Supporting Information

Dirhodium Catalyzed Phenol and Aniline Oxidations with T-HYDRO. Substrate Scope and Mechanism of Oxidation

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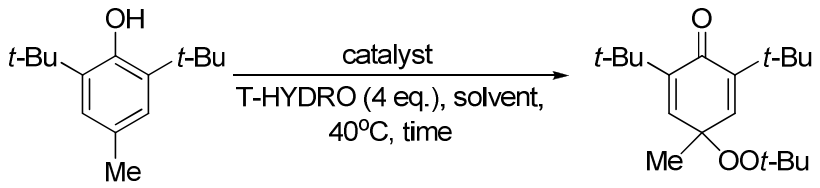
Kinetic Data of Transition Metal Catalyzed 2,6-di-*tert*-Butyl-4-methylphenol Oxidation with T-HYDRO



1 **2**

Table 1. Percent Conversions for Transition Metal Catalyzed Oxidations of 2,6-di-*tert*-Butyl-4-methylphenol (**1**) by T-HYDRO.

catalyst	loading, mol %	solvent	equiv. of T-HYDRO	time, h						
				0	0.1	0.5	1	3	24	48
$Rh_2(cap)_4$	0.1	DCE	4	0	-	-	38.6	49.7	78.6	99
$Rh_2(cap)_4$	0.05	PhCl	4	0	100	-	-	-	-	-
$Rh_2(cap)_4$	0.01	PhCl	4	0	-	-	31.6	49.7	78.6	99
$Rh_2(cap)_4$	0.03	PhCl	4	0	-	89.7	96.6	100	-	-
$Rh_2(cap)_4$	0.03	PhCl	2	0	-	63.1	69	77.1	91.9	-
CuI	1.0	DCE	4	0	-	-	14.9	28.8	100	-
CuI	1.0	PhCl	4	0	-	-	27.8	61.4	100	-
CuI	0.1	DCE	4	0	-	-	8.3	19	79.5	100
CuI	0.1	PhCl	4	0	-	-	17.7	35.1	100	-
CuI	0.05	PhCl	4	0	-	-	0.7	6.3	26.5	34.8
CuBr	0.1	PhCl	4	0	-	-	0.1	8	79.6	-
CuCl	0.1	PhCl	4	0	-	-	0.1	1.7	78.9	-
$RuCl_2(PPh_3)_3$	0.1	DCE	4	0	-	79.4	100	-	-	-
$RuCl_2(PPh_3)_3$	0.1	PhCl	4	0	-	-	100	-	-	-
$RuCl_2(PPh_3)_3$	0.05	PhCl	4	0	-	44.5	78.9	100	-	-

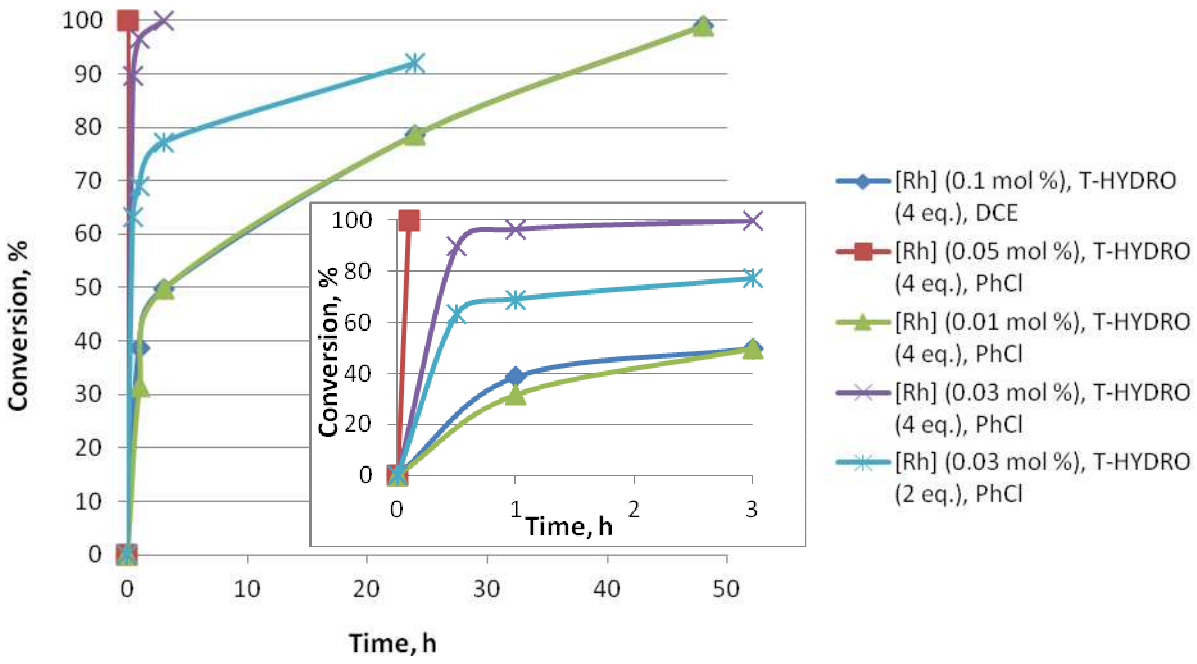


Figure 1. Comparative Time Courses for $Rh_2(cap)_4$ Catalyzed Oxidations of **1** by T-HYDRO at 40°C.

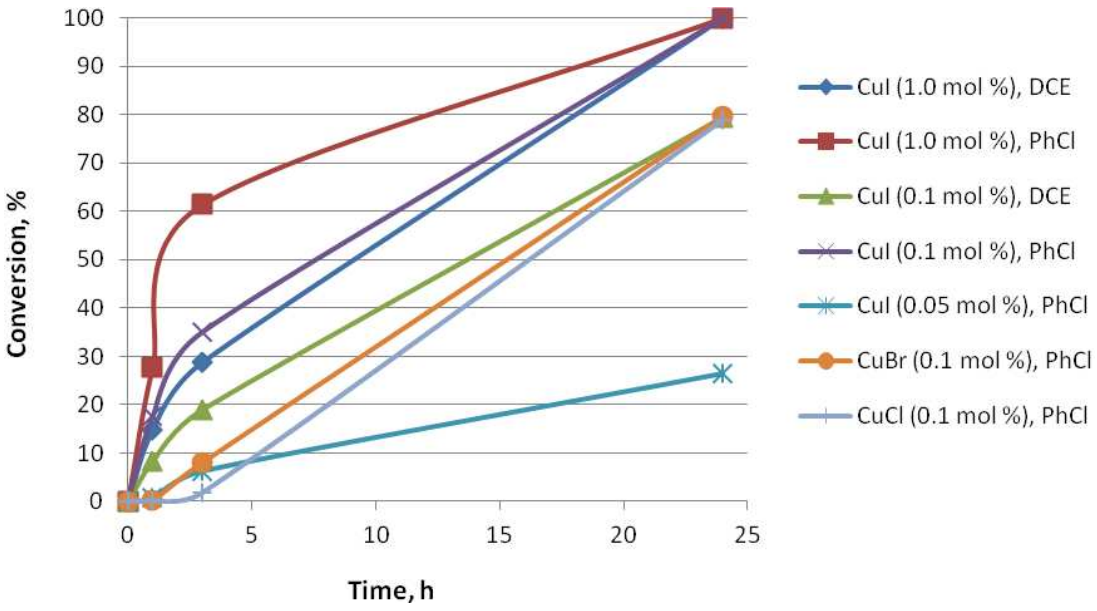


Figure 2. Comparative Time Courses for Copper(I) Halide Catalyzed Oxidation of **1** by 4.0 Equiv. of T-HYDRO at 40°C.

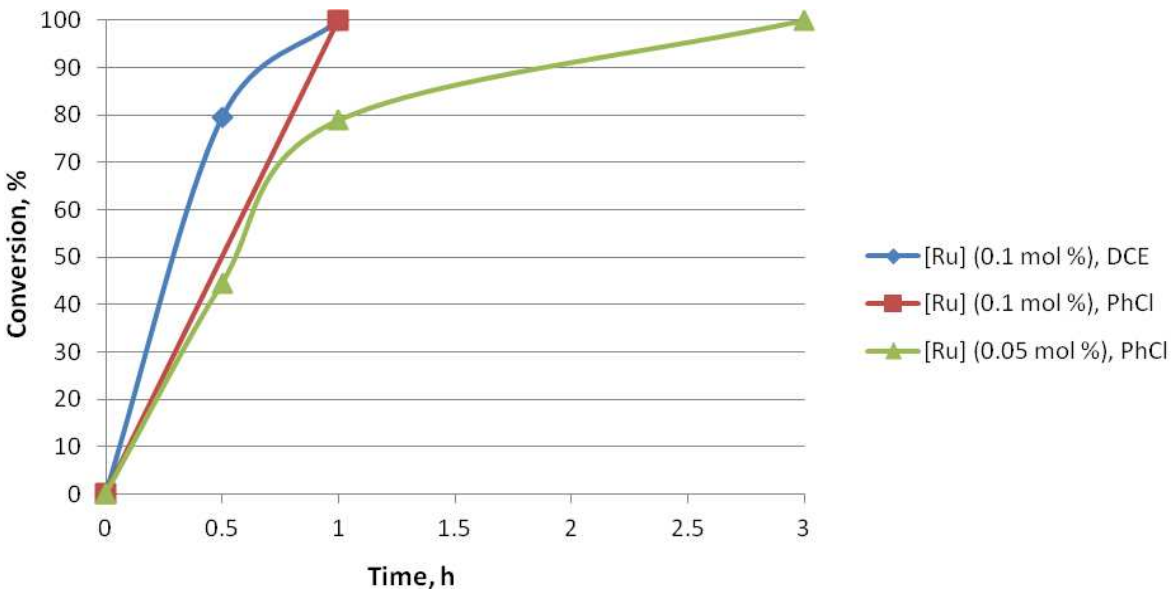
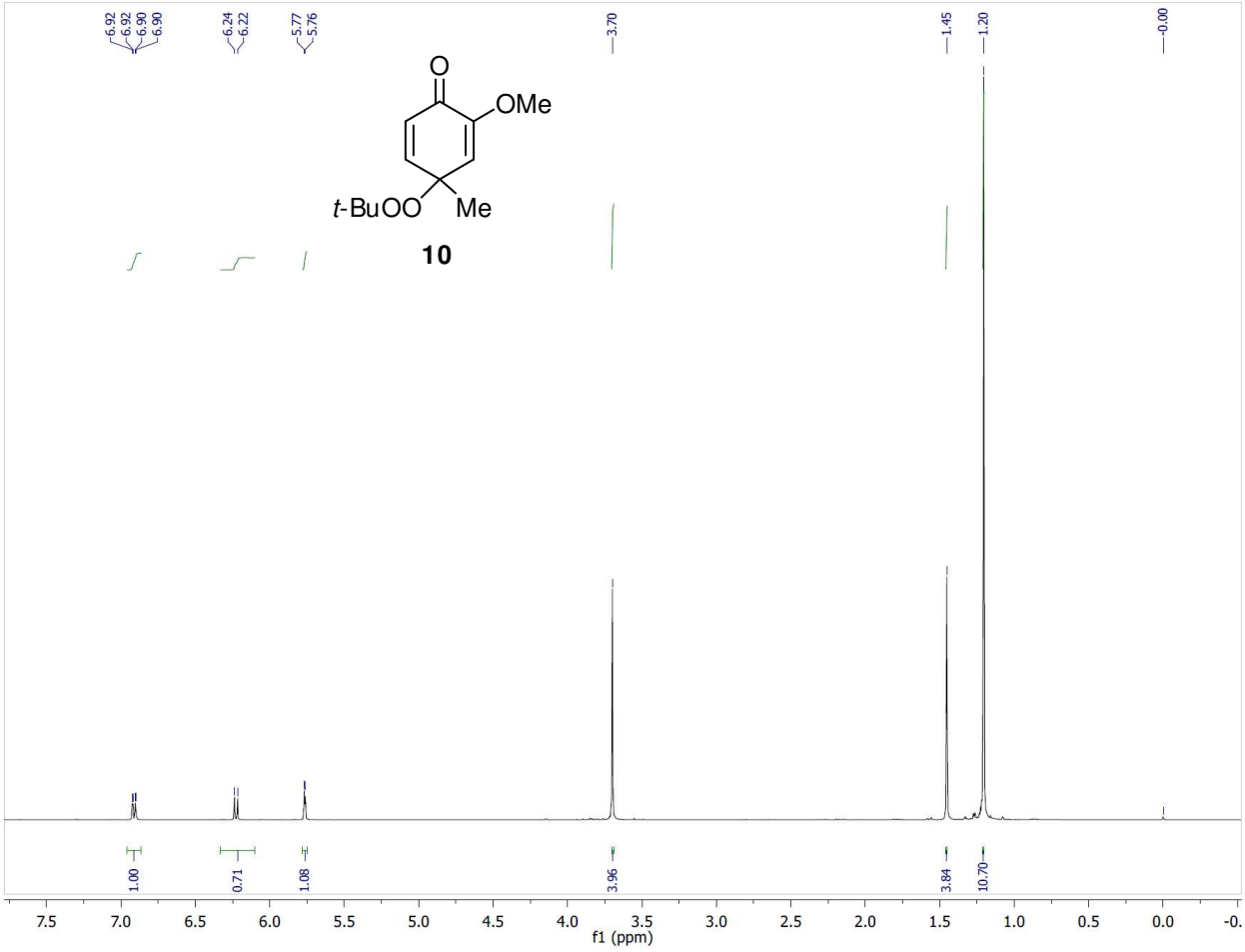
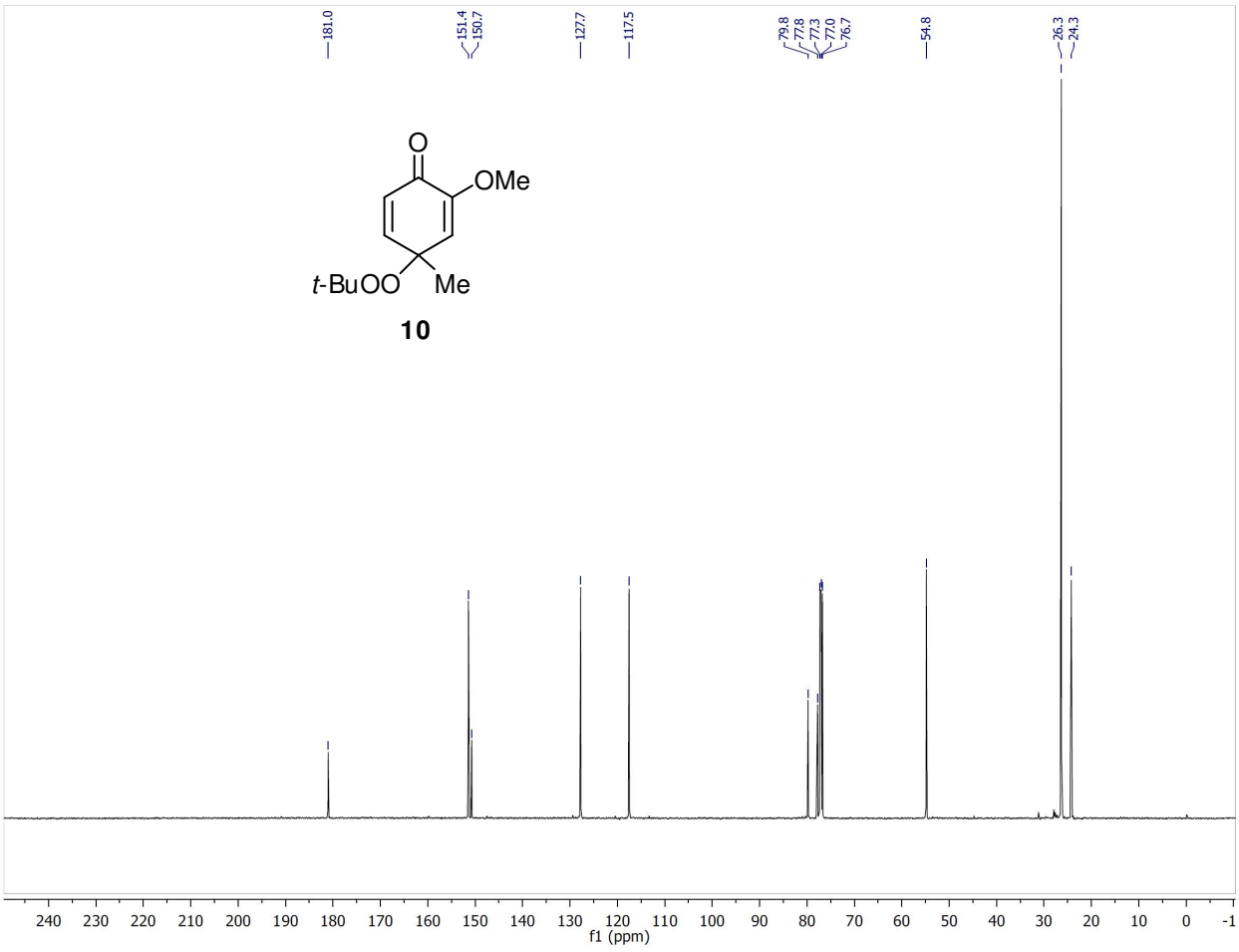
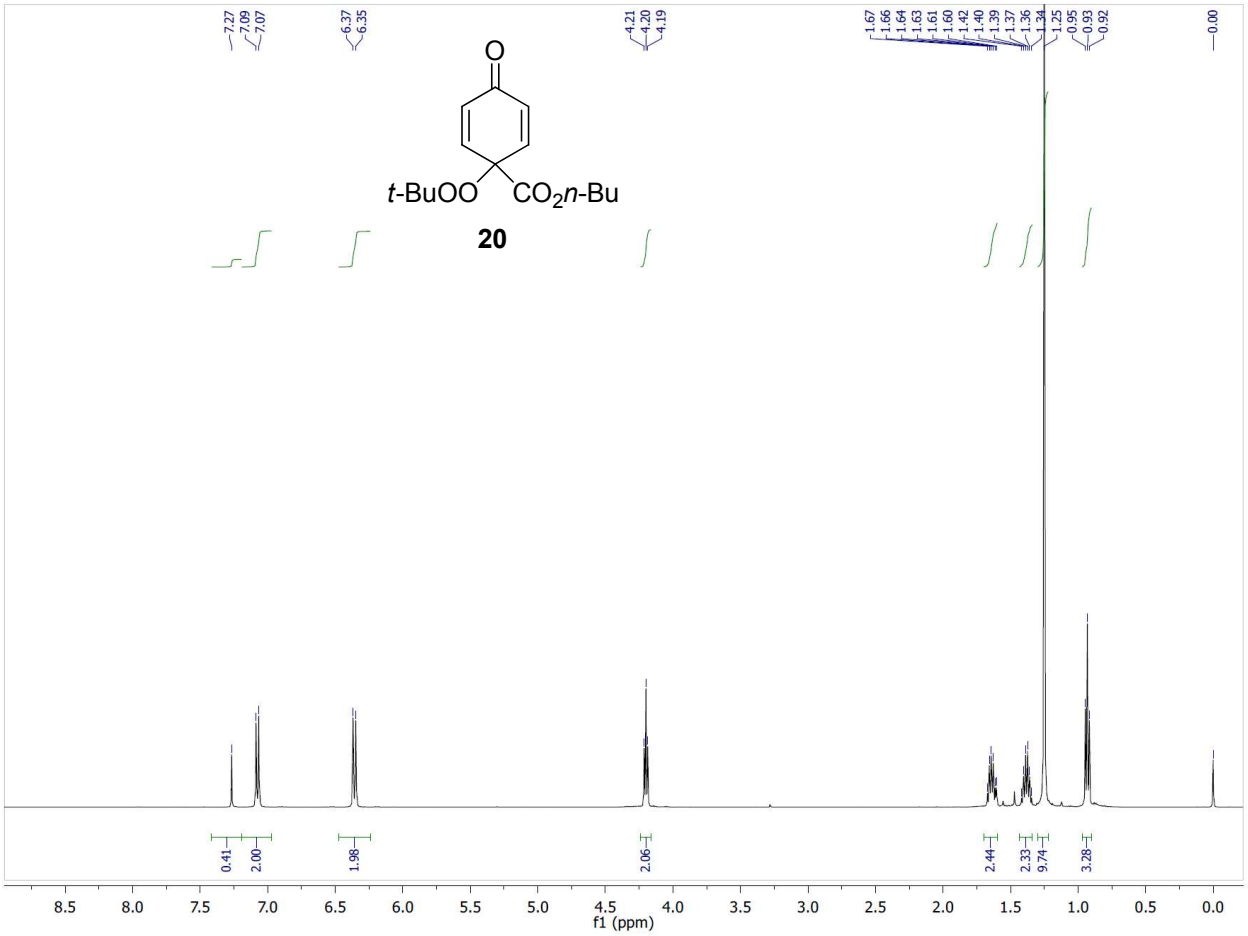


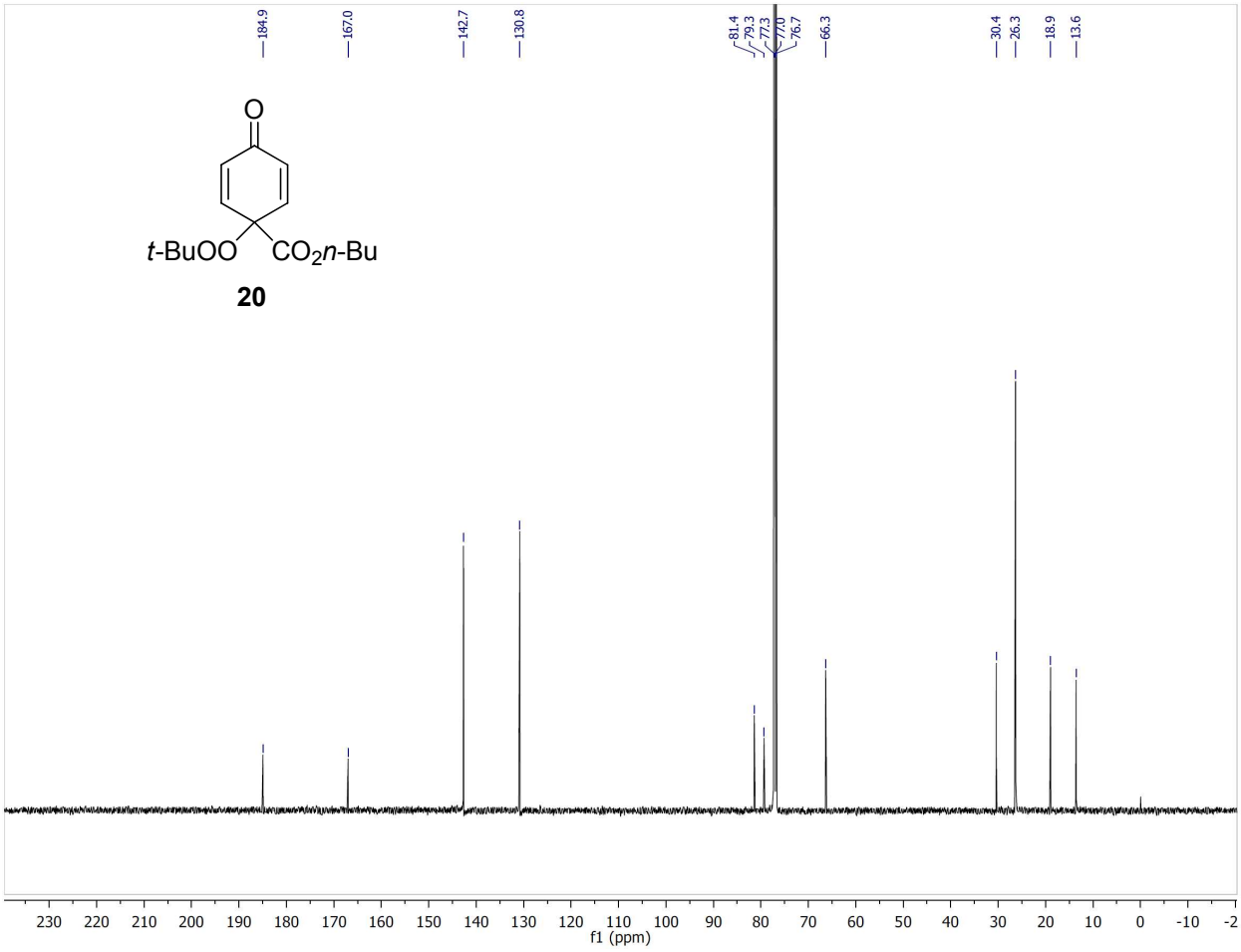
Figure 3. Comparative Time Courses for $RuCl_2(PPh_3)_3$ Catalyzed Oxidation of **1** by 4.0 Equiv. of T-HYDRO at 40°C.

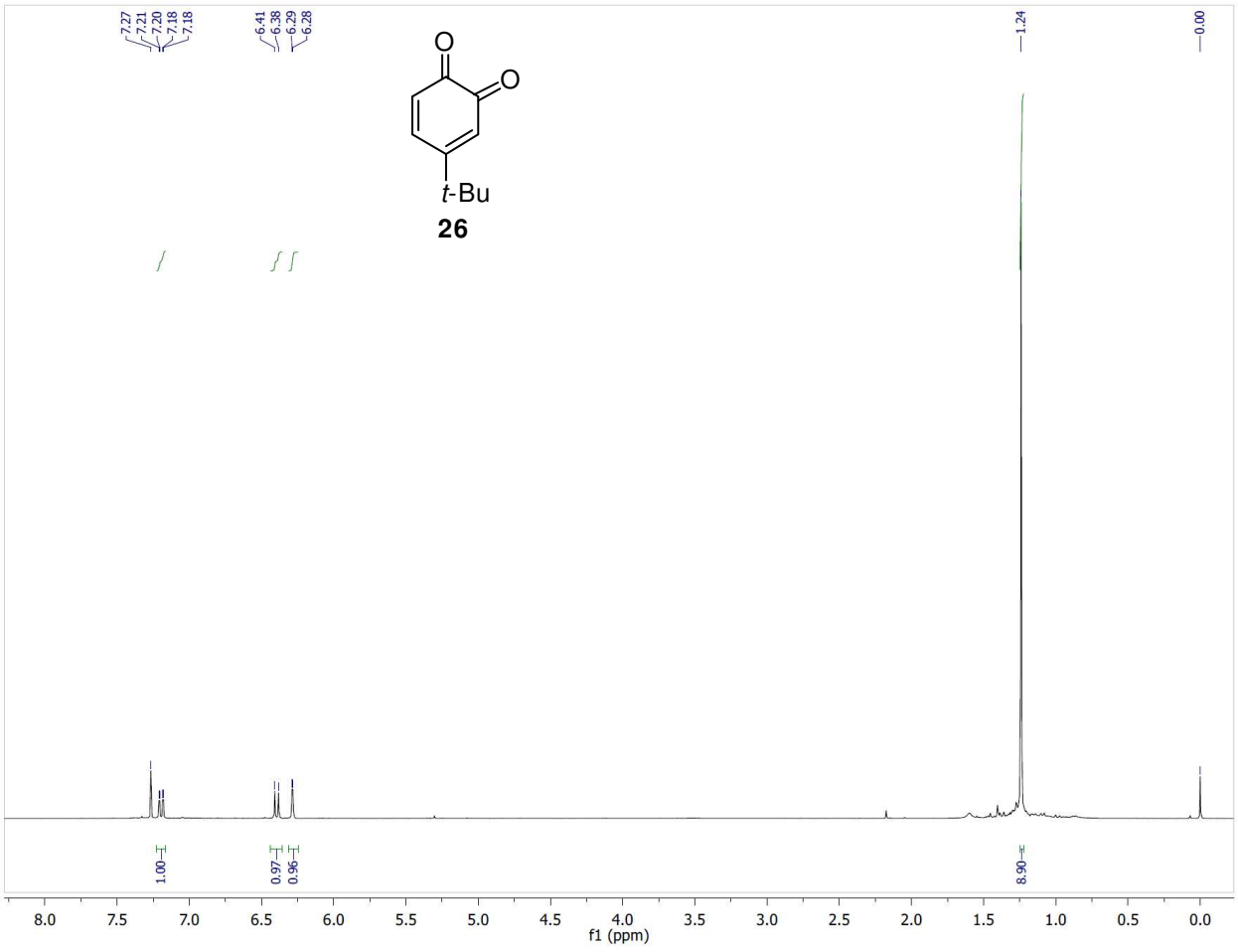
^{1}H and ^{13}C Spectra of New Compounds

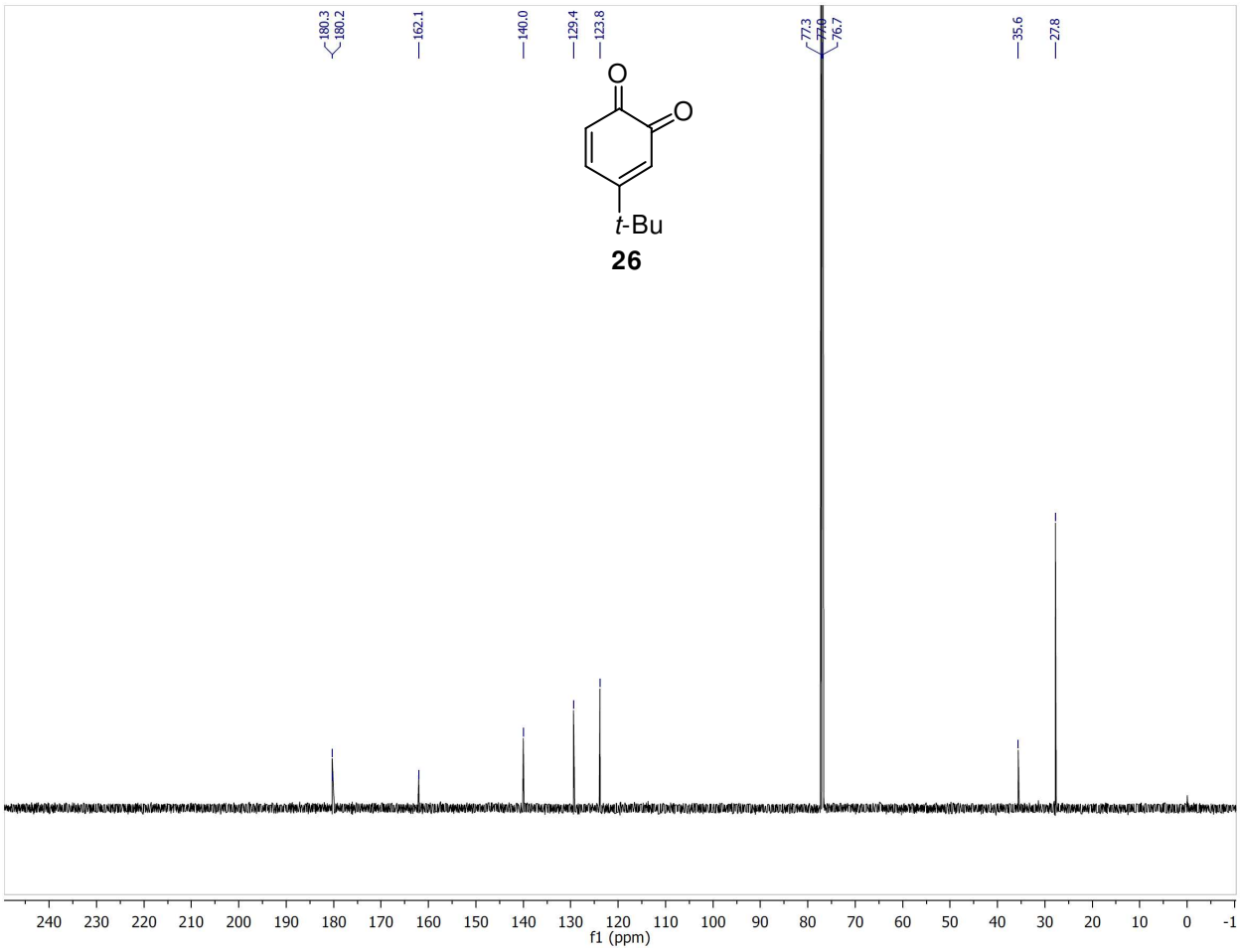


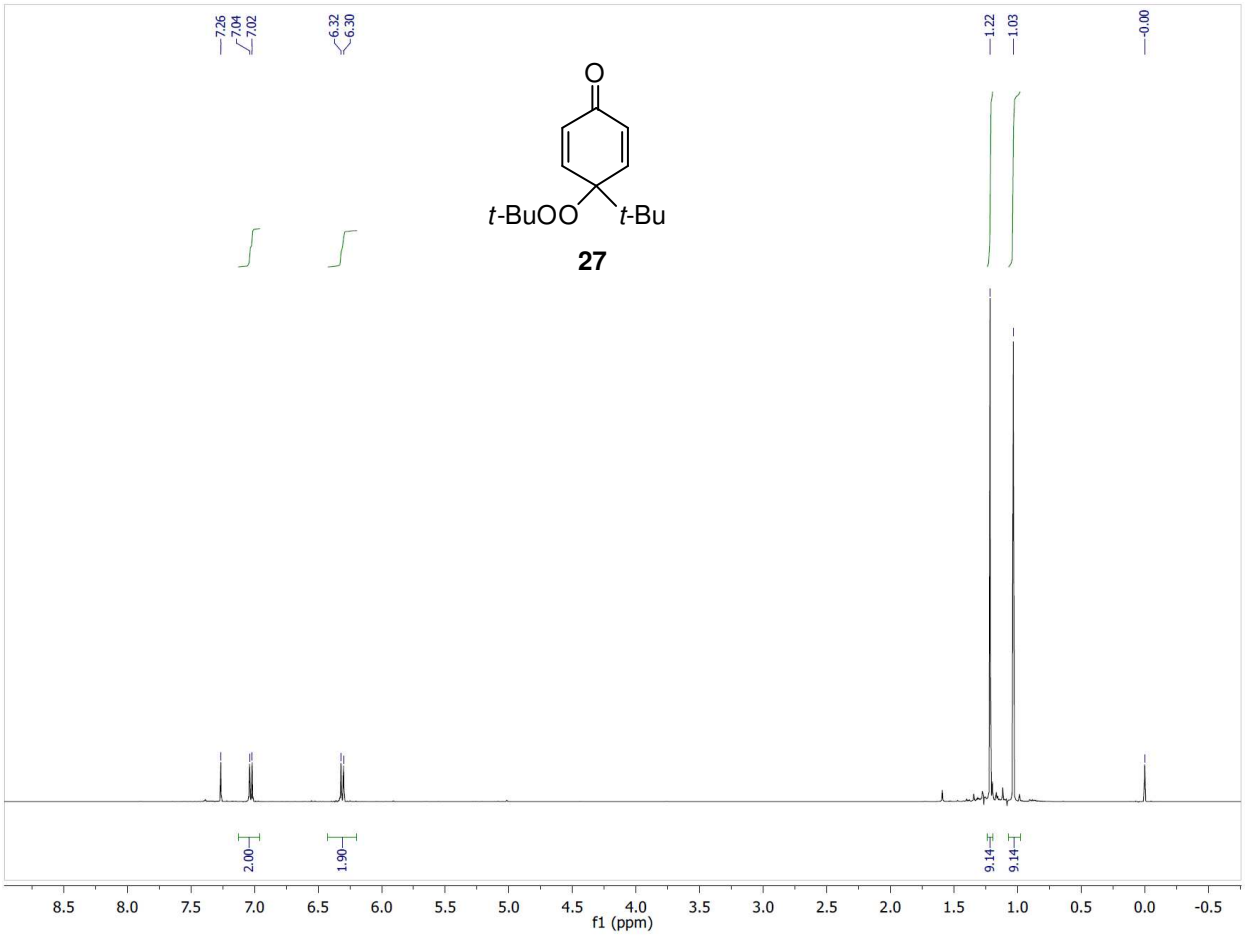

181.0
151.4
150.7
127.7
117.5
79.8
77.8
77.3
77.0
76.7
54.8
26.3
24.3
O
OMe
t-BuOO
Me
10
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

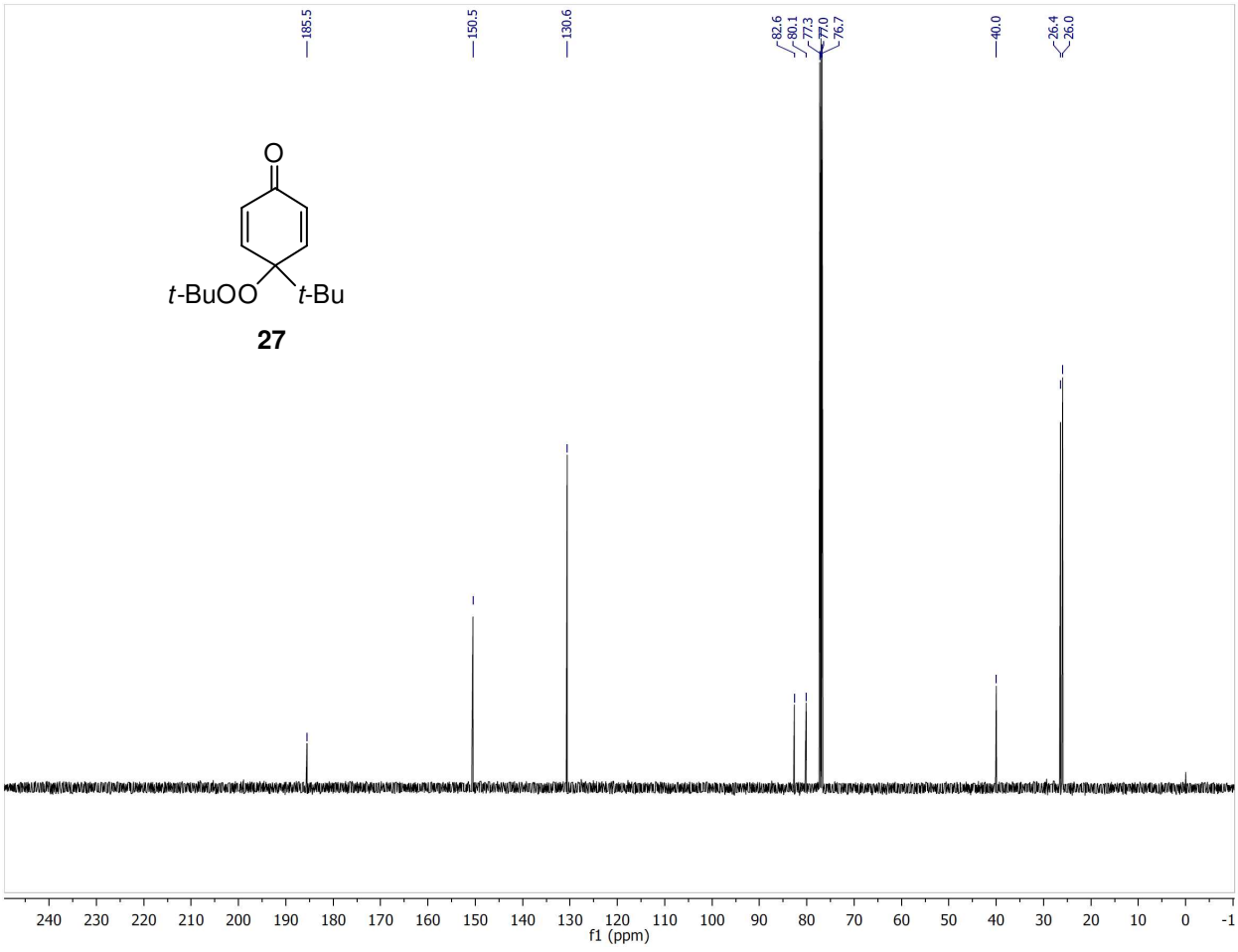

7.27
7.09
7.07
6.37
6.35
4.21
4.20
4.19
1.67
1.66
1.64
1.63
1.61
1.60
1.42
1.40
1.39
1.37
1.36
1.34
1.25
0.95
0.93
0.92
0.00
O
t-BuOO
CO2n-Bu
20
0.41
2.00
1.98
2.06
2.44
2.33
9.74
3.28
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

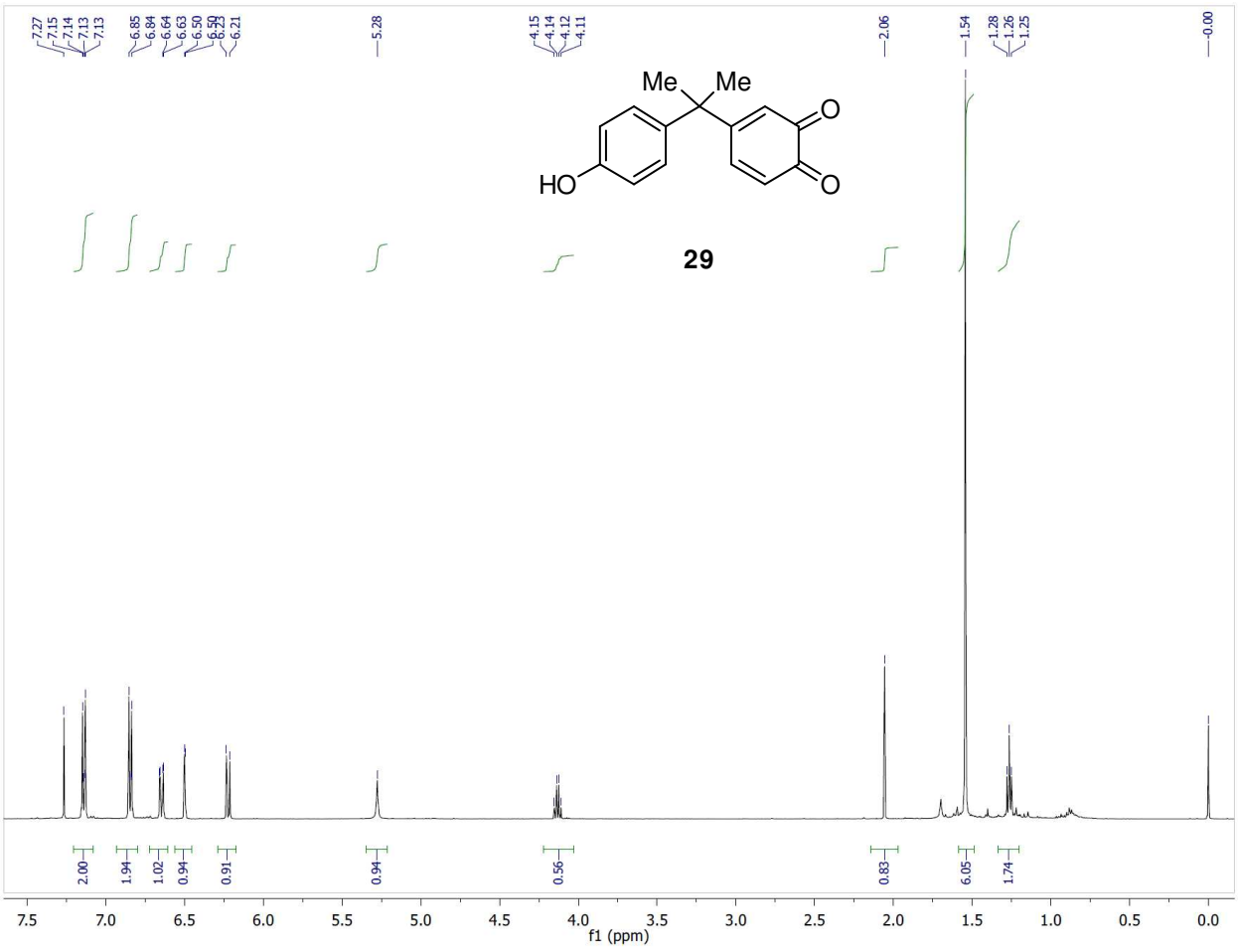

184.9
167.0
142.7
130.8
81.4
79.3
77.3
77.0
76.7
66.3
30.4
26.3
18.9
13.6
O
t-BuOO
CO2n-Bu
20
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)

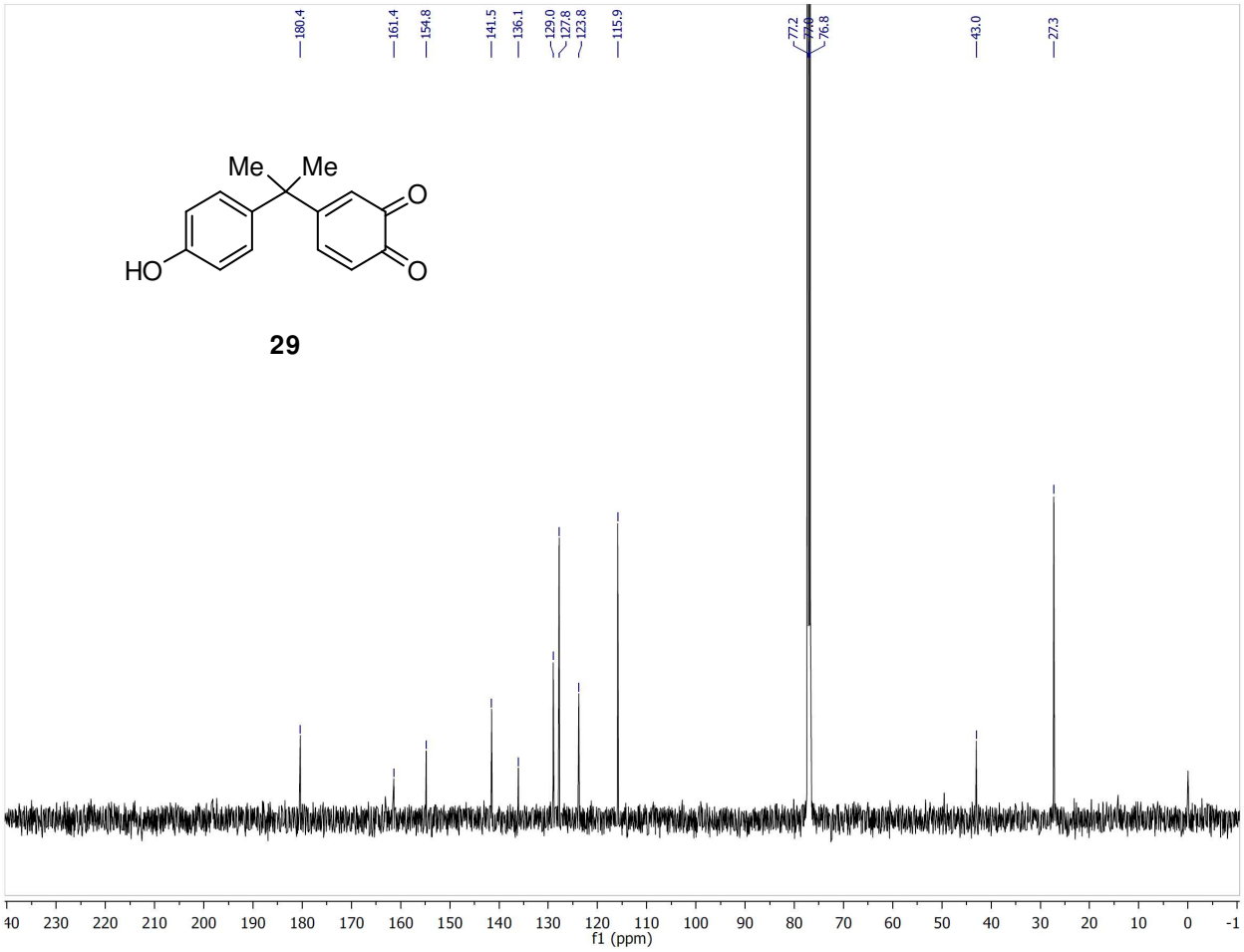

7.27
7.21
7.20
7.18
7.18
6.41
6.38
6.29
6.28
1.24
0.00
O
O
t-Bu
26
1.00
0.97
0.96
8.90
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


180.3
180.2
162.1
140.0
129.4
123.8
77.3
77.0
76.7
35.6
27.8
O
O
t-Bu
26
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


7.26
7.04
7.02
6.32
6.30
1.22
1.03
0.00
O
t-BuOO
t-Bu
27
2.00
1.90
9.14
9.14
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
-0.5
f1 (ppm)


185.5
150.5
130.6
82.6
80.1
77.3
77.0
76.7
40.0
26.4
26.0
O
t-BuOO
t-Bu
27
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


Me
Me
O
O
HO
29
f1 (ppm)


180.4
161.4
154.8
141.5
136.1
129.0
127.8
123.8
115.9
77.2
76.8
43.0
27.3
Me
Me
O
O
HO
f1 (ppm)

29