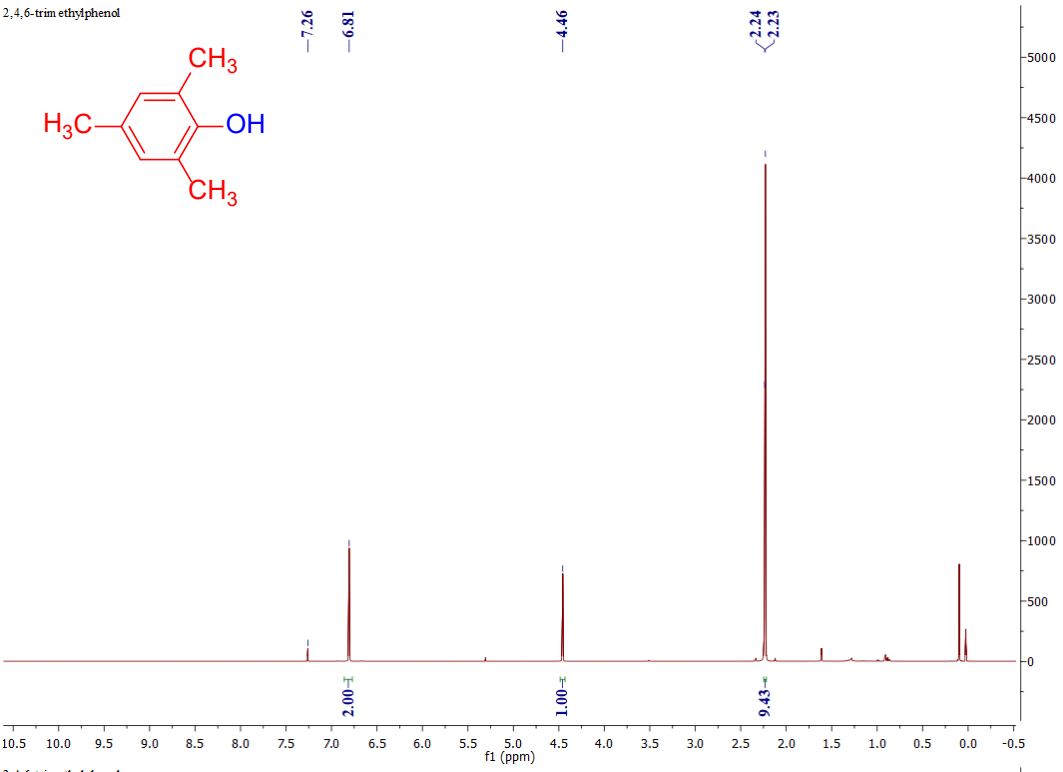

p-Cl
154.13
129.65
125.77
116.81
77.37
77.16
76.95
f1 (ppm)

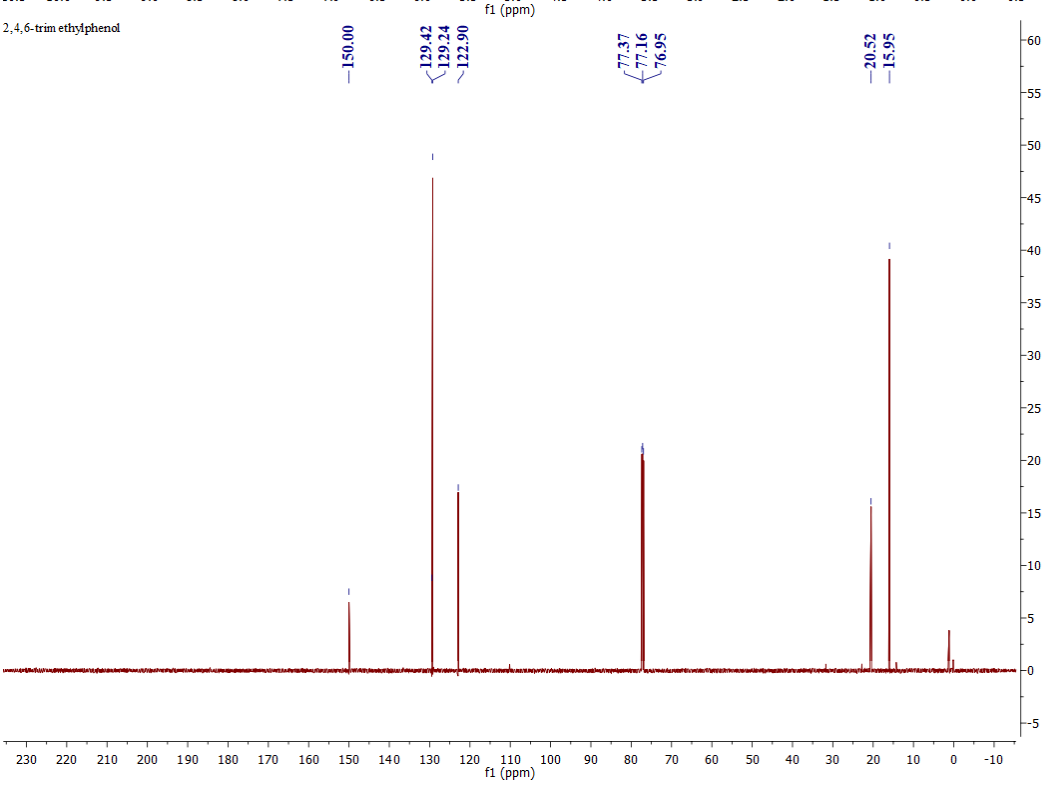

p-Br
Br
OH
7.34
7.33
7.26
6.73
6.72
4.76
2.00
2.08
1.08
f1 (ppm)

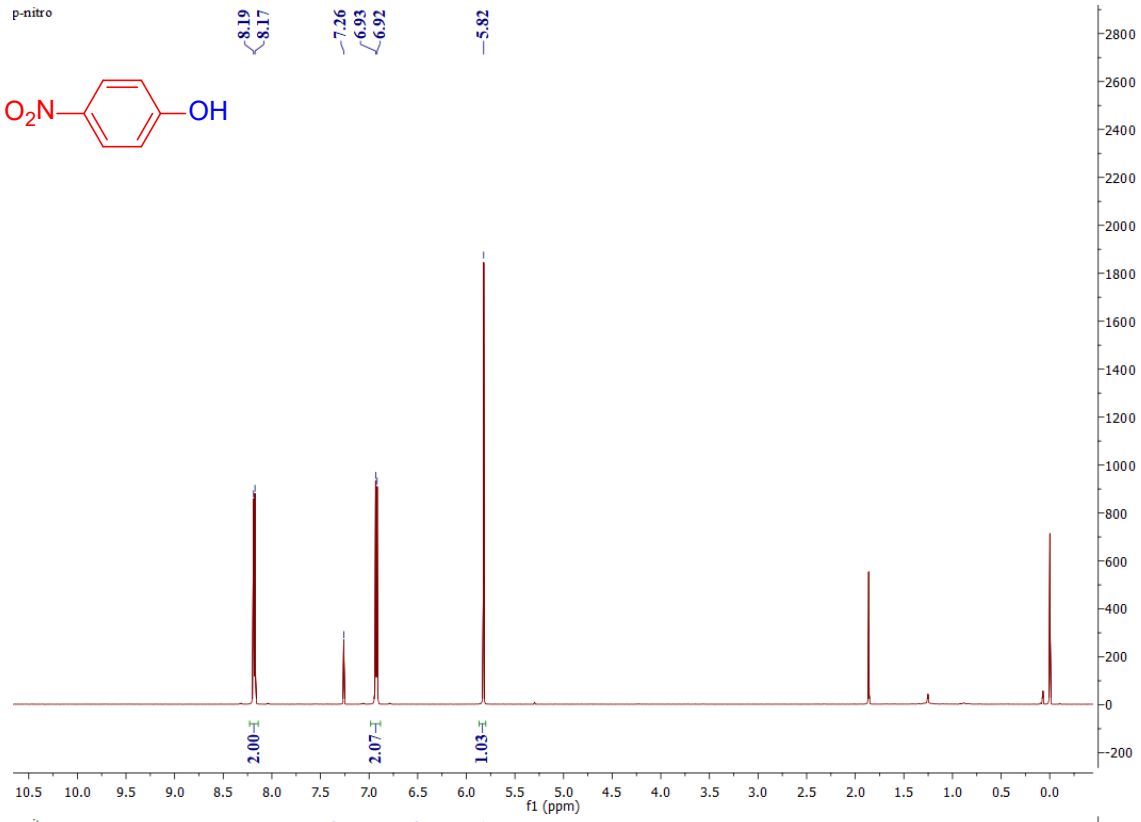

p-Br
154.76
132.63
117.33
113.06
77.37
77.16
76.95
f1 (ppm)

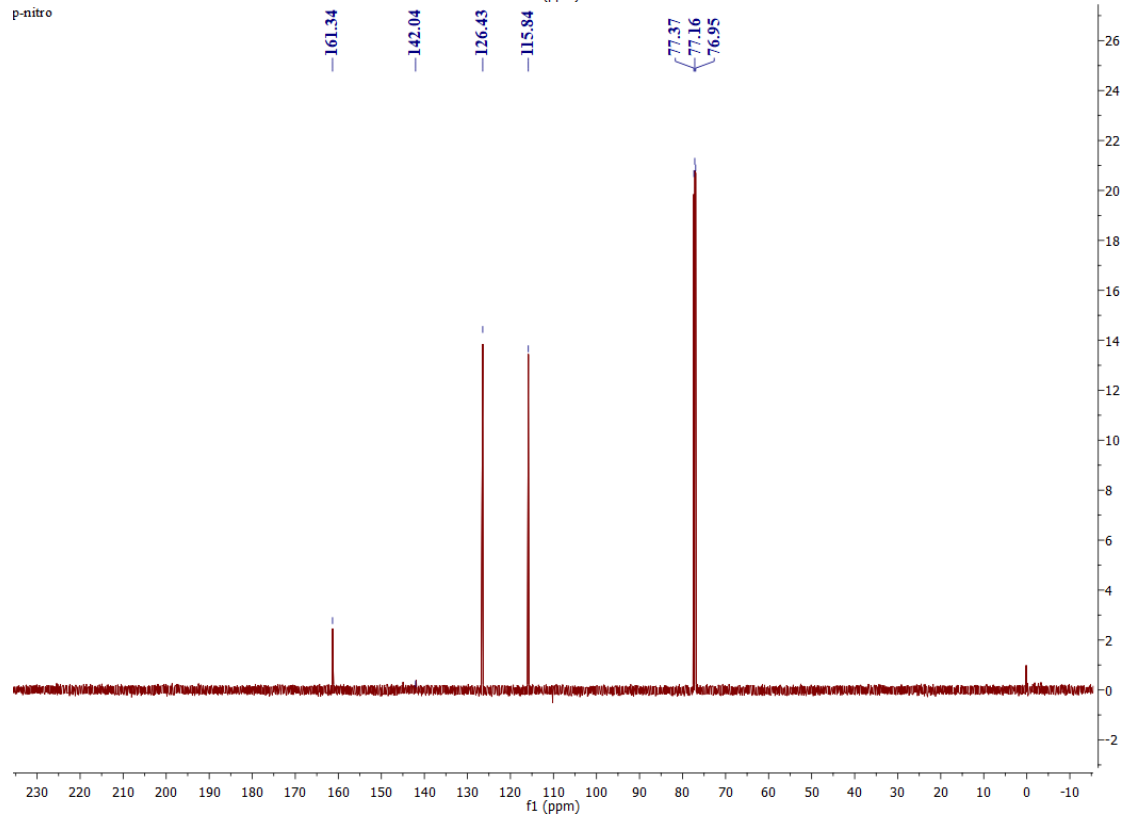

[1,1'-biphenyl]-4,4'-diol
HO
OH
7.37
7.36
6.83
6.81
4.87
4.00
3.97
f1 (ppm)

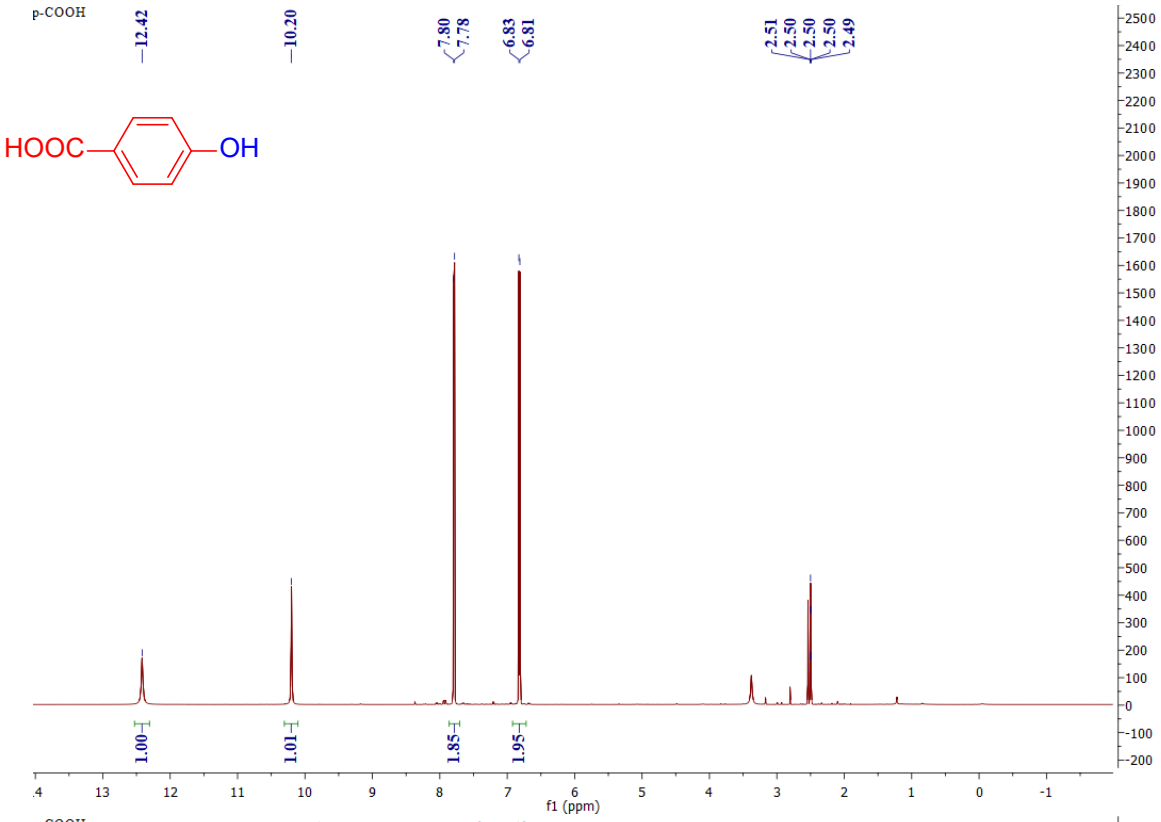

[1,1'-biphenyl]-4,4'-diol
157.51
134.14
128.60
116.61
49.58
49.43
49.29
49.15
49.01
48.87
48.72
f1 (ppm)


2,4,6-trim ethylphenol
CH3
H3C
OH
CH3
7.26
6.81
4.46
2.24
2.23
2.00
1.00
9.43
f1 (ppm)


2,4,6-trim ethylphenol
150.00
129.42
129.24
122.90
77.37
77.16
76.95
20.52
15.95
f1 (ppm)


p-nitro
8.19
8.17
7.26
6.93
6.92
5.82
2.00
2.07
1.03
f1 (ppm)


p-nitro
161.34
142.04
126.43
115.84
77.37
77.16
76.95
f1 (ppm)


p-COOH
12.42
10.20
7.80
7.78
6.83
6.81
2.51
2.50
2.50
2.50
2.49
HOOC
OH
1.00
1.01
1.85
1.95
f1 (ppm)

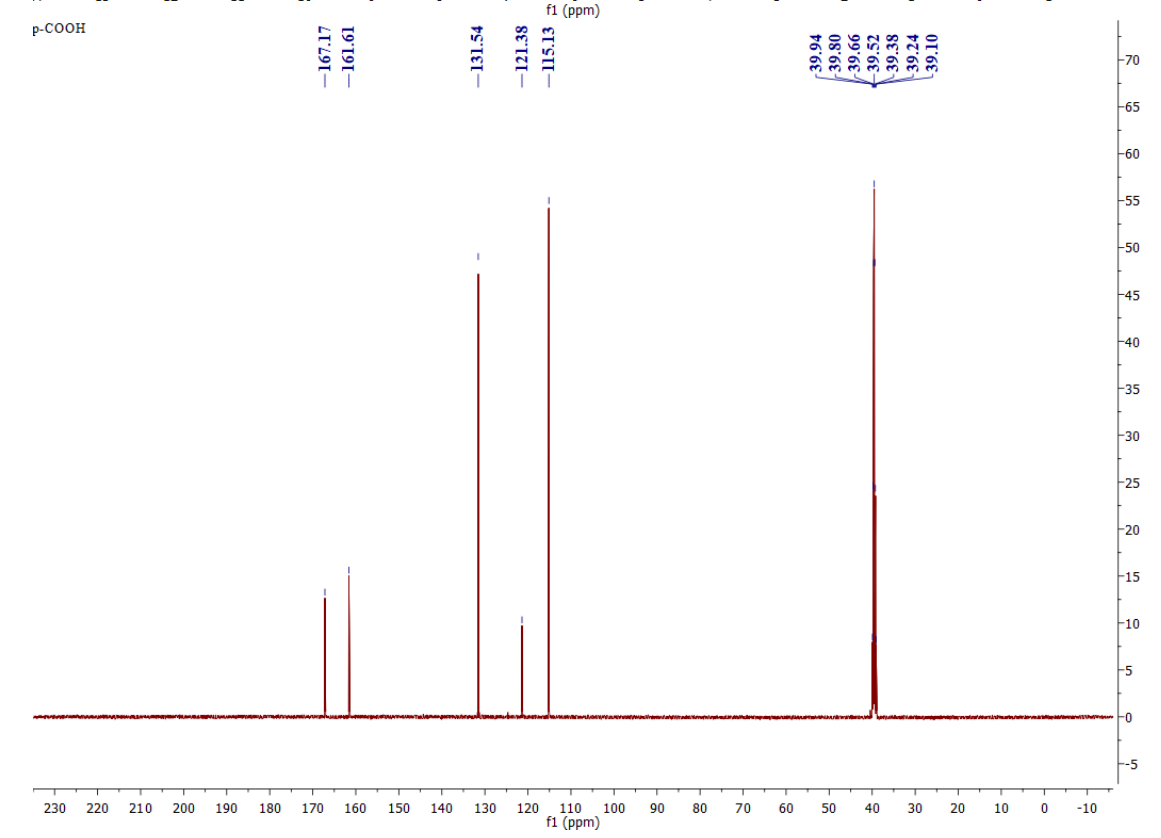

p-COOH
167.17
161.61
131.54
121.38
115.13
39.94
39.80
39.66
39.52
39.38
39.24
39.10
f1 (ppm)

Table S1 Comparison of the catalyst with typical Cu(I) salts

Entry	Catalyst	Ligand	Loading	Temperature	Condition	Reference
1	CuI	50 mol% 1,3-diketone	10 mol%	110-130°C	Under N_2	[S1]
2	CuI	20 mol% 1,10-phenanthroline	10 mol%	100 °C	Under N_2	[S2]
3	CuI	20 mol% lithium pipecolinate	10 mol%	130 °C	20 mol% $(n\text{-}Bu)_4NF$, in air	[S3]
4	CuI	40 mol% 8-hydroxyquinoline-N-oxide	10 mol%	110-130°C	Under Ar	[S4]
5	CuI	20 mol% 8-Hydroxyquinoline	20 mol%	100 °C	t-BuOH, under Ar	[S5]
6	Cu_2O	10 mol% pyridine-2-aldoxime	5 mol%	100-110°C	20 mol% $(n\text{-}Bu)_4NBr$, under N_2	[S6]
7	CuI	20 mol% 8-hydroxyquinalidine	10 mol%	100 °C	300 mol % $n\text{-}Bu_4NOH{\cdot}5H_2O$	[S7]
8	Cu-ZnO-ZrO_2	No	1.24 mol %	110°C	Under air	This work

References

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