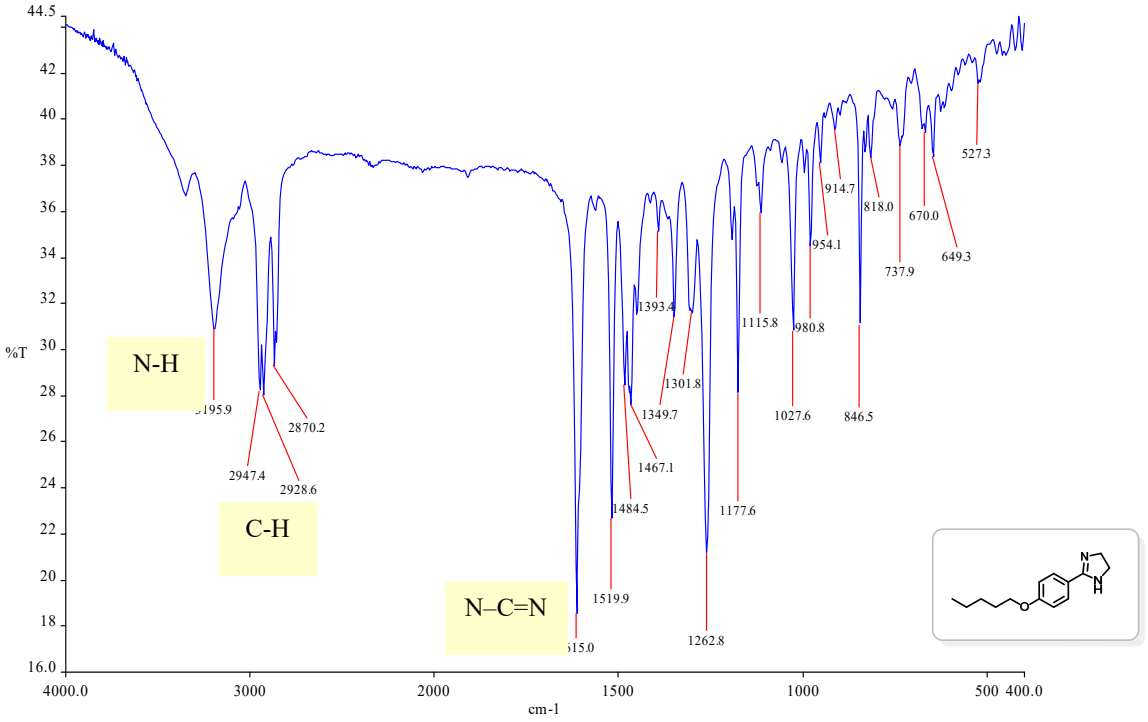
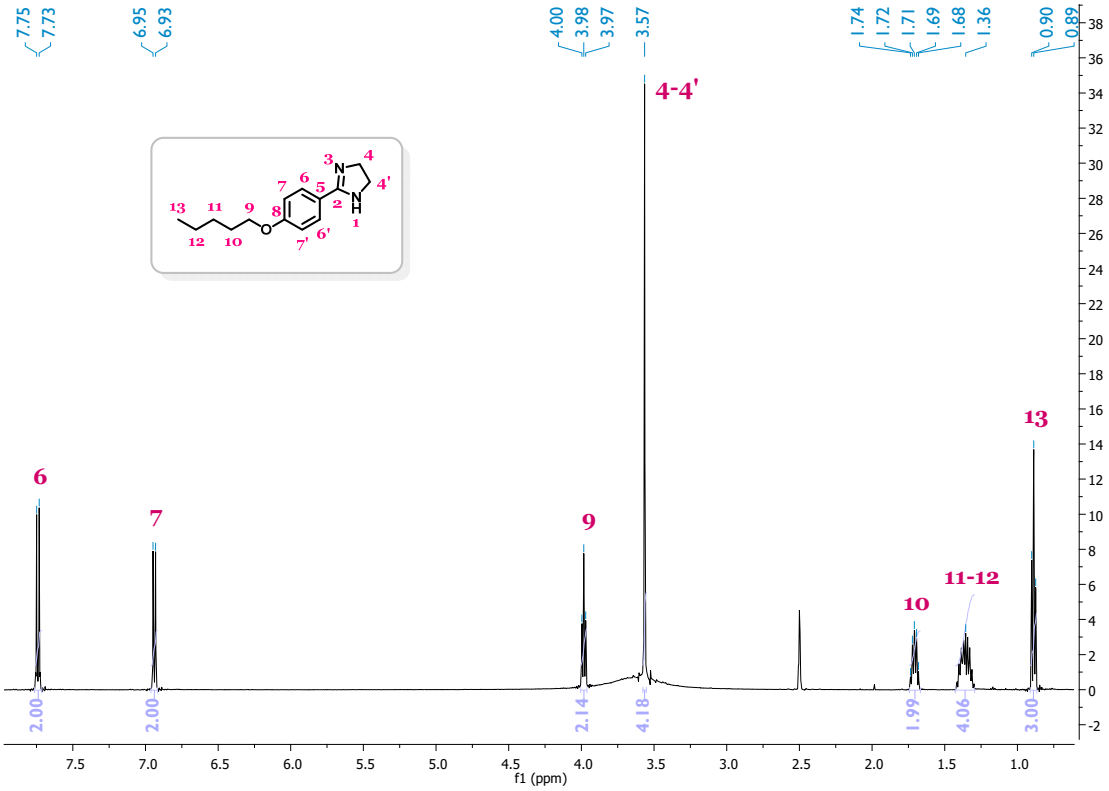
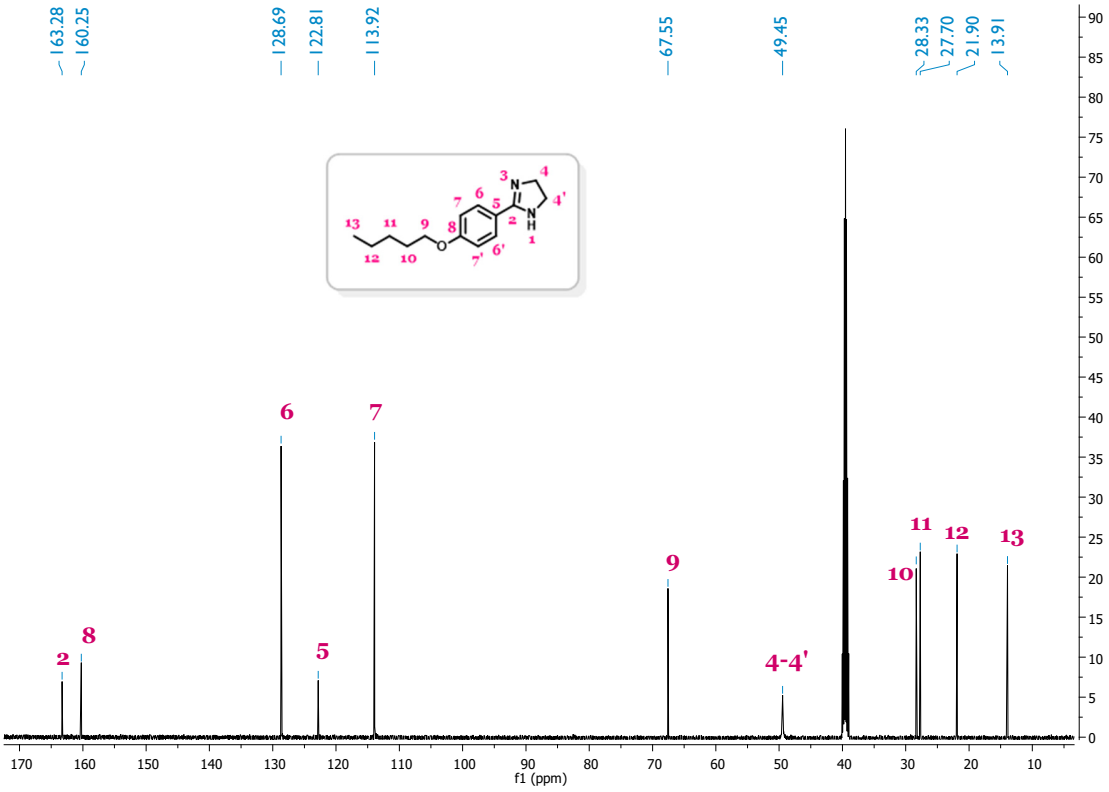
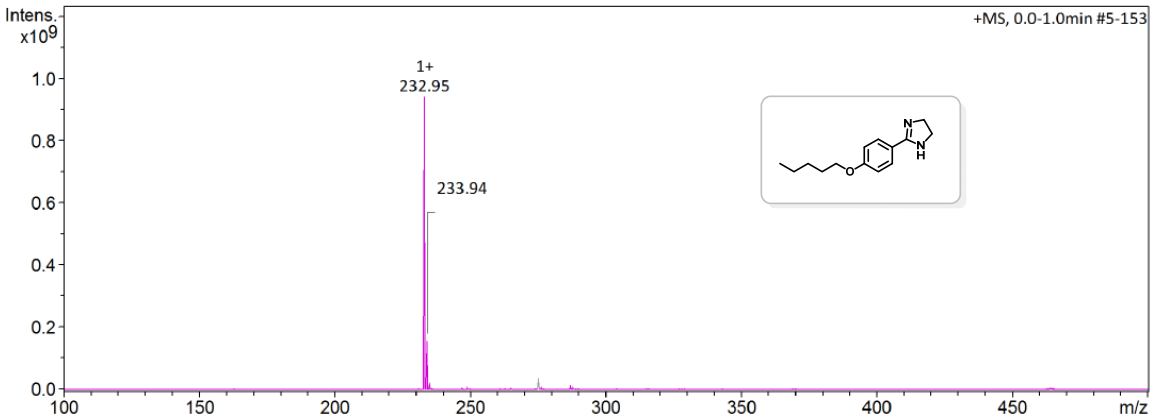
Supplementary material

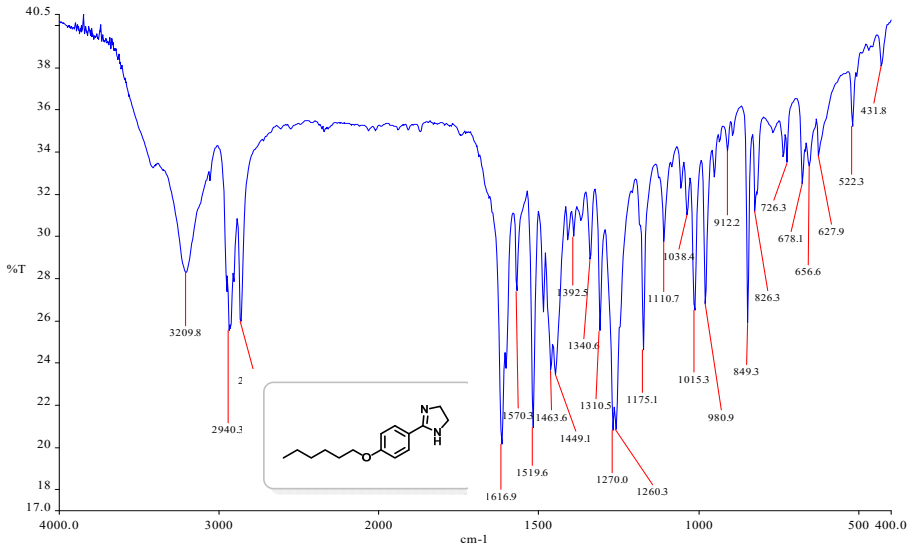
Selected Spectra

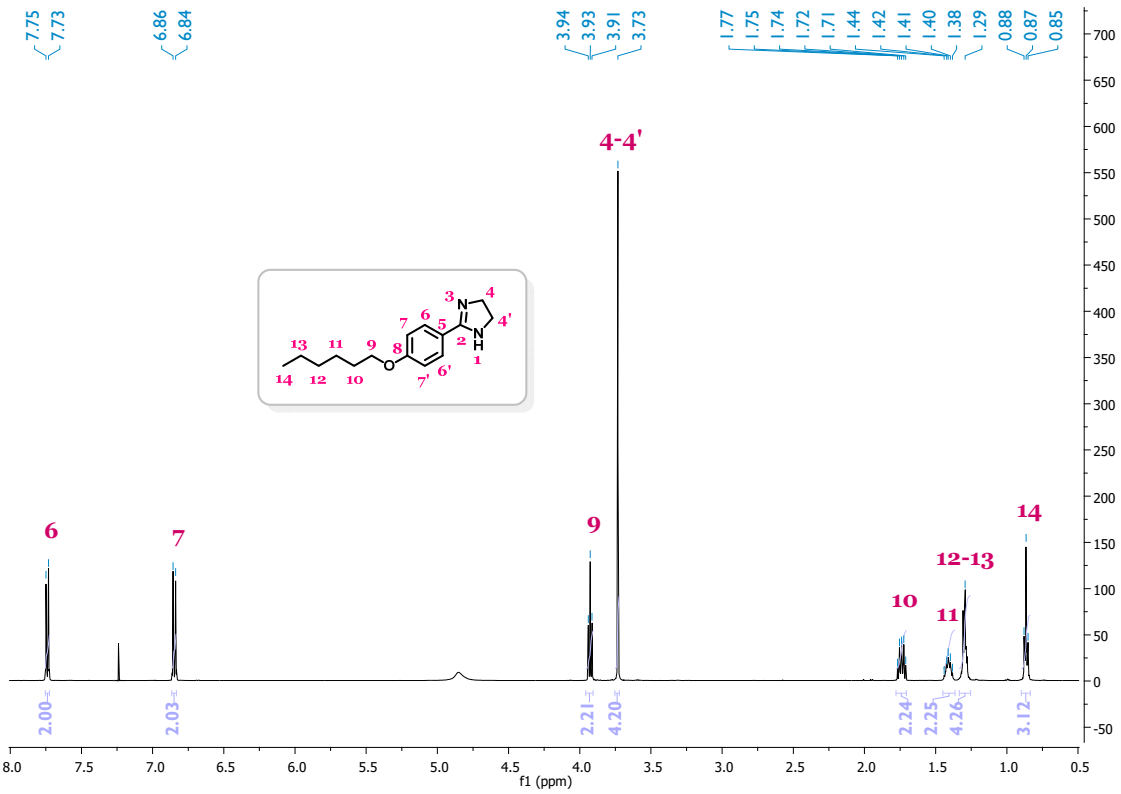


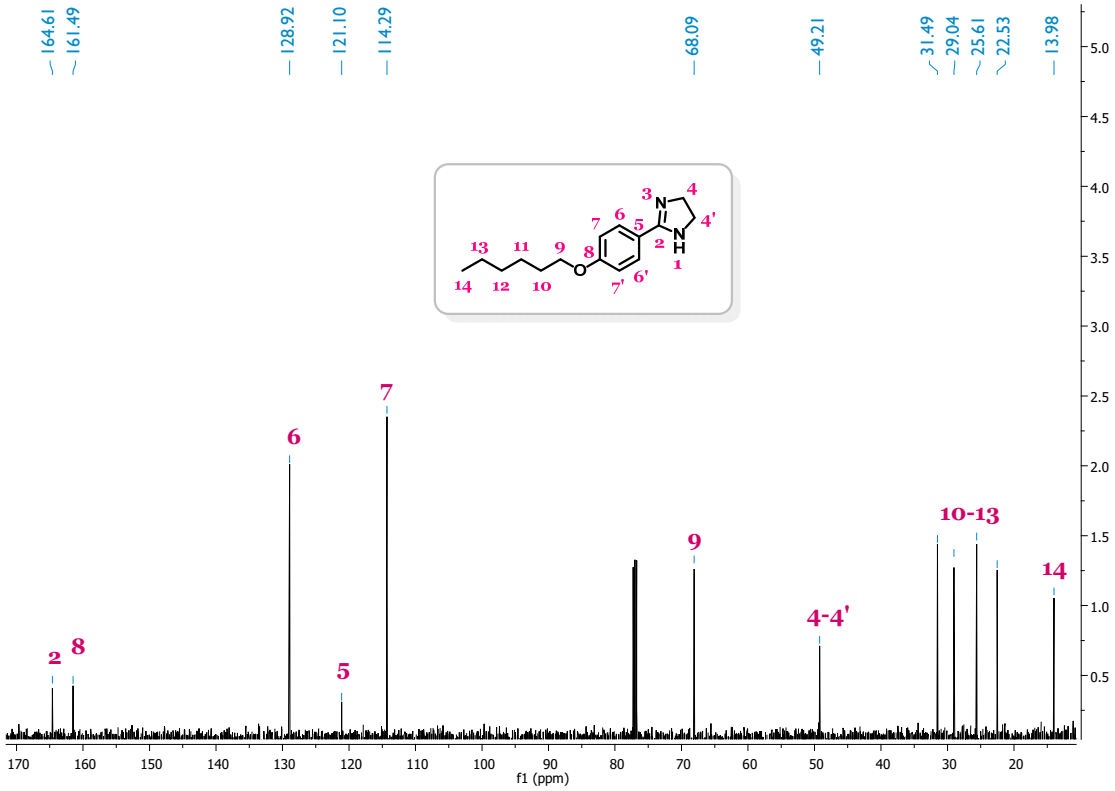

7.75
7.73
6.95
6.93
4.00
3.98
3.97
3.57
1.74
1.72
1.71
1.69
1.68
1.36
0.90
0.89
4-4'
6
7
9
10
11-12
13
2.00
2.00
2.14
4.18
1.99
4.06
3.00
f1 (ppm)

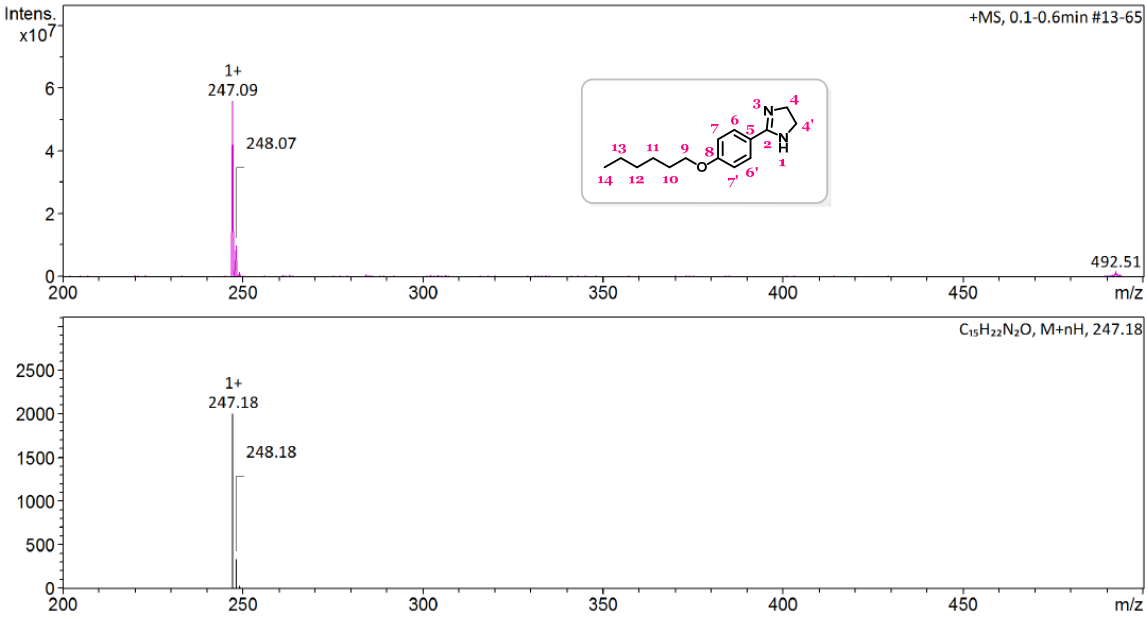

163.28
160.25
128.69
122.81
113.92
67.55
49.45
28.33
27.70
21.90
13.91
6
7
9
11
12
13
10
2
8
5
4-4'
f1 (ppm)

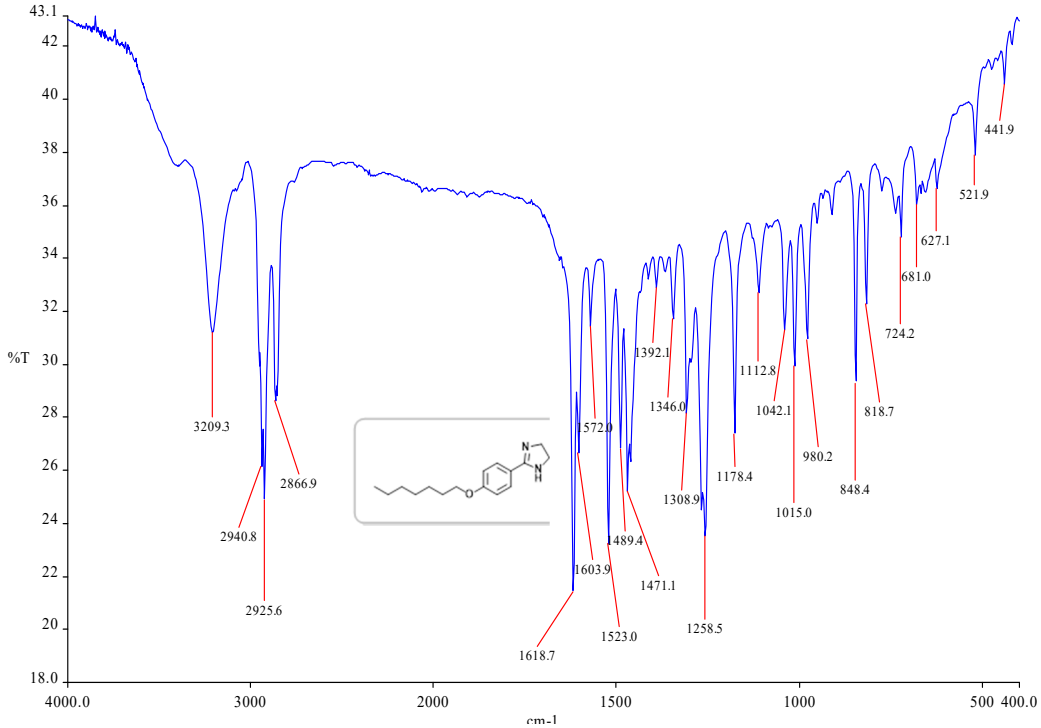

Intens.
x10^9
+MS, 0.0-1.0min #5-153
1+
232.95
233.94
m/z

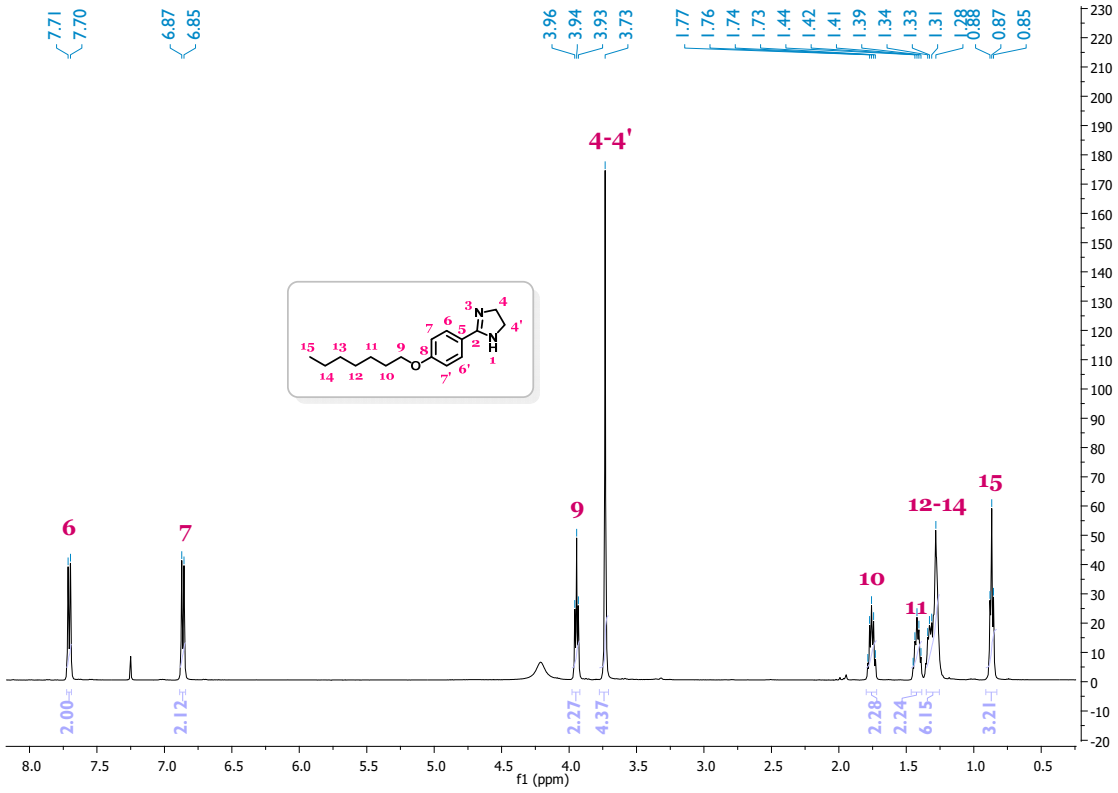

%T
cm-1
3209.8
2940.3
1616.9
1570.3
1519.6
1463.6
1449.1
1392.5
1340.6
1310.5
1270.0
1260.3
1175.1
1110.7
1038.4
1015.3
980.9
912.2
849.3
826.3
726.3
678.1
656.6
627.9
522.3
431.8

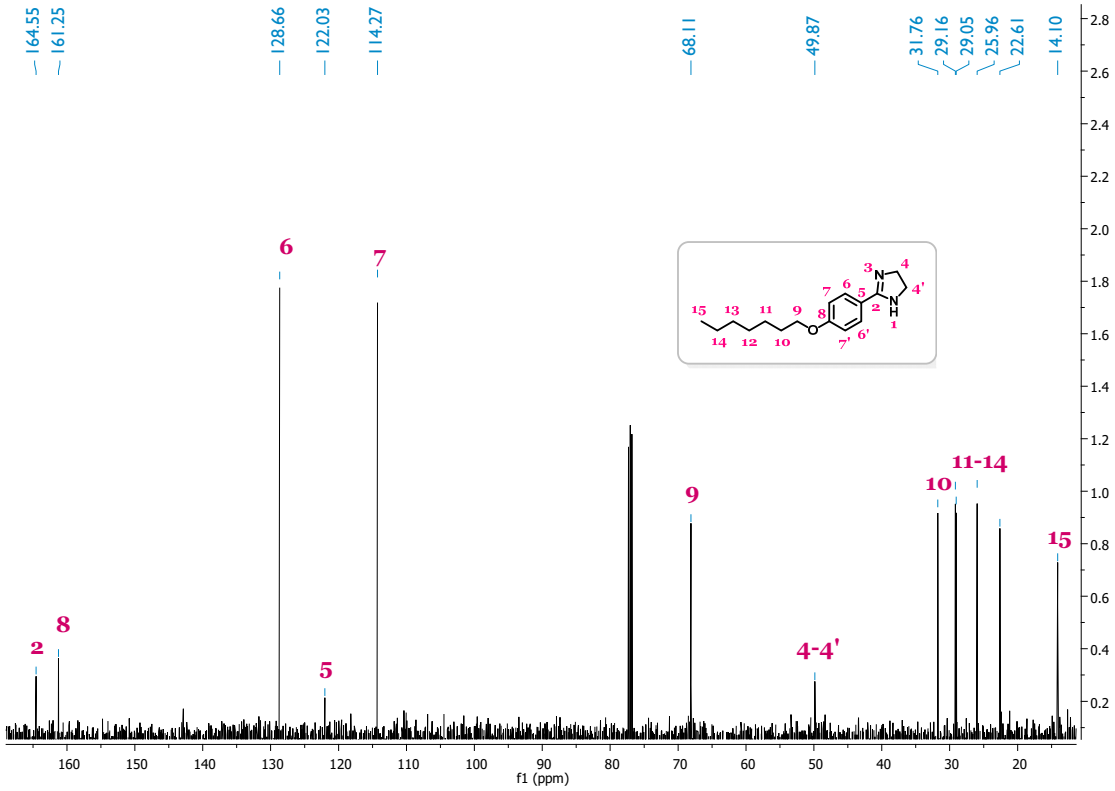

7.75
7.73
6.86
6.84
3.94
3.93
3.91
3.73
1.77
1.75
1.74
1.72
1.71
1.44
1.42
1.41
1.40
1.38
1.29
0.88
0.87
0.85
4-4'
6
7
9
10
11
12-13
14
2.00
2.03
2.21
4.20
2.24
2.25
4.26
3.12
f1 (ppm)

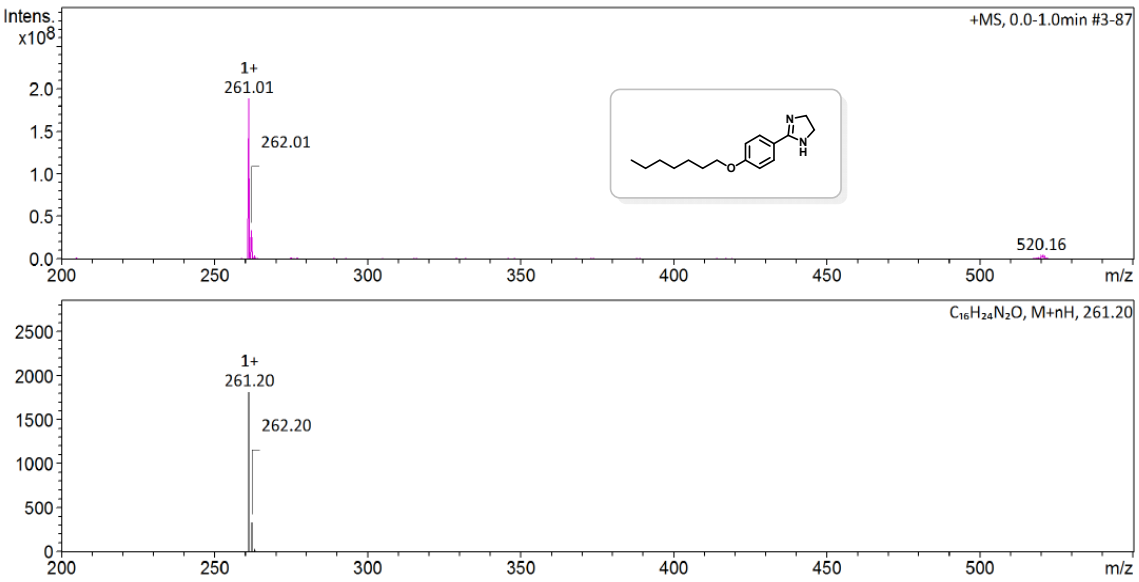

164.61
161.49
128.92
121.10
114.29
68.09
49.21
31.49
29.04
25.61
22.53
13.98
2
8
5
6
7
9
4-4'
10-13
14
f1 (ppm)


Intens.
x10^7
+MS, 0.1-0.6min #13-65
1+
247.09
248.07
492.51
m/z
C15H22N2O, M+nH, 247.18
1+
247.18
248.18
m/z

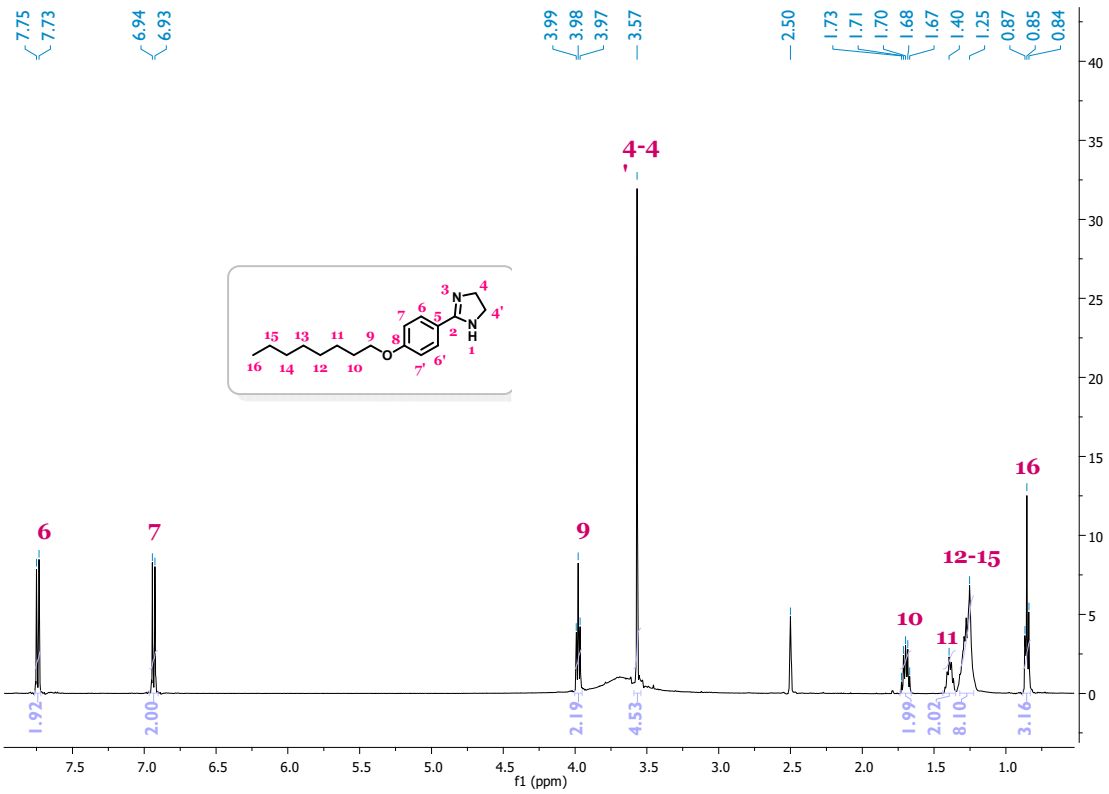

%T
cm-1
3209.3
2940.8
2925.6
2866.9
1618.7
1603.9
1572.0
1523.0
1489.4
1471.1
1392.1
1346.0
1308.9
1258.5
1178.4
1112.8
1042.1
1015.0
980.2
848.4
818.7
724.2
681.0
627.1
521.9
441.9

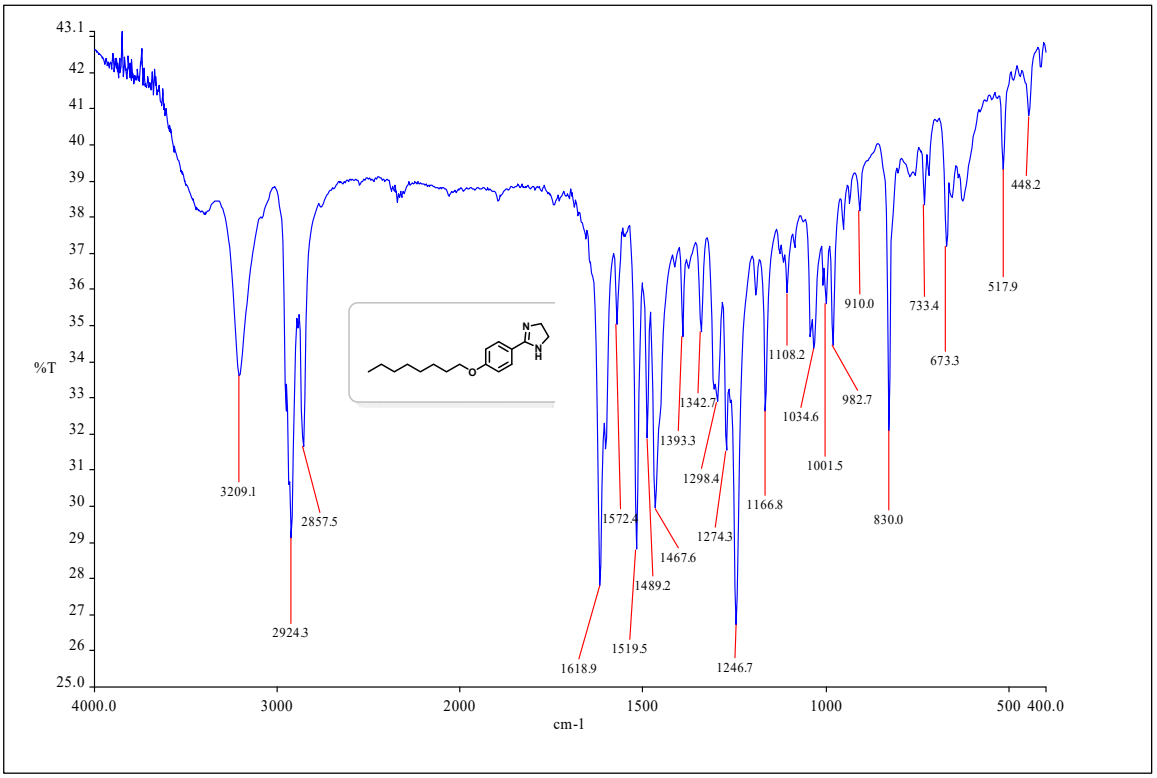

7.71
7.70
6.87
6.85
3.96
3.94
3.93
3.73
1.77
1.76
1.74
1.73
1.44
1.42
1.41
1.39
1.34
1.33
1.31
0.87
0.85
4-4'
6
7
9
10
11
12-14
15
2.00
2.12
2.27
4.37
2.28
2.24
6.15
3.21
f1 (ppm)

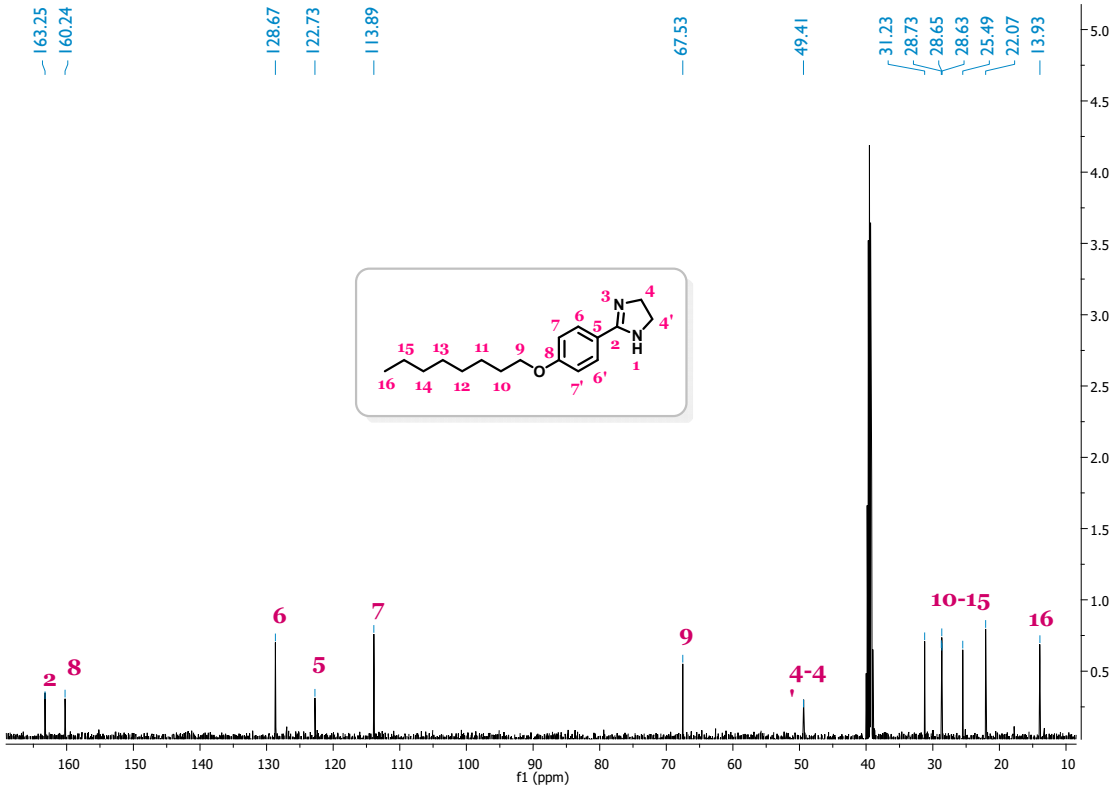

164.55
161.25
128.66
122.03
114.27
68.11
49.87
31.76
29.16
29.05
25.96
22.61
14.10
2
8
6
5
7
9
4-4'
10
11-14
15
f1 (ppm)

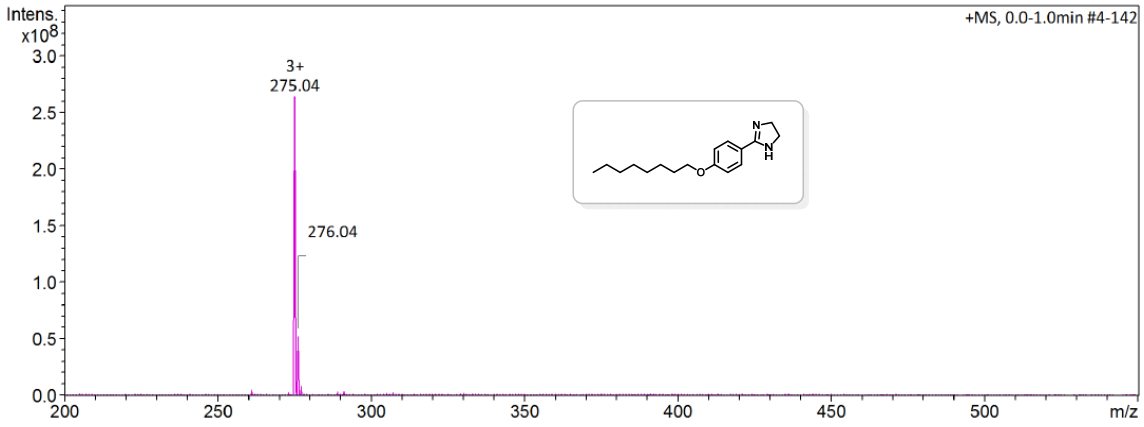

Intens.
x10^8
+MS, 0.0-1.0min #3-87
1+
261.01
262.01
520.16
m/z

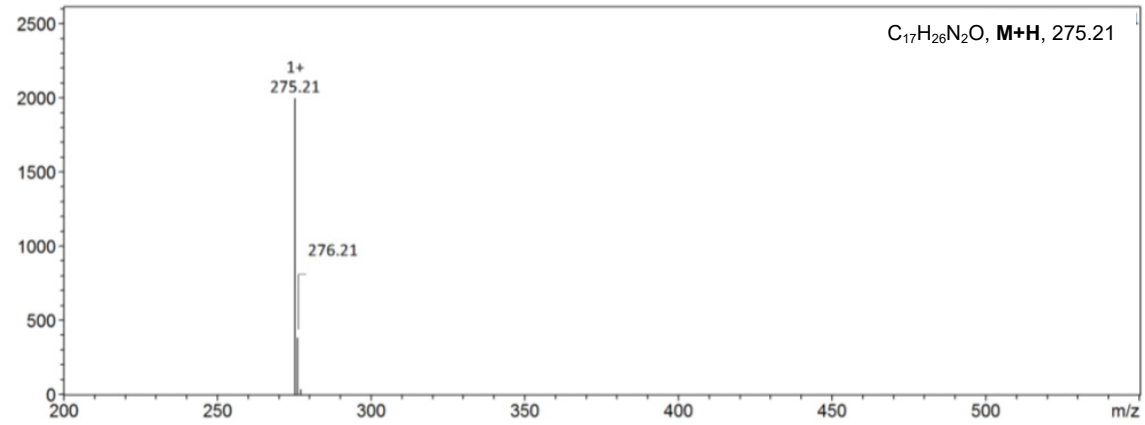
C16H24N2O, M+nH, 261.20
1+
261.20
262.20
m/z

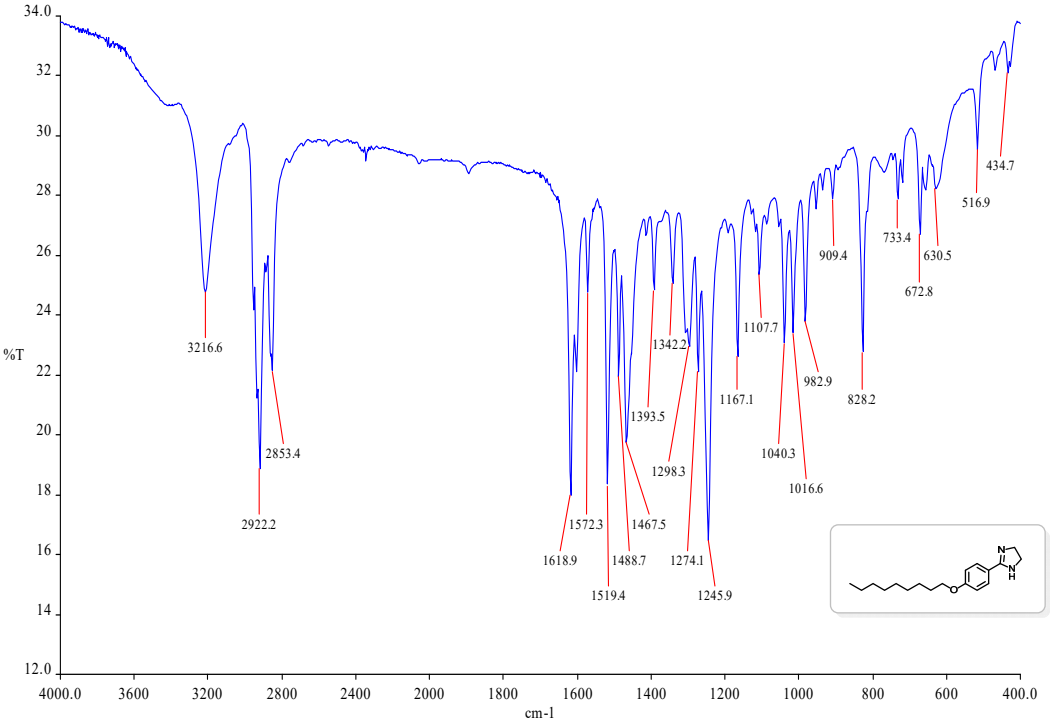

7.75
7.73
6.94
6.93
3.99
3.98
3.97
3.57
2.50
1.73
1.71
1.70
1.68
1.67
1.40
1.25
0.87
0.85
0.84
4-4'
6
7
9
10
11
12-15
16
1.92
2.00
2.19
4.53
1.99
2.02
8.10
3.16
f1 (ppm)

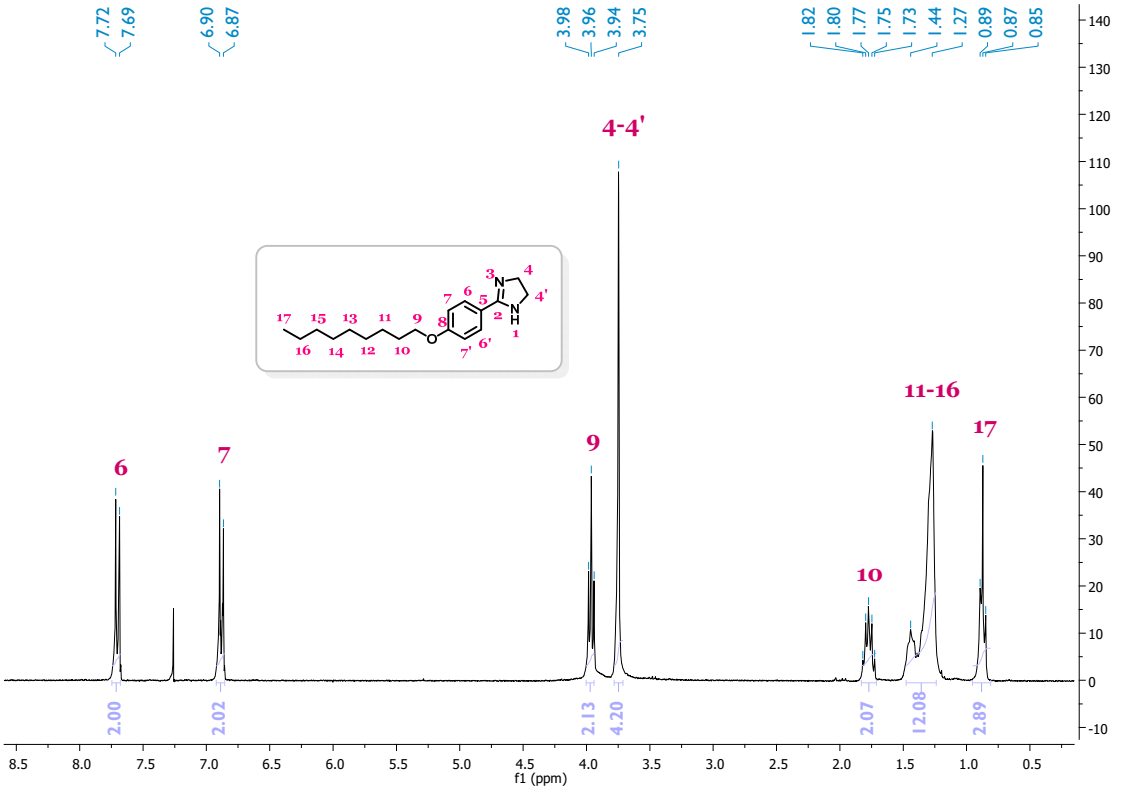

%T
cm-1
3209.1
2924.3
2857.5
1618.9
1572.4
1519.5
1489.2
1467.6
1393.3
1342.7
1298.4
1274.3
1246.7
1166.8
1108.2
1034.6
1001.5
982.7
910.0
830.0
733.4
673.3
517.9
448.2

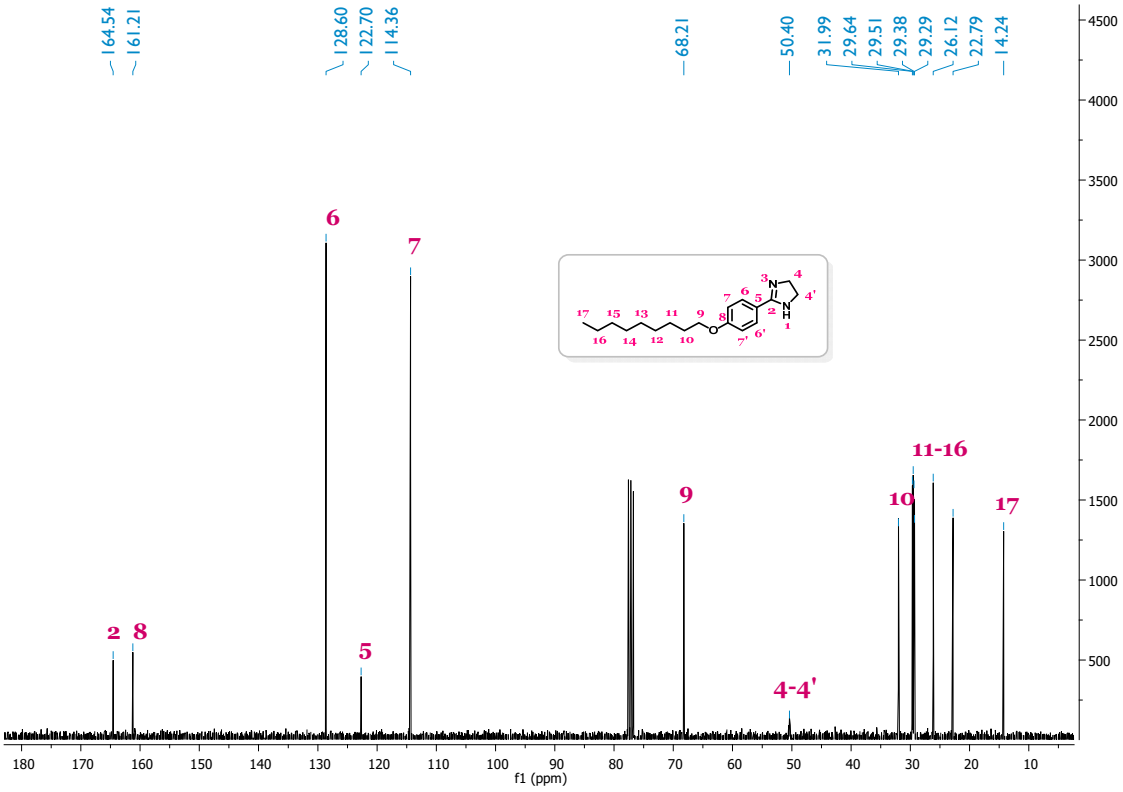

163.25
160.24
128.67
122.73
113.89
67.53
49.41
31.23
28.73
28.65
28.63
25.49
22.07
13.93
2
8
6
5
7
9
4-4'
10-15
16
f1 (ppm)

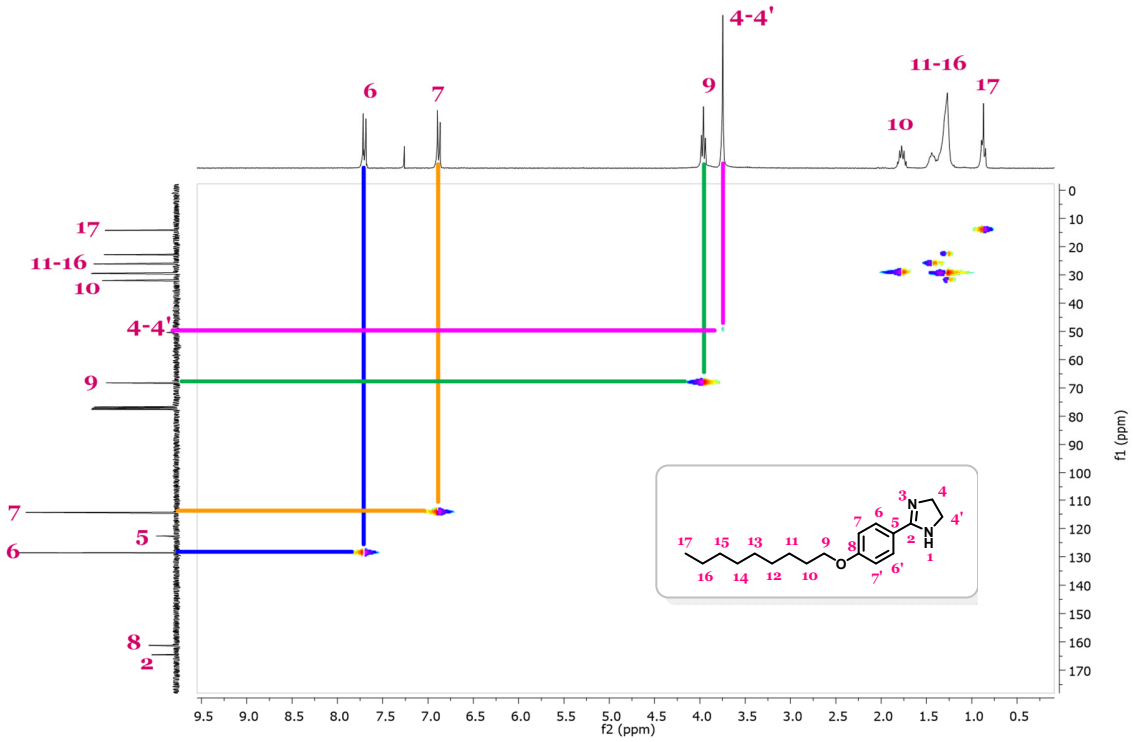

Intens.
x10^8
+MS, 0.0-1.0min #4-142
3+
275.04
276.04
m/z

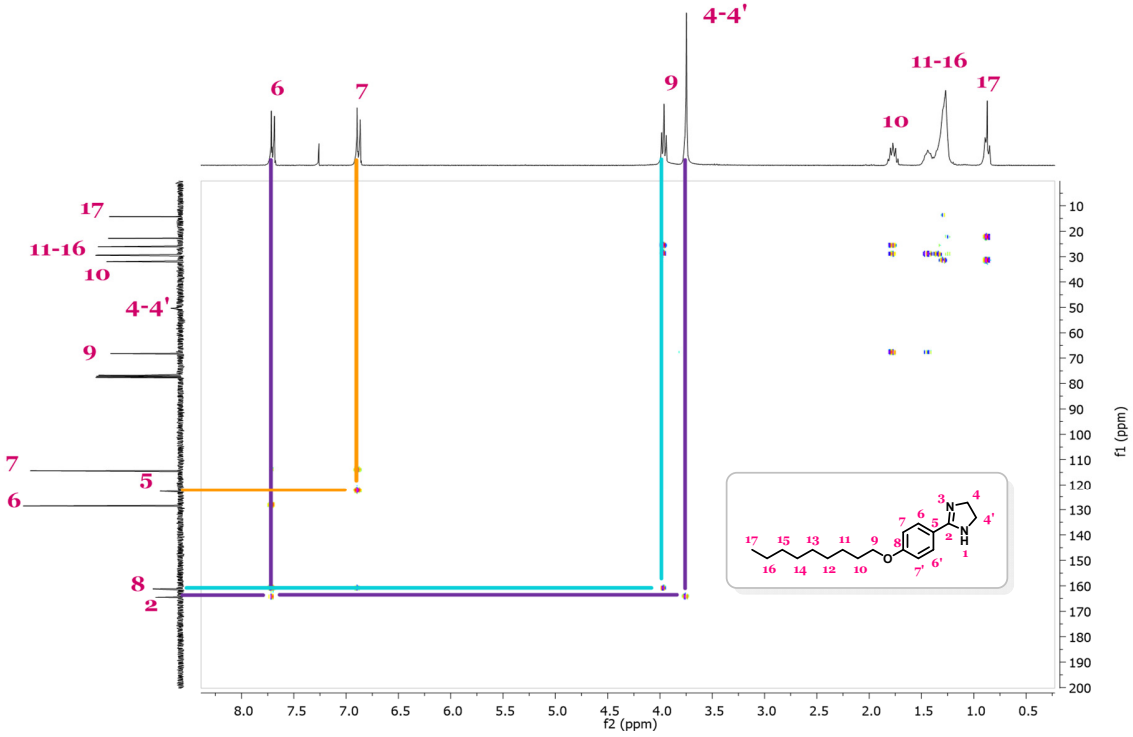

C17H26N2O, M+H, 275.21
1+
275.21
276.21
m/z

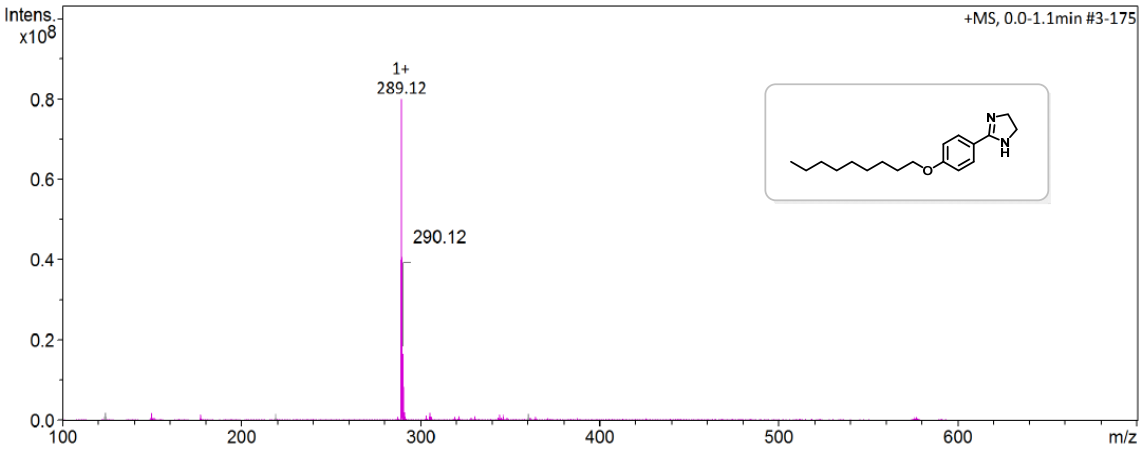

%T
cm-1
3216.6
2922.2
2853.4
1618.9
1572.3
1519.4
1488.7
1467.5
1393.5
1342.2
1298.3
1274.1
1245.9
1167.1
1107.7
1040.3
1016.6
982.9
909.4
828.2
733.4
672.8
630.5
516.9
434.7

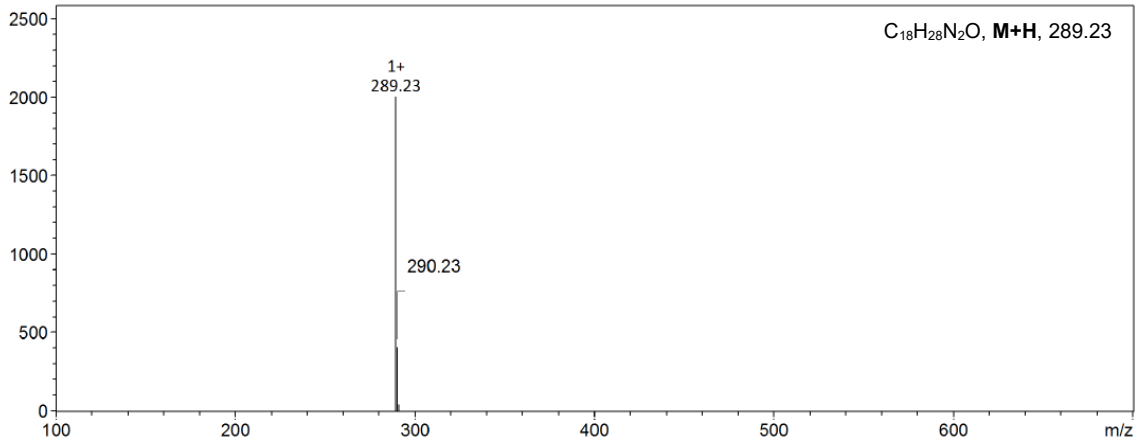

7.72
7.69
6.90
6.87
3.98
3.96
3.94
3.75
1.82
1.80
1.77
1.75
1.73
1.44
1.27
0.89
0.87
0.85
4-4'
6
7
9
10
11-16
17
2.00
2.02
2.13
4.20
2.07
12.08
2.89
f1 (ppm)

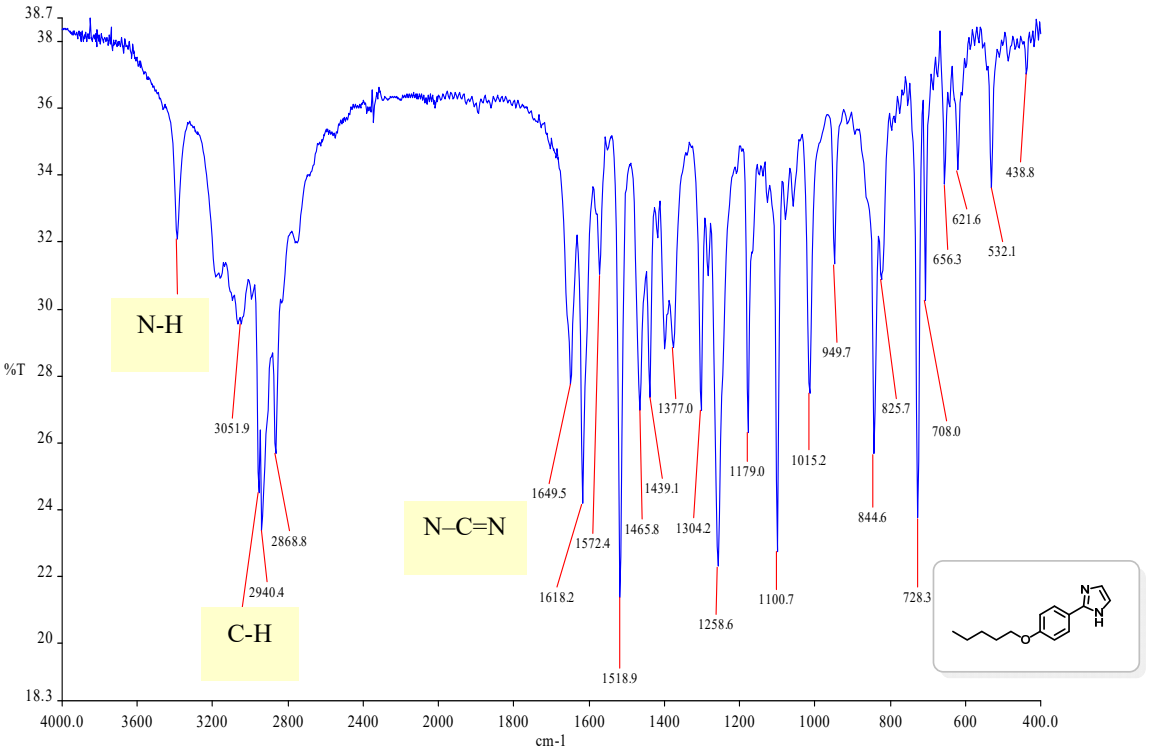

164.54
161.21
128.60
122.70
114.36
68.21
50.40
31.99
29.64
29.51
29.38
29.29
26.12
22.79
14.24
6
7
2
8
5
4-4'
9
10
11-16
17
f1 (ppm)

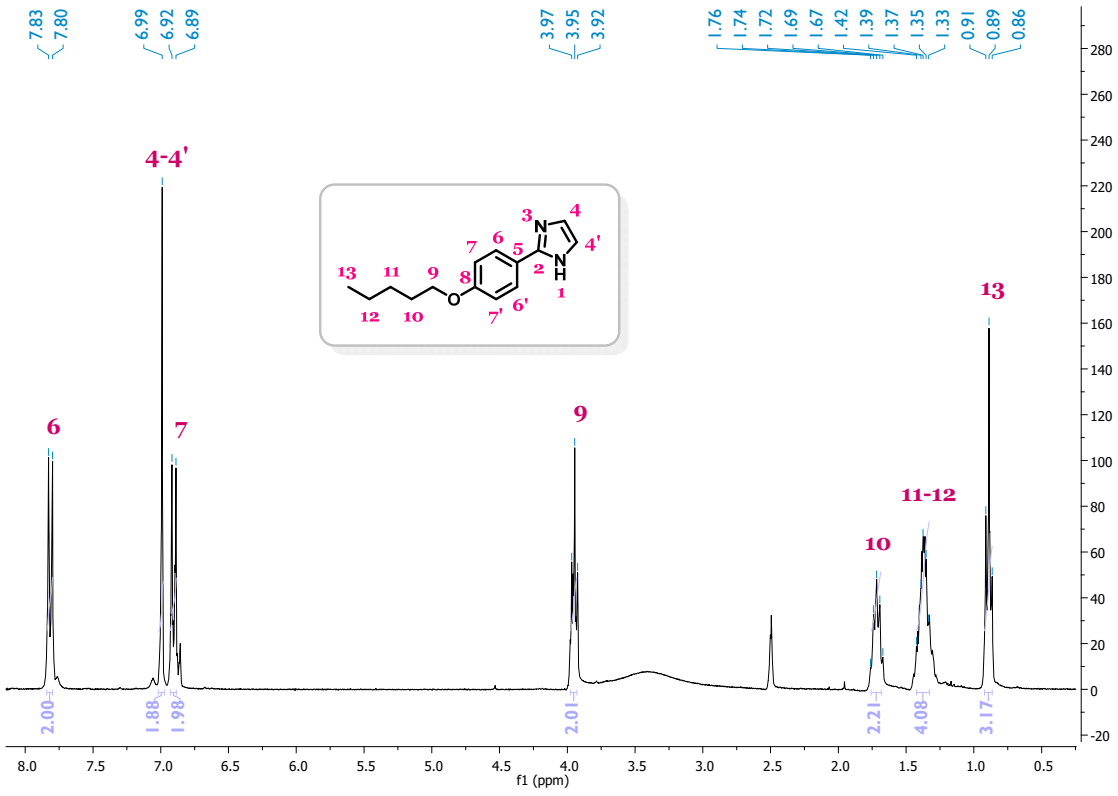

4-4'
6
7
9
11-16
17
10
17
11-16
10
4-4'
9
7
5
6
8
2
f2 (ppm)
f1 (ppm)

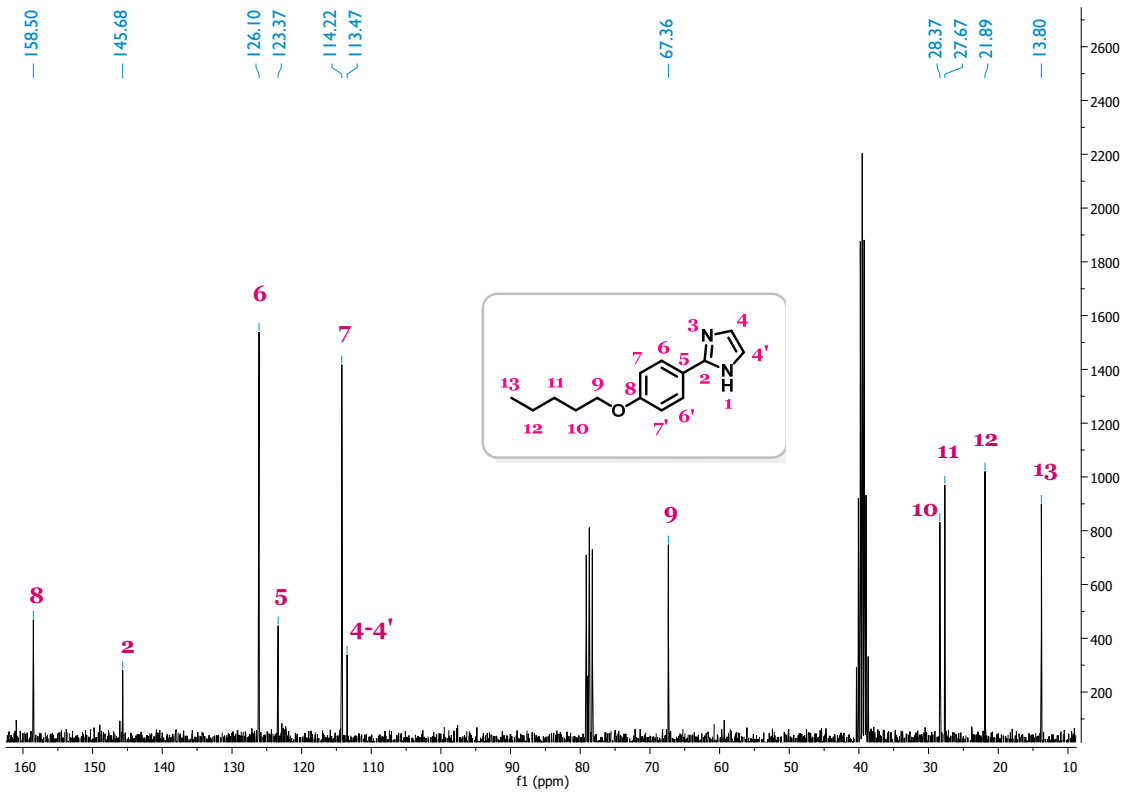

4-4'
6
7
9
11-16
17
10
17
11-16
10
4-4'
9
7
5
6
8
2
f2 (ppm)
f1 (ppm)

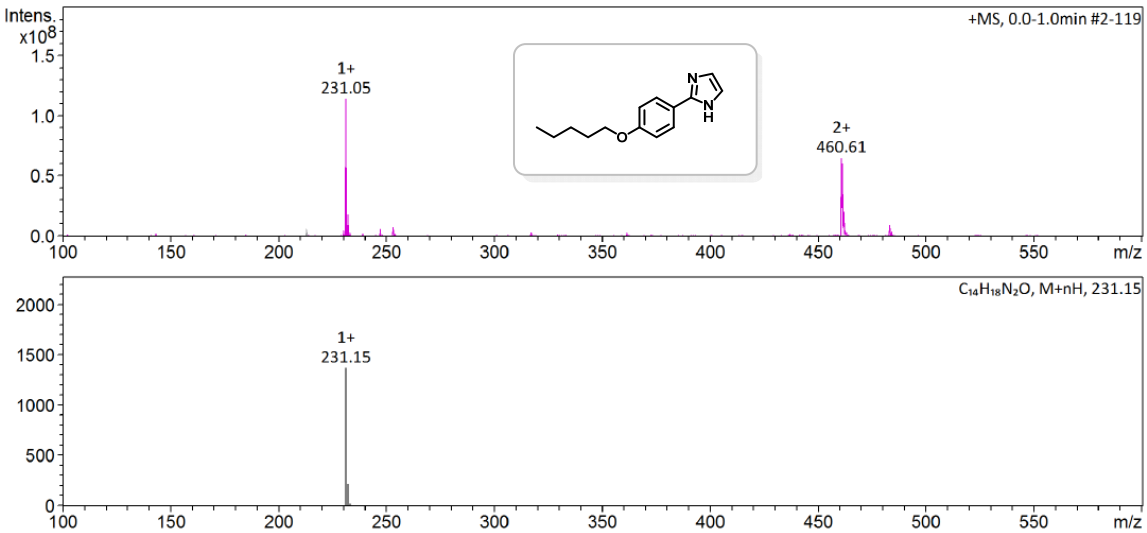

Intens.
x10^8
+MS, 0.0-1.1min #3-175
1+
289.12
290.12
0.8
0.6
0.4
0.2
0.0
100
200
300
400
500
600
m/z
N
N
H
O


$C_{18}H_{28}N_2O$, **M+H**, 289.23
1+
289.23
290.23
2500
2000
1500
1000
500
0
100
200
300
400
500
600
m/z

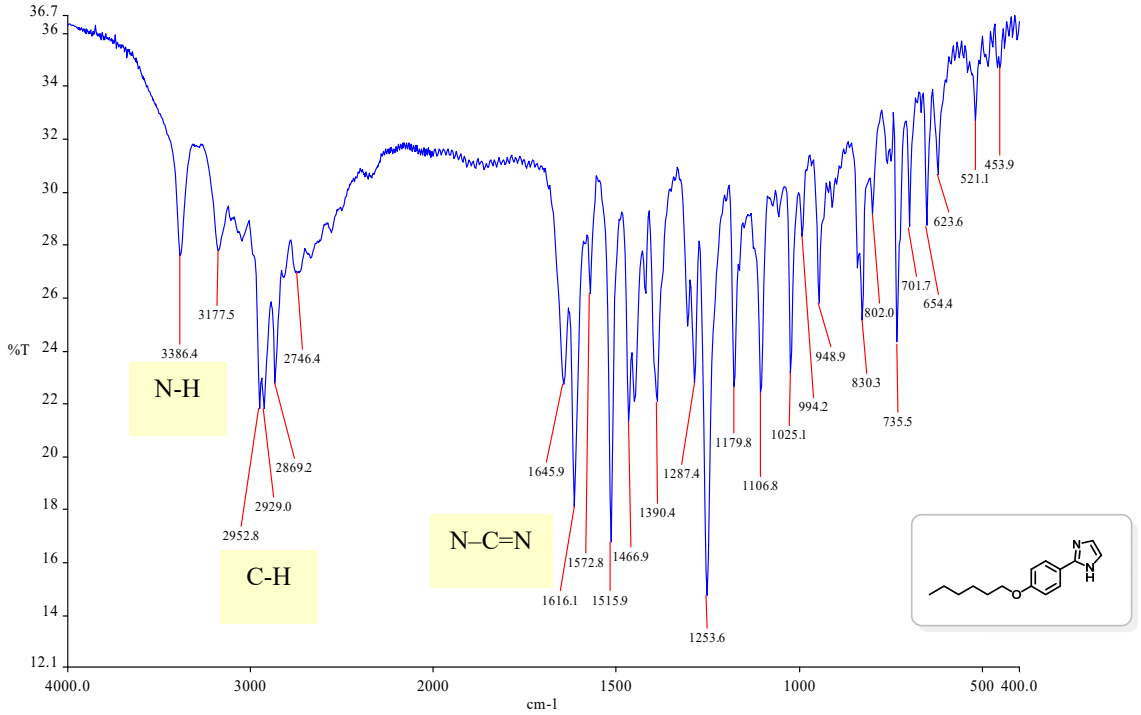

N-H
C-H
N–C=N
3051.9
2940.4
2868.8
1649.5
1618.2
1572.4
1518.9
1465.8
1439.1
1377.0
1304.2
1258.6
1179.0
1100.7
1015.2
949.7
844.6
825.7
728.3
708.0
656.3
621.6
532.1
438.8
%T
cm-1

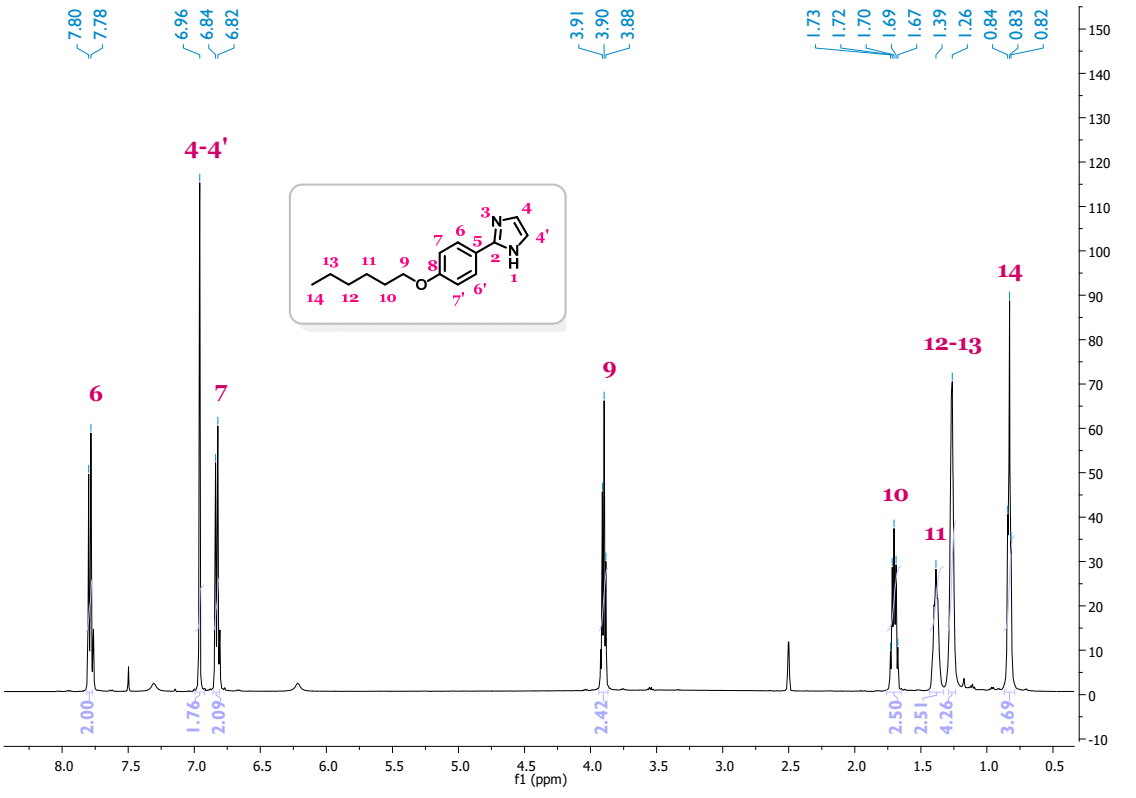

7.83
7.80
6.99
6.92
6.89
3.97
3.95
3.92
1.76
1.74
1.72
1.69
1.67
1.42
1.39
1.37
1.35
1.33
0.91
0.89
0.86
4-4'
6
7
9
10
11-12
13
2.00
1.88
1.98
2.01
2.21
4.08
3.17
f1 (ppm)

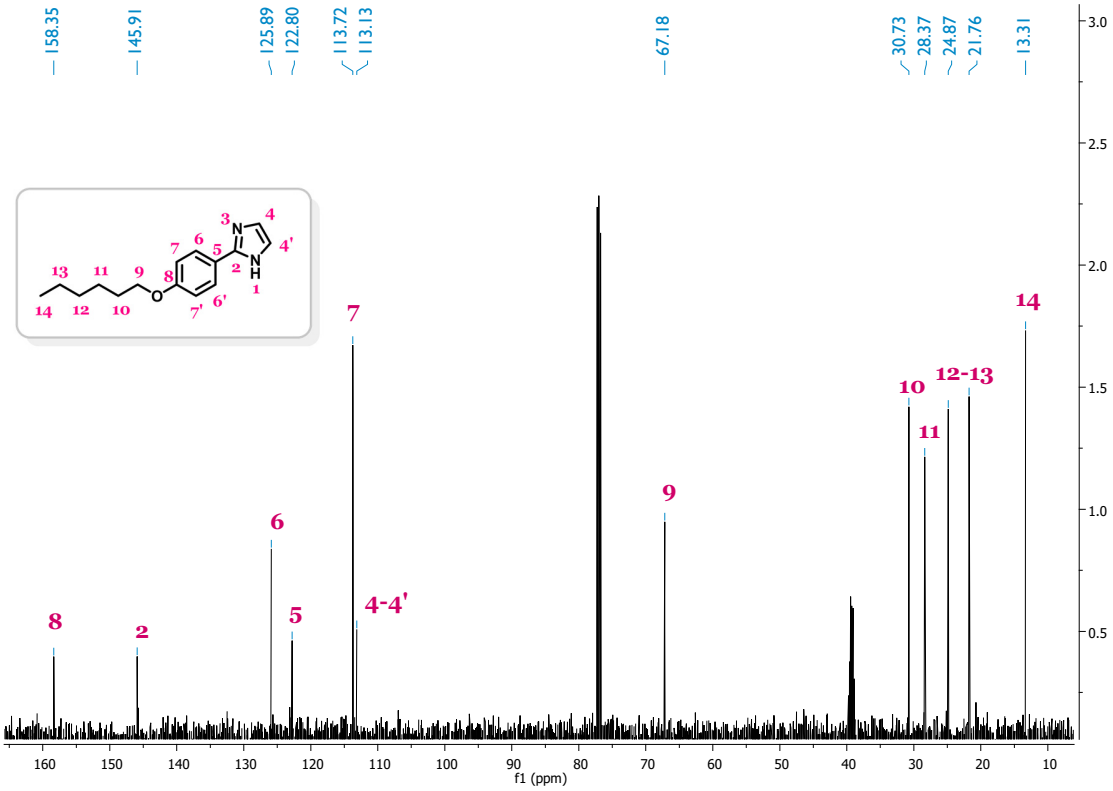

158.50
145.68
126.10
123.37
114.22
113.47
67.36
28.37
27.67
21.89
13.80
8
2
6
5
7
4-4'
9
10
11
12
13
f1 (ppm)

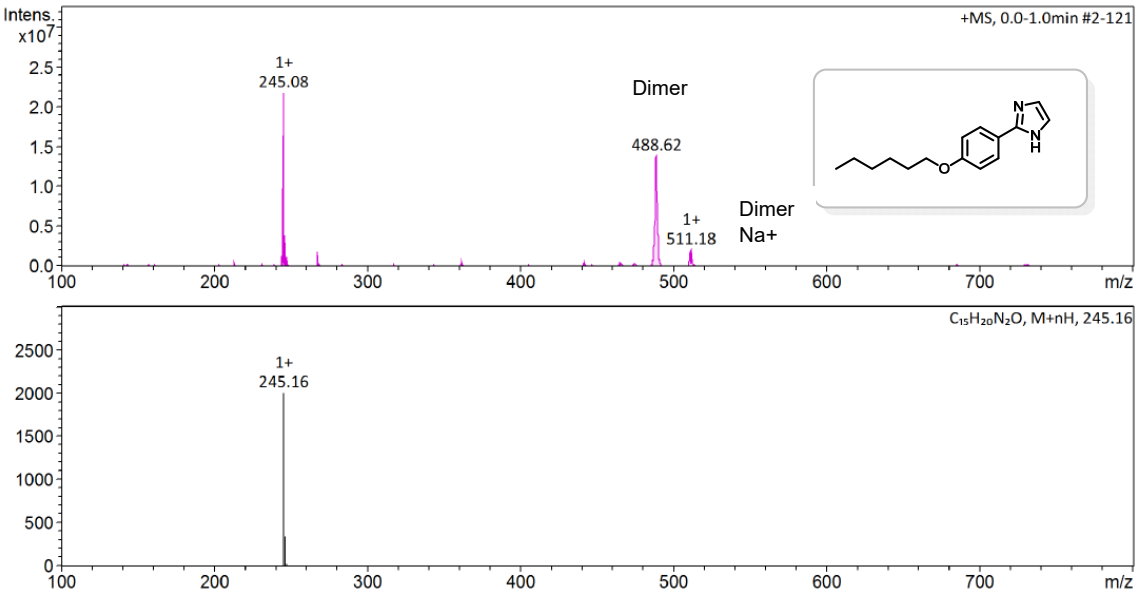

Intens.
x10^8
+MS, 0.0-1.0min #2-119
1+
231.05
2+
460.61
m/z

C14H18N2O, M+nH, 231.15
1+
231.15
m/z

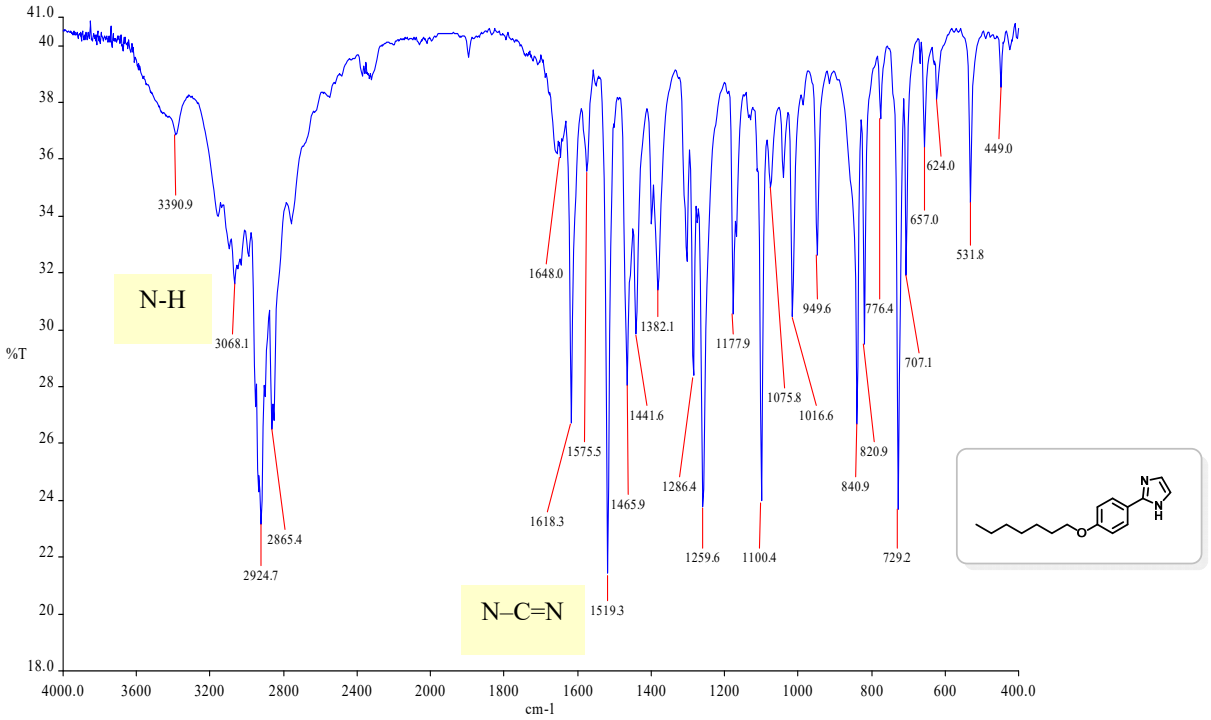

%T
cm-1
3386.4
3177.5
2952.8
2929.0
2869.2
2746.4
1645.9
1616.1
1572.8
1515.9
1466.9
1390.4
1287.4
1253.6
1179.8
1106.8
1025.1
994.2
948.9
830.3
802.0
735.5
701.7
654.4
623.6
521.1
453.9
N-H
C-H
N–C=N

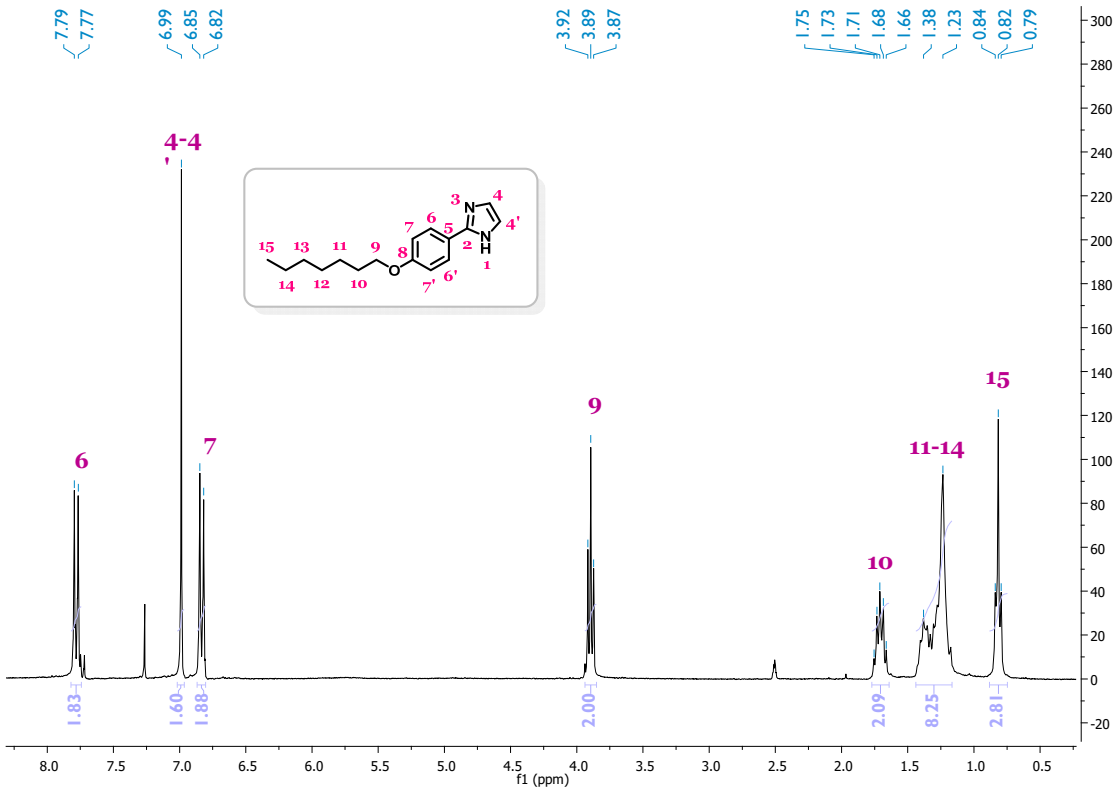

4-4'
6
7
9
10
11
12-13
14
f1 (ppm)

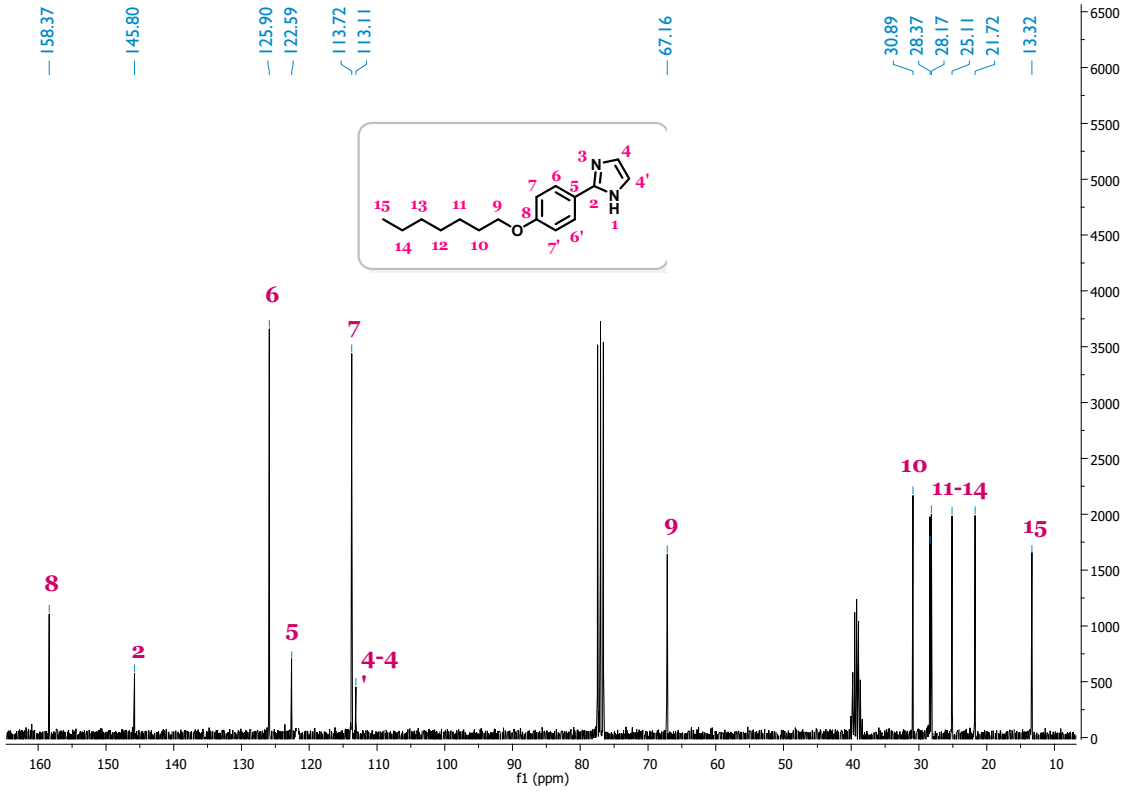

158.35
145.91
125.89
122.80
113.72
113.13
67.18
30.73
28.37
24.87
21.76
13.31
8
2
6
5
4-4'
7
9
10
11
12-13
14
f1 (ppm)

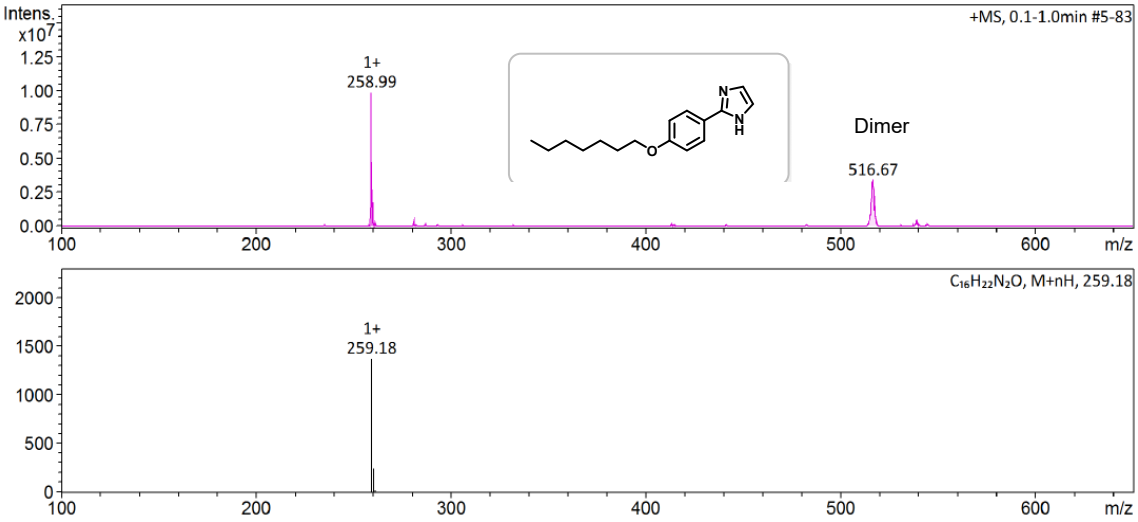

Intens.
x10^7
+MS, 0.0-1.0min #2-121
1+
245.08
Dimer
488.62
1+
511.18
Dimer
Na+
m/z

C15H20N2O, M+nH, 245.16
1+
245.16
m/z

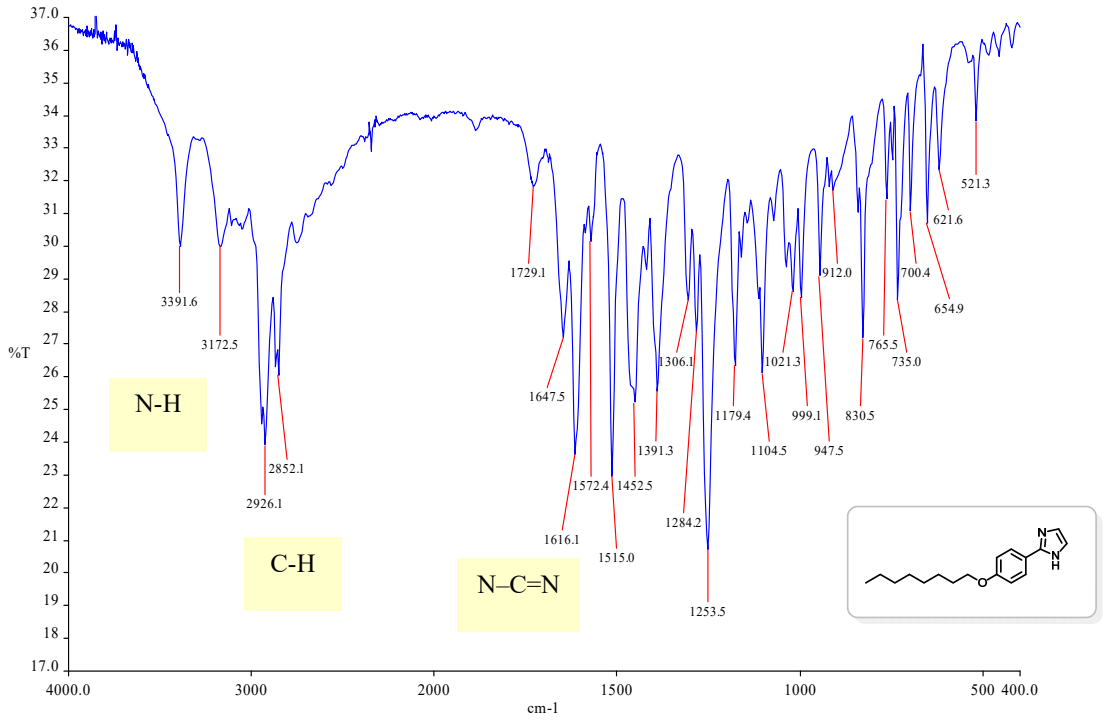

N-H
N–C=N
%T
cm-1
3390.9
3068.1
2924.7
2865.4
1648.0
1618.3
1575.5
1519.3
1465.9
1441.6
1382.1
1286.4
1259.6
1177.9
1100.4
1075.8
1016.6
949.6
840.9
820.9
776.4
729.2
707.1
657.0
624.0
531.8
449.0

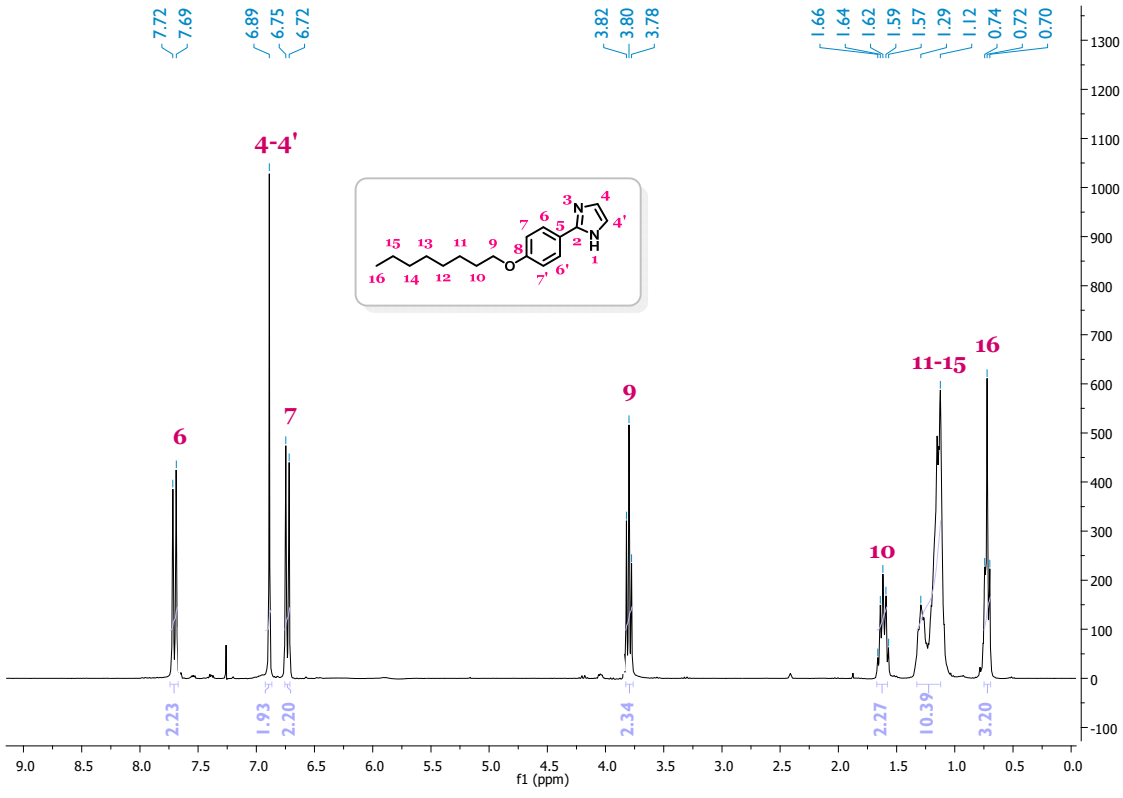

7.79
7.77
6.99
6.85
6.82
3.92
3.89
3.87
1.75
1.73
1.71
1.68
1.66
1.38
1.23
0.84
0.82
0.79
4-4'
6
7
9
10
11-14
15
1.83
1.60
1.88
2.00
2.09
8.25
2.81
f1 (ppm)

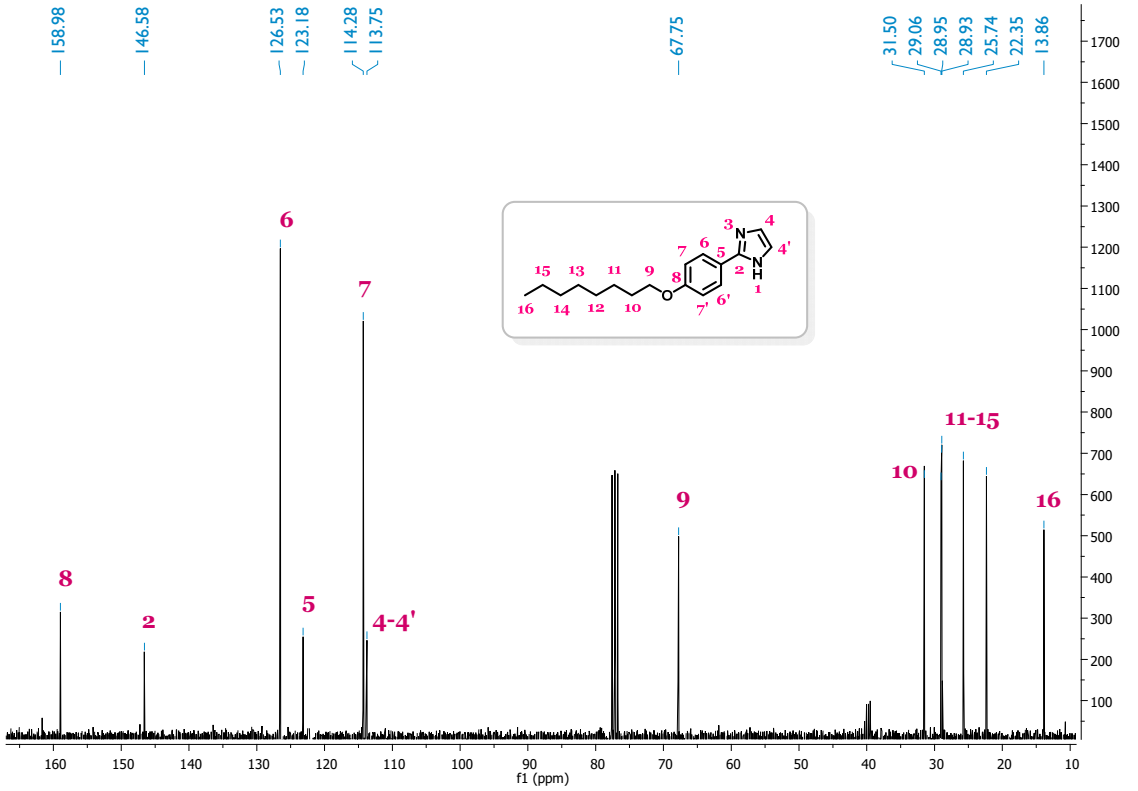

158.37
145.80
125.90
122.59
113.72
113.11
67.16
30.89
28.37
28.17
25.11
21.72
13.32
6
7
8
2
5
4-4'
9
10
11-14
15
f1 (ppm)

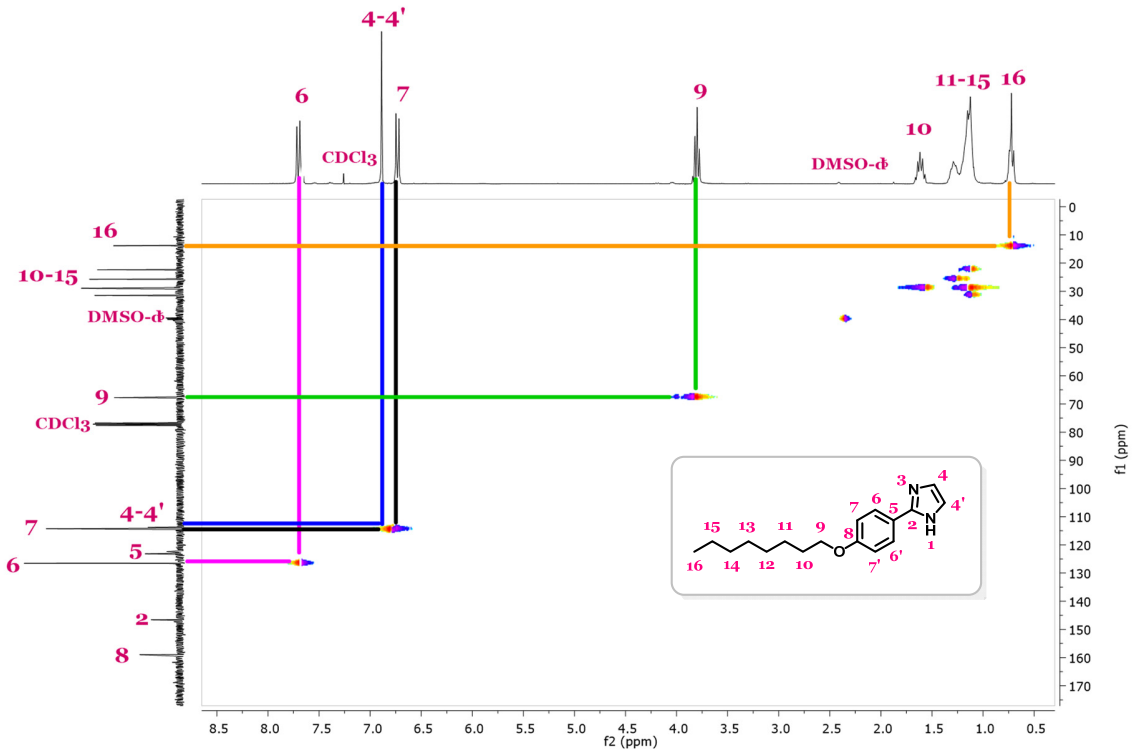

Intens.
x10^7
+MS, 0.1-1.0min #5-83
1+
258.99
Dimer
516.67
m/z

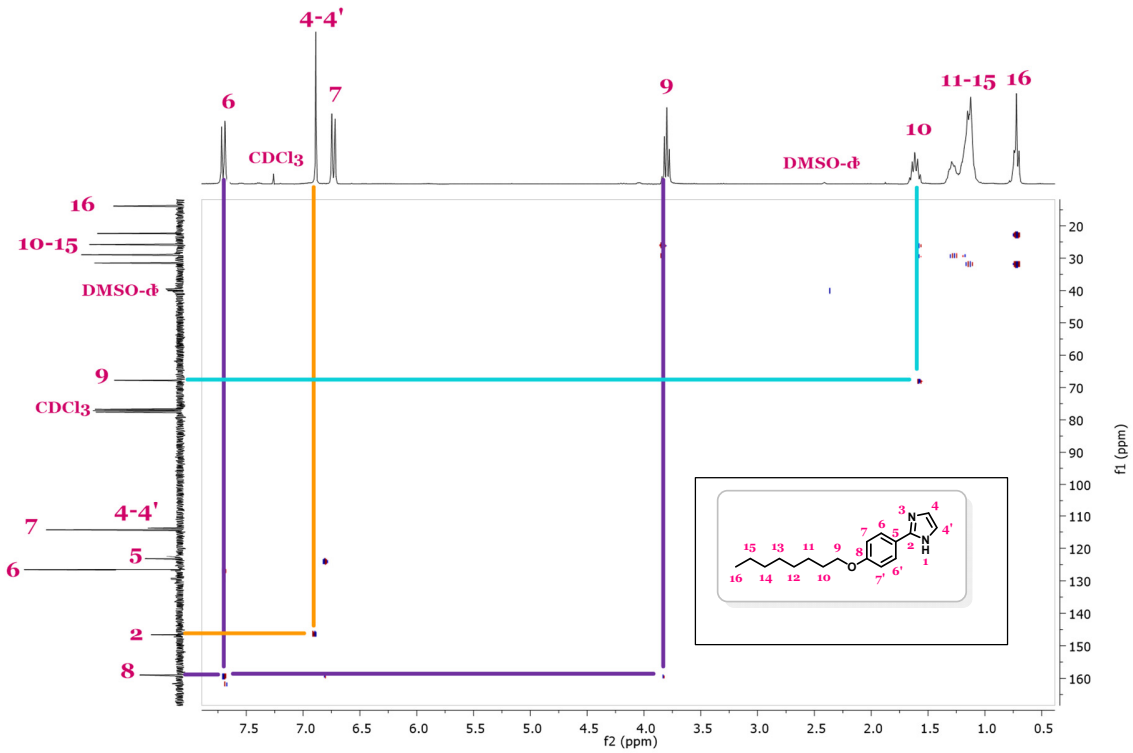
C16H22N2O, M+nH, 259.18
1+
259.18
m/z

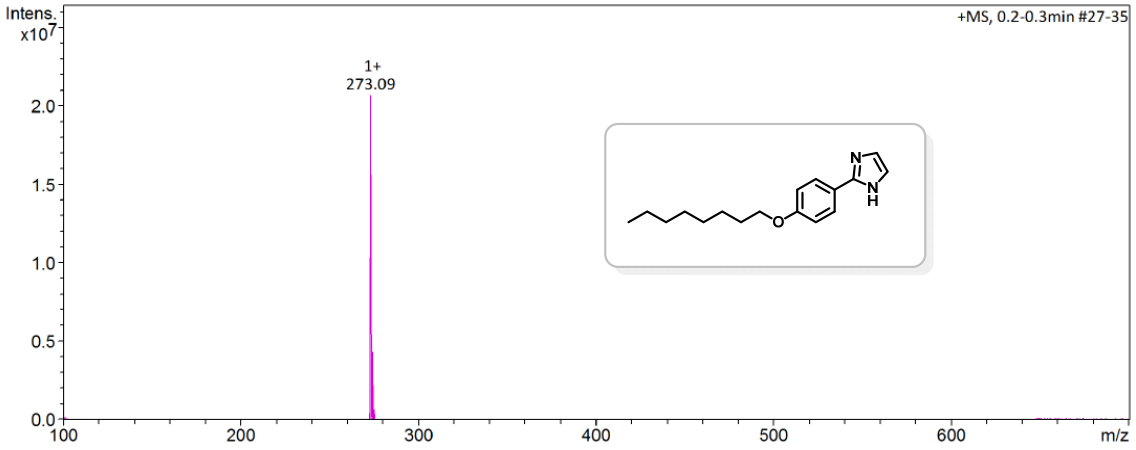

%T
cm-1
3391.6
3172.5
2926.1
2852.1
1729.1
1647.5
1616.1
1572.4
1515.0
1452.5
1391.3
1306.1
1284.2
1253.5
1179.4
1104.5
1021.3
999.1
947.5
912.0
830.5
765.5
735.0
700.4
654.9
621.6
521.3
N-H
C-H
N–C=N

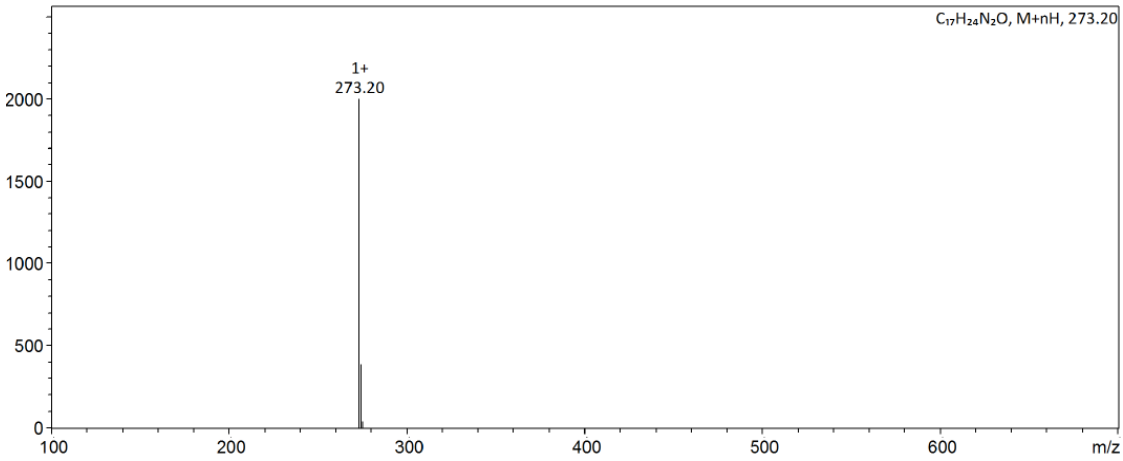

7.72
7.69
6.89
6.75
6.72
3.82
3.80
3.78
1.66
1.64
1.62
1.59
1.57
1.29
1.12
0.74
0.72
0.70
4-4'
6
7
9
10
11-15
16
2.23
1.93
2.20
2.34
2.27
10.39
3.20
f1 (ppm)

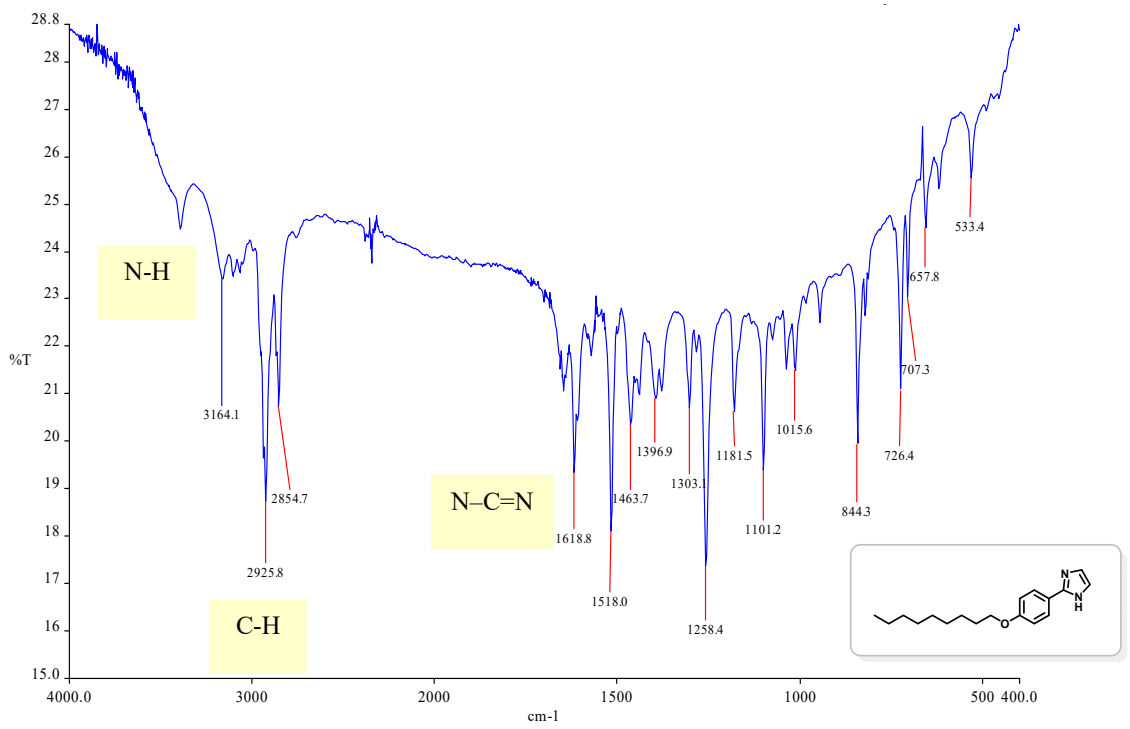

158.98
146.58
126.53
123.18
114.28
113.75
67.75
31.50
29.06
28.95
28.93
25.74
22.35
13.86
8
2
6
5
7
4-4'
9
10
11-15
16
f1 (ppm)

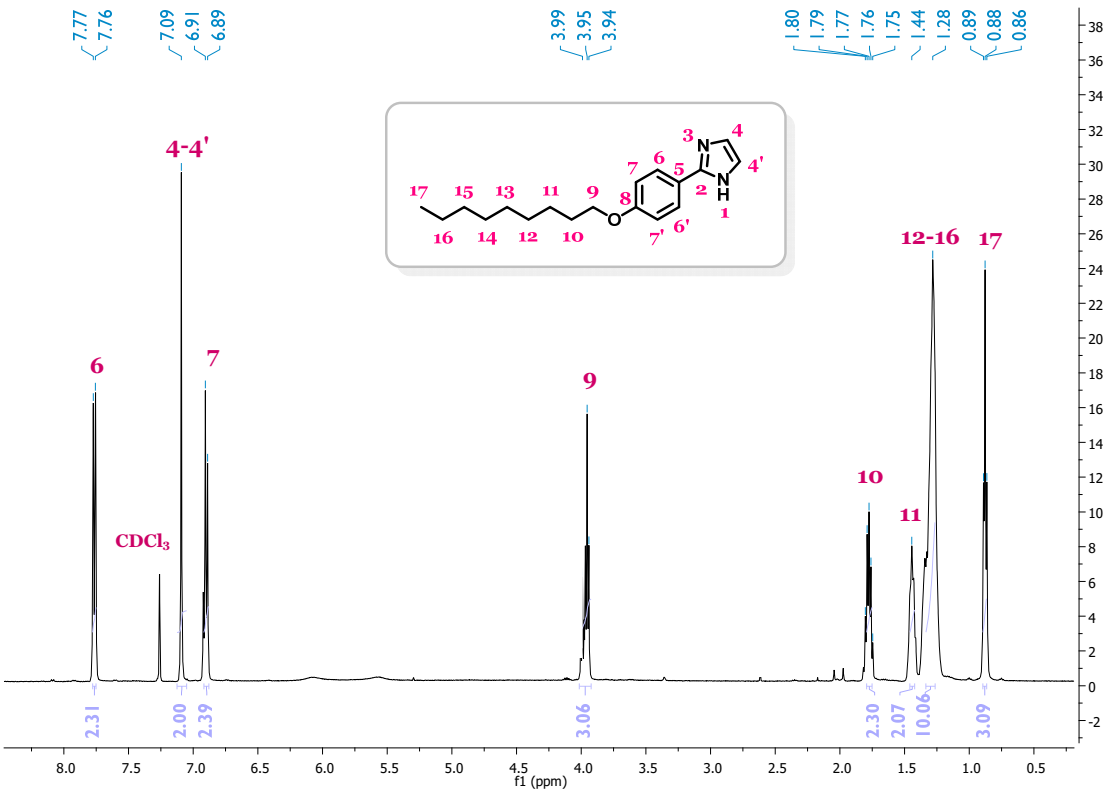

4-4'
6
7
9
11-15
16
10
CDCl3
DMSO-d
16
10-15
DMSO-d
9
CDCl3
4-4'
7
5
6
2
8
f2 (ppm)
f1 (ppm)

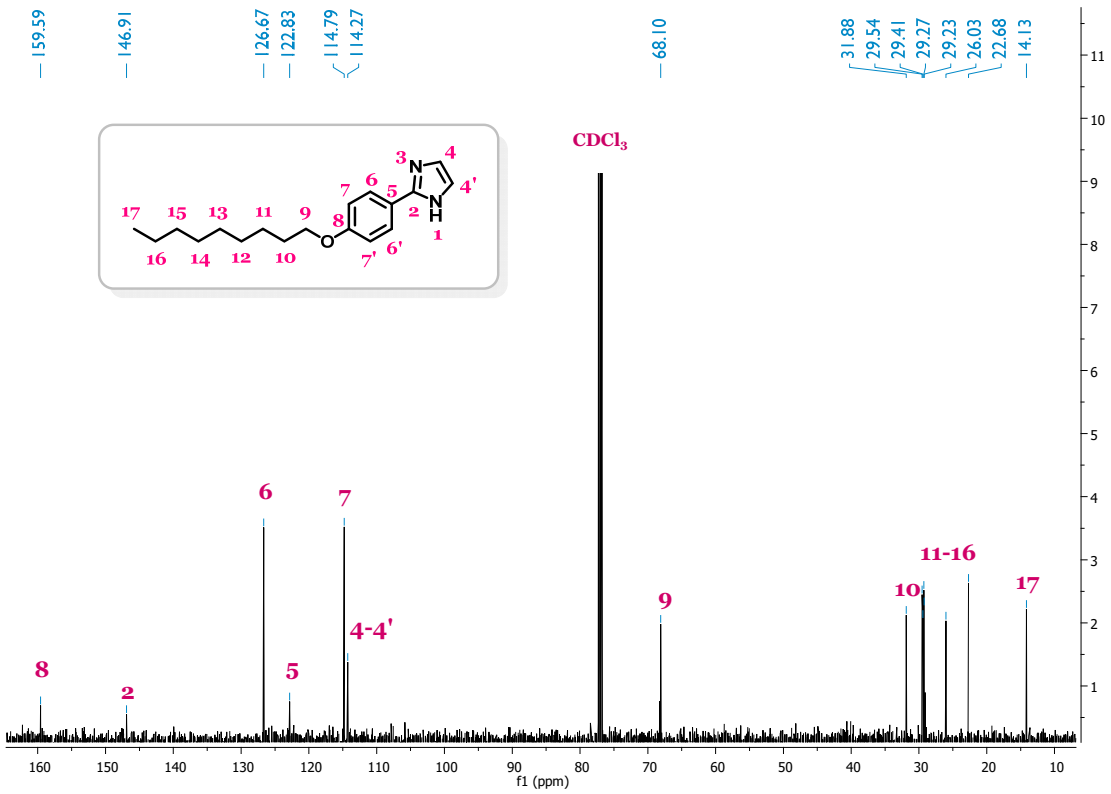

4-4'
6
7
9
11-15
16
10
CDCl3
DMSO-d6
16
10-15
DMSO-d6
9
CDCl3
7
4-4'
5
6
2
8
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
f1 (ppm)

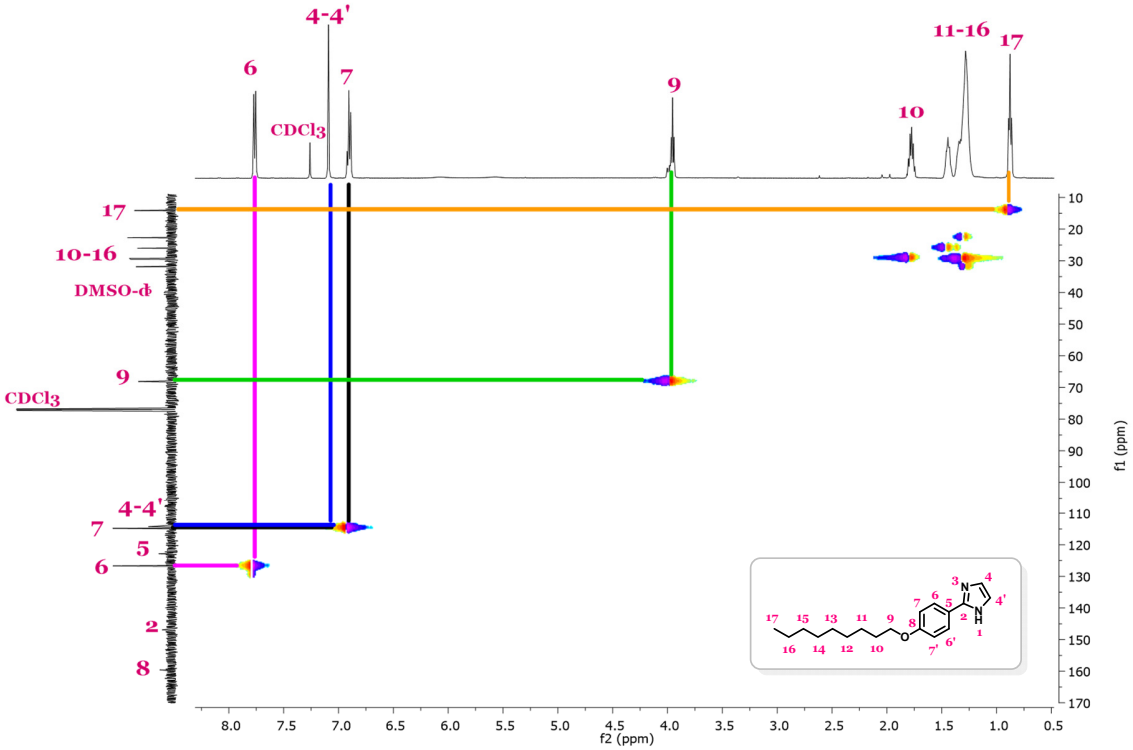

Intens.
x10^7
+MS, 0.2-0.3min #27-35
1+
273.09
2.0
1.5
1.0
0.5
0.0
100
200
300
400
500
600
m/z
N
N
H
O

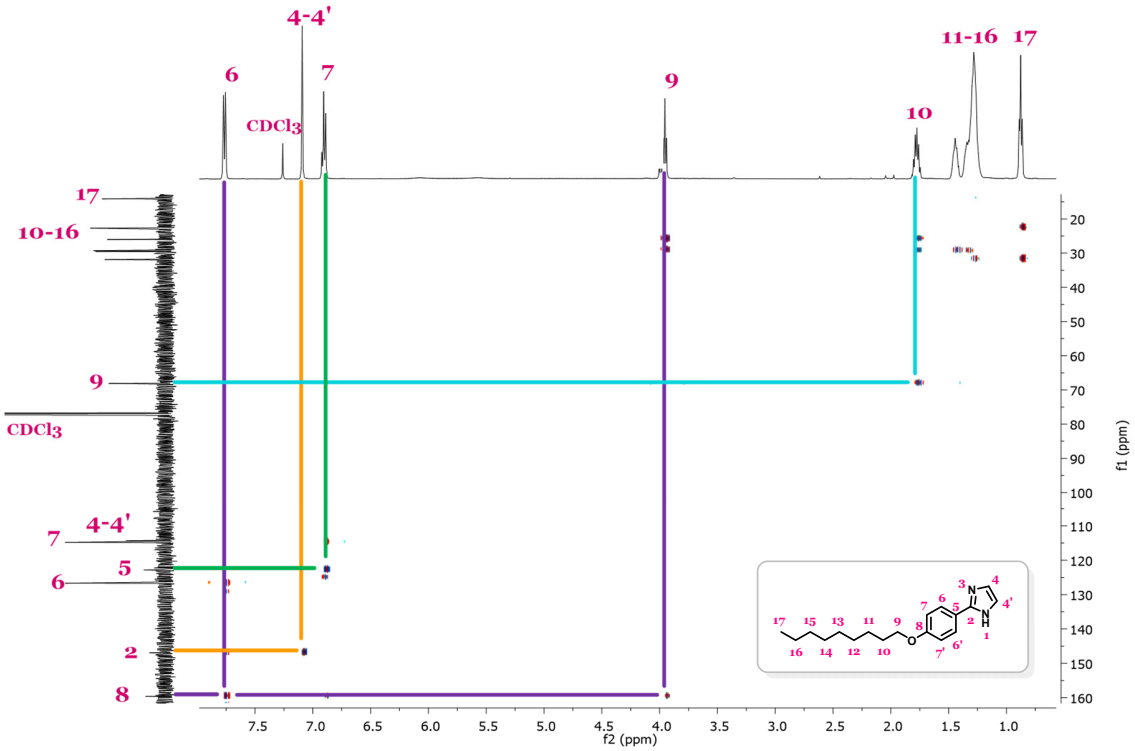

C17H24N2O, M+nH, 273.20
1+
273.20
2000
1500
1000
500
0
100
200
300
400
500
600
m/z

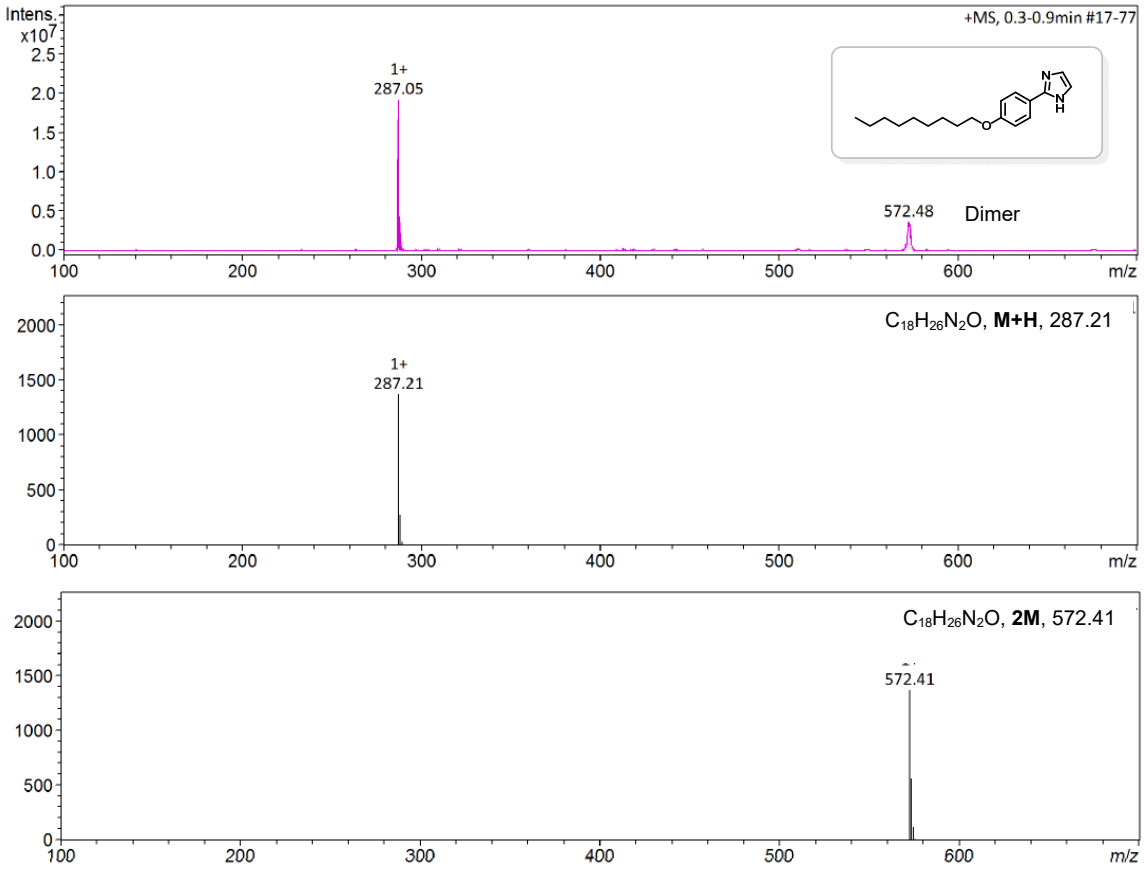

N-H
N–C=N
C-H
%T
cm-1
3164.1
2925.8
2854.7
1618.8
1518.0
1463.7
1396.9
1303.1
1258.4
1181.5
1101.2
1015.6
844.3
726.4
707.3
657.8
533.4


4-4'
6
7
9
10
11
12-16
17
CDCl3


159.59
146.91
126.67
122.83
114.79
114.27
68.10
31.88
29.54
29.41
29.27
29.23
26.03
22.68
14.13
CDCl3
8
2
6
5
7
4-4'
9
10
11-16
17
f1 (ppm)


4-4'
6
7
CDCl3
9
10
11-16
17
17
10-16
DMSO-d6
9
CDCl3
4-4'
7
5
6
2
8
f2 (ppm)
f1 (ppm)


4-4'
6
7
CDCl3
9
10
11-16
17
17
10-16
9
CDCl3
7
4-4'
5
6
2
8
f2 (ppm)
f1 (ppm)


Intens.
x10^7
2.5
2.0
1.5
1.0
0.5
0.0
+MS, 0.3-0.9min #17-77
1+
287.05
572.48
Dimer
100
200
300
400
500
600
m/z
2000
1500
1000
500
0
C18H26N2O, M+H, 287.21
1+
287.21
C18H26N2O, 2M, 572.41
572.41