Supporting Information

Gold-Catalyzed Tandem [3,3] Propargyl Ester Rearrangement Leading to *E*-1*H*-Inden-1-ones

Li-Jing Wang, Hai-Tao Zhu, An-Qi Wang, Yi-Feng Qiu, Xue-Yuan Liu and Yong-Min Liang*

State Key Laboratory of Applied Organic Chemistry, Lanzhou University, 730000, P.R. China.
e-mail: *liangym@lzu.edu.cn*

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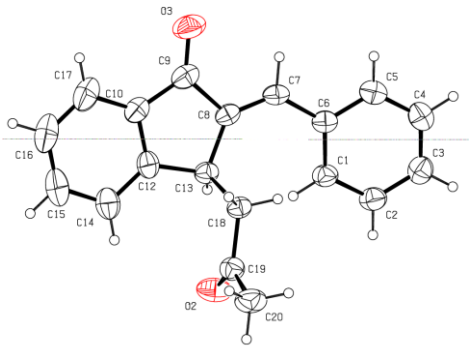
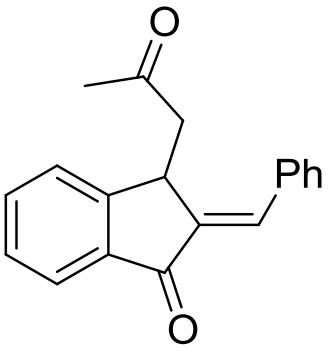




X-ray structure of 2a (CCDC 960618)

Bond precision: C-C = 0.0073 A Wavelength=0.71070

Cell: a=11.2513(11) b=16.593(2) c=8.0237(9)
alpha=90 beta=90 gamma=90

Temperature: 292 K

	Calculated	Reported
Volume	1498.0(3)	1498.0(3)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C19 H16 O2	C19 H16 O2
Sum formula	C19 H16 O2	C19 H16 O2
Mr	276.32	276.32
Dx,g cm-3	1.225	1.225
Z	4	4
Mu (mm-1)	0.078	0.078
F000	584.0	584.0
F000'	584.27	
h,k,lmax	14,20,10	14,20,10
Nref	3042[1639]	2648
Tmin,Tmax	0.978,0.991	0.325,1.000
Tmin'	0.975	

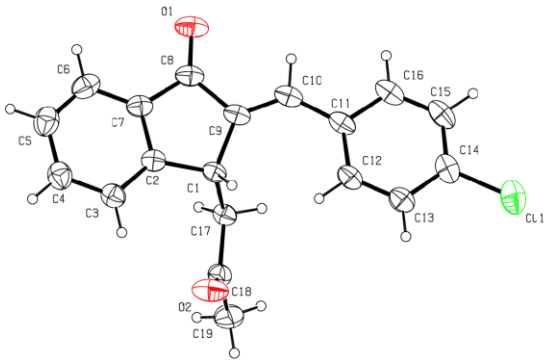
Correction method= MULTI-SCAN

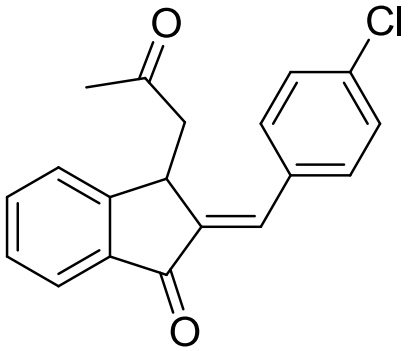
Data completeness= 1.62/0.87 Theta(max)= 26.370

R(reflections)= 0.0699(1419) wR2(reflections)= 0.1565(2648)

S = 1.070 Npar= 192

X-ray Diffraction Analysis of Compound 2d





X-ray structure of 2d

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: a=5.9699(3) b=8.9969(6) c=28.9795(15)
alpha=90 beta=95.309(6) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	1549.83(15)	1549.81(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C19 H15 Cl O2	C19 H15 Cl O2
Sum formula	C19 H15 Cl O2	C19 H15 Cl O2
Mr	310.76	310.76
Dx,g cm-3	1.332	1.332
Z	4	4
Mu (mm-1)	0.251	0.251
F000	648.0	648.0
F000'	648.86	
h,k,lmax	7,11,35	7,11,35
Nref	3059	3045
Tmin,Tmax	0.909,0.921	0.540,1.000
Tmin'	0.909	

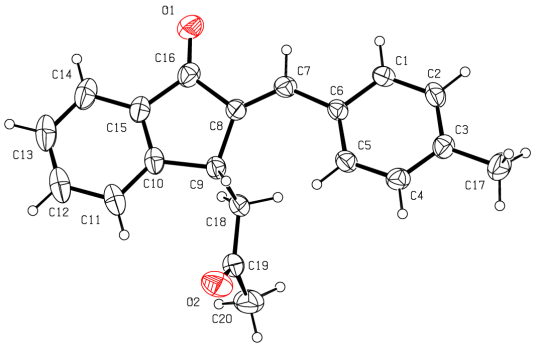
Correction method= MULTI-SCAN

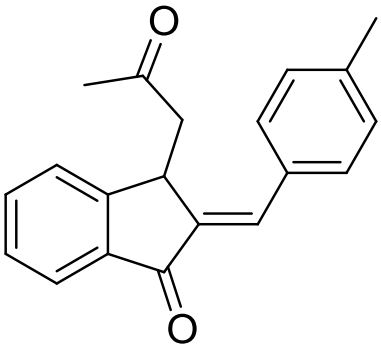
Data completeness= 0.995 Theta(max)= 26.021

R(reflections)= 0.0506(2151) wR2(reflections)= 0.1376(3045)

S = 1.049 Npar= 200

X-ray Diffraction Analysis of Compound 2f

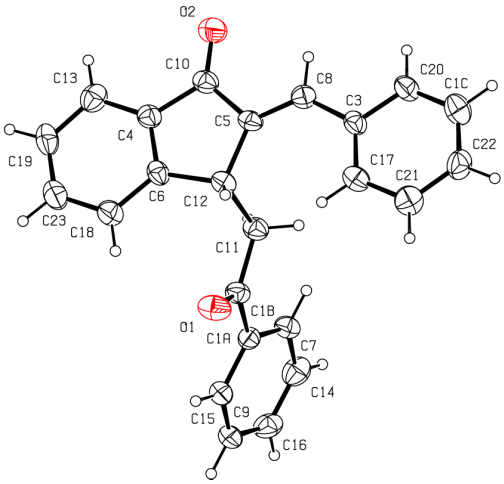


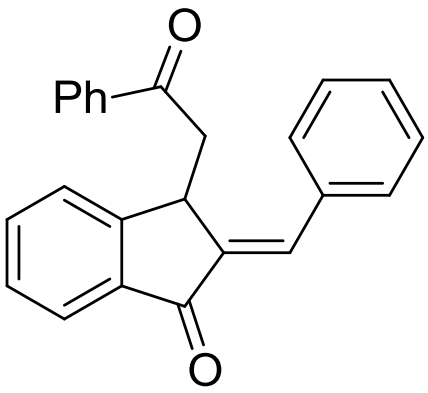


X-ray structure of 2f

Bond precision: C-C = 0.0059 A Wavelength=0.71073
Cell: a=5.5429(6) b=8.4278(9) c=34.013(3)
alpha=90 beta=90 gamma=90
Temperature: 293 K
Calculated Reported
Volume 1588.9(3) 1588.9(3)
Space group P 21 21 21 P 21 21 21
Hall group P 2ac 2ab P 2ac 2ab
Moiety formula C20 H18 O2 C20 H18 O2
Sum formula C20 H18 O2 C20 H18 O2
Mr 290.34 290.34
Dx,g cm-3 1.214 1.214
Z 4 4
Mu (mm-1) 0.077 0.077
F000 616.0 616.0
F000’ 616.28
h,k,lmax 6,10,41 6,10,41
Nref 3125[1860] 2949
Tmin,Tmax
Tmin’
Correction method= Not given
Data completeness= 1.59/0.94 Theta(max)= 26.020
R(reflections)= 0.0664(1941) wR2(reflections)= 0.1653(2949)
S = 1.077 Npar= 202

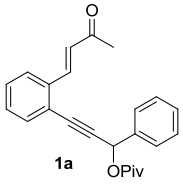
X-ray Diffraction Analysis of Compound 2o





X-ray structure of 2o

Bond precision: C-C = 0.0062 A Wavelength=0.71070
Cell: a=14.712(3) b=5.8398(14) c=20.996(6)
alpha=90 beta=105.27(3) gamma=90
Temperature: 293 K
Calculated Reported
Volume 1740.2(8) 1740.2(8)
Space group P 21/c P 1 21/c 1
Hall group -P 2ybc -P 2ybc
Moiety formula C24 H18 O2 C24 H18 O2
Sum formula C24 H18 O2 C24 H18 O2
Mr 338.38 338.38
Dx,g cm-3 1.292 1.292
Z 4 4
Mu (mm-1) 0.081 0.081
F000 712.0 712.0
F000’ 712.32
h,k,lmax 18,7,25 18,7,25
Nref 3425 3399
Tmin,Tmax 0.982,0.994 0.071,1.000
Tmin’ 0.981
Correction method= MULTI-SCAN
Data completeness= 0.992 Theta(max)= 26.020
R(reflections)= 0.0755(1295) wR2(reflections)= 0.1987(3399)
S = 0.964 Npar= 236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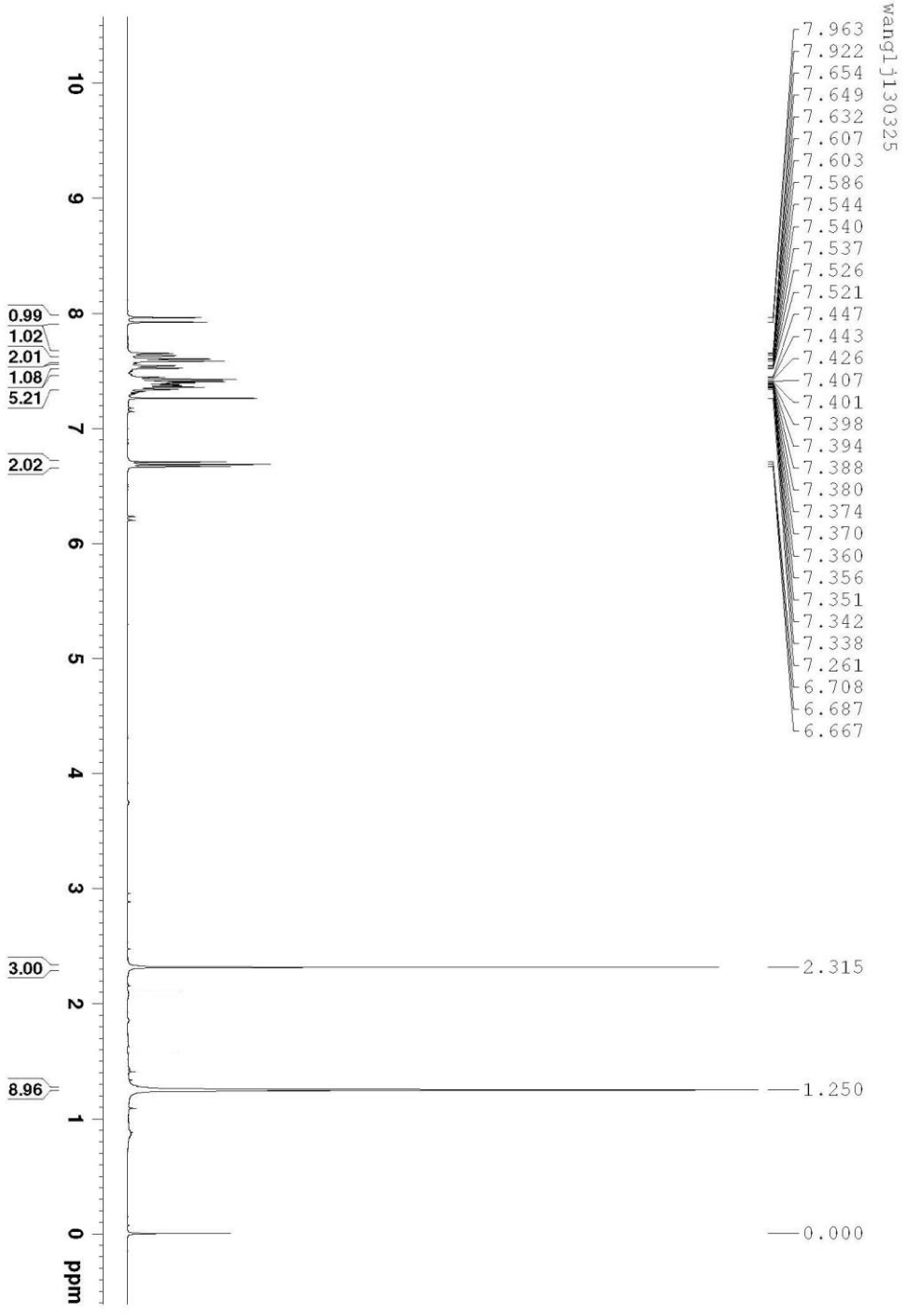
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7.526
7.521
7.447
7.443
7.426
7.407
7.401
7.398
7.394
7.388
7.380
7.374
7.370
7.360
7.356
7.351
7.342
7.338
7.261
6.708
6.687
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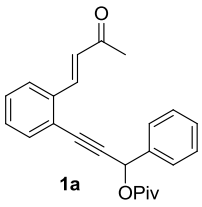
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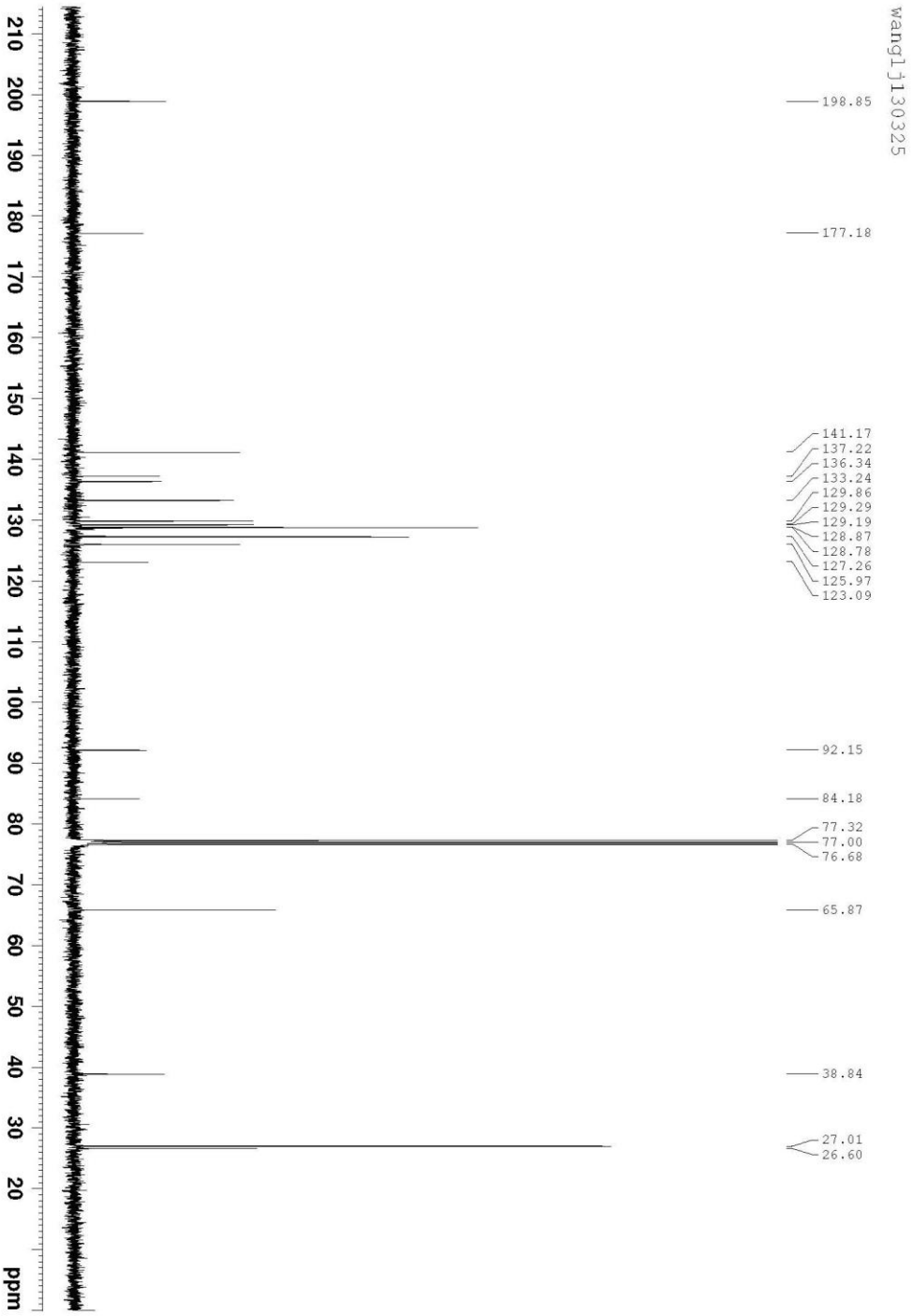
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128.78
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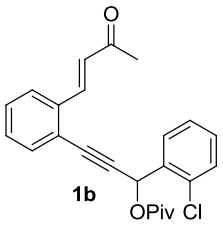
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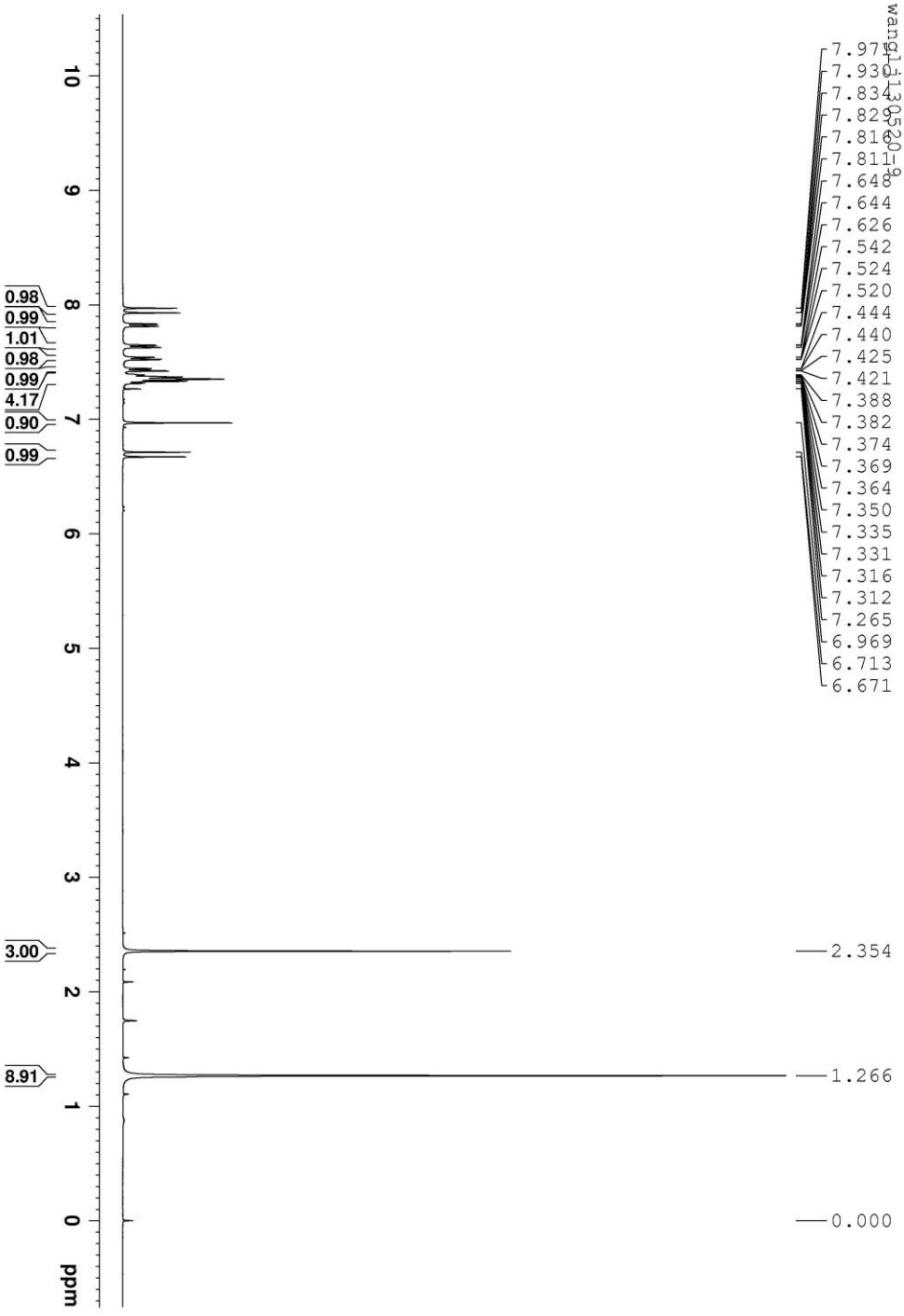
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7.542
7.524
7.520
7.444
7.440
7.425
7.421
7.388
7.382
7.374
7.369
7.364
7.350
7.335
7.331
7.316
7.312
7.265
6.969
6.713
6.671
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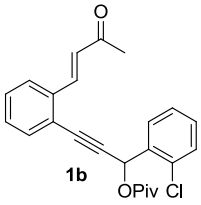
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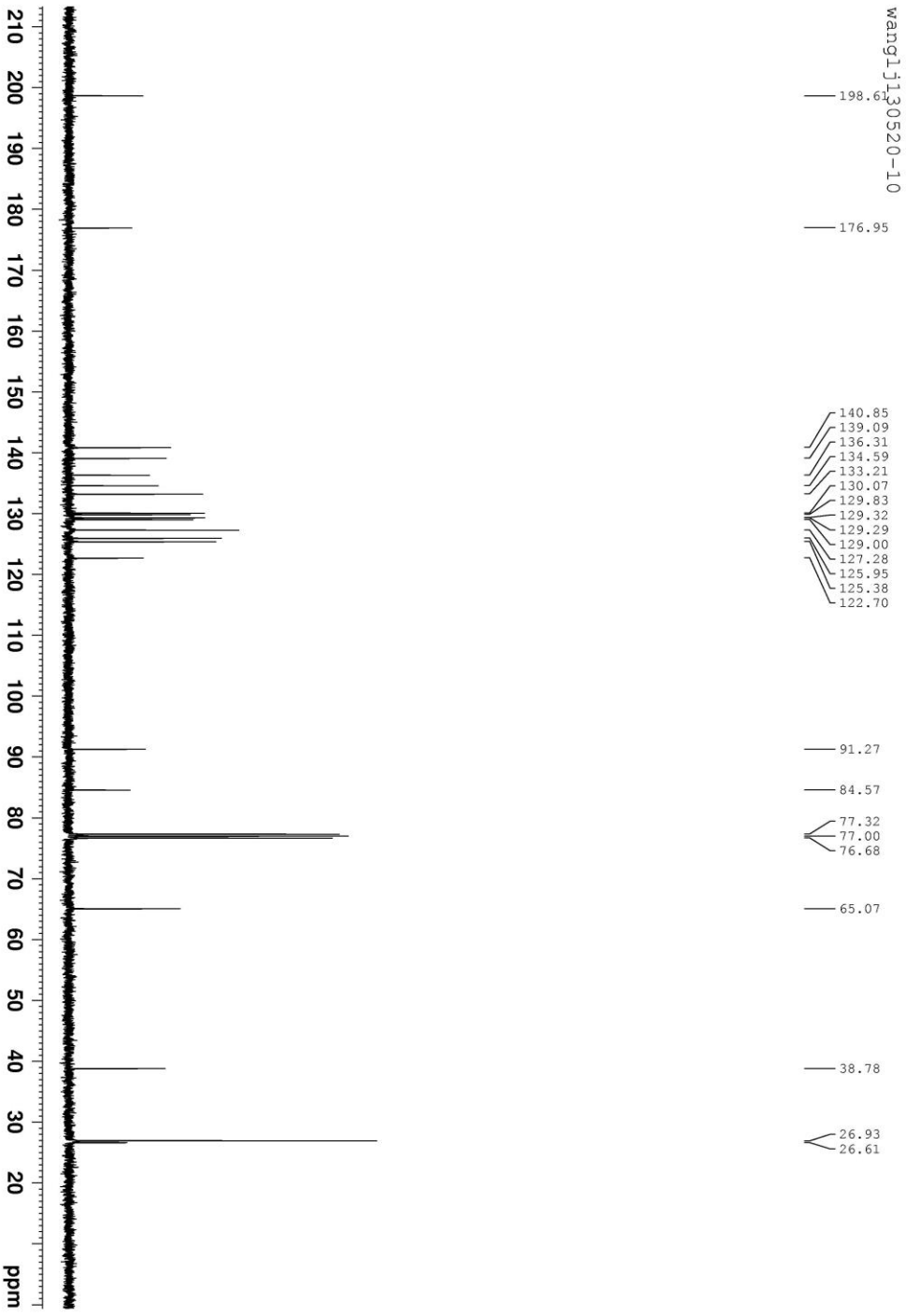
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136.31
134.59
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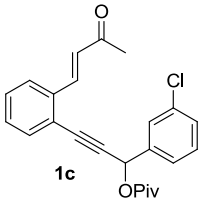
129.83
129.32
129.29
129.00
127.28
125.95
125.38
122.70
91.27
84.57
77.32
77.00
76.68
65.07
38.78
26.93
26.61
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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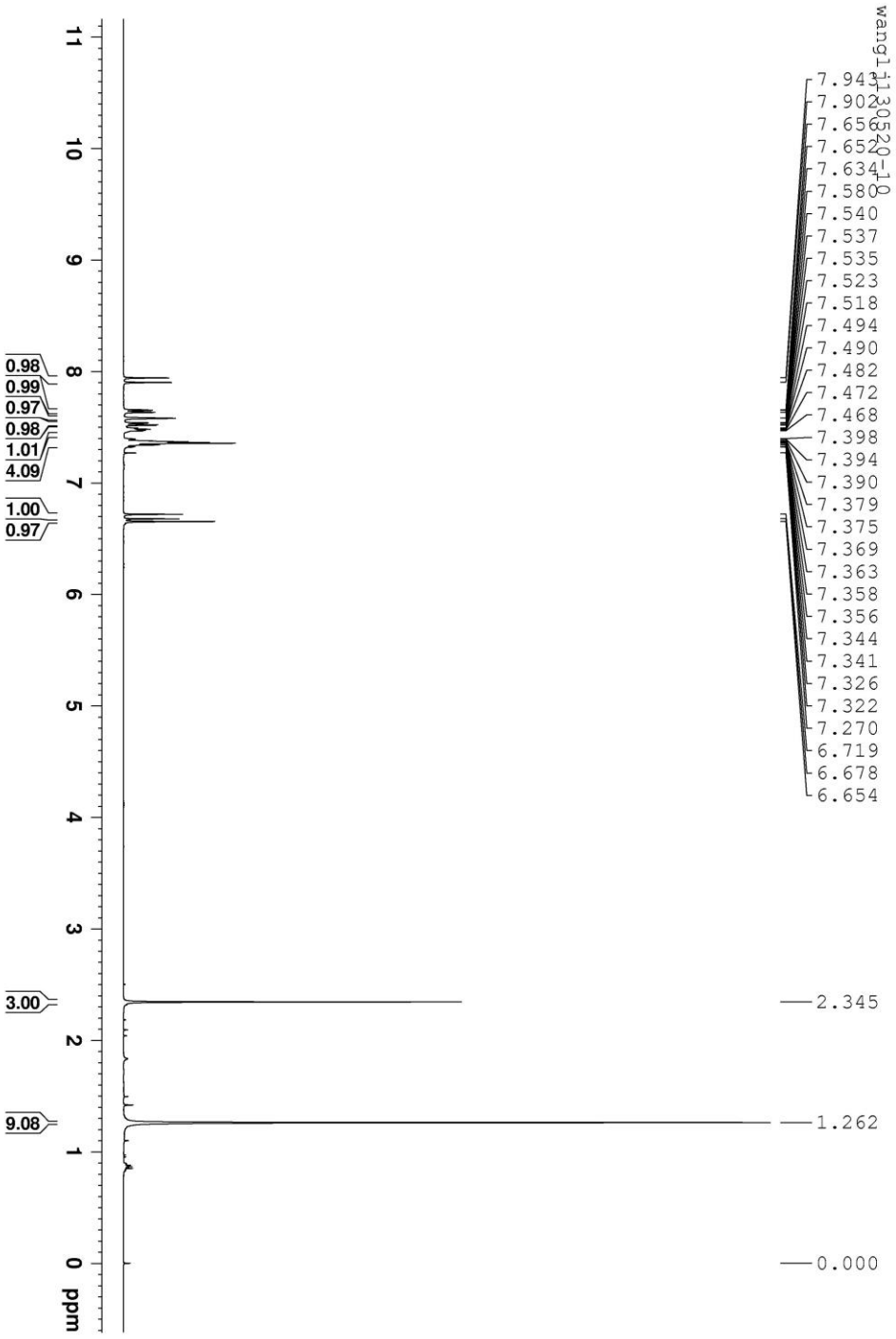
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7.494
7.490
7.482
7.472
7.468
7.398
7.394
7.390
7.379
7.375
7.369
7.363
7.358
7.356
7.344
7.341
7.326
7.322
7.270
6.719
6.678
6.654
0.98
0.99
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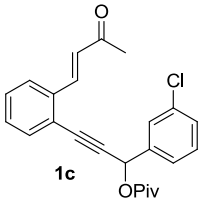
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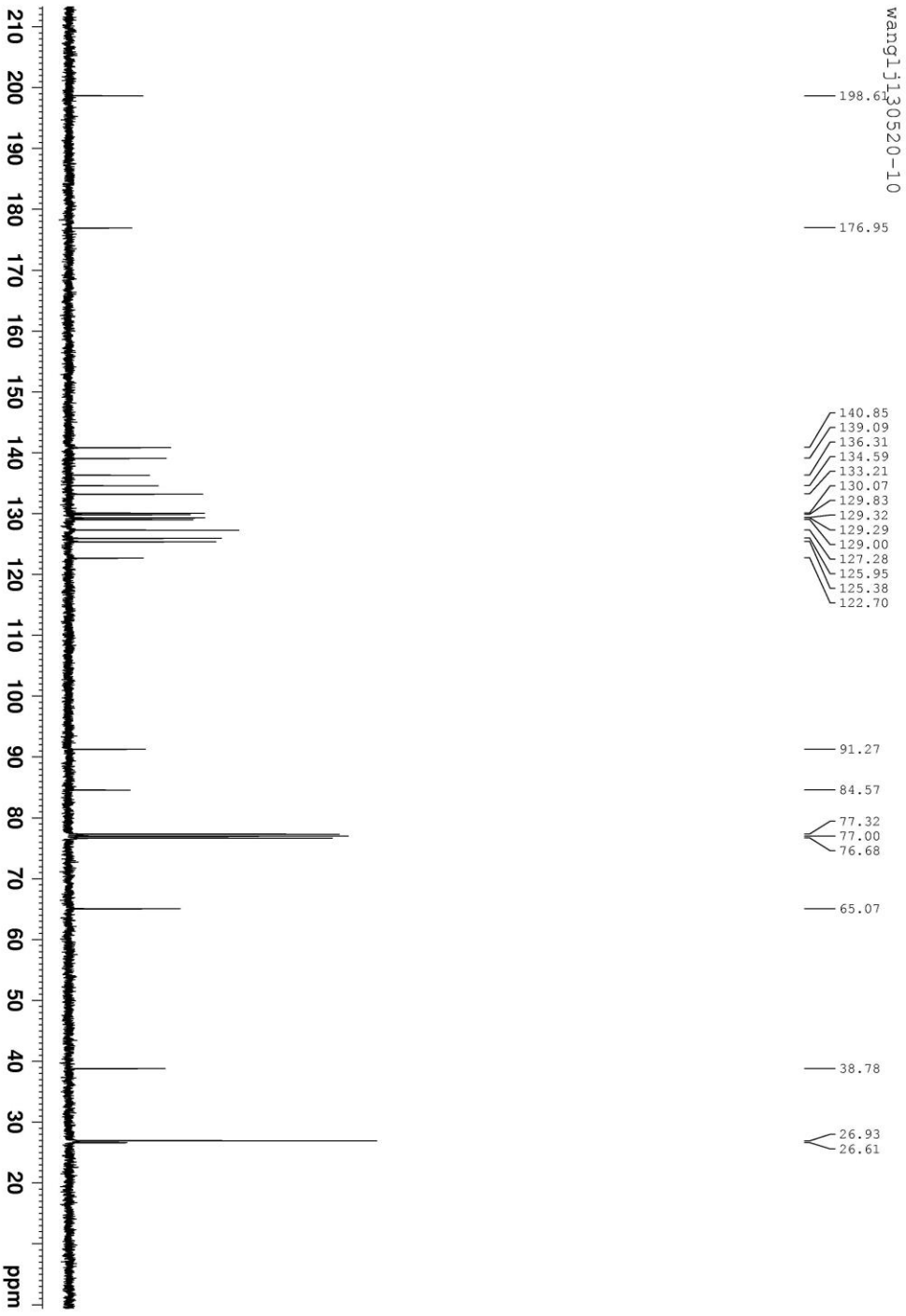
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129.00
127.28
125.95
125.38
122.70
91.27
84.57
77.32
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76.68
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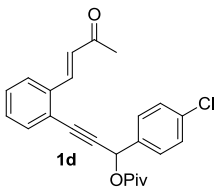
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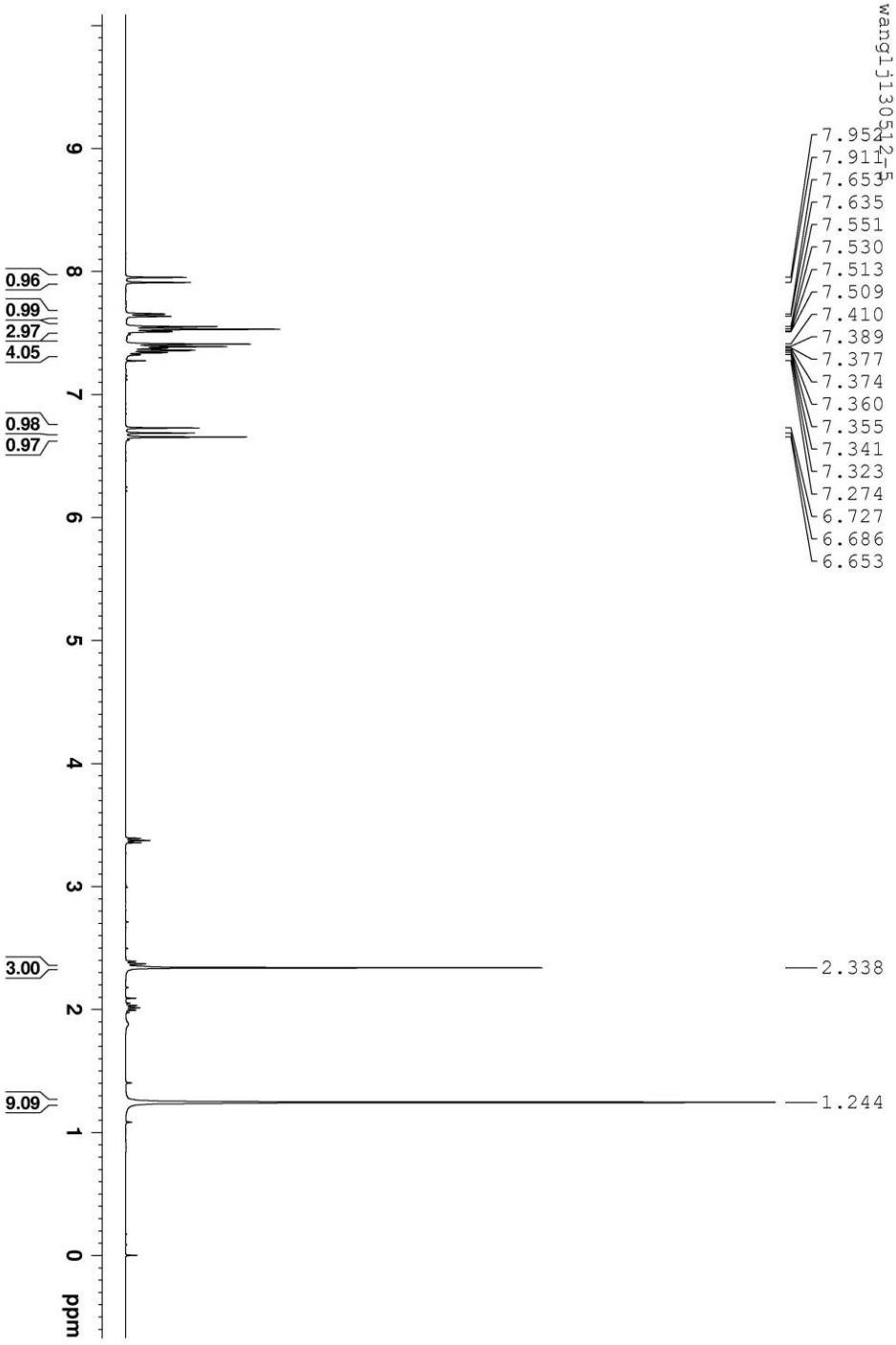
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7.635
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7.530
7.513
7.509
7.410
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7.377
7.374
7.360
7.355
7.341
7.323
7.274
6.727
6.686
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9.09
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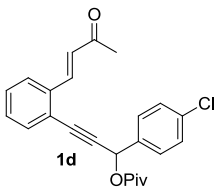
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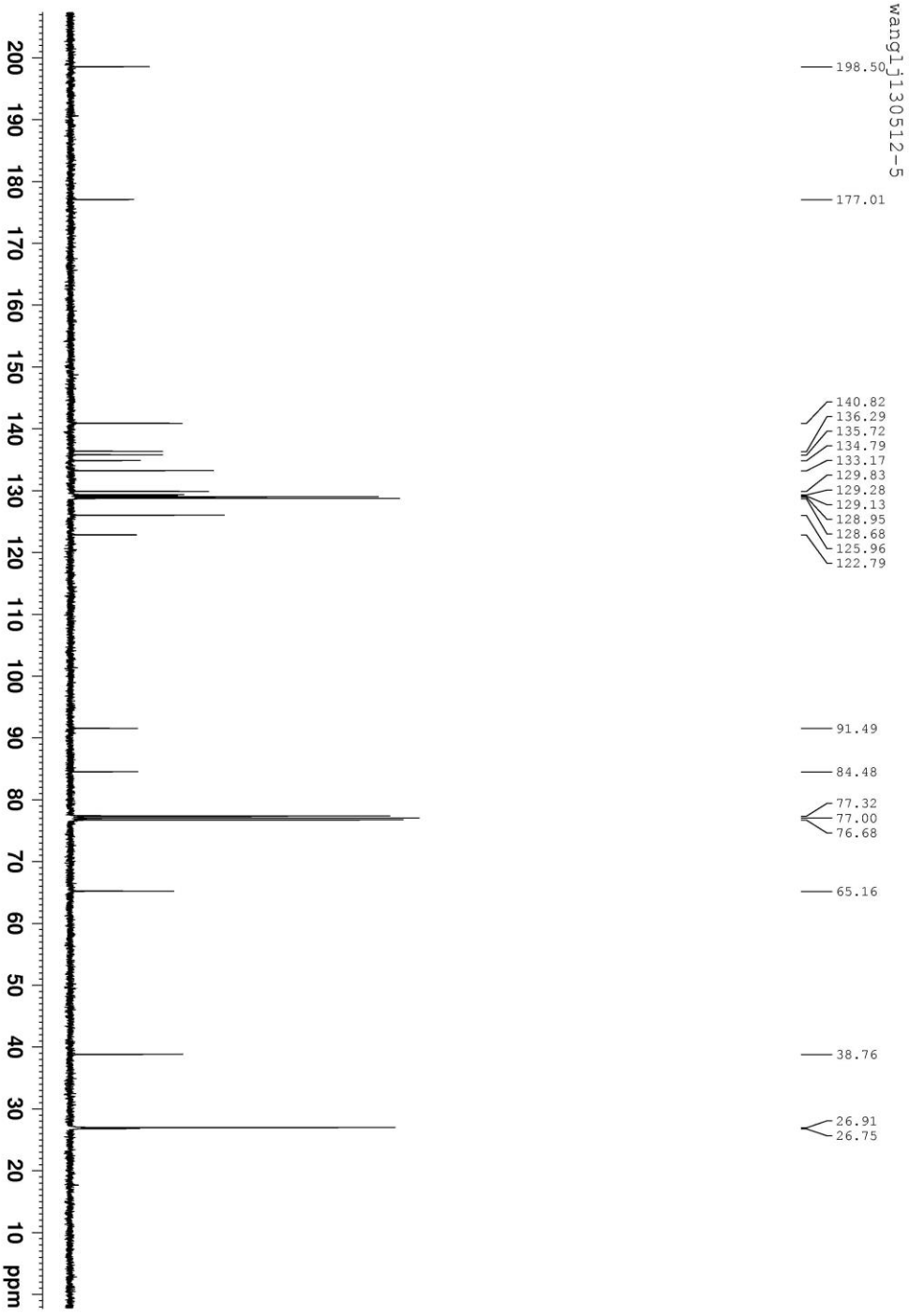
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134.79
133.17
129.83
129.28
129.13
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128.68
125.96
122.79
91.49
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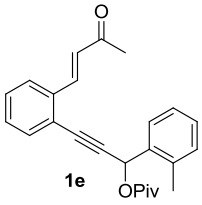
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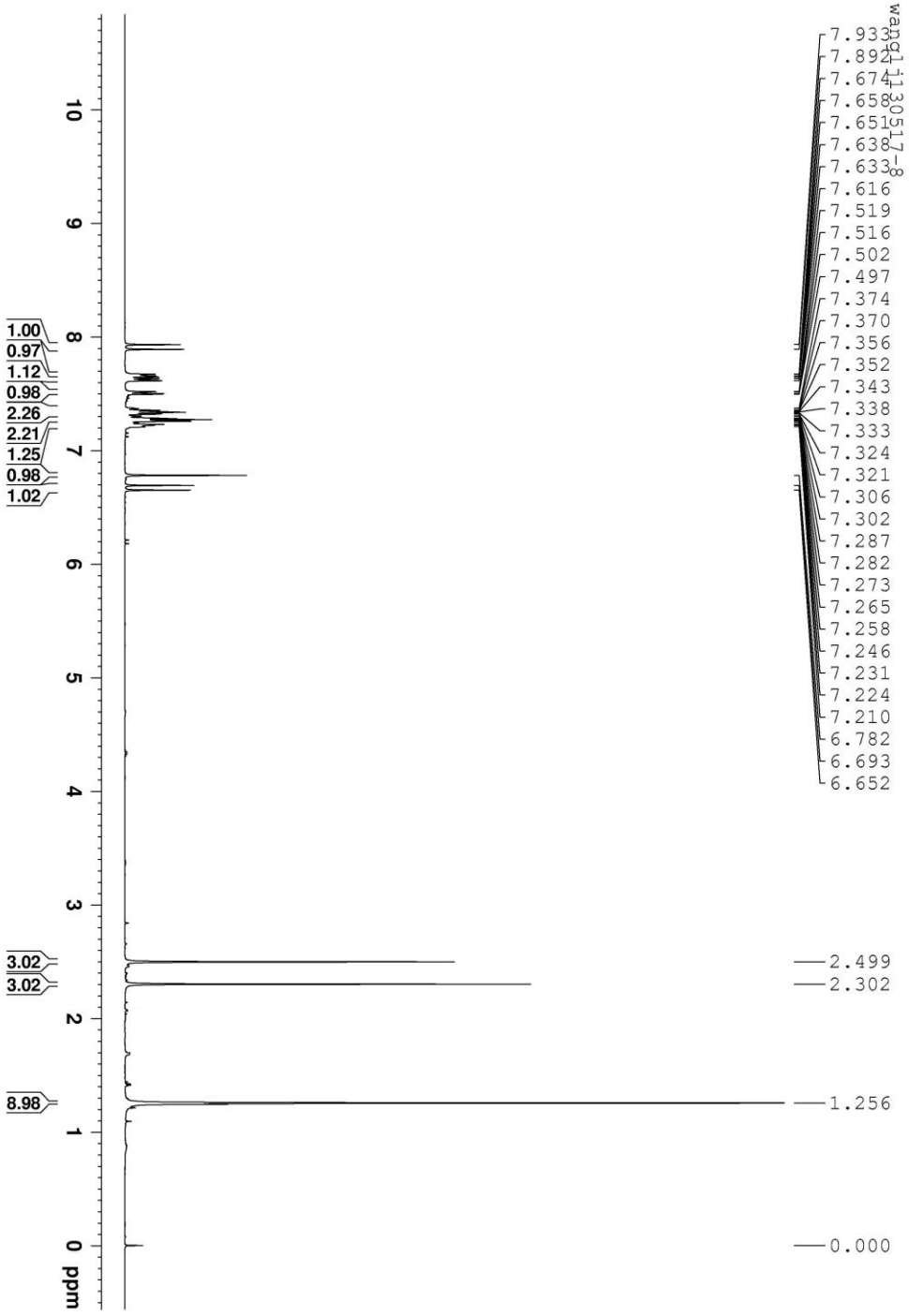
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7.616
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7.497
7.374
7.370
7.356
7.352
7.343
7.338
7.333
7.324
7.321
7.306
7.302
7.287
7.282
7.273
7.265
7.258
7.246
7.231
7.224
7.210
6.782
6.693
6.652
1.00
0.97
1.12
0.98
2.26
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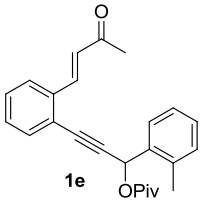
ppm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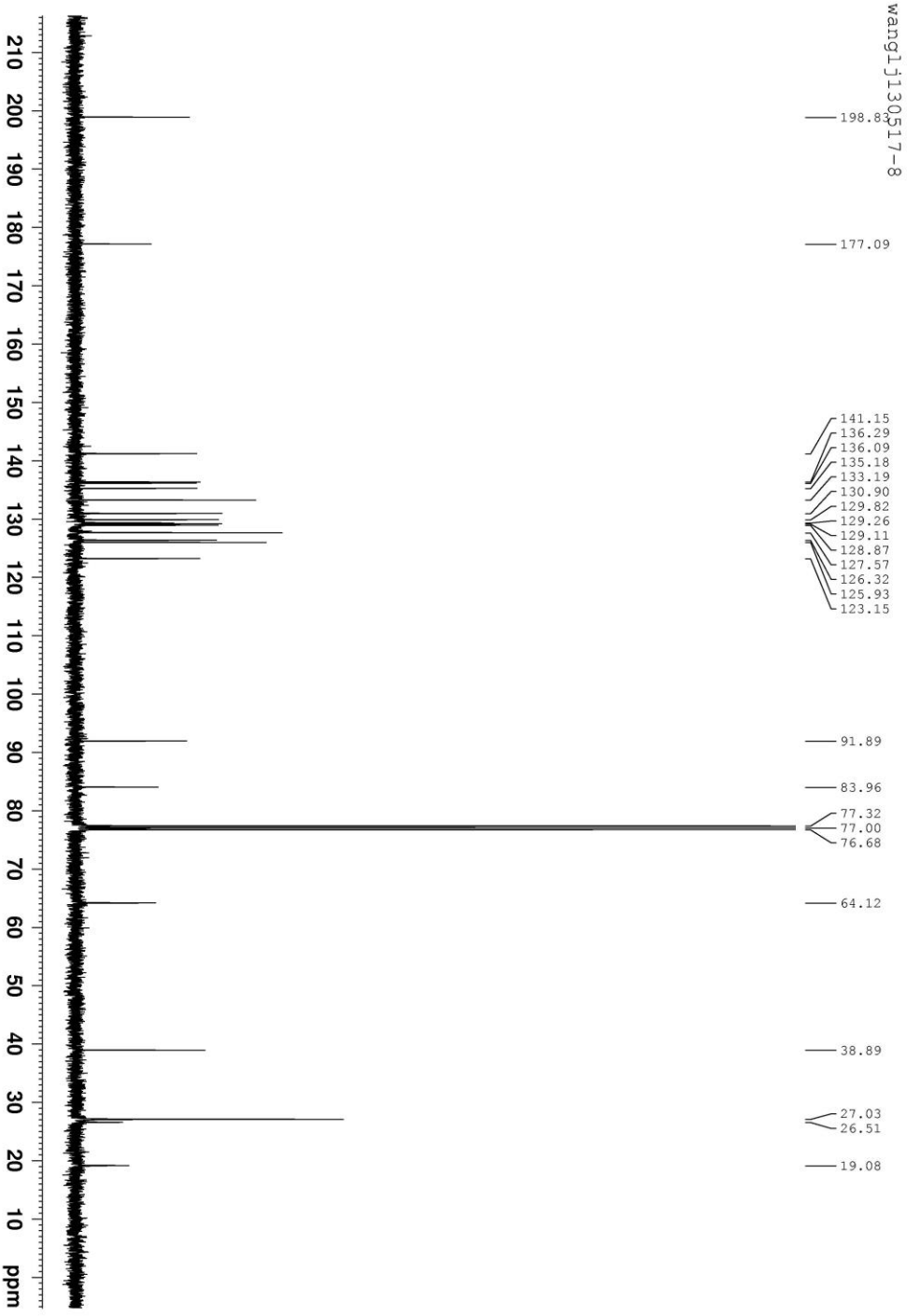
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136.29
136.09
135.18
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128.87
127.57
126.32
125.93
123.15
91.89
83.96
77.32
77.00
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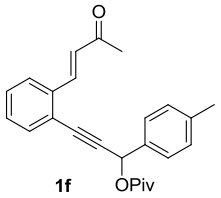
19.08
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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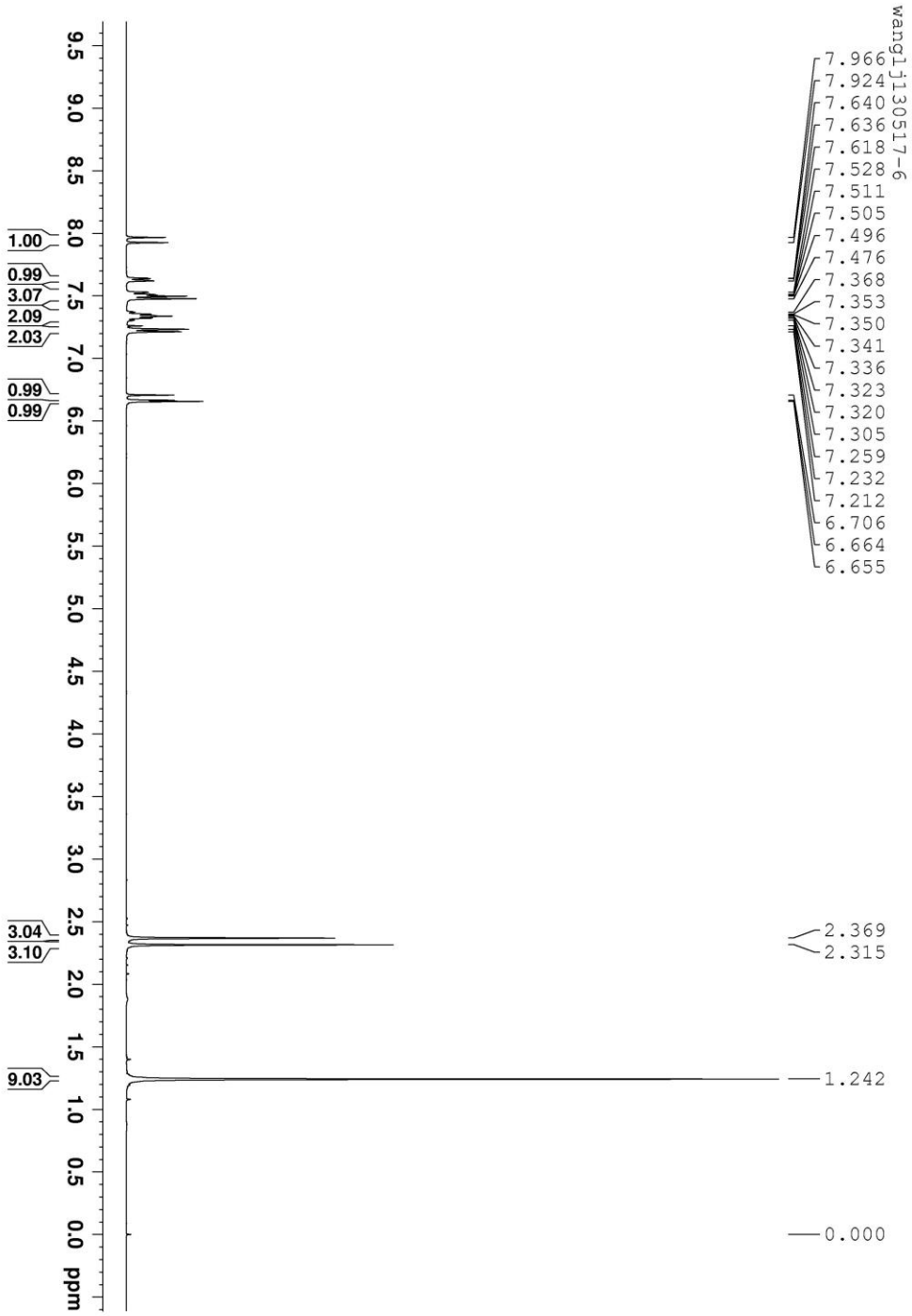
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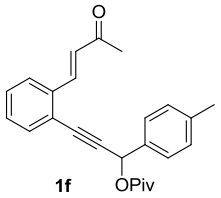
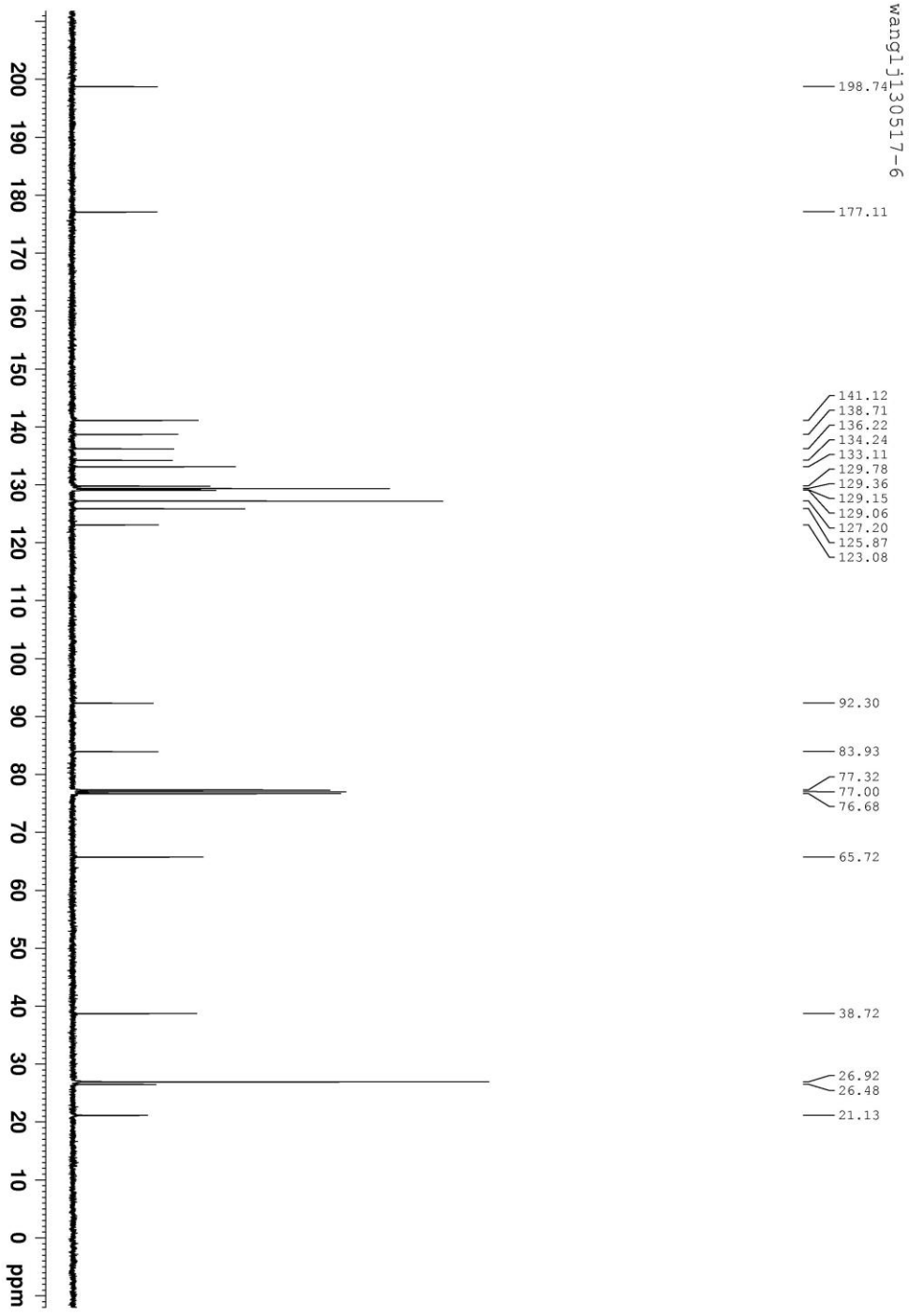
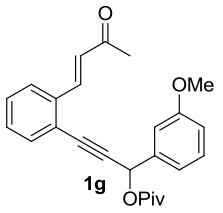
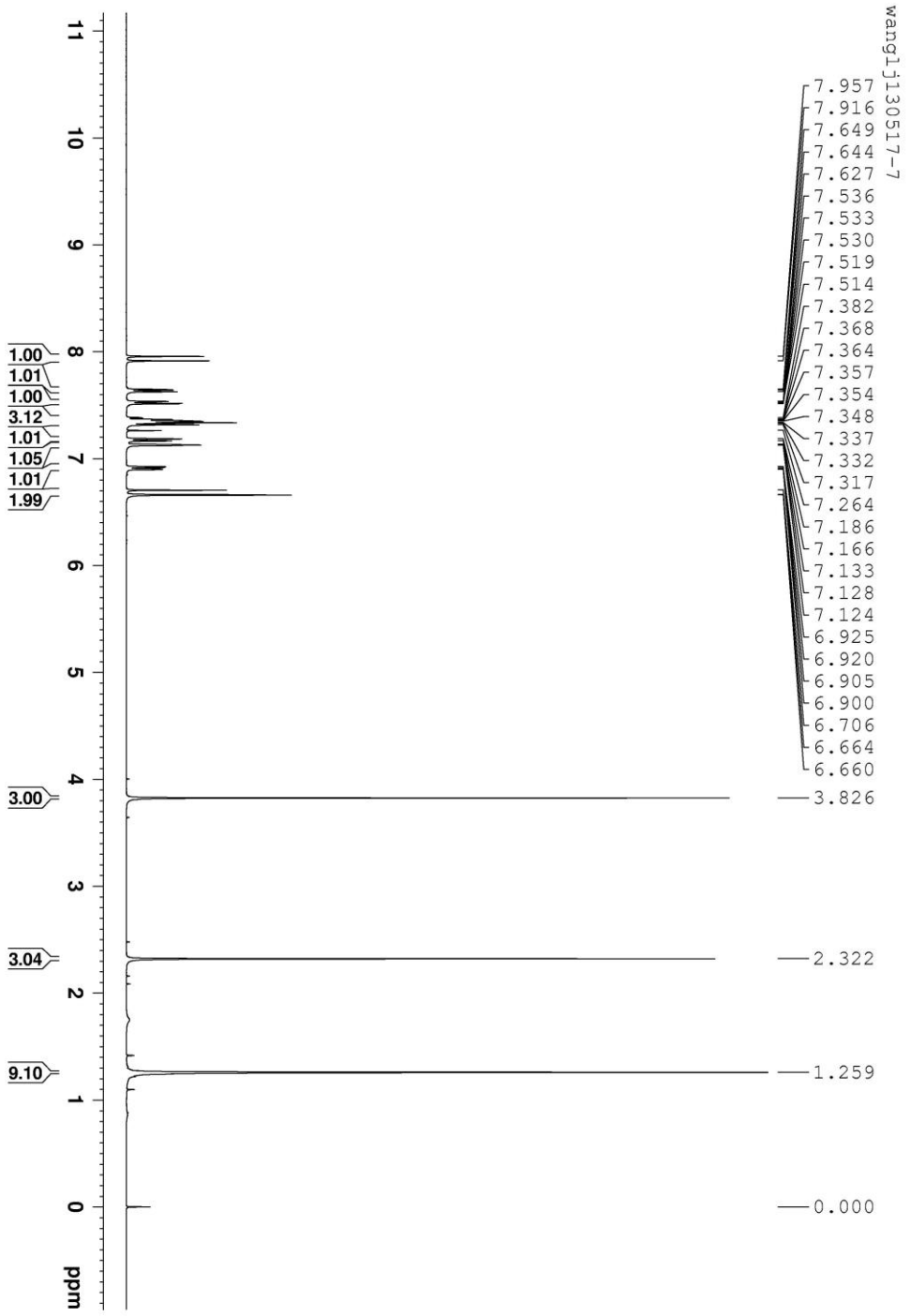
7.353
7.350
7.341
7.336
7.323
7.320
7.305
7.259
7.232
7.212
6.706
6.664
6.655
2.369
2.315
1.242
0.000
1.00
0.99
3.07
2.09
2.03
0.99
0.99
3.04
3.10
9.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


O
1f
OPiv


wangli130517-6
198.74
177.11
141.12
138.71
136.22
134.24
133.11
129.78
129.36
129.15
129.06
127.20
125.87
123.08
92.30
83.93
77.32
77.00
76.68
65.72
38.72
26.92
26.48
21.13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
OMe
1g
OPiv


wangji130517-7
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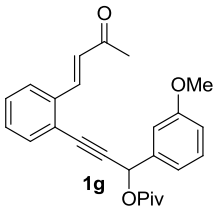
7.916
7.649
7.644
7.627
7.536
7.533
7.530
7.519
7.514
7.382
7.368
7.364
7.357
7.354
7.348
7.337
7.332
7.317
7.264
7.186
7.166
7.133
7.128
7.124
6.925
6.920
6.905
6.900
6.706
6.664
6.660
3.826
2.322
1.259
0.000
1.00
1.01
1.00
3.12
1.01
1.05
1.01
1.99
3.00
3.04
9.10
ppm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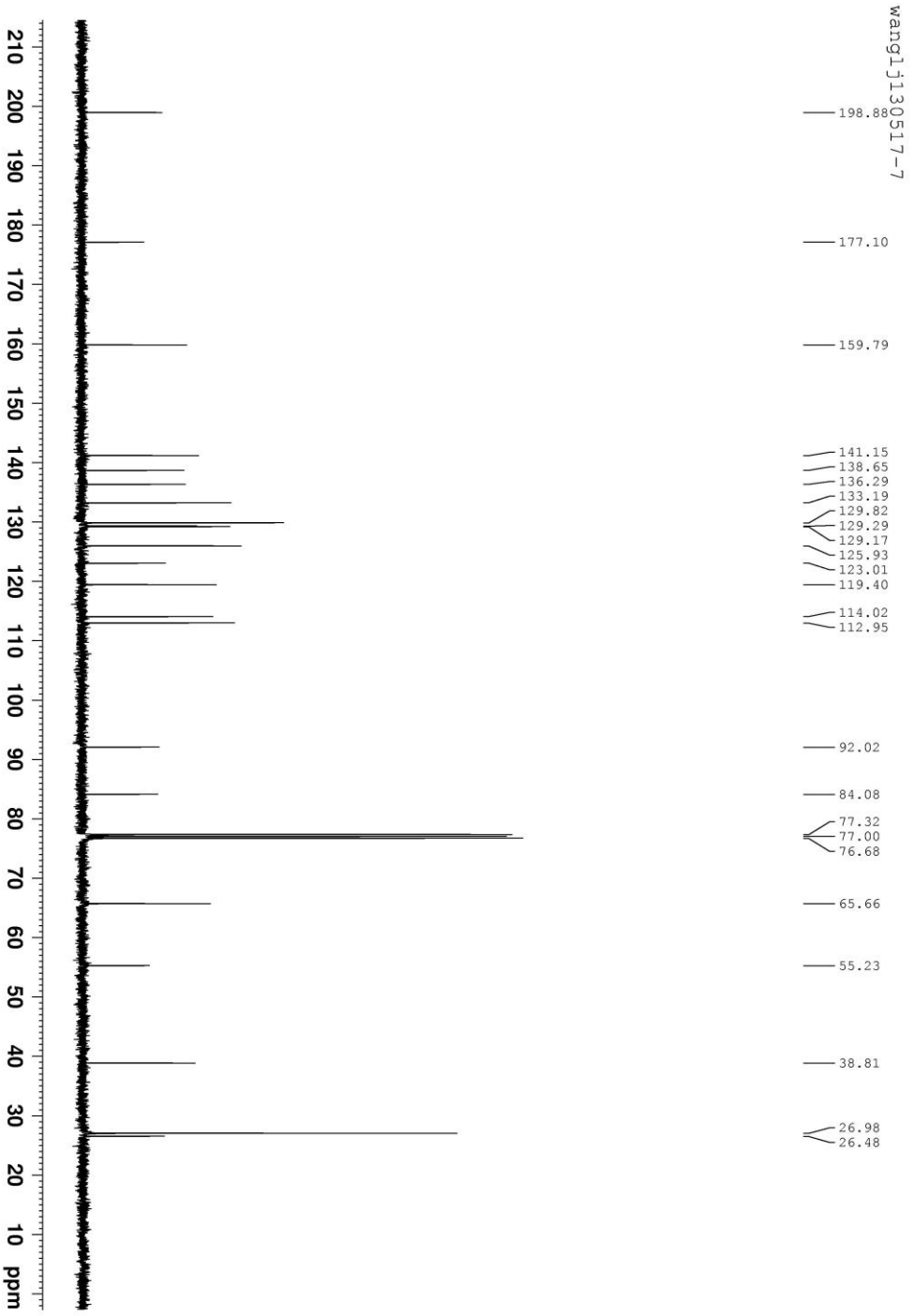
OMe
1g
OPiv


wangji130517-7
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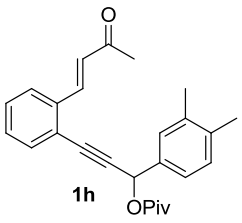
177.10
159.79
141.15
138.65
136.29
133.19
129.82
129.29
129.17
125.93
123.01
119.40
114.02
112.95
92.02
84.08
77.32
77.00
76.68
65.66
55.23
38.81
26.98
26.48
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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1h
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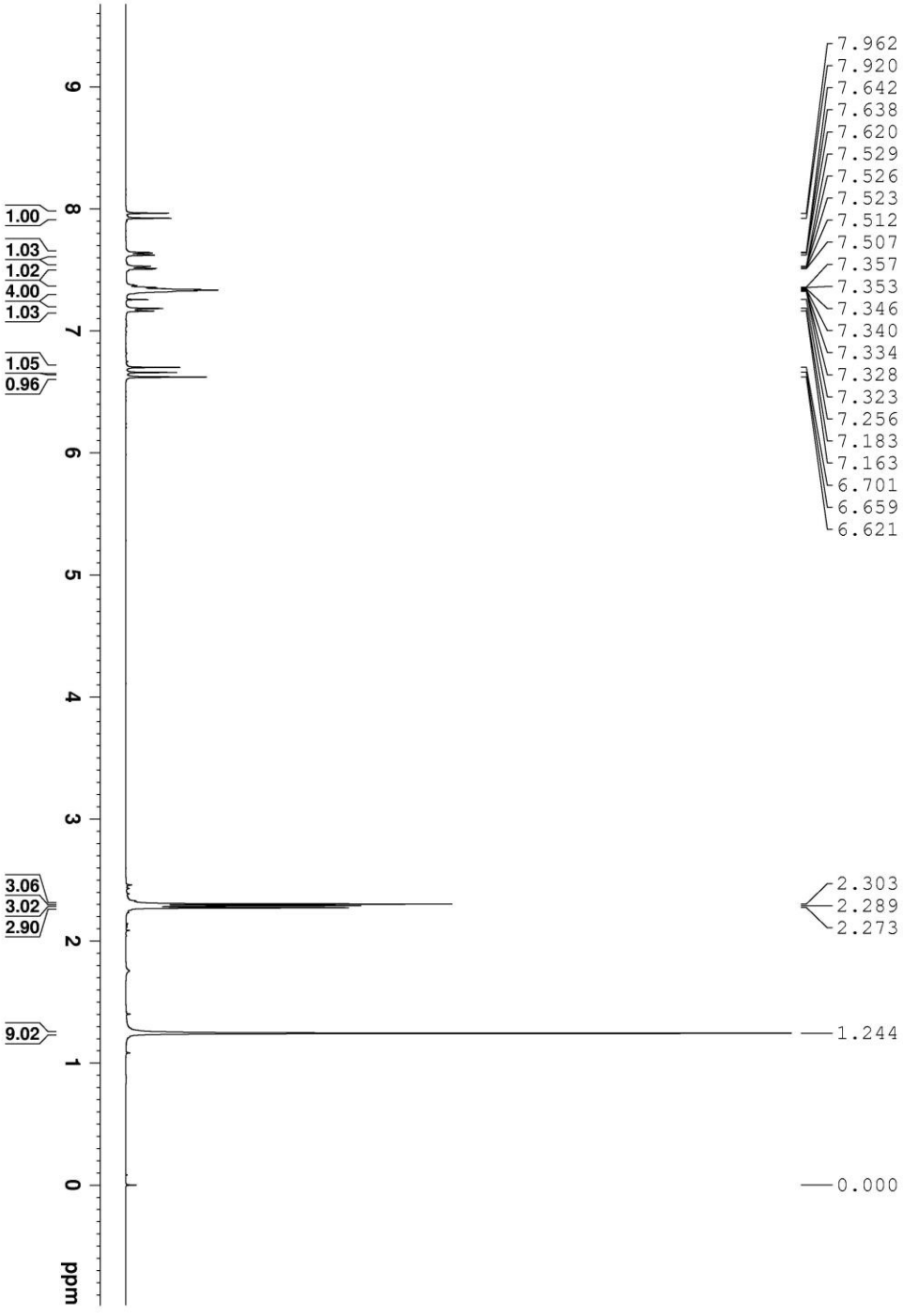
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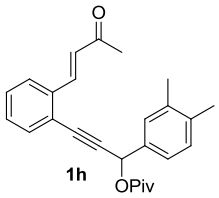
7.920
7.642
7.638
7.620
7.529
7.526
7.523
7.512
7.507
7.357
7.353
7.346
7.340
7.334
7.328
7.323
7.256
7.183
7.163
6.701
6.659
6.621
2.303
2.289
2.273
1.244
0.000
1.00
1.03
1.02
4.00
1.03
1.05
0.96
3.06
3.02
2.90
9.02
ppm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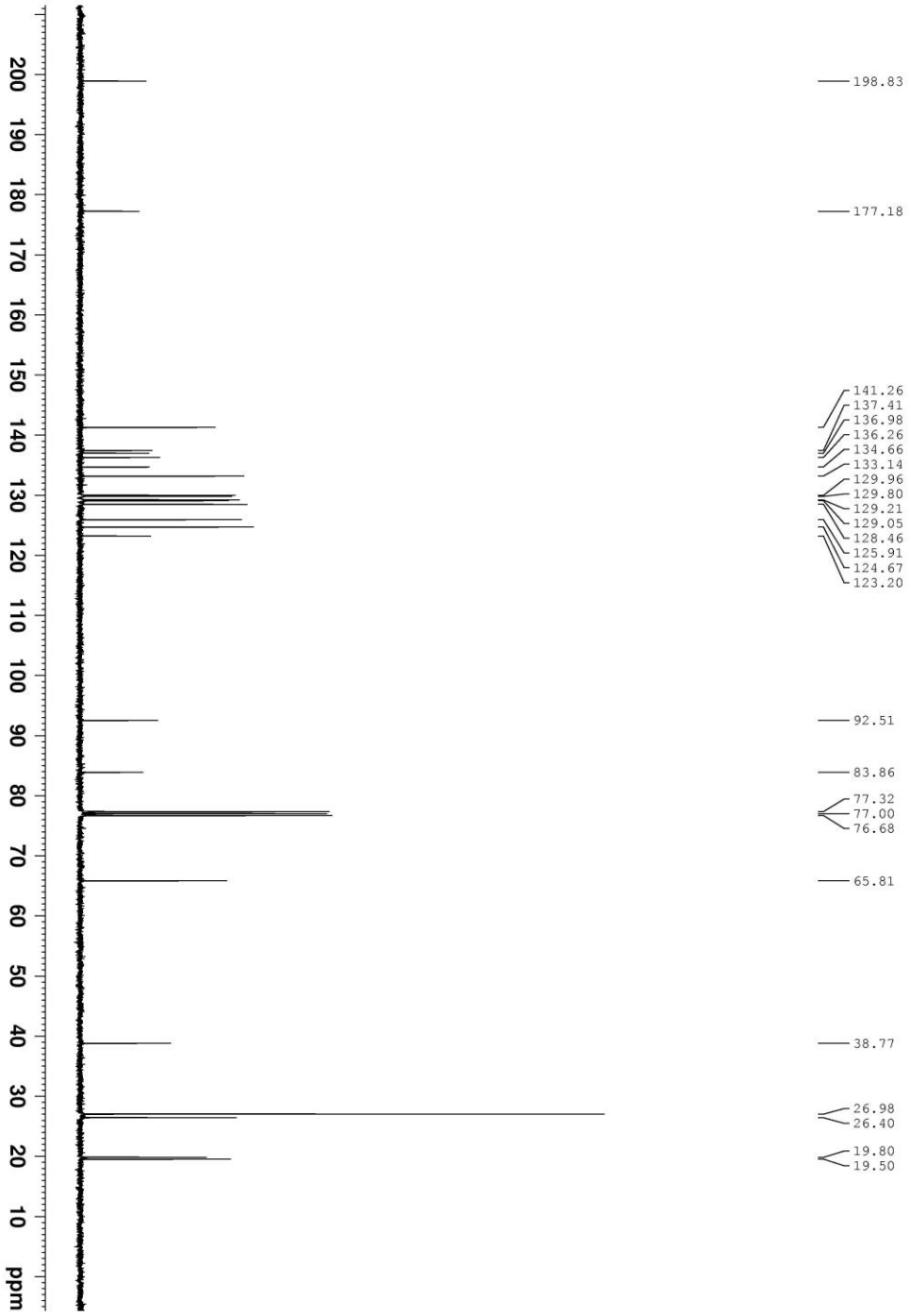
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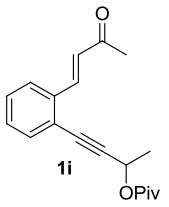
141.26
137.41
136.98
136.26
134.66
133.14
129.96
129.80
129.21
129.05
128.46
125.91
124.67
123.20
92.51
83.86
77.32
77.00
76.68
65.81
38.77
26.98
26.40
19.80
19.50
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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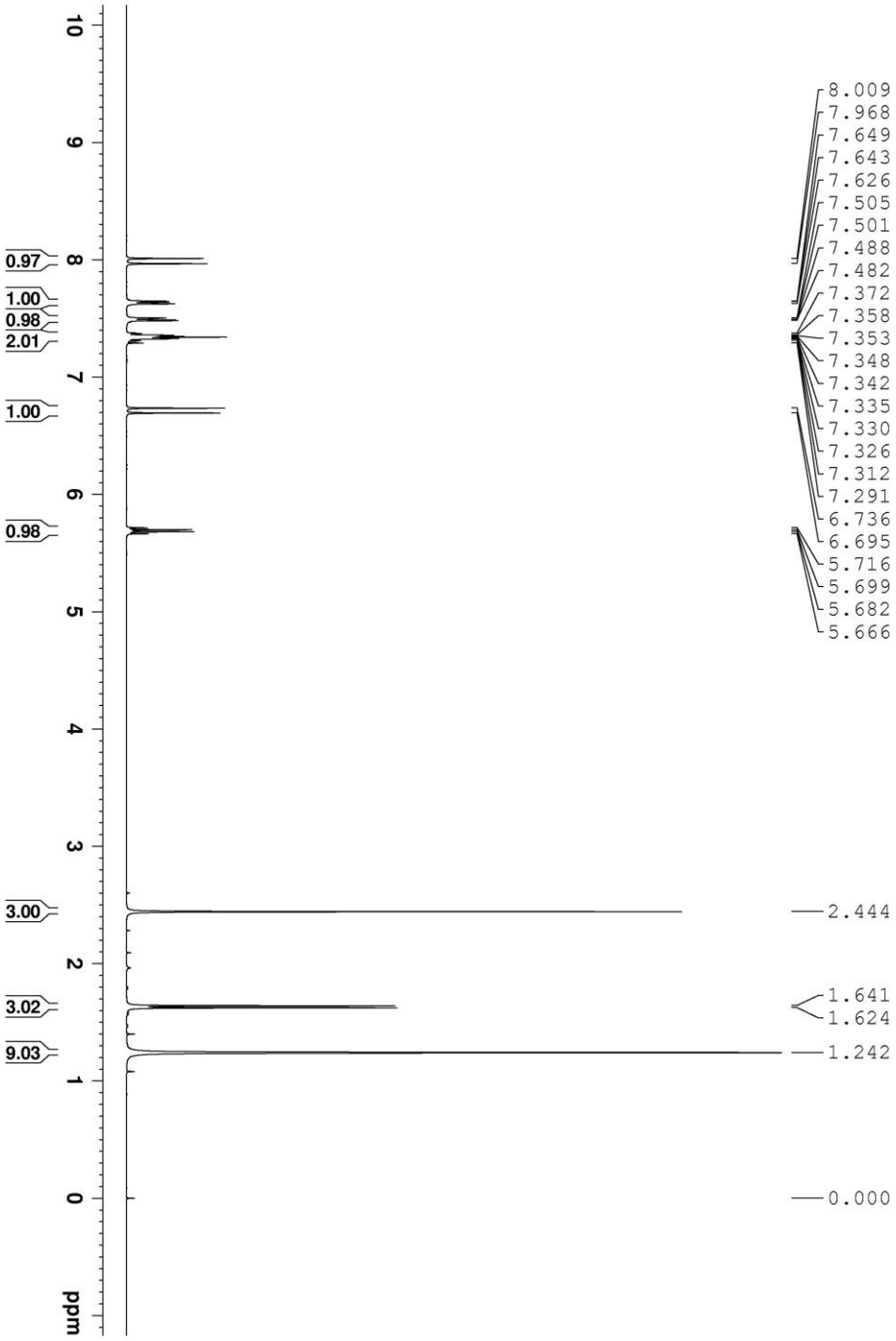
1i
OPiv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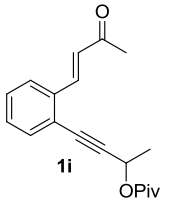
7.968
7.649
7.643
7.626
7.505
7.501
7.488
7.482
7.372
7.358
7.353
7.348
7.342
7.335
7.330
7.326
7.312
7.291
6.736
6.695
5.716
5.699
5.682
5.666
2.444
1.641
1.624
1.242
0.000
0.97
1.00
0.98
2.01
1.00
0.98
3.00
3.02
9.03
ppm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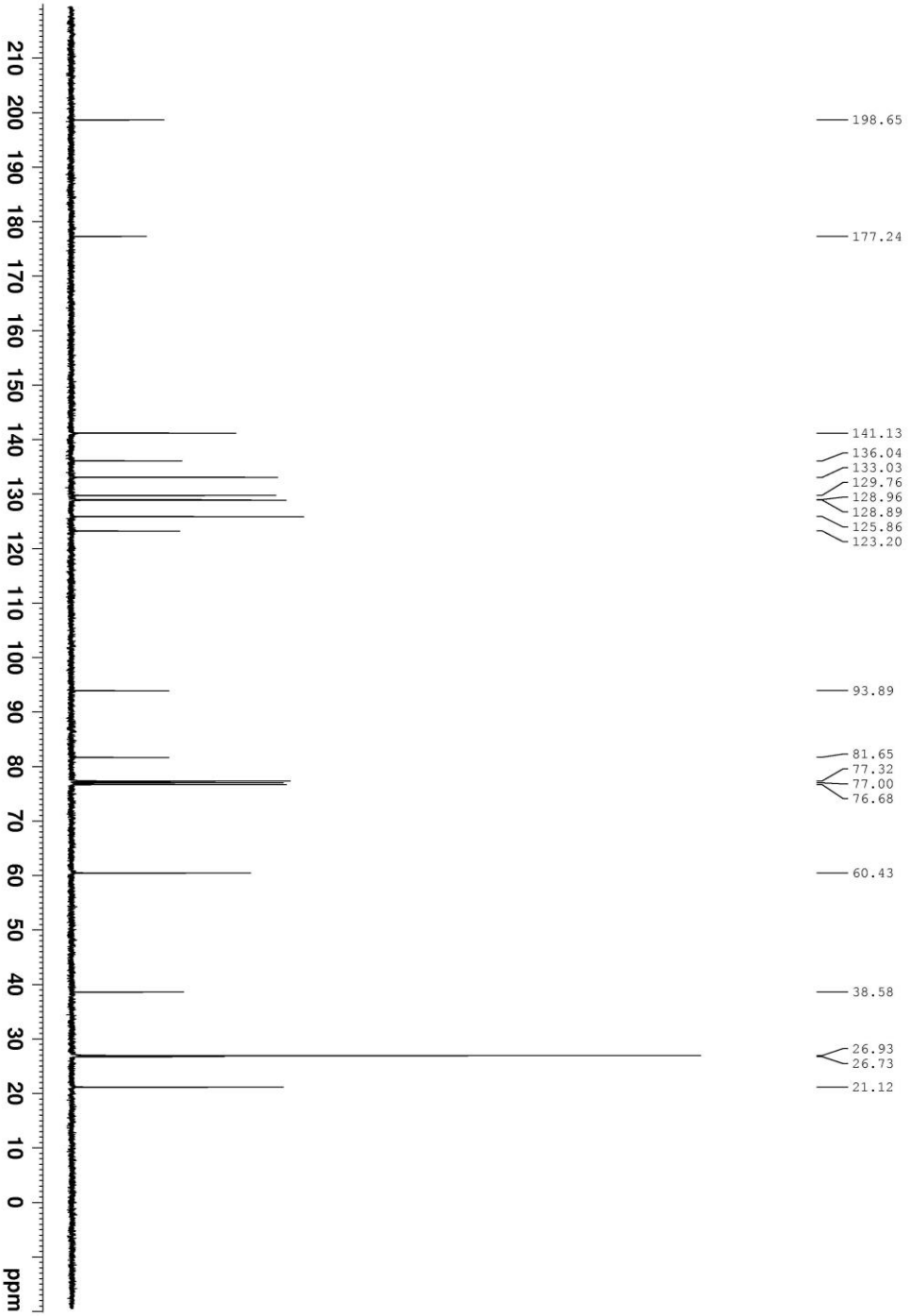
1i
OPiv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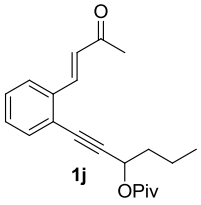
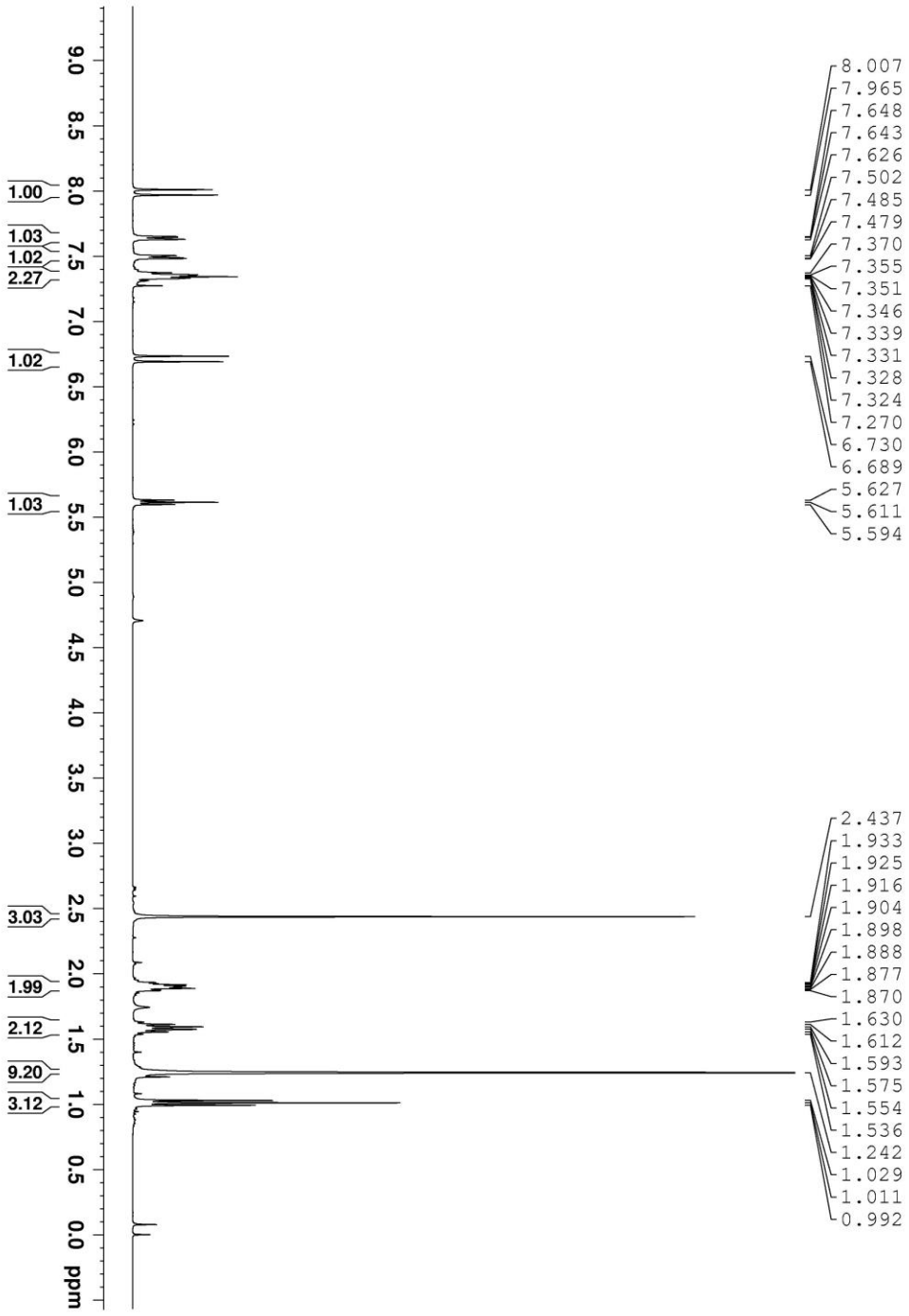
177.24
141.13
136.04
133.03
129.76
128.96
128.89
125.86
123.20
93.89
81.65
77.32
77.00
76.68
60.43
38.58
26.93
26.73
21.12
ppm


O
1j
OPiv


1.00
1.03
1.02
2.27
1.02
1.03
3.03
1.99
2.12
9.20
3.12
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
ppm
8.007
7.965
7.648
7.643
7.626
7.502
7.485
7.479
7.370
7.355
7.351
7.346
7.339
7.331
7.328
7.324
7.270
6.730
6.689
5.627
5.611
5.594
2.437
1.933
1.925
1.916
1.904
1.898
1.888
1.877
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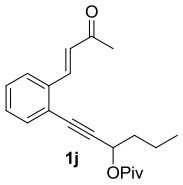
1.630
1.612
1.593
1.575
1.554
1.536
1.242
1.029
1.011
0.992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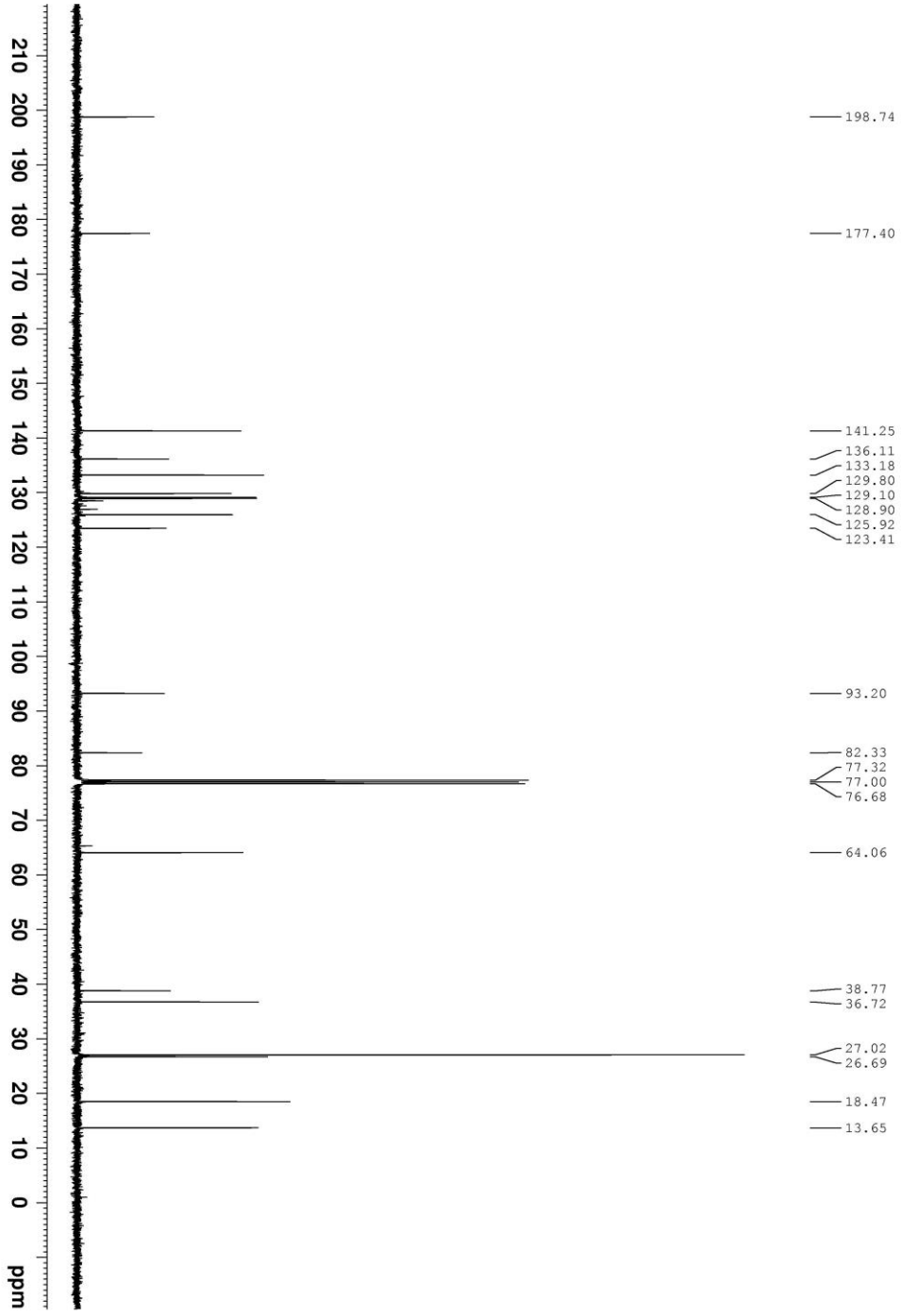
1j
OPiv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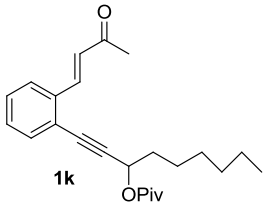
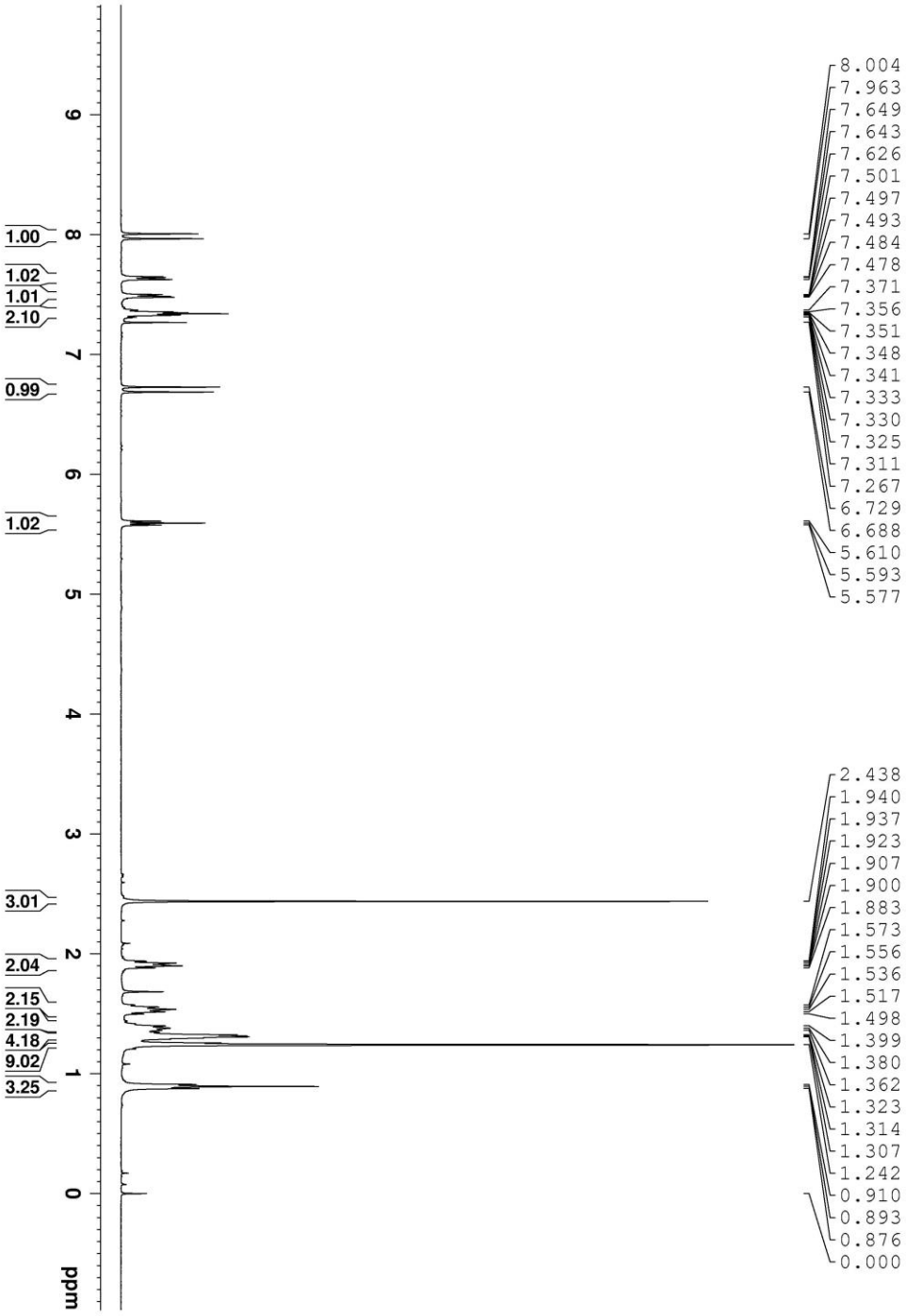
177.40
141.25
136.11
133.18
129.80
129.10
128.90
125.92
123.41
93.20
82.33
77.32
77.00
76.68
64.06
38.77
36.72
27.02
26.69
18.47
13.65
ppm


O
1k
OPiv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1.02
1.01
2.10
0.99
1.02
3.01
2.04
2.15
2.19
4.18
9.02
3.25
ppm
8.004
7.963
7.649
7.643
7.626
7.501
7.497
7.493
7.484
7.478
7.371
7.356
7.351
7.348
7.341
7.333
7.330
7.325
7.311
7.267
6.729
6.688
5.610
5.593
5.577
2.438
1.940
1.937
1.923
1.907
1.900
1.883
1.573
1.556
1.536
1.517
1.498
1.399
1.380
1.362
1.323
1.314
1.307
1.242
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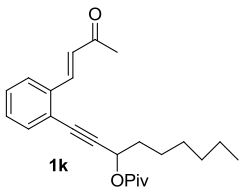
0.893
0.876
0.000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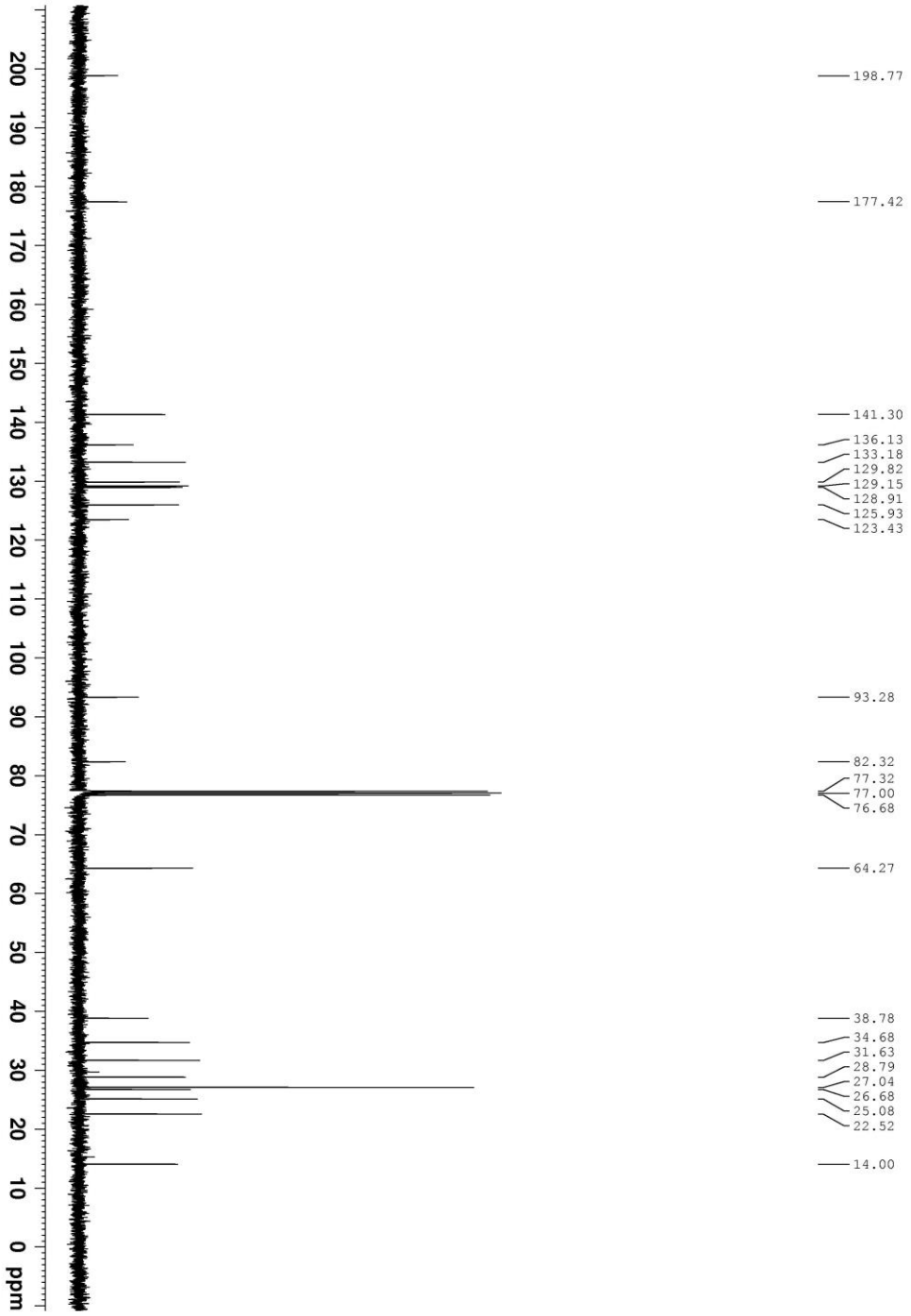
1k
OPiv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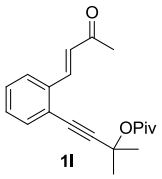
136.13
133.18
129.82
129.15
128.91
125.93
123.43
93.28
82.32
77.32
77.00
76.68
64.27
38.78
34.68
31.63
28.79
27.04
26.68
25.08
22.52
14.00
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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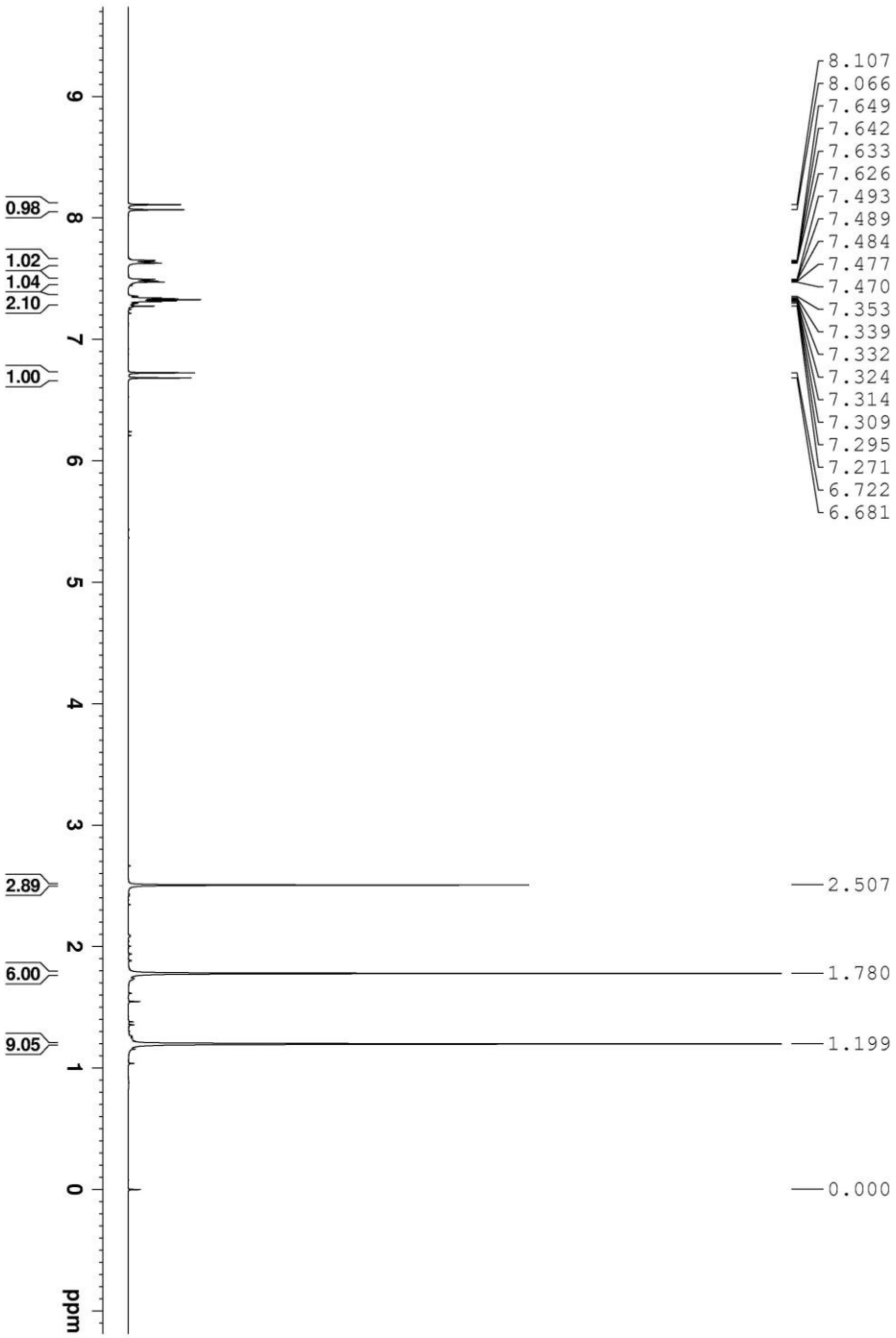
OPiv

1l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7.626
7.493
7.489
7.484
7.477
7.470
7.353
7.339
7.332
7.324
7.314
7.309
7.295
7.271
6.722
6.681
0.98
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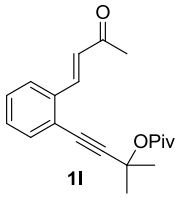
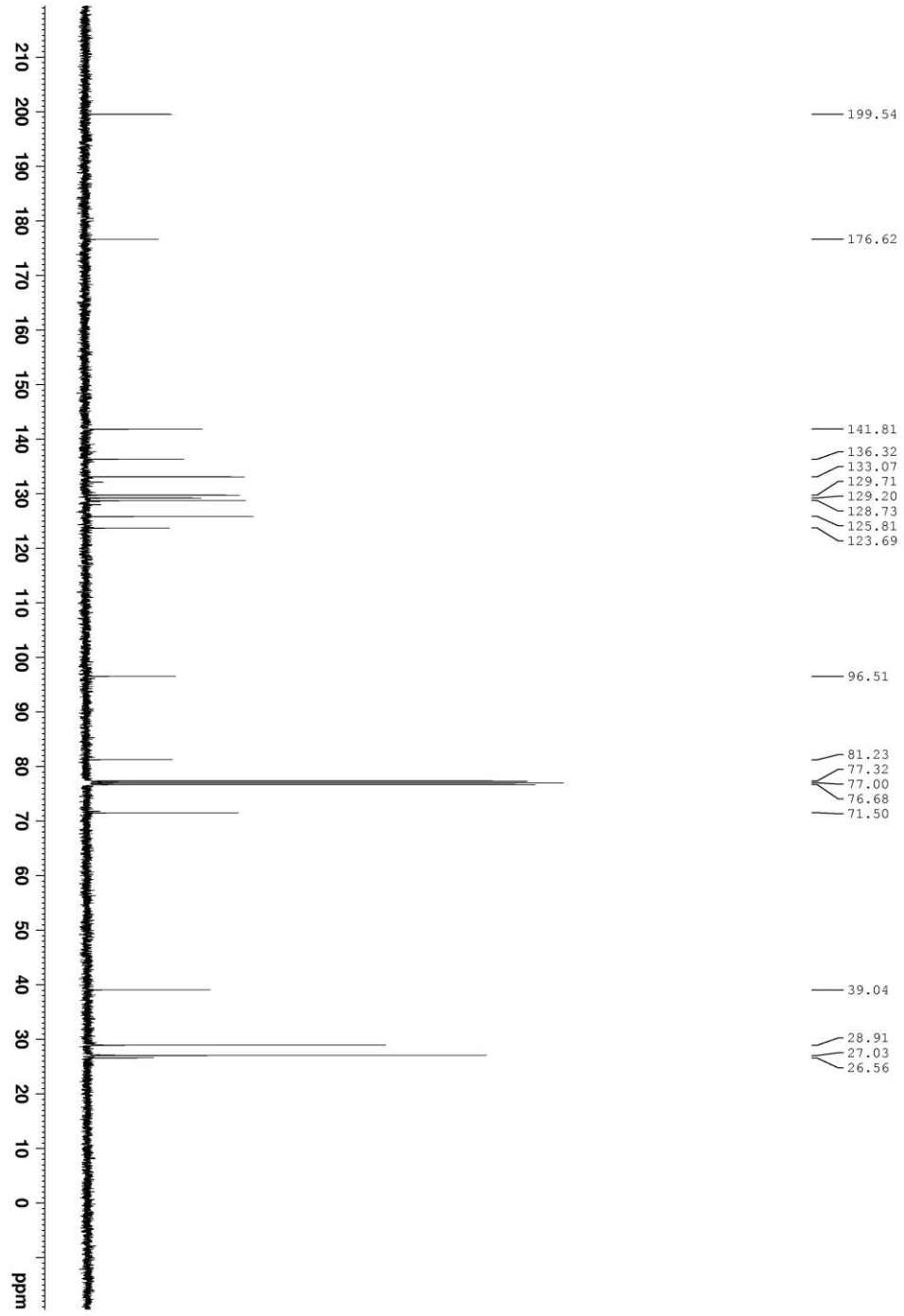
1.04
2.10
1.00
2.89
6.00
9.05
2.507
1.780
1.199
0.000
ppm


O
OPiv

1l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136.32
133.07
129.71
129.20
128.73
125.81
123.69
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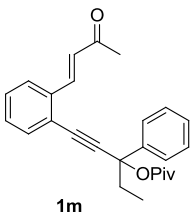
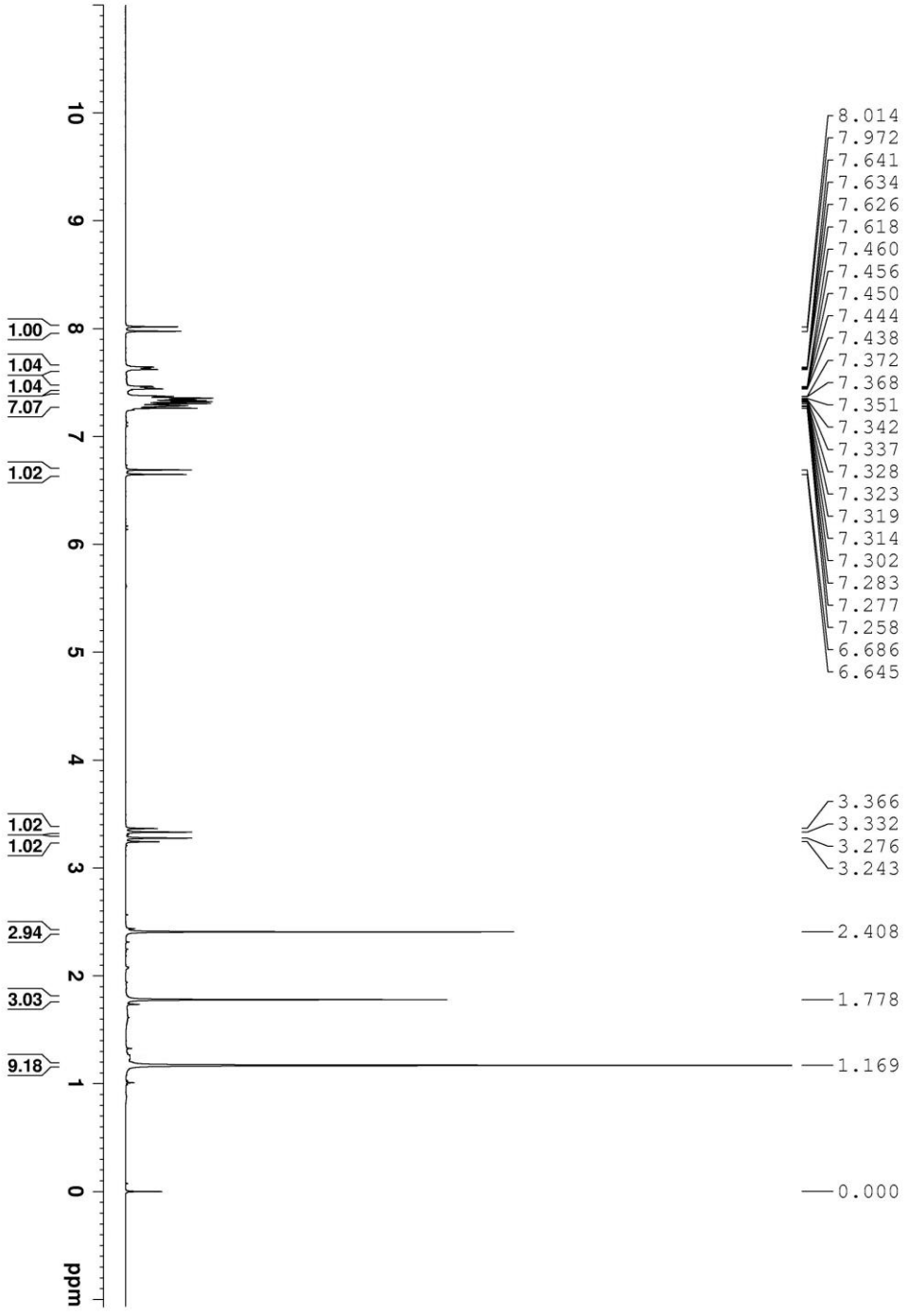
81.23
77.32
77.00
76.68
71.50
39.04
28.91
27.03
26.56
ppm


O
OPiv

1m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7.444
7.438
7.372
7.368
7.351
7.342
7.337
7.328
7.323
7.319
7.314
7.302
7.283
7.277
7.258
6.686
6.645
3.366
3.332
3.276
3.243
2.408
1.778
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1.04
1.04
7.07
1.02
1.02
1.02
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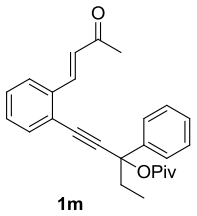
3.03
9.18
ppm


O
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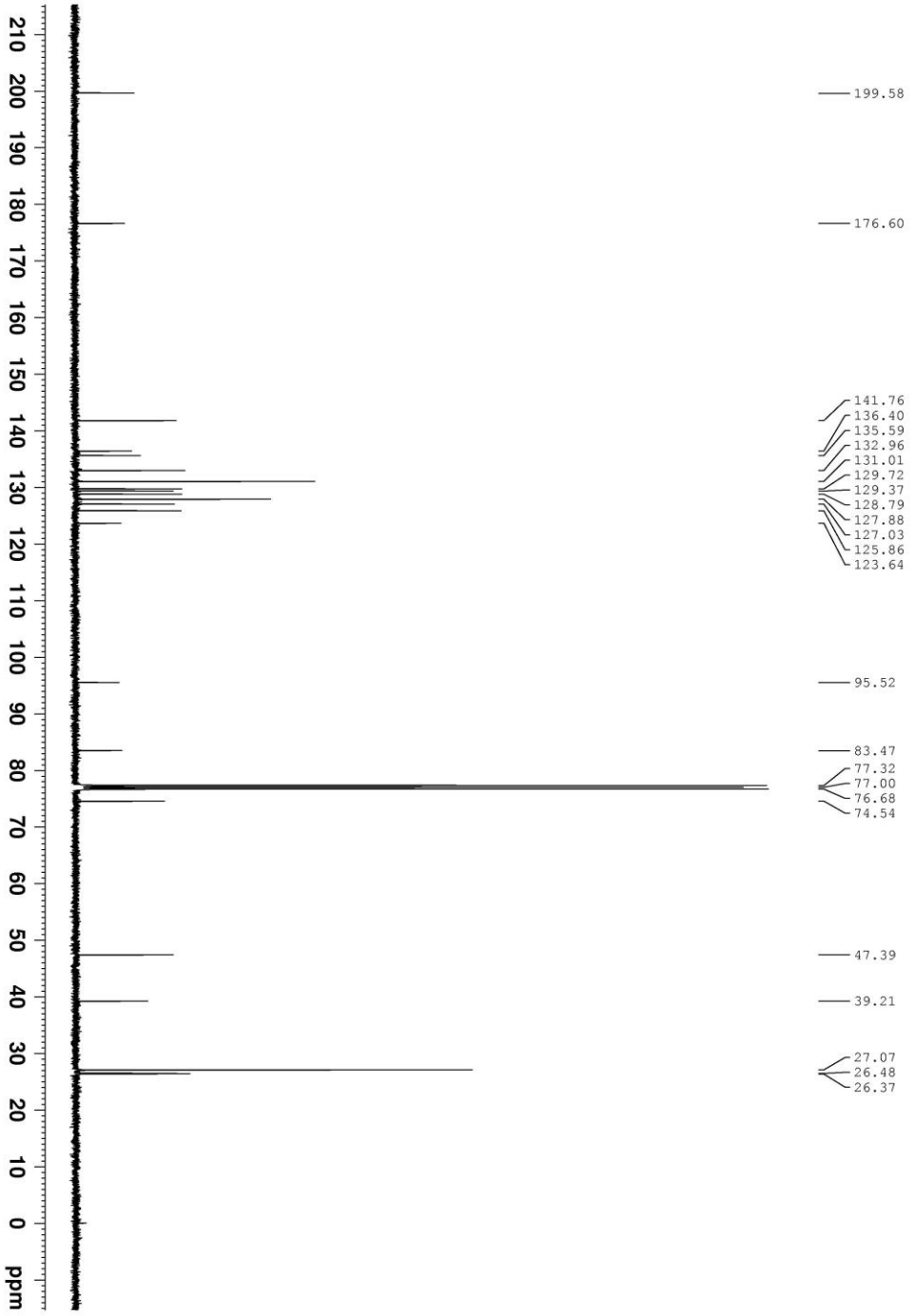
1m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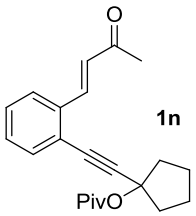
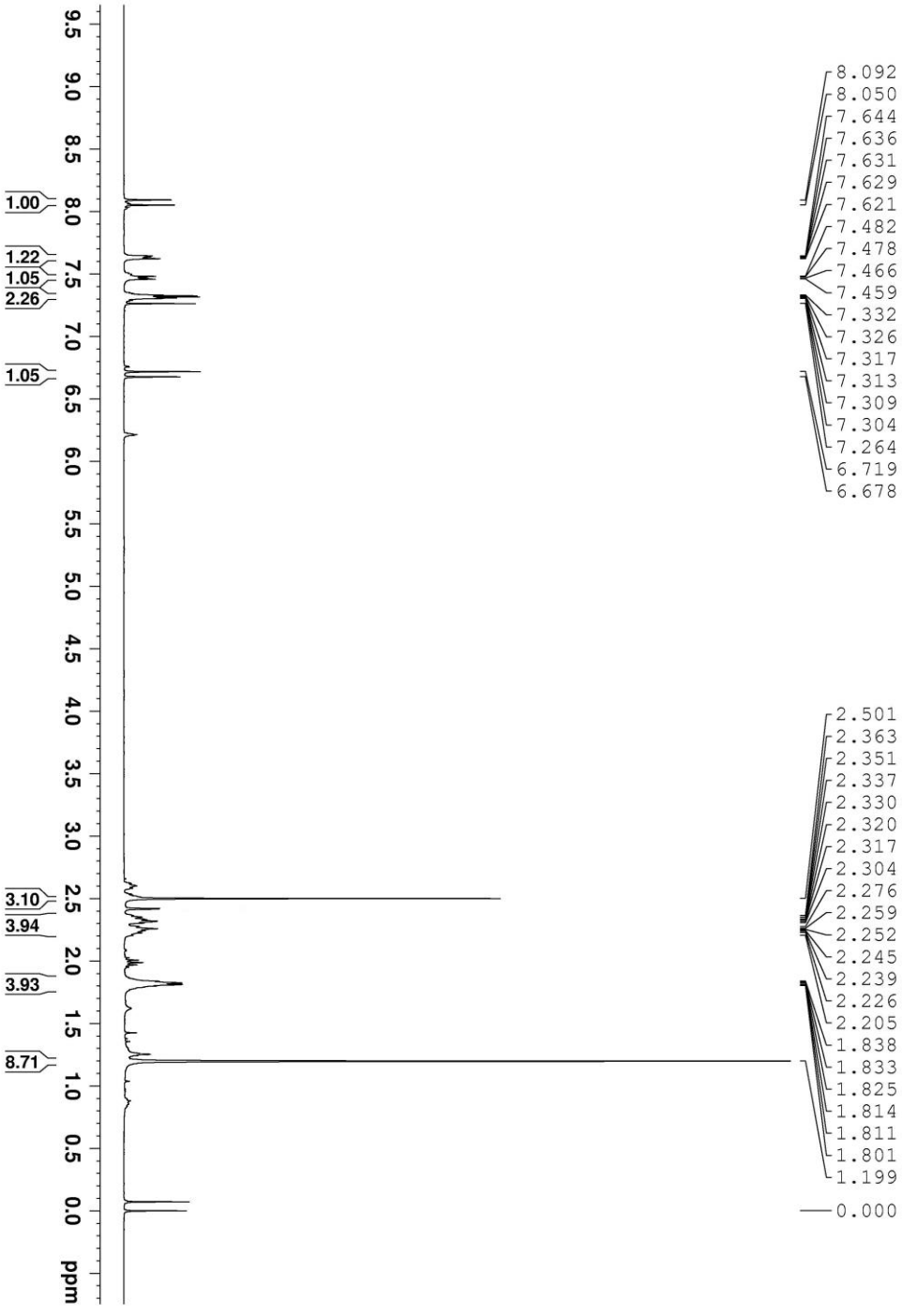
131.01
129.72
129.37
128.79
127.88
127.03
125.86
123.64
95.52
83.47
77.32
77.00
76.68
74.54
47.39
39.21
27.07
26.48
26.37
ppm


O
1n
PivO


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 ppm
1.00
1.22
1.05
2.26
1.05
3.10
3.94
3.93
8.71
8.092
8.050
7.644
7.636
7.631
7.629
7.621
7.482
7.478
7.466
7.459
7.332
7.326
7.317
7.313
7.309
7.304
7.264
6.719
6.678
2.501
2.363
2.351
2.337
2.330
2.320
2.317
2.304
2.276
2.259
2.252
2.245
2.239
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2.205
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1.833
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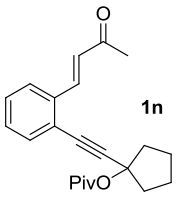
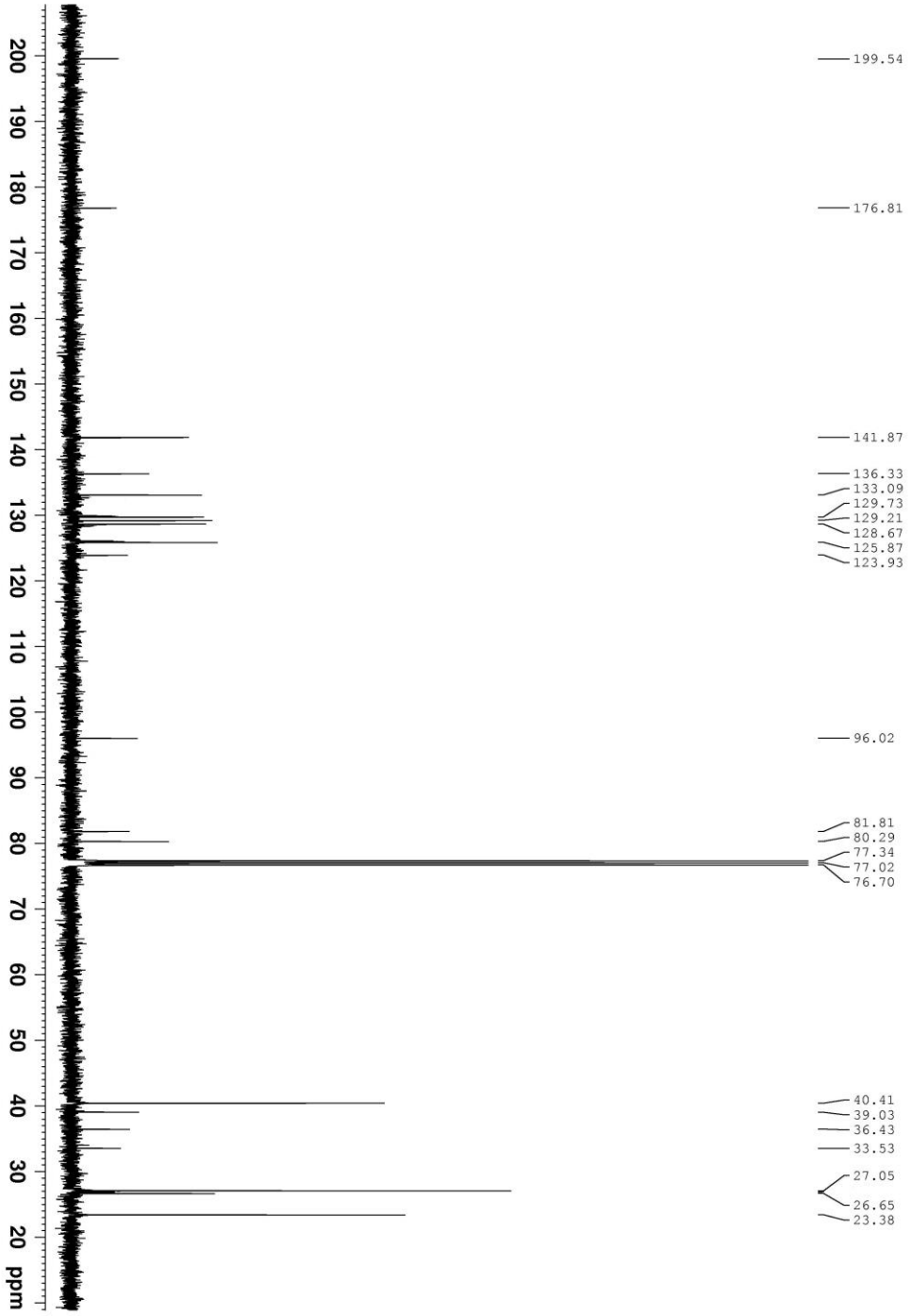
1.811
1.801
1.199
0.000


O
1n
PivO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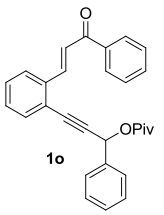
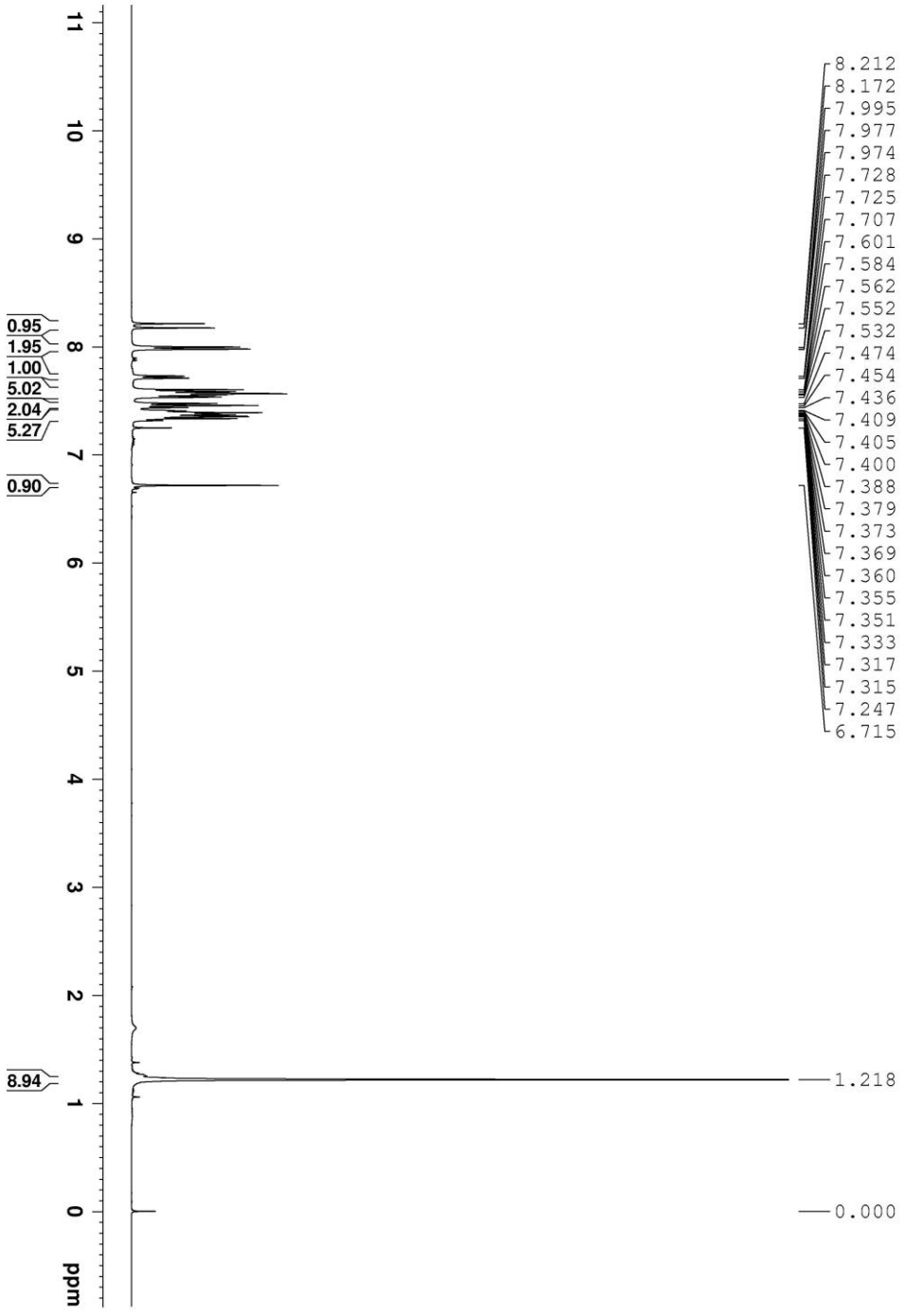
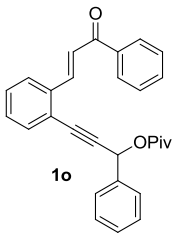
176.81
141.87
136.33
133.09
129.73
129.21
128.67
125.87
123.93
96.02
81.81
80.29
77.34
77.02
76.70
40.41
39.03
36.43
33.53
27.05
26.65
23.38
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

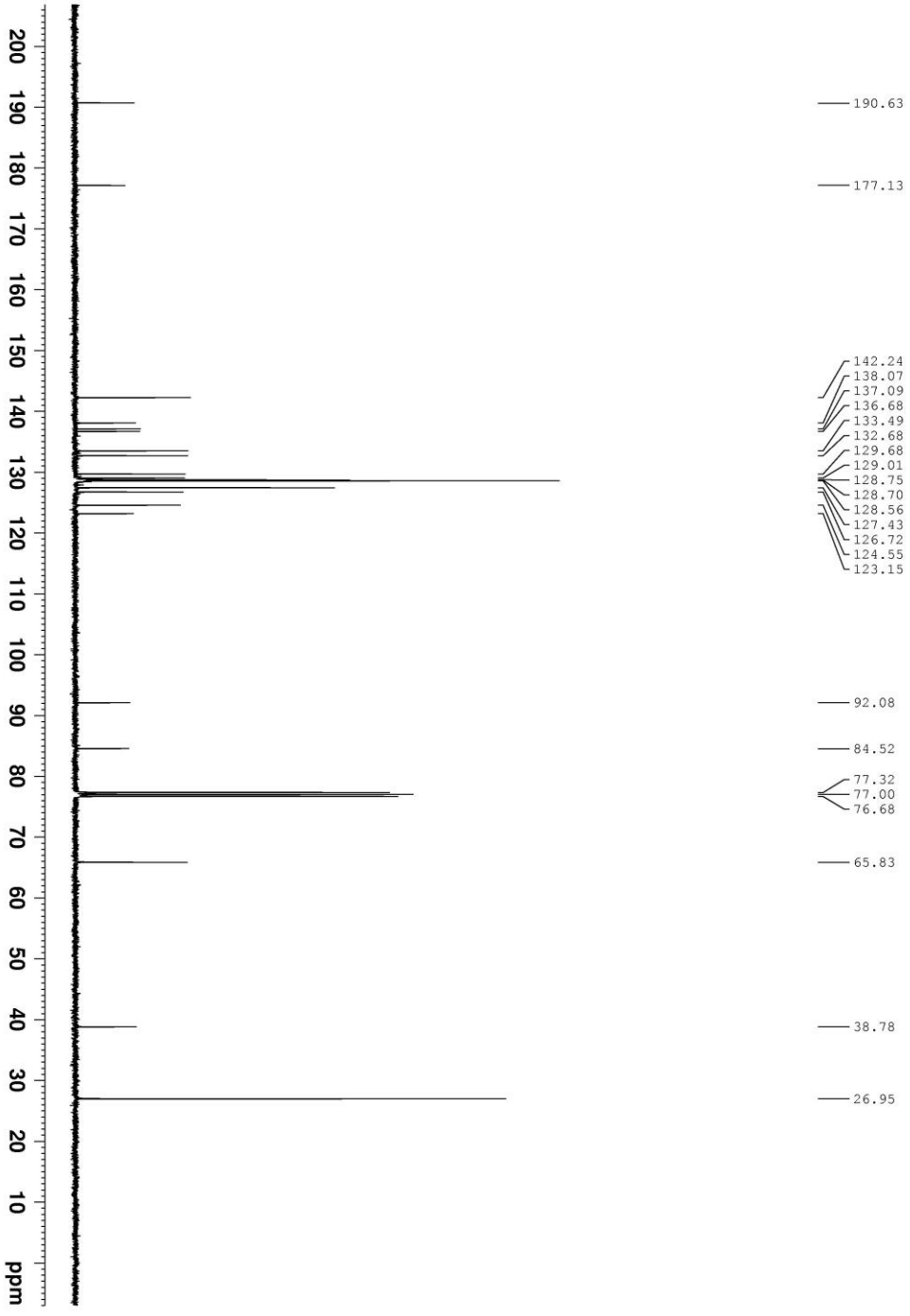

O
OPiv

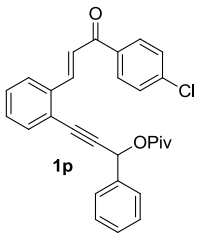
1o

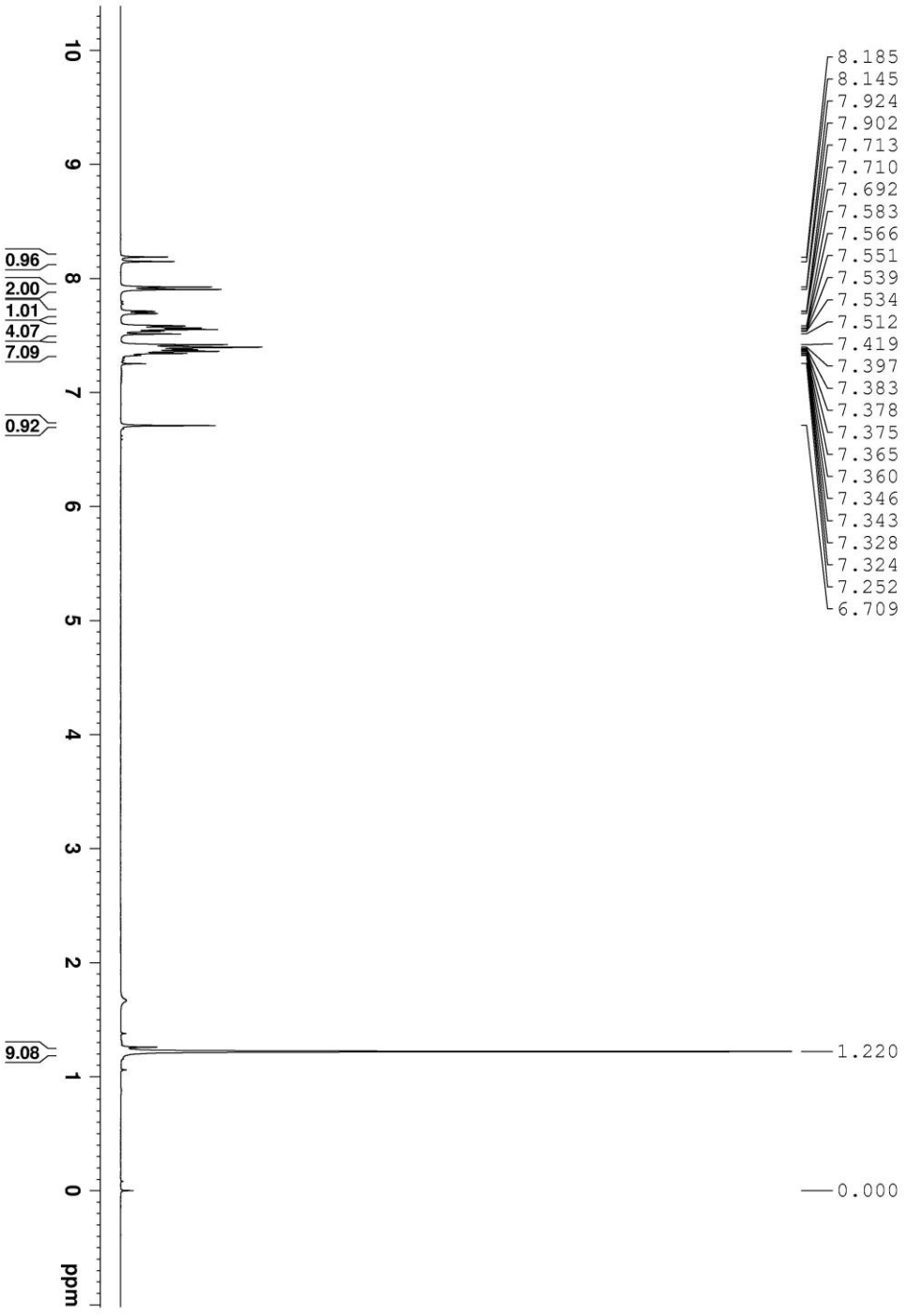

11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.95
1.95
1.00
5.02
2.04
5.27
0.90
8.94
8.212
8.172
7.995
7.977
7.974
7.728
7.725
7.707
7.601
7.584
7.562
7.552
7.532
7.474
7.454
7.436
7.409
7.405
7.400
7.388
7.379
7.373
7.369
7.360
7.355
7.351
7.333
7.317
7.315
7.247
6.715
1.218
0.000

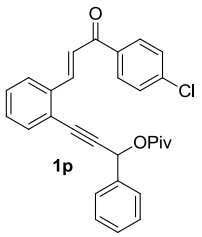

O
OPiv

1o


190.63
177.13
142.24
138.07
137.09
136.68
133.49
132.68
129.68
129.01
128.75
128.70
128.56
127.43
126.72
124.55
123.15
92.08
84.52
77.32
77.00
76.68
65.83
38.78
26.95
ppm


O
Cl
OPiv
1p


0.96
2.00
1.01
4.07
7.09
0.92
9.08
8.185
8.145
7.924
7.902
7.713
7.710
7.692
7.583
7.566
7.551
7.539
7.534
7.512
7.419
7.397
7.383
7.378
7.375
7.365
7.360
7.346
7.343
7.328
7.324
7.252
6.709
1.220
0.000
ppm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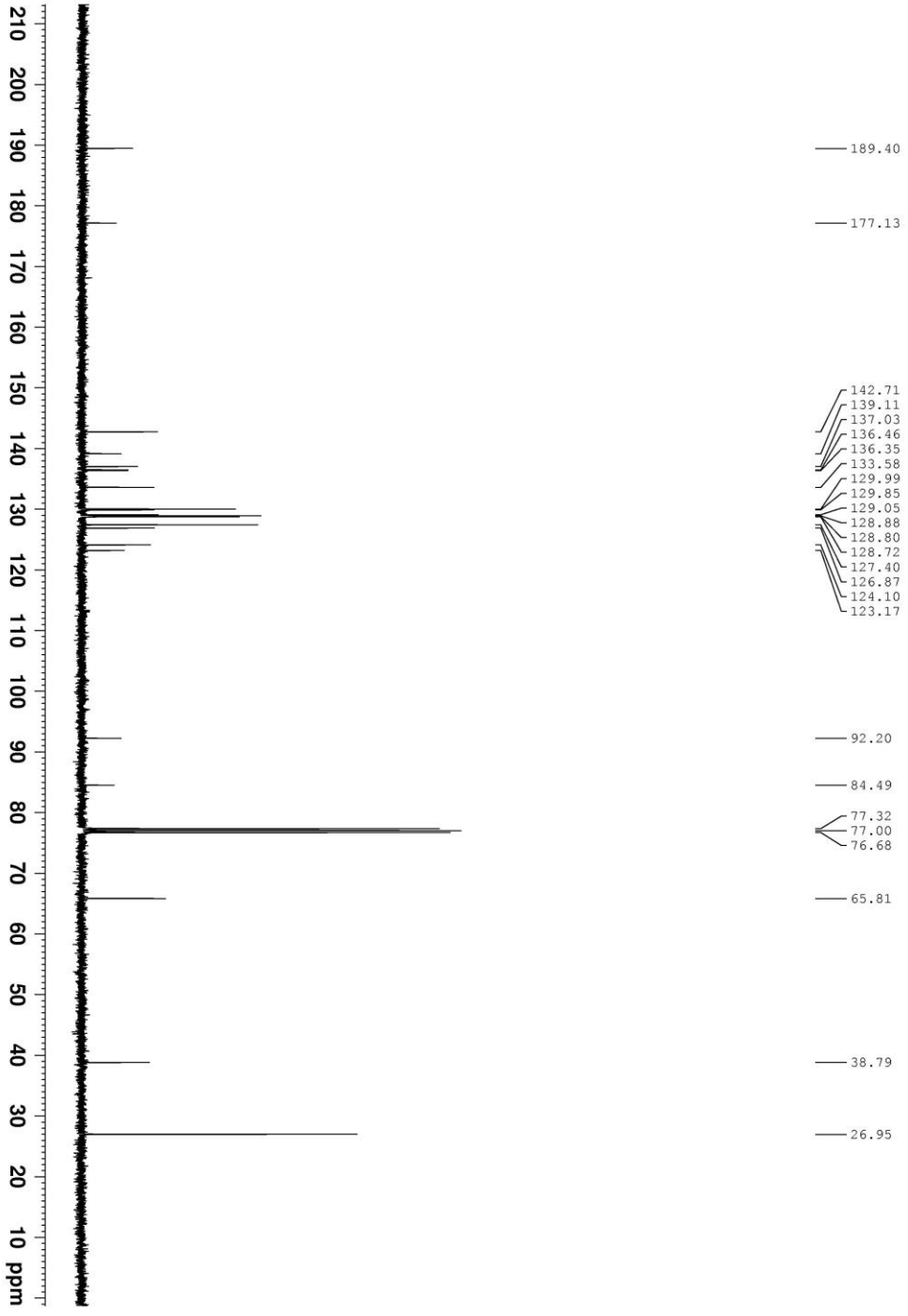
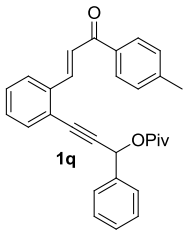
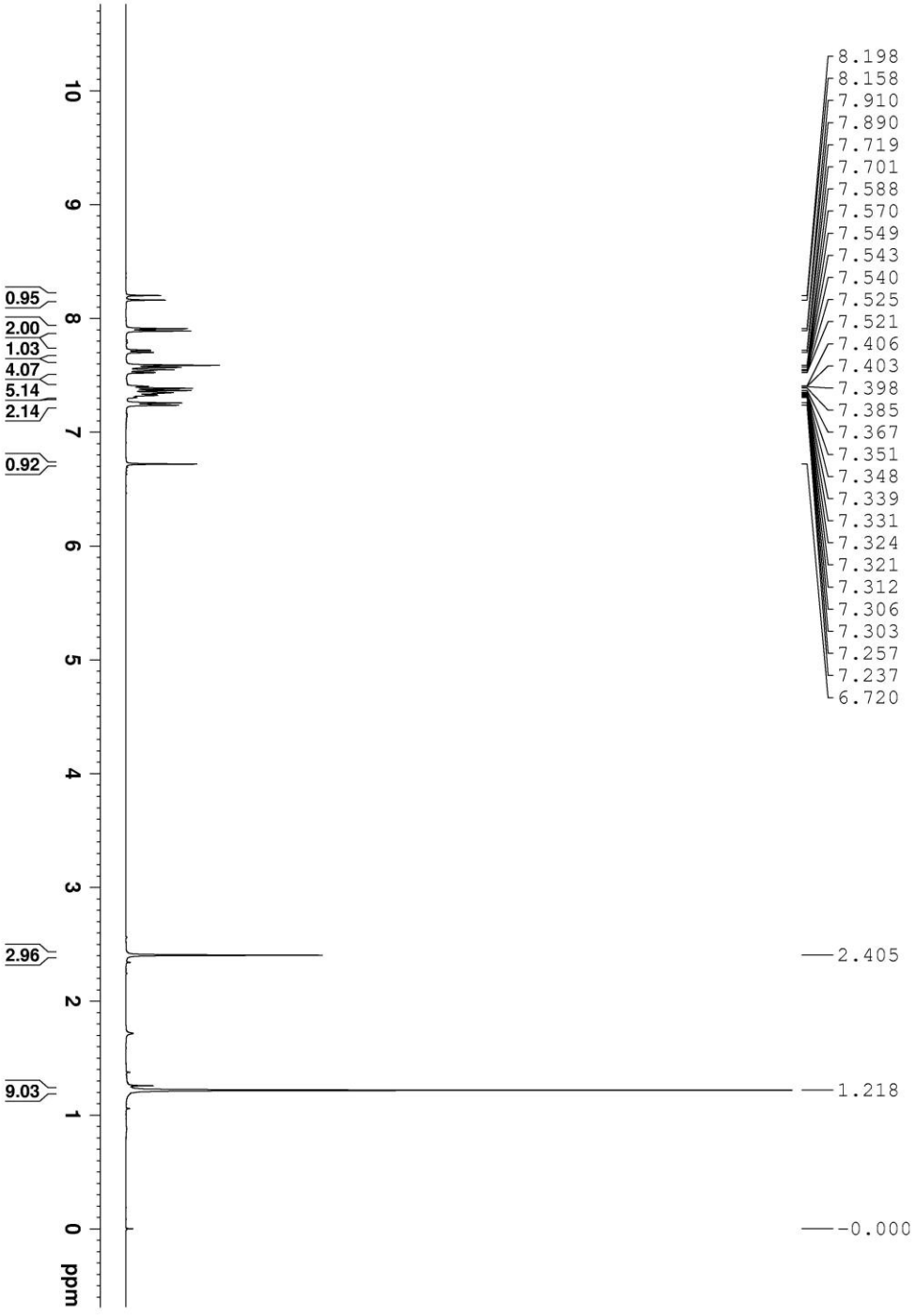
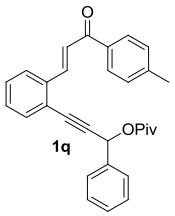
Cl
OPiv

1p


189.40
177.13
142.71
139.11
137.03
136.46
136.35
133.58
129.99
129.85
129.05
128.88
128.80
128.72
127.40
126.87
124.10
123.17
92.20
84.49
77.32
77.00
76.68
65.81
38.79
26.95
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


O
OPiv
1q


0.95
2.00
1.03
4.07
5.14
2.14
0.92
2.96
9.03
10
9
8
7
6
5
4
3
2
1
0
ppm
8.198
8.158
7.910
7.890
7.719
7.701
7.588
7.570
7.549
7.543
7.540
7.525
7.521
7.406
7.403
7.398
7.385
7.367
7.351
7.348
7.339
7.331
7.324
7.321
7.312
7.306
7.303
7.257
7.237
6.720
2.405
1.218
-0.000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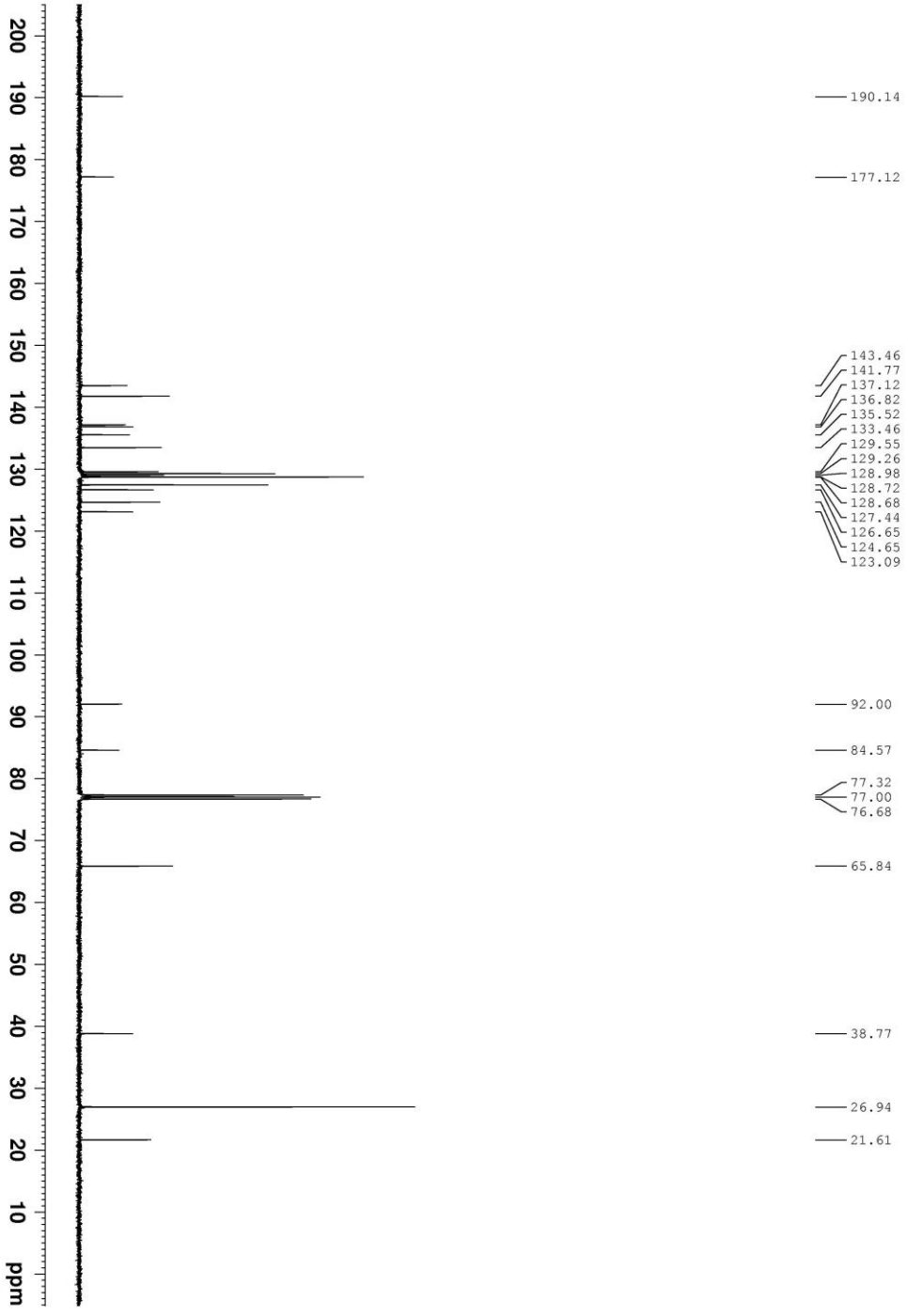
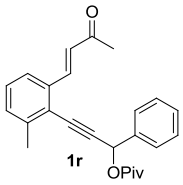
OPiv

1q


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
190.14
177.12
143.46
141.77
137.12
136.82
135.52
133.46
129.55
129.26
128.98
128.72
128.68
127.44
126.65
124.65
123.09
92.00
84.57
77.32
77.00
76.68
65.84
38.77
26.94
21.61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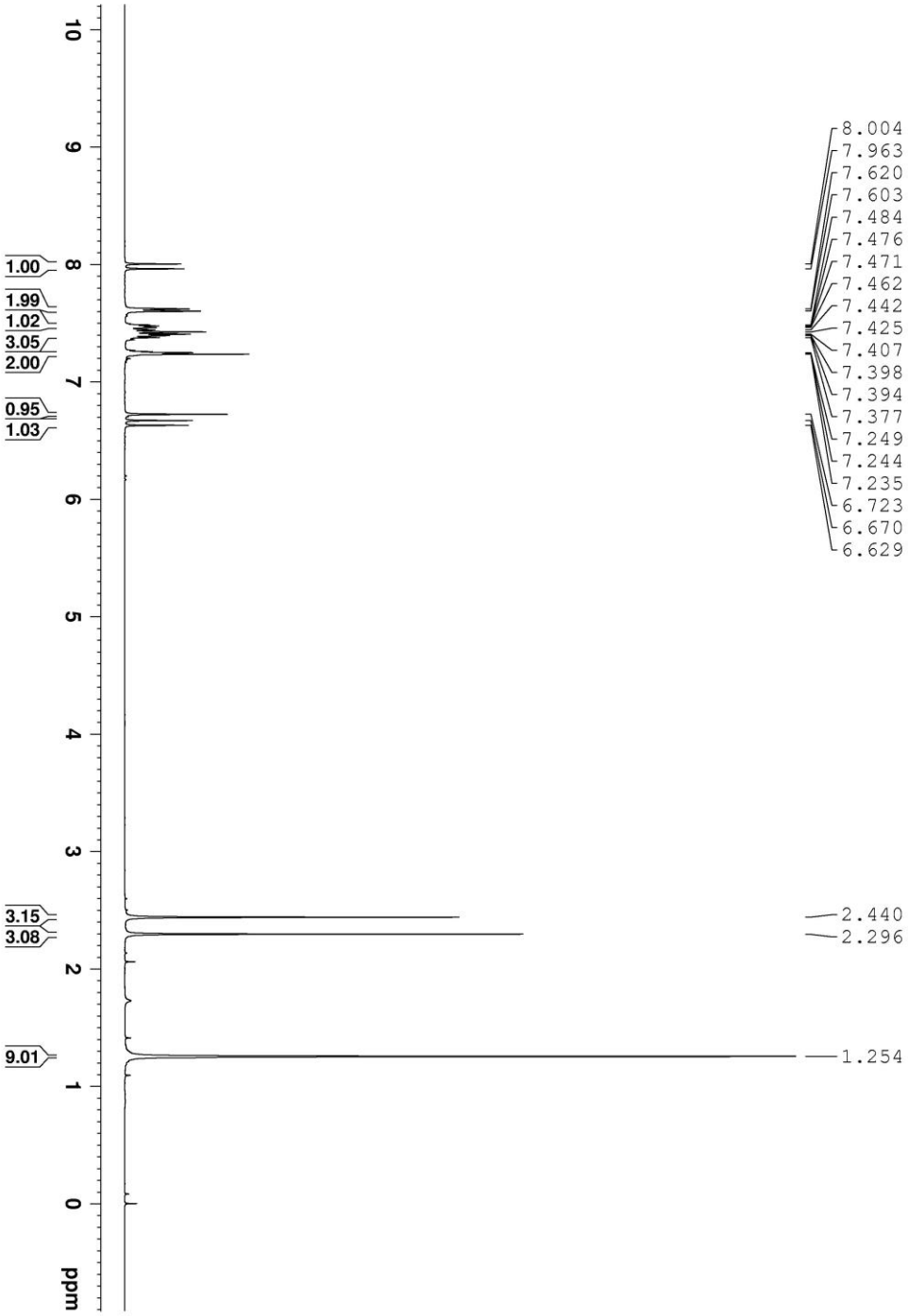
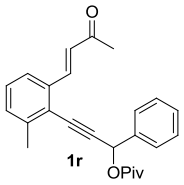
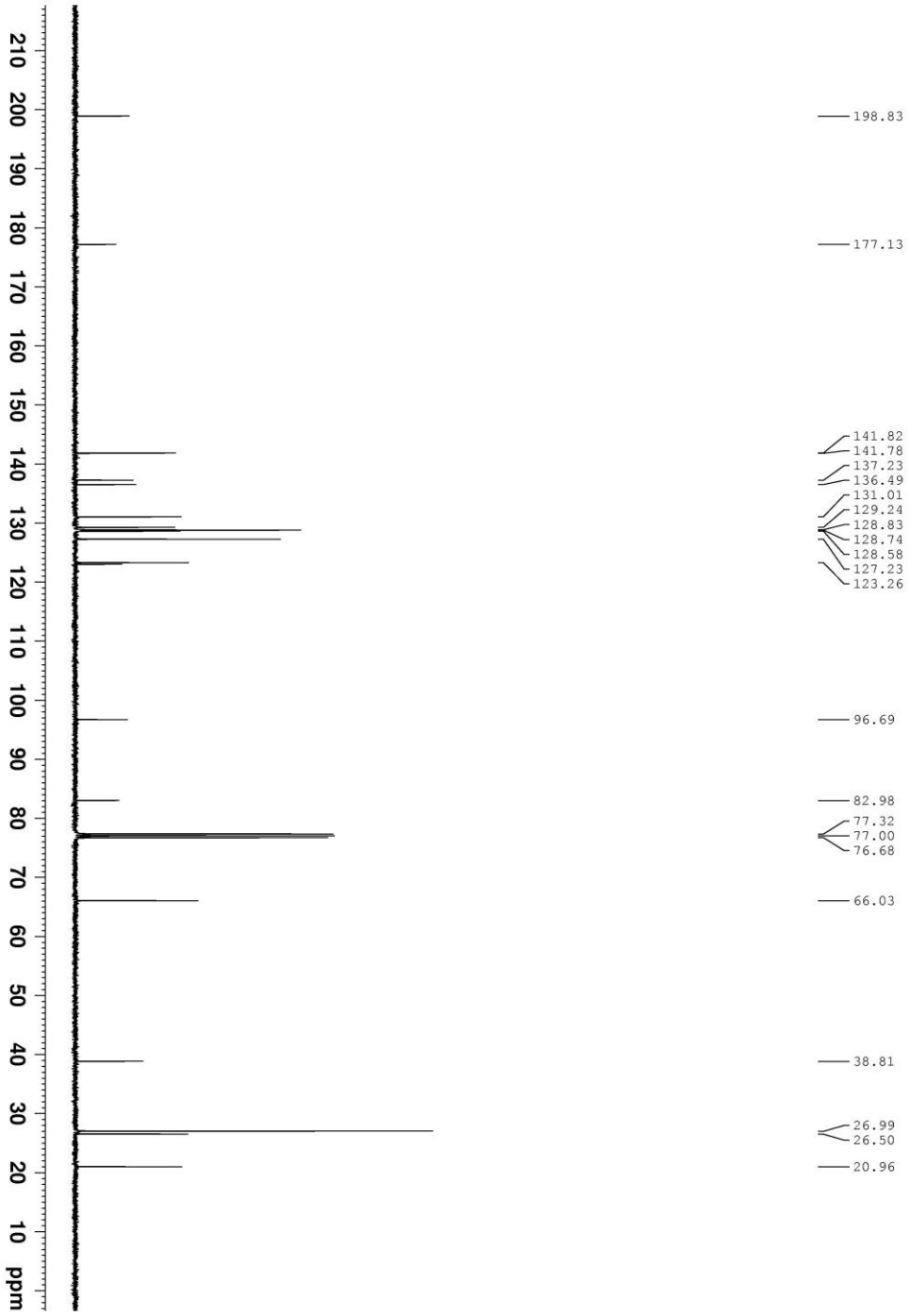
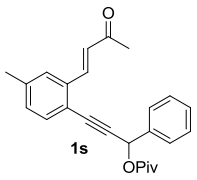
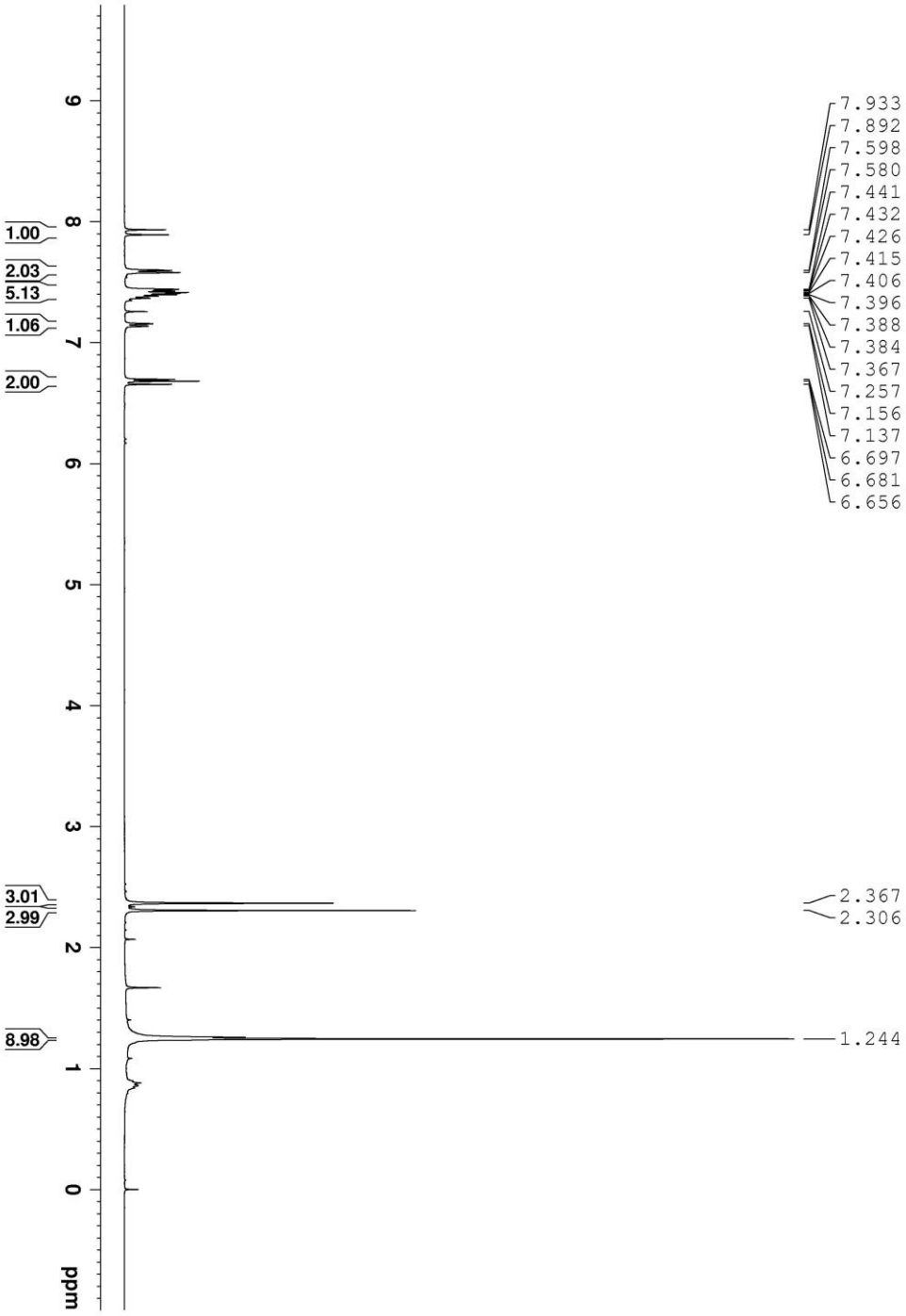
1r
OPiv

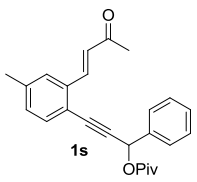

8.004
7.963
7.620
7.603
7.484
7.476
7.471
7.462
7.442
7.425
7.407
7.398
7.394
7.377
7.249
7.244
7.235
6.723
6.670
6.629
2.440
2.296
1.254
1.00
1.99
1.02
3.05
2.00
0.95
1.03
3.15
3.08
9.01
ppm

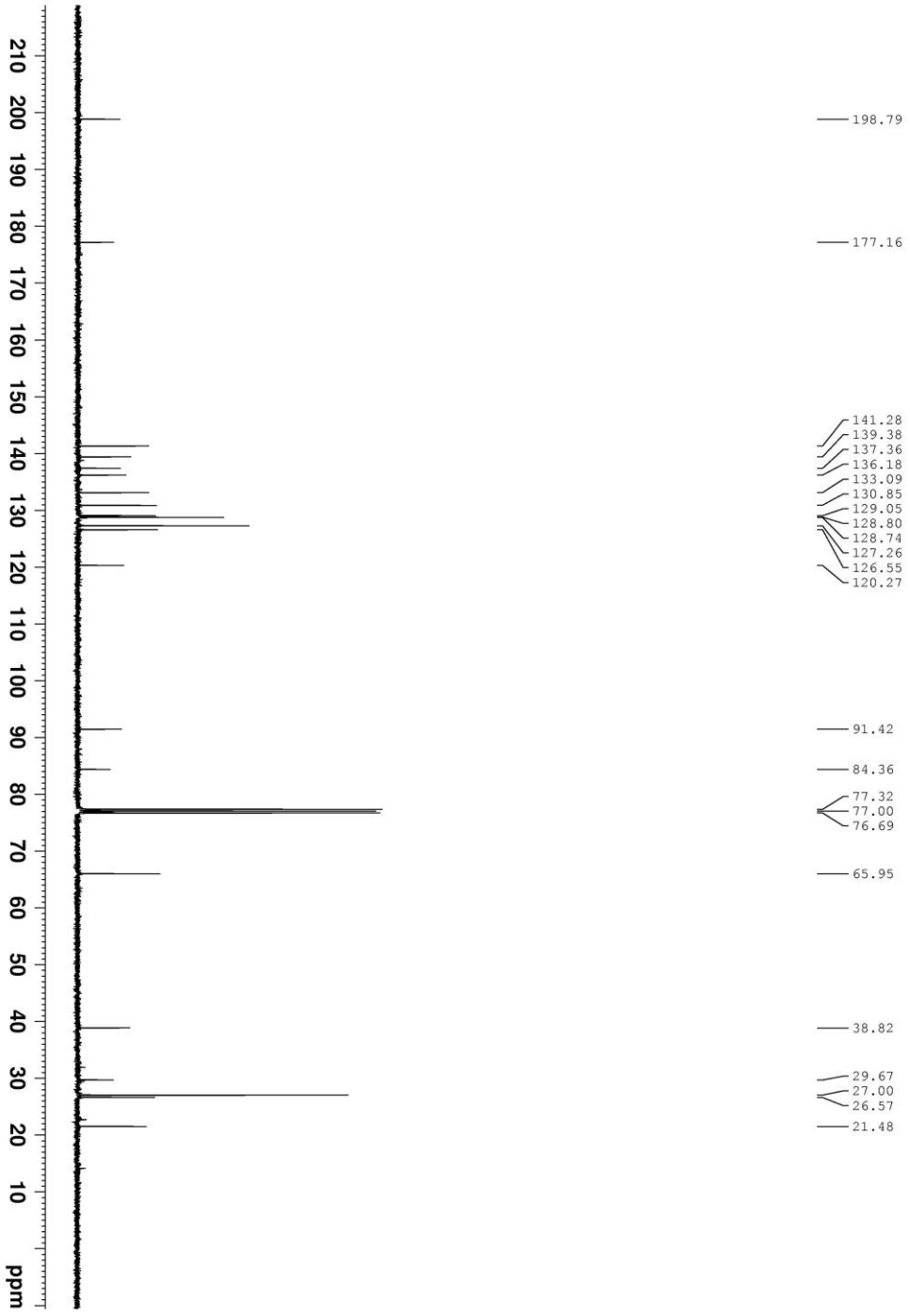

O
1r
OPiv

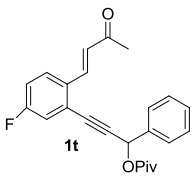

198.83
177.13
141.82
141.78
137.23
136.49
131.01
129.24
128.83
128.74
128.58
127.23
123.26
96.69
82.98
77.32
77.00
76.68
66.03
38.81
26.99
26.50
20.96
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
1s
OPiv

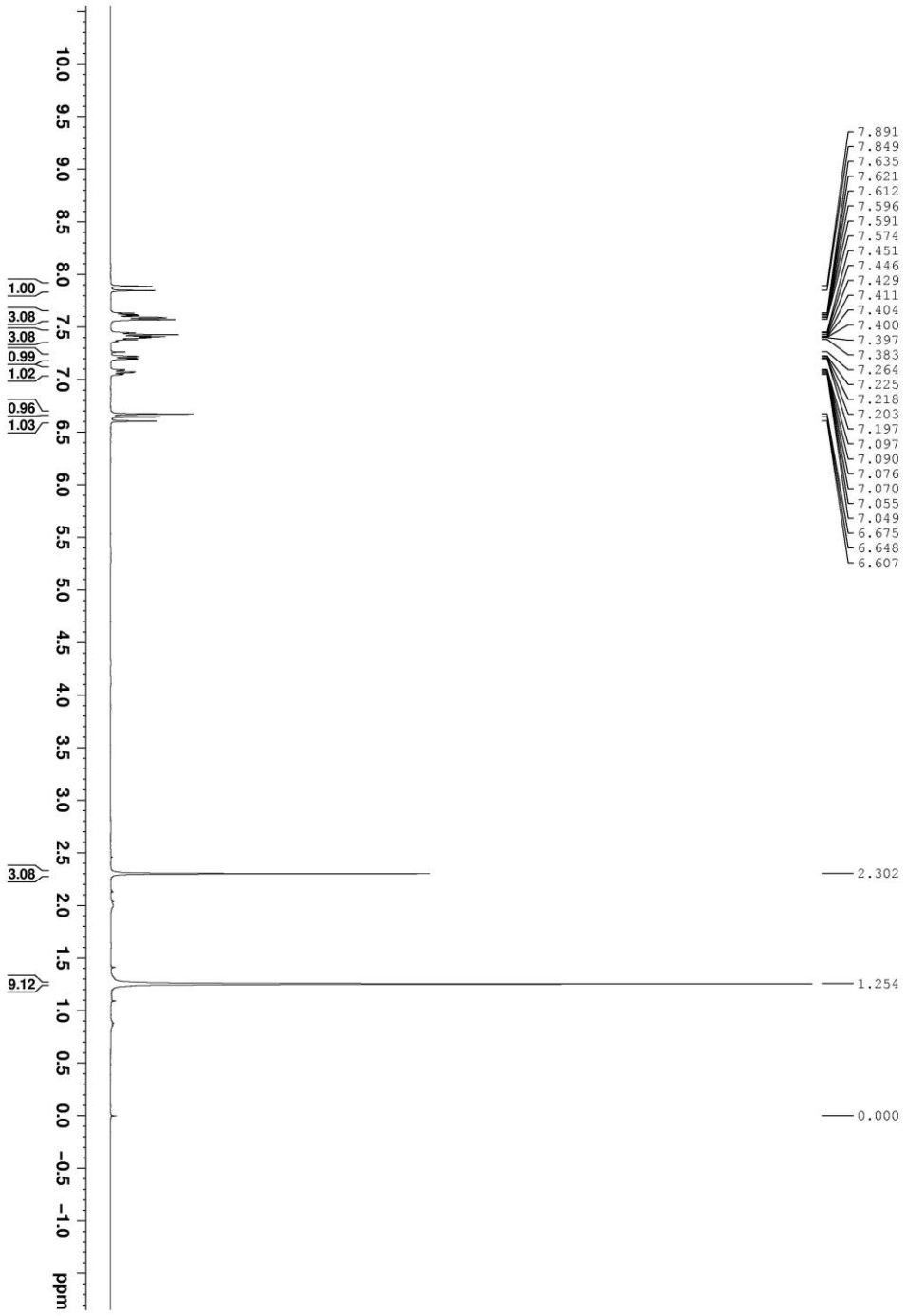

7.933
7.892
7.598
7.580
7.441
7.432
7.426
7.415
7.406
7.396
7.388
7.384
7.367
7.257
7.156
7.137
6.697
6.681
6.656
2.367
2.306
1.244
1.00
2.03
5.13
1.06
2.00
3.01
2.99
8.98
ppm

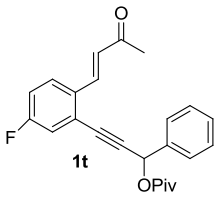

O
1s
OPiv

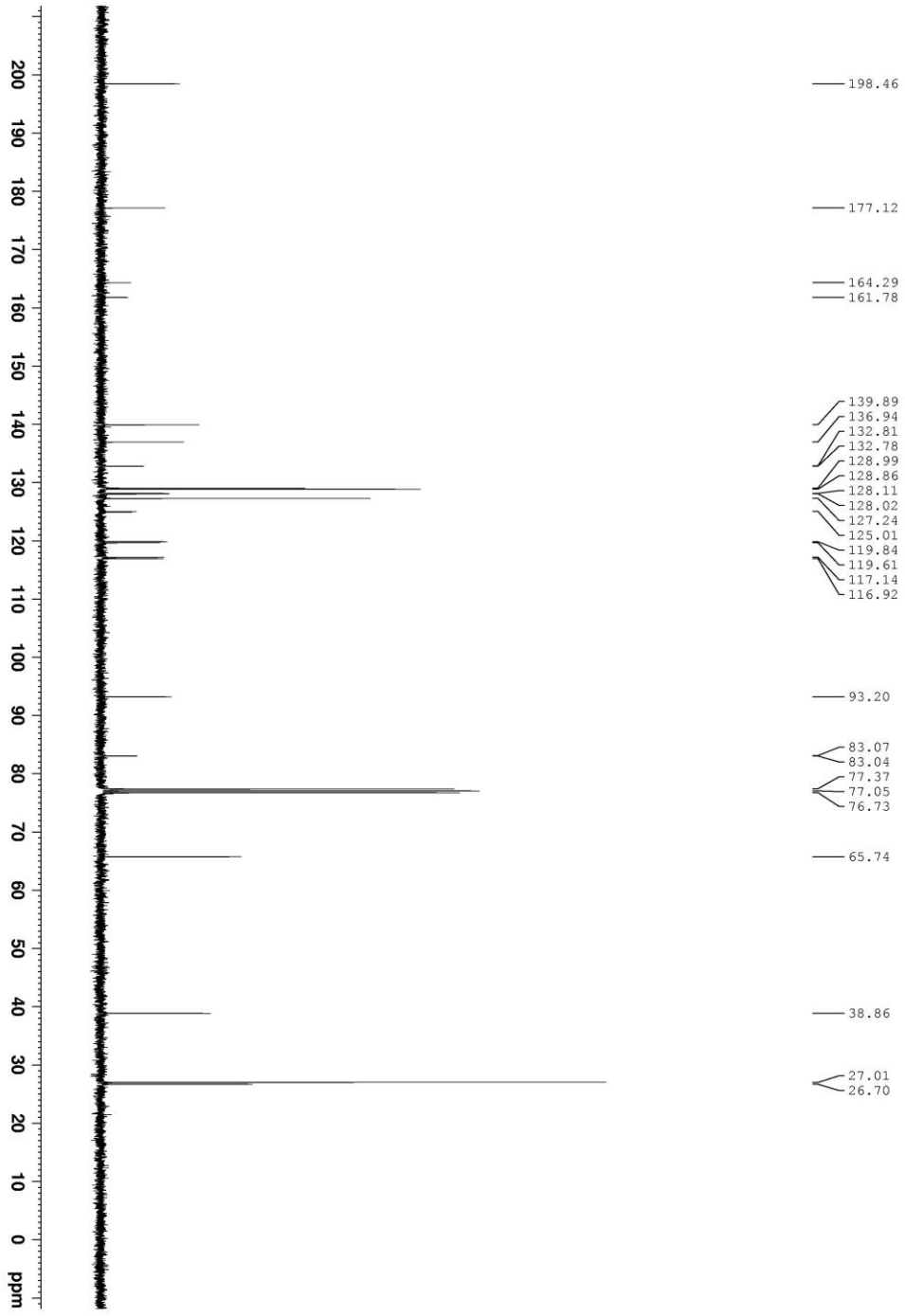

198.79
177.16
141.28
139.38
137.36
136.18
133.09
130.85
129.05
128.80
128.74
127.26
126.55
120.27
91.42
84.36
77.32
77.00
76.69
65.95
38.82
29.67
27.00
26.57
21.48
ppm

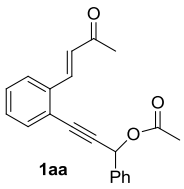

O
F
OPiv

1t

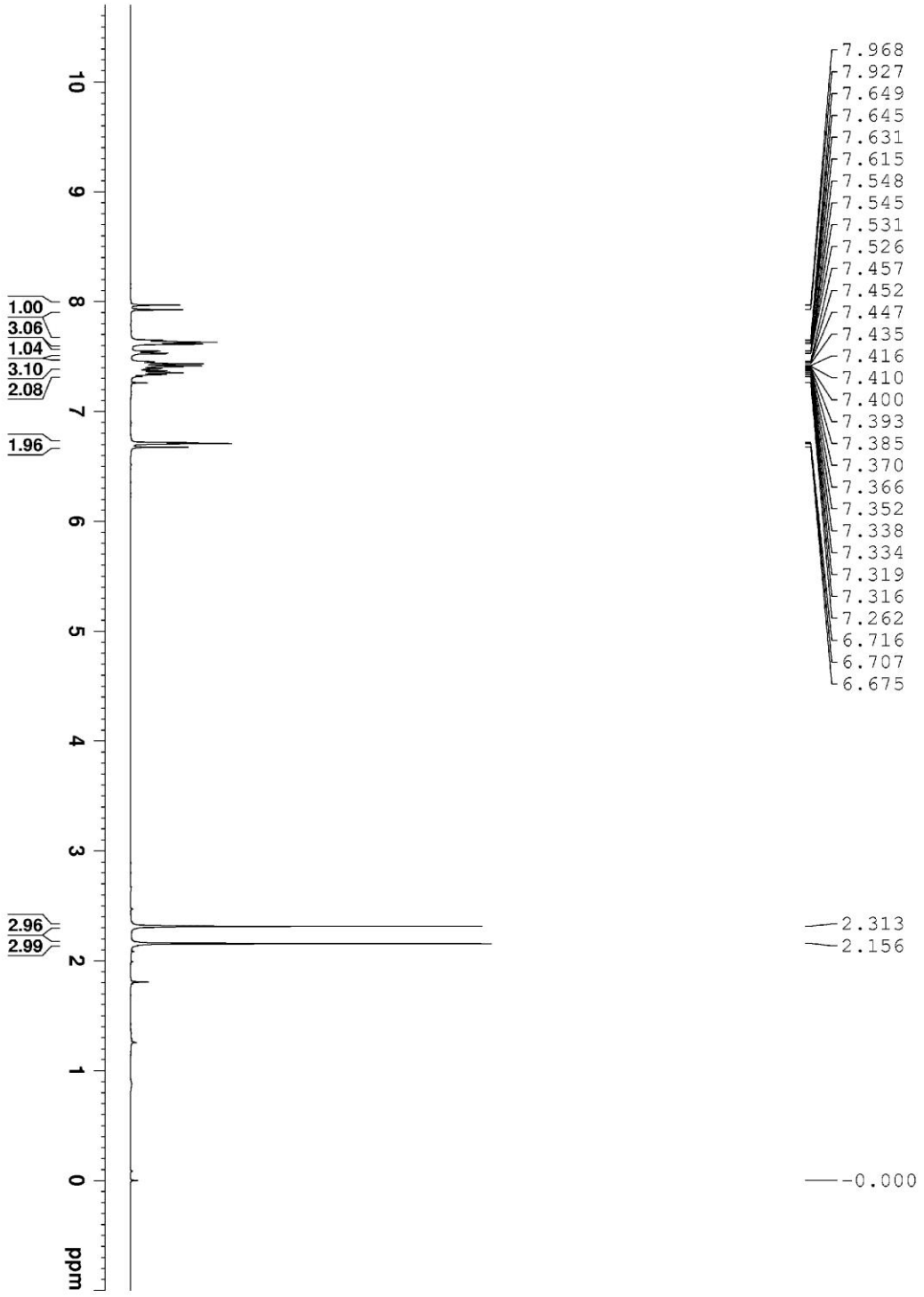

1.00
3.08
3.08
0.99
1.02
0.96
1.03
3.08
9.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 ppm
7.891
7.849
7.635
7.621
7.612
7.596
7.591
7.574
7.451
7.446
7.429
7.411
7.404
7.400
7.397
7.383
7.264
7.225
7.218
7.203
7.197
7.097
7.090
7.076
7.070
7.055
7.049
6.675
6.648
6.607
2.302
1.254
0.000

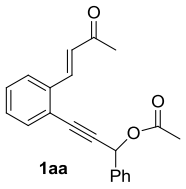

O
F
1t
OPiv


198.46
177.12
164.29
161.78
139.89
136.94
132.81
132.78
128.99
128.86
128.11
128.02
127.24
125.01
119.84
119.61
117.14
116.92
93.20
83.07
83.04
77.37
77.05
76.73
65.74
38.86
27.01
26.70
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

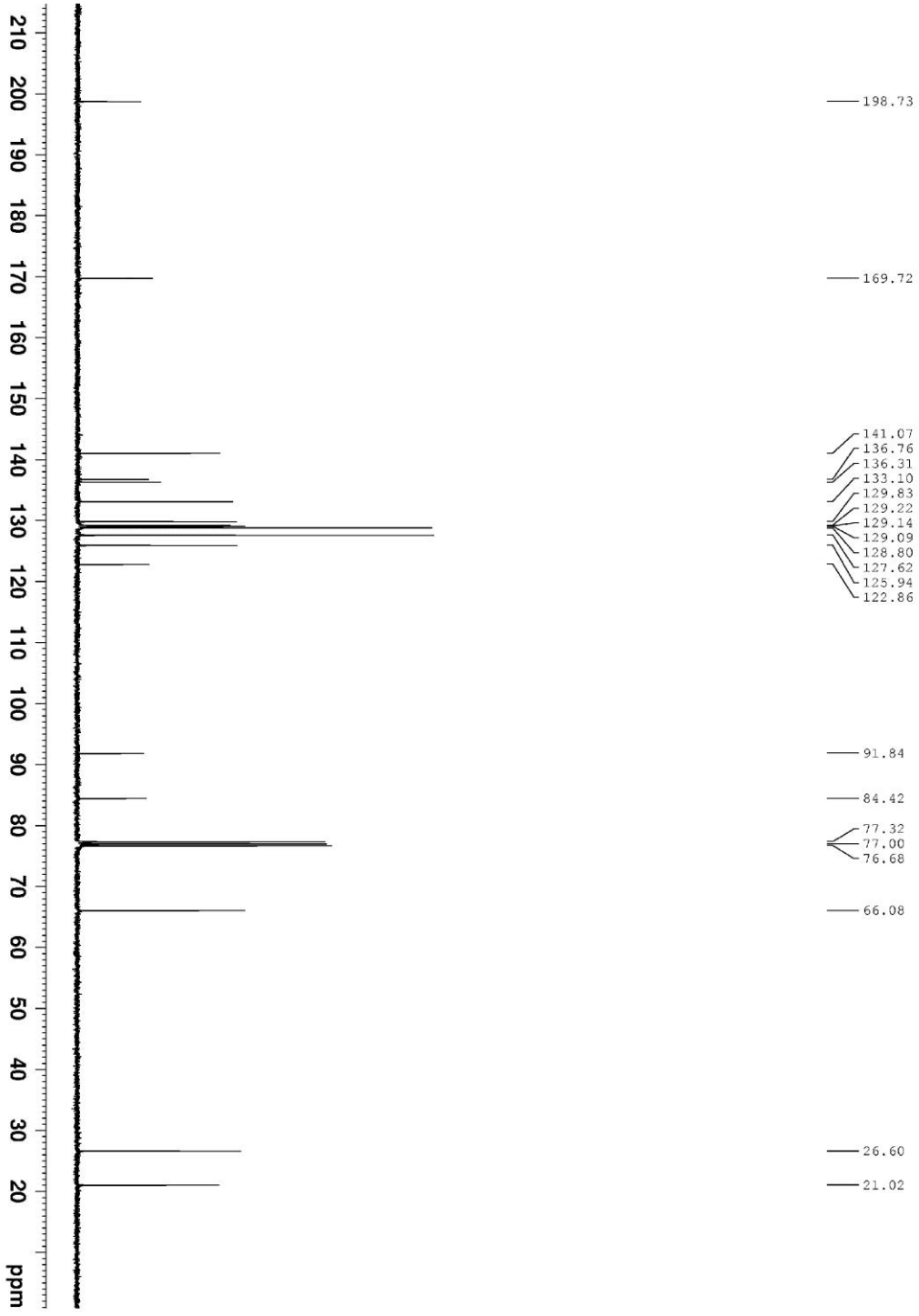

O
O
O
Ph

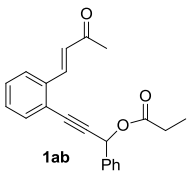
1aa

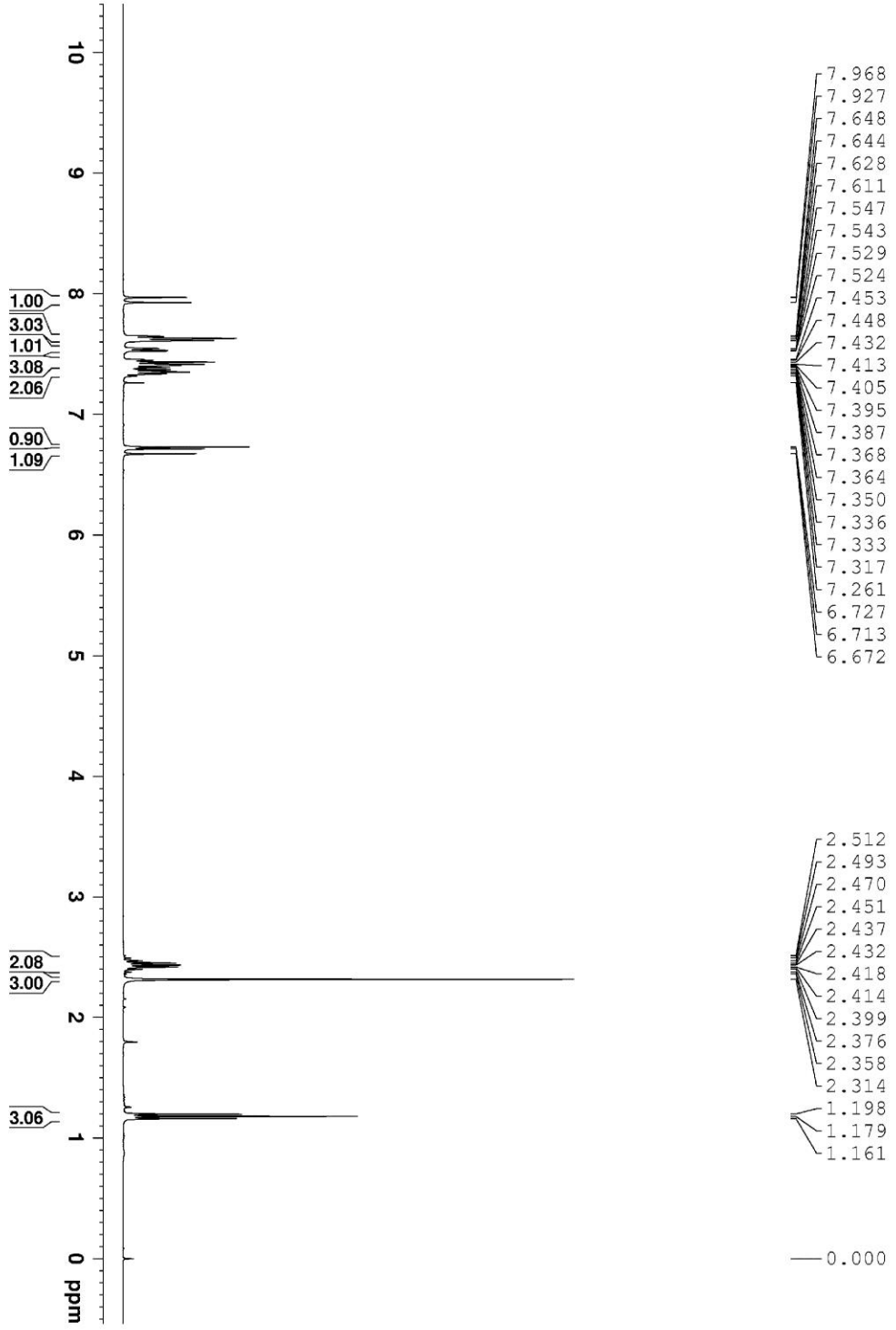

7.968
7.927
7.649
7.645
7.631
7.615
7.548
7.545
7.531
7.526
7.457
7.452
7.447
7.435
7.416
7.410
7.400
7.393
7.385
7.370
7.366
7.352
7.338
7.334
7.319
7.316
7.262
6.716
6.707
6.675
2.313
2.156
-0.000
1.00
3.06
1.04
3.10
2.08
1.96
2.96
2.99
ppm

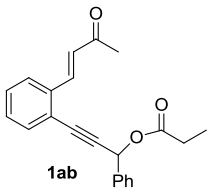

O
O
O
Ph

1aa

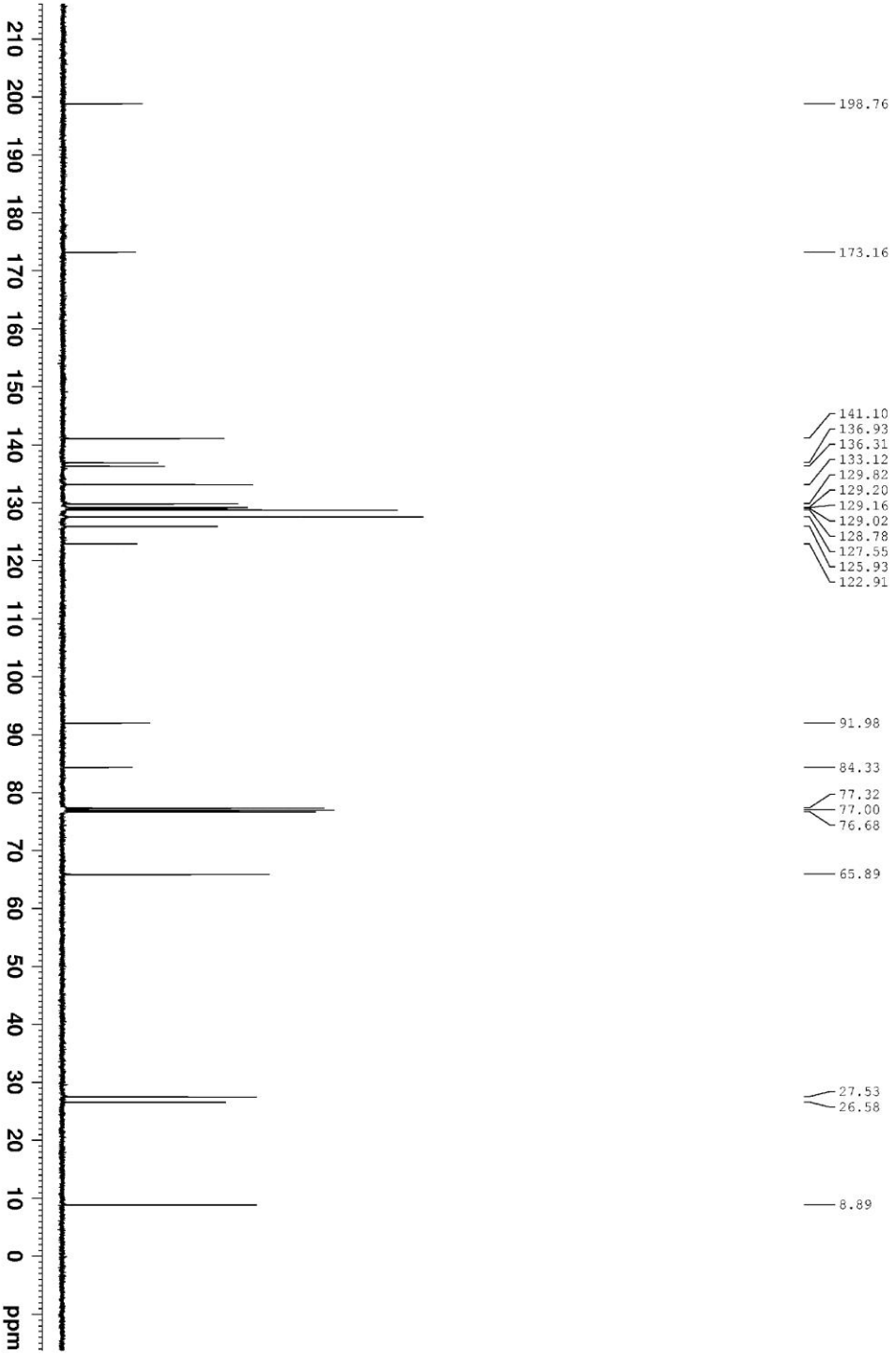

198.73
169.72
141.07
136.76
136.31
133.10
129.83
129.22
129.14
129.09
128.80
127.62
125.94
122.86
91.84
84.42
77.32
77.00
76.68
66.08
26.60
21.02
ppm

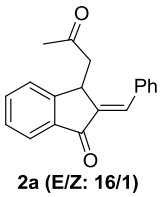

O
O
O
1ab
Ph


10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.03
1.01
3.08
2.06
0.90
1.09
2.08
3.00
3.06
7.968
7.927
7.648
7.644
7.628
7.611
7.547
7.543
7.529
7.524
7.453
7.448
7.432
7.413
7.405
7.395
7.387
7.368
7.364
7.350
7.336
7.333
7.317
7.261
6.727
6.713
6.672
2.512
2.493
2.470
2.451
2.437
2.432
2.418
2.414
2.399
2.376
2.358
2.314
1.198
1.179
1.161
0.000

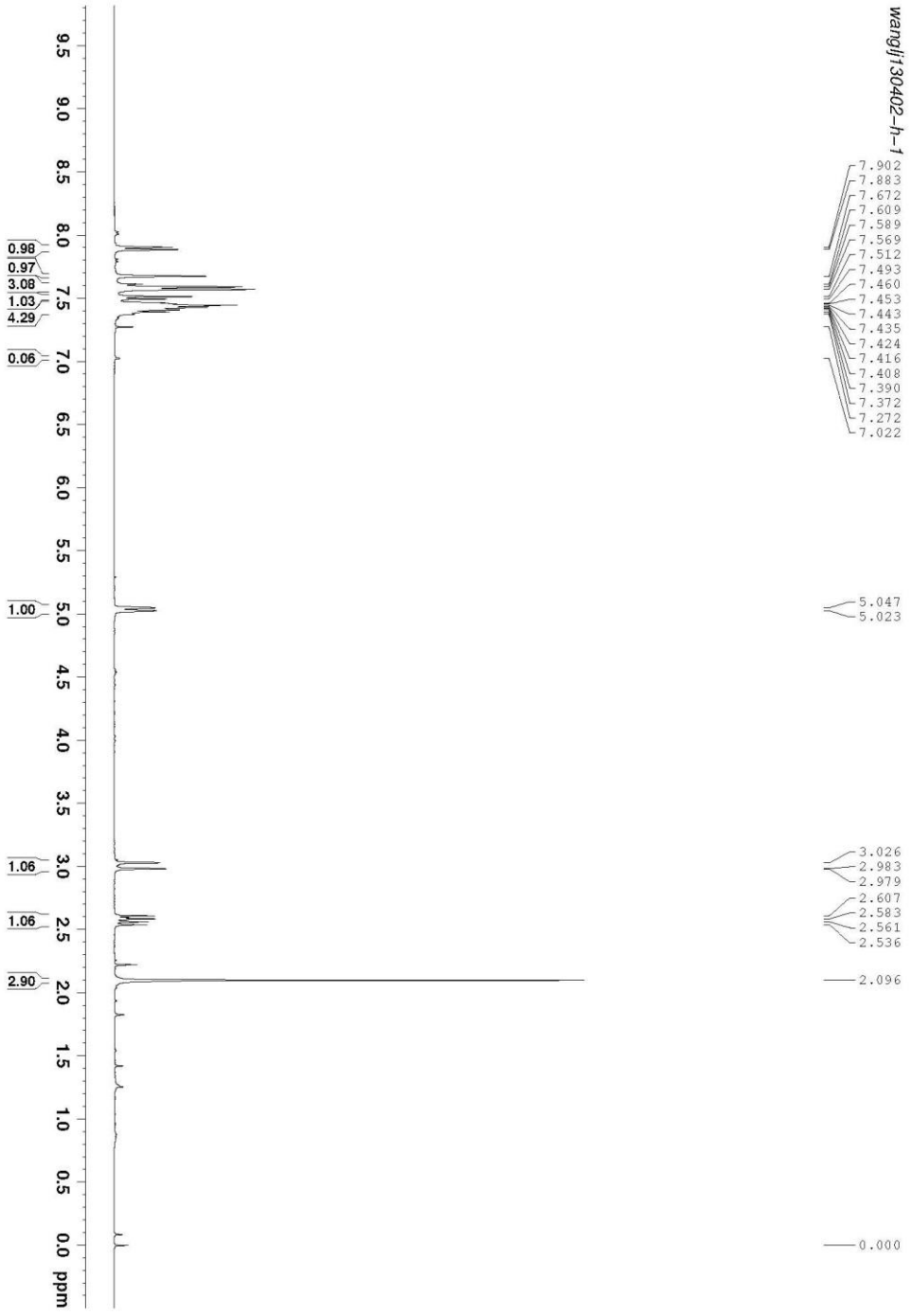

O
O
O
Ph

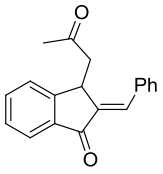
1ab


198.76
173.16
141.10
136.93
136.31
133.12
129.82
129.20
129.16
129.02
128.78
127.55
125.93
122.91
91.98
84.33
77.32
77.00
76.68
65.89
27.53
26.58
8.89
ppm

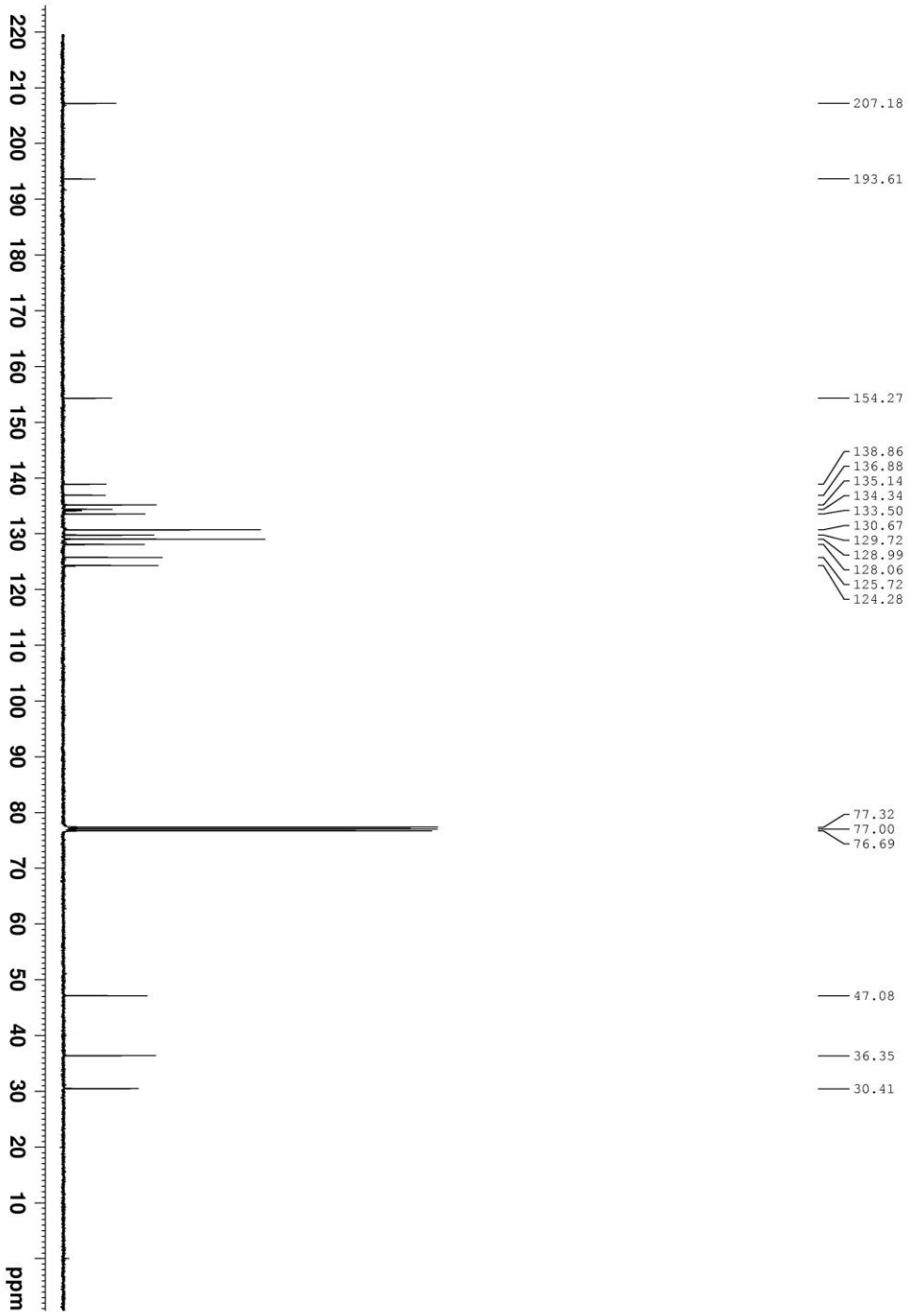

O
Ph
O

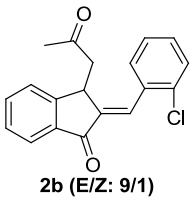
2a (E/Z: 16/1)


wangjf130402-h-1
7.902
7.883
7.672
7.609
7.589
7.569
7.512
7.493
7.460
7.453
7.443
7.435
7.424
7.416
7.408
7.390
7.372
7.272
7.022
5.047
5.023
3.026
2.983
2.979
2.607
2.583
2.561
2.536
2.096
0.000
0.98
0.97
3.08
1.03
4.29
0.06
1.00
1.06
1.06
2.90
ppm

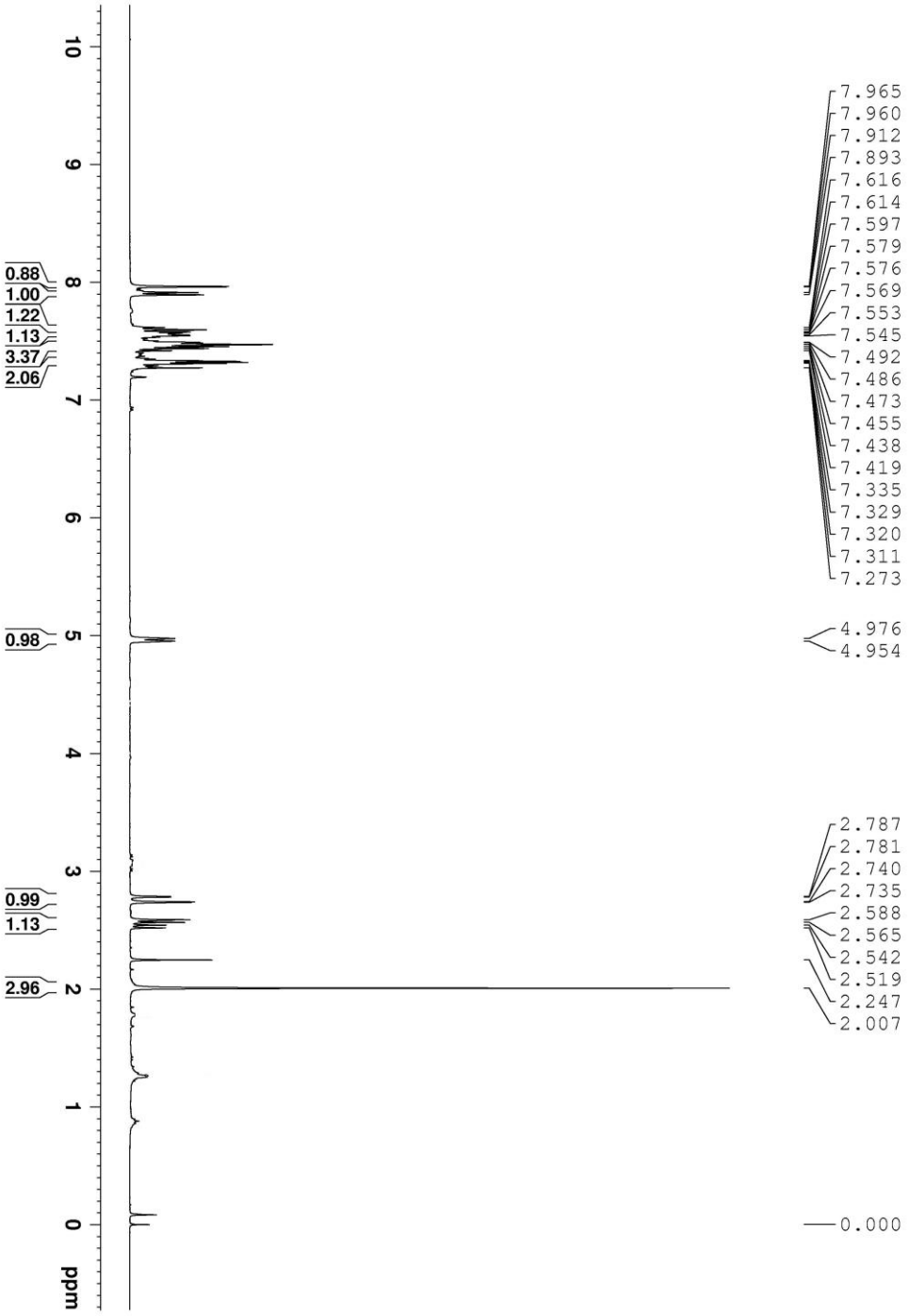

O
Ph
O

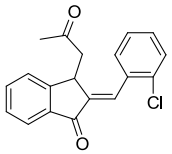
2a (E/Z: 16/1)


207.18
193.61
154.27
138.86
136.88
135.14
134.34
133.50
130.67
129.72
128.99
128.06
125.72
124.28
77.32
77.00
76.69
47.08
36.35
30.41
ppm

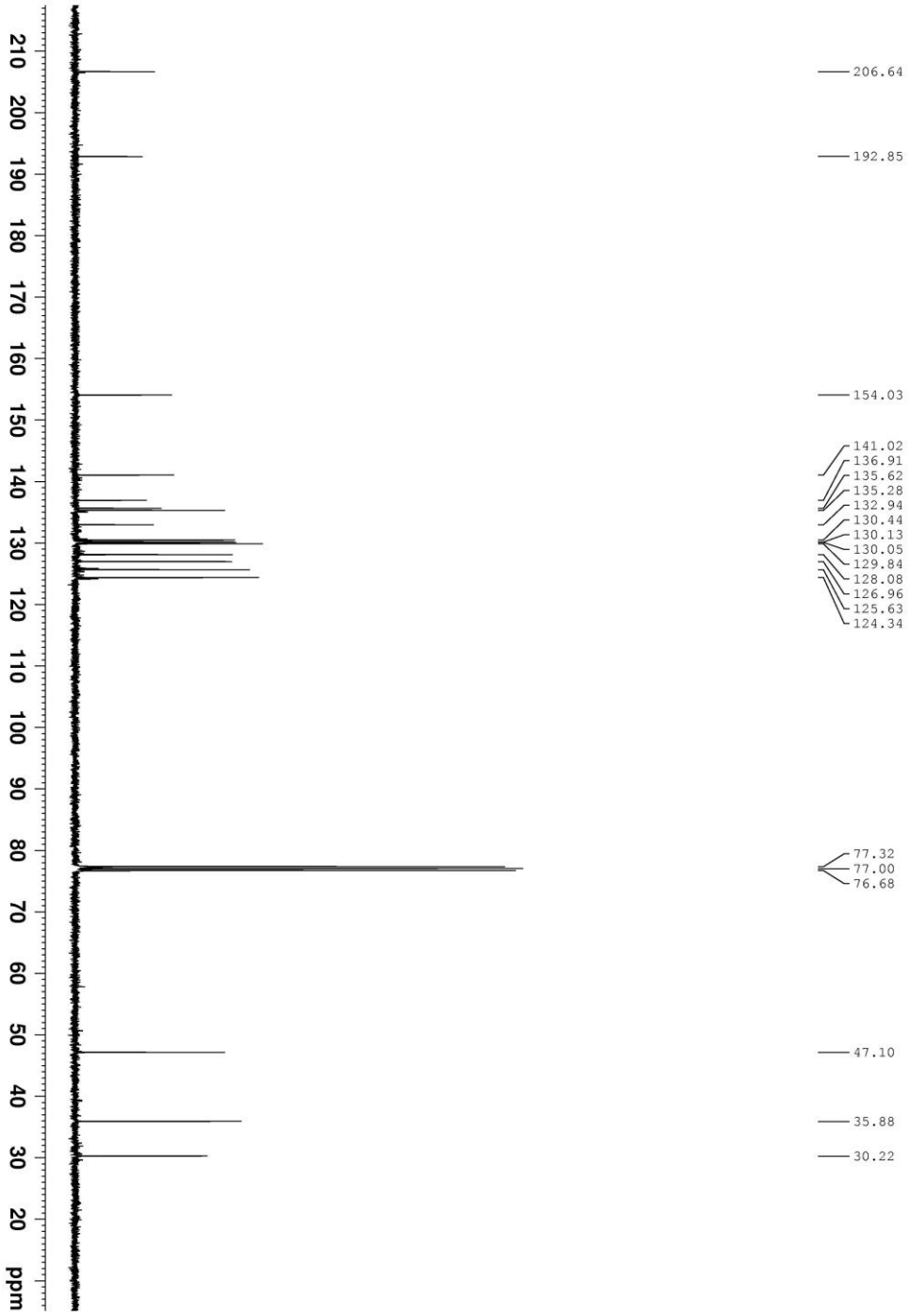

O
Cl
O

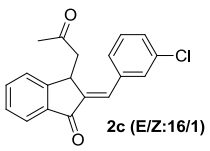
2b (E/Z: 9/1)


0.88
1.00
1.22
1.13
3.37
2.06
0.98
0.99
1.13
2.96
7.965
7.960
7.912
7.893
7.616
7.614
7.597
7.579
7.576
7.569
7.553
7.545
7.492
7.486
7.473
7.455
7.438
7.419
7.335
7.329
7.320
7.311
7.273
4.976
4.954
2.787
2.781
2.740
2.735
2.588
2.565
2.542
2.519
2.247
2.007
0.000
ppm

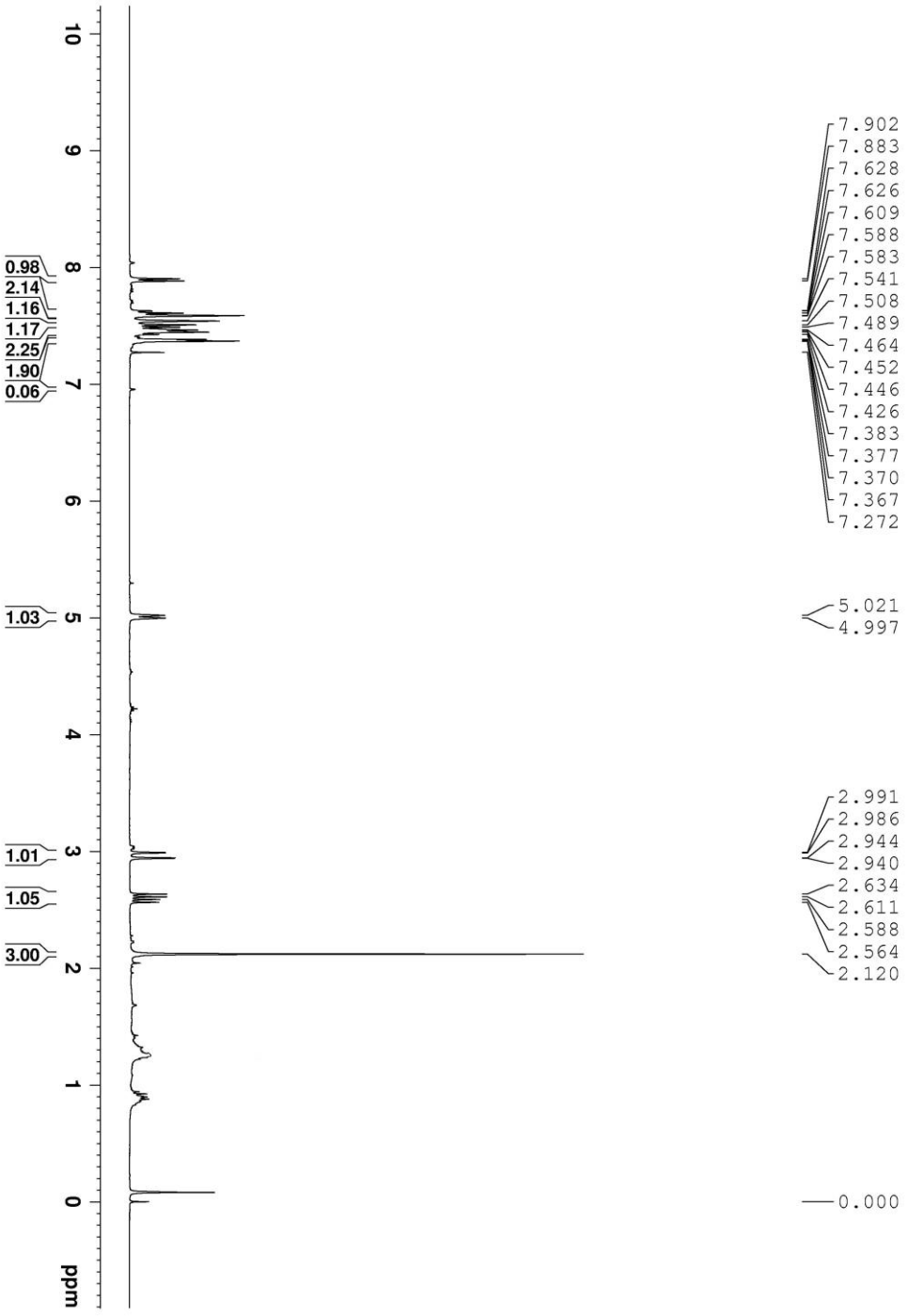

O
Cl
O

2b E/Z: 9/1)


206.64
192.85
154.03
141.02
136.91
135.62
135.28
132.94
130.44
130.13
130.05
129.84
128.08
126.96
125.63
124.34
77.32
77.00
76.68
47.10
35.88
30.22
ppm


O
Cl
O

2c (E/Z:16/1)


0.98
2.14
1.16
1.17
2.25
1.90
0.06
1.03
1.01
1.05
3.00
ppm
7.902
7.883
7.628
7.626
7.609
7.588
7.583
7.541
7.508
7.489
7.464
7.452
7.446
7.426
7.383
7.377
7.370
7.367
7.272
5.021
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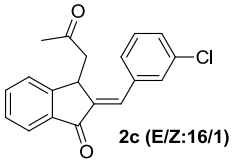
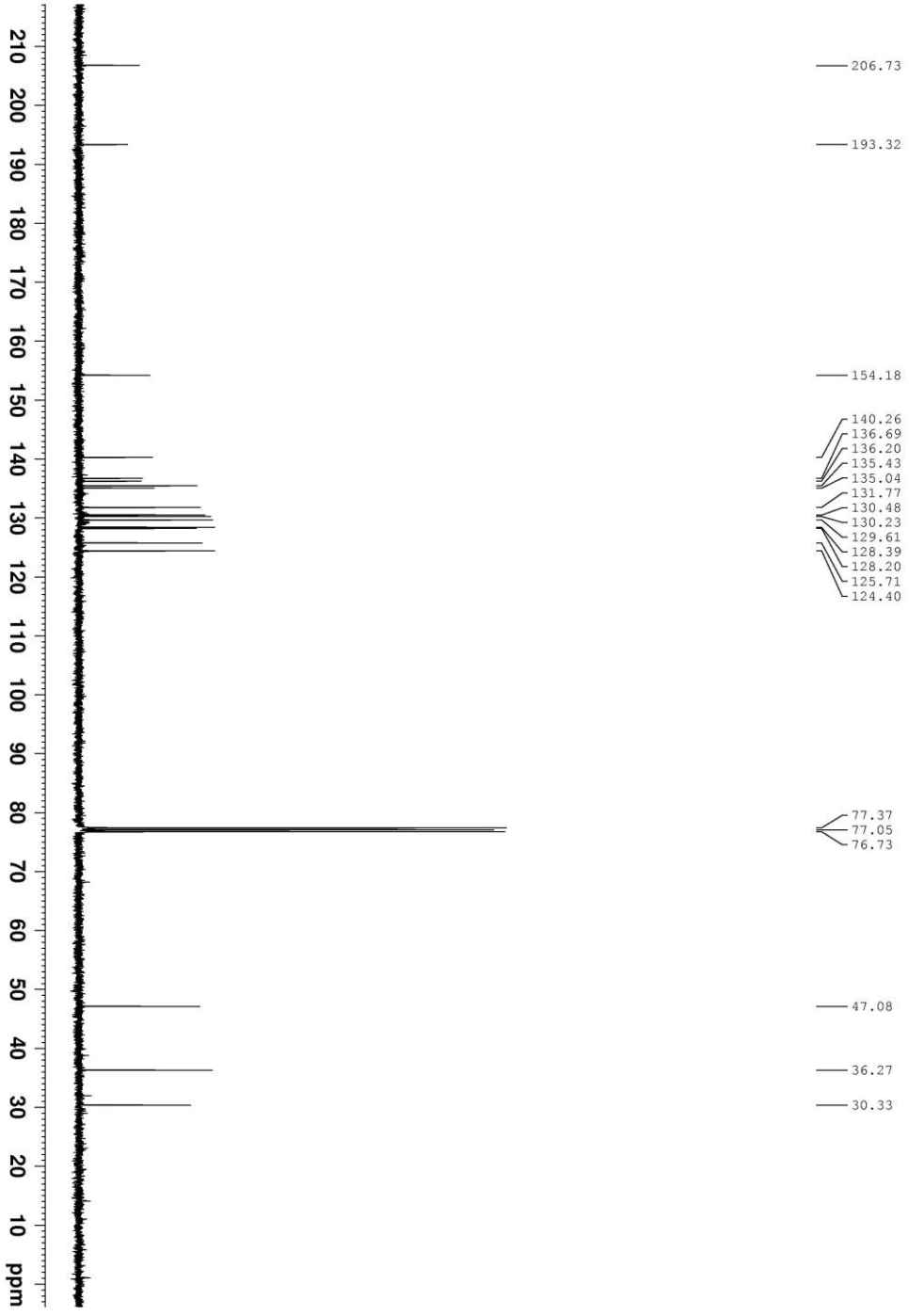
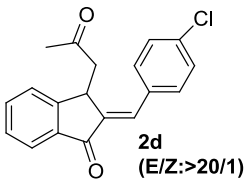
2.940
2.634
2.611
2.588
2.564
2.120
0.000

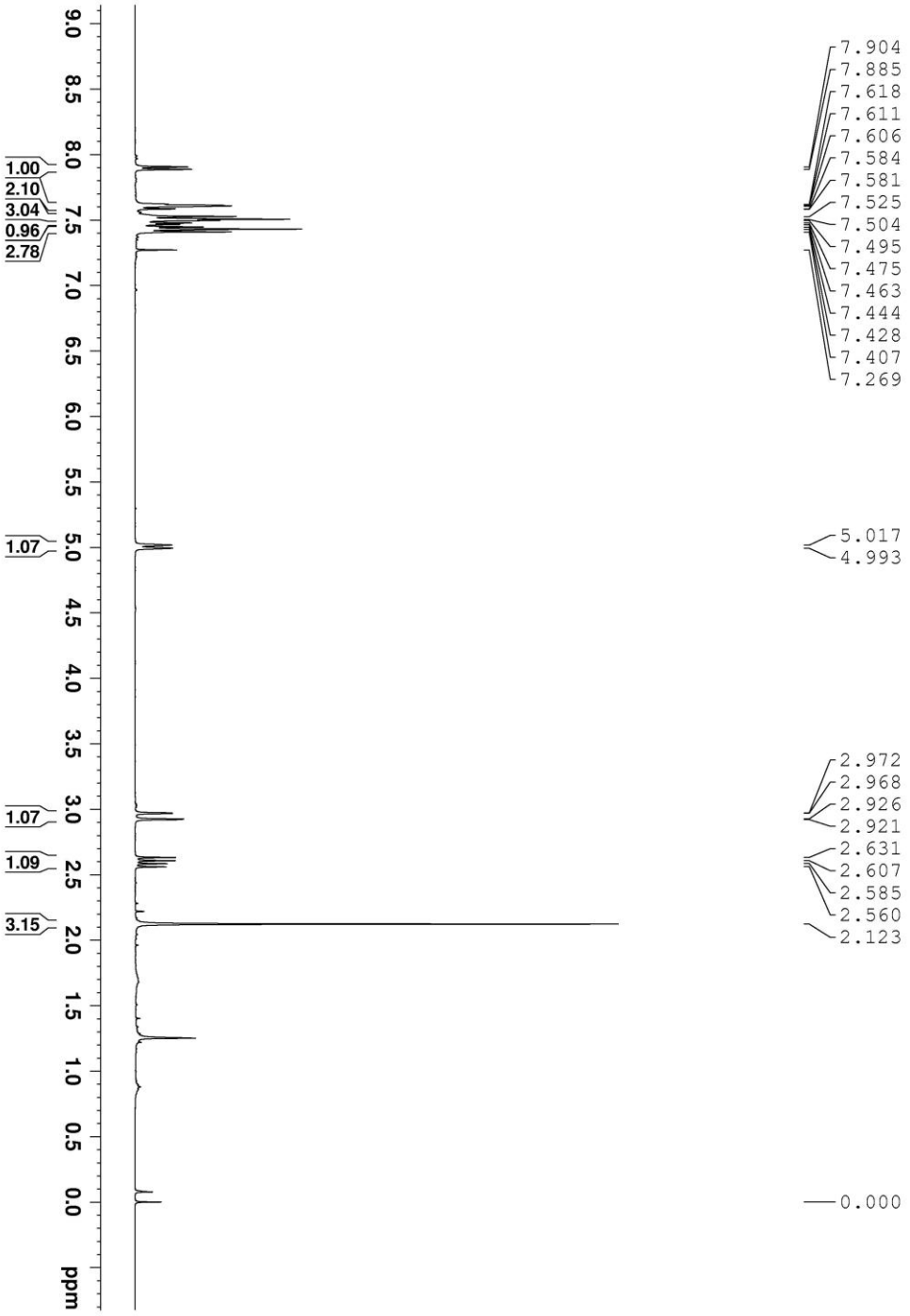

O
Cl
O

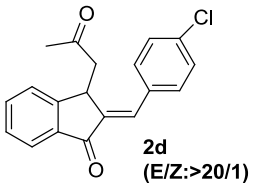
2c (E/Z:16/1)


206.73
193.32
154.18
140.26
136.69
136.20
135.43
135.04
131.77
130.48
130.23
129.61
128.39
128.20
125.71
124.40
77.37
77.05
76.73
47.08
36.27
30.33
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

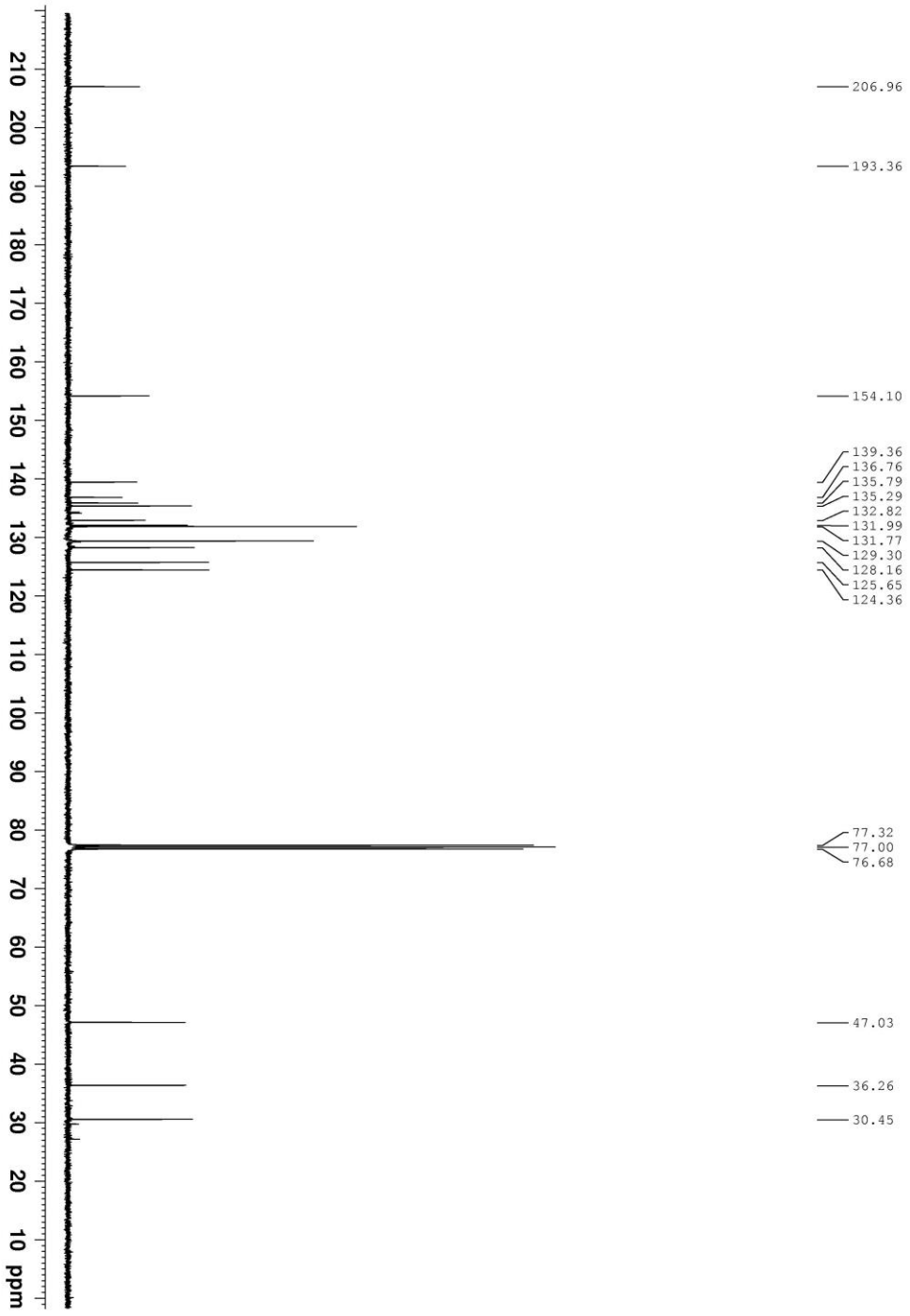

O
Cl
O

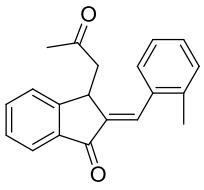
2d
(E/Z:>20/1)


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
ppm
1.00
2.10
3.04
0.96
2.78
1.07
1.07
1.09
3.15
7.904
7.885
7.618
7.611
7.606
7.584
7.581
7.525
7.504
7.495
7.475
7.463
7.444
7.428
7.407
7.269
5.017
4.993
2.972
2.968
2.926
2.921
2.631
2.607
2.585
2.560
2.123
0.000

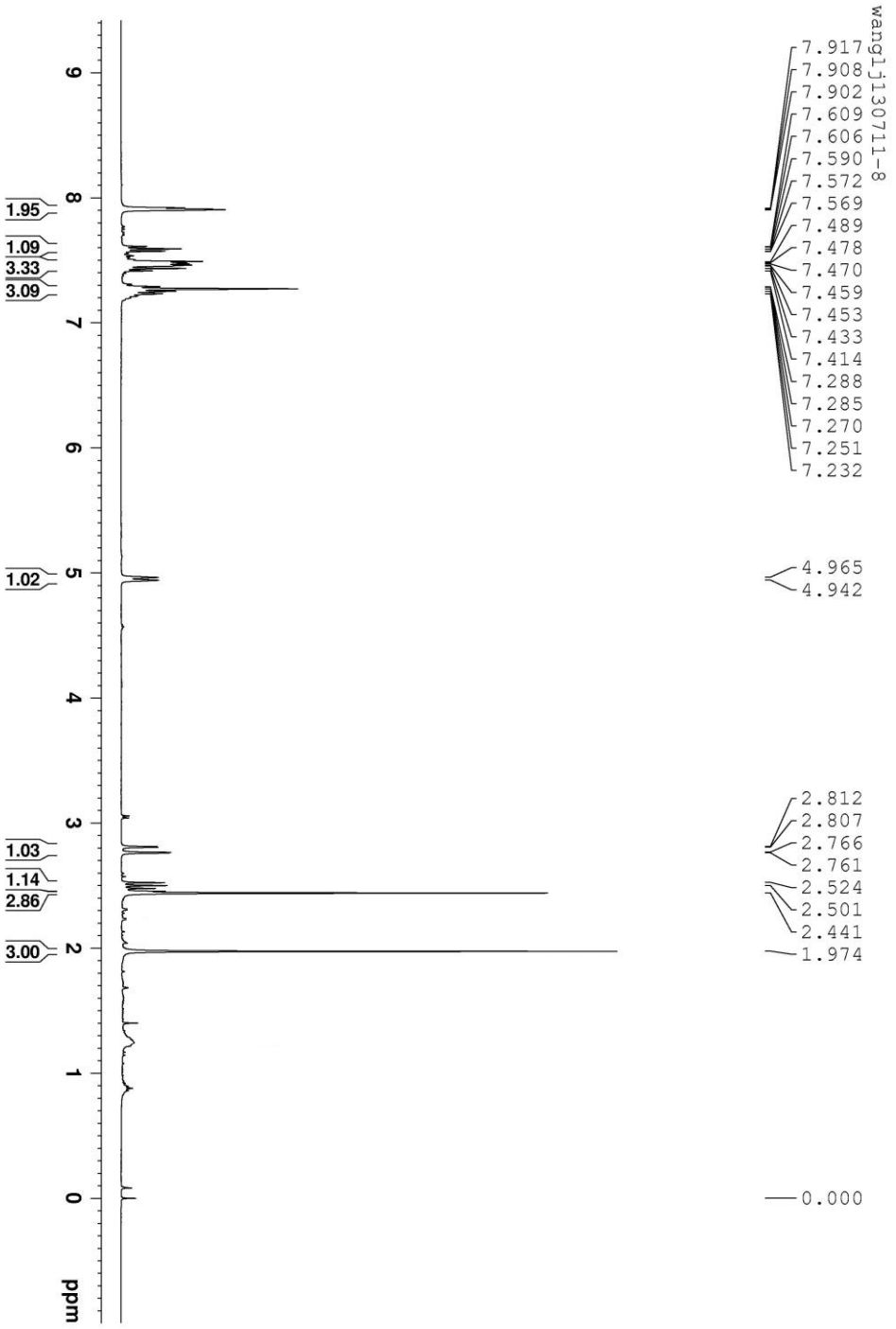

O
Cl
O

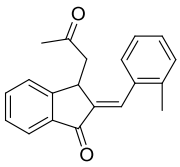
2d
(E/Z:>20/1)


206.96
193.36
154.10
139.36
136.76
135.79
135.29
132.82
131.99
131.77
129.30
128.16
125.65
124.36
77.32
77.00
76.68
47.03
36.26
30.45
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

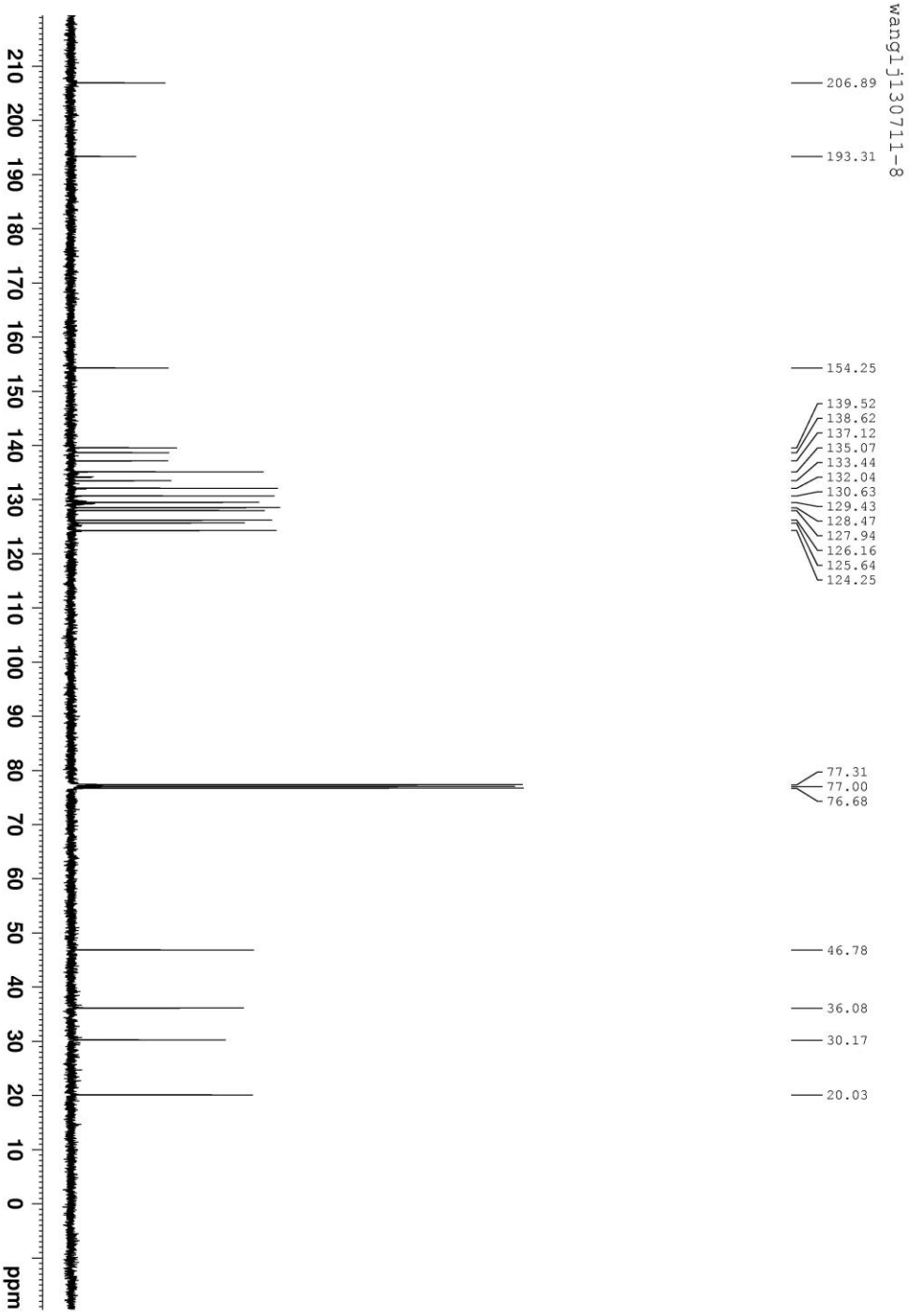


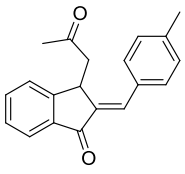
2e (E/Z:>20/1)


wangli130711-8
7.917
7.908
7.902
7.609
7.606
7.590
7.572
7.569
7.489
7.478
7.470
7.459
7.453
7.433
7.414
7.288
7.285
7.270
7.251
7.232
4.965
4.942
2.812
2.807
2.766
2.761
2.524
2.501
2.441
1.974
0.000
1.95
1.09
3.33
3.09
1.02
1.03
1.14
2.86
3.00
ppm

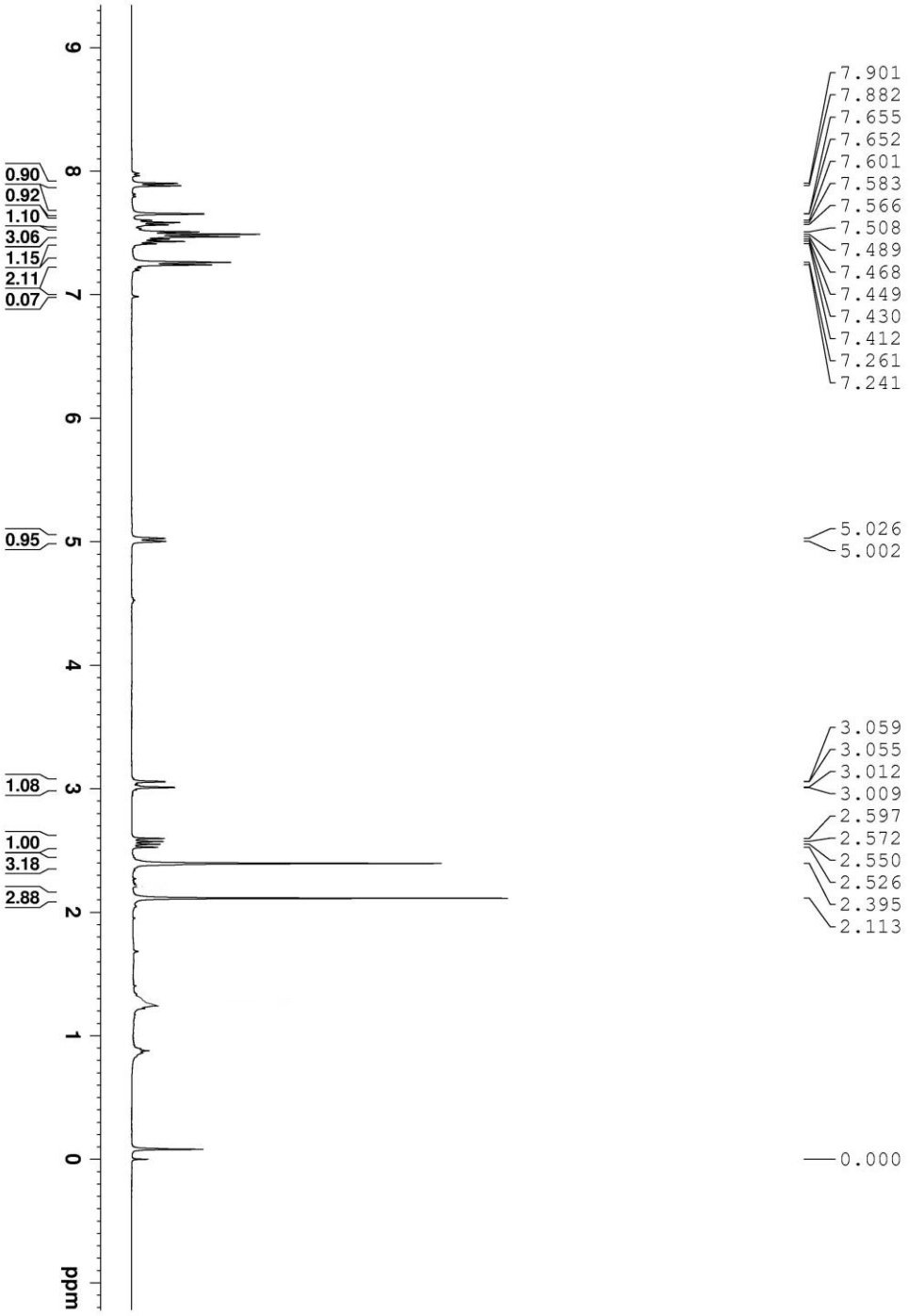


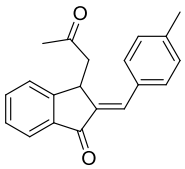
2e (E/Z:>20/1)


wangljl30711-8
206.89
193.31
154.25
139.52
138.62
137.12
135.07
133.44
132.04
130.63
129.43
128.47
127.94
126.16
125.64
124.25
77.31
77.00
76.68
46.78
36.08
30.17
20.03
ppm

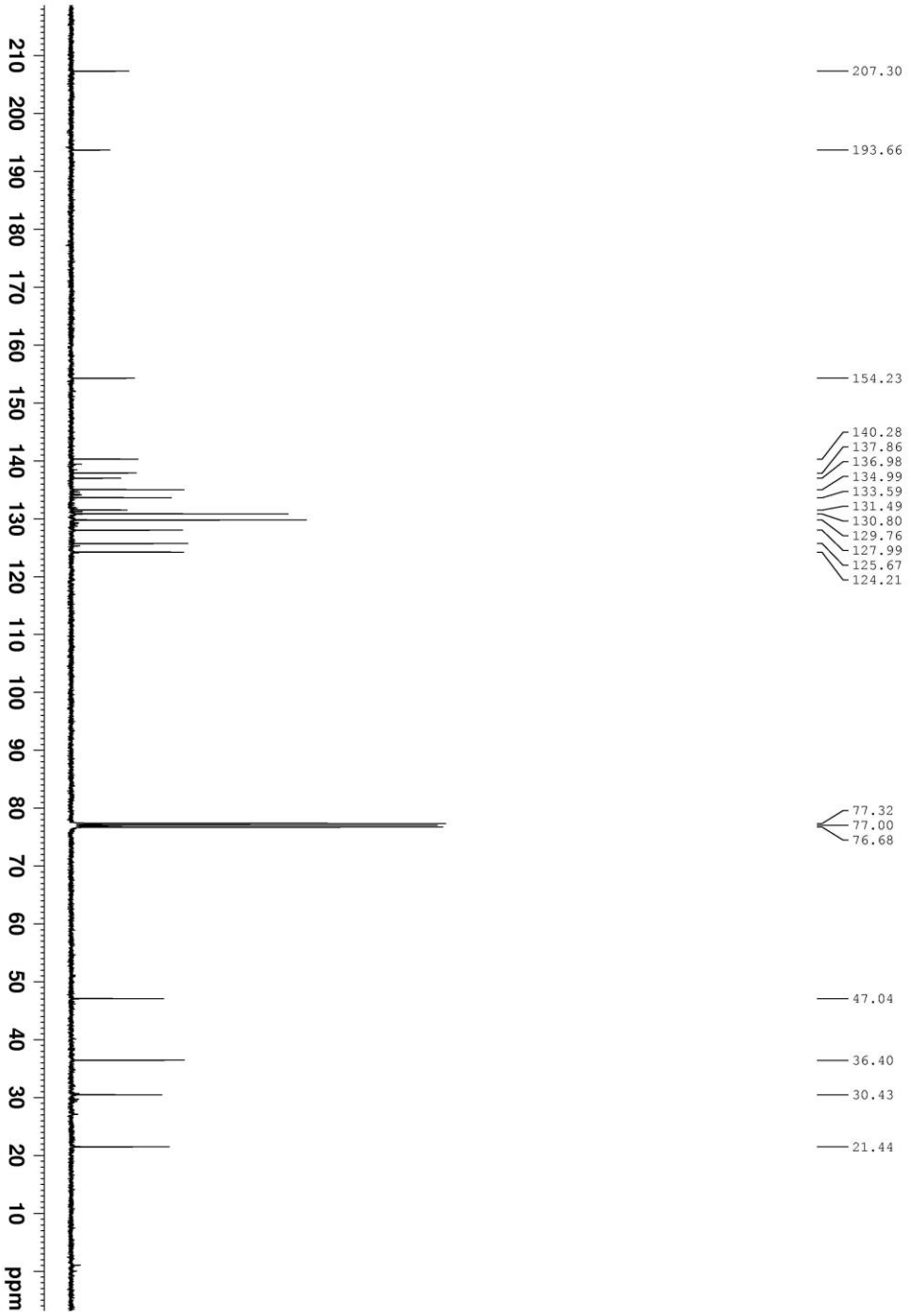


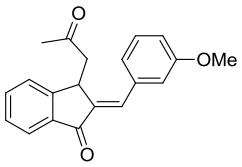
2f (E/Z:13/1)


0.90
0.92
1.10
3.06
1.15
2.11
0.07
0.95
1.08
1.00
3.18
2.88
9
8
7
6
5
4
3
2
1
0
ppm
7.901
7.882
7.655
7.652
7.601
7.583
7.566
7.508
7.489
7.468
7.449
7.430
7.412
7.261
7.241
5.026
5.002
3.059
3.055
3.012
3.009
2.597
2.572
2.550
2.526
2.395
2.113
0.000

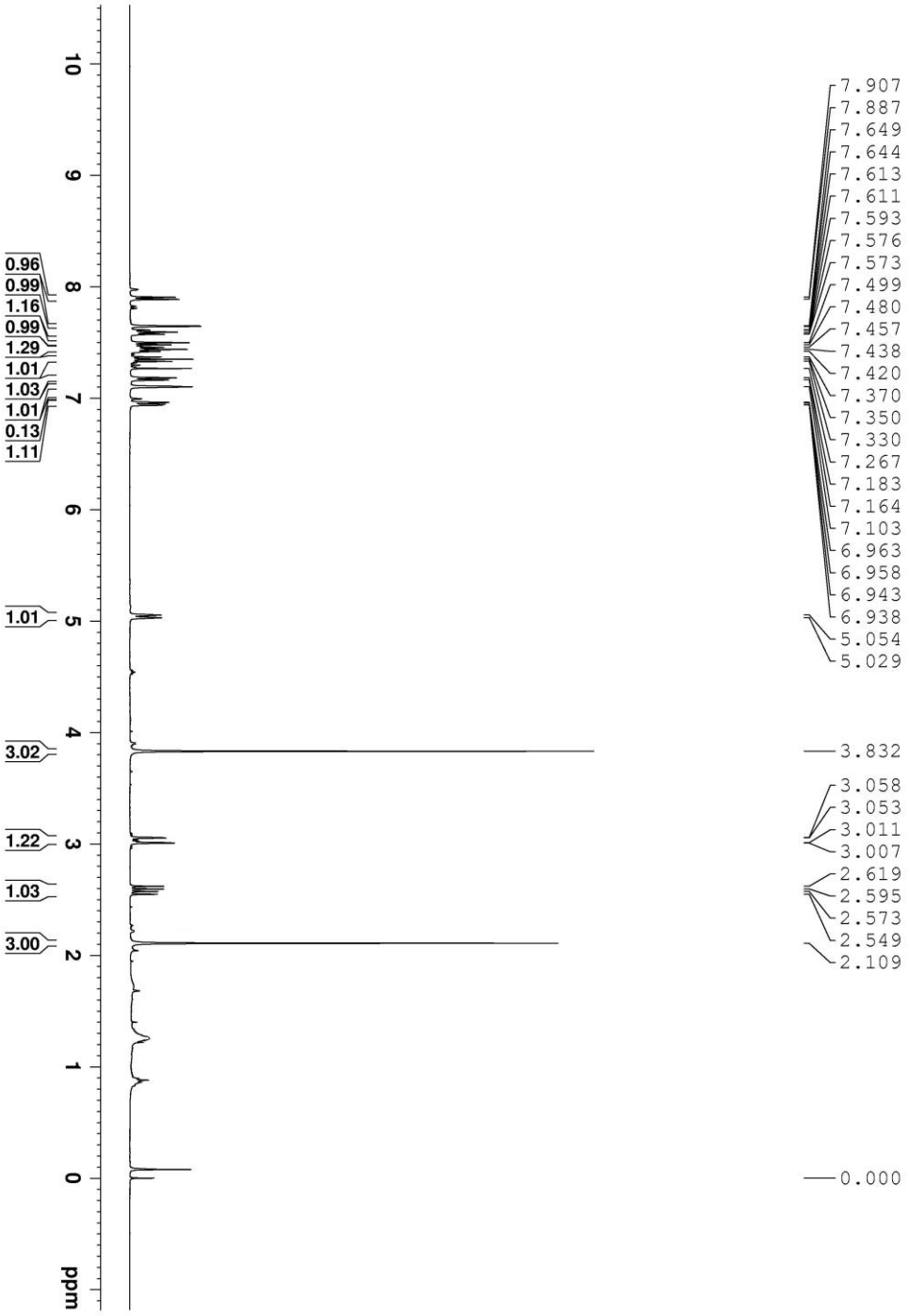


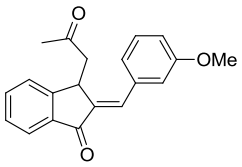
2f (E/Z:13/1)


207.30
193.66
154.23
140.28
137.86
136.98
134.99
133.59
131.49
130.80
129.76
127.99
125.67
124.21
77.32
77.00
76.68
47.04
36.40
30.43
21.44
ppm

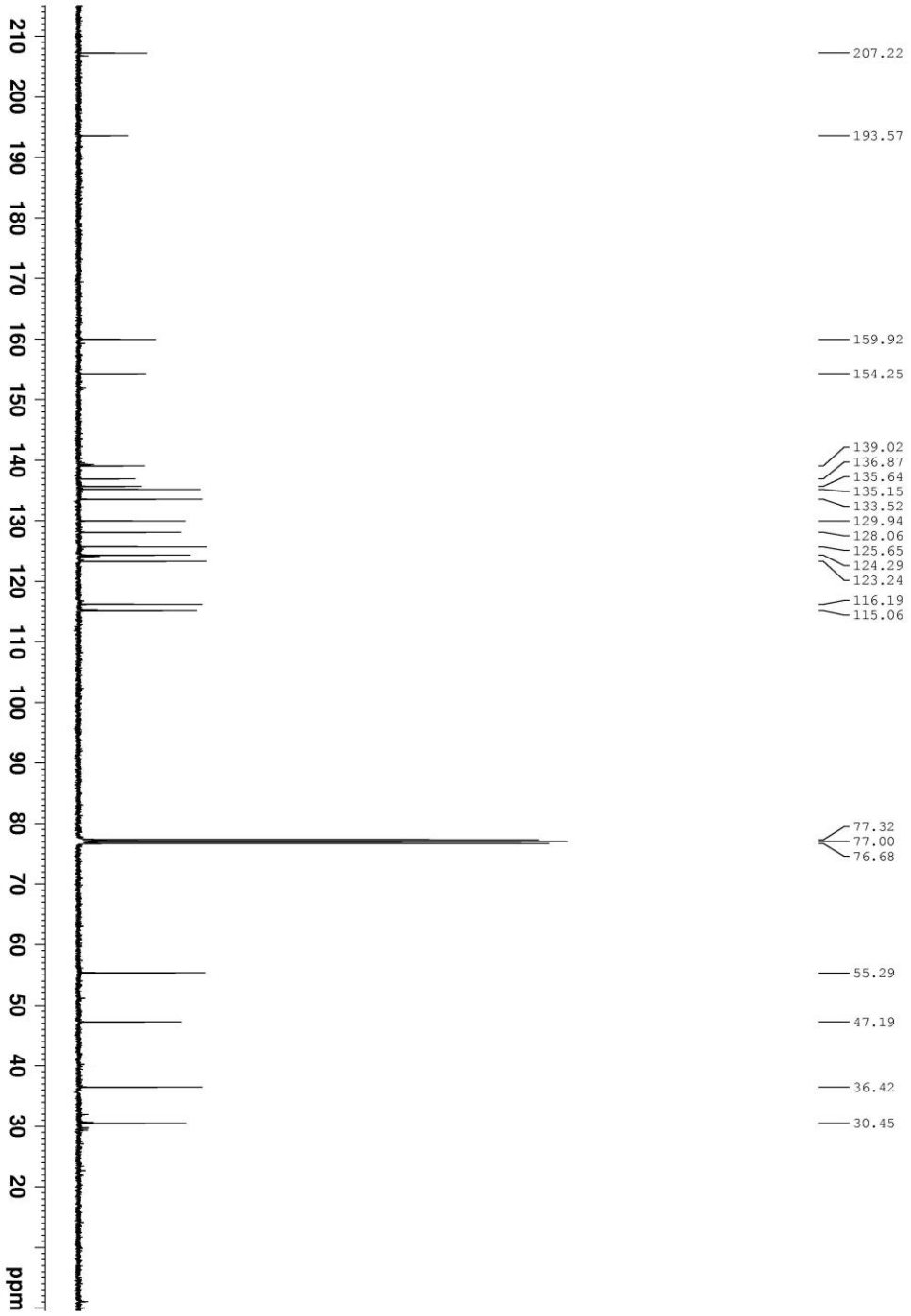

O
OMe
O

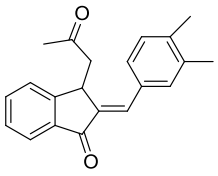
2g (E/Z:8/1)


0.96
0.99
1.16
0.99
1.29
1.01
1.03
1.01
0.13
1.11
1.01
3.02
1.22
1.03
3.00
ppm
7.907
7.887
7.649
7.644
7.613
7.611
7.593
7.576
7.573
7.499
7.480
7.457
7.438
7.420
7.370
7.350
7.330
7.267
7.183
7.164
7.103
6.963
6.958
6.943
6.938
5.054
5.029
3.832
3.058
3.053
3.011
3.007
2.619
2.595
2.573
2.549
2.109
0.000

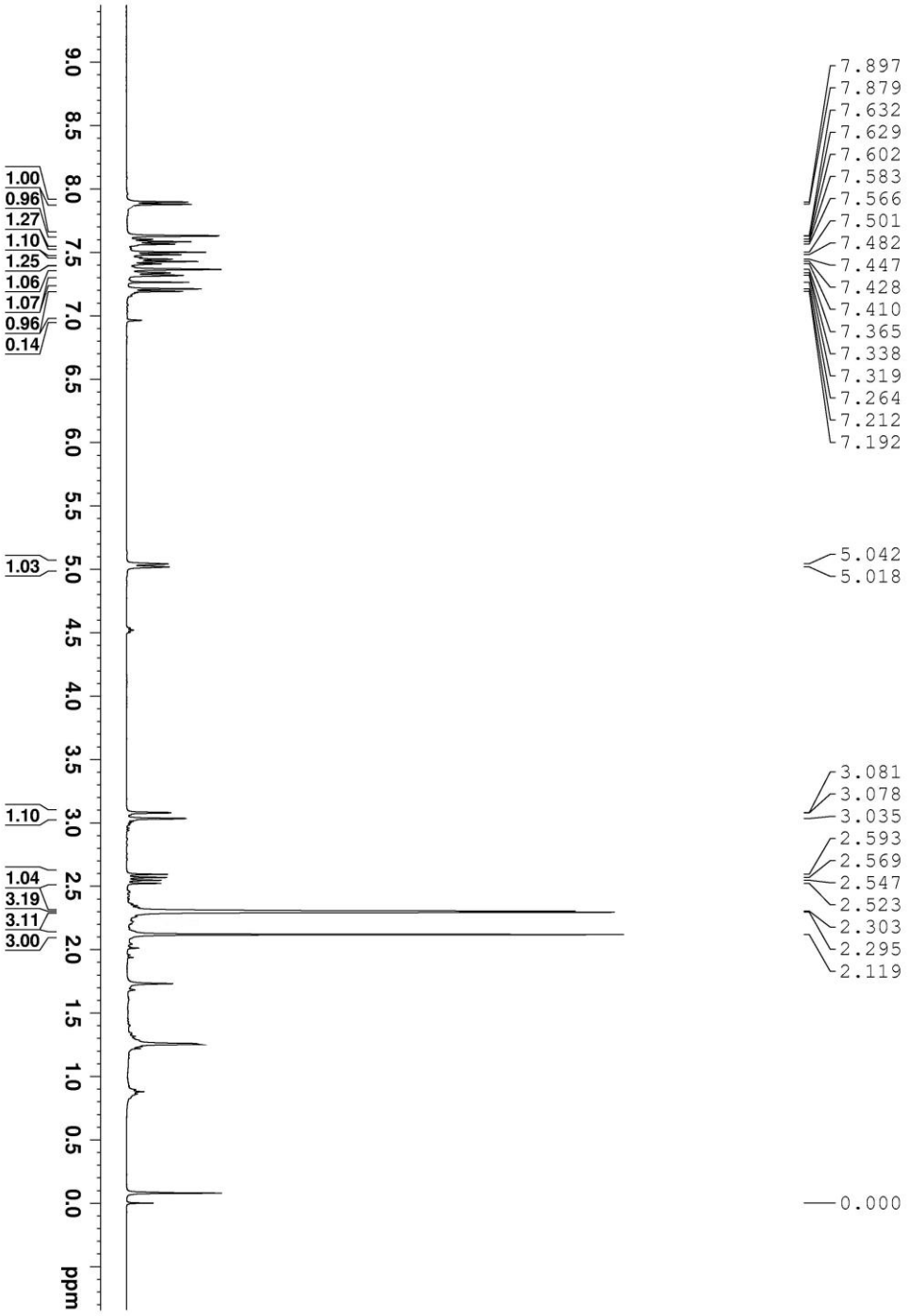

O
OMe
O

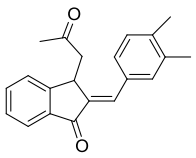
2g (E/Z:8/1)


207.22
193.57
159.92
154.25
139.02
136.87
135.64
135.15
133.52
129.94
128.06
125.65
124.29
123.24
116.19
115.06
77.32
77.00
76.68
55.29
47.19
36.42
30.45
ppm

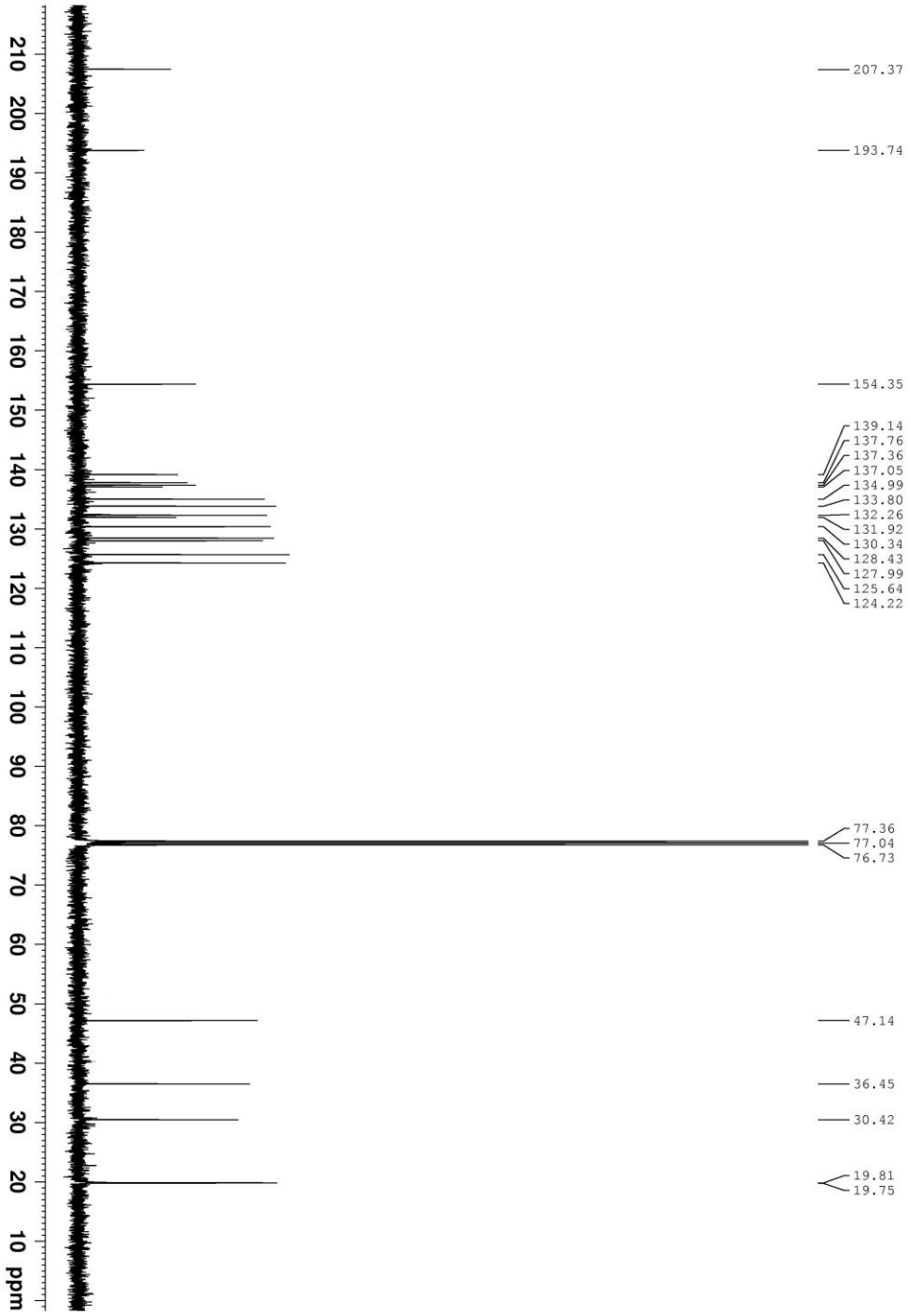


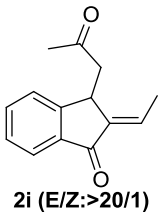
2h (E/Z:7/1)


1.00
0.96
1.27
1.10
1.25
1.06
1.07
0.96
0.14
1.03
1.10
1.04
3.19
3.11
3.00
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
ppm
7.897
7.879
7.632
7.629
7.602
7.583
7.566
7.501
7.482
7.447
7.428
7.410
7.365
7.338
7.319
7.264
7.212
7.192
5.042
5.018
3.081
3.078
3.035
2.593
2.569
2.547
2.523
2.303
2.295
2.119
0.000

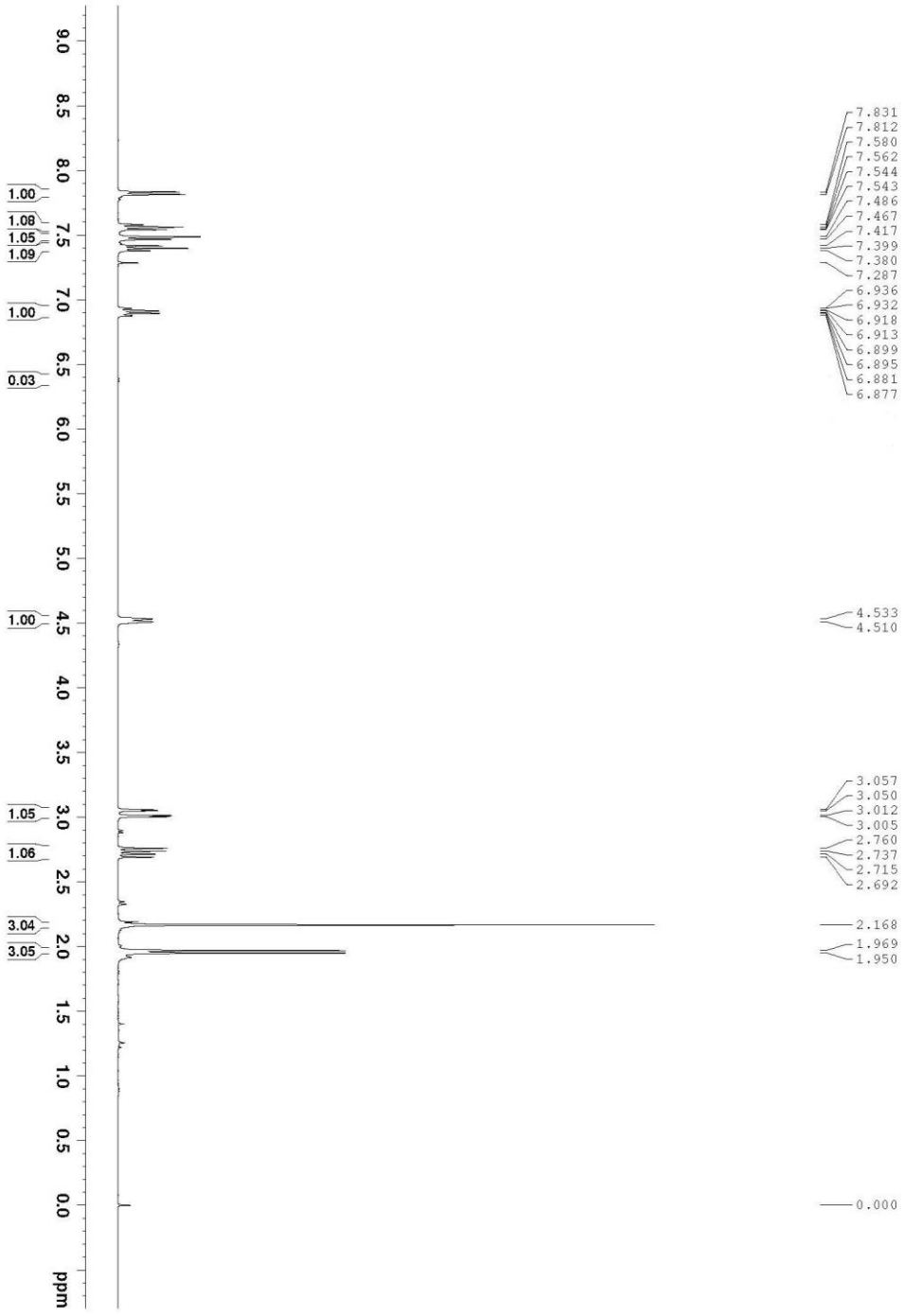


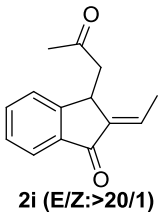
2h (E/Z:7/1)


207.37
193.74
154.35
139.14
137.76
137.36
137.05
134.99
133.80
132.26
131.92
130.34
128.43
127.99
125.64
124.22
77.36
77.04
76.73
47.14
36.45
30.42
19.81
19.75
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



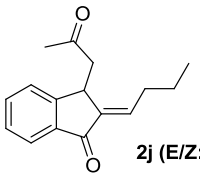
2i (E/Z:>20/1)


7.831
7.812
7.580
7.562
7.544
7.543
7.486
7.467
7.417
7.399
7.380
7.287
6.936
6.932
6.918
6.913
6.899
6.895
6.881
6.877
4.533
4.510
3.057
3.050
3.012
3.005
2.760
2.737
2.715
2.692
2.168
1.969
1.950
0.000
1.00
1.08
1.05
1.09
1.00
0.03
1.00
1.05
1.06
3.04
3.05
ppm

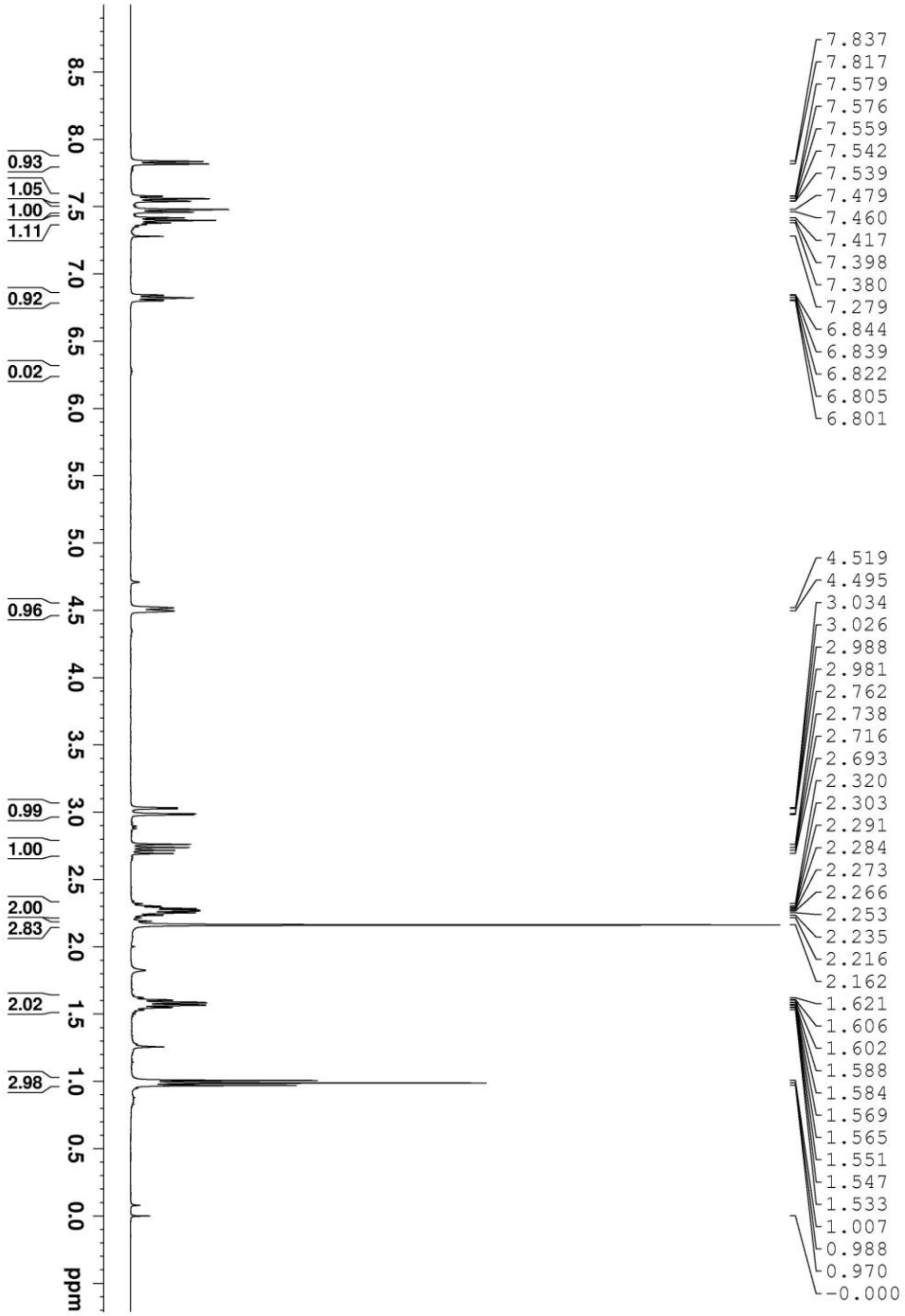


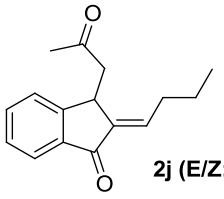
2i (E/Z:>20/1)


206.63
192.61
153.60
141.19
137.41
134.86
132.81
127.92
125.84
124.15
77.32
77.00
76.68
48.71
35.60
30.52
14.88
ppm

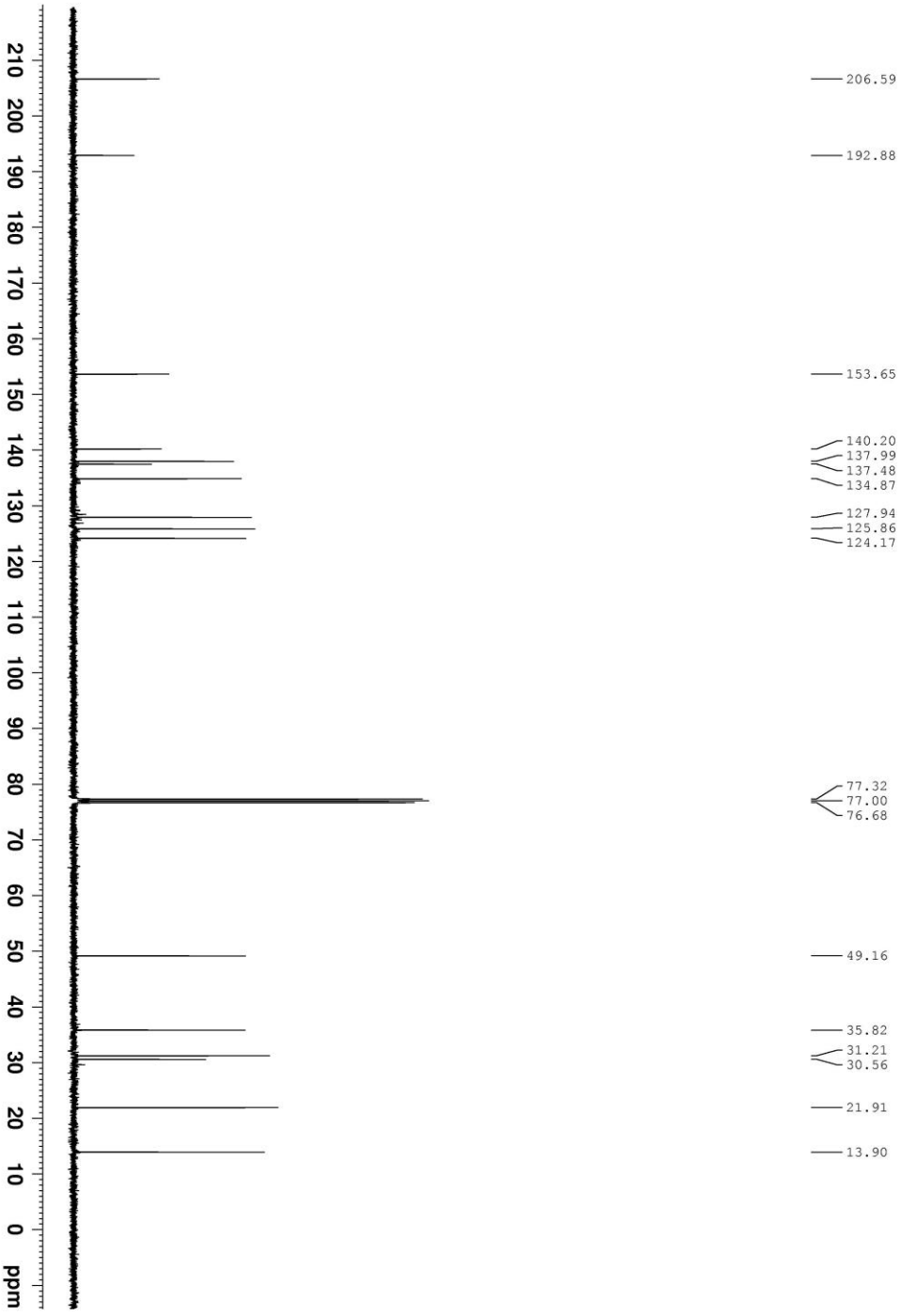


2j (E/Z:>20/1)


0.93
1.05
1.00
1.11
0.92
0.02
0.96
0.99
1.00
2.00
2.83
2.02
2.98
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
ppm
7.837
7.817
7.579
7.576
7.559
7.542
7.539
7.479
7.460
7.417
7.398
7.380
7.279
6.844
6.839
6.822
6.805
6.801
4.519
4.495
3.034
3.026
2.988
2.981
2.762
2.738
2.716
2.693
2.320
2.303
2.291
2.284
2.273
2.266
2.253
2.235
2.216
2.162
1.621
1.606
1.602
1.588
1.584
1.569
1.565
1.551
1.547
1.533
1.007
0.988
0.970
-0.000



2j (E/Z:>20/1)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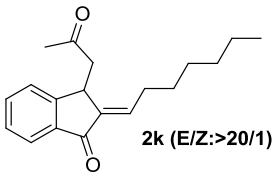
192.88
153.65
140.20
137.99
137.48
134.87
127.94
125.86
124.17
77.32
77.00
76.68
49.16
35.82
31.21
30.56
21.91
13.90
ppm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O
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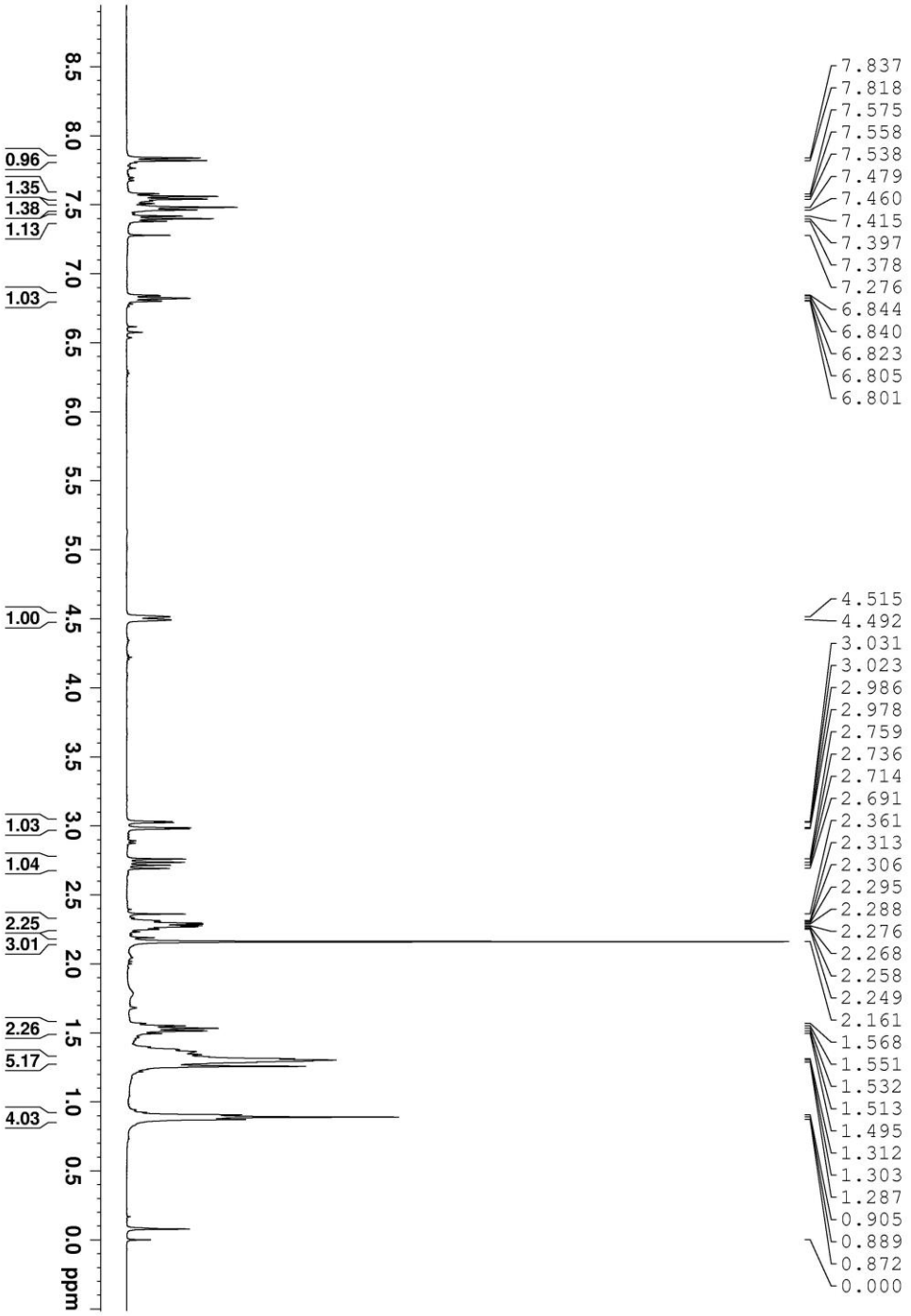
2k (E/Z:>20/1)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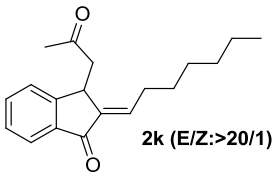
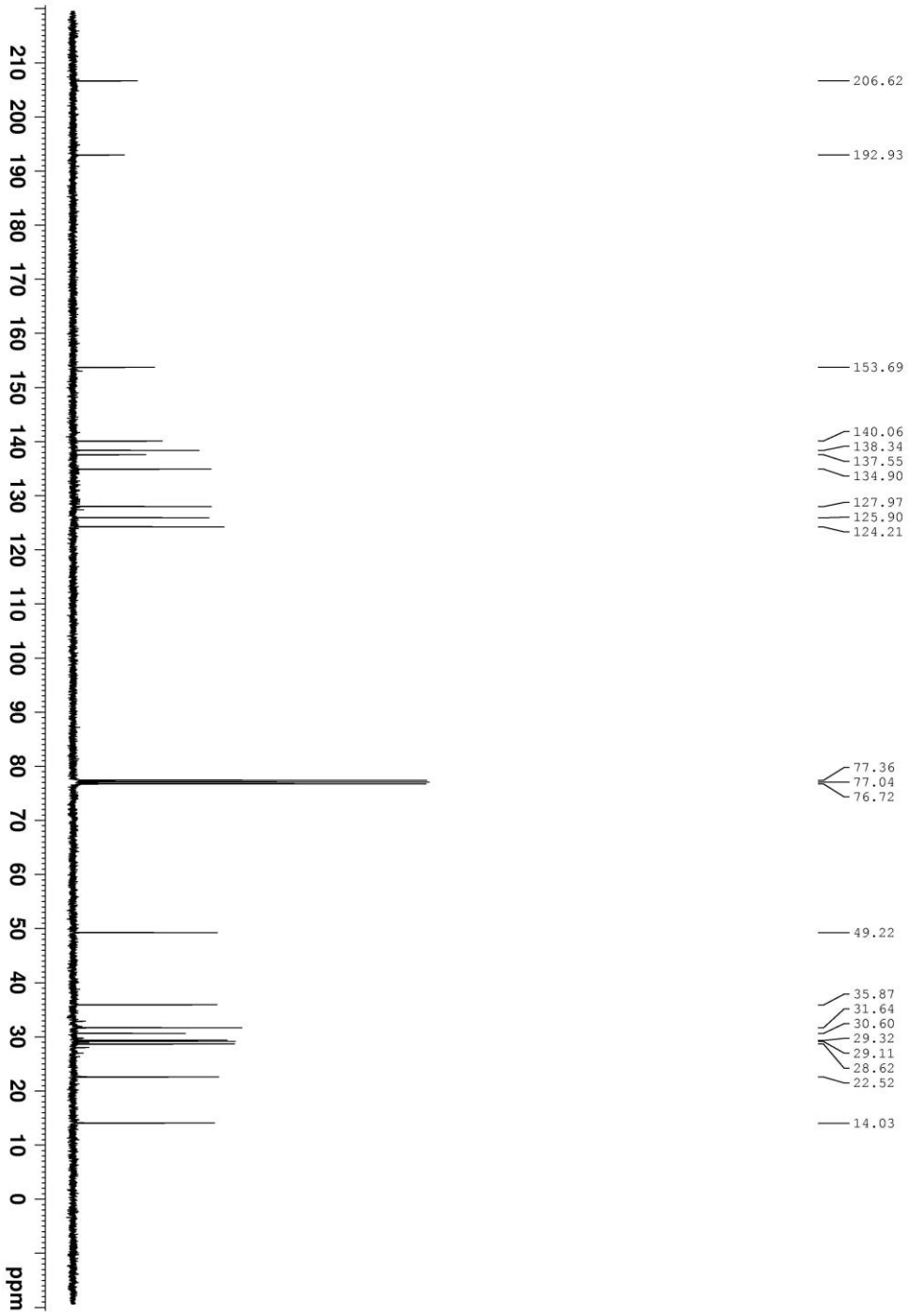
1.35
1.38
1.13
1.03
1.00
1.03
1.04
2.25
3.01
2.26
5.17
4.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
7.837
7.818
7.575
7.558
7.538
7.479
7.460
7.415
7.397
7.378
7.276
6.844
6.840
6.823
6.805
6.801
4.515
4.492
3.031
3.023
2.986
2.978
2.759
2.736
2.714
2.691
2.361
2.313
2.306
2.295
2.288
2.276
2.268
2.258
2.249
2.161
1.568
1.551
1.532
1.513
1.495
1.312
1.303
1.287
0.905
0.889
0.872
0.000



2k (E/Z:>20/1)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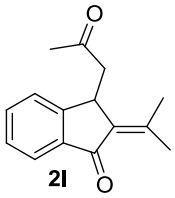
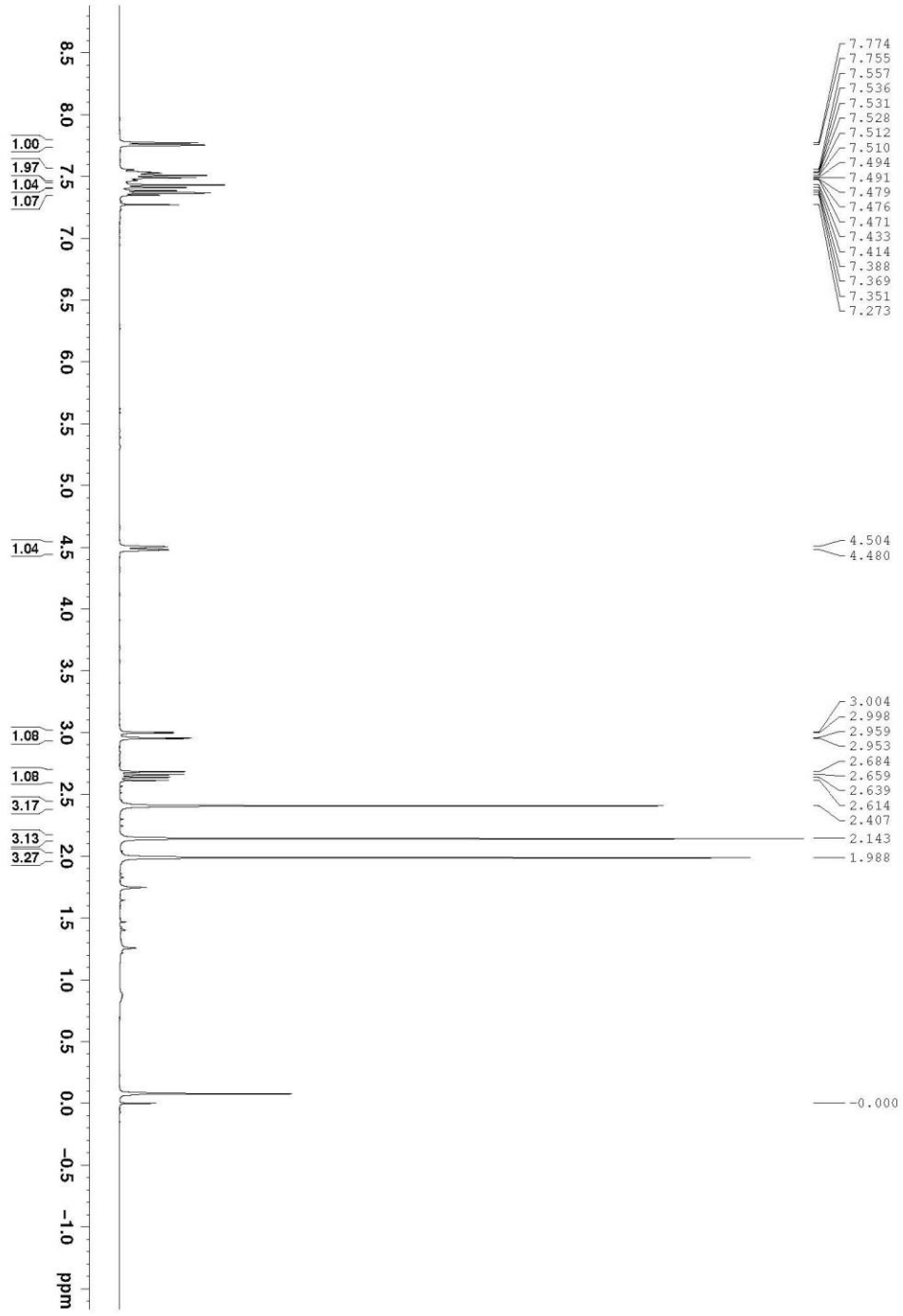
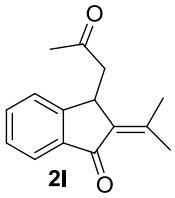
192.93
153.69
140.06
138.34
137.55
134.90
127.97
125.90
124.21
77.36
77.04
76.72
49.22
35.87
31.64
30.60
29.32
29.11
28.62
22.52
14.03
ppm


O
O
2l


7.774
7.755
7.557
7.536
7.531
7.528
7.512
7.510
7.494
7.491
7.479
7.476
7.471
7.433
7.414
7.388
7.369
7.351
7.273
4.504
4.480
3.004
2.998
2.959
2.953
2.684
2.659
2.639
2.614
2.407
2.143
1.988
-0.000
1.00
1.97
1.04
1.07
1.04
1.08
1.08
3.17
3.13
3.27
ppm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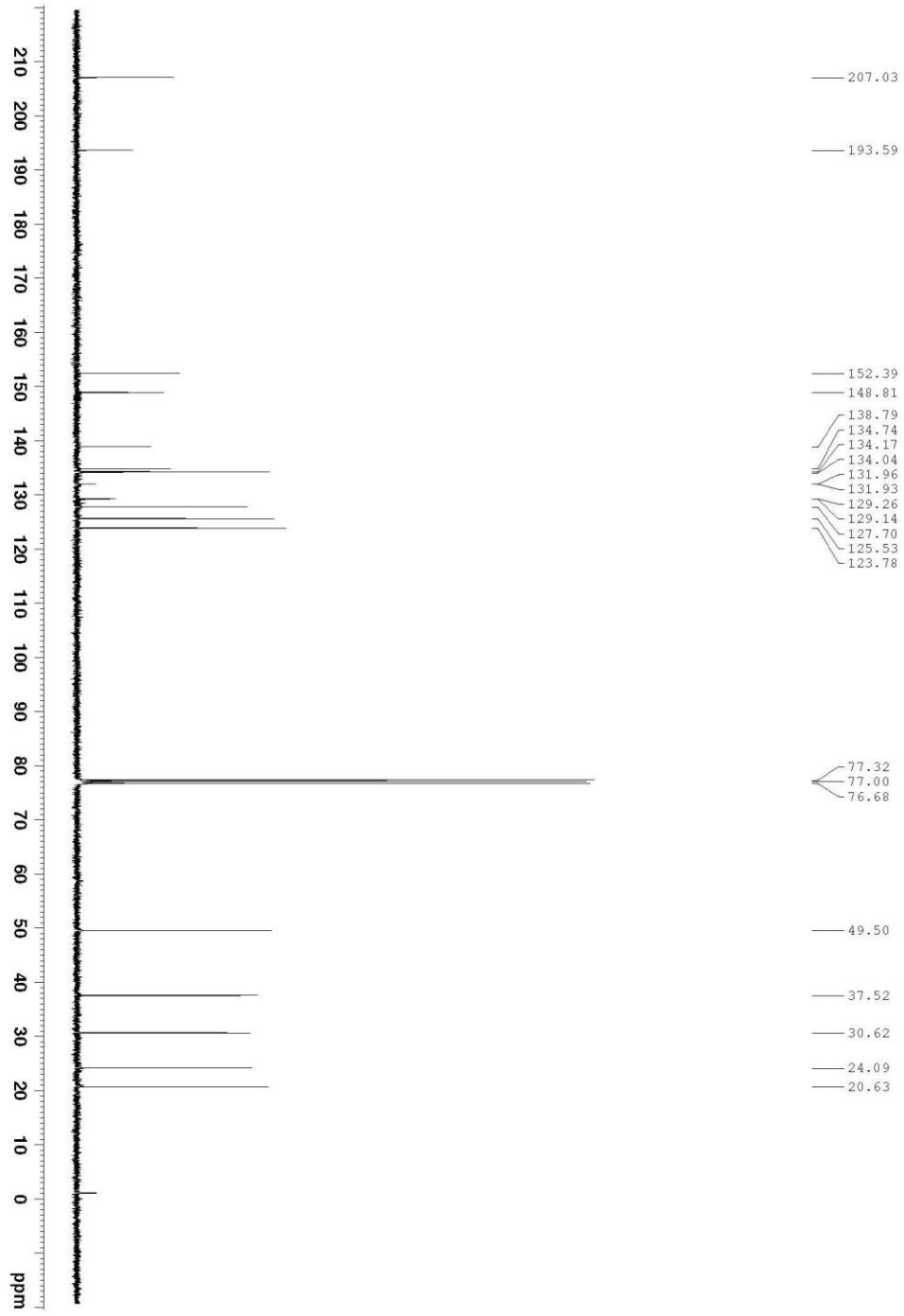
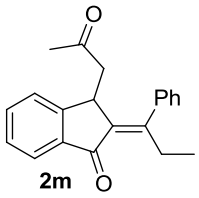
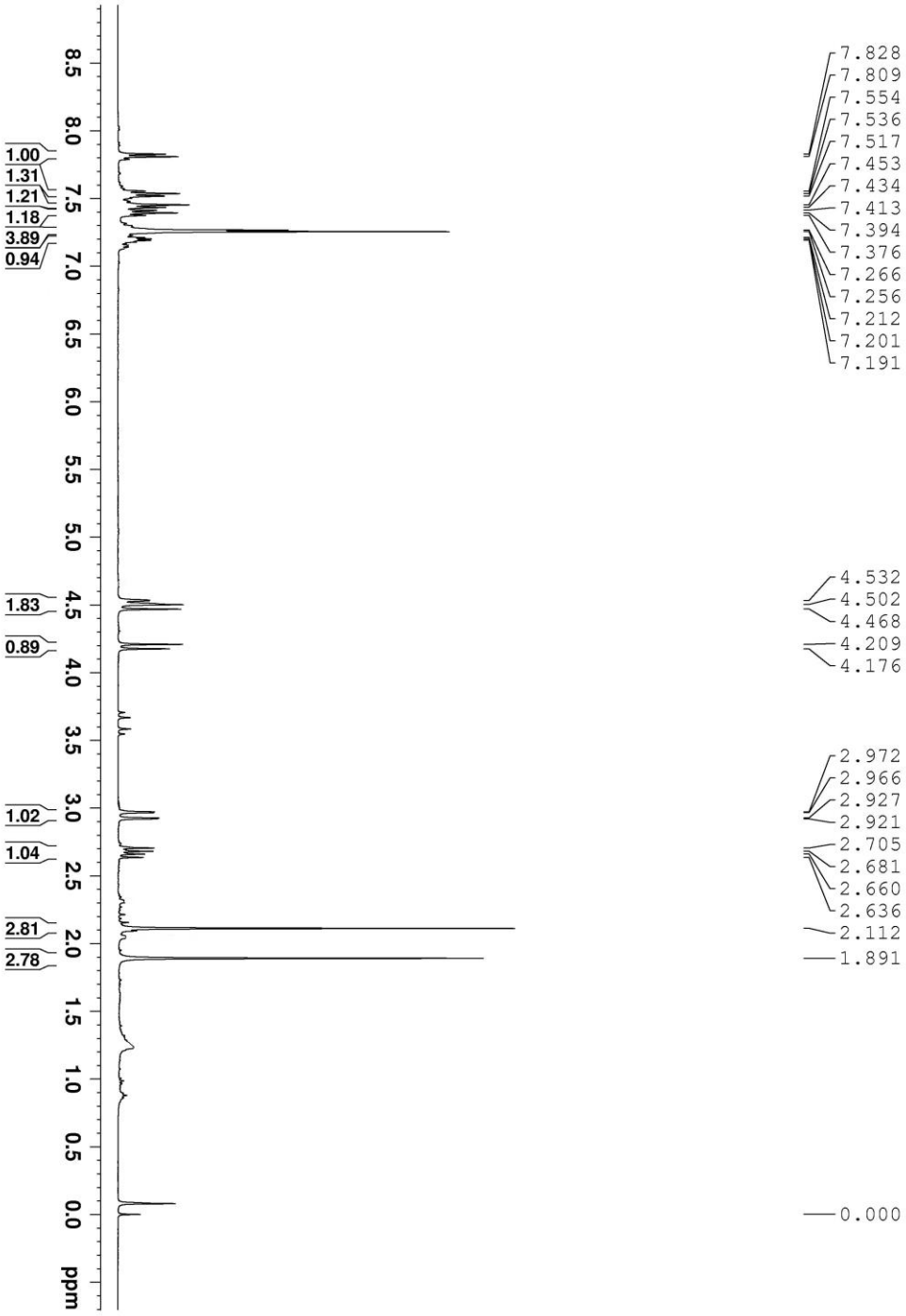
O

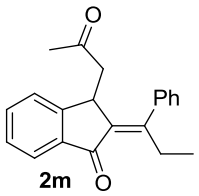
2l


207.03
193.59
152.39
148.81
138.79
134.74
134.17
134.04
131.96
131.93
129.26
129.14
127.70
125.53
123.78
77.32
77.00
76.68
49.50
37.52
30.62
24.09
20.63
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

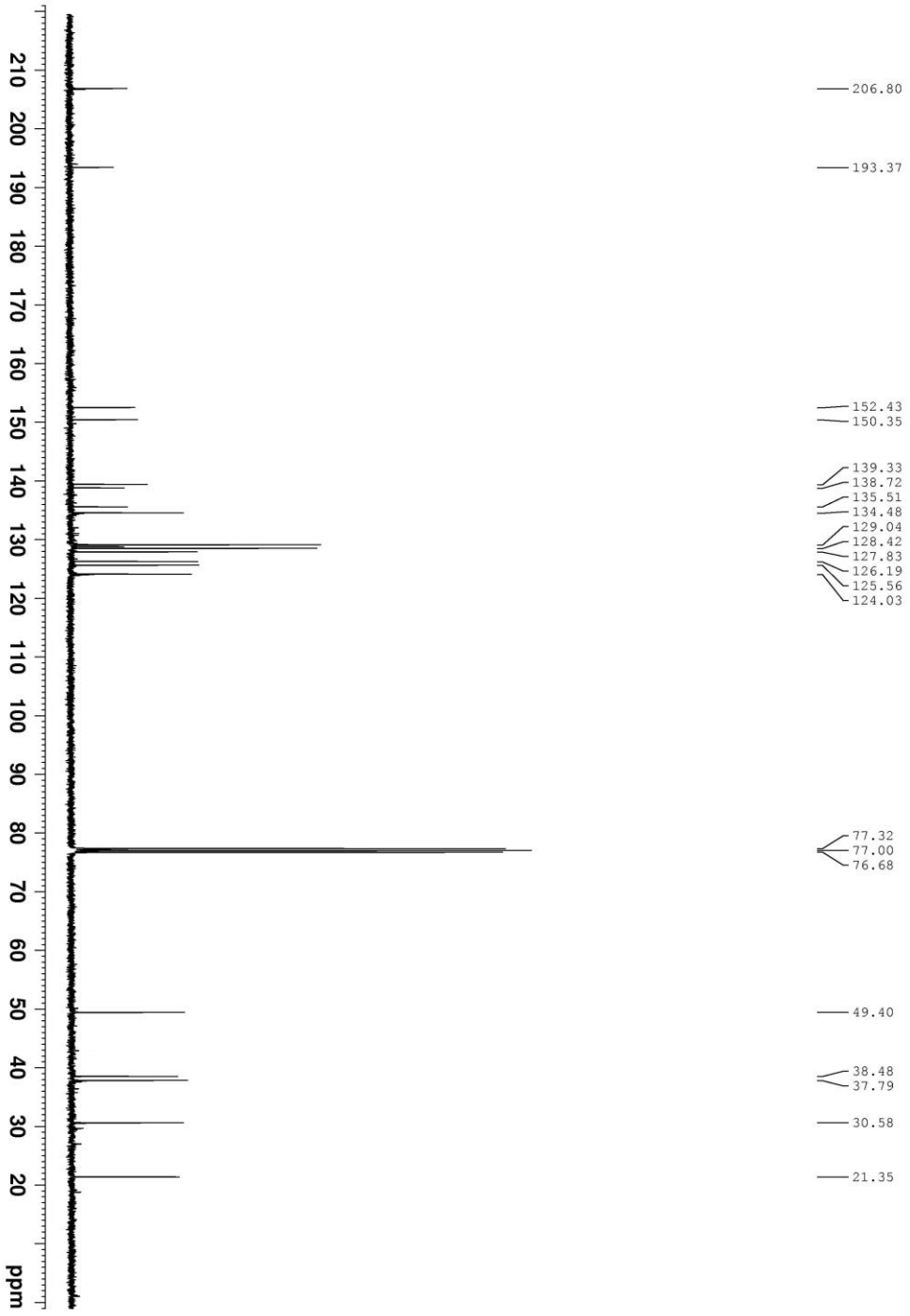

O
Ph
O

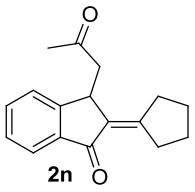
2m

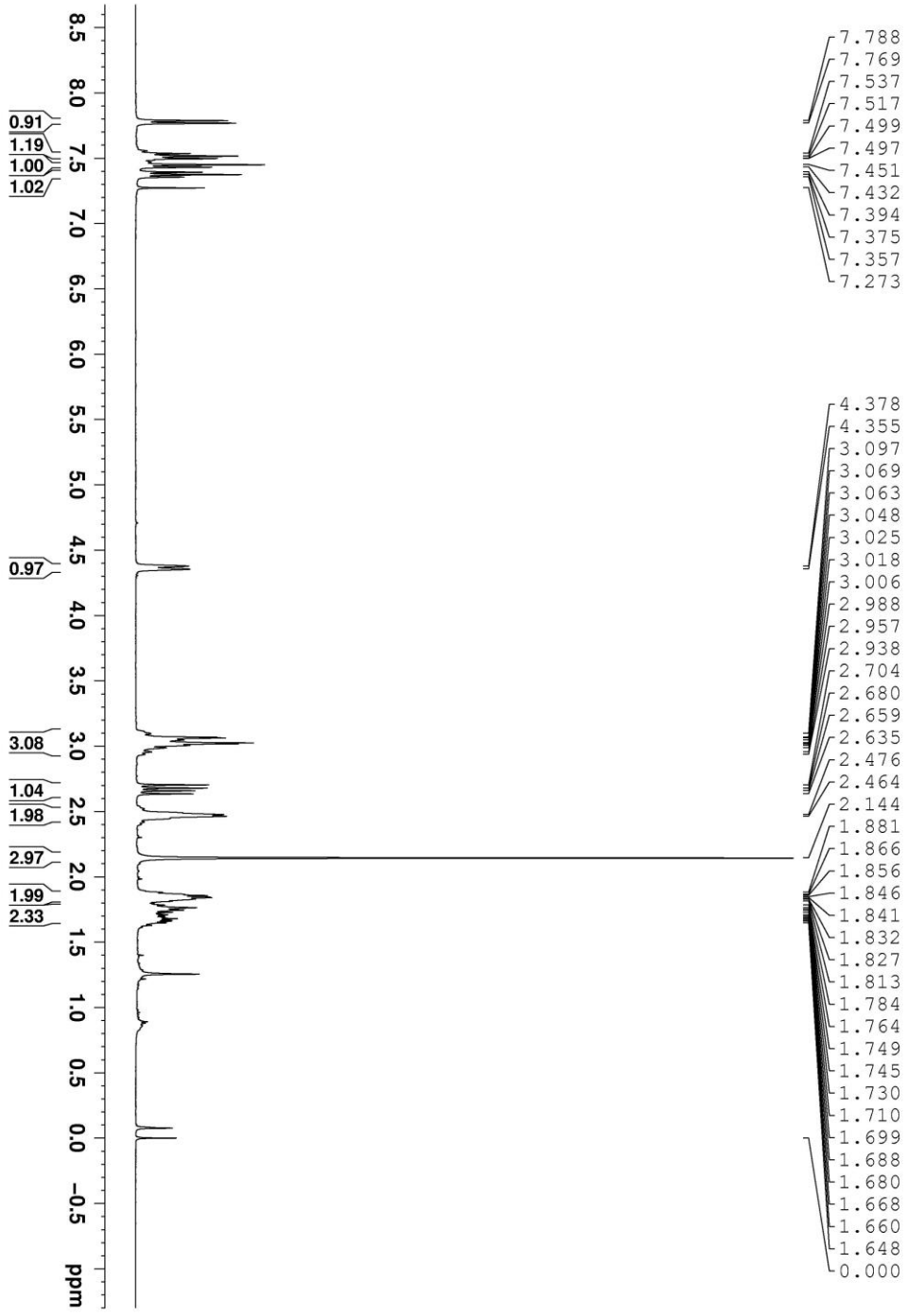

1.00
1.31
1.21
1.18
3.89
0.94
1.83
0.89
1.02
1.04
2.81
2.78
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
7.828
7.809
7.554
7.536
7.517
7.453
7.434
7.413
7.394
7.376
7.266
7.256
7.212
7.201
7.191
4.532
4.502
4.468
4.209
4.176
2.972
2.966
2.927
2.921
2.705
2.681
2.660
2.636
2.112
1.891
0.000

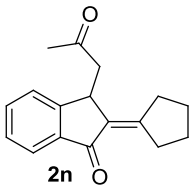

O
Ph
O

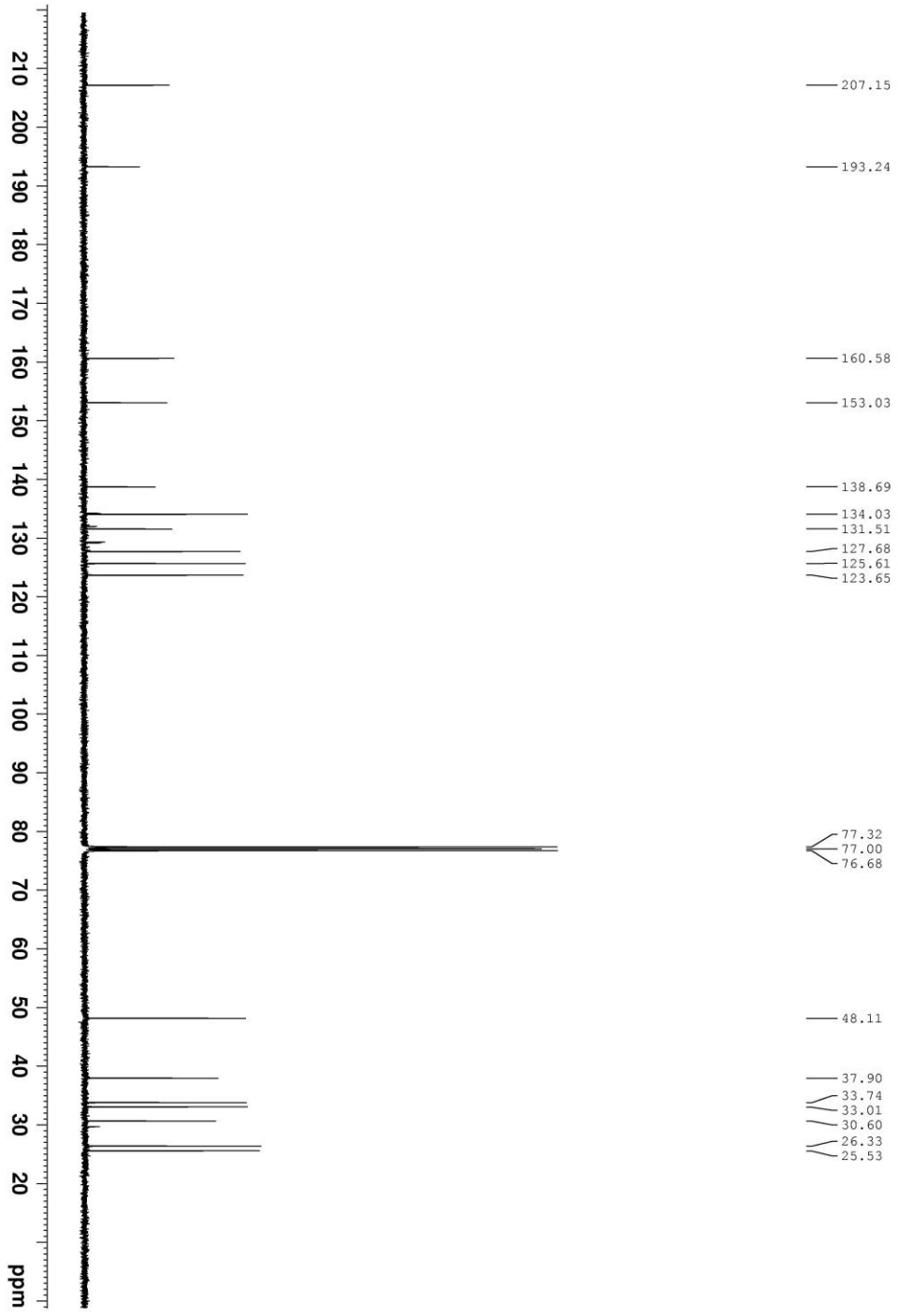
2m

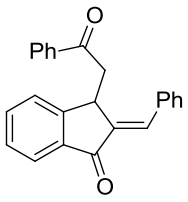

206.80
193.37
152.43
150.35
139.33
138.72
135.51
134.48
129.04
128.42
127.83
126.19
125.56
124.03
77.32
77.00
76.68
49.40
38.48
37.79
30.58
21.35
ppm


O
O
2n

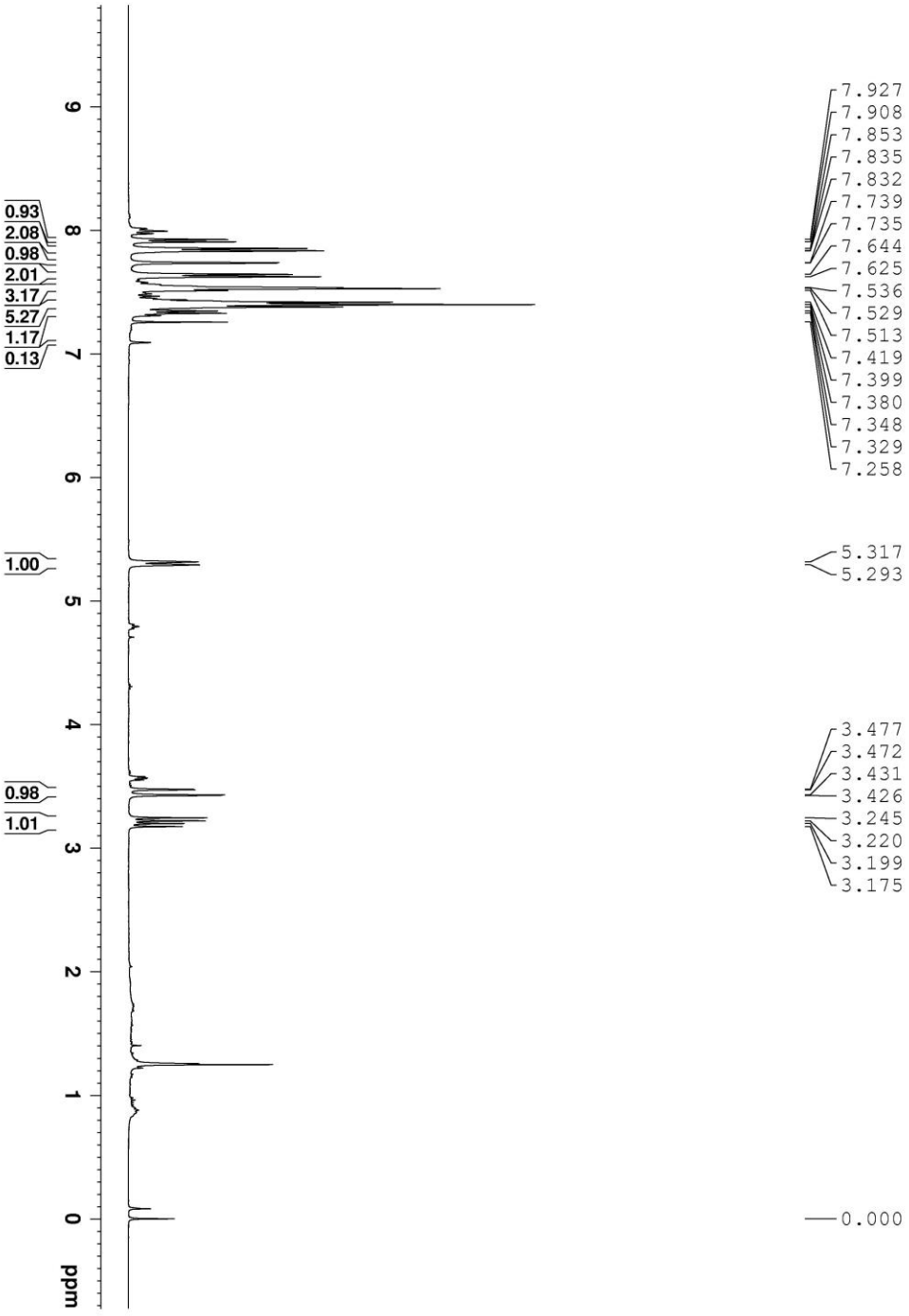

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
ppm
0.91
1.19
1.00
1.02
0.97
3.08
1.04
1.98
2.97
1.99
2.33
7.788
7.769
7.537
7.517
7.499
7.497
7.451
7.432
7.394
7.375
7.357
7.273
4.378
4.355
3.097
3.069
3.063
3.048
3.025
3.018
3.006
2.988
2.957
2.938
2.704
2.680
2.659
2.635
2.476
2.464
2.144
1.881
1.866
1.856
1.846
1.841
1.832
1.827
1.813
1.784
1.764
1.749
1.745
1.730
1.710
1.699
1.688
1.680
1.668
1.660
1.648
0.000

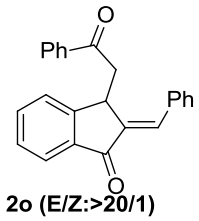

O
O
2n


207.15
193.24
160.58
153.03
138.69
134.03
131.51
127.68
125.61
123.65
77.32
77.00
76.68
48.11
37.90
33.74
33.01
30.60
26.33
25.53
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

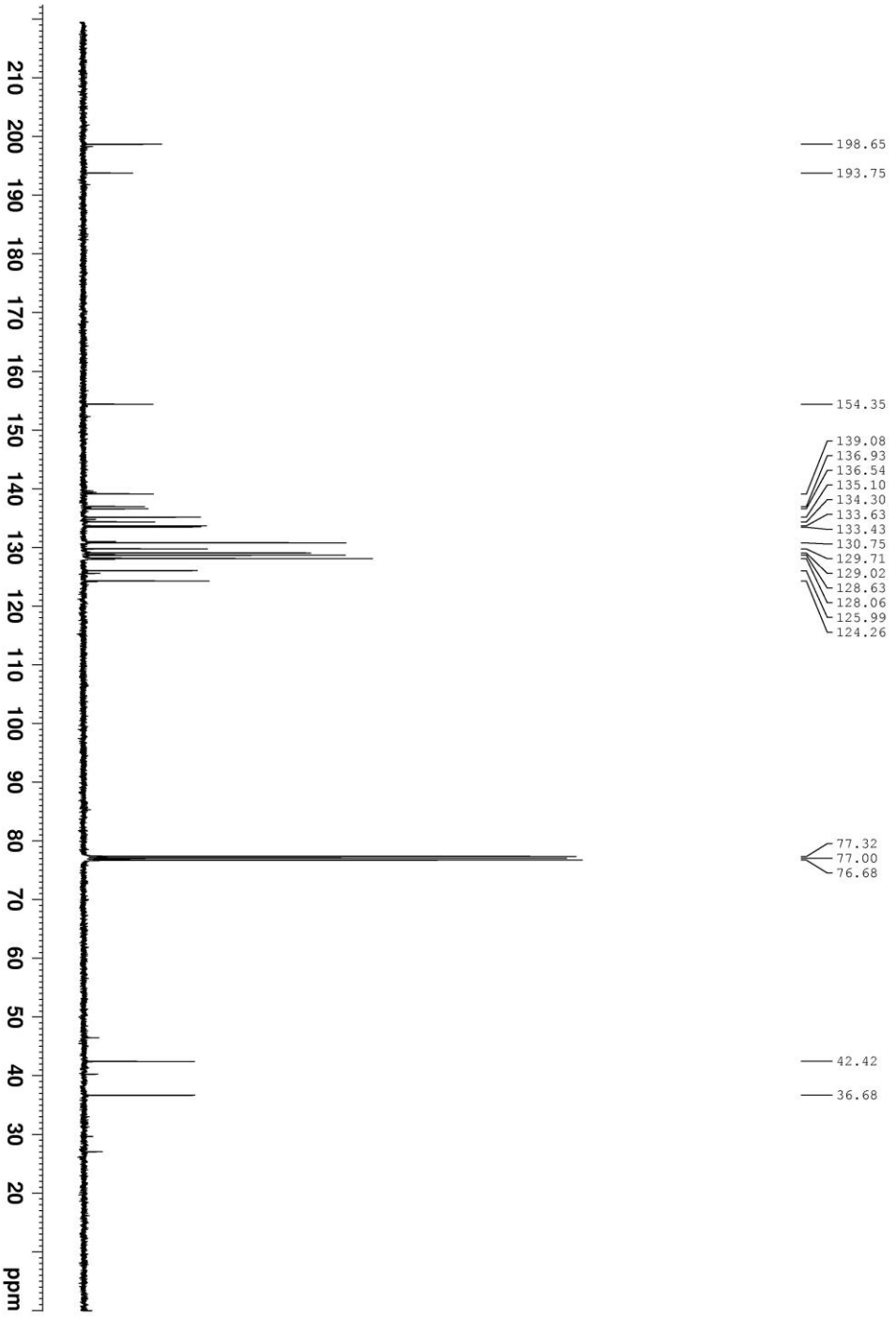

O
Ph
Ph
O

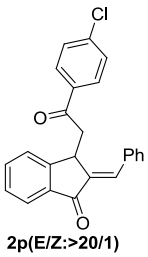
2o (E/Z:8/1)


0.93
2.08
0.98
2.01
3.17
5.27
1.17
0.13
1.00
0.98
1.01
9
8
7
6
5
4
3
2
1
0
ppm
7.927
7.908
7.853
7.835
7.832
7.739
7.735
7.644
7.625
7.536
7.529
7.513
7.419
7.399
7.380
7.348
7.329
7.258
5.317
5.293
3.477
3.472
3.431
3.426
3.245
3.220
3.199
3.175
0.000

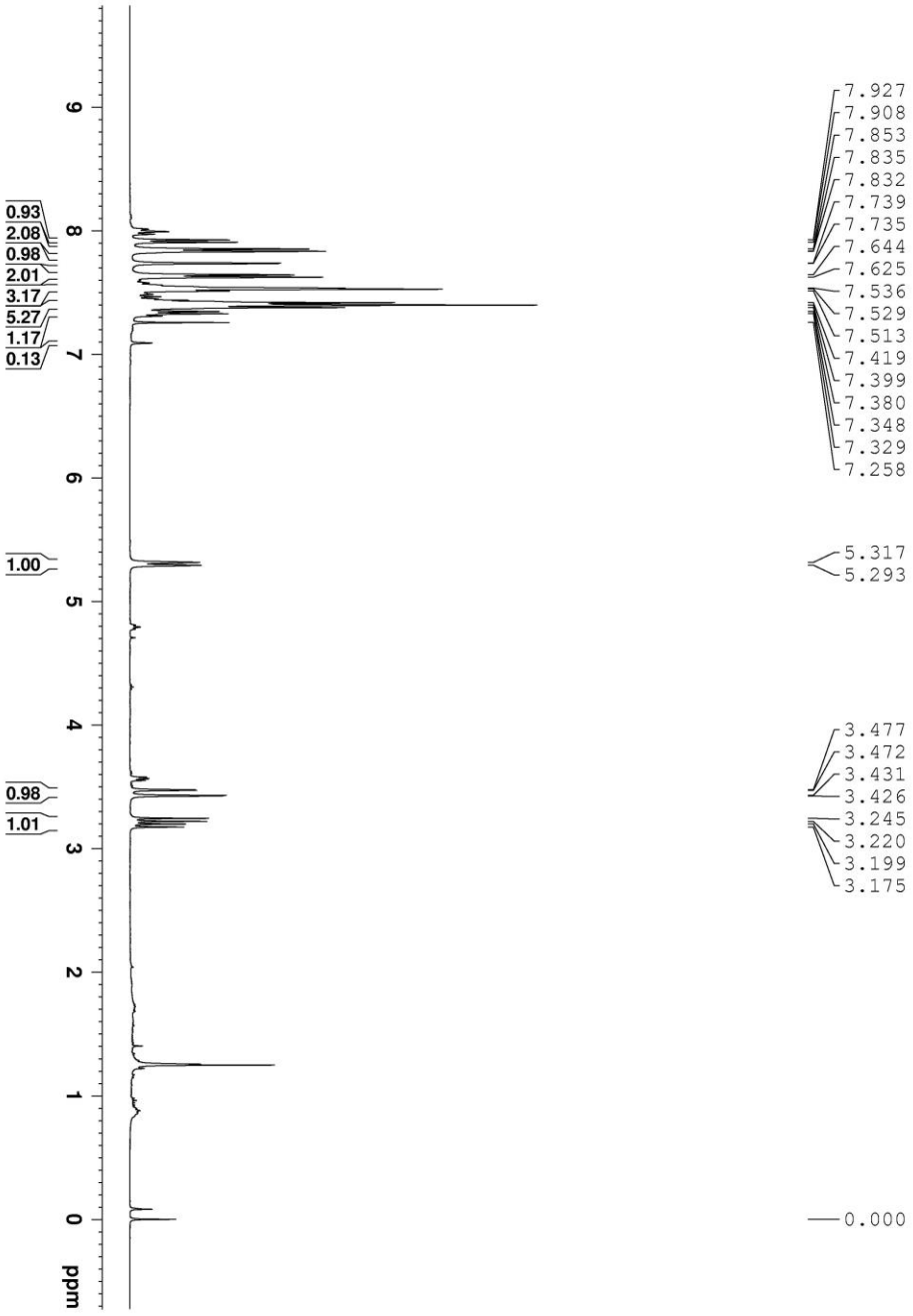

O
Ph
Ph
O

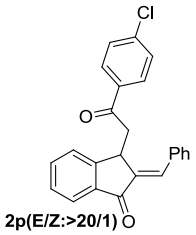
2o (E/Z:>20/1)


198.65
193.75
154.35
139.08
136.93
136.54
135.10
134.30
133.63
133.43
130.75
129.71
129.02
128.63
128.06
125.99
124.26
77.32
77.00
76.68
42.42
36.68
ppm

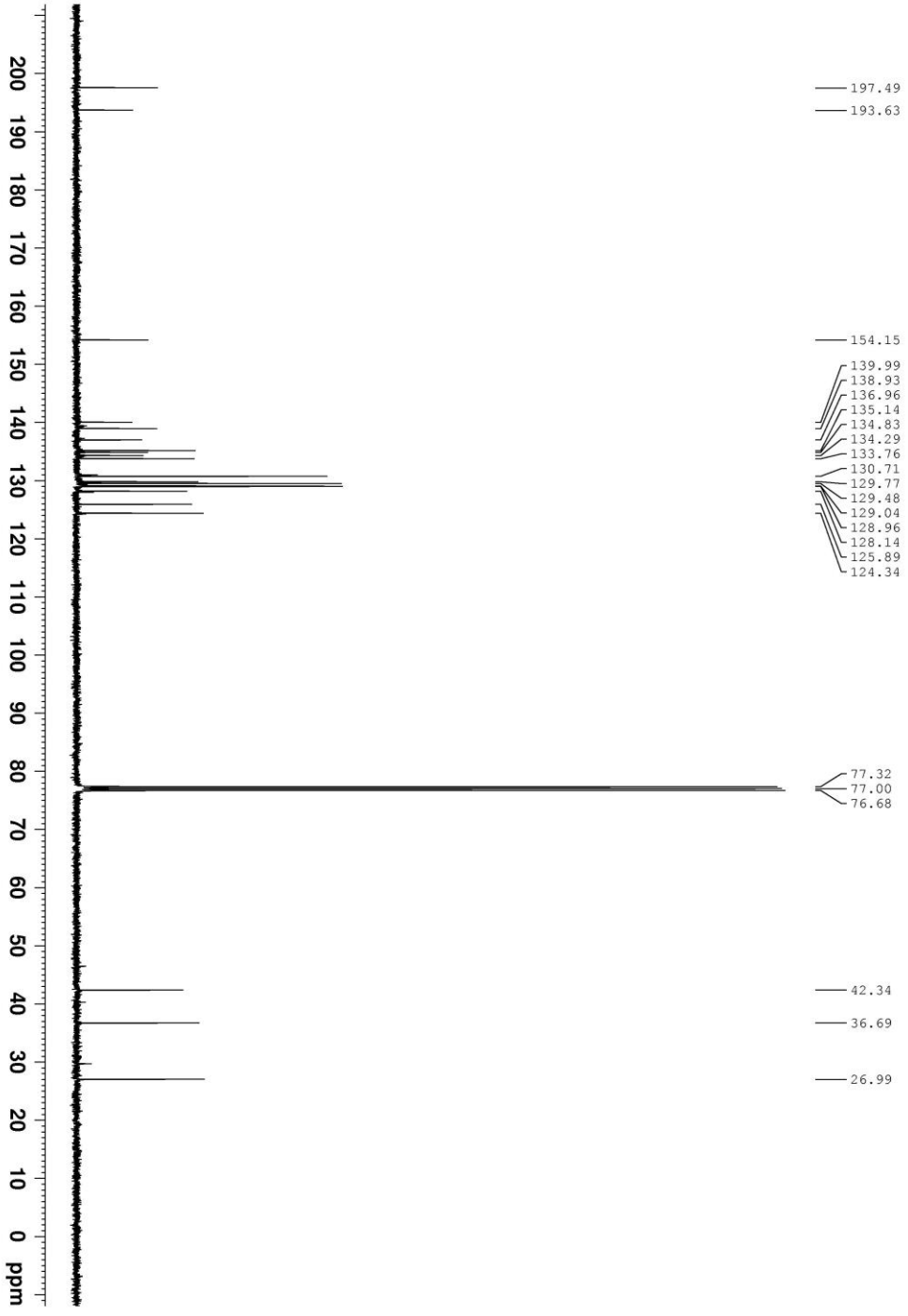

Cl
O
Ph
O

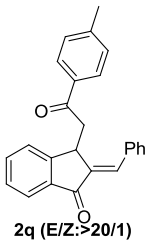
2p(E/Z:>20/1)


0.93
2.08
0.98
2.01
3.17
5.27
1.17
0.13
1.00
0.98
1.01
9
8
7
6
5
4
3
2
1
0
ppm
7.927
7.908
7.853
7.835
7.832
7.739
7.735
7.644
7.625
7.536
7.529
7.513
7.419
7.399
7.380
7.348
7.329
7.258
5.317
5.293
3.477
3.472
3.431
3.426
3.245
3.220
3.199
3.175
0.000

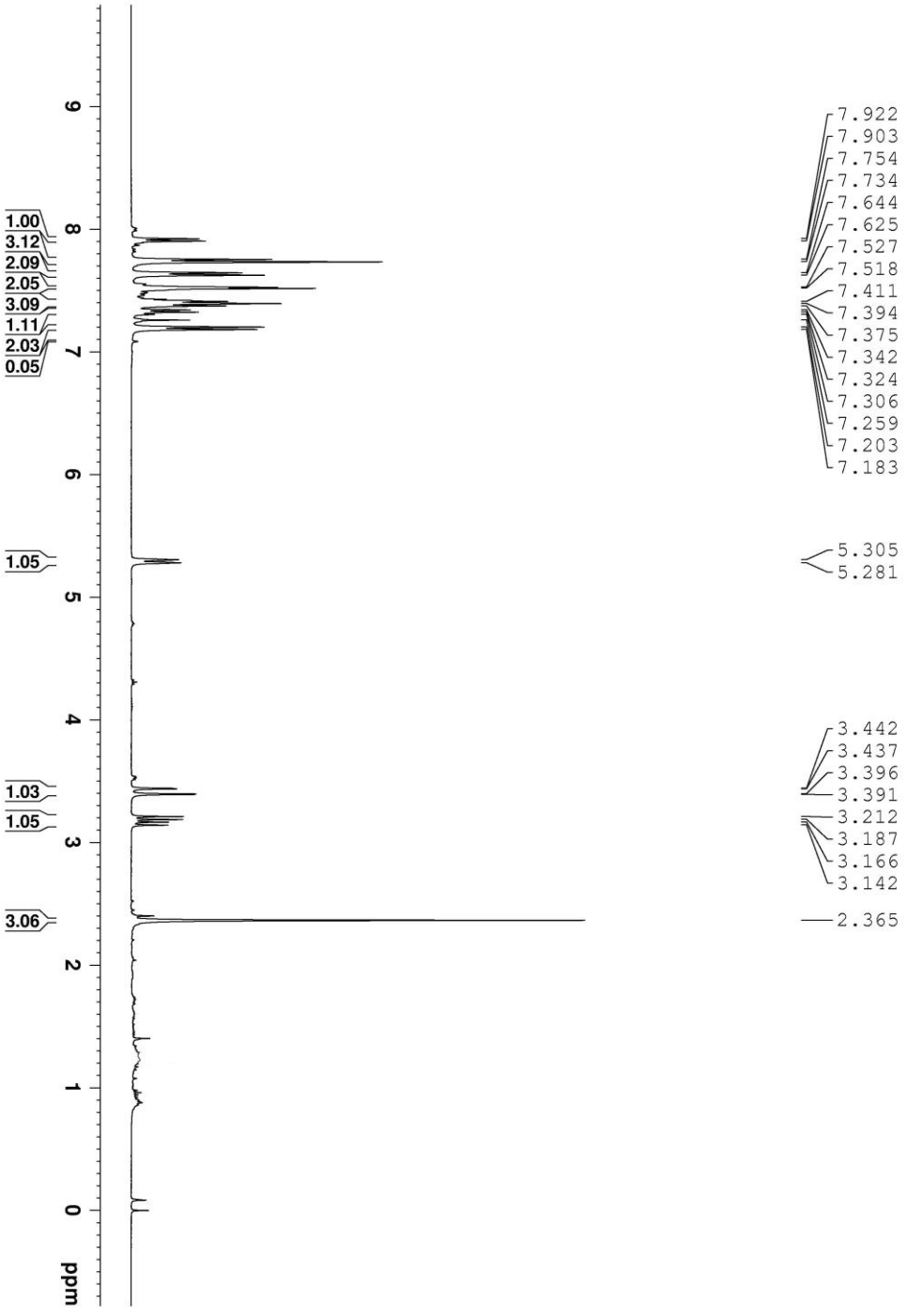

Cl
O
Ph
O

2p(E/Z:>20/1)


197.49
193.63
154.15
139.99
138.93
136.96
135.14
134.83
134.29
133.76
130.71
129.77
129.48
129.04
128.96
128.14
125.89
124.34
77.32
77.00
76.68
42.34
36.69
26.99
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
Ph
O

2q (E/Z:>20/1)


1.00
3.12
2.09
2.05
3.09
1.11
2.03
0.05
1.05
1.03
1.05
3.06
9
8
7
6
5
4
3
2
1
0
ppm
7.922
7.903
7.754
7.734
7.644
7.625
7.527
7.518
7.411
7.394
7.375
7.342
7.324
7.306
7.259
7.203
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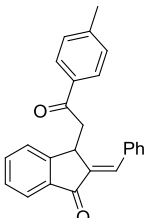
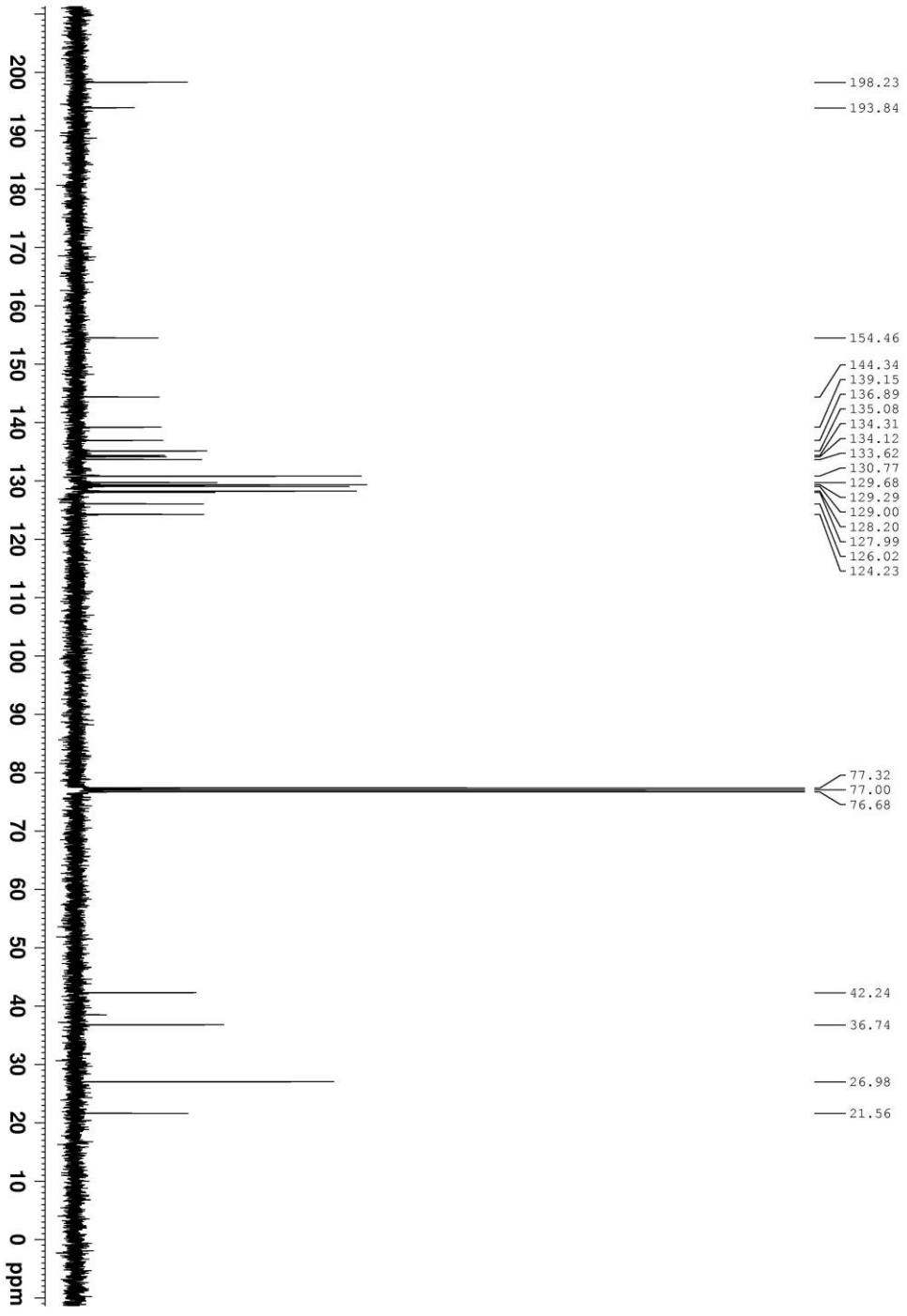
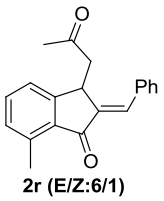
3.391
3.212
3.187
3.166
3.142
2.365

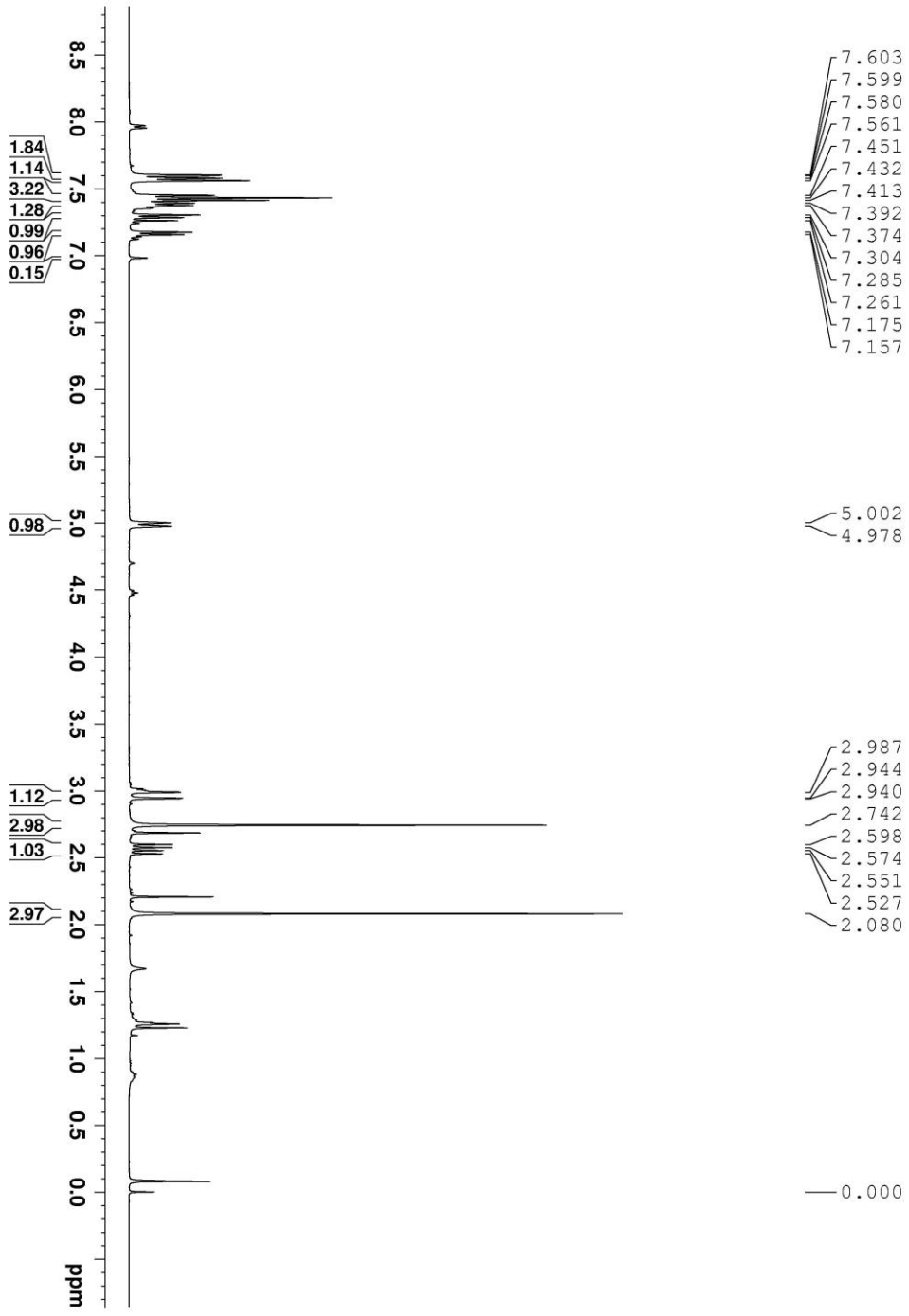

O
Ph
O

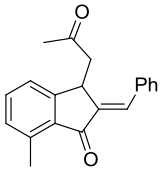
2q (E/Z:>20/1)


198.23
193.84
154.46
144.34
139.15
136.89
135.08
134.31
134.12
133.62
130.77
129.68
129.29
129.00
128.20
127.99
126.02
124.23
77.32
77.00
76.68
42.24
36.74
26.98
21.56
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

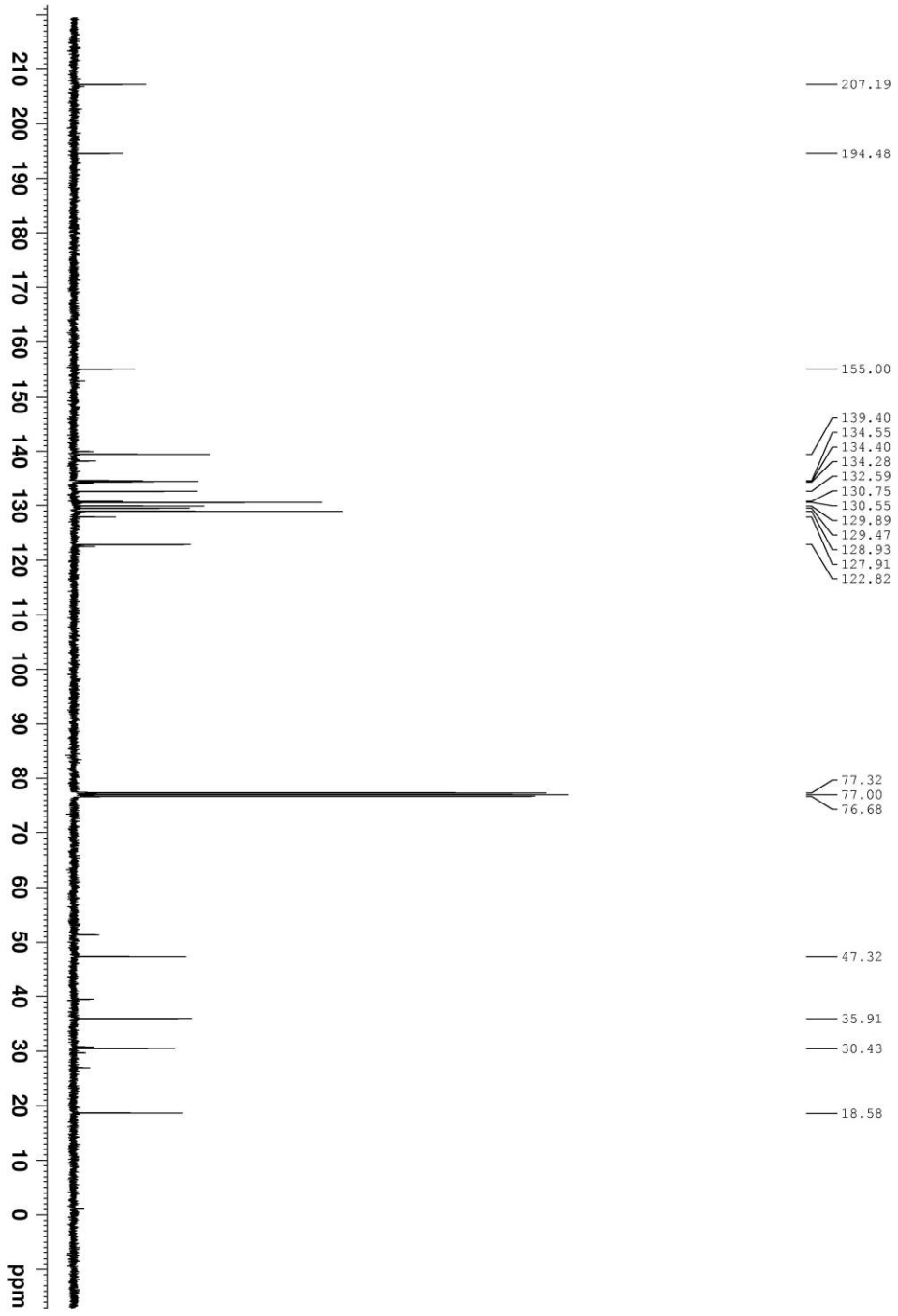

O
Ph
O

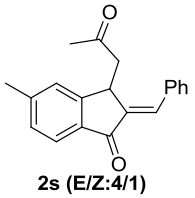
2r (E/Z:6/1)


1.84
1.14
3.22
1.28
0.99
0.96
0.15
0.98
1.12
2.98
1.03
2.97
7.603
7.599
7.580
7.561
7.451
7.432
7.413
7.392
7.374
7.304
7.285
7.261
7.175
7.157
5.002
4.978
2.987
2.944
2.940
2.742
2.598
2.574
2.551
2.527
2.080
0.000
ppm

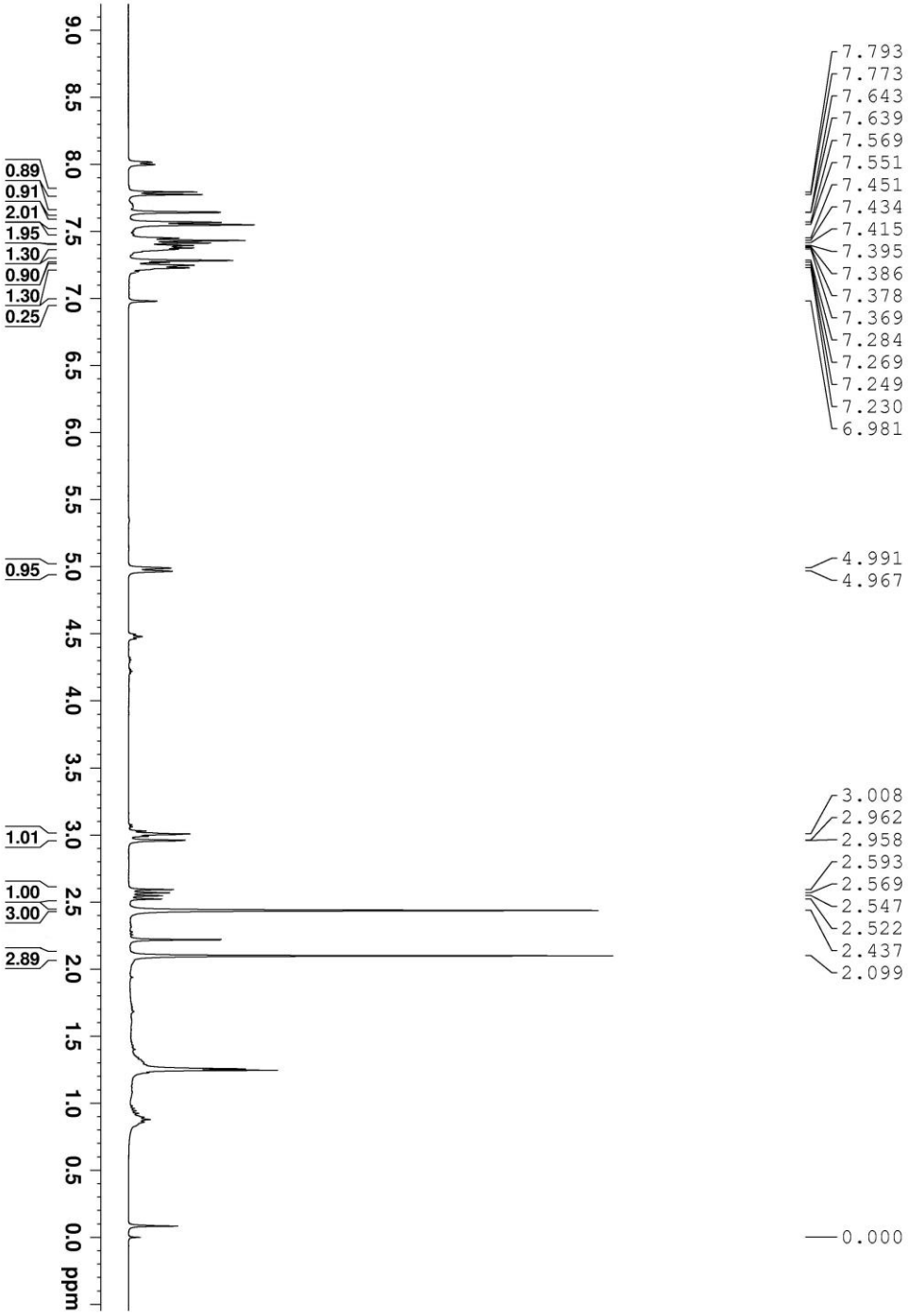

O
Ph
O

2r (E/Z:6/1)


207.19
194.48
155.00
139.40
134.55
134.40
134.28
132.59
130.75
130.55
129.89
129.47
128.93
127.91
122.82
77.32
77.00
76.68
47.32
35.91
30.43
18.58
ppm


O
Ph
O

2s (E/Z:4/1)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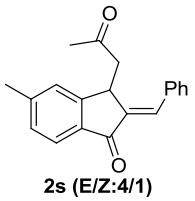
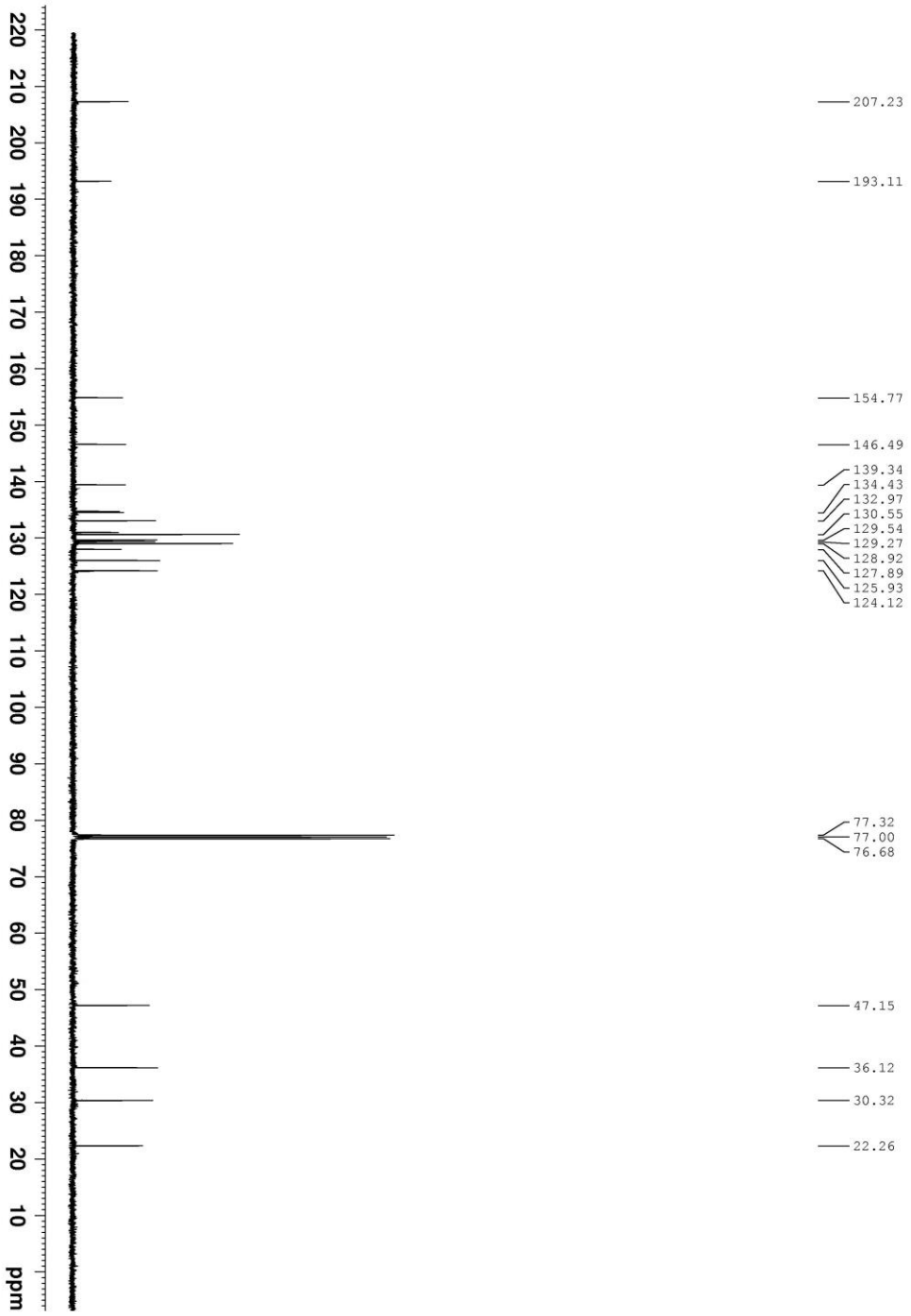
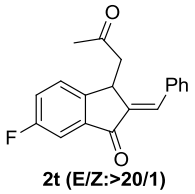
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.89
0.91
2.01
1.95
1.30
0.90
1.30
0.25
0.95
1.01
1.00
3.00
2.89
7.793
7.773
7.643
7.639
7.569
7.551
7.451
7.434
7.415
7.395
7.386
7.378
7.369
7.284
7.269
7.249
7.230
6.981
4.991
4.967
3.008
2.962
2.958
2.593
2.569
2.547
2.522
2.437
2.099
0.000

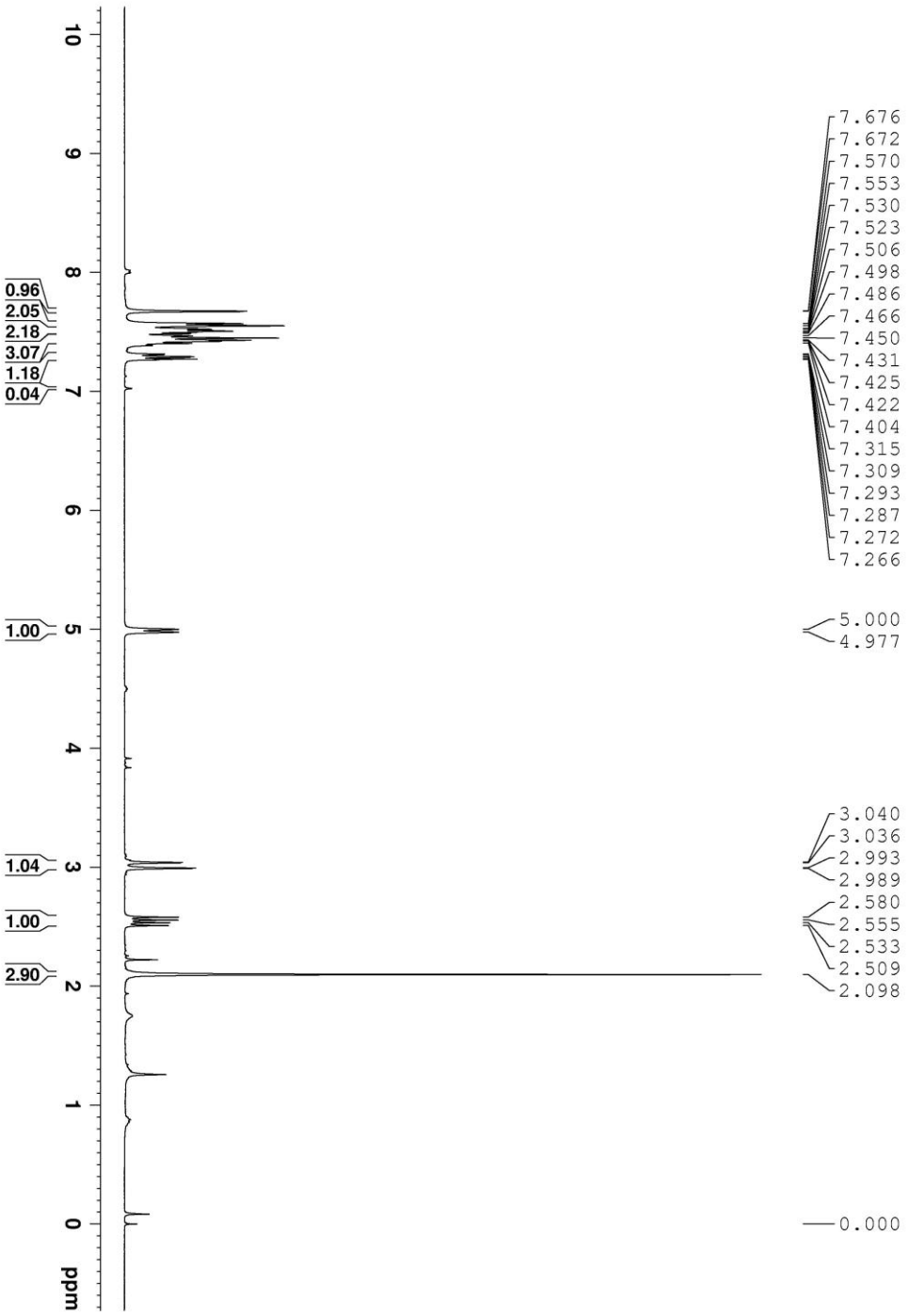

O
Ph
O

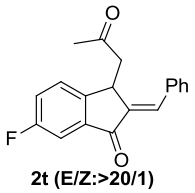
2s (E/Z:4/1)


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
207.23
193.11
154.77
146.49
139.34
134.43
132.97
130.55
129.54
129.27
128.92
127.89
125.93
124.12
77.32
77.00
76.68
47.15
36.12
30.32
22.26

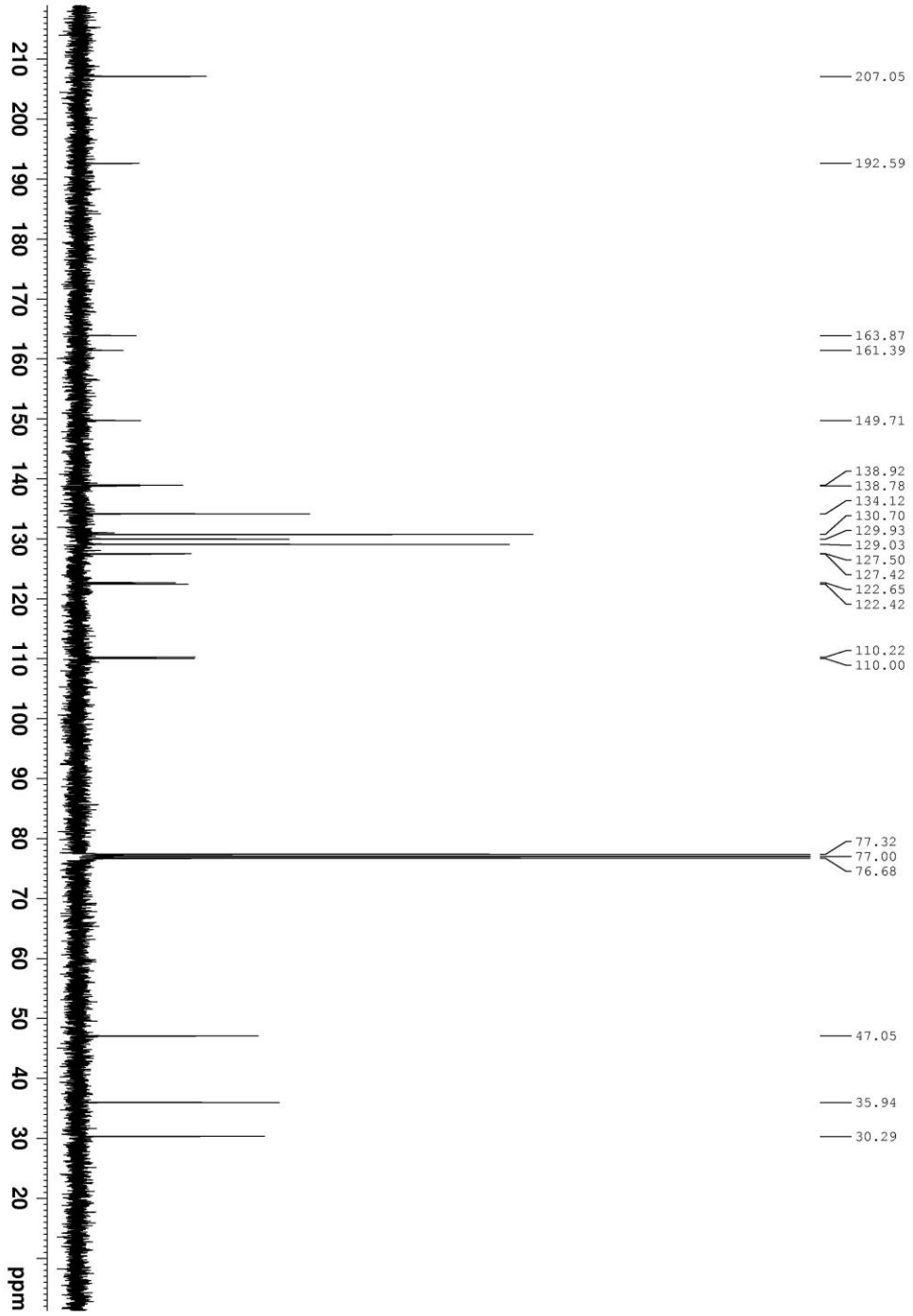

O
Ph
F
O

2t (E/Z:>20/1)


10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
2.05
2.18
3.07
1.18
0.04
1.00
1.04
1.00
2.90
7.676
7.672
7.570
7.553
7.530
7.523
7.506
7.498
7.486
7.466
7.450
7.431
7.425
7.422
7.404
7.315
7.309
7.293
7.287
7.272
7.266
5.000
4.977
3.040
3.036
2.993
2.989
2.580
2.555
2.533
2.509
2.098
0.000


O
Ph
F
O

2t (E/Z:>20/1)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163.87
161.39
149.71
138.92
138.78
134.12
130.70
129.93
129.03
127.50
127.42
122.65
122.42
110.22
110.00
77.32
77.00
76.68
47.05
35.94
30.29
ppm