Electronic Supplementary Material (ESI) for Green Chemistry.


# Supplementary Information

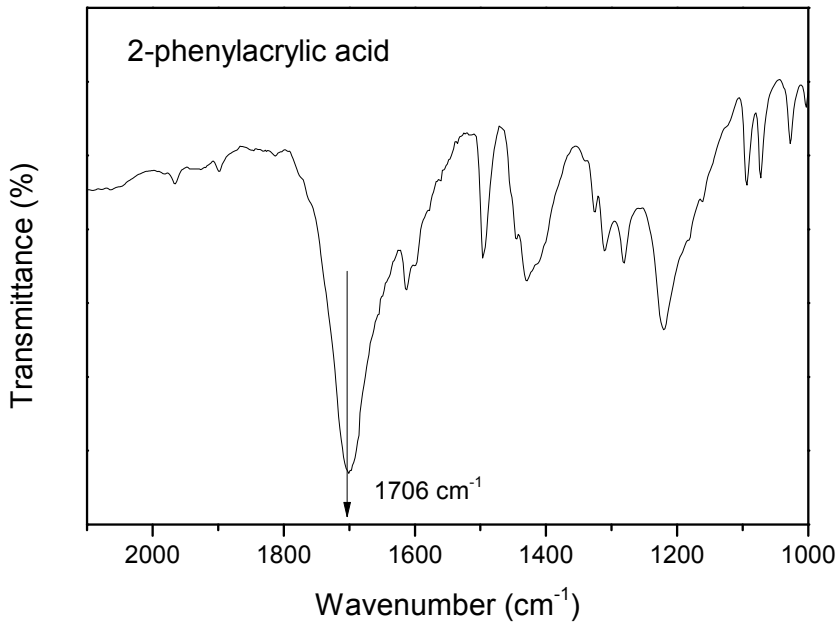
## 1. Characterization

### 1.1 FT-IR spectral characterization

### 1.2 $^{1}H/^{31}P$ NMR data for Pd-L1

### 1.3 $^{1}H/^{13}C$ NMR data for the products of hydroxycarbonyltion of phenylacetylene derivatives

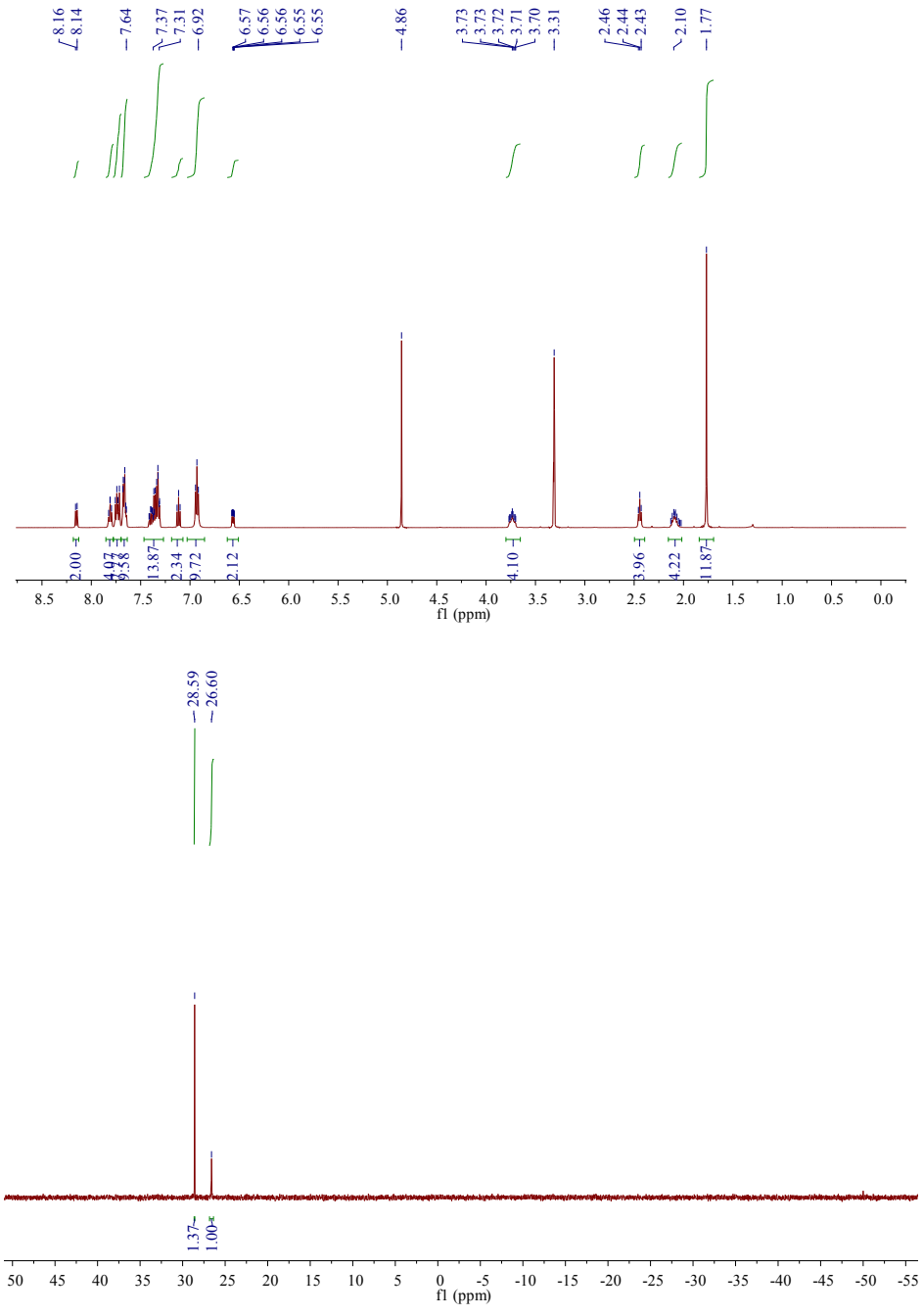
## 1.1 FT-IR spectral characterization




**S. Fig. 1** The FT-IR spectra of 2-phenylarylic acid recorded at room temperature in air atmosphere (KBr pellet)

## 1.2 $^{1}H/^{31}P$ NMR data for Pd-L1

**Pd-L1**: $^{1}H$ NMR (500 MHz, $CD_3OD$): $\delta$ = 8.15 (d, $J$ = 10 Hz, 2H, $2P^{+}Ph_2CCH$), 7.80-7.82 (m, 4H, phenyl), 7.72-7.76 (m, 8H, phenyl), 7.64-7.68 (m, 10H, phenyl), 7.31-7.40 (m, 14H, phenyl), 7.12 (t, $J$ = 10 Hz, 2H, phenyl), 6.93 (t, $J$ = 10 Hz, 10H, phenyl), 6.55-6.58 (m, 2H, phenyl), 3.70-3.77 (m, 4H, $2P^{+}CH_2$), 2.43-2.46 (m, 4H, $2CH_2SO_3^{-}$), 2.02-2.10 (m, 4H, $2CH_2CH_2CH_2$), 1.77 (s, 12H, $4CH_3$). $^{31}P$ NMR (202 MHz, $CD_3OD$): $\delta$ = 26.60 (s, $P^{+}Ph_2$), 28.59 (s, $PdPPh_2$).



## 1.3 $^{1}H/^{13}C$ NMR data and spectra for the products of alkoxycarbonylation of the phenylacetylene derivatives listed in Table 3

**2-phenylacrylic acid** (Entry 1)

$^{1}H$ NMR (400 M, $CDCl_3$): $\delta$ = 7.43-7.47 (m, 2H, $C_6H_5$), 7.35-7.41 (m, 3H, $C_6H_5$), 6.56 (s, 1H, $CCH_2$), 6.04 (s, 1H, $CCH_2$).

$^{13}C$ NMR (100 M, $CDCl_3$): $\delta$ = 172.22, 140.78, 136.25, 129.55, 128.59, 128.50, 128.28.

**2-(*p*-tolyl)acrylic acid** (Entry 2)

$^{1}H$ NMR (400 M, $CDCl_3$): $\delta$ = 7.32-7.34 (m, 2H, $C_6H_4$), 7.17-7.18 (m, 2H, $C_6H_4$), 6.48 (s, 1H, $CCH_2$), 5.98 (s, 1H, $CCH_2$), 2.36 (s, 3H, $CH_3$).

$^{13}C$ NMR (100 M, $CDCl_3$): $\delta$ = 171.74, 140.60, 138.43, 133.43, 129.52, 129.01, 128.65, 128.46, 126.99, 21.34.

**2-(*m*-tolyl)acrylic acid** (Entry 3)

$^{1}H$ NMR (400 M, $CDCl_3$): $\delta$ = 7.24-7.33 (m, 3H, $C_6H_4$), 7.17-7.19 (m, 1H, $C_6H_4$), 6.53 (s, 1H, $CCH_2$), 6.01 (s, 1H, $CCH_2$), 2.39 (s, 3H, $CH_3$).

**(*E*)-3-(*m*-tolyl)acrylic acid** (Entry 3)

$^{1}H$ NMR (400 M, $CDCl_3$): $\delta$ = 7.78 (d, $J$ = 16.0 Hz, 1H, PhC*H*), 6.45 (d, $J$ = 16.0 Hz, 1H, C*H*COOH).

**2-(*o*-tolyl)acrylic acid** (Entry 4)

$^{1}H$ NMR (400 M, $CDCl_3$): $\delta$ = 7.13-7.25 (m, 4H, $C_6H_4$), 6.64 (s, 1H, $CCH_2$), 5.84 (s, 1H, $CCH_2$), 2.24 (s, 3H, $CH_3$).

$^{13}C$ NMR (100 M, $CDCl_3$): $\delta$ = 171.97, 141.31, 136.63, 136.34, 130.95, 130.07, 129.68, 128.52, 125.82, 20.00.

**2-(4-(*tert*-butyl)phenyl)acrylic acid** (Entry 5)

$^{1}H$ NMR (400 M, $CDCl_3$): $\delta$ = 7.36-7.42 (m, 4H, $C_6H_4$), 6.51 (s, 1H, $CCH_2$), 6.02 (s, 1H, $CCH_2$), 1.34 (s, 9H, $C(CH_3)_3$).

$^{13}C$ NMR (100 M, $CDCl_3$): $\delta$ = 172.21, 151.58, 140.53, 133.33, 128.83, 128.42, 128.26, 126.10, 125.27, 34.76, 31.43, 31.29, 31.24.

**2-(4-methoxyphenyl)acrylic acid** (Entry 6)

$^{1}H$ NMR (400 M, $CDCl_3$): $\delta$ = 7.39-7.41 (m, 2H, $C_6H_4$), 6.90-6.92 (m, 2H, $C_6H_4$), 6.46 (s, 1H, $CCH_2$), 5.96 (s, 1H, $CCH_2$), 3.83 (s, 3H, $OCH_3$).

**(*E*)-3-(4-methoxyphenyl)acrylic acid** (Entry 6)

$^{1}$H NMR (400 M, $CDCl_3$): $\delta$ = 7.76 (d, $J$ = 16.0 Hz, 1H, PhC*H*), 6.33 (d, $J$ = 16.0 Hz, 1H, C*H*COOH).

**2-(4-fluorophenyl)acrylic acid** (Entry 7)

$^{1}$H NMR (400 M, $CDCl_3$): $\delta$ = 7.40-7.44 (m, 2H, $C_6H_4$), 7.03-7.07 (m, 2H, $C_6H_4$), 6.54 (s, 1H, $CCH_2$), 6.00 (s, 1H, $CCH_2$).

$^{13}$C NMR (100 M, $CDCl_3$): $\delta$ = 172.06, 164.20, 161.74, 139.72, 130.46, 130.38, 129.66, 115.36, 115.14.

**2-(4-chlorophenyl)acrylic acid** (Entry 8)

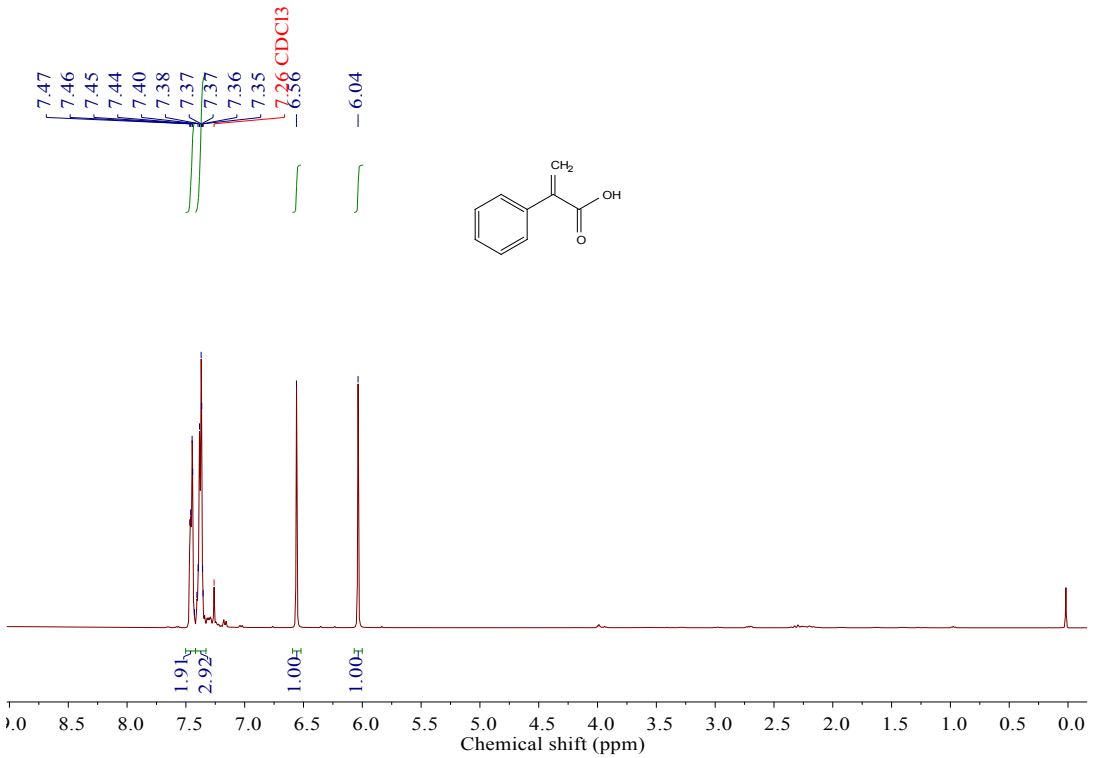
$^{1}$H NMR (400 M, $CDCl_3$): $\delta$ = 7.33-7.39 (m, 4H, $C_6H_4$), 6.56 (s, 1H, $CCH_2$), 6.03 (s, 1H, $CCH_2$).

$^{13}$C NMR (100 M, $CDCl_3$): $\delta$ = 171.50, 139.66, 134.63, 129.98, 129.95, 129.68, 129.44, 128.51, 117.82.

**2-(4-bromophenyl)acrylic acid** (Entry 9)

$^{1}$H NMR (400 M, $CDCl_3$): $\delta$ = 7.49-7.51 (m, 2H, $C_6H_4$), 7.31-7.33 (m, 2H, $C_6H_4$), 6.57 (s, 1H, $CCH_2$), 6.04 (s, 1H, $CCH_2$).

$^{13}$C NMR (100 M, $CDCl_3$): $\delta$ = 171.60, 139.71, 135.08, 131.47, 130.25, 130.08, 122.84.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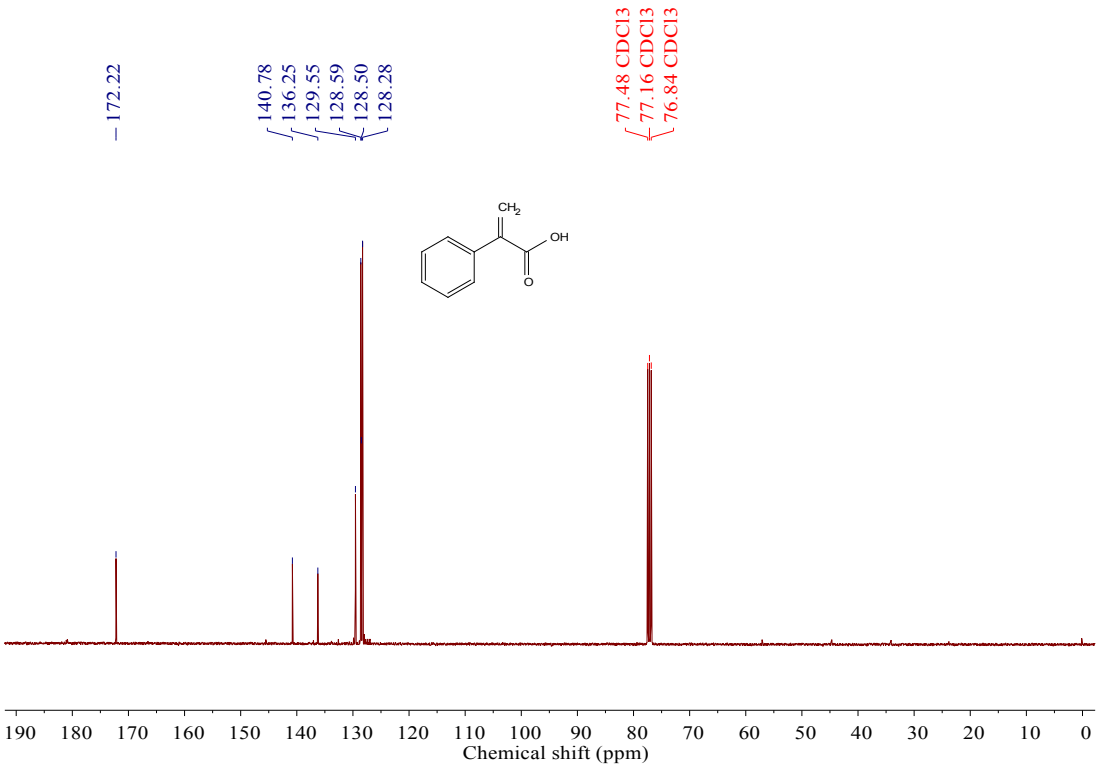
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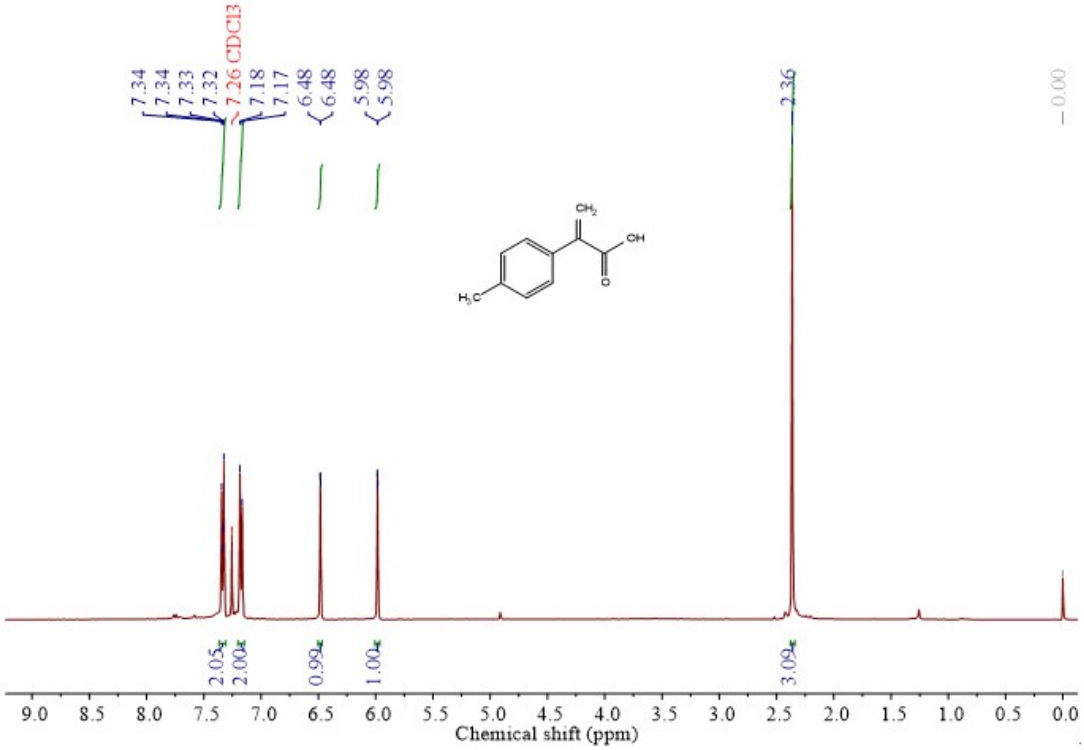
128.28
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
CH2
OH
O
Chemical shift (ppm)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6.48
5.98
5.98
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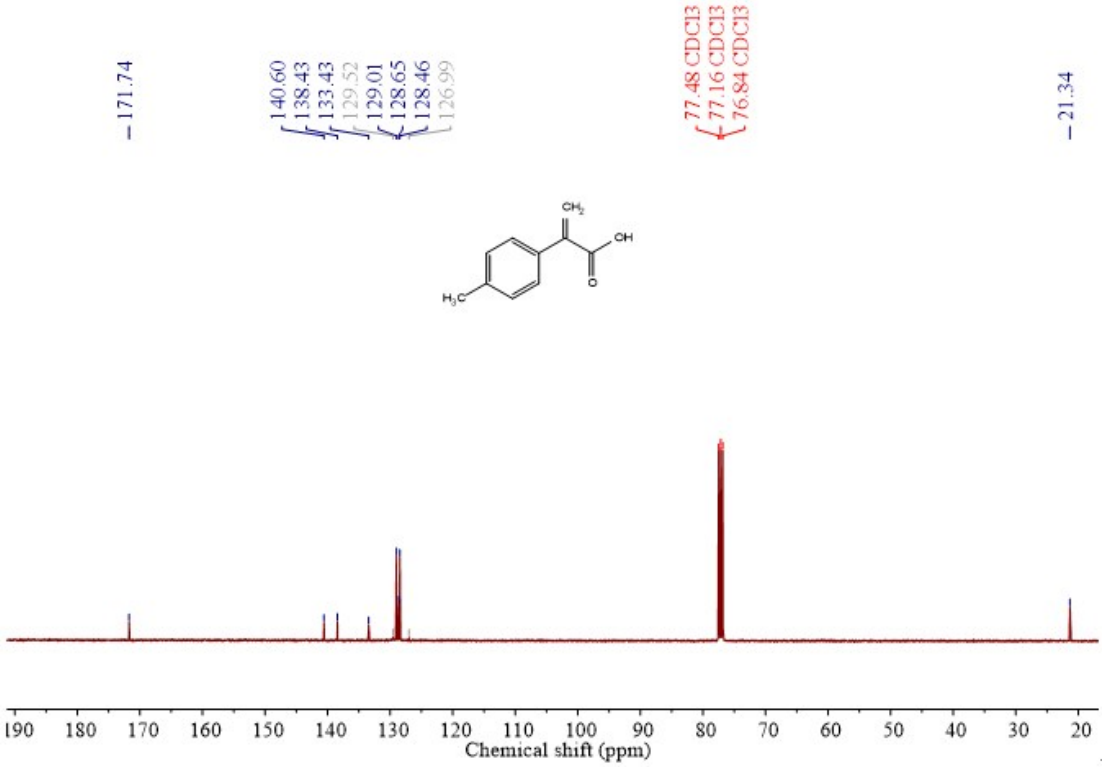
2.05
2.00
0.99
1.00
3.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical shift (ppm)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133.43
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128.65
128.46
126.99
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
21.34
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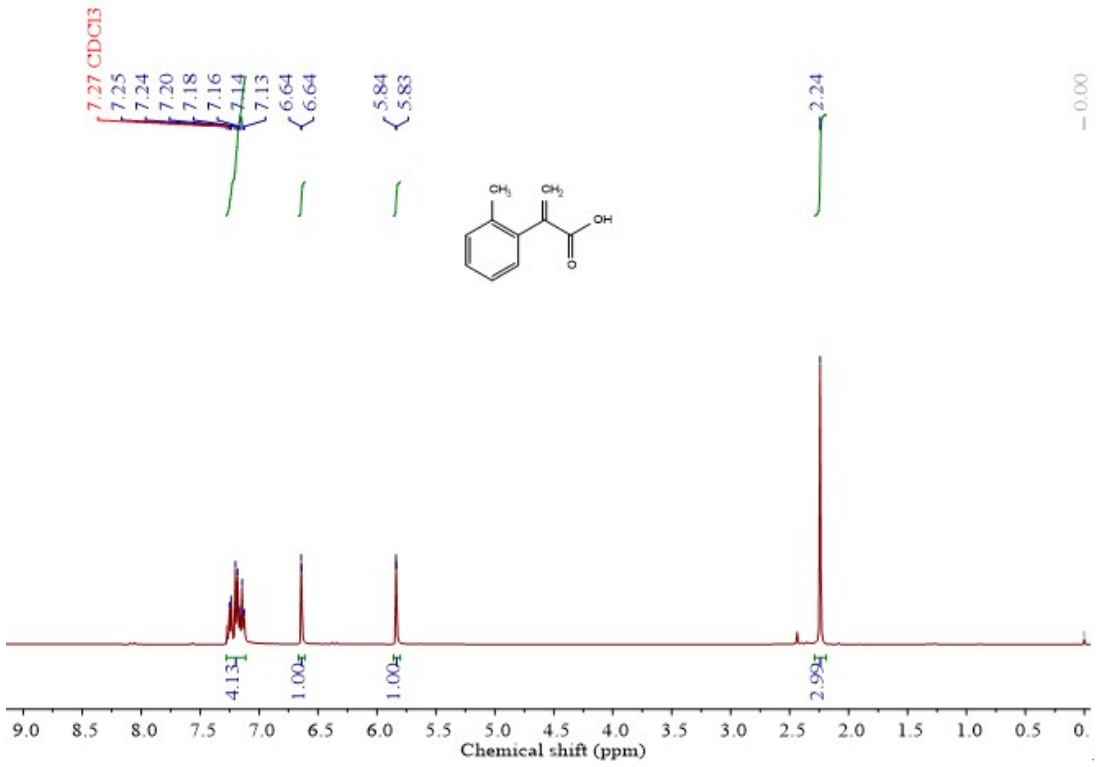
Chemical shift (ppm)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6.64
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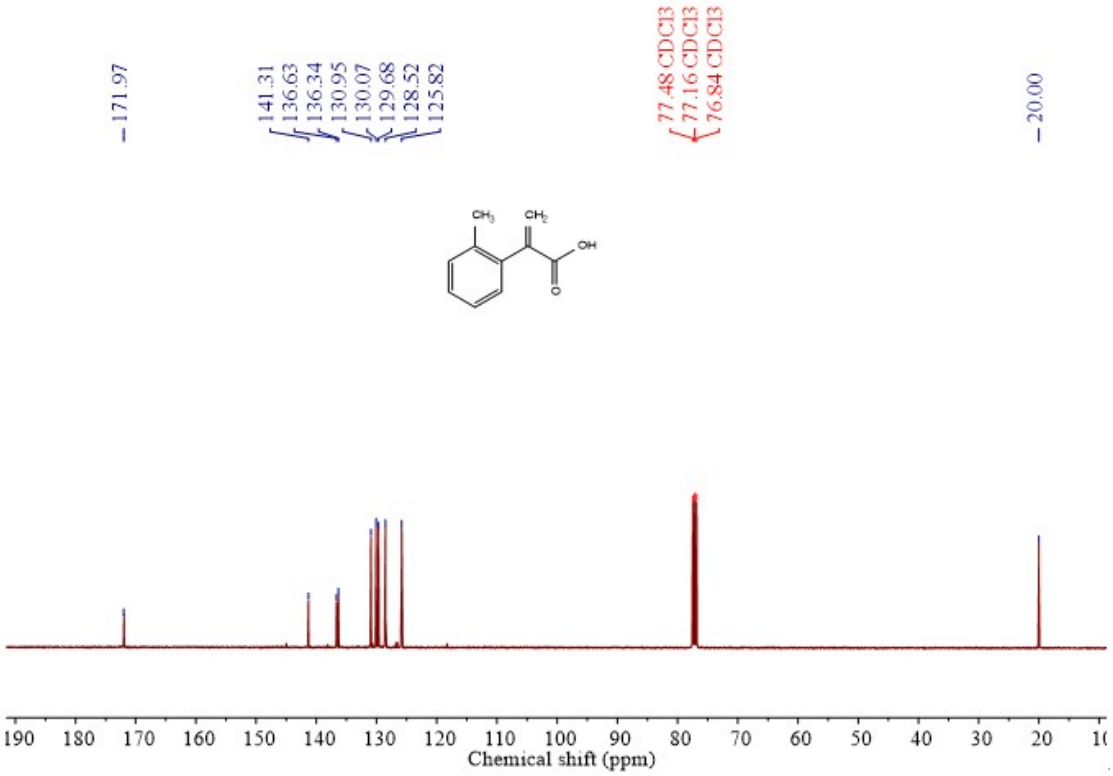
5.83
2.24
0.00
CH3
CH2
OH
O
4.13
1.00
1.00
2.99
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
Chemical shift (ppm)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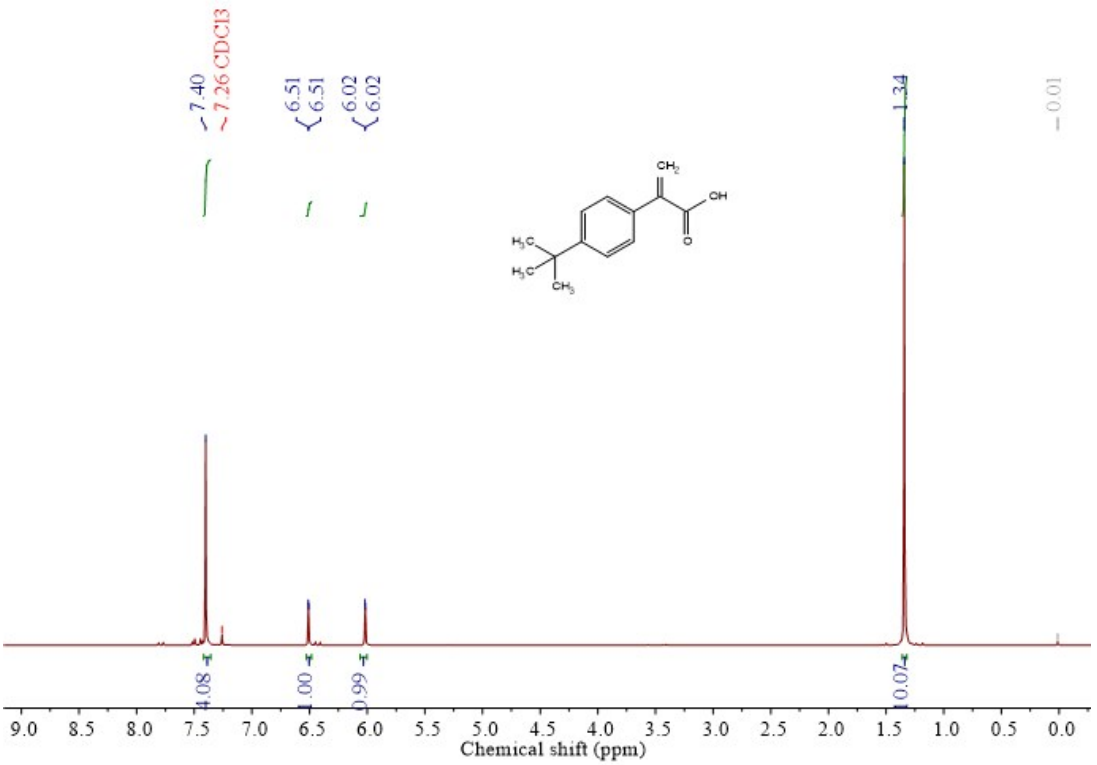
129.68
128.52
125.82
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
20.00
CH3
CH2
OH
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
Chemical shift (ppm)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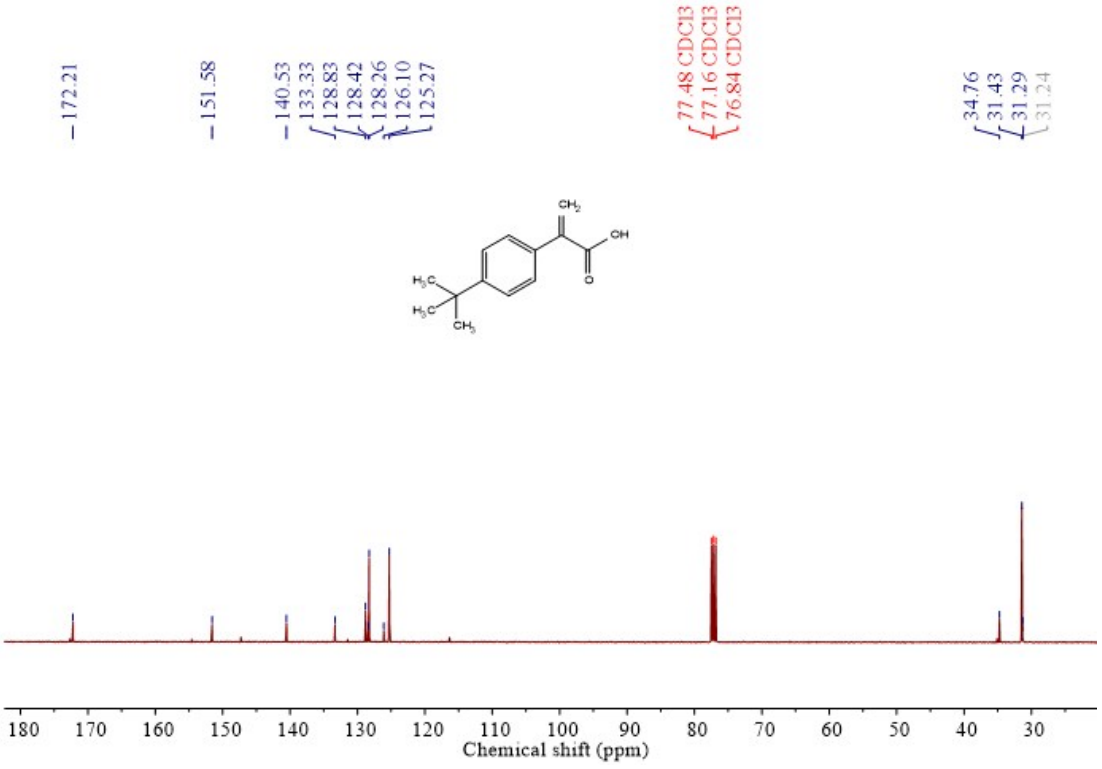
Chemical shift (ppm)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128.26
126.10
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77.16 CDCl3
76.84 CDCl3
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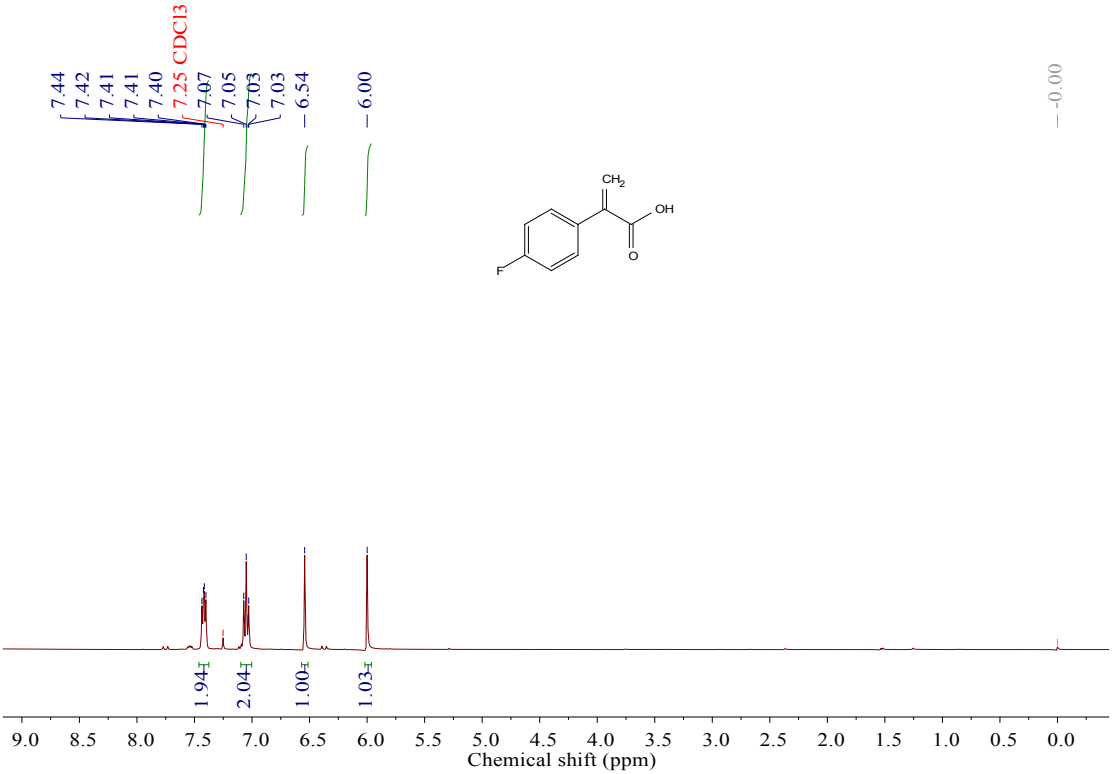
31.43
31.29
31.24
Chemical shift (ppm)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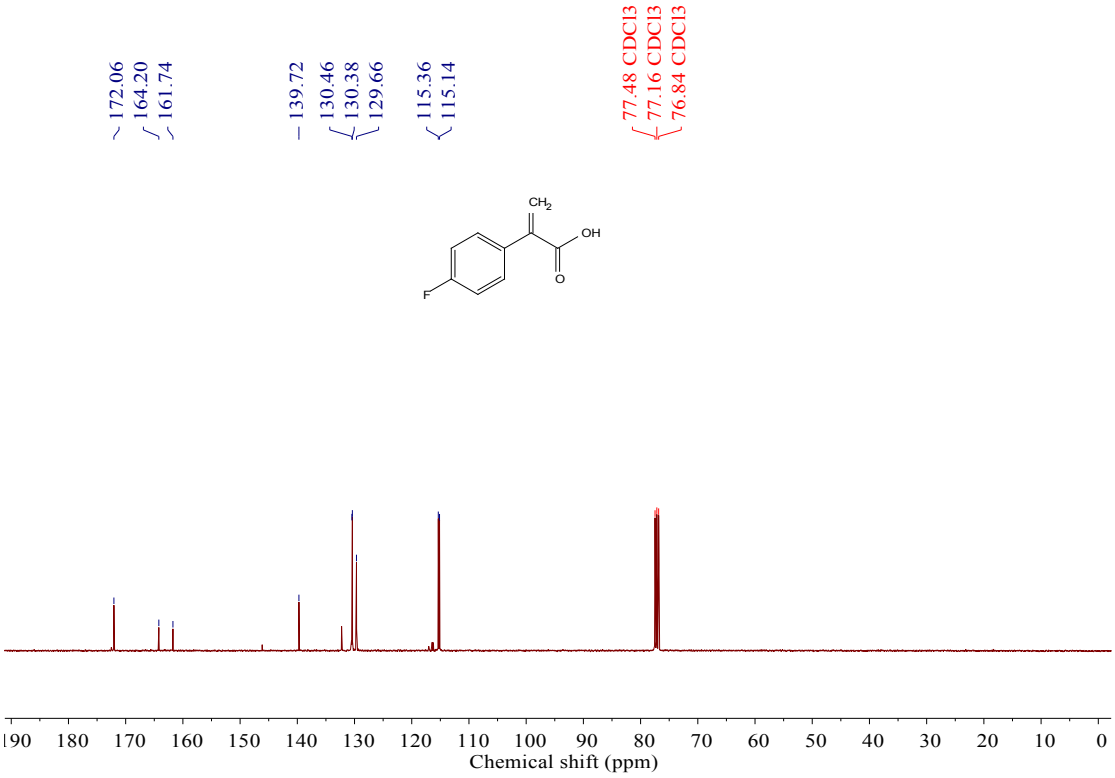
7.03
7.03
6.54
6.00
-0.00
CH2
OH
O
F
1.94
2.04
1.00
1.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical shift (ppm)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139.72
130.46
130.38
129.66
115.36
115.14
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
CH2
OH
O
F
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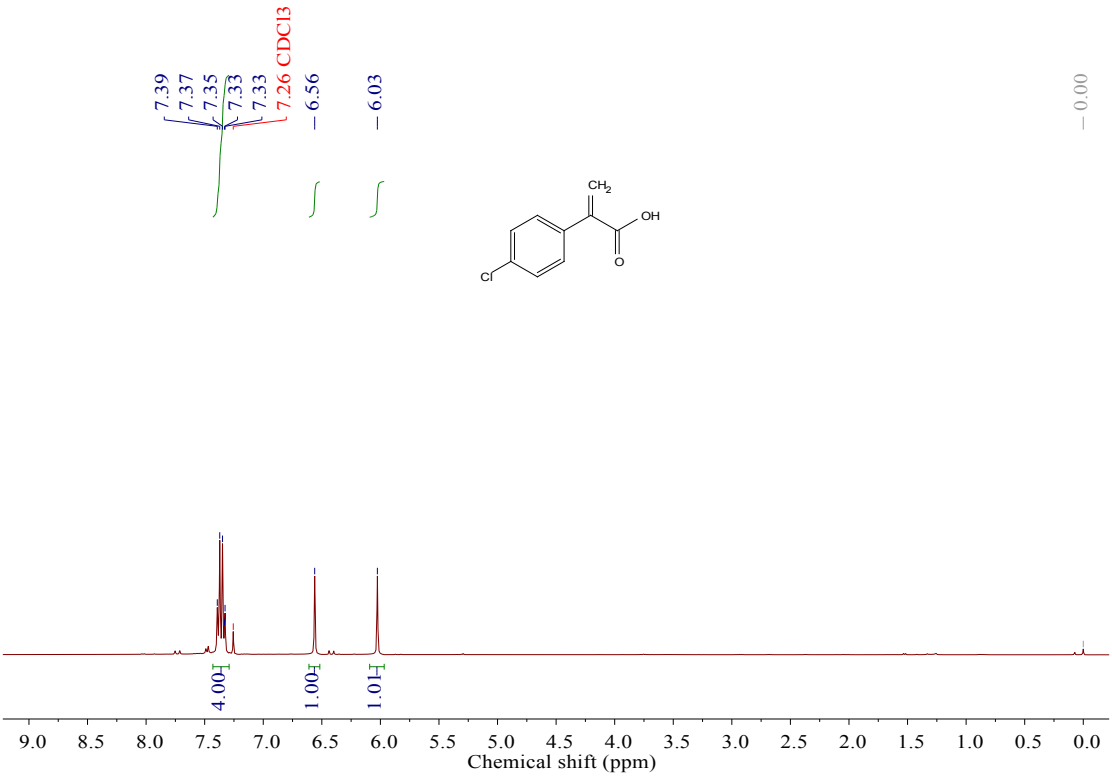
Chemical shift (ppm)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7.33
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OH
O
Cl
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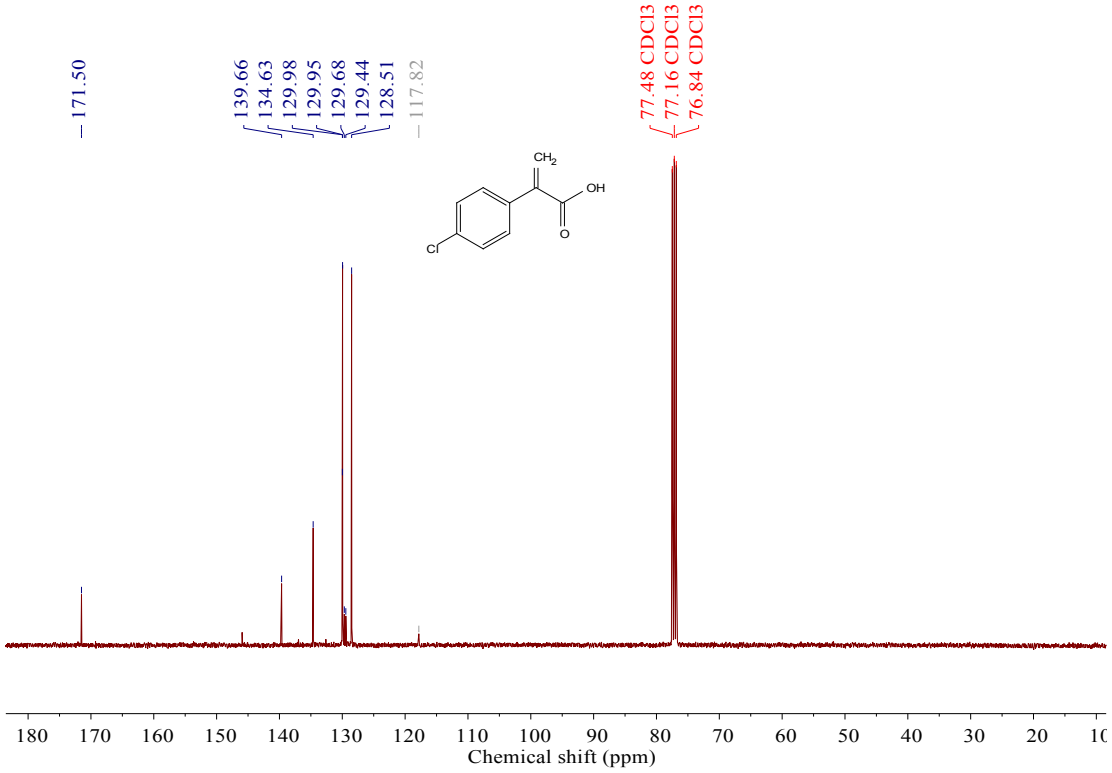
1.00
1.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical shift (ppm)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OH
O
Cl
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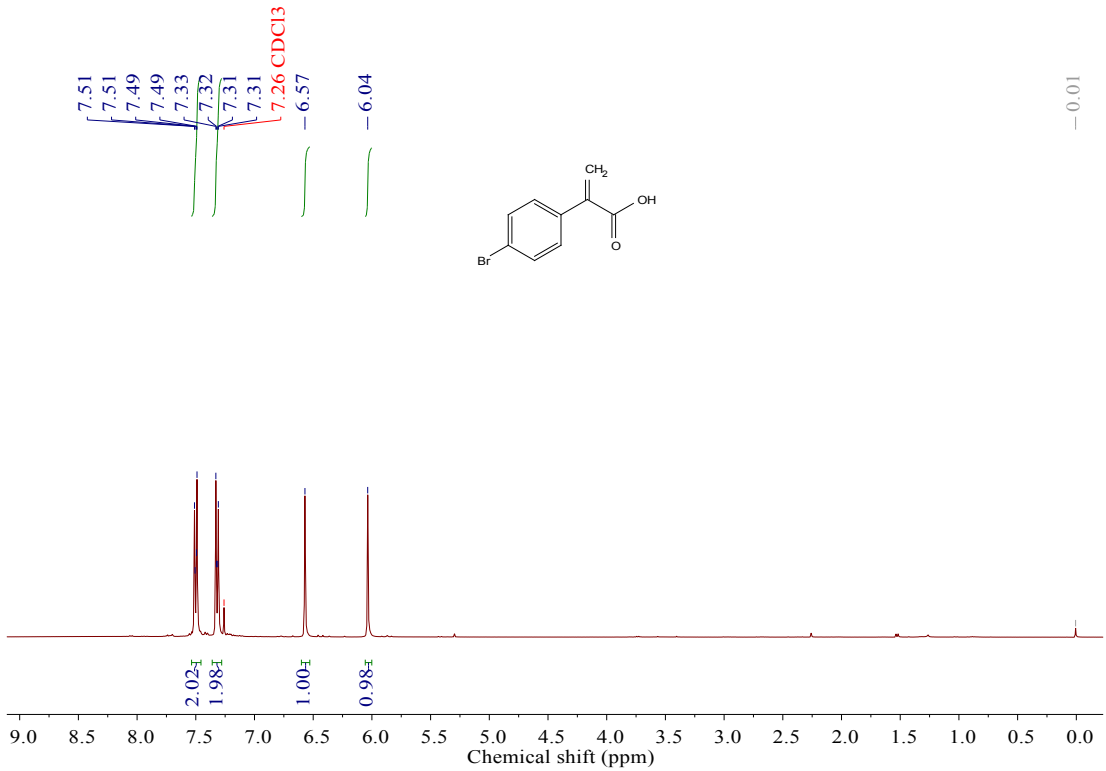
Chemical shift (ppm)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7.31
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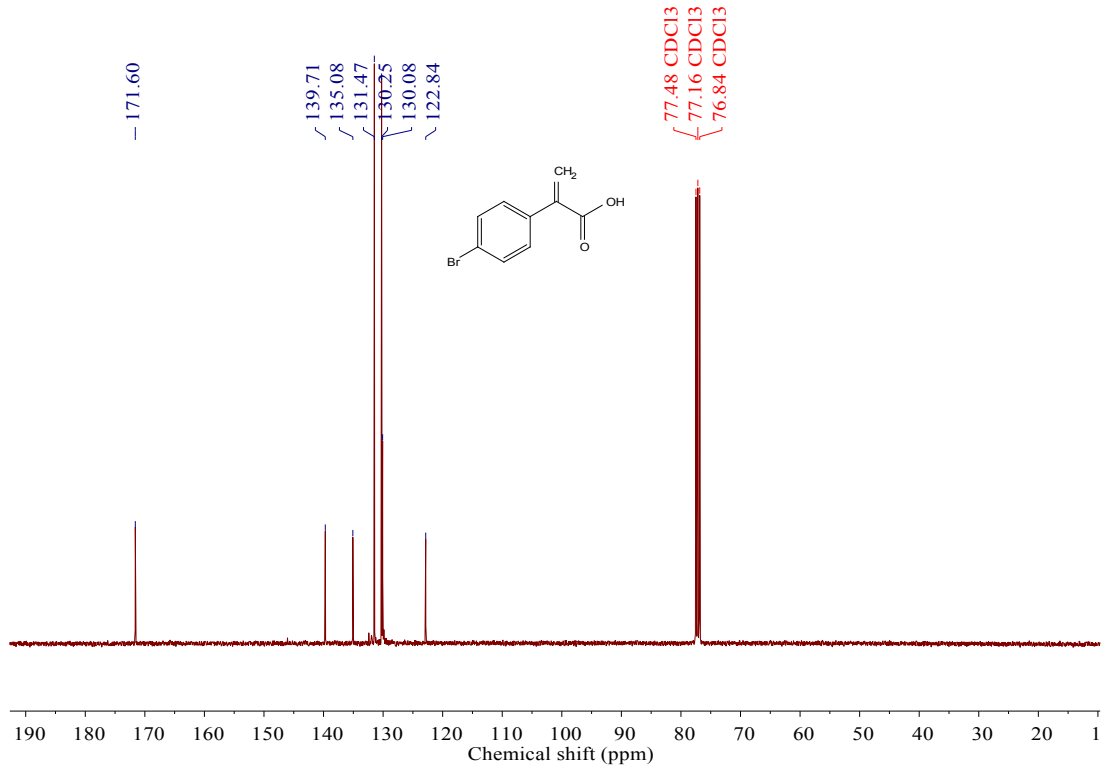
6.57
6.04
0.01
CH2
OH
O
Br
2.02
1.98
1.00
0.98
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical shift (ppm)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OH
O
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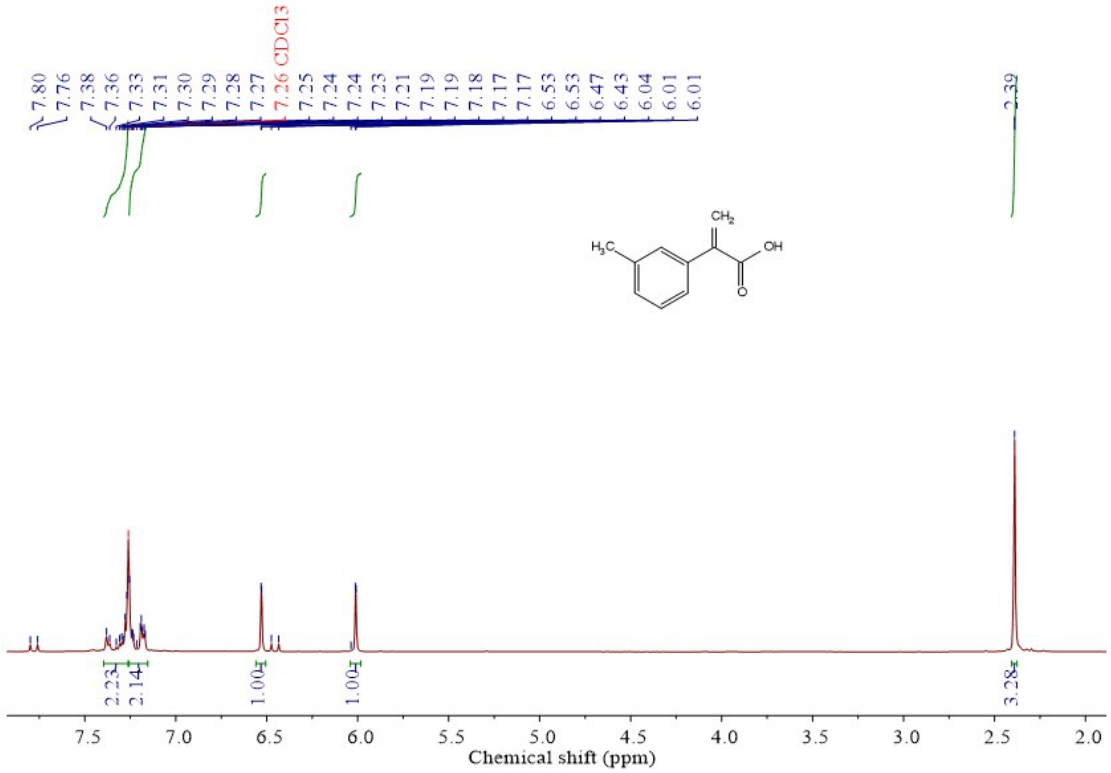
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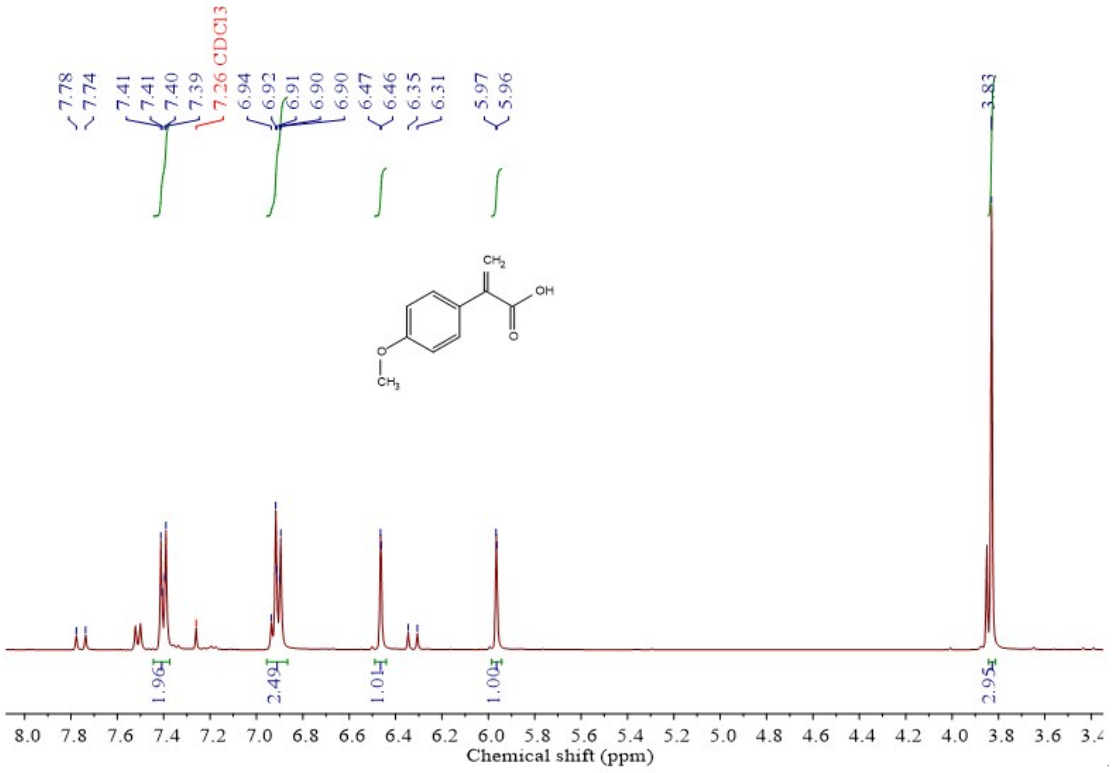
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6.47
6.46
6.35
6.31
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7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
Chemical shift (ppm)