Synthesis of α-Fluoro-β-hydroxy Ketones *via* Electrophilic Fluorination of Tertiary Propargyl Alcohols Using Selectfluor

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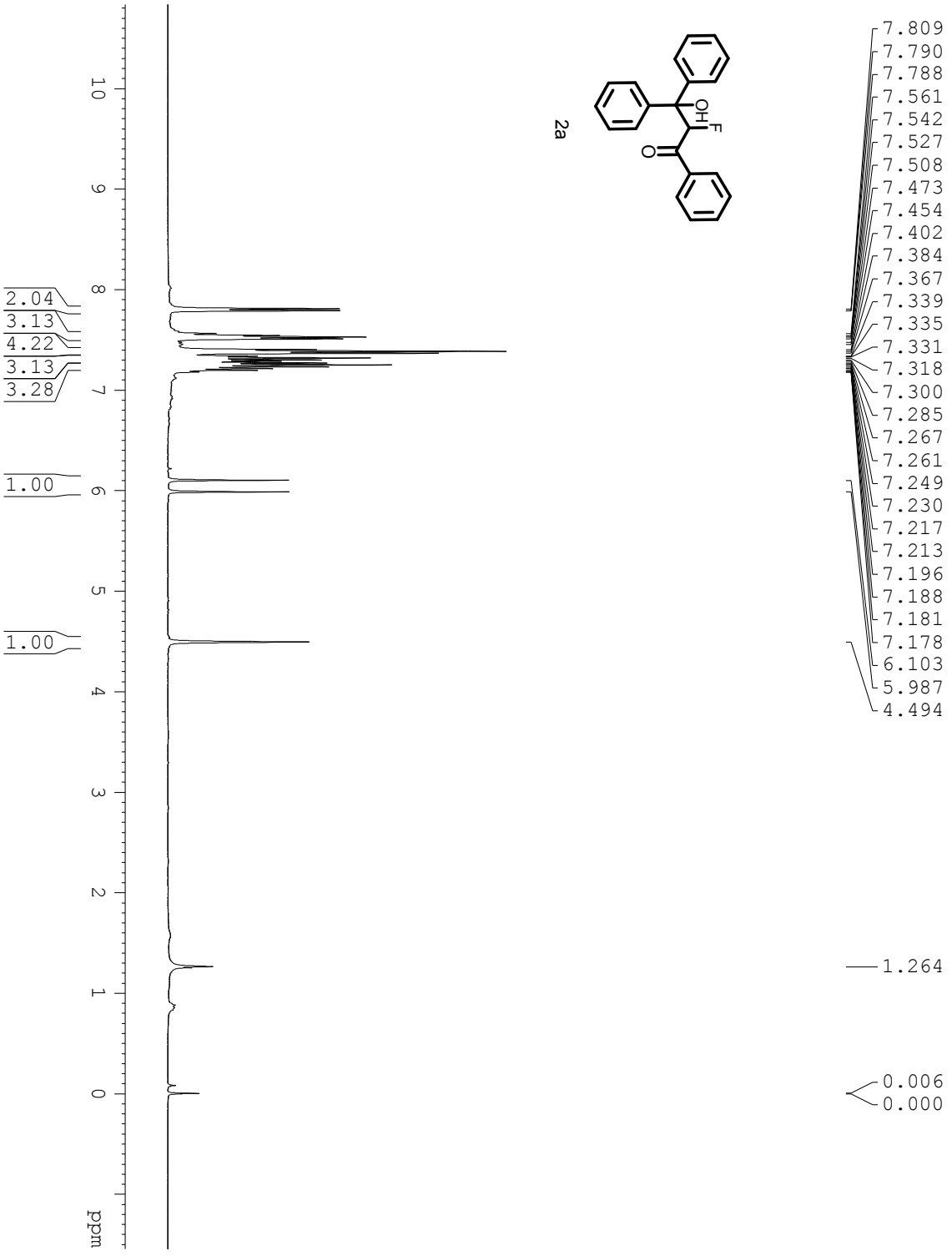
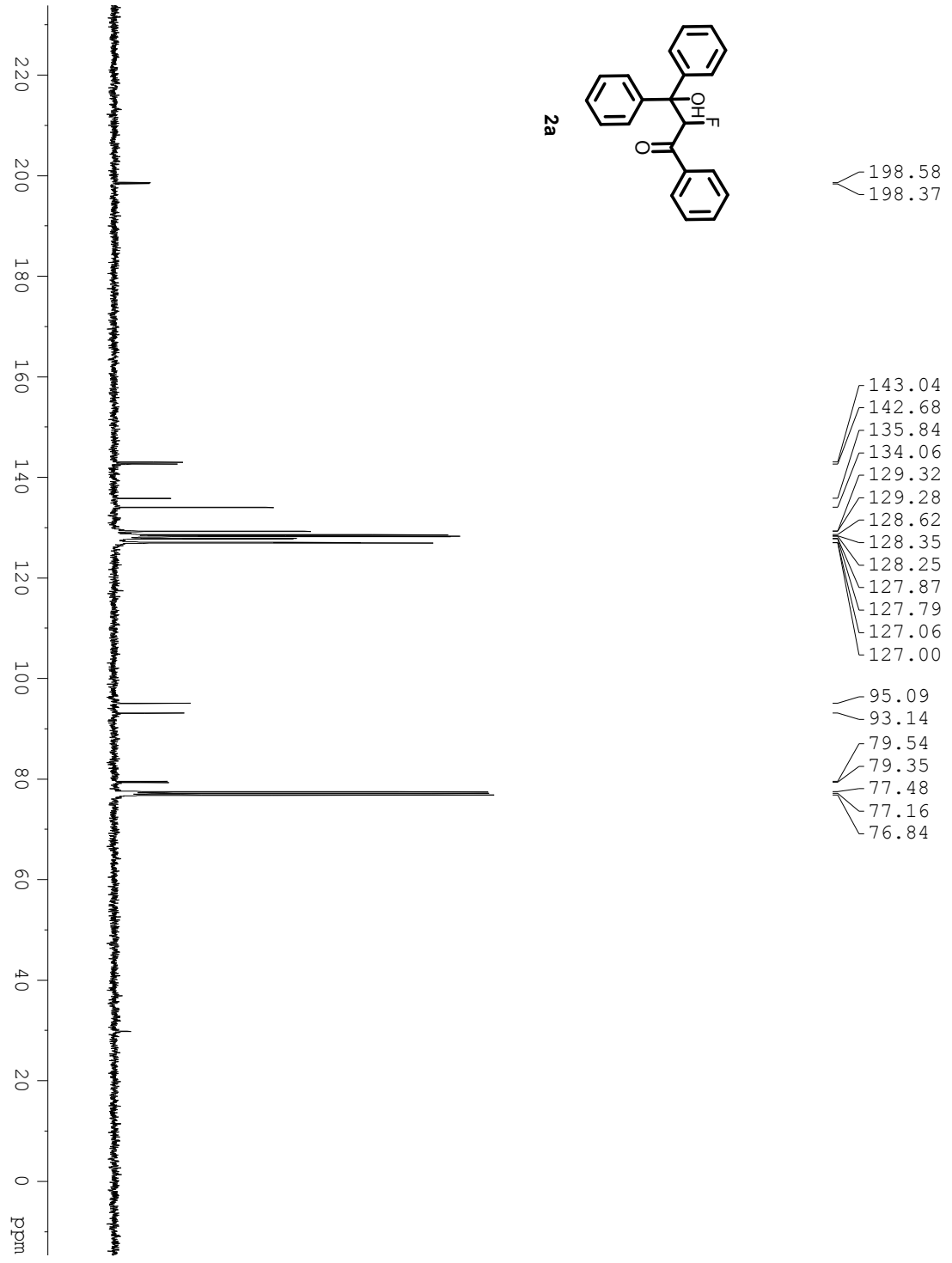
Supporting Information

1. NMR spectra of synthesized compounds

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127.87
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127.06
127.00
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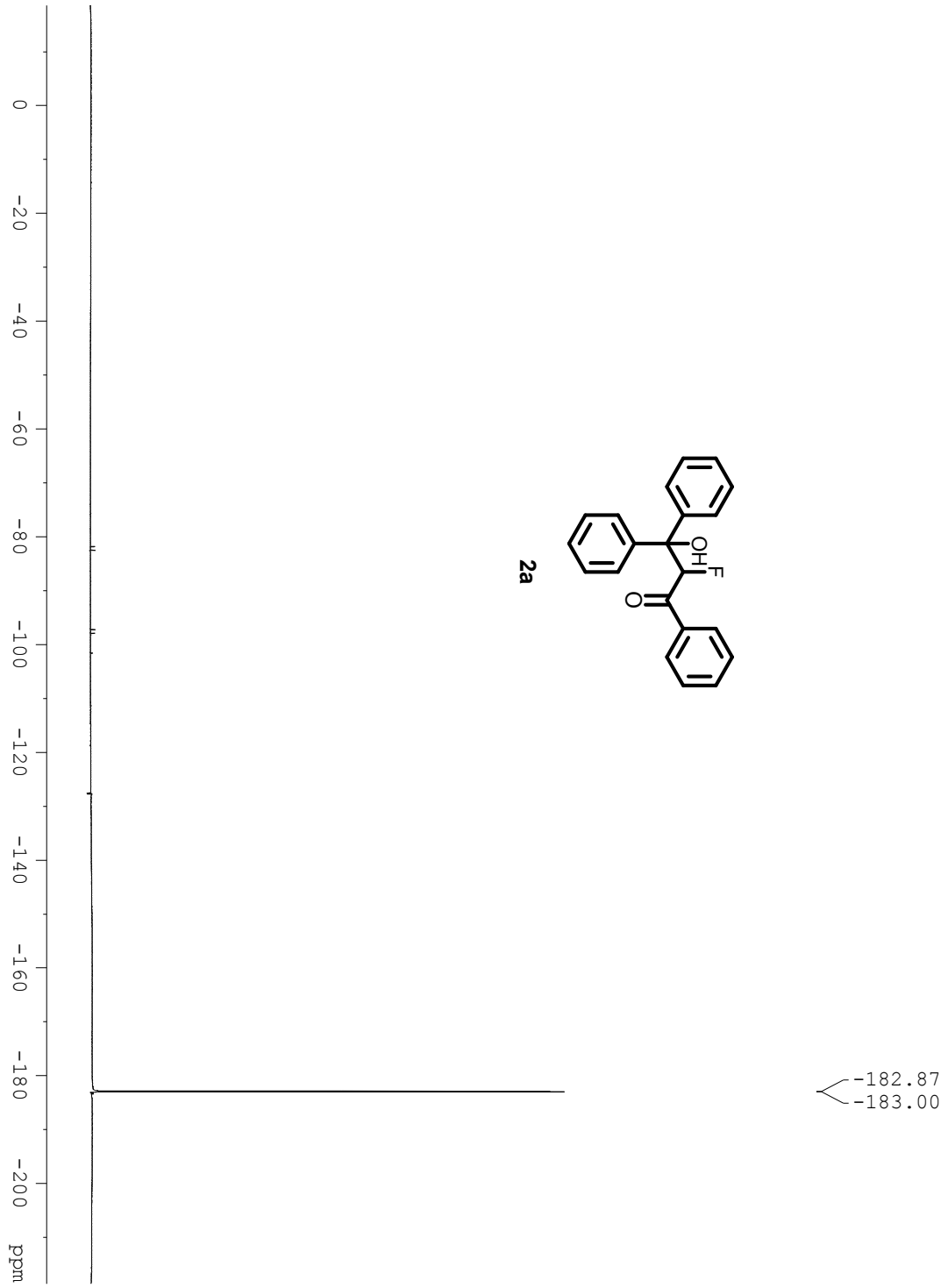
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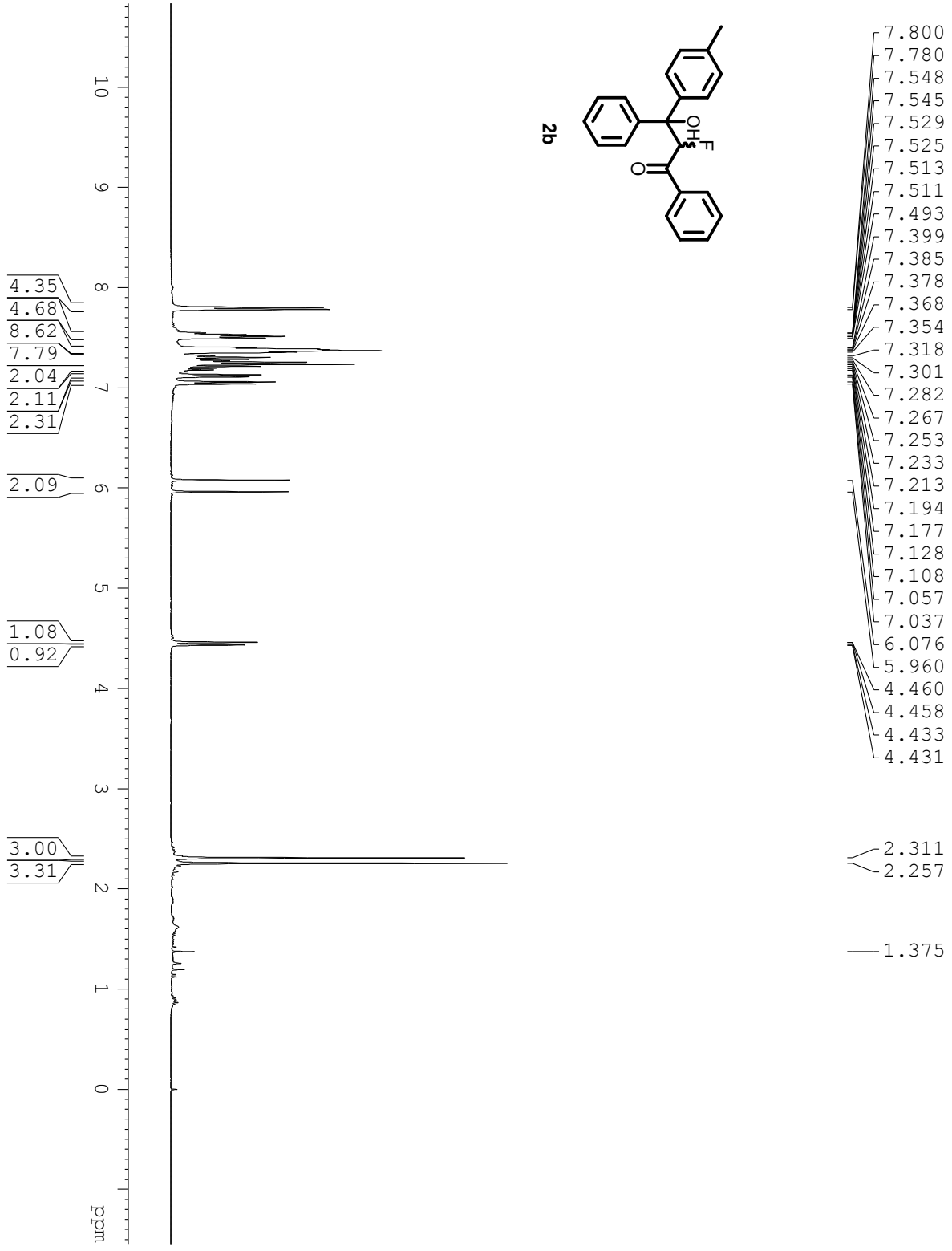
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7.385
7.378
7.368
7.354
7.318
7.301
7.282
7.267
7.253
7.233
7.213
7.194
7.177
7.128
7.108
7.057
7.037
6.076
5.960
4.460
4.458
4.433
4.431
2.311
2.257
1.375
4.35
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8.62
7.79
2.04
2.11
2.31
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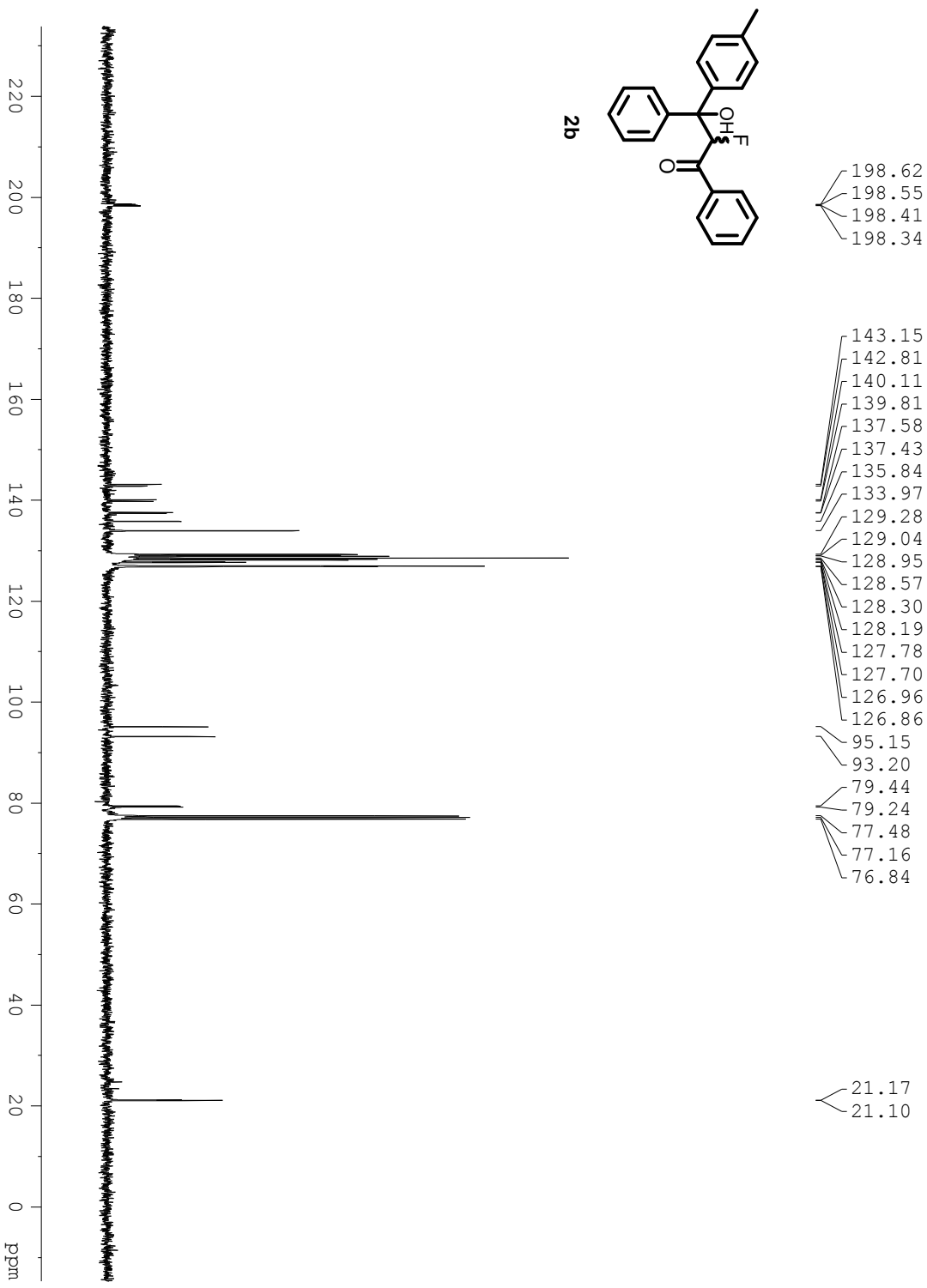
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133.97
129.28
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128.30
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127.70
126.96
126.86
95.15
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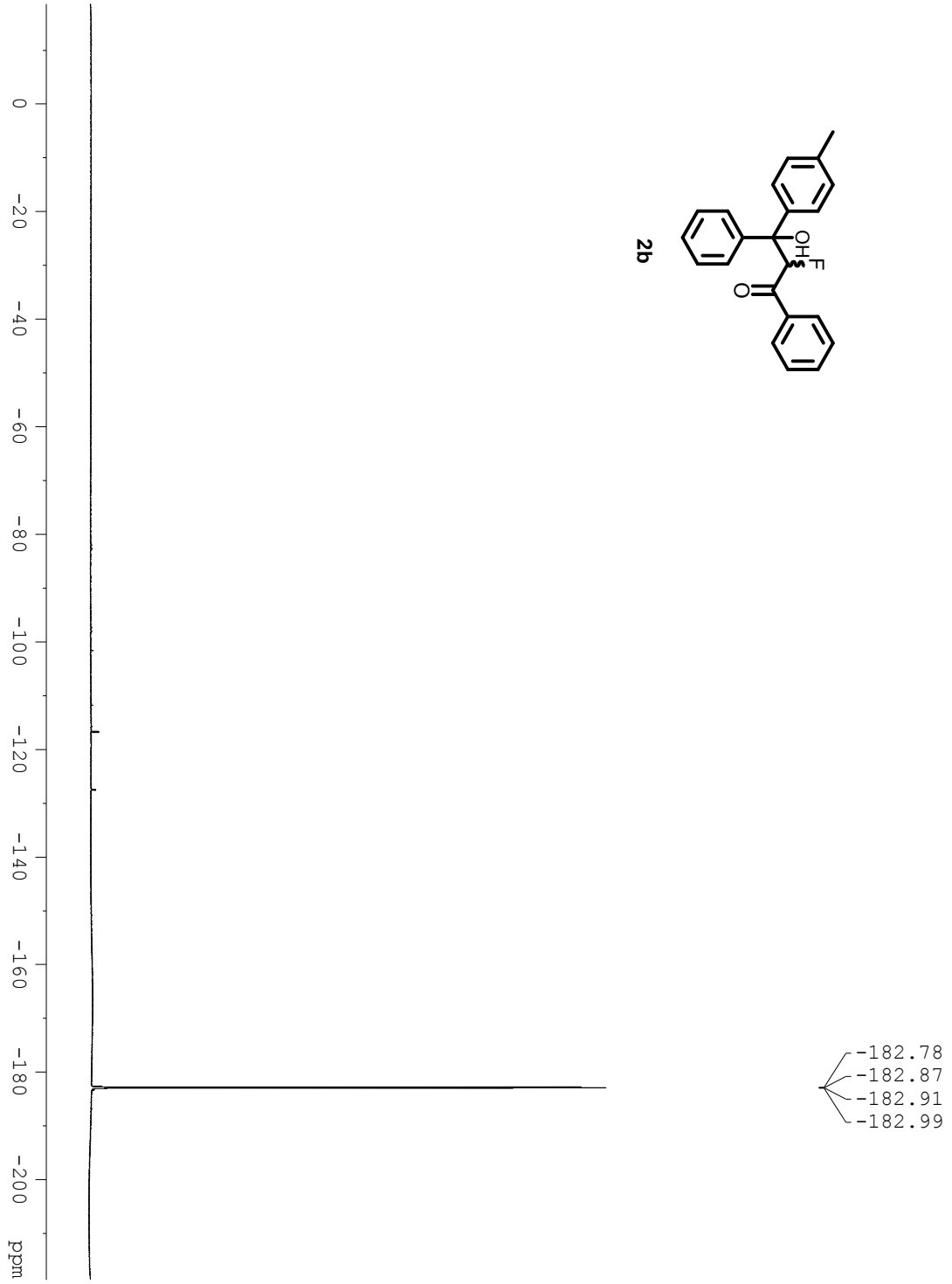
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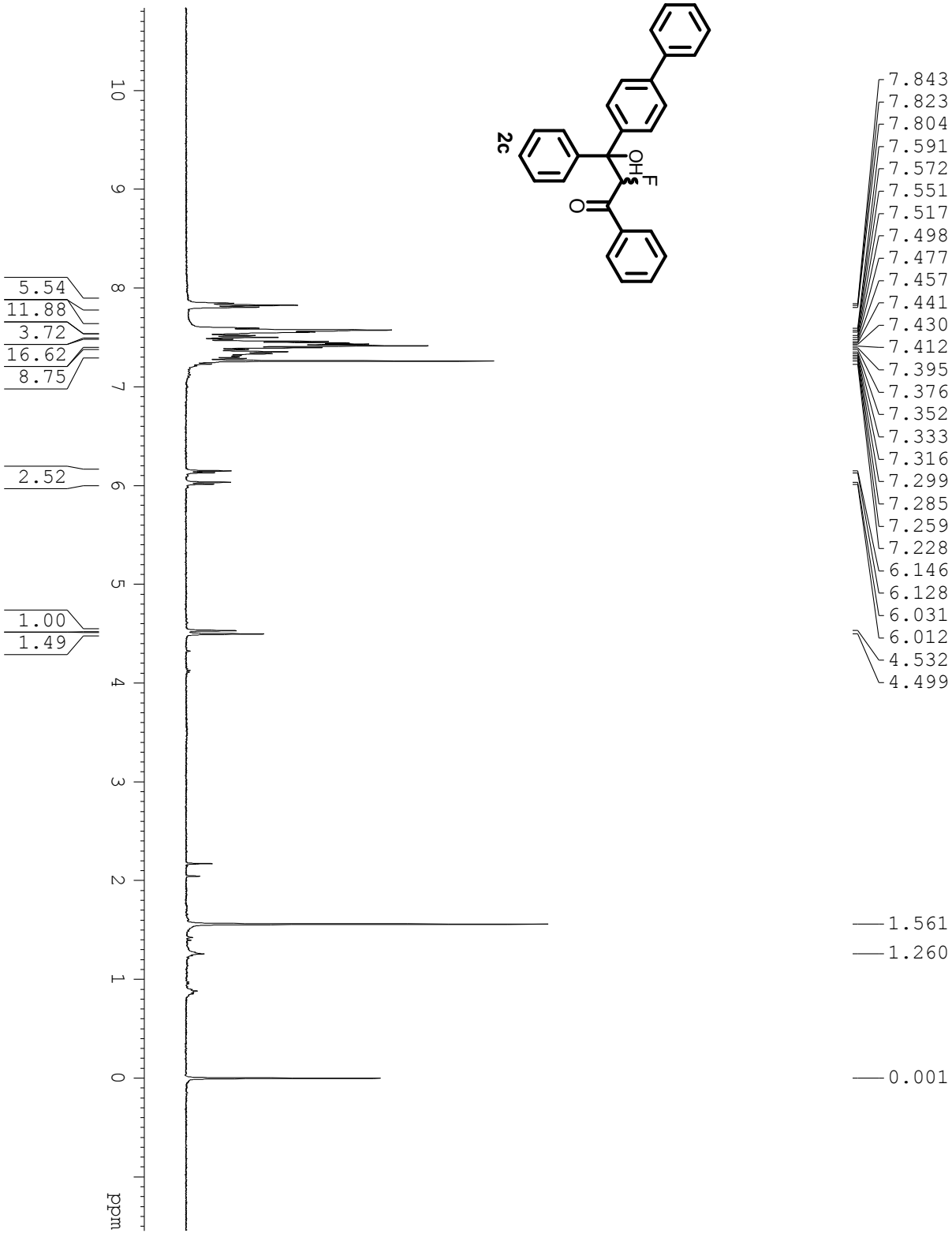
F
O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7.551
7.517
7.498
7.477
7.457
7.441
7.430
7.412
7.395
7.376
7.352
7.333
7.316
7.299
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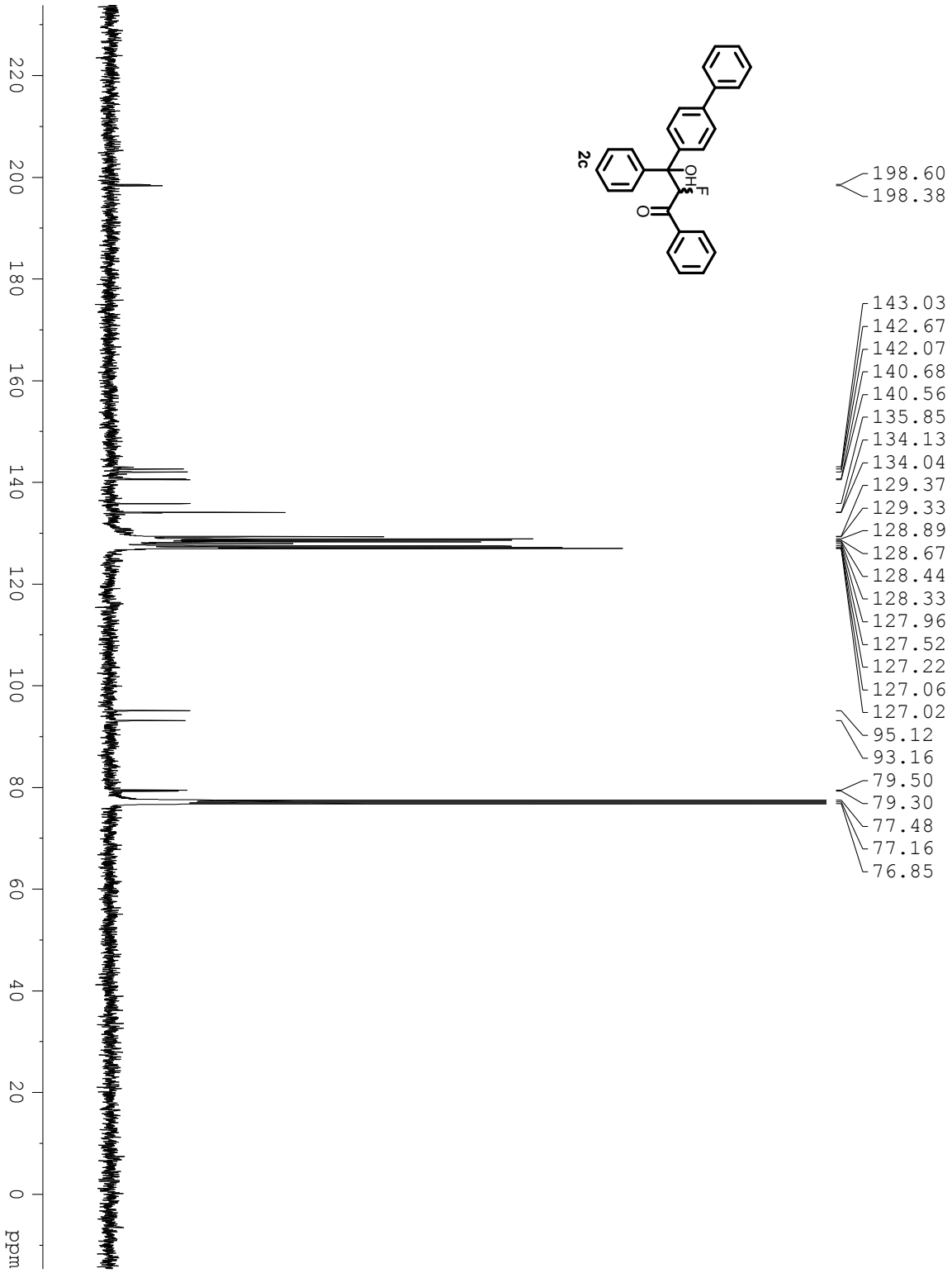
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F
O
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142.07
140.68
140.56
135.85
134.13
134.04
129.37
129.33
128.89
128.67
128.44
128.33
127.96
127.52
127.22
127.06
127.02
95.12
93.16
79.50
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76.85
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200
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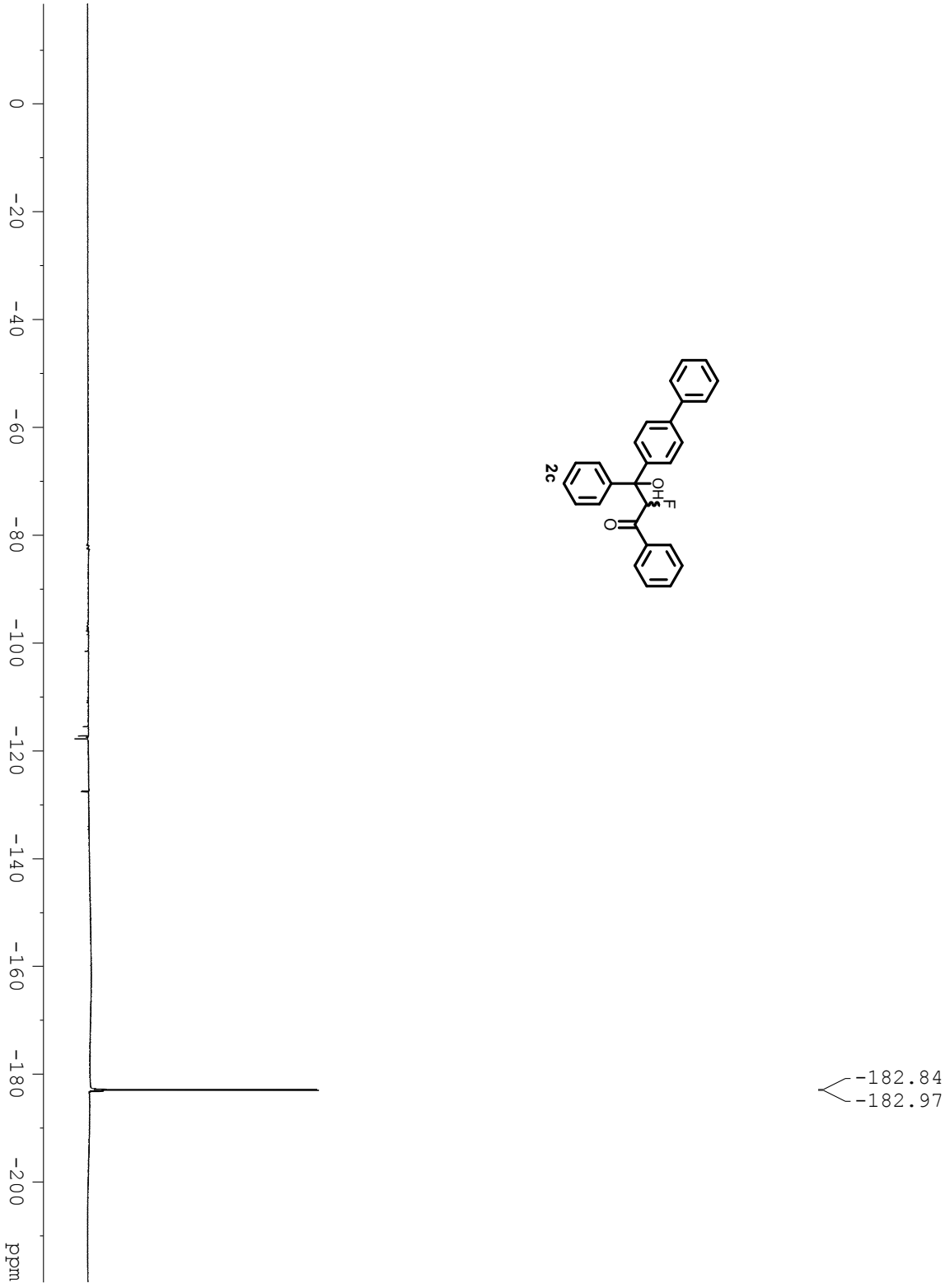
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-20
-40
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-180
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ppm
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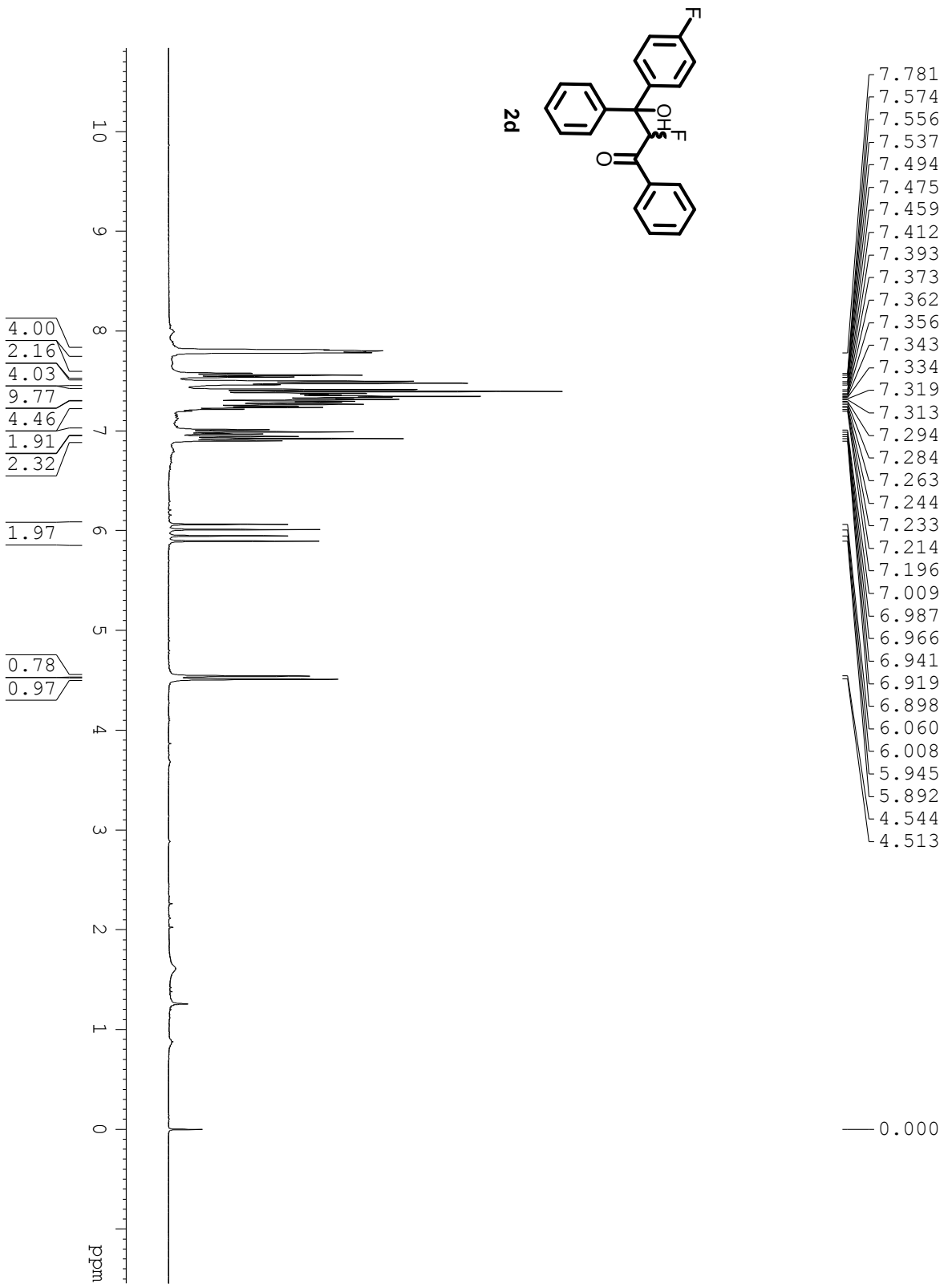
F
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O
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ppm
7.781
7.574
7.556
7.537
7.494
7.475
7.459
7.412
7.393
7.373
7.362
7.356
7.343
7.334
7.319
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7.284
7.263
7.244
7.233
7.214
7.196
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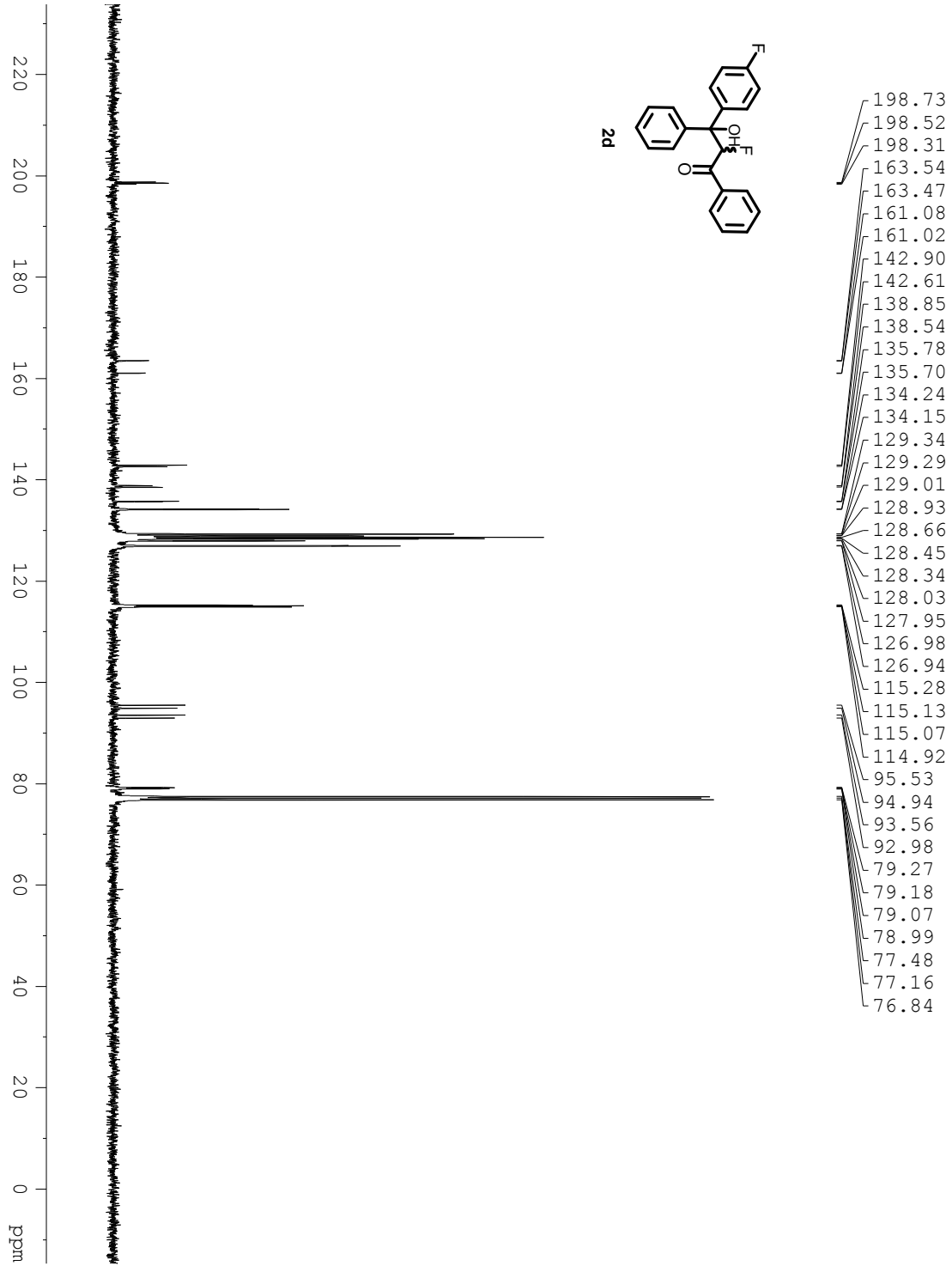
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F
O
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161.02
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138.85
138.54
135.78
135.70
134.24
134.15
129.34
129.29
129.01
128.93
128.66
128.45
128.34
128.03
127.95
126.98
126.94
115.28
115.13
115.07
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95.53
94.94
93.56
92.98
79.27
79.18
79.07
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77.16
76.84
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200
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140
120
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80
60
40
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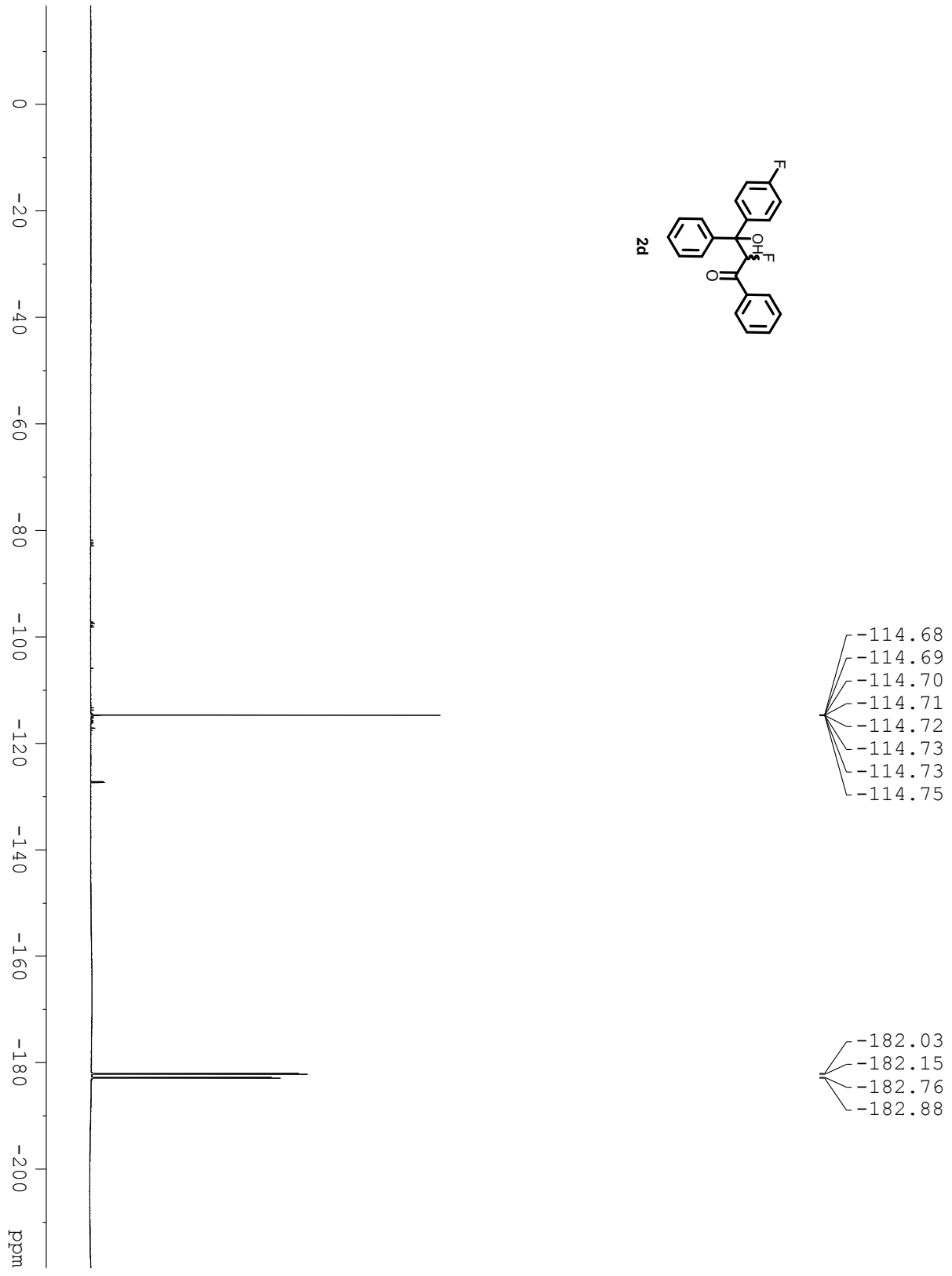
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-200
ppm
F
OH
F
O
2d
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-114.73
-114.75
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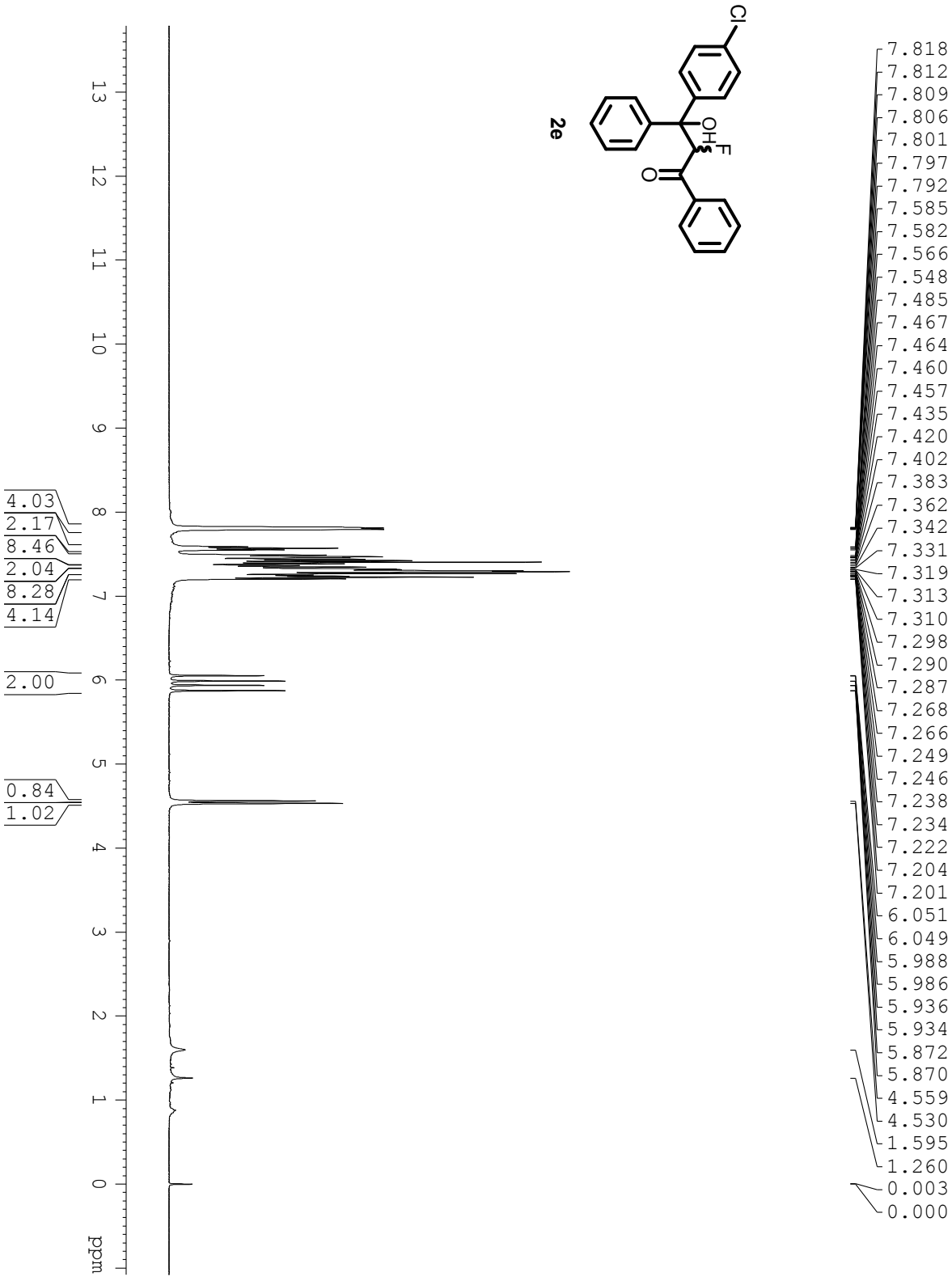
-182.76
-182.88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7.566
7.548
7.485
7.467
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7.460
7.457
7.435
7.420
7.402
7.383
7.362
7.342
7.331
7.319
7.313
7.310
7.298
7.290
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7.268
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7.246
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7.234
7.222
7.204
7.201
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5.936
5.934
5.872
5.870
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4.530
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1.260
0.003
0.000
4.03
2.17
8.46
2.04
8.28
4.14
2.00
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13
12
11
10
9
8
7
6
5
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3
2
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0
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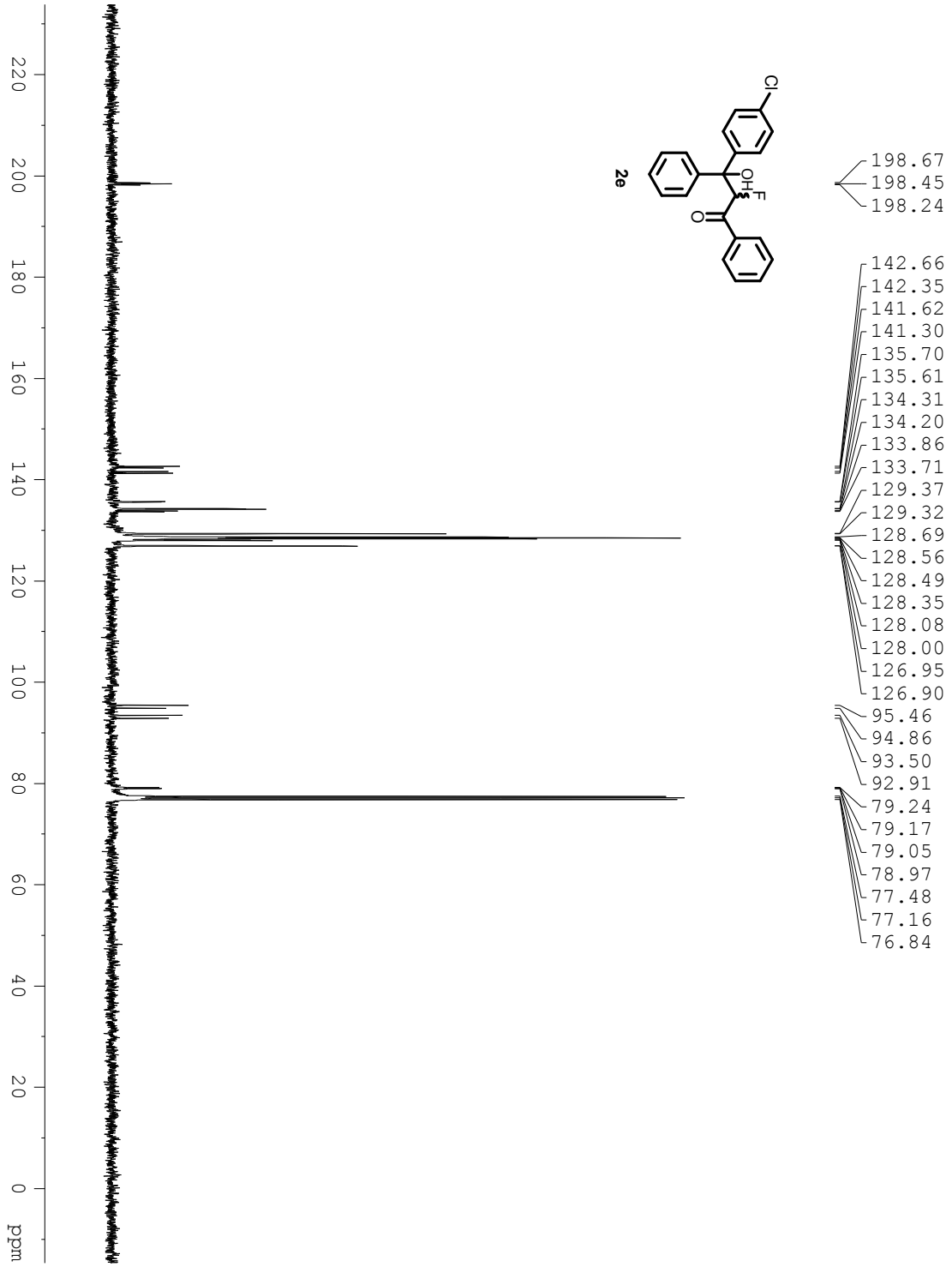
220
200
180
160
140
120
100
80
60
40
20
0
ppm
2e
Cl
OH
F
O
198.67
198.45
198.24
142.66
142.35
141.62
141.30
135.70
135.61
134.31
134.20
133.86
133.71
129.37
129.32
128.69
128.56
128.49
128.35
128.08
128.00
126.95
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79.05
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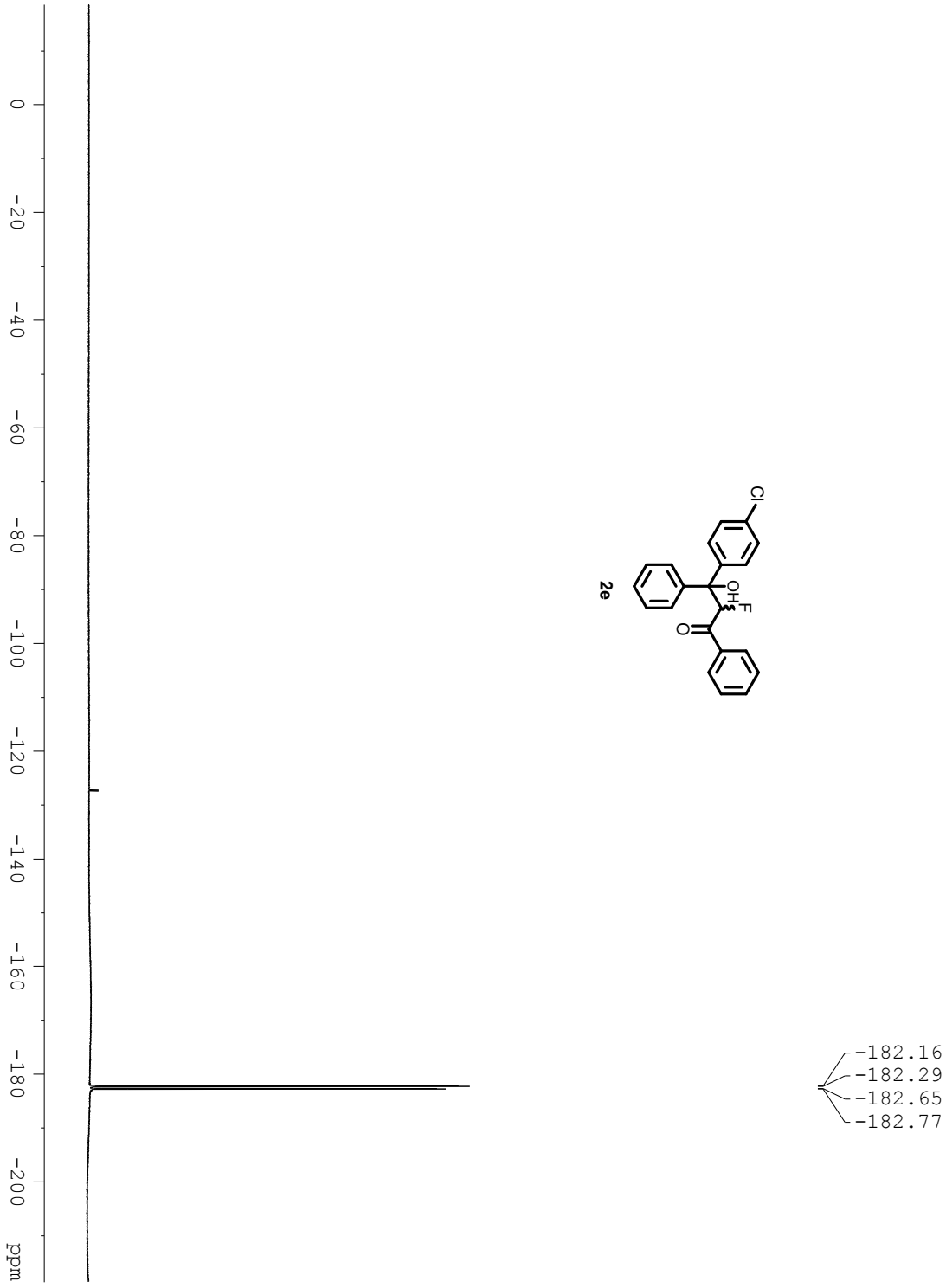
77.48
77.16
76.84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-100
-120
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-200
ppm
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OH
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2e
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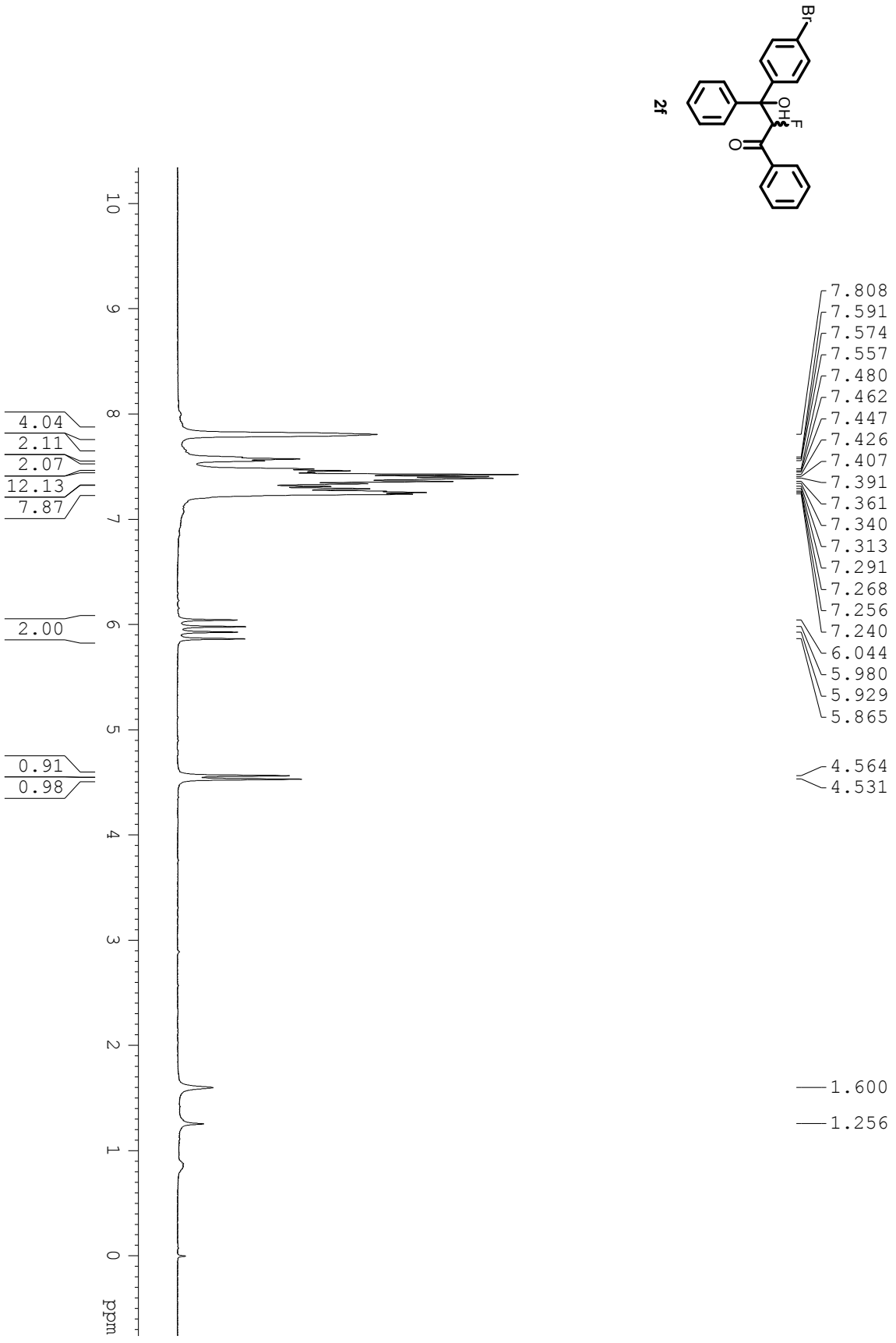
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O
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7.447
7.426
7.407
7.391
7.361
7.340
7.313
7.291
7.268
7.256
7.240
6.044
5.980
5.929
5.865
4.564
4.531
1.600
1.256
4.04
2.11
2.07
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6
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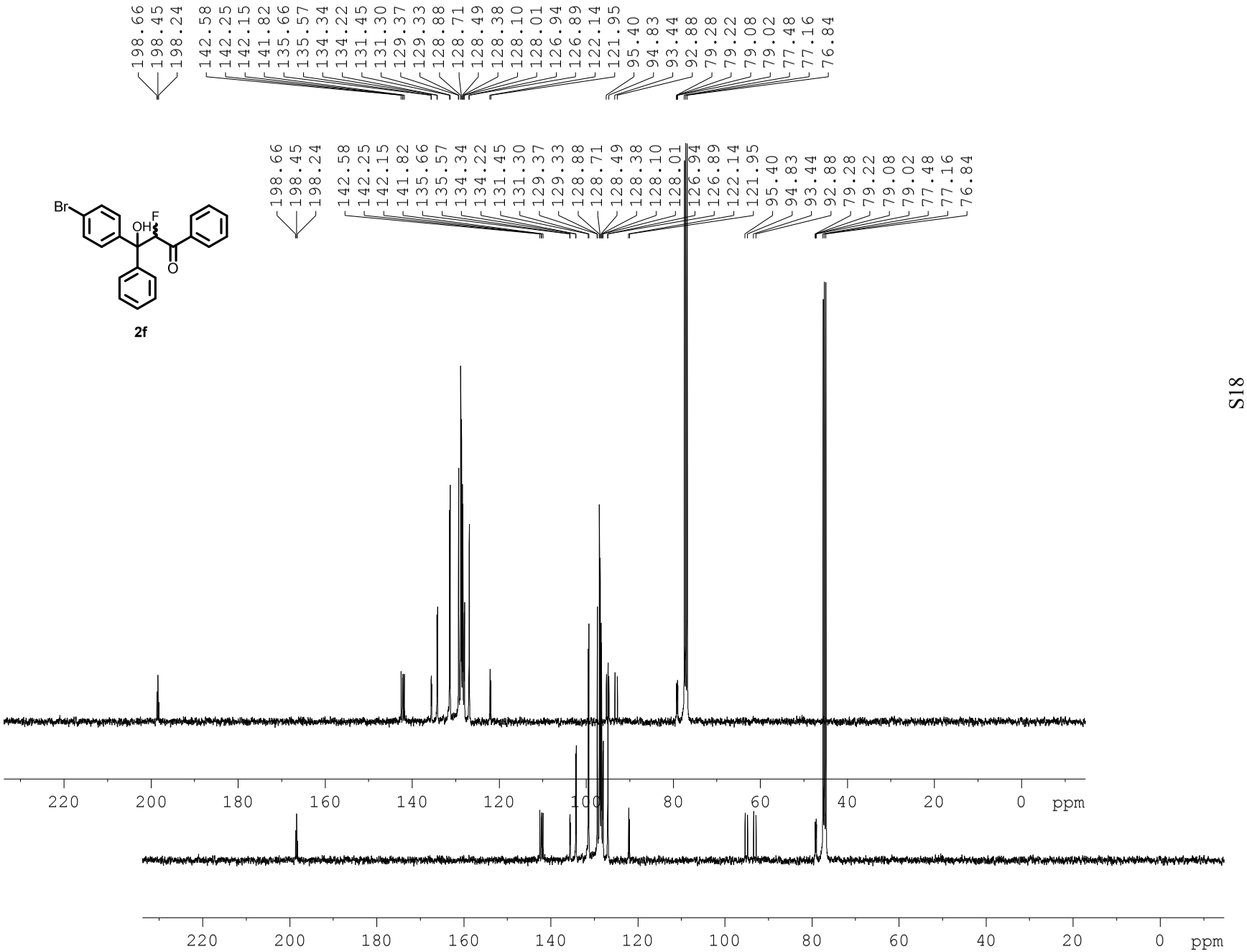
ppm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129.33
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126.89
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121.95
95.40
94.83
93.44
92.88
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79.22
79.08
79.02
77.48
77.16
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O
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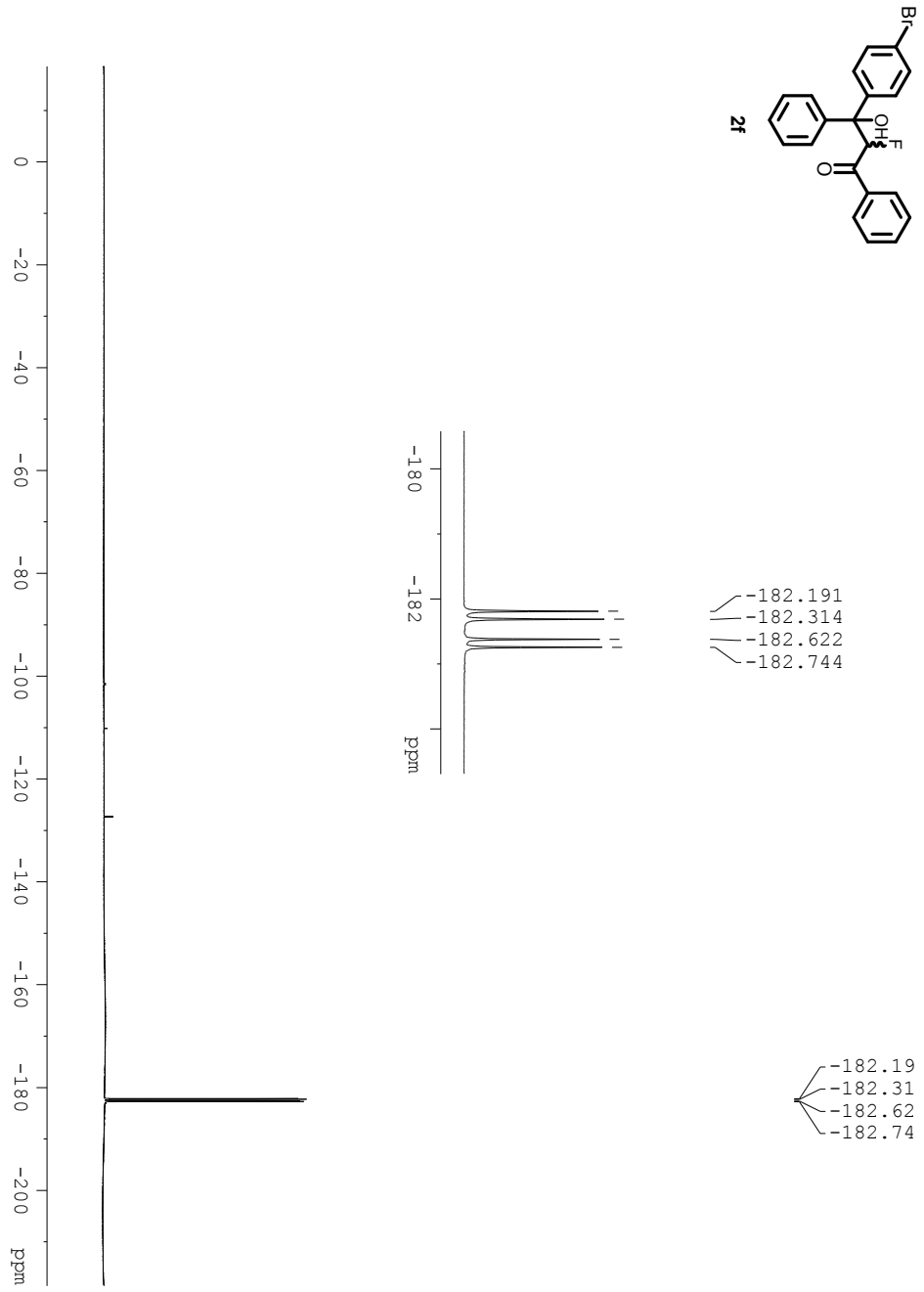
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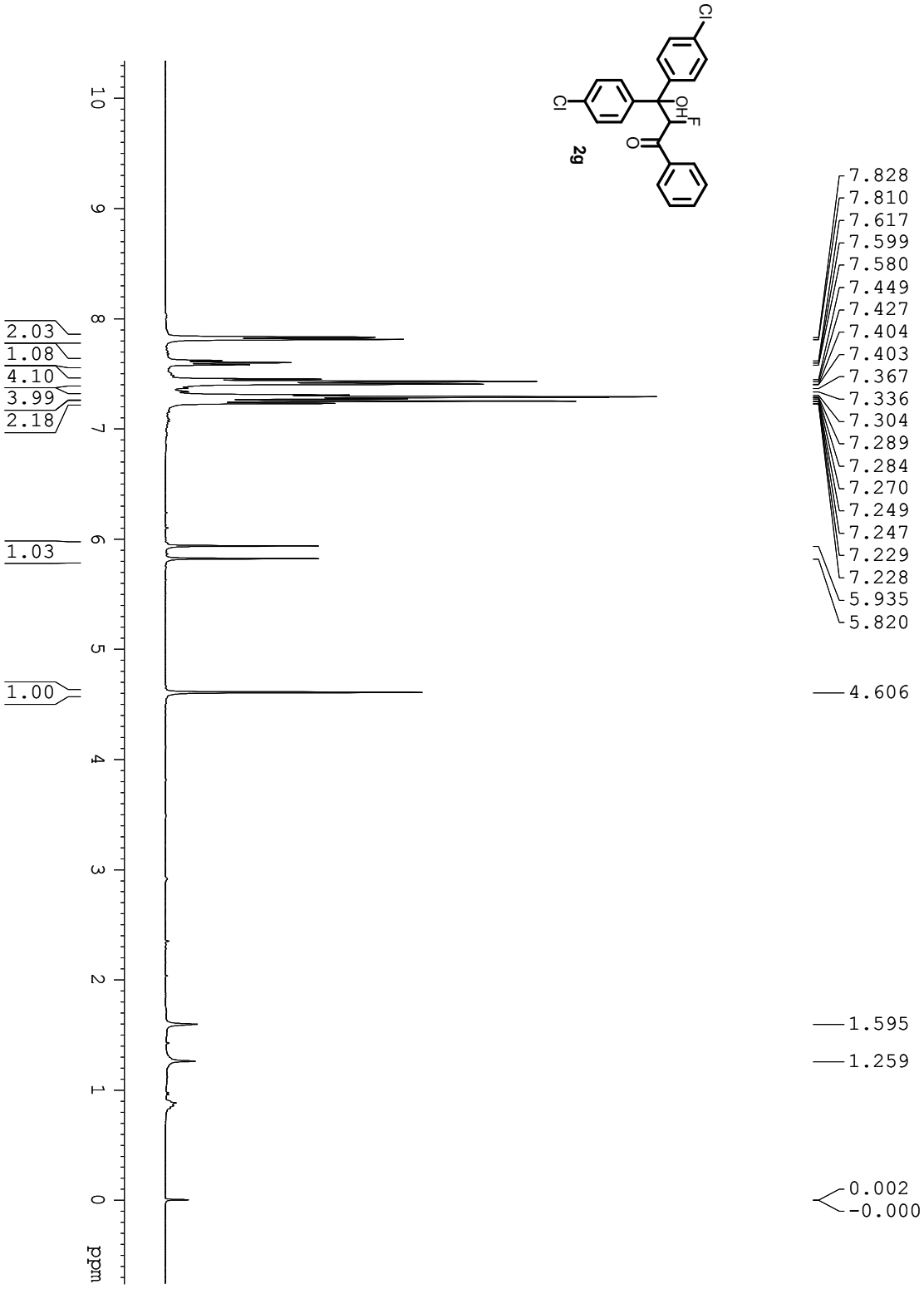
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Cl
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7.403
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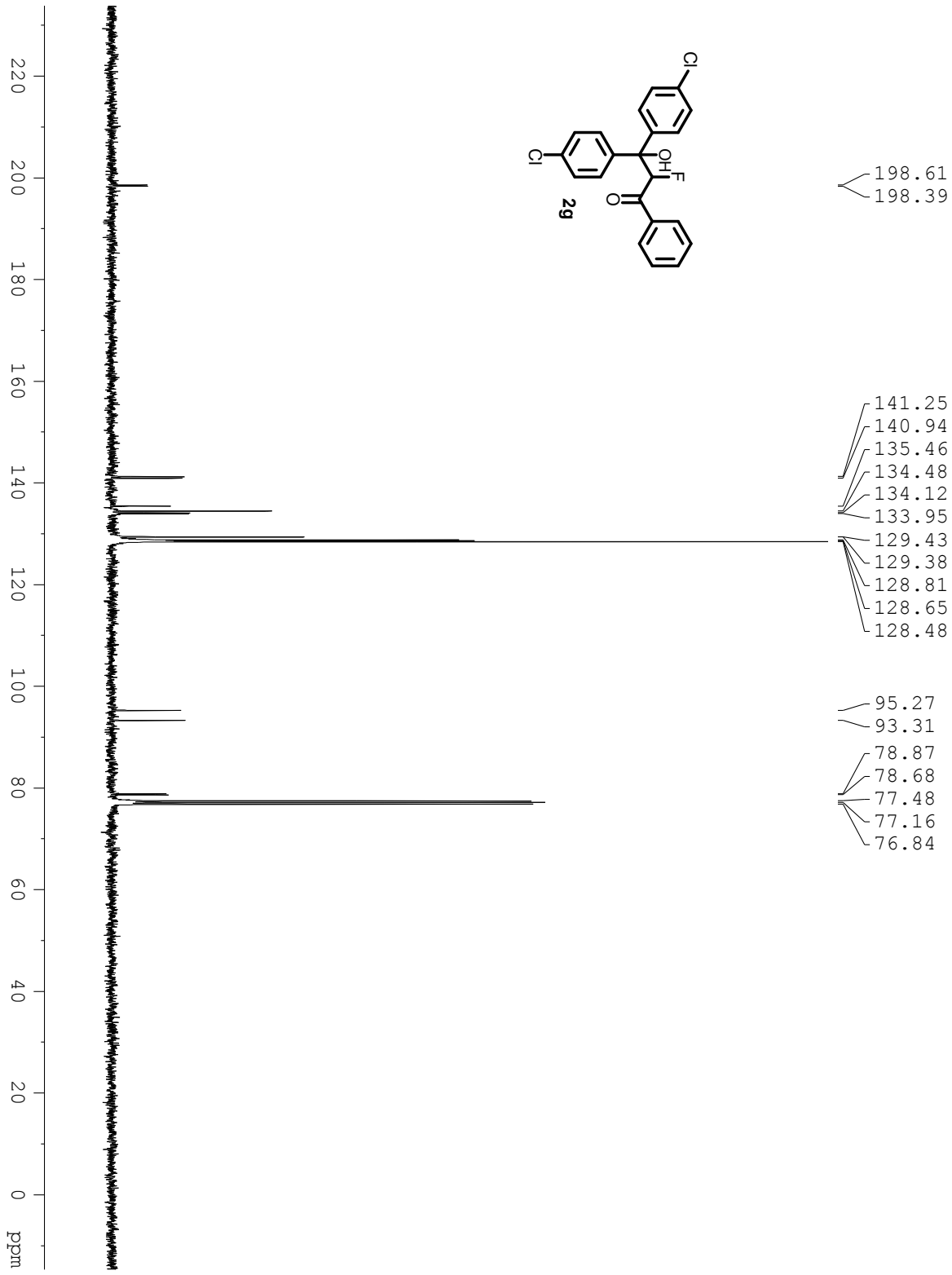
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Cl
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F
O
2g
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128.65
128.48
95.27
93.31
78.87
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76.84
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200
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120
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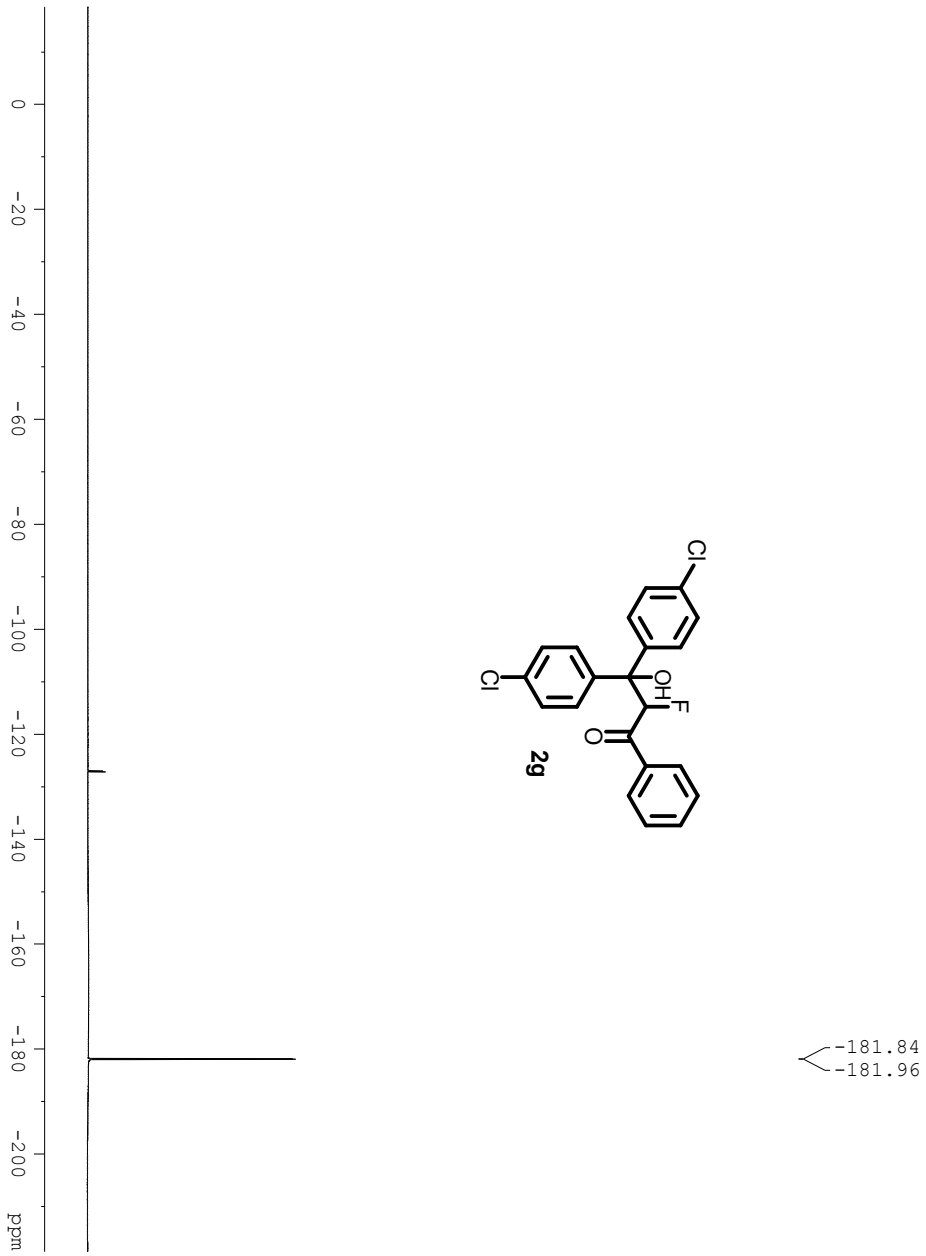
0
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ppm
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Cl
OH
F
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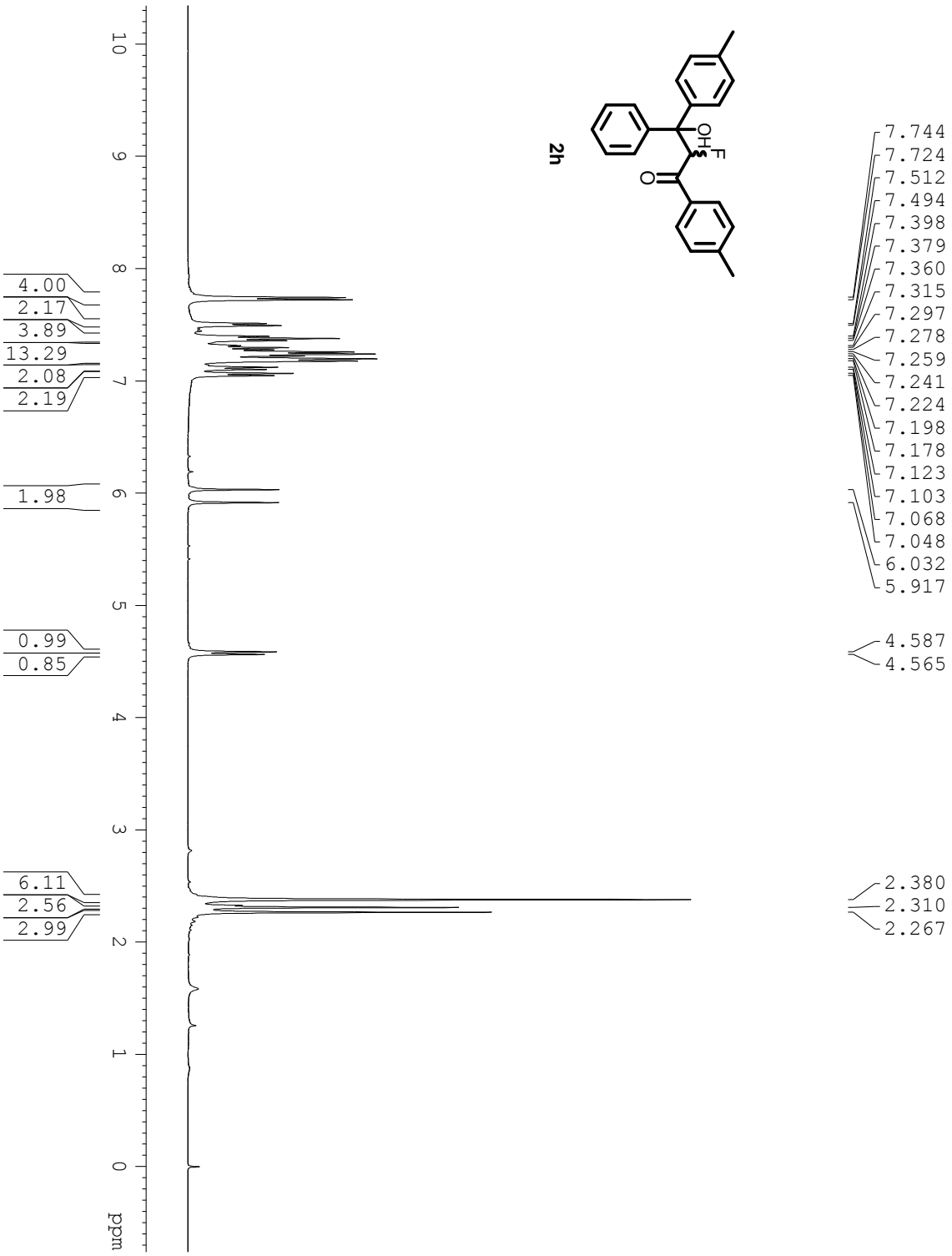
-181.96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F
O
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7.259
7.241
7.224
7.198
7.178
7.123
7.103
7.068
7.048
6.032
5.917
4.587
4.565
2.380
2.310
2.267
4.00
2.17
3.89
13.29
2.08
2.19
1.98
0.99
0.85
6.11
2.56
2.99
10
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8
7
6
5
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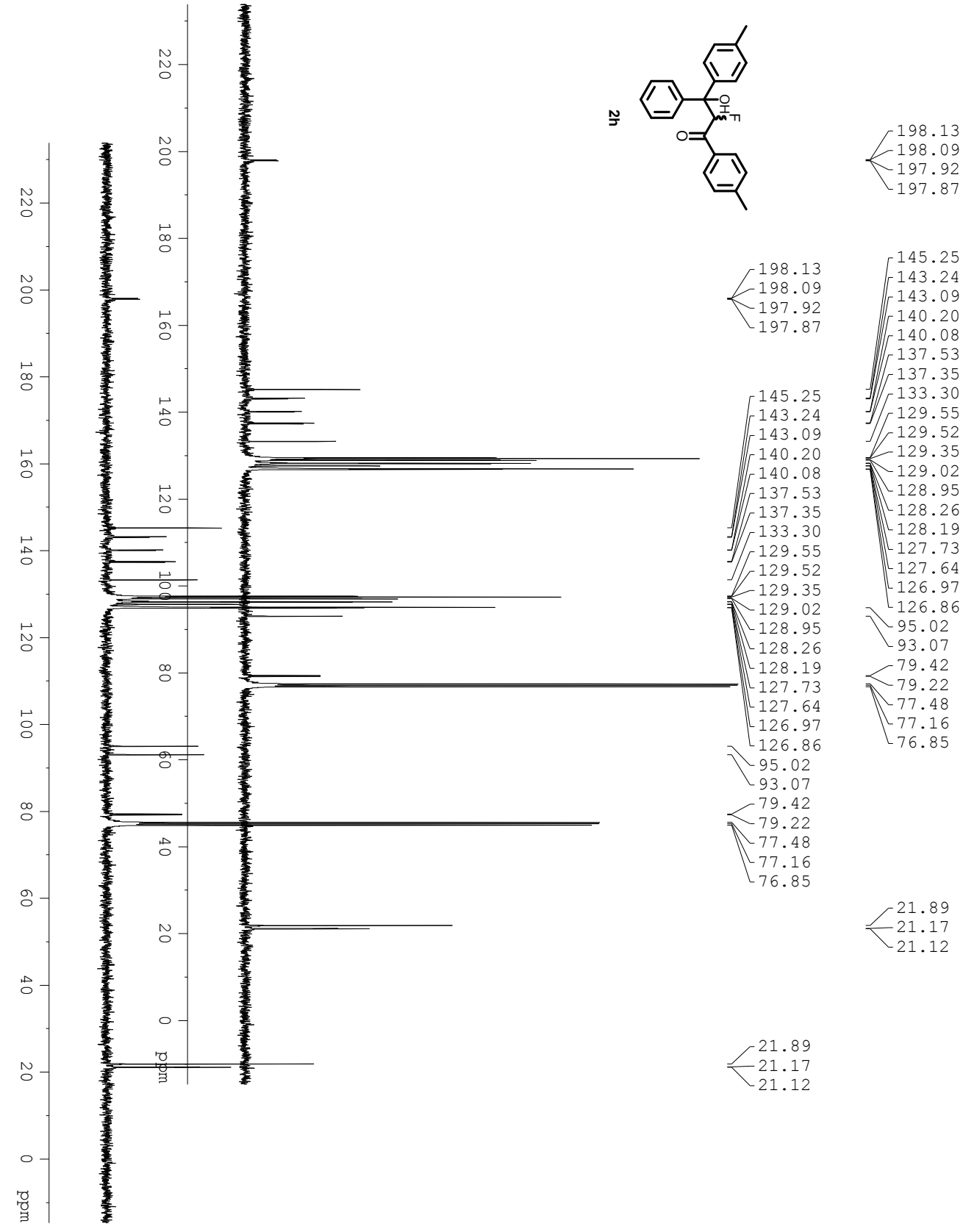
ppm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143.09
140.20
140.08
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137.35
133.30
129.55
129.52
129.35
129.02
128.95
128.26
128.19
127.73
127.64
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126.86
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93.07
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77.16
76.85
21.89
21.17
21.12
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-200
ppm

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ppm
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2h
OH
F
O

-182.55
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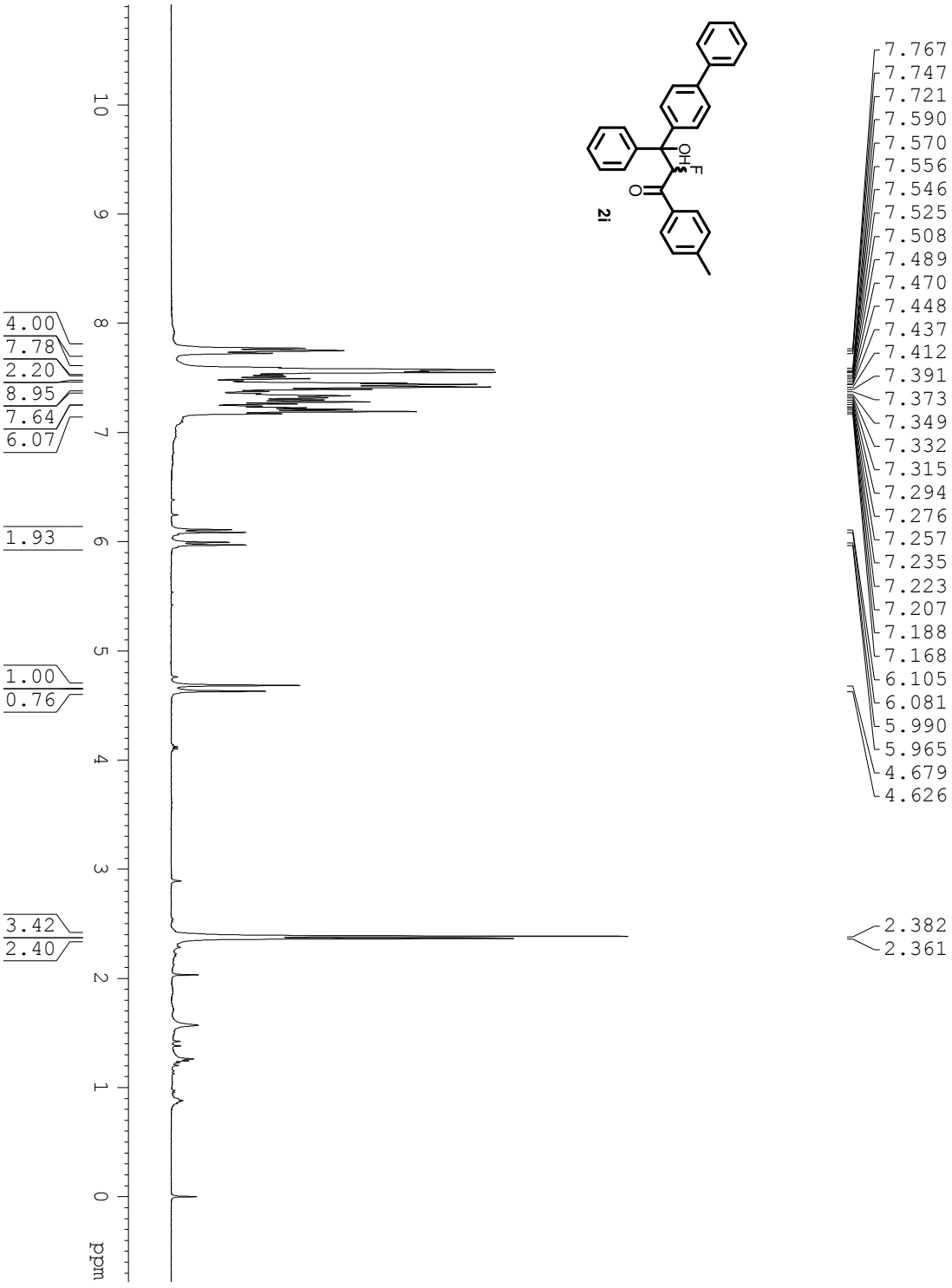
-182.67
-182.71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8
7
6
5
4
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2
1
0
ppm
OH
F
O
2i
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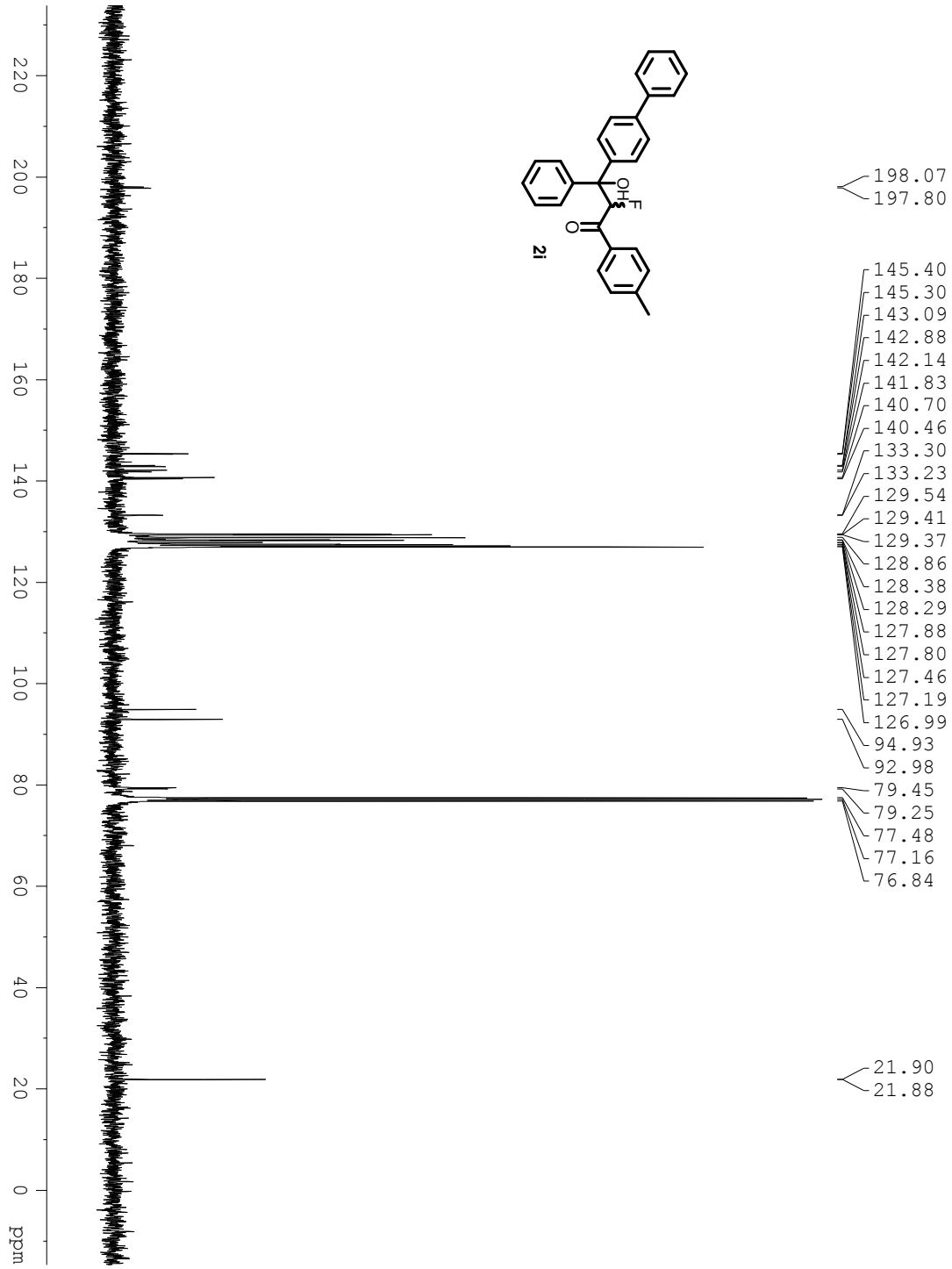
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142.14
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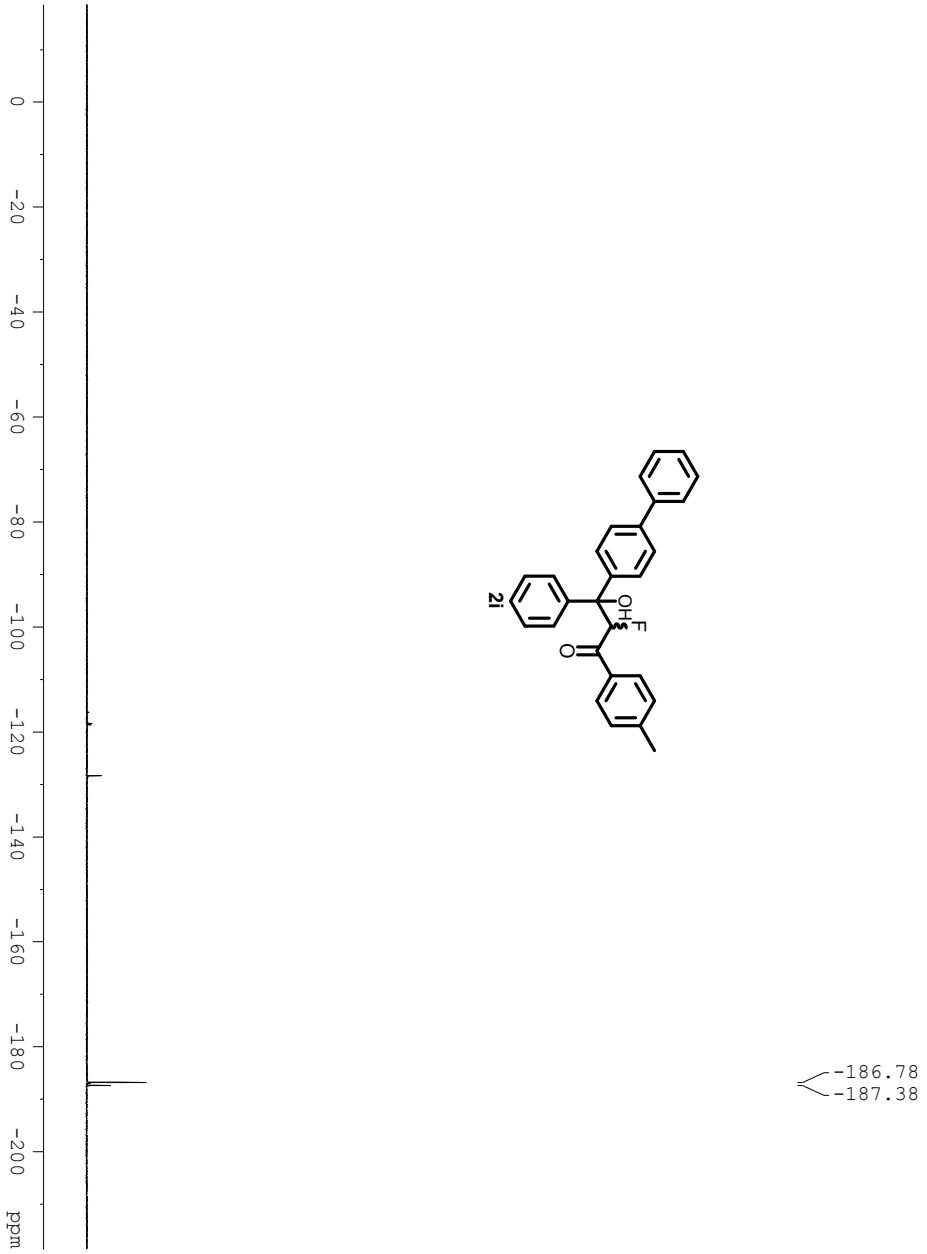
140.46
133.30
133.23
129.54
129.41
129.37
128.86
128.38
128.29
127.88
127.80
127.46
127.19
126.99
94.93
92.98
79.45
79.25
77.48
77.16
76.84
21.90
21.88
OH
F
O
2i
220
200
180
160
140
120
100
80
60
40
20
0
ppm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-20
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-60
-80
-100
-120
-140
-160
-180
-200
ppm
21
OH
F
O
-186.78
-187.38


Br
OH
F
O
2j
7.747
7.730
7.714
7.477
7.459
7.430
7.409
7.388
7.372
7.367
7.351
7.341
7.314
7.297
7.278
7.271
7.264
7.252
7.231
7.224
7.210
7.190
6.001
5.946
5.886
5.830
4.705
4.651
2.386
1.259
4.00
2.46
9.32
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0.98
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10
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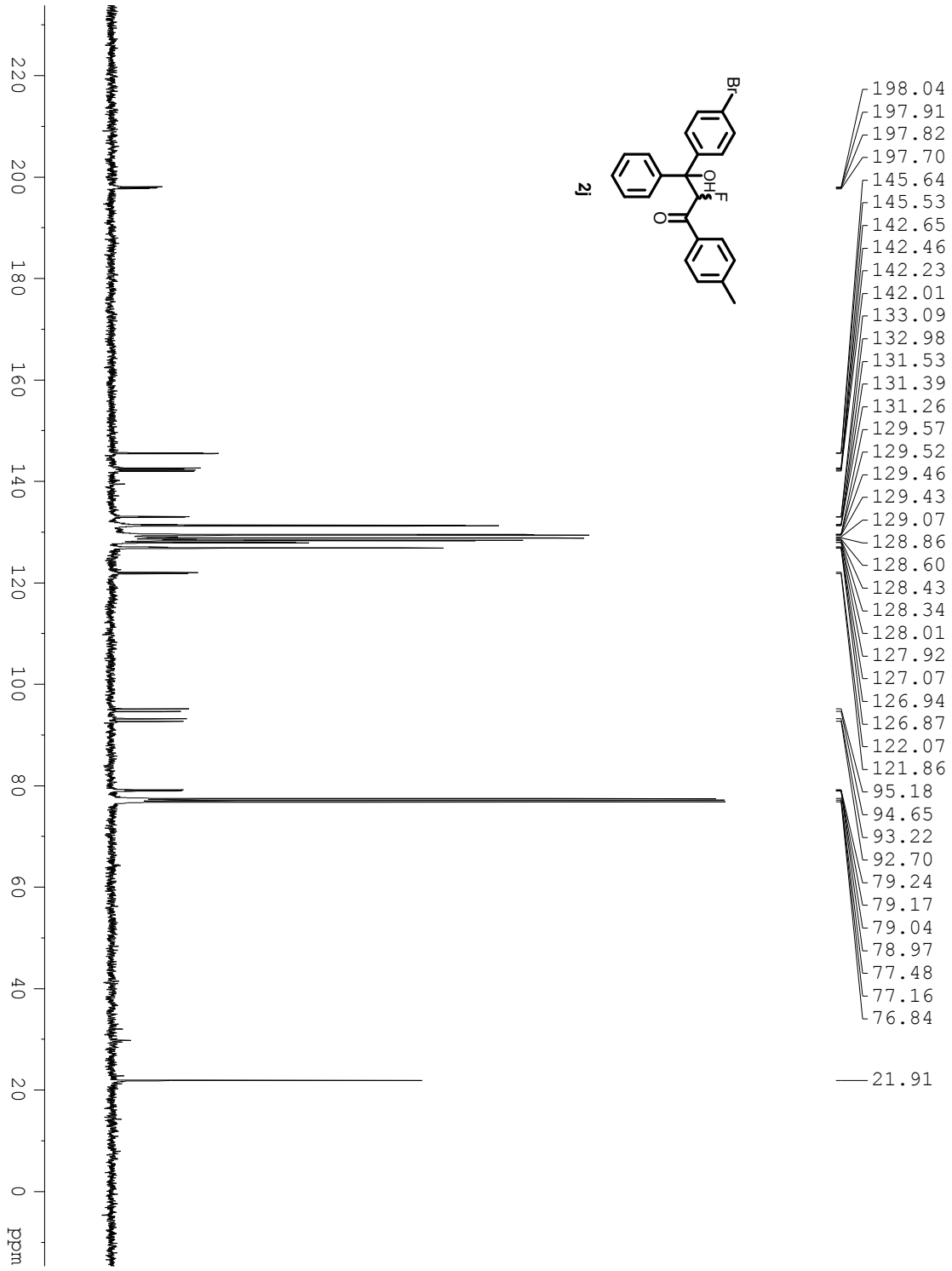
7
6
5
4
3
2
1
ppm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197.91
197.82
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145.53
142.65
142.46
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142.01
133.09
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131.53
131.39
131.26
129.57
129.52
129.46
129.43
129.07
128.86
128.60
128.43
128.34
128.01
127.92
127.07
126.94
126.87
122.07
121.86
95.18
94.65
93.22
92.70
79.24
79.17
79.04
78.97
77.48
77.16
76.84
21.91
Br
OH
F
O
2j
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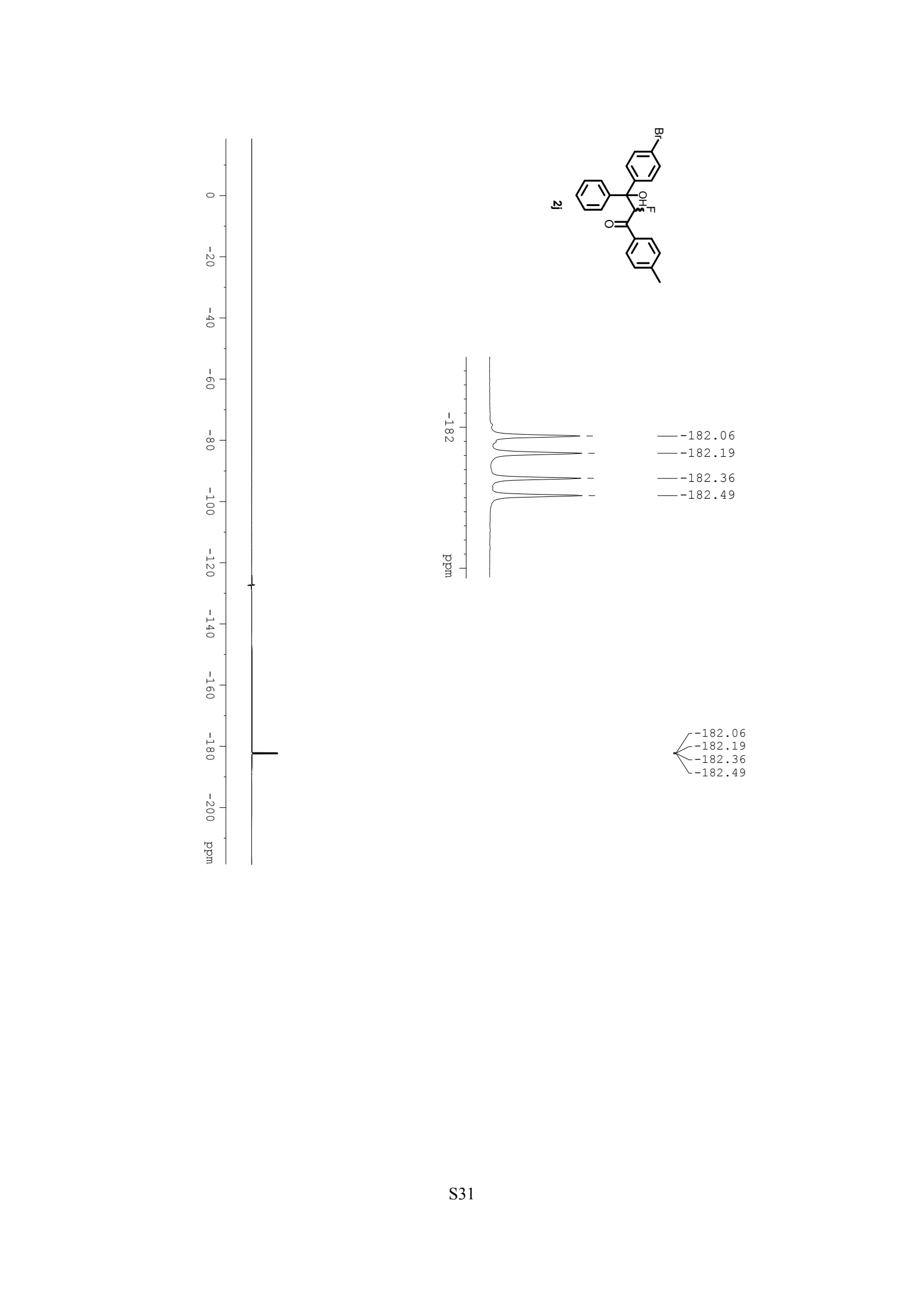
120
100
80
60
40
20
0
ppm


Br
OH
F
O
2i
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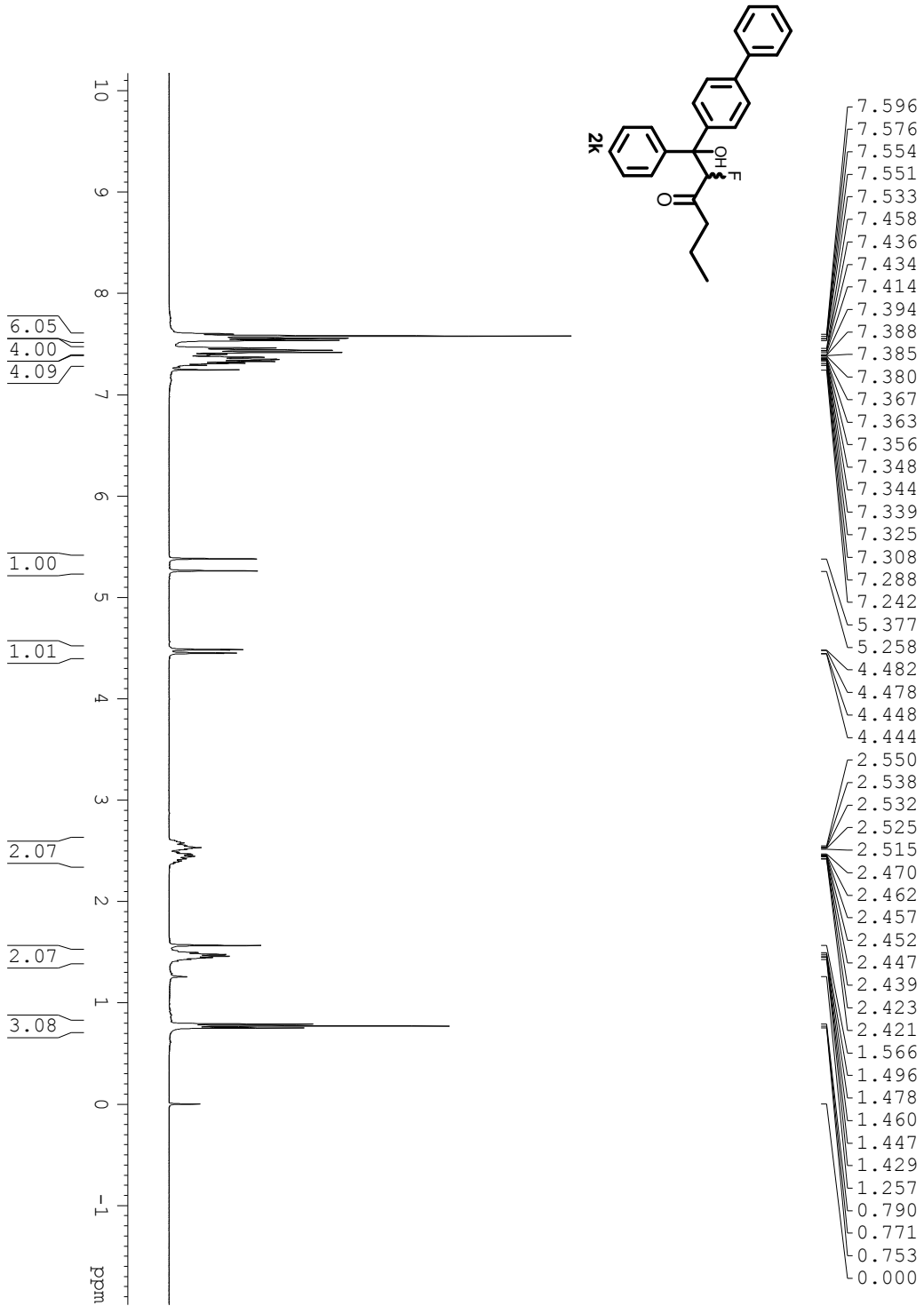
-182.19
-182.36
-182.49
-182
ppm
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-182.06
-182.19
-182.36
-182.49


2k
OH
F
O
6.05
4.00
4.09
1.00
1.01
2.07
2.07
3.08
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
7.596
7.576
7.554
7.551
7.533
7.458
7.436
7.434
7.414
7.394
7.388
7.385
7.380
7.367
7.363
7.356
7.348
7.344
7.339
7.325
7.308
7.288
7.242
5.377
5.258
4.482
4.478
4.448
4.444
2.550
2.538
2.532
2.525
2.515
2.470
2.462
2.457
2.452
2.447
2.439
2.423
2.421
1.566
1.496
1.478
1.460
1.447
1.429
1.257
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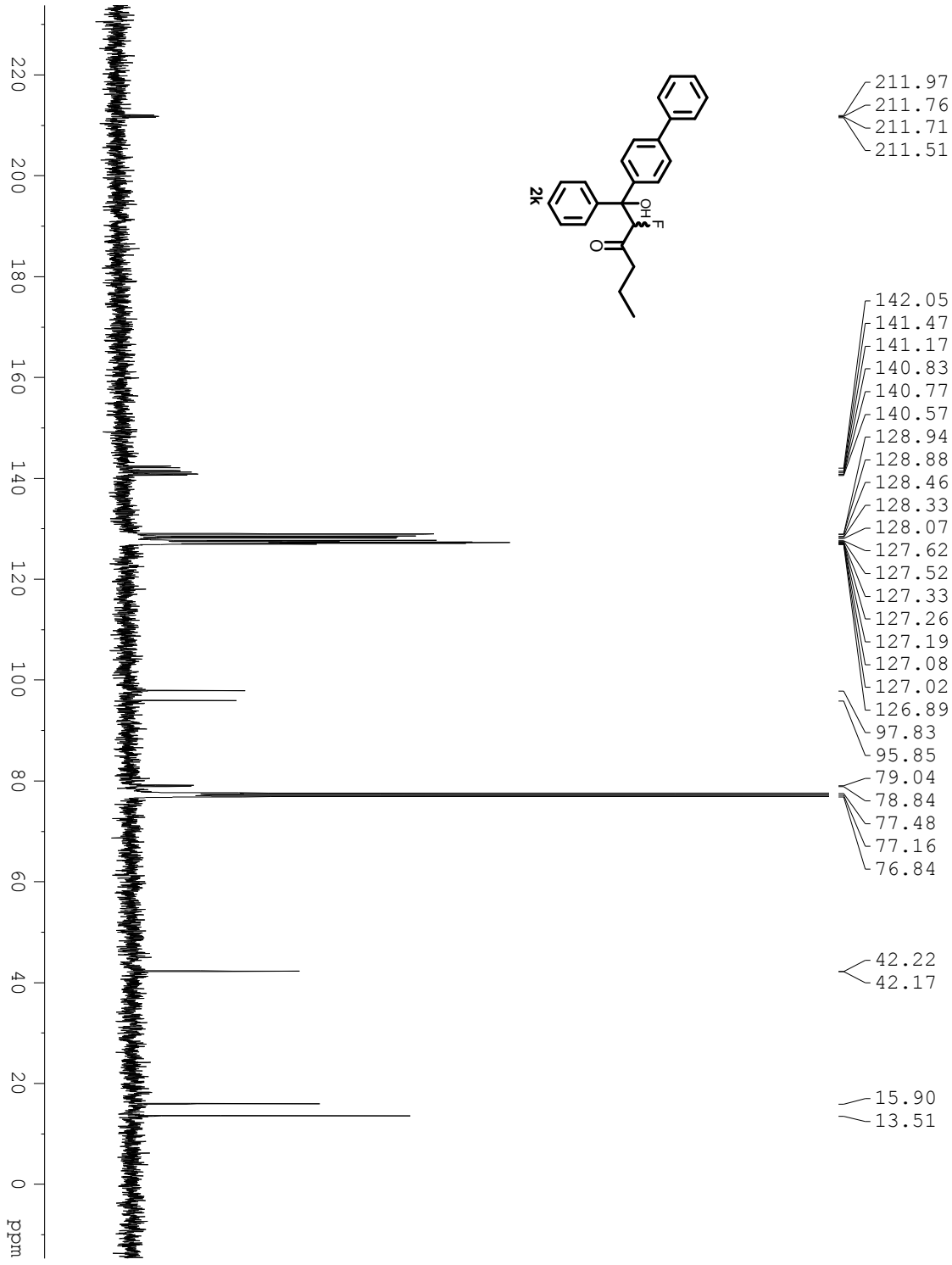
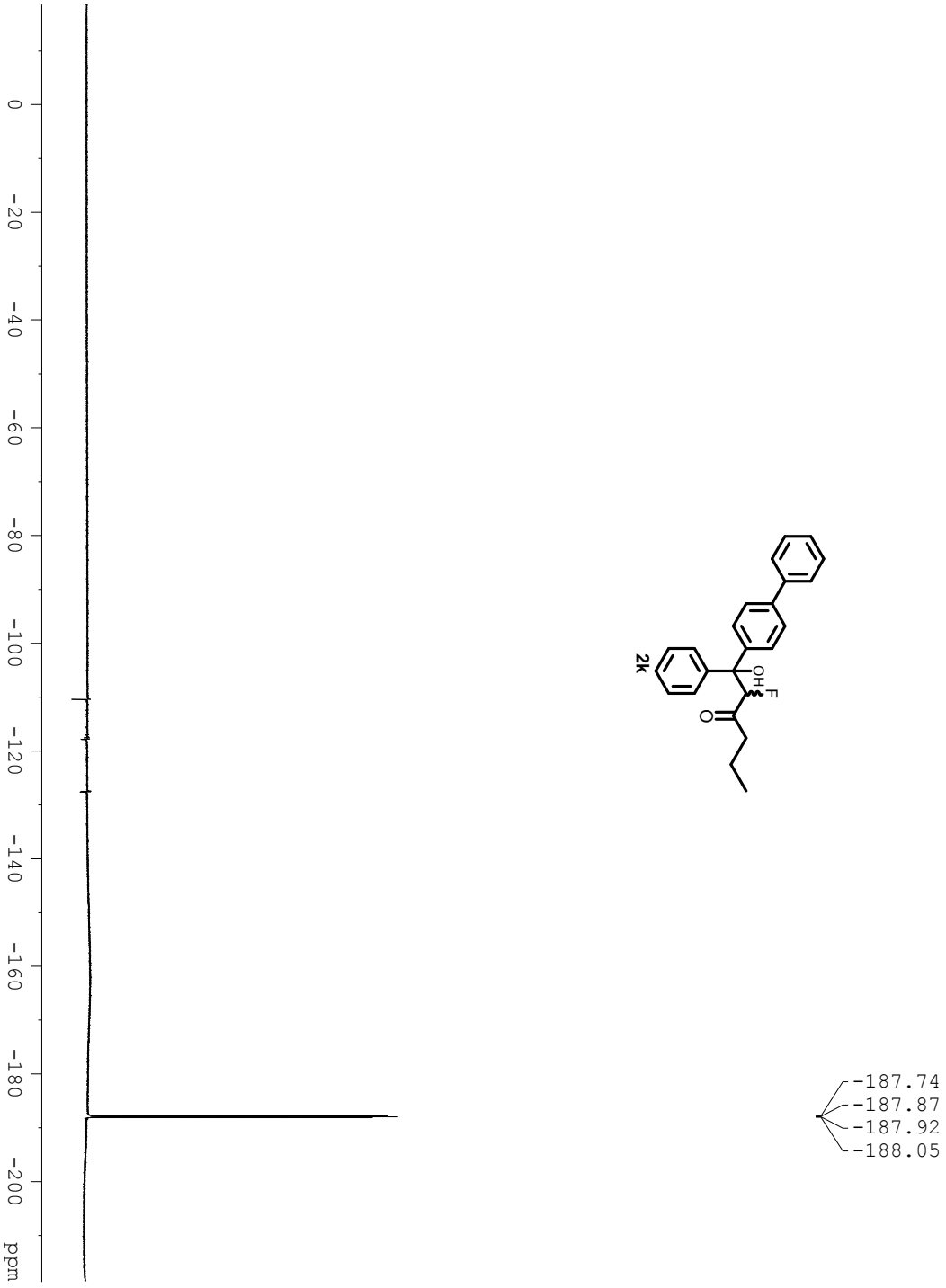
0.771
0.753
0.000


211.97
211.76
211.71
211.51
142.05
141.47
141.17
140.83
140.77
140.57
128.94
128.88
128.46
128.33
128.07
127.62
127.52
127.33
127.26
127.19
127.08
127.02
126.89
97.83
95.85
79.04
78.84
77.48
77.16
76.84
42.22
42.17
15.90
13.51
2k
OH
F
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm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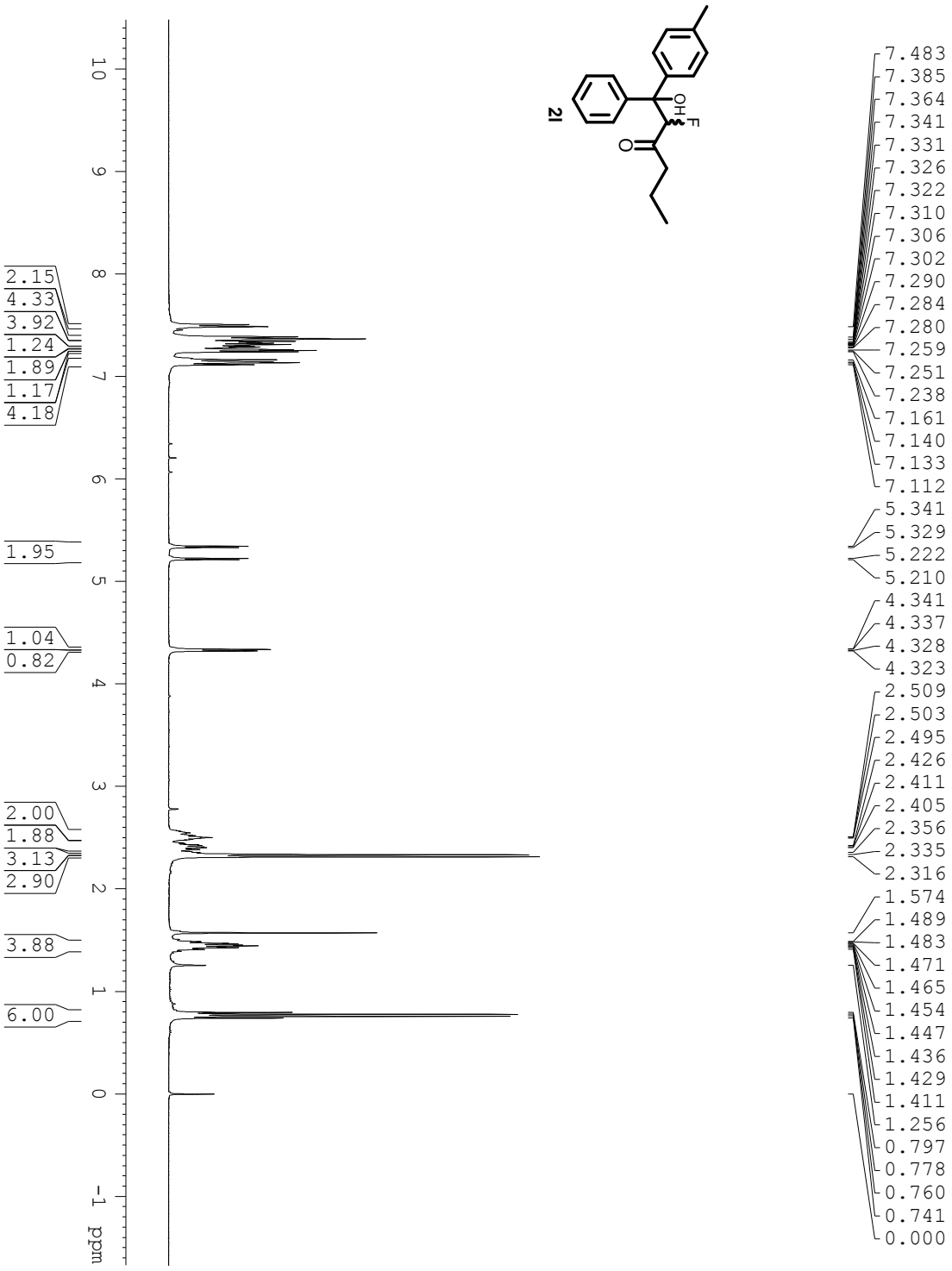
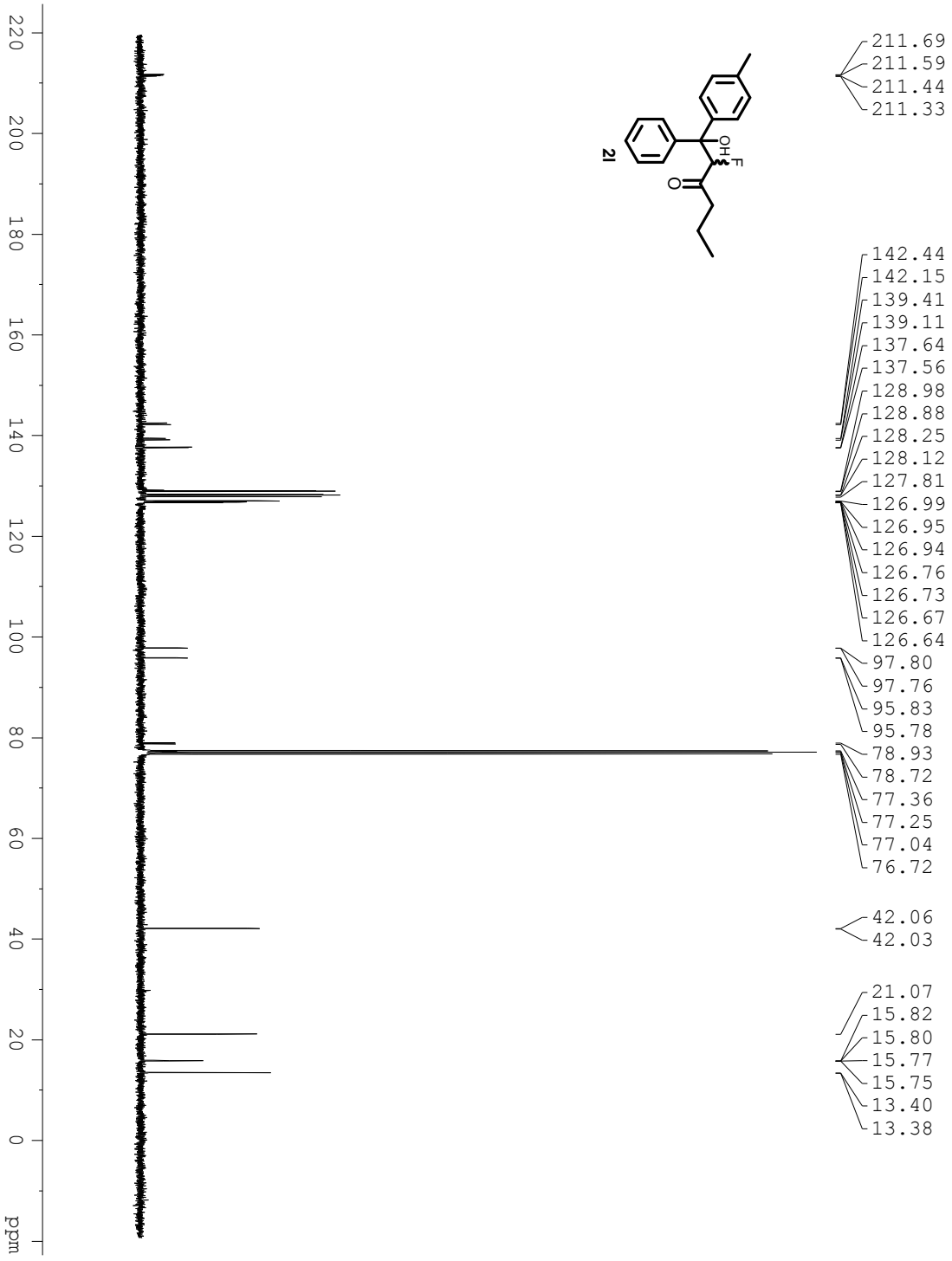
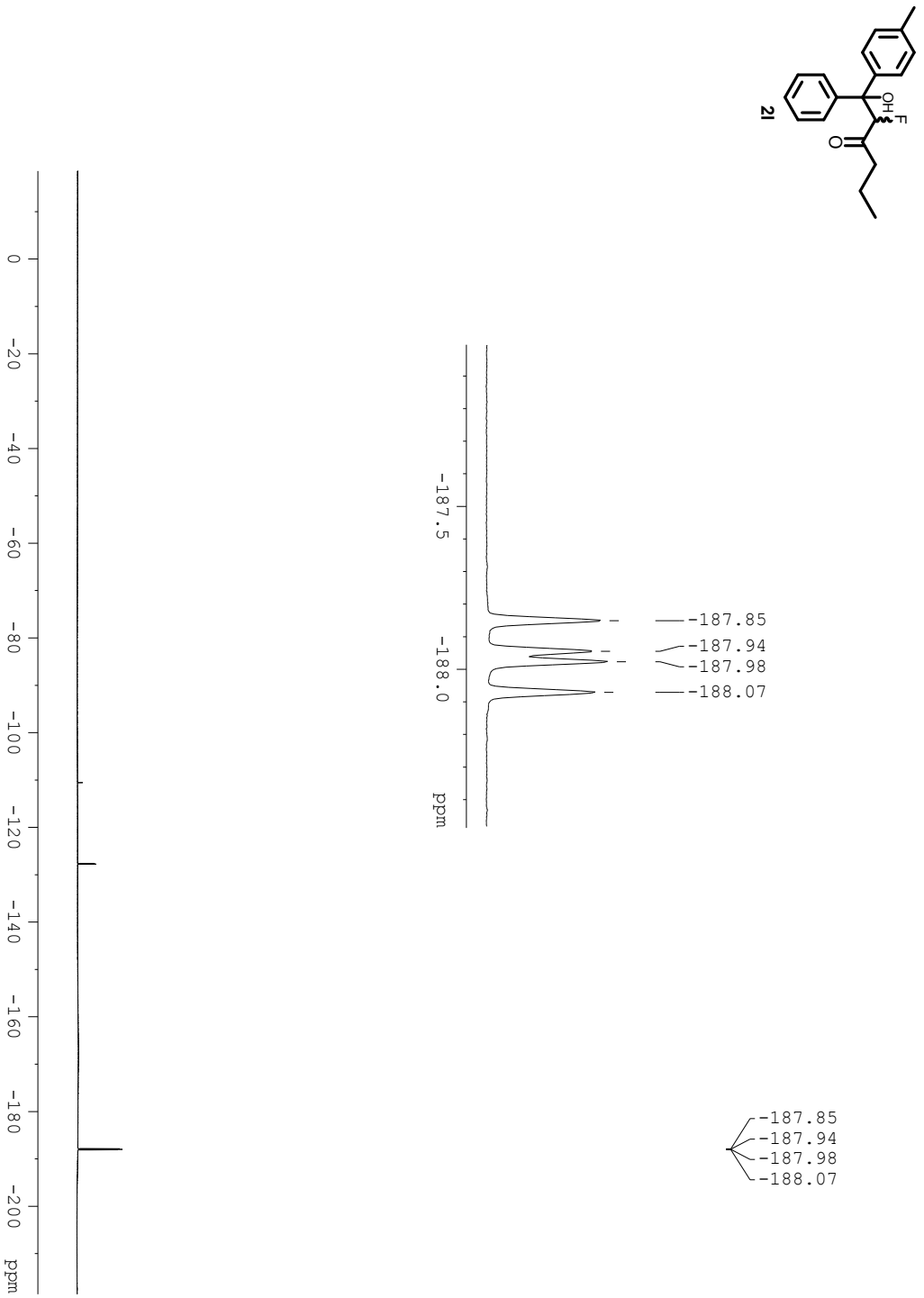
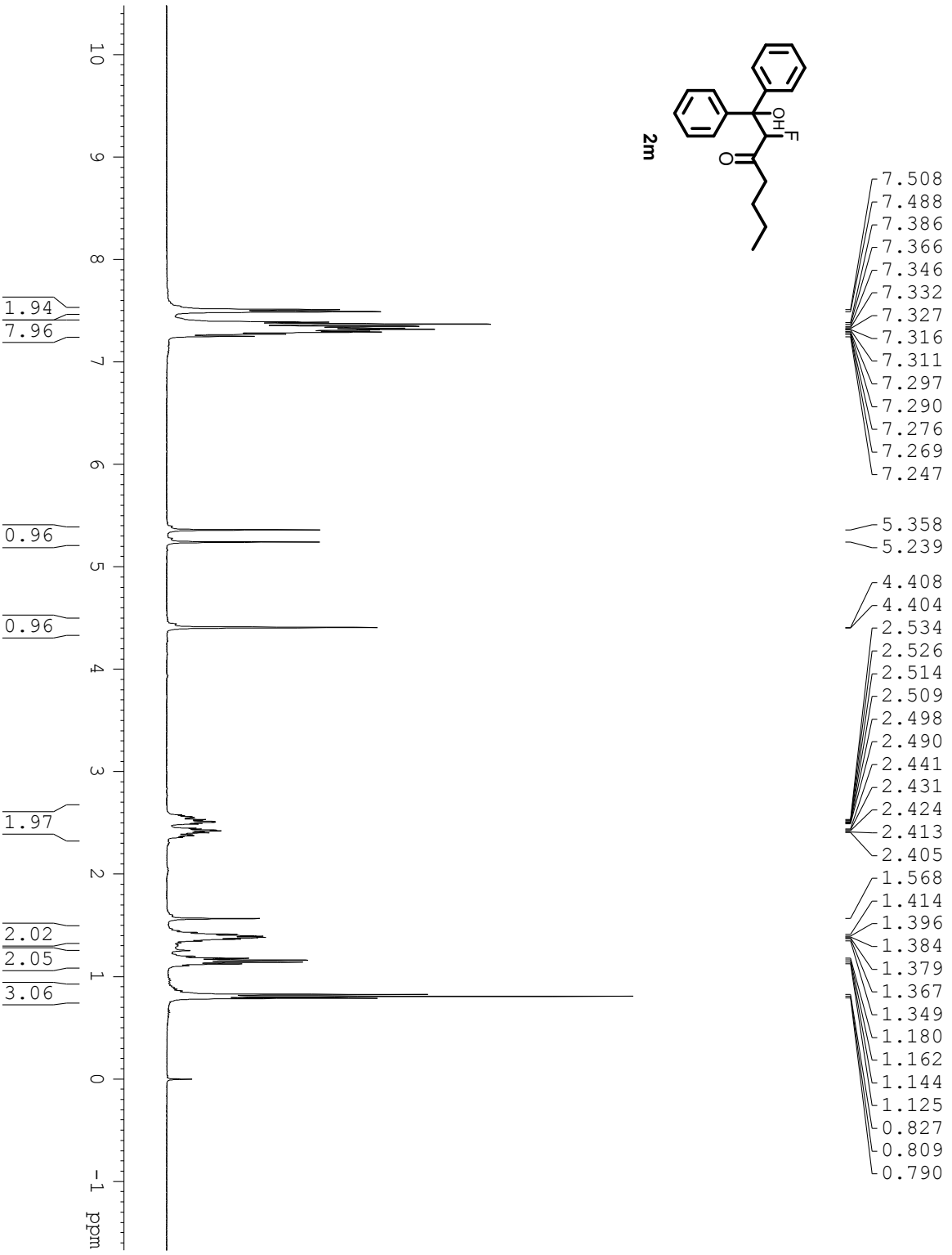
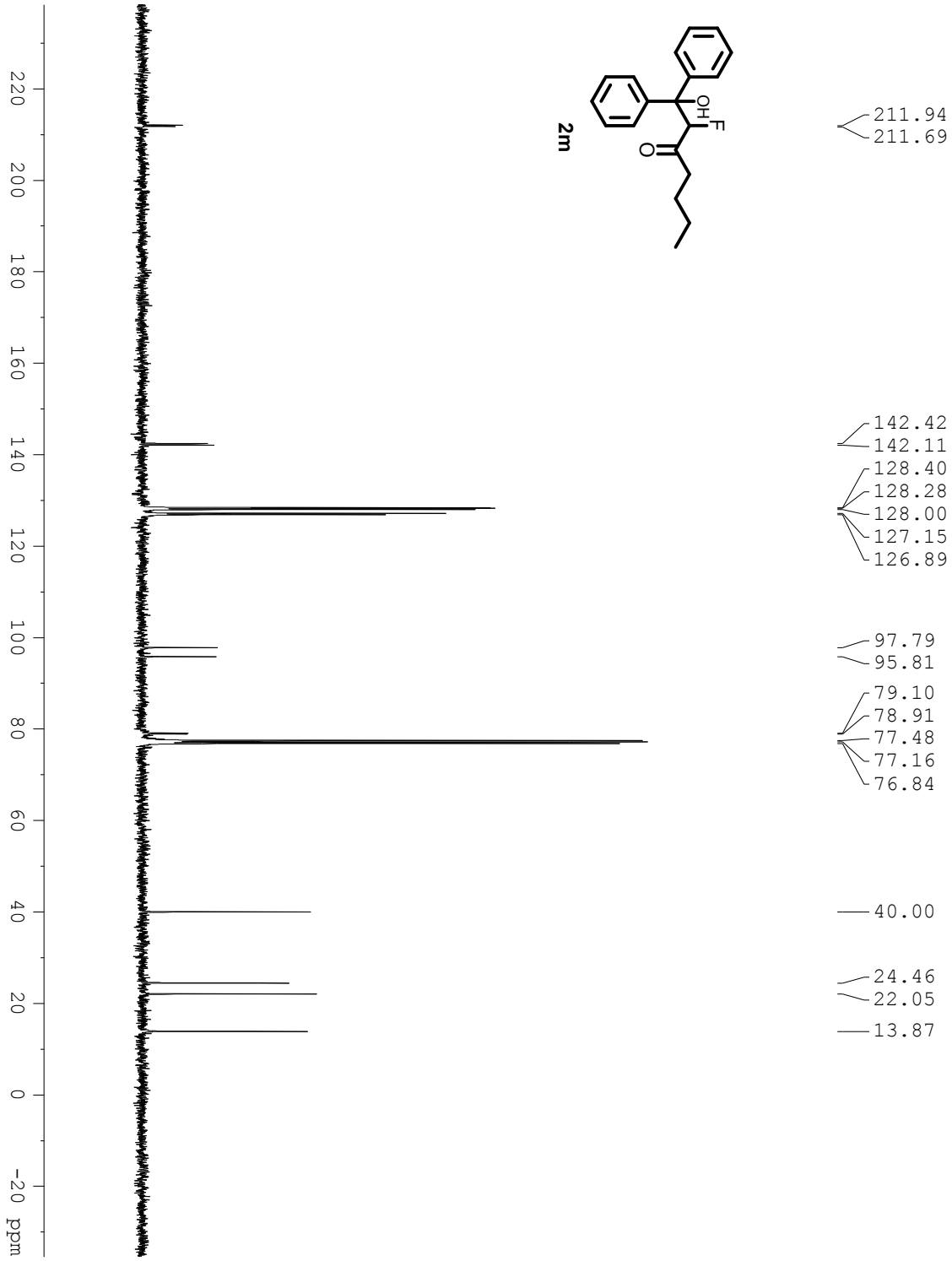
-80
-100
-120
-140
-160
-180
-200
ppm
2k
OH
F
O
-187.74
-187.87
-187.92
-188.05


21
OH
F
O
2.15
4.33
3.92
1.24
1.89
1.17
4.18
1.95
1.04
0.82
2.00
1.88
3.13
2.90
3.88
6.00
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
7.483
7.385
7.364
7.341
7.331
7.326
7.322
7.310
7.306
7.302
7.290
7.284
7.280
7.259
7.251
7.238
7.161
7.140
7.133
7.112
5.341
5.329
5.222
5.210
4.341
4.337
4.328
4.323
2.509
2.503
2.495
2.426
2.411
2.405
2.356
2.335
2.316
1.574
1.489
1.483
1.471
1.465
1.454
1.447
1.436
1.429
1.411
1.256
0.797
0.778
0.760
0.741
0.000


211.69
211.59
211.44
211.33
142.44
142.15
139.41
139.11
137.64
137.56
128.98
128.88
128.25
128.12
127.81
126.99
126.95
126.94
126.76
126.73
126.67
126.64
97.80
97.76
95.83
95.78
78.93
78.72
77.36
77.25
77.04
76.72
42.06
42.03
21.07
15.82
15.80
15.77
15.75
13.40
13.38
21
OH
F
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm


21
OH
F
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-187.5
-188.0
ppm
-187.85
-187.94
-187.98
-188.07
-187.85
-187.94
-187.98
-188.07


2m
OH
F
O
7.508
7.488
7.386
7.366
7.346
7.332
7.327
7.316
7.311
7.297
7.290
7.276
7.269
7.247
5.358
5.239
4.408
4.404
2.534
2.526
2.514
2.509
2.498
2.490
2.441
2.431
2.424
2.413
2.405
1.568
1.414
1.396
1.384
1.379
1.367
1.349
1.180
1.162
1.144
1.125
0.827
0.809
0.790
1.94
7.96
0.96
0.96
1.97
2.02
2.05
3.06
10
9
8
7
6
5
4
3
2
1
0
-1
ppm


2m
OH
F
O
211.94
211.69
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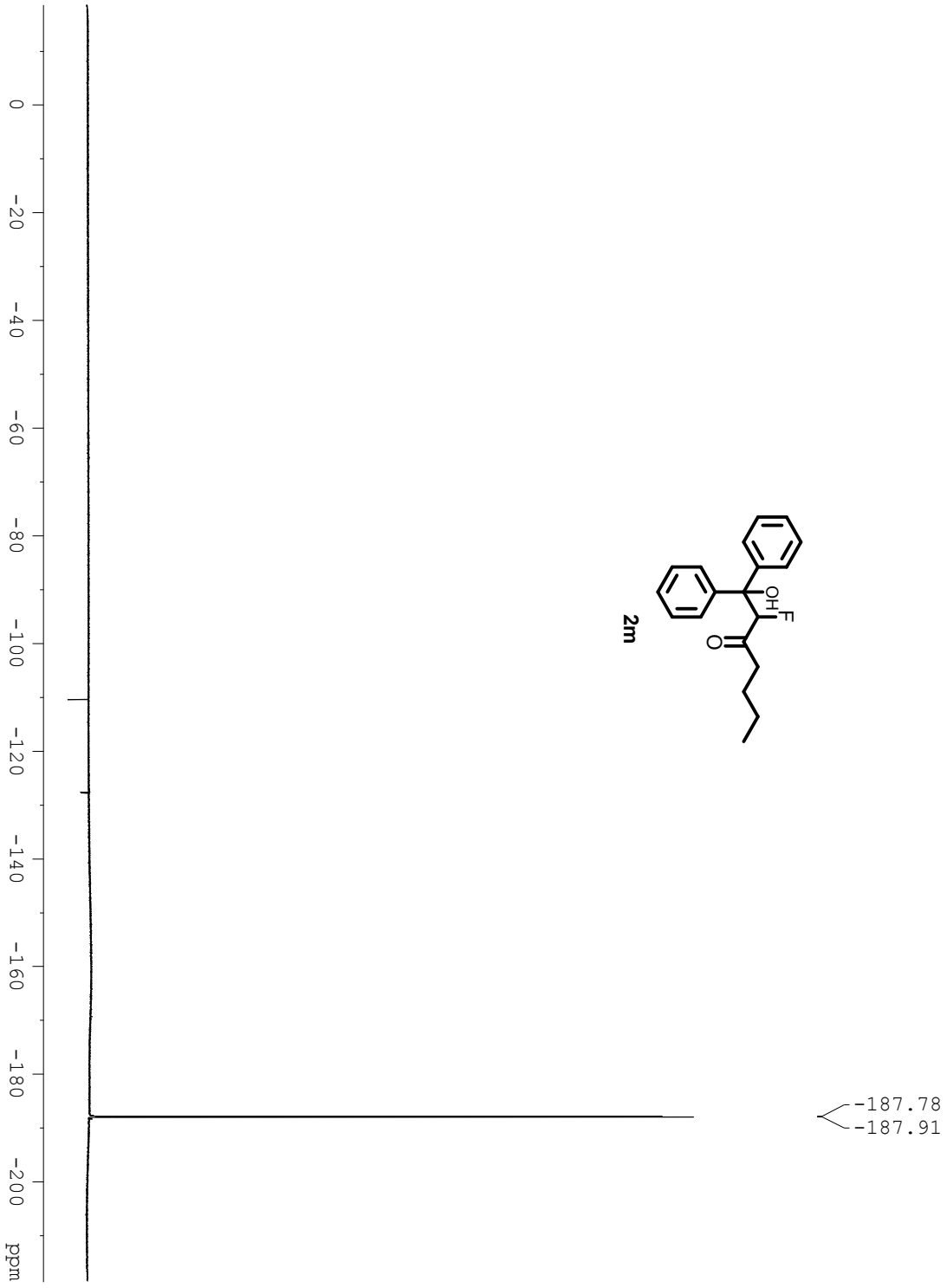
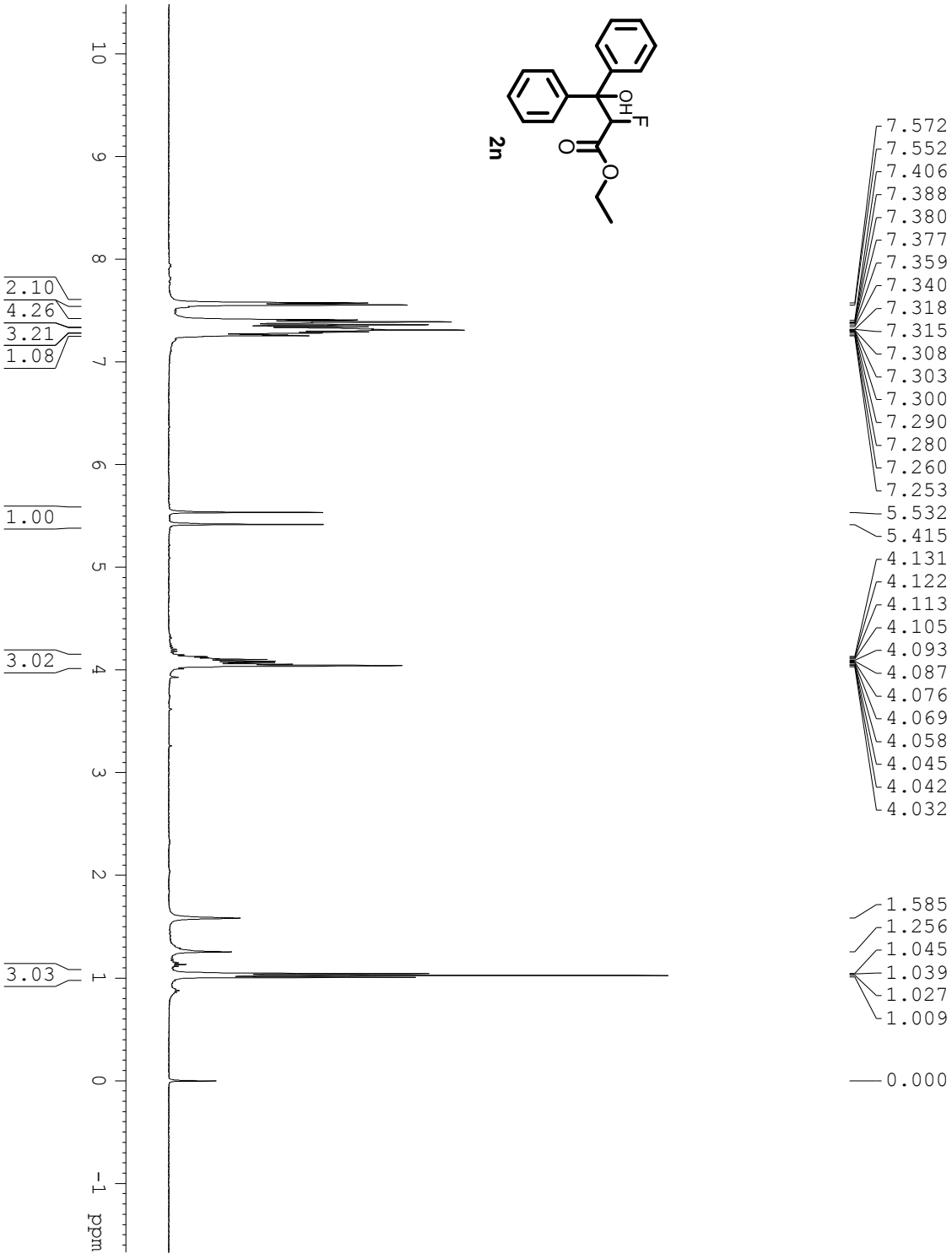
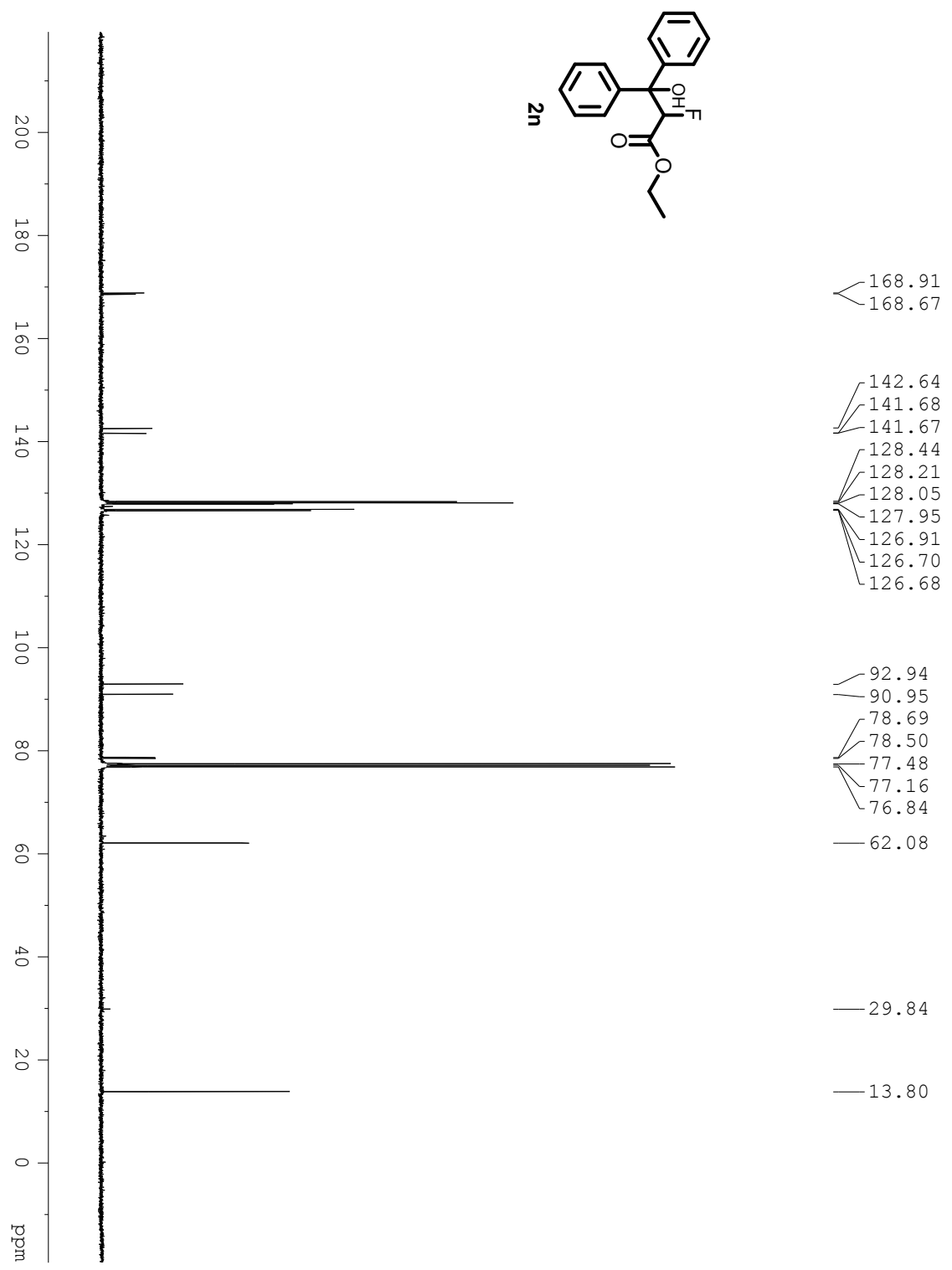
142.11
128.40
128.28
128.00
127.15
126.89
97.79
95.81
79.10
78.91
77.48
77.16
76.84
40.00
24.46
22.05
13.87
220
200
180
160
140
120
100
80
60
40
20
0
-20
ppm

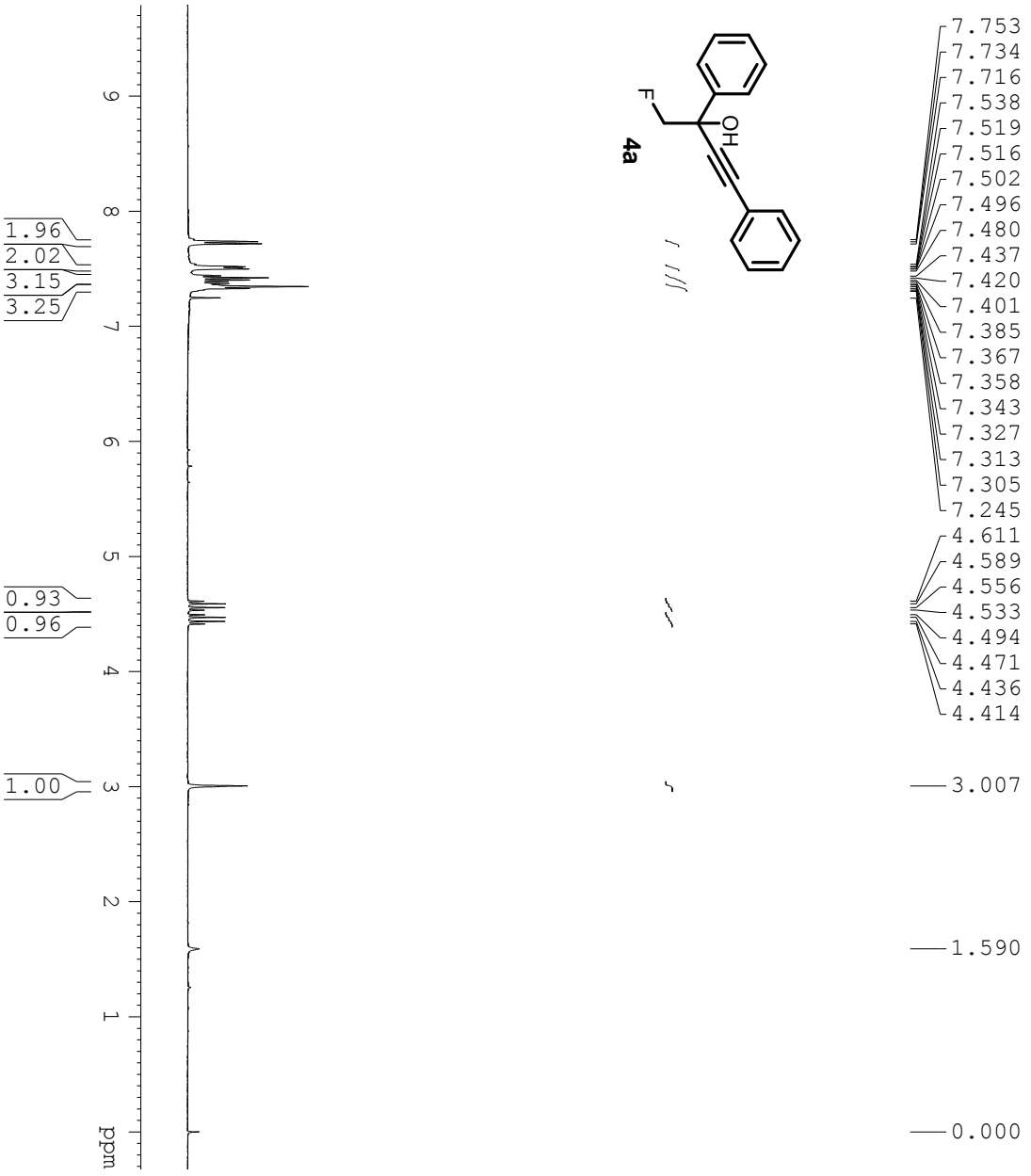

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-187.78
-187.91
OH
F
O
2m


2n
OH
F
O
O
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.10
4.26
3.21
1.08
1.00
3.02
3.03
7.572
7.552
7.406
7.388
7.380
7.377
7.359
7.340
7.318
7.315
7.308
7.303
7.300
7.290
7.280
7.260
7.253
5.532
5.415
4.131
4.122
4.113
4.105
4.093
4.087
4.076
4.069
4.058
4.045
4.042
4.032
1.585
1.256
1.045
1.039
1.027
1.009
0.000


2n
OH
F
O
O
200
180
160
140
120
100
80
60
40
20
0
ppm
168.91
168.67
142.64
141.68
141.67
128.44
128.21
128.05
127.95
126.91
126.70
126.68
92.94
90.95
78.69
78.50
77.48
77.16
76.84
62.08
29.84
13.80

2n

-189.00
-189.13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7.716
7.538
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7.516
7.502
7.496
7.480
7.437
7.420
7.401
7.385
7.367
7.358
7.343
7.327
7.313
7.305
7.245
4.611
4.589
4.556
4.533
4.494
4.471
4.436
4.414
3.007
1.590
0.000
F
OH
4a
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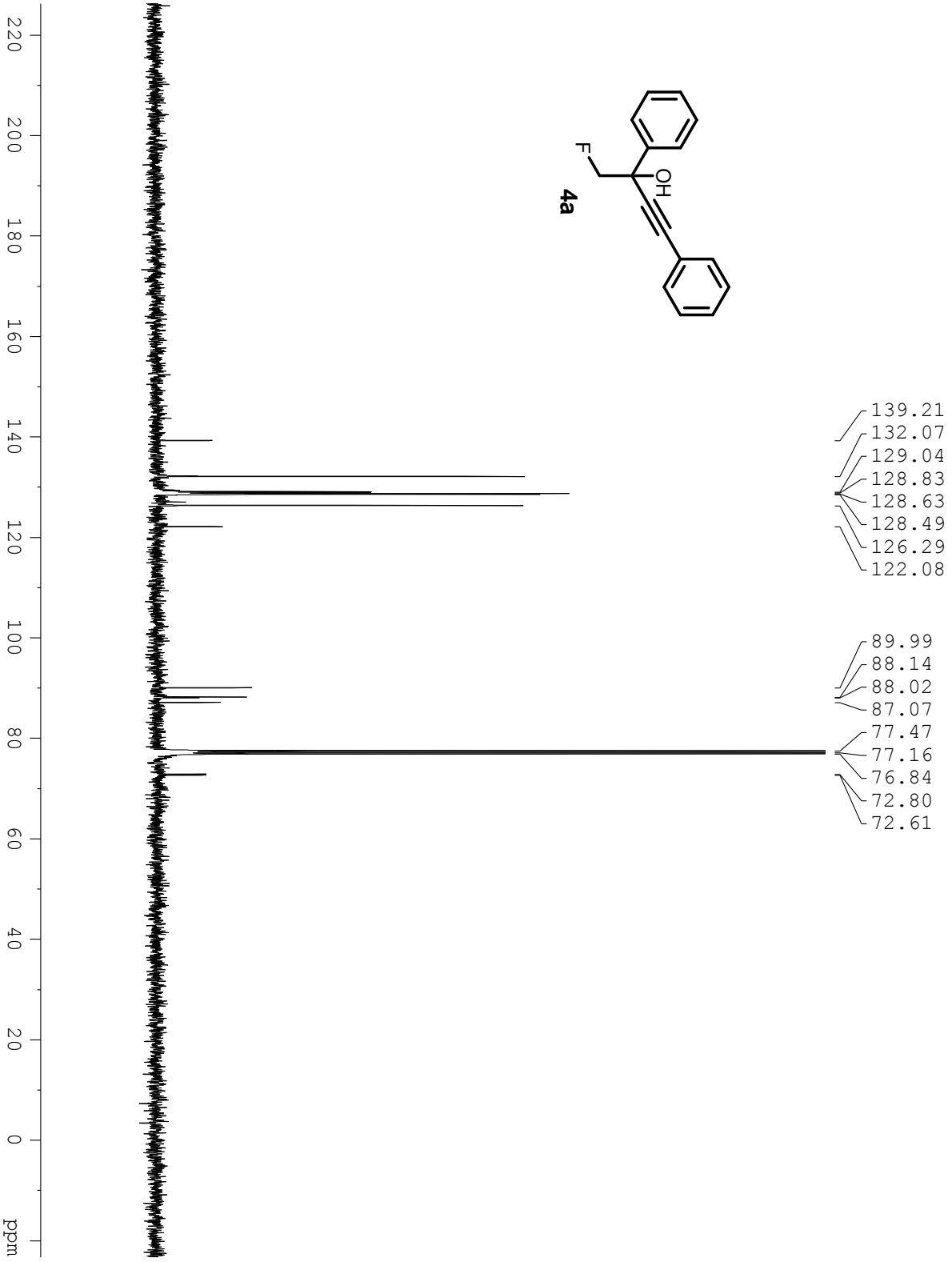
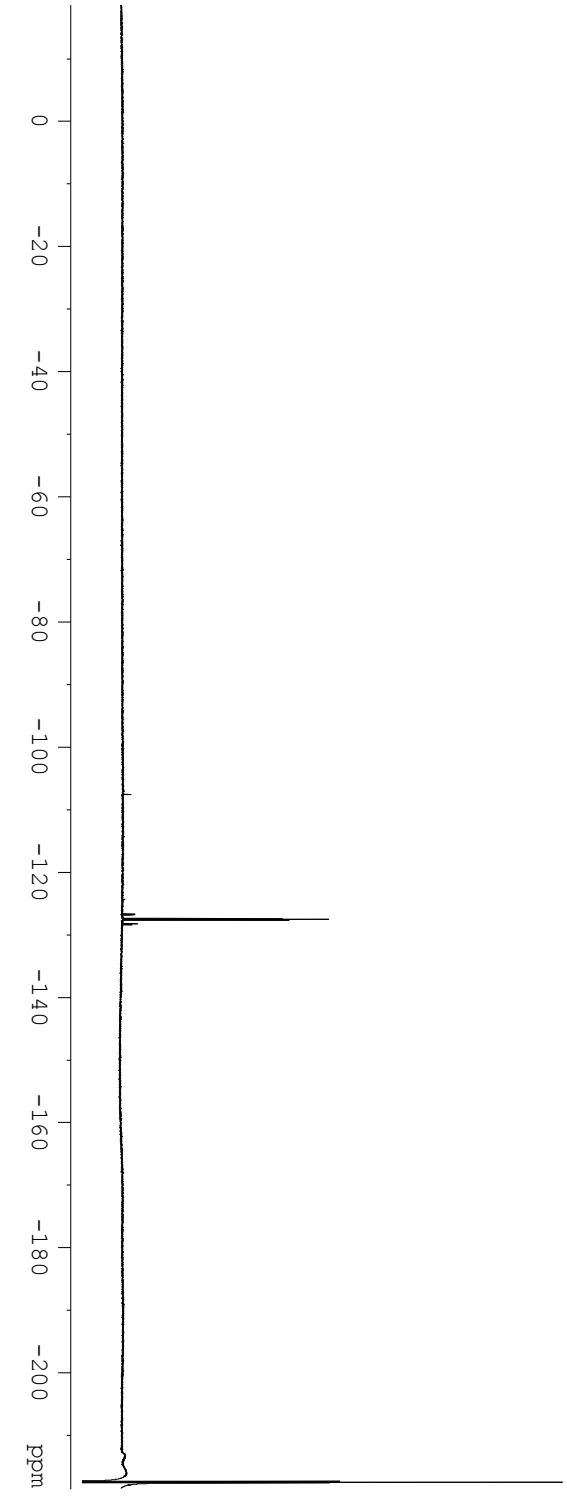
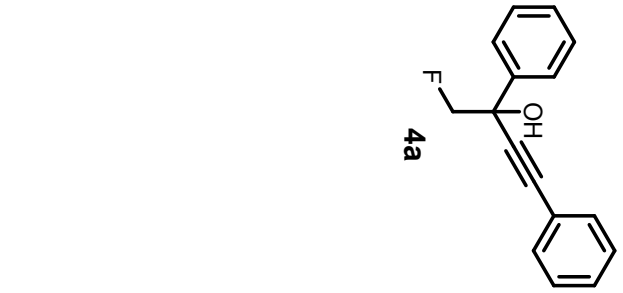
2.02
3.15
3.25
0.93
0.96
1.00
ppm

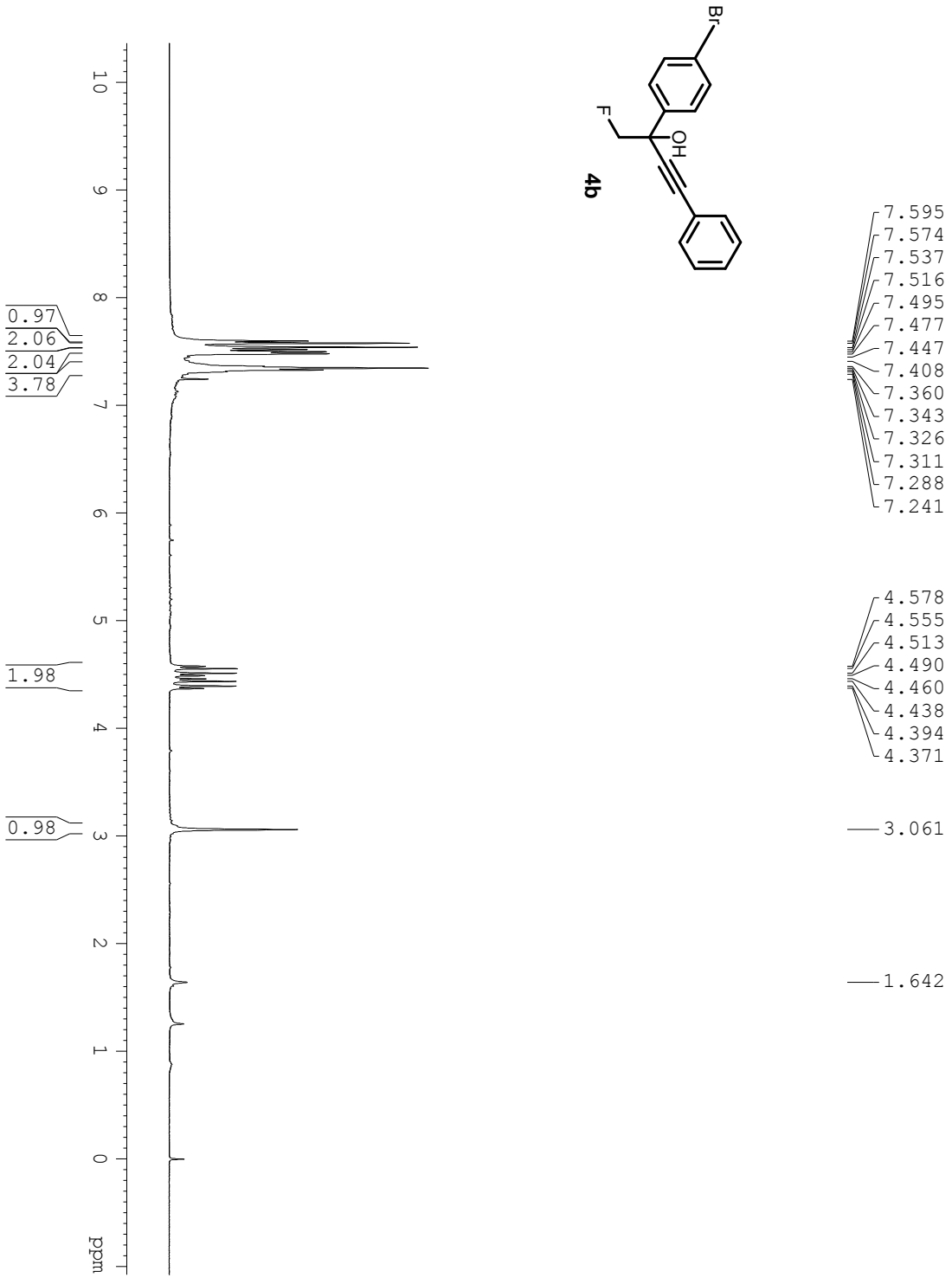

F
OH
4a
139.21
132.07
129.04
128.83
128.63
128.49
126.29
122.08
89.99
88.14
88.02
87.07
77.47
77.16
76.84
72.80
72.61
220
200
180
160
140
120
100
80
60
40
20
0
ppm

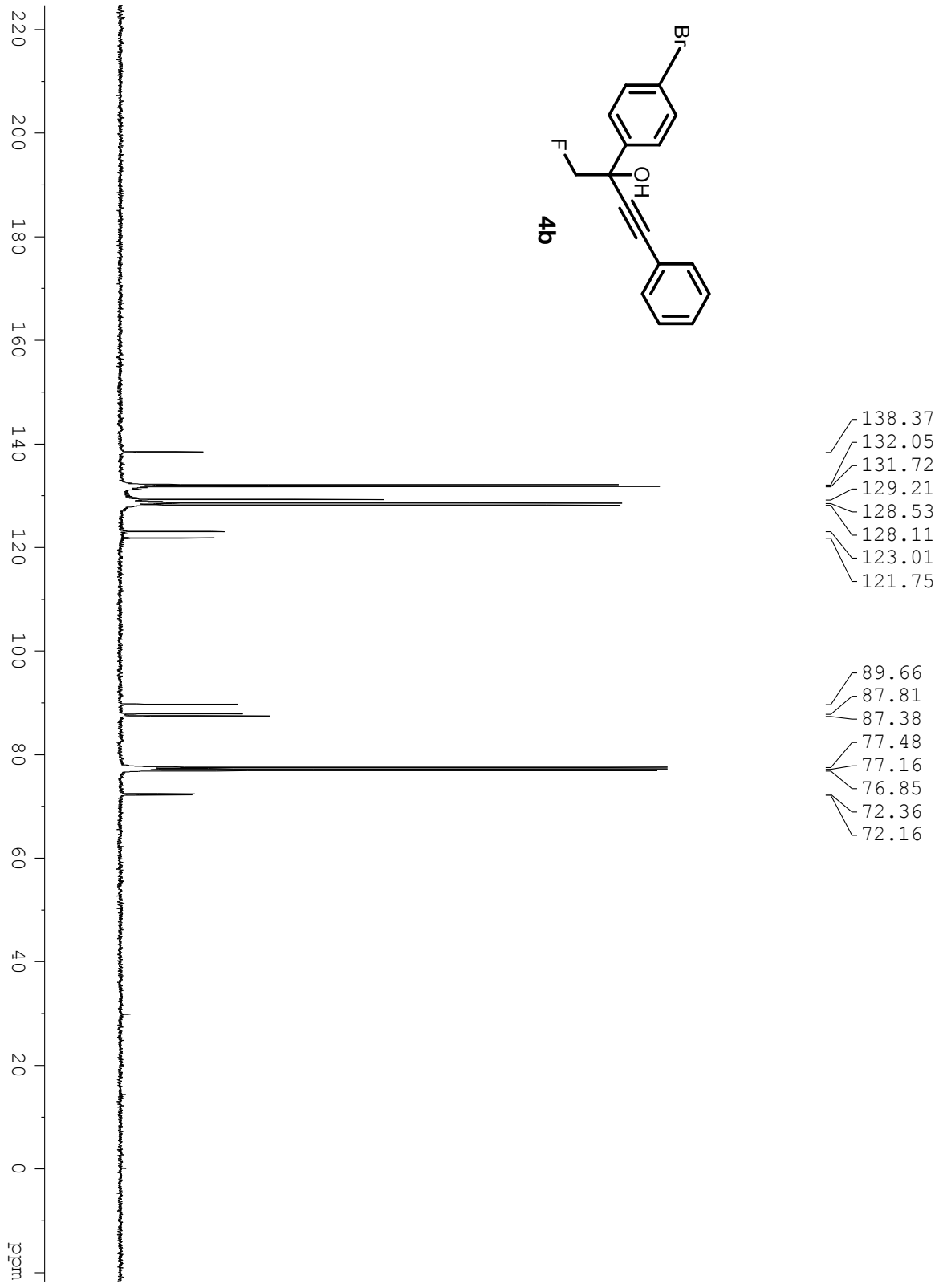




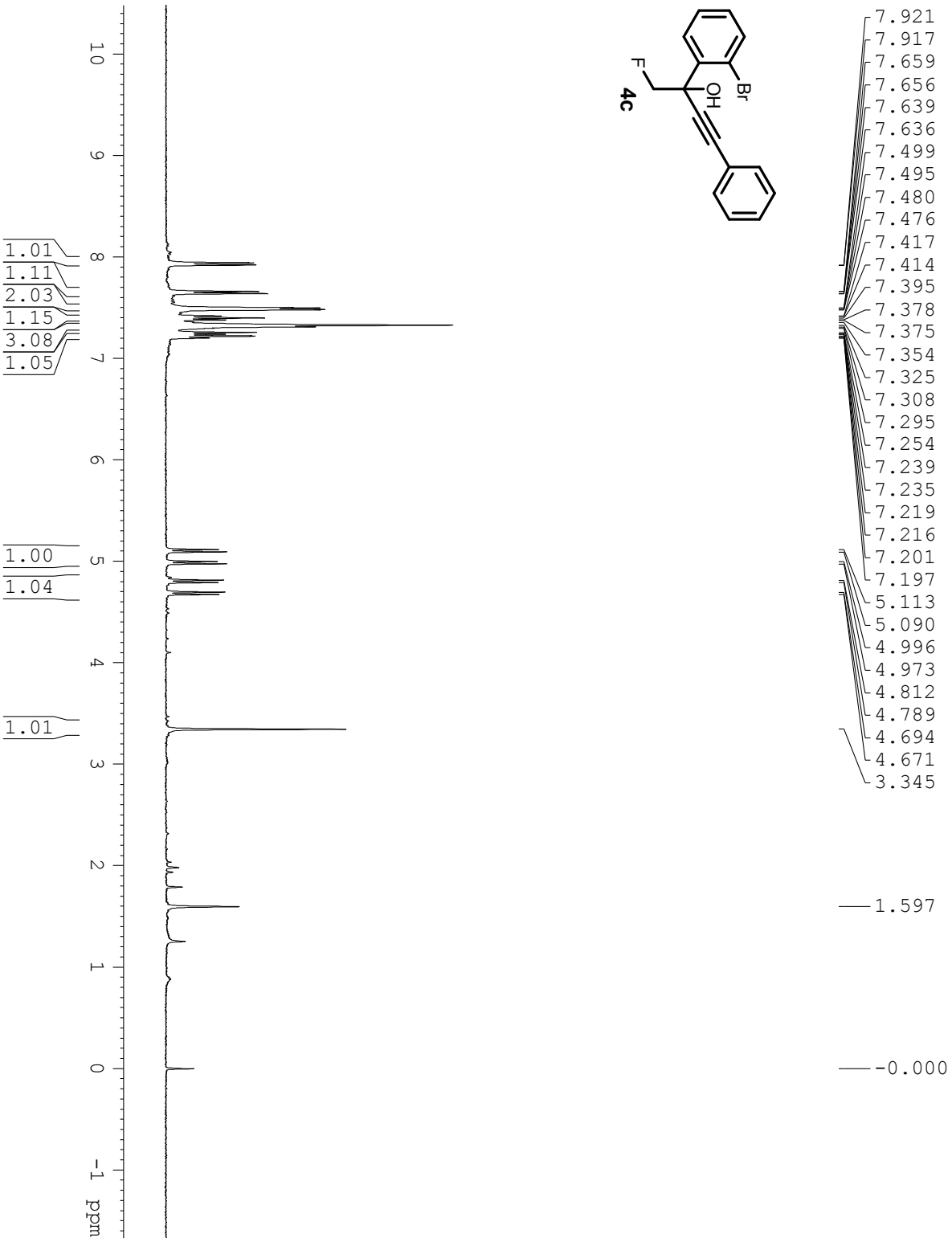
4a

-127.35
-127.45
-127.49
-127.60


Br
F
OH
4b
7.595
7.574
7.537
7.516
7.495
7.477
7.447
7.408
7.360
7.343
7.326
7.311
7.288
7.241
4.578
4.555
4.513
4.490
4.460
4.438
4.394
4.371
3.061
1.642
0.97
2.06
2.04
3.78
1.98
0.98
ppm


Br
F
OH
4b
138.37
132.05
131.72
129.21
128.53
128.11
123.01
121.75
89.66
87.81
87.38
77.48
77.16
76.85
72.36
72.16
220
200
180
160
140
120
100
80
60
40
20
0
ppm


0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
Br
F
OH
4b
-127.32
-127.34
-127.47
-127.49


4c
F
OH
Br
7.921
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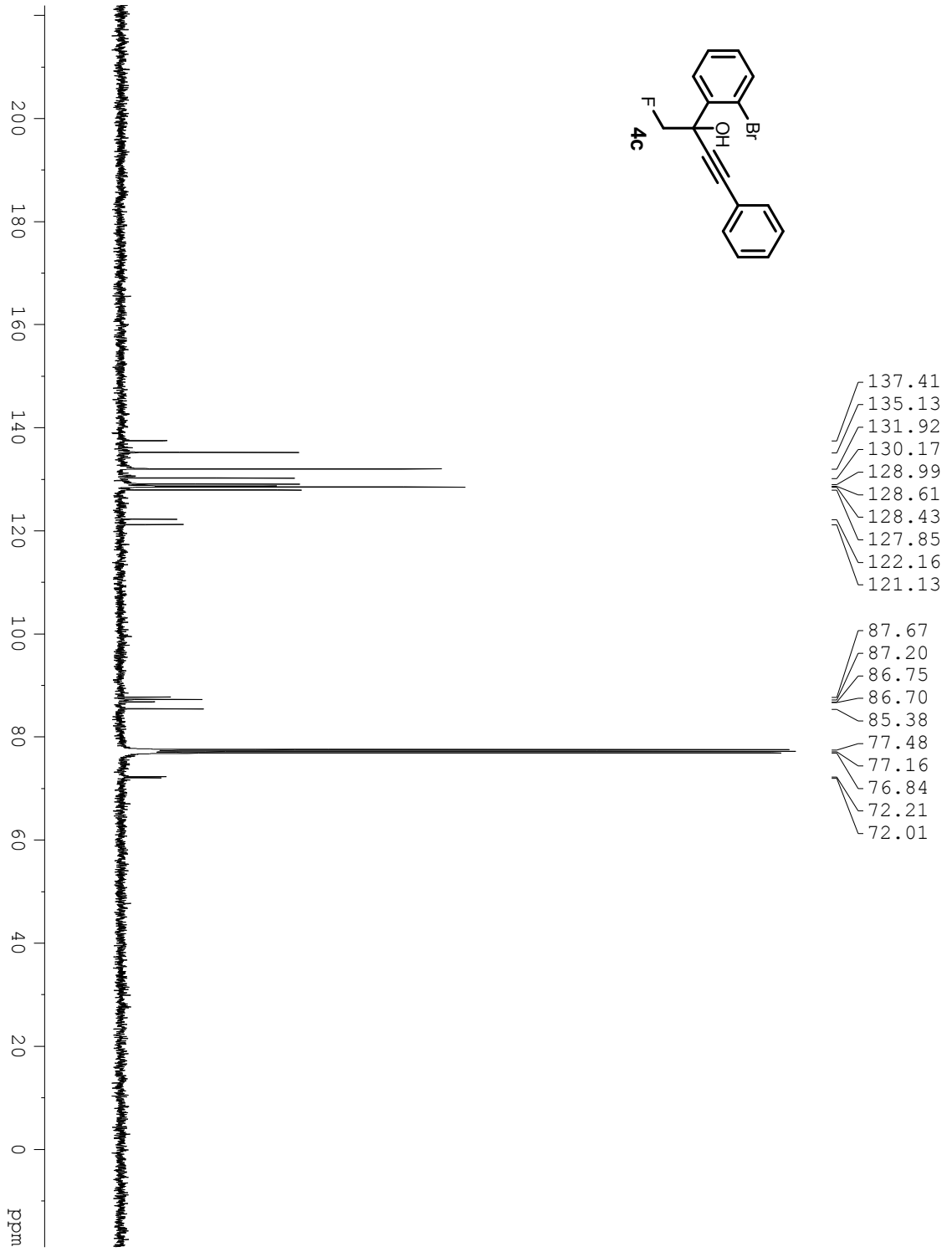
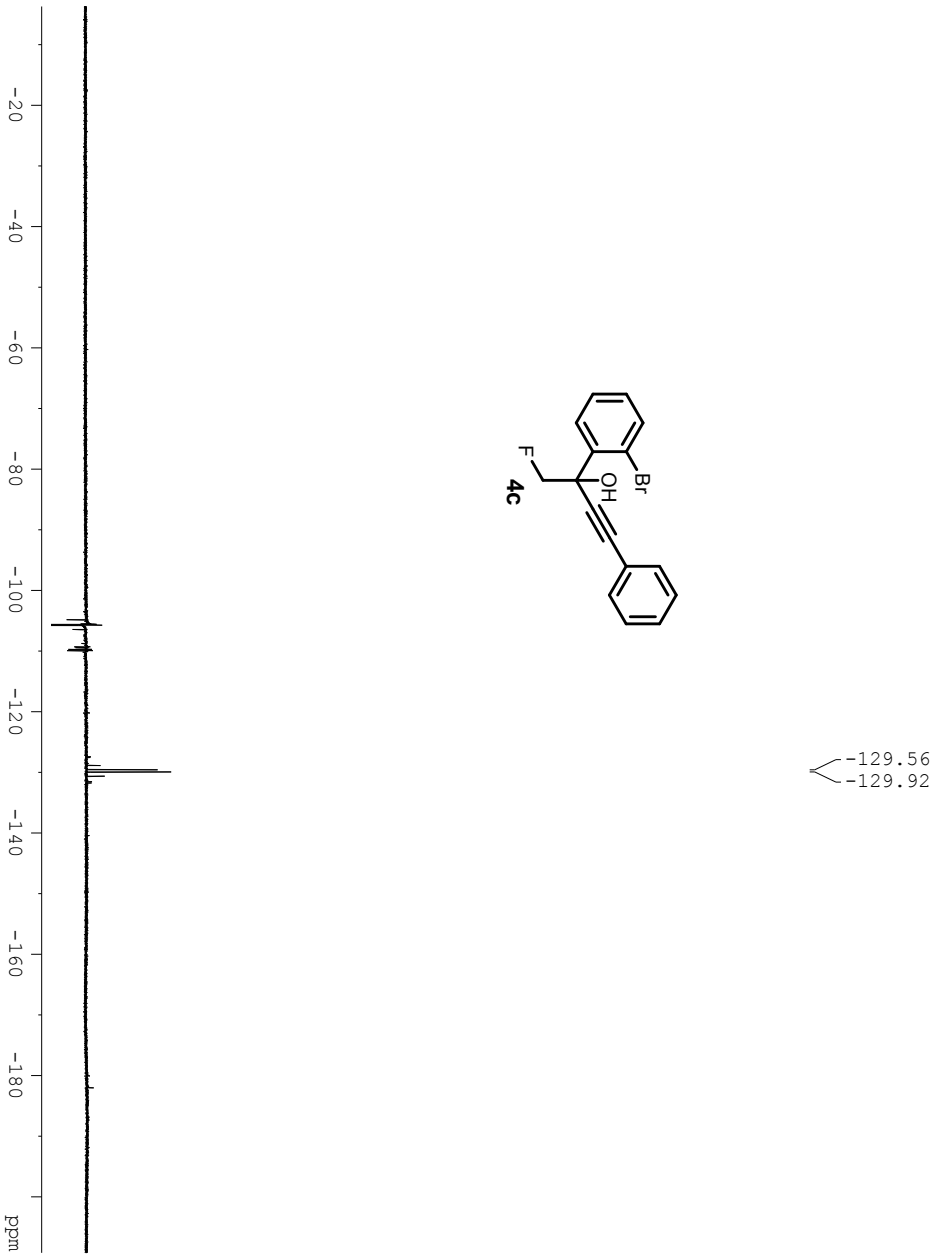
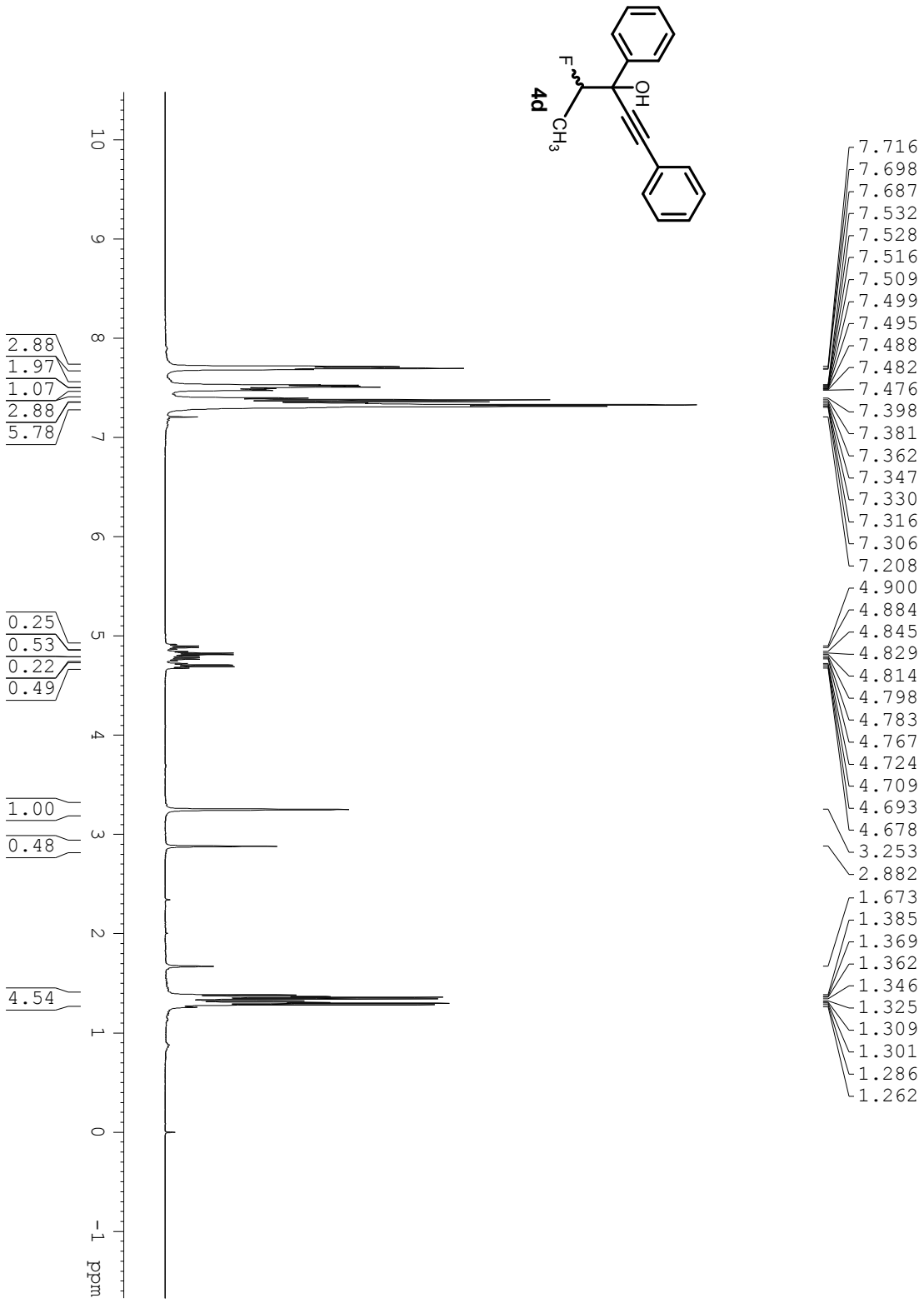
7.659
7.656
7.639
7.636
7.499
7.495
7.480
7.476
7.417
7.414
7.395
7.378
7.375
7.354
7.325
7.308
7.295
7.254
7.239
7.235
7.219
7.216
7.201
7.197
5.113
5.090
4.996
4.973
4.812
4.789
4.694
4.671
3.345
1.597
-0.000
1.01
1.11
2.03
1.15
3.08
1.05
1.00
1.04
1.01
10
9
8
7
6
5
4
3
2
1
0
-1
ppm


F
OH
Br
4c
137.41
135.13
131.92
130.17
128.99
128.61
128.43
127.85
122.16
121.13
87.67
87.20
86.75
86.70
85.38
77.48
77.16
76.84
72.21
72.01
200
180
160
140
120
100
80
60
40
20
0
ppm


-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm
F
OH
Br
4c
-129.56
-129.92


4d
F
OH
CH3
7.716
7.698
7.687
7.532
7.528
7.516
7.509
7.499
7.495
7.488
7.482
7.476
7.398
7.381
7.362
7.347
7.330
7.316
7.306
7.208
4.900
4.884
4.845
4.829
4.814
4.798
4.783
4.767
4.724
4.709
4.693
4.678
3.253
2.882
1.673
1.385
1.369
1.362
1.346
1.325
1.309
1.301
1.286
1.262
2.88
1.97
1.07
2.88
5.78
0.25
0.53
0.22
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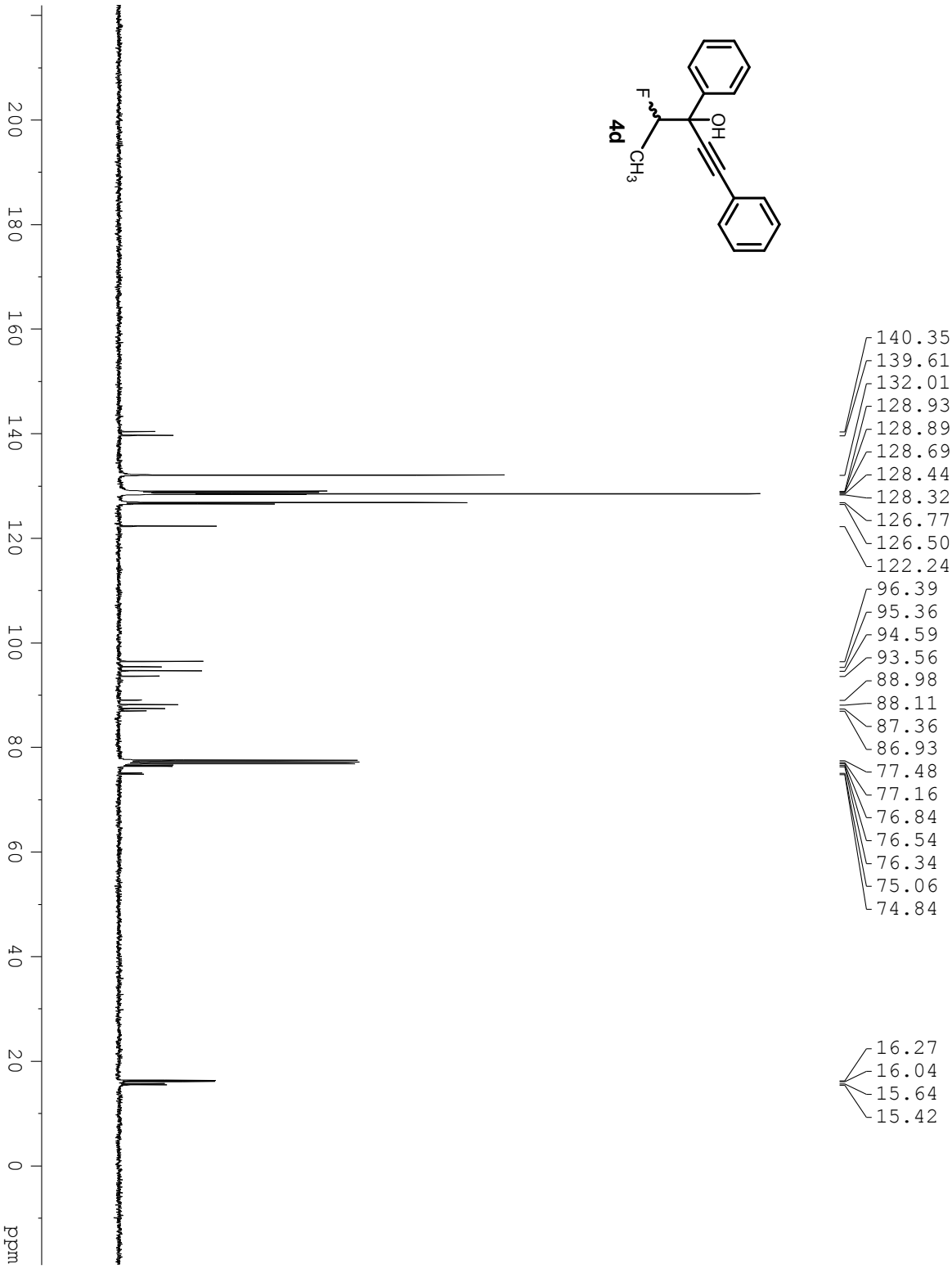
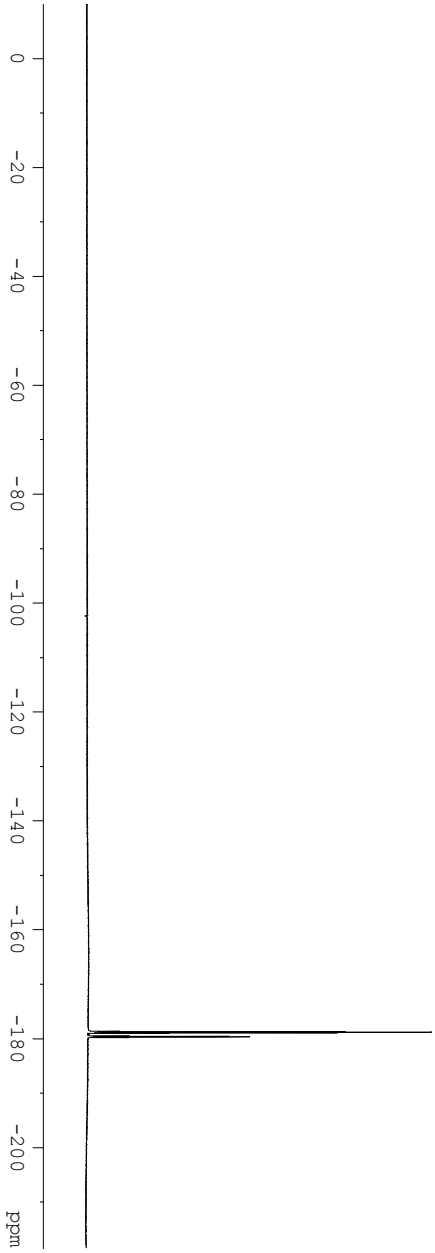
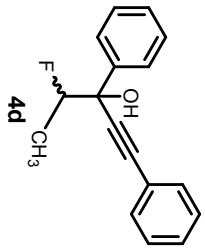
1.00
0.48
4.54
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

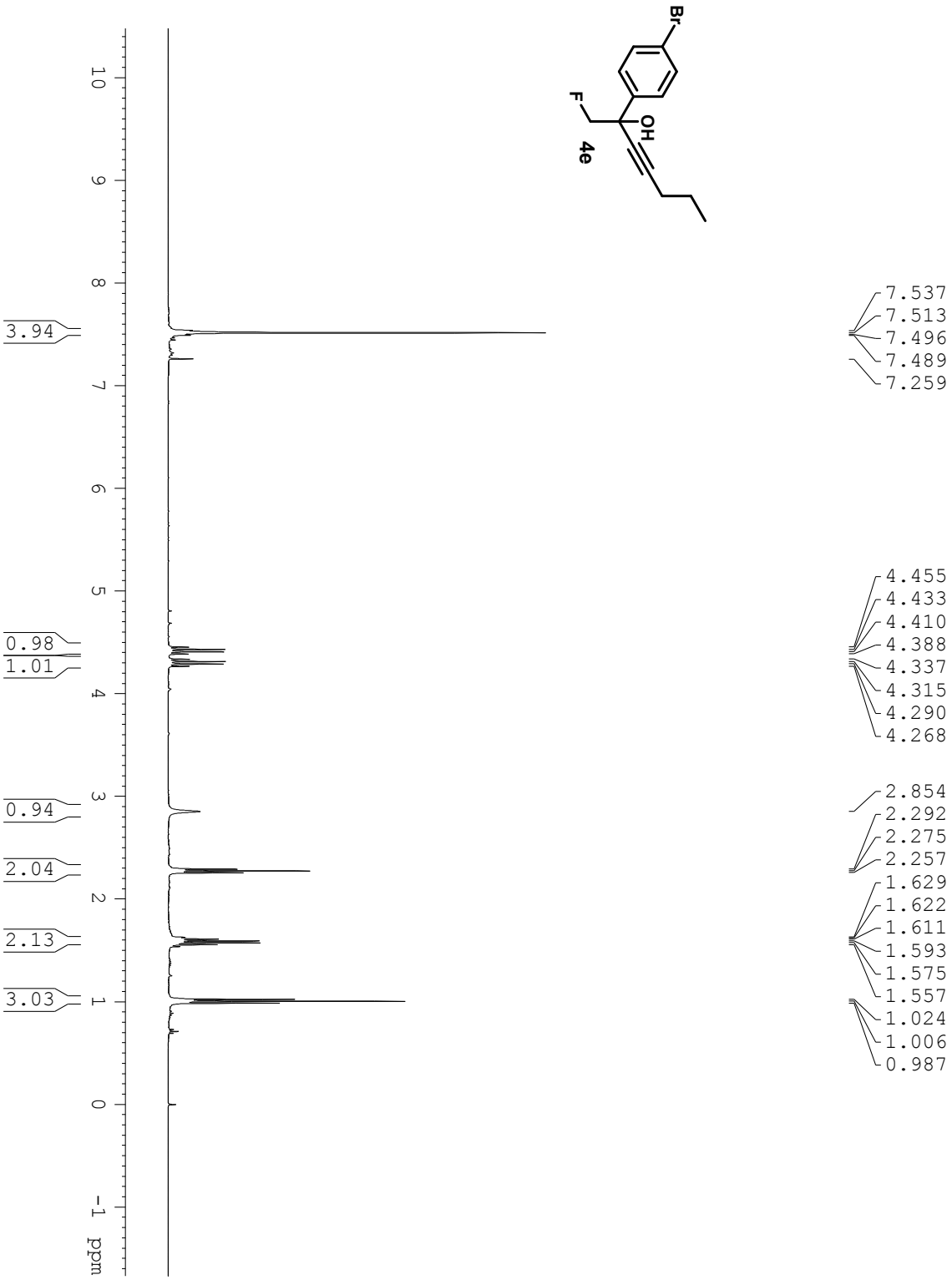

4d
F
OH
CH3
140.35
139.61
132.01
128.93
128.89
128.69
128.44
128.32
126.77
126.50
122.24
96.39
95.36
94.59
93.56
88.98
88.11
87.36
86.93
77.48
77.16
76.84
76.54
76.34
75.06
74.84
16.27
16.04
15.64
15.42
200
180
160
140
120
100
80
60
40
20
0
ppm

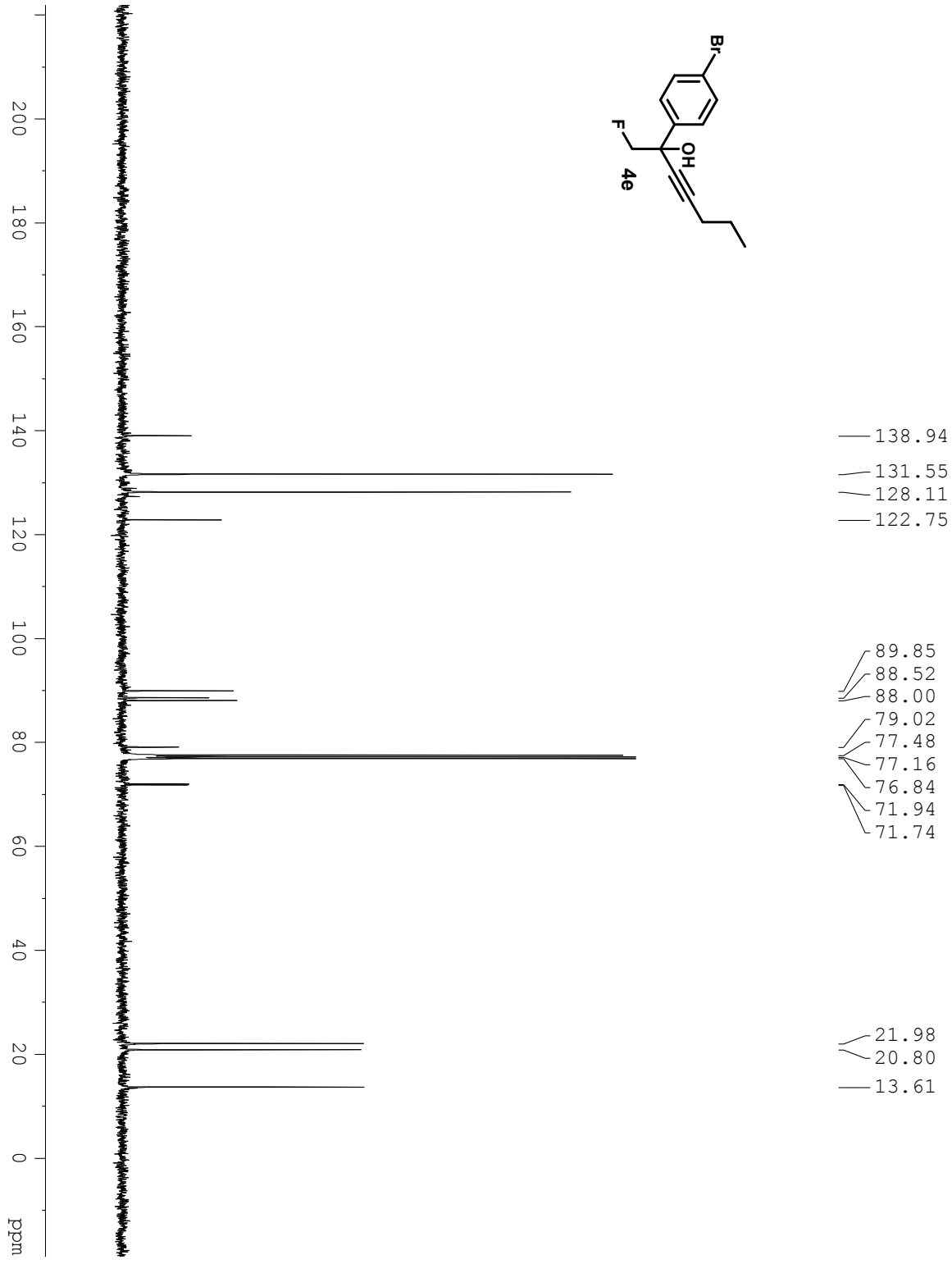


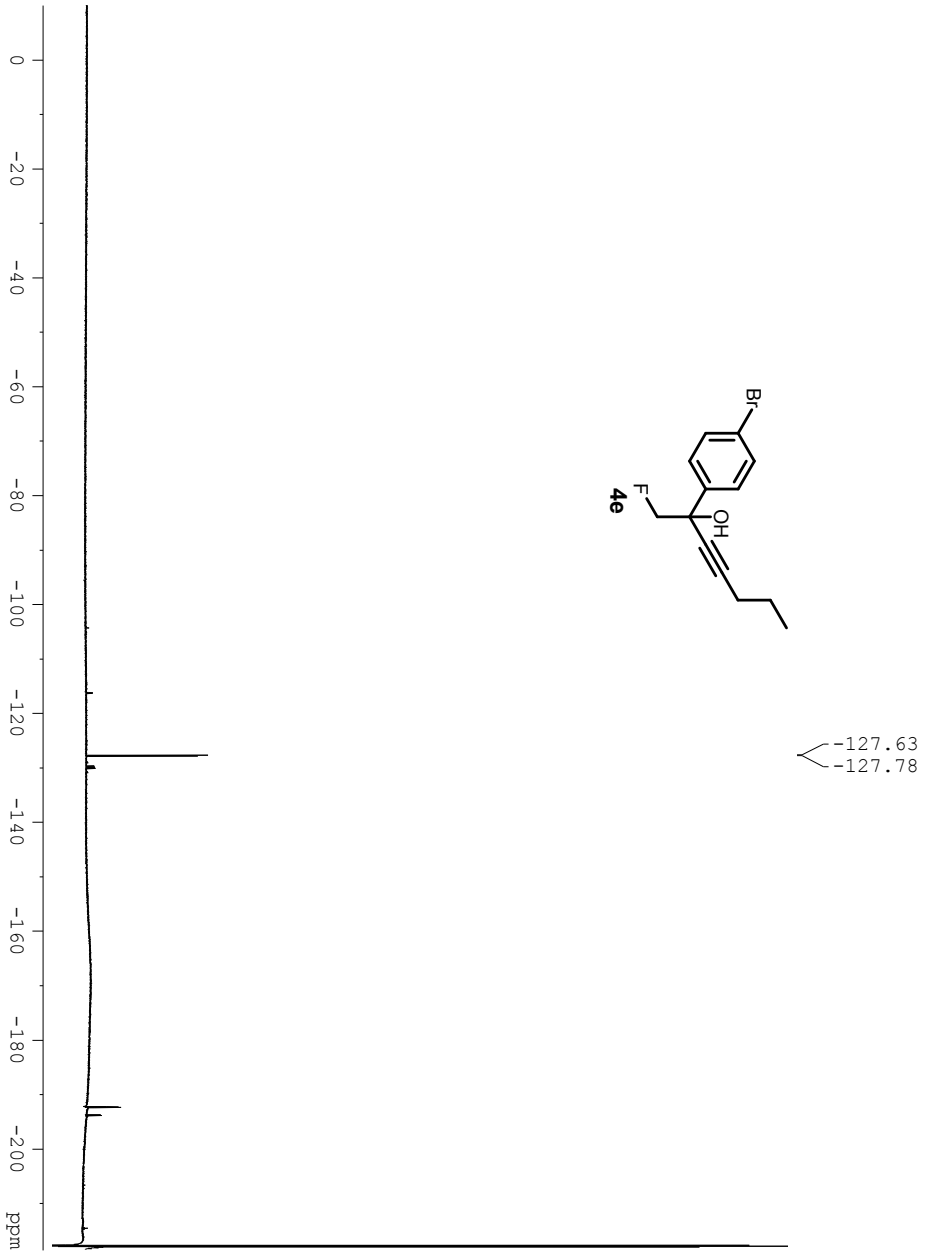


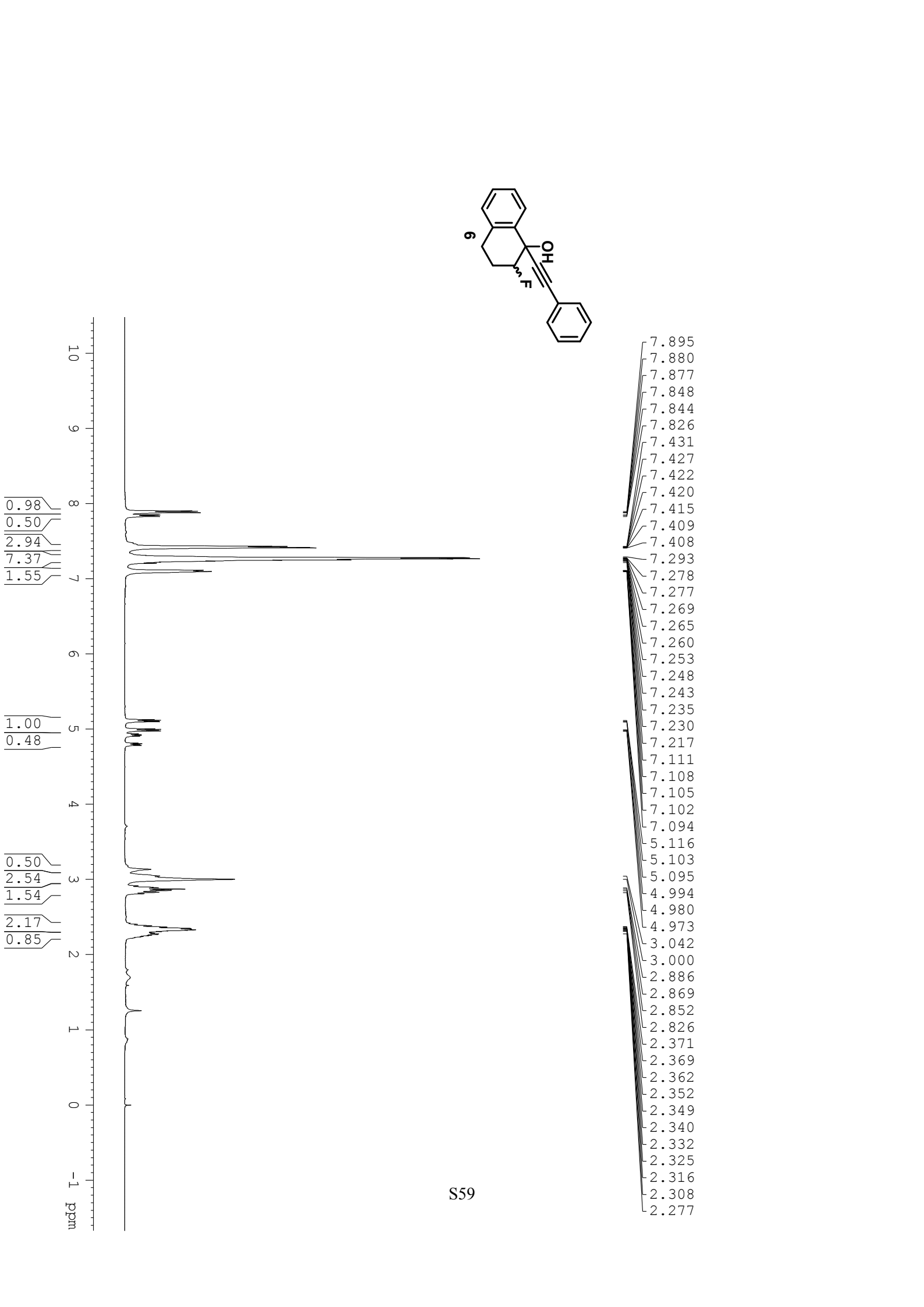
4d

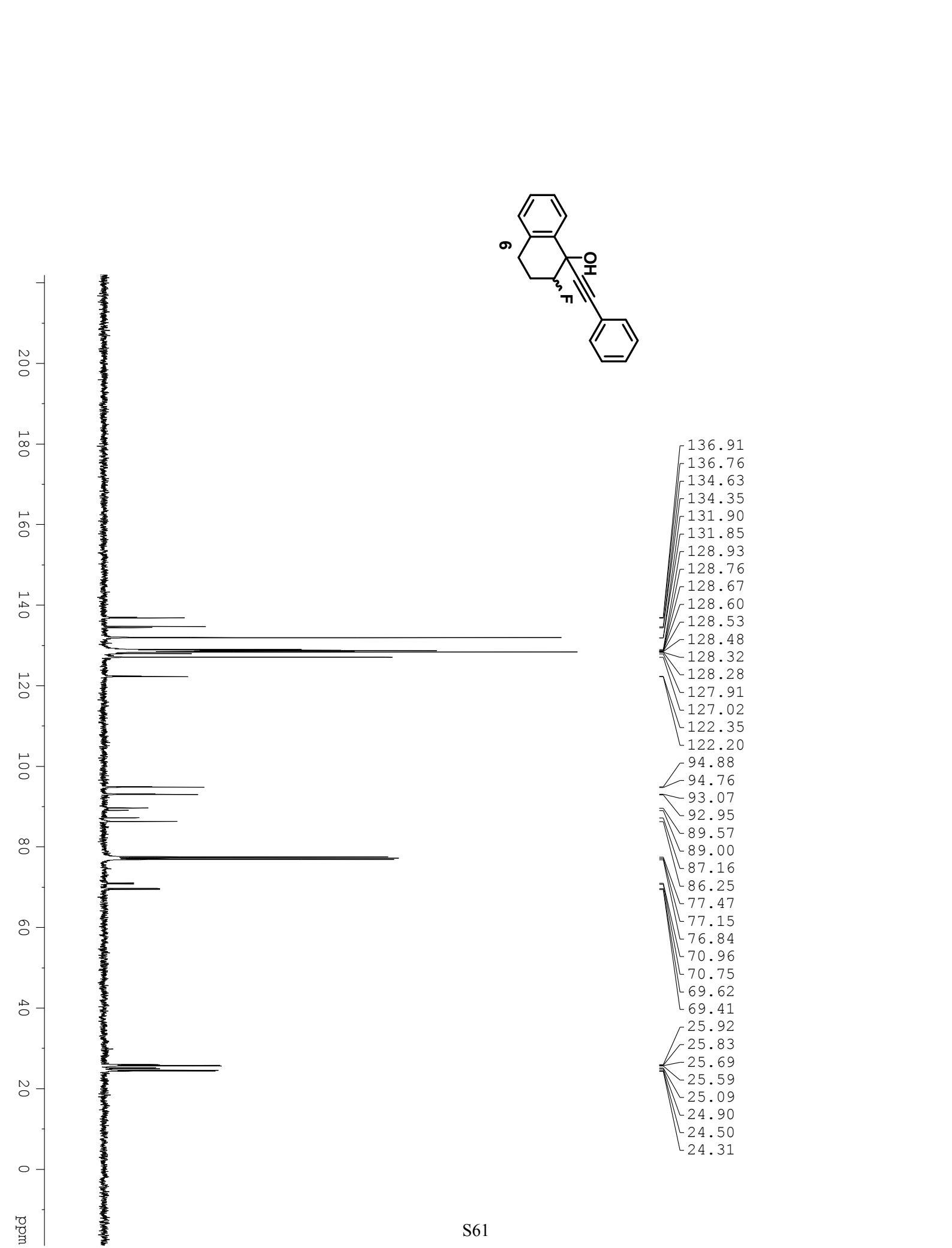
-178.64
-178.71
-178.77
-178.83
-178.90
-178.96
-179.45
-179.51
-179.57
-179.64
-179.70
-179.76

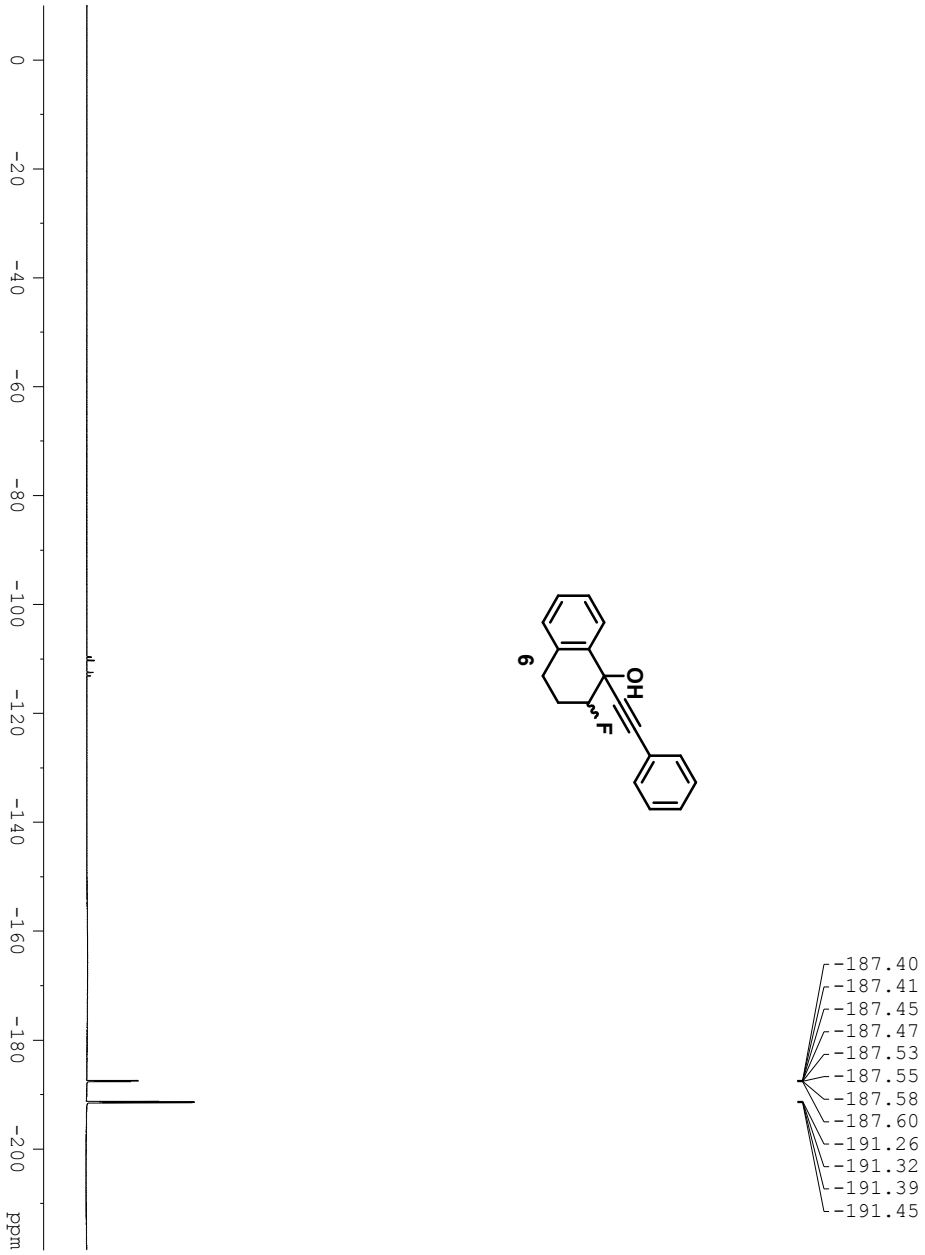

Br
F
OH
4e
7.537
7.513
7.496
7.489
7.259
4.455
4.433
4.410
4.388
4.337
4.315
4.290
4.268
2.854
2.292
2.275
2.257
1.629
1.622
1.611
1.593
1.575
1.557
1.024
1.006
0.987
3.94
0.98
1.01
0.94
2.04
2.13
3.03
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

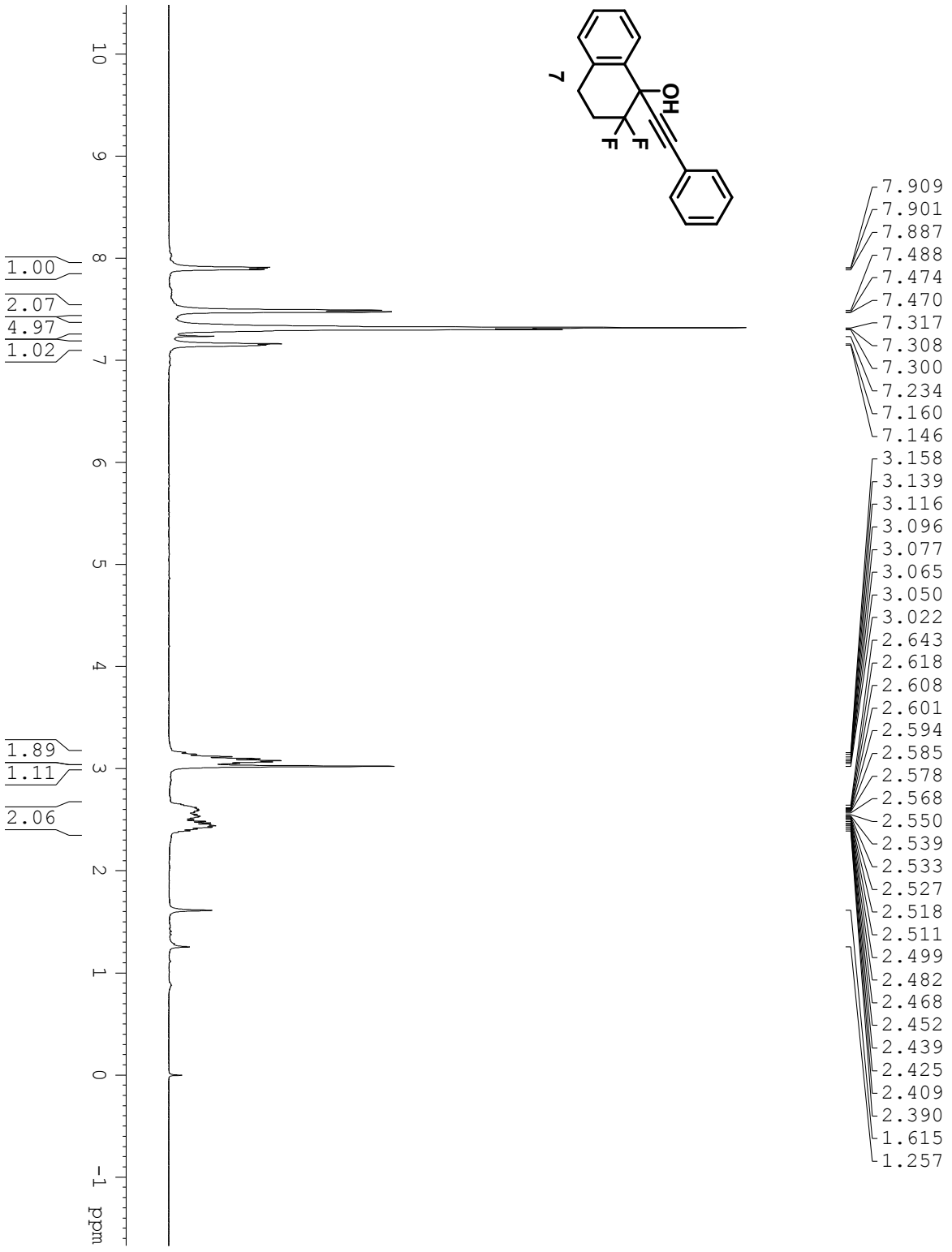

Br
F
OH
4e
138.94
131.55
128.11
122.75
89.85
88.52
88.00
79.02
77.48
77.16
76.84
71.94
71.74
21.98
20.80
13.61
200
180
160
140
120
100
80
60
40
20
0
ppm

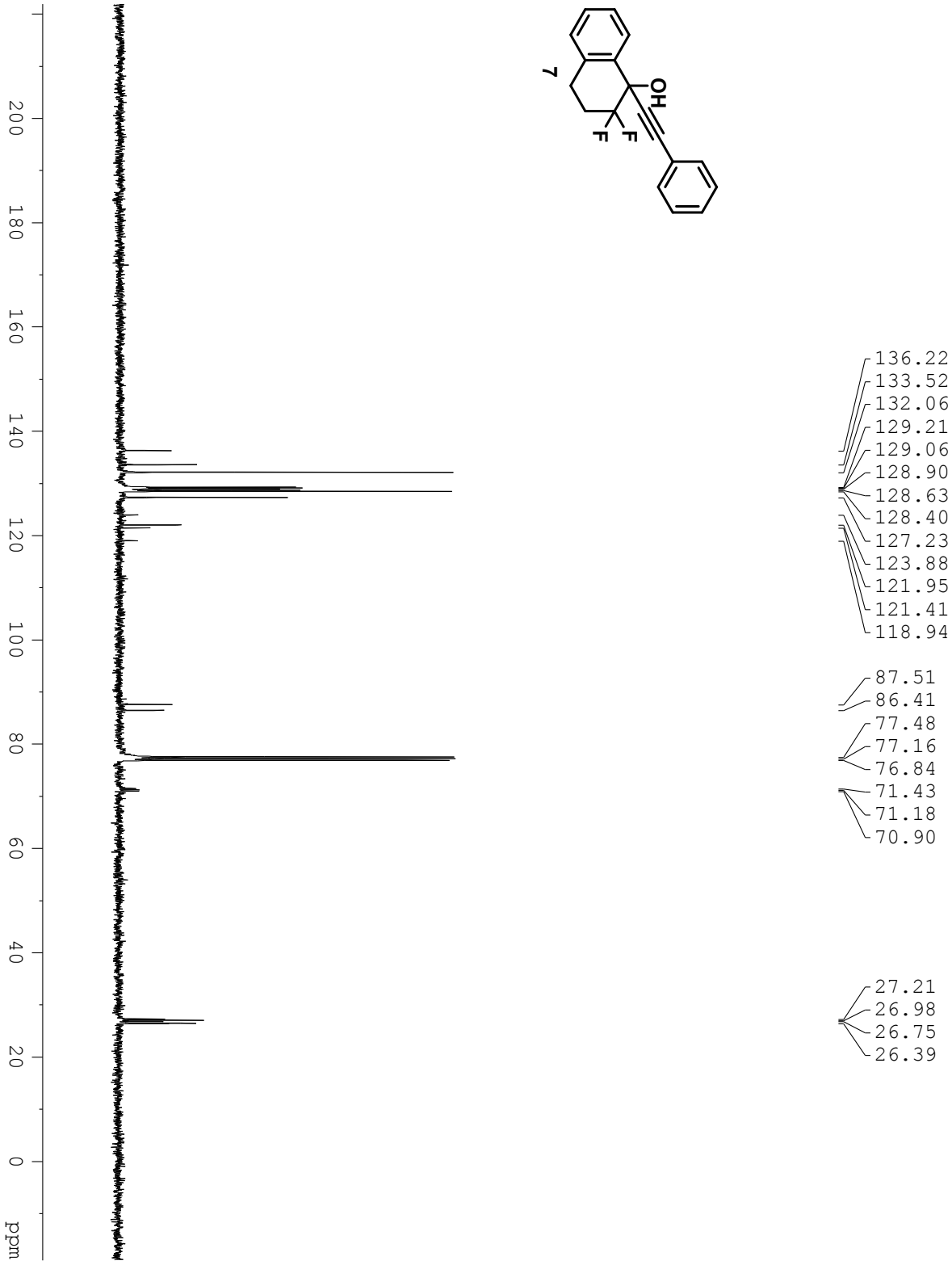

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
Br
F
OH
4e
-127.63
-127.78

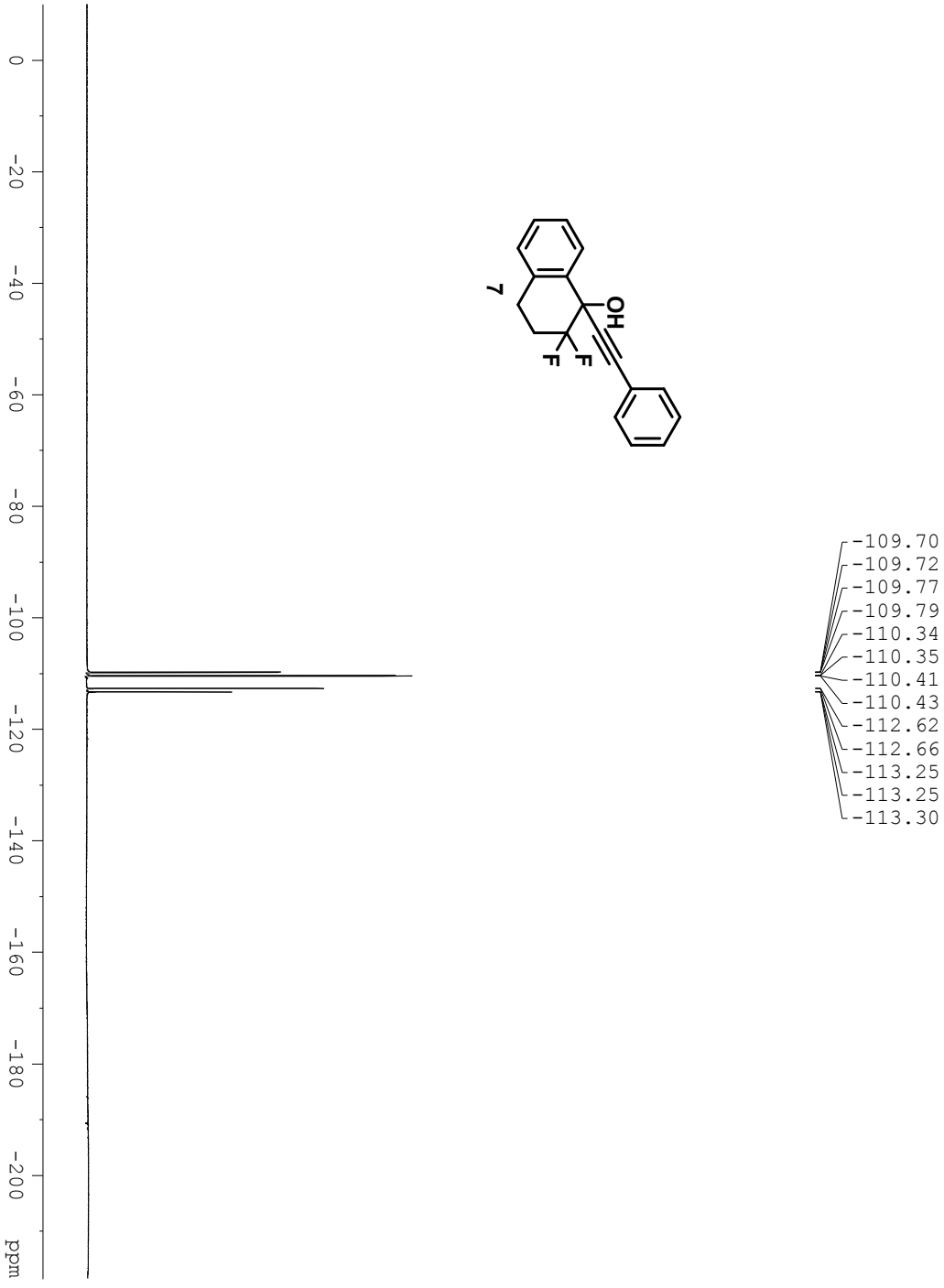

6
OH
F
7.895
7.880
7.877
7.848
7.844
7.826
7.431
7.427
7.422
7.420
7.415
7.409
7.408
7.293
7.278
7.277
7.269
7.265
7.260
7.253
7.248
7.243
7.235
7.230
7.217
7.111
7.108
7.105
7.102
7.094
5.116
5.103
5.095
4.994
4.980
4.973
3.042
3.000
2.886
2.869
2.852
2.826
2.371
2.369
2.362
2.352
2.349
2.340
2.332
2.325
2.316
2.308
2.277
0.98
0.50
2.94
7.37
1.55
1.00
0.48
0.50
2.54
1.54
2.17
0.85
10
9
8
7
6
5
4
3
2
1
0
−1
ppm


6
OH
F
136.91
136.76
134.63
134.35
131.90
131.85
128.93
128.76
128.67
128.60
128.53
128.48
128.32
128.28
127.91
127.02
122.35
122.20
94.88
94.76
93.07
92.95
89.57
89.00
87.16
86.25
77.47
77.15
76.84
70.96
70.75
69.62
69.41
25.92
25.83
25.69
25.59
25.09
24.90
24.50
24.31
200
180
160
140
120
100
80
60
40
20
0
ppm

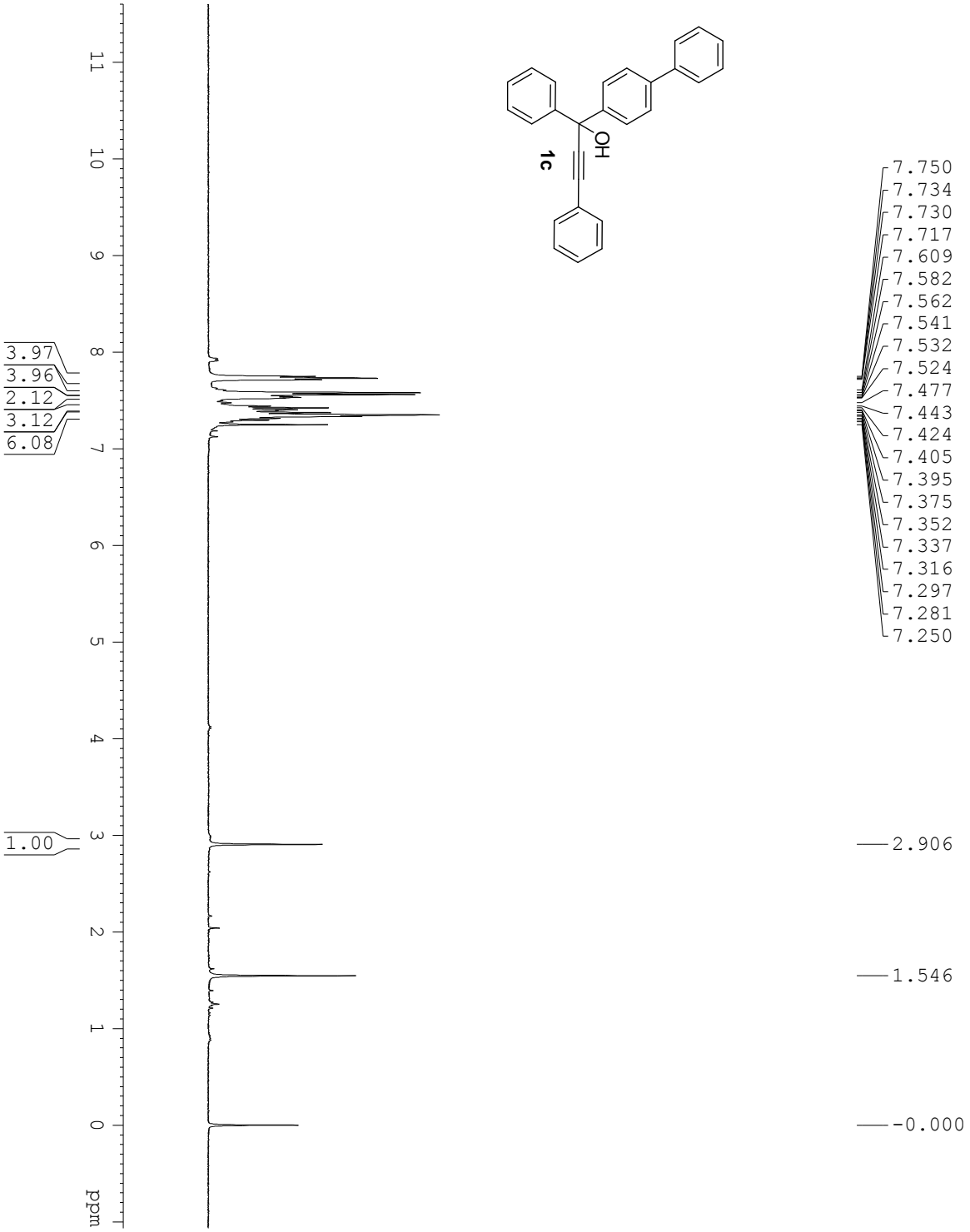

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
6
OH
F
-187.40
-187.41
-187.45
-187.47
-187.53
-187.55
-187.58
-187.60
-191.26
-191.32
-191.39
-191.45

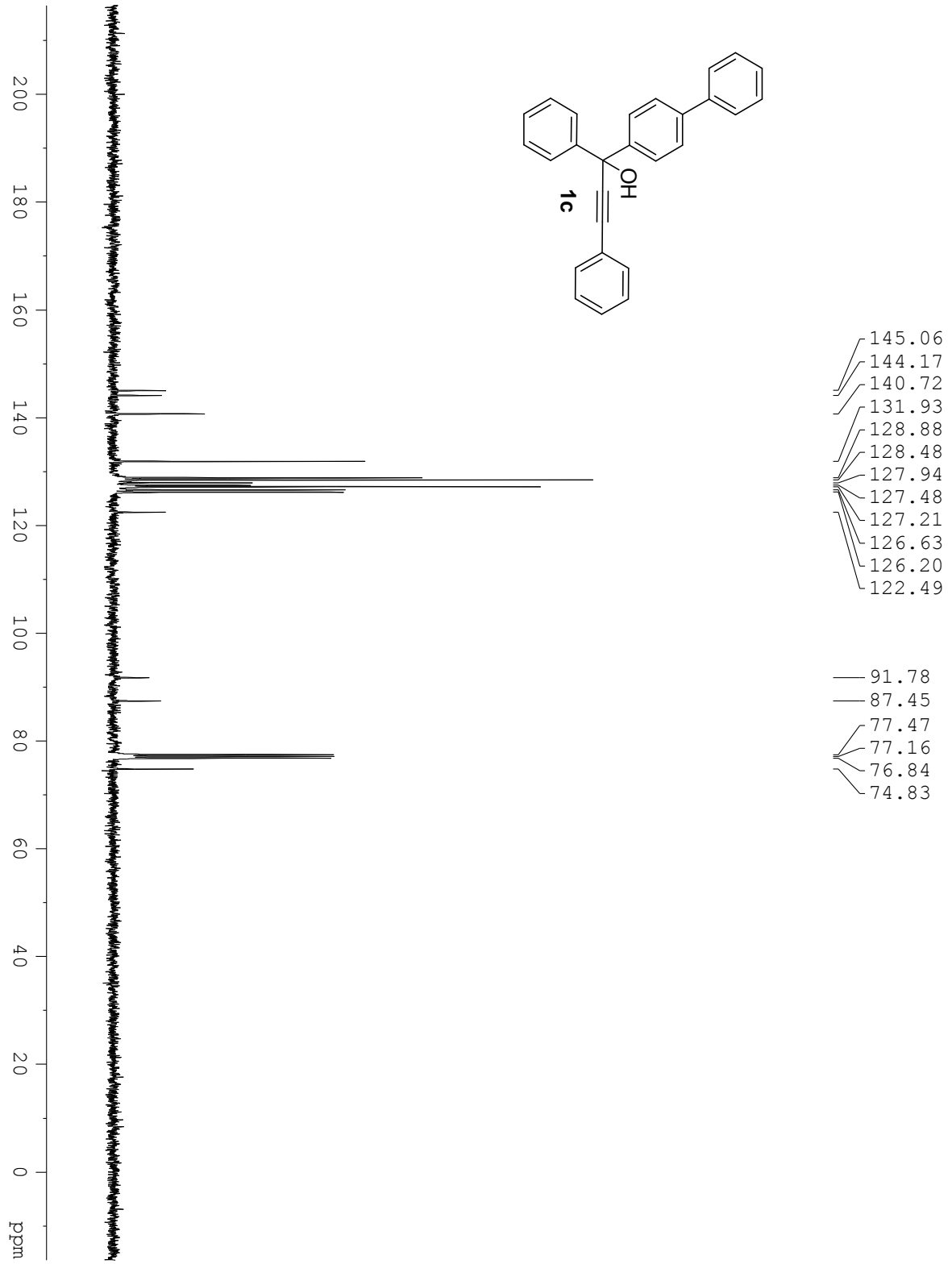

7
OH
F
F
1.00
2.07
4.97
1.02
1.89
1.11
2.06
7.909
7.901
7.887
7.488
7.474
7.470
7.317
7.308
7.300
7.234
7.160
7.146
3.158
3.139
3.116
3.096
3.077
3.065
3.050
3.022
2.643
2.618
2.608
2.601
2.594
2.585
2.578
2.568
2.550
2.539
2.533
2.527
2.518
2.511
2.499
2.482
2.468
2.452
2.439
2.425
2.409
2.390
1.615
1.257
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

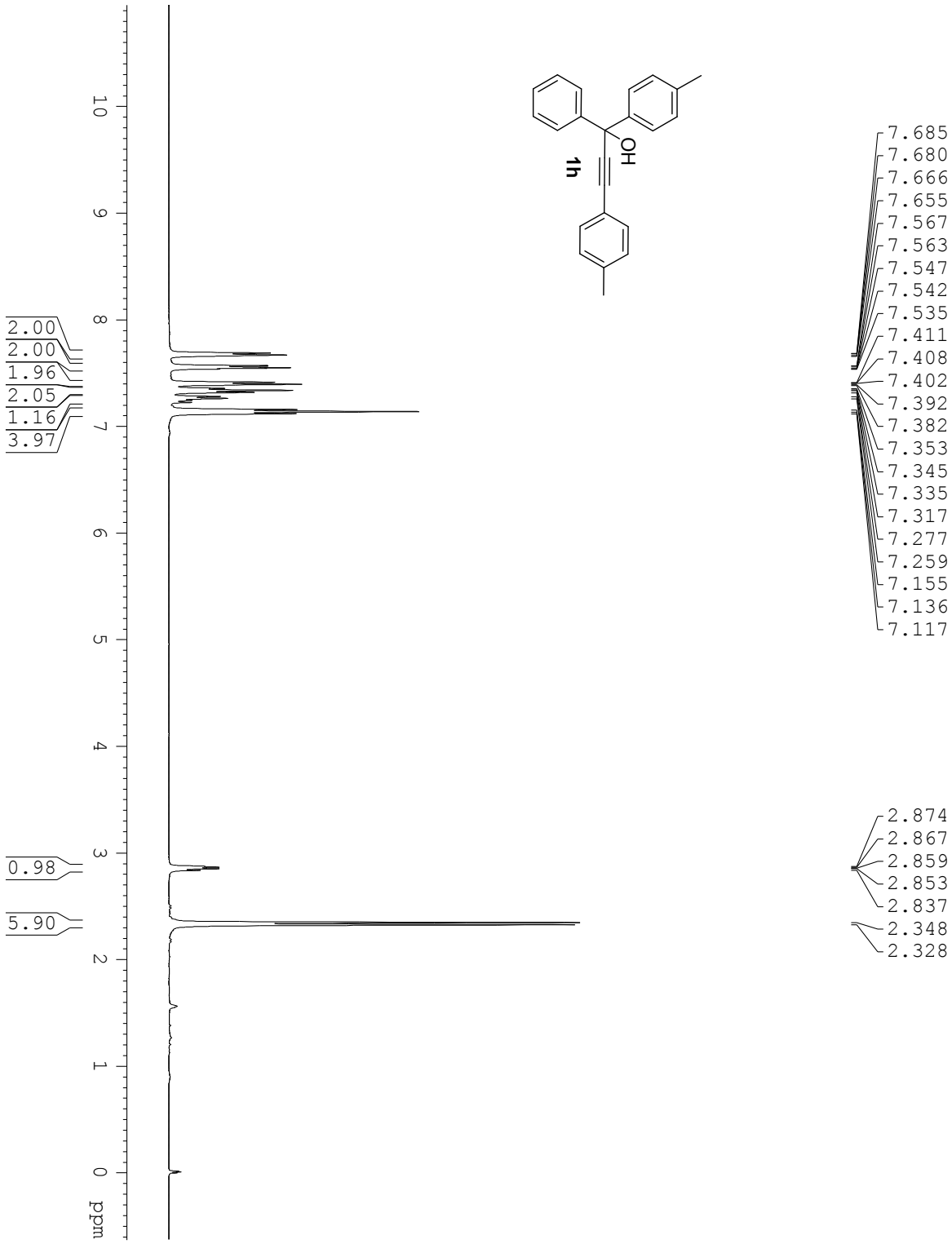

7
OH
F
F
200
180
160
140
120
100
80
60
40
20
0
ppm
136.22
133.52
132.06
129.21
129.06
128.90
128.63
128.40
127.23
123.88
121.95
121.41
118.94
87.51
86.41
77.48
77.16
76.84
71.43
71.18
70.90
27.21
26.98
26.75
26.39

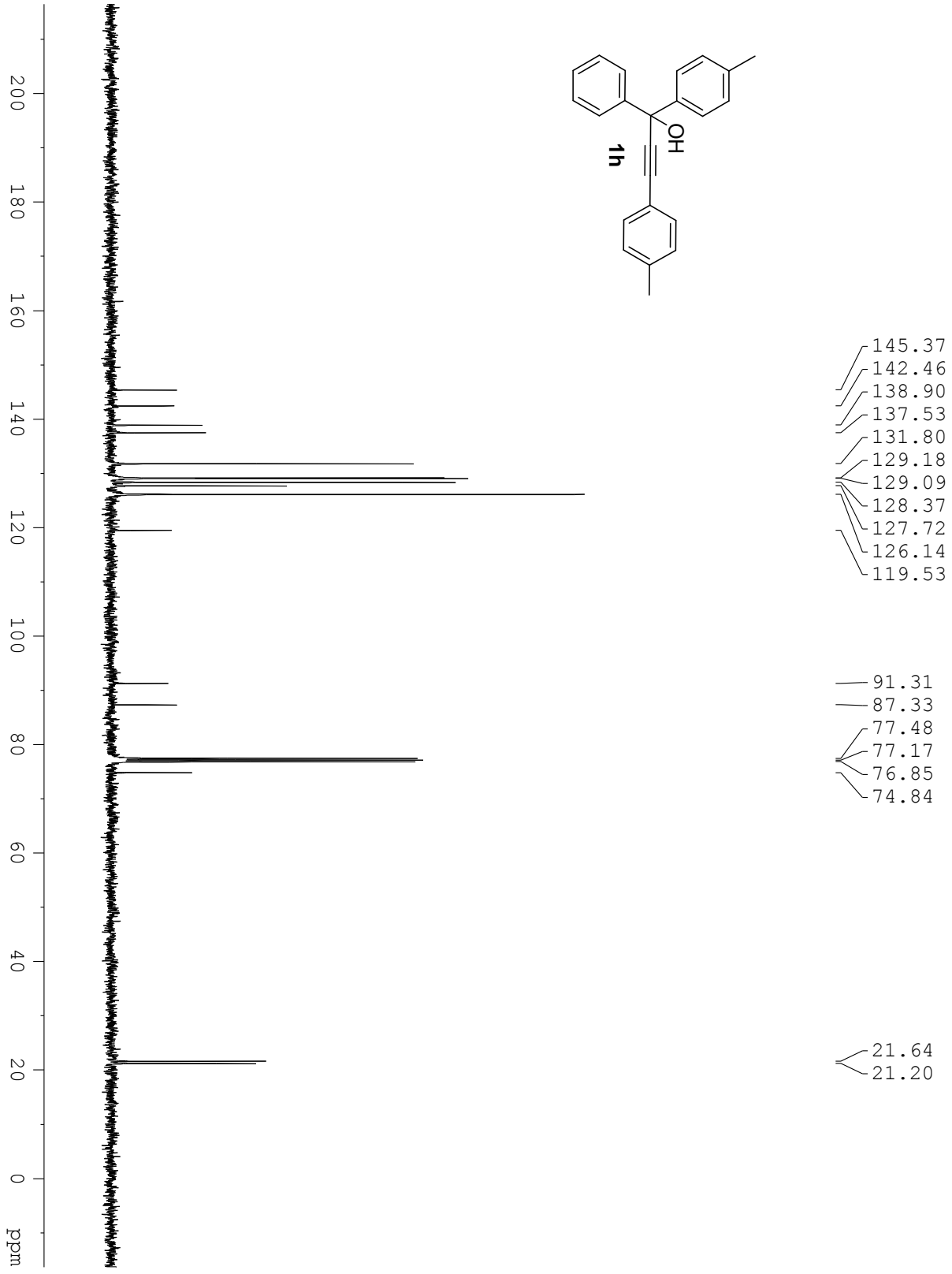

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
7
OH
F
F
-109.70
-109.72
-109.77
-109.79
-110.34
-110.35
-110.41
-110.43
-112.62
-112.66
-113.25
-113.25
-113.30

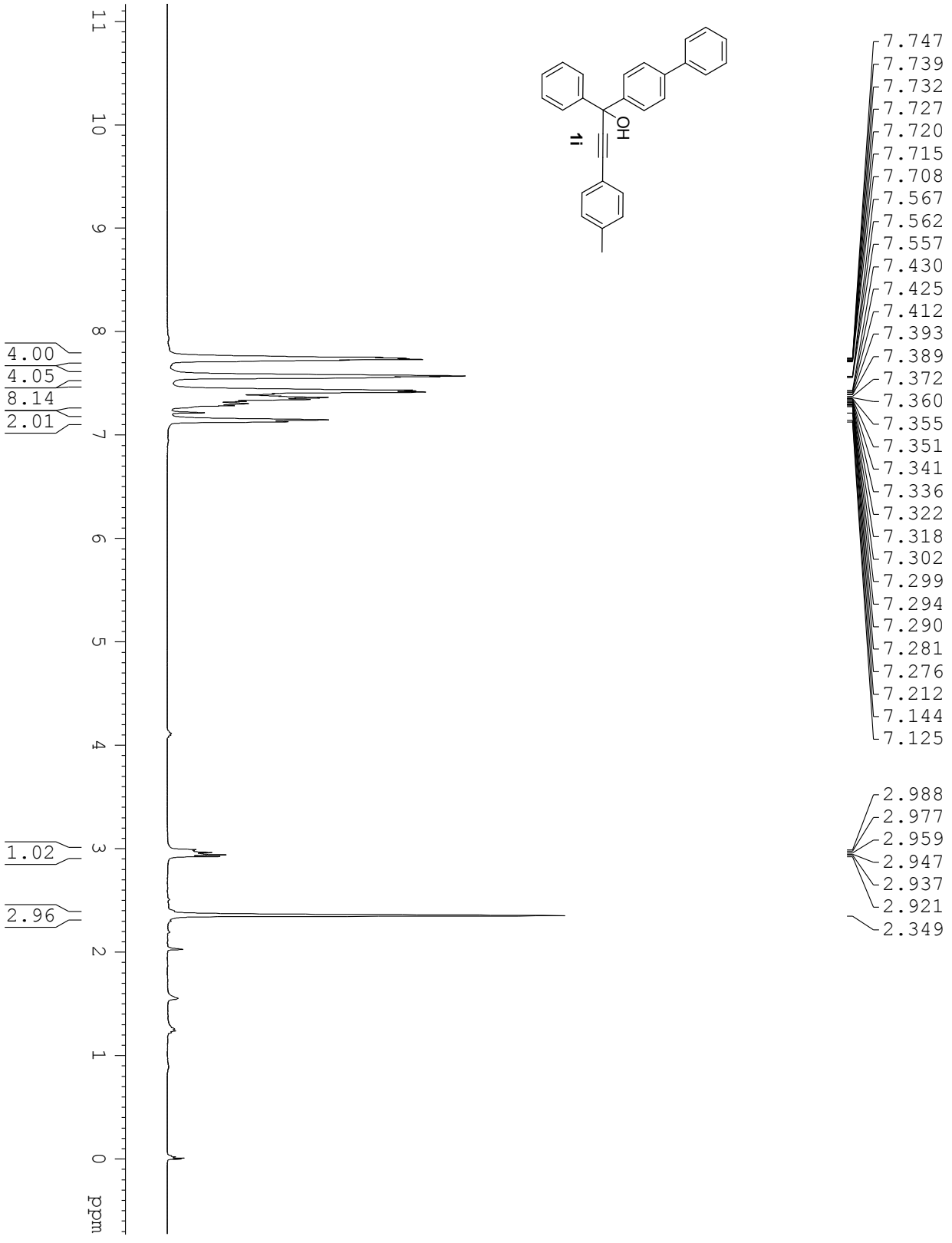
1.1 ^{1}H NMR, ^{13}C NMR spectra of tertiary propargyl alcohols

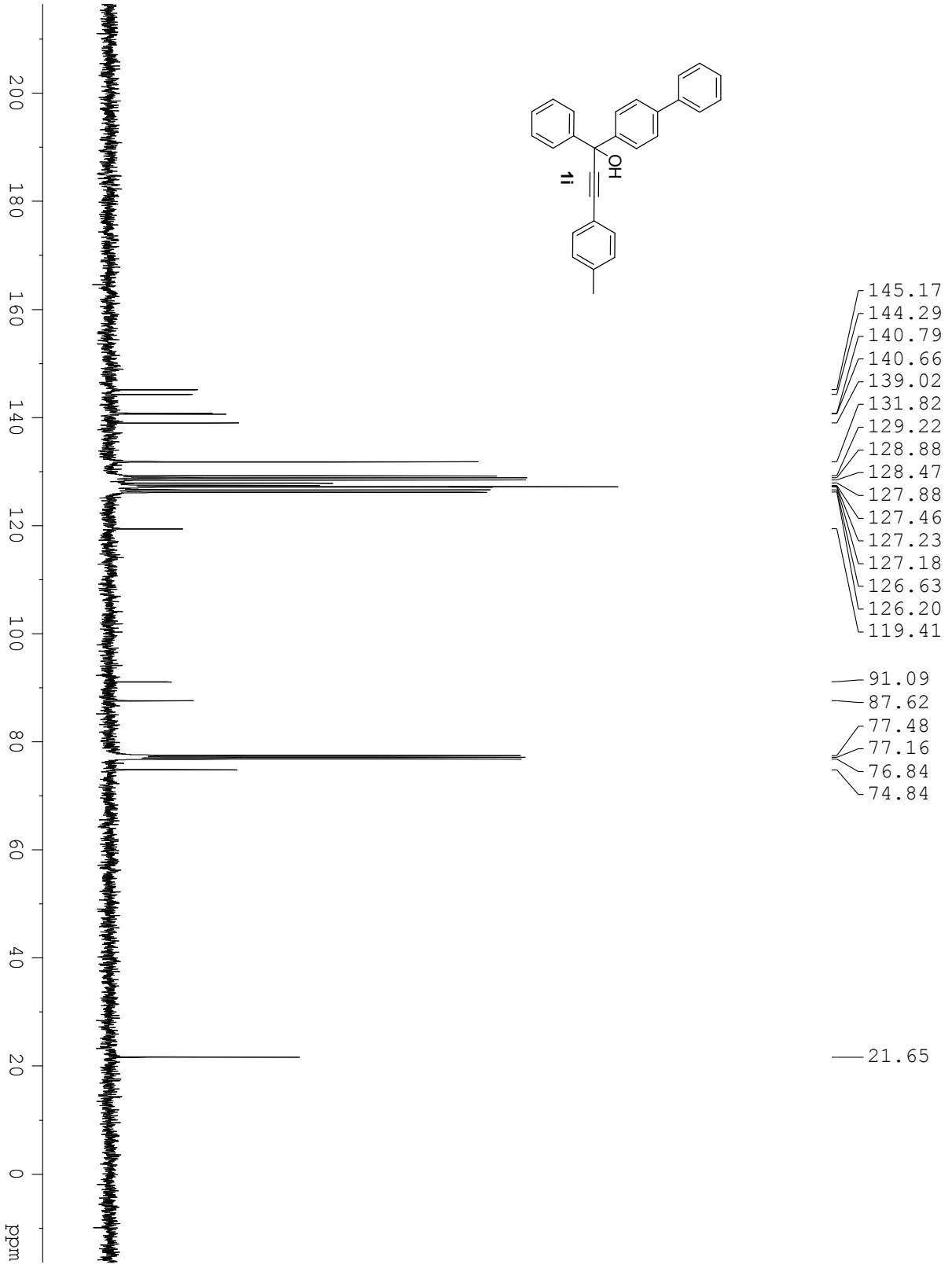


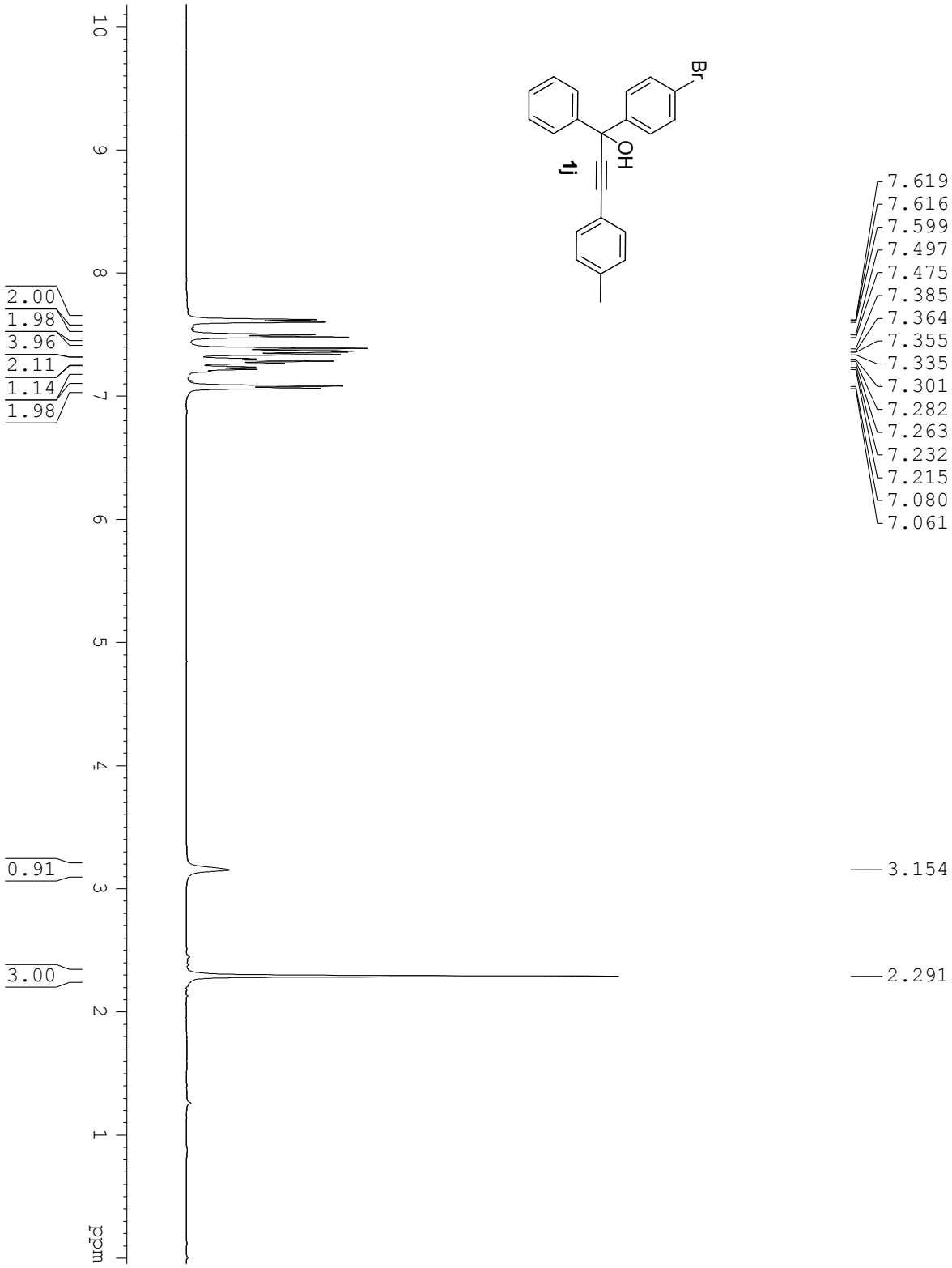

OH
1c
145.06
144.17
140.72
131.93
128.88
128.48
127.94
127.48
127.21
126.63
126.20
122.49
91.78
87.45
77.47
77.16
76.84
74.83
200
180
160
140
120
100
80
60
40
20
0
ppm

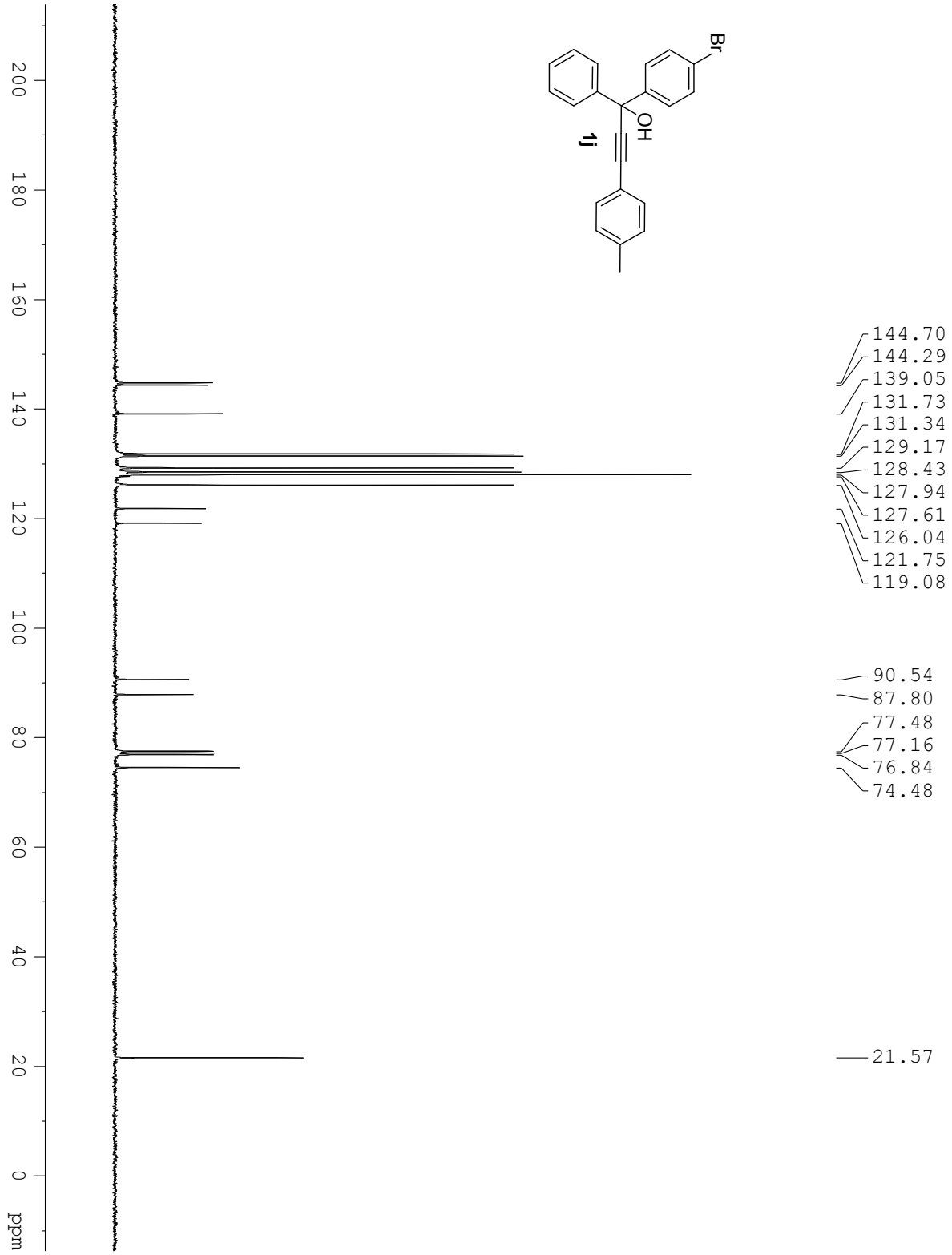

1h
OH
7.685
7.680
7.666
7.655
7.567
7.563
7.547
7.542
7.535
7.411
7.408
7.402
7.392
7.382
7.353
7.345
7.335
7.317
7.277
7.259
7.155
7.136
7.117
2.874
2.867
2.859
2.853
2.837
2.348
2.328
2.00
2.00
1.96
2.05
1.16
3.97
0.98
5.90
ppm

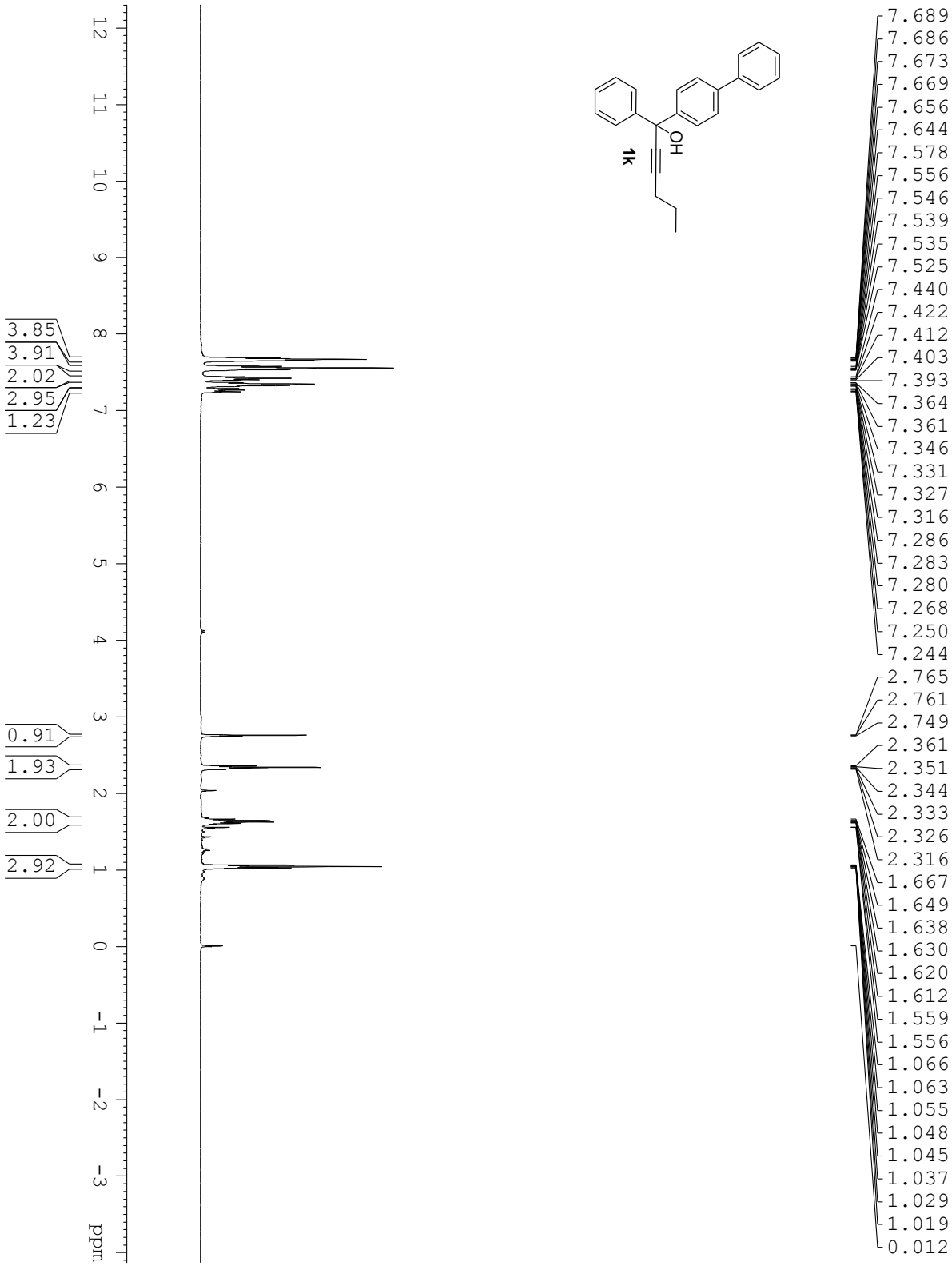

OH
1h
145.37
142.46
138.90
137.53
131.80
129.18
129.09
128.37
127.72
126.14
119.53
91.31
87.33
77.48
77.17
76.85
74.84
21.64
21.20
200
180
160
140
120
100
80
60
40
20
0
ppm

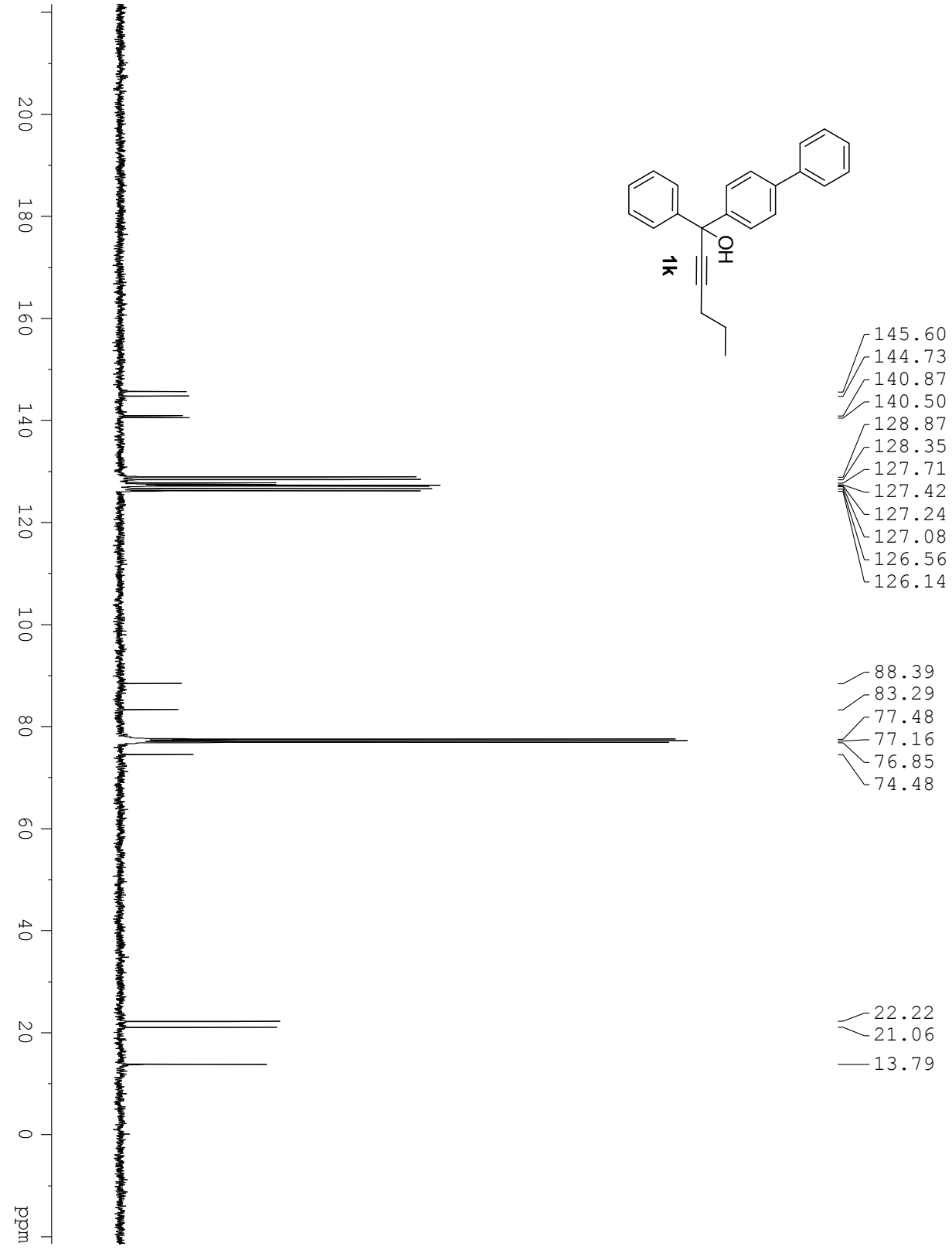

11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
4.05
8.14
2.01
1.02
2.96
OH
1i
7.747
7.739
7.732
7.727
7.720
7.715
7.708
7.567
7.562
7.557
7.430
7.425
7.412
7.393
7.389
7.372
7.360
7.355
7.351
7.341
7.336
7.322
7.318
7.302
7.299
7.294
7.290
7.281
7.276
7.212
7.144
7.125
2.988
2.977
2.959
2.947
2.937
2.921
2.349

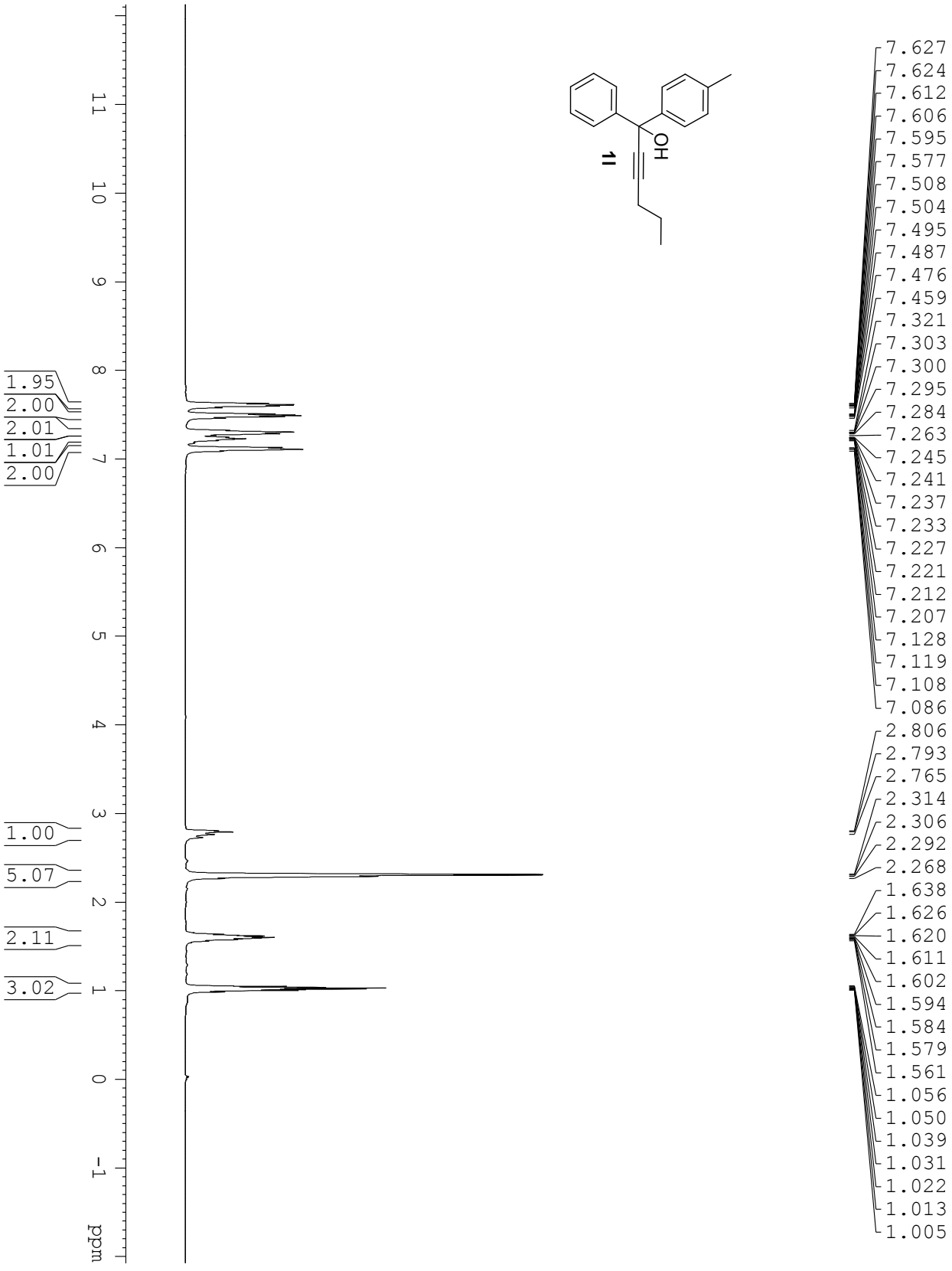

OH
1i
145.17
144.29
140.79
140.66
139.02
131.82
129.22
128.88
128.47
127.88
127.46
127.23
127.18
126.63
126.20
119.41
91.09
87.62
77.48
77.16
76.84
74.84
21.65
200
180
160
140
120
100
80
60
40
20
0
ppm

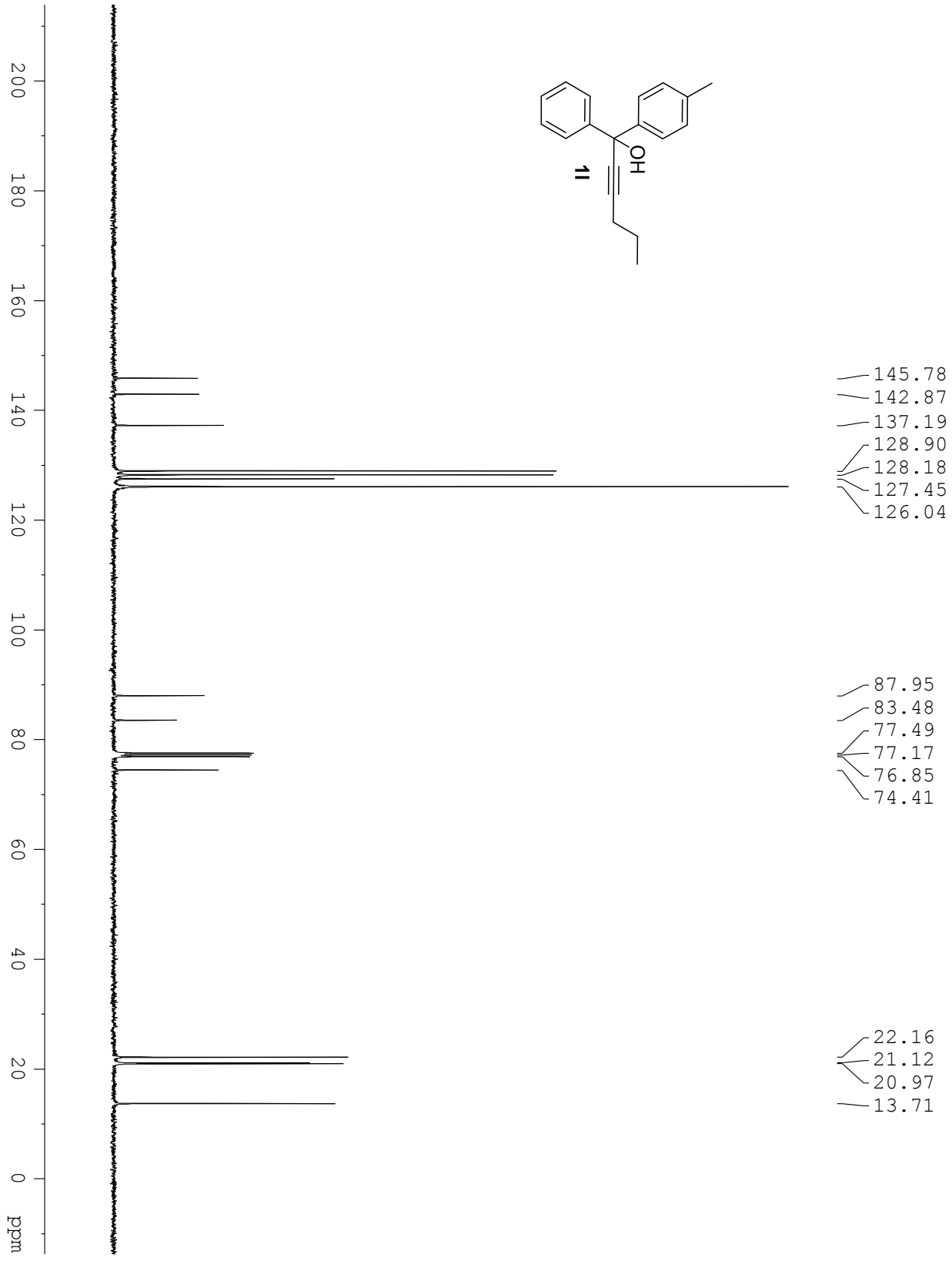

Br
OH
1j
7.619
7.616
7.599
7.497
7.475
7.385
7.364
7.355
7.335
7.301
7.282
7.263
7.232
7.215
7.080
7.061
3.154
2.291
2.00
1.98
3.96
2.11
1.14
1.98
0.91
3.00
10
9
8
7
6
5
4
3
2
1
ppm

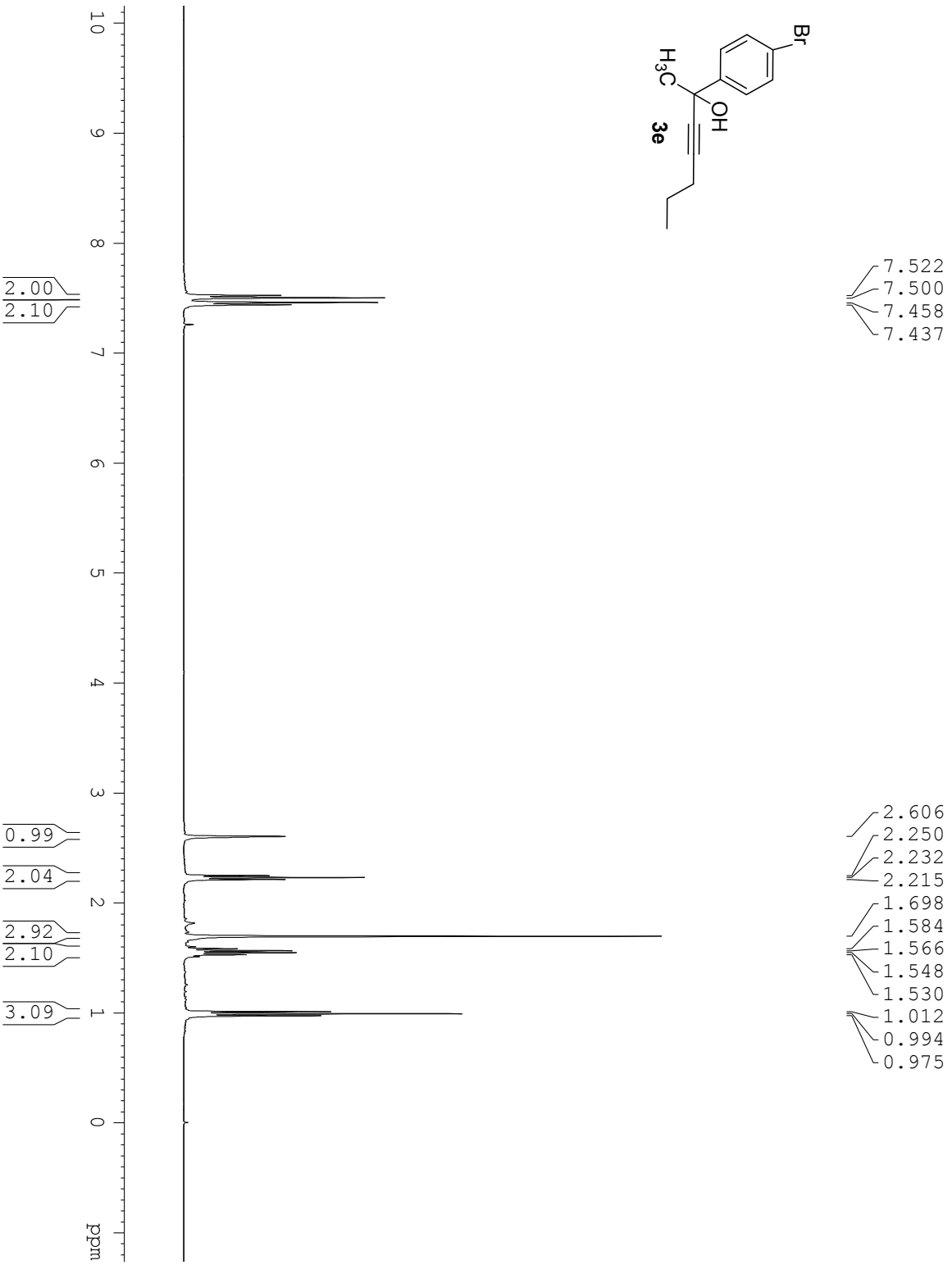

Br
OH
1j
144.70
144.29
139.05
131.73
131.34
129.17
128.43
127.94
127.61
126.04
121.75
119.08
90.54
87.80
77.48
77.16
76.84
74.48
21.57
200
180
160
140
120
100
80
60
40
20
0
ppm

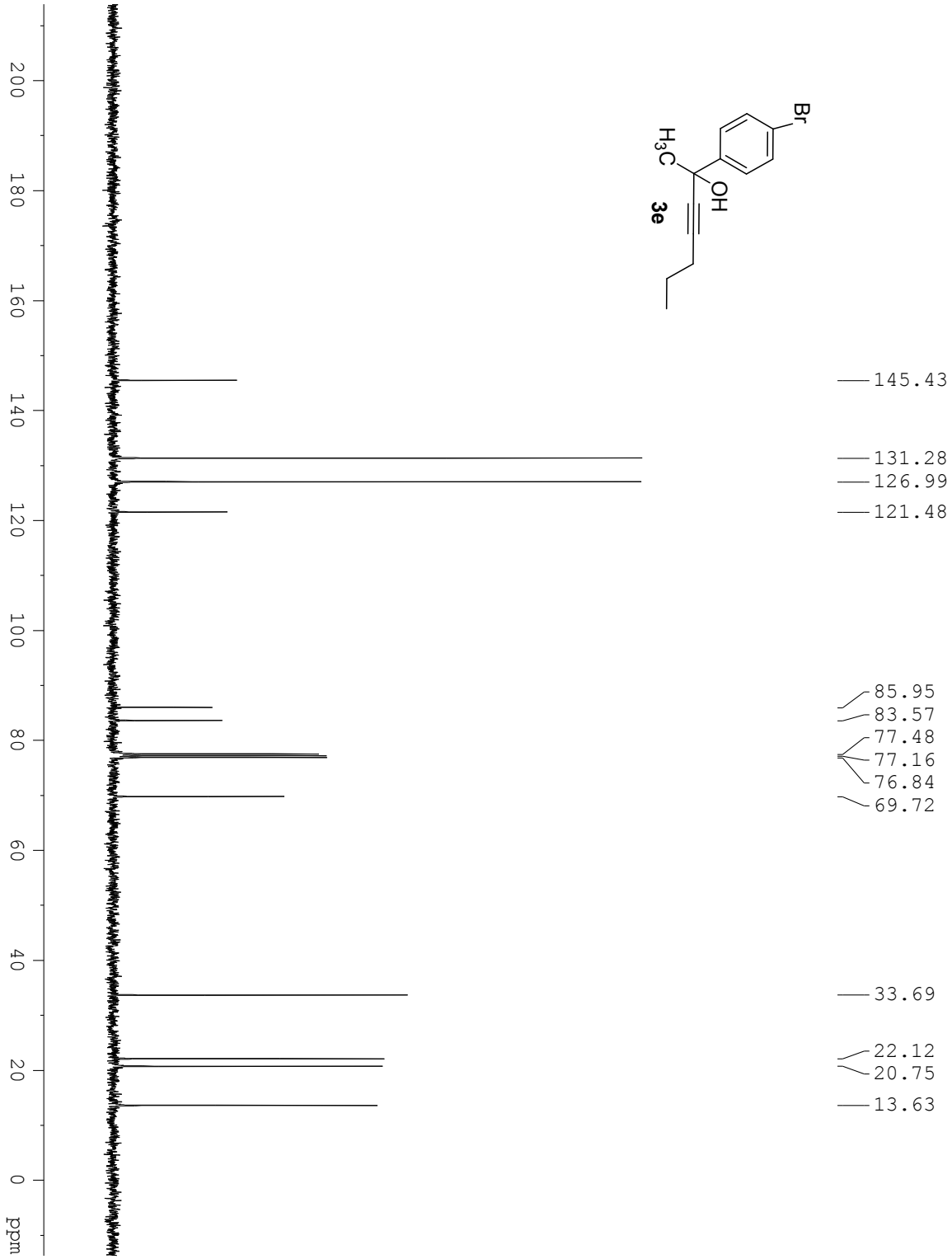

7.689
7.686
7.673
7.669
7.656
7.644
7.578
7.556
7.546
7.539
7.535
7.525
7.440
7.422
7.412
7.403
7.393
7.364
7.361
7.346
7.331
7.327
7.316
7.286
7.283
7.280
7.268
7.250
7.244
2.765
2.761
2.749
2.361
2.351
2.344
2.333
2.326
2.316
1.667
1.649
1.638
1.630
1.620
1.612
1.559
1.556
1.066
1.063
1.055
1.048
1.045
1.037
1.029
1.019
0.012
OH
1k
3.85
3.91
2.02
2.95
1.23
0.91
1.93
2.00
2.92
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm


OH
1k
145.60
144.73
140.87
140.50
128.87
128.35
127.71
127.42
127.24
127.08
126.56
126.14
88.39
83.29
77.48
77.16
76.85
74.48
22.22
21.06
13.79
200
180
160
140
120
100
80
60
40
20
0
ppm

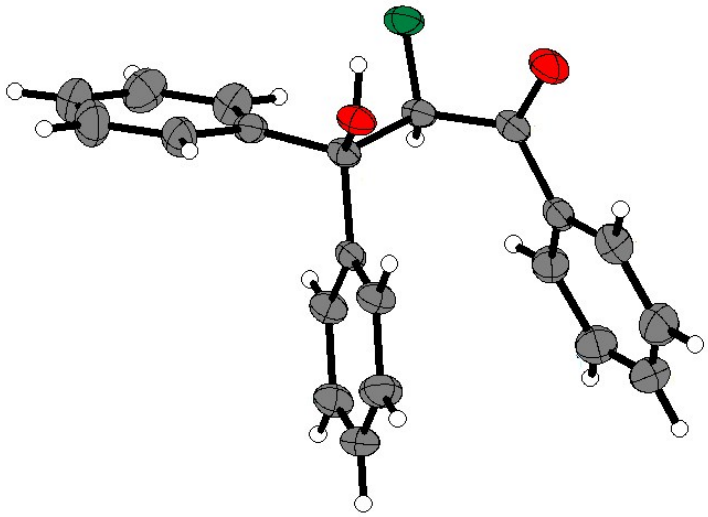

11
OH
7.627
7.624
7.612
7.606
7.595
7.577
7.508
7.504
7.495
7.487
7.476
7.459
7.321
7.303
7.300
7.295
7.284
7.263
7.245
7.241
7.237
7.233
7.227
7.221
7.212
7.207
7.128
7.119
7.108
7.086
2.806
2.793
2.765
2.314
2.306
2.292
2.268
1.638
1.626
1.620
1.611
1.602
1.594
1.584
1.579
1.561
1.056
1.050
1.039
1.031
1.022
1.013
1.005
1.95
2.00
2.01
1.01
2.00
1.00
5.07
2.11
3.02
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm


OH
1l
145.78
142.87
137.19
128.90
128.18
127.45
126.04
87.95
83.48
77.49
77.17
76.85
74.41
22.16
21.12
20.97
13.71
200
180
160
140
120
100
80
60
40
20
0
ppm


Br
H3C
OH
3e
7.522
7.500
7.458
7.437
2.606
2.250
2.232
2.215
1.698
1.584
1.566
1.548
1.530
1.012
0.994
0.975
2.00
2.10
0.99
2.04
2.92
2.10
3.09
ppm


Br
H3C
OH
3e
145.43
131.28
126.99
121.48
85.95
83.57
77.48
77.16
76.84
69.72
33.69
22.12
20.75
13.63
200
180
160
140
120
100
80
60
40
20
0
ppm

2. ORTEP diagram of **2a**



Crystal parameters

Identification code	rbnnk2	
Empirical formula	C_{21} H_{17} F O_2	
Formula weight	320.35	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal system	'Monoclinic'	
Space group	'P121/n1'	
Unit cell dimensions	a = 15.0818(3) Å	α= 90°.
	b = 5.99520(10) Å	β= 102.281(2)°.
	c = 18.5272(4) Å	γ = 90°.
Volume	1636.86(6) $Å^3$	
Z	4	
Density (calculated)	1.300 Mg/m^3	
Absorption coefficient	0.734 mm^{-1}	
F(000)	672	
Crystal size	0.28 x 0.12 x 0.12 mm^3	
Theta range for data collection	3.441 to 71.438°.	
Index ranges	-18<=h<=16, -3<=k<=7, -22<=l<=19	
Reflections collected	5097	
Independent reflections	3106 [R(int) = 0.0121]	

Completeness to theta = 25.00°	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3106 / 0 / 218
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1172
R indices (all data)	R1 = 0.0472, wR2 = 0.1223
Largest diff. peak and hole	0.164 and -0.245 e.$Å^{-3}$
CCDC	**1033721**