Supporting Information

[4+2] Cyclization/Retro-Mannich Reaction Cascade of *para*-Quinone Methide Derivatives with Pd-Containing 1,4-Dipoles

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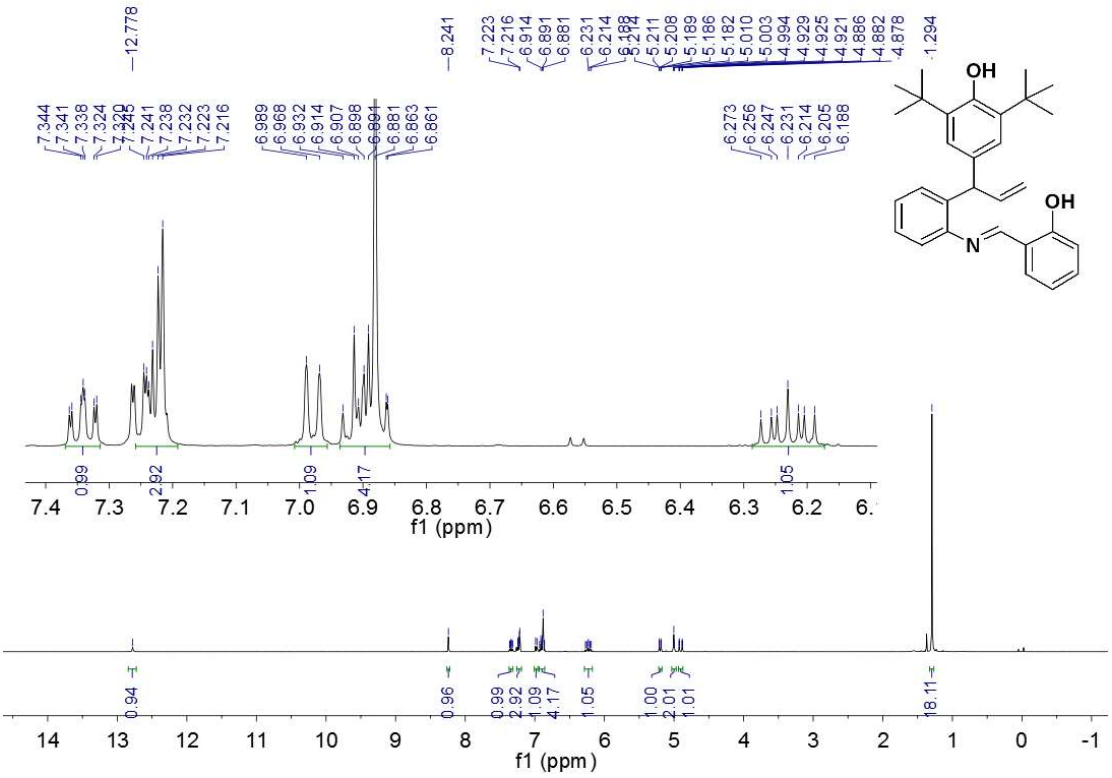
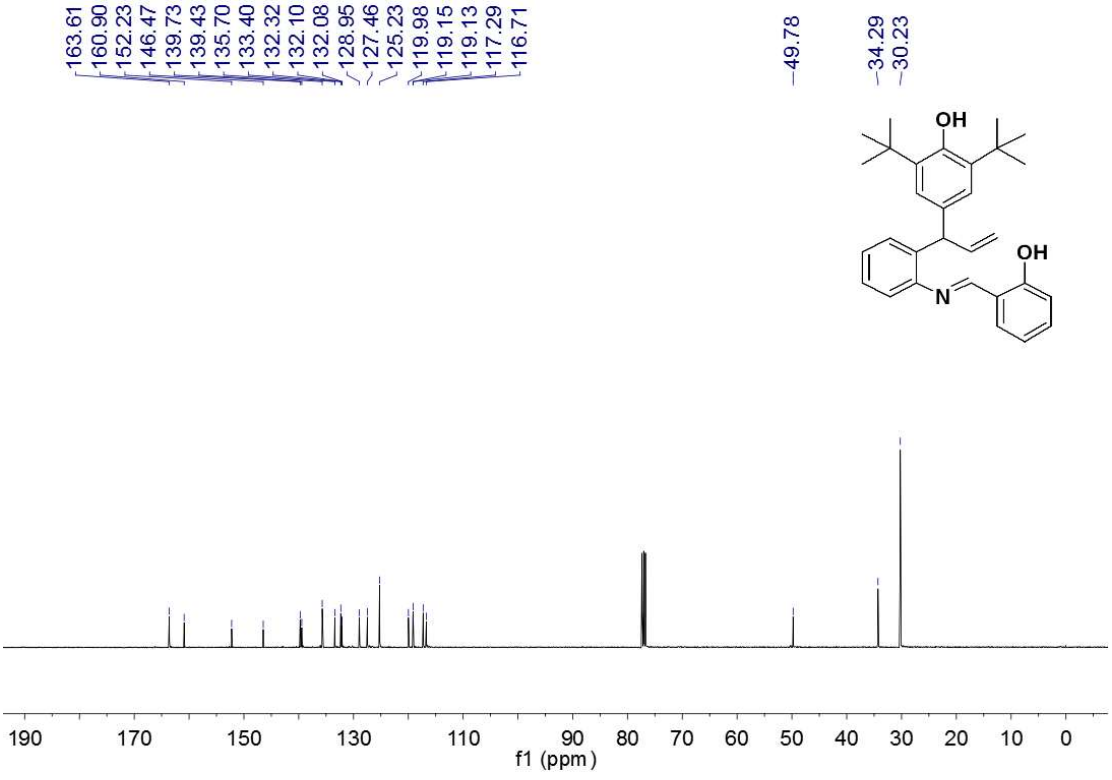
1. ^{1}H and ^{13}C NMR spectra of products 3

3aa





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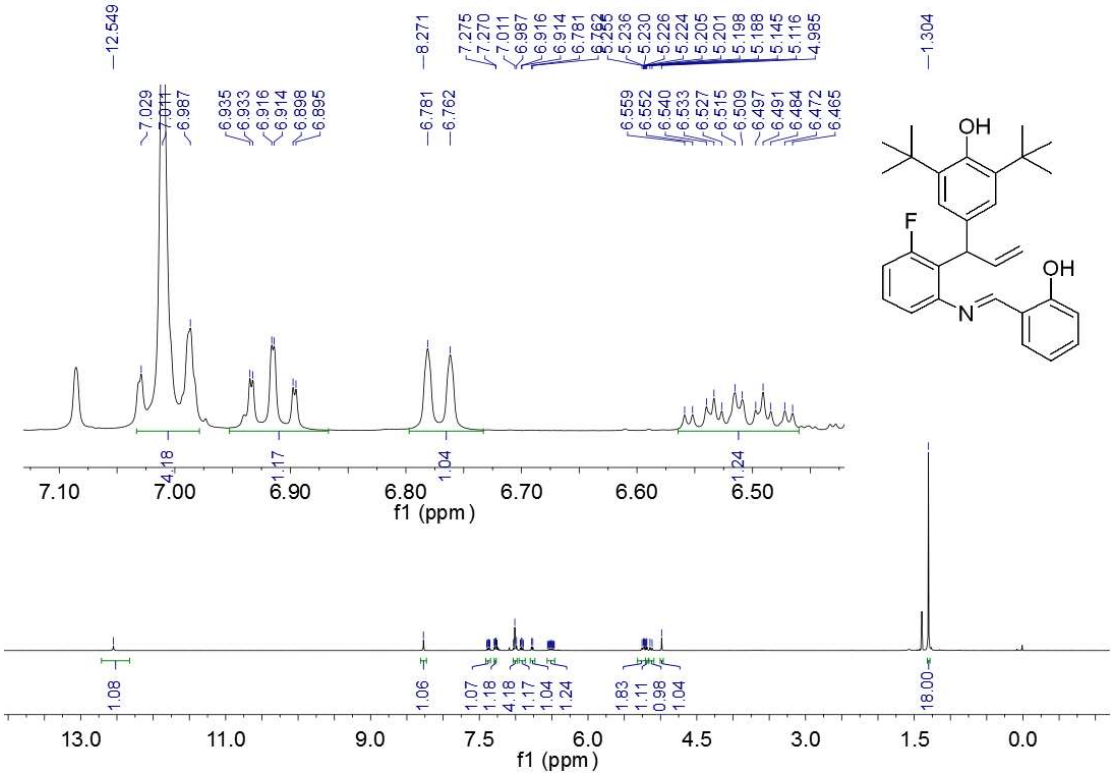
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OH
N
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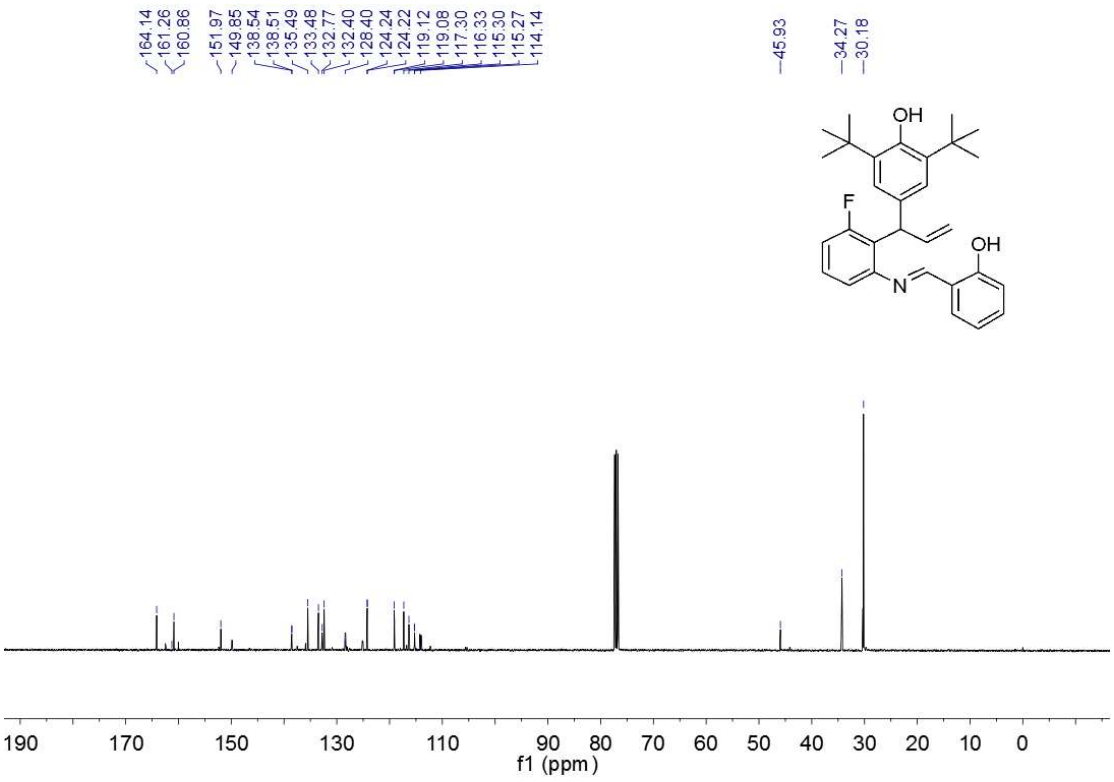
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F
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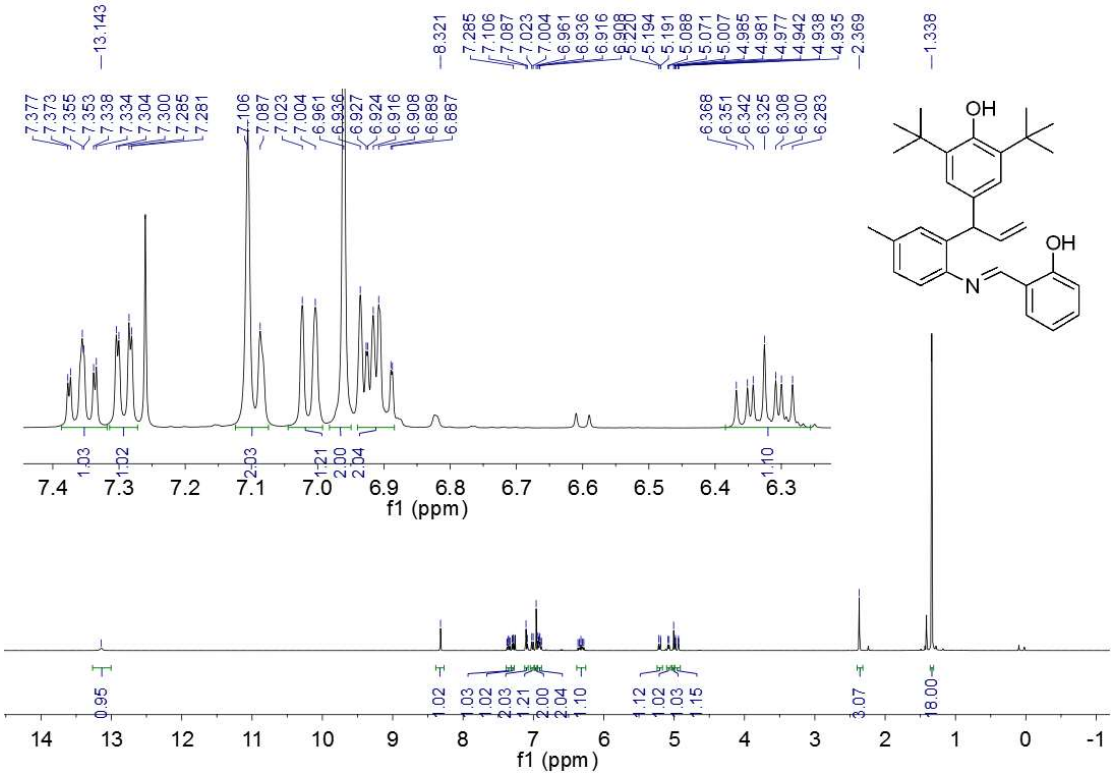
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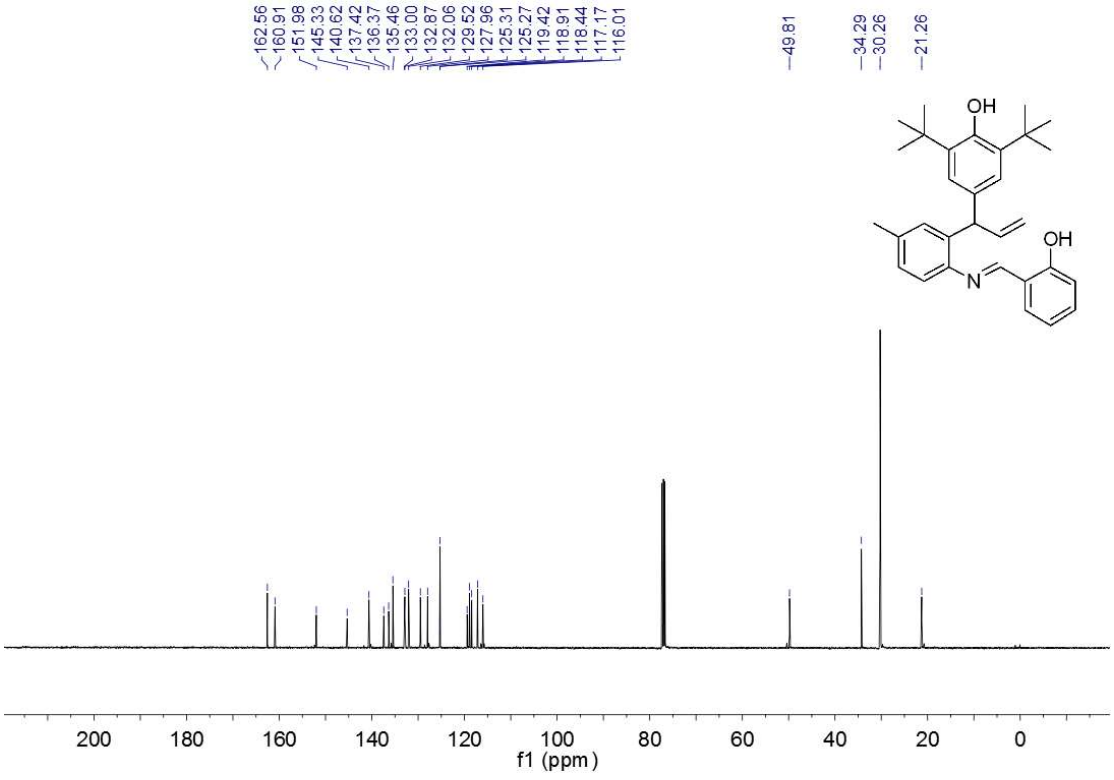
f1 (ppm)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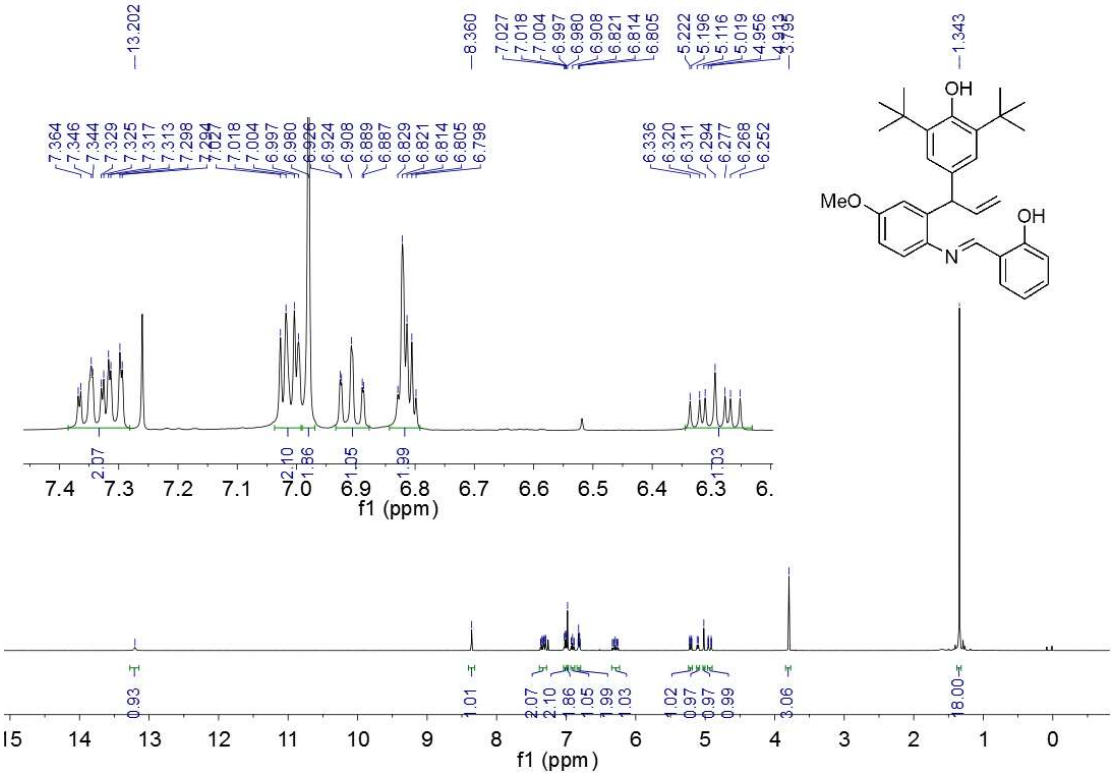
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6.887
6.829
6.821
6.814
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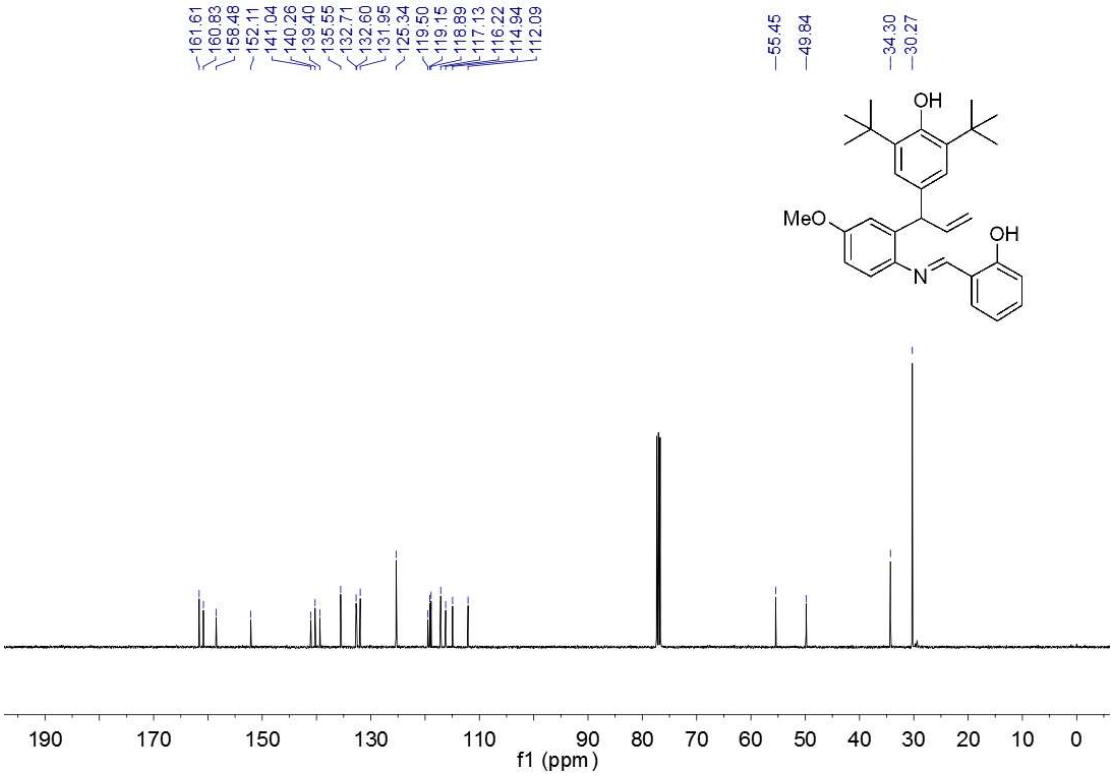
f1 (ppm)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117.13
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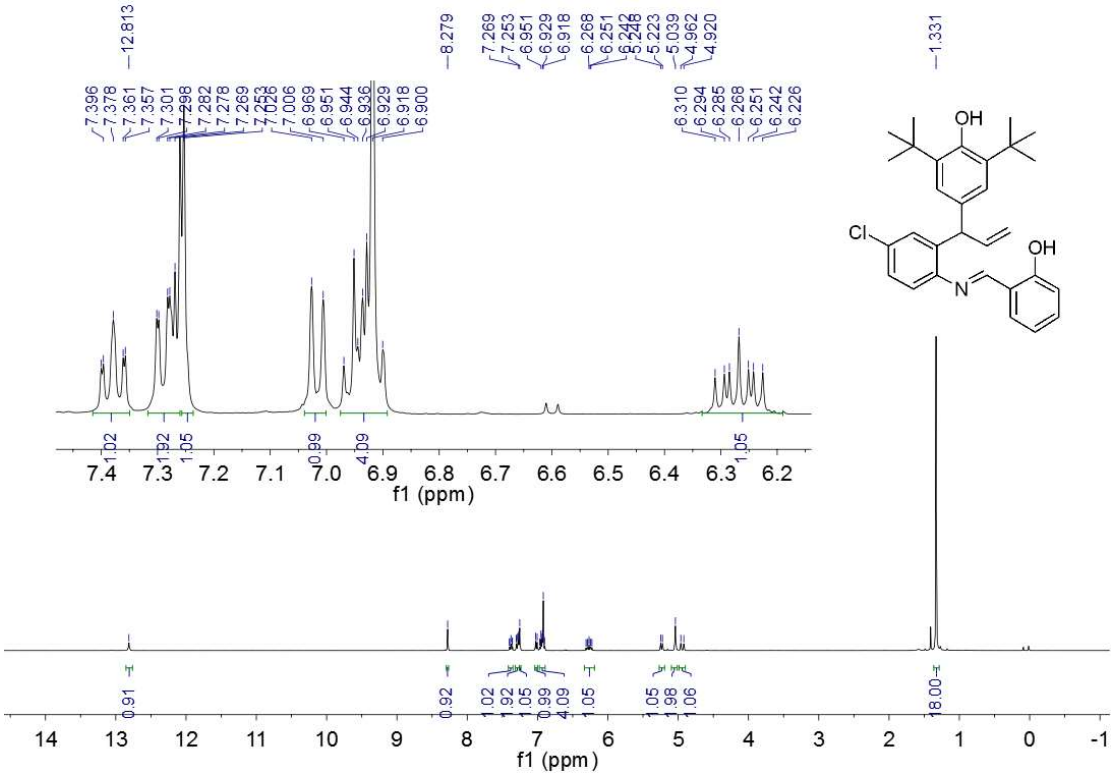
MeO
OH
N
f1 (ppm)

3ae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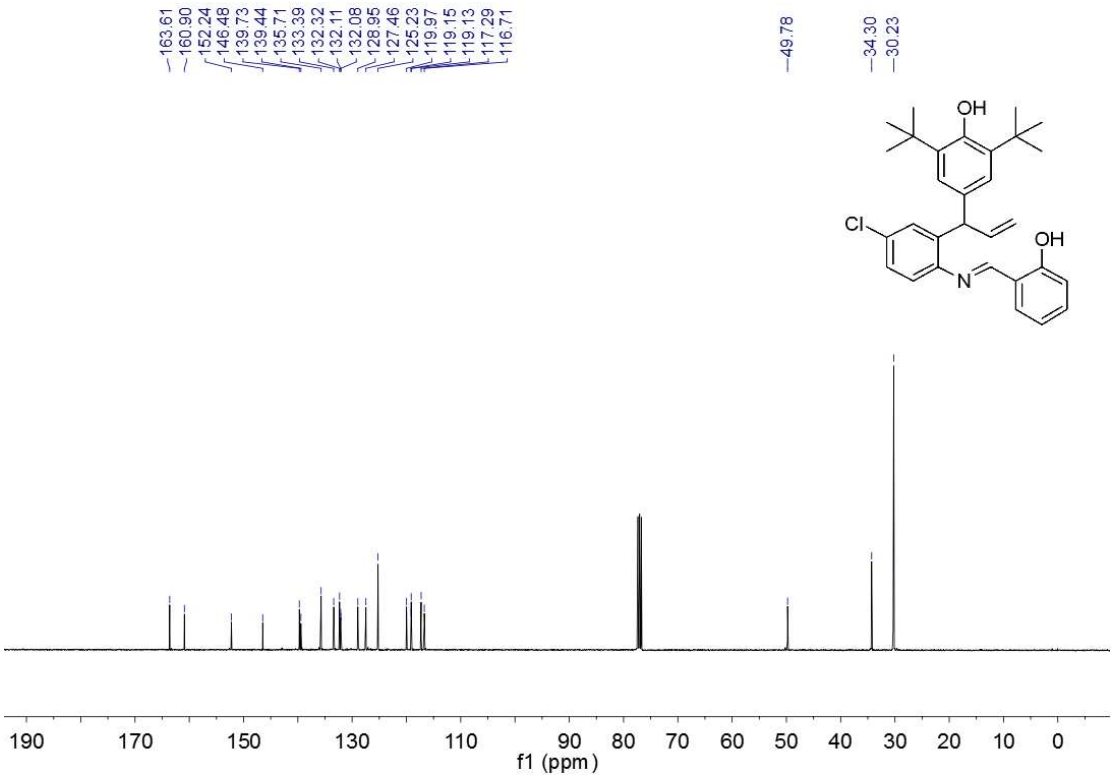
f1 (ppm)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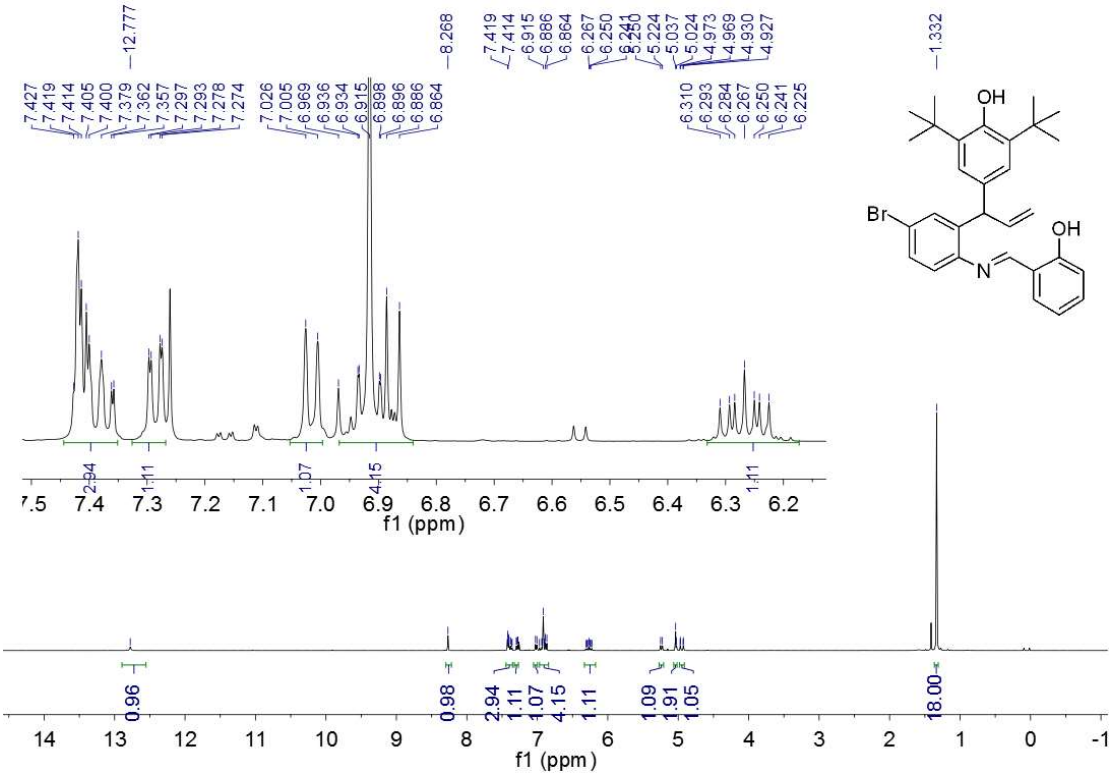
OH
Cl
OH
N
f1 (ppm)

3af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4.930
4.927
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6.241
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Br
OH
N
2.94
1.11
1.07
4.15
1.11
f1 (ppm)
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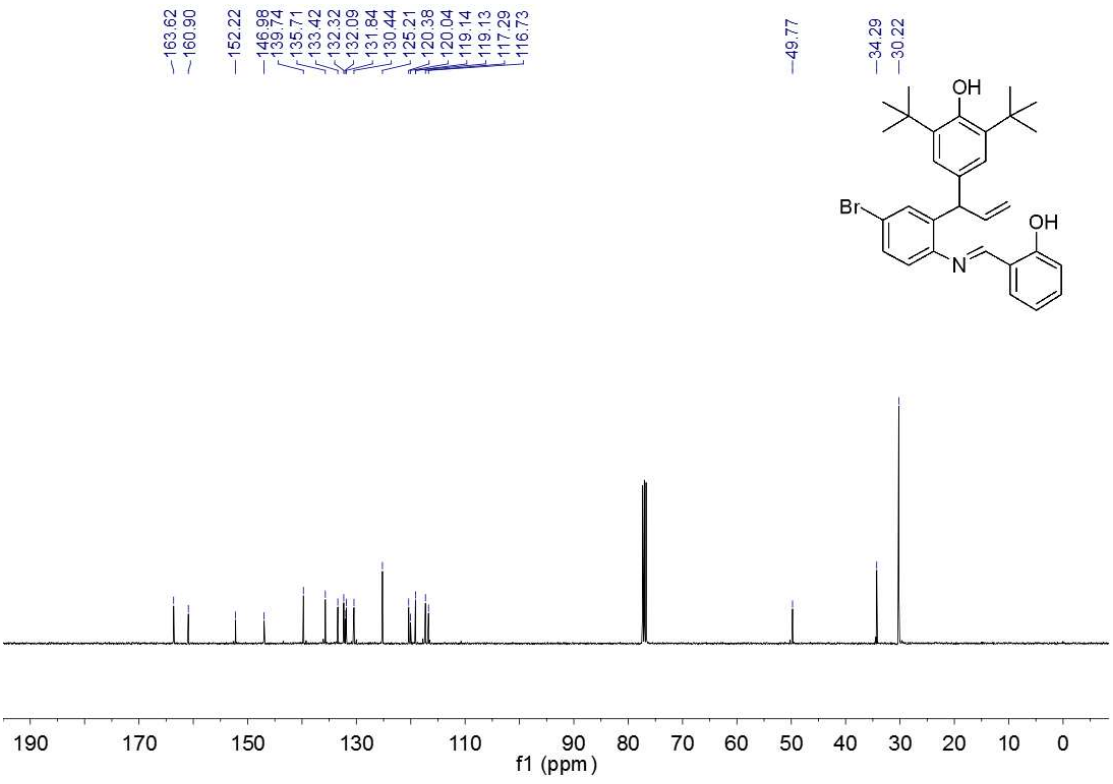
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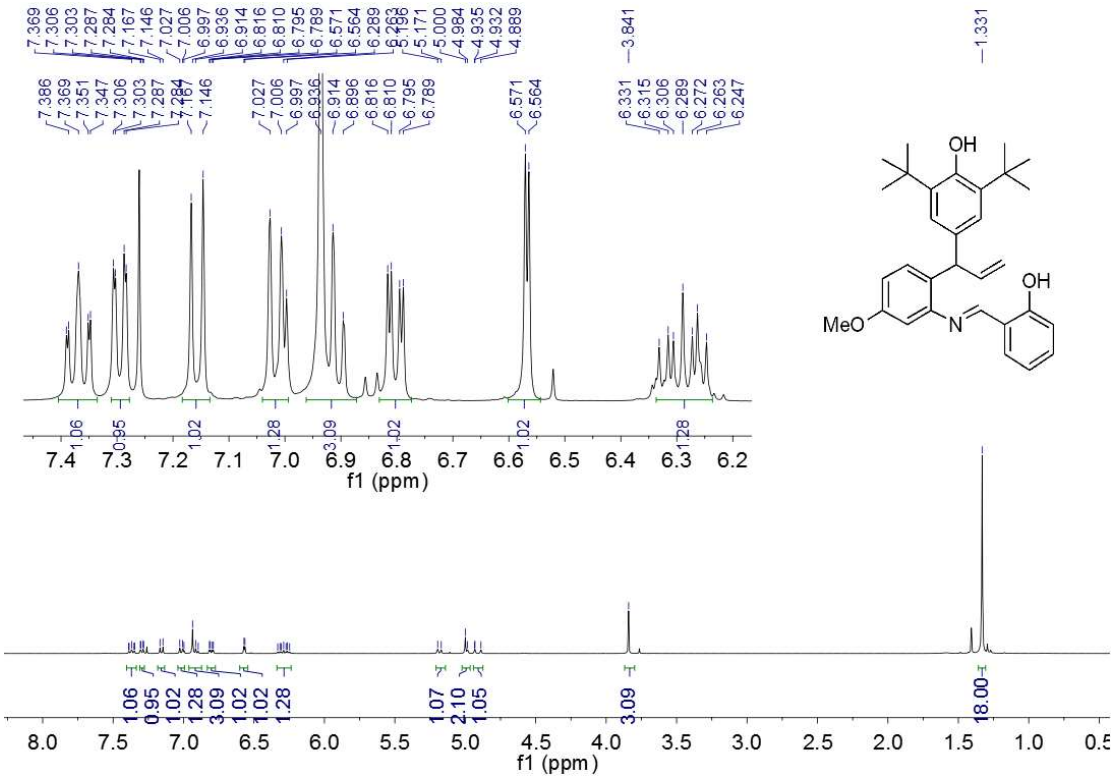
Br
OH
N
f1 (ppm)

3ag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OH
MeO
N
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3.09
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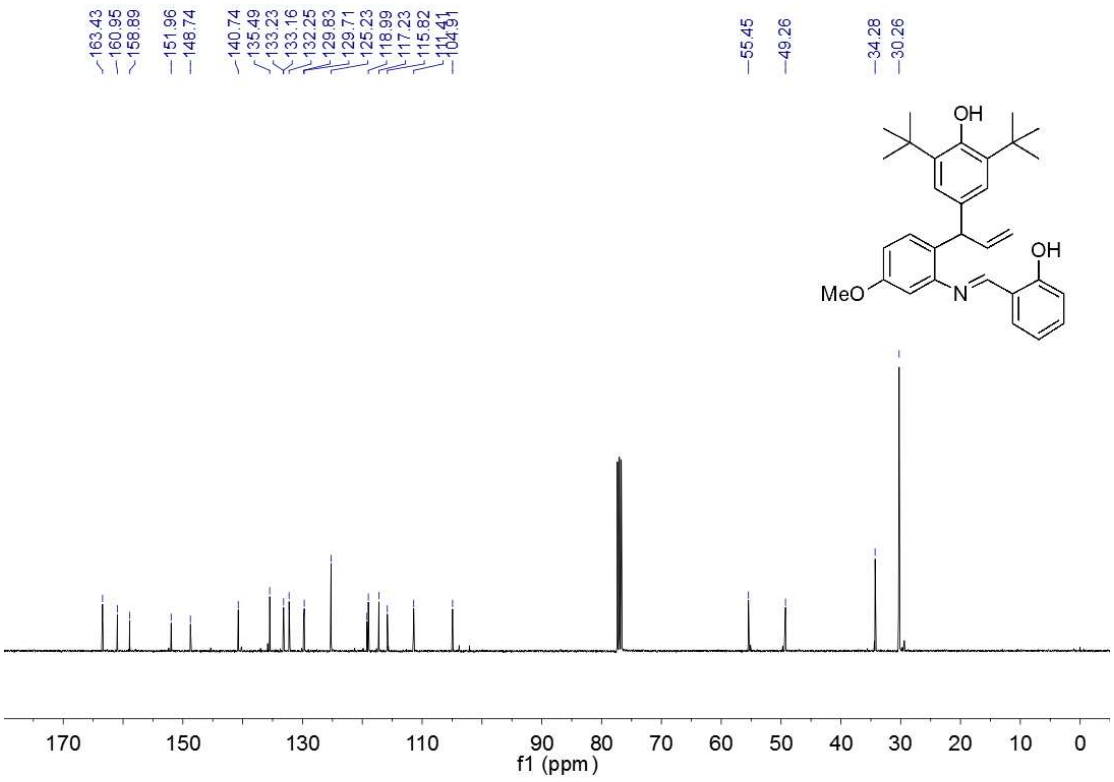
f1 (ppm)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117.23
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OH
MeO
N
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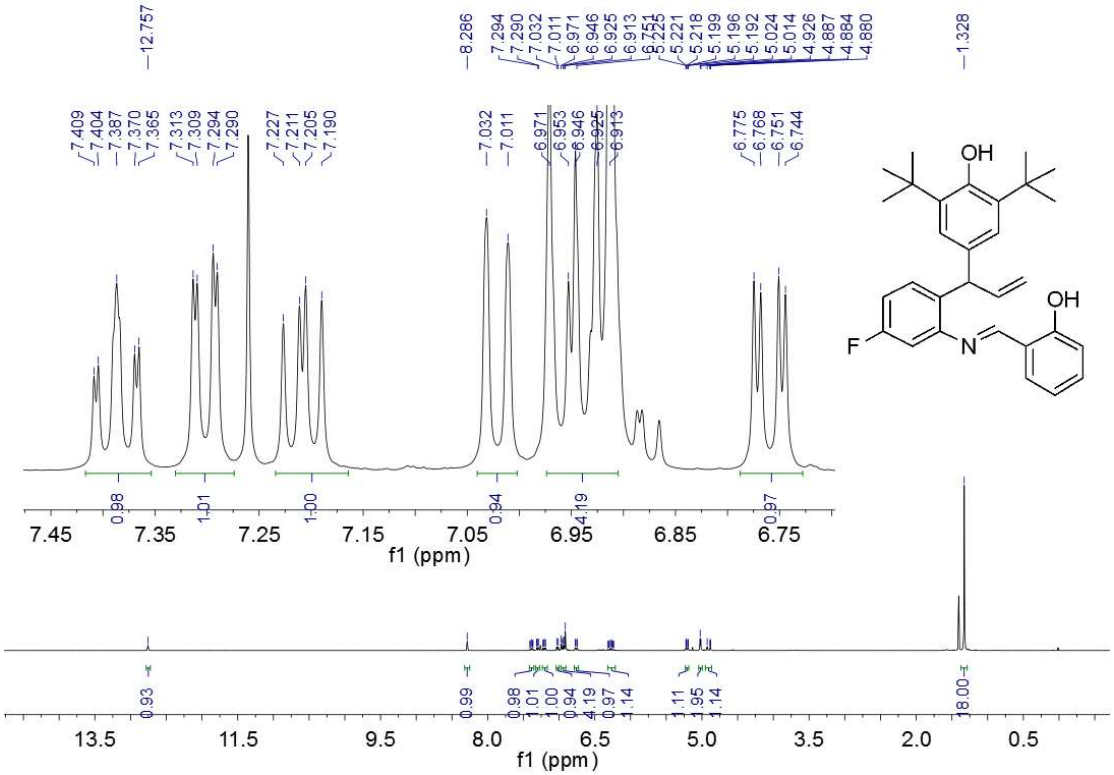
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OH
F
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1.00
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4.19
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7.25
7.15
7.05
6.95
6.85
6.75
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0.99
0.98
1.01
1.00
0.94
4.19
0.97
1.14
1.11
1.95
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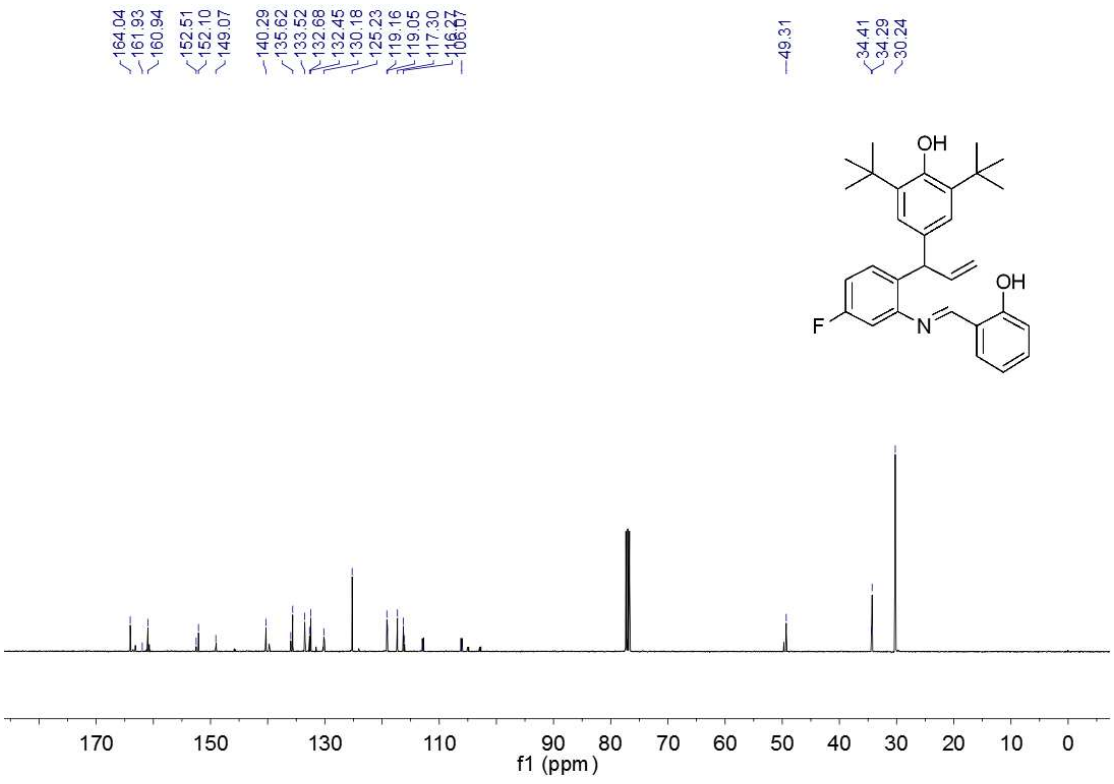
f1 (ppm)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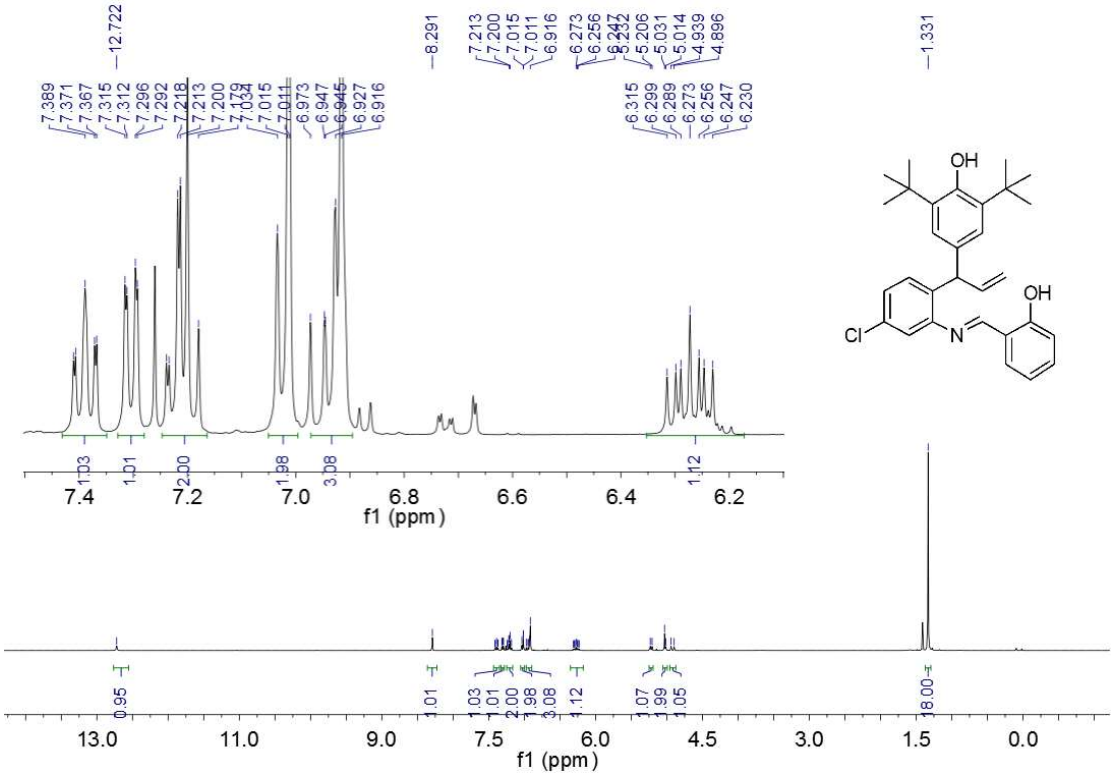
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OH
Cl
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2.00
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7.4
7.2
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6.8
6.6
6.4
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3.08
1.12
1.07
1.99
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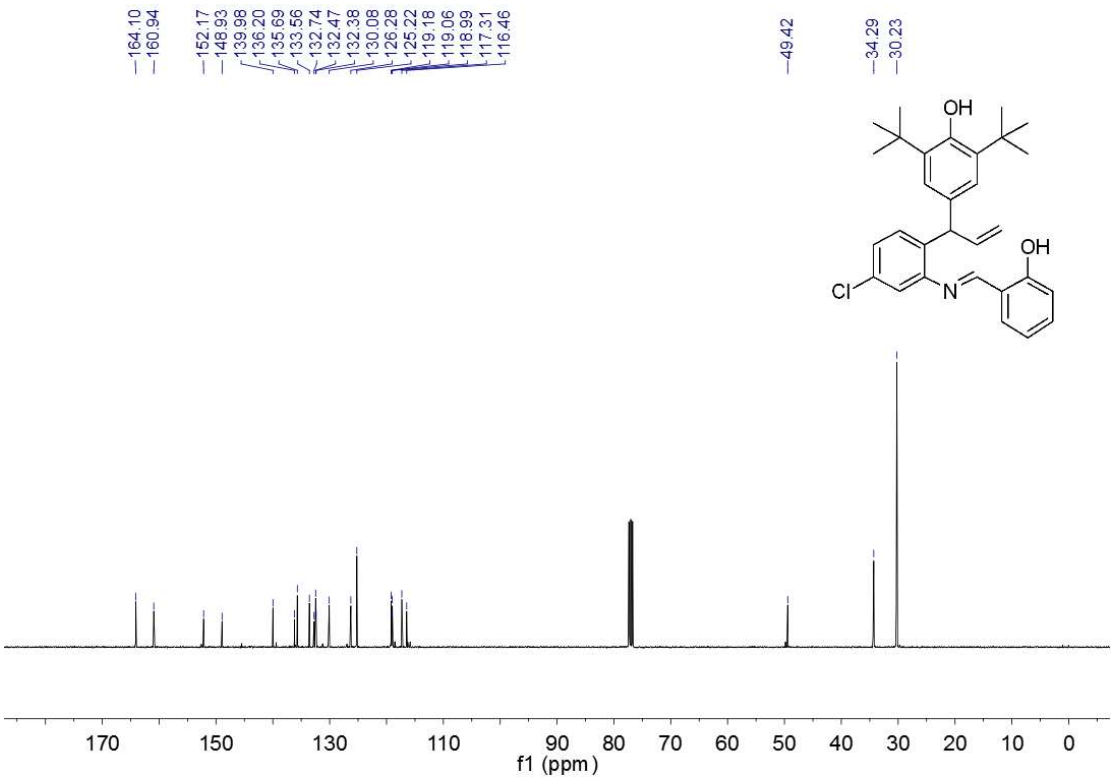
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30.23
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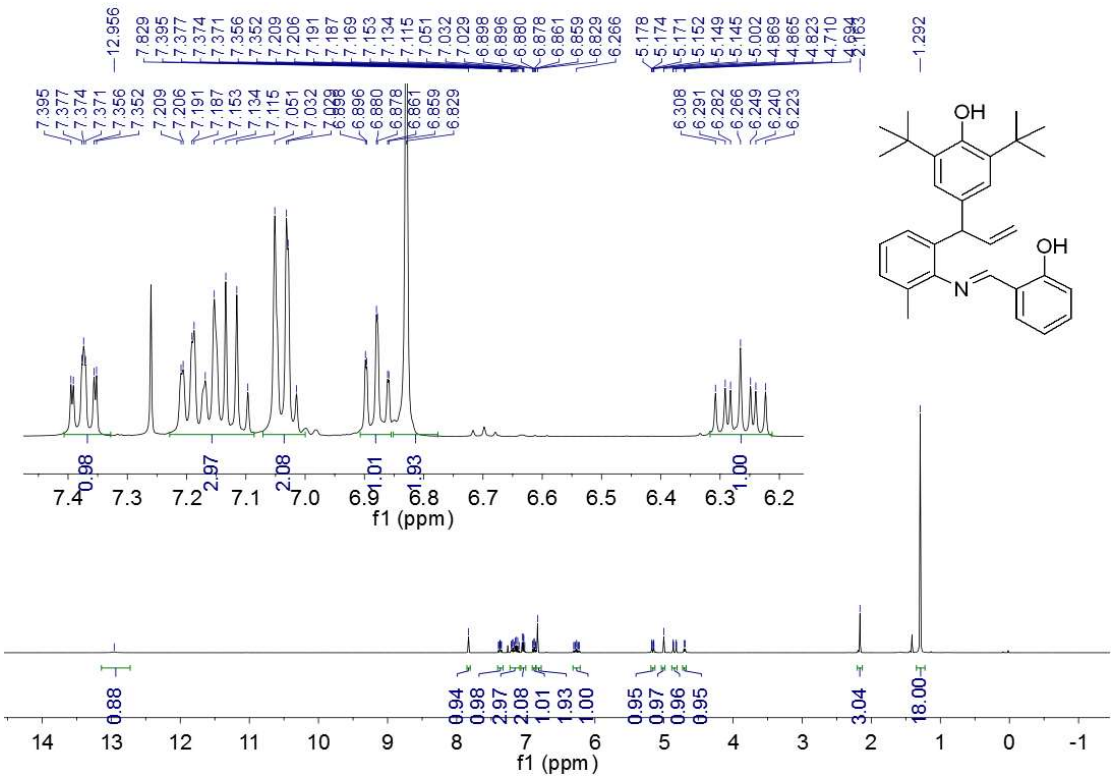

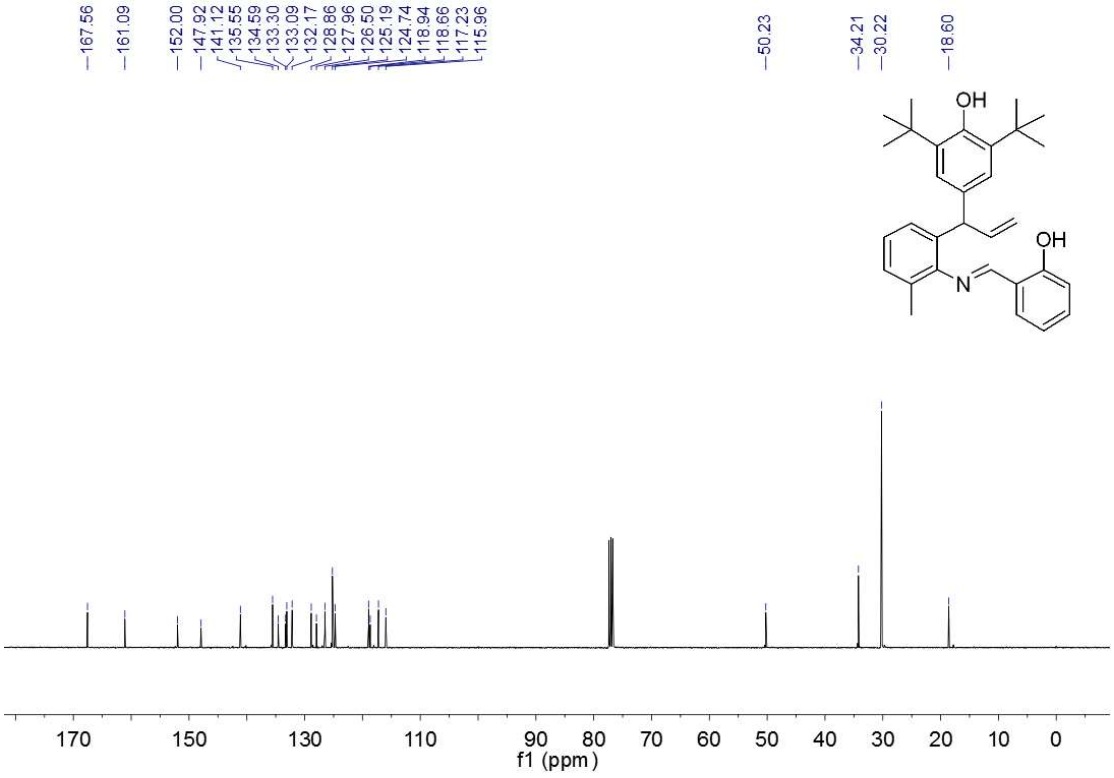

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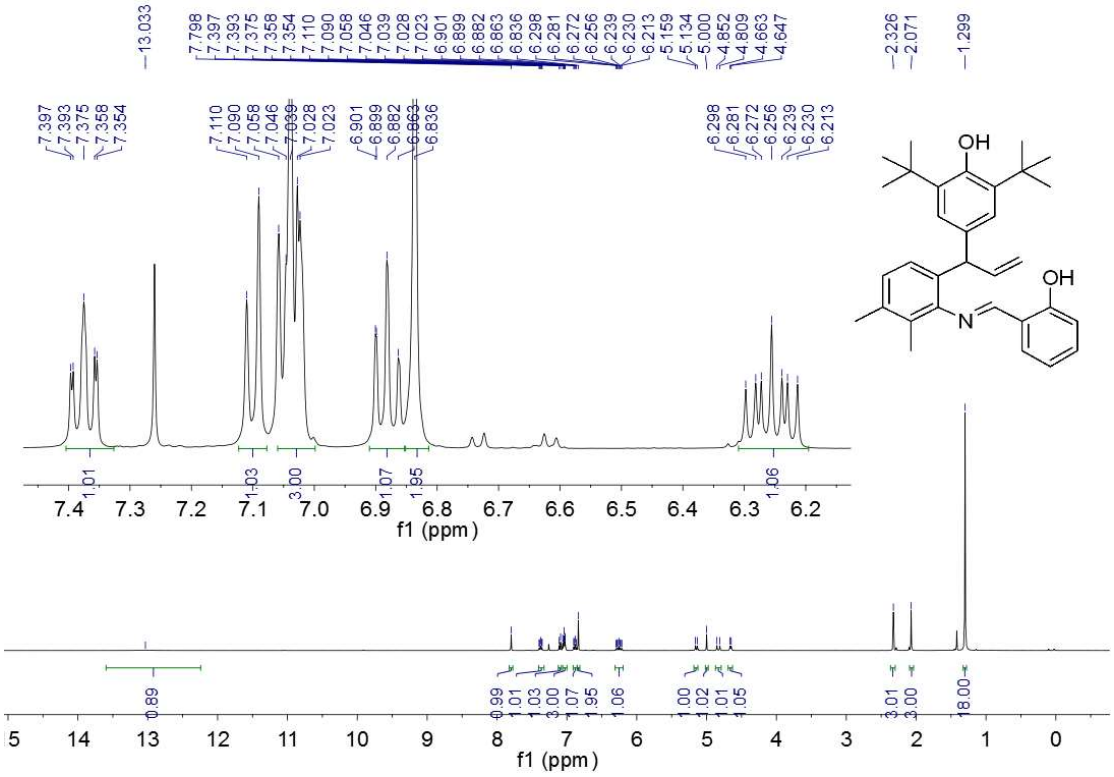
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7.023
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6.836
6.298
6.281
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6.230
6.213
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2.071
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OH
OH
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1.01
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3.00
1.07
1.95
1.06
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1.03
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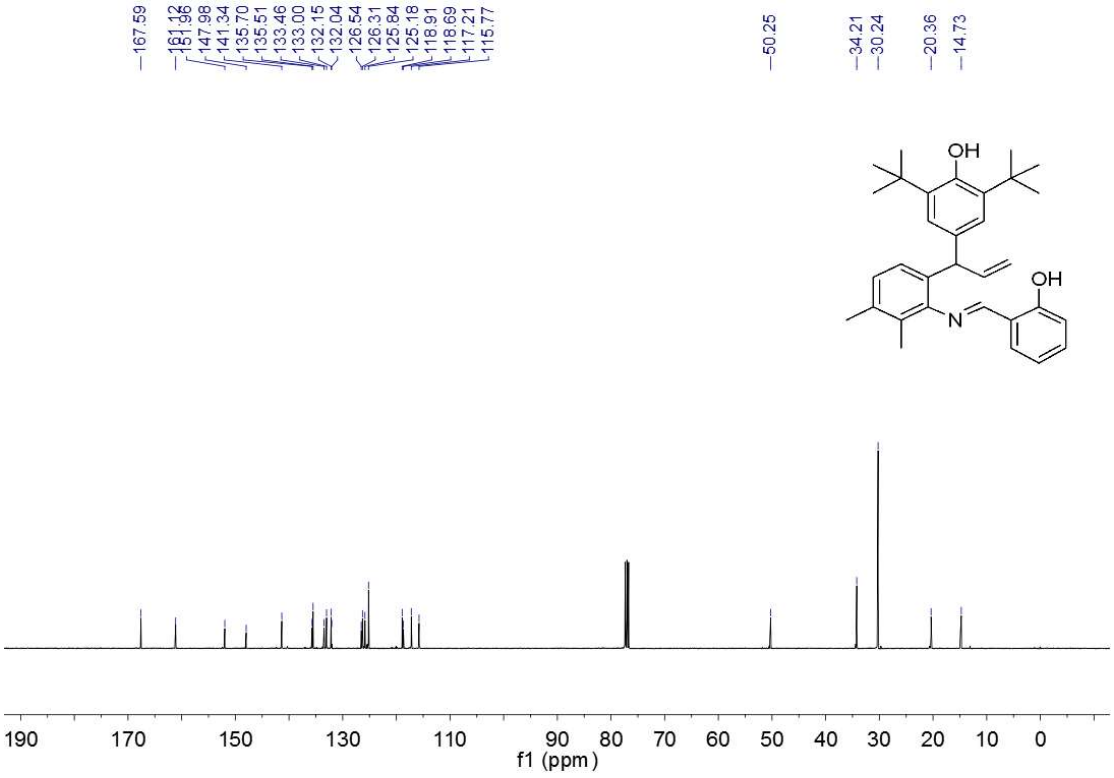
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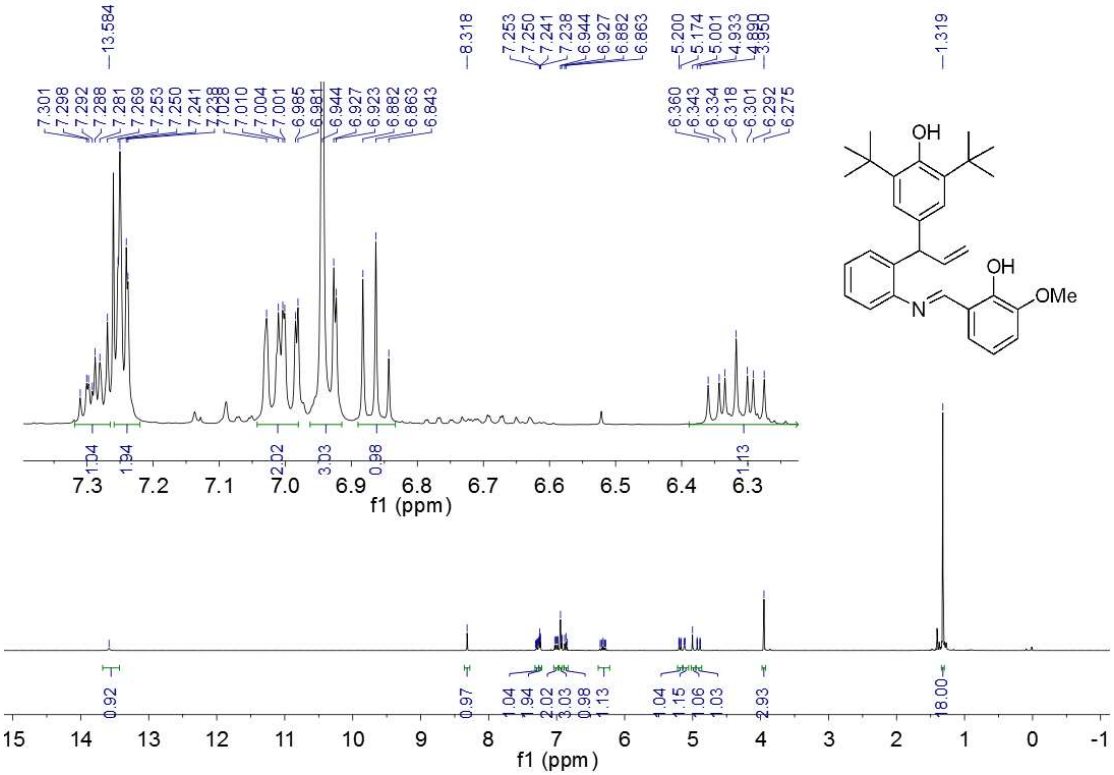
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1.319
7.301
7.298
7.292
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7.001
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6.927
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OH
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6.4
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f1 (ppm)
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2.02
3.03
0.98
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1.04
1.15
1.06
1.03
2.93
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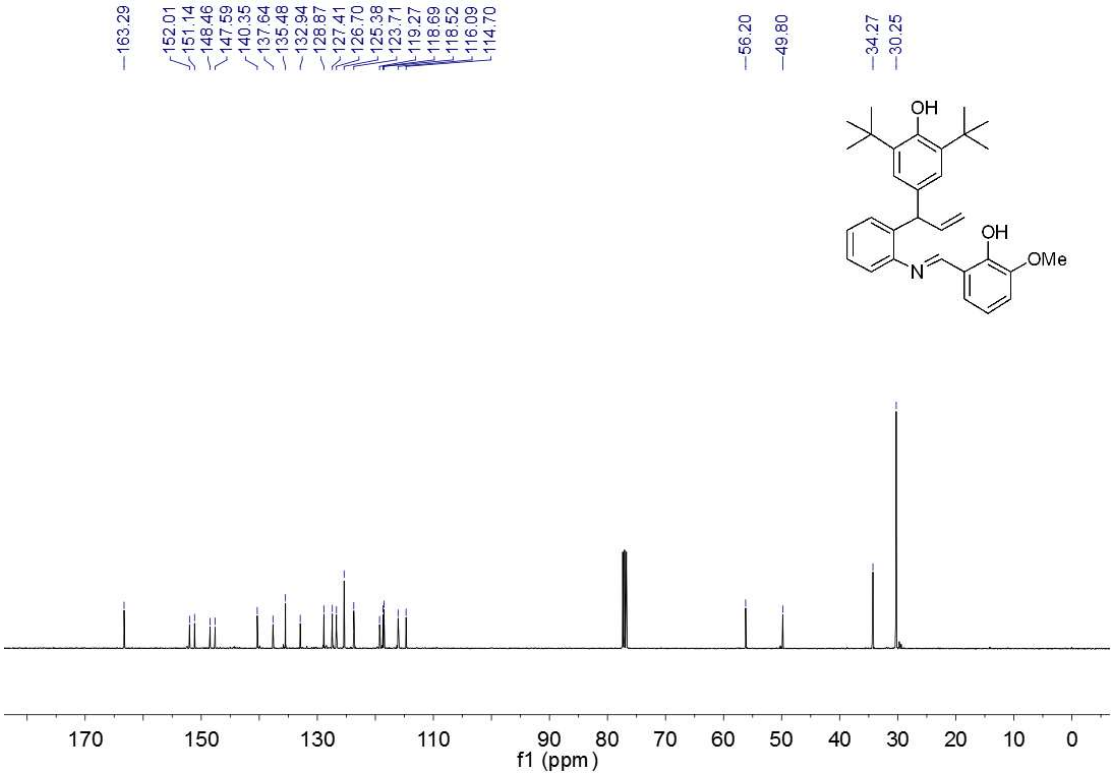
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125.38
123.71
119.27
118.69
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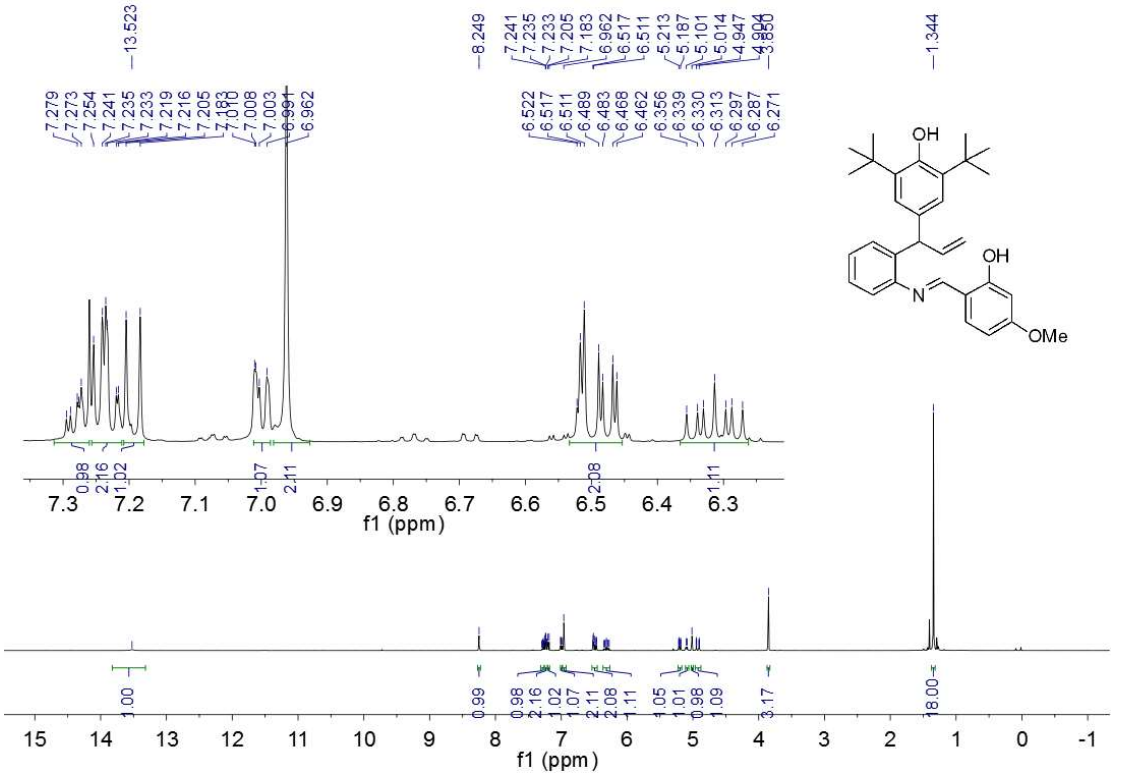
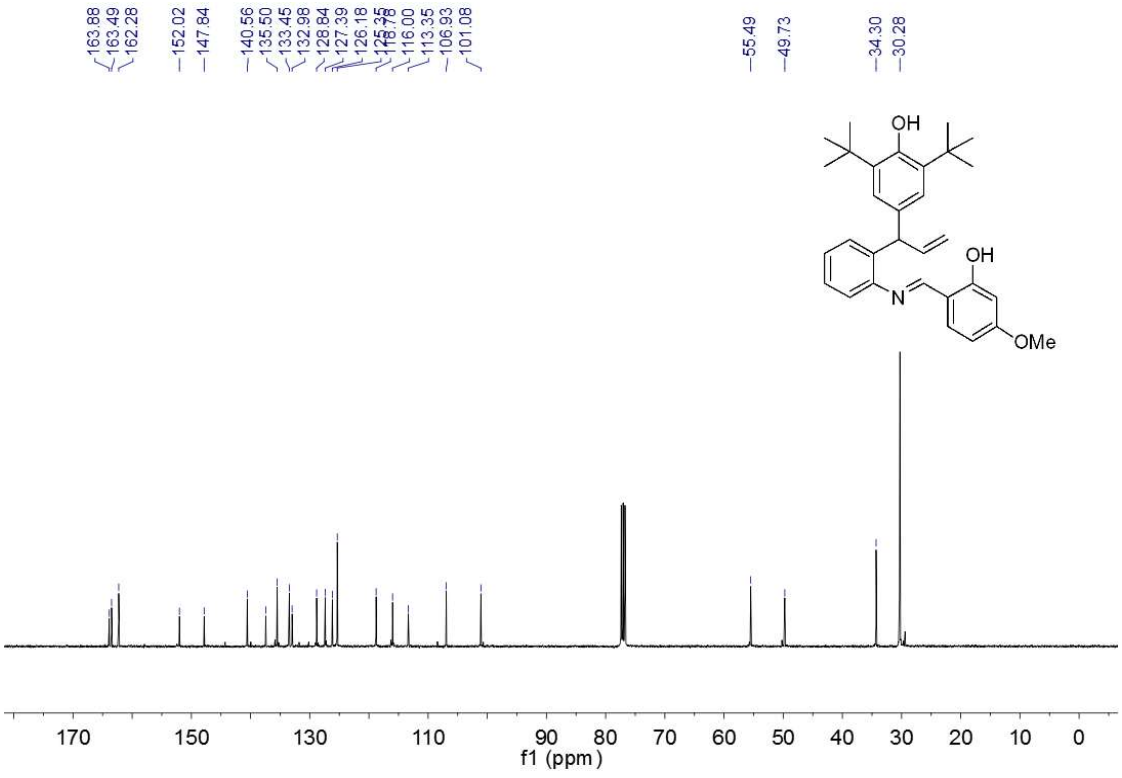
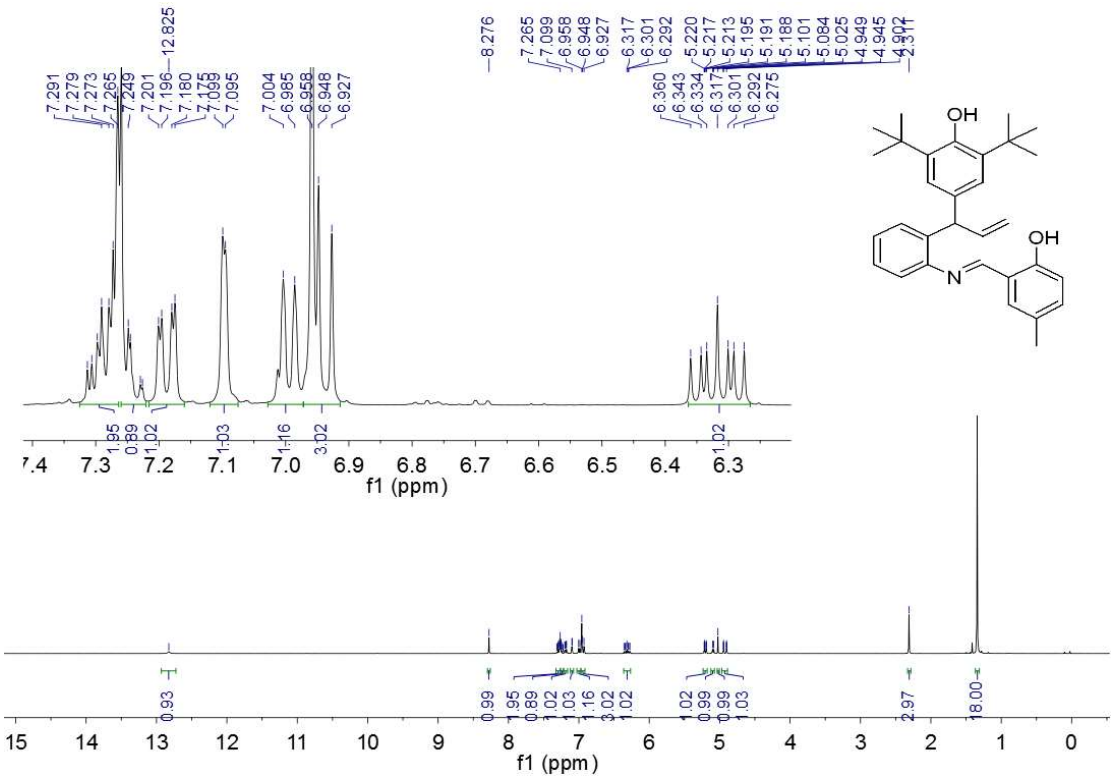
116.09
114.70
56.20
49.80
34.27
30.25
OH
OH
OMe
N
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

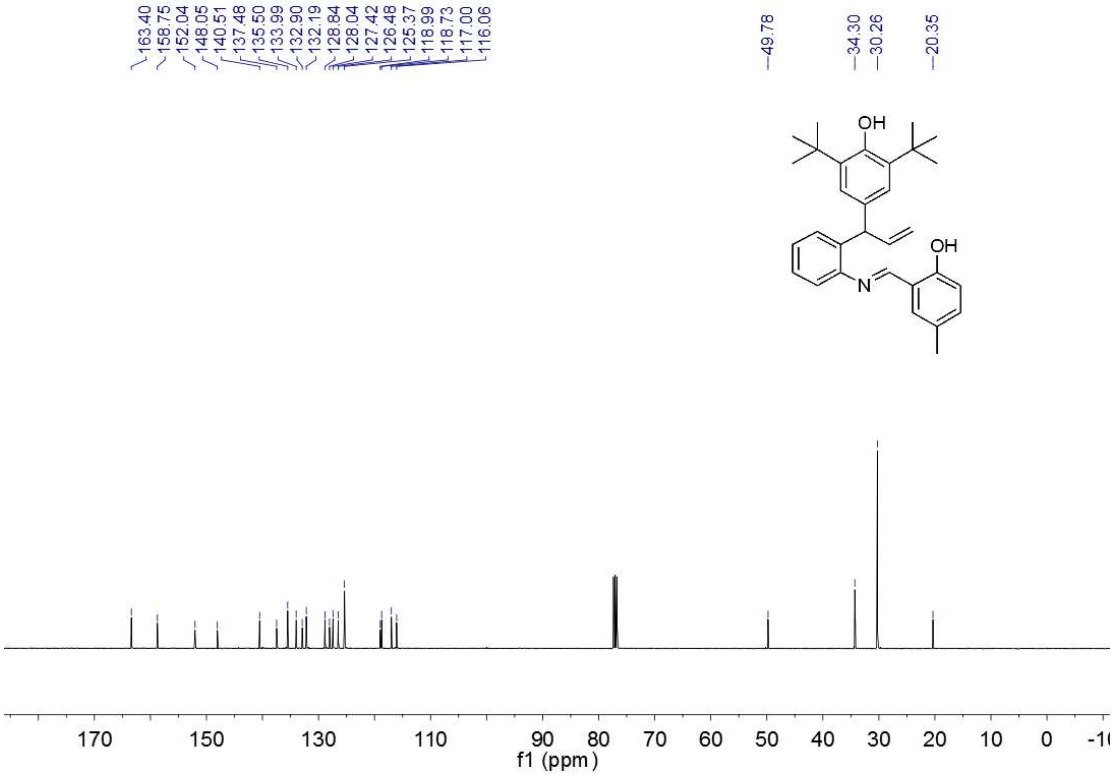
3ca


13.523
8.249
7.241
7.235
7.233
7.205
7.183
6.962
6.517
6.511
5.213
5.187
5.101
5.014
4.947
4.904
4.850
1.344
7.279
7.273
7.254
7.241
7.235
7.233
7.219
7.216
7.205
7.183
7.010
7.008
7.003
6.991
6.962
6.522
6.517
6.511
6.489
6.483
6.468
6.462
6.356
6.339
6.330
6.313
6.297
6.287
6.271
OH
OH
N
OMe
0.98
2.16
1.02
1.07
2.11
2.08
1.11
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
f1 (ppm)
1.00
0.99
0.98
2.16
1.02
1.07
2.11
2.08
1.11
1.05
1.01
0.98
1.09
3.17
18.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

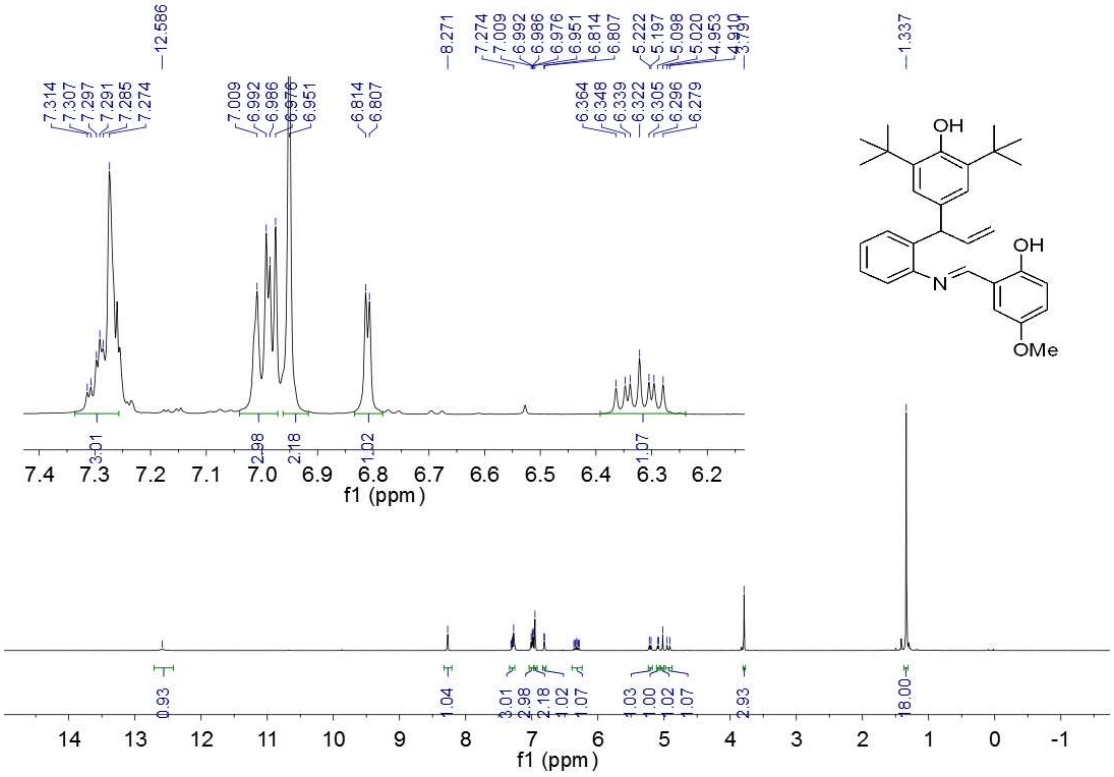

163.88
163.49
162.28
152.02
147.84
140.56
135.50
133.45
132.98
128.84
127.39
126.18
116.00
113.35
106.93
101.08
55.49
49.73
34.30
30.28
OH
OH
N
OMe
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

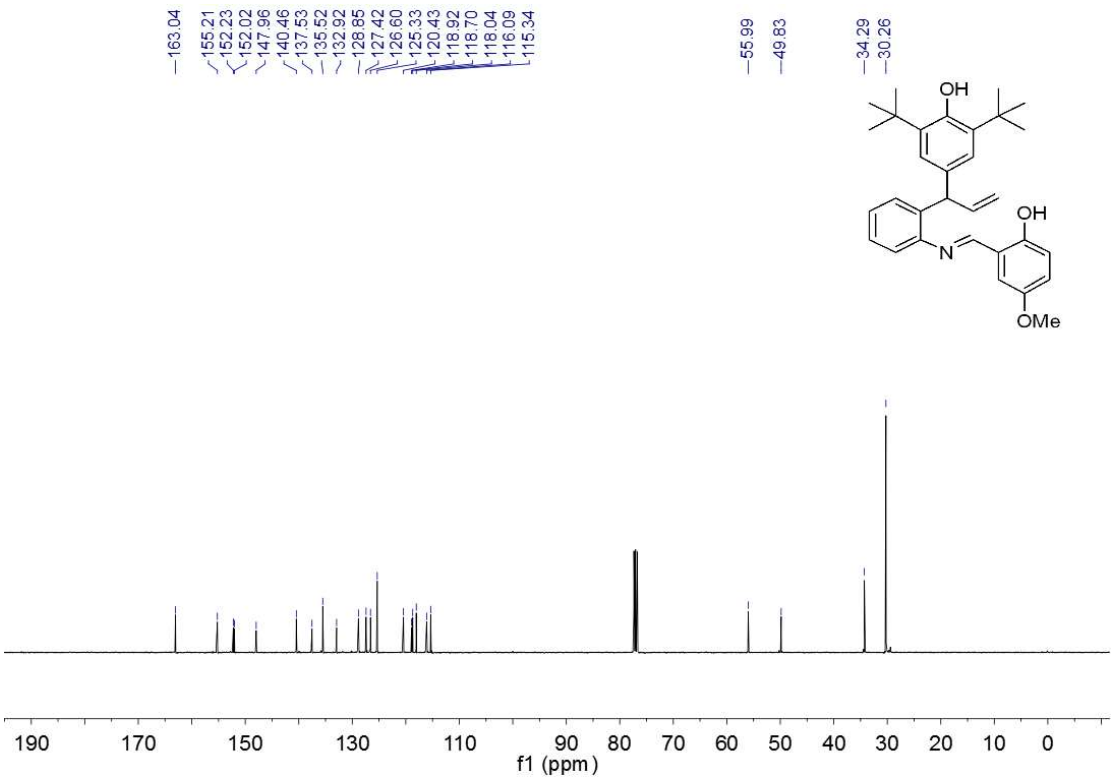
3da



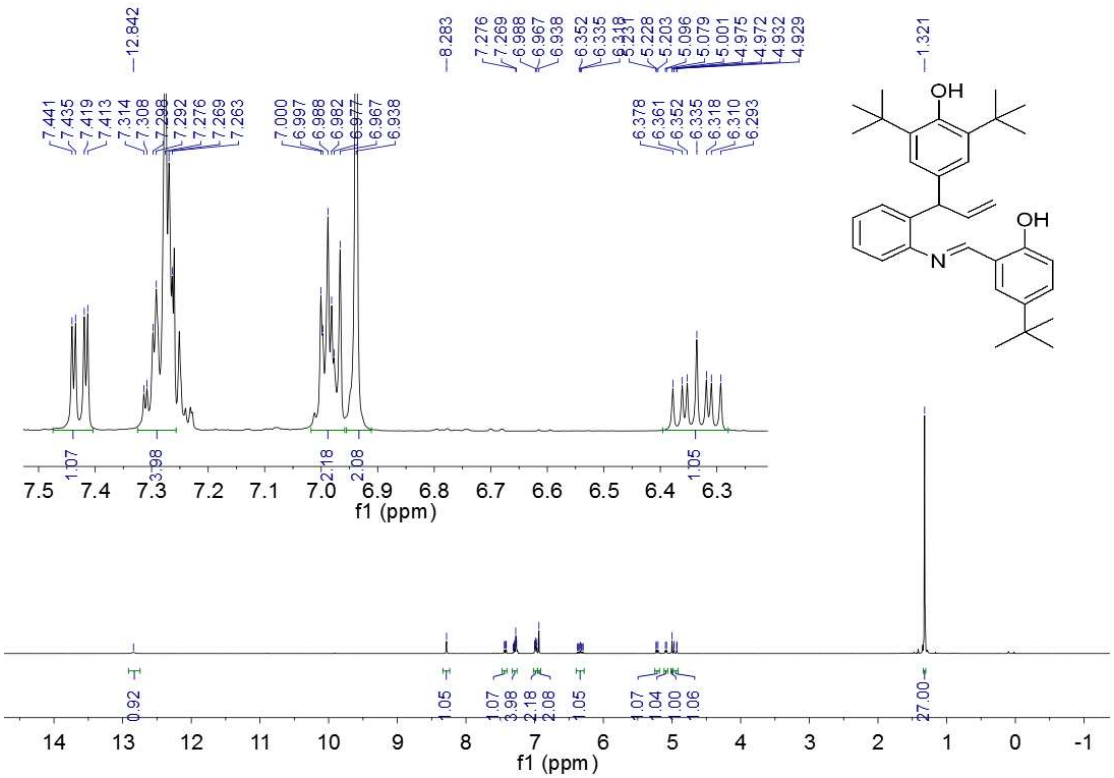


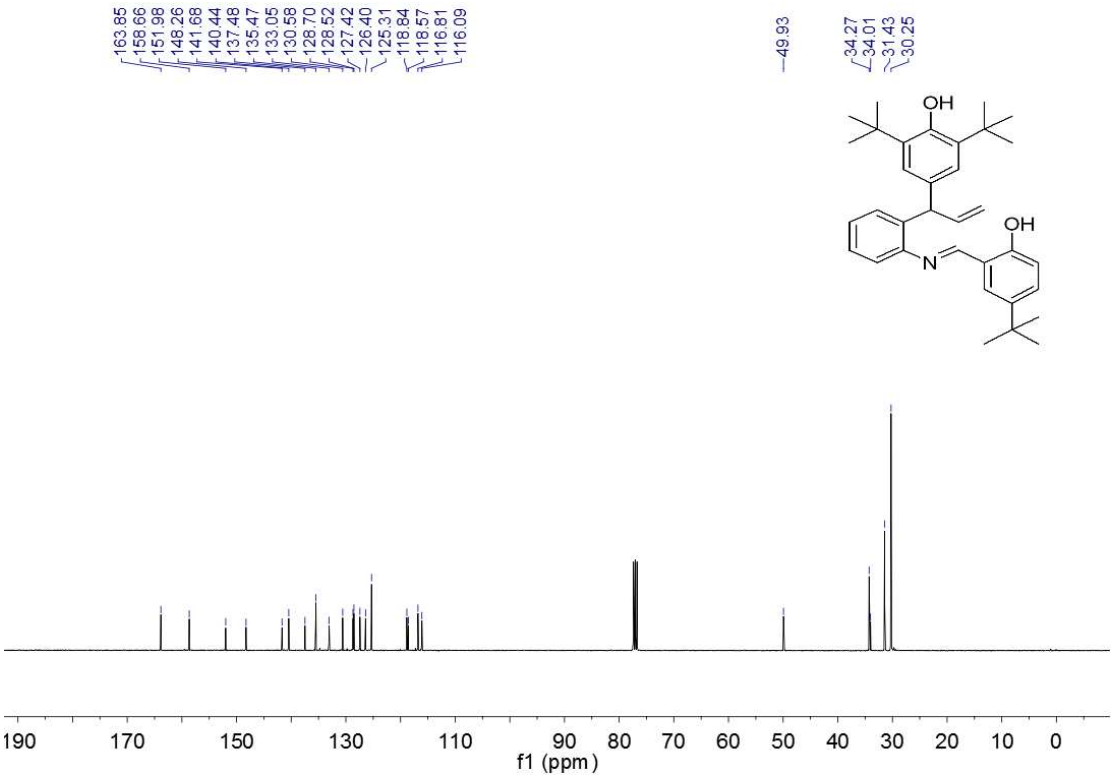
3ea


12.586
8.271
7.274
7.009
6.992
6.986
6.976
6.951
6.814
6.807
5.222
5.197
5.098
5.020
4.953
4.910
4.791
1.337
7.314
7.307
7.297
7.291
7.285
7.274
6.364
6.348
6.339
6.322
6.305
6.296
6.279
OH
OH
N
OMe
3.01
2.98
2.18
1.02
1.07
f1 (ppm)
0.93
1.04
3.01
2.98
2.18
1.02
1.07
1.03
1.00
1.02
1.07
2.93
18.00
f1 (ppm)

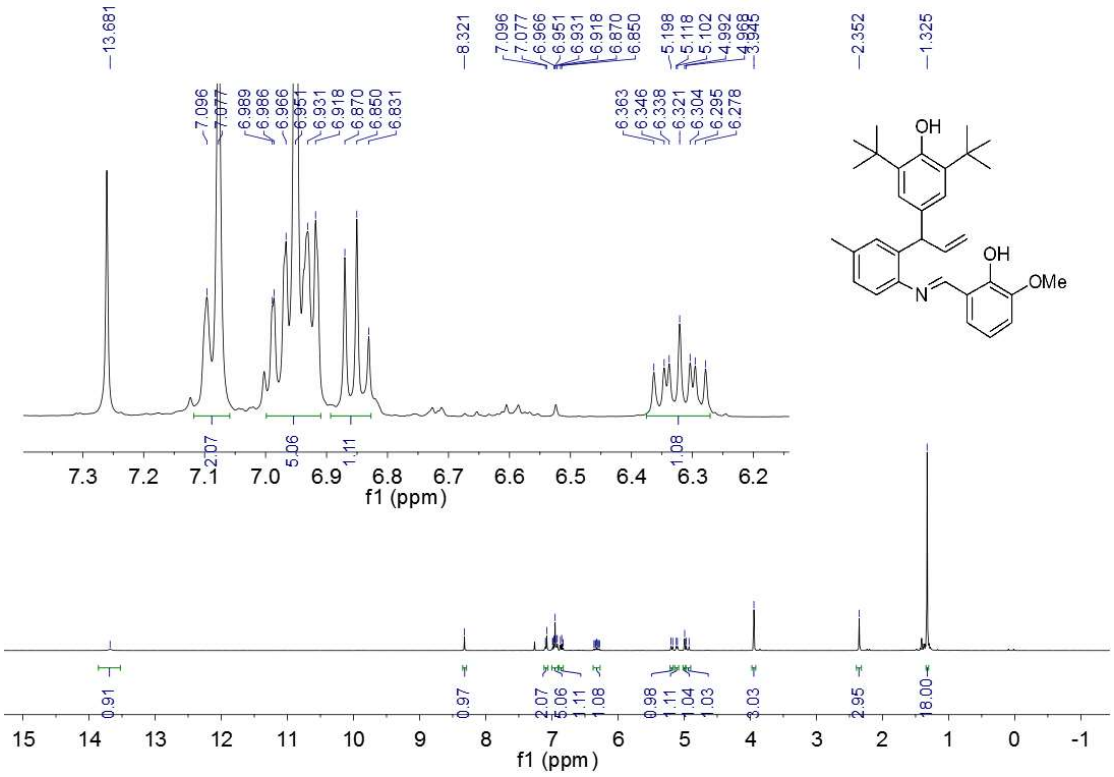

163.04
155.21
152.23
152.02
147.96
140.46
137.53
135.52
132.92
128.85
127.42
126.60
125.33
120.43
118.92
118.70
118.04
116.09
115.34
55.99
49.83
34.29
30.26
OH
OH
N
OMe
f1 (ppm)

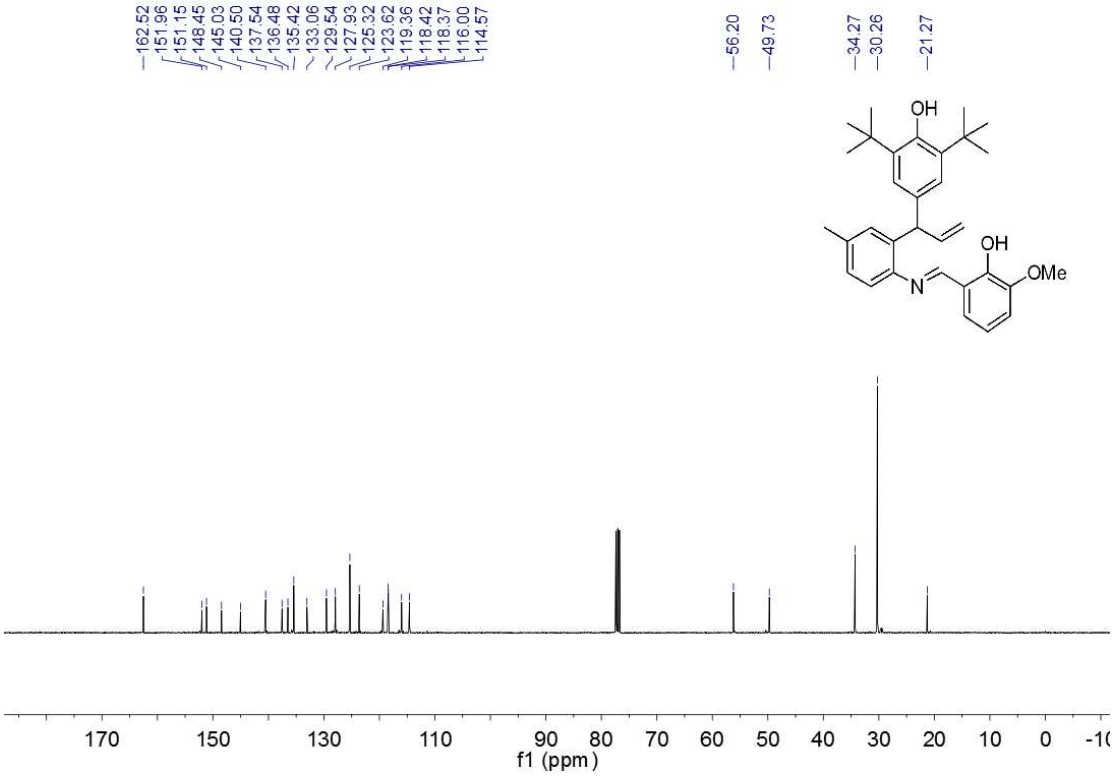
3fa


12.842
8.283
7.276
7.269
6.988
6.967
6.938
6.352
6.335
6.318
5.228
5.203
5.096
5.079
5.001
4.975
4.972
4.932
4.929
1.321
7.441
7.435
7.419
7.413
7.314
7.308
7.298
7.292
7.276
7.269
7.263
7.000
6.997
6.988
6.982
6.977
6.967
6.938
6.378
6.361
6.352
6.335
6.318
6.310
6.293
OH
OH
N
1.07
3.98
2.18
2.08
1.05
f1 (ppm)
0.92
1.05
1.07
3.98
2.18
2.08
1.05
1.07
1.04
1.00
1.06
27.00
f1 (ppm)

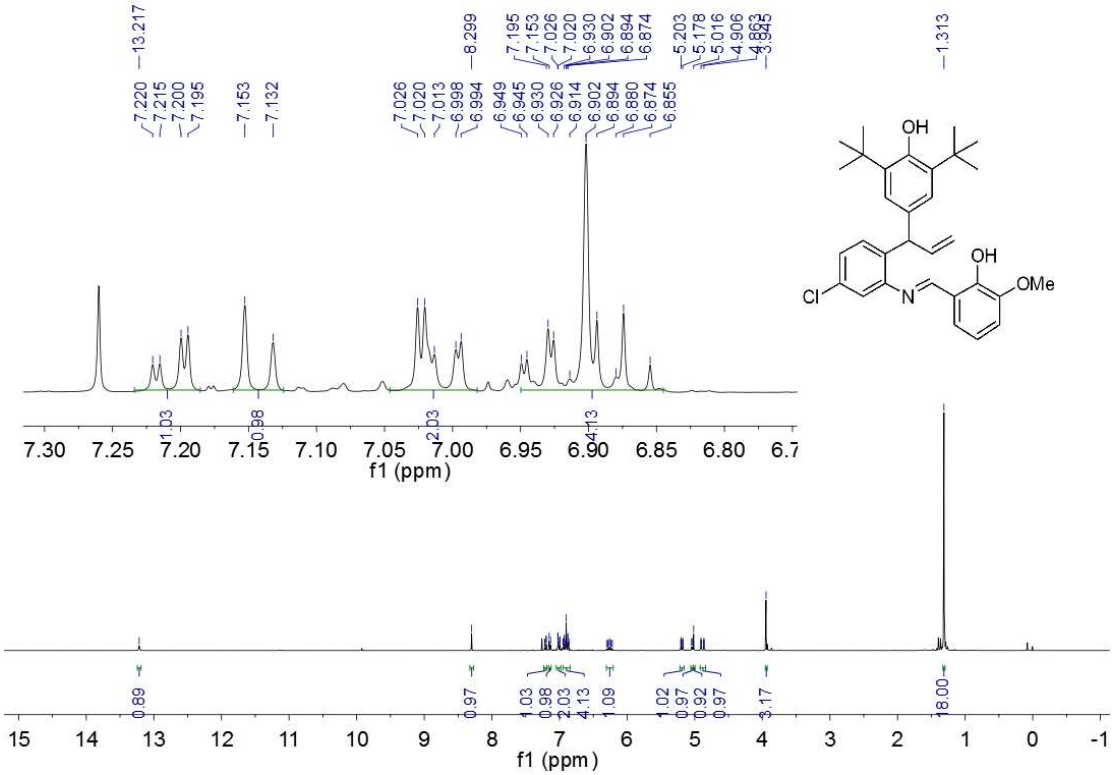

163.85
158.66
151.98
148.26
141.68
140.44
137.48
135.47
133.05
130.58
128.70
128.52
127.42
126.40
125.31
118.84
118.57
116.81
116.09
49.93
34.27
34.01
31.43
30.25
OH
OH
N
f1 (ppm)

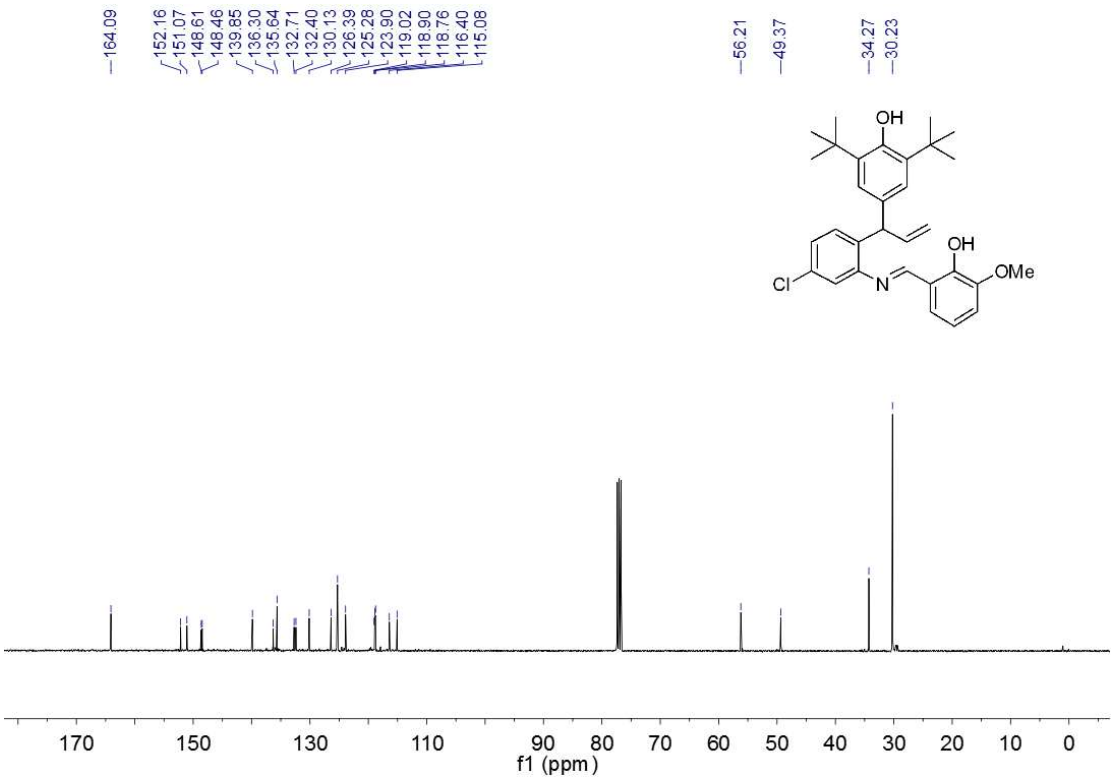
3bc


13.681
8.321
7.096
7.077
6.966
6.951
6.931
6.918
6.870
6.850
5.198
5.118
5.102
4.992
2.352
1.325
6.363
6.346
6.338
6.321
6.304
6.295
6.278
6.989
6.986
6.831
OH
OH
OMe
N
2.07
5.06
1.11
1.08
f1 (ppm)
0.91
0.97
2.07
5.06
1.11
1.08
0.98
1.11
1.04
1.03
3.03
2.95
18.00

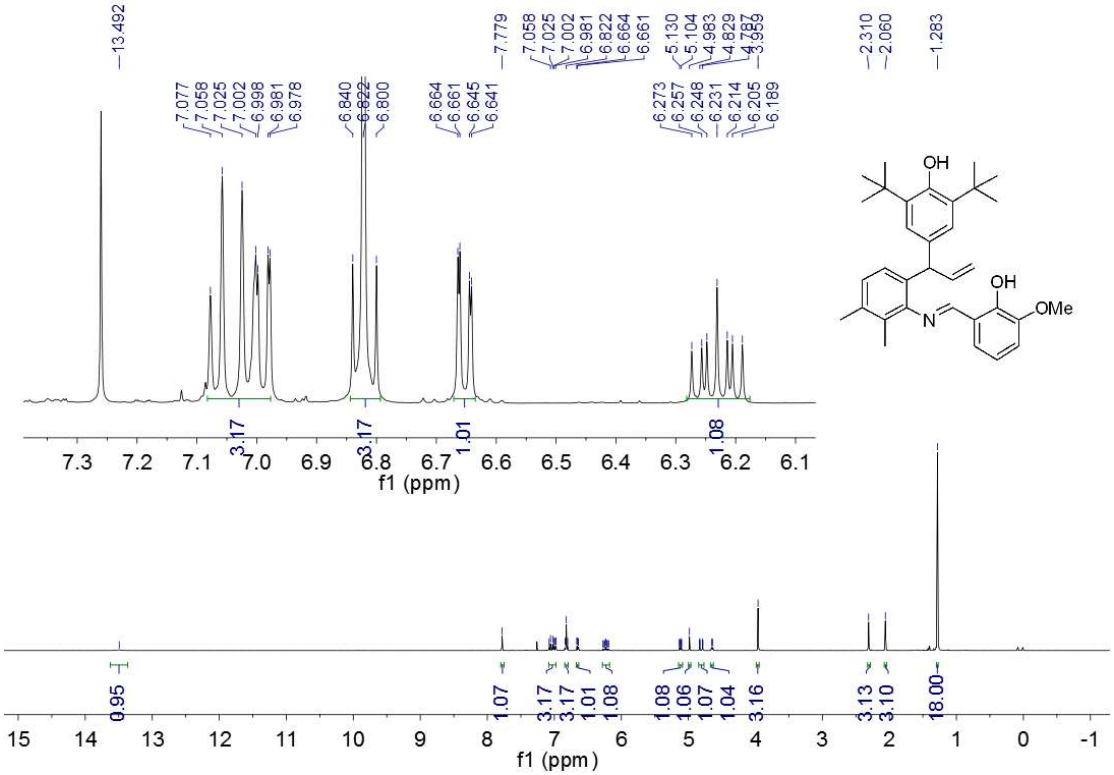

162.52
151.96
151.15
148.45
145.03
140.50
137.54
136.48
135.42
133.06
129.54
127.93
125.32
123.62
119.36
118.42
118.37
116.00
114.57
56.20
49.73
34.27
30.26
21.27
OH
OH
OMe
N
f1 (ppm)

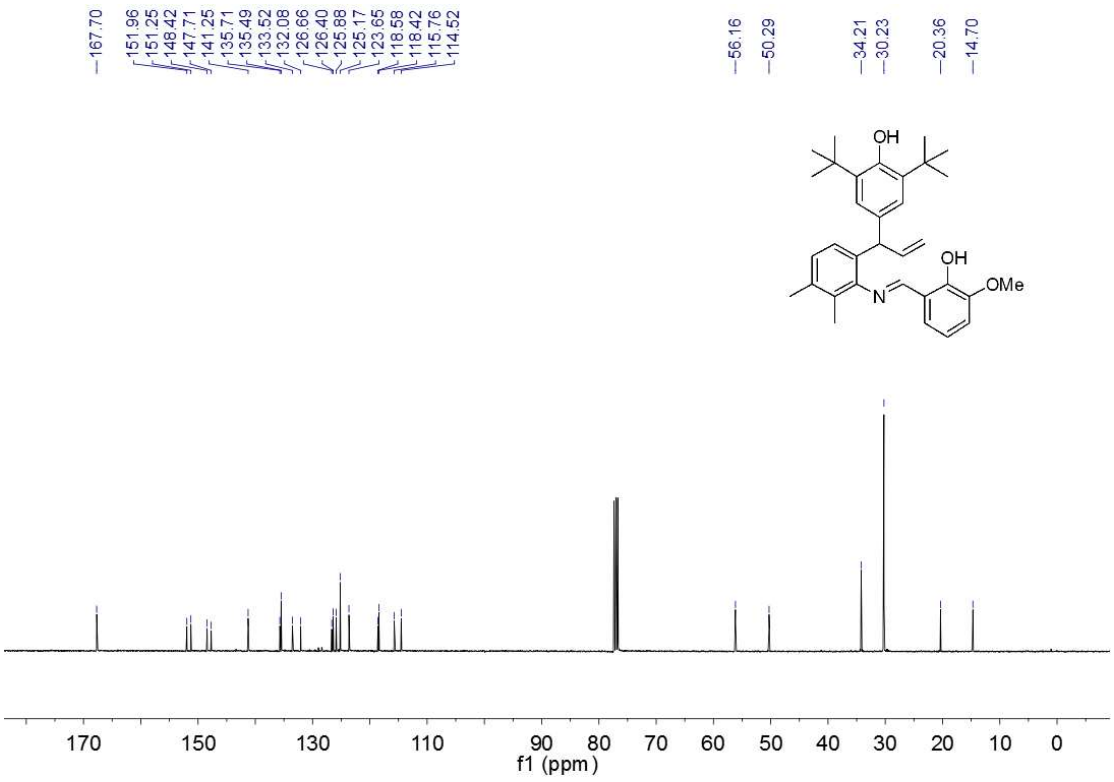
3bi


13.217
8.299
7.220
7.215
7.200
7.195
7.153
7.132
7.026
7.020
7.013
6.998
6.994
6.949
6.945
6.930
6.926
6.914
6.902
6.894
6.880
6.874
6.855
5.203
5.178
5.016
4.906
1.313
OH
OH
OMe
Cl
N
f1 (ppm)

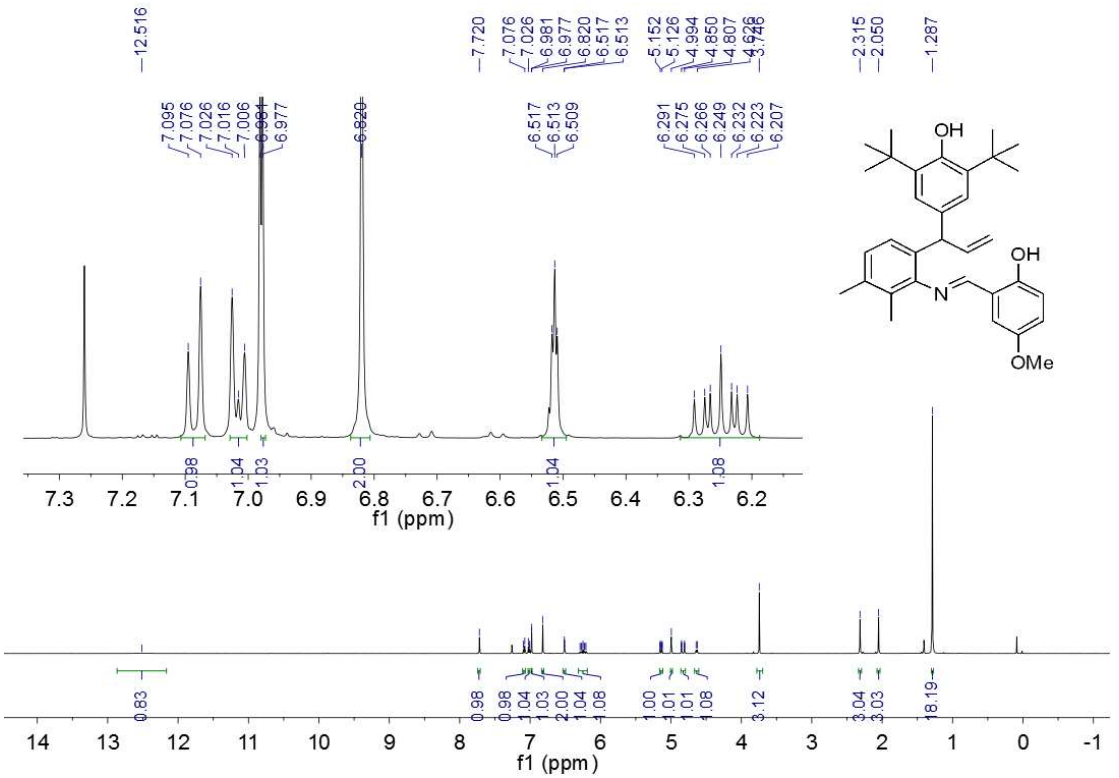

164.09
152.16
151.07
148.61
148.46
139.85
136.30
135.64
132.71
132.40
130.13
126.39
125.28
123.90
119.02
118.90
118.76
116.40
115.08
56.21
49.37
34.27
30.23
OH
OH
OMe
Cl
N
f1 (ppm)

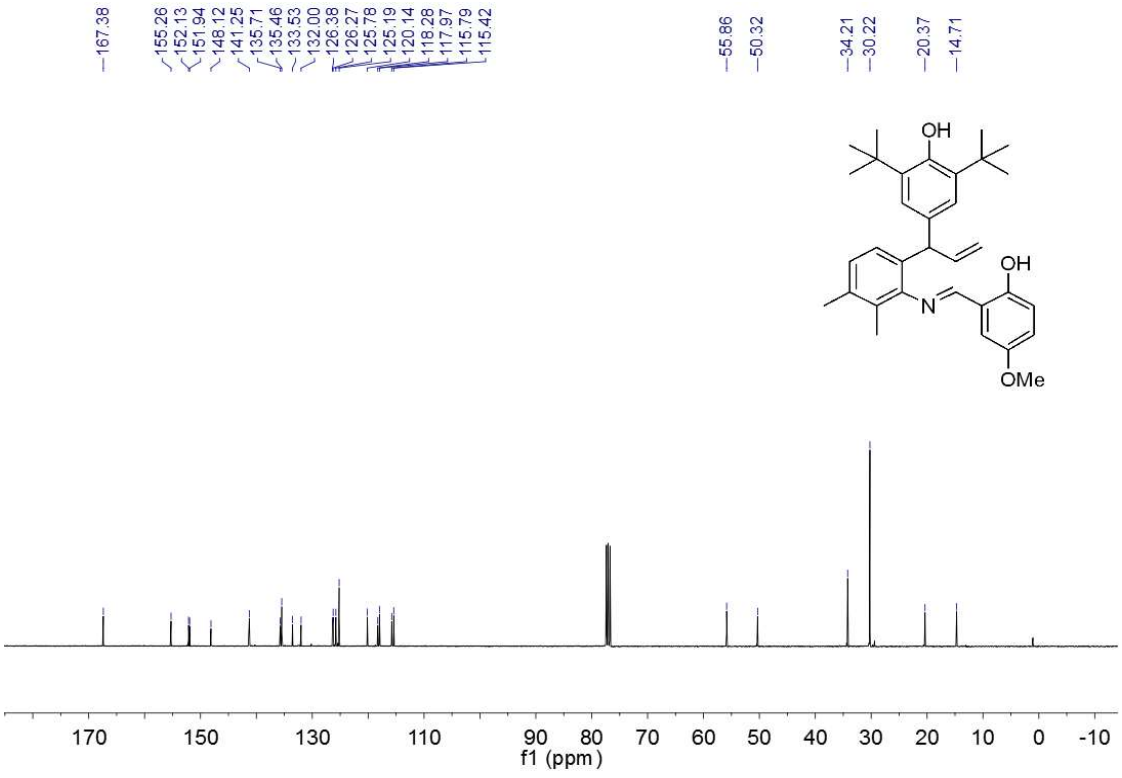
3bk


13.492
7.779
7.077
7.058
7.025
7.002
6.998
6.981
6.978
6.840
6.832
6.800
6.664
6.661
6.645
6.641
7.058
7.025
7.002
6.981
6.822
6.664
6.661
6.273
6.257
6.248
6.231
6.214
6.205
6.189
5.130
5.104
4.983
4.829
4.827
3.959
2.310
2.060
1.283
OH
OH
OMe
N
3.17
3.17
1.01
1.08
f1 (ppm)
0.95
1.07
3.17
3.17
1.01
1.08
1.08
1.06
1.07
1.04
3.16
3.13
3.10
18.00
f1 (ppm)

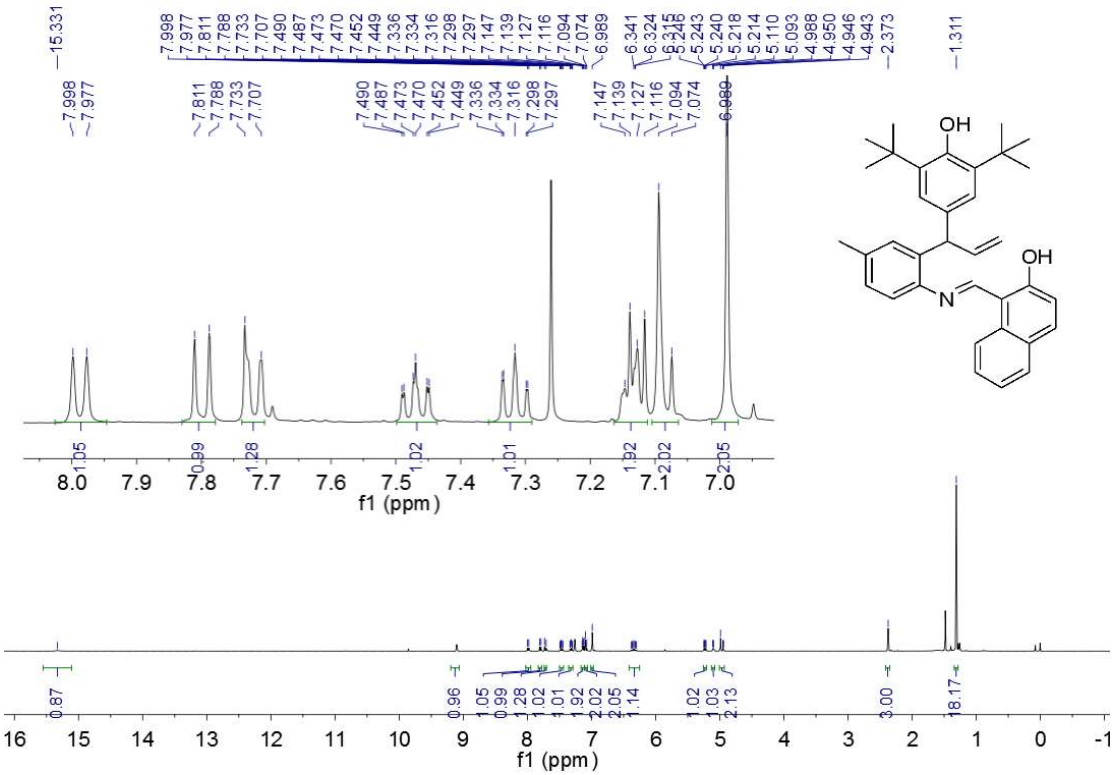

167.70
151.96
151.25
148.42
147.71
141.25
135.71
135.49
133.52
132.08
126.66
126.40
125.88
125.17
123.65
118.58
118.42
115.76
114.52
56.16
50.29
34.21
30.23
20.36
14.70
OH
OH
OMe
N
f1 (ppm)

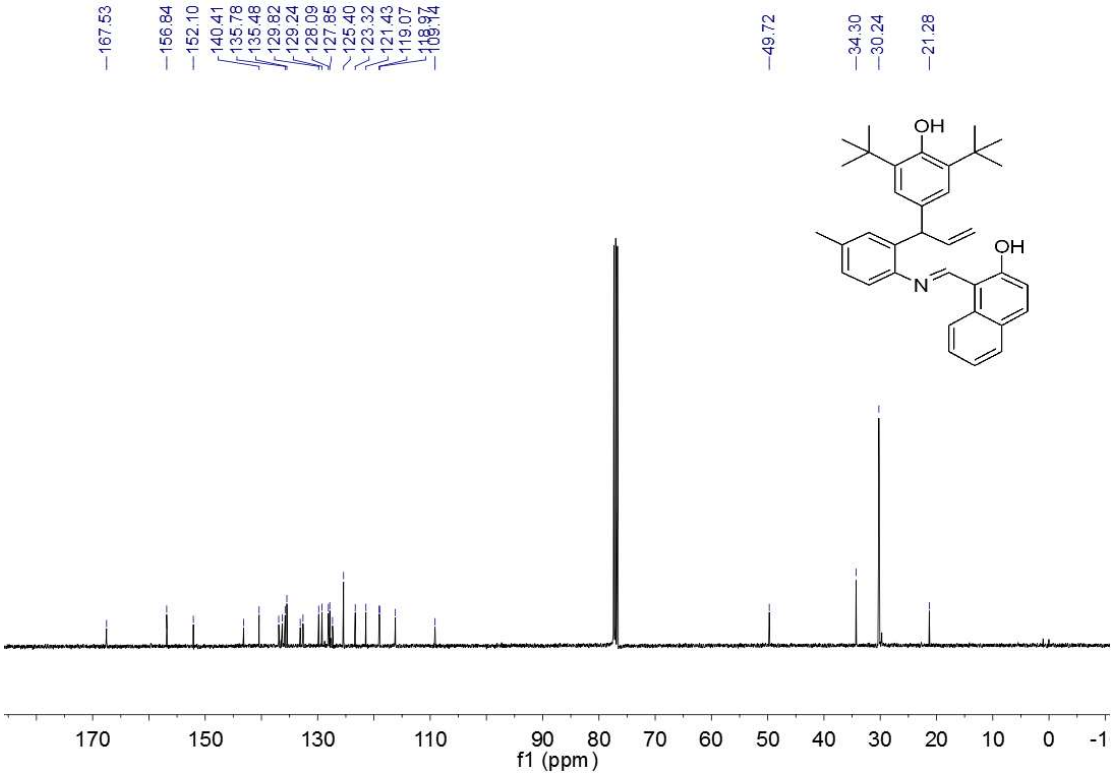
3ek


12.516
7.720
7.095
7.076
7.026
7.016
7.006
6.977
6.820
6.517
6.513
6.509
6.291
6.275
6.266
6.249
6.232
6.223
6.207
5.152
5.126
4.994
4.850
4.807
3.748
2.315
2.050
1.287
OH
OH
N
OMe
f1 (ppm)

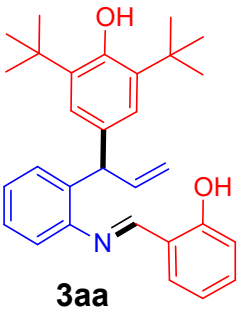

167.38
155.26
152.13
151.94
148.12
141.25
135.71
135.46
133.53
132.00
126.38
126.27
125.78
125.19
120.14
118.28
117.97
115.79
115.42
55.86
50.32
34.21
30.22
20.37
14.71
OH
OH
N
OMe
f1 (ppm)

3jc

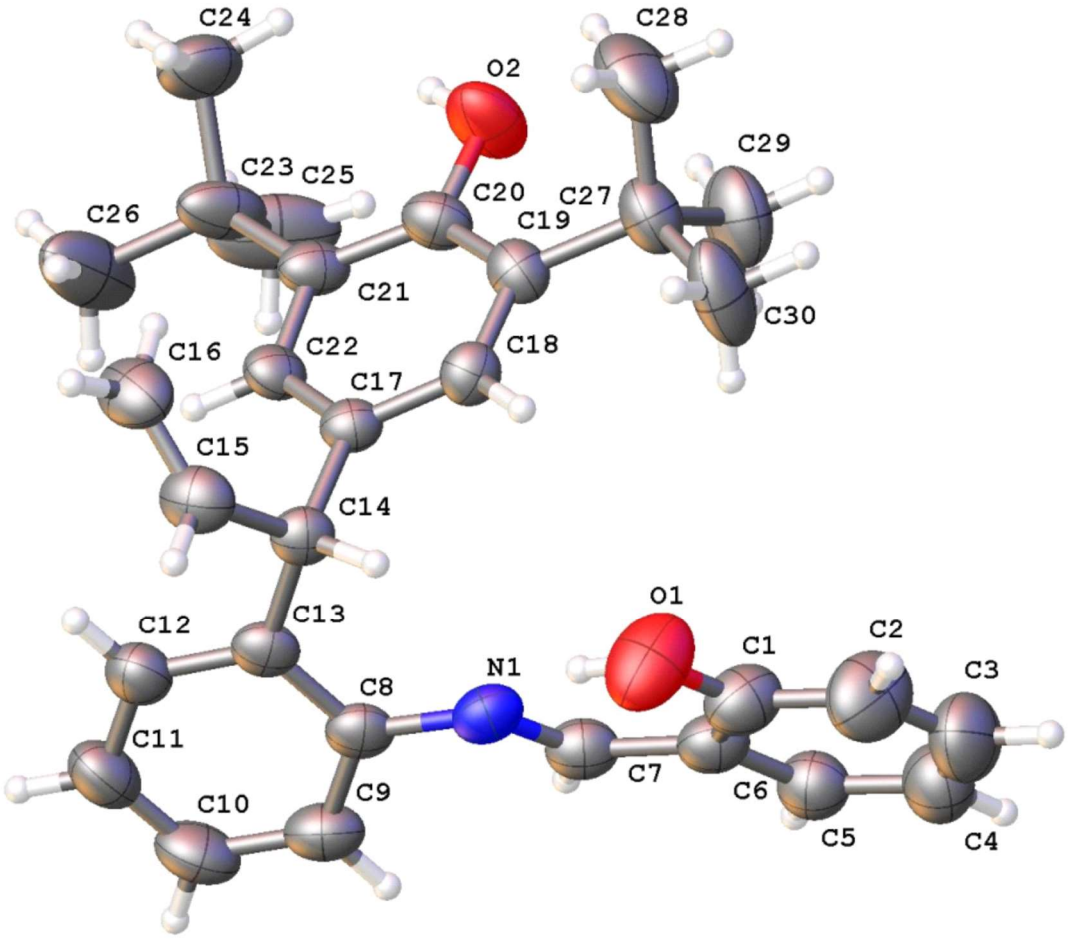

15.331
7.998
7.977
7.811
7.788
7.733
7.707
7.490
7.487
7.473
7.470
7.452
7.449
7.336
7.334
7.316
7.298
7.297
7.147
7.139
7.127
7.116
7.094
7.074
6.989
6.341
6.324
6.315
6.246
5.243
5.240
5.218
5.214
5.110
5.093
4.988
4.950
4.946
4.943
2.373
1.311
OH
OH
N
f1 (ppm)


167.53
156.84
152.10
140.41
135.78
135.48
129.82
129.24
128.09
127.85
125.40
123.32
121.43
119.07
49.72
34.30
30.24
21.28
OH
OH
N
f1 (ppm)

2. Single crystal data of product 3aa



3aa



The thermal ellipsoid was drawn at the 30% probability level.

Empirical formula	C30 H35 N O2	
Formula weight	441.59	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.229(13) Å	α= 88.979(15)°.

	b = 10.292(13) Å	β= 78.134(14)°.
	c = 12.452(16) Å	γ = 86.738(14)°.
Volume	1281(3) Å^3	
Z	2	
Density (calculated)	1.145 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	476	
Crystal size	0.3 x 0.3 x 0.16 mm^3	
Theta range for data collection	2.356 to 25.998°.	
Index ranges	-12<=h<=12, -12<=k<=12, -12<=l<=15	
Reflections collected	8334	
Independent reflections	4937 [R(int) = 0.0889]	
Completeness to theta = 25.242°	98.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4937 / 1 / 309	
Goodness-of-fit on F^2	0.984	
Final R indices [I>2sigma(I)]	R1 = 0.0638, wR2 = 0.1701	
R indices (all data)	R1 = 0.0900, wR2 = 0.1889	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.238 and -0.297 e.Å^{-3}	