Copies of spectra

Pd-Mediated new synthesis of pyrroles: Their evalution as potential inhibitors of phosphodiesterase 4

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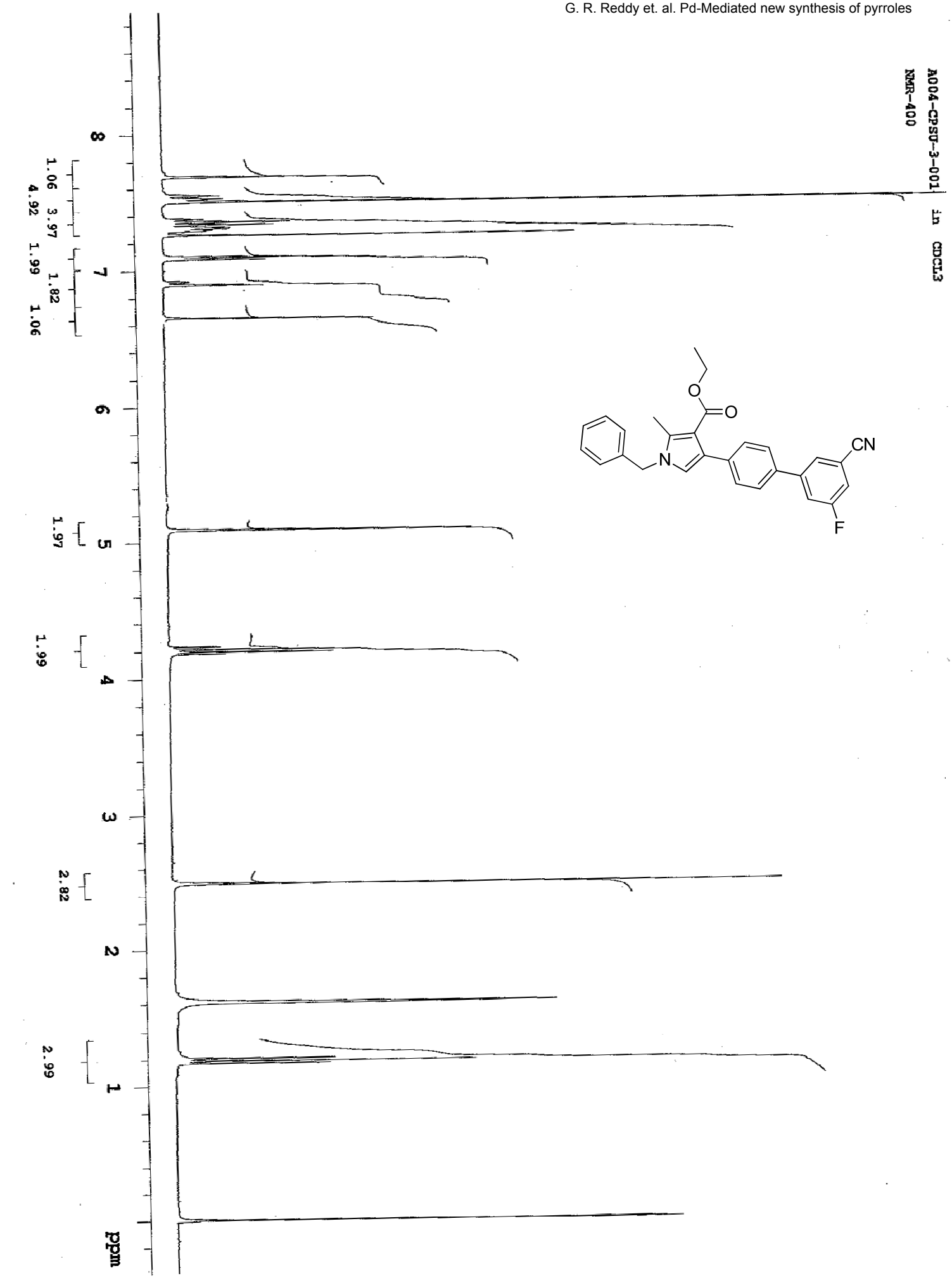
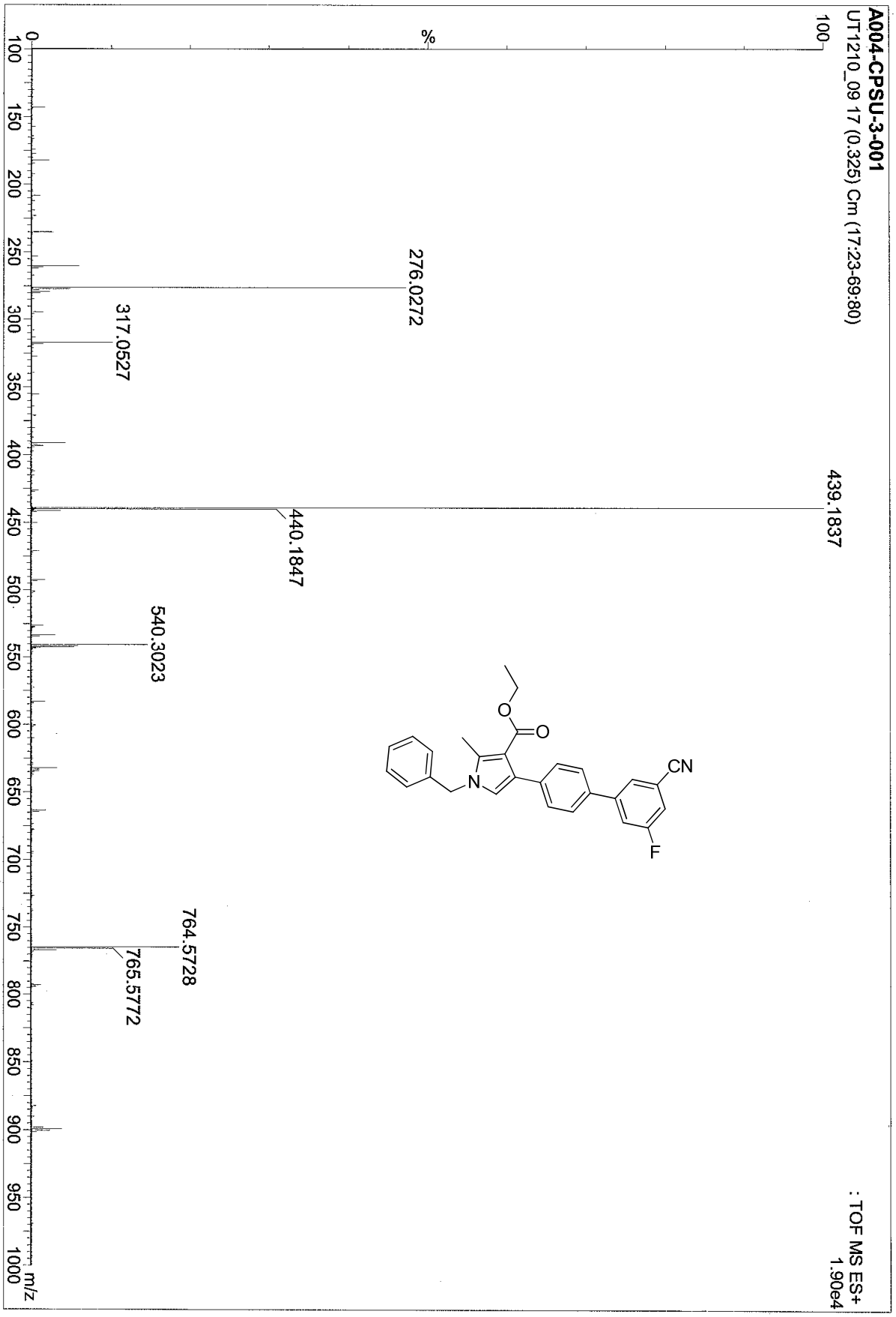

A004-CPSU-3-001
NMR-400
in CDCL3
8
7
6
5
4
3
2
1
ppm
1.06
3.97
1.82
4.92
1.99
1.06
1.97
1.99
2.82
2.99
O
O
N
CN
F


A004-CPSU-3-001
UT1210_09 17 (0.325) Cm (17:23-69:80)
: TOF MS ES+
1.90e4
%
100
0
276.0272
317.0527
439.1837
440.1847
540.3023
764.5728
765.5772
m/z
O
O
N
CN
F

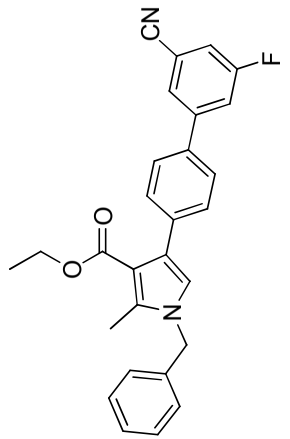
Elemental Composition Report

Single Mass Analysis

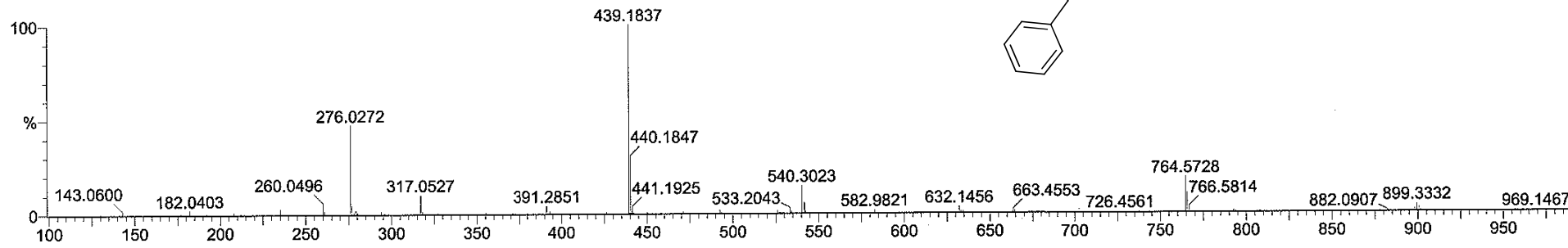
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
239 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-4 O: 0-4 F: 0-1

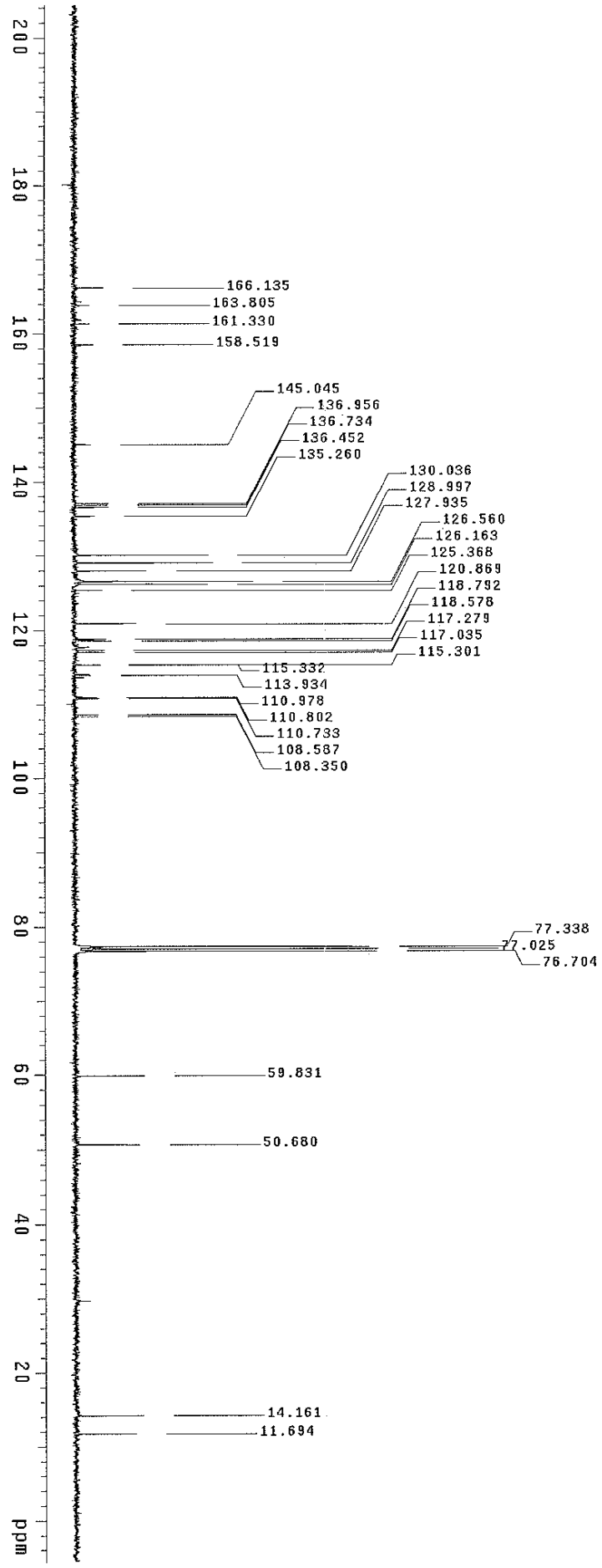
A004-CPSU-3-001
UT1210_09 17 (0.325) Cm (17:23-69:80)

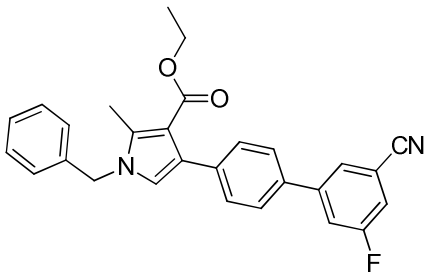


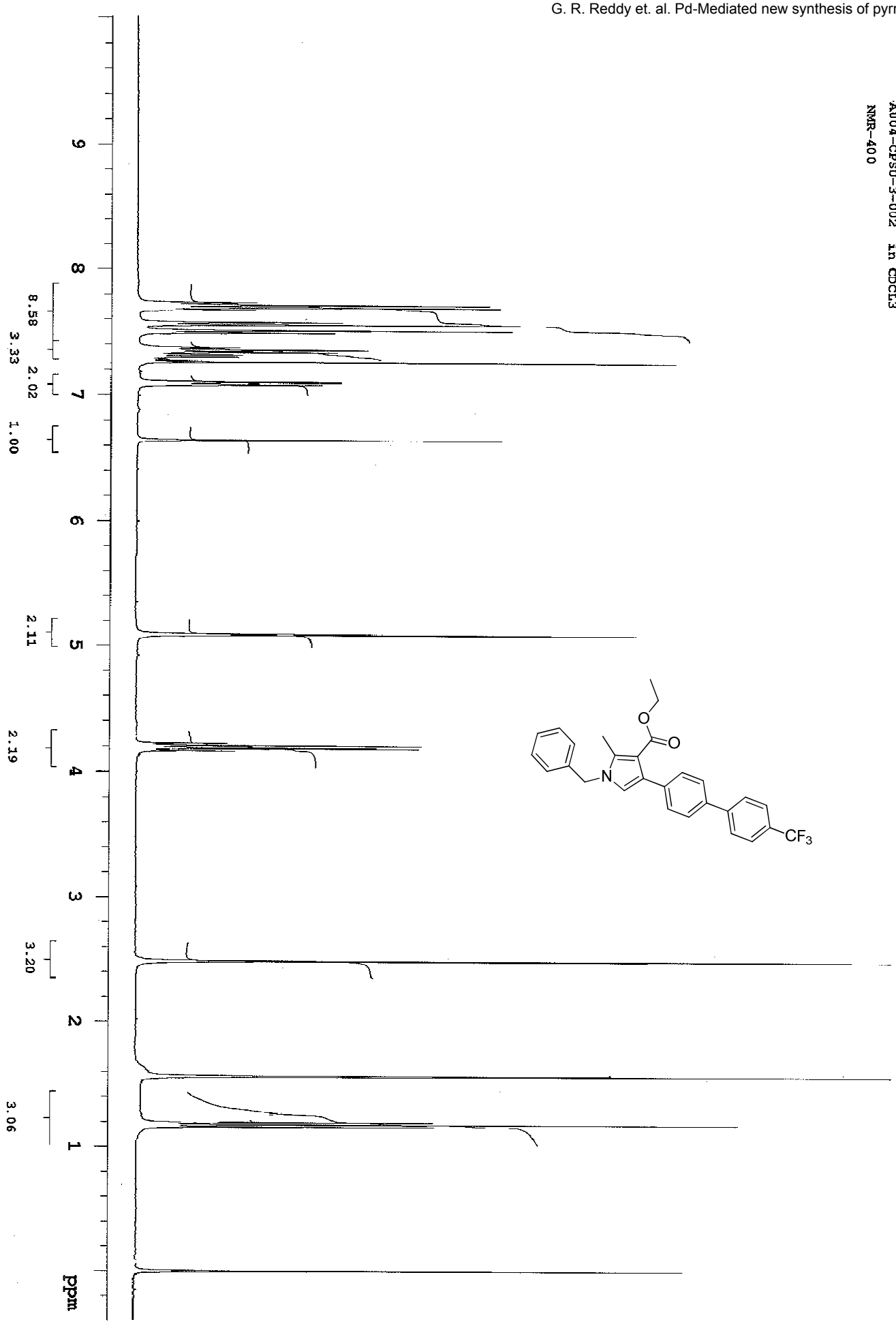
1: TOF

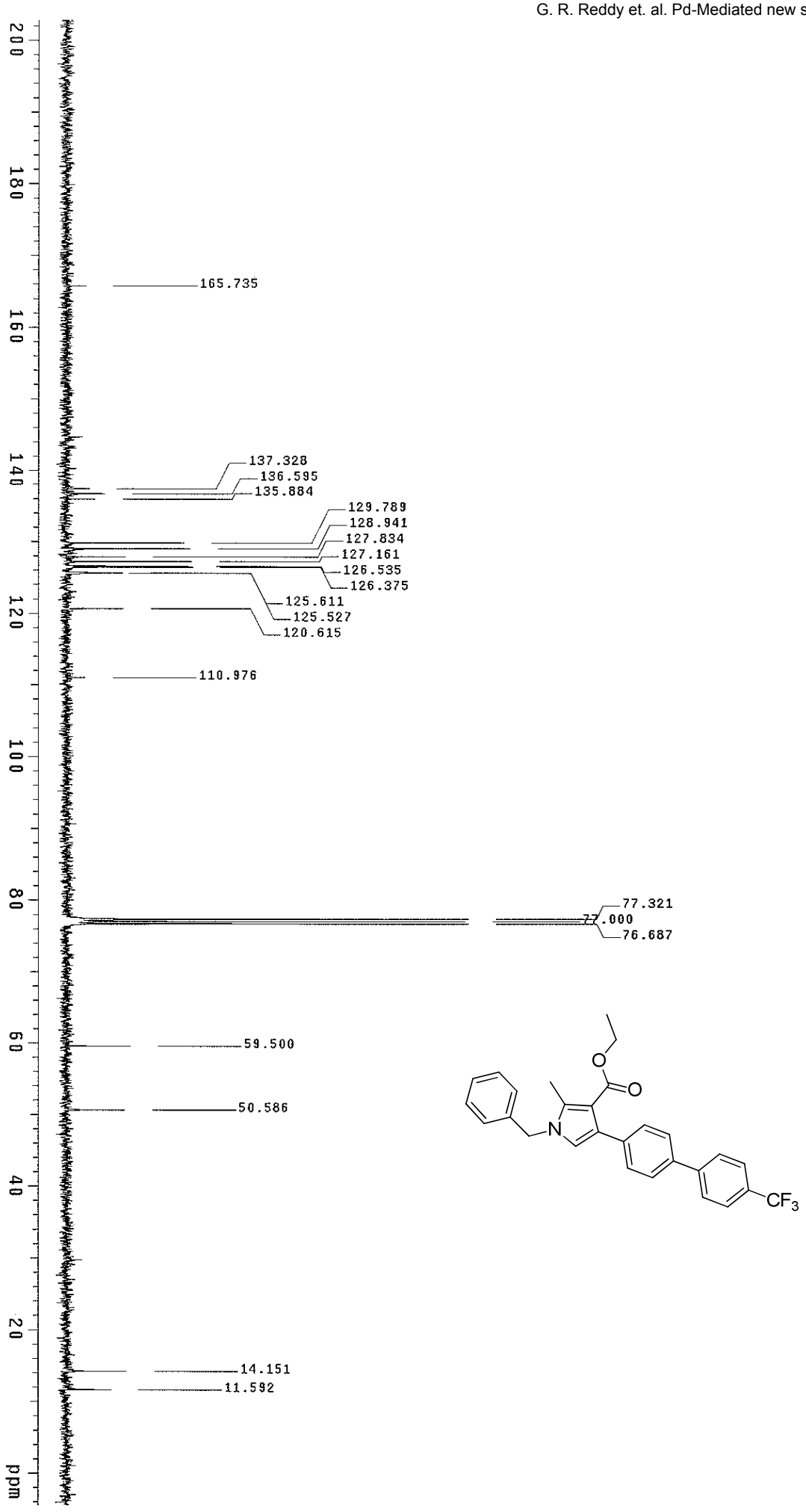


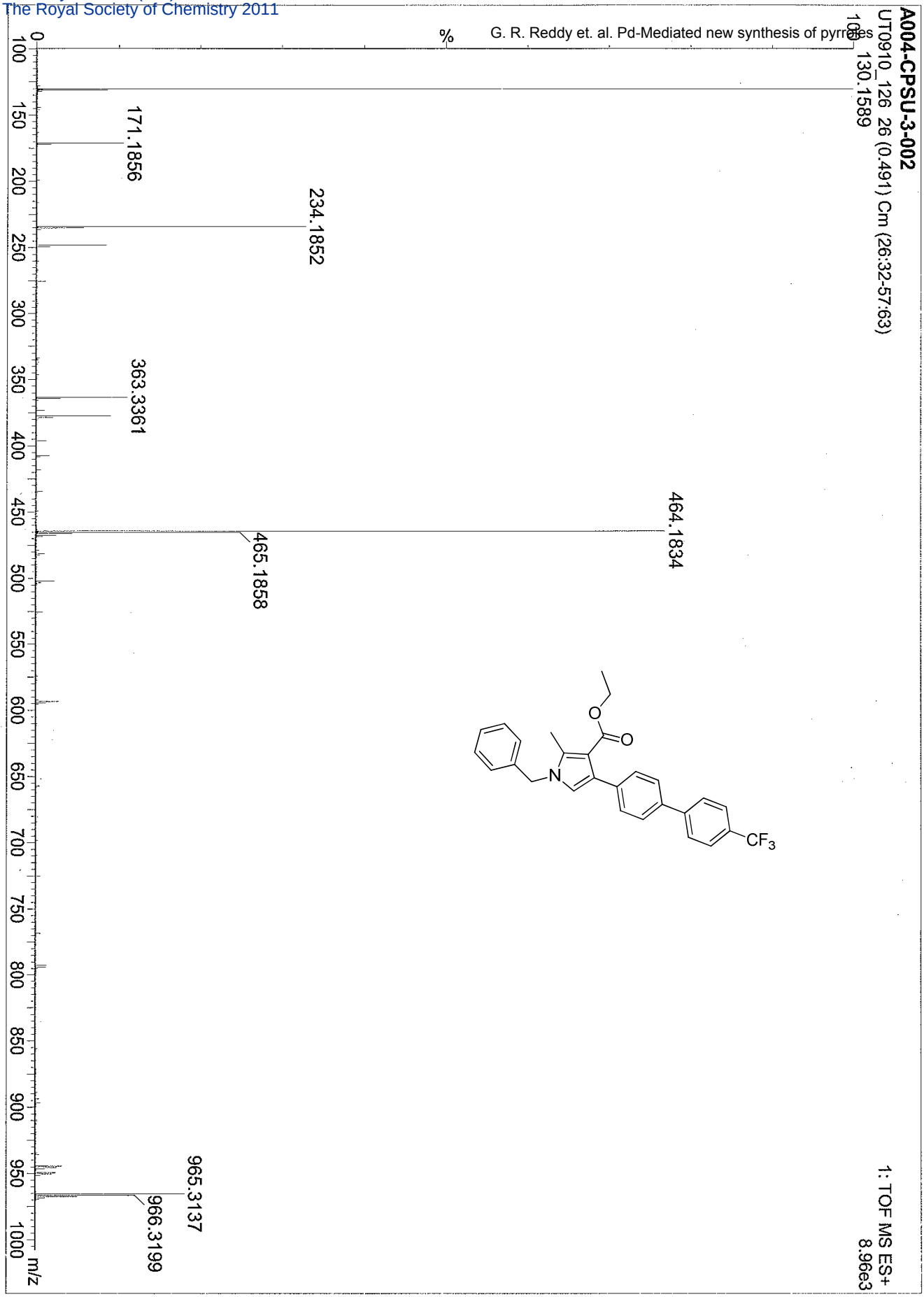
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
439.1837	439.1822	1.5	3.4	17.5	76.5	C28 H24 N2 O2 F


A004-CPSU-3-001 in CDCl3
NMR-400
166.135
163.805
161.330
158.519
145.045
136.956
136.734
136.452
135.260
130.036
128.997
127.935
126.560
126.163
125.368
120.869
118.792
118.578
117.279
117.035
115.301
115.332
113.934
110.978
110.802
110.733
108.587
108.350
77.338
77.025
76.704
59.831
50.680
14.161
11.694
200
180
160
140
120
100
80
60
40
20
ppm


O
O
N
CN
F


AU04-CPSU-3-002 in CDCl3
NMR-400
8.58
2.02
3.33
1.00
2.11
2.19
3.20
3.06
ppm
O
O
N
CF3


A004/CPSU-3/002 in CDCl3
NMR-400
165.735
137.328
136.595
135.884
129.789
128.941
127.834
127.161
126.535
126.375
125.611
125.527
120.615
110.976
77.321
77.000
76.687
59.500
50.586
14.151
11.592
ppm
O
O
N
CF3

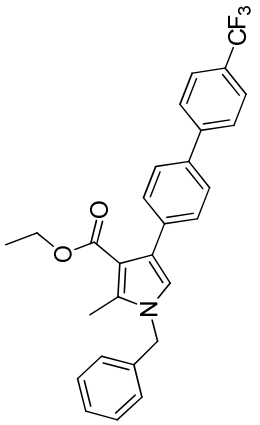


Elemental Composition Report

Single Mass Analysis

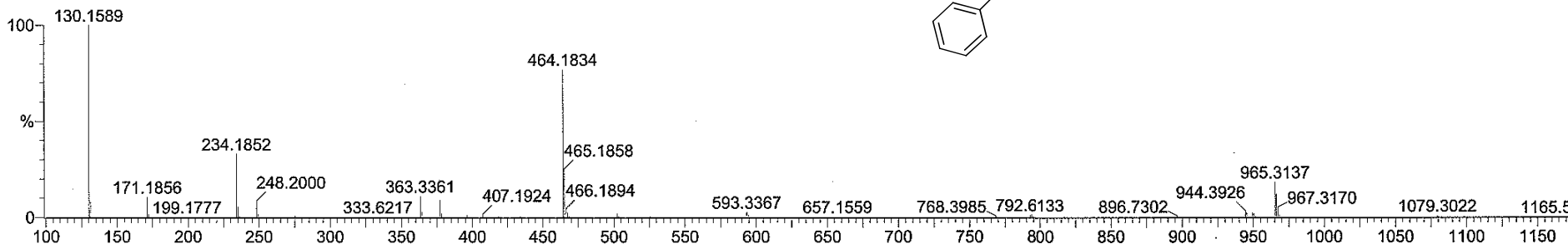
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
395 formula(e) evaluated with 3 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-35 H: 0-60 N: 0-3 O: 0-4 F: 0-3

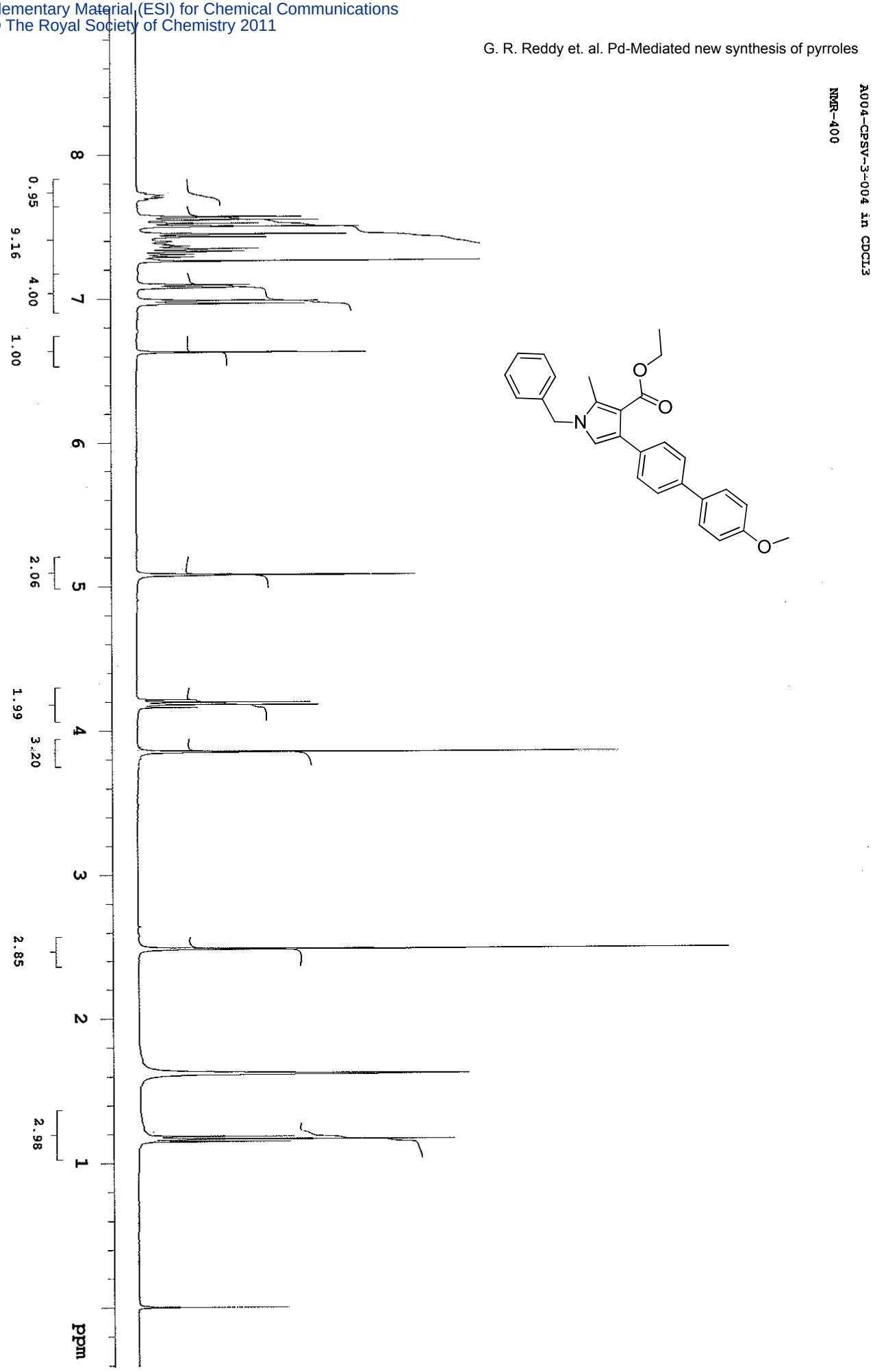


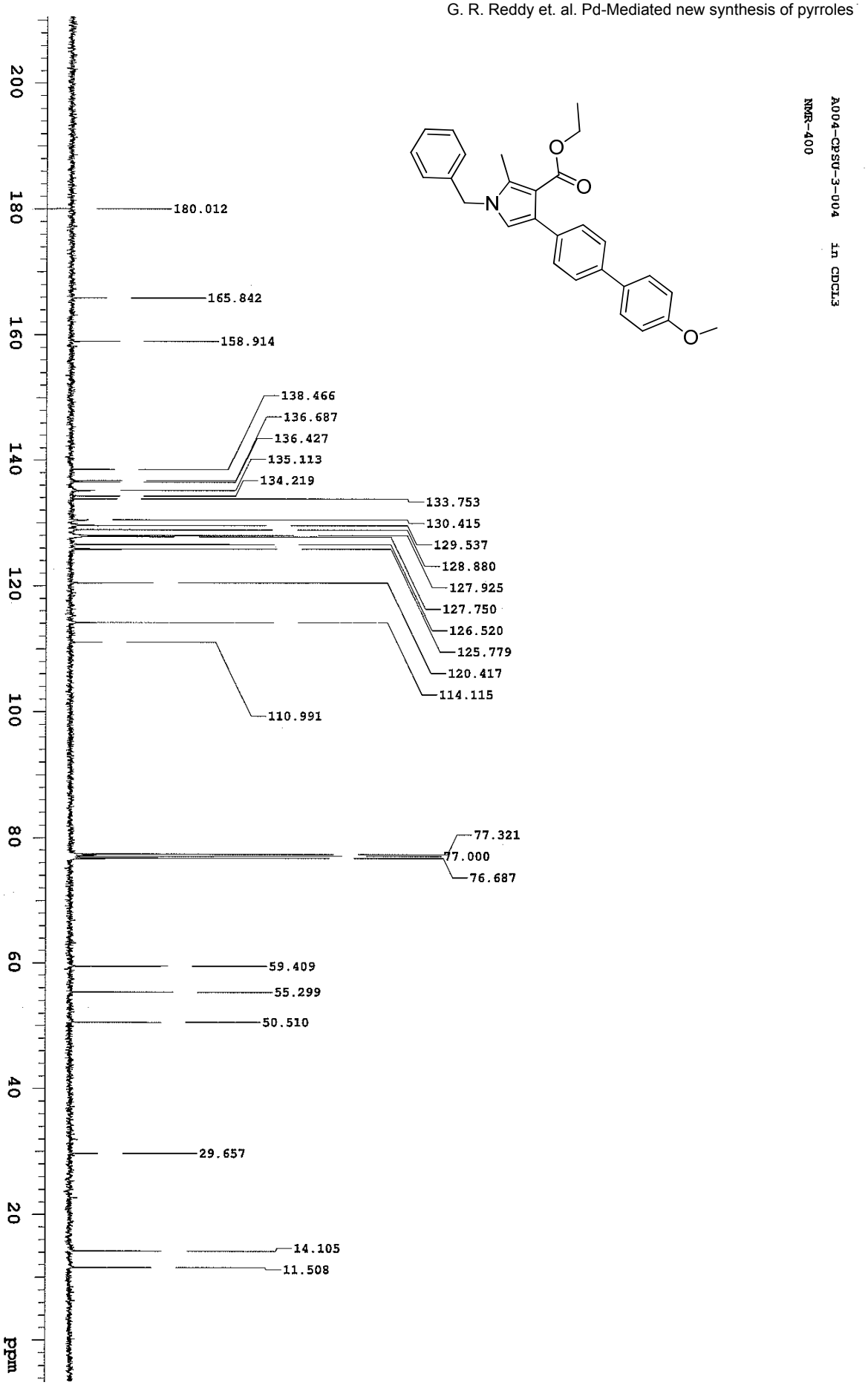
A004-CPSU-3-002
UT0910_126 26 (0.491) Cm (26:32-57:63)

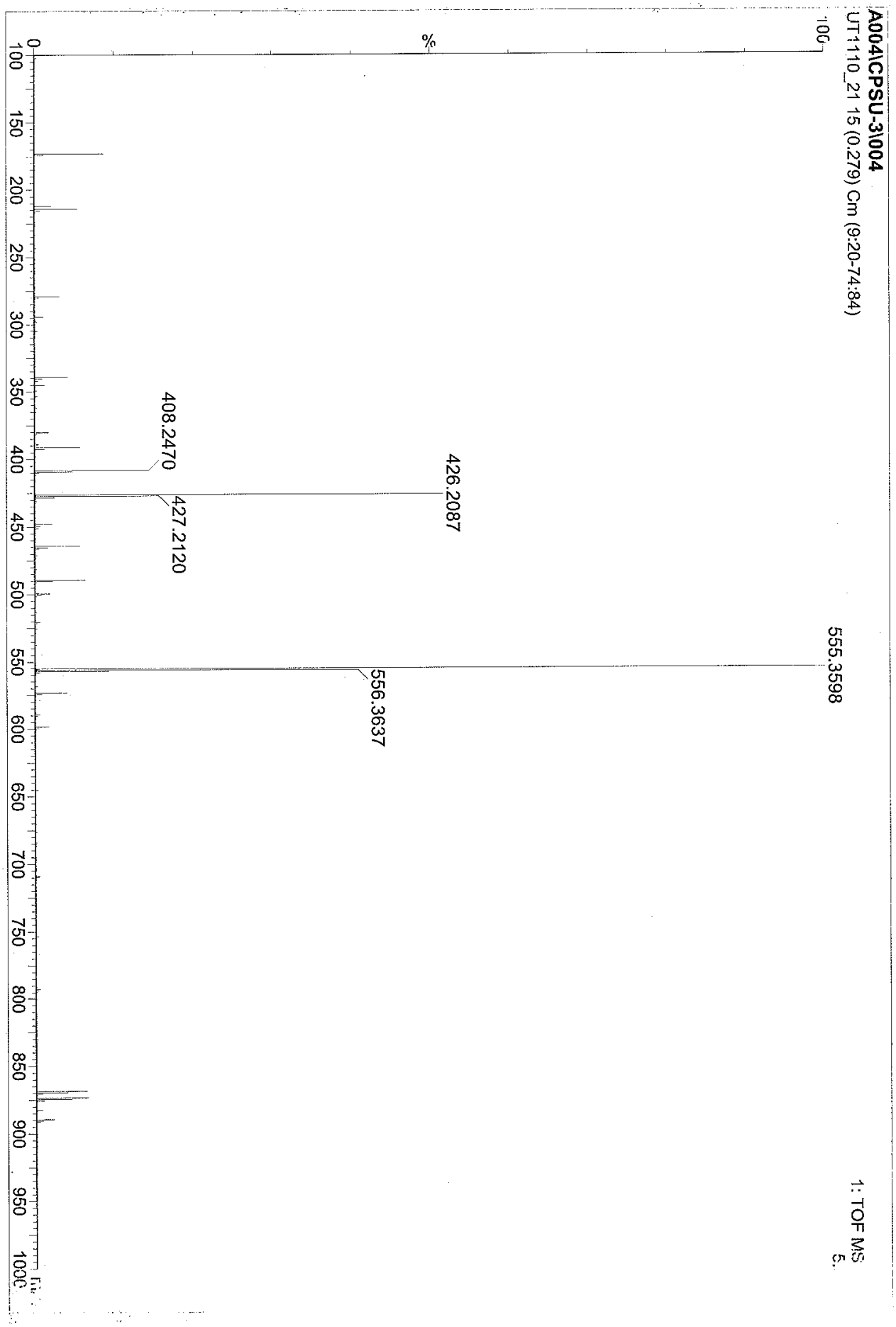
1: TO



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
464.1834	464.1837	-0.3	-0.6	15.5	0.2	C28 H25 N O2 F3
	464.1826	0.8	1.7	19.5	6.4	C31 H24 N O F2
	464.1815	1.9	4.1	23.5	28.0	C34 H23 N F




A004-CPSU-3-004 in CDCL3
NMR-400
O
O
N
O
180.012
165.842
158.914
138.466
136.687
136.427
135.113
134.219
133.753
130.415
129.537
128.880
127.925
127.750
126.520
125.779
120.417
114.115
110.991
77.321
77.000
76.687
59.409
55.299
50.510
29.657
14.105
11.508
200
180
160
140
120
100
80
60
40
20
ppm

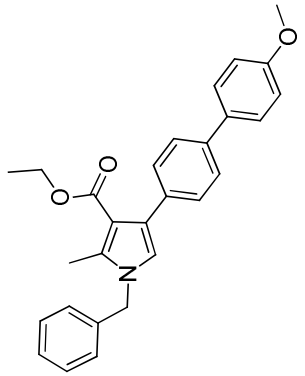

A004\CPSU-3\004
UT1110_21 15 (0.279) Cm (9:20-74:84)
%
100
0
408.2470
426.2087
427.2120
555.3598
556.3637
1: TOF MS
5.

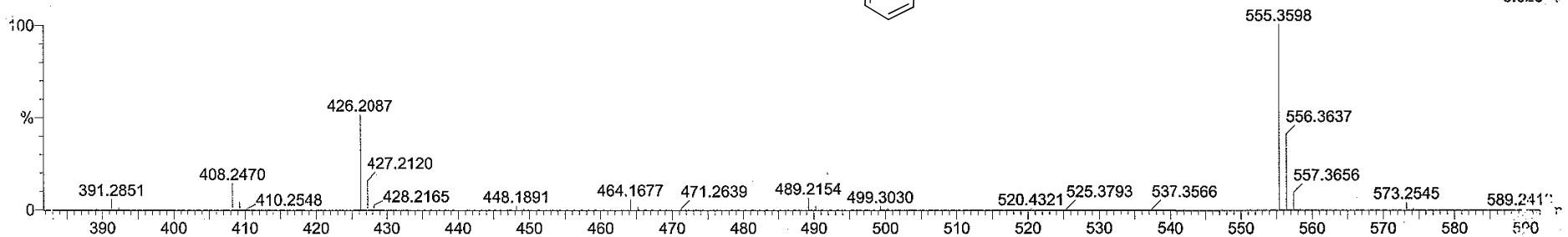
Elemental Composition Report

Single Mass Analysis

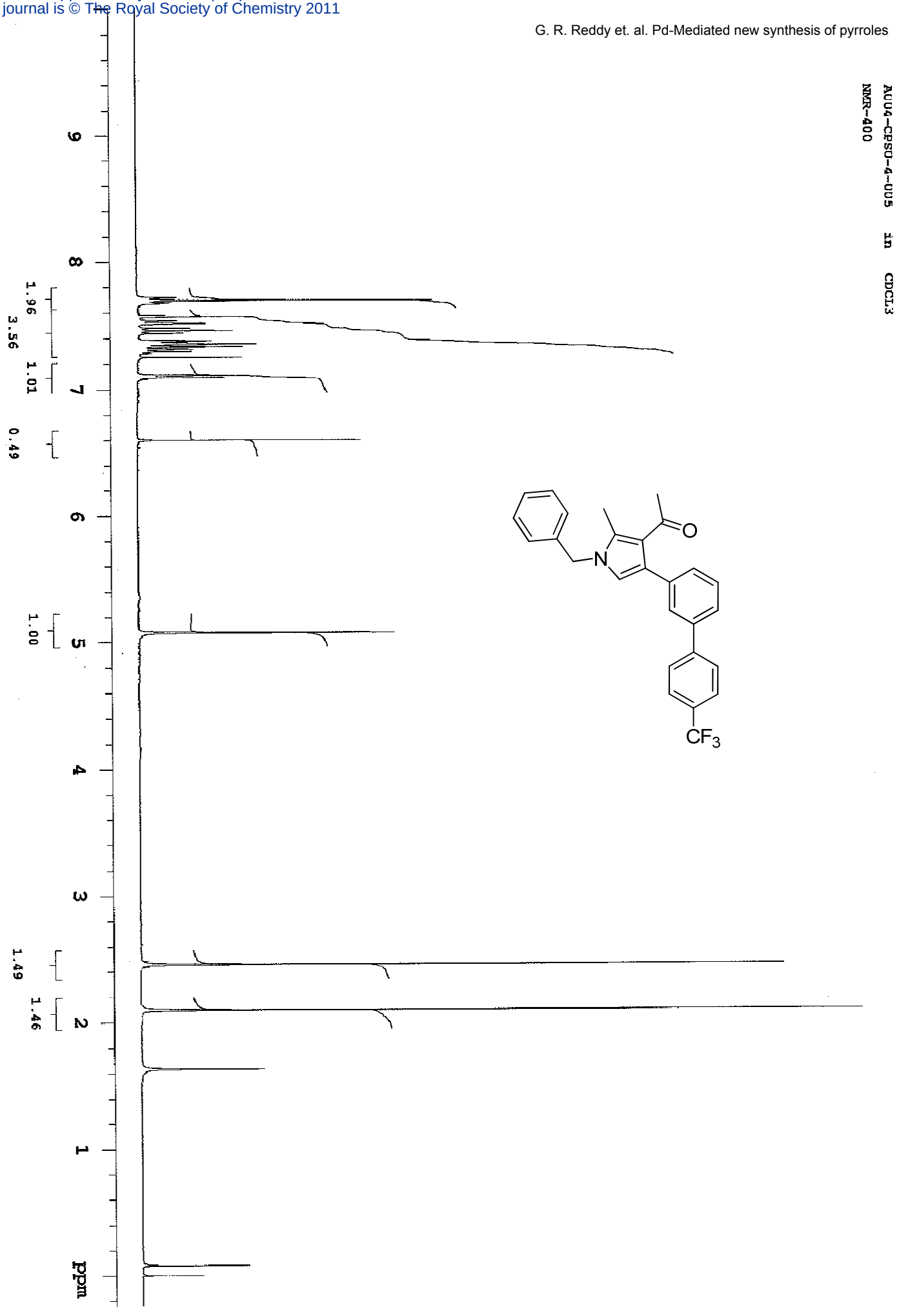
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

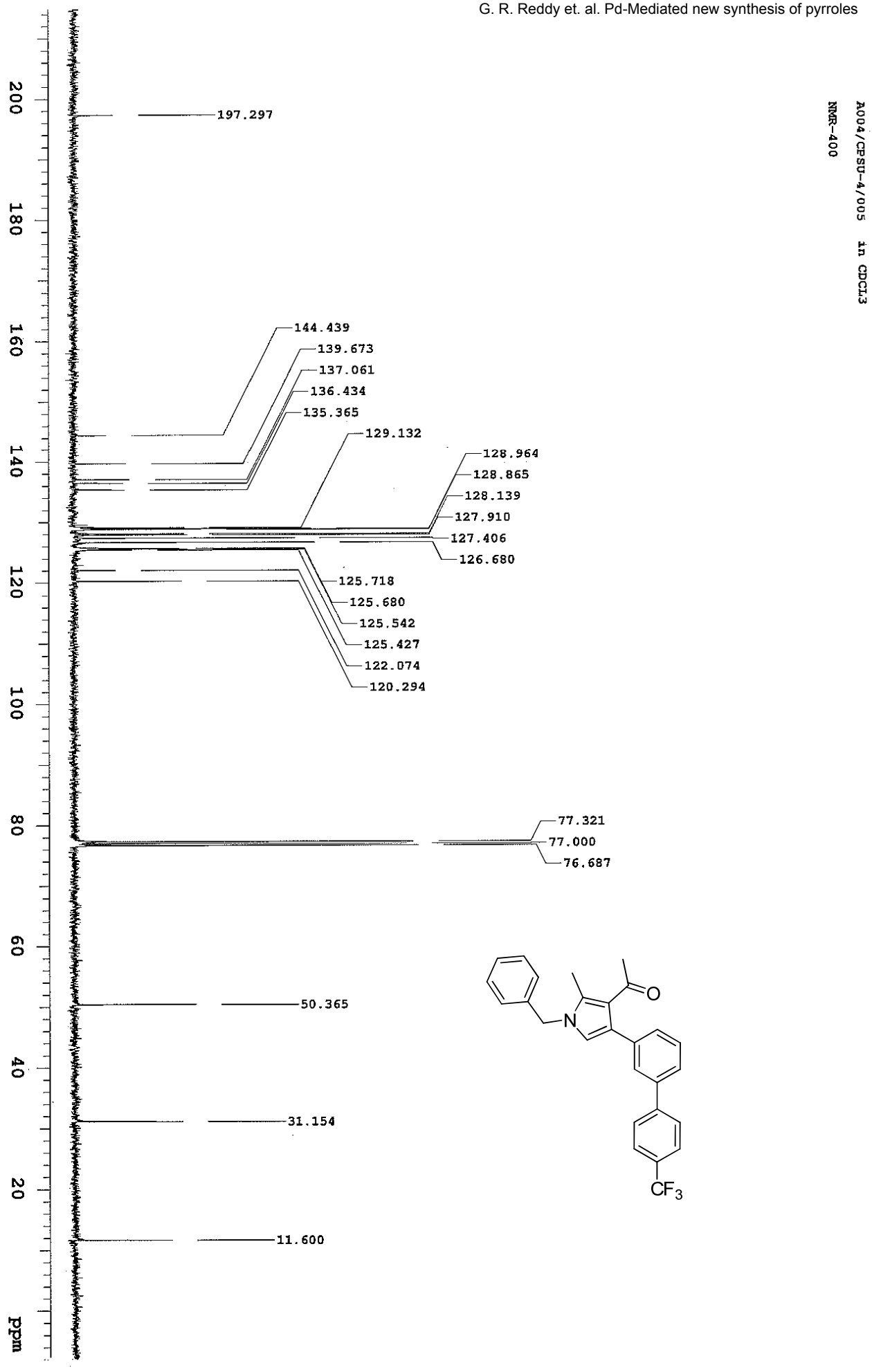
Monoisotopic Mass, Even Electron Ions
138 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-5 O: 0-5
A004\CPSU-3\004
UT1110_21 15 (0.279) Cm (9:20-74:84)

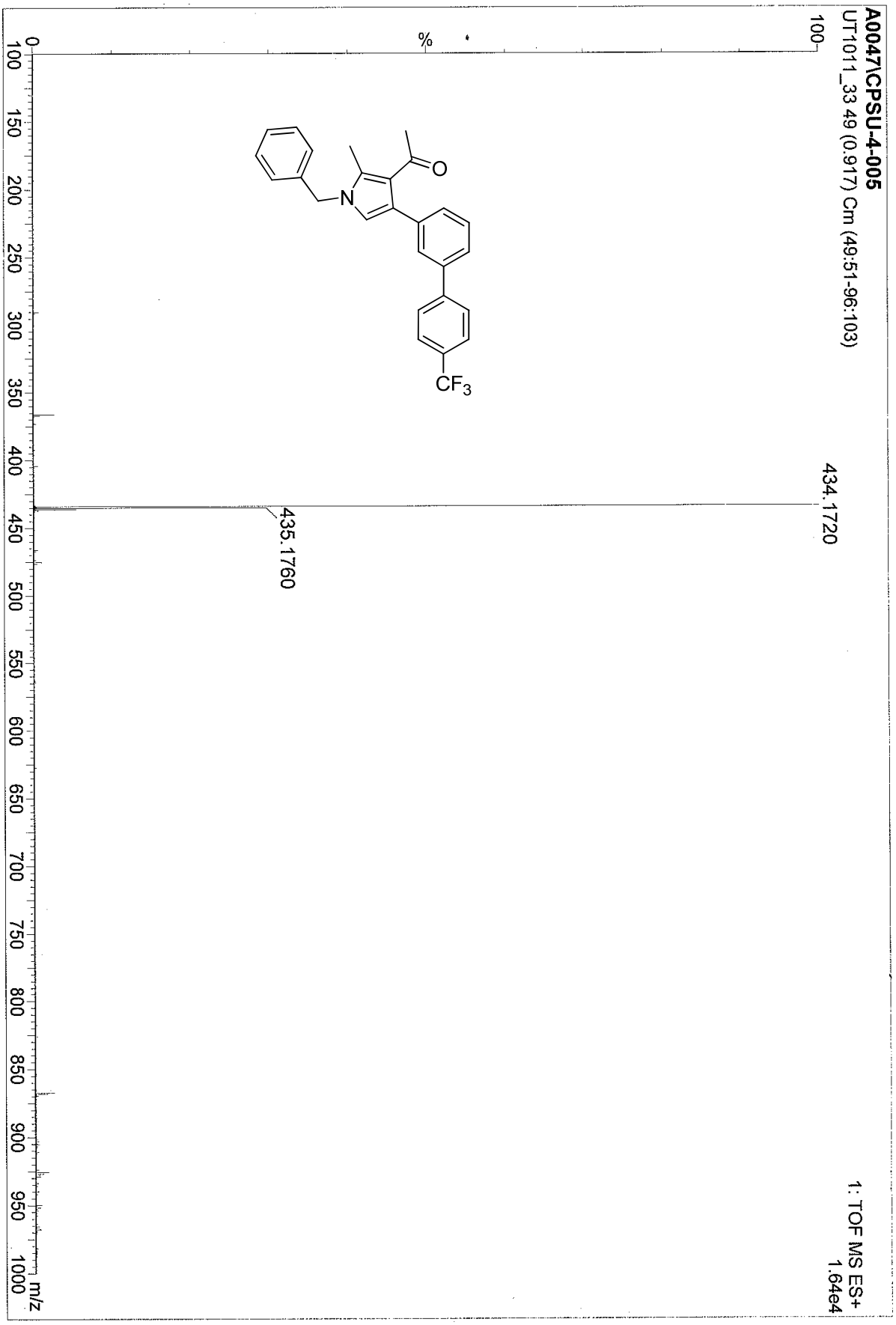




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
426.2087	426.2069	1.8	4.2	15.5	2.4	C28 H28 N O3


AUU4-CRSU-4-UU5 in CDCL3
NMR-400
1.96
3.56
1.01
0.49
1.00
1.49
1.46
O
N
CF3
ppm


A004/CPSU-4/005 in CDCL3
NMR-400
197.297
144.439
139.673
137.061
136.434
135.365
129.132
128.964
128.865
128.139
127.910
127.406
126.680
125.718
125.680
125.542
125.427
122.074
120.294
77.321
77.000
76.687
50.365
31.154
11.600
200
180
160
140
120
100
80
60
40
20
Ppm
O
N
CF3


A0047\CPSU-4-005
UT1011_33 49 (0.917) Cm (49:51-96:103)
%
100
0
434.1720
435.1760
O
N
CF3
1: TOF MS ES+
1.64e4
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z

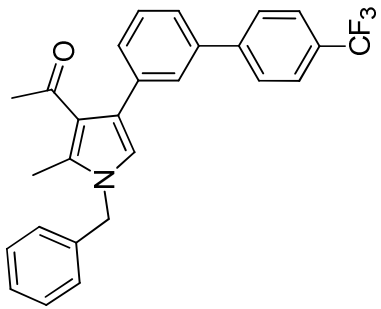
Elemental Composition Report

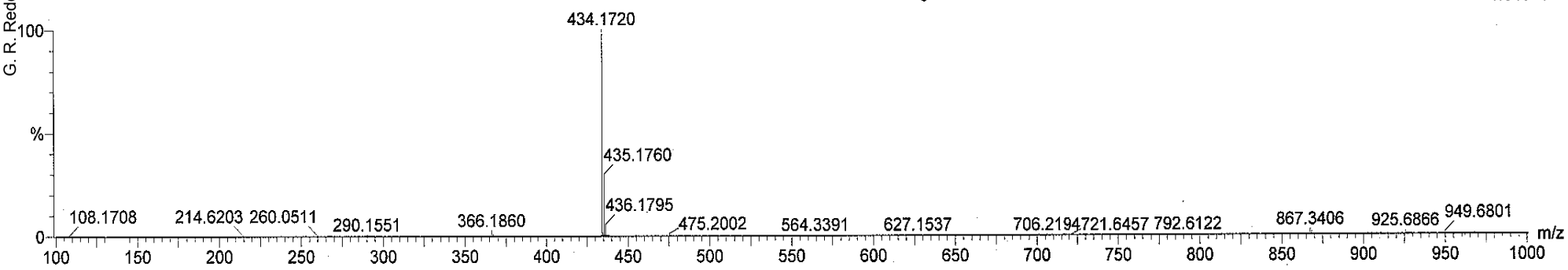
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

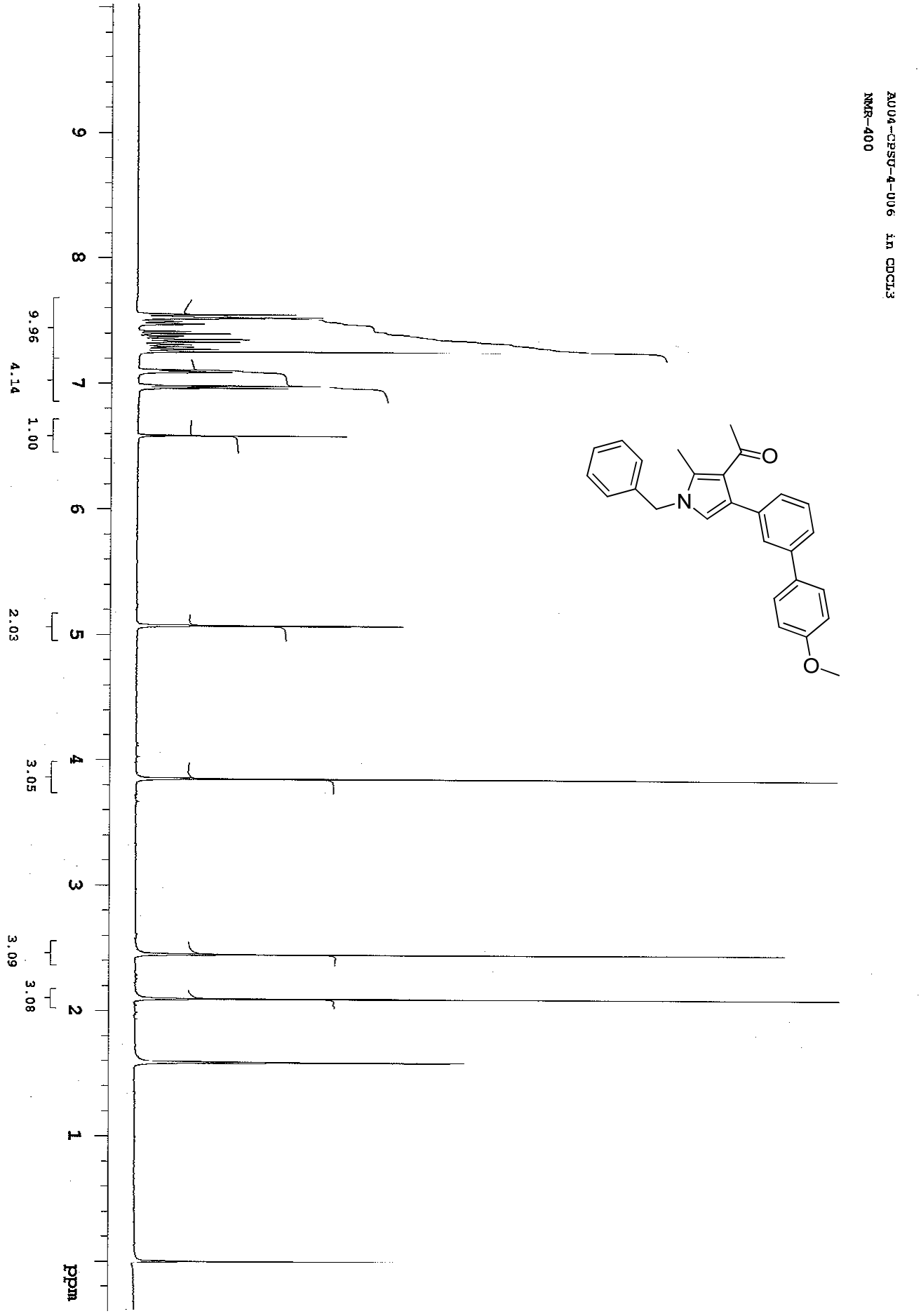
Monoisotopic Mass, Even Electron Ions
111 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-5 O: 0-6 F: 3-3

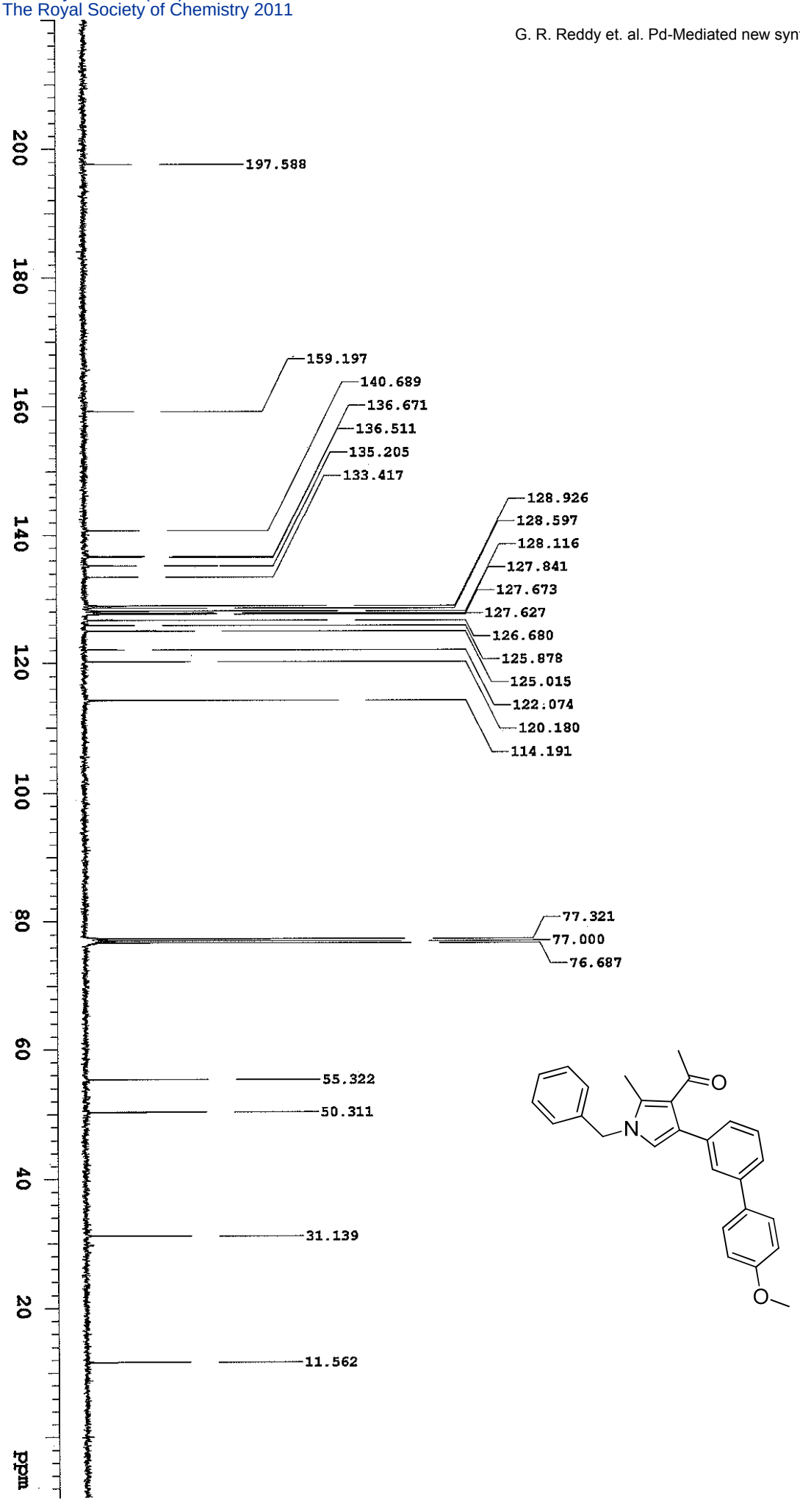
A0047\CPSU-4-005
UT1011_33 49 (0.917) Cm (49:51-96:103)

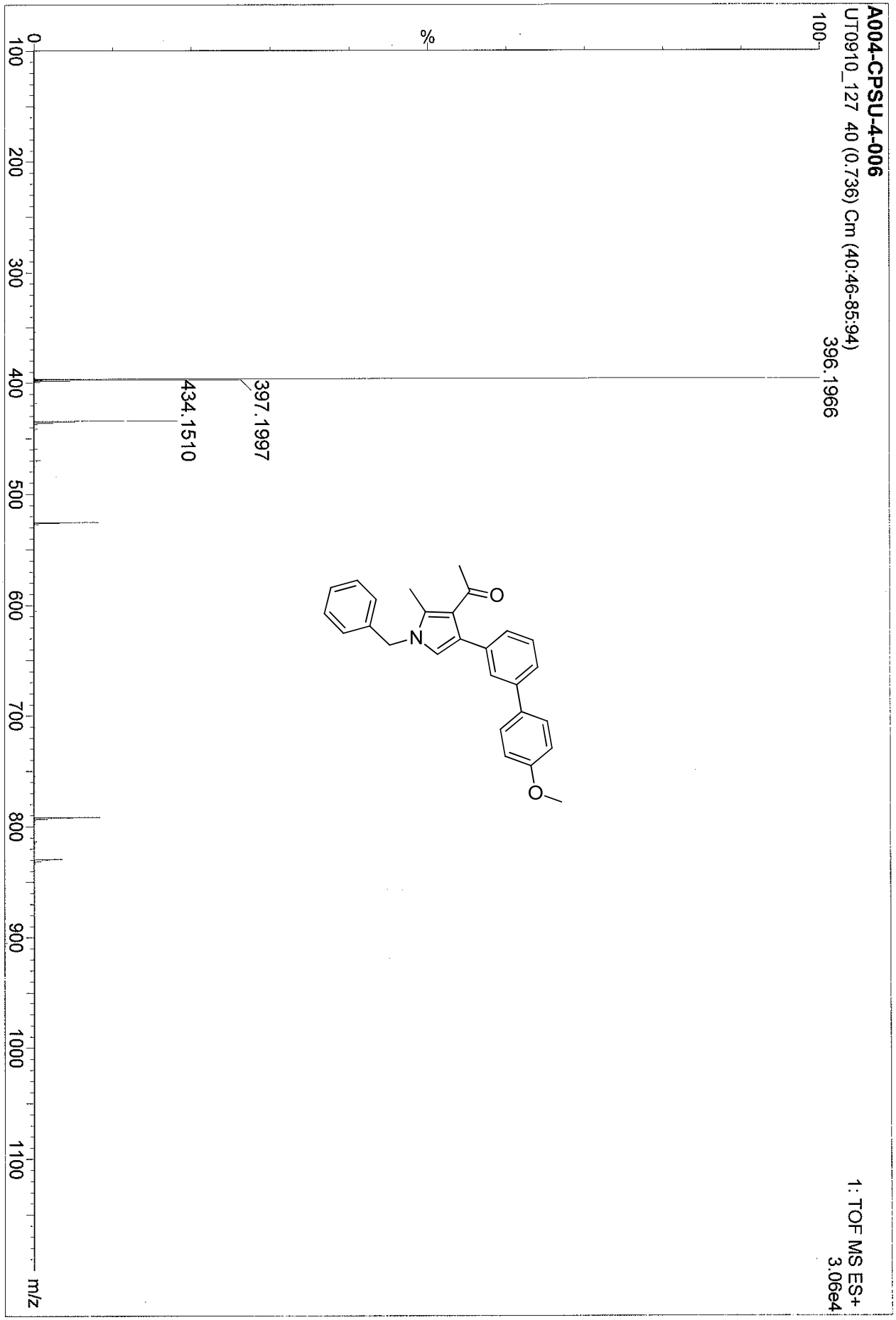




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
434.1720	434.1732	-1.2	-2.8	15.5	3.3	C27 H23 N O F3


AU04-CESU-4-006 in CDCL3
NMR-400
9.96
4.14
1.00
2.03
3.05
3.09
3.08
ppm
O
N
O



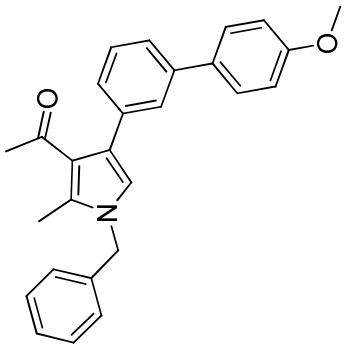

A004-CPSU-4-006
UT0910_127 40 (0.736) Cm (40:46-85:94)
%
100
0
396.1966
397.1997
434.1510
100
200
300
400
500
600
700
800
900
1000
1100
m/z
1: TOF MS ES+
3.06e4
O
N
O

Elemental Composition Report

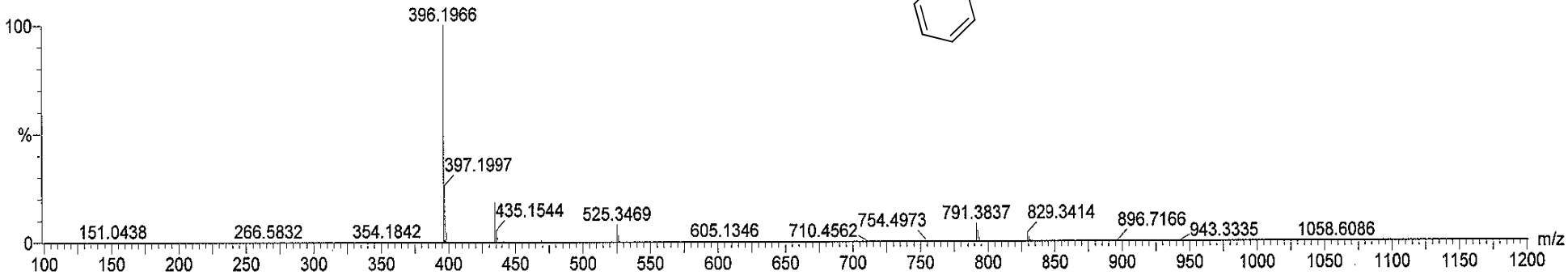
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

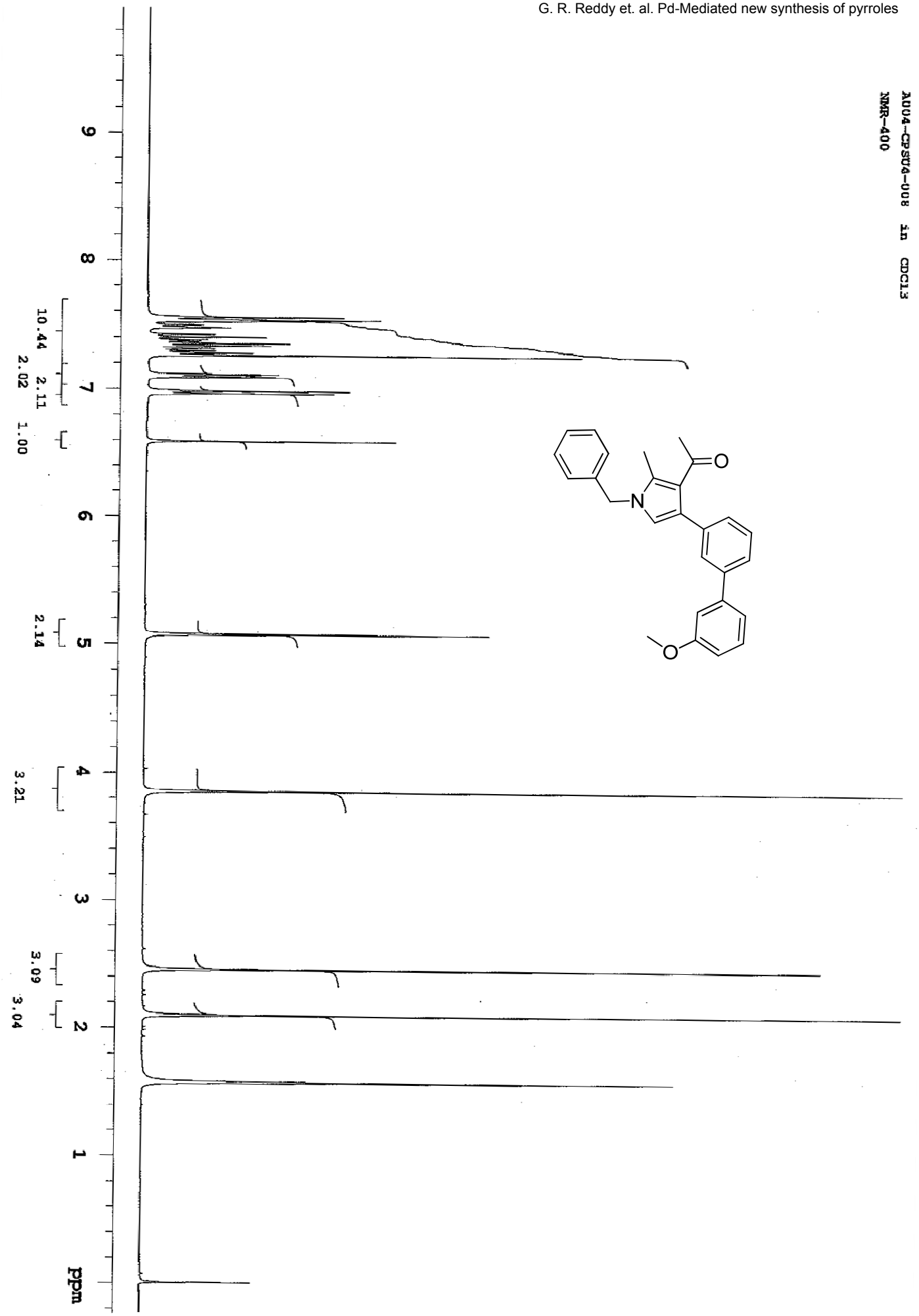
Monoisotopic Mass, Even Electron Ions
286 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-40 H: 0-60 N: 0-6 O: 0-8
A004-CPSU-4-006
UT0910_127 40 (0.736) Cm (40:46-85:94)

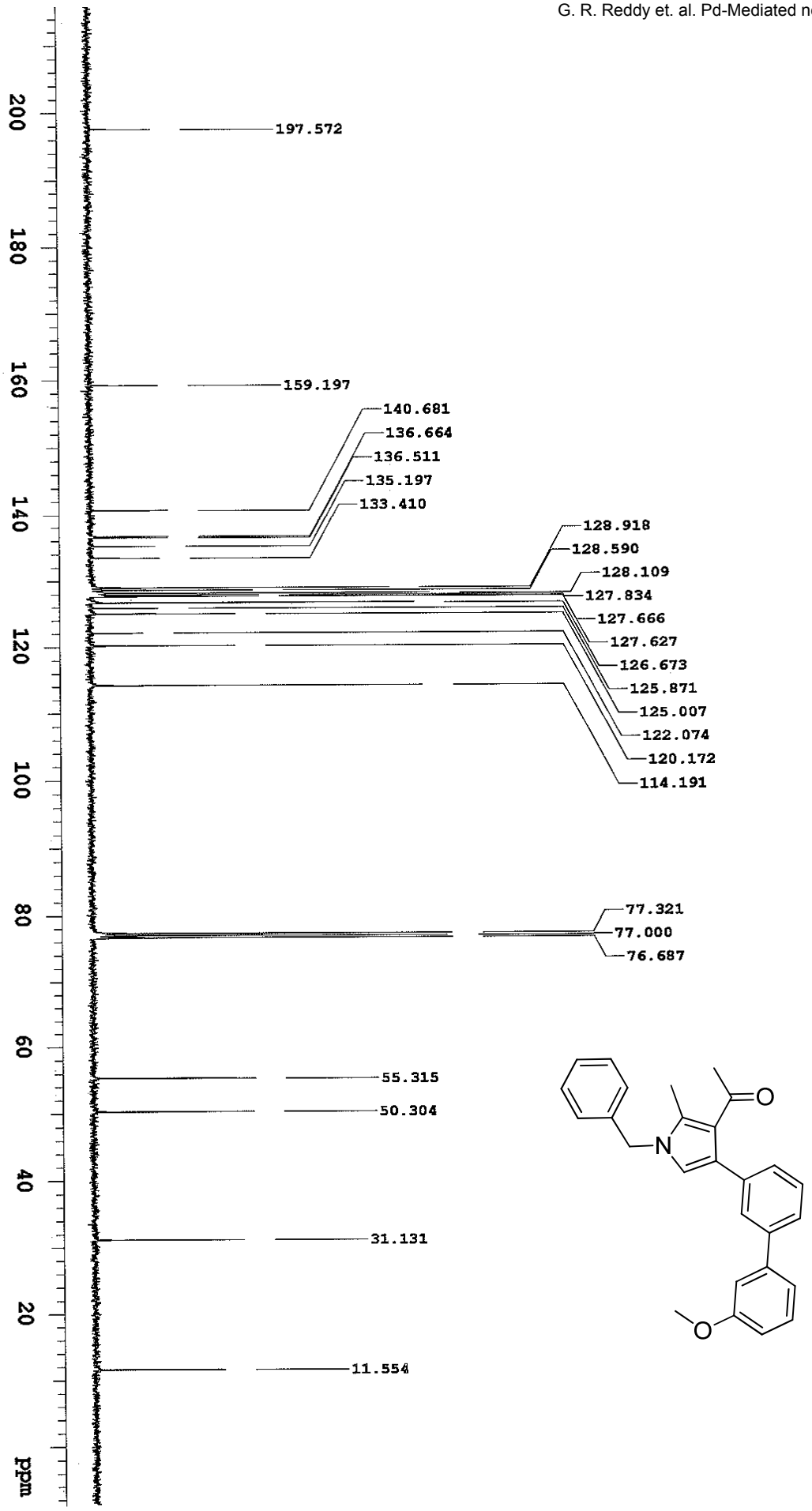


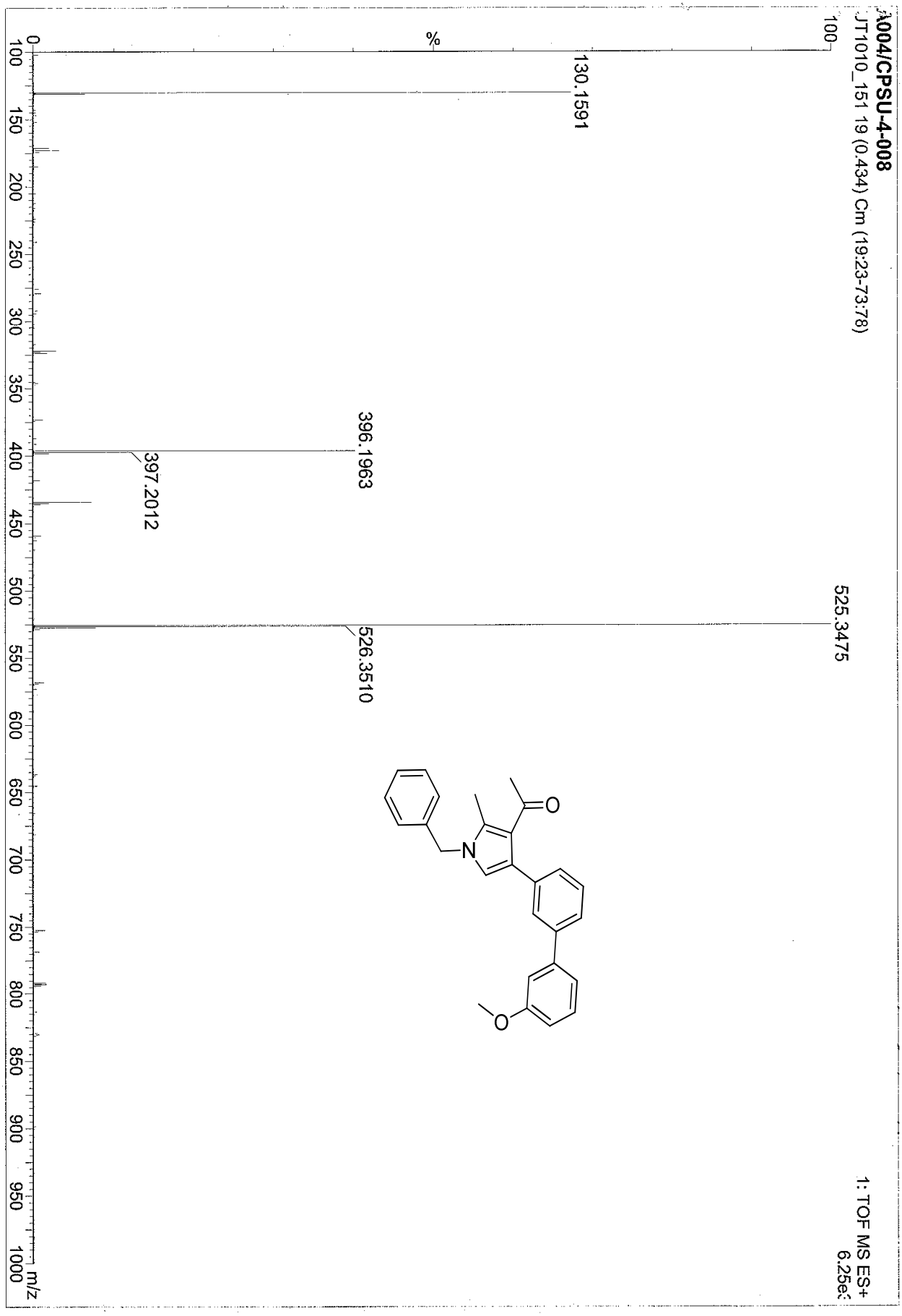
1: TOF MS ES+
3.06e+004



Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
396.1966	396.1964	0.2	0.5	15.5	91.8	C27 H26 N O2


AU04-CPSU4-008 in CDCl3
NMR-400
10.44
2.11
2.02
1.00
2.14
3.21
3.09
3.04
ppm
O
N
O


A004-CPSU-4-008 in CDCl3
NMR-400
197.572
159.197
140.681
136.664
136.511
135.197
133.410
128.918
128.590
128.109
127.834
127.666
127.627
126.673
125.871
125.007
122.074
120.172
114.191
77.321
77.000
76.687
55.315
50.304
31.131
11.554
200
180
160
140
120
100
80
60
40
20
ppm
O
N
O

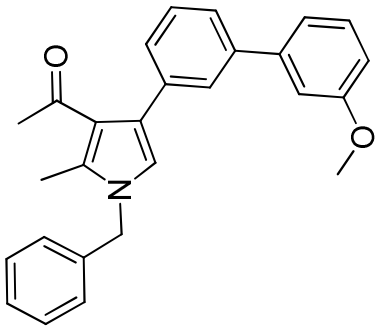

004/CPSU-4-008
JT1010_151 19 (0.434) Cm (19:23-73:78)
%
100
0
130.1591
396.1963
397.2012
525.3475
526.3510
O
N
O
1: TOF MS ES+
6.25e
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z

Elemental Composition Report

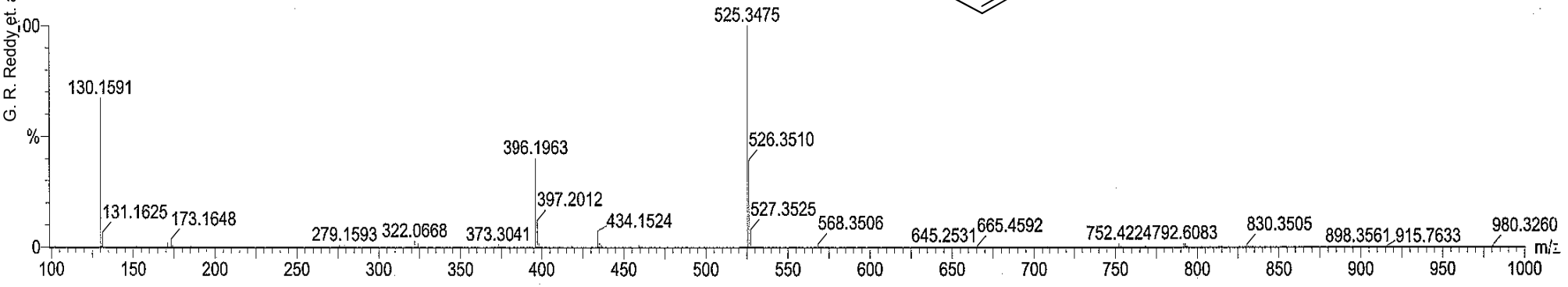
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

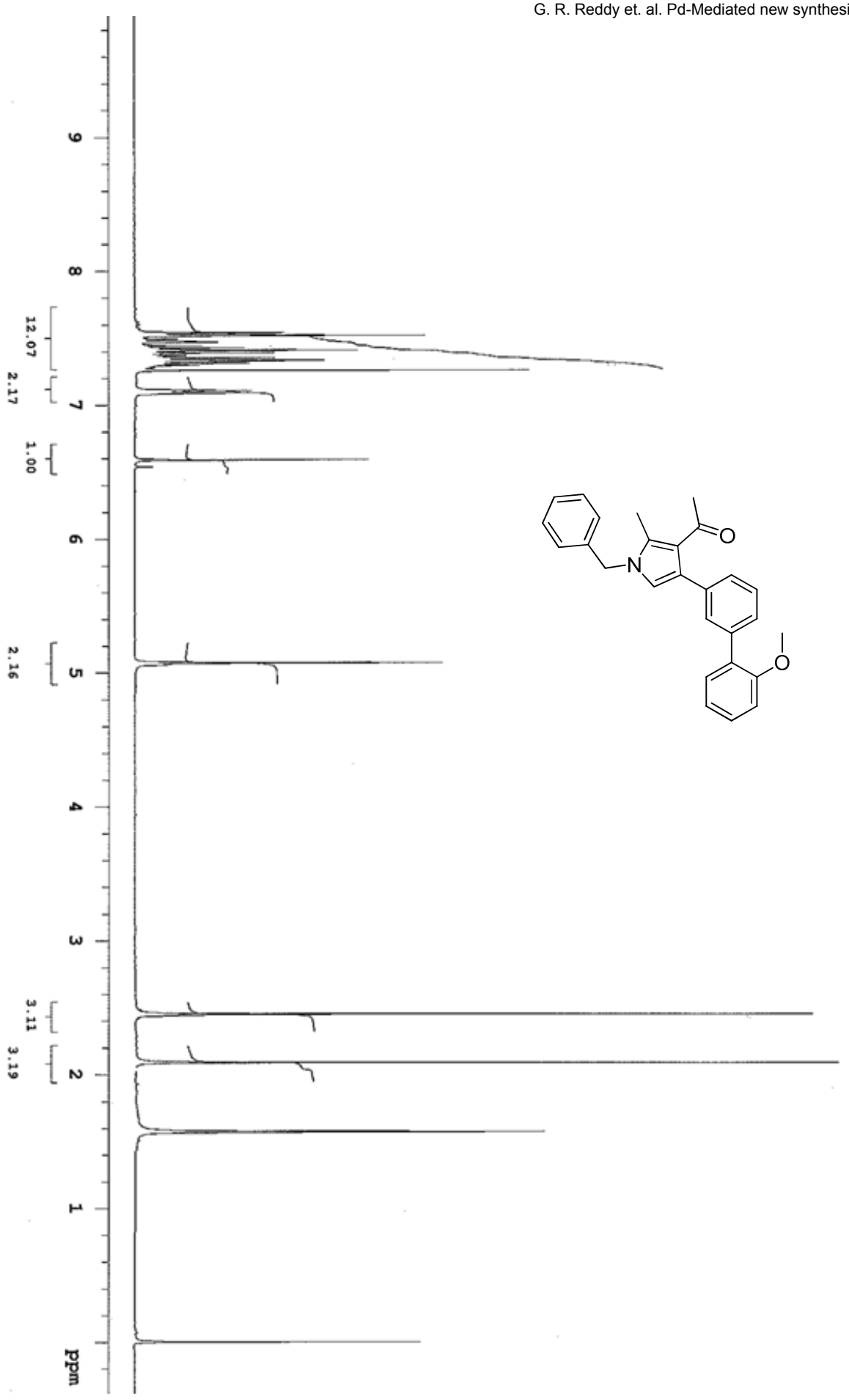
Monoisotopic Mass, Even Electron Ions
304 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-6 O: 0-6
A004/CPSU-4-008
UT1010_151 19 (0.434) Cm (19:23-73:78)

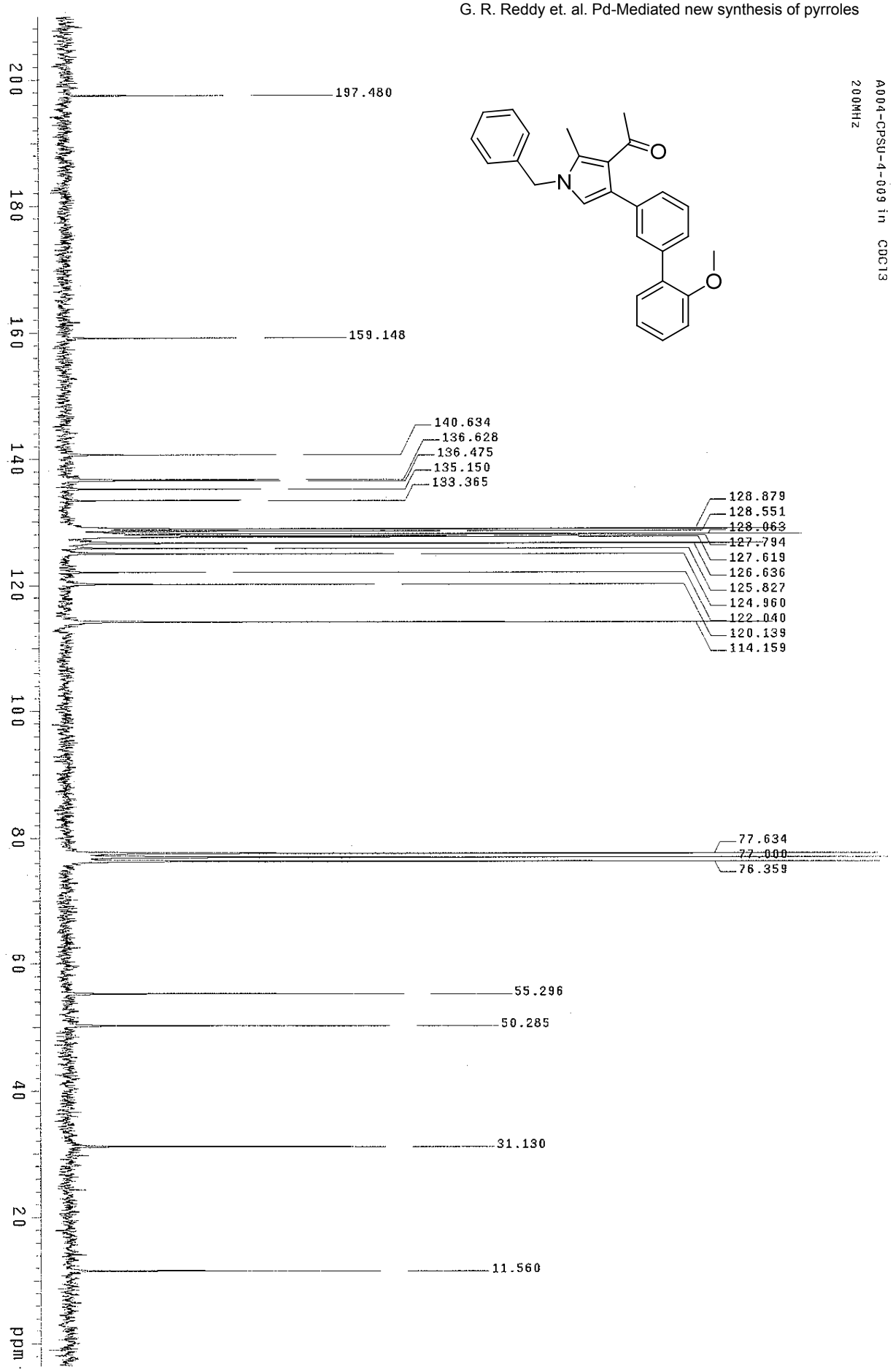


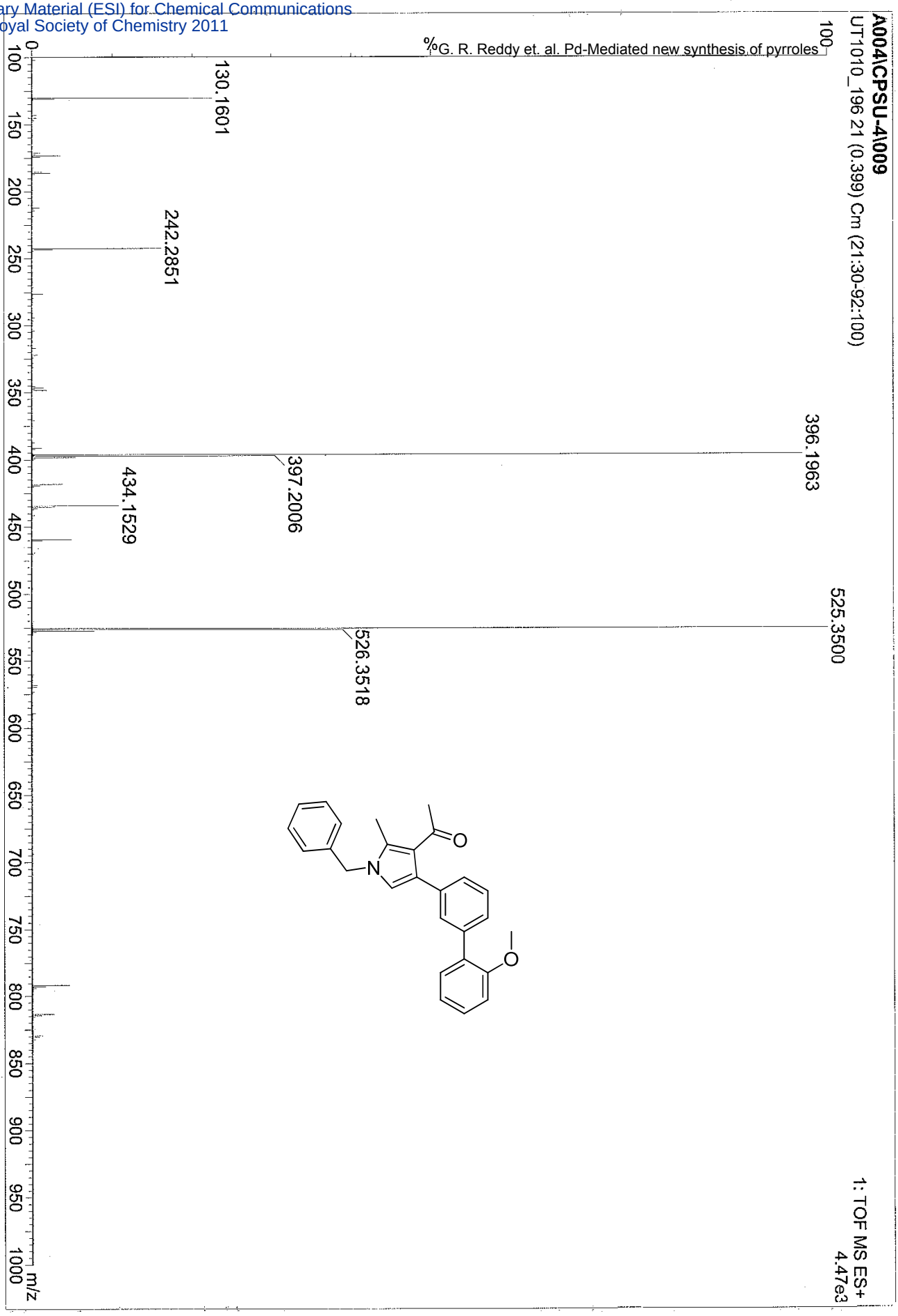
1: TOF MS ES+
6.26e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
396.1963	396.1964	-0.1	-0.3	15.5	0.2	C27 H26 N O2


A004-CPSU-4-009 in CDCL3
NMR-400
12.07
2.17
1.00
2.16
3.11
3.19
ppm
O
N
O


A004-CPSU-4-009 in CDCl3
200MHz
197.480
159.148
140.634
136.628
136.475
135.150
133.365
128.879
128.551
128.063
127.794
127.619
126.636
125.827
124.960
122.040
120.139
114.159
77.634
77.000
76.359
55.296
50.285
31.130
11.560
O
N
O
200
180
160
140
120
100
80
60
40
20
ppm



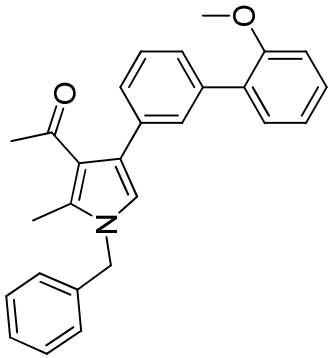
Elemental Composition Report

Single Mass Analysis

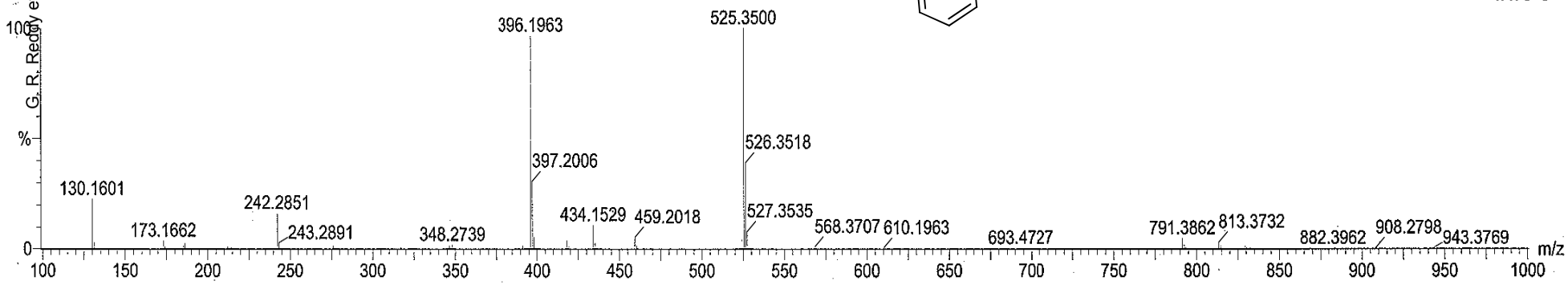
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
81 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-3 O: 0-3

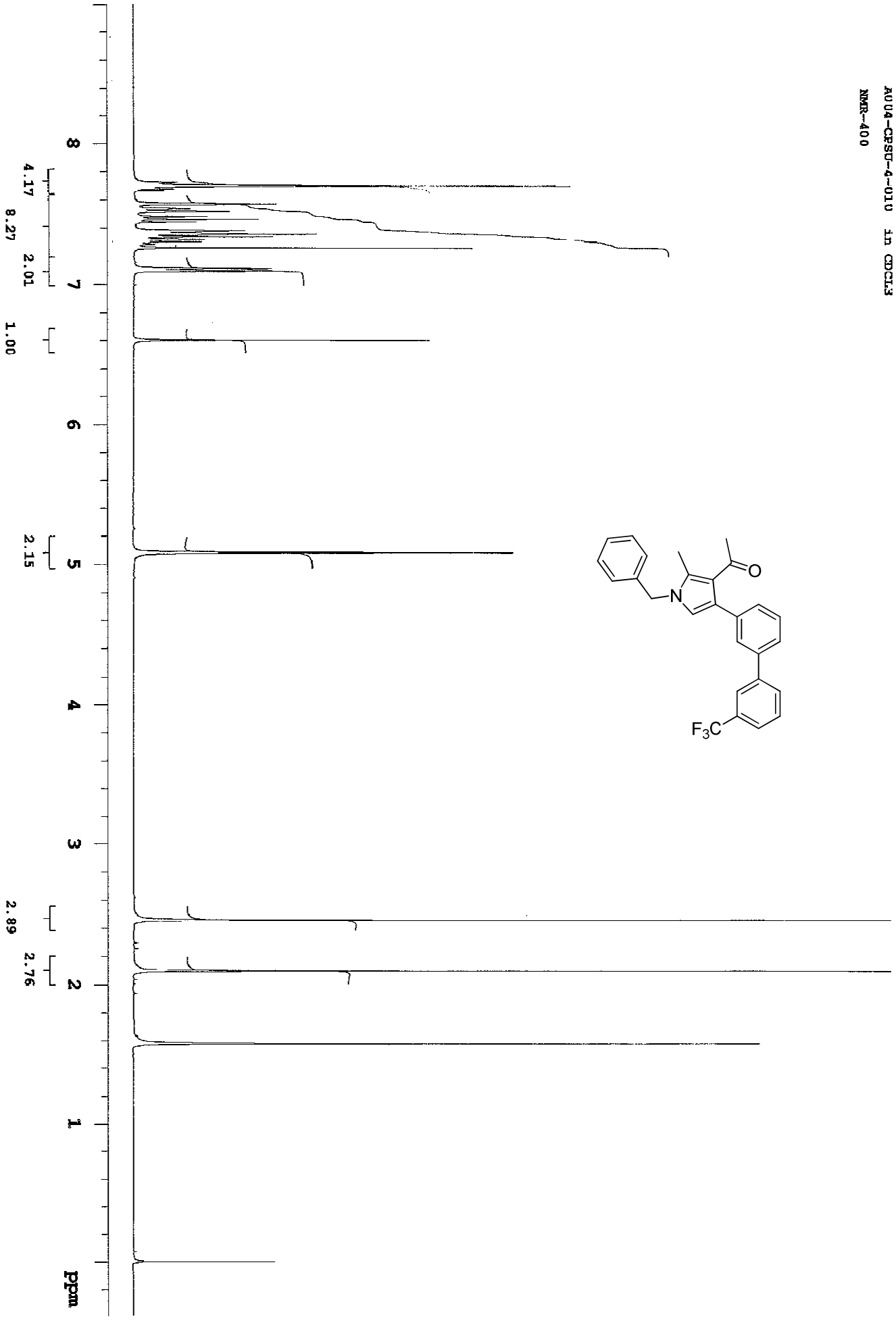
A0[illegible]\CPSU-4\009
UT1010_196 21 (0.399) Cm (21:30-92:100)

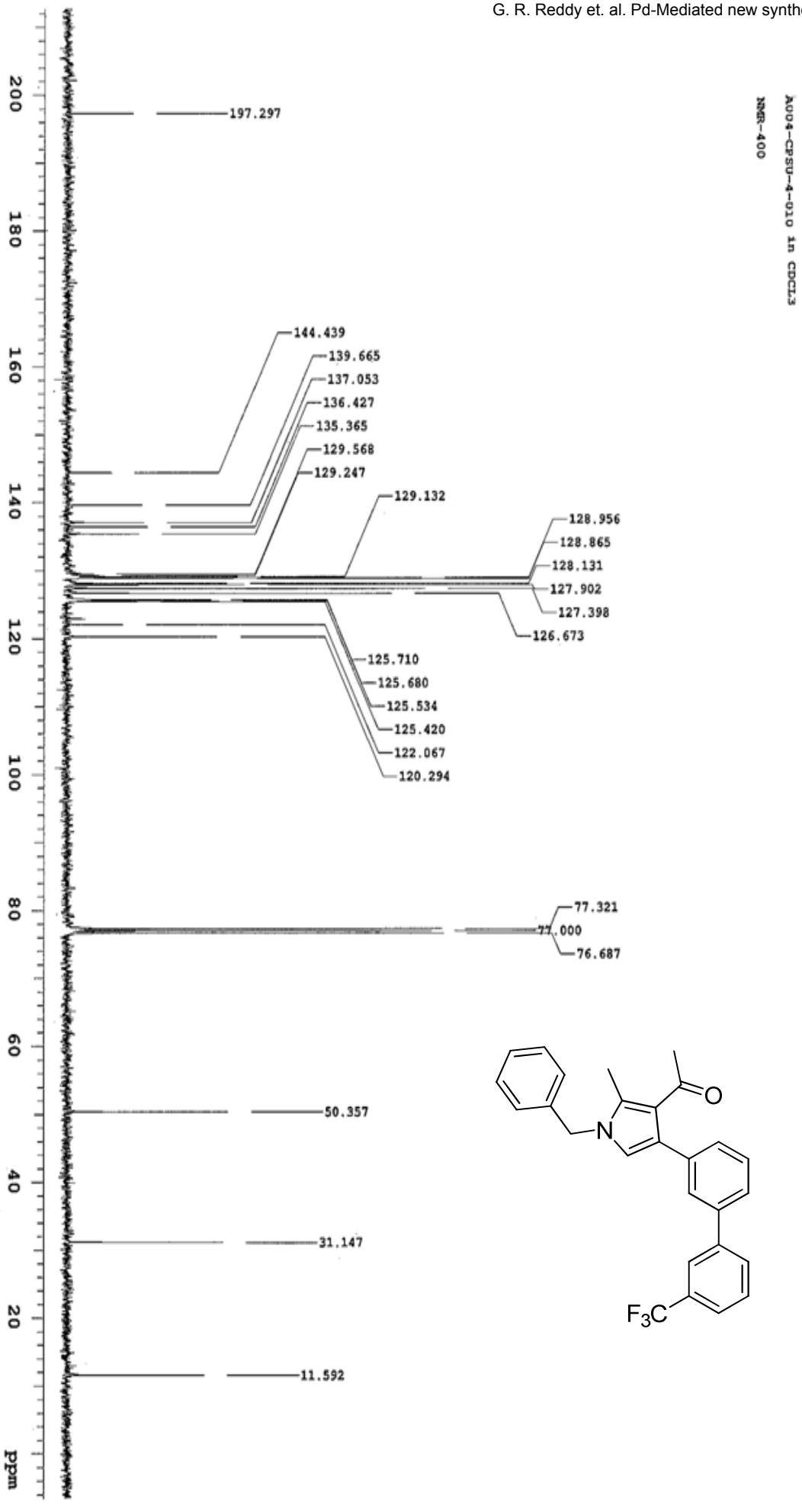


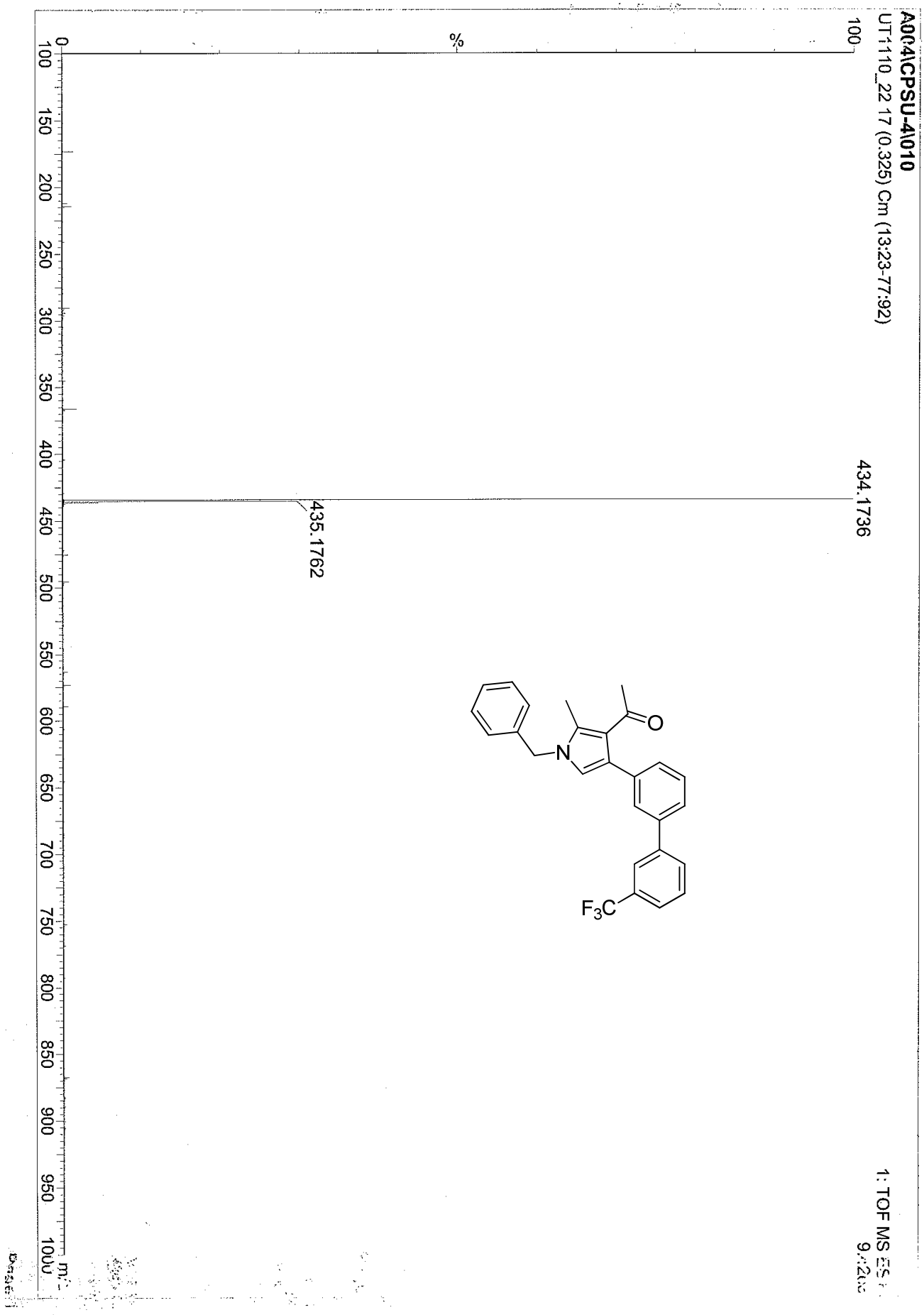
1: TOF MS ES
4.47e+0



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
396.1963	396.1964	-0.1	-0.3	15.5	1.5	C27 H26 N O2


AU04-CRSU-4-010 in CDCL3
NMR-400
8
7
6
5
4
3
2
1
Ppm
4.17
8.27
2.01
1.00
2.15
2.89
2.76
N
O
F3C


A004-CPSU-4-010 in CDCL3
NMR-400
197.297
144.439
139.665
137.053
136.427
135.365
129.568
129.247
129.132
128.956
128.865
128.131
127.902
127.398
126.673
125.710
125.680
125.534
125.420
122.067
120.294
77.321
77.000
76.687
50.357
31.147
11.592
ppm
200
180
160
140
120
100
80
60
40
20
O
N
F3C

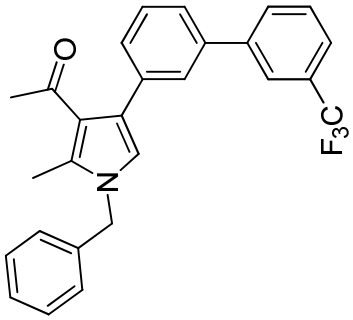

A0(4\CPSU-4\010
UT1110_22 17 (0.325) Cm (13:23-77:92)
%
100
0
434.1736
435.1762
O
N
F3C
1: TOF MS ES
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000

Elemental Composition Report

Single Mass Analysis

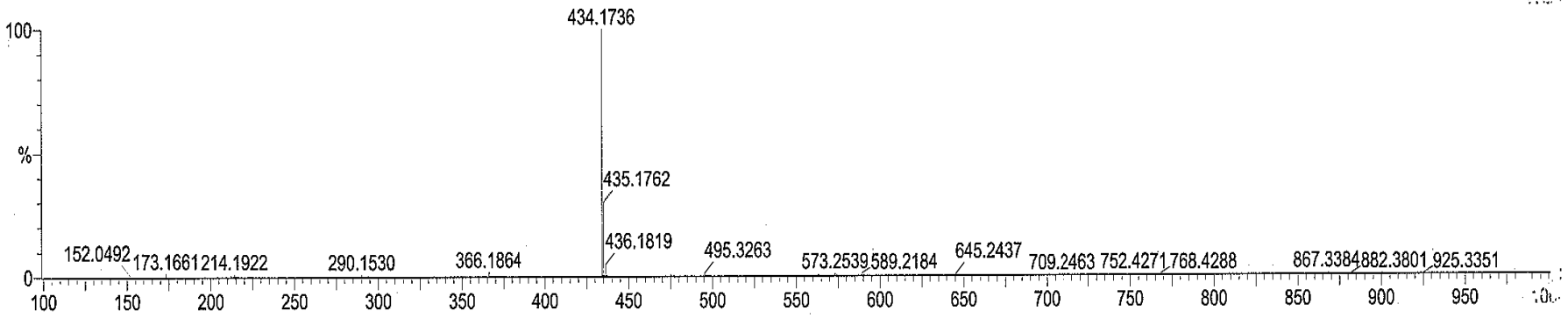
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
140 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-2 O: 0-2 F: 0-3

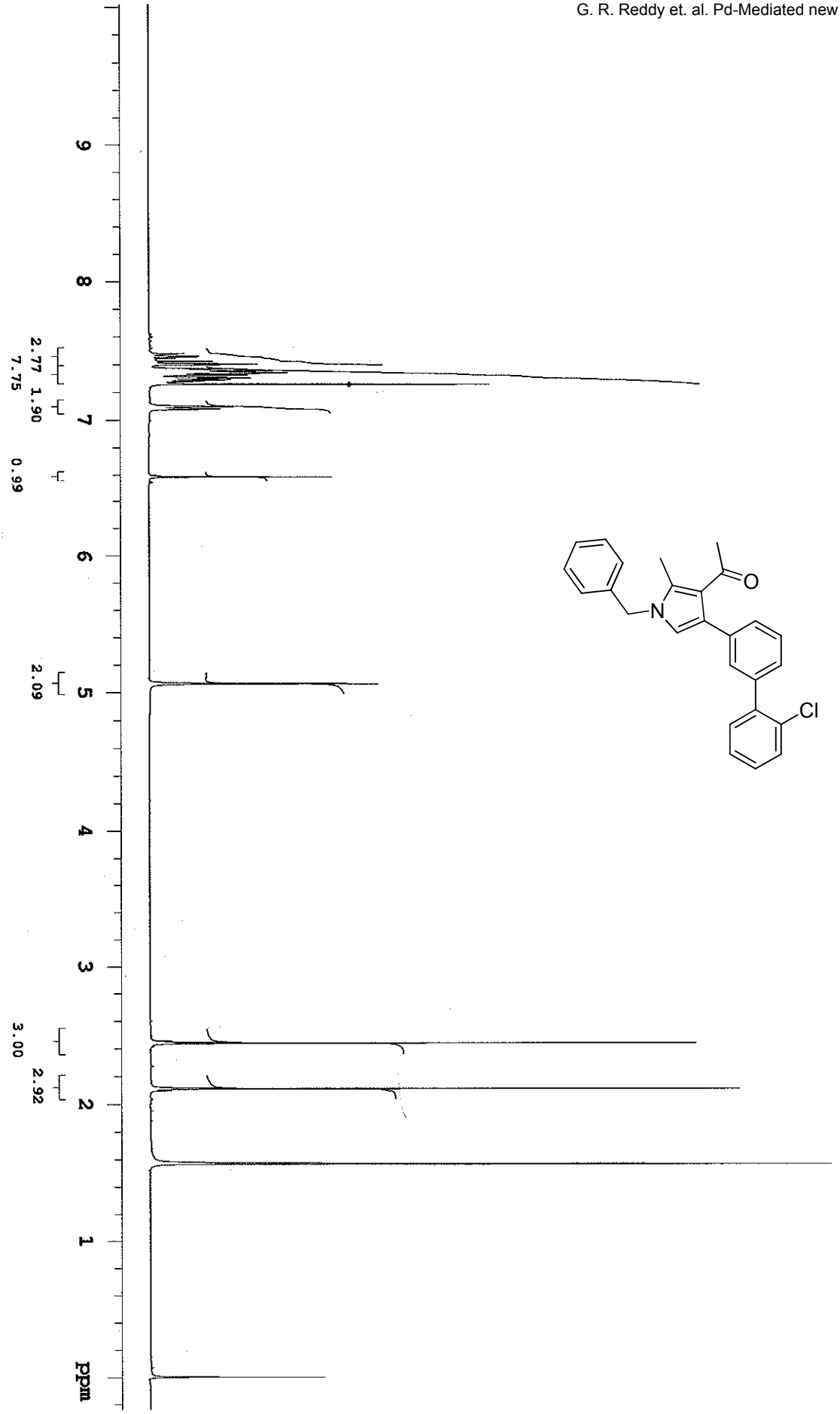


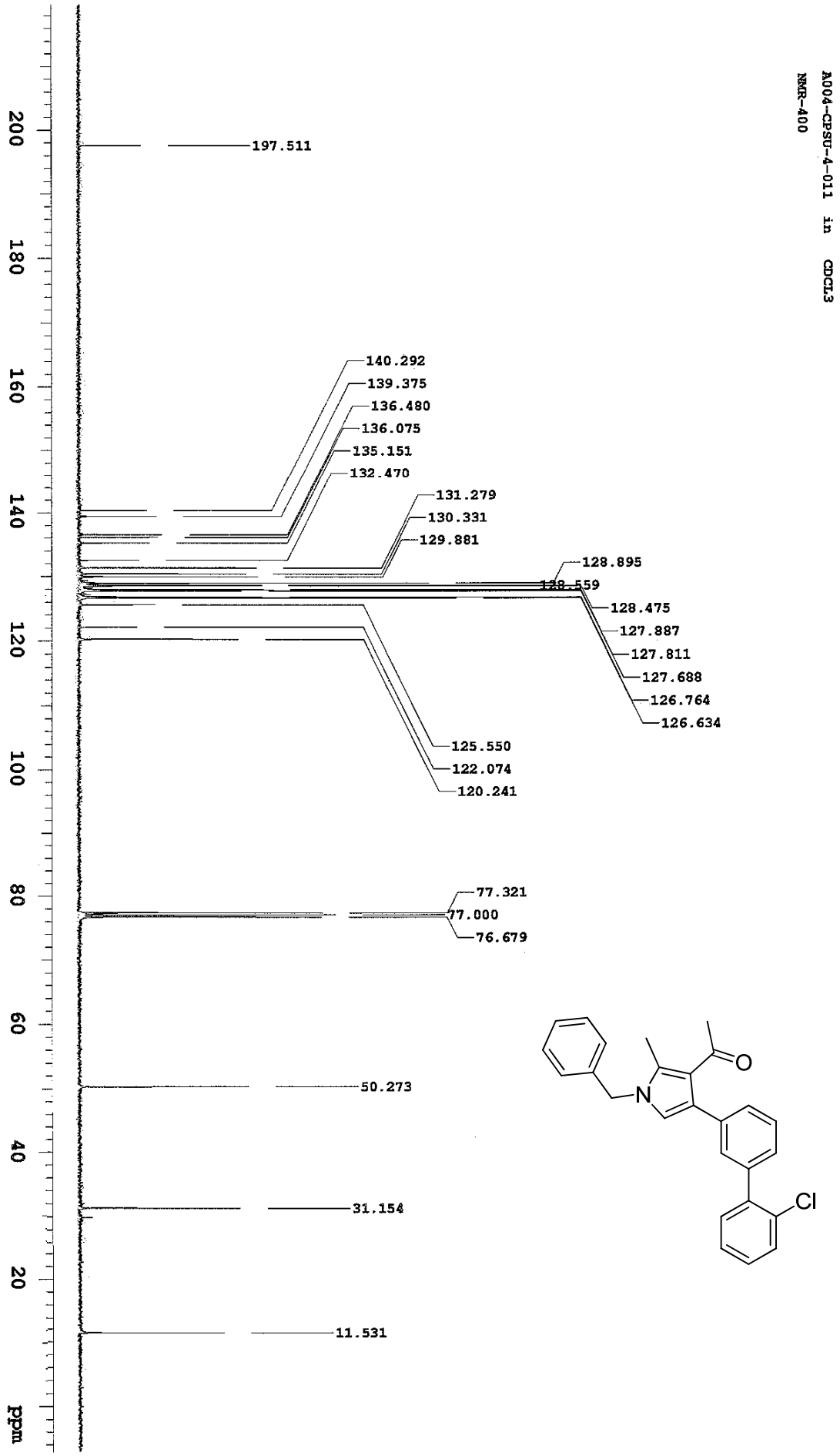
A004\CPSU-4\010
UT1110_22 17 (0.325) Cm (13:23-77:92)

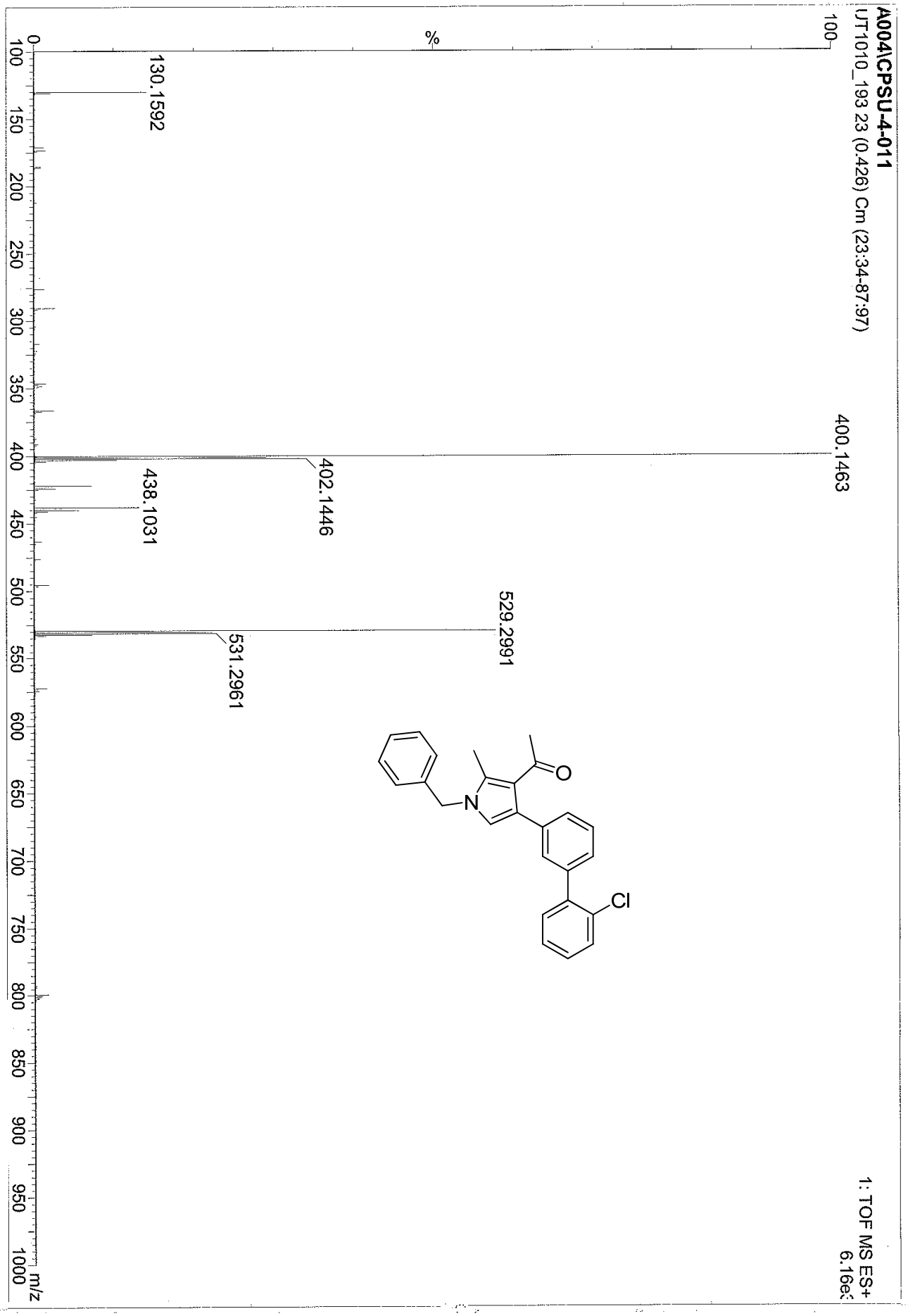
1: TOF MS ES



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
434.1736	434.1732	0.4	0.9	15.5	1.9	C27 H23 N O F3


AU04/CPSU-4/U1.1 in CDCl3
NMR-400
9
8
7
6
5
4
3
2
1
ppm
2.77 1.90
7.75
0.99
2.09
3.00
2.92
O
N
Cl


A004-CPSU-4-011 in CDCL3
NMR-400
197.511
140.292
139.375
136.480
136.075
135.151
132.470
131.279
130.331
129.881
128.895
128.559
128.475
127.887
127.811
127.688
126.764
126.634
125.550
122.074
120.241
77.321
77.000
76.679
50.273
31.154
11.531
200
180
160
140
120
100
80
60
40
20
ppm
O
N
Cl


A004\CPSU-4-011
UT1010_193 23 (0.426) Cm (23:34-87:97)
%
100
0
130.1592
400.1463
402.1446
438.1031
529.2991
531.2961
O
N
Cl
m/z
1: TOF MS ES+
6.16e

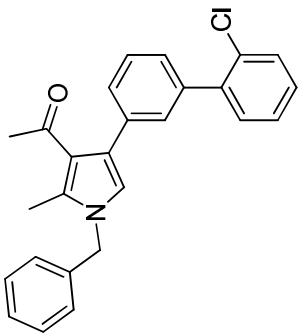
Elemental Composition Report

Single Mass Analysis

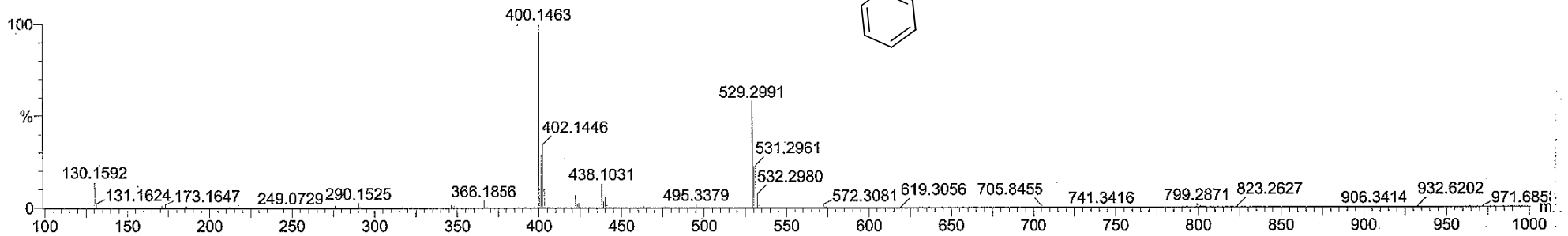
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
161 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-3 O: 0-3 Cl: 0-1

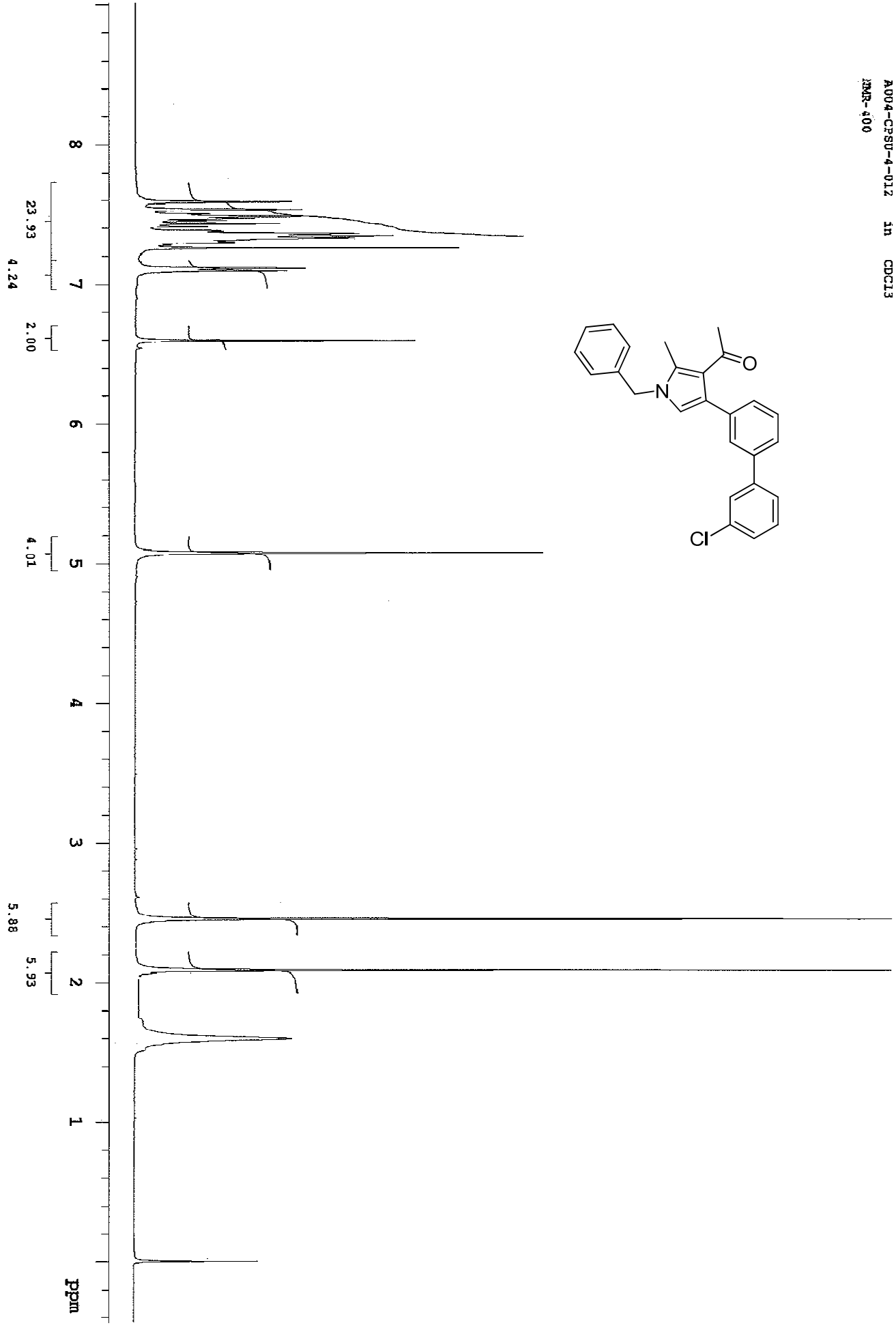
A: 04\CPSU-4-011
UT1010_193 23 (0.426) Cm (23:34-87:97)

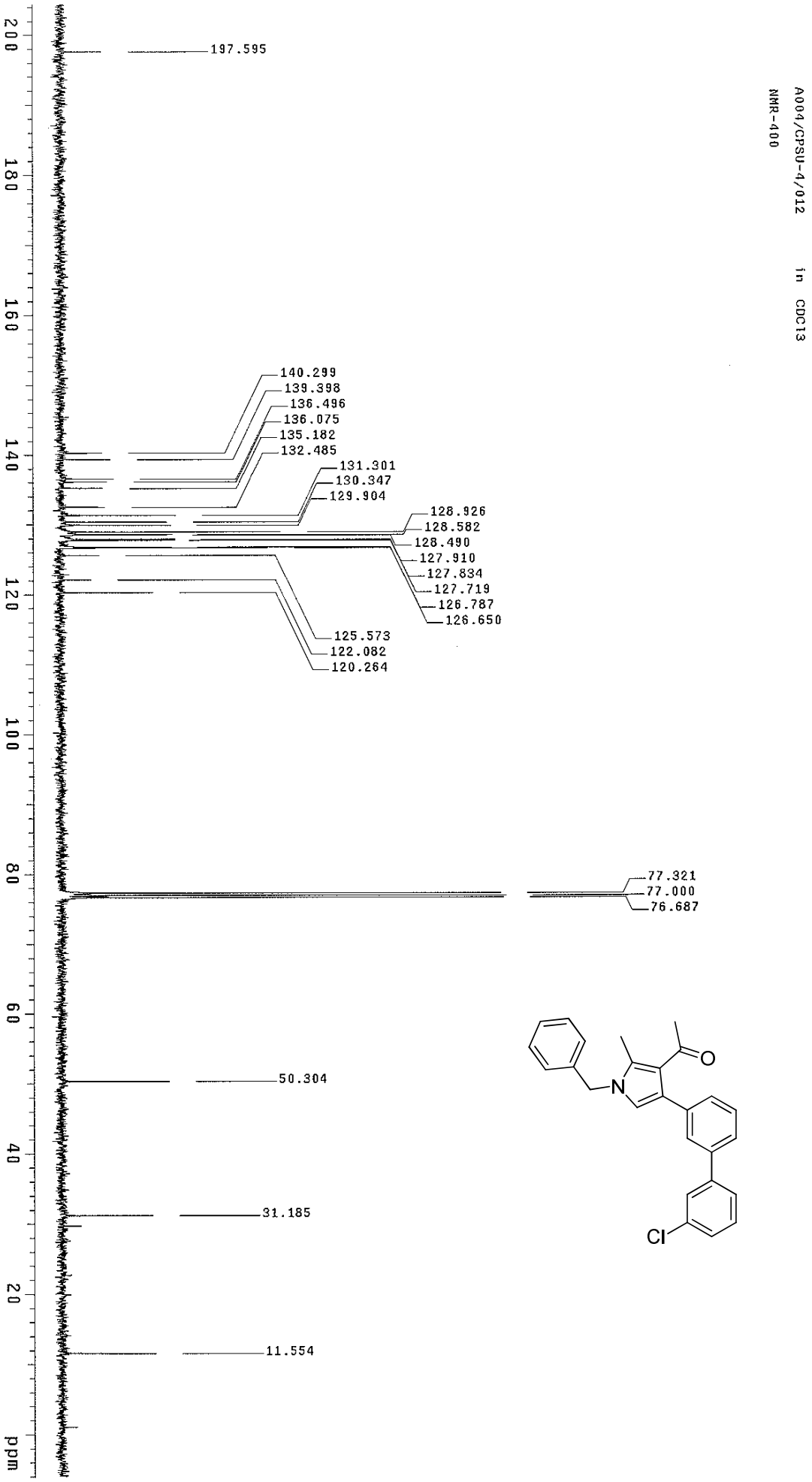


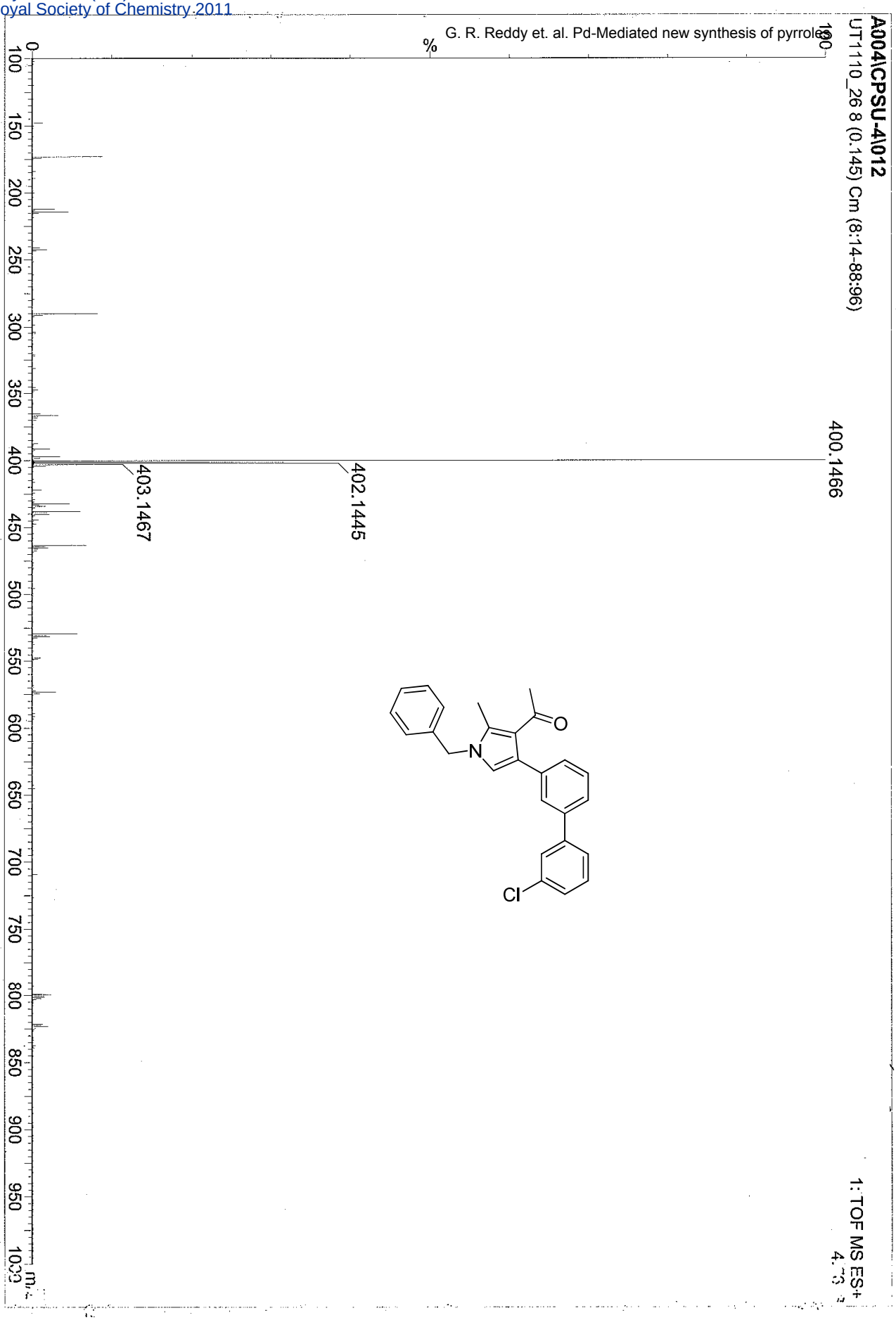
1: TOF MS ES
6.16e+0



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
400.1463	400.1468	-0.5	-1.2	15.5	3.8	C26 H23 N O Cl


A004-CPSU-4-012 in CDCl3
NMR-400
23.93
4.24
2.00
4.01
5.88
5.93
8
7
6
5
4
3
2
1
ppm
O
N
Cl


A004/CPSU-4/012
NMR-400
in CDC13
197.595
140.299
139.398
136.496
136.075
135.182
132.485
131.301
130.347
129.904
128.926
128.582
128.490
127.910
127.834
127.719
126.787
126.650
125.573
122.082
120.264
77.321
77.000
76.687
50.304
31.185
11.554
200
180
160
140
120
100
80
60
40
20
ppm
O
N
Cl



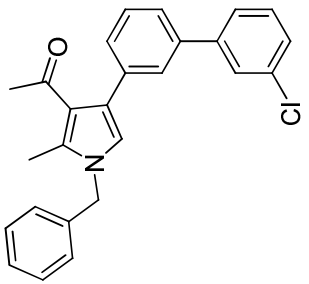
Elemental Composition Report

Single Mass Analysis

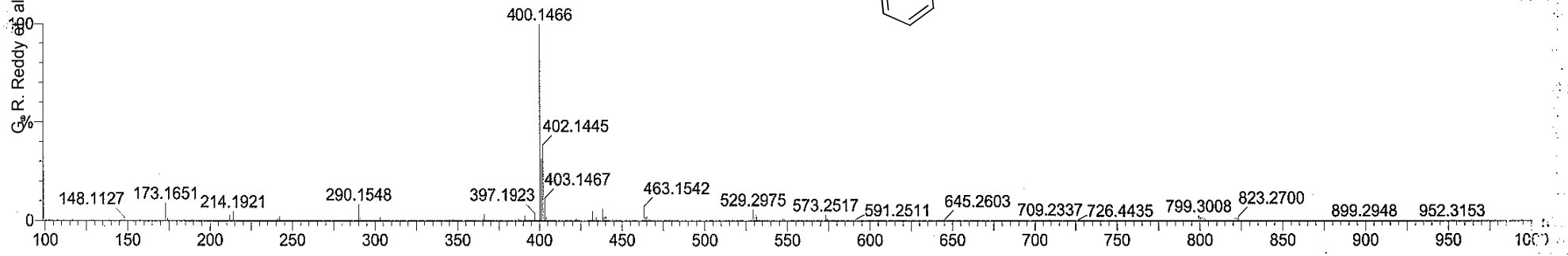
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
71 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-2 O: 0-2 Cl: 0-1

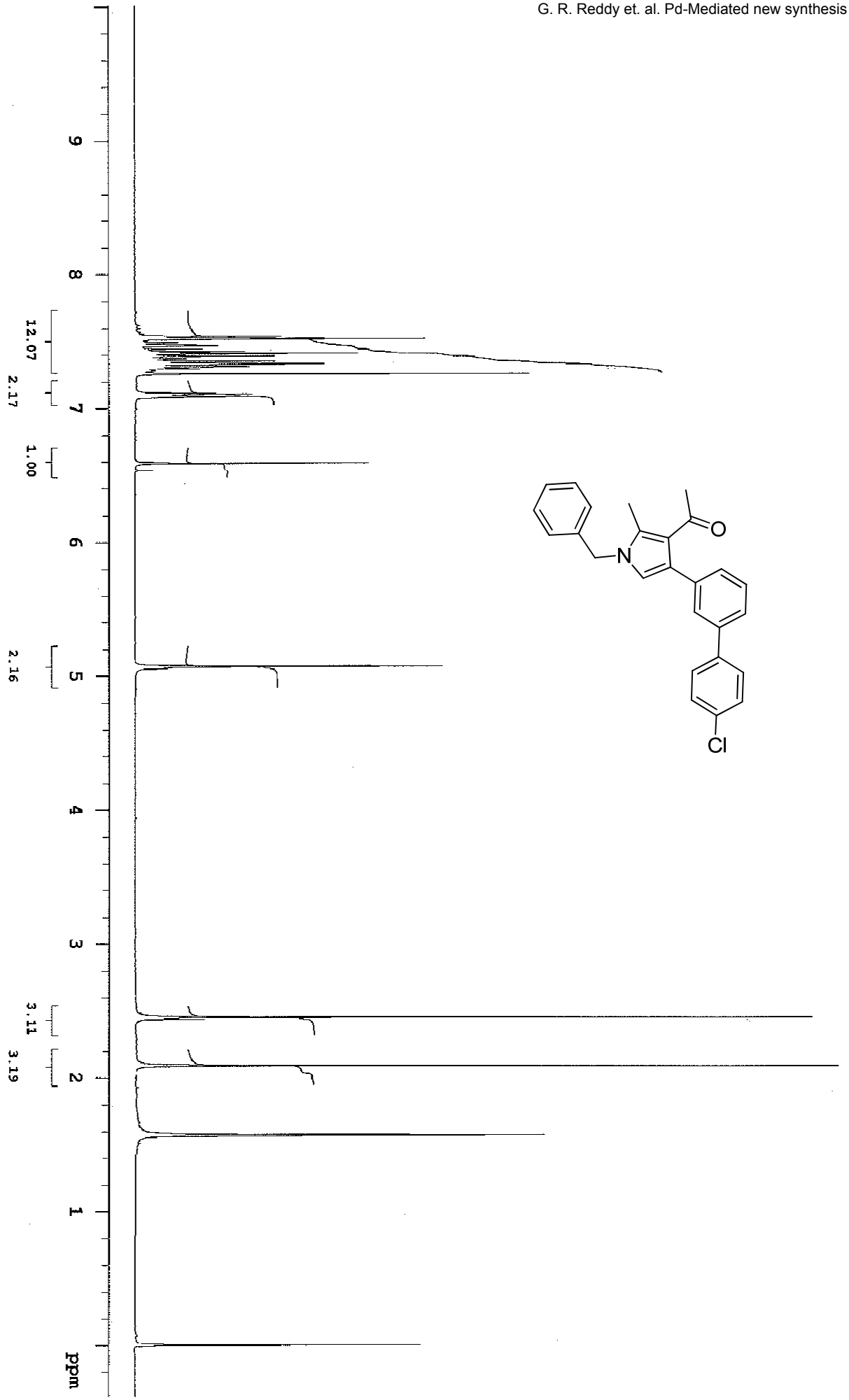
AE04\CPSU-4\012
UP1110_26 8 (0.145) Cm (8:14-88:96)

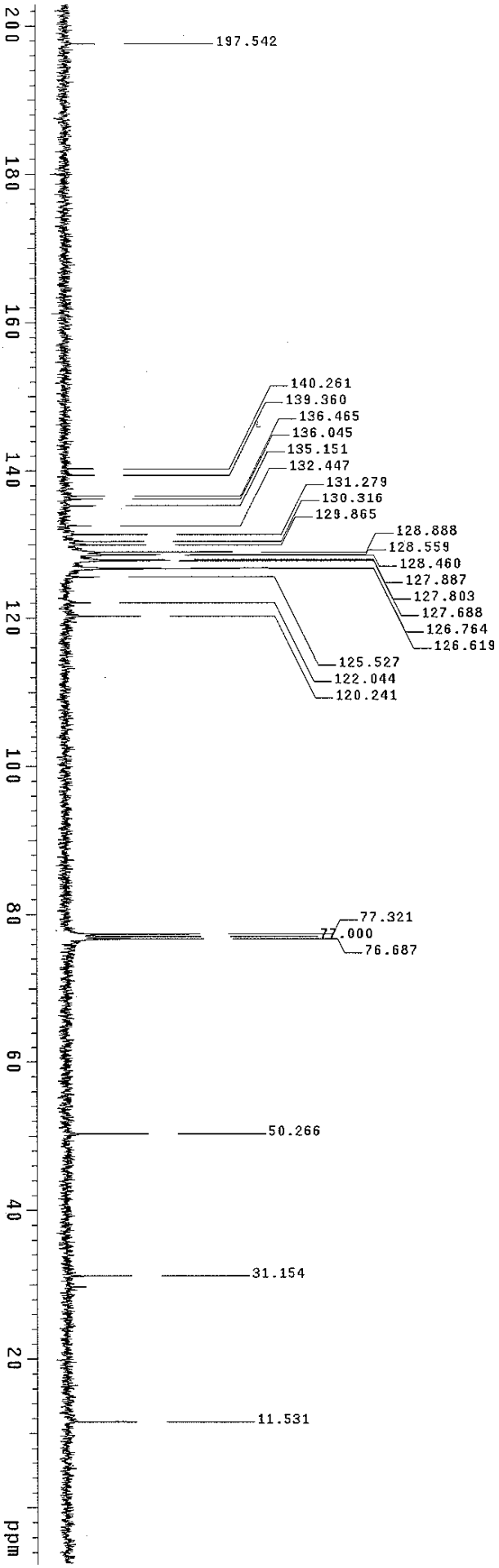


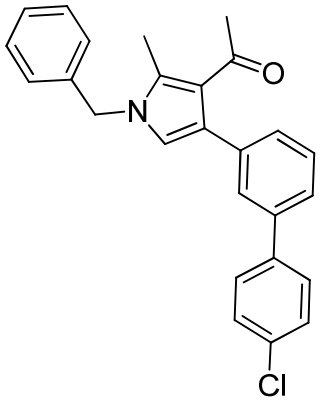
1: TOF MS ES+
4.76e+0

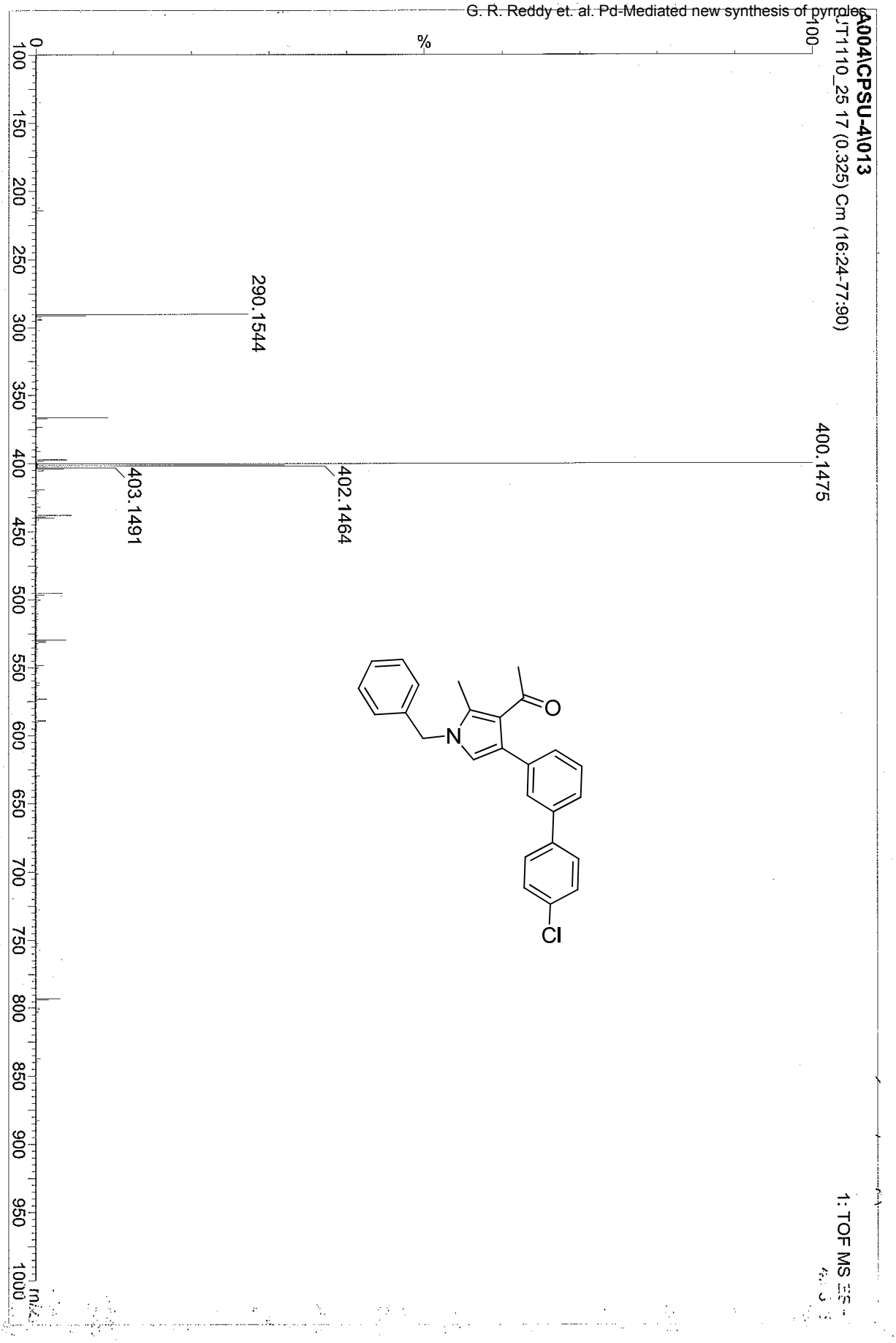


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
400.1466	400.1468	-0.2	-0.5	15.5	3.5	C26 H23 N O Cl


A004-CPSU-4-013 in CDCL3
NMR-400
12.07
2.17
1.00
2.16
3.11
3.19
ppm
O
N
Cl


A004/CPSU-4/013
NMR-400
in CDCl3
197.542
140.261
139.360
136.465
136.045
135.151
132.447
131.279
130.316
129.865
128.888
128.559
128.460
127.887
127.803
127.688
126.764
126.619
125.527
122.044
120.241
77.321
77.000
76.687
50.266
31.154
11.531
200
180
160
140
120
100
80
60
40
20
ppm


O
N
Cl



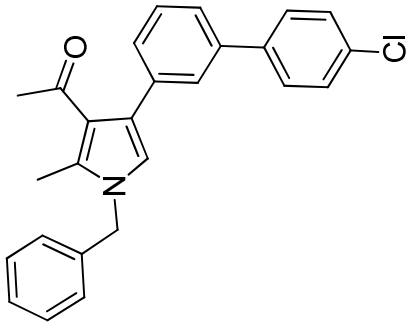
Elemental Composition Report

Single Mass Analysis

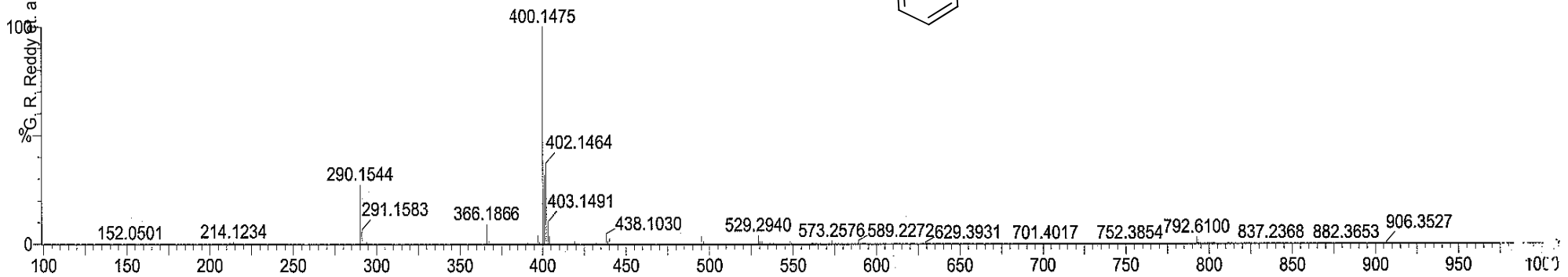
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
71 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-2 O: 0-2 Cl: 0-1

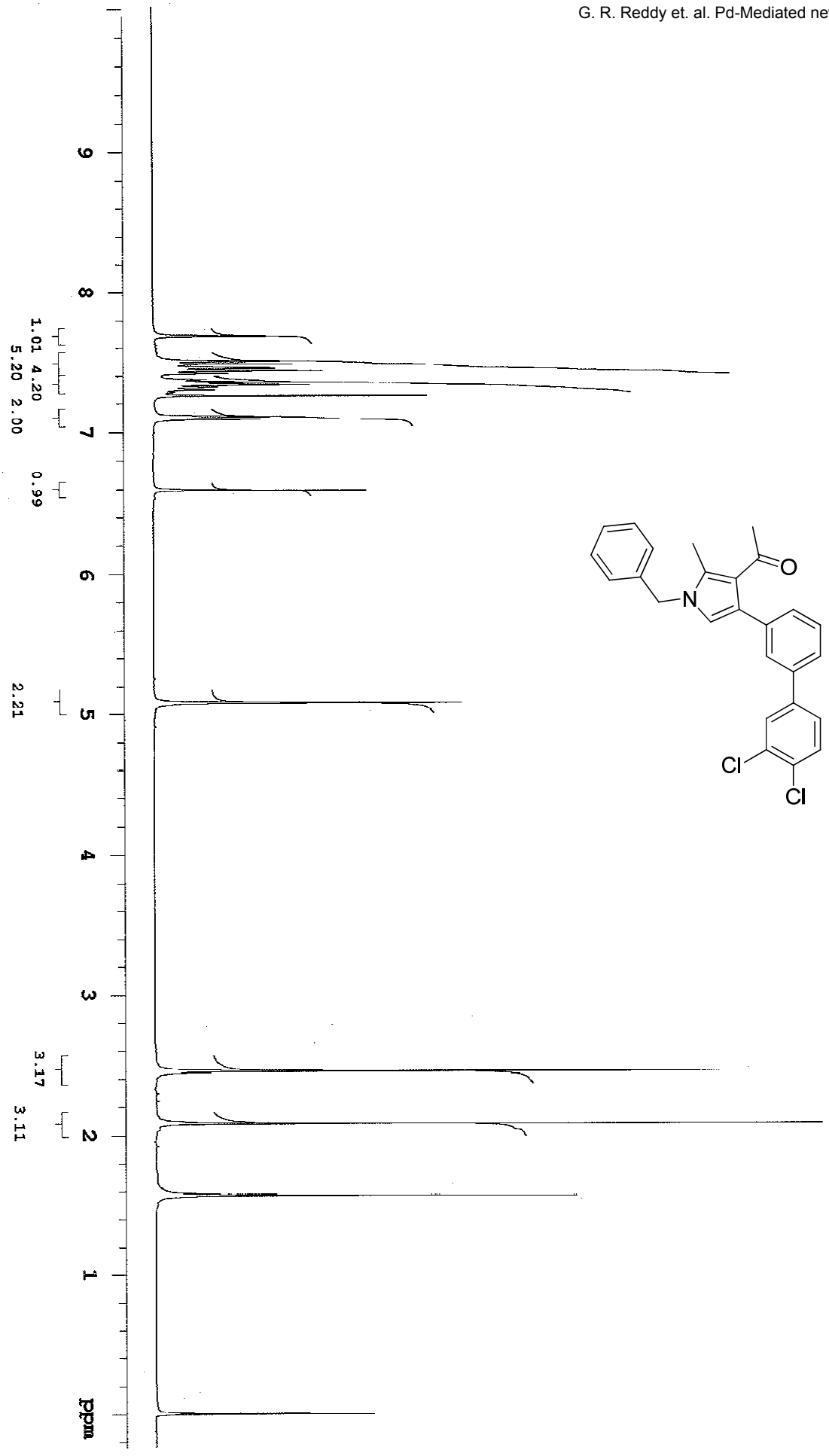
A0[illegible]\CPSU-4\013
UT1110_25 17 (0.325) Cm (16:24-77:90)

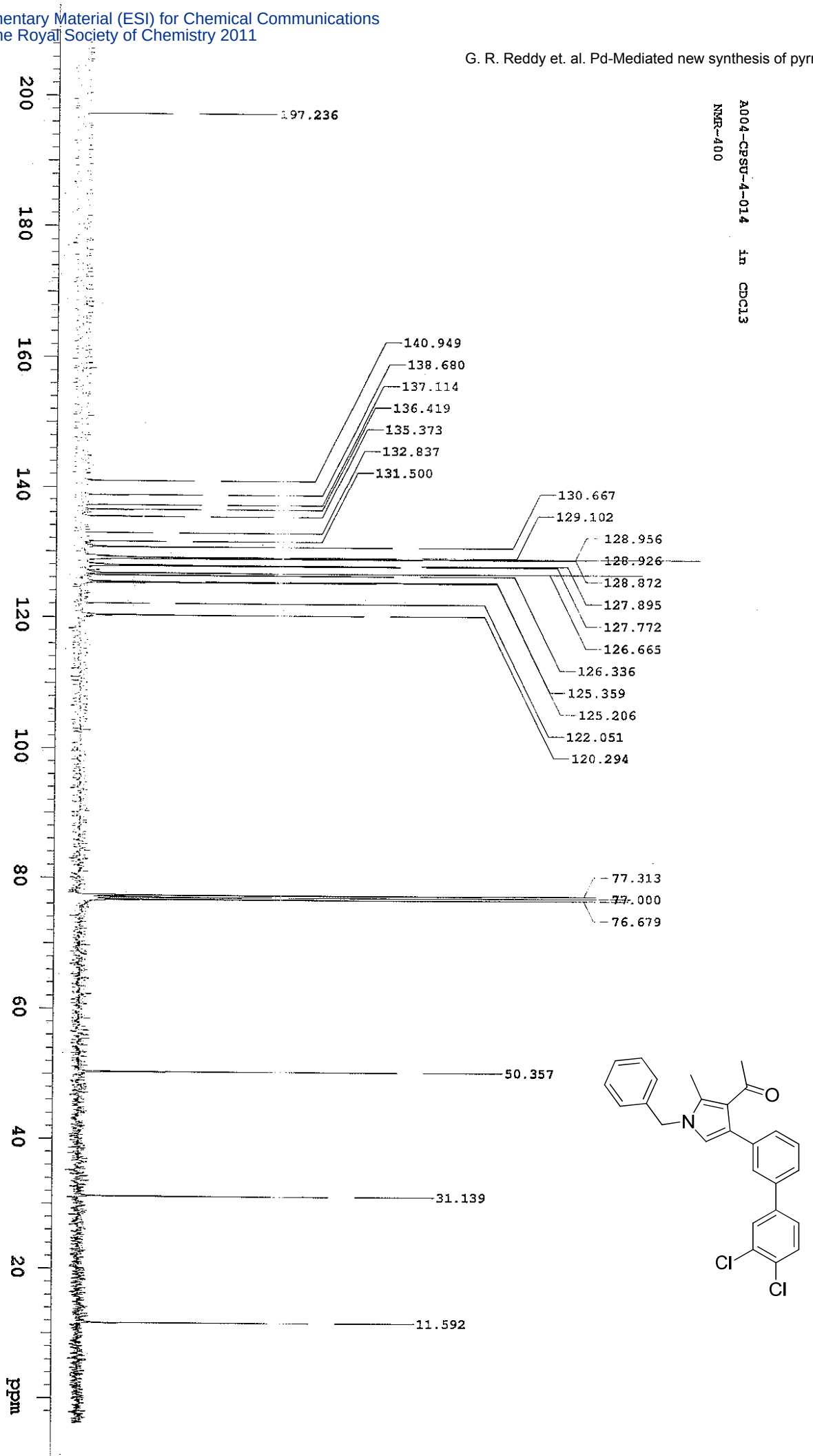


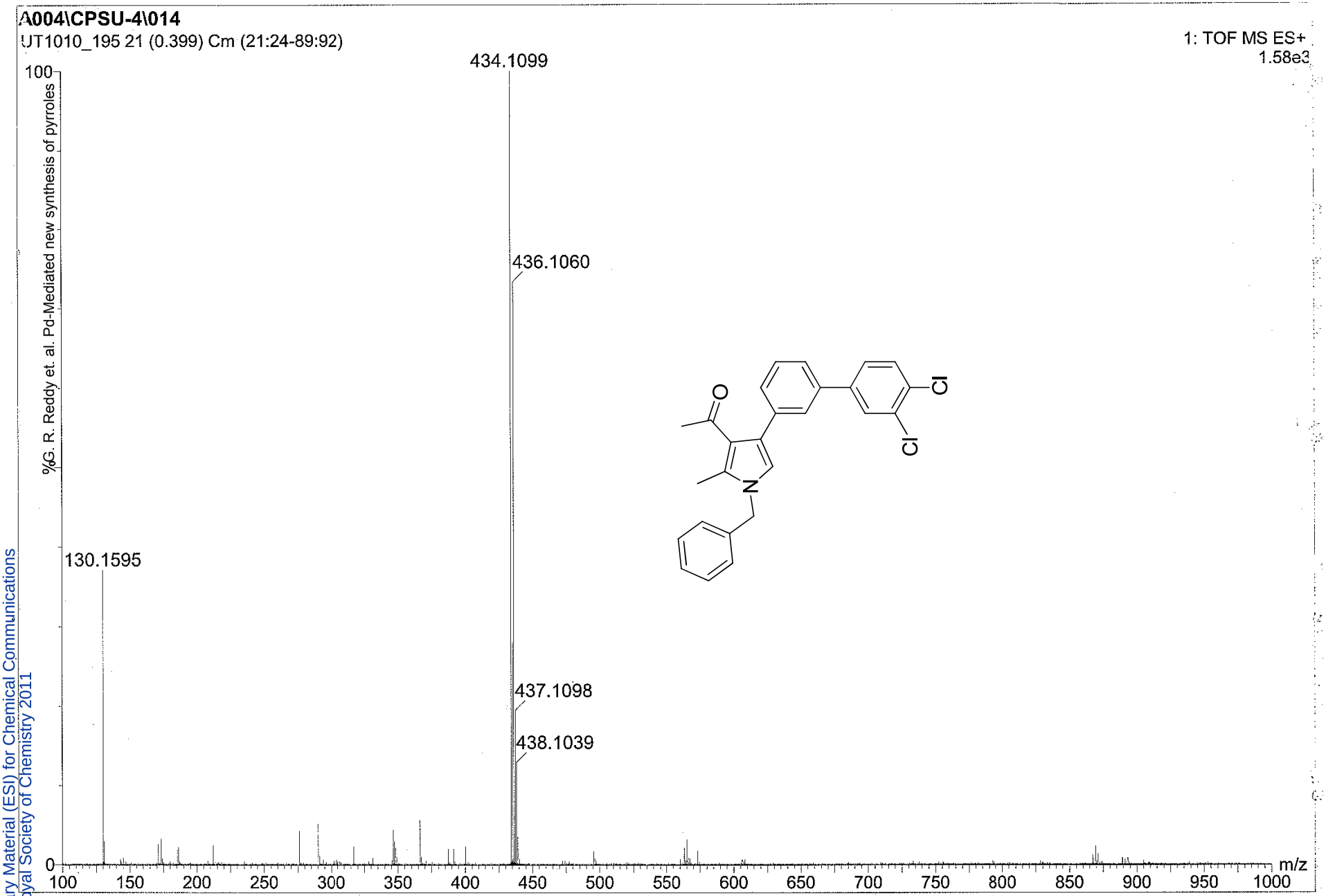
1: TOF [illegible]
4.08e+0[illegible]



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
400.1475	400.1468	0.7	1.7	15.5	3.0	C26 H23 N O Cl


AU04/CPSU-4/014 in CDCl3
NMR-400
1.01 4.20
5.20 2.00
0.99
2.21
3.17
3.11
ppm
O
N
Cl
Cl


A004-CPSU-4-014 in CDCl3
NMR-400
197.236
140.949
138.680
137.114
136.419
135.373
132.837
131.500
130.667
129.102
128.956
128.926
128.872
127.895
127.772
126.665
126.336
125.359
125.206
122.051
120.294
77.313
77.000
76.679
50.357
31.139
11.592
200
180
160
140
120
100
80
60
40
20
ppm
O
N
Cl
Cl



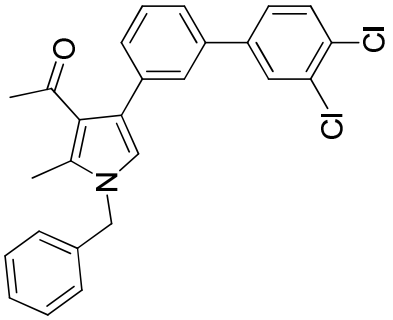
Elemental Composition Report

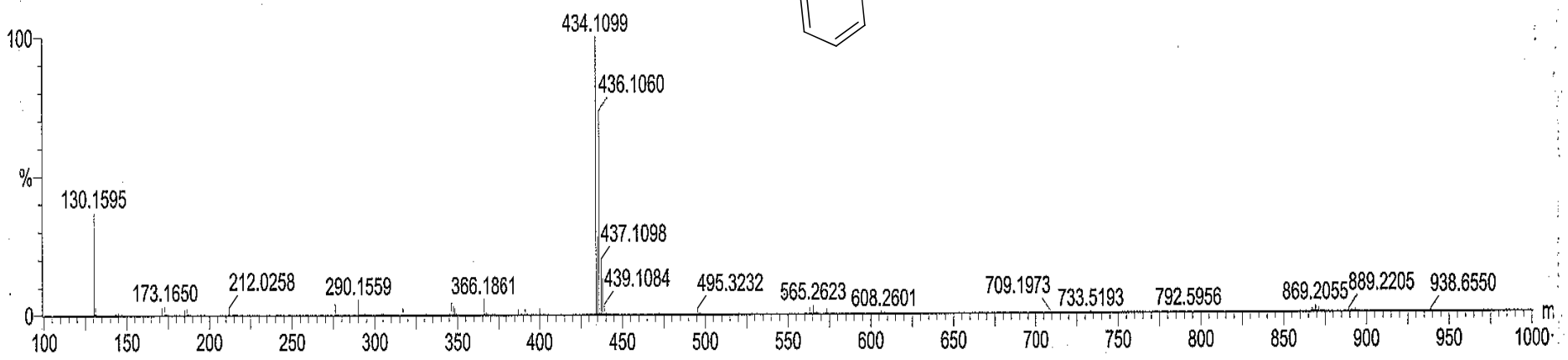
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

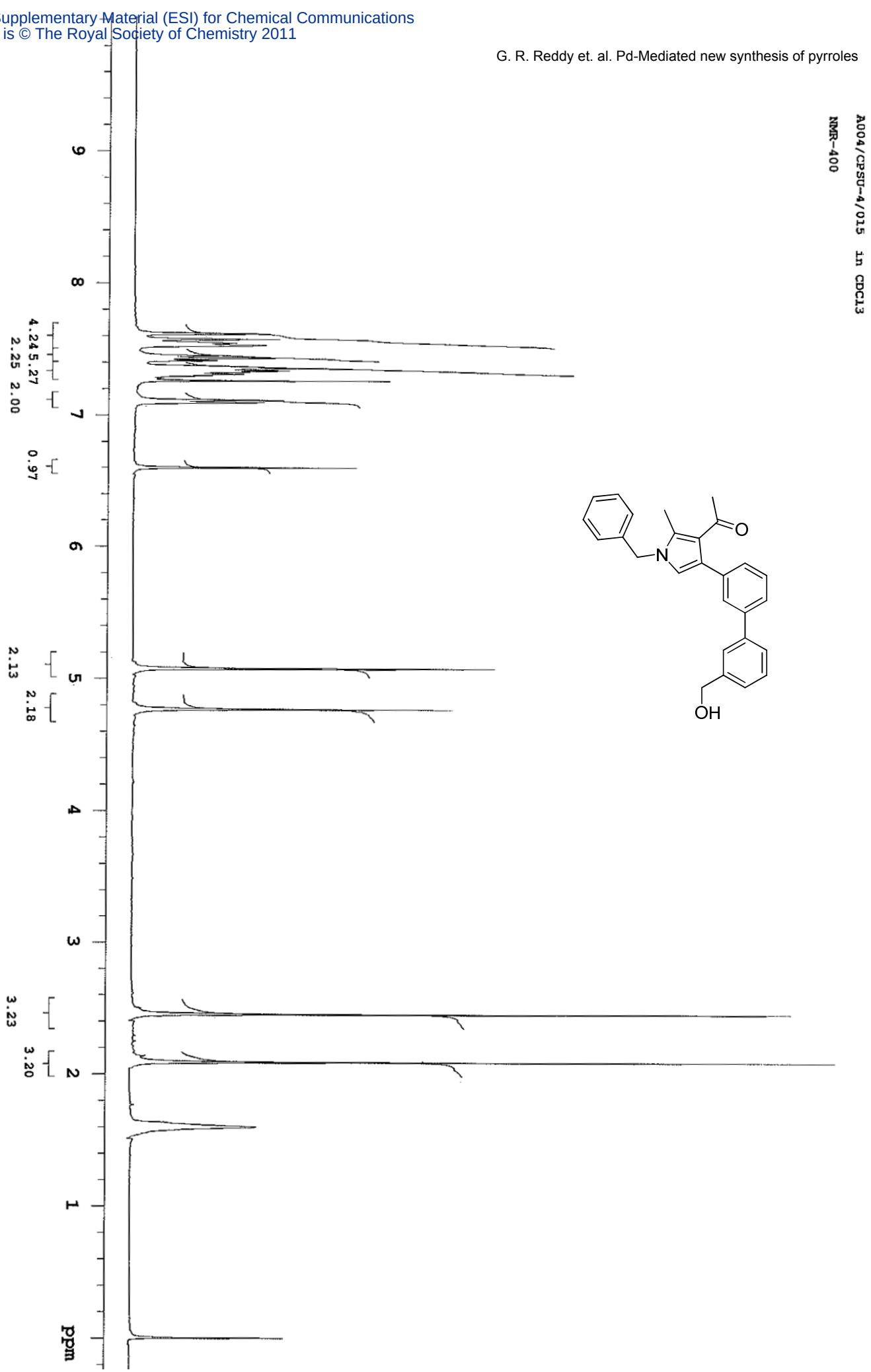
Monoisotopic Mass, Even Electron Ions
250 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-3 O: 0-3 Cl: 0-2

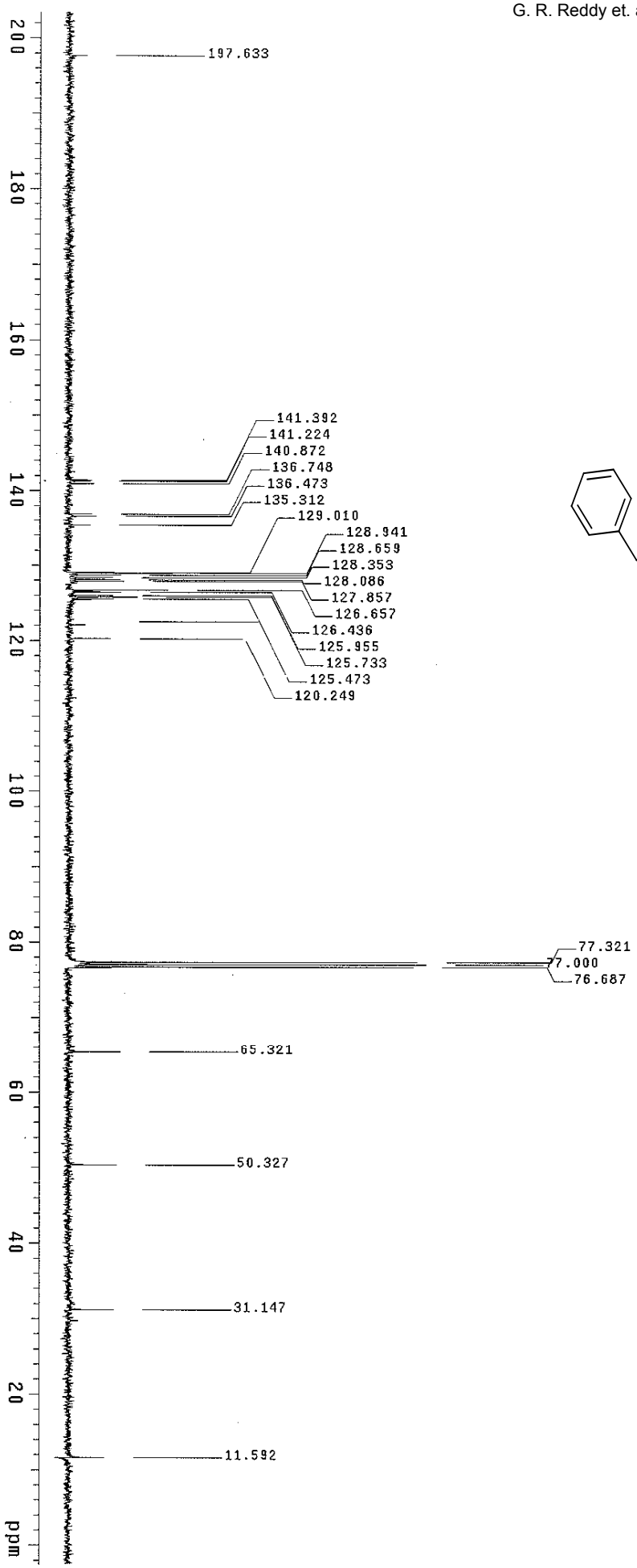
A004\CPSU-4\014
UT1010_195 21 (0.399) Cm (21:24-89:92)

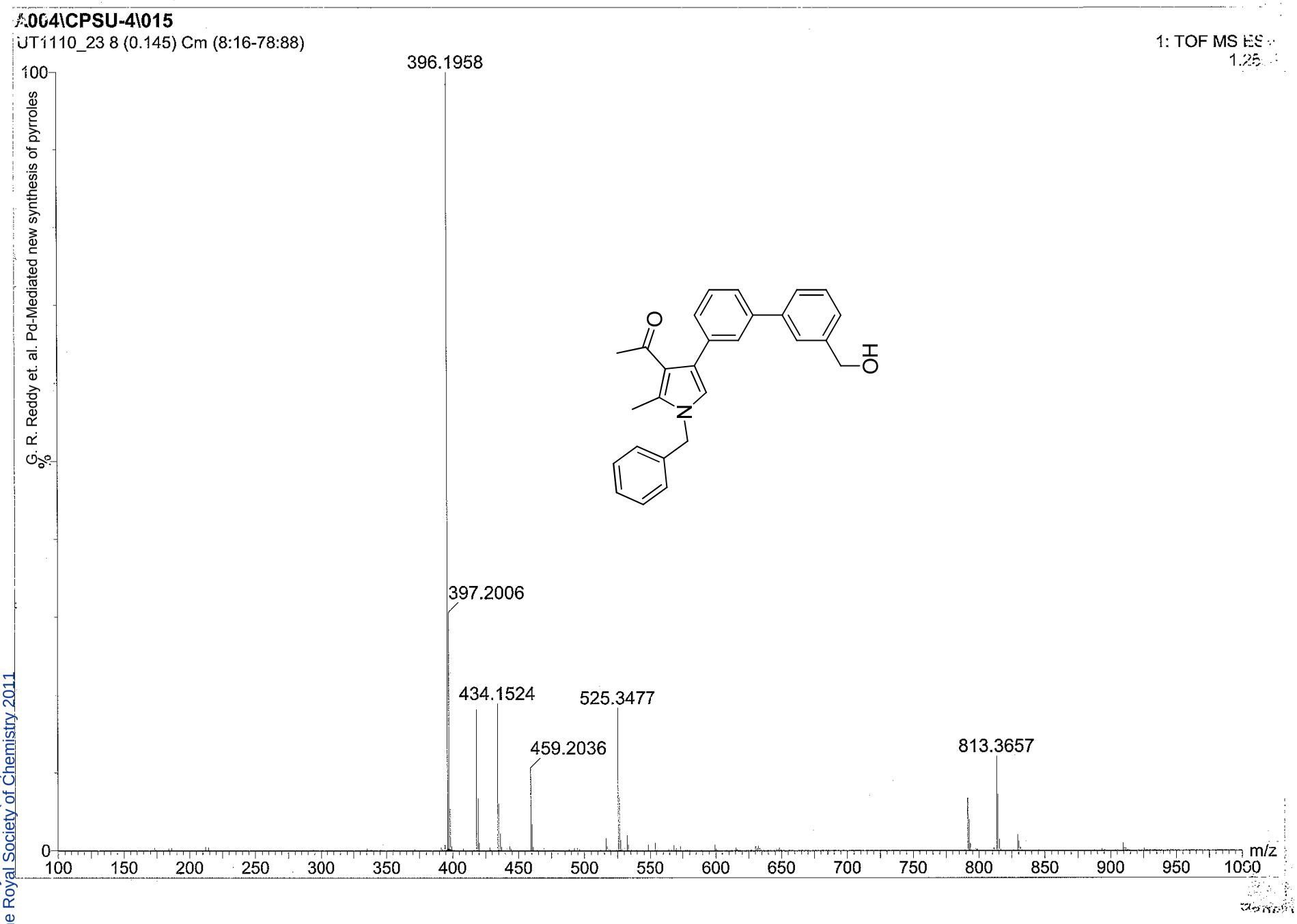




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
434.1099	434.1078	2.1	4.8	15.5	3.1	C26 H22 N O Cl2


A004/CPSU-4/015 in CDCl3
NMR-400
4.24 5.27
2.25 2.00
0.97
2.13
2.18
3.23
3.20
ppm
N
O
OH


A004/CPSU-4/015 in CDCl3
NMR-400
197.633
141.392
141.224
140.872
136.748
136.473
135.312
129.010
128.941
128.659
128.353
128.086
127.857
126.657
126.436
125.955
125.733
125.473
120.249
77.321
77.000
76.687
65.321
50.327
31.147
11.592
ppm
200
180
160
140
120
100
80
60
40
20
N
O
OH

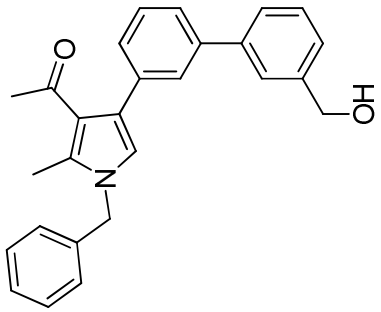


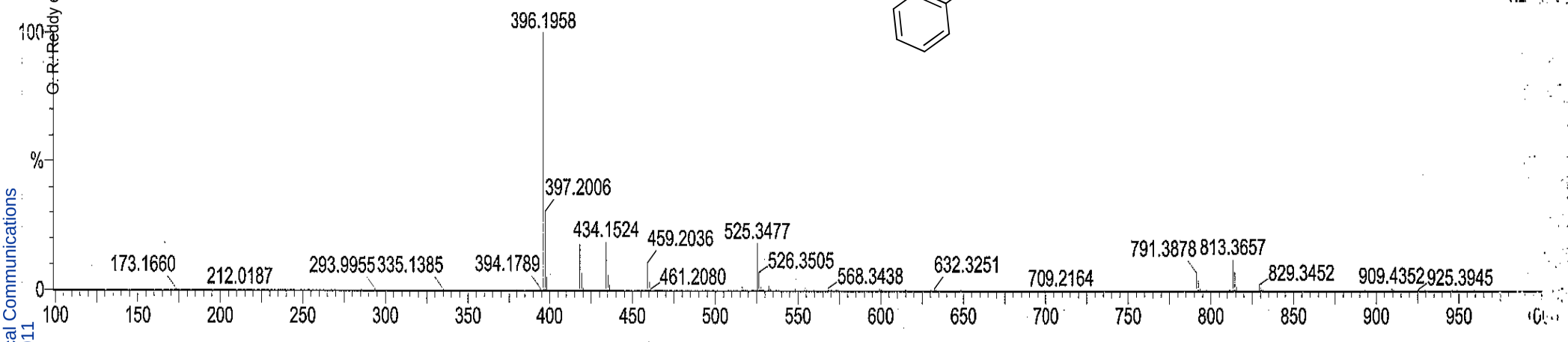
Elemental Composition Report

Single Mass Analysis

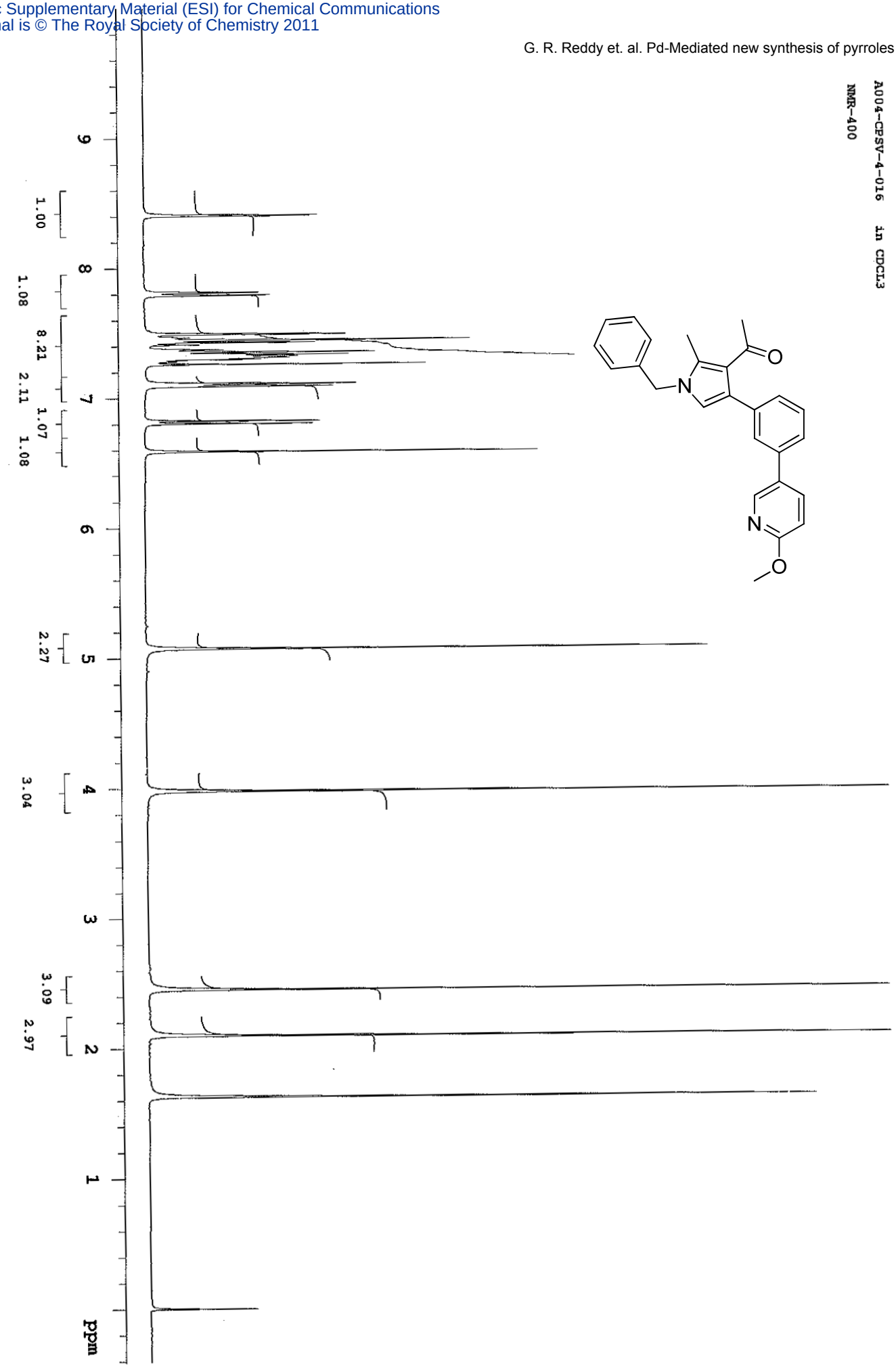
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

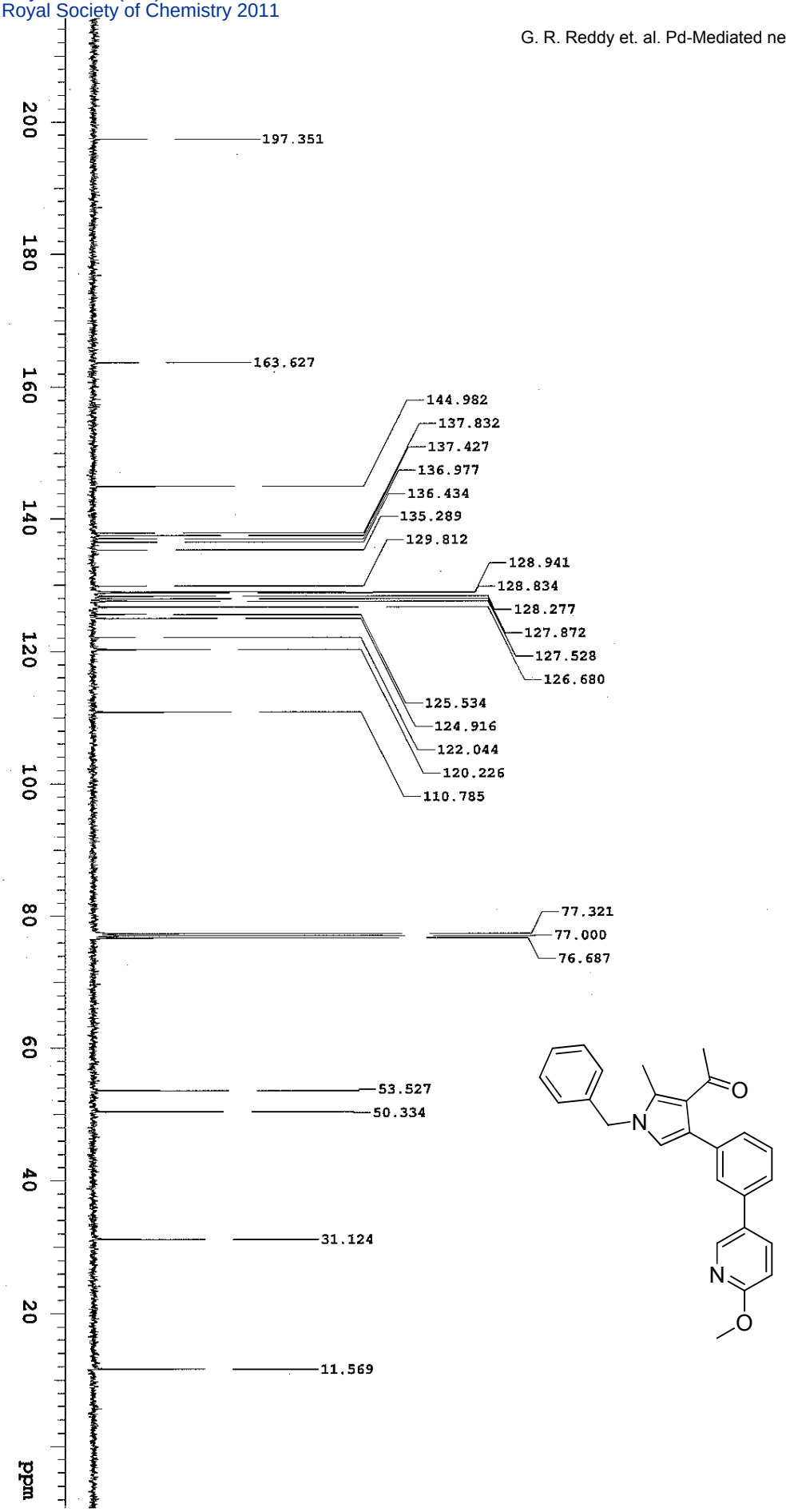
Monoisotopic Mass, Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-2 O: 0-2
A004\CPSU-4\015
UT11a0_23 8 (0.145) Cm (8:16-78:88)

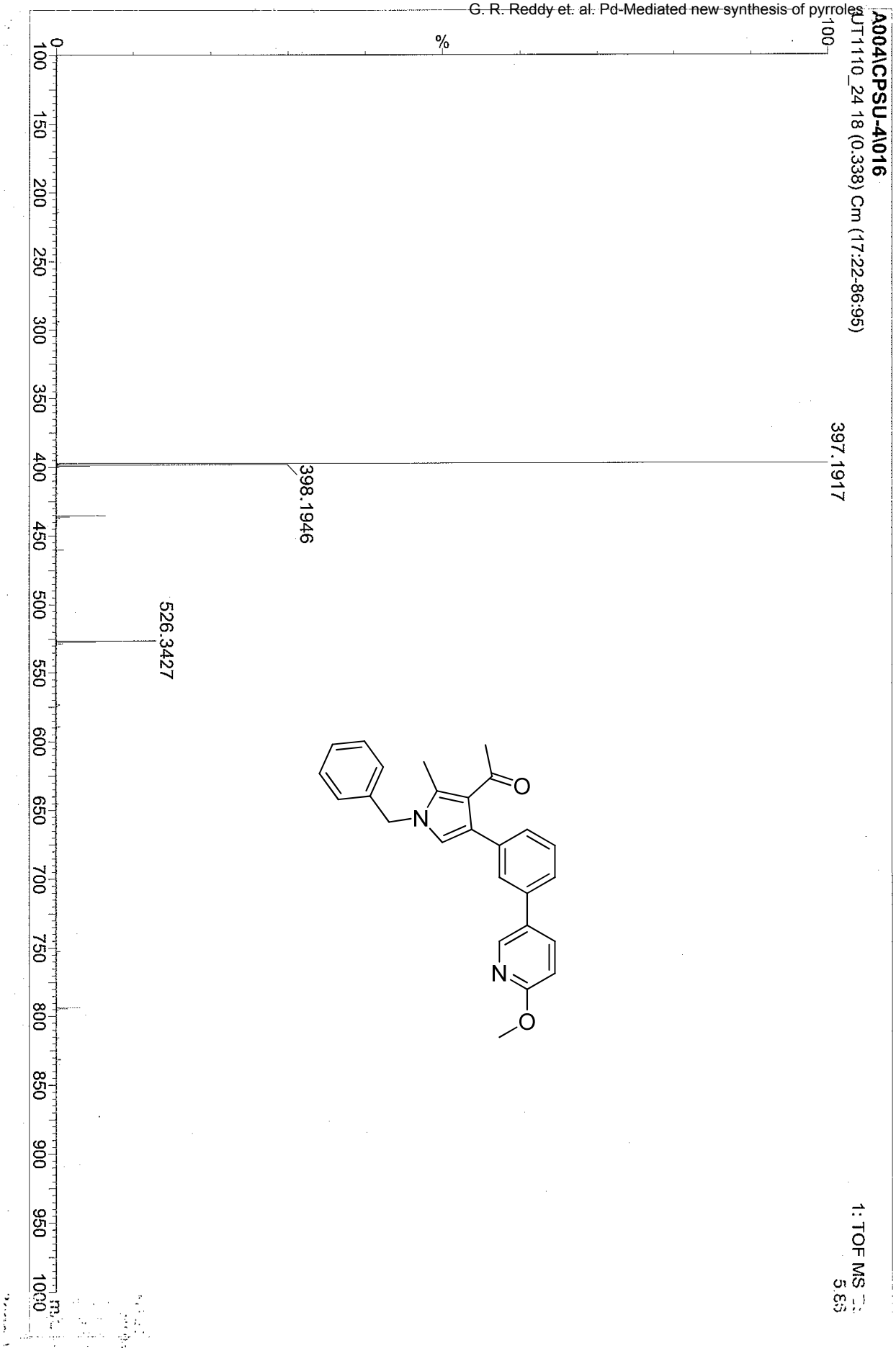




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
396.1958	396.1964	-0.6	-1.5	15.5	1.5	C27 H26 N O2


A004-CPSV-4-016 in CDCL3
NMR-400
9
8
7
6
5
4
3
2
1
ppm
1.00
1.08
8.21
2.11
1.07
1.08
2.27
3.04
3.09
2.97
N
O
N
O


AD04/CPSU-4/016 in CDCl3
NMR-400
197.351
163.627
144.982
137.832
137.427
136.977
136.434
135.289
129.812
128.941
128.834
128.277
127.872
127.528
126.680
125.534
124.916
122.044
120.226
110.785
77.321
77.000
76.687
53.527
50.334
31.124
11.569
200
180
160
140
120
100
80
60
40
20
ppm
O
N
N
O

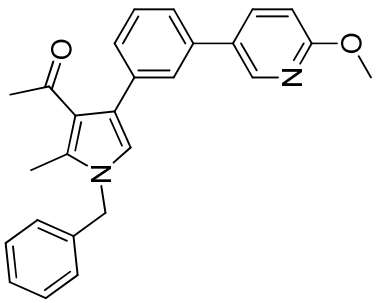

A004\CPSU-4\016
UT1110_24 18 (0.338) Cm (17:22-86:95)
%
100
0
397.1917
398.1946
526.3427
1: TOF MS
5.83
O
N
N
O

Elemental Composition Report

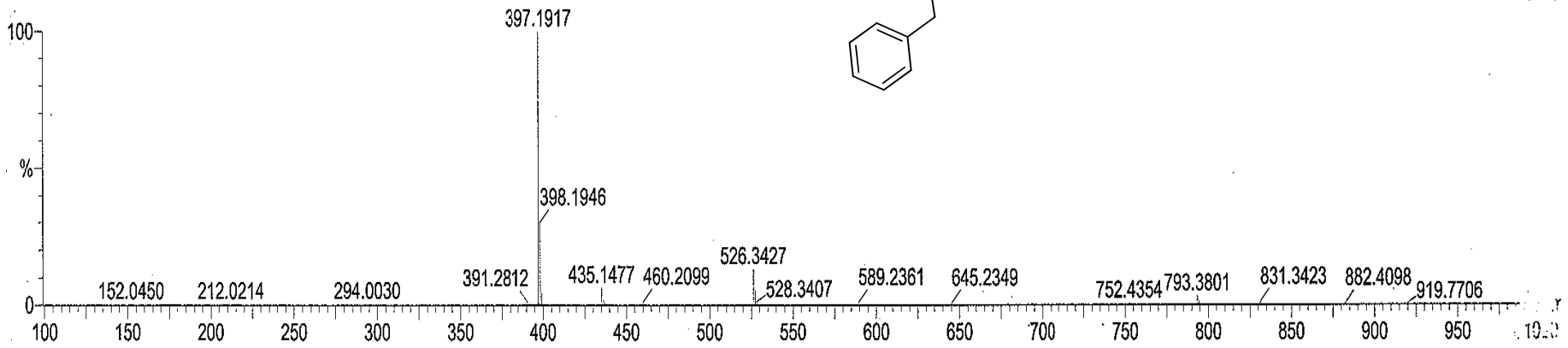
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

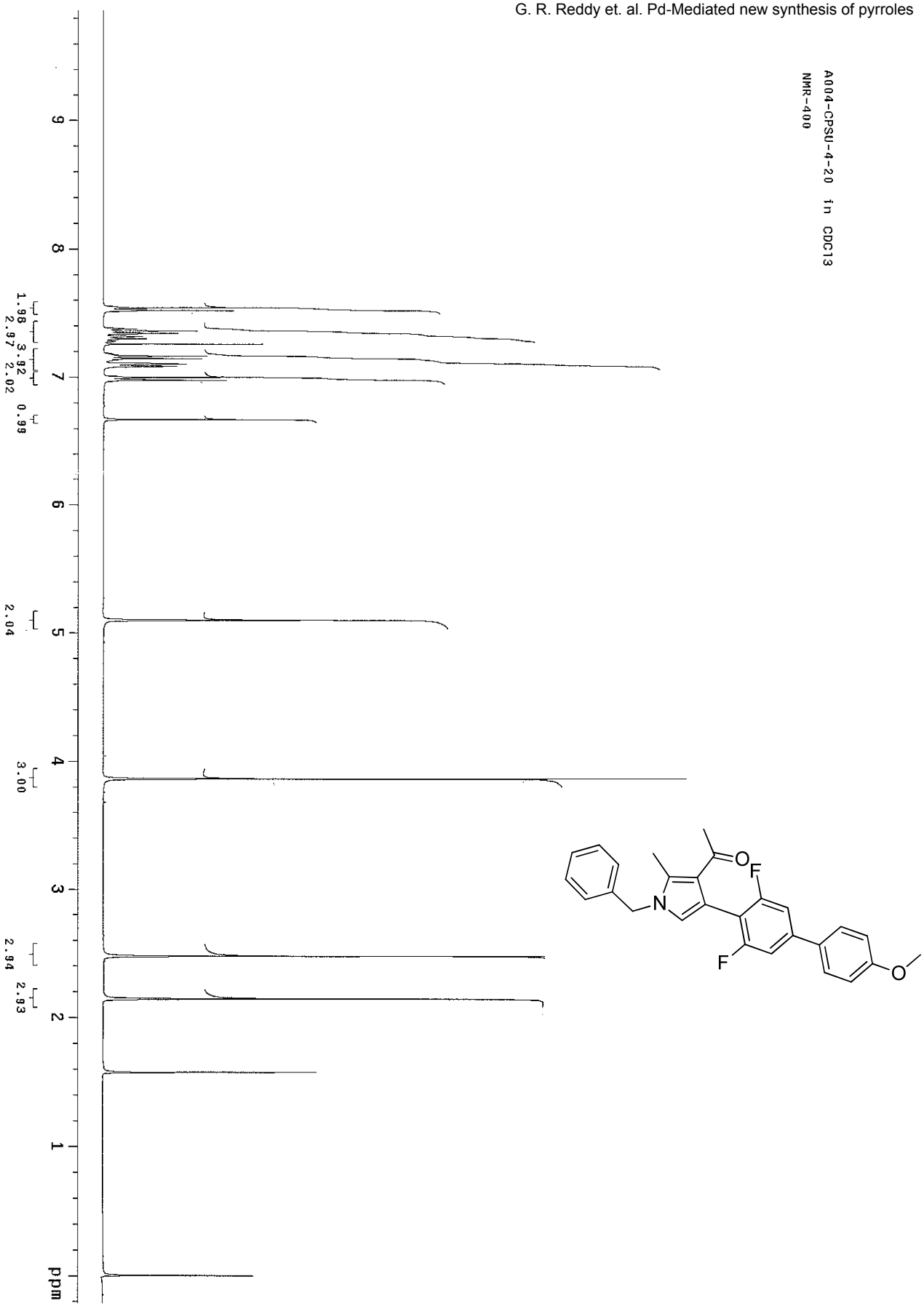
Monoisotopic Mass, Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-2 O: 0-2
A004\CPSU-4\016
UT1110_24 18 (0.338) Cm (17:22-86:95)

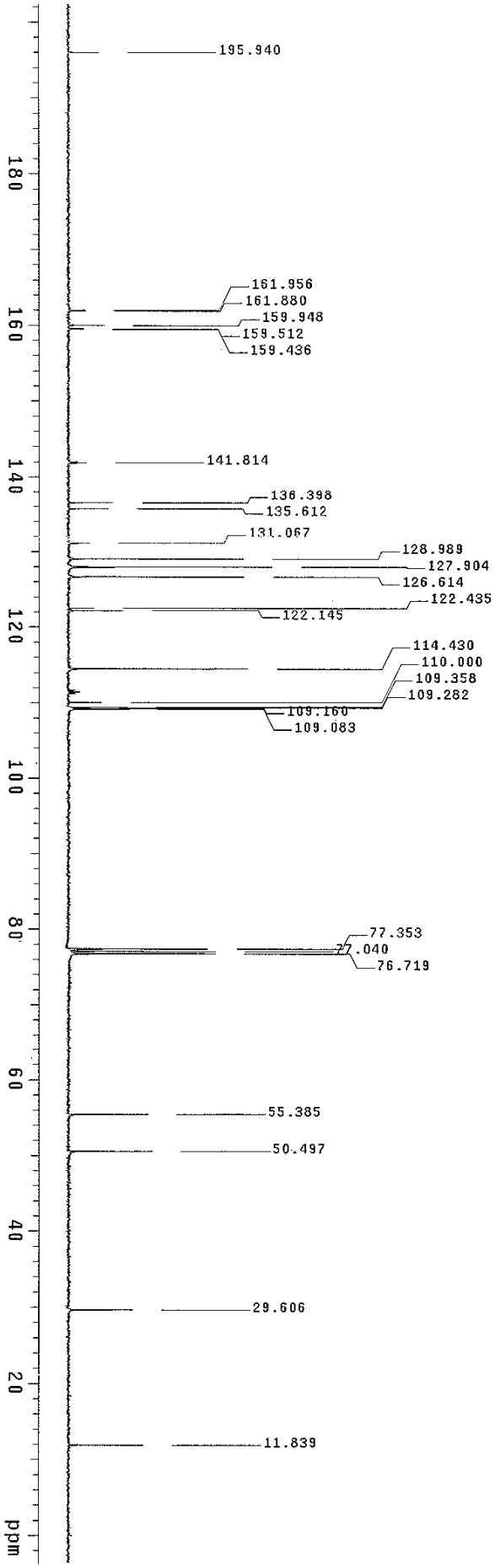


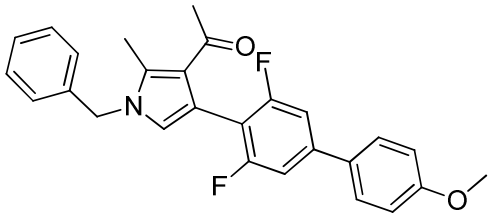
1: TOF MS
5.86e+0

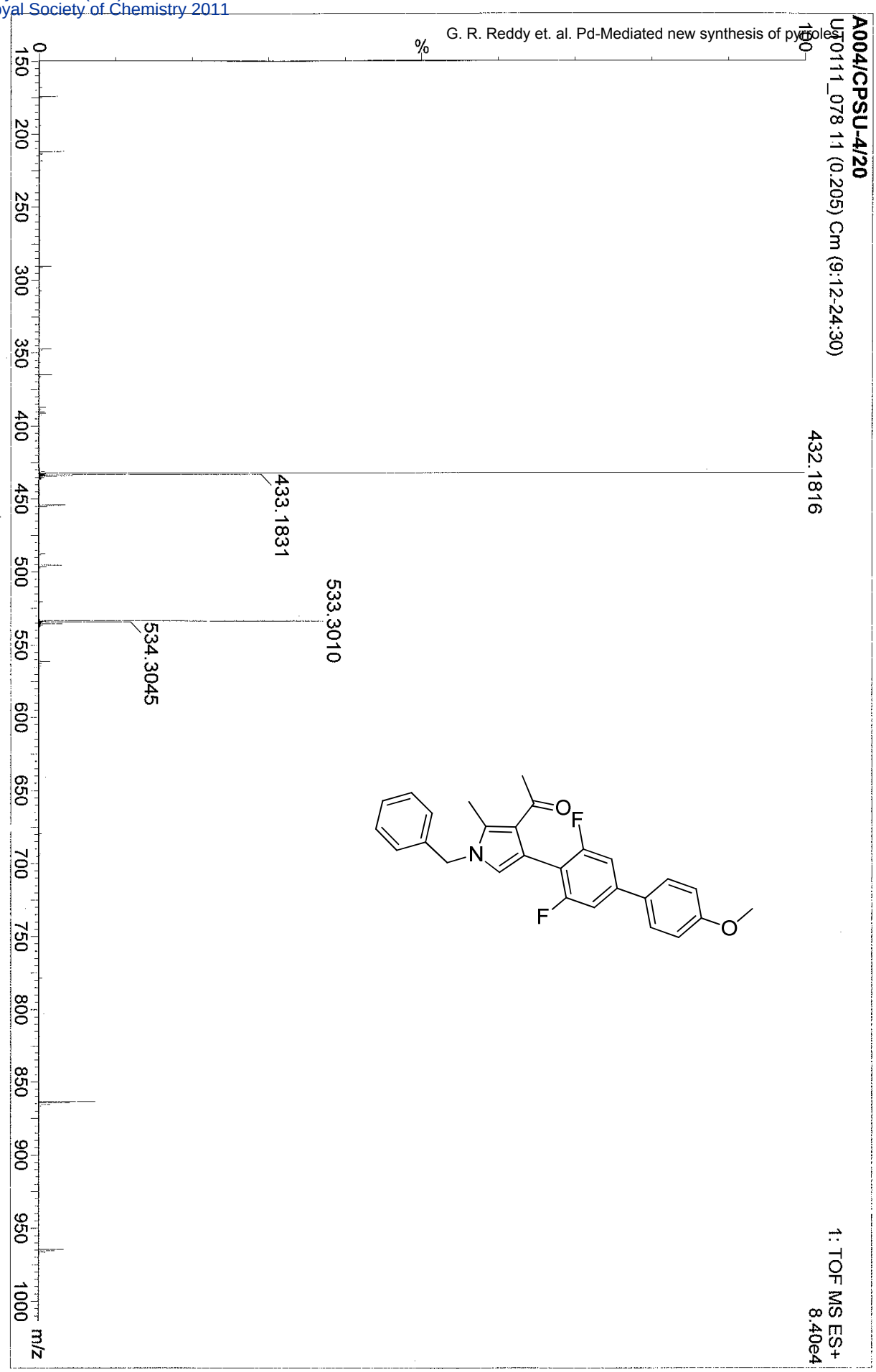


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
397.1917	397.1916	0.1	0.3	15.5	1.1	C26 H25 N2 O2


A004-CPSU-4-20 in CDCl3
NMR-400
1.98
3.92
2.97
2.02
0.99
2.04
3.00
2.94
2.93
ppm
O
F
N
F
O


195.940
161.956
161.880
159.948
159.512
159.436
141.814
136.398
135.612
131.067
128.989
127.904
126.614
122.435
122.145
114.430
110.000
109.358
109.282
109.160
109.083
77.353
77.040
76.719
55.385
50.497
29.606
11.839
ppm
A004/CPSU-4/020 in CDCl3
NMR-400


O
F
N
F
O

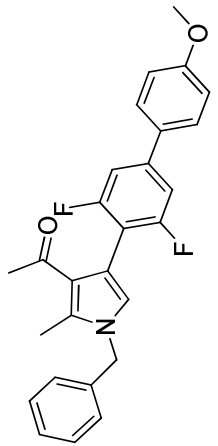


Elemental Composition Report

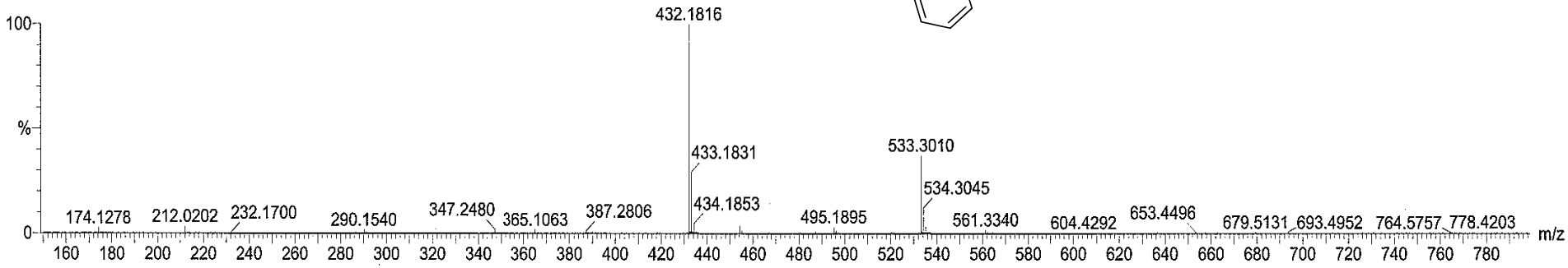
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

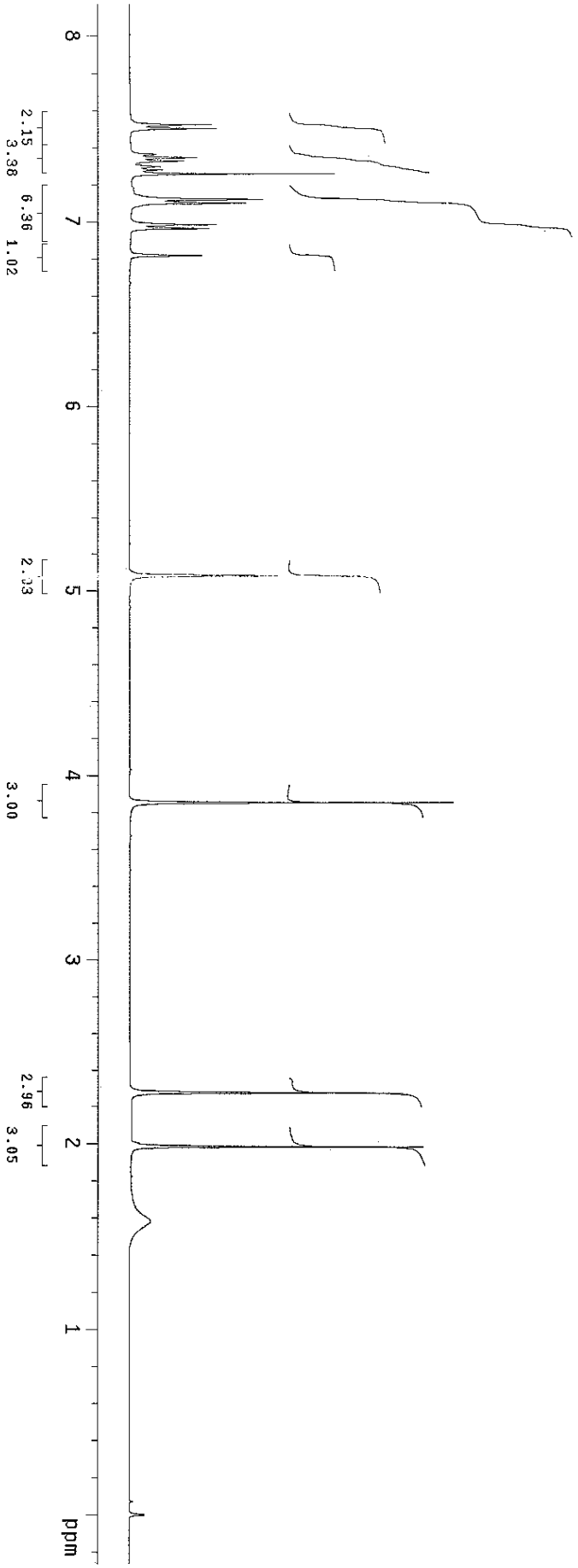
Monoisotopic Mass, Even Electron Ions
149 formula(e) evaluated with 2 results within limits (up to 15 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-5 F: 0-2
A004/CPSU-4/20
UT0111_078 11 (0.205) Cm (9:12-24:30)

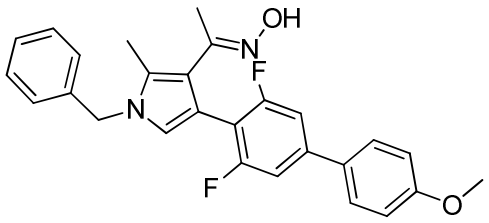


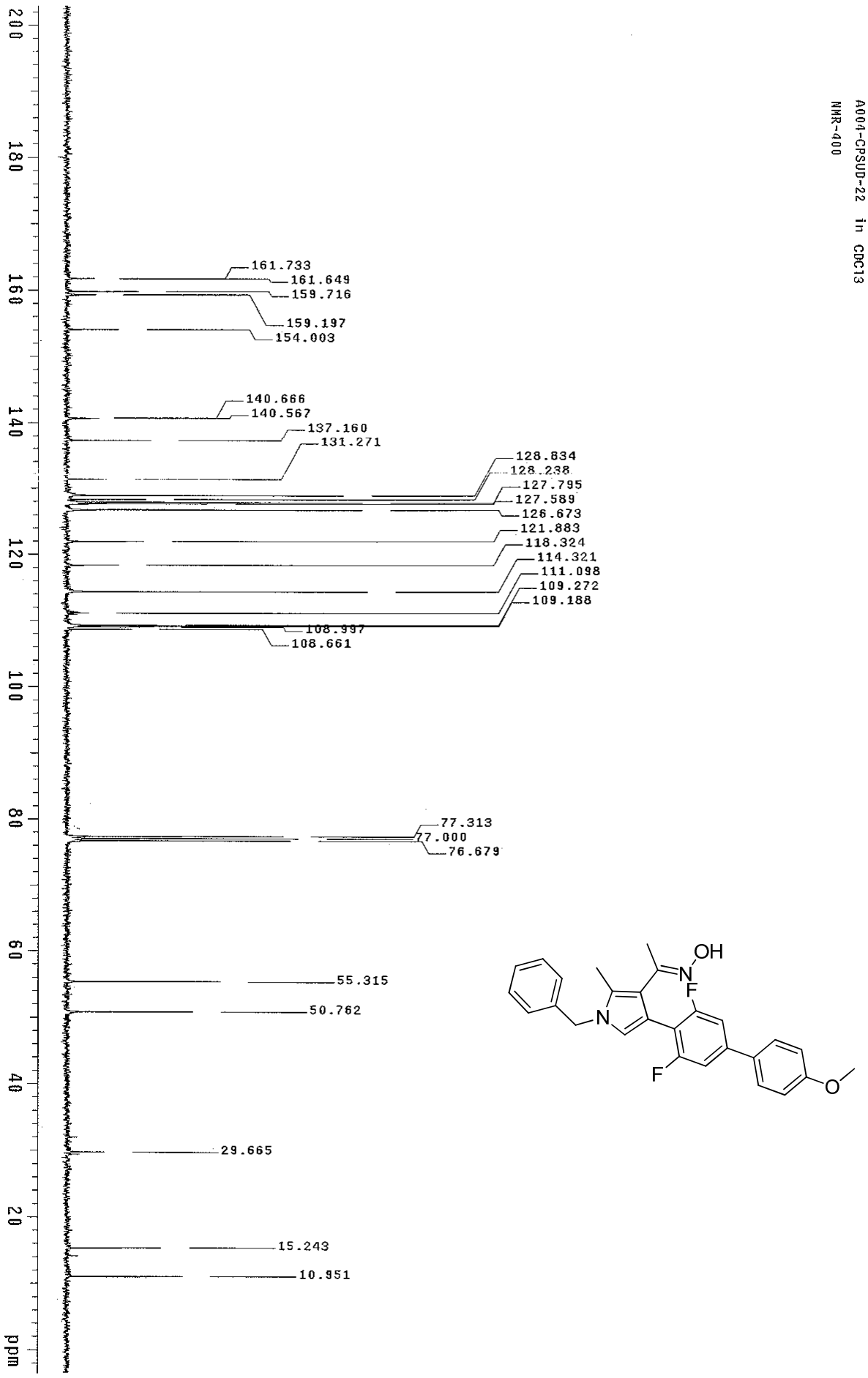
TOF MS ES+
8.40e+004

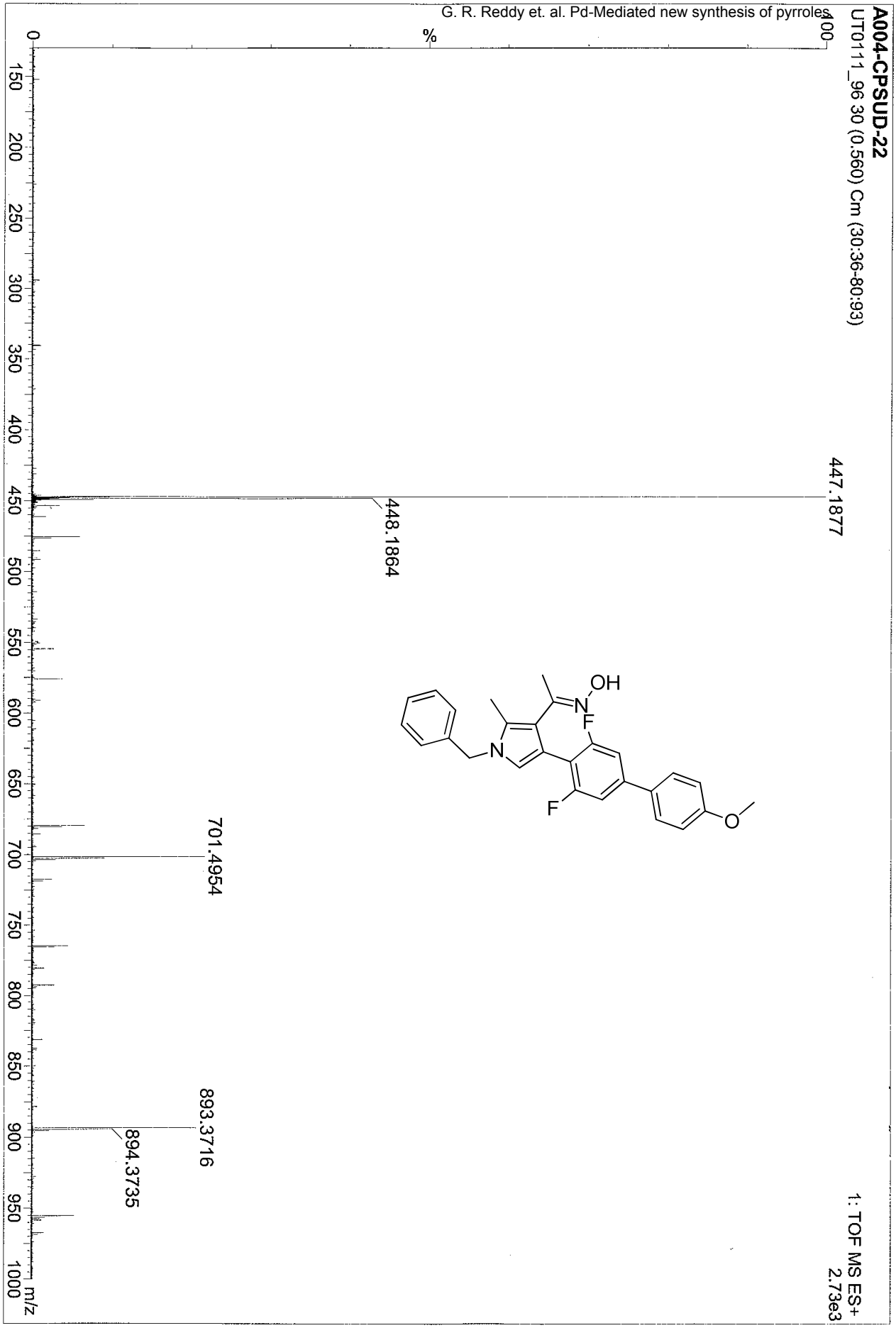


Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
432.1816	432.1775	4.1	9.5	15.5	77.7	C27 H24 N O2 F2

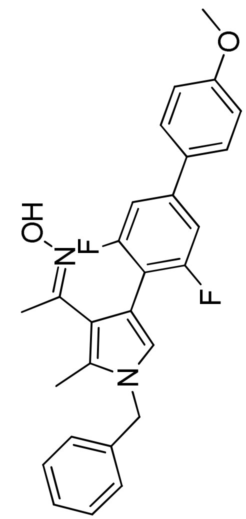

A004-CPSUD-22 in CDCl3
NMR-400
8
7
6
5
4
3
2
1
ppm
2.15
3.38
6.36
1.02
2.13
3.00
2.96
3.05


OH
N
F
N
F
O


A004-CPSUD-22 in CDC13
NMR-400
161.733
161.649
159.716
159.197
154.003
140.666
140.567
137.160
131.271
128.834
128.238
127.795
127.589
126.673
121.883
118.324
114.321
111.098
109.272
109.188
108.997
108.661
77.313
77.000
76.679
55.315
50.762
29.665
15.243
10.951
ppm
200
180
160
140
120
100
80
60
40
20
OH
N
F
N
F
O



Elemental Composition Report

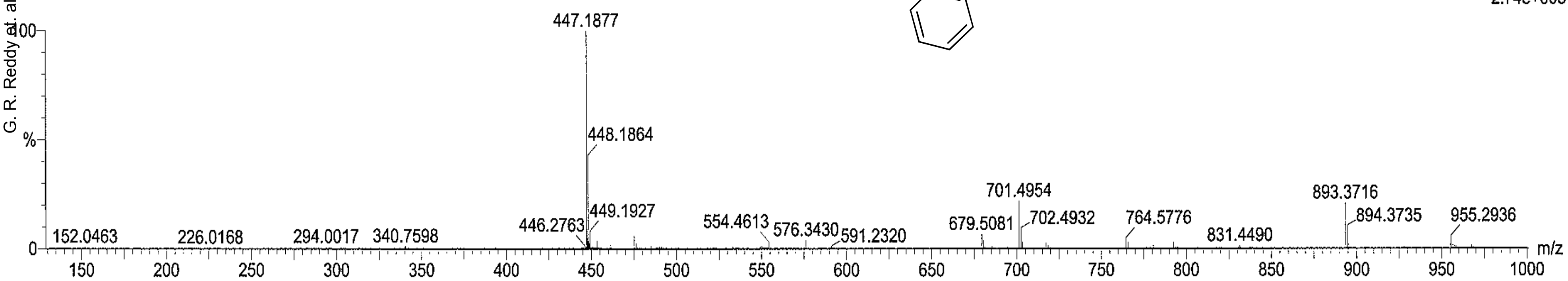


Single Mass Analysis

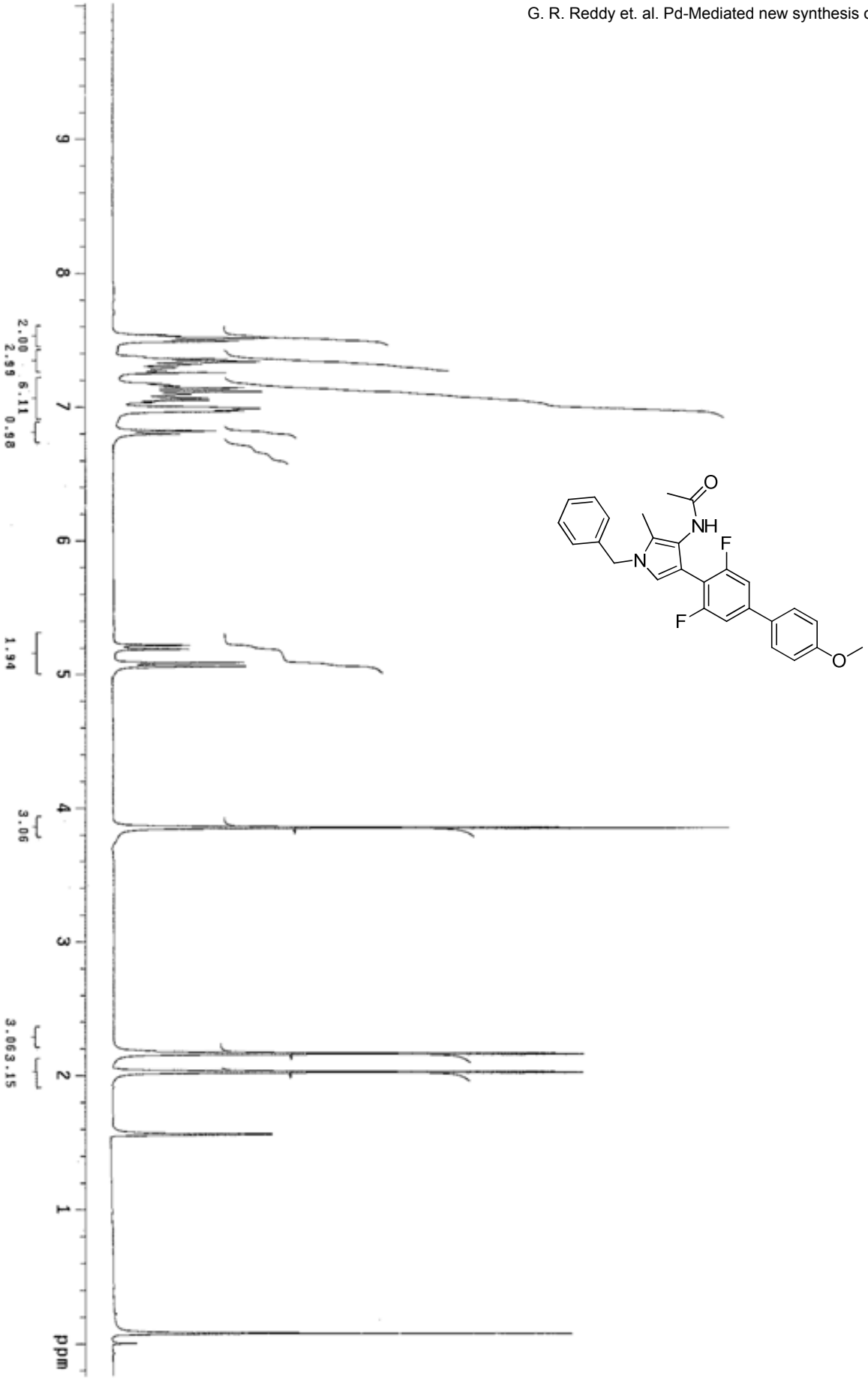
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

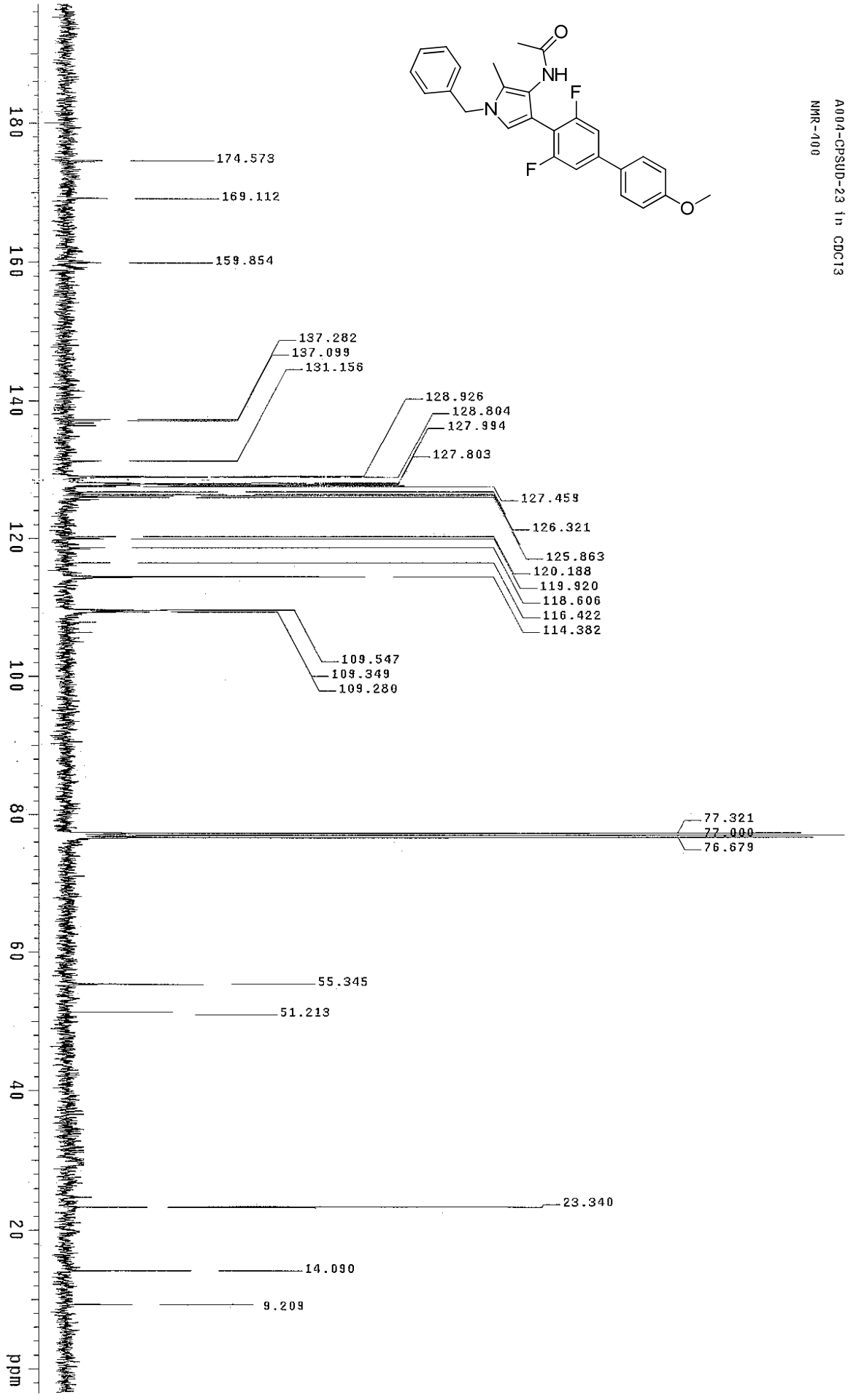
Monoisotopic Mass, Even Electron Ions
237 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-55 N: 0-4 O: 0-4 F: 1-2

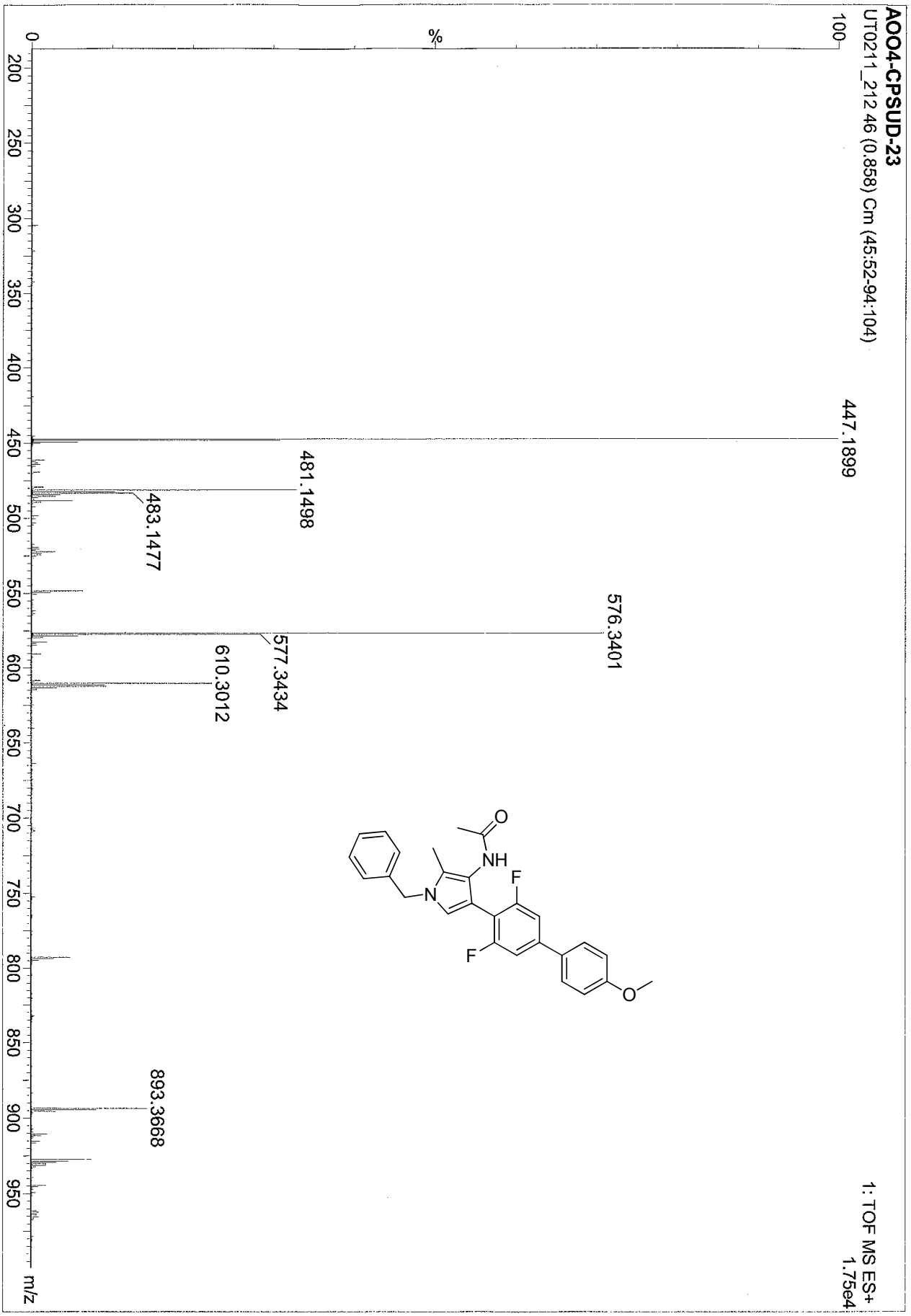
A004-CPSUD-22
GT0111_96 30 (0.560) Cm (30:36-80:93)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
447.1877	447.1884	-0.7	-1.6	15.5	44.6	C27 H25 N2 O2 F2


A004/CPSUD/23 fn CDCl3
NMR-400
2.00
2.99
6.11
0.98
1.94
3.06
3.06
3.15
ppm
O
NH
N
F
F
O


A004-CPSUD-23 in CDCl3
NMR-100
O
NH
N
F
F
O
174.573
169.112
159.854
137.282
137.099
131.156
128.926
128.804
127.994
127.803
127.459
126.321
125.863
120.188
119.920
118.606
116.422
114.382
109.547
109.349
109.280
77.321
77.000
76.679
55.345
51.213
23.340
14.090
9.209
180
160
140
120
100
80
60
40
20
ppm

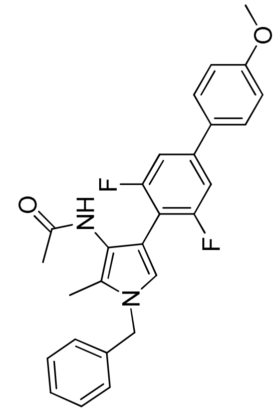

AO04-CPSUD-23
UT0211_212 46 (0.858) Cm (45:52-94:104)
1: TOF MS ES+
1.75e4
%
m/z
447.1899
481.1498
483.1477
576.3401
577.3434
610.3012
893.3668
O
NH
F
F
N
O

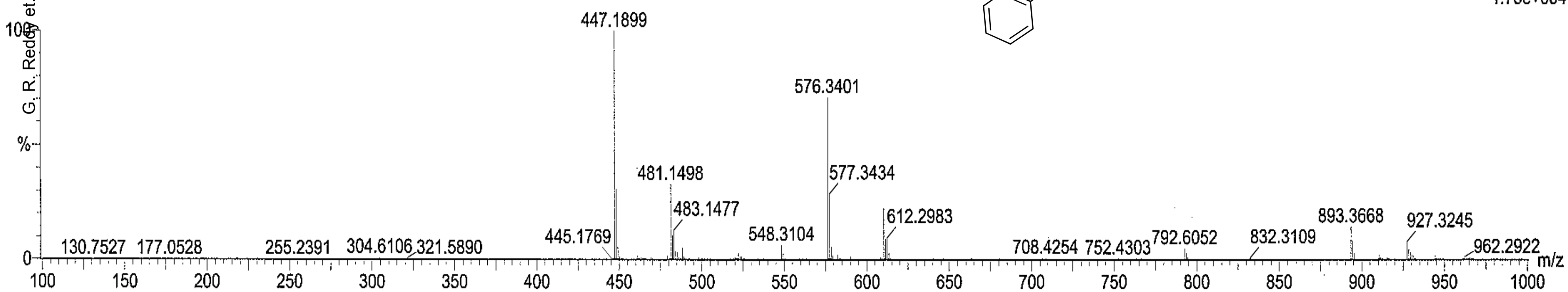
Elemental Composition Report

Single Mass Analysis

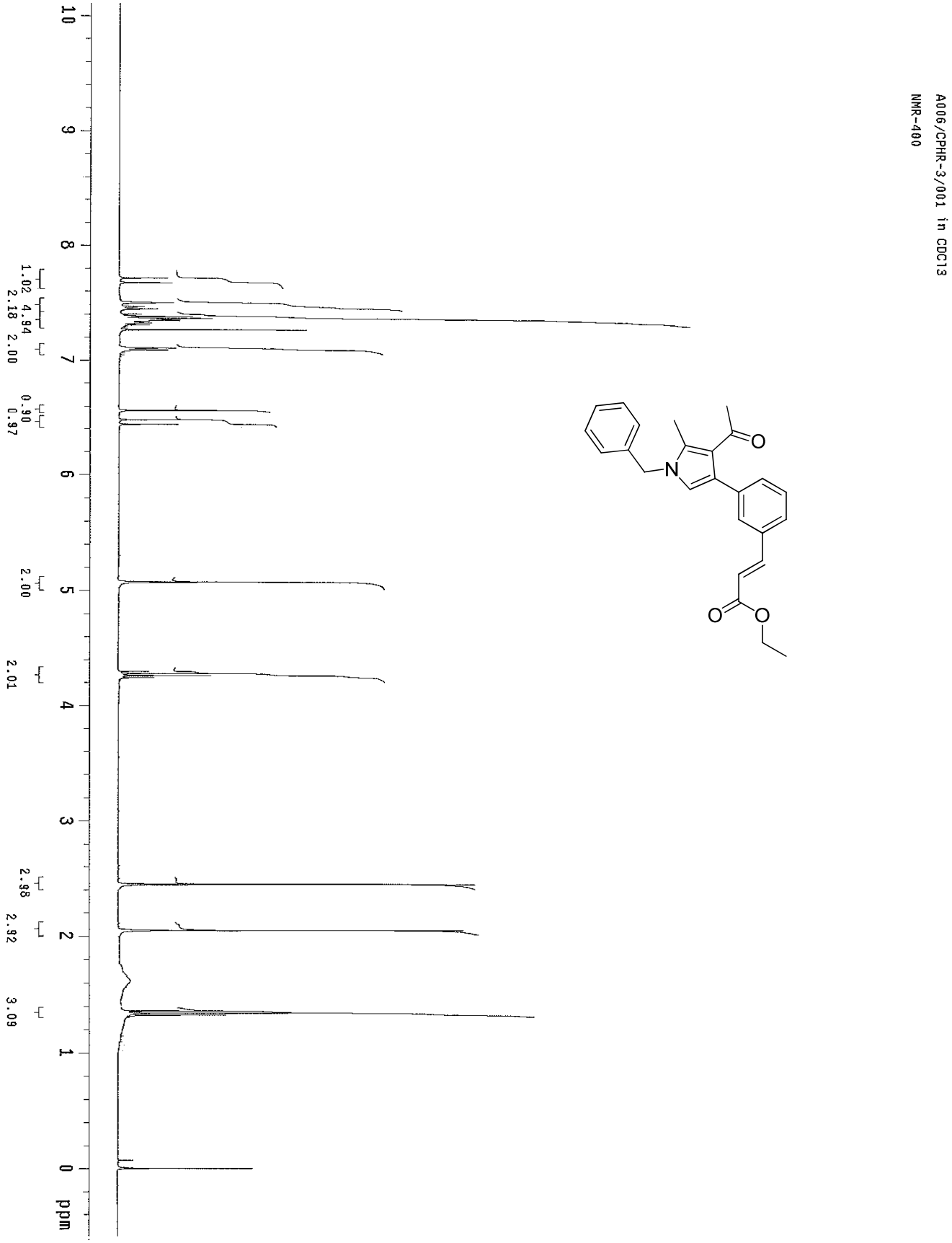
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

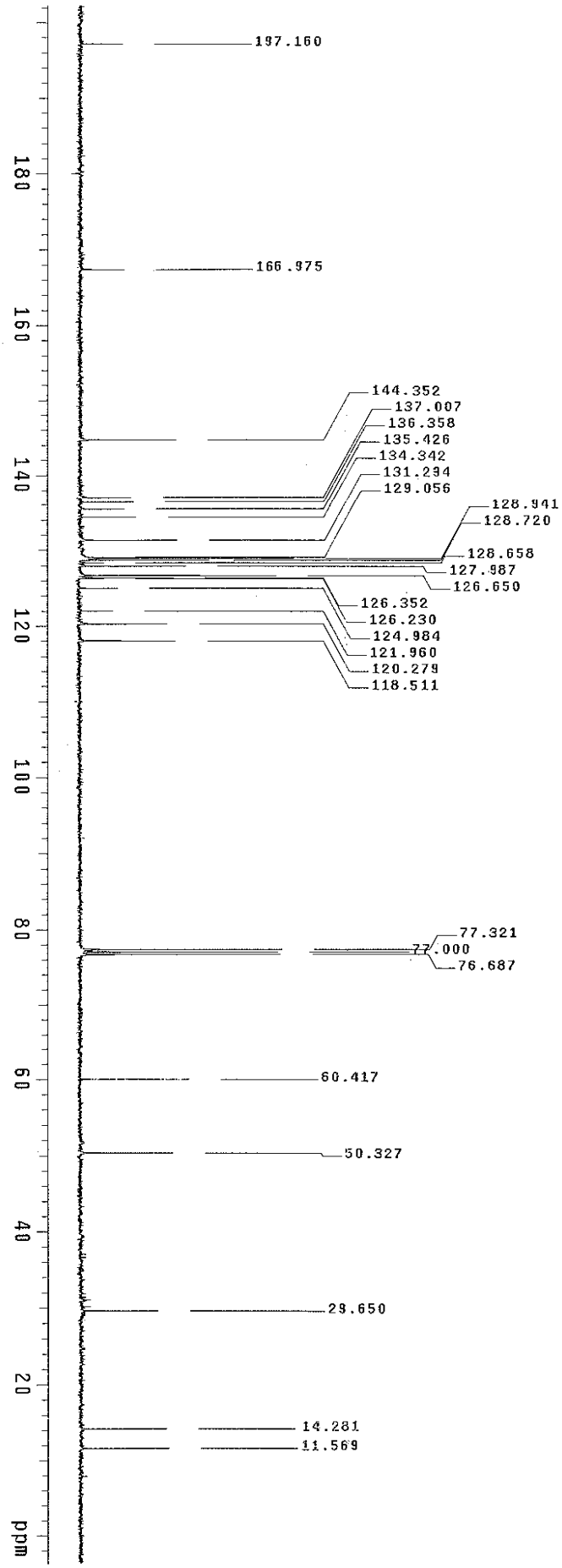
Monoisotopic Mass, Even Electron Ions
293 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-4 O: 0-4 F: 0-2
AO04-CPSUD-23
UT0211_212 46 (0.858) Cm (45:52-94:104)



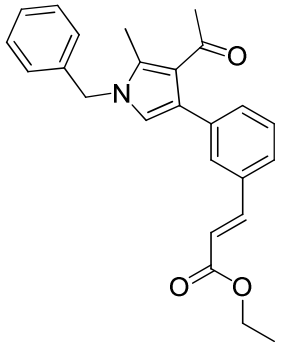


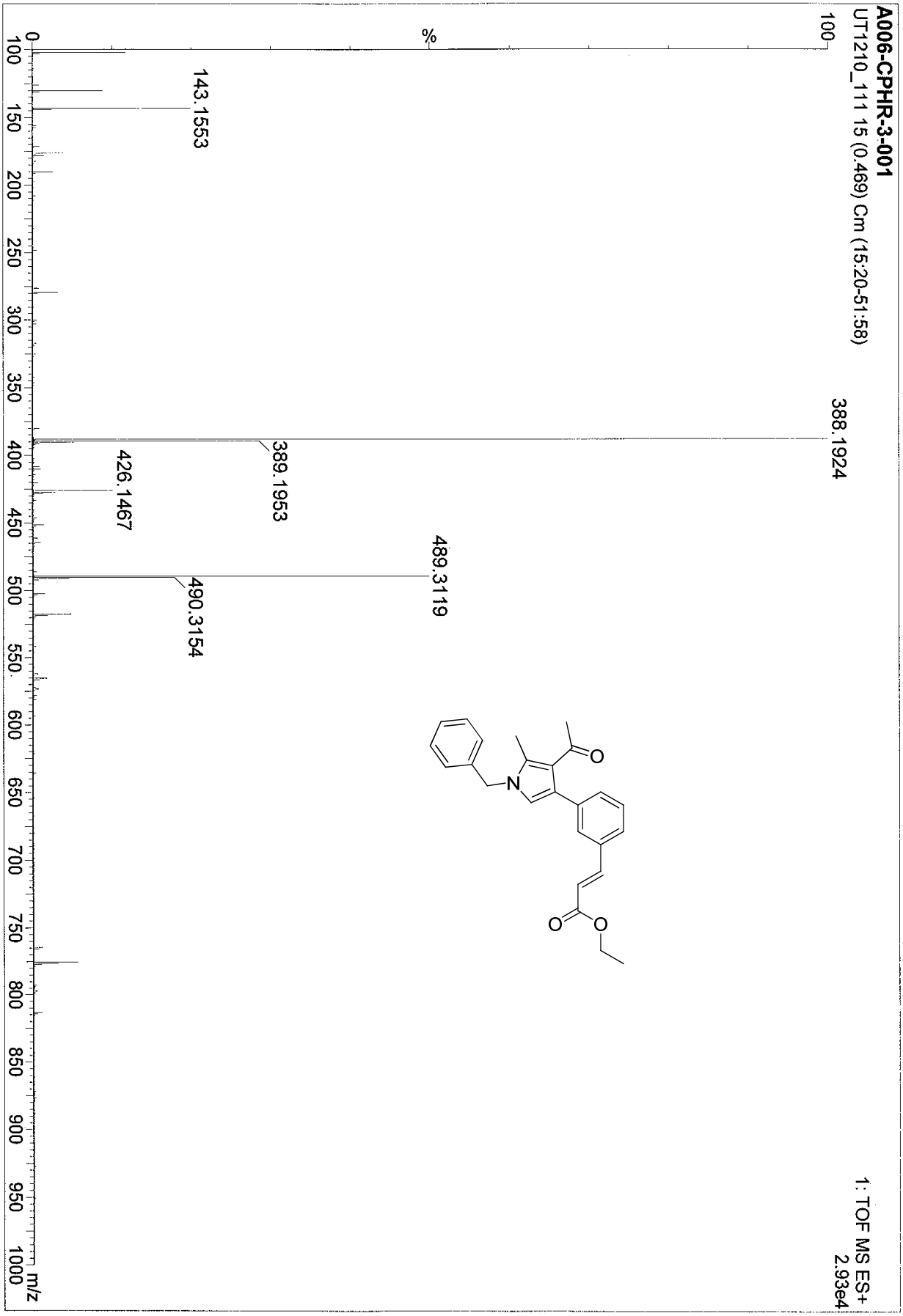
Minimum:	80.00				-1.0		
Maximum:	100.00		5.0	5.0	80.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
447.1899	100.00	447.1884	1.5	3.4	15.5	7.0	C27 H25 N2 O2 F2


A006/CPHR-3/001 in CDCl3
NMR-400
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
4.94
2.18
2.00
0.90
0.97
2.00
2.01
2.98
2.92
3.09
N
O
O
O


197.160
166.975
144.352
137.007
136.358
135.426
134.342
131.294
129.056
128.941
128.720
128.658
127.987
126.650
126.352
126.230
124.984
121.960
120.279
118.511
77.321
77.000
76.687
60.417
50.327
29.650
14.281
11.569
180
160
140
120
100
80
60
40
20
ppm


A006-CPHR-3-002 in CDC13
NMR-400


N
O
O
O


A006-CPHR-3-001
UT1210_111 15 (0.469) Cm (15:20-51:58)
1: TOF MS ES+
2.93e4
%
m/z
143.1553
388.1924
389.1953
426.1467
489.3119
490.3154
O
N
O
O

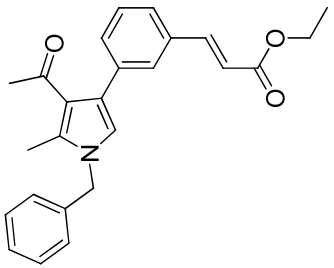
Elemental Composition Report

Single Mass Analysis

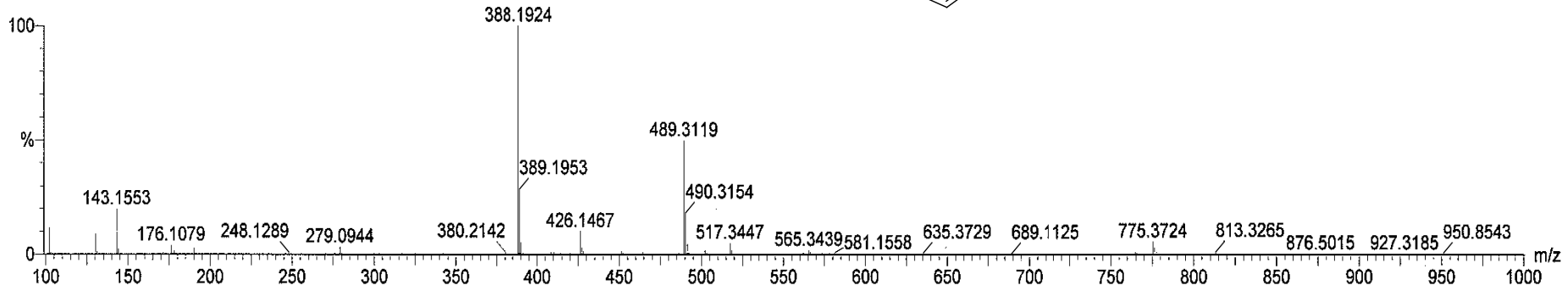
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
220 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-6 O: 0-6

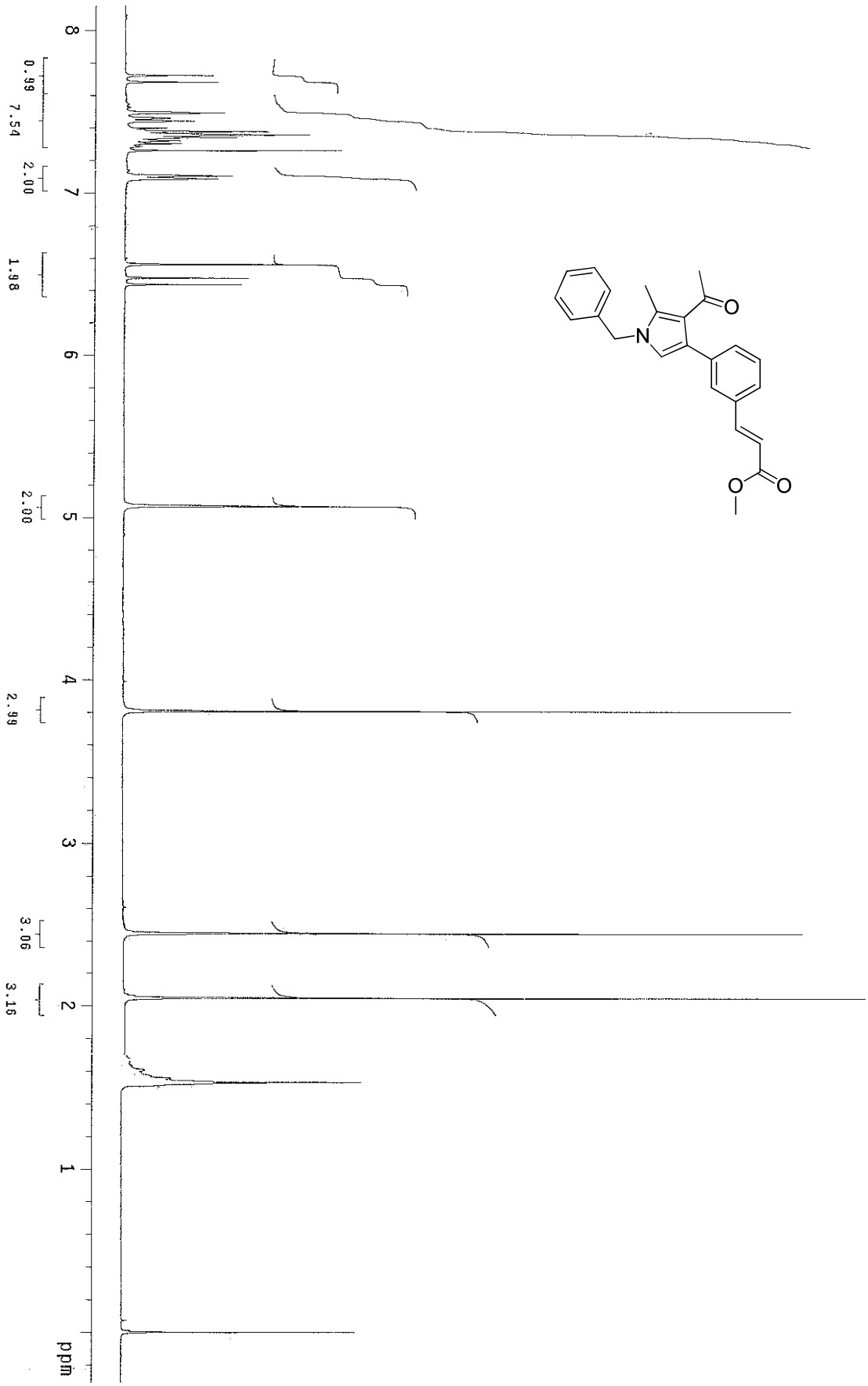
A006-CPHR-3-001
UT1210_111 15 (0.469) Cm (15:20-51:58)

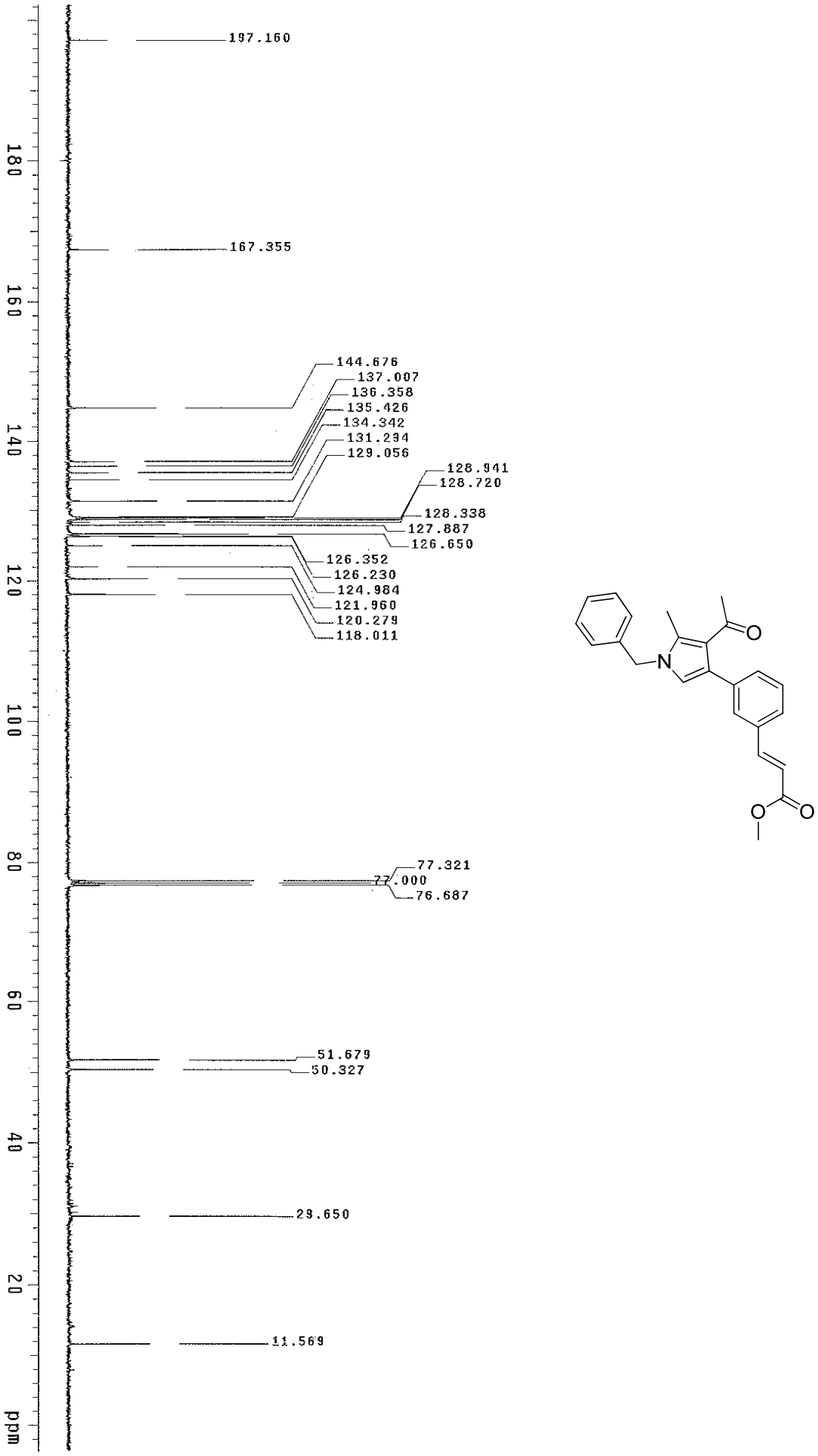


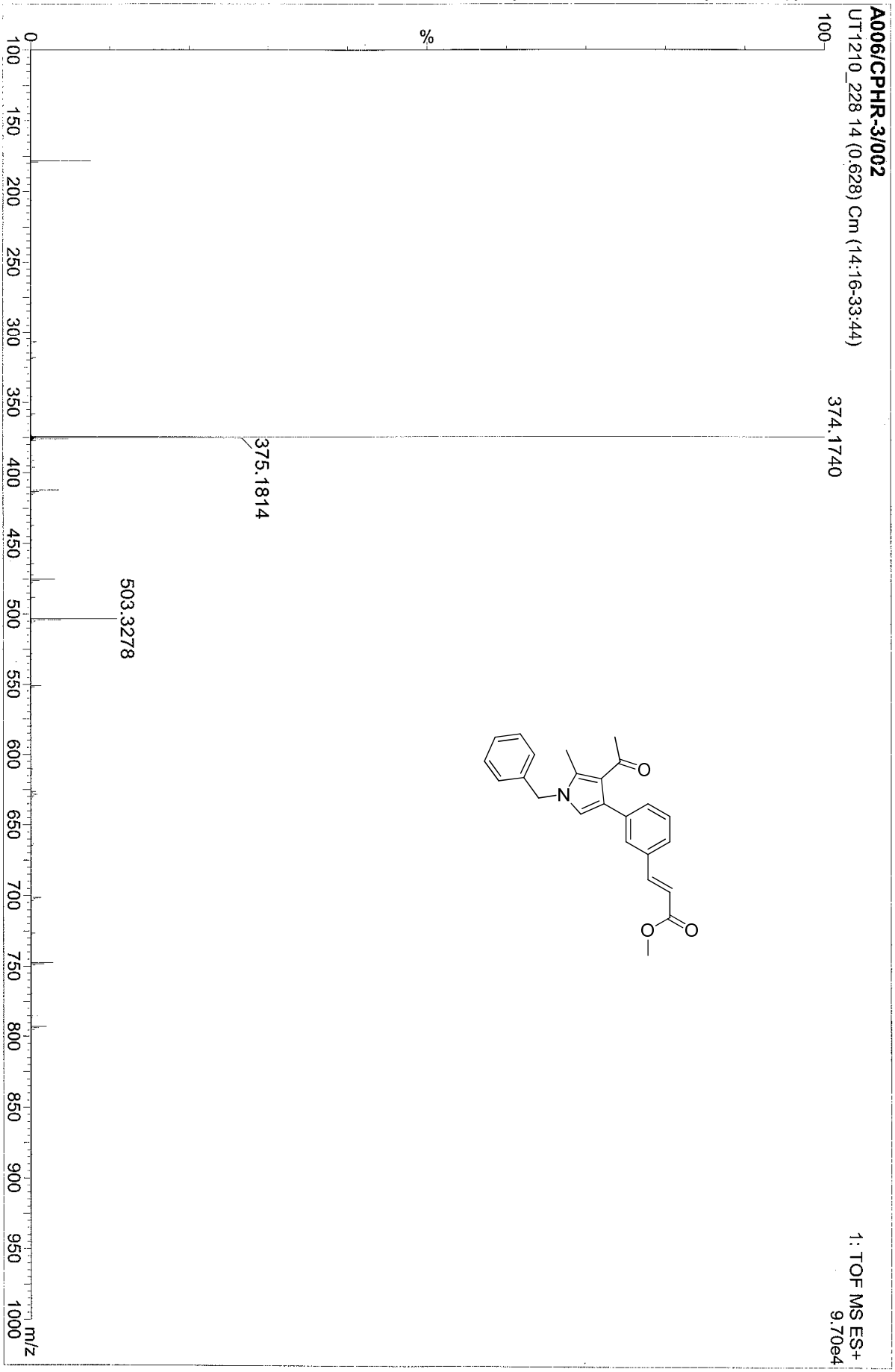
1: TOF MS ES+
2.93e+004



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
388.1924	388.1913	1.1	2.8	13.5	12.4	C25 H26 N O3


A006-CPHR-3-002 in CDCl3
NMR-400
0.99
7.54
2.00
1.98
2.00
2.99
3.06
3.16
ppm
O
N
O
O


197.160
167.355
144.676
137.007
136.358
135.426
134.342
131.294
129.056
128.941
128.720
128.338
127.887
126.650
126.352
126.230
124.984
121.960
120.279
118.011
77.321
77.000
76.687
51.679
50.327
29.650
11.569
ppm
A006-CPHR-3-002 in CDCl3
NMR-400
O
N
O
O

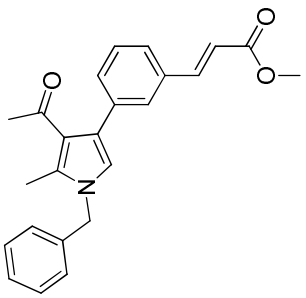

A006/CPHR-3/002
UT1210_228 14 (0.628) Cm (14:16-33:44)
%
100
0
374.1740
375.1814
503.3278
m/z
1: TOF MS ES+
9.70e4
N
O
O
O

Elemental Composition Report

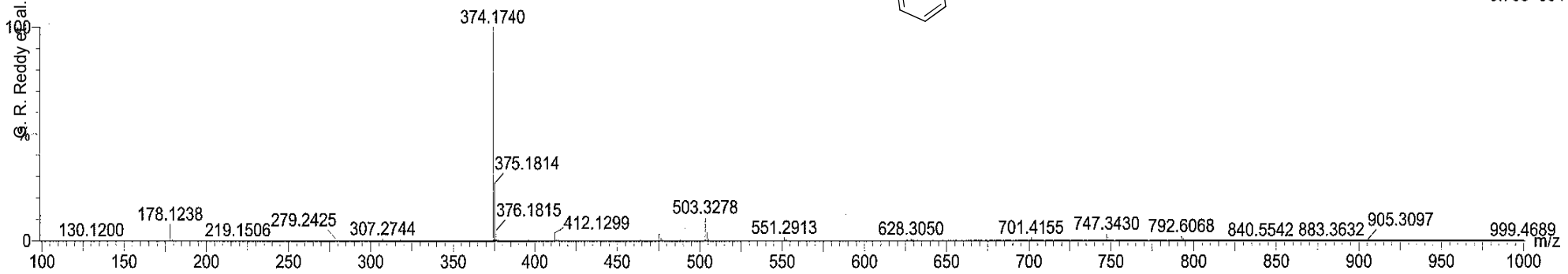
Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

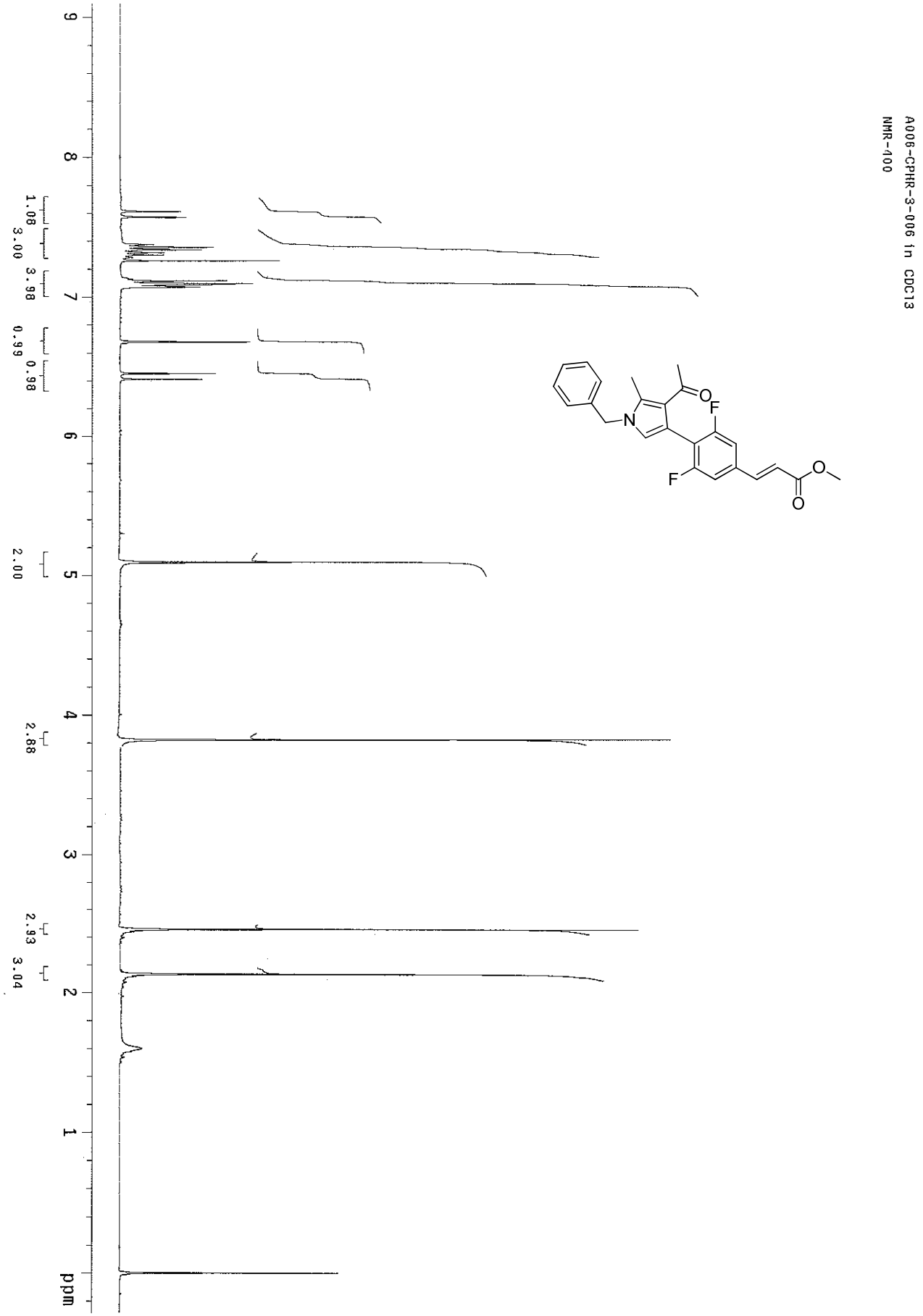
Monoisotopic Mass, Even Electron Ions
79 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-430 N: 0-3 O: 0-3
AQ06/CPHR-3/002
UT1210_228 14 (0.628) Cm (14:16-33:44)

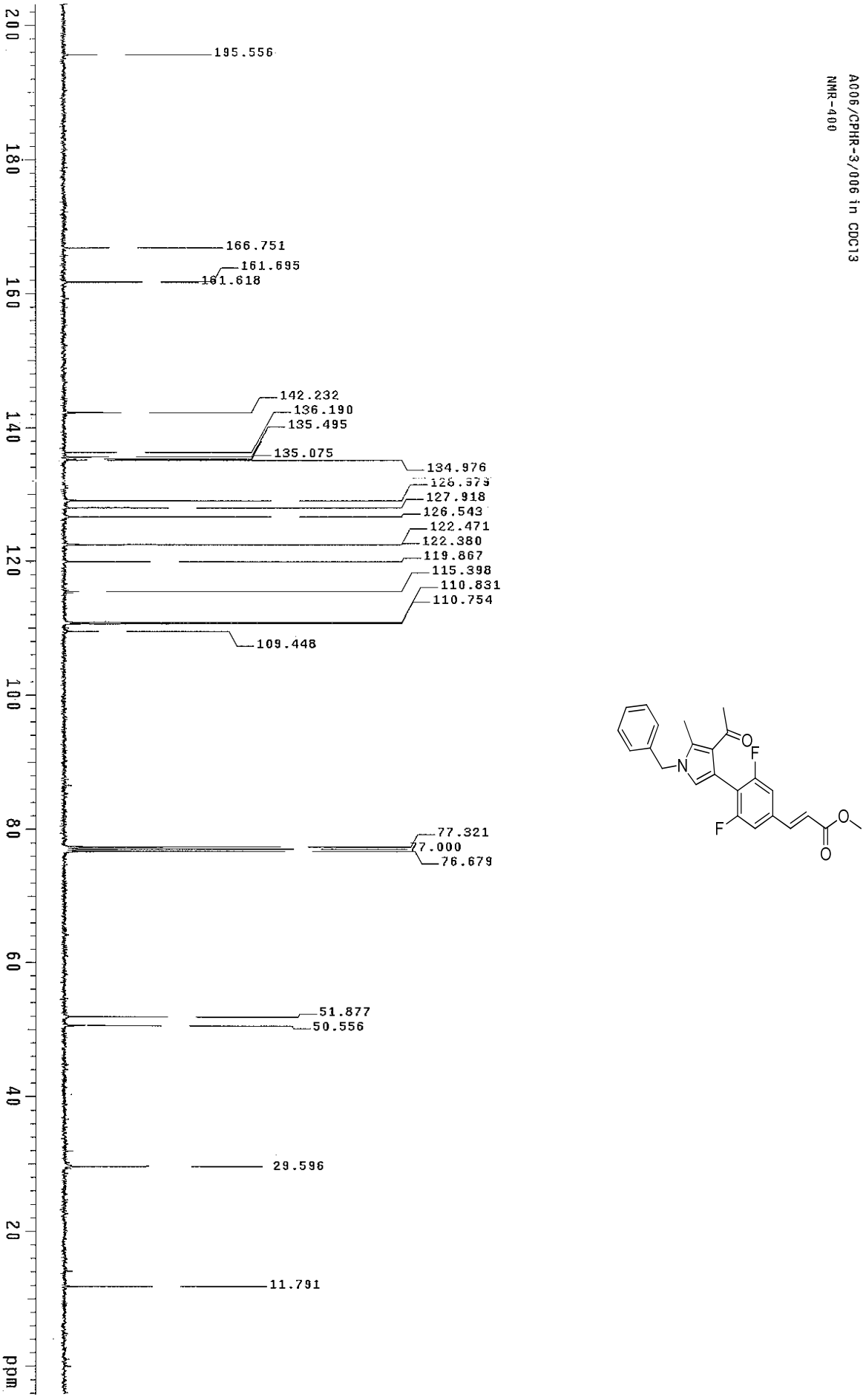


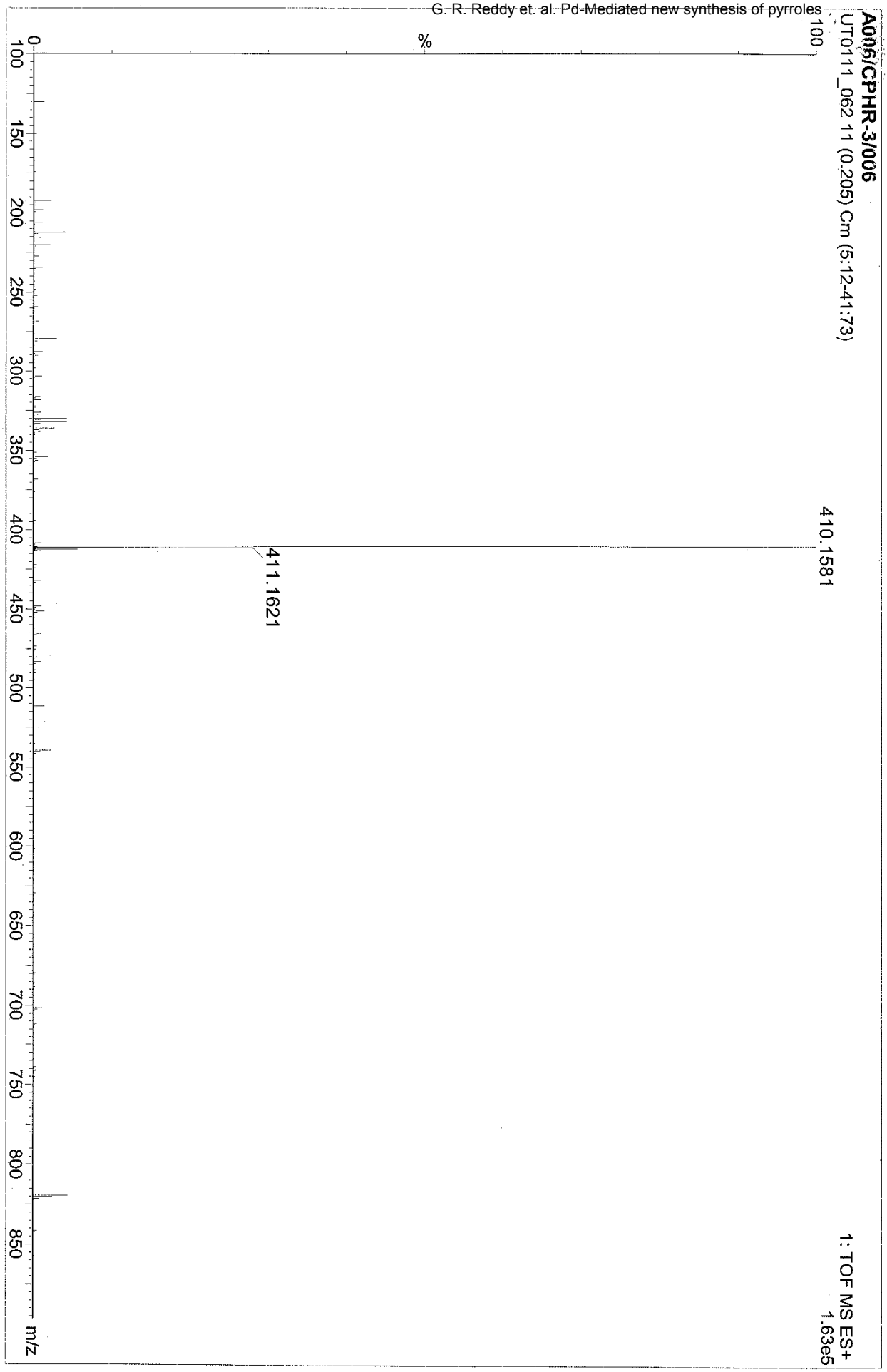
1: TOF MS ES+
9.70e+004



Minimum:				-1.0		
Maximum:		5.0	20.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
374.1740	374.1756	-1.6	-4.3	13.5	49.0	C24 H24 N O3


A006-CPHR-3-006 in CDCl3
NMR-400
1.08
3.00
3.98
0.99
0.98
2.00
2.88
2.93
3.04
ppm
O
F
N
F
O
O


A006/CPHR-3/006 in CDC13
NMR-400
195.556
166.751
161.695
161.618
142.232
136.190
135.495
135.075
134.976
126.575
127.918
126.543
122.471
122.380
119.867
115.398
110.831
110.754
109.448
77.321
77.000
76.679
51.877
50.556
29.596
11.791
ppm
200
180
160
140
120
100
80
60
40
20
N
O
F
F
O
O



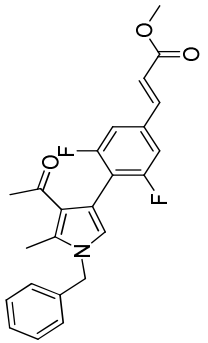
Elemental Composition Report

Single Mass Analysis

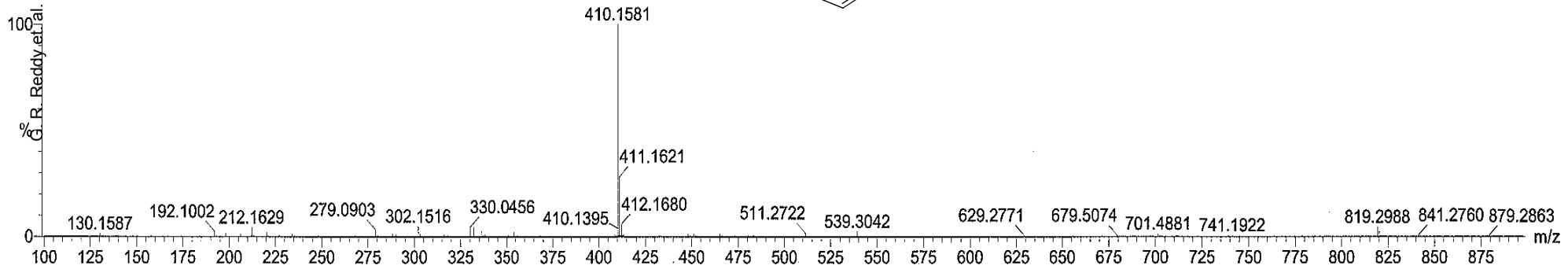
Tolerance = 15.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
156 formula(e) evaluated with 2 results within limits (up to 15 closest results for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-5 O: 0-5

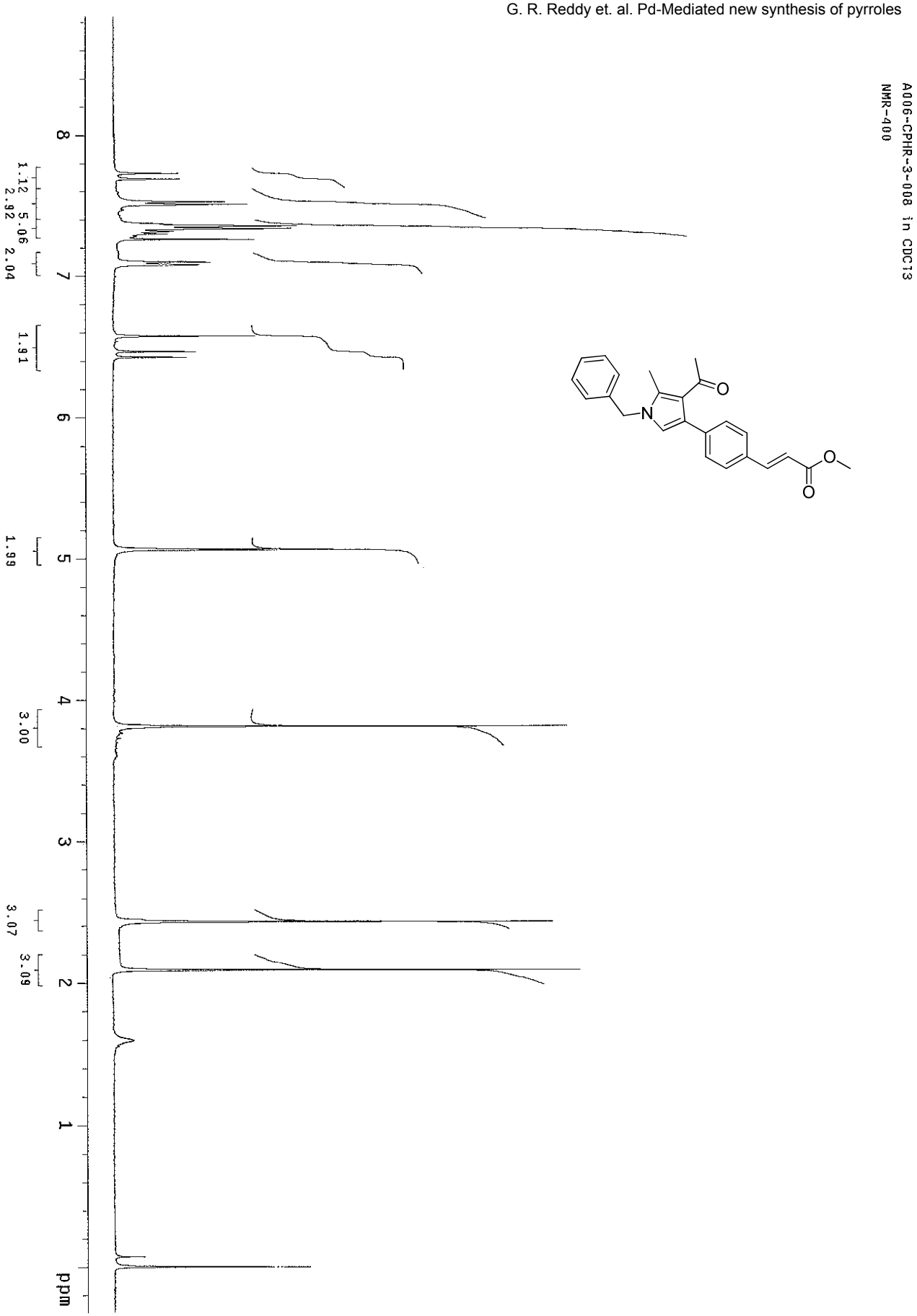
A008/CPHR-3/006
UT0111_062 11 (0.205) Cm (5:12-41:73)

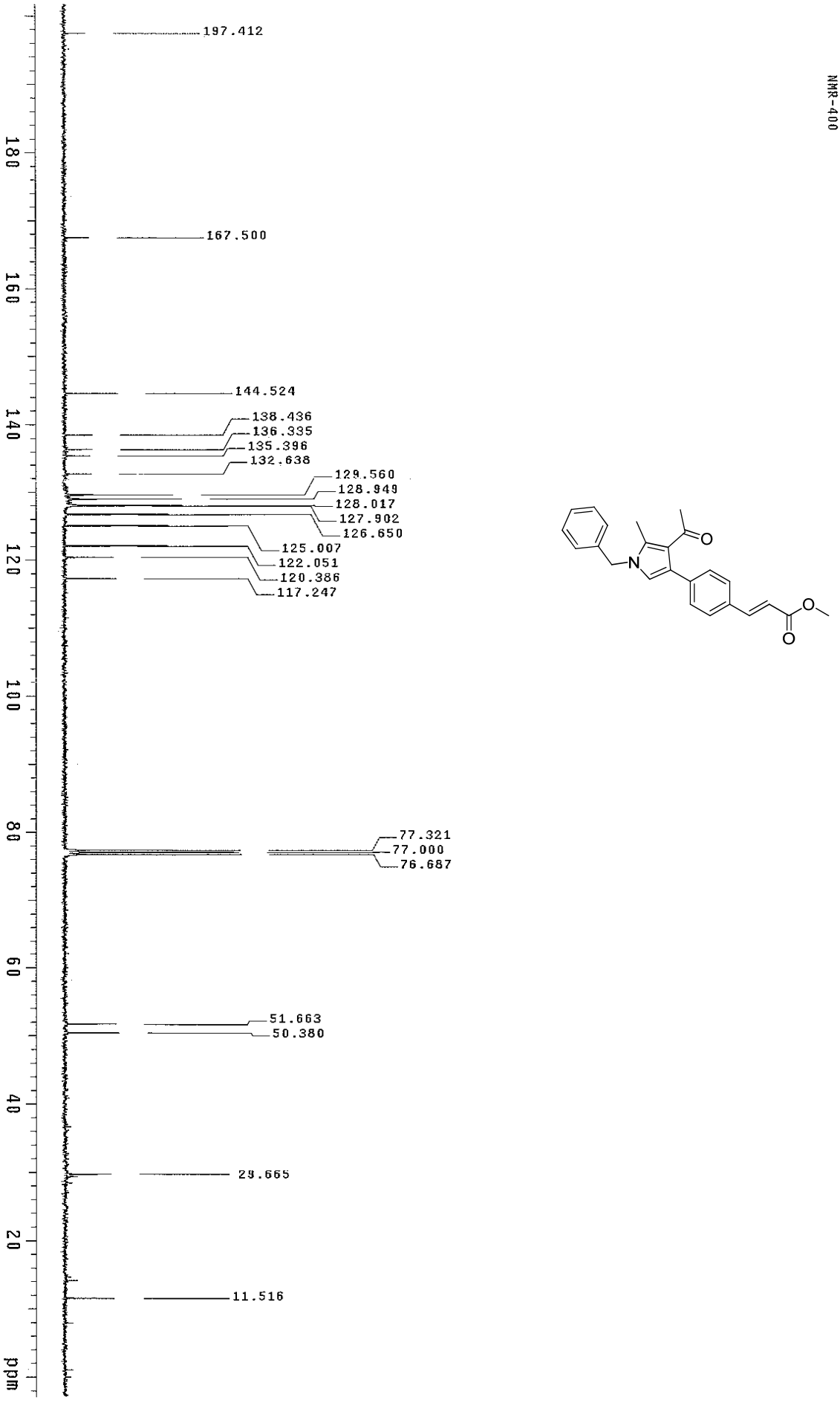


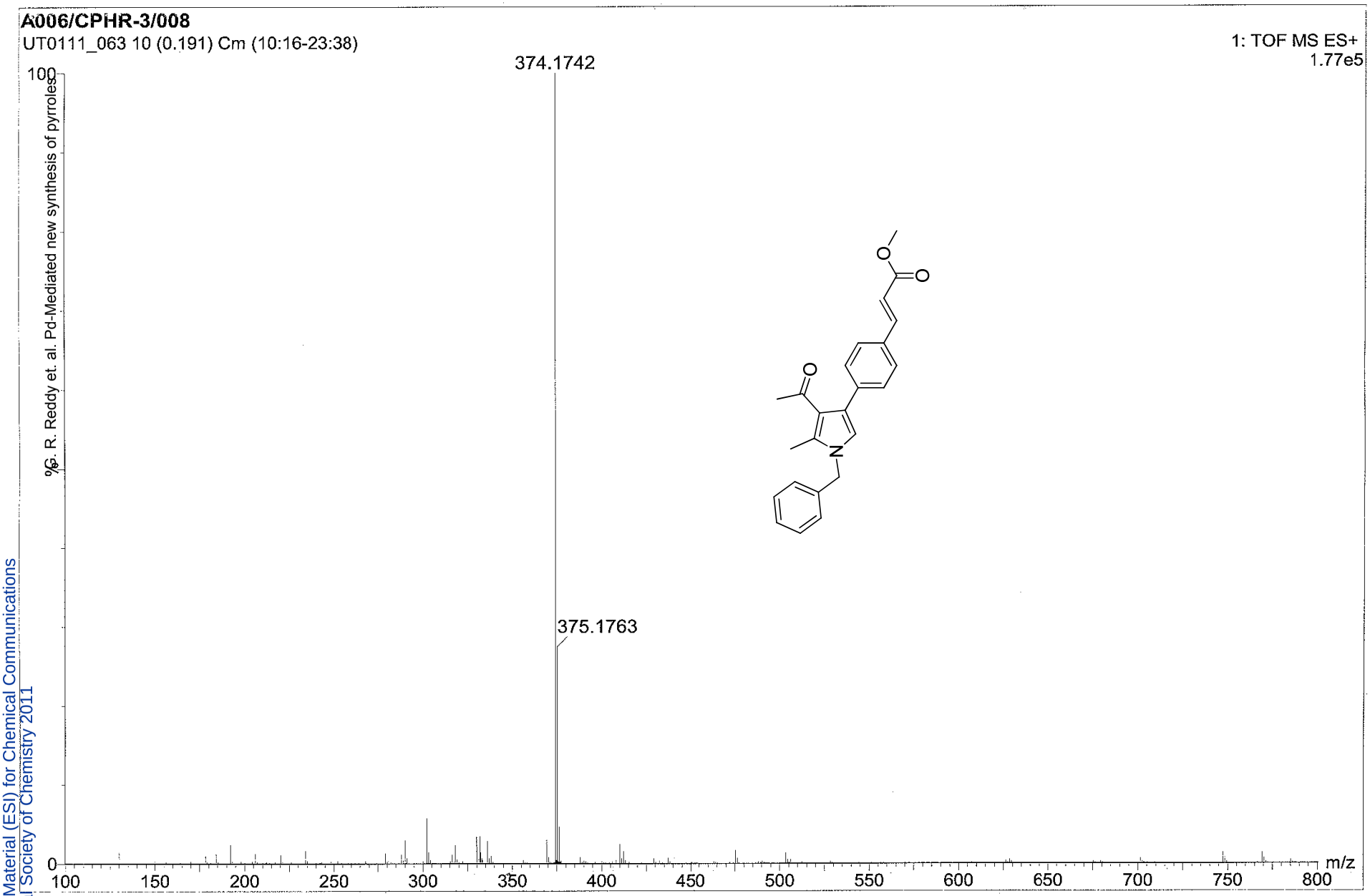
1: TOF MS ES+
1.63e+005



Minimum:				-1.0		
Maximum:		5.0	15.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
410.1581	410.1545	3.6	8.8	21.5	877.7	C24 H22 N O3 F2


A006-CPHR-3-008 in CDCl3
NMR-400
1.12
5.06
2.92
2.04
1.91
1.99
3.00
3.07
3.09
O
N
O
O
8
7
6
5
4
3
2
1
ppm


A006/CPHR-3/008 in CDCl3
NMR-400
197.412
167.500
144.524
138.436
136.335
135.396
132.638
129.560
128.949
128.017
127.902
126.650
125.007
122.051
120.386
117.247
77.321
77.000
76.687
51.663
50.380
29.665
11.516
ppm
180
160
140
120
100
80
60
40
20
N
O
O
O

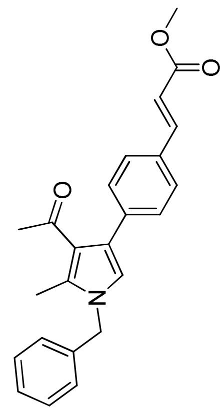


Elemental Composition Report

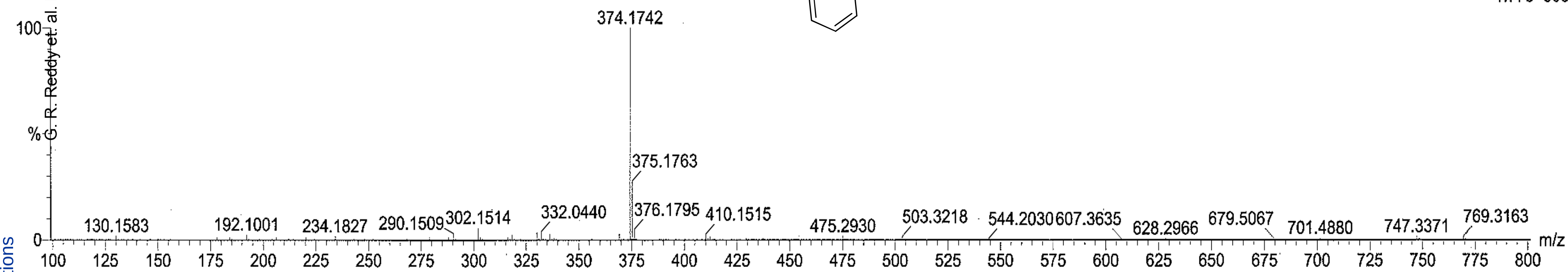
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

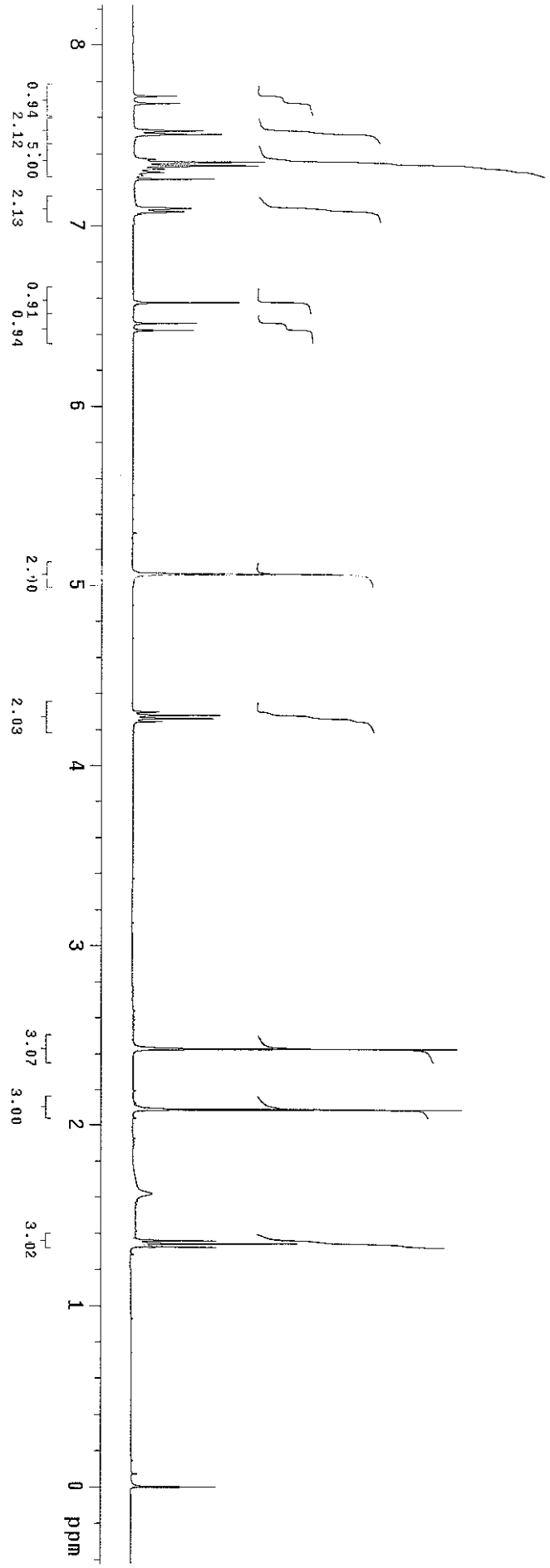
Monoisotopic Mass, Even Electron Ions
456 formula(e) evaluated with 5 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-5 O: 0-5 F: 0-2

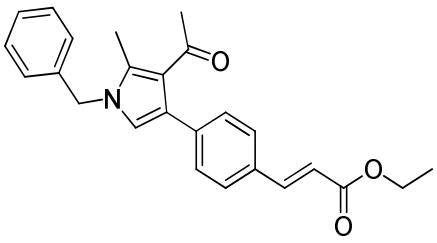


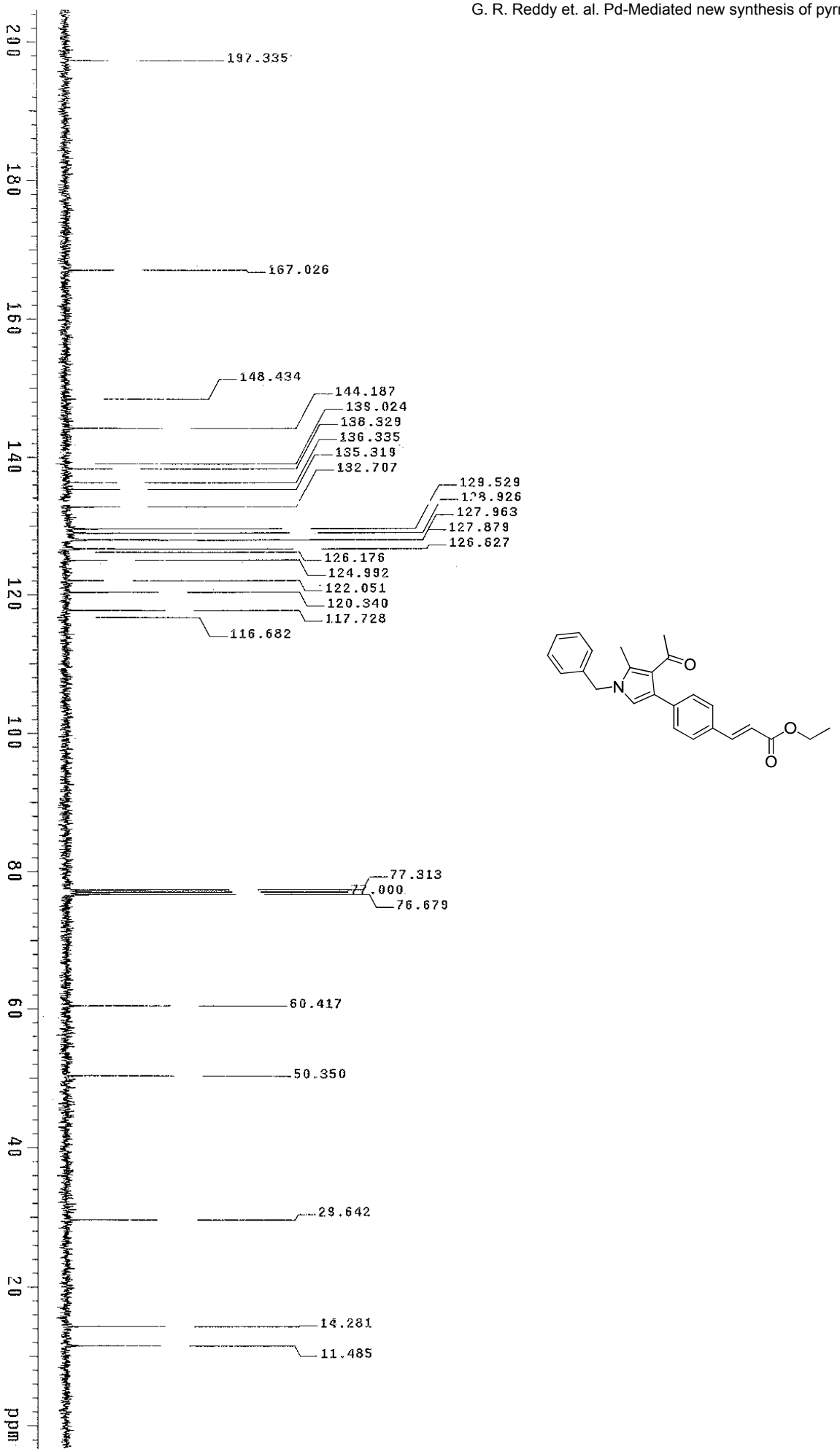
A006CPHR-3/008
UT0111_063 10 (0.191) Cm (10:16-23:38)

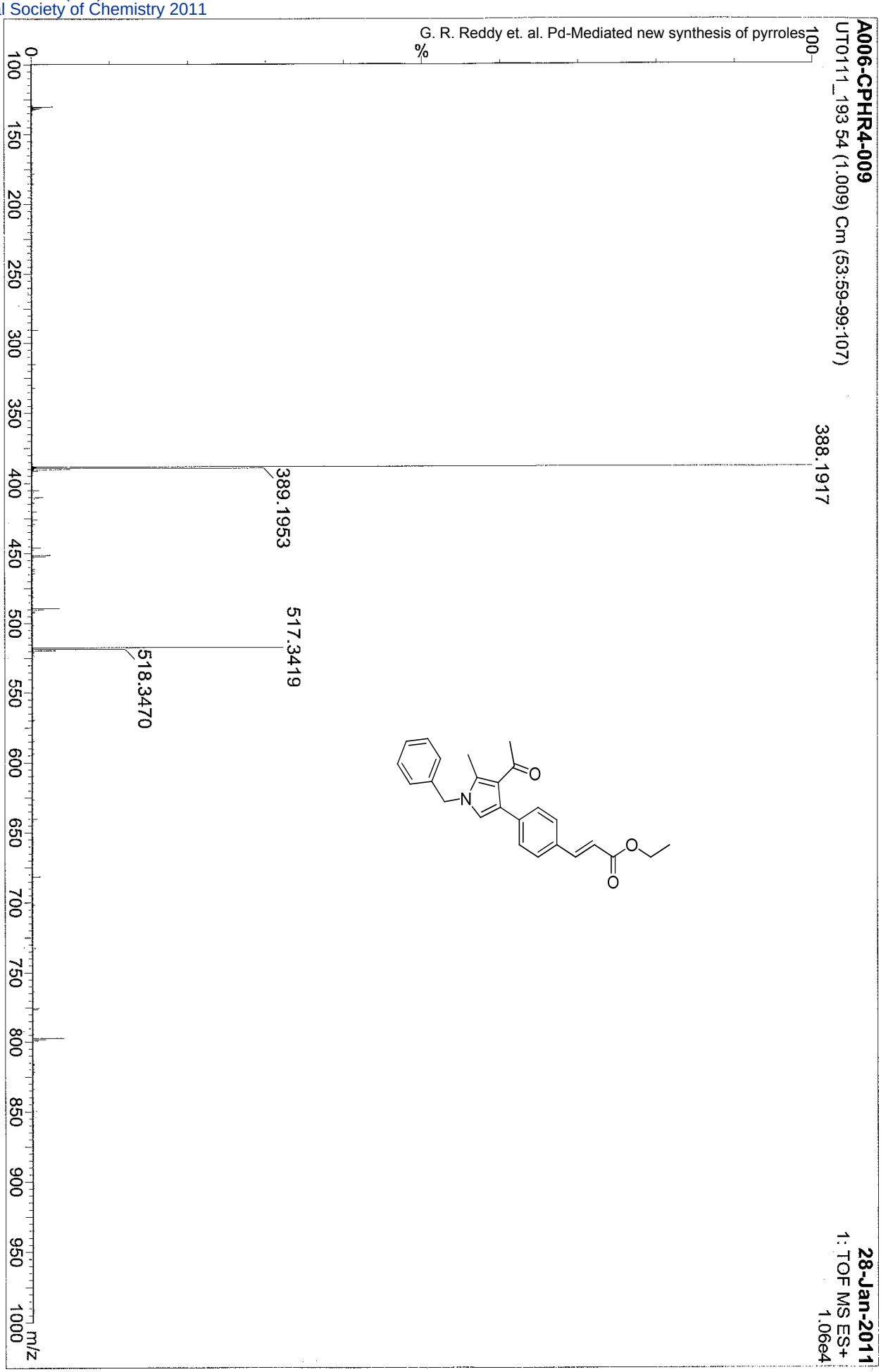


Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
374.1742	374.1756	-1.4	-3.7	13.5	91.2	C24 H24 N O3


A006-CPHR-4-009 in CDCl3
NMR-400
8
7
6
5
4
3
2
1
0
ppm
0.94
5.00
2.12
2.13
0.91
0.94
2.10
2.03
3.07
3.00
3.02


O
N
O
O


A006-CPHR-4-009 in CDCl3
NMR-400
197.335
167.026
148.434
144.187
138.024
138.329
136.335
135.319
132.707
129.529
128.926
127.963
127.879
126.627
126.176
124.992
122.051
120.340
117.728
116.682
77.313
77.000
76.679
60.417
50.350
29.642
14.281
11.485
ppm
200
180
160
140
120
100
80
60
40
20
N
O
O
O

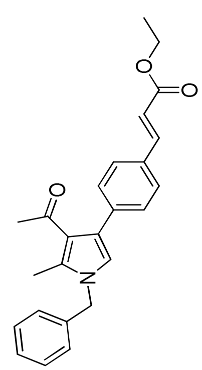


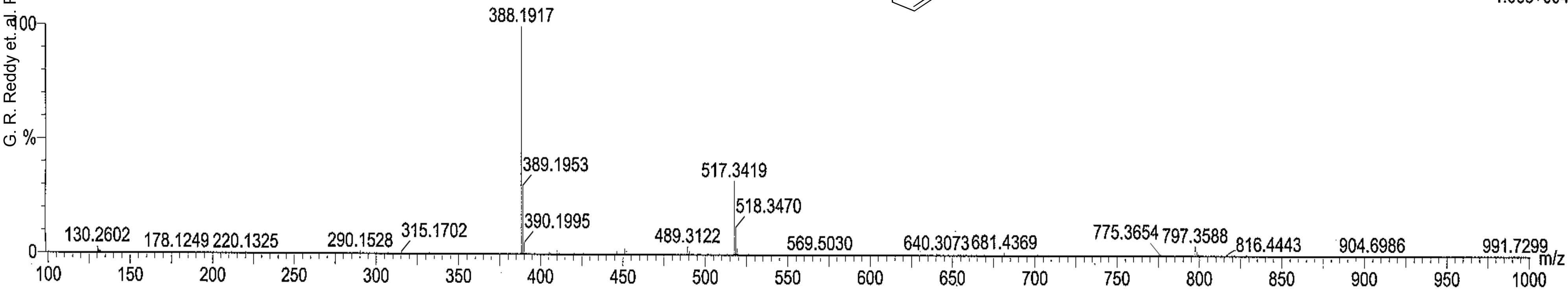
Elemental Composition Report

Single Mass Analysis

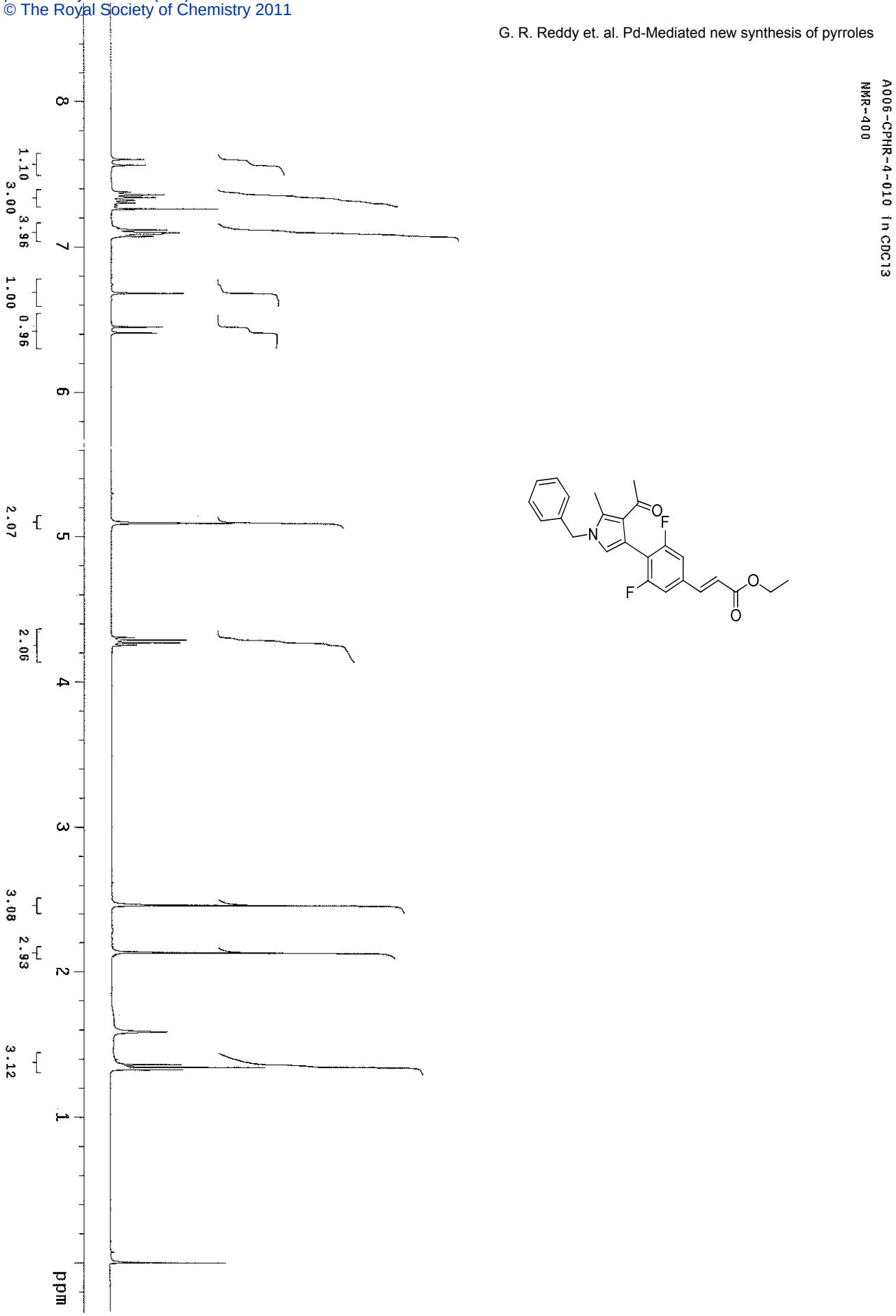
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

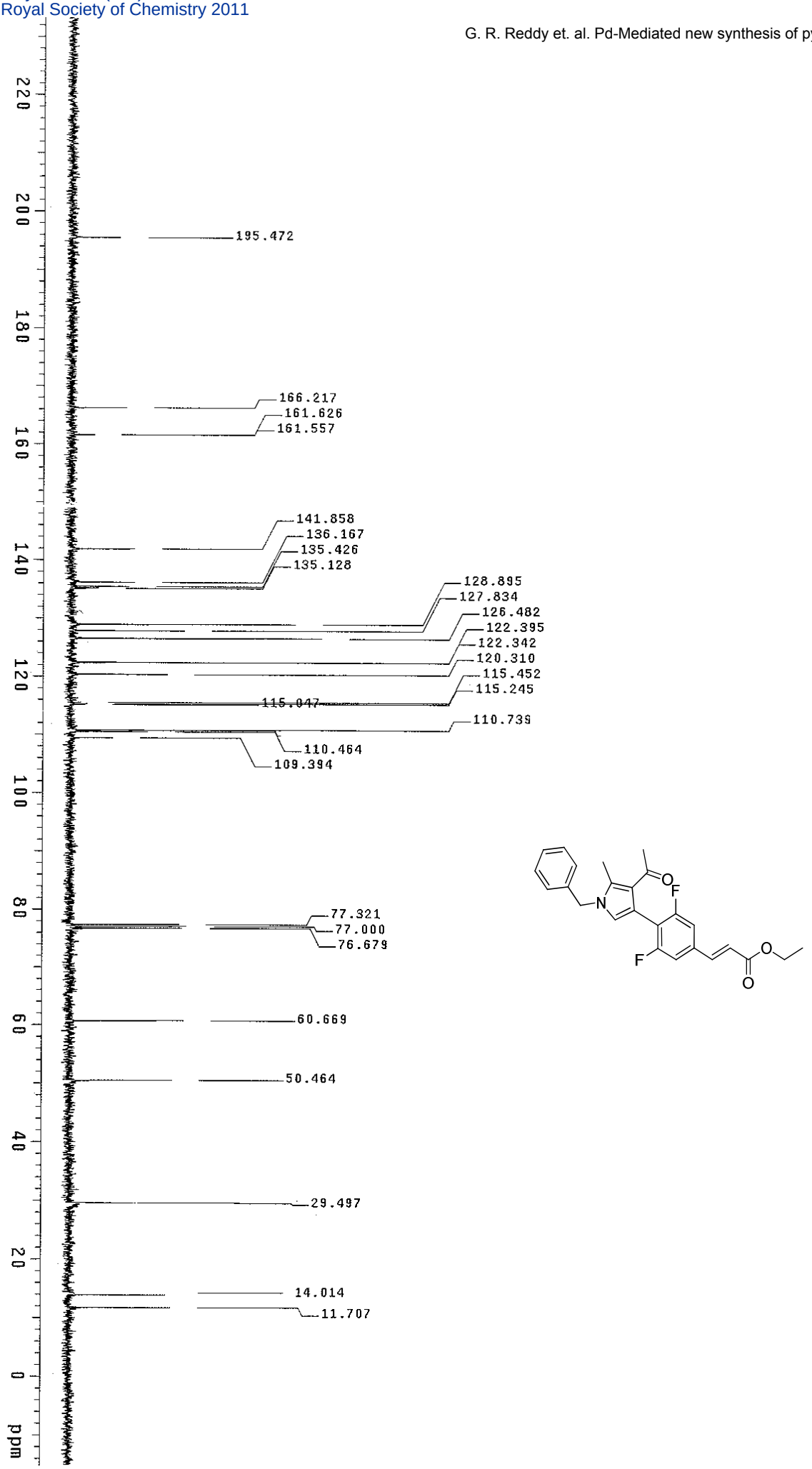
Monoisotopic Mass, Even Electron Ions
133 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-60 N: 0-3 O: 0-6
A006-CPHR4-009
GT0111_193 54 (1.009) Cm (53:59-99:107)

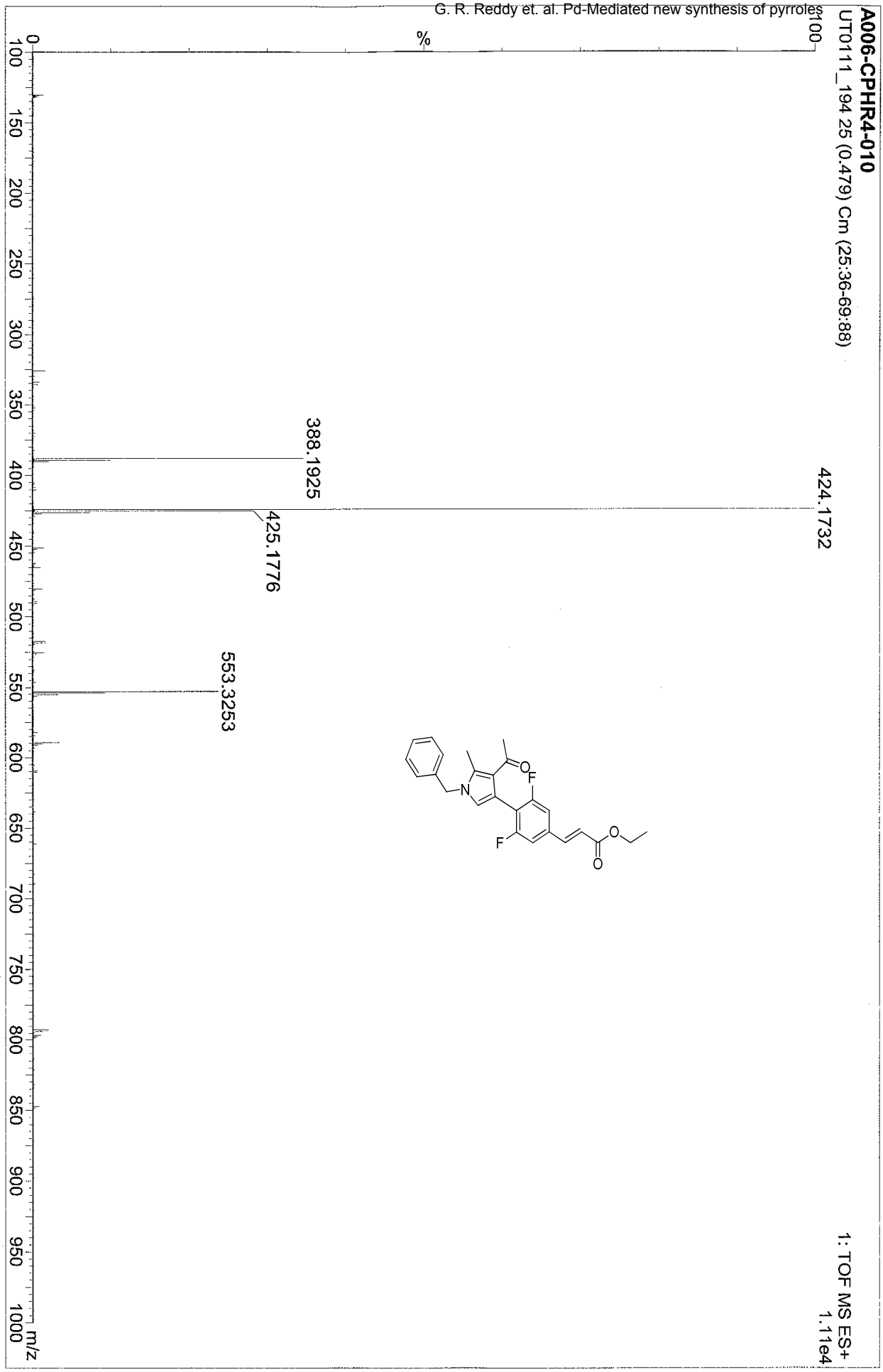




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
388.1917	388.1913	0.4	1.0	13.5	2.7	C25 H26 N O3







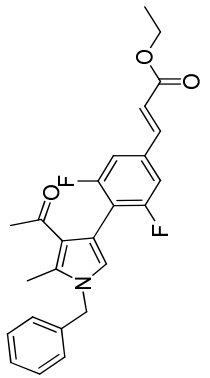
Elemental Composition Report

Single Mass Analysis

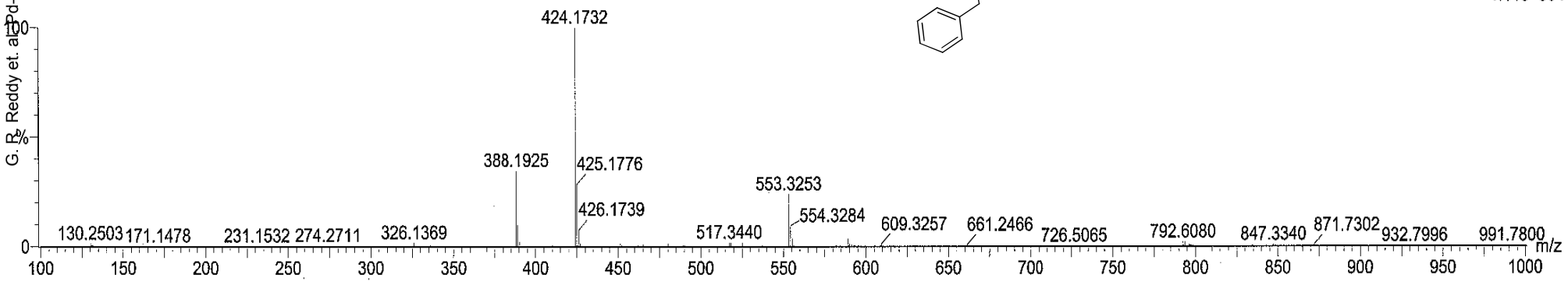
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
451 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-50 N: 0-4 O: 0-6 F: 0-2

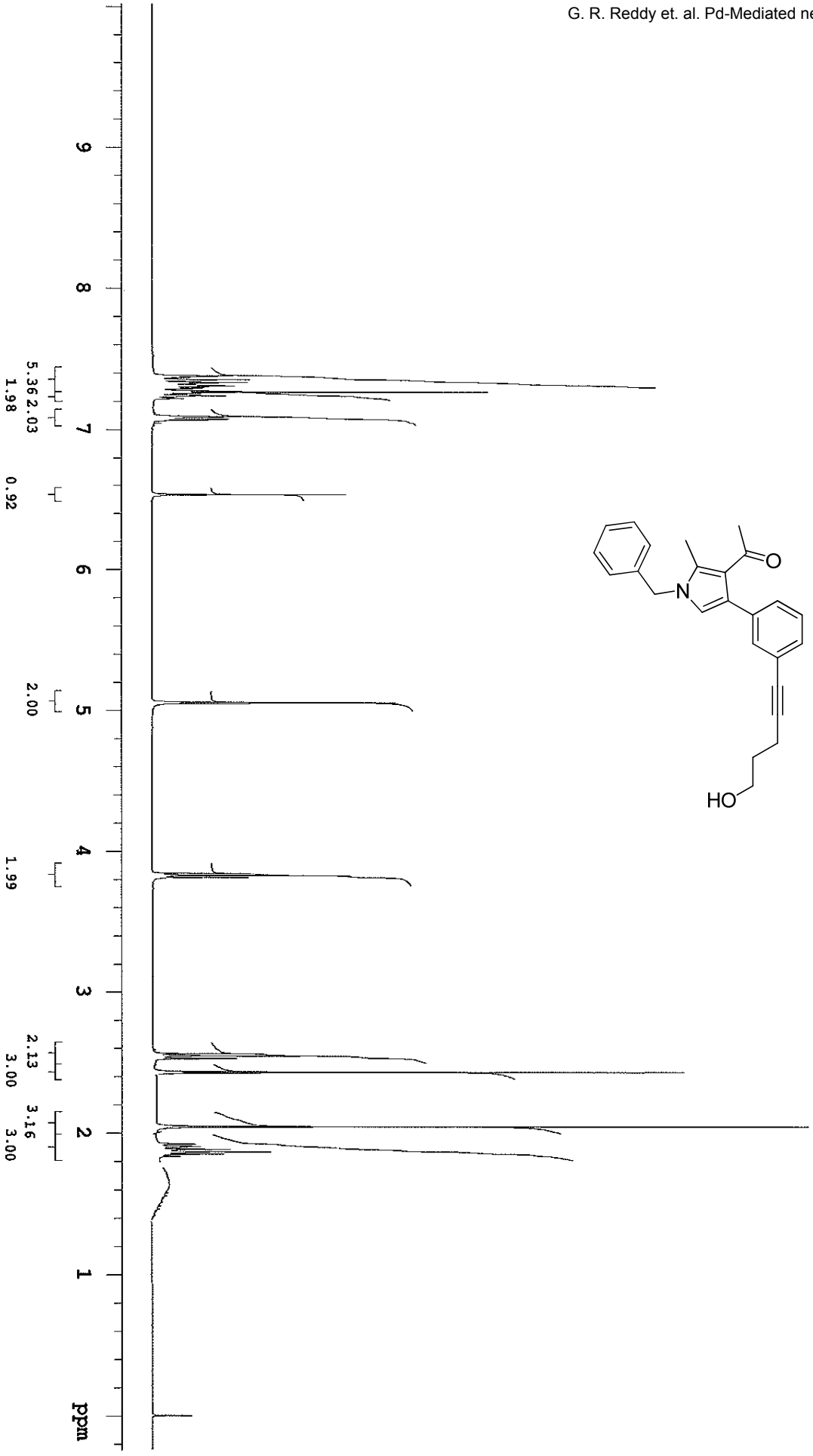
A006-CPHR4-010
U10111_194 25 (0.479) Cm (25:36-69:88)

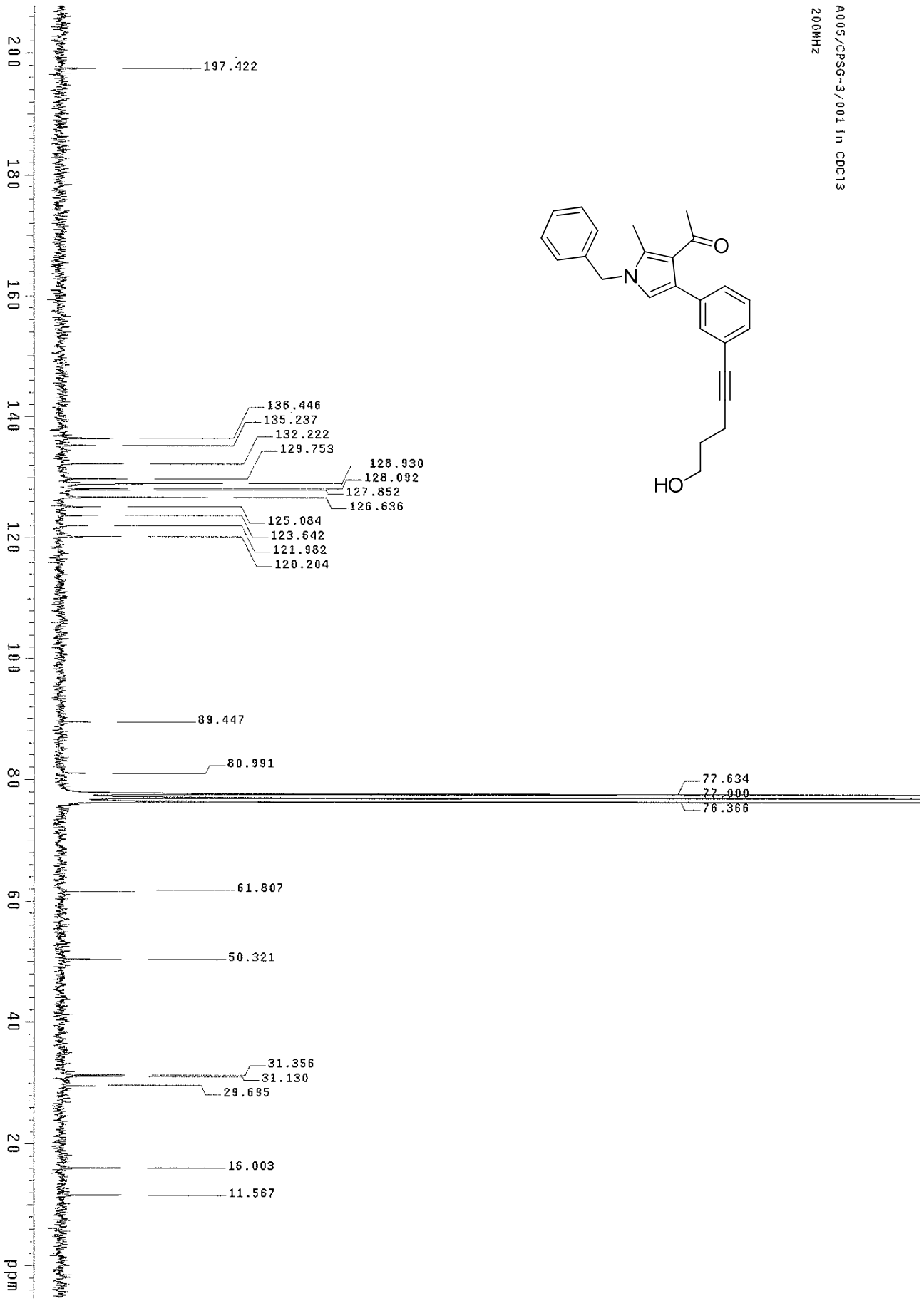


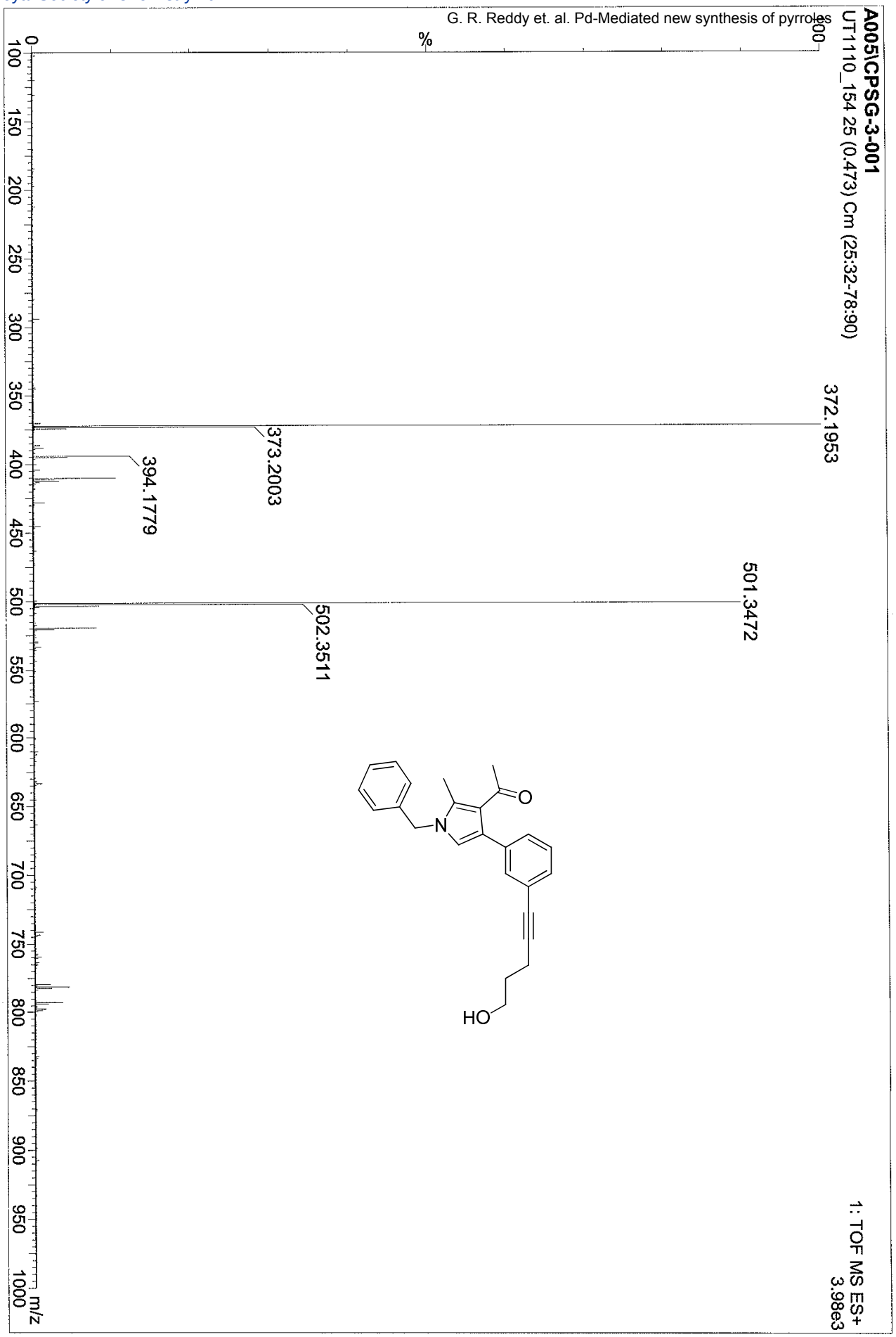
1: TOF MS ES+
1.11e+004



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
424.1732	424.1724	0.8	1.9	13.5	58.1	C25 H24 N O3 F2


A005/CPSQ-3/001 1n CDCl3
NMR-400
9
8
7
6
5
4
3
2
1
ppm
5.36 2.03
1.98
0.92
2.00
1.99
2.13
3.00
3.16
3.00
O
N
HO



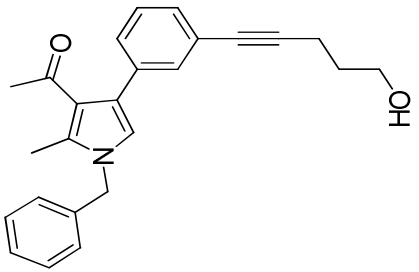

A005\CPSG-3-001
UT1110_154 25 (0.473) Cm (25:32-78:90)
%
100
0
372.1953
373.2003
394.1779
501.3472
502.3511
O
N
HO
1: TOF MS ES+
3.98e3
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z

Elemental Composition Report

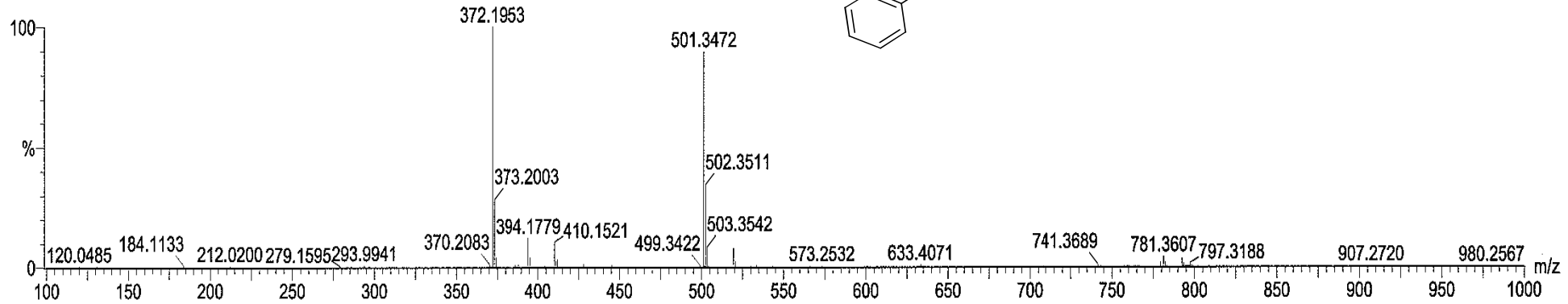
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

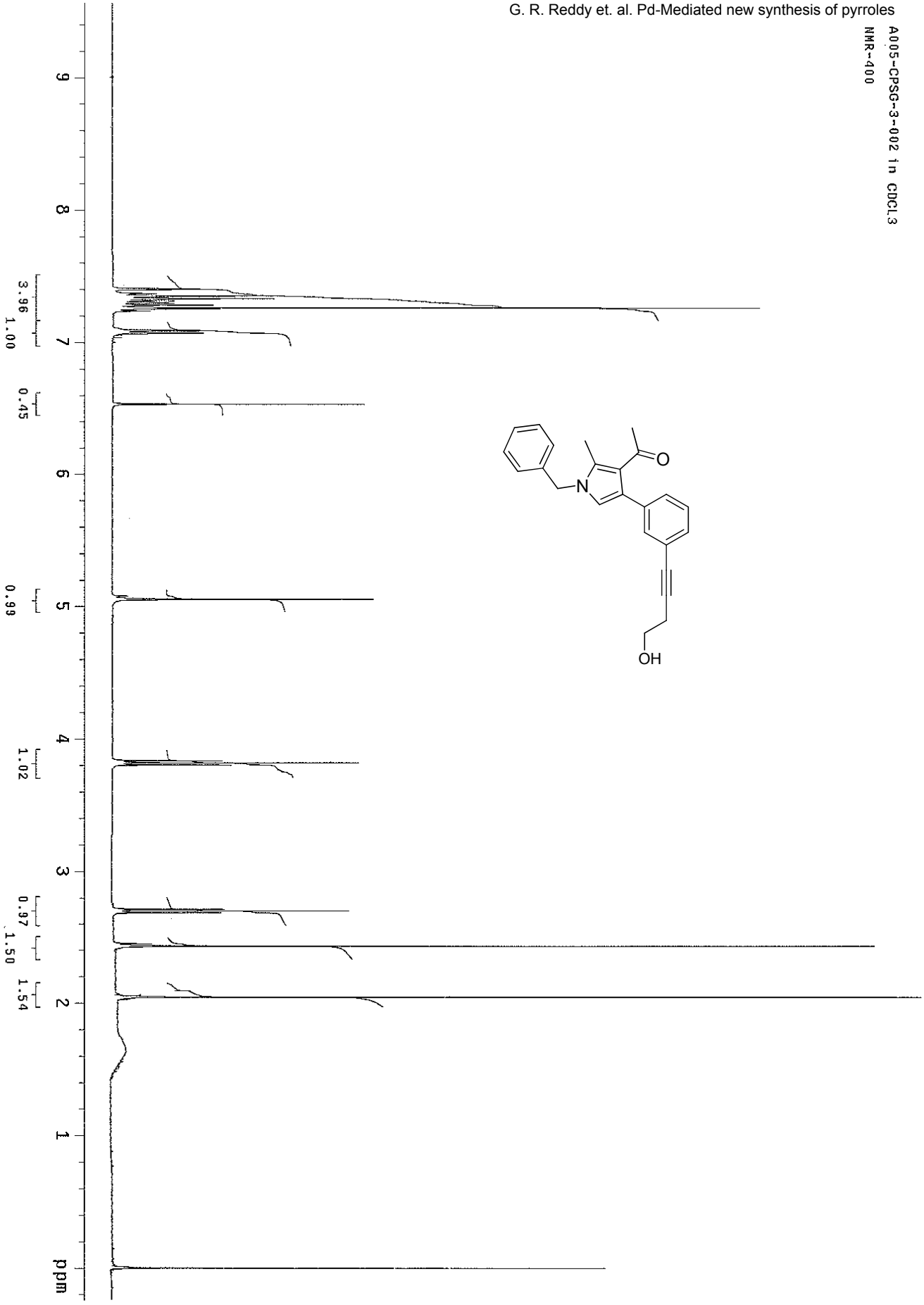
Monoisotopic Mass, Even Electron Ions
87 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-65 N: 0-5 O: 0-2
A005\CPSG-3-001
UT1110_154 25 (0.473) Cm (25:32-78:90)

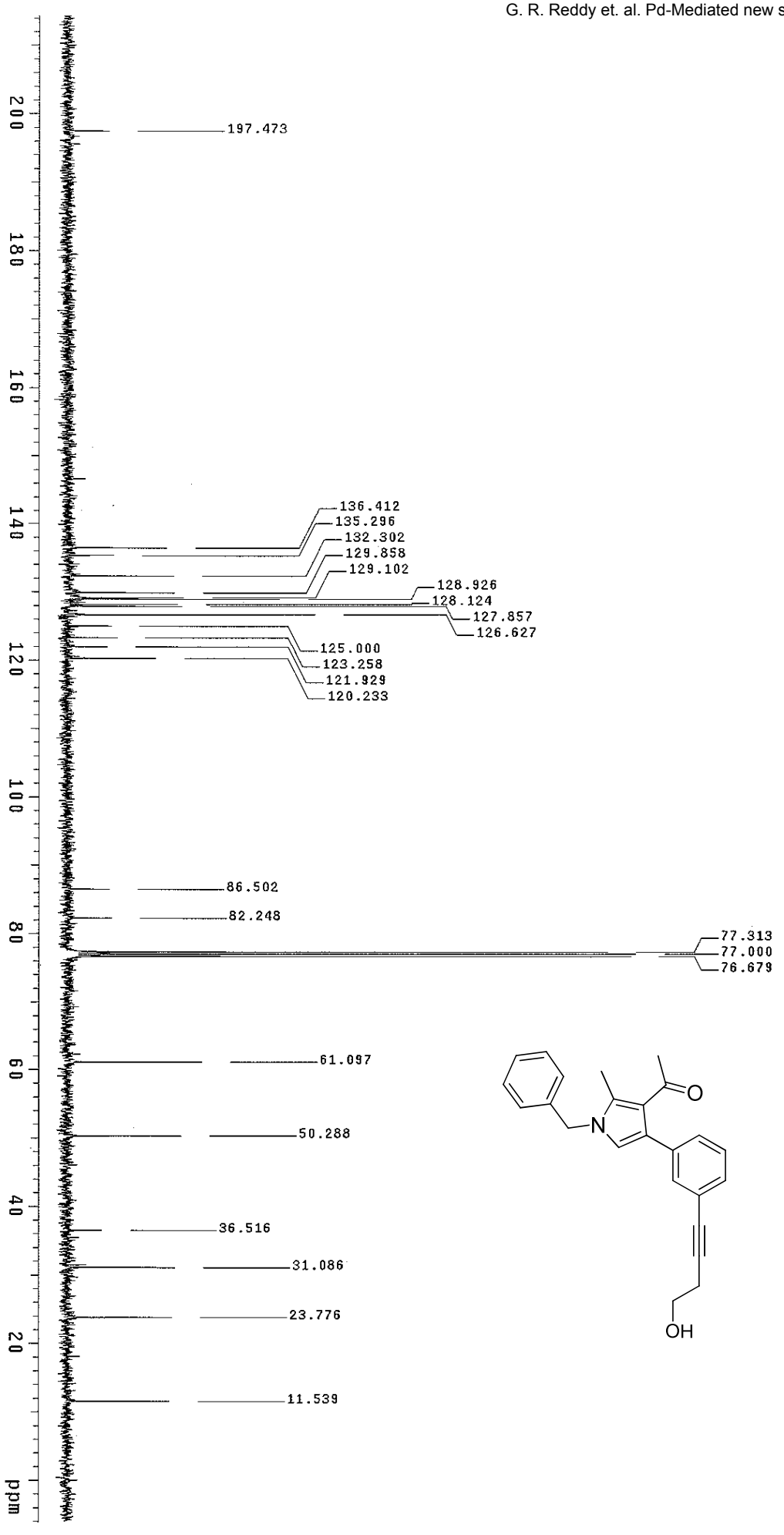


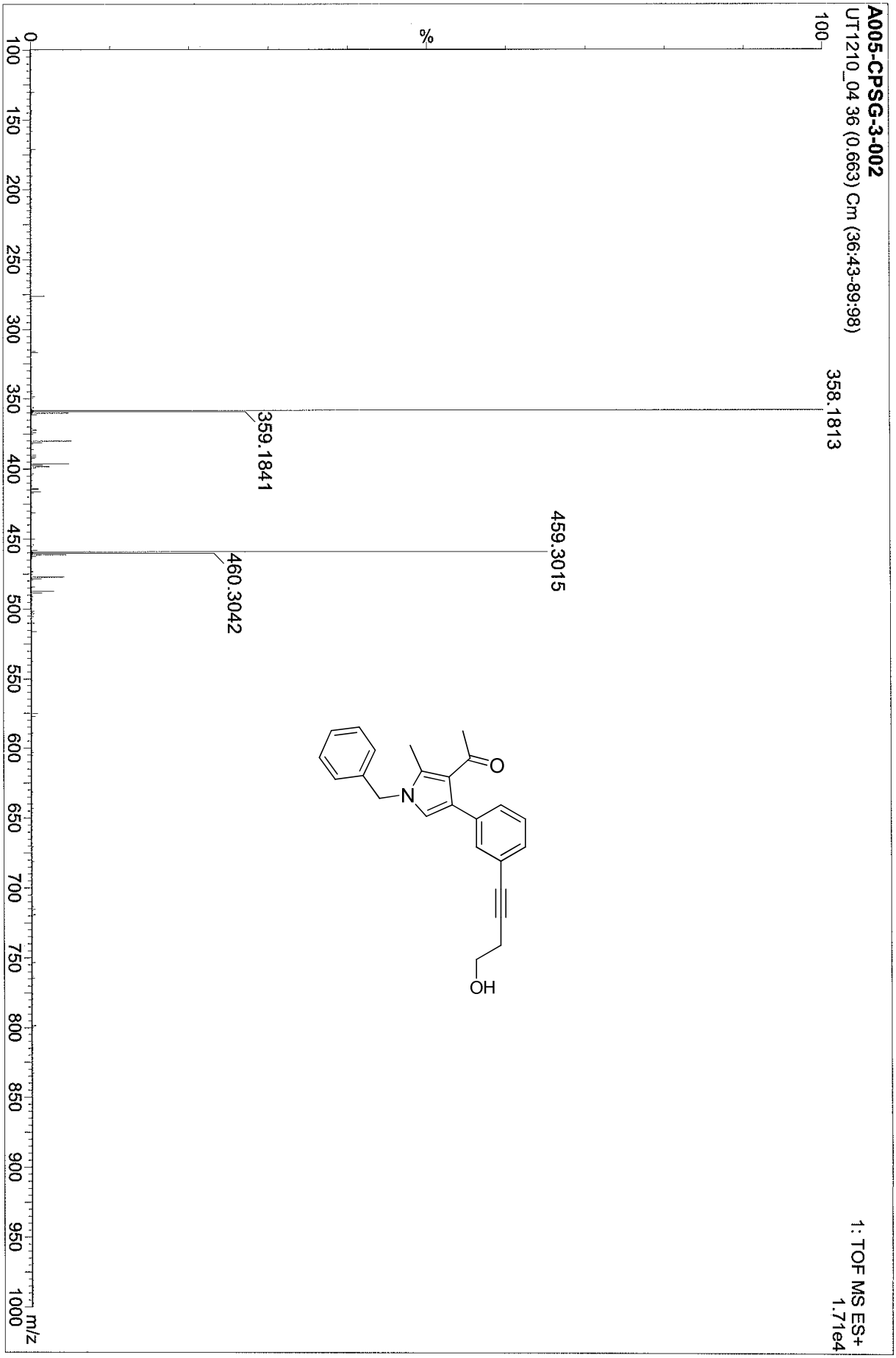
1: TOF MS ES+
3.98e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.1953	372.1964	-1.1	-3.0	13.5	0.3	C25 H26 N O2


A005-CPSG-3-002 in CDCl3
NMR-400
9
8
7
6
5
4
3
2
1
ppm
3.96
1.00
0.45
0.99
1.02
0.97
1.50
1.54
N
O
OH


A005/CPSG-3/002 in CDC13
NMR-400
197.473
136.412
135.296
132.302
129.858
129.102
128.926
128.124
127.857
126.627
125.000
123.258
121.929
120.233
86.502
82.248
77.313
77.000
76.679
61.097
50.288
36.516
31.086
23.776
11.539
ppm
200
180
160
140
120
100
80
60
40
20
O
N
OH

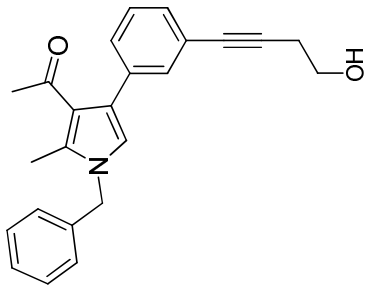

A005-CPSG-3-002
UT1210_04 36 (0.663) Cm (36:43-89:98)
%
100
0
358.1813
359.1841
459.3015
460.3042
O
N
OH
1: TOF MS ES+
1.71e4
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z

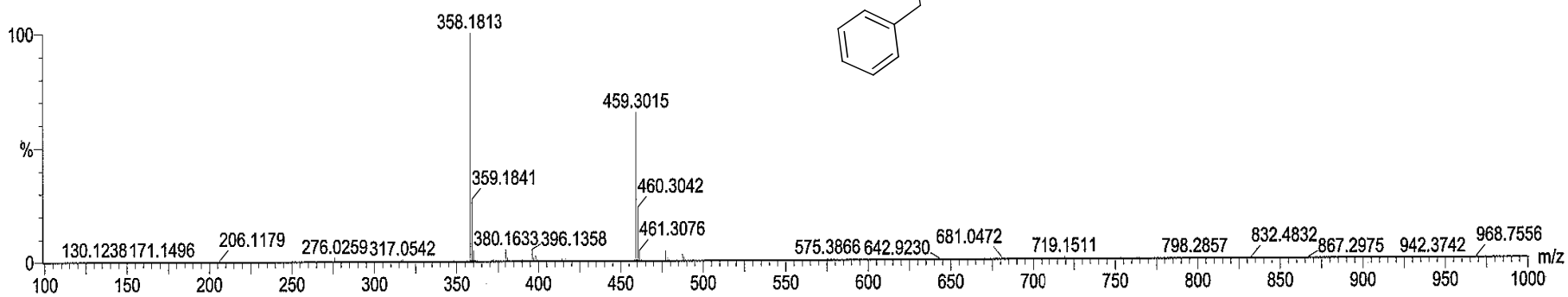
Elemental Composition Report

Single Mass Analysis

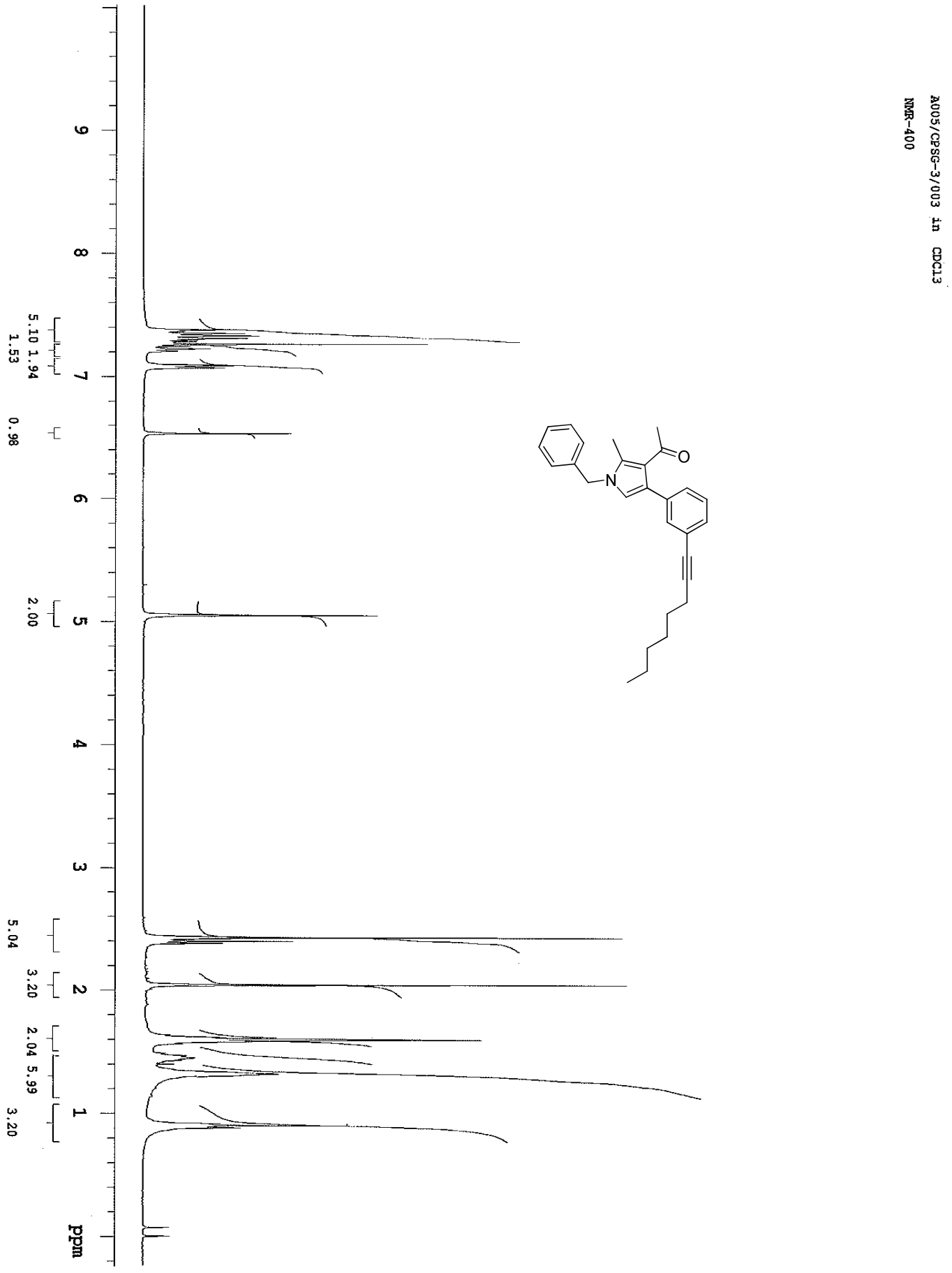
Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

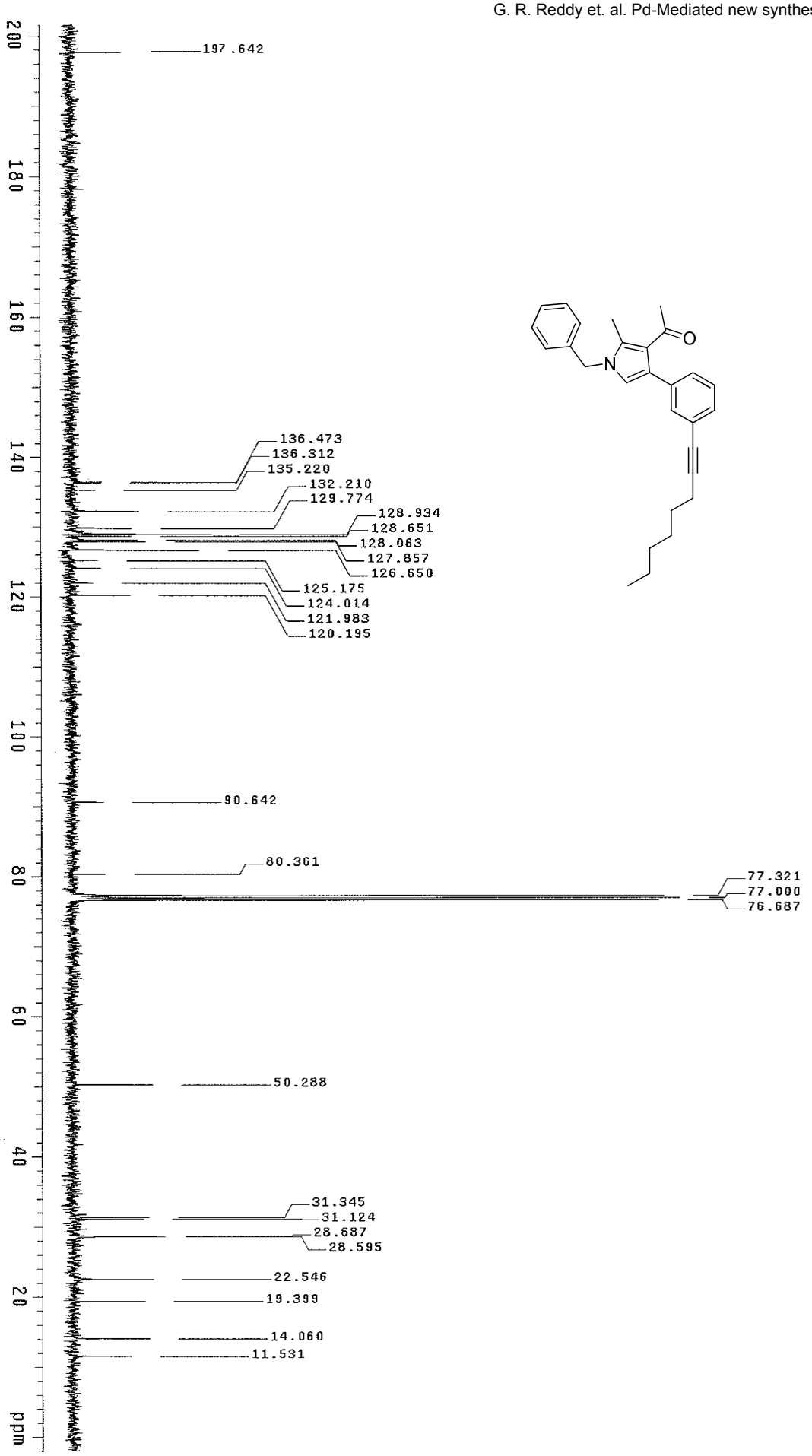
Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-3 O: 0-4
A005-CPSG-3-002
UT1210_04 36 (0.663) Cm (36:43-89:98)

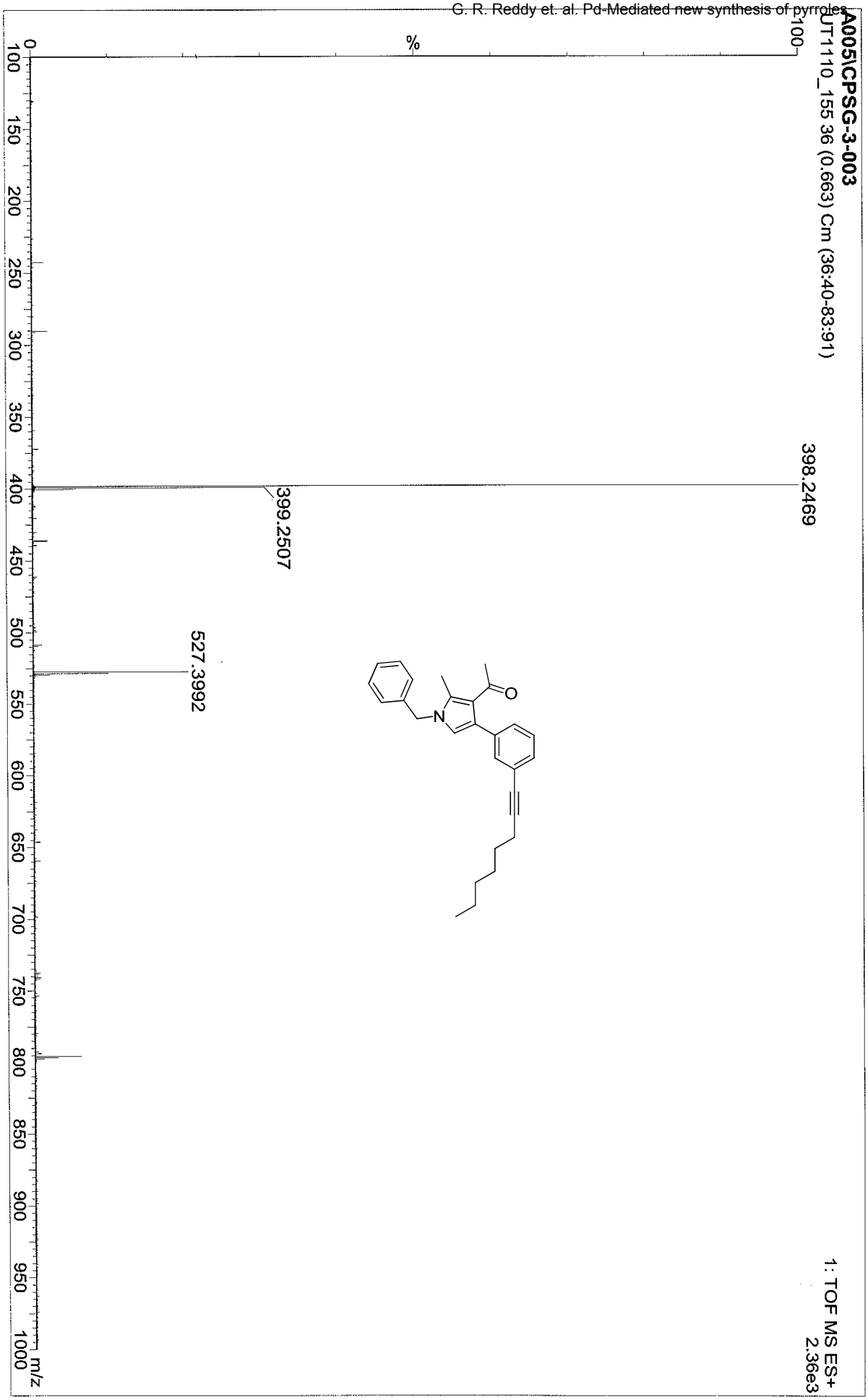




Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.1813	358.1807	0.6	1.7	13.5	10.4	C24 H24 N O2


A005/CPSG-3/003 in CDCl3
NMR-400
O
N
9
8
7
6
5
4
3
2
1
ppm
5.10 1.94
1.53
0.98
2.00
5.04
3.20
2.04 5.99
3.20


A005/CPSG-3/003 in CDC13
NMR-400
197.642
136.473
136.312
135.220
132.210
129.774
128.934
128.651
128.063
127.857
126.650
125.175
124.014
121.983
120.195
90.642
80.361
77.321
77.000
76.687
50.288
31.345
31.124
28.687
28.595
22.546
19.399
14.060
11.531
O
N
200
180
160
140
120
100
80
60
40
20
ppm


A005\CPSG-3-003
UT1110_155 36 (0.663) Cm (36:40-83:91)
%
100
0
398.2469
399.2507
527.3992
O
N
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z
1: TOF MS ES+
2.36e3

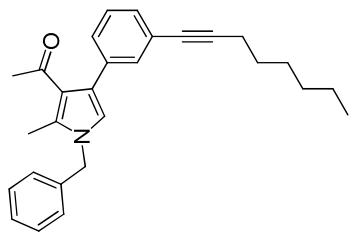
Elemental Composition Report

Single Mass Analysis

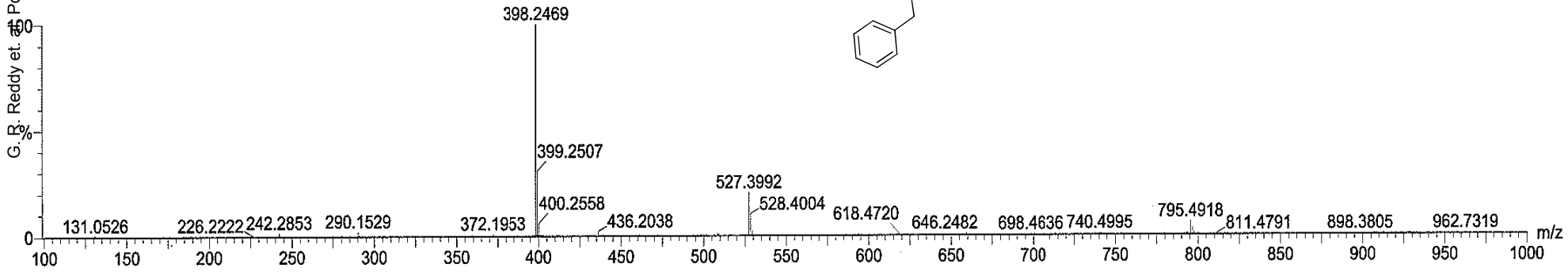
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
91 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-65 N: 0-5 O: 0-2

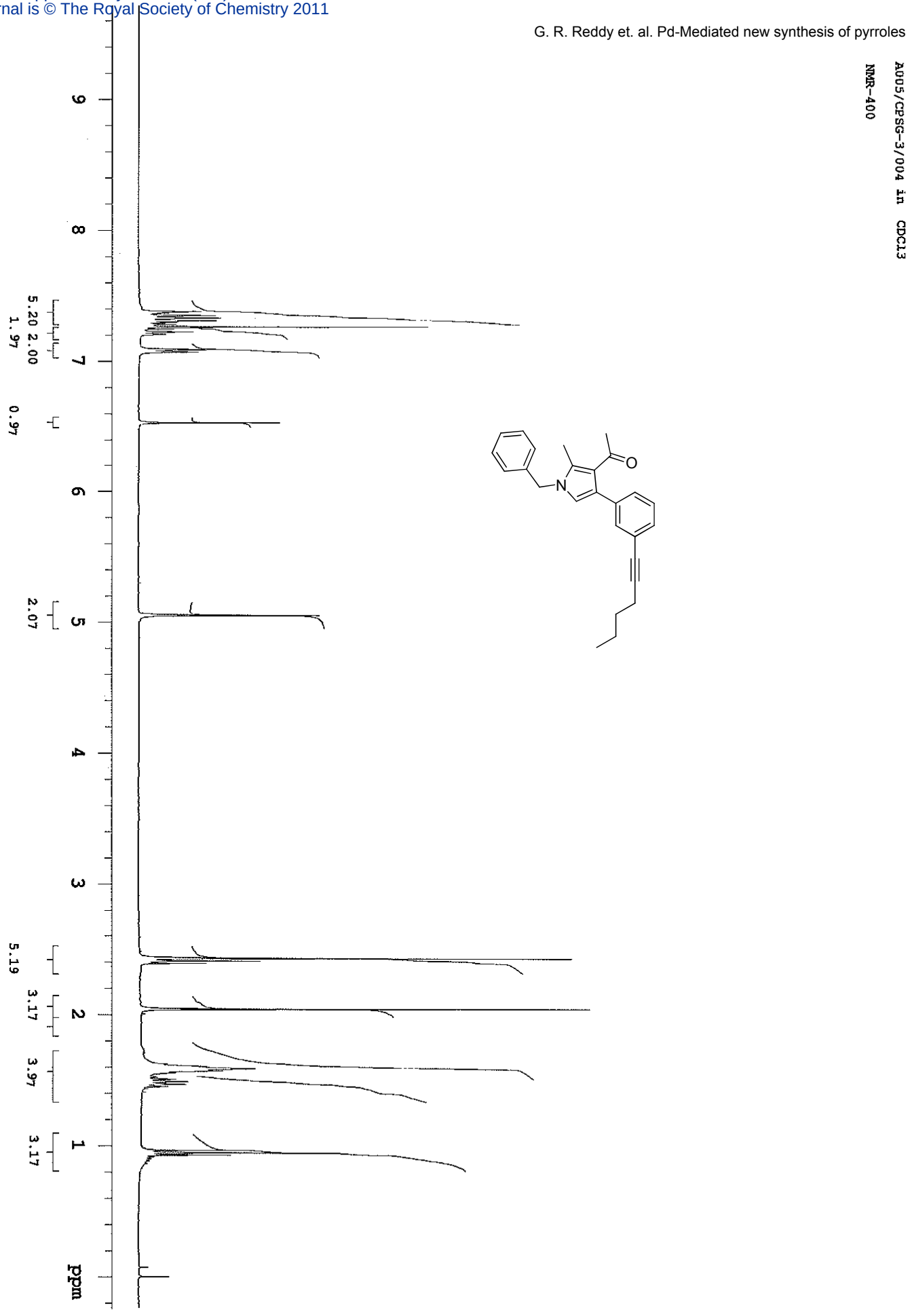
A005\CPSG-3-003
UT1110_155 36 (0.663) Cm (36:40-83:91)

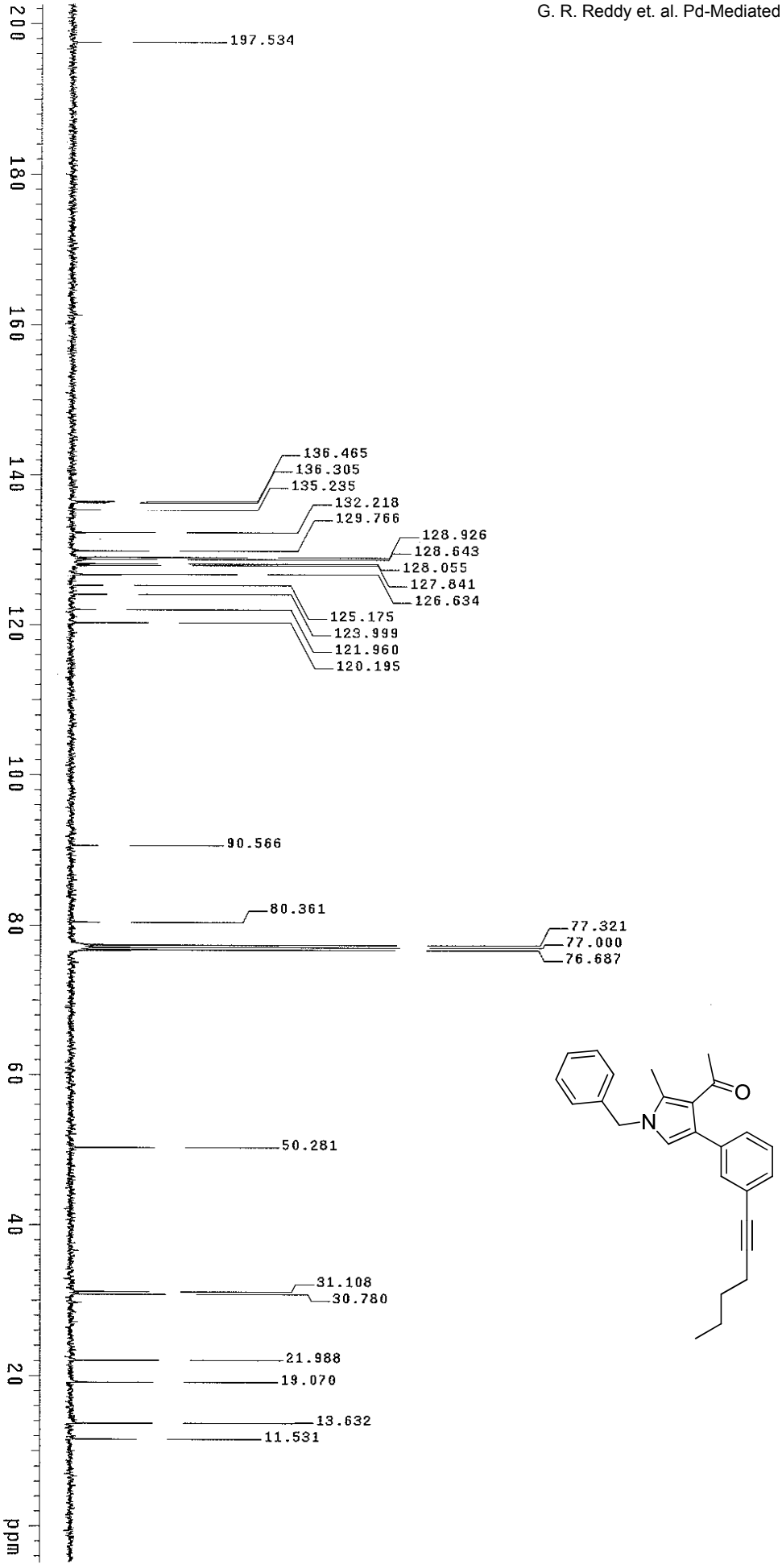


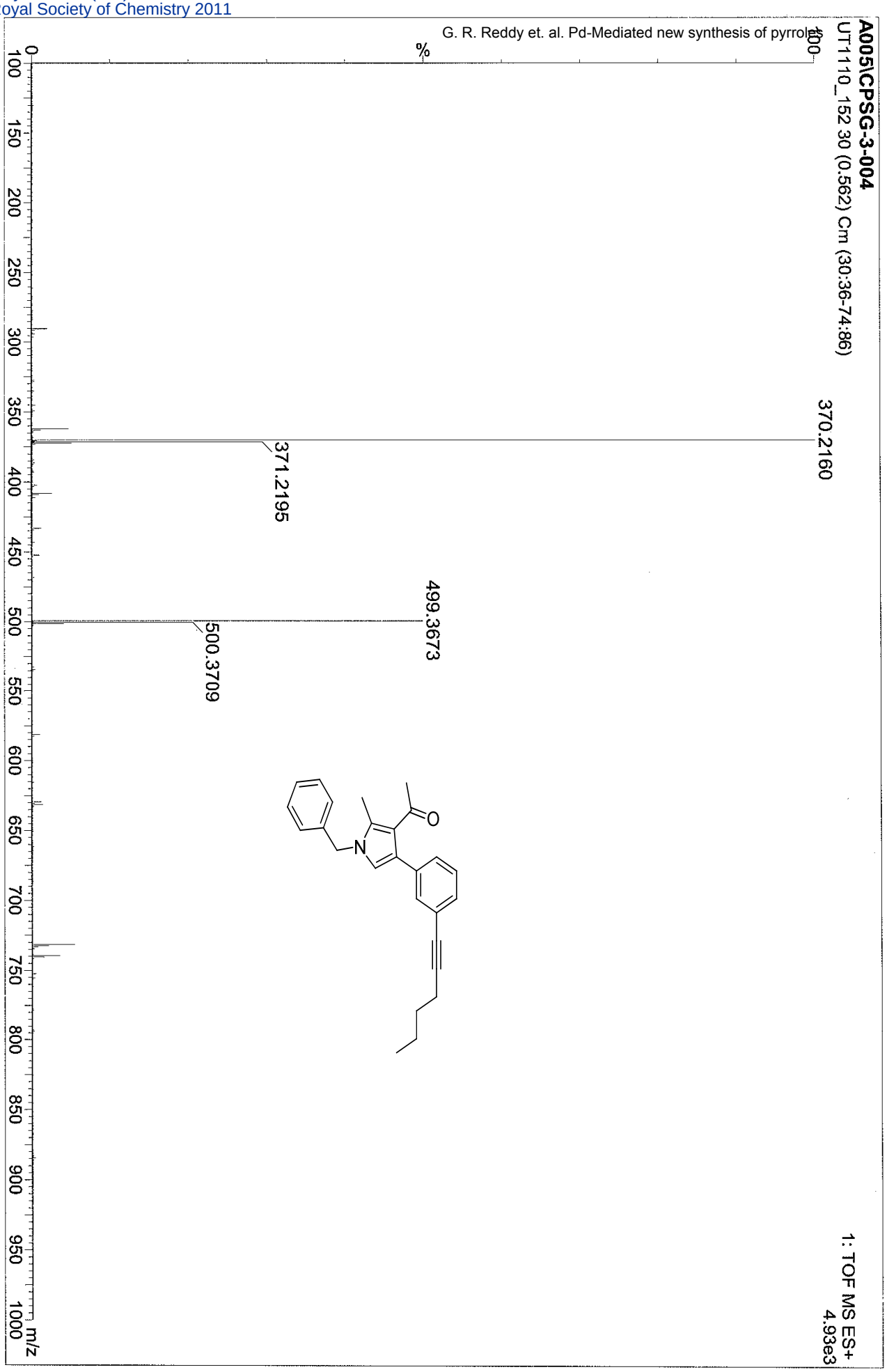
1: TOF MS ES+
2.36e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
398.2469	398.2484	-1.5	-3.8	13.5	0.9	C28 H32 N O


A005/CPSG-3/004 in CDCl3
NMR-400
9
8
7
6
5
4
3
2
1
ppm
5.20 2.00
1.97
0.97
2.07
5.19
3.17
3.97
3.17
N
O


A005/CPSG-3/004 in CDC13
NMR-400
197.534
136.465
136.305
135.235
132.218
129.766
128.926
128.643
128.055
127.841
126.634
125.175
123.999
121.960
120.195
90.566
80.361
77.321
77.000
76.687
50.281
31.108
30.780
21.988
19.070
13.632
11.531
200
180
160
140
120
100
80
60
40
20
ppm
N
O

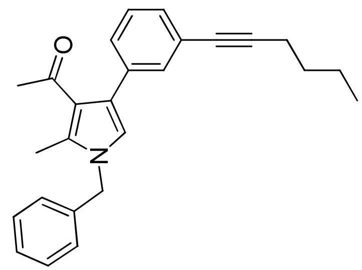


Elemental Composition Report

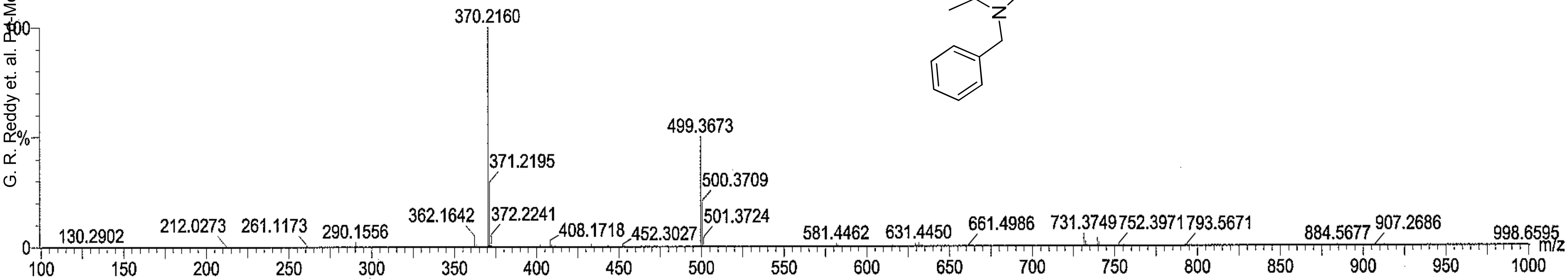
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

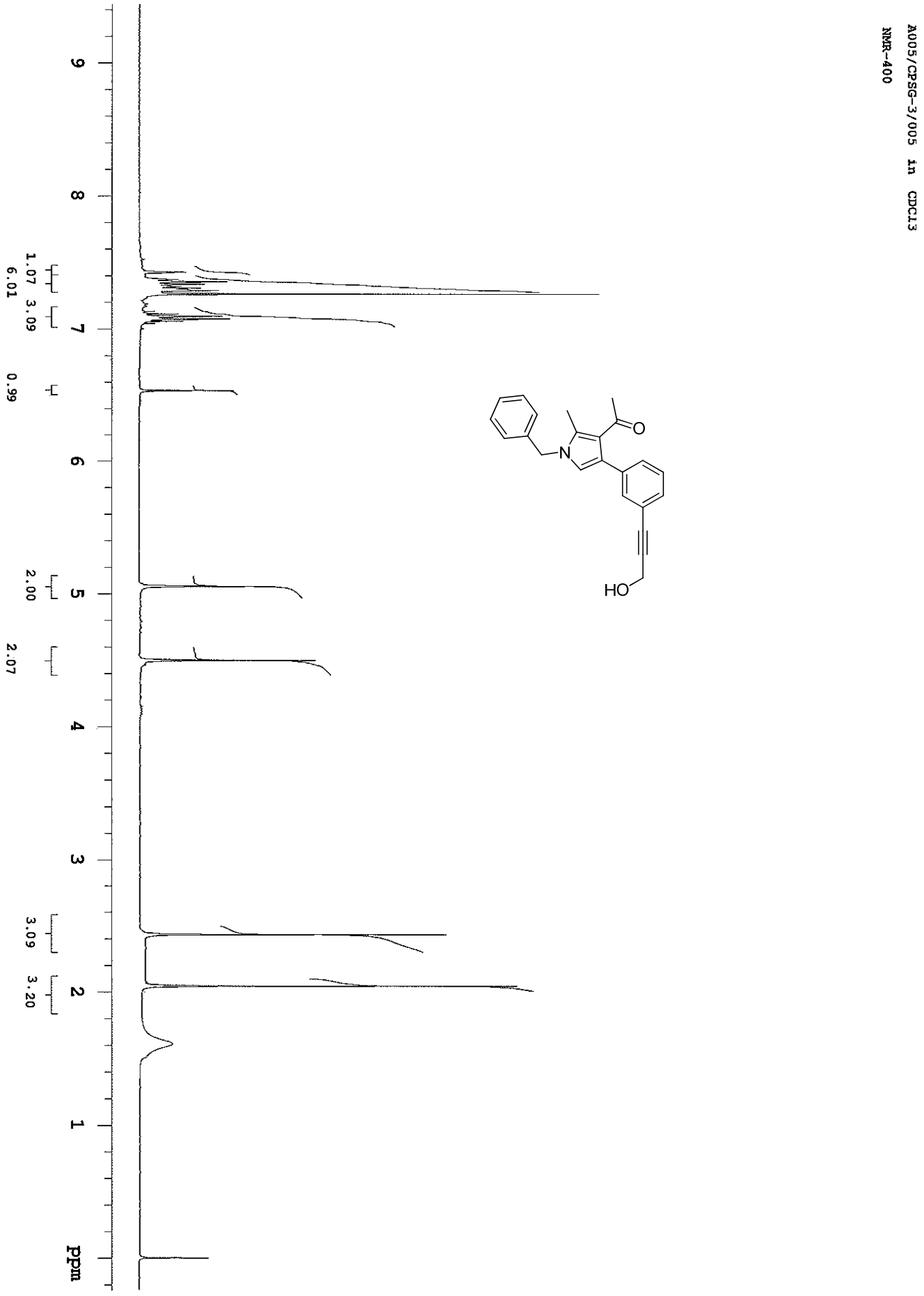
Monoisotopic Mass, Even Electron Ions
85 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-65 N: 0-5 O: 0-2
A005\CPSG-3-004
GT1110_152 30 (0.562) Cm (30:36-74:86)

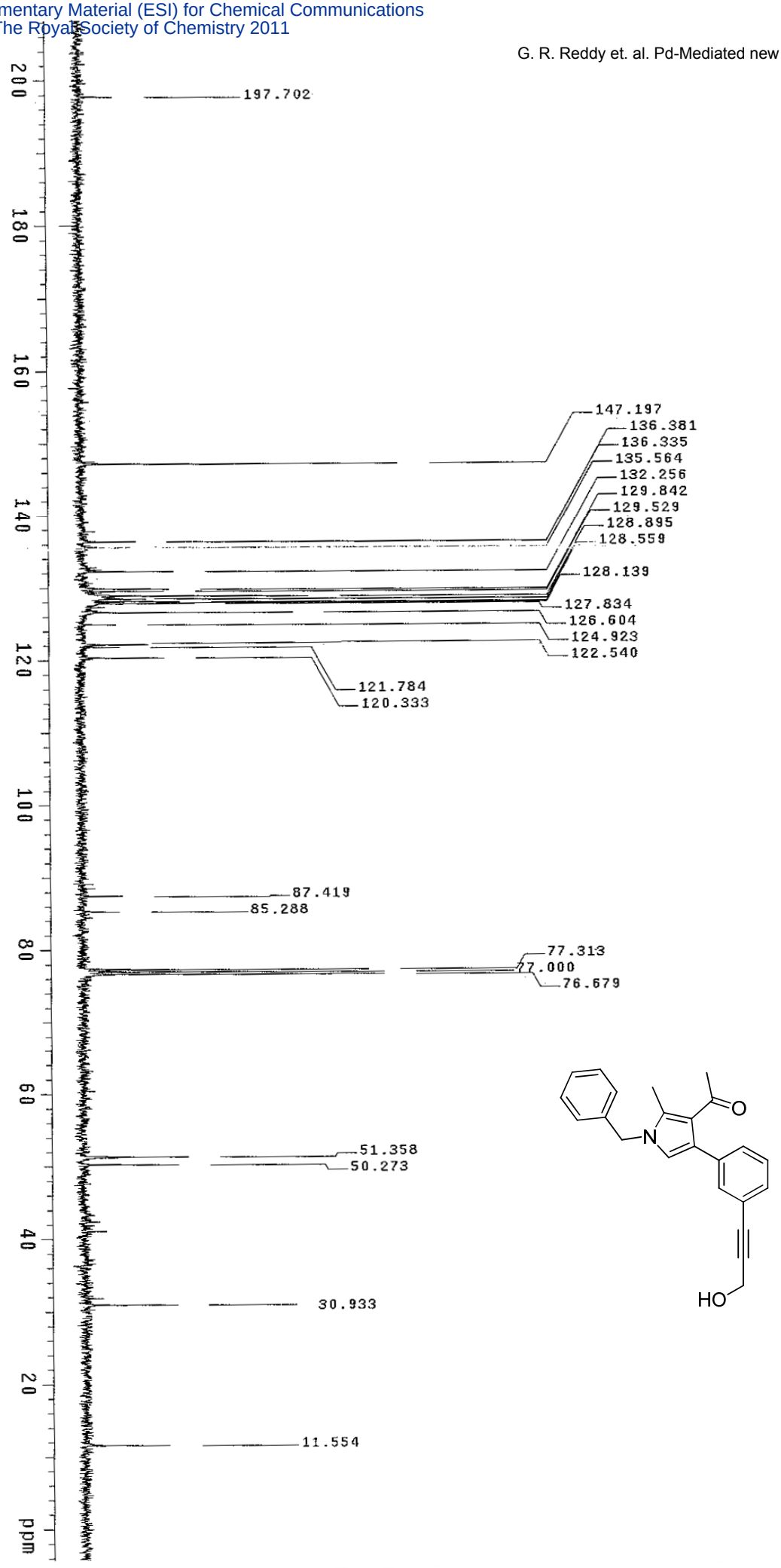


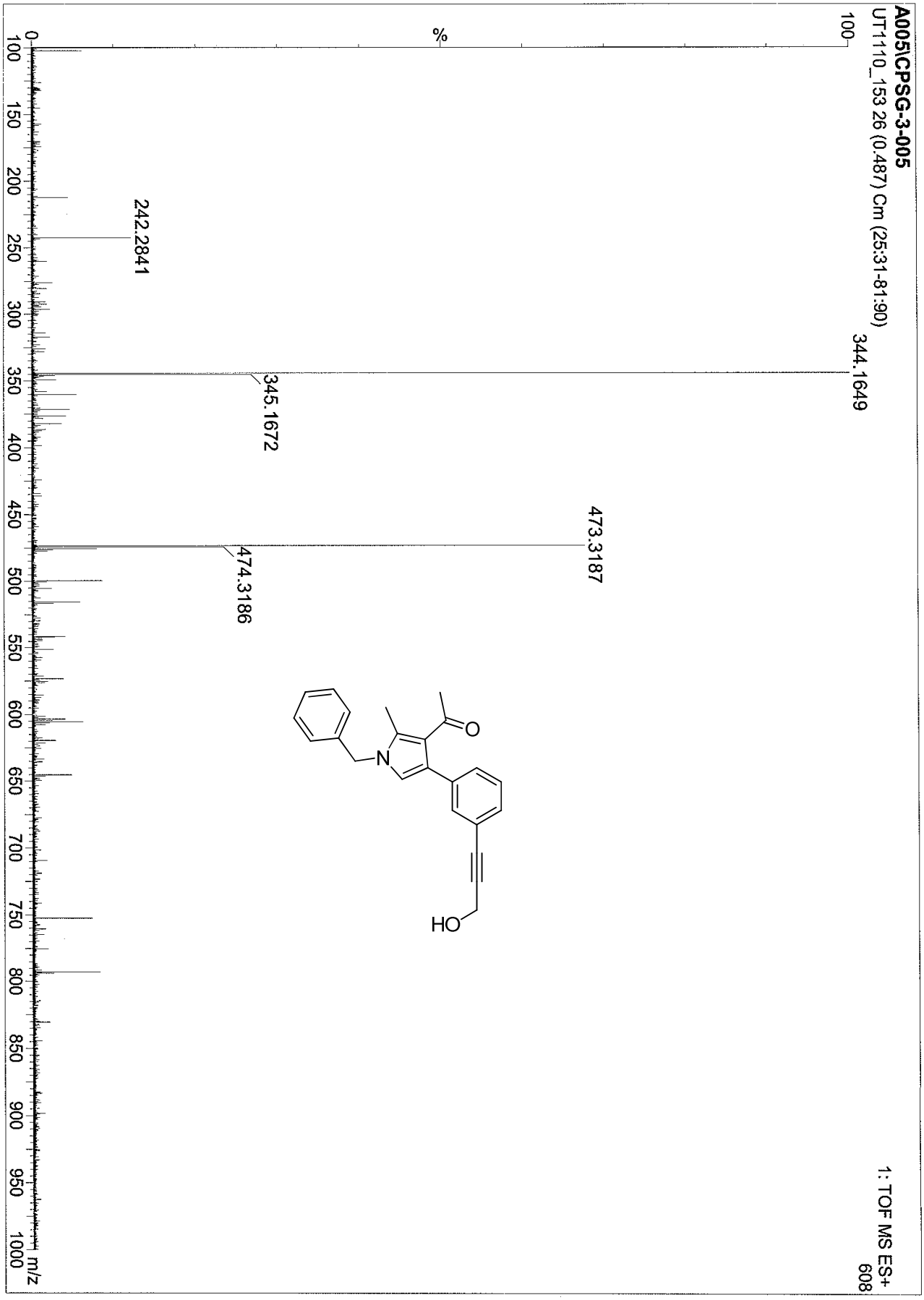
1: TOF MS ES+
4.93e+003



Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
370.2160	370.2171	-1.1	-3.0	13.5	0.2	C26 H28 N O


A005/CPSG-3/005 1n CDCL3
NMR-400
9
8
7
6
5
4
3
2
1
ppm
1.07
3.09
6.01
0.99
2.00
2.07
3.09
3.20
O
N
HO


A005-CPSG3-005 in CDCl3
NMR-400
197.702
147.197
136.381
136.335
135.564
132.256
129.842
129.529
128.895
128.559
128.139
127.834
126.604
124.923
122.540
121.784
120.333
87.419
85.288
77.313
77.000
76.679
51.358
50.273
30.933
11.554
ppm
200
180
160
140
120
100
80
60
40
20
O
N
HO


A005\CPSG-3-005
UT1110_153 26 (0.487) Cm (25:31-81:90)
1: TOF MS ES+
608
%
100
0
242.2841
345.1672
344.1649
473.3187
474.3186
O
N
HO
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z

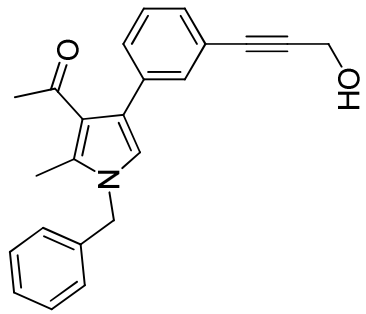
Elemental Composition Report

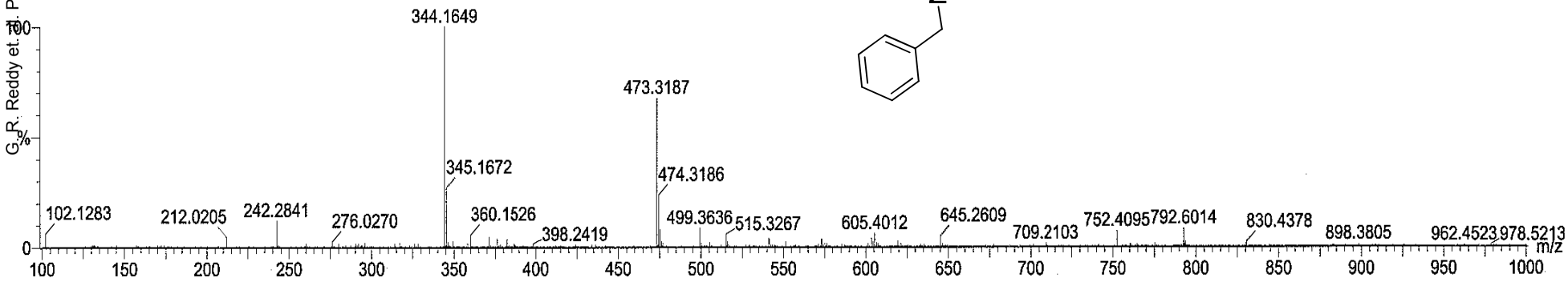
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

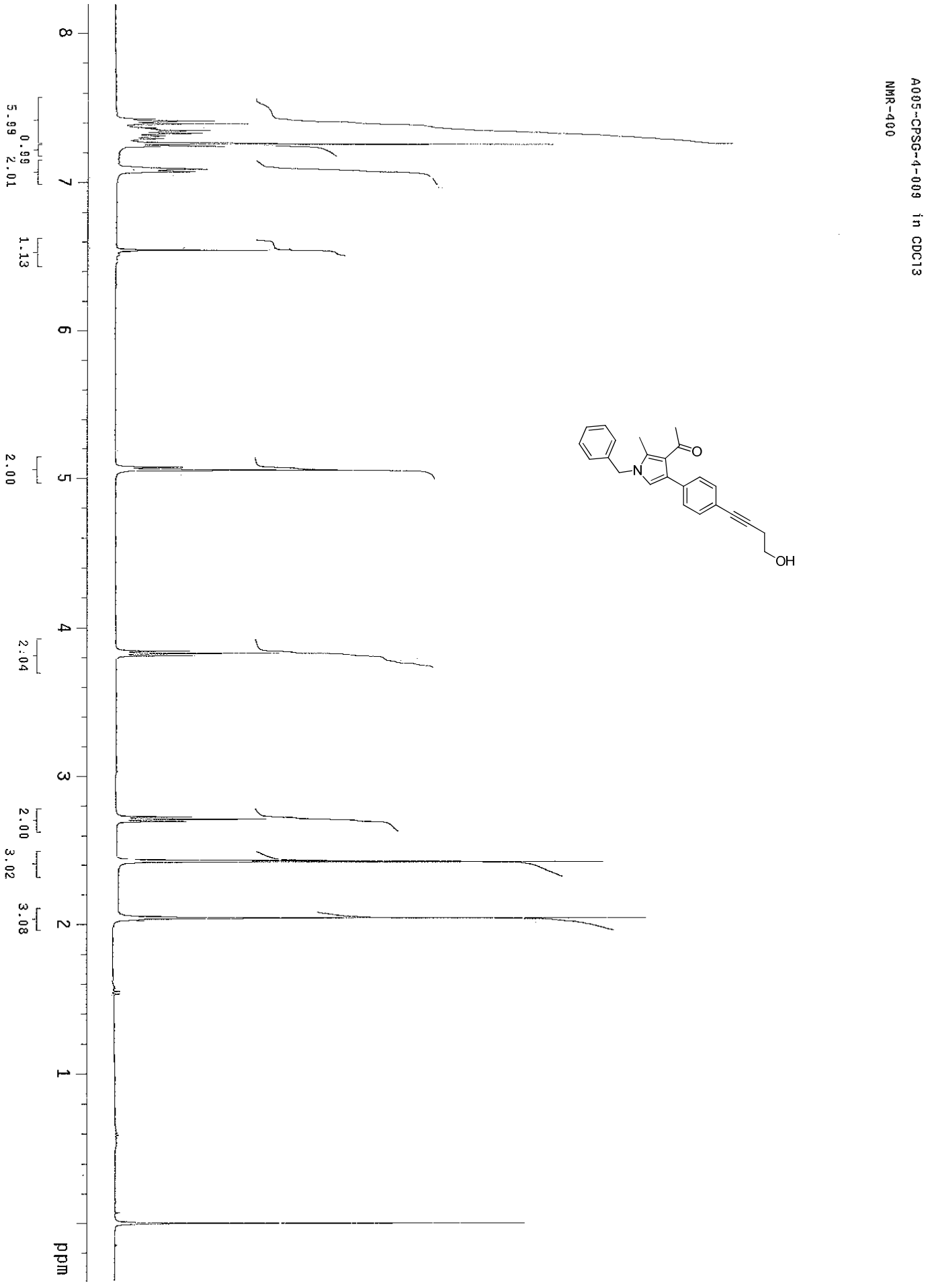
Monoisotopic Mass, Even Electron Ions
84 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-65 N: 0-5 O: 0-2

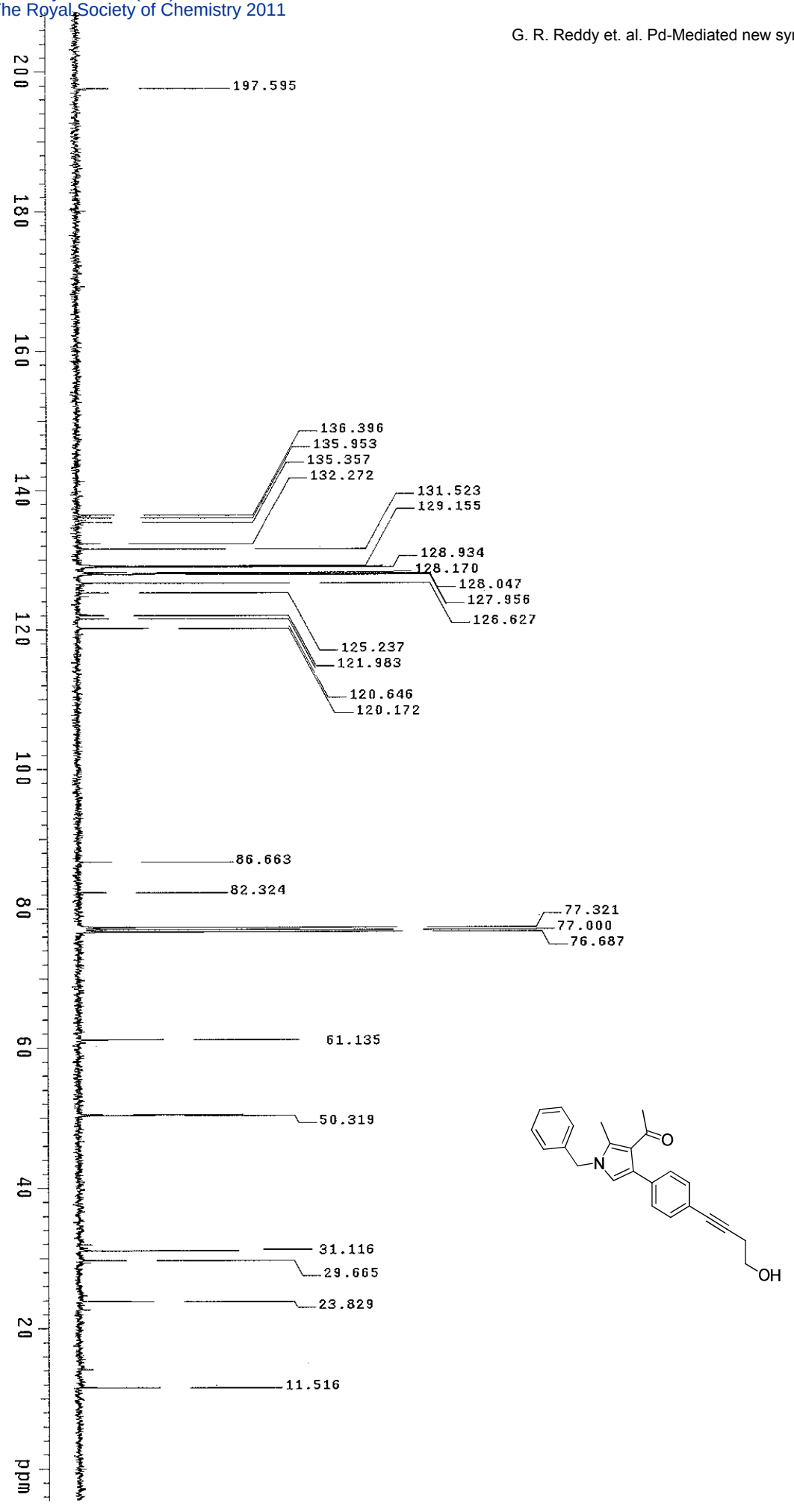
A005\CPSG-3-005
071110_153 26 (0.487) Cm (25:31-81:90)

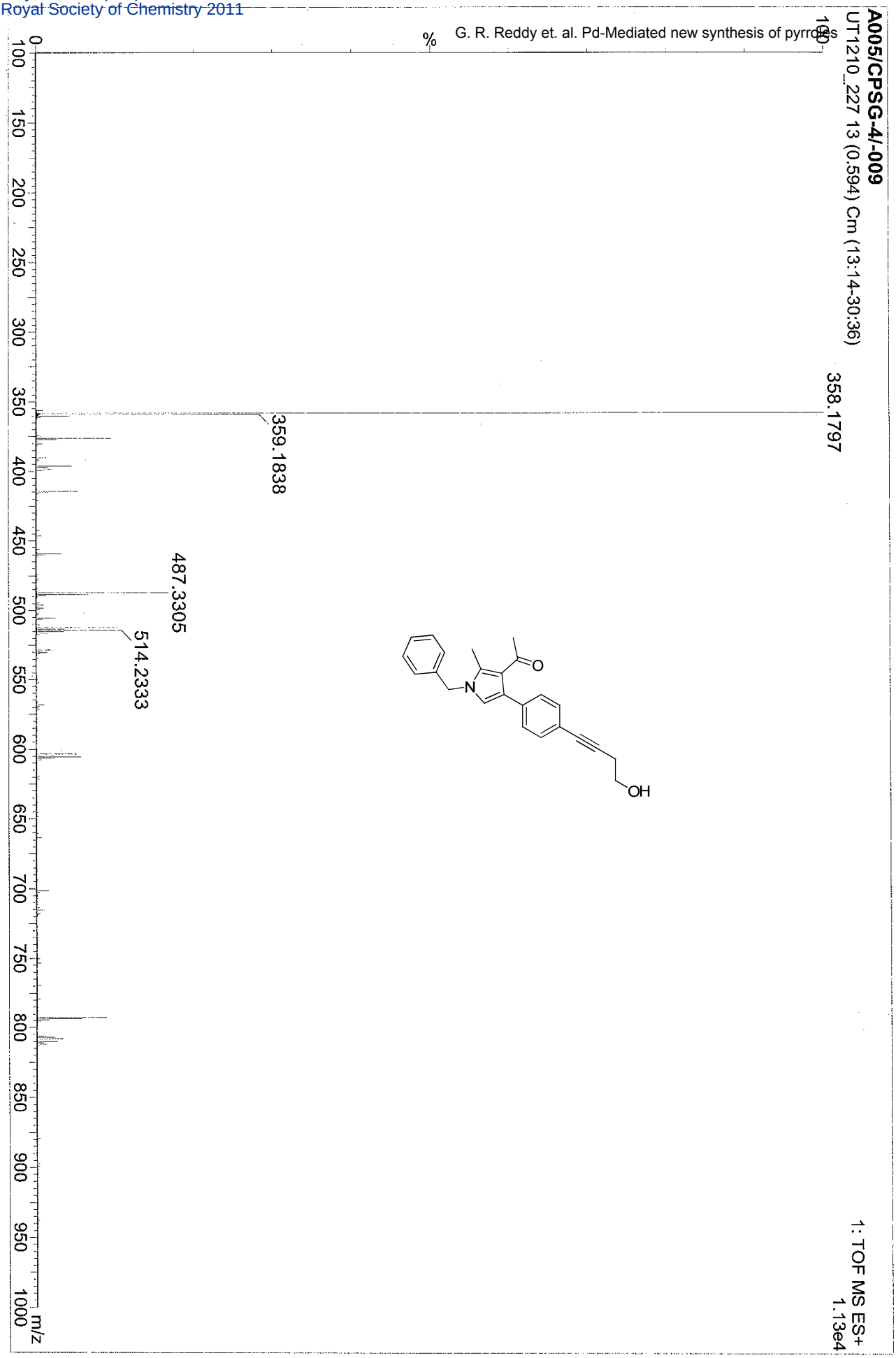




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
344.1649	344.1651	-0.2	-0.6	13.5	0.0	C23 H22 N O2


A005-CPSG-4-009 in CDCl3
NMR-400
8
7
6
5
4
3
2
1
ppm
5.99
0.99
2.01
1.13
2.00
2.04
2.00
3.02
3.08
N
O
OH


A005-CPSG-4-009 in CDCl3
NMR-400
197.595
136.396
135.953
135.357
132.272
131.523
129.155
128.934
128.170
128.047
127.956
126.627
125.237
121.983
120.646
120.172
86.663
82.324
77.321
77.000
76.687
61.135
50.319
31.116
29.665
23.829
11.516
200
180
160
140
120
100
80
60
40
20
ppm
O
N
OH

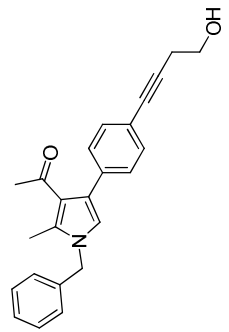


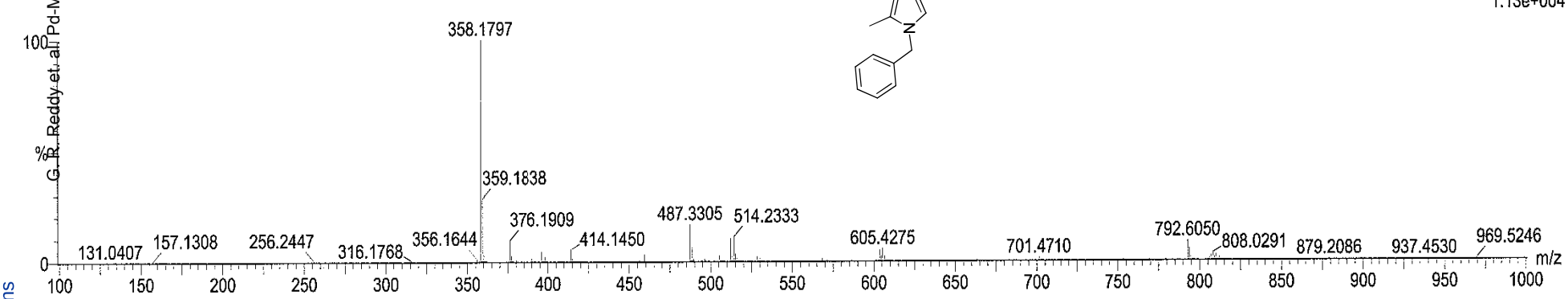
Elemental Composition Report

Single Mass Analysis

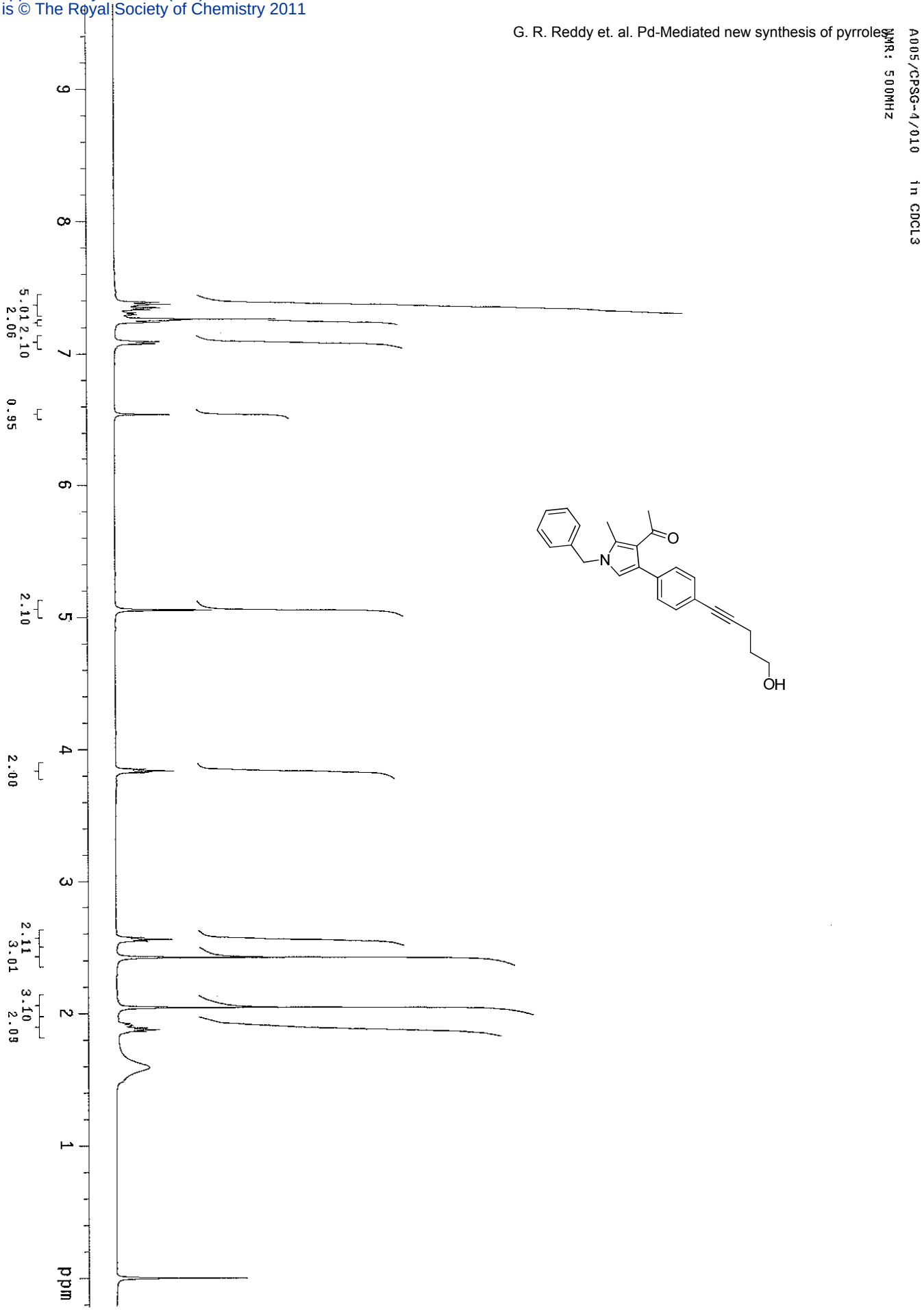
Tolerance = 20.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

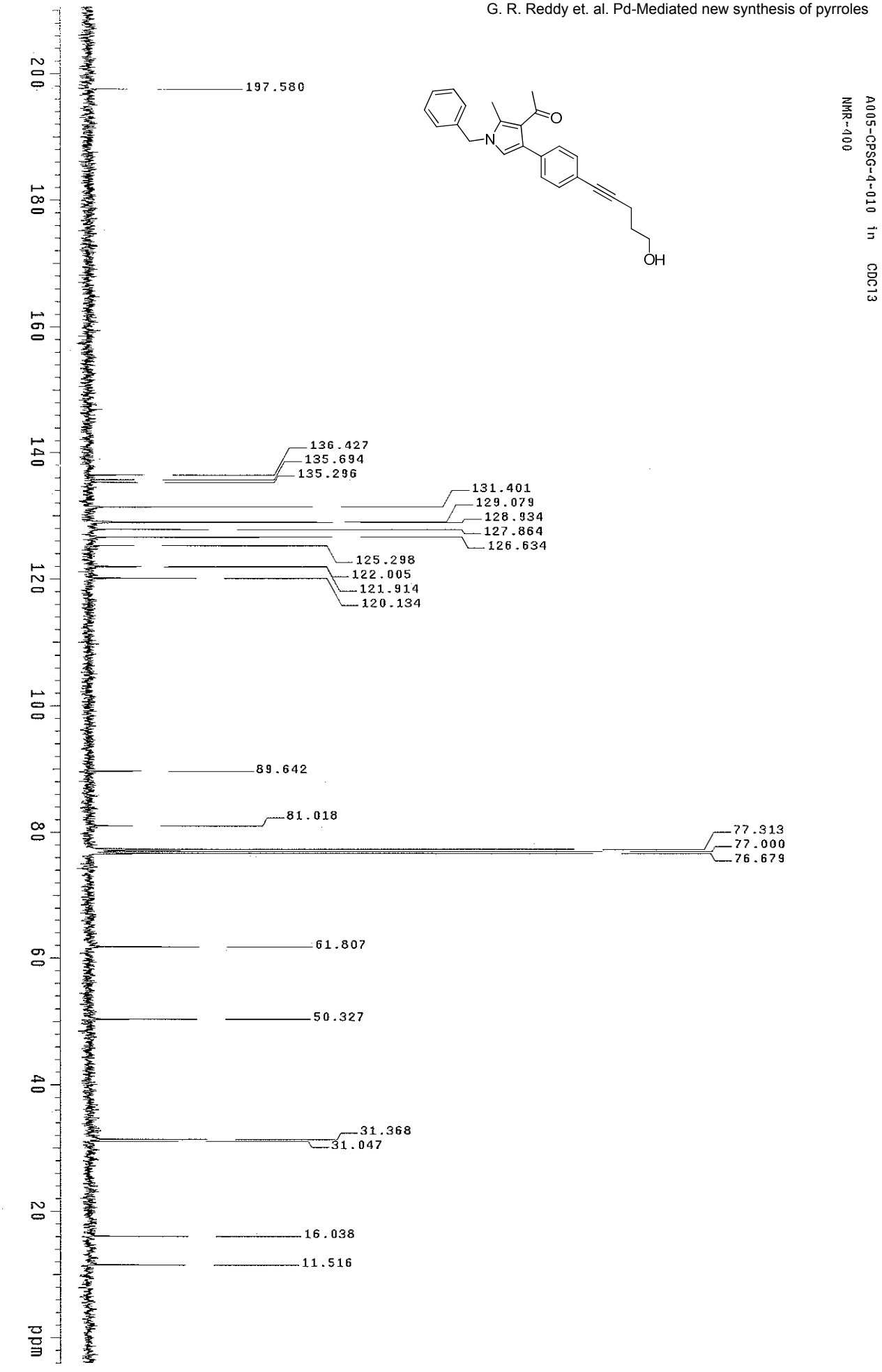
Monoisotopic Mass, Even Electron Ions
74 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-430 N: 0-3 O: 0-3
A005ICPSG-4/-009
UT1210_227 13 (0.594) Cm (13:14-30:36)

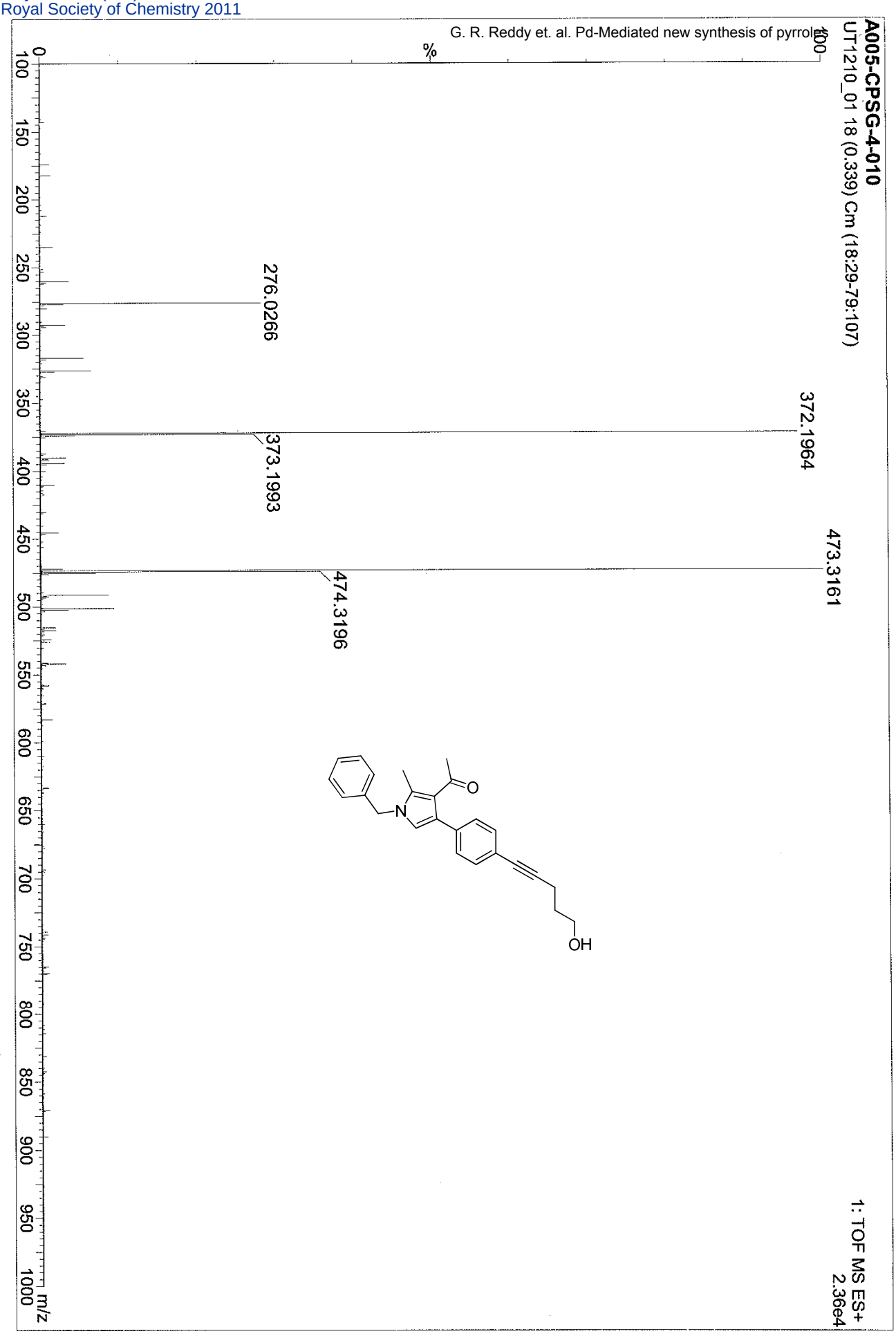




Minimum:				-1.0		
Maximum:		5.0	20.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.1797	358.1807	-1.0	-2.8	13.5	1.5	C24 H24 N O2


A005/CPSG-4/010 in CDCL3
NMR: 500MHz
5.01 2.10
2.06
0.95
2.10
2.00
2.11
3.01
3.10
2.09
ppm
O
N
OH


A005-CPSG-4-010 in CDC13
NMR-400
O
N
OH
197.580
136.427
135.694
135.296
131.401
129.079
128.934
127.864
126.634
125.298
122.005
121.914
120.134
89.642
81.018
77.313
77.000
76.679
61.807
50.327
31.368
31.047
16.038
11.516
200
180
160
140
120
100
80
60
40
20
ppm

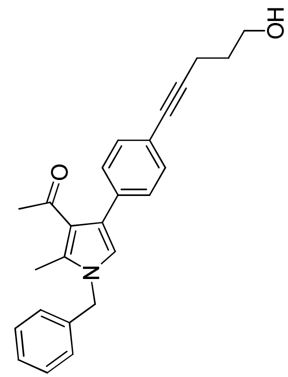


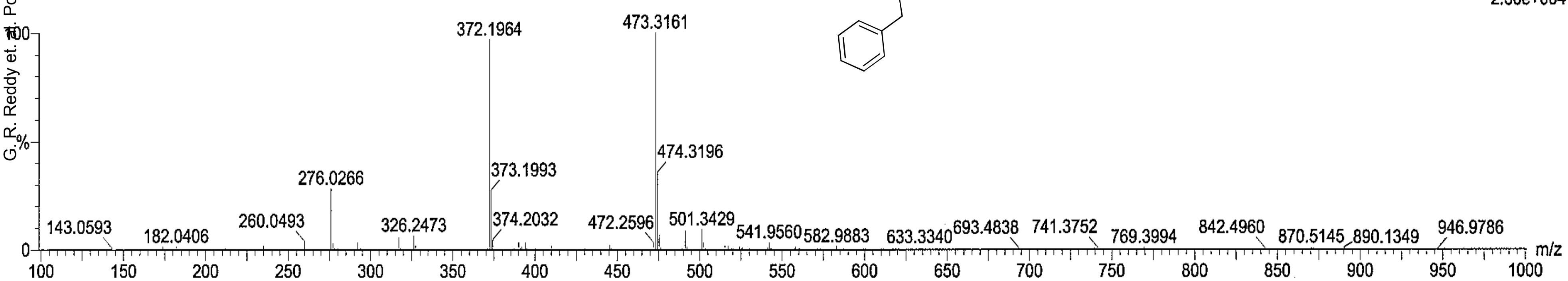
Elemental Composition Report

Single Mass Analysis

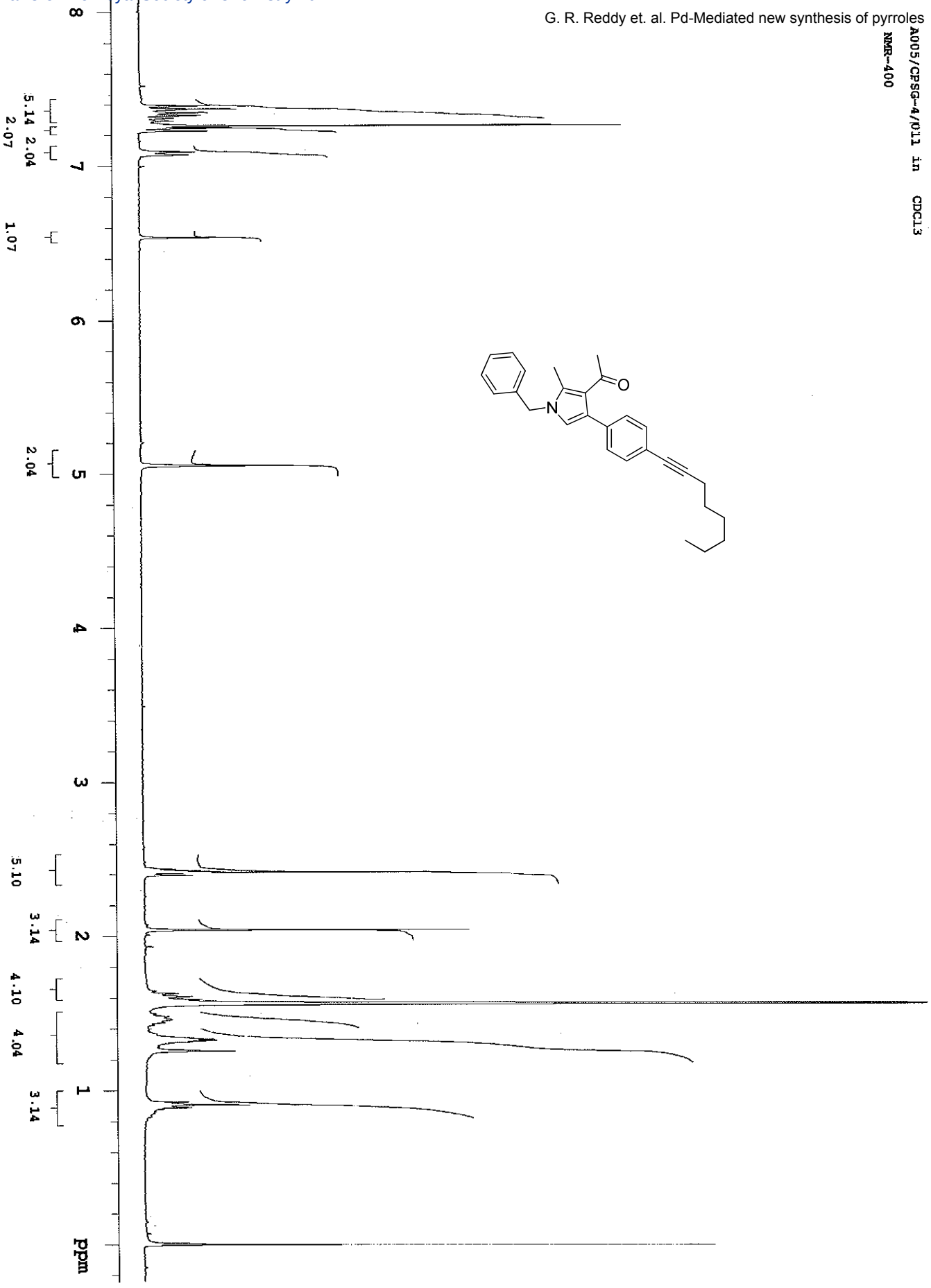
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

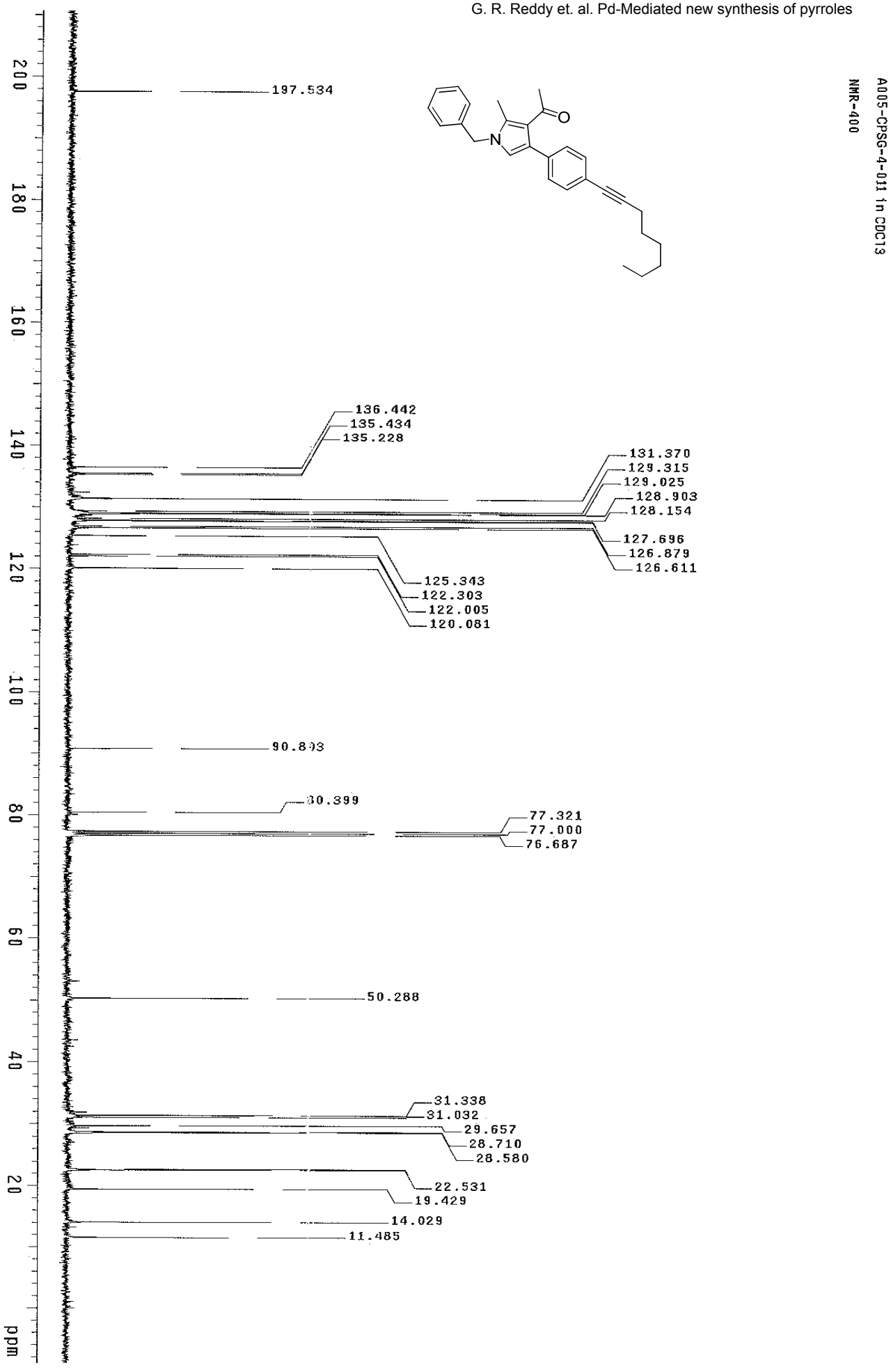
Monoisotopic Mass, Even Electron Ions
99 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-3 O: 0-4
A005-CPSG-4-010
UT1210_01 18 (0.339) Cm (18:29-79:107)

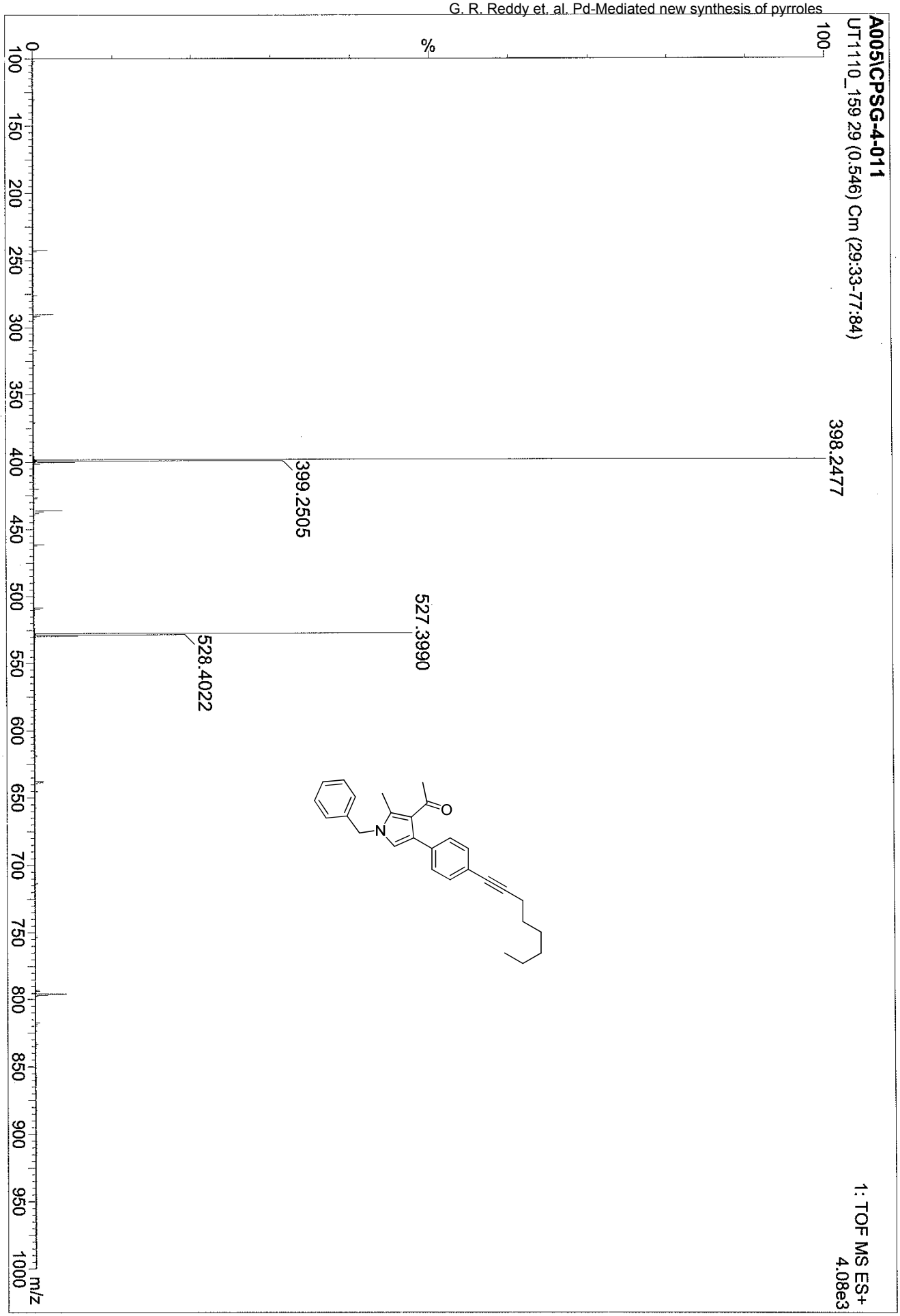




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.1964	372.1964	0.0	0.0	13.5	2.3	C25 H26 N O2


A005/CPSG-4/011 in CDCl3
NMR-400
8
7
6
5
4
3
2
1
ppm
5.14
2.04
2.07
1.07
2.04
5.10
3.14
4.10
4.04
3.14
N
O


A005-CPSG-4-011 in CDCl3
NMR-400
197.534
136.442
135.434
135.228
131.370
129.315
129.025
128.903
128.154
127.696
126.879
126.611
125.343
122.303
122.005
120.081
90.893
80.399
77.321
77.000
76.687
50.288
31.338
31.032
29.657
28.710
28.580
22.531
19.429
14.029
11.485
O
N
200
180
160
140
120
100
80
60
40
20
ppm



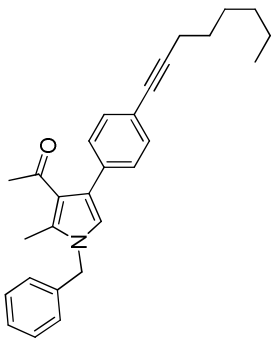
Elemental Composition Report

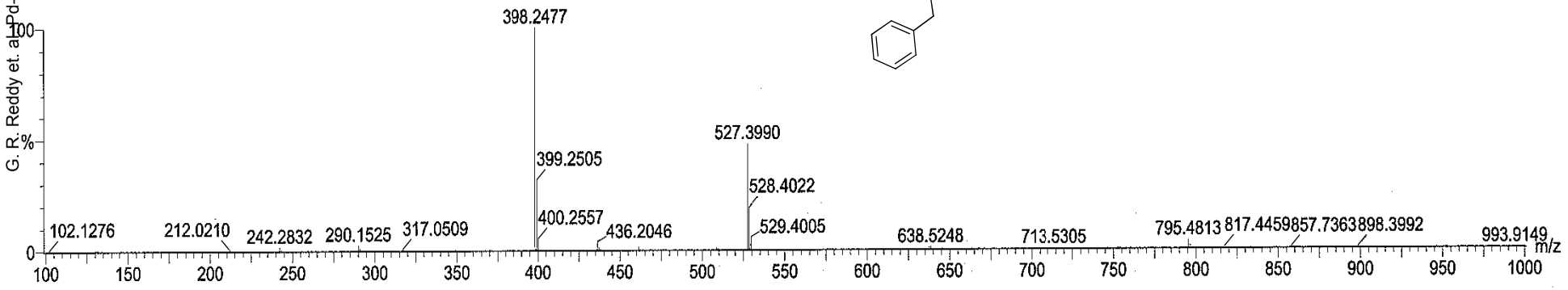
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

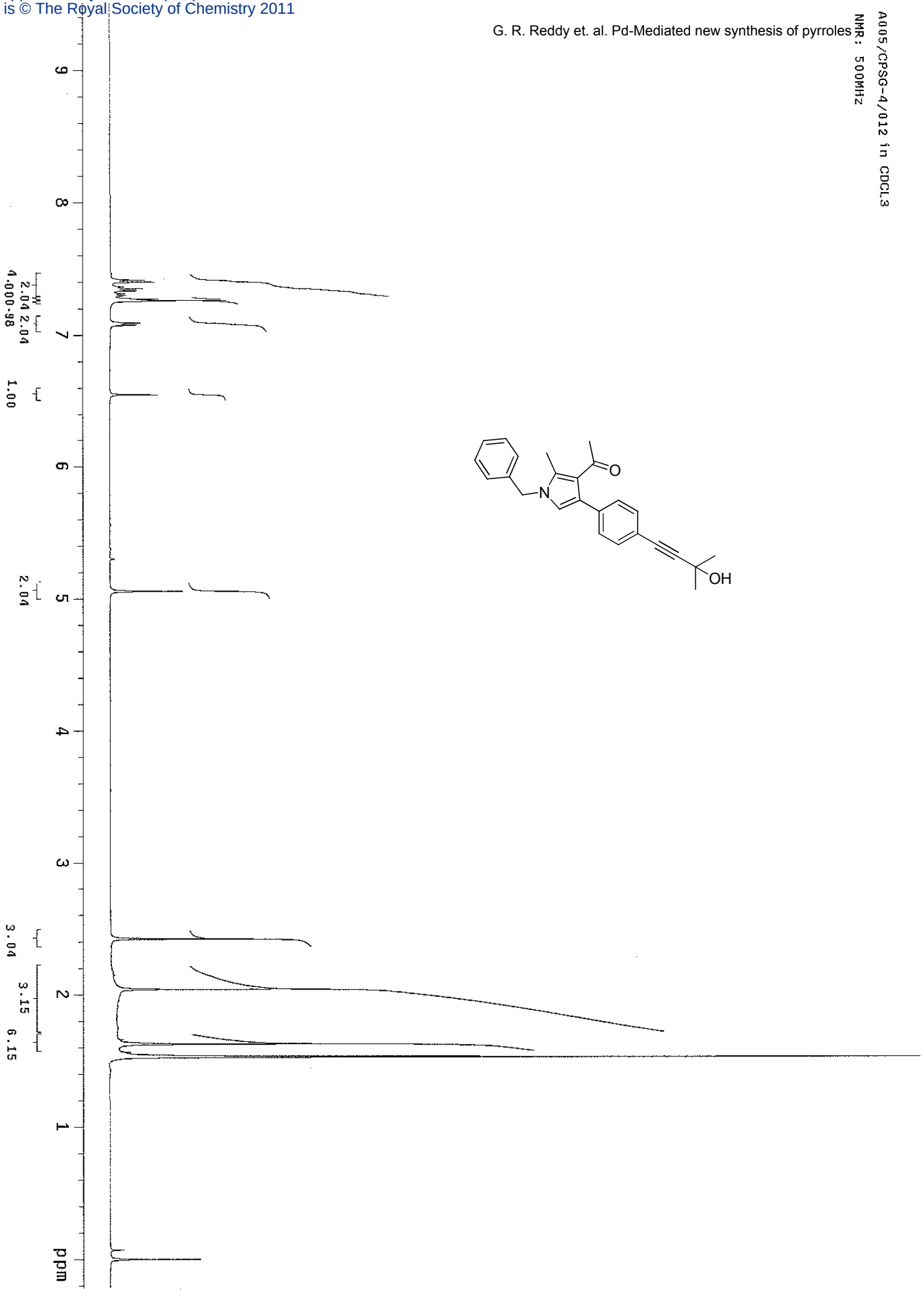
Monoisotopic Mass, Even Electron Ions
177 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-65 N: 0-5 O: 0-5

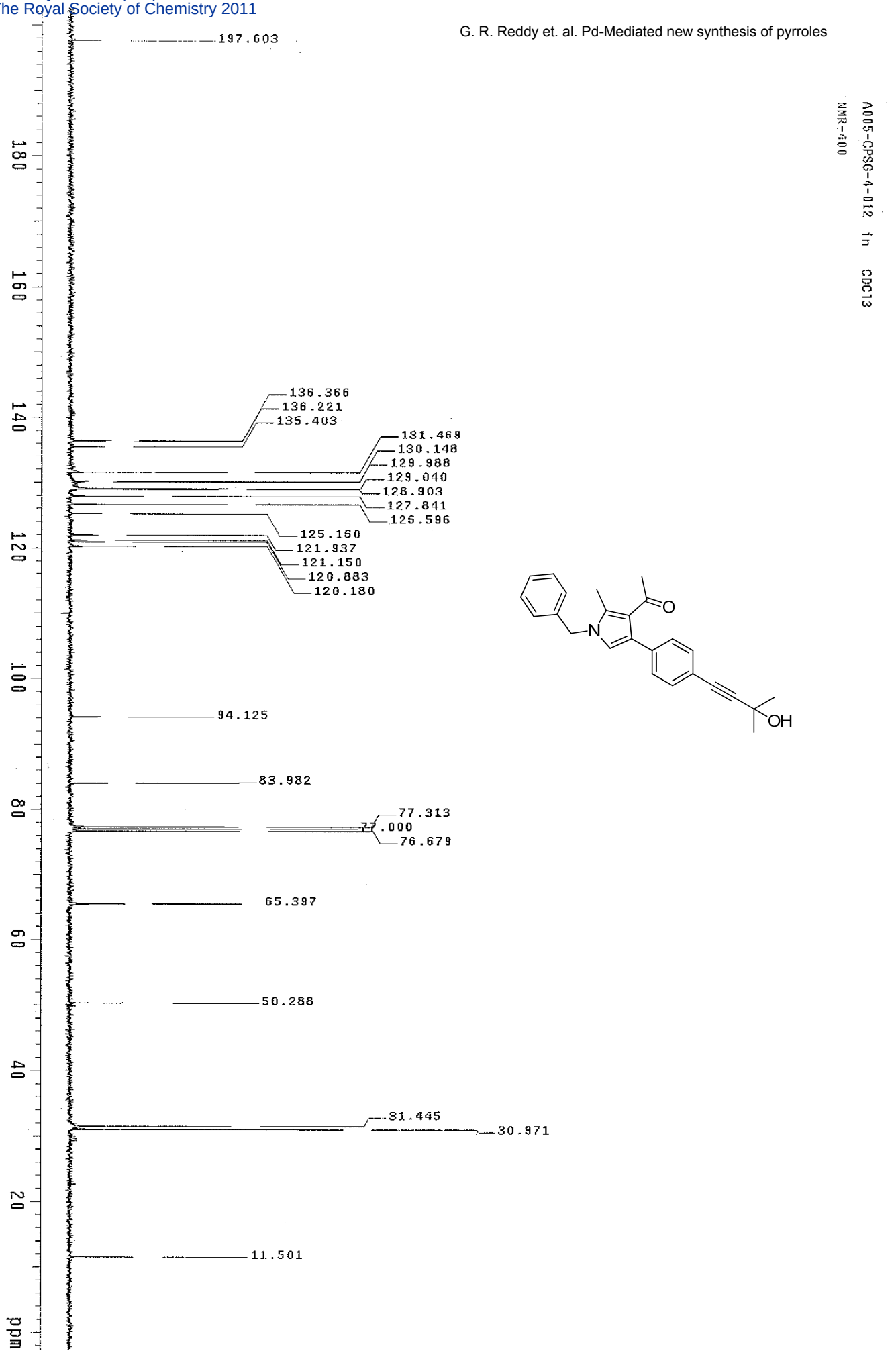
A005\CPSG-4-011
GT1110_159 29 (0.546) Cm (29:33-77:84)

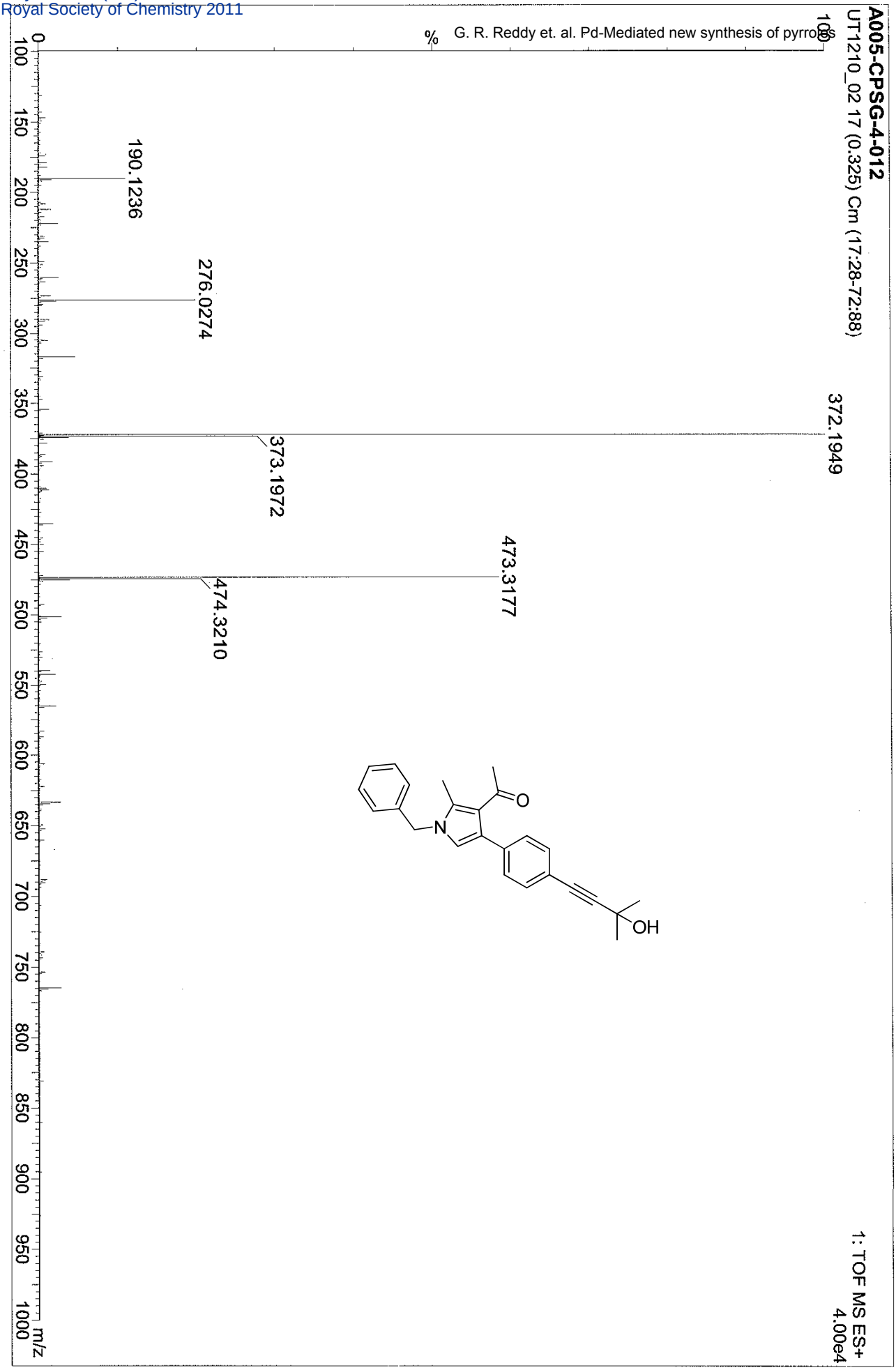




Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
398.2477	398.2484	-0.7	-1.8	13.5	0.3	C28 H32 N O


A005/CPSG-4/012 in CDCL3
NMR: 500MHz
O
N
OH
ppm
9
8
7
6
5
4
3
2
1
4.000
2.04
2.04
98
1.00
2.04
3.04
3.15
6.15





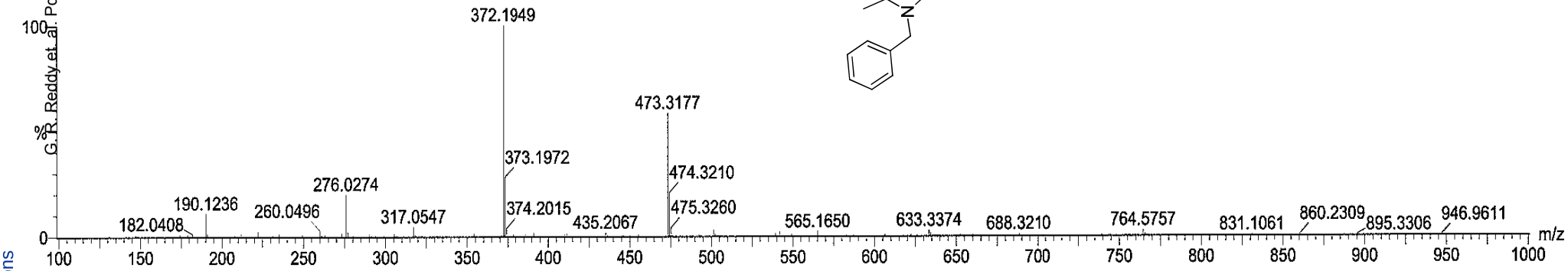
Elemental Composition Report

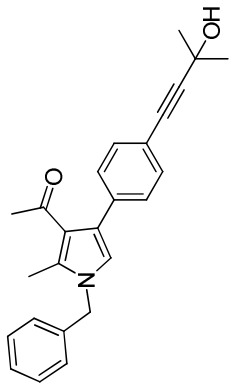
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-3 O: 0-4

A005-CPSG-4-012
UT1010_02 17 (0.325) Cm (17:28-72:88)





Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.1949	372.1964	-1.5	-4.0	13.5	24.1	C25 H26 N O2