catalysts

MDPI

Supplementary Materials

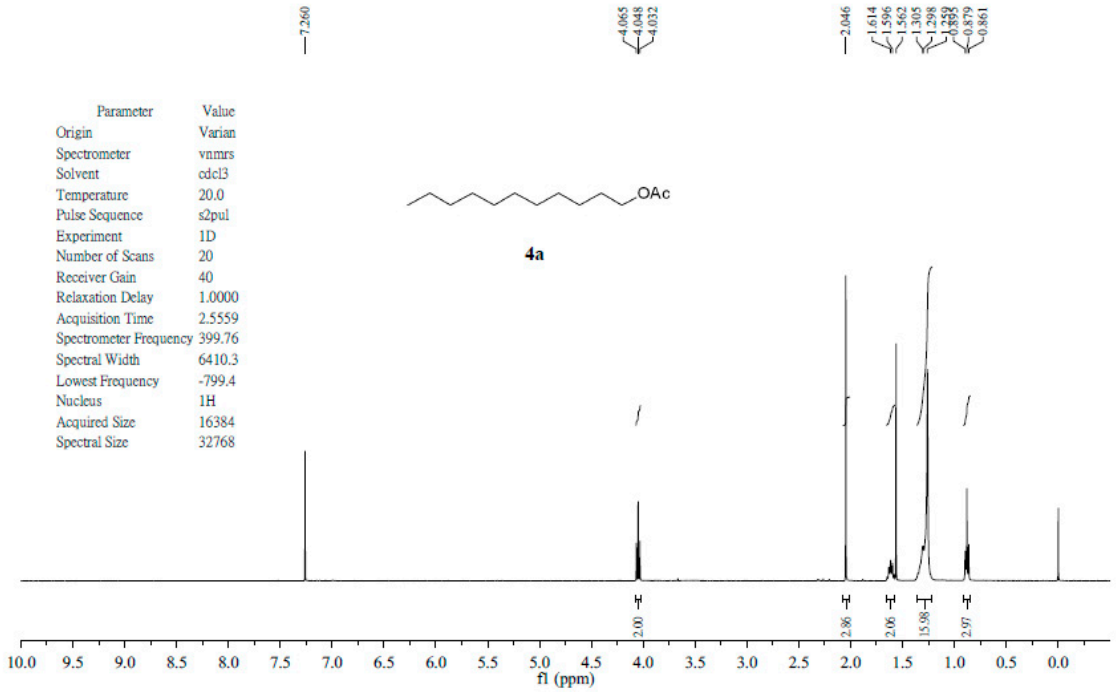
Mild and Efficient Tunable Brønsted Acidic Ionic Liquid Catalyzed *O*-Acetylation and *O*-Trimethylsilylation with Trimethylsilyl Acetate (TMSOAc) and Hexamethyldisilazane (HMDS)

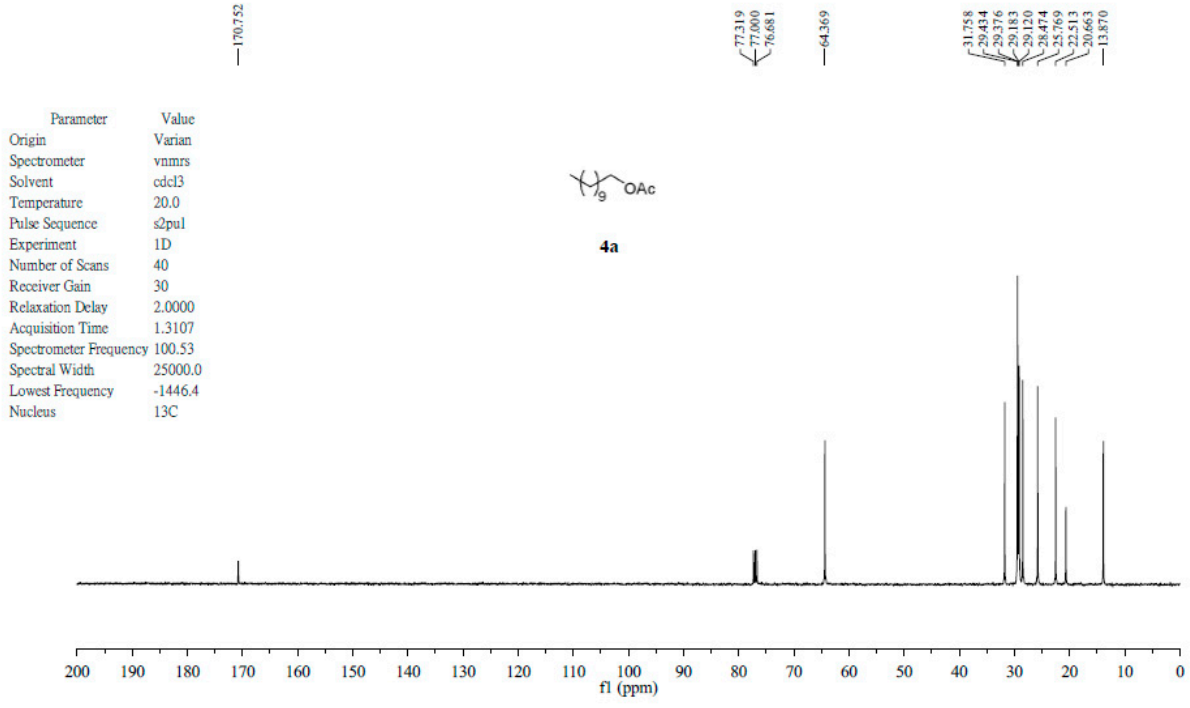
Amit Ravindra Pantawane [1,†], Mayur Thul [1,†], Yi-Jyun Lin [1], Michelle Lin [2], Wesley Lin [2], Satyanarayana Reddy Julakanti [3], Hsin-Ru Wu [4] and Shun-Yuan Luo [1,*]

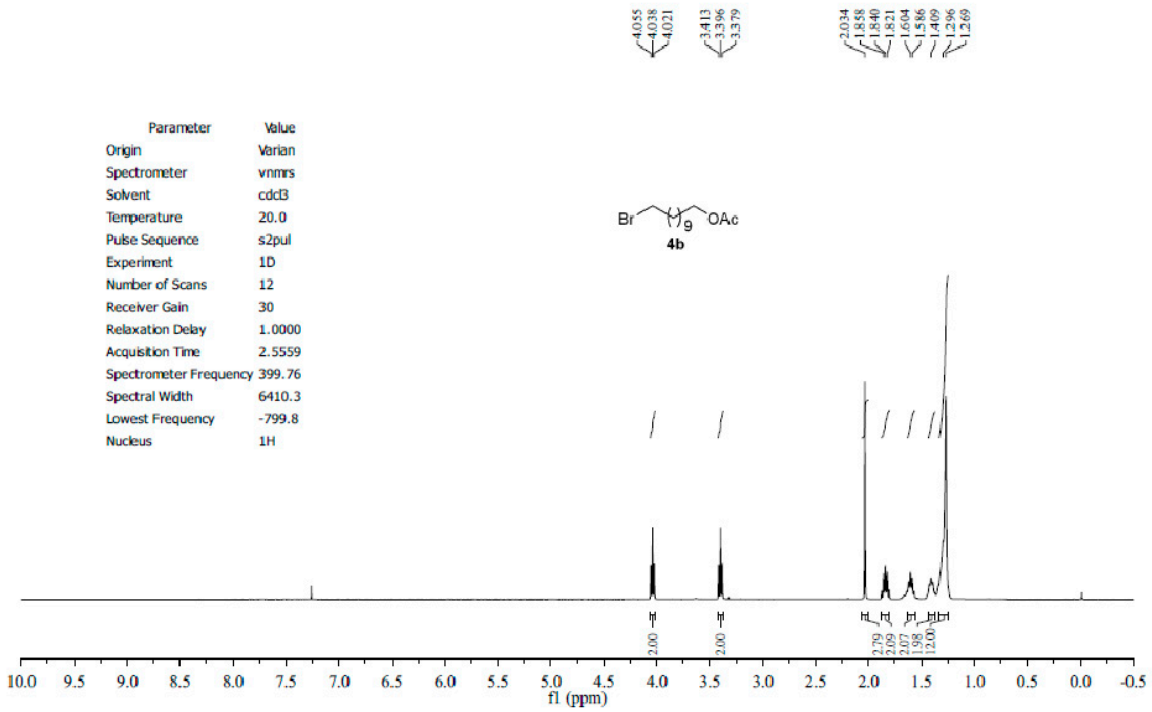
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[3] Institute of Biotechnology and Pharmaceutical Research, National Health Research Institutes, 35 Keyan Road, Zhunan, Miaoli County 35053, Taiwan; sjsnreddy@gmail.com
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† A.R.P. and M.T. contributed equally.

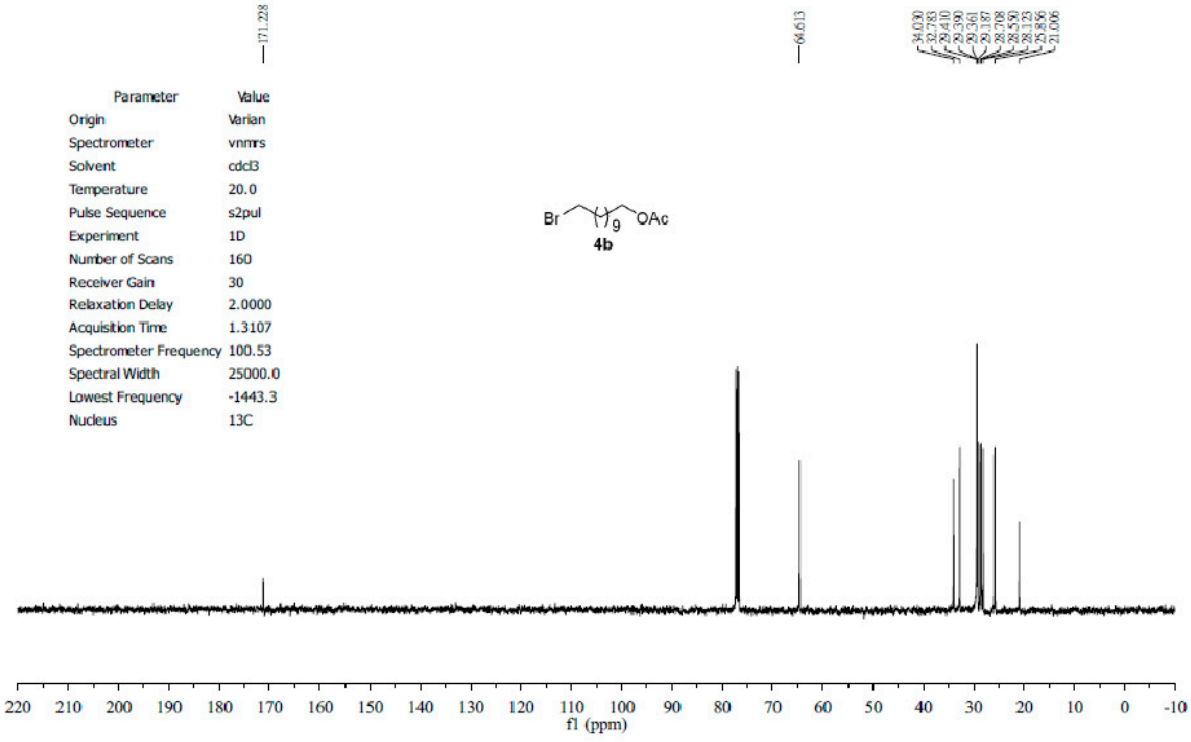
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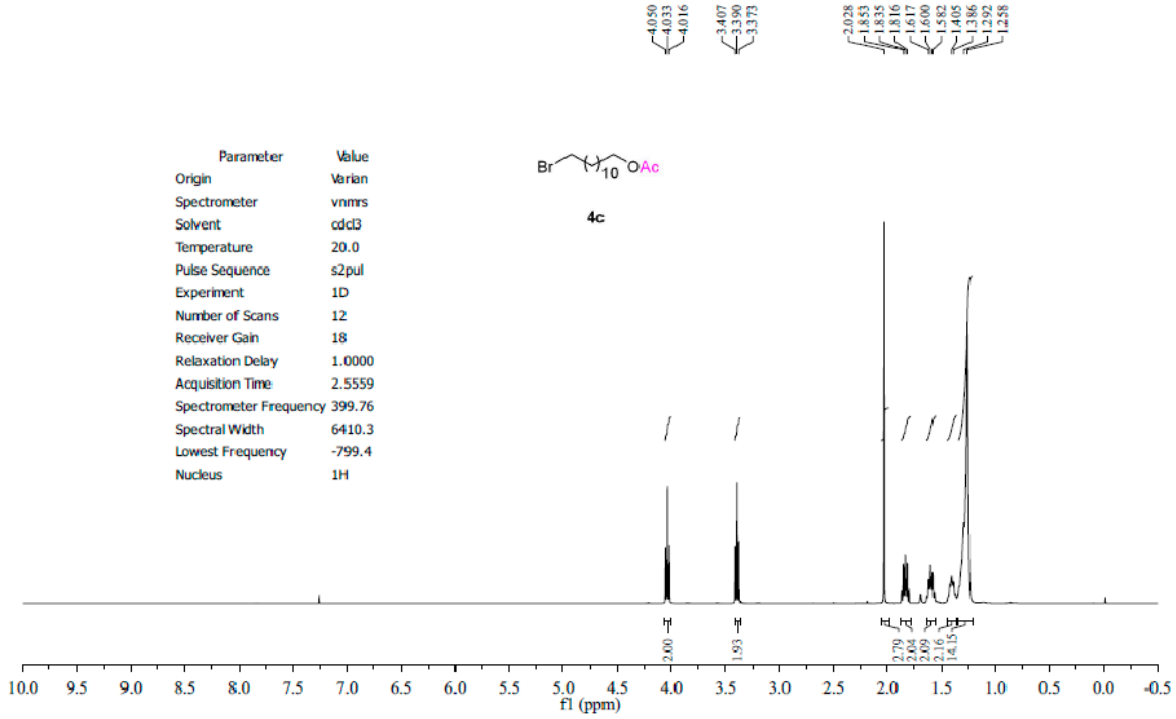
[1]HNMR and [13]C NMR of all compounds 2–20

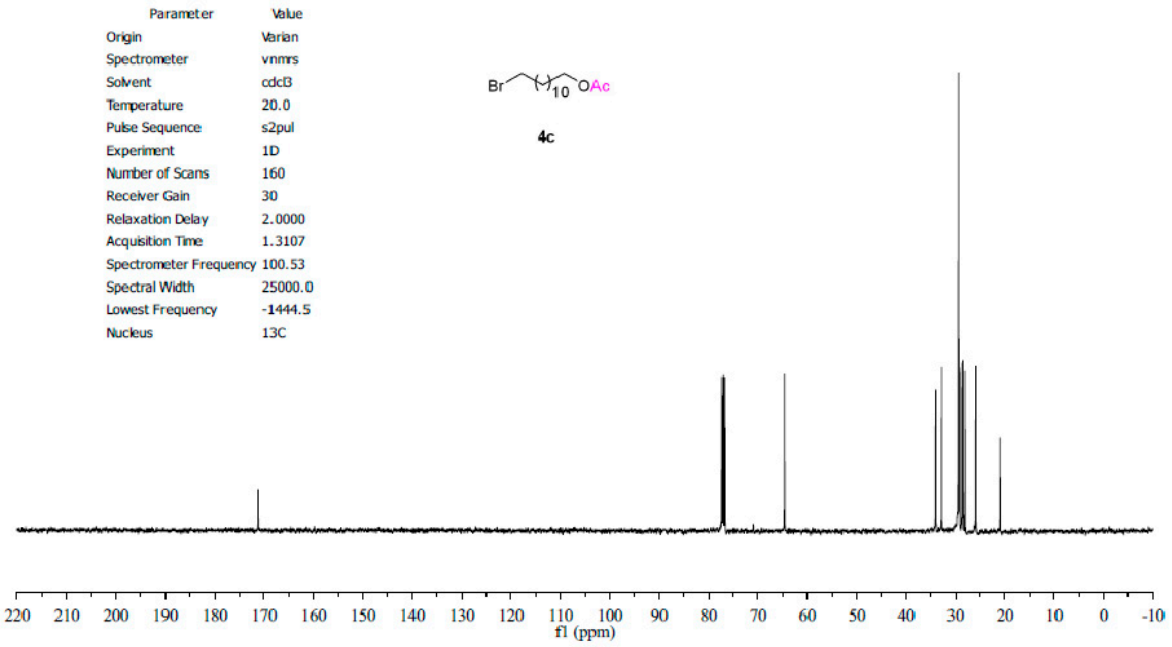


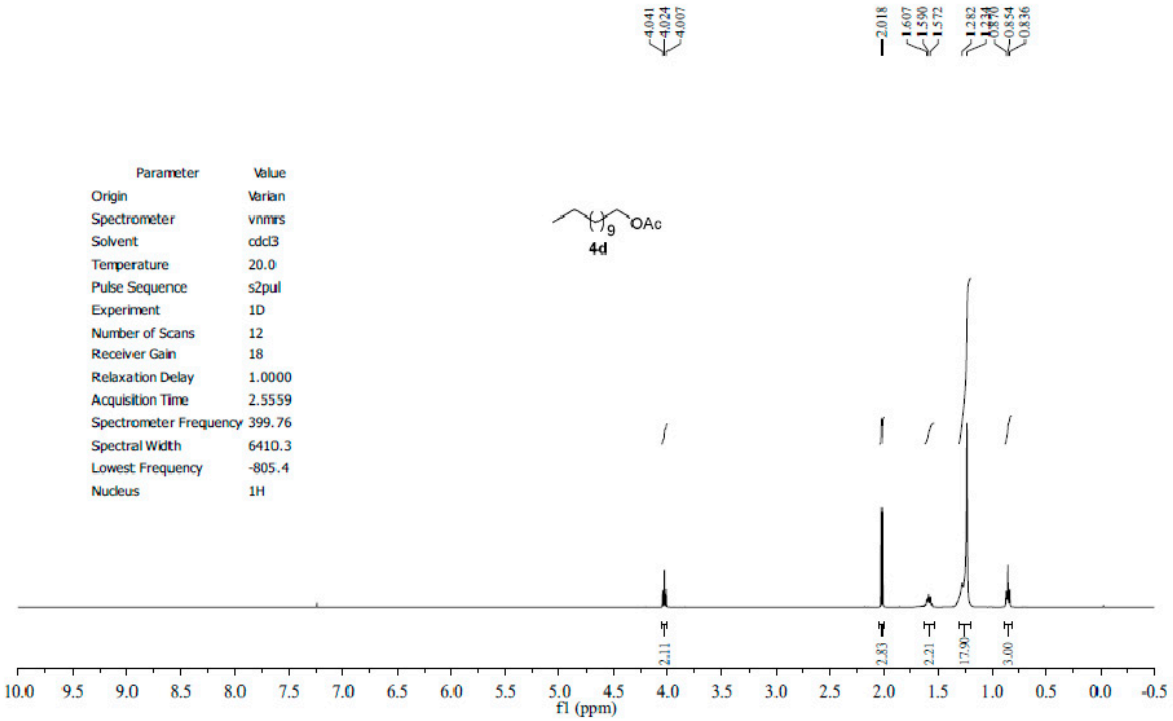


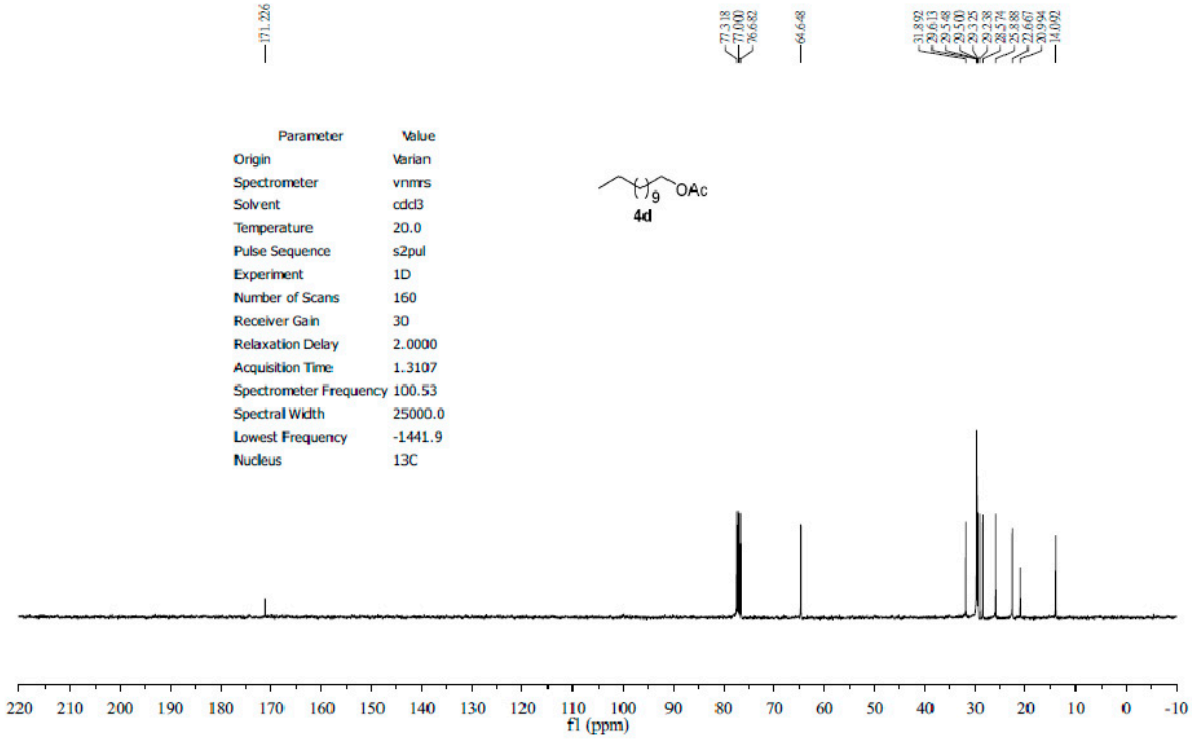

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3.413
3.396
3.379
2.034
1.858
1.840
1.821
1.604
1.586
1.409
1.296
1.269
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Solvent cdcl3
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Pulse Sequence s2pul
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Number of Scans 12
Receiver Gain 30
Relaxation Delay 1.0000
Acquisition Time 2.5559
Spectrometer Frequency 399.76
Spectral Width 6410.3
Lowest Frequency -799.8
Nucleus 1H
Br
9
OAc
4b
2.00
2.00
2.79
2.09
2.07
1.98
12.00
10.0 9.5 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 -0.5
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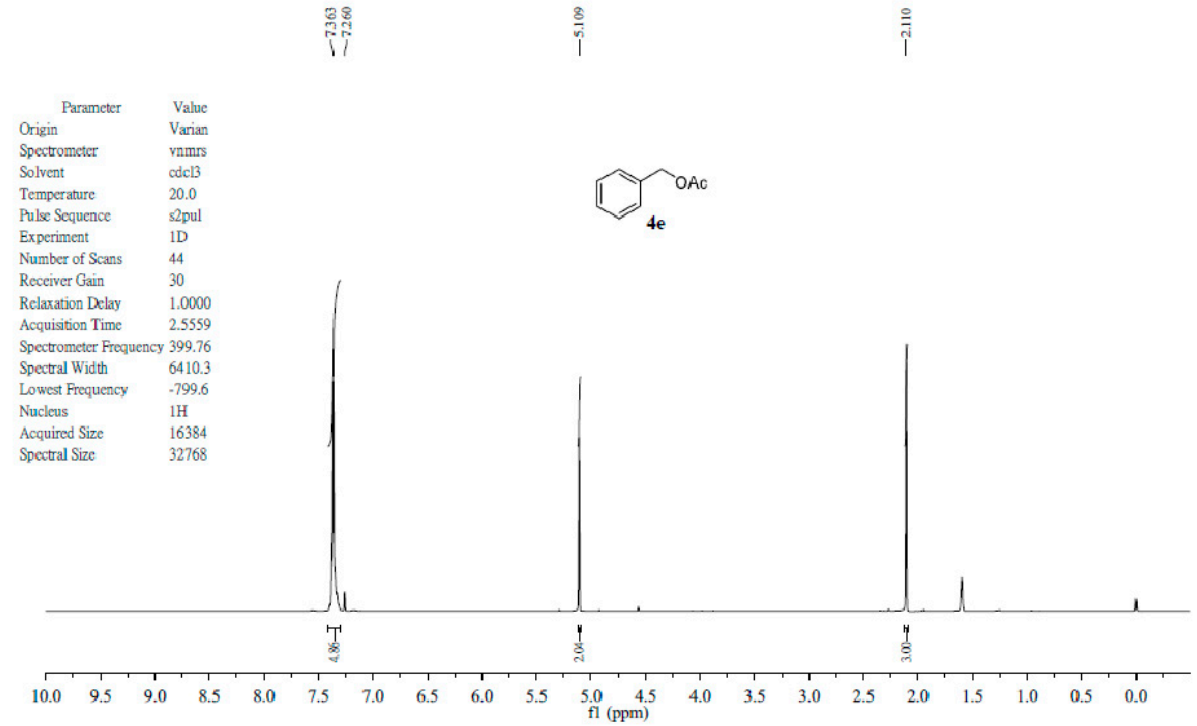

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32.783
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29.390
29.361
29.187
28.708
28.550
28.123
25.856
21.006
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Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 160
Receiver Gain 30
Relaxation Delay 2.0000
Acquisition Time 1.3107
Spectrometer Frequency 100.53
Spectral Width 25000.0
Lowest Frequency -1443.3
Nucleus 13C
Br
9
OAc
4b
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f1 (ppm)

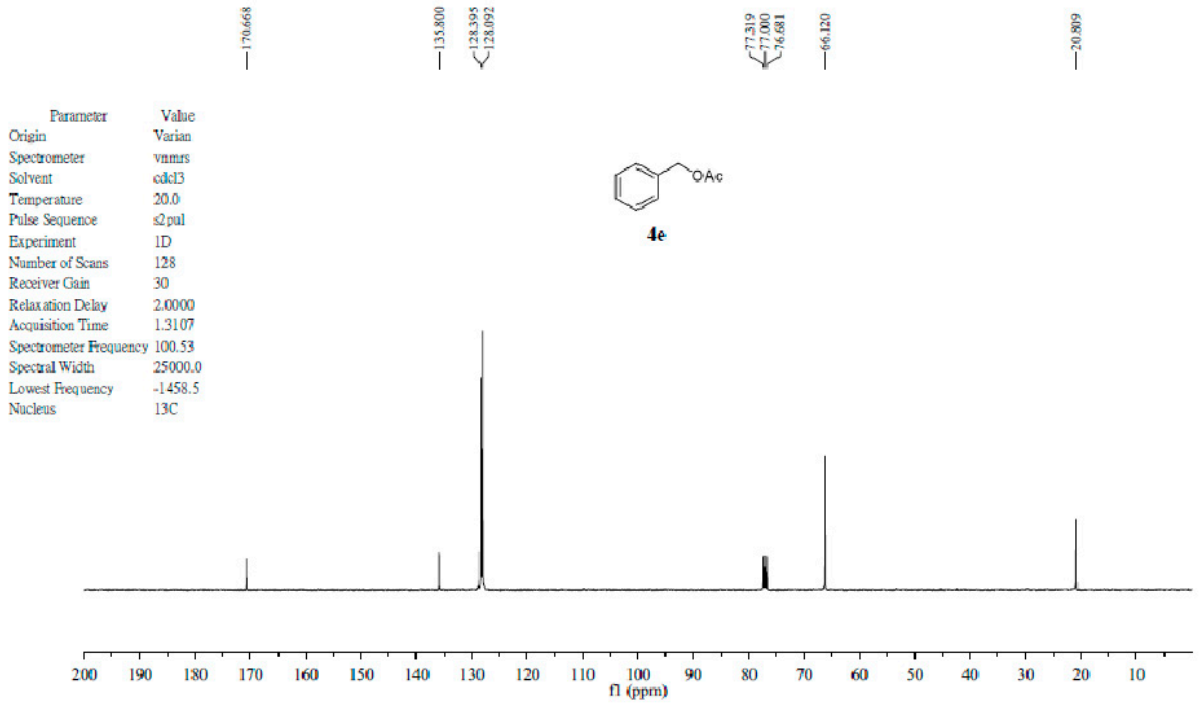

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3.390
3.373
2.028
1.853
1.835
1.816
1.617
1.600
1.582
1.405
1.386
1.292
1.258
Parameter Value
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 12
Receiver Gain 18
Relaxation Delay 1.0000
Acquisition Time 2.5559
Spectrometer Frequency 399.76
Spectral Width 6410.3
Lowest Frequency -799.4
Nucleus 1H
Br
10
OAc
4c
2.00
1.93
2.79
2.04
2.09
2.16
14.15
10.0 9.5 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 -0.5
f1 (ppm)

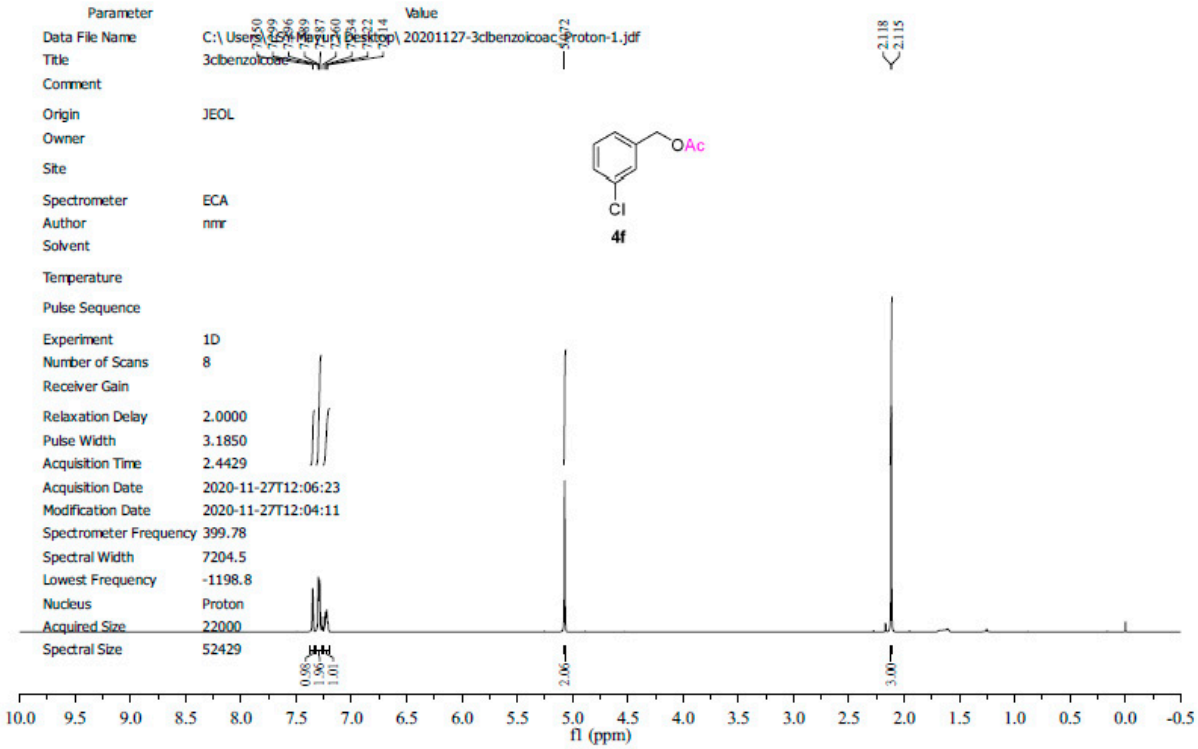

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Spectrometer vnmrs
Solvent cdcl3
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Pulse Sequence s2pul
Experiment 1D
Number of Scans 160
Receiver Gain 30
Relaxation Delay 2.0000
Acquisition Time 1.3107
Spectrometer Frequency 100.53
Spectral Width 25000.0
Lowest Frequency -1444.5
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Br
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OAc
4c
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f1 (ppm)

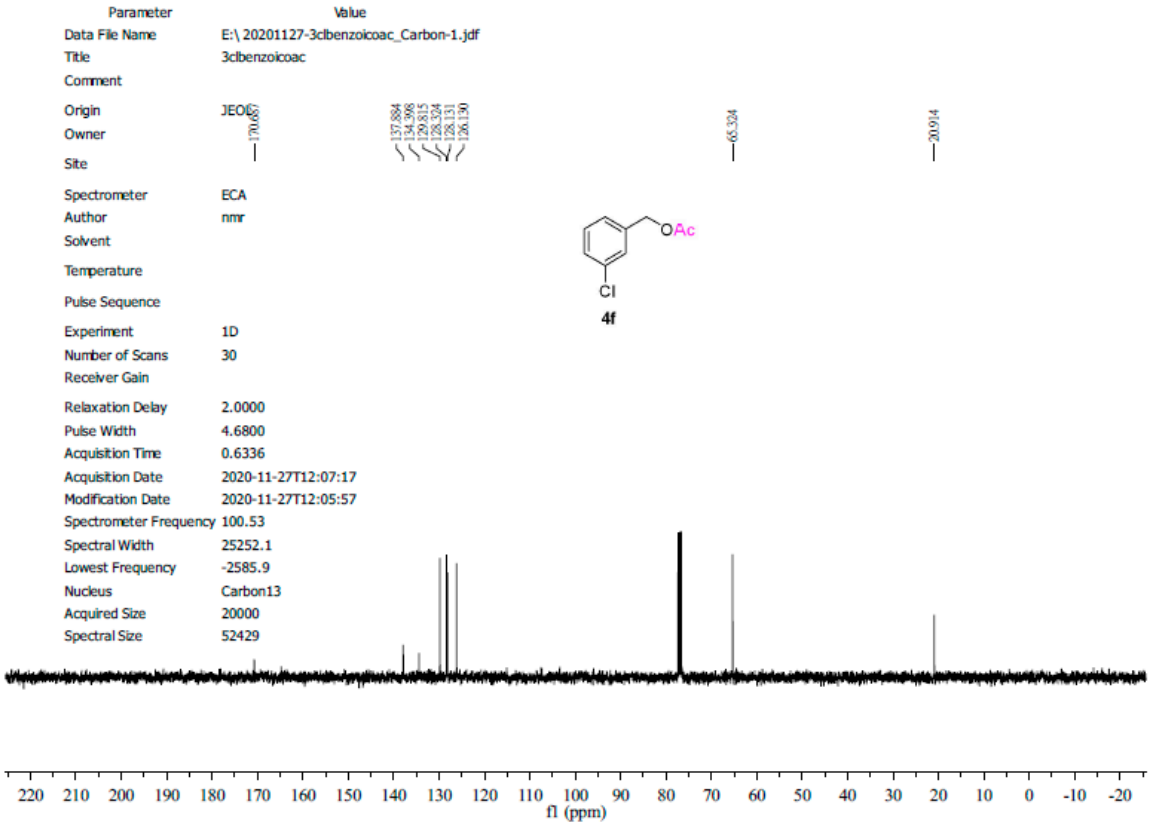

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0.836
Parameter Value
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 12
Receiver Gain 18
Relaxation Delay 1.0000
Acquisition Time 2.5559
Spectrometer Frequency 399.76
Spectral Width 6410.3
Lowest Frequency -805.4
Nucleus 1H
OAc
9
4d
2.11
2.83
2.21
17.99
3.00
10.0 9.5 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 -0.5
f1 (ppm)

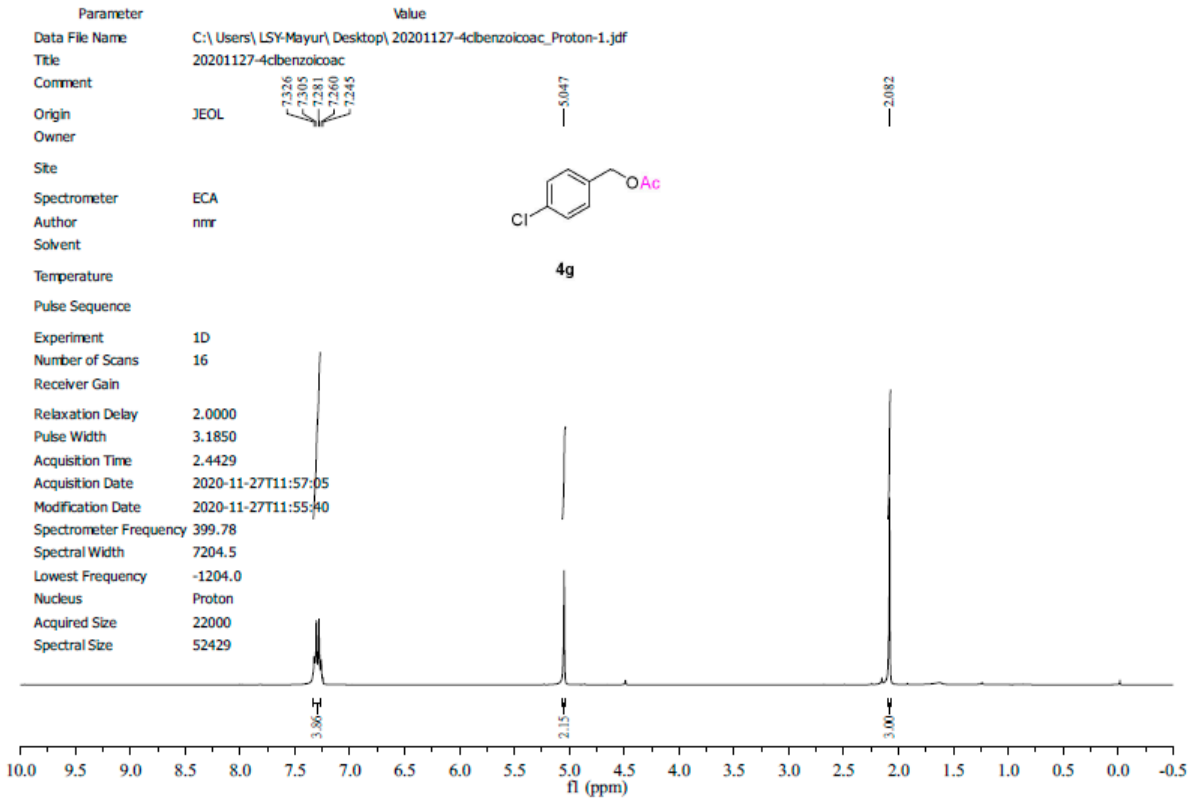

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77.000
76.682
66.648
31.892
29.613
29.548
29.500
29.325
29.238
28.574
25.888
22.667
20.994
14.092
Parameter Value
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 160
Receiver Gain 30
Relaxation Delay 2.0000
Acquisition Time 1.3107
Spectrometer Frequency 100.53
Spectral Width 25000.0
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Nucleus 13C
OAc
9
4d
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f1 (ppm)

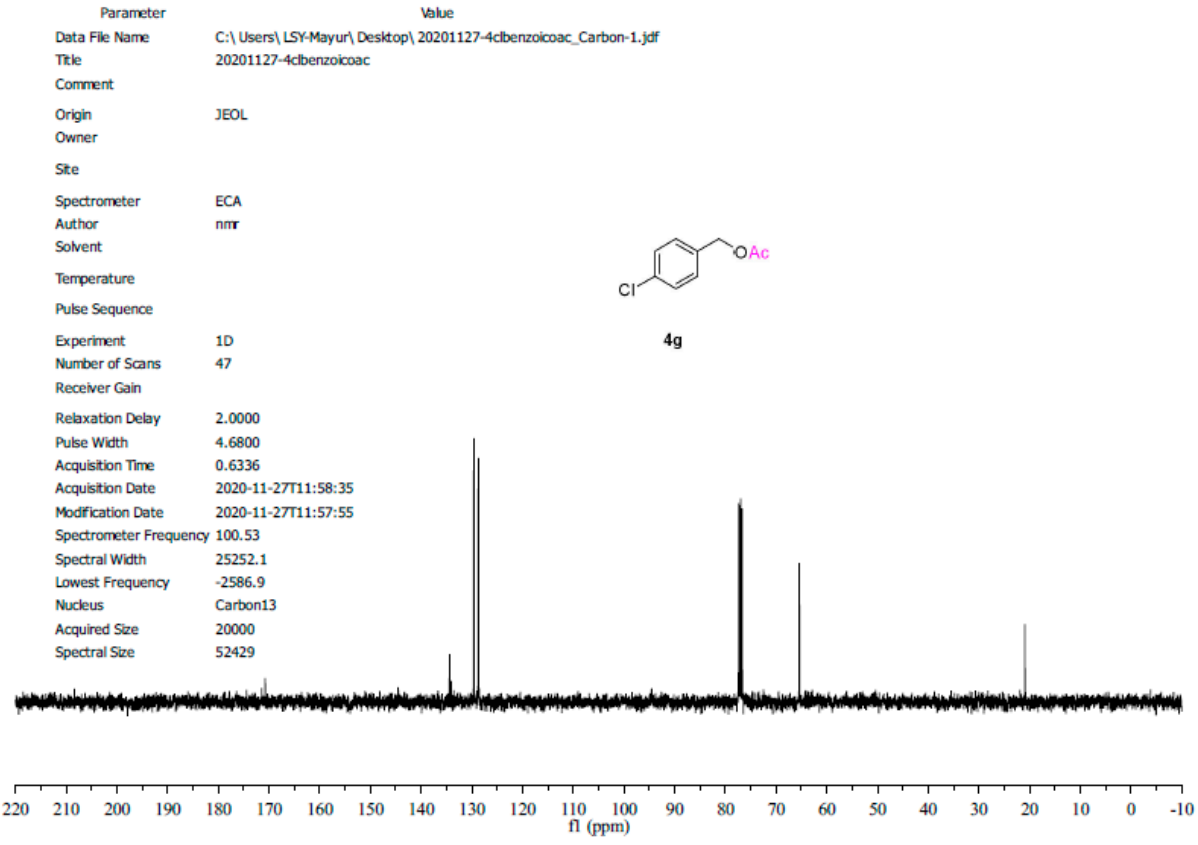

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Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
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Acquisition Time 2.5559
Spectrometer Frequency 399.76
Spectral Width 6410.3
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3.00
f1 (ppm)

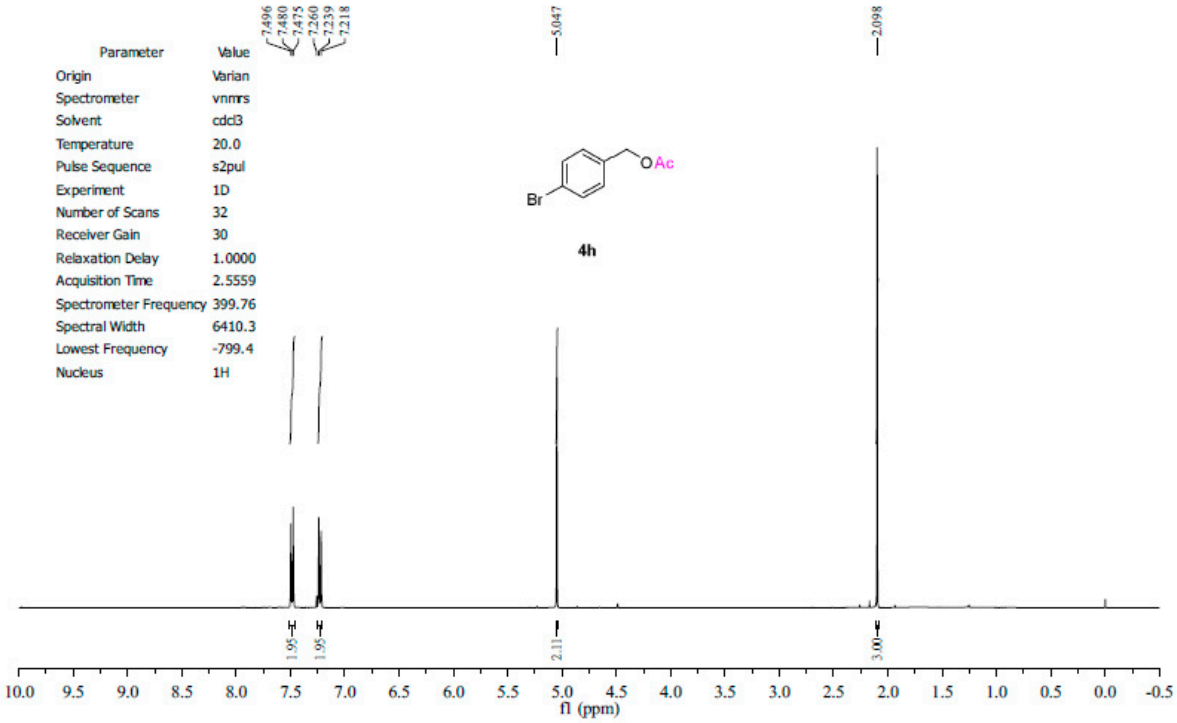

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135.800
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128.092
77.319
77.000
76.681
66.120
20.809
Parameter Value
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 128
Receiver Gain 30
Relaxation Delay 2.0000
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Nucleus 13C
OAc
4e
f1 (ppm)

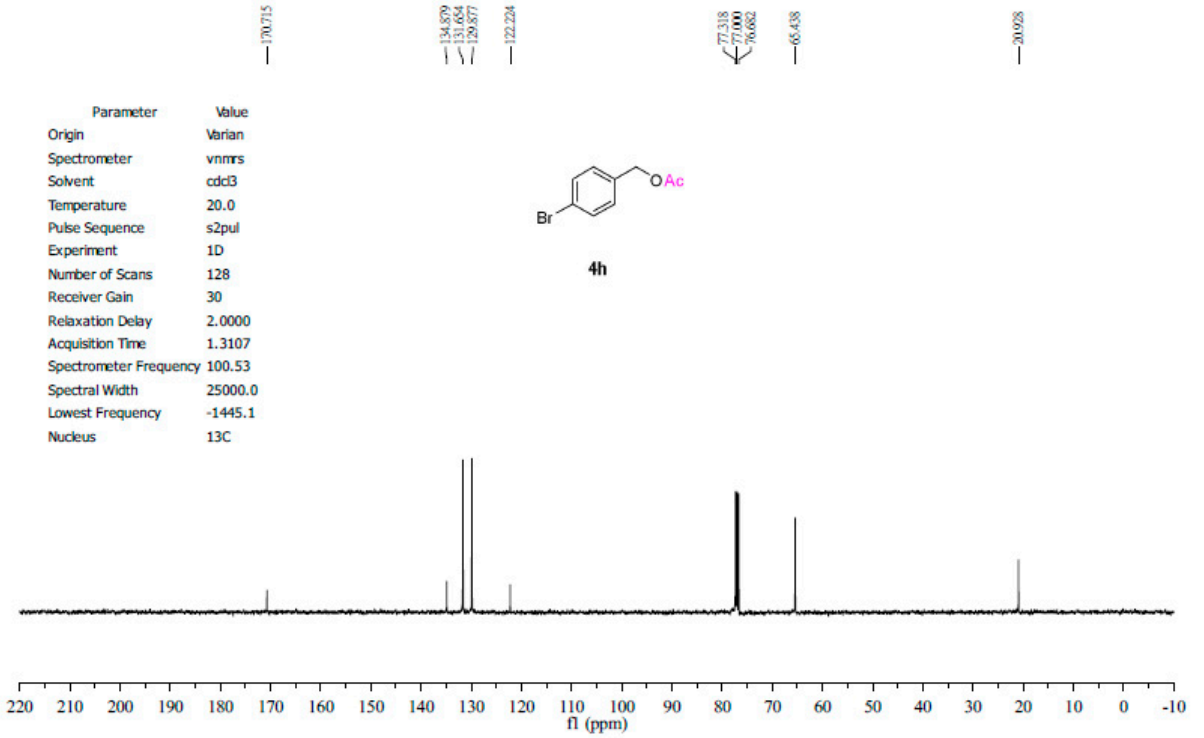

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Solvent
Temperature
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Spectral Size 52429
OAc
Cl
4f
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7.596
7.589
7.587
7.560
7.534
7.522
7.514
5.072
2.118
2.115
0.99
1.96
1.03
2.06
3.00
10.0 9.5 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 -0.5
f1 (ppm)

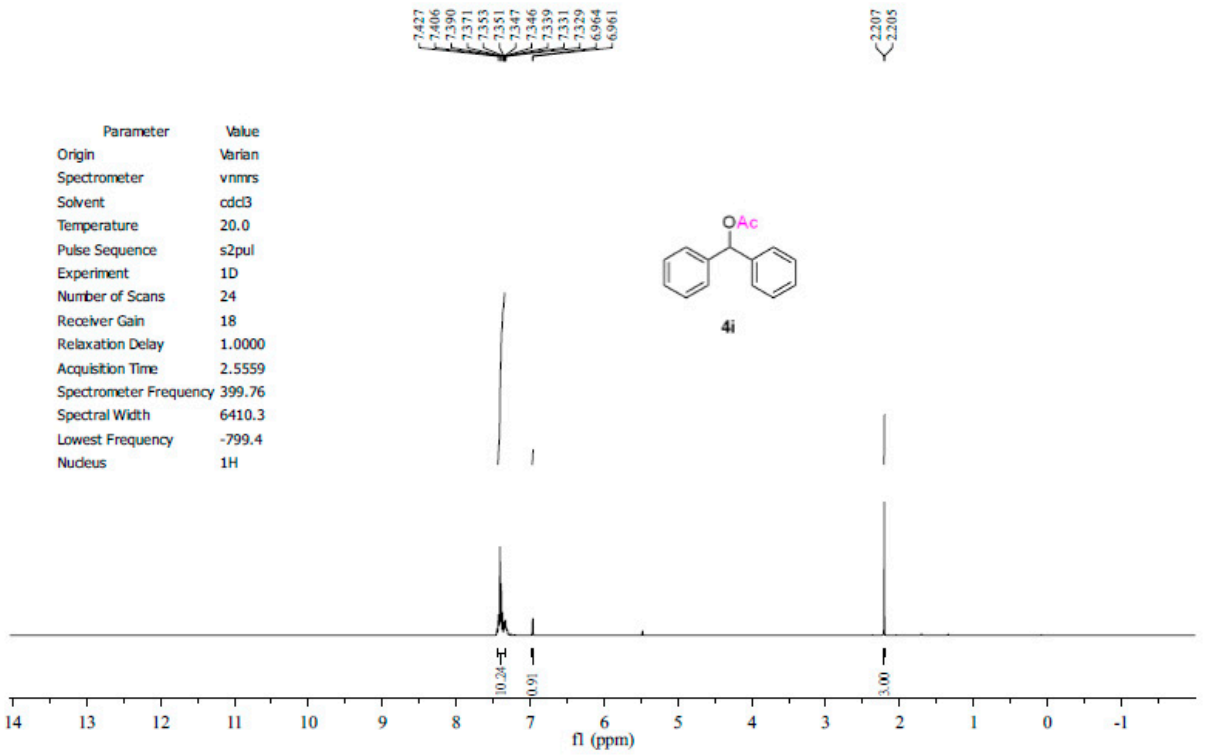

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Solvent
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Spectral Size 52429
OAc
Cl
4f
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134.396
129.815
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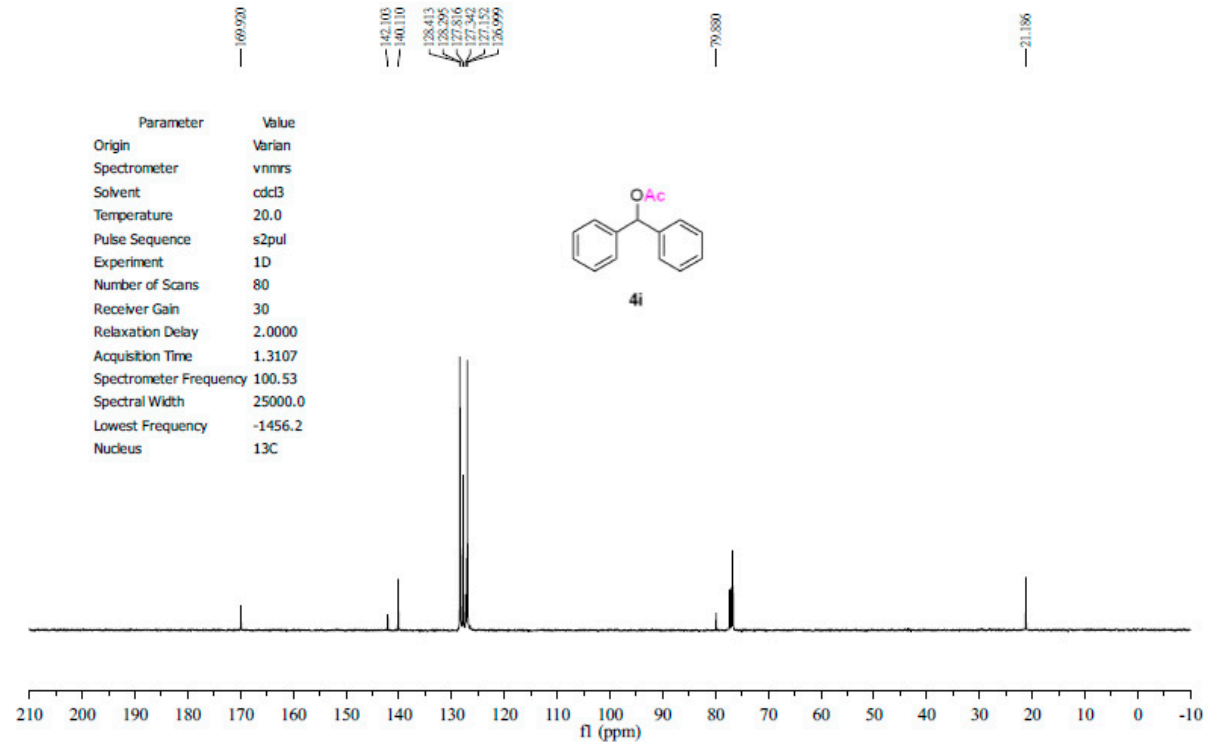

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Site
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Author nmr
Solvent
Temperature
Pulse Sequence
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Relaxation Delay 2.0000
Pulse Width 3.1850
Acquisition Time 2.4429
Acquisition Date 2020-11-27T11:57:05
Modification Date 2020-11-27T11:55:40
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Lowest Frequency -1204.0
Nucleus Proton
Acquired Size 22000
Spectral Size 52429
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7.281
7.260
7.245
5.047
2.082
OAc
Cl
4g
3.86
2.15
3.00
10.0 9.5 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 -0.5
f1 (ppm)

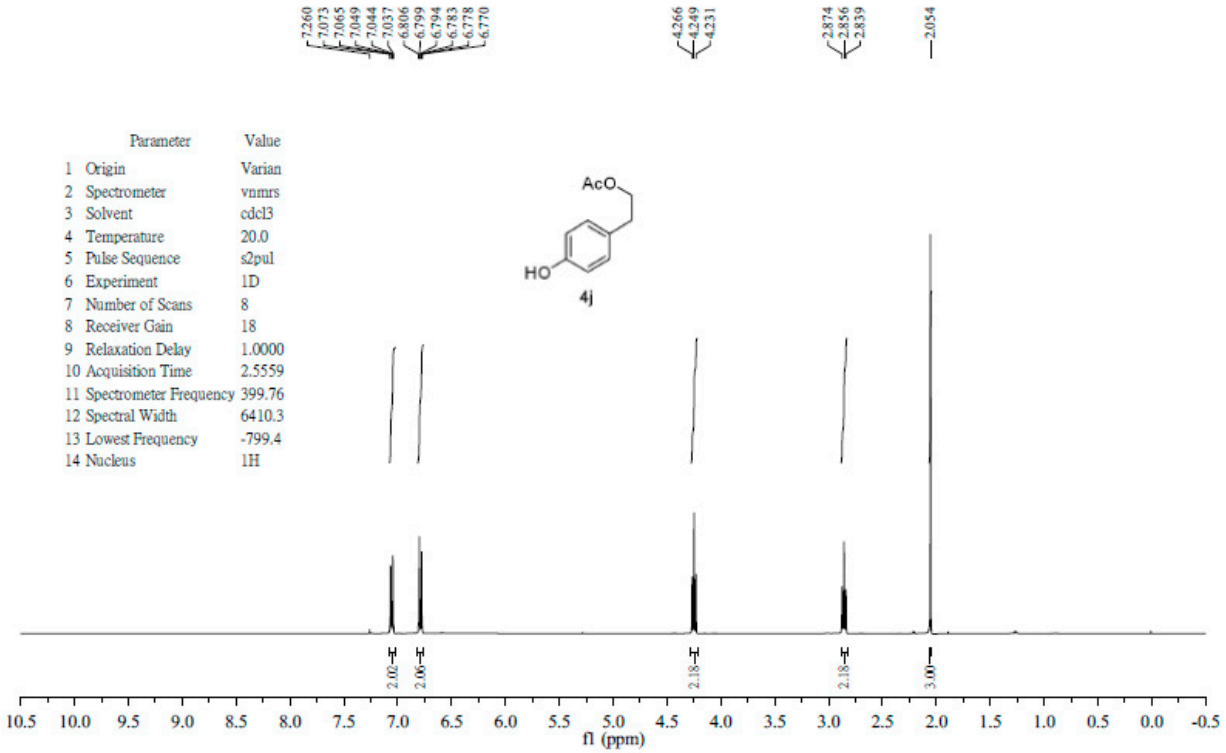

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Author nmr
Solvent
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Cl
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f1 (ppm)

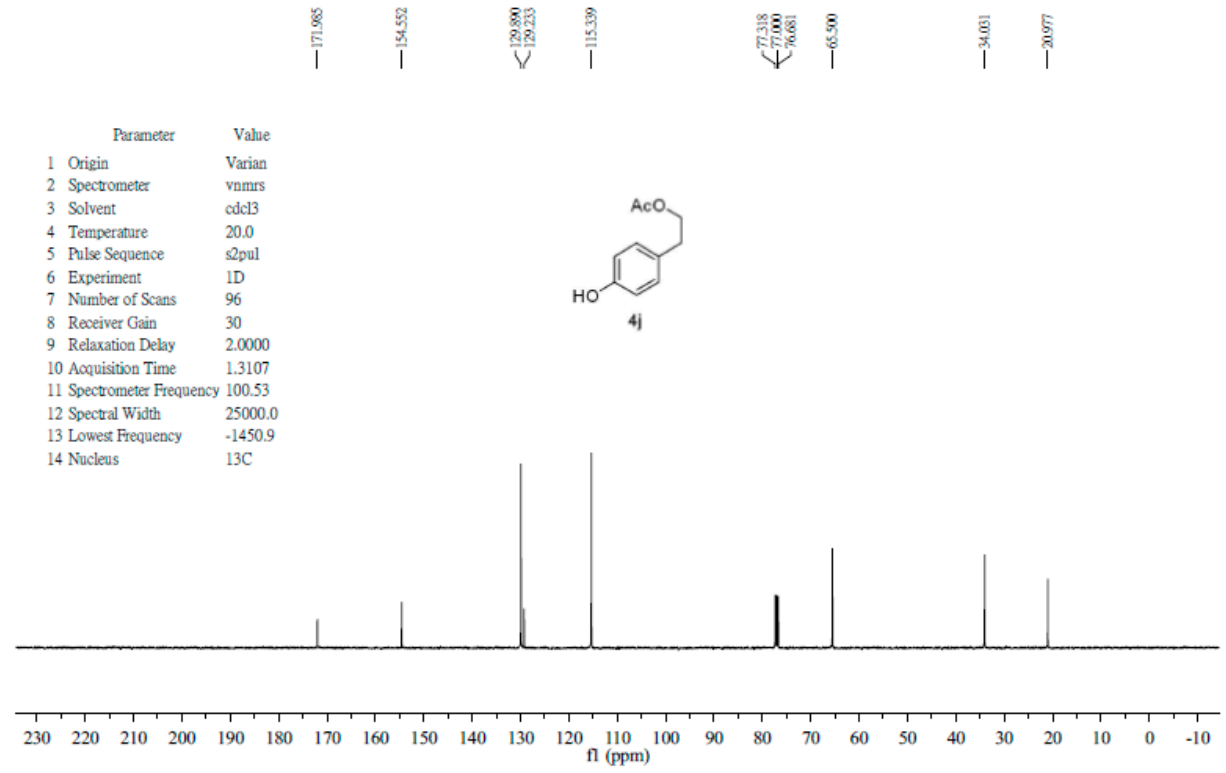

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7.260
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7.218
5.047
2.098
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Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
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Acquisition Time 2.5559
Spectrometer Frequency 399.76
Spectral Width 6410.3
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Nucleus 1H
OAc
Br
4h
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1.95
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3.00
f1 (ppm)

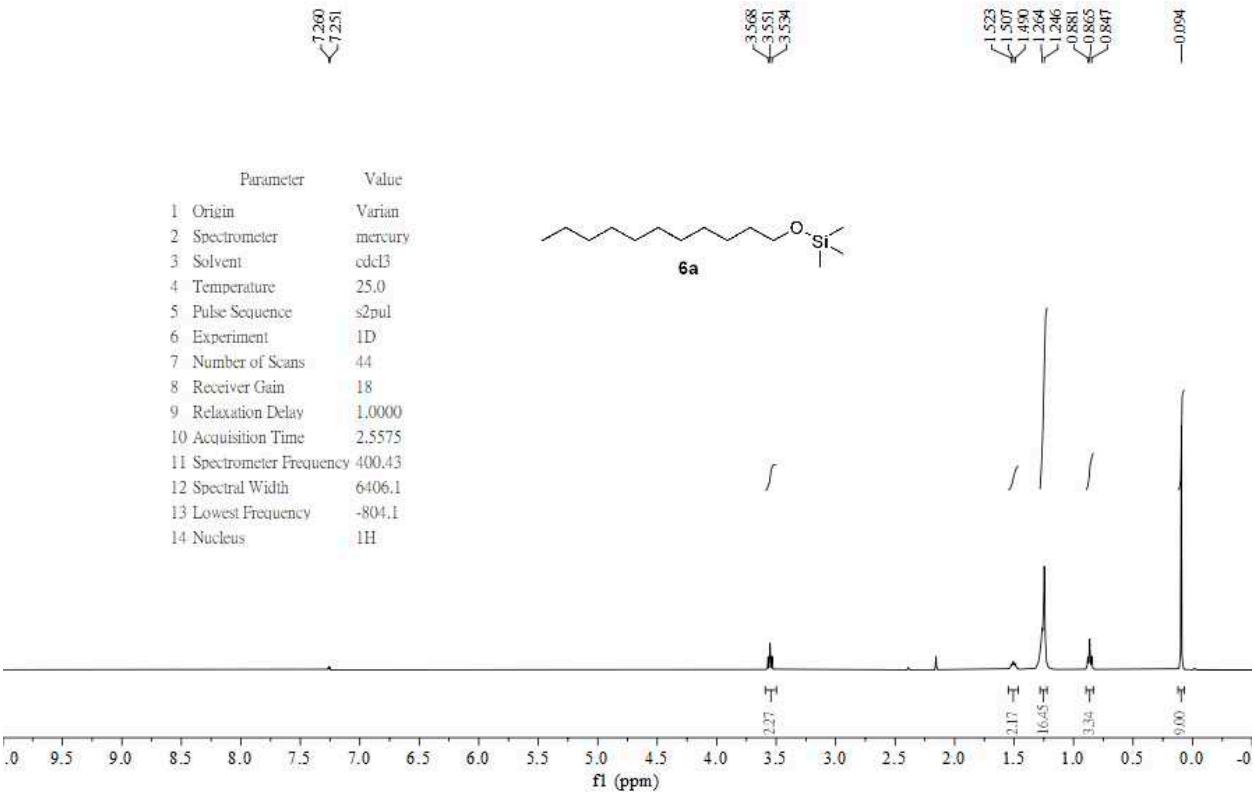

170.715
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131.654
129.877
122.224
77.318
77.000
76.682
65.438
20.928
Parameter Value
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Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 128
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Relaxation Delay 2.0000
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OAc
Br
4h
f1 (ppm)

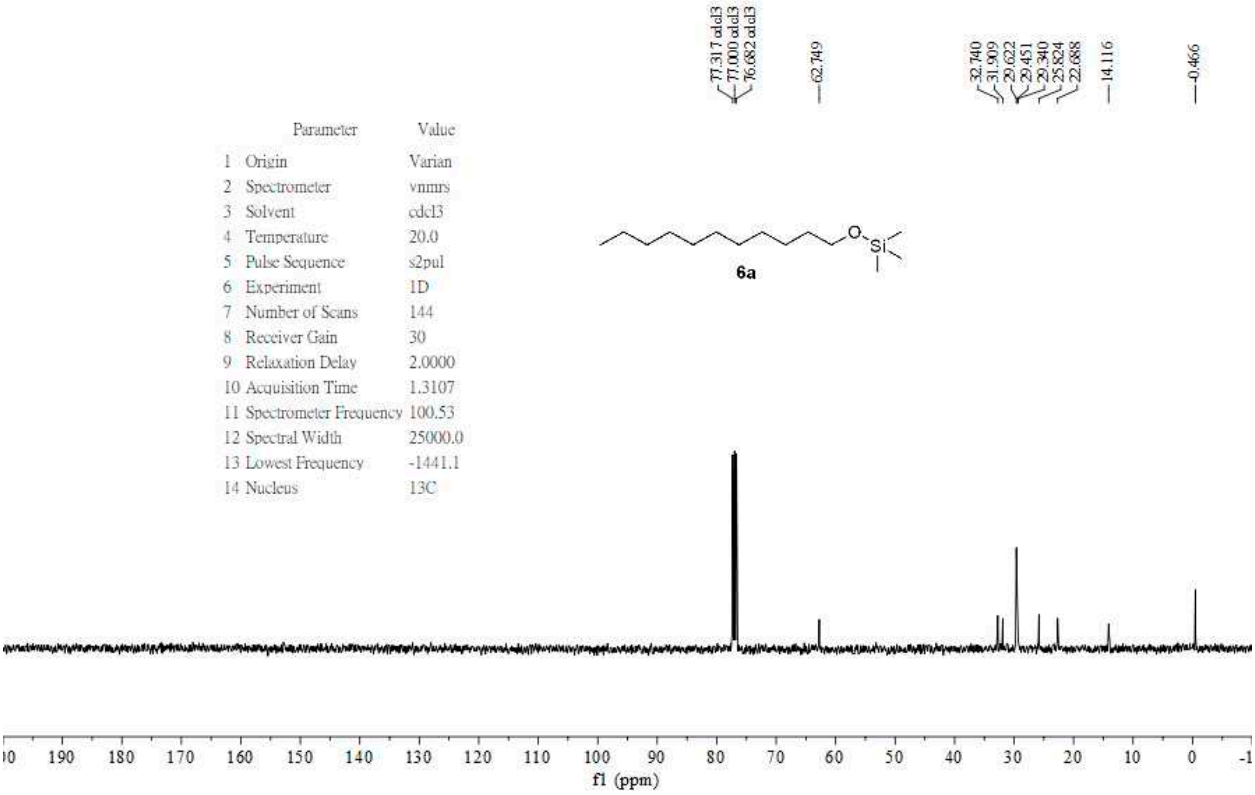

7.427
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7.390
7.371
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7.351
7.347
7.346
7.339
7.331
7.329
6.964
6.961
2.207
2.205
Parameter Value
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 24
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Acquisition Time 2.5559
Spectrometer Frequency 399.76
Spectral Width 6410.3
Lowest Frequency -799.4
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f1 (ppm)

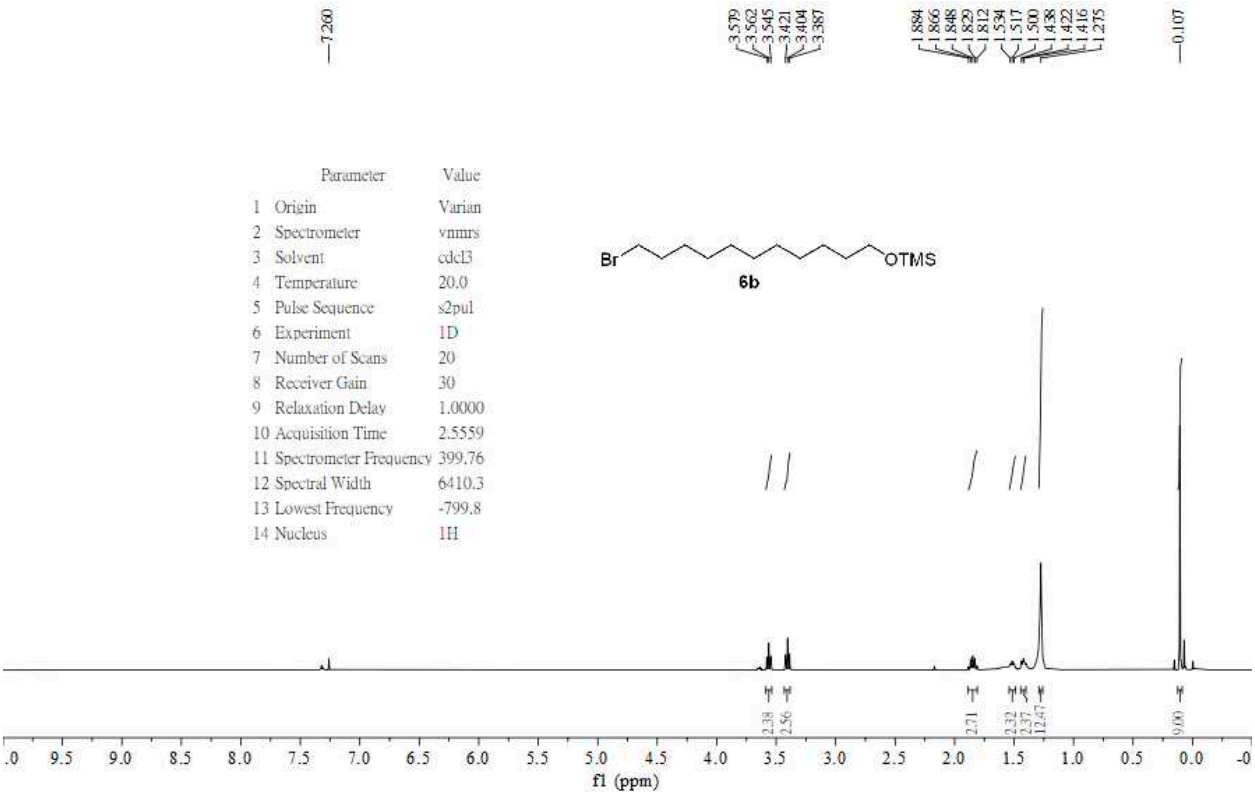

169.920
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128.413
128.295
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127.342
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Spectrometer vnmrs
Solvent cdcl3
Temperature 20.0
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Acquisition Time 1.3107
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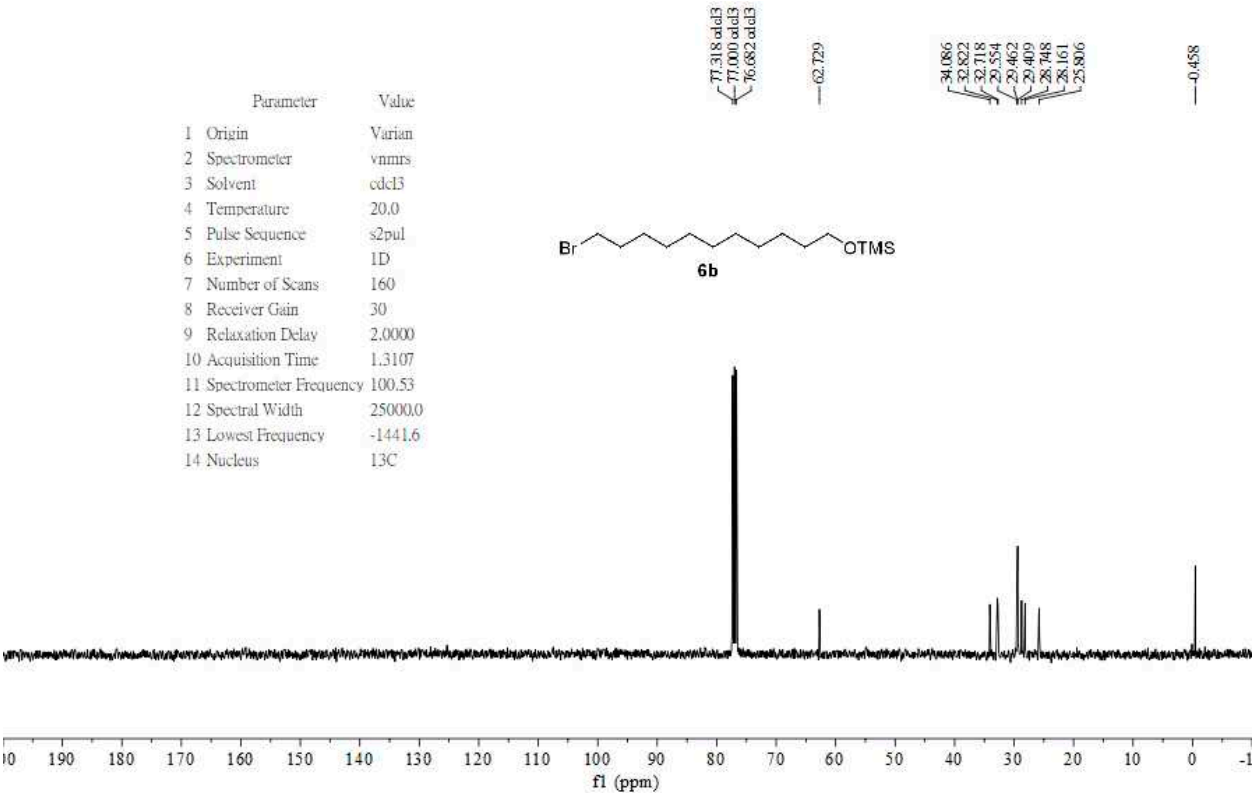

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7.044
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4.249
4.231
2.874
2.856
2.839
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Parameter Value
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3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 8
8 Receiver Gain 18
9 Relaxation Delay 1.0000
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HO
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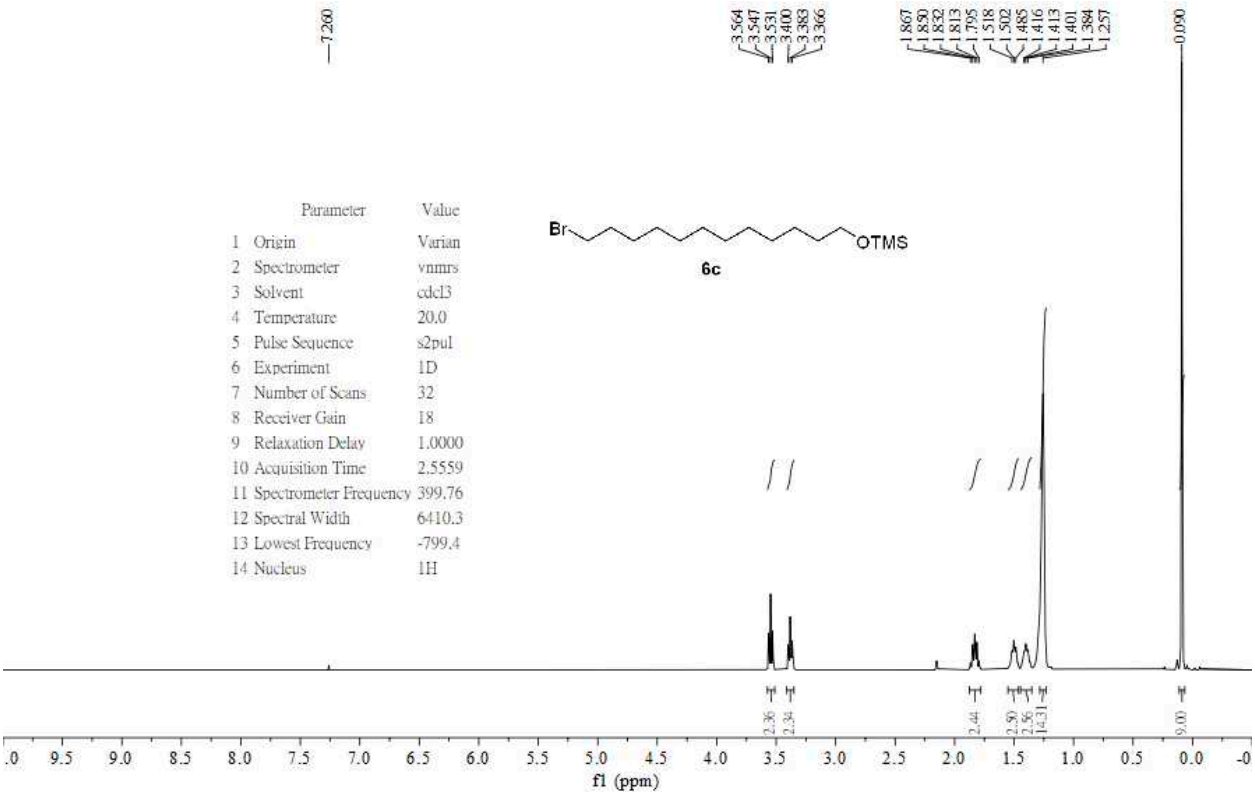

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129.233
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77.318
77.000
76.681
65.500
34.011
20.977
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3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
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8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1450.9
14 Nucleus 13C
AcO
HO
4j
f1 (ppm)

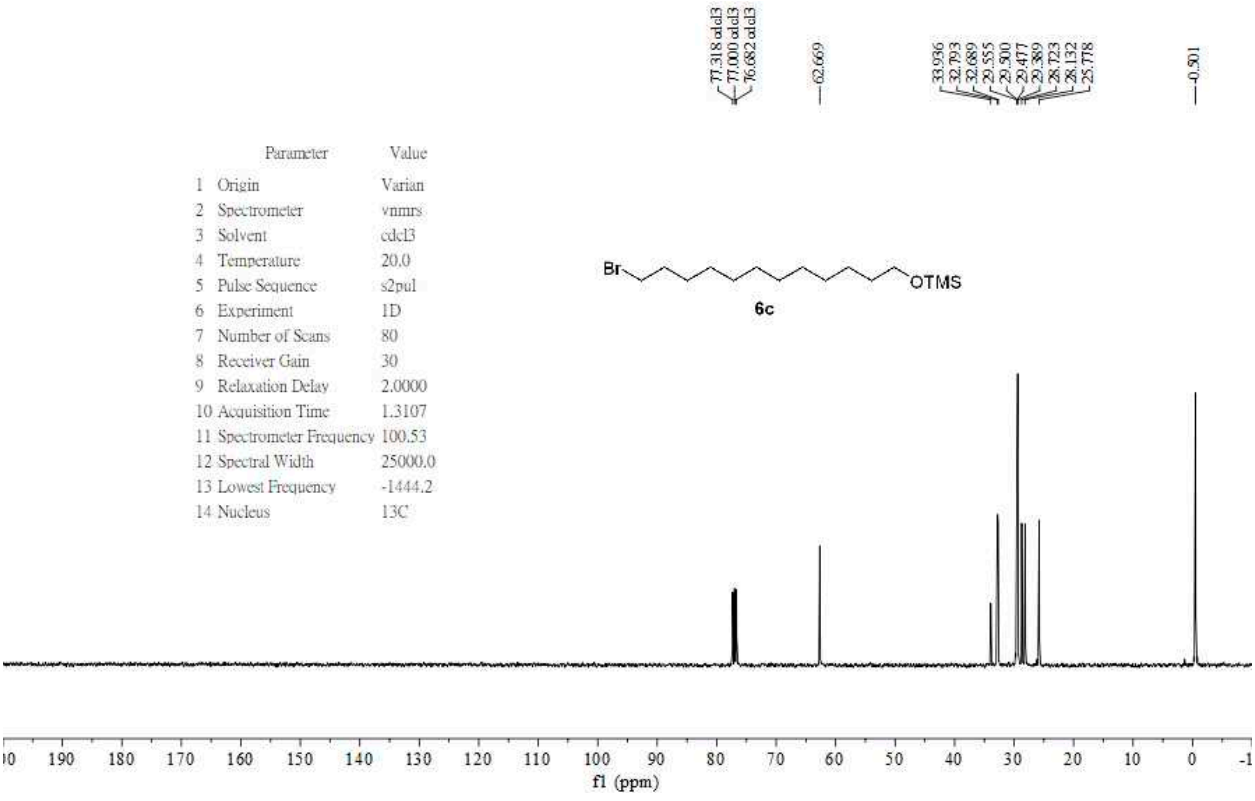

7.260
7.251
3.568
3.551
3.534
1.523
1.507
1.490
1.264
1.246
0.881
0.865
0.847
0.094
Parameter Value
1 Origin Varian
2 Spectrometer mercury
3 Solvent cdcl3
4 Temperature 25.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 44
8 Receiver Gain 18
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5575
11 Spectrometer Frequency 400.43
12 Spectral Width 6406.1
13 Lowest Frequency -804.1
14 Nucleus 1H
O
Si
6a
2.27
2.17
16.65
3.34
9.00
f1 (ppm)

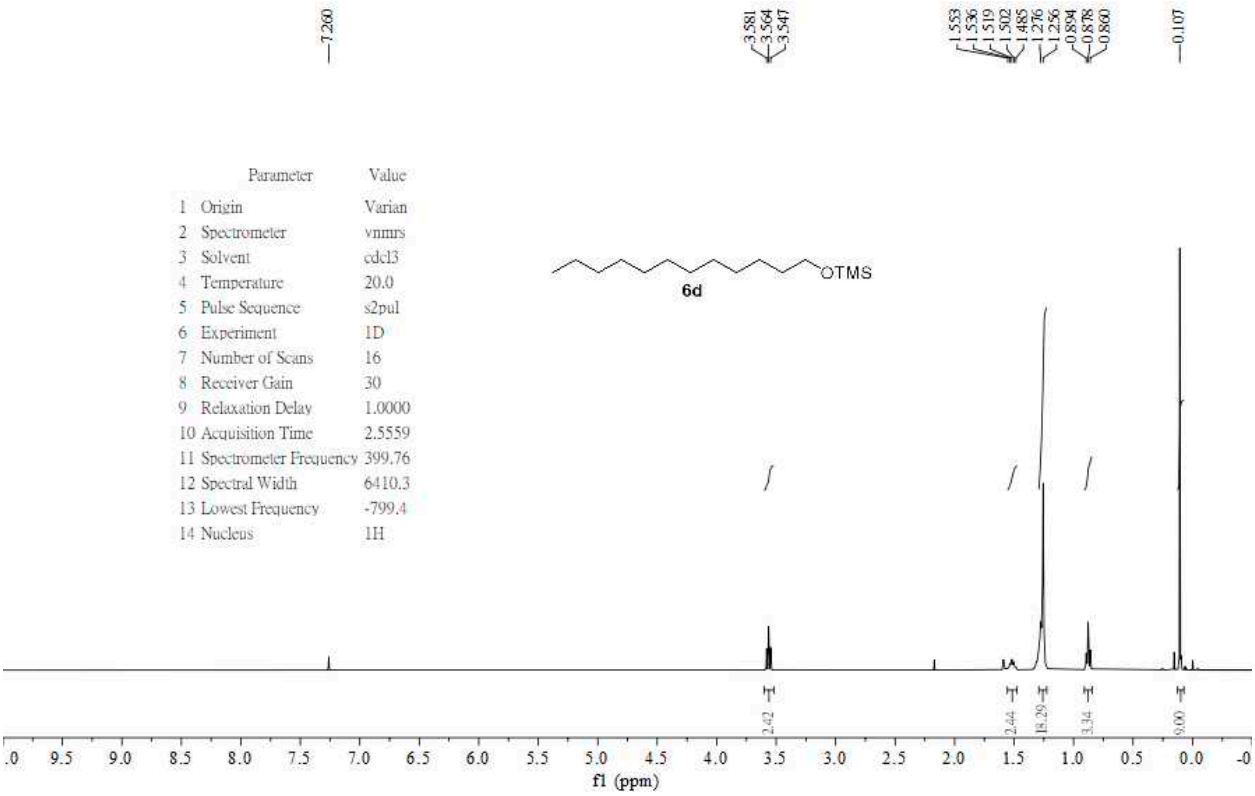

77.317 cdcl3
77.000 cdcl3
76.682 cdcl3
62.749
32.740
31.909
29.622
29.451
29.340
25.824
22.688
14.116
-0.466
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 144
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1441.1
14 Nucleus 13C
O
Si
6a
f1 (ppm)

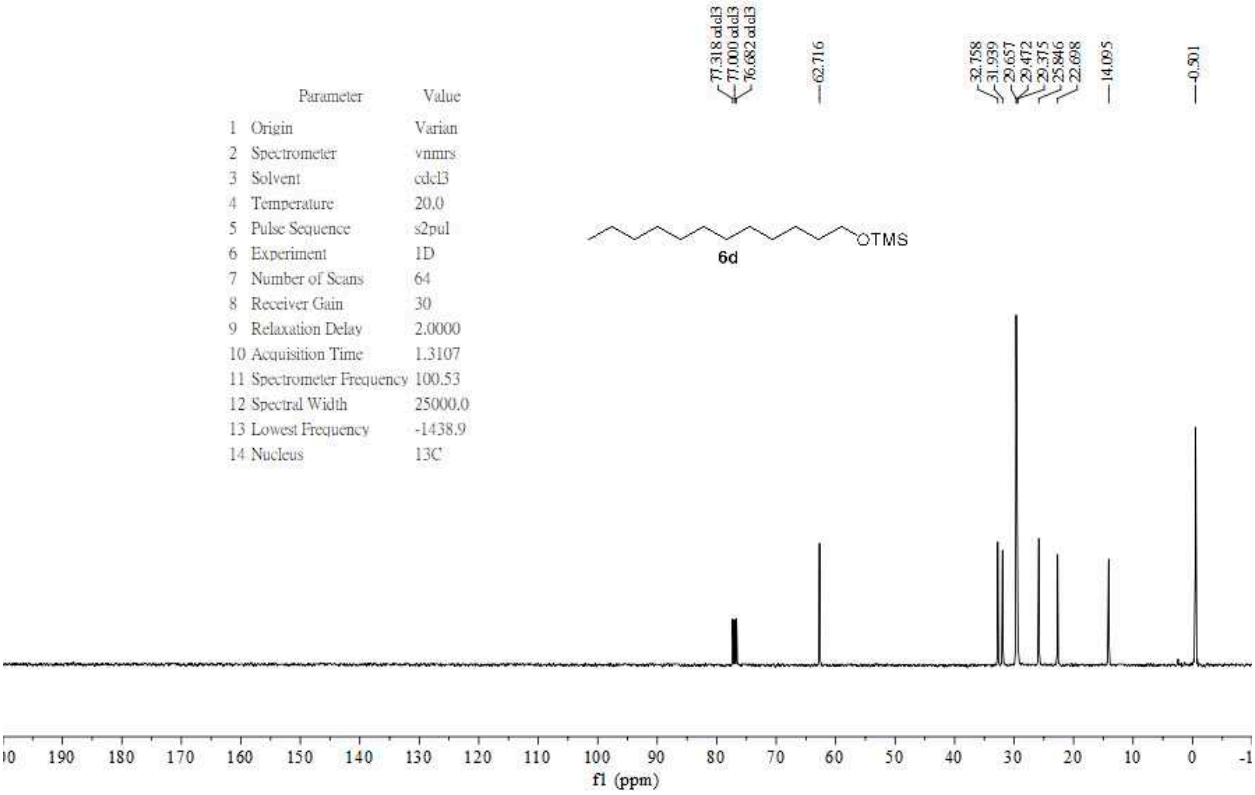

7.260
3.579
3.562
3.545
3.421
3.404
3.387
1.884
1.866
1.848
1.829
1.812
1.534
1.517
1.500
1.438
1.422
1.416
1.275
0.107
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 20
8 Receiver Gain 30
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5559
11 Spectrometer Frequency 399.76
12 Spectral Width 6410.3
13 Lowest Frequency -799.8
14 Nucleus 1H
Br
OTMS
6b
2.38
2.56
2.71
2.32
2.37
12.47
9.00
f1 (ppm)

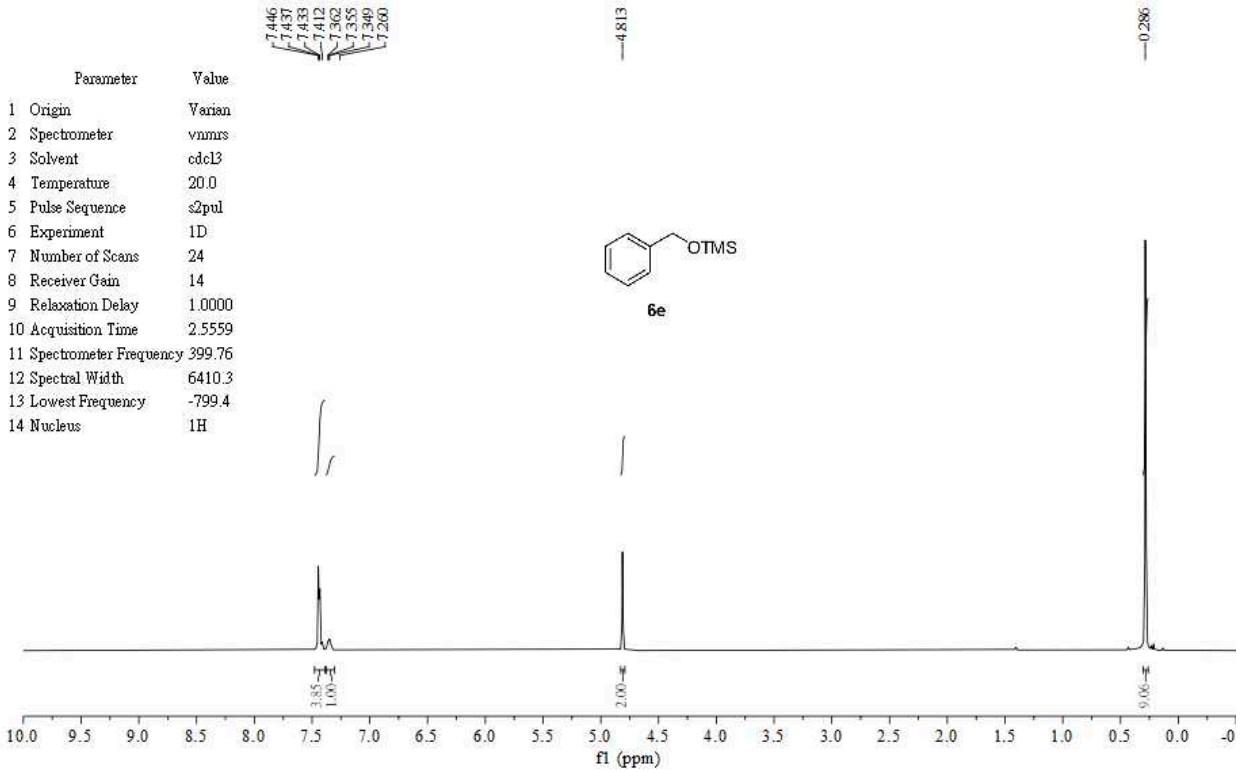

77.318 cdcl3
77.000 cdcl3
76.682 cdcl3
62.729
34.086
32.822
32.718
29.554
29.462
29.409
28.748
28.161
25.806
0.458
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 160
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1441.6
14 Nucleus 13C
Br
OTMS
6b
f1 (ppm)

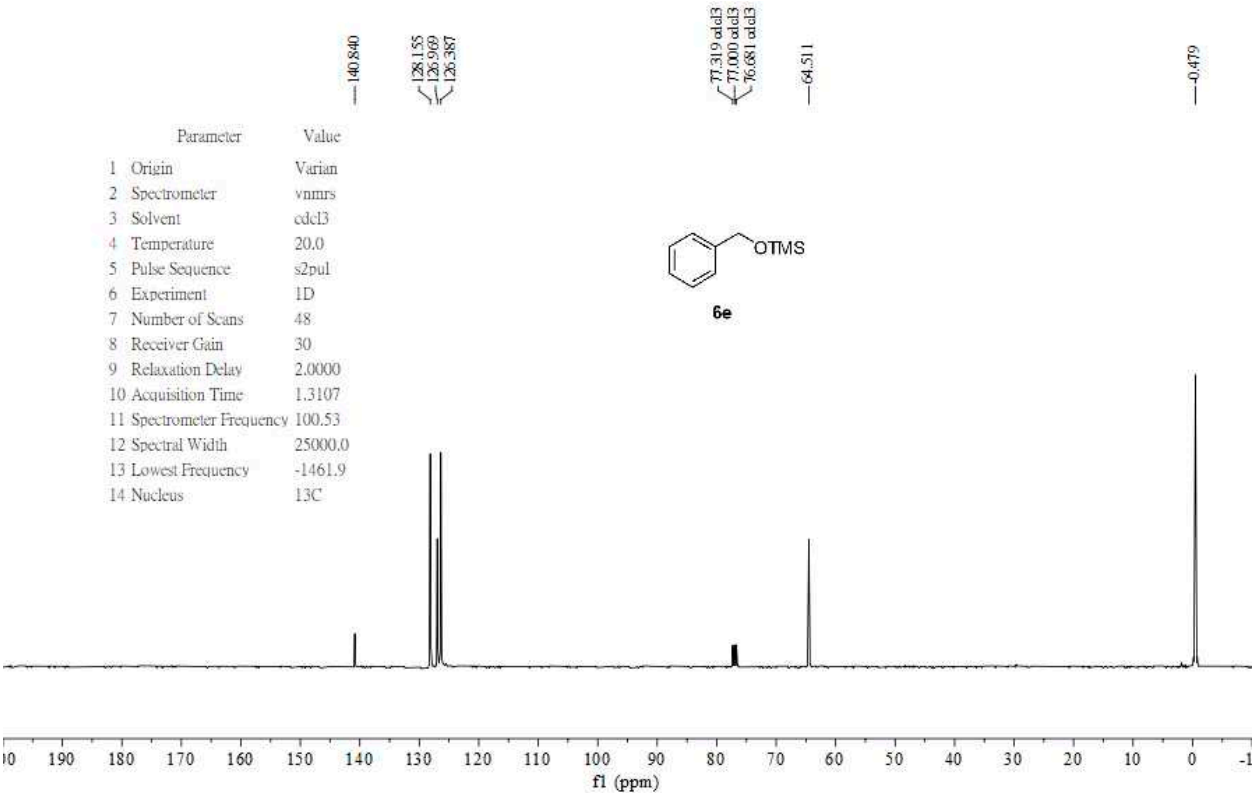

7.260
3.564
3.547
3.531
3.400
3.383
3.366
1.867
1.850
1.832
1.813
1.795
1.518
1.502
1.485
1.416
1.413
1.401
1.384
1.257
0.090
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 18
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5559
11 Spectrometer Frequency 399.76
12 Spectral Width 6410.3
13 Lowest Frequency -799.4
14 Nucleus 1H
Br
OTMS
6c
2.36
2.34
2.44
2.50
2.56
14.31
9.00
f1 (ppm)

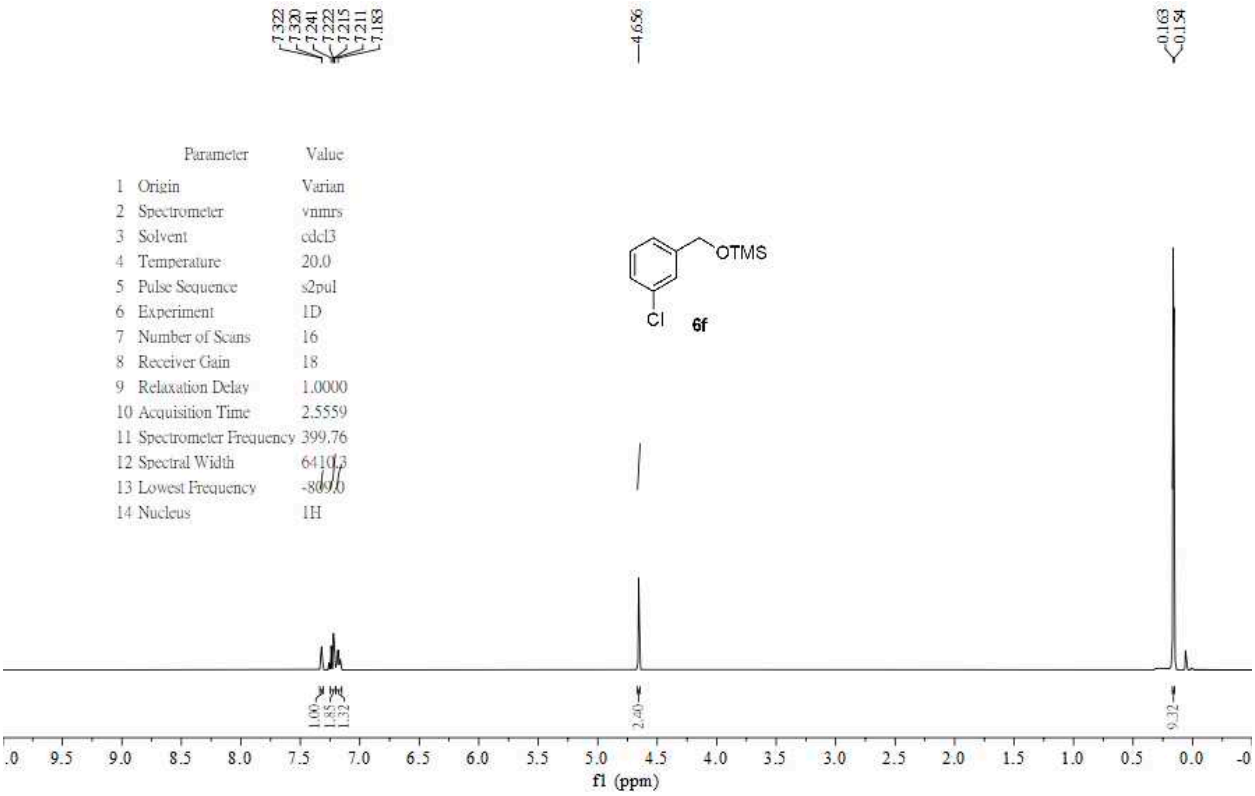

77.318 cdcl3
77.000 cdcl3
76.682 cdcl3
62.669
33.936
32.793
32.689
29.555
29.500
29.477
29.389
28.723
28.132
25.778
0.901
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 80
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1444.2
14 Nucleus 13C
Br
OTMS
6c
f1 (ppm)

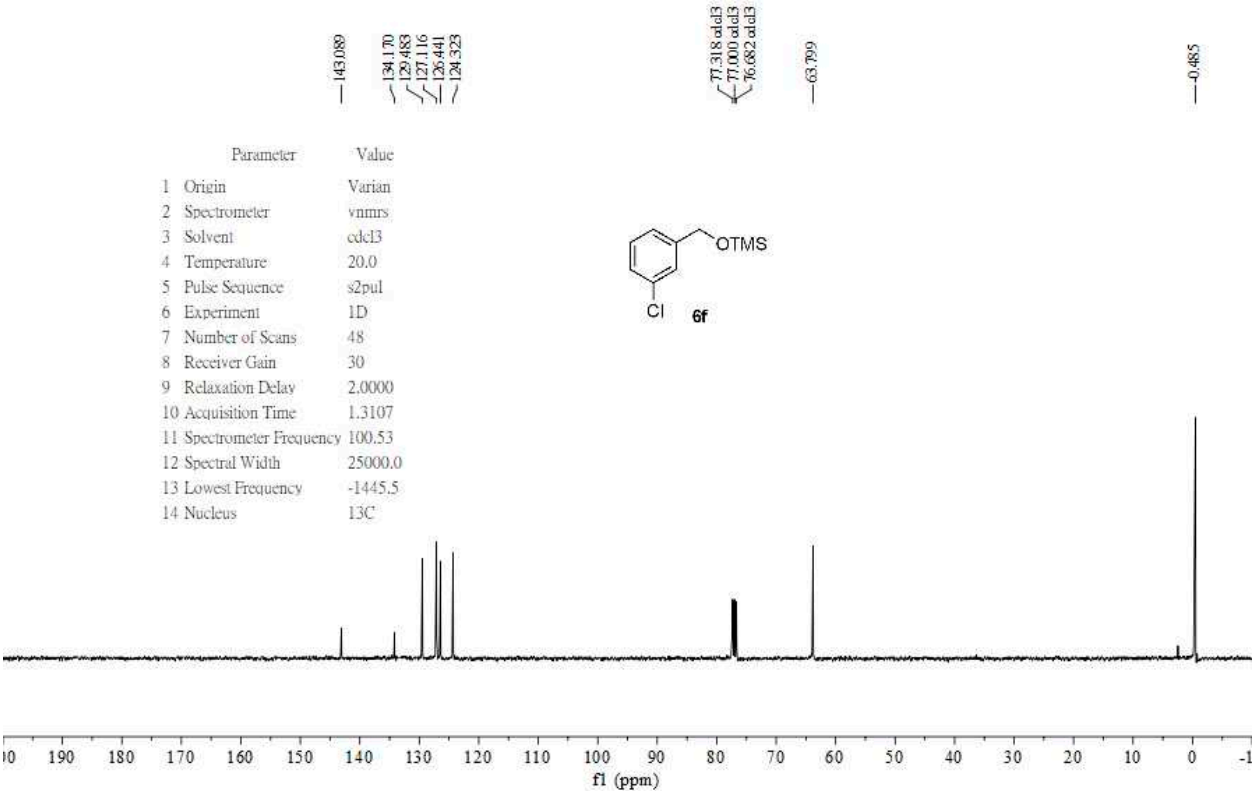

7.260
3.581
3.564
3.547
1.553
1.536
1.519
1.502
1.485
1.276
1.256
0.894
0.878
0.860
0.107
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 30
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5559
11 Spectrometer Frequency 399.76
12 Spectral Width 6410.3
13 Lowest Frequency -799.4
14 Nucleus 1H
OTMS
6d
2.42
2.44
18.29
3.34
9.00
f1 (ppm)

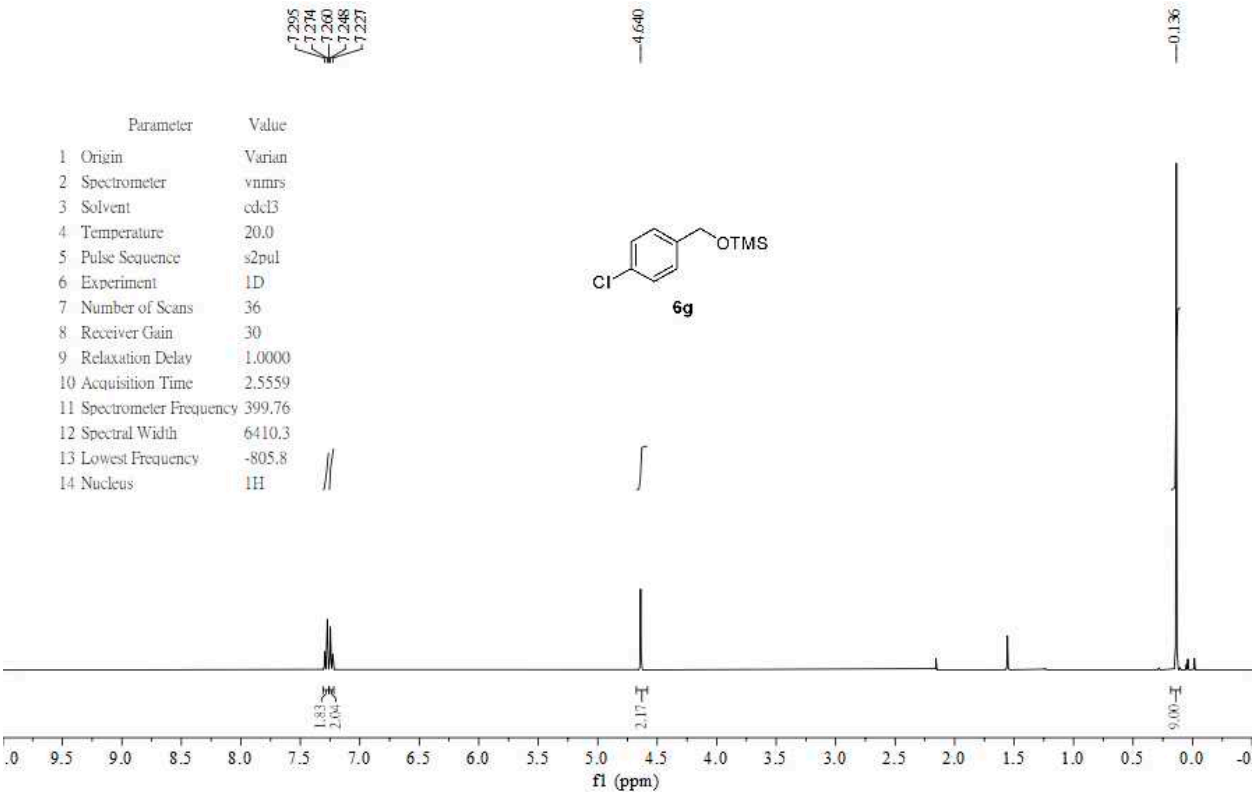

77.318 ddd3
77.000 ddd3
76.682 ddd3
62.716
32.758
31.939
29.657
29.472
29.375
25.846
22.698
14.095
0.501
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 64
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1438.9
14 Nucleus 13C
OTMS
6d
f1 (ppm)

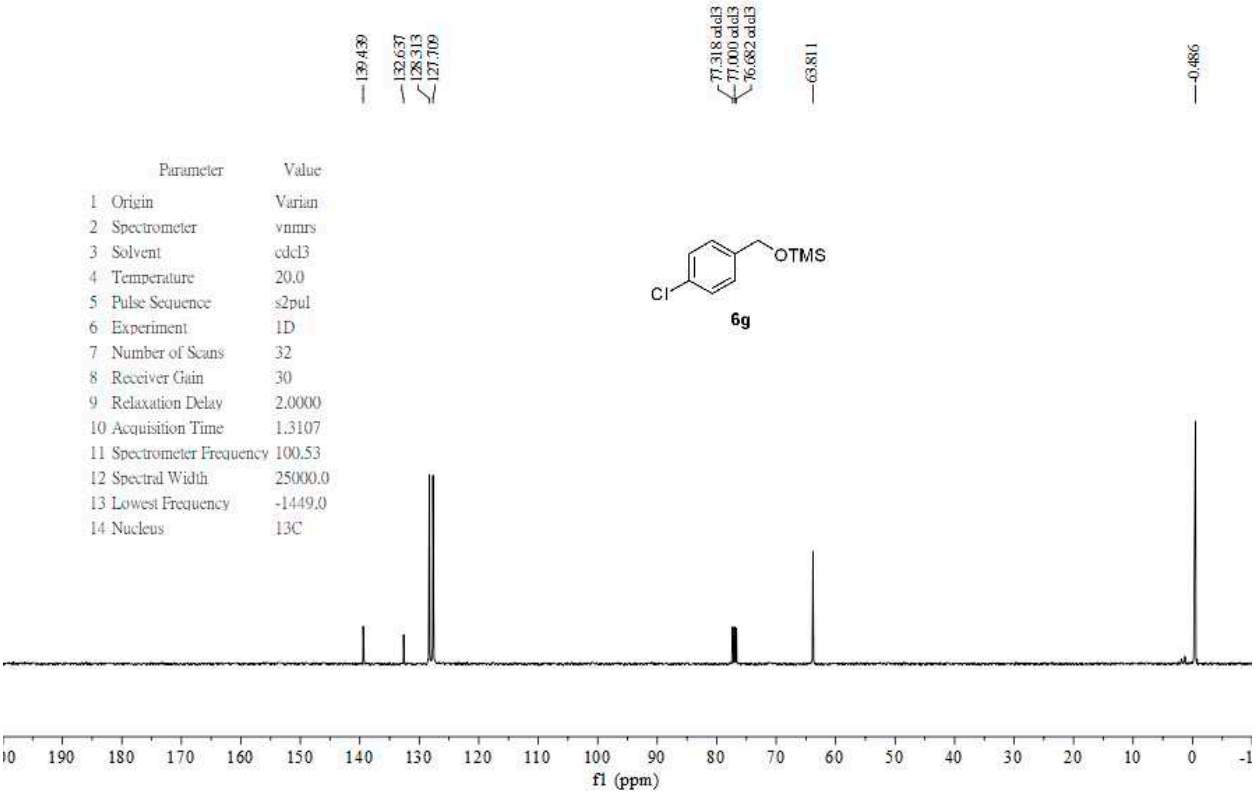

7.446
7.437
7.433
7.412
7.362
7.355
7.349
7.260
4.813
0.286
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 24
8 Receiver Gain 14
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5559
11 Spectrometer Frequency 399.76
12 Spectral Width 6410.3
13 Lowest Frequency -799.4
14 Nucleus 1H
OTMS
6e
3.85
1.00
2.00
9.06
f1 (ppm)

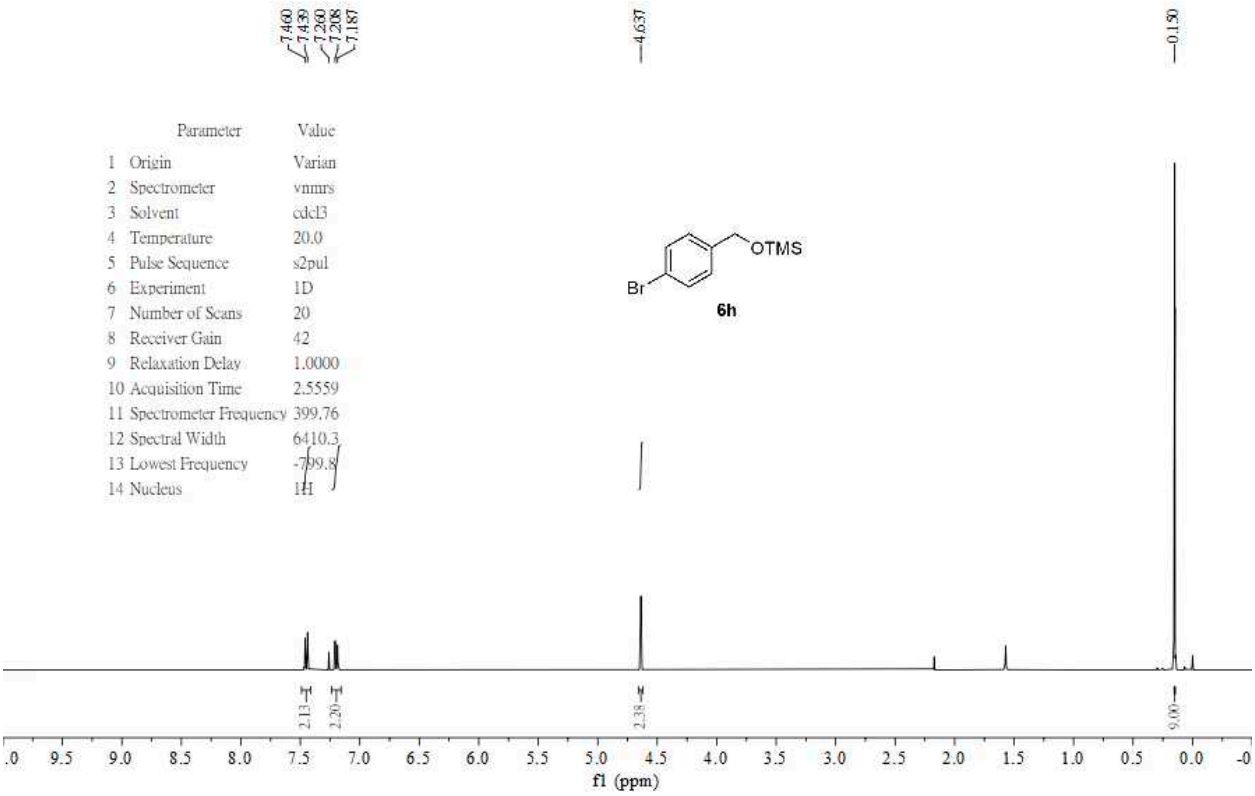

140.840
128.155
126.969
126.387
77.319 cdcl3
77.000 cdcl3
76.681 cdcl3
64.511
0.479
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 48
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1461.9
14 Nucleus 13C
OTMS
6e
f1 (ppm)

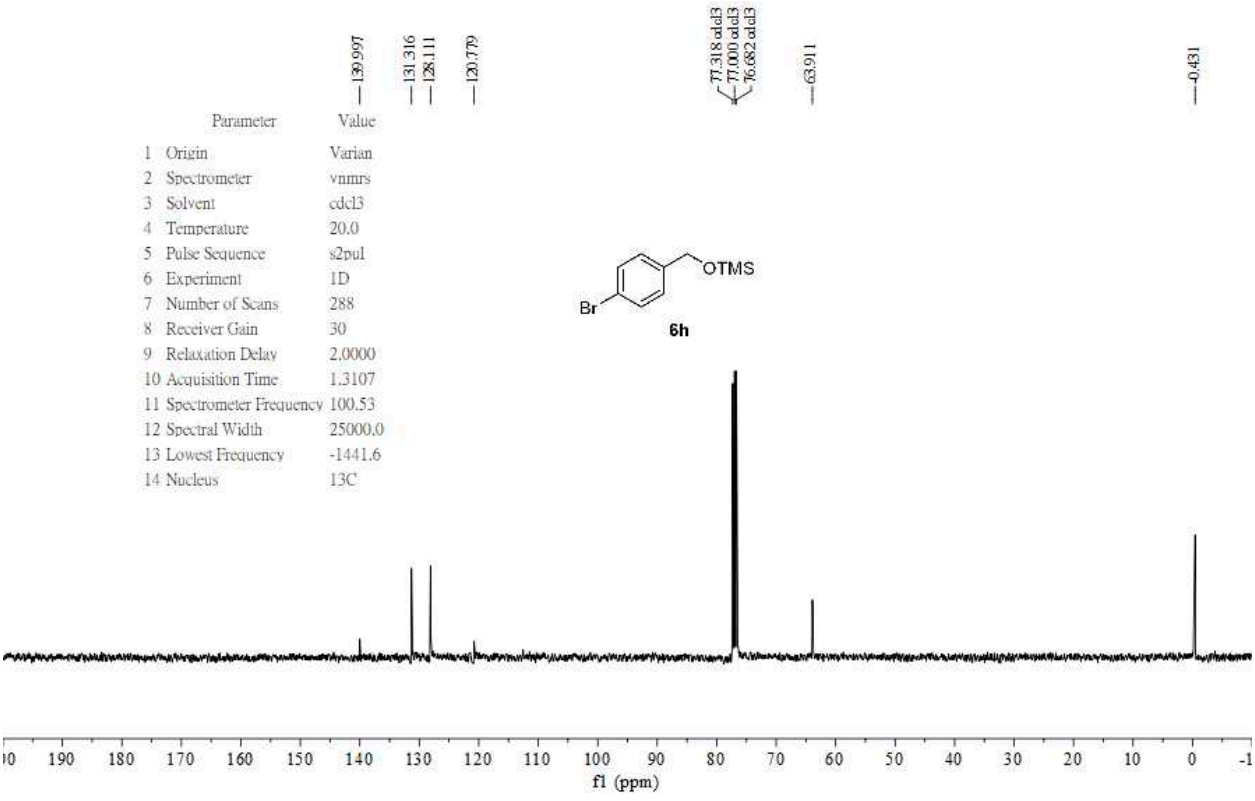

7.322
7.330
7.241
7.222
7.215
7.211
7.183
4.656
0.163
0.154
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 18
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5559
11 Spectrometer Frequency 399.76
12 Spectral Width 6410.3
13 Lowest Frequency -800.0
14 Nucleus 1H
OTMS
Cl
6f
1.00
1.85
1.32
2.00
9.32
f1 (ppm)

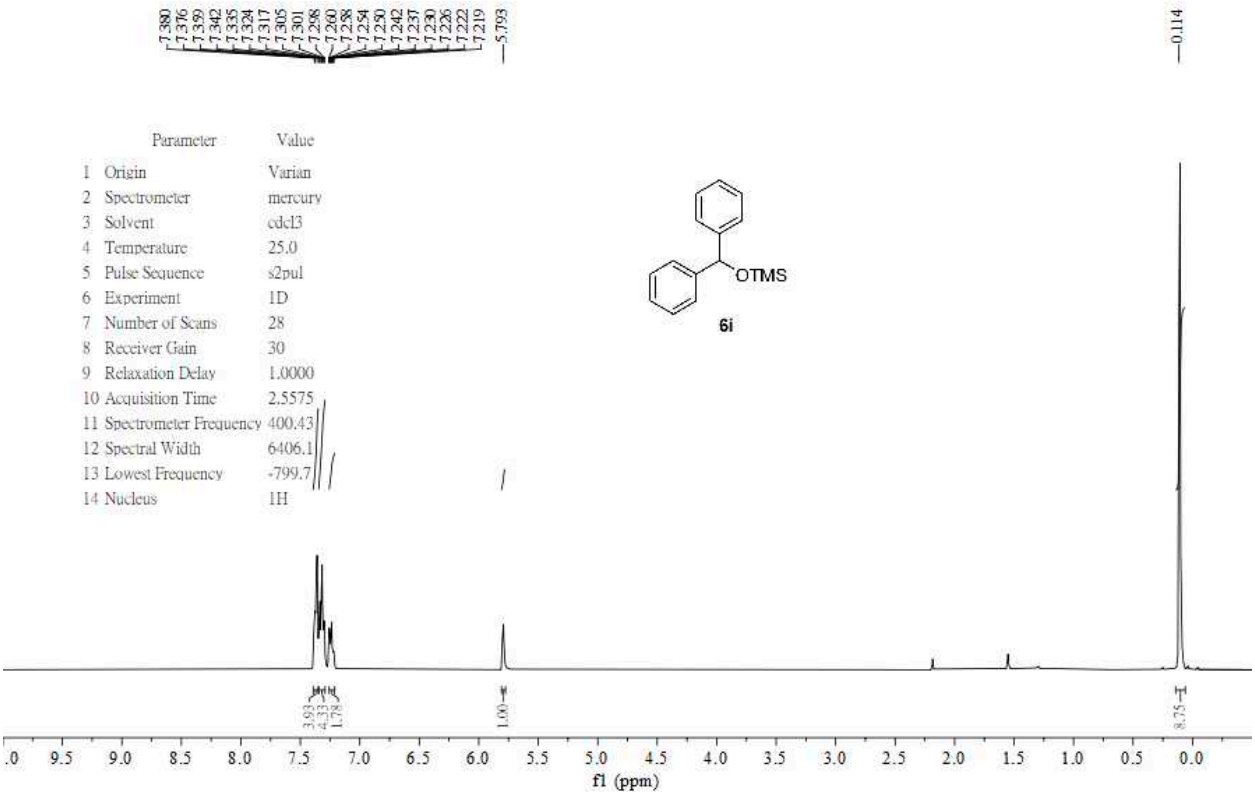

143.089
134.170
129.483
127.116
126.441
124.323
77.318 cdcl3
77.000 cdcl3
76.682 cdcl3
63.799
0.485
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 48
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1445.5
14 Nucleus 13C
OTMS
Cl
6f
f1 (ppm)

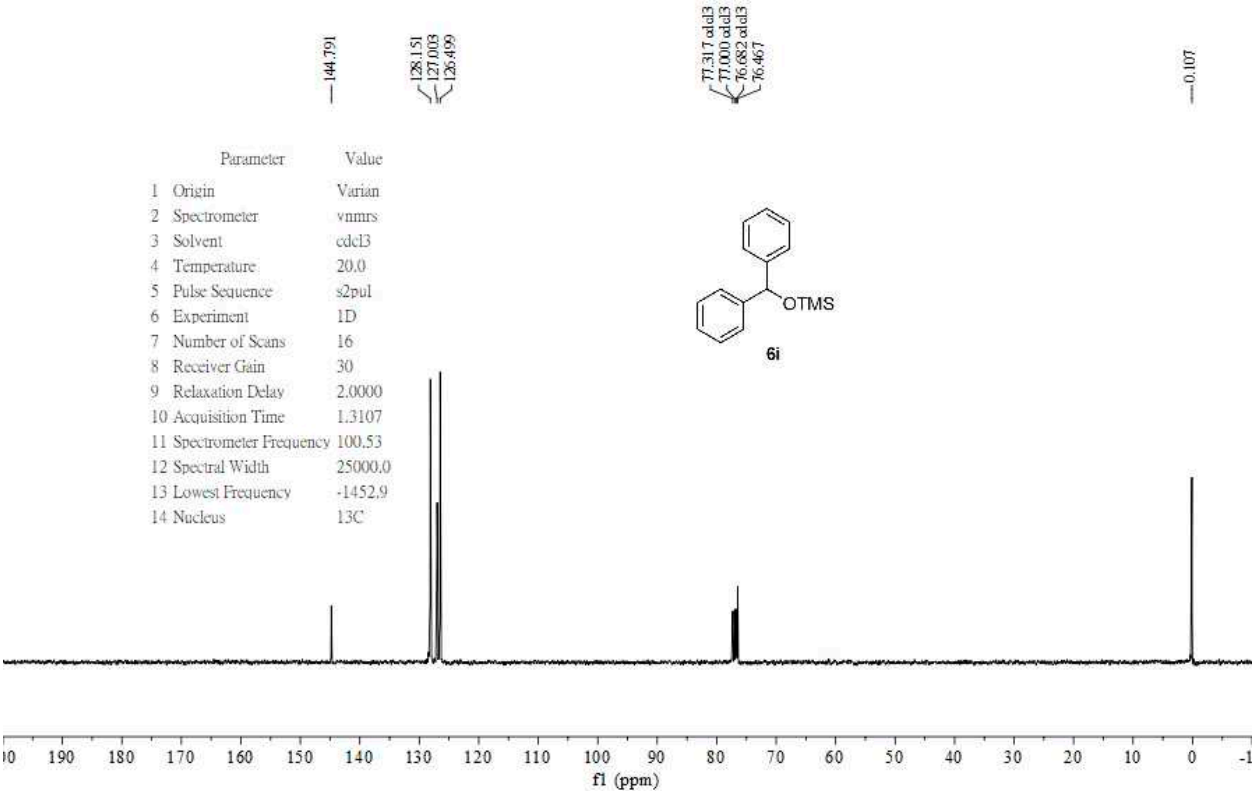

7.295
7.274
7.260
7.248
7.227
4.640
0.136
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 36
8 Receiver Gain 30
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5559
11 Spectrometer Frequency 399.76
12 Spectral Width 6410.3
13 Lowest Frequency -805.8
14 Nucleus 1H
OTMS
Cl
6g
1.83
2.04
2.17
9.00
f1 (ppm)


139.439
132.637
128.313
127.709
77.318 cdcl3
77.000 cdcl3
76.682 cdcl3
63.811
0.486
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1449.0
14 Nucleus 13C
OTMS
Cl
6g
f1 (ppm)


7.460
7.439
7.260
7.208
7.187
4.637
0.150
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 20
8 Receiver Gain 42
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5559
11 Spectrometer Frequency 399.76
12 Spectral Width 6410.3
13 Lowest Frequency -799.8
14 Nucleus 1H
OTMS
Br
6h
2.13
2.20
2.38
9.00
f1 (ppm)


139.997
131.316
128.111
120.779
77.318 cdcl3
77.000 cdcl3
76.682 cdcl3
63.911
0.431
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 288
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1441.6
14 Nucleus 13C
OTMS
Br
6h
f1 (ppm)


7.380
7.376
7.359
7.342
7.335
7.324
7.317
7.305
7.301
7.298
7.260
7.238
7.234
7.230
7.242
7.237
7.230
7.226
7.222
7.219
5.793
0.114
Parameter Value
1 Origin Varian
2 Spectrometer mercury
3 Solvent cdcl3
4 Temperature 25.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 28
8 Receiver Gain 30
9 Relaxation Delay 1.0000
10 Acquisition Time 2.5575
11 Spectrometer Frequency 400.43
12 Spectral Width 6406.1
13 Lowest Frequency -799.7
14 Nucleus 1H
OTMS
6i
3.93
4.33
1.78
1.00
8.75
f1 (ppm)


144.791
128.151
127.003
126.499
77.317 cdcl3
77.000 cdcl3
76.682 cdcl3
76.467
0.107
Parameter Value
1 Origin Varian
2 Spectrometer vnmrs
3 Solvent cdcl3
4 Temperature 20.0
5 Pulse Sequence s2pul
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 30
9 Relaxation Delay 2.0000
10 Acquisition Time 1.3107
11 Spectrometer Frequency 100.53
12 Spectral Width 25000.0
13 Lowest Frequency -1452.9
14 Nucleus 13C
OTMS
6i
f1 (ppm)