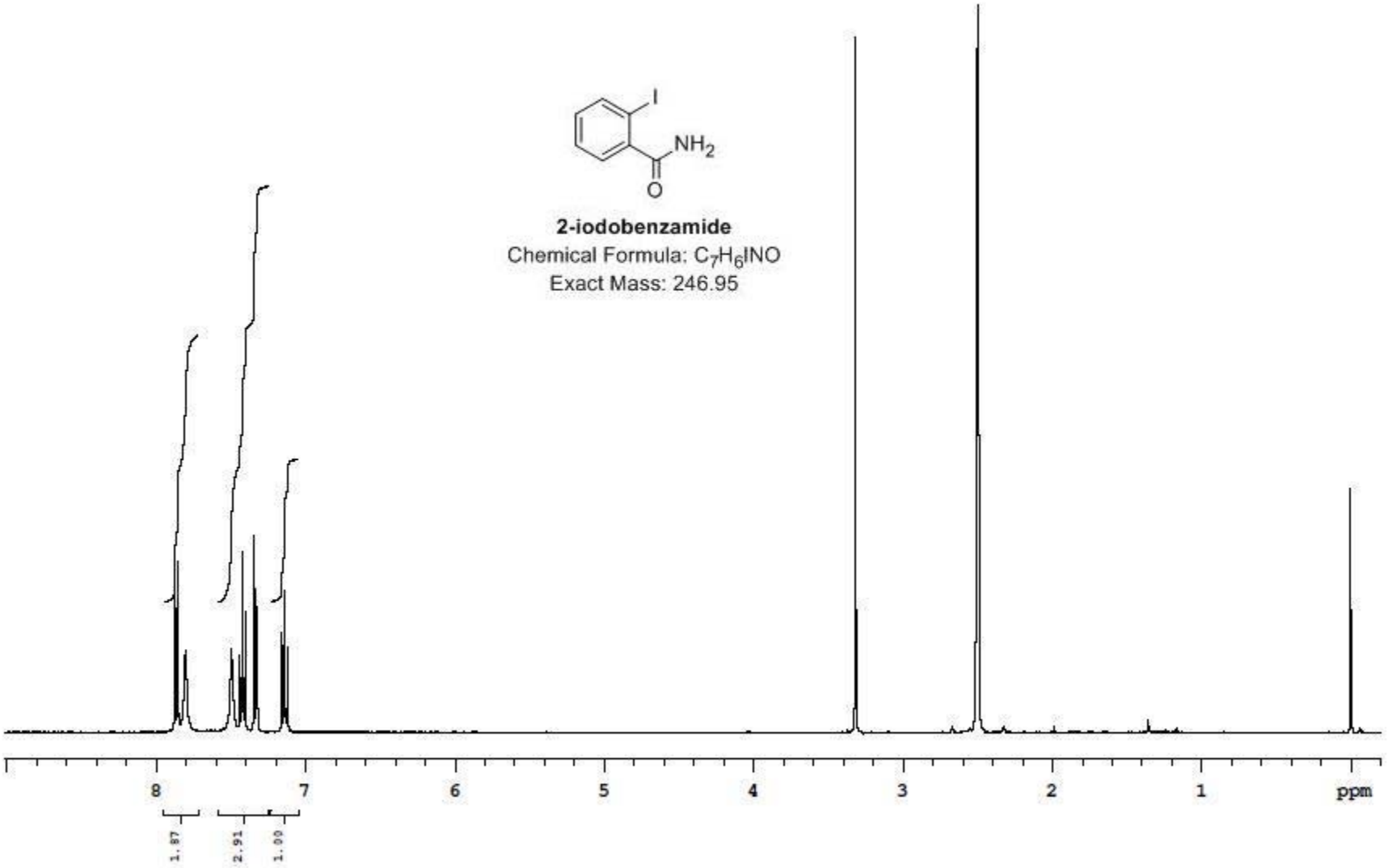
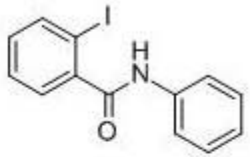
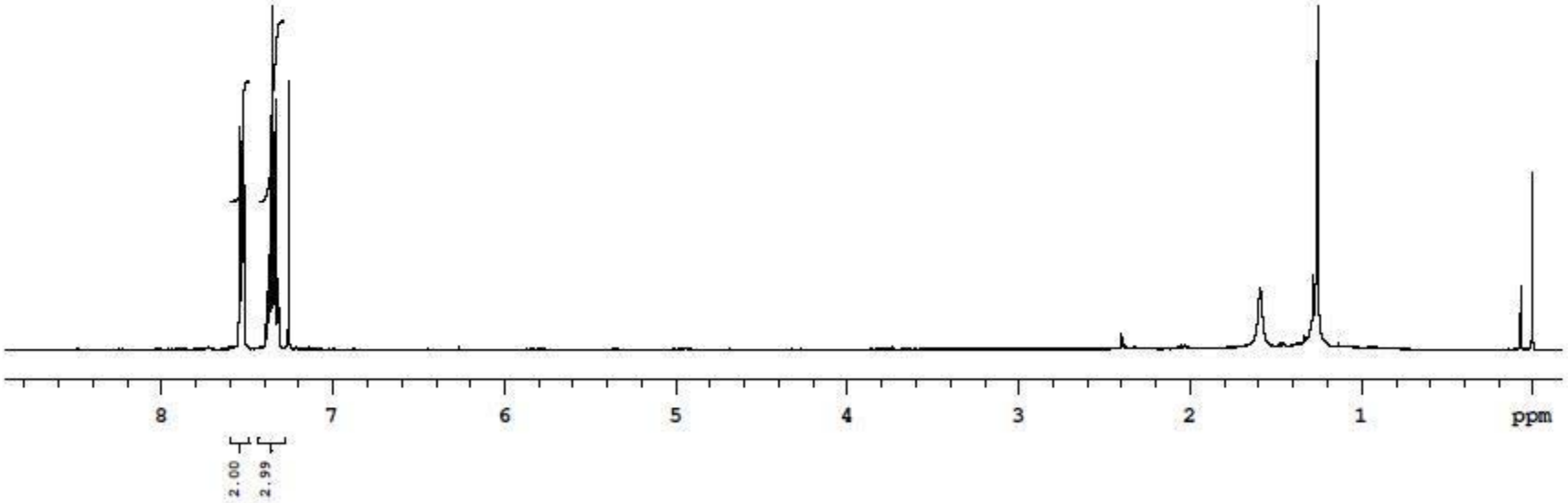
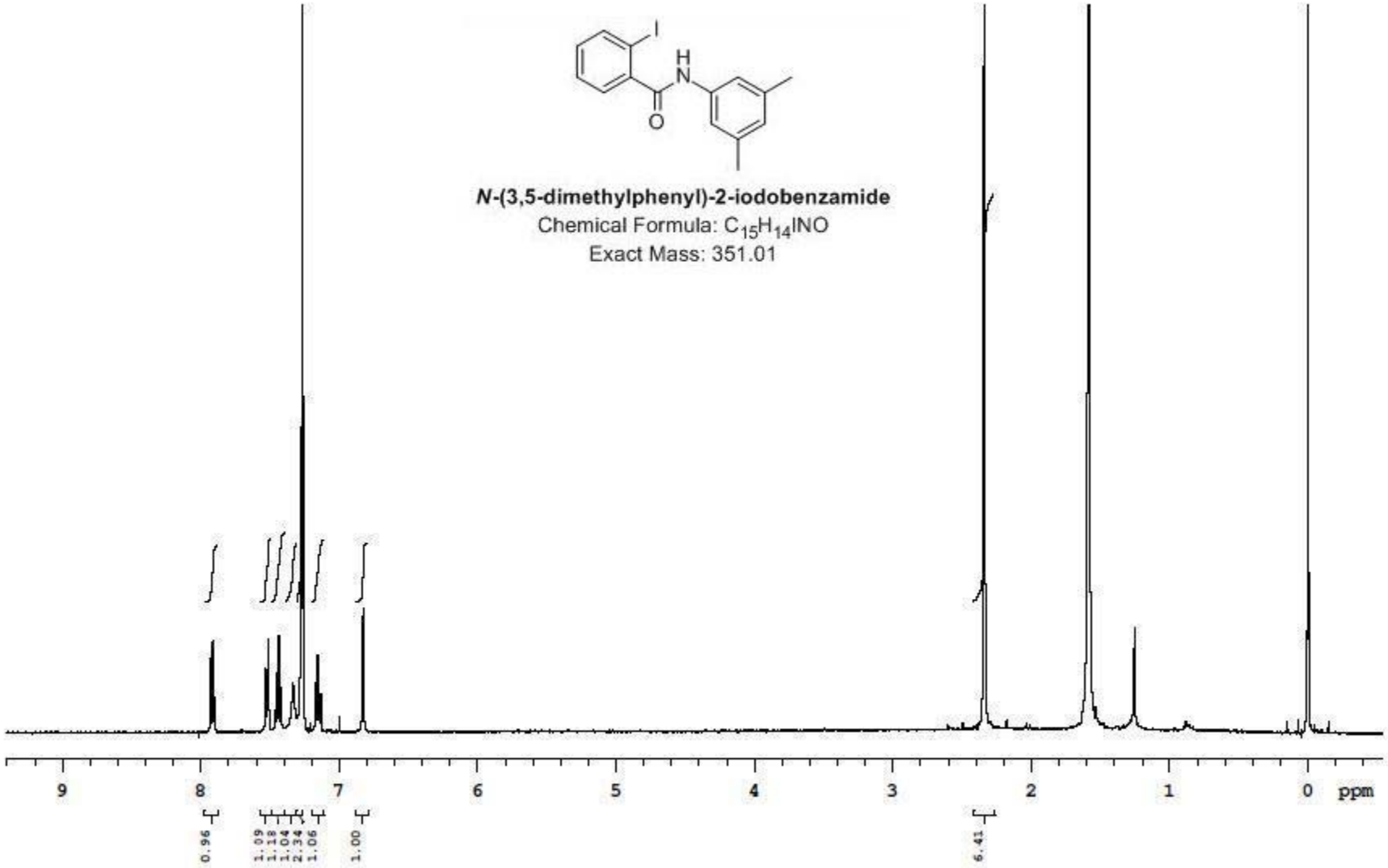
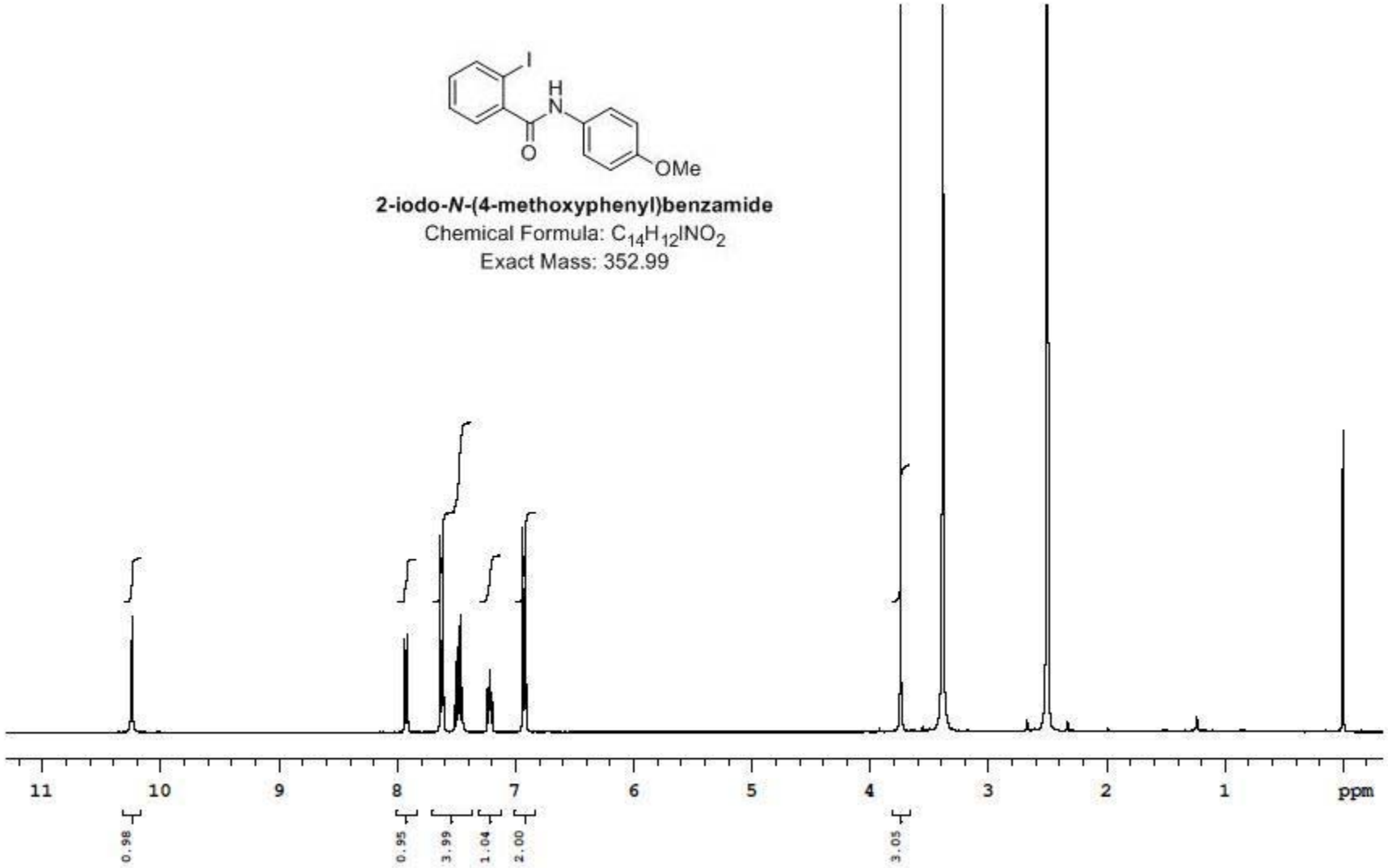


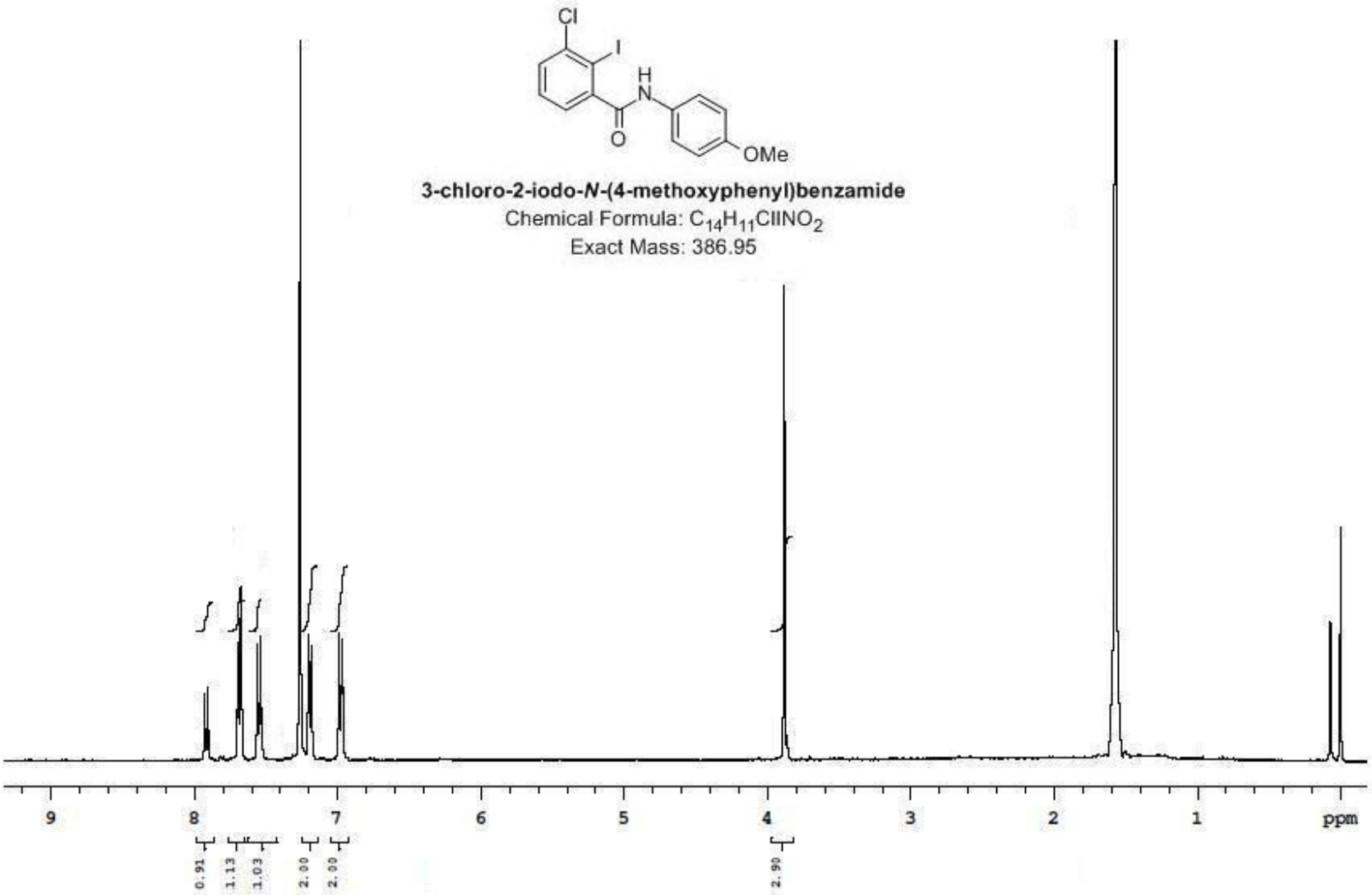


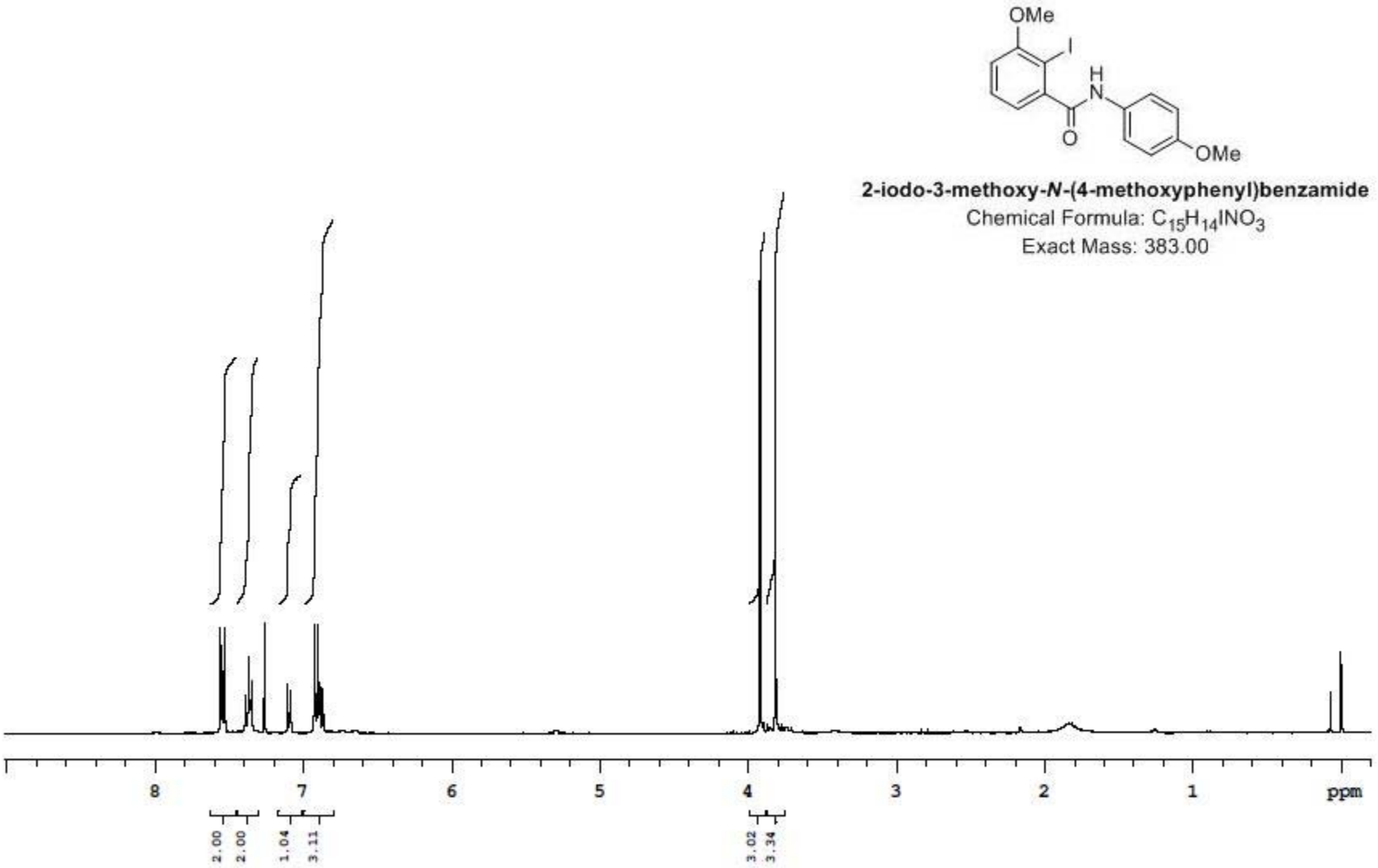
2-iodo-*N*-phenylbenzamide
Chemical Formula: $C_{13}H_{10}INO$
Exact Mass: 322.98




I
H
N
O
N-(3,5-dimethylphenyl)-2-iodobenzamide
Chemical Formula: C15H14INO
Exact Mass: 351.01
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.09
1.18
1.04
2.34
1.06
1.00
6.41


I
H
N
O
OMe
2-iodo-N-(4-methoxyphenyl)benzamide
Chemical Formula: C14H12INO2
Exact Mass: 352.99
11
10
9
8
7
6
5
4
3
2
1
ppm
0.98
0.95
3.99
1.04
2.00
3.05

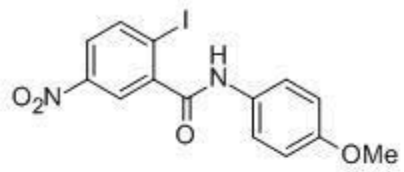

Cl
I
H
N
O
OMe
3-chloro-2-iodo-N-(4-methoxyphenyl)benzamide
Chemical Formula: C14H11ClINO2
Exact Mass: 386.95
9
8
7
6
5
4
3
2
1
ppm
0.91
1.13
1.03
2.00
2.00
2.90



2-iodo-3-methoxy-*N*-(4-methoxyphenyl)benzamide

Chemical Formula: $C_{15}H_{14}INO_3$

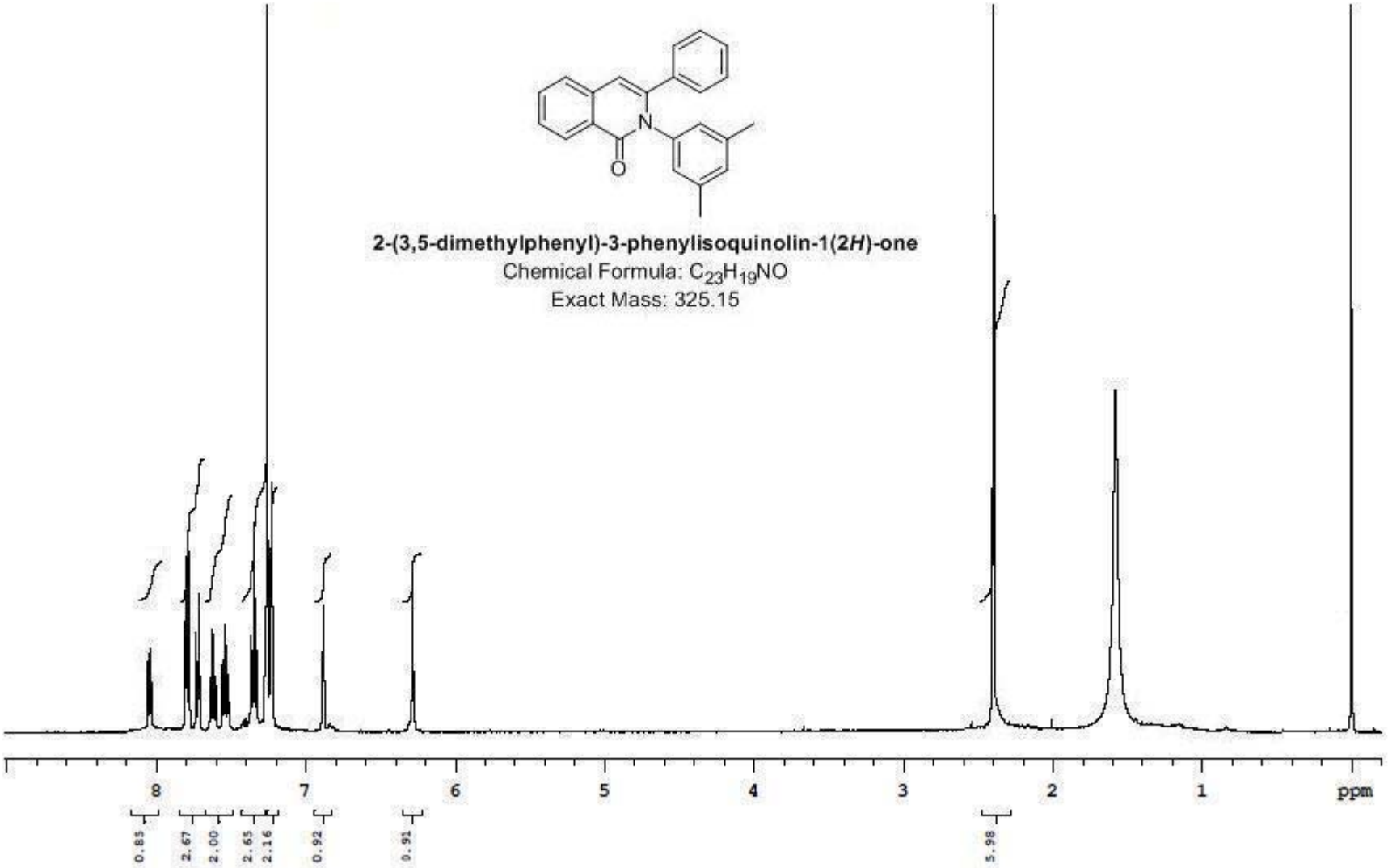
Exact Mass: 383.00



2-iodo-*N*-(4-methoxyphenyl)-5-nitrobenzamide

Chemical Formula: $C_{14}H_{11}IN_2O_4$

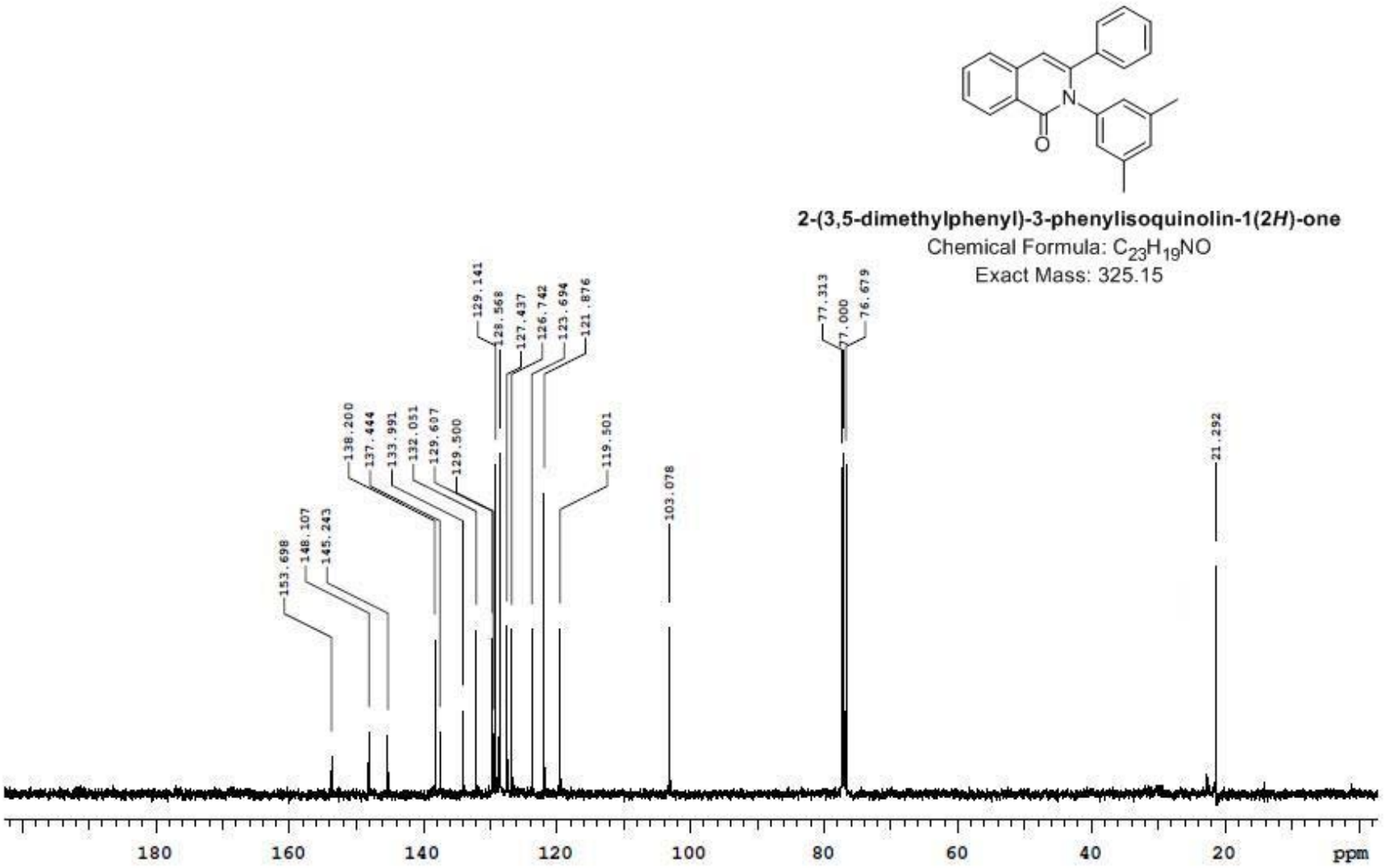
Exact Mass: 397.98



2-(3,5-dimethylphenyl)-3-phenylisoquinolin-1(2*H*)-one

Chemical Formula: $C_{23}H_{19}NO$

Exact Mass: 325.15


2-(3,5-dimethylphenyl)-3-phenylisoquinolin-1(2H)-one
Chemical Formula: C23H19NO
Exact Mass: 325.15
153.698
148.107
145.243
138.200
137.444
133.991
132.051
129.607
129.500
129.141
128.568
127.437
126.742
123.694
121.876
119.501
103.078
77.313
77.000
76.679
21.292
180
160
140
120
100
80
60
40
20
ppm

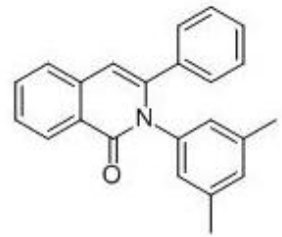
Elemental Composition Report

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-2 O: 0-3

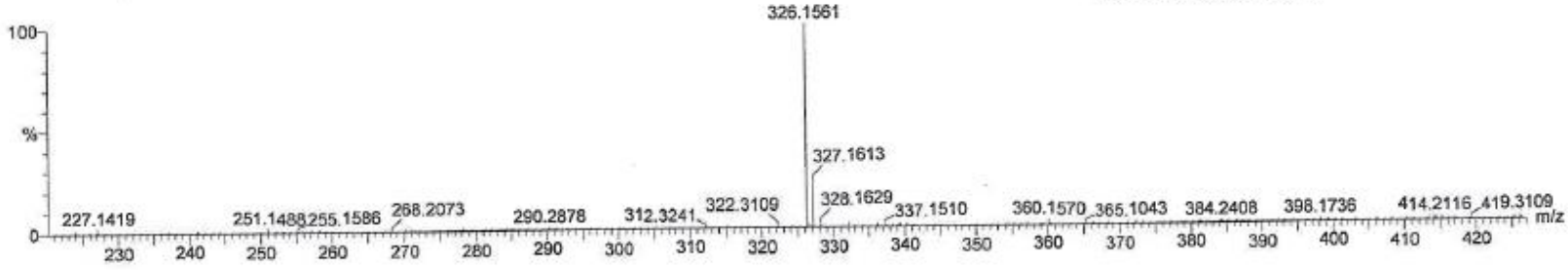
B036/CDMA/015
131202008 17 (0.620) Cm (15:17-26:28)



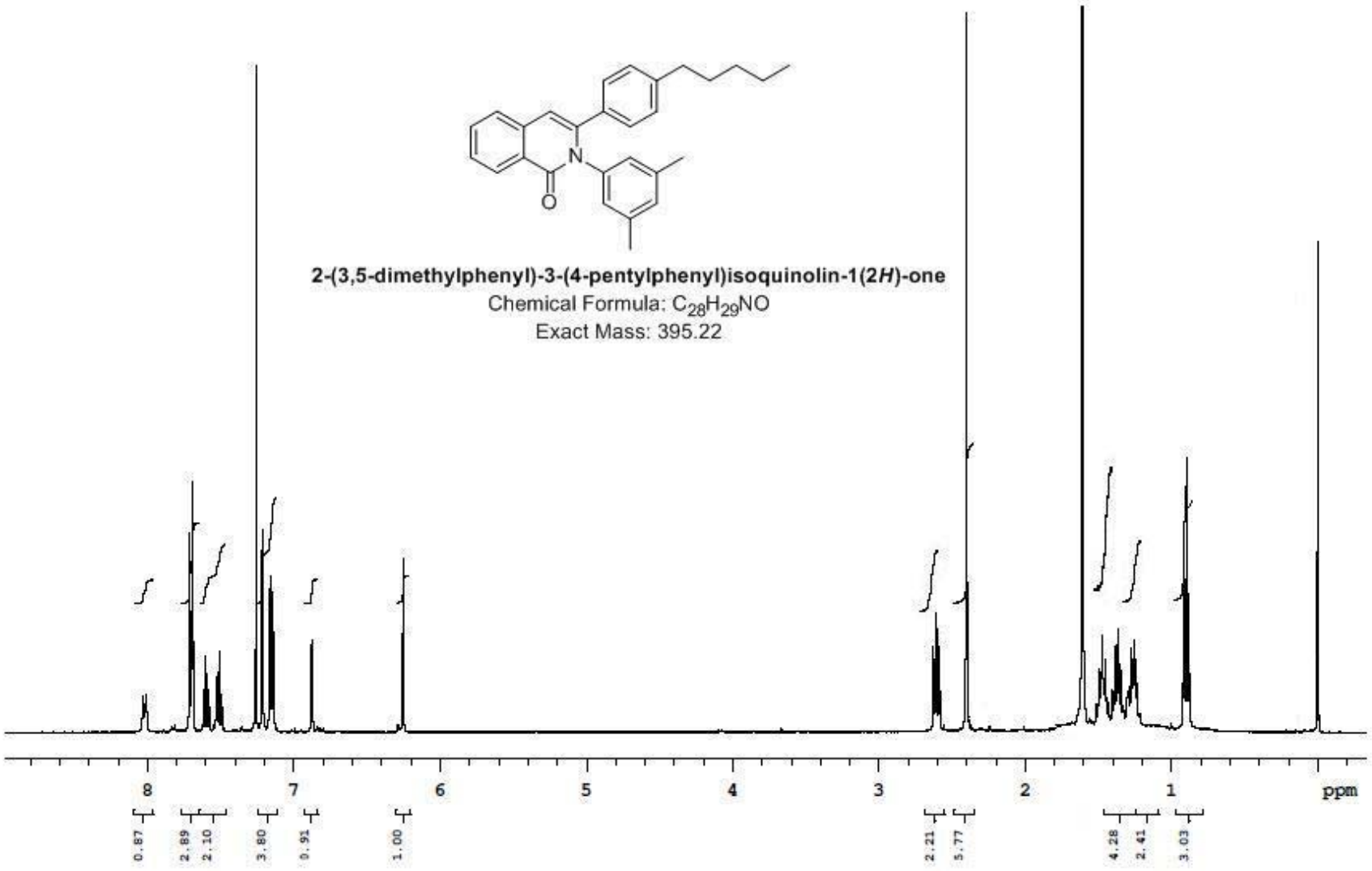
2-(3,5-dimethylphenyl)-3-phenylisoquinolin-1(2*H*)-one

Chemical Formula: $C_{23}H_{19}NO$
Exact Mass: 325.15

1: TOF MS ES+
1.07e+003



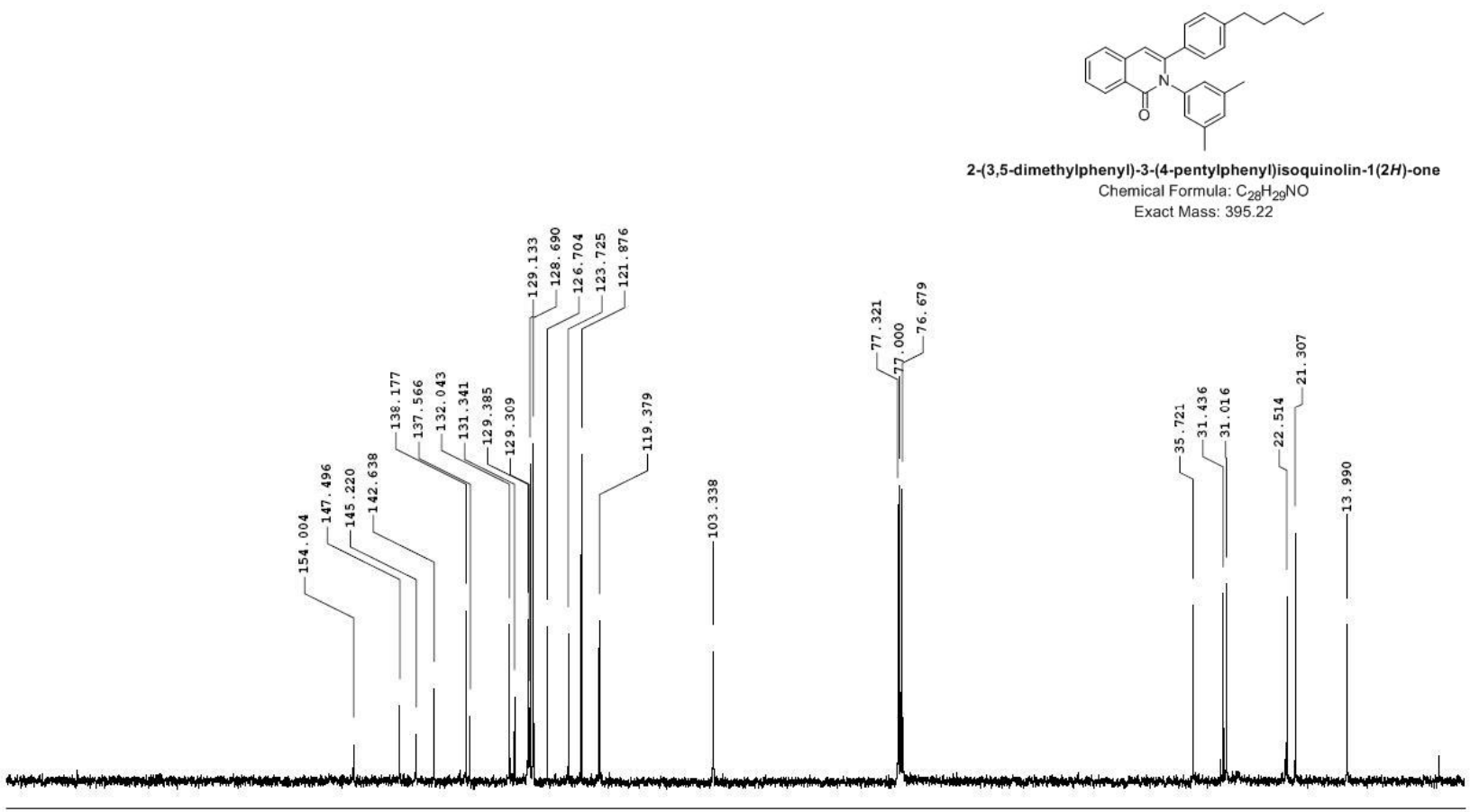
Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.1561	326.1545	1.6	4.9	14.5	0.7	C23 H20 N O



2-(3,5-dimethylphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{28}H_{29}NO$

Exact Mass: 395.22



2-(3,5-dimethylphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{28}H_{29}NO$

Exact Mass: 395.22

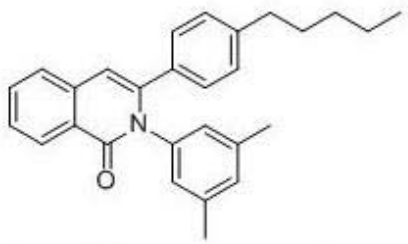
Elemental Composition Report

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-3

B036/CDMA/016
131202009 4 (0.138) Cm (4-1:2)

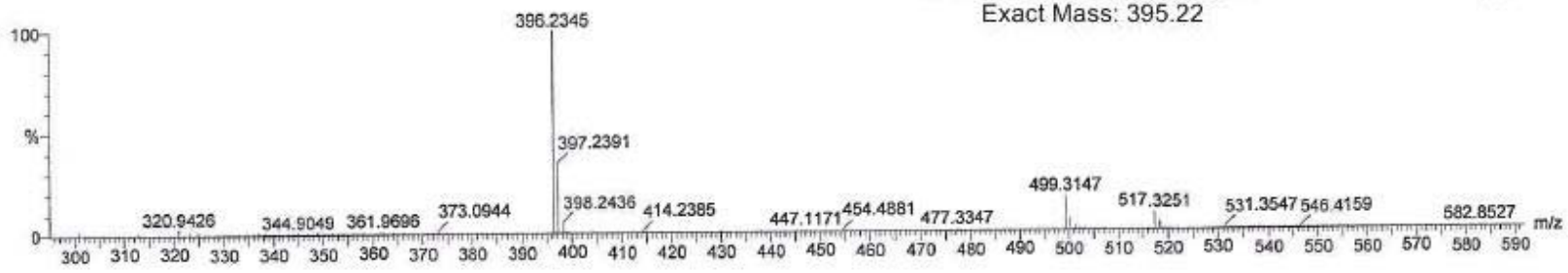


2-(3,5-dimethylphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

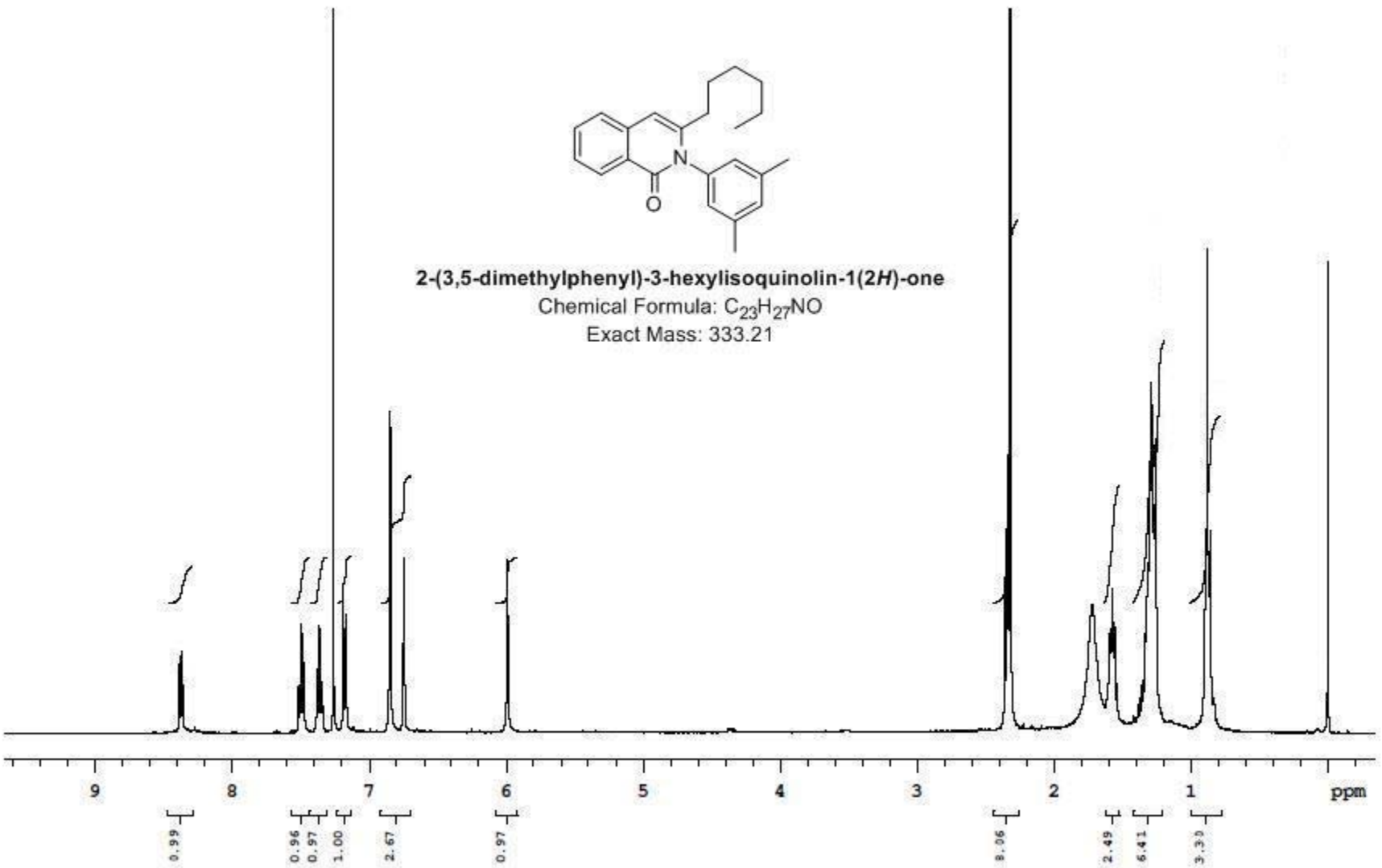
Chemical Formula: $C_{28}H_{29}NO$

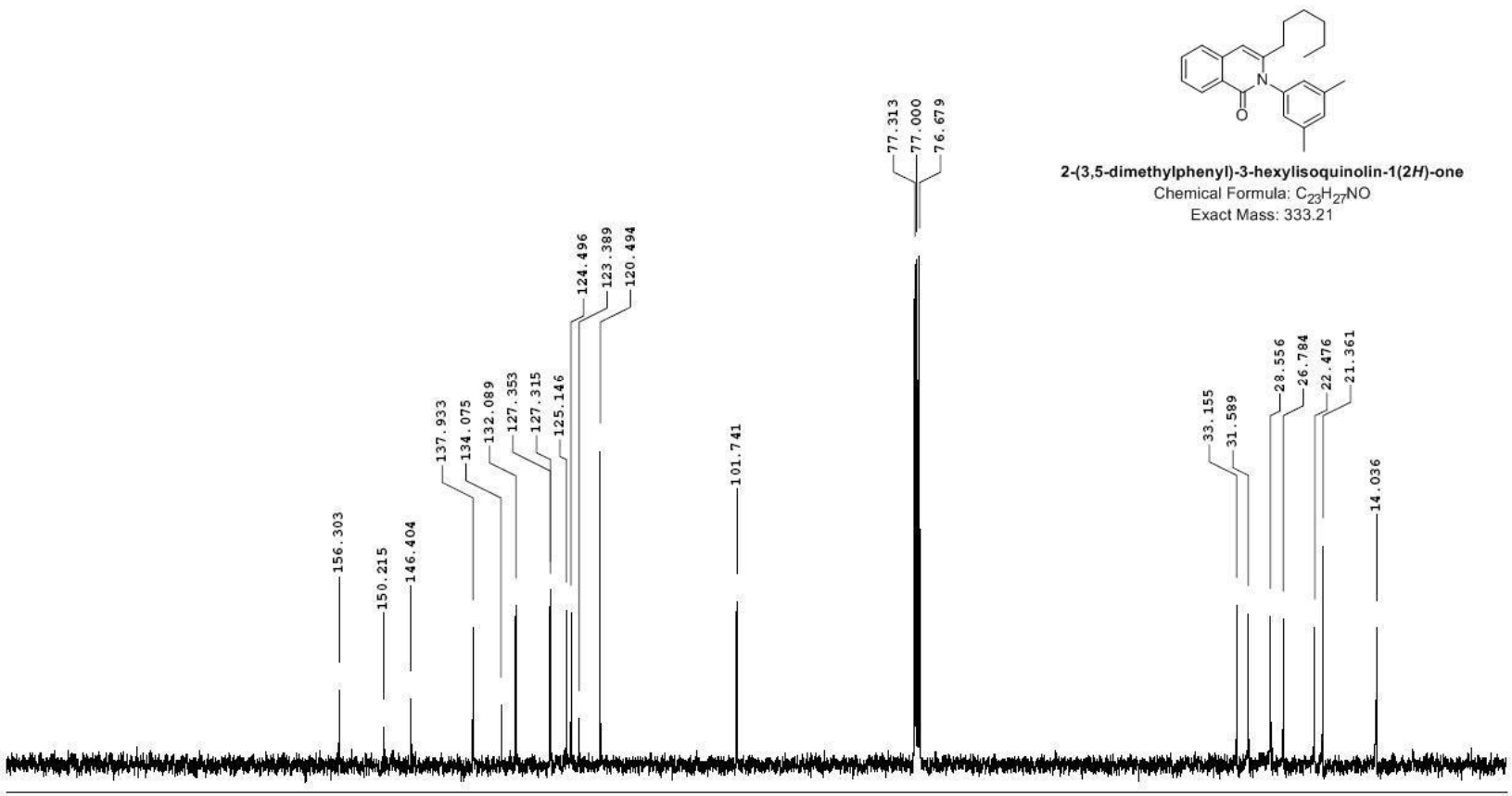
Exact Mass: 395.22

1: TOF MS ES+
2.17e+003



Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
396.2345	396.2327	1.8	4.5	14.5	2.4	C28 H30 N O


2-(3,5-dimethylphenyl)-3-hexylisoquinolin-1(2H)-one
Chemical Formula: C23H27NO
Exact Mass: 333.21
9
8
7
6
5
4
3
2
1
ppm
0.99
0.96
0.97
1.00
2.67
0.97
8.06
2.49
6.41
3.30


156.303
150.215
146.404
137.933
134.075
132.089
127.353
127.315
125.146
124.496
123.389
120.494
101.741
77.313
77.000
76.679
33.155
31.589
28.556
26.784
22.476
21.361
14.036
2-(3,5-dimethylphenyl)-3-hexylisoquinolin-1(2H)-one
Chemical Formula: C23H27NO
Exact Mass: 333.21

Elemental Composition Report

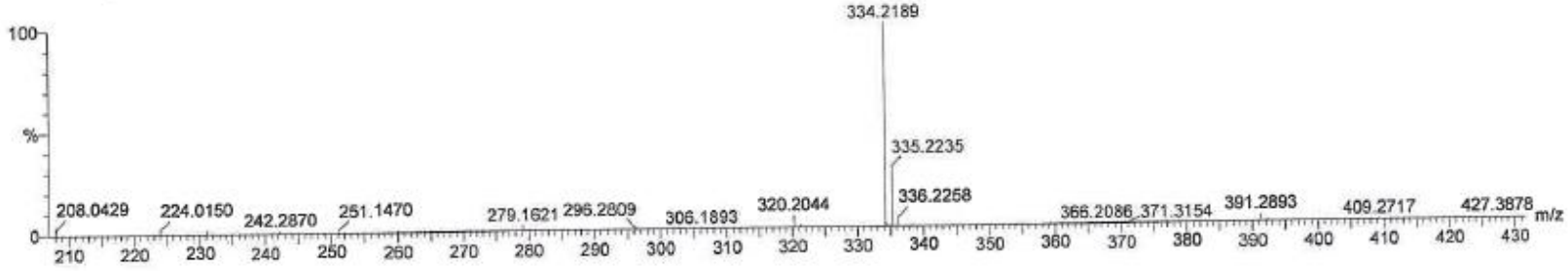
Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

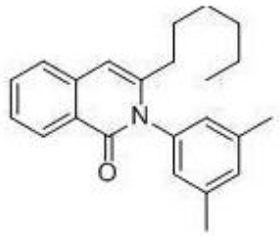
Monoisotopic Mass, Even Electron Ions
42 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-3

B036/CDMA/017
131202010 8 (0.279) Cm (8)

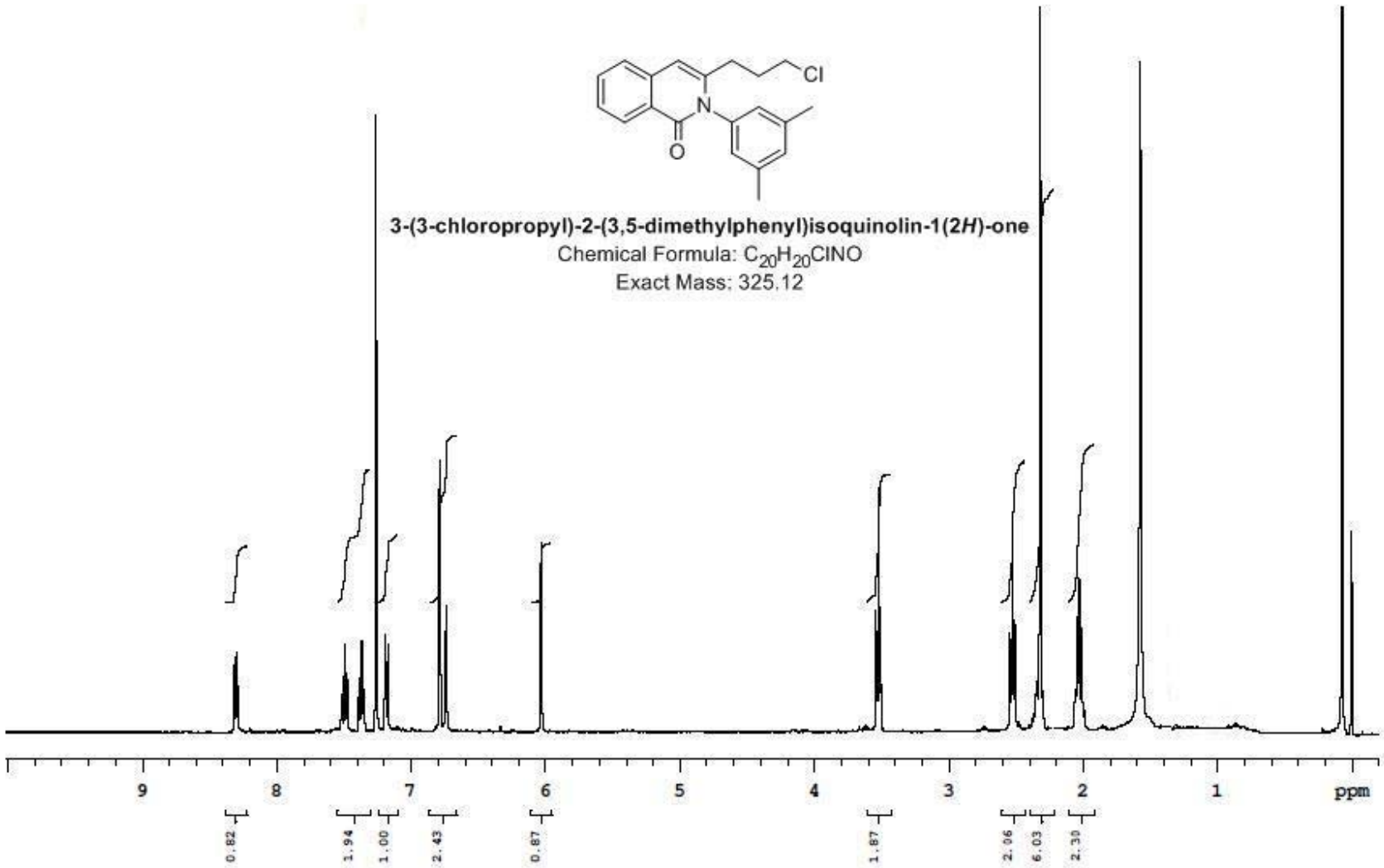
1: TOF MS ES+
6.23e+003

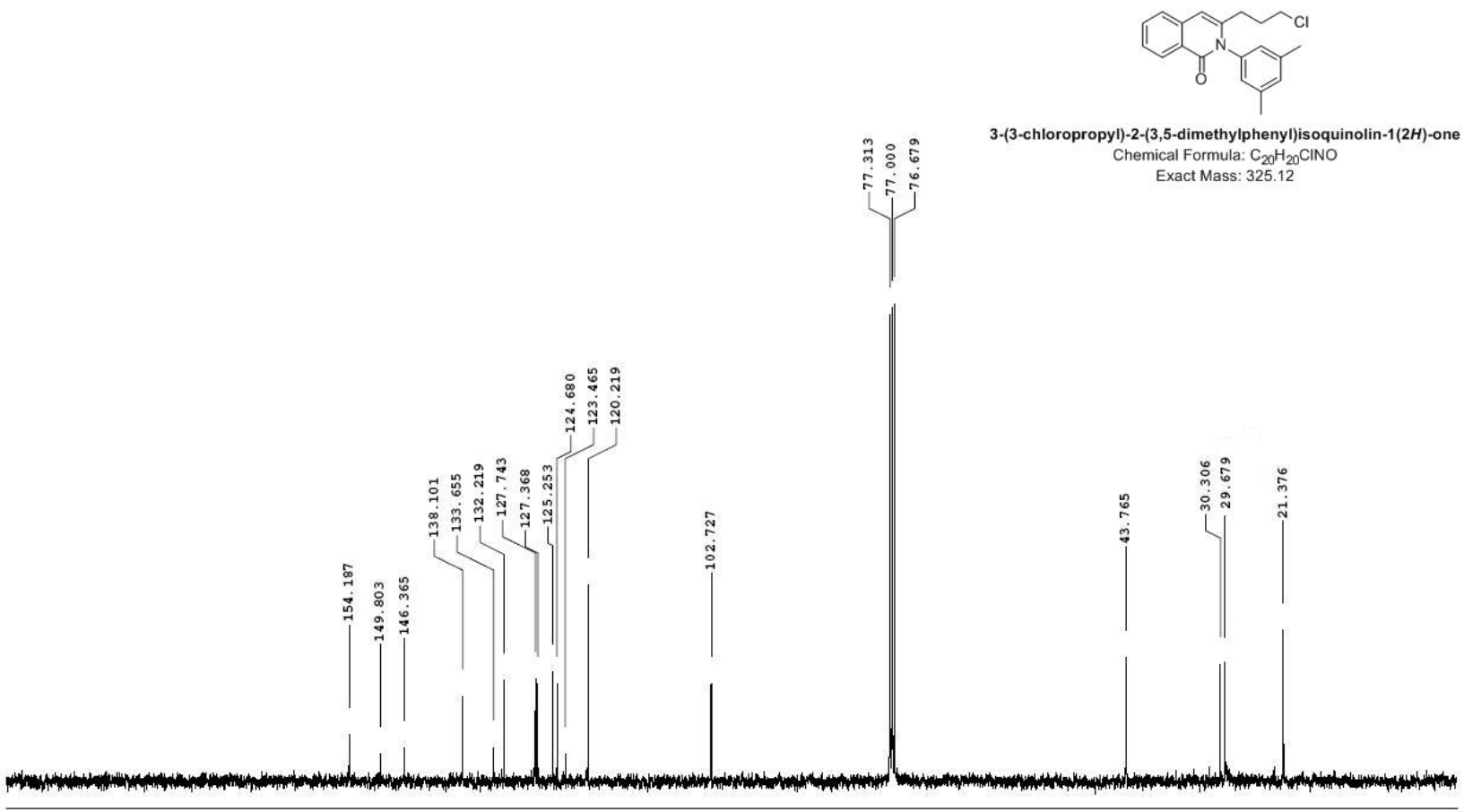


Minimum:				-5.0		
Maximum:		5.0	6.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
334.2189	334.2171	1.8	5.4	10.5	8.6	C23 H28 N O



2-(3,5-dimethylphenyl)-3-hexylisoquinolin-1(2*H*)-one
Chemical Formula: $C_{23}H_{27}NO$
Exact Mass: 333.21


Cl
N
O
3-(3-chloropropyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2H)-one
Chemical Formula: C20H20ClNO
Exact Mass: 325.12
9
8
7
6
5
4
3
2
1
ppm
0.82
1.94
1.00
2.43
0.87
1.87
2.06
6.03
2.30


Cl
N
O
3-(3-chloropropyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2H)-one
Chemical Formula: C20H20ClNO
Exact Mass: 325.12
77.313
77.000
76.679
154.187
149.803
146.365
138.101
133.655
132.219
127.743
127.368
125.253
124.680
123.465
120.219
102.727
43.765
30.306
29.679
21.376

Elemental Composition Report

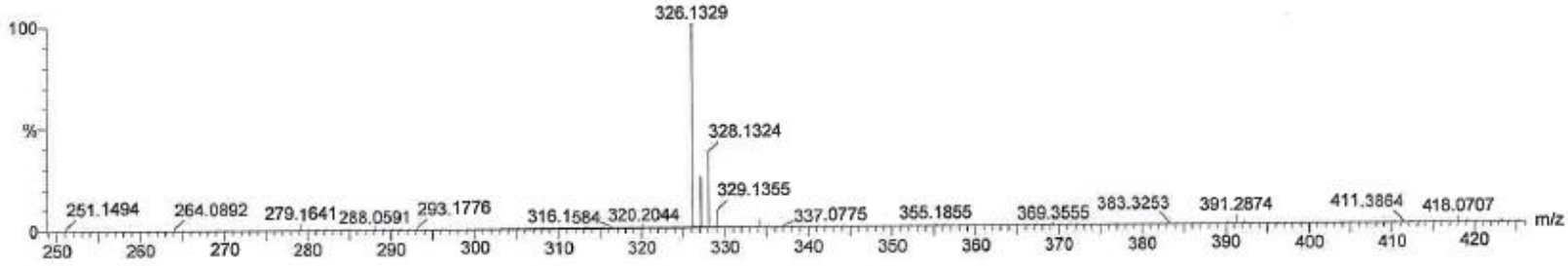
Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

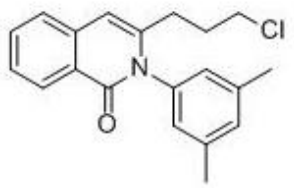
Monoisotopic Mass, Even Electron Ions
85 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-3 Cl: 0-1

B036/CDMA/018
131202011 16 (0.561) Cm (16)

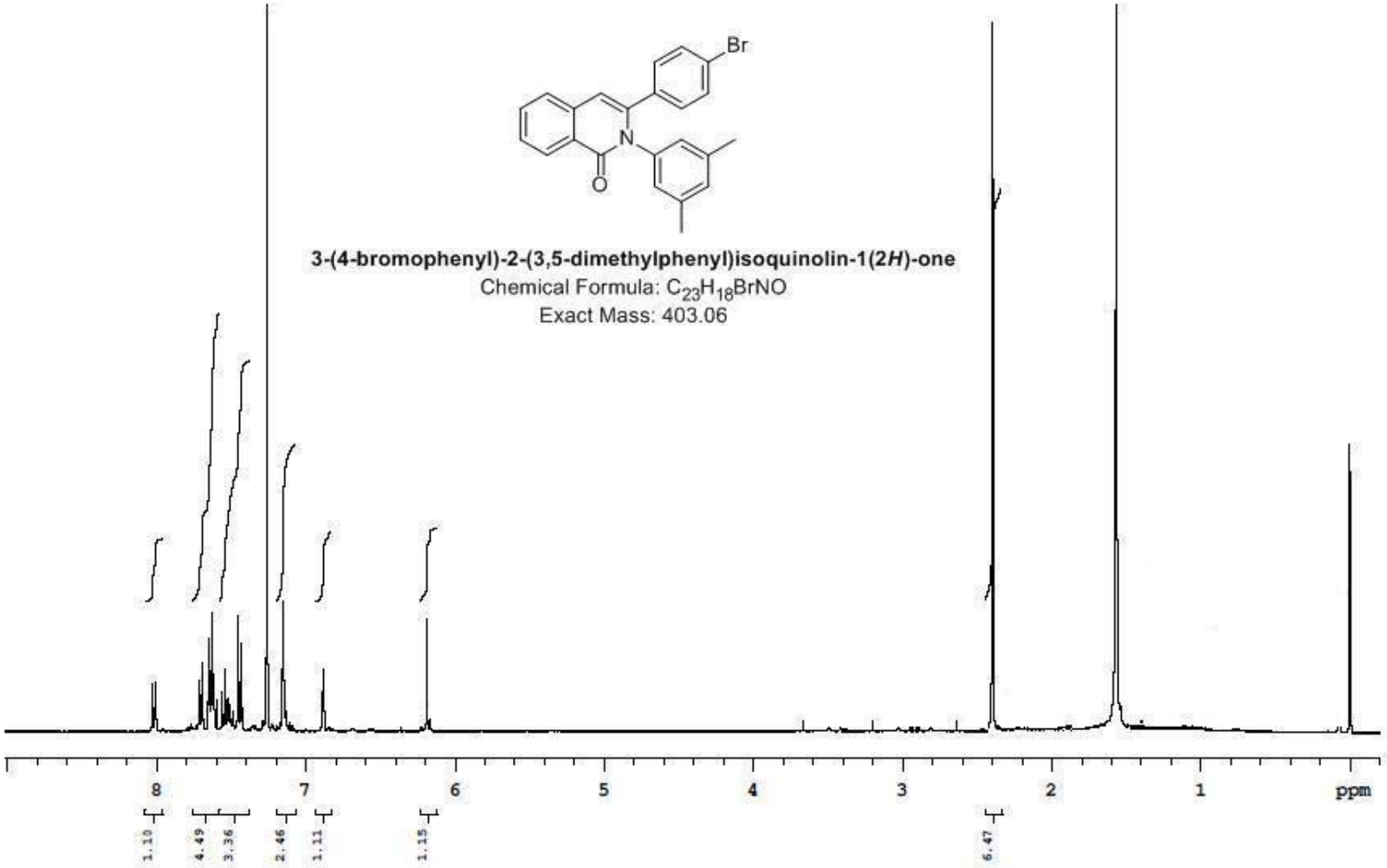
1: TOF MS ES+
4.64e+003

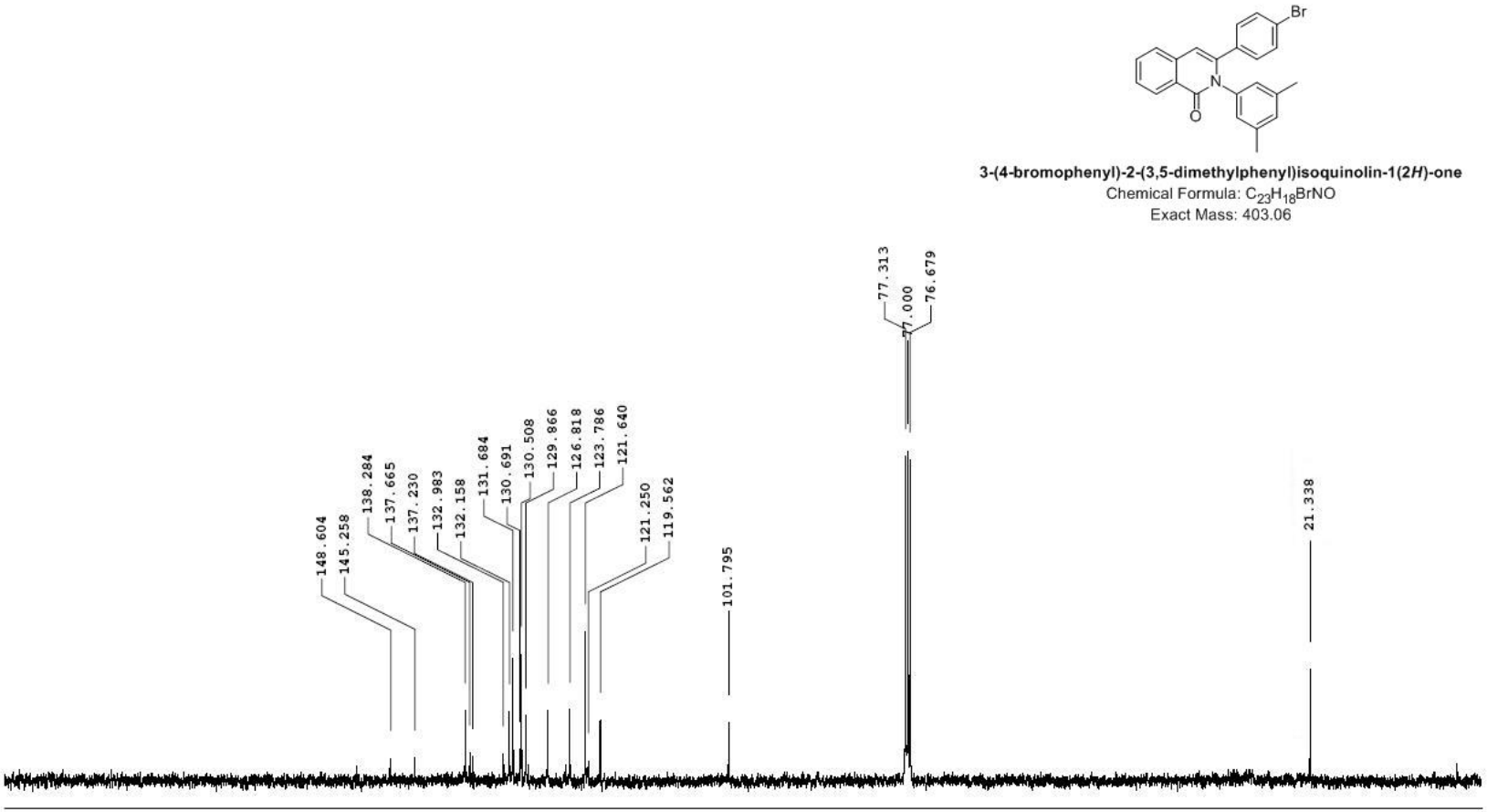


Minimum:				-5.0		
Maximum:		5.0	6.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.1329	326.1312	1.7	5.2	10.5	6.5	C20 H21 N O Cl



3-(3-chloropropyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{20}H_{20}ClNO$
Exact Mass: 325.12


Br
N
O
3-(4-bromophenyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2H)-one
Chemical Formula: C23H18BrNO
Exact Mass: 403.06
8
7
6
5
4
3
2
1
ppm
1.10
4.49
3.36
2.46
1.11
1.15
6.47



3-(4-bromophenyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{23}H_{18}BrNO$

Exact Mass: 403.06

Elemental Composition Report

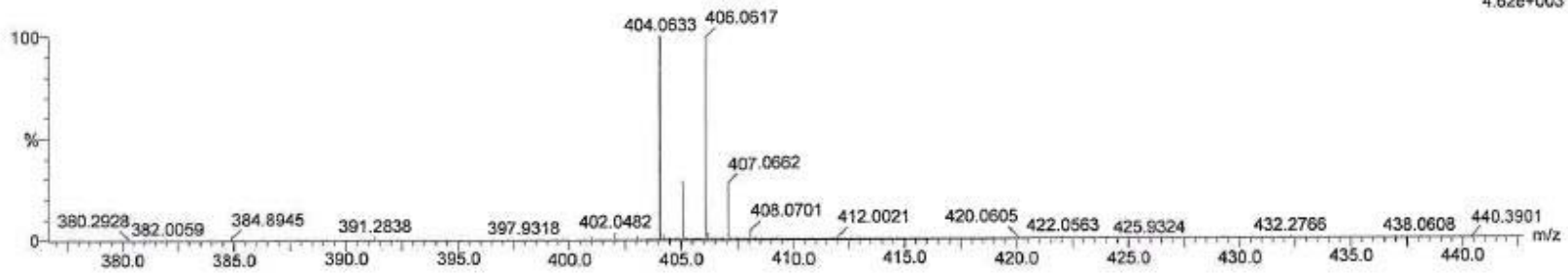
Single Mass Analysis

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

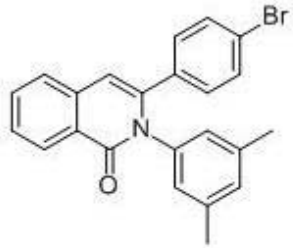
Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-2 O: 0-2 Br: 0-1

B036/CDMA1/019
131129004 8 (0.279) Cm (8:9-15:21)

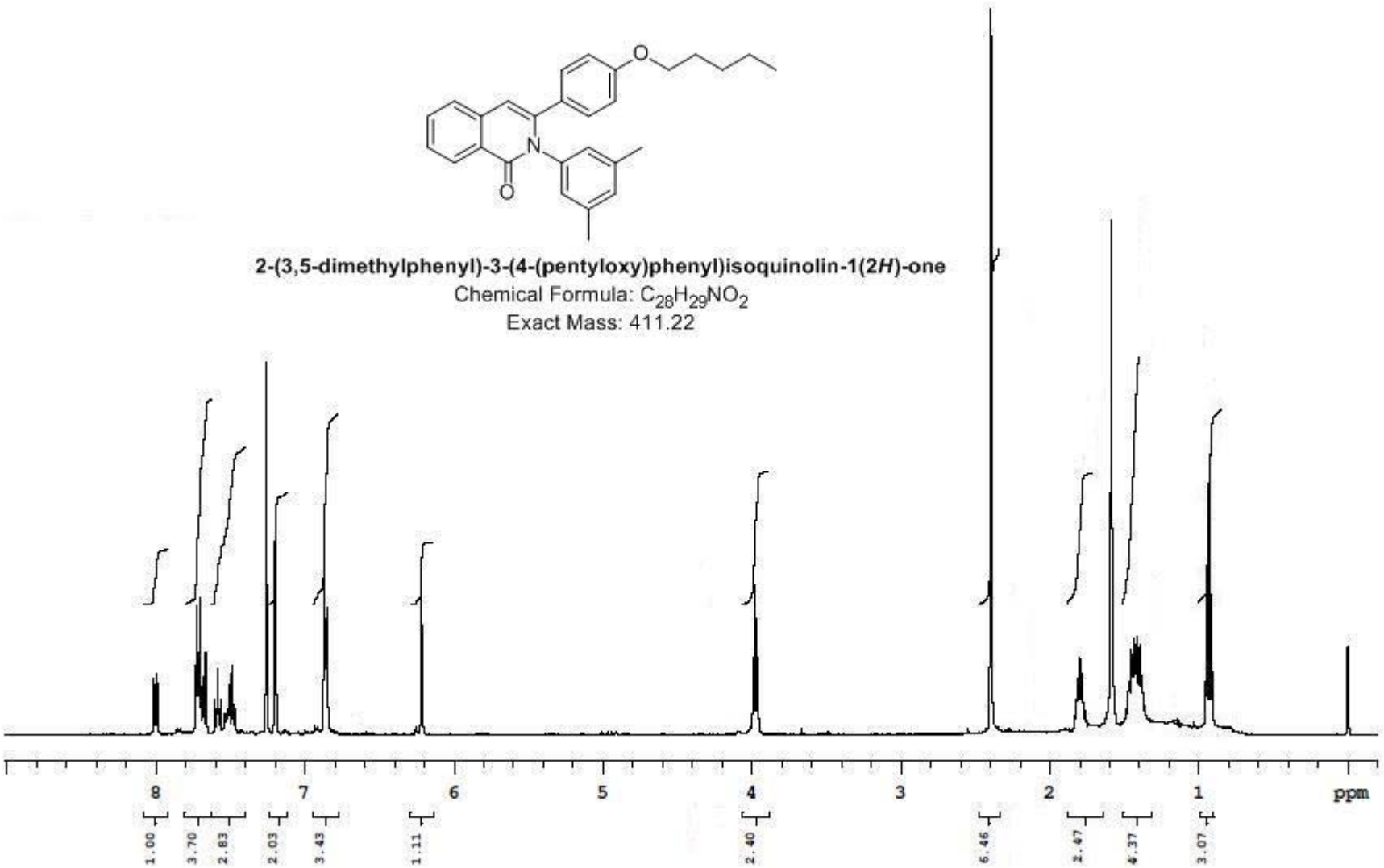
1: TOF MS ES+
4.62e+003



Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
404.0633	404.0650	-1.7	-4.2	14.5	5.4	C23 H19 N O Br



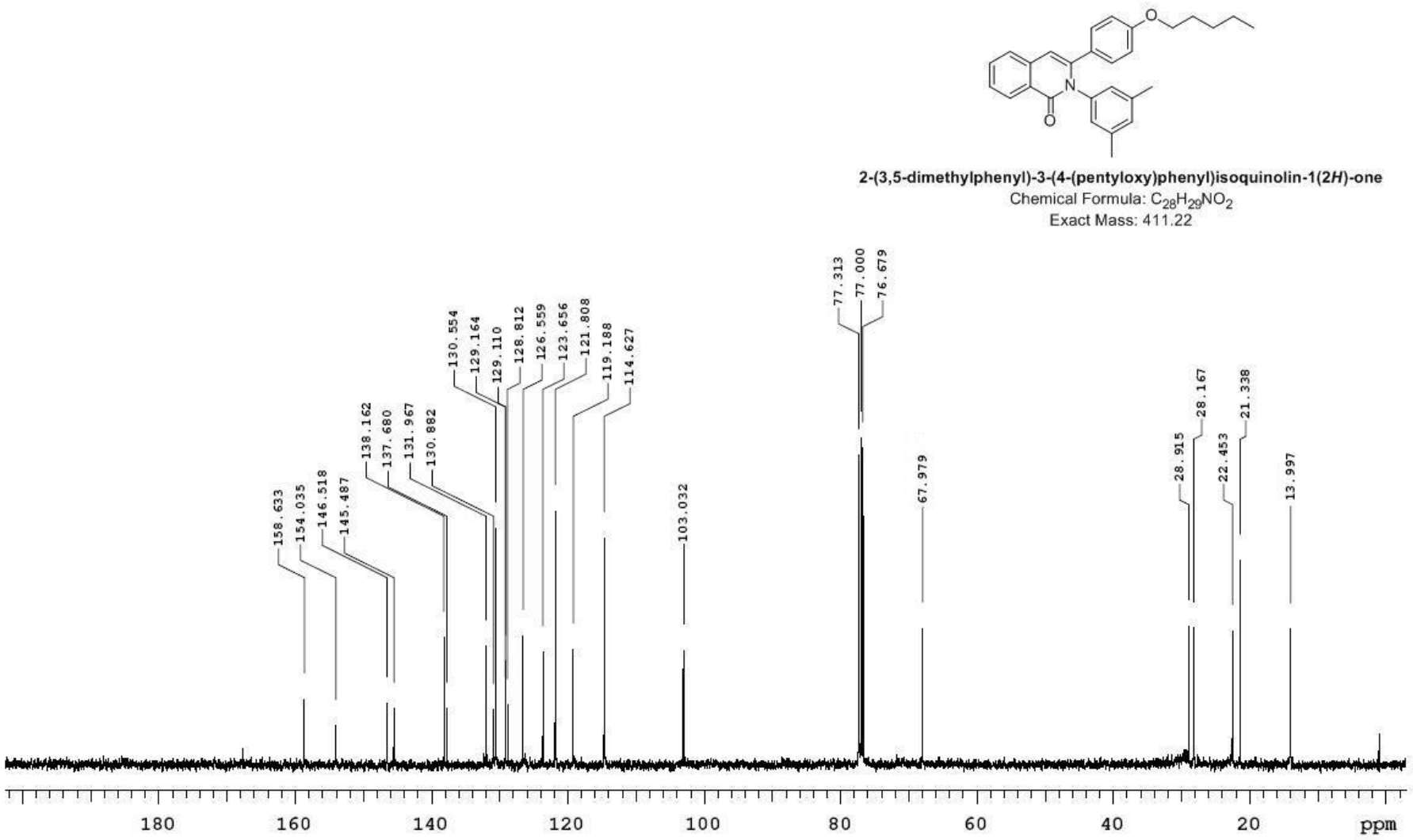
3-(4-bromophenyl)-2-(3,5-dimethylphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{23}H_{18}BrNO$
Exact Mass: 403.06



2-(3,5-dimethylphenyl)-3-(4-(pentyloxy)phenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{28}H_{29}NO_2$

Exact Mass: 411.22


O
N
O
2-(3,5-dimethylphenyl)-3-(4-(pentyloxy)phenyl)isoquinolin-1(2H)-one
Chemical Formula: C28H29NO2
Exact Mass: 411.22
158.633
154.035
146.518
145.487
138.162
137.680
131.967
130.882
130.554
129.164
129.110
128.812
126.559
123.656
121.808
119.188
114.627
103.032
77.313
77.000
76.679
67.979
28.915
28.167
22.453
21.338
13.997
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

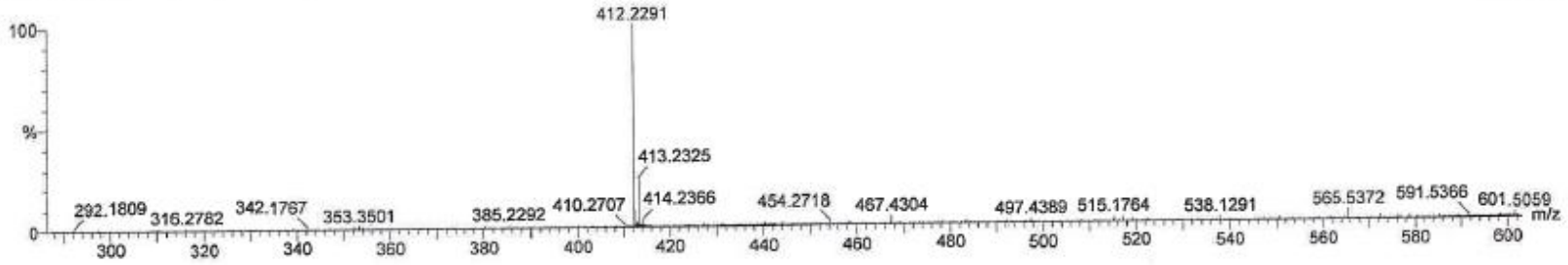
Single Mass Analysis

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

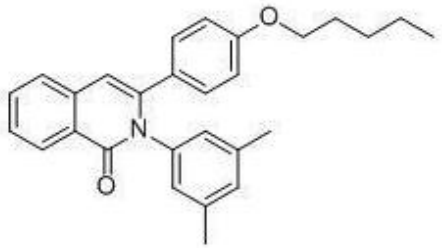
Monoisotopic Mass, Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-3

B036/CDMA/020
131202012 21 (0.760) Cm (21:23-29:35)

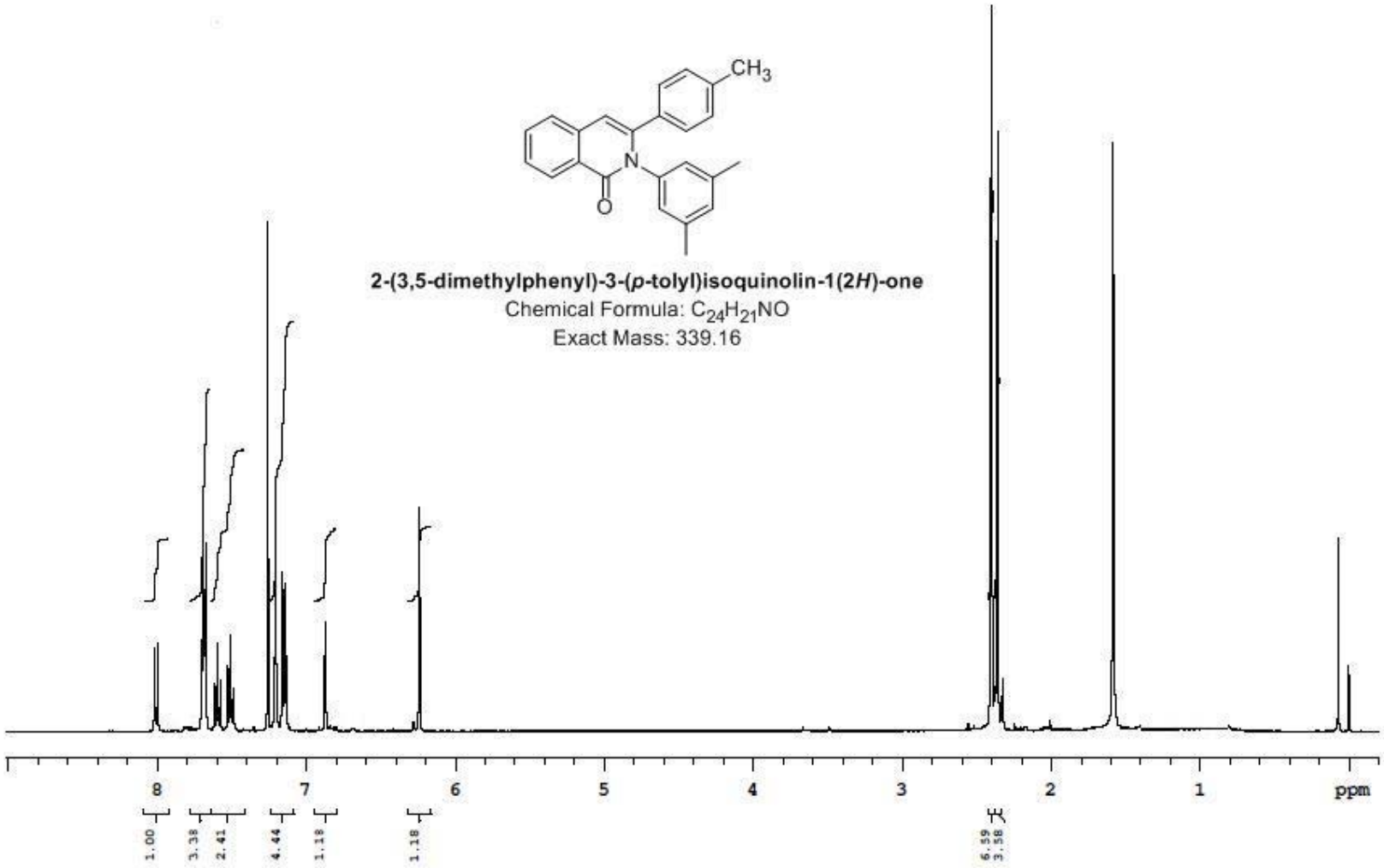
1: TOF MS ES+
1.24e+003



Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
412.2291	412.2277	1.4	3.4	14.5	13.5	C28 H30 N O2



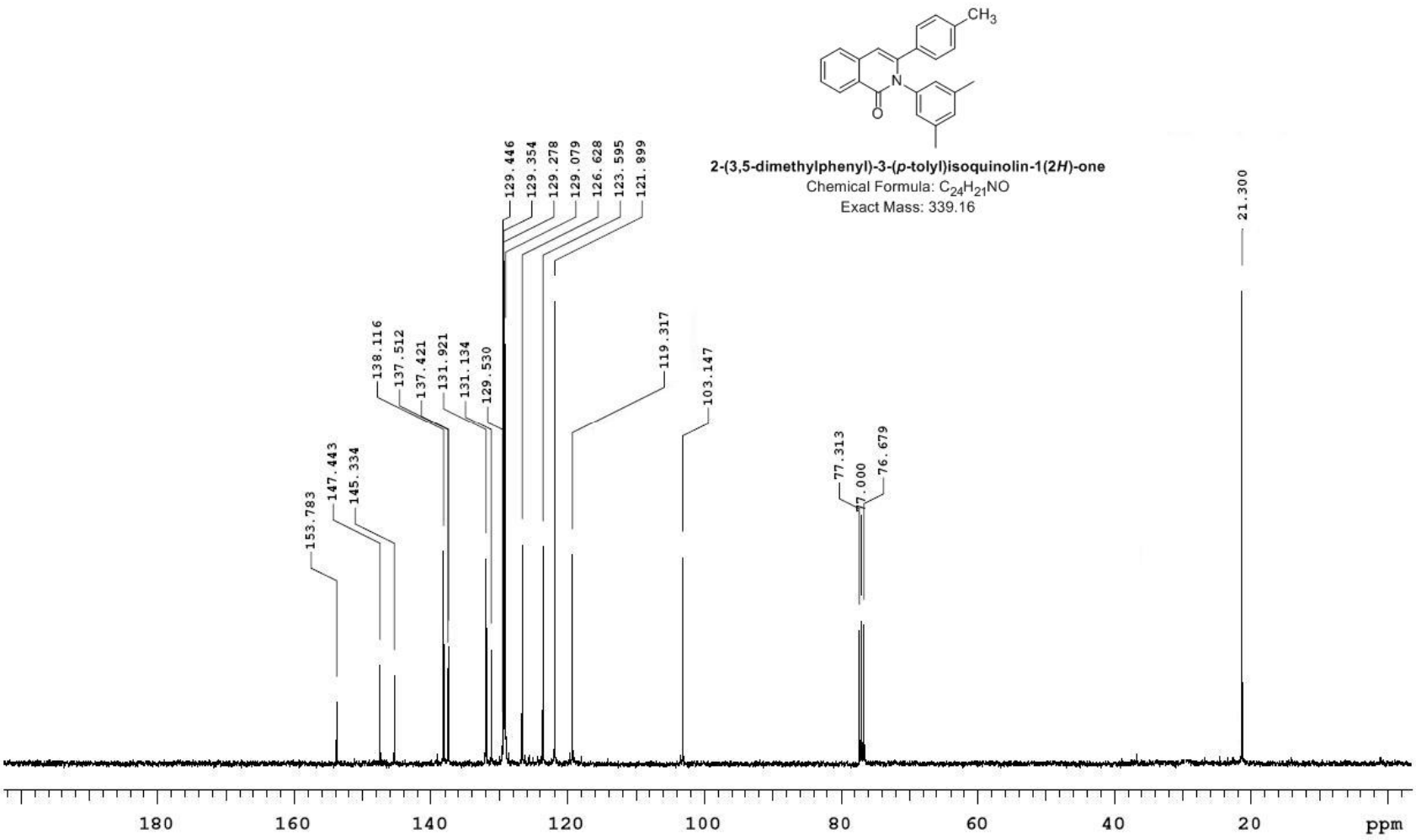
2-(3,5-dimethylphenyl)-3-(4-(pentyloxy)phenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{28}H_{29}NO_2$
Exact Mass: 411.22



2-(3,5-dimethylphenyl)-3-(*p*-tolyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{24}H_{21}NO$

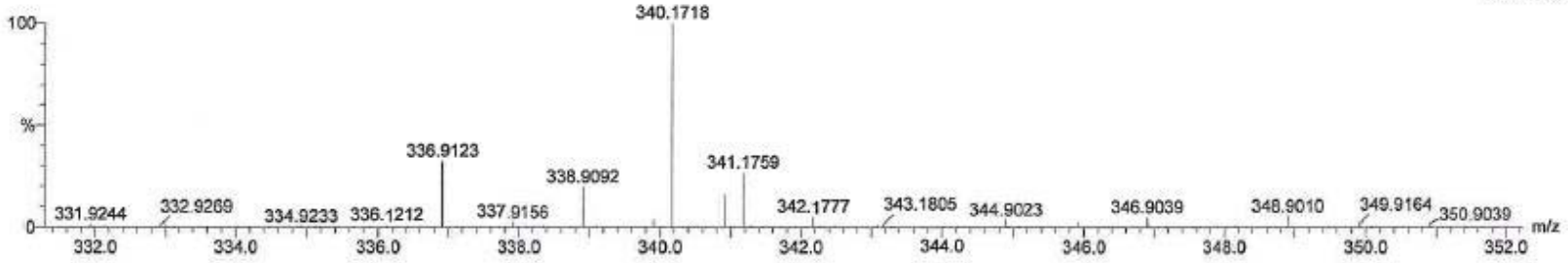
Exact Mass: 339.16


CH3
N
O
2-(3,5-dimethylphenyl)-3-(p-tolyl)isoquinolin-1(2H)-one
Chemical Formula: C24H21NO
Exact Mass: 339.16
153.783
147.443
145.334
138.116
137.512
137.421
131.921
131.134
129.530
129.446
129.354
129.278
129.079
126.628
123.595
121.899
119.317
103.147
77.313
77.000
76.679
21.300
180
160
140
120
100
80
60
40
20
ppm

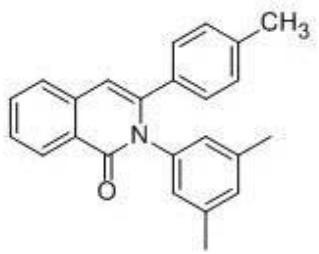
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-3
B036/CDMA/021
131203001 4 (0.138) Cm (4:6)

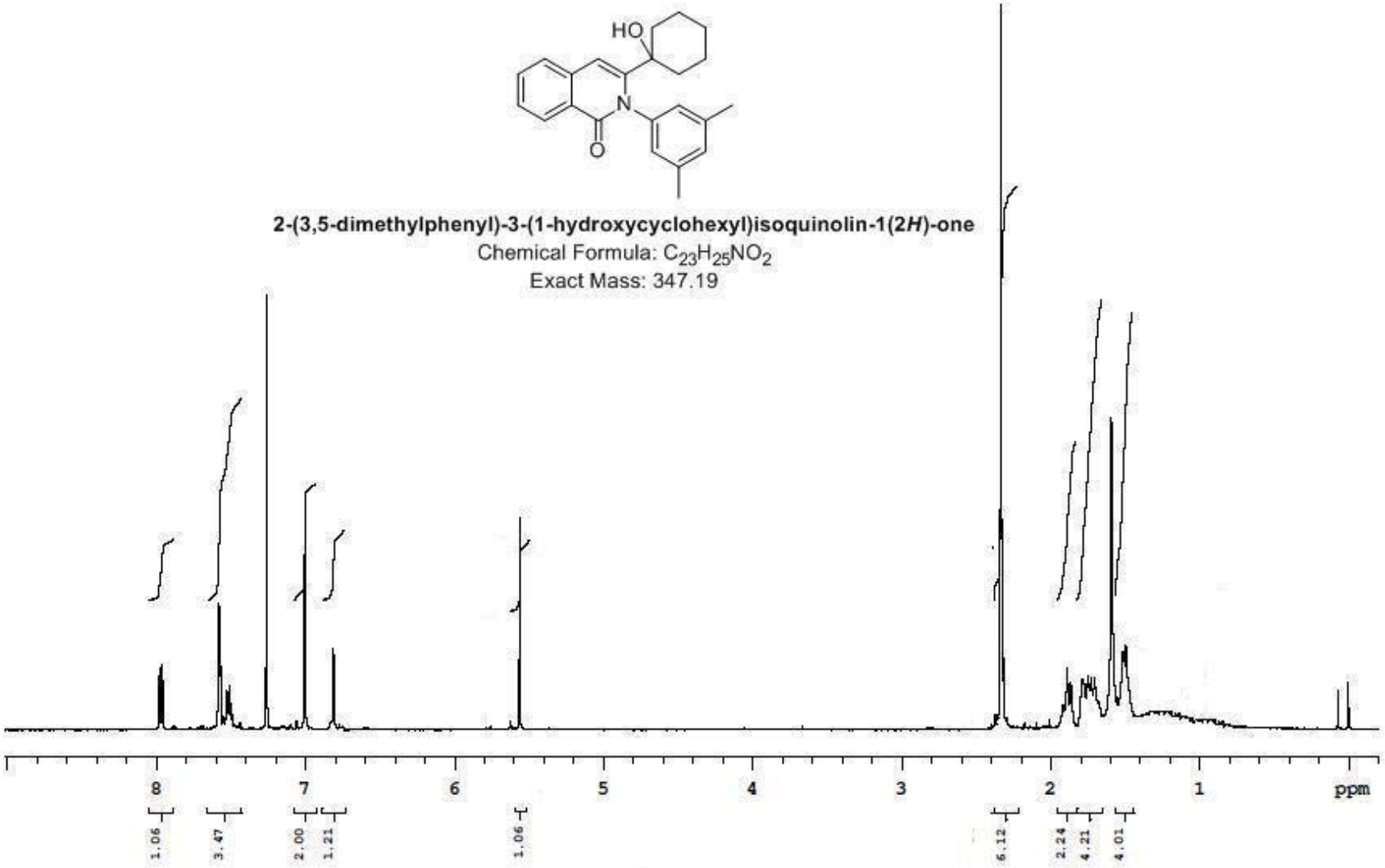
1: TOF MS ES+
1.61e+003



Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
340.1718	340.1701	1.7	5.0	14.5	2.4	C24 H22 N O



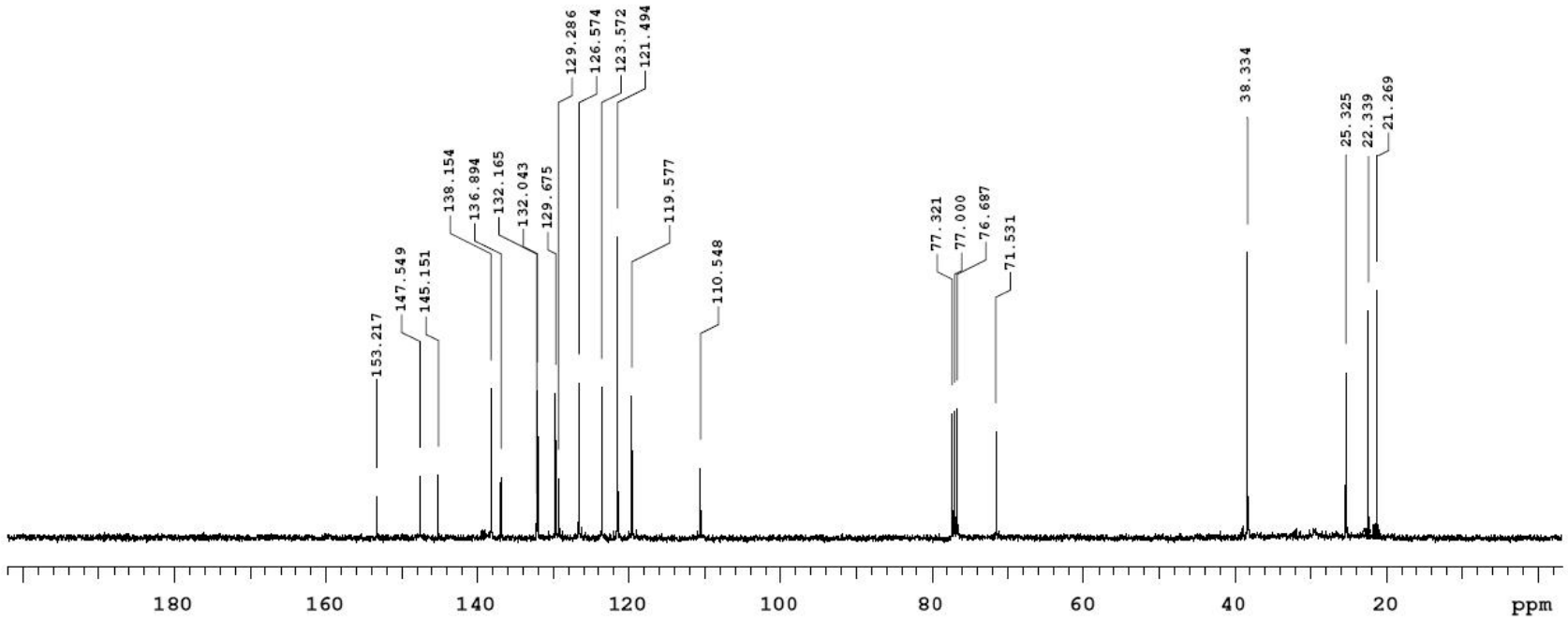
2-(3,5-dimethylphenyl)-3-(*p*-tolyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{24}H_{21}NO$
Exact Mass: 339.16


HO
N
O
2-(3,5-dimethylphenyl)-3-(1-hydroxycyclohexyl)isoquinolin-1(2H)-one
Chemical Formula: C23H25NO2
Exact Mass: 347.19
8
7
6
5
4
3
2
1
ppm
1.06
3.47
2.00
1.21
1.06
6.12
2.24
4.21
4.01

2-(3,5-dimethylphenyl)-3-(1-hydroxycyclohexyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{23}H_{25}NO_2$

Exact Mass: 347.19



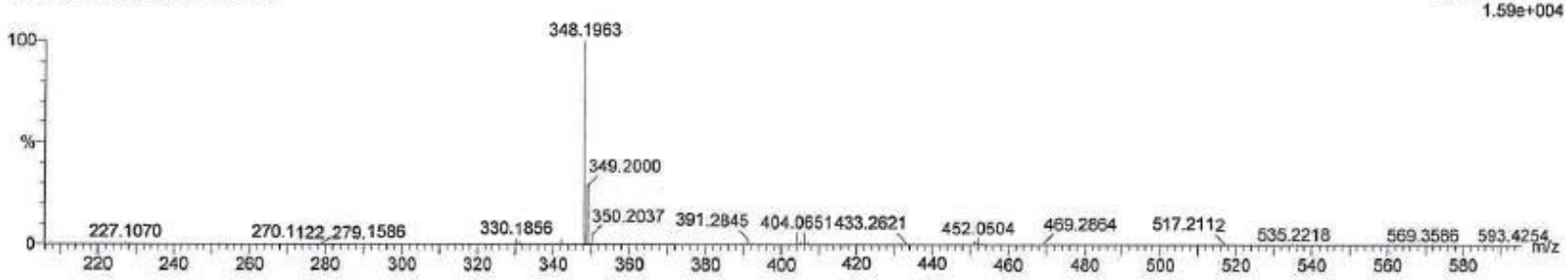
Elemental Composition Report

Single Mass Analysis

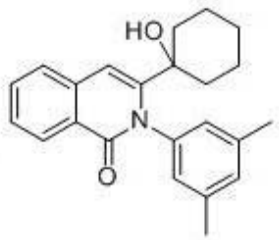
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-30 N: 0-2 O: 0-2
B036/CDMA1/022
131129007 9 (0.338) Cm (9:11-1:2)

1: TOF MS ES+
1.59e+004

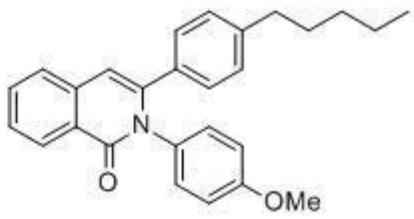


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.1963	348.1964	-0.1	-0.3	11.5	19.6	C23 H26 N O2



2-(3,5-dimethylphenyl)-3-(1-hydroxycyclohexyl)isoquinolin-1(2*H*)-one

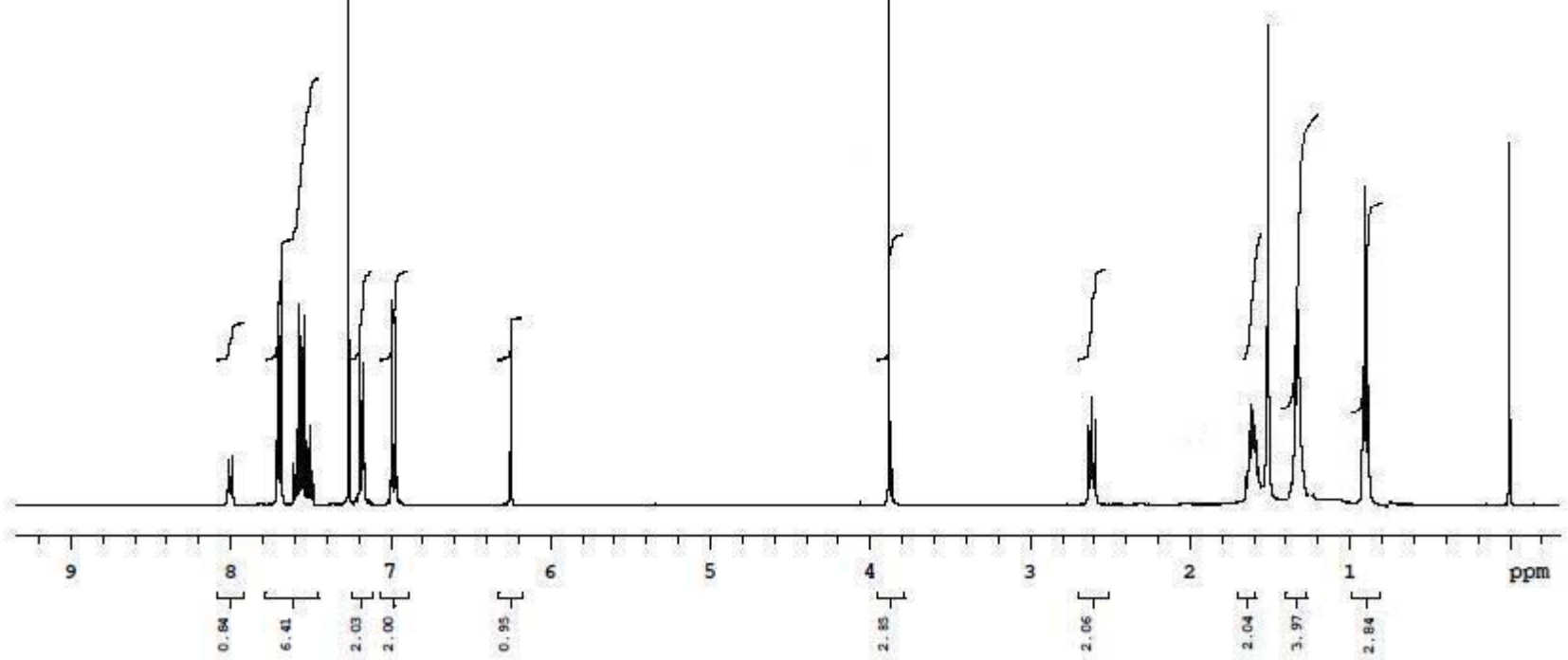
Chemical Formula: $C_{23}H_{25}NO_2$
Exact Mass: 347.19

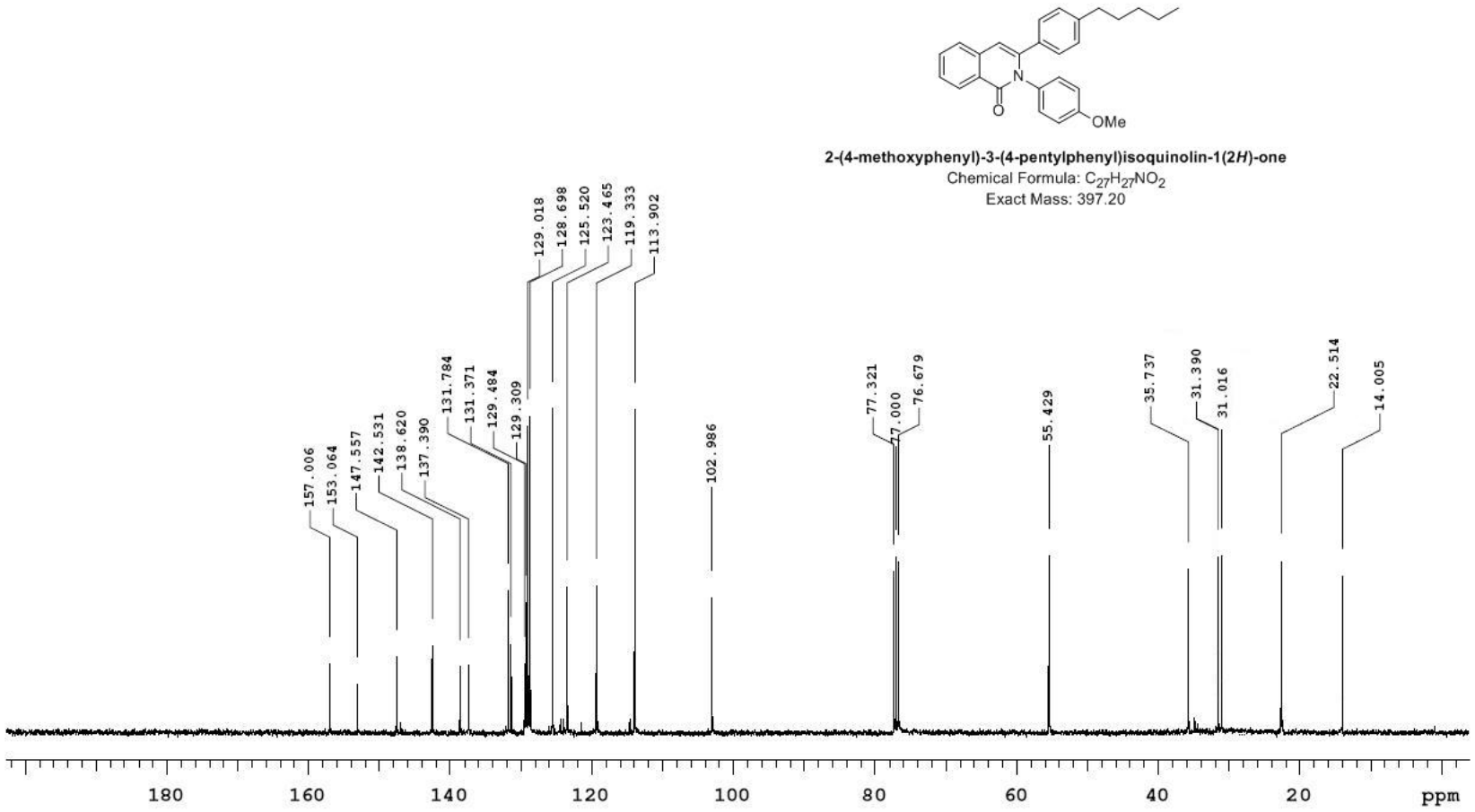


2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{27}H_{27}NO_2$

Exact Mass: 397.20



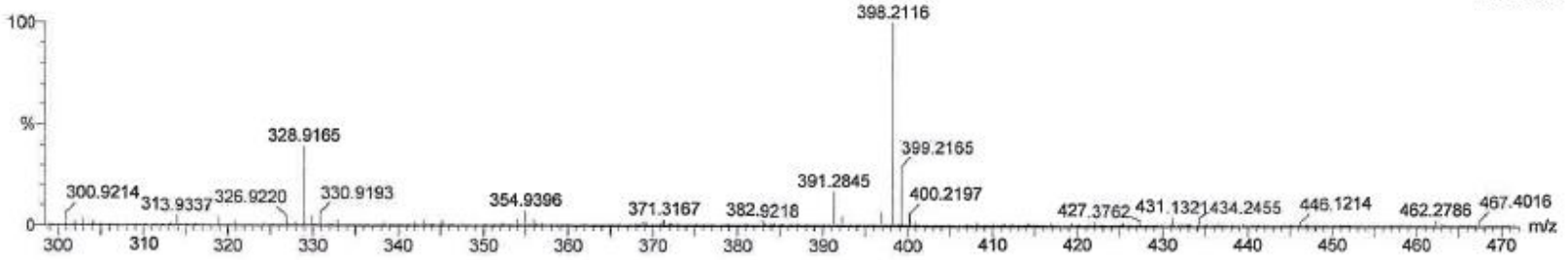

OMe
2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2H)-one
Chemical Formula: C27H27NO2
Exact Mass: 397.20
157.006
153.064
147.557
142.531
138.620
137.390
131.784
131.371
129.484
129.309
129.018
128.698
125.520
123.465
119.333
113.902
102.986
77.321
77.000
76.679
55.429
35.737
31.390
31.016
22.514
14.005
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

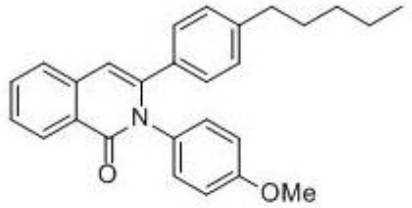
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-2 O: 0-2
B036/CVIG1/031
131202002 10 (0.365) Cm (9:14-1:5)

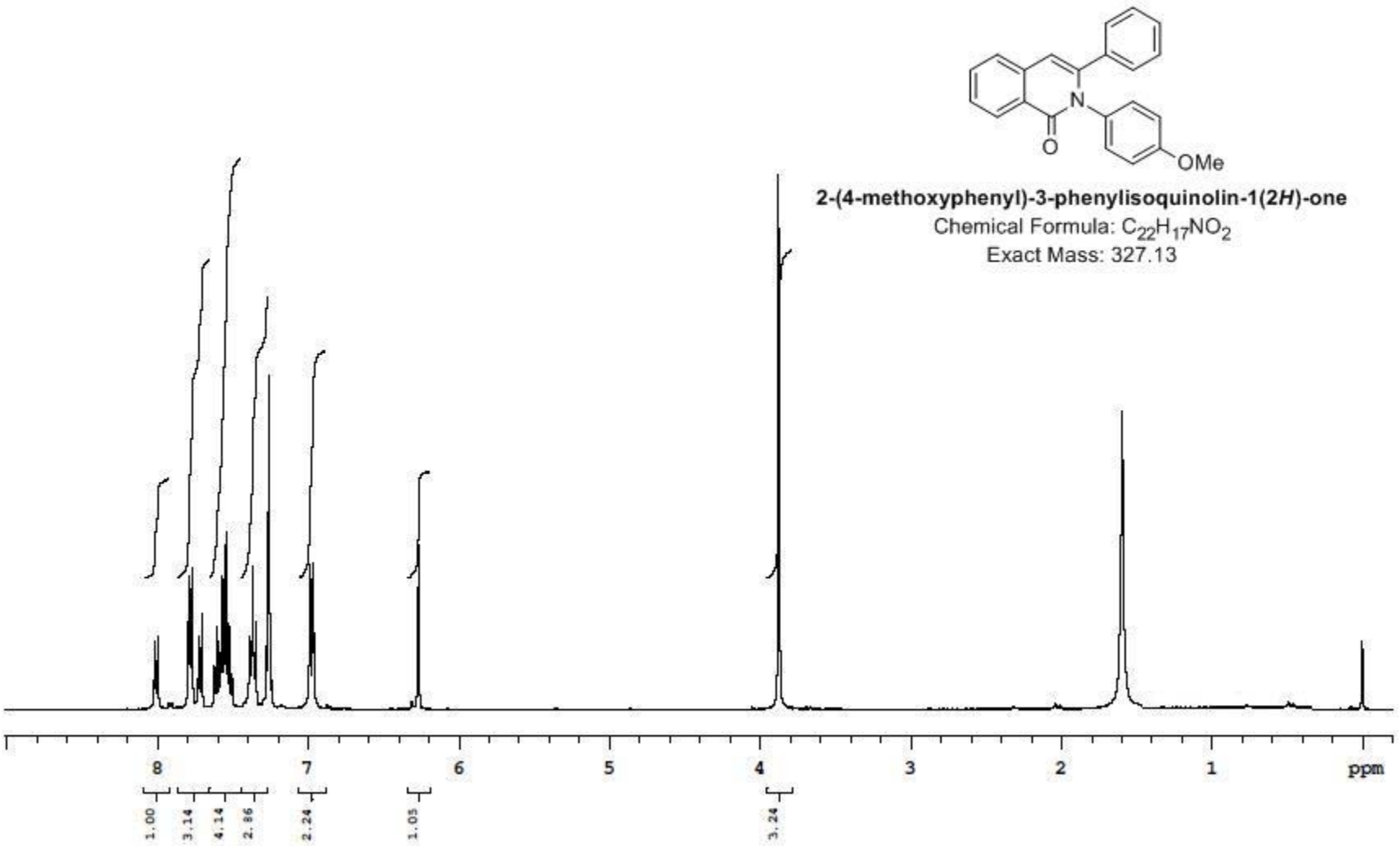
1: TOF MS ES+
2.99e+003

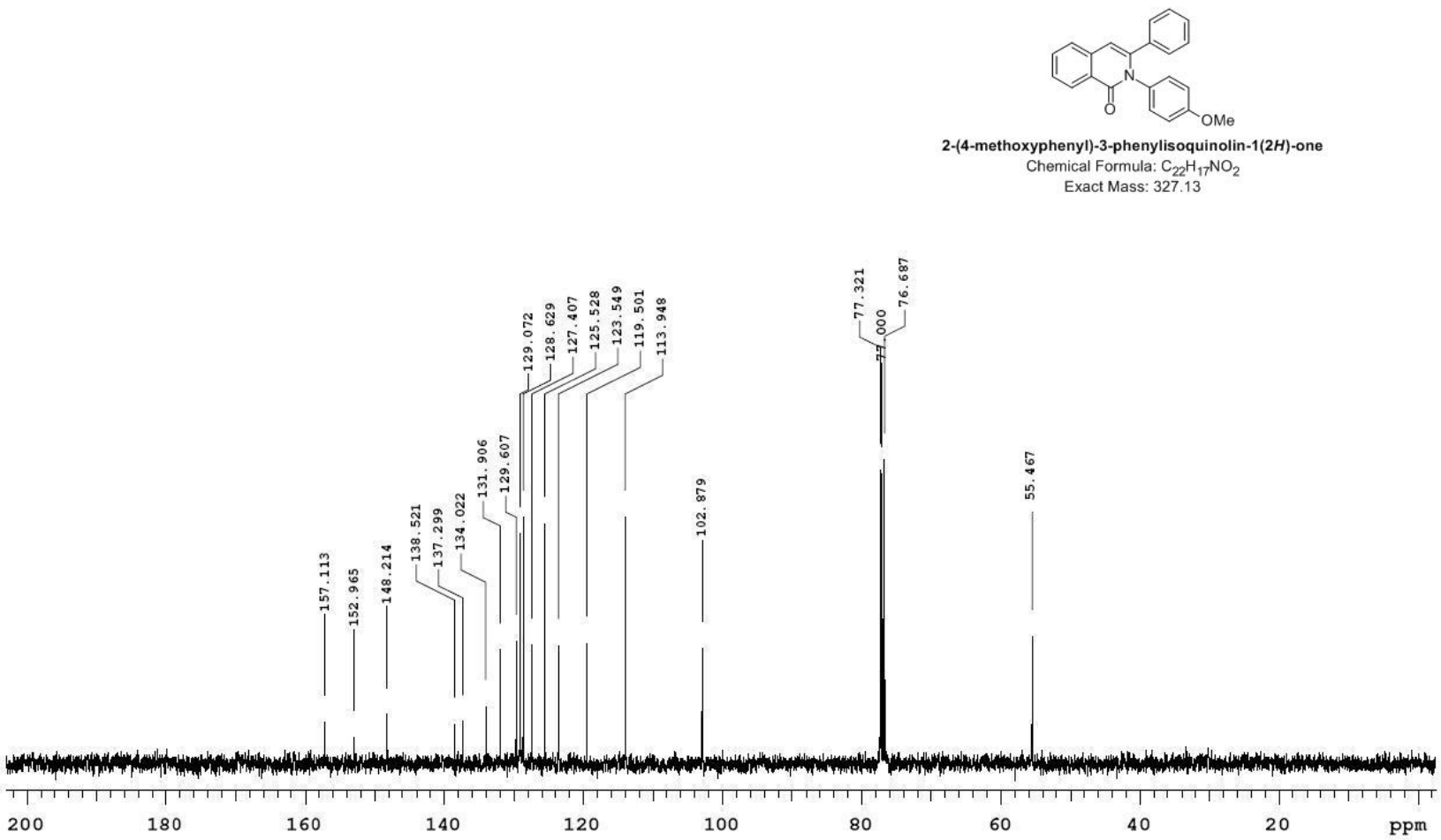


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
398.2116	398.2120	-0.4	-1.0	14.5	3.1	C27 H28 N O2



2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{27}H_{27}NO_2$
Exact Mass: 397.20


N
O
OMe
2-(4-methoxyphenyl)-3-phenylisoquinolin-1(2H)-one
Chemical Formula: C22H17NO2
Exact Mass: 327.13
8
7
6
5
4
3
2
1
ppm
1.00
3.14
4.14
2.86
2.24
1.05
3.24


OMe
2-(4-methoxyphenyl)-3-phenylisoquinolin-1(2H)-one
Chemical Formula: C22H17NO2
Exact Mass: 327.13
157.113
152.965
148.214
138.521
137.299
134.022
131.906
129.607
129.072
128.629
127.407
125.528
123.549
119.501
113.948
102.879
77.321
77.000
76.687
55.467
200
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

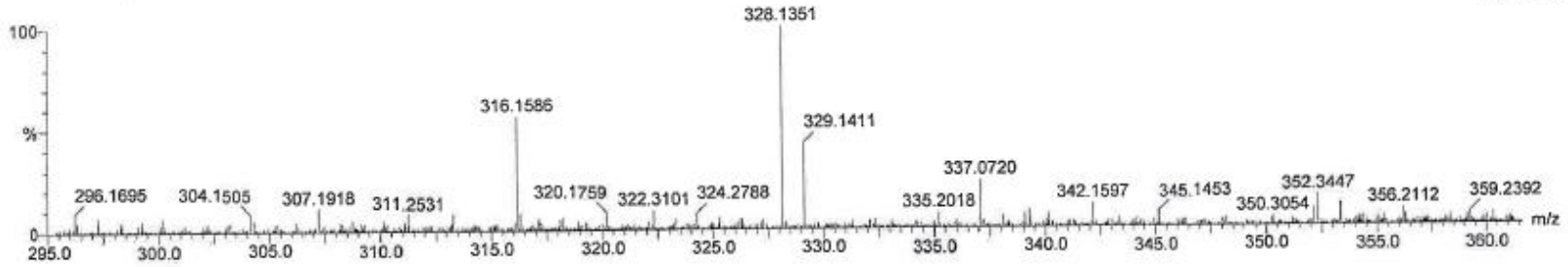
Single Mass Analysis

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

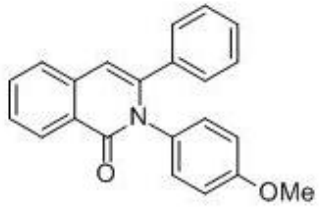
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-2 O: 0-2

B036/CVIG1/032
131202003 22 (0.788) Cm (19:23-31:33)

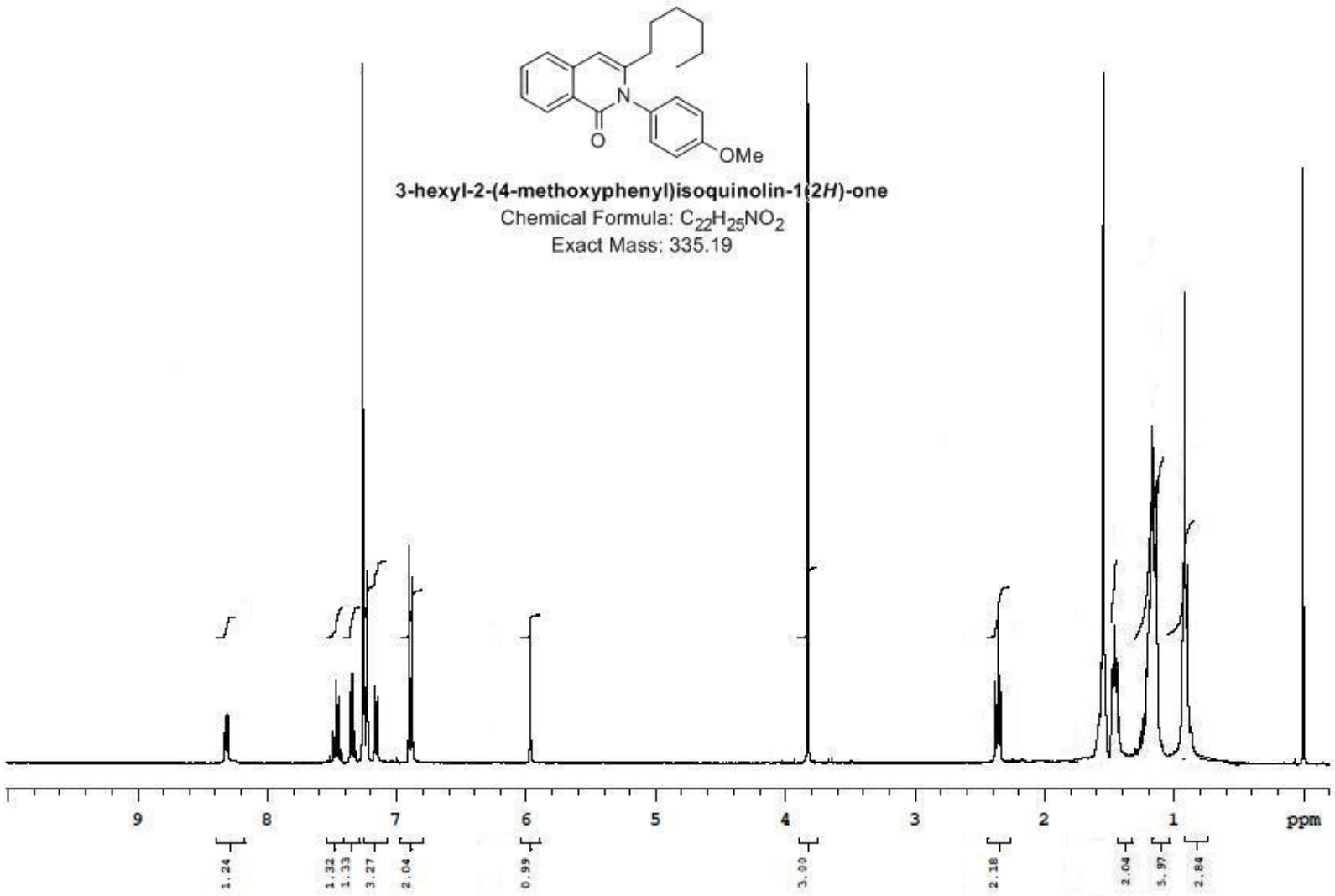
1: TOF MS ES+
2.53e+002

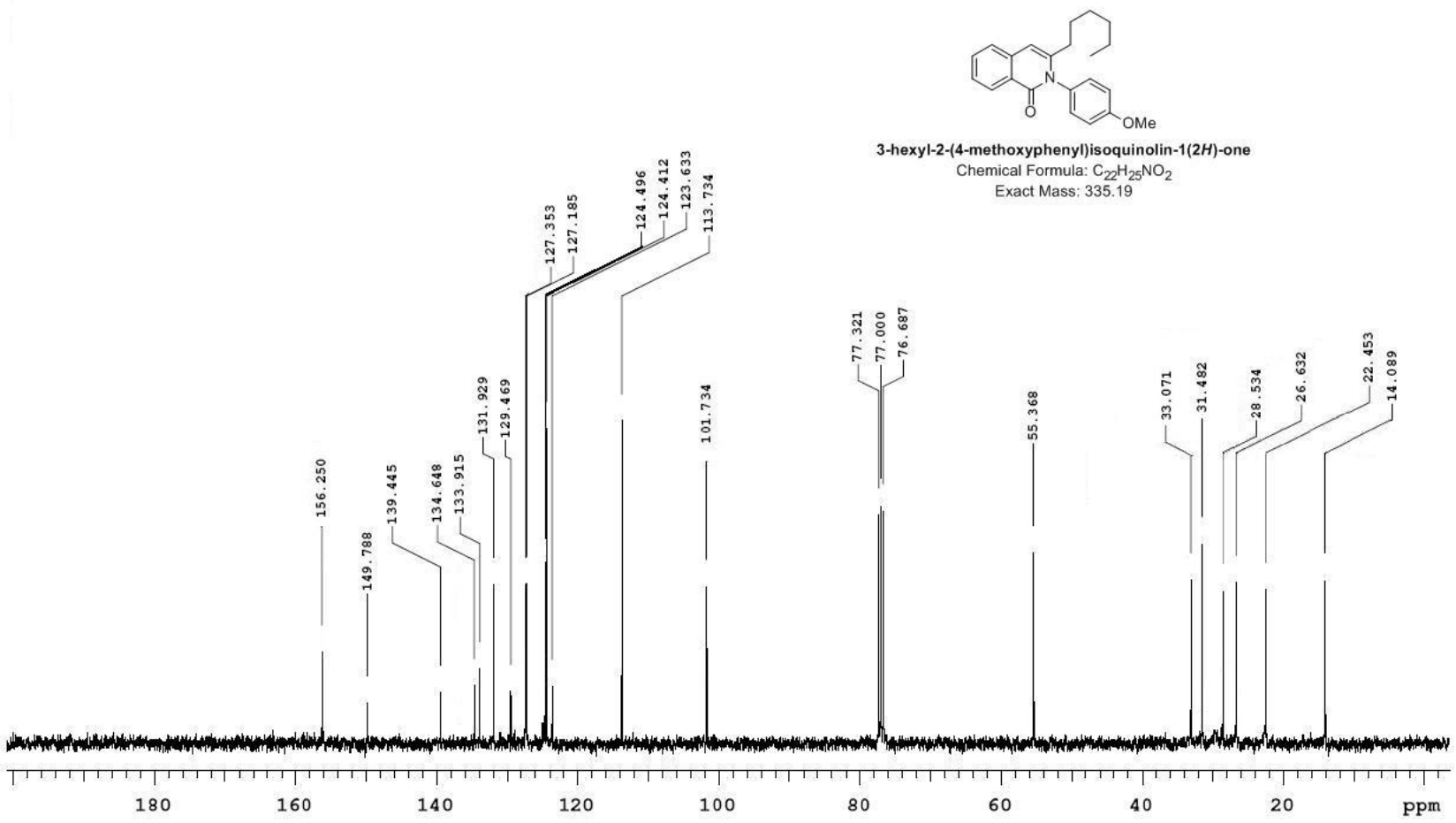


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.1351	328.1338	1.3	4.0	14.5	8.8	C22 H18 N O2



2-(4-methoxyphenyl)-3-phenylisoquinolin-1(2*H*)-one
Chemical Formula: $C_{22}H_{17}NO_2$
Exact Mass: 327.13


O
N
OMe
3-hexyl-2-(4-methoxyphenyl)isoquinolin-1(2H)-one
Chemical Formula: C22H25NO2
Exact Mass: 335.19
9
8
7
6
5
4
3
2
1
ppm
1.24
1.32
1.33
3.27
2.04
0.99
3.00
2.18
2.04
5.97
2.84


OMe
3-hexyl-2-(4-methoxyphenyl)isoquinolin-1(2H)-one
Chemical Formula: C22H25NO2
Exact Mass: 335.19
156.250
149.788
139.445
134.648
133.915
131.929
129.469
127.353
127.185
124.496
124.412
123.633
113.734
101.734
77.321
77.000
76.687
55.368
33.071
31.482
28.534
26.632
22.453
14.089
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

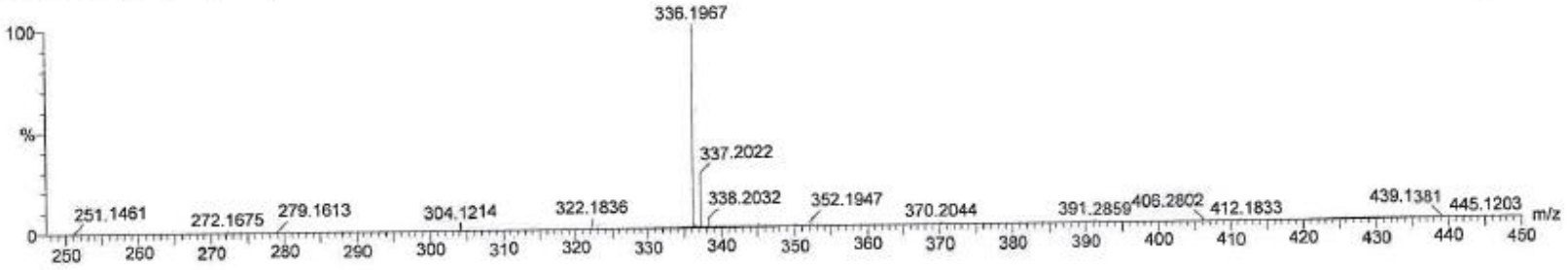
Single Mass Analysis

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

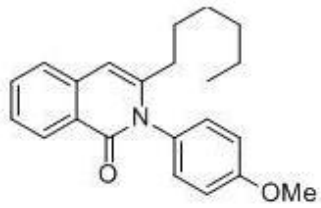
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-2 O: 0-2

B036/CVIG1/033
131202004 14 (0.506) Cm (14:15-1)

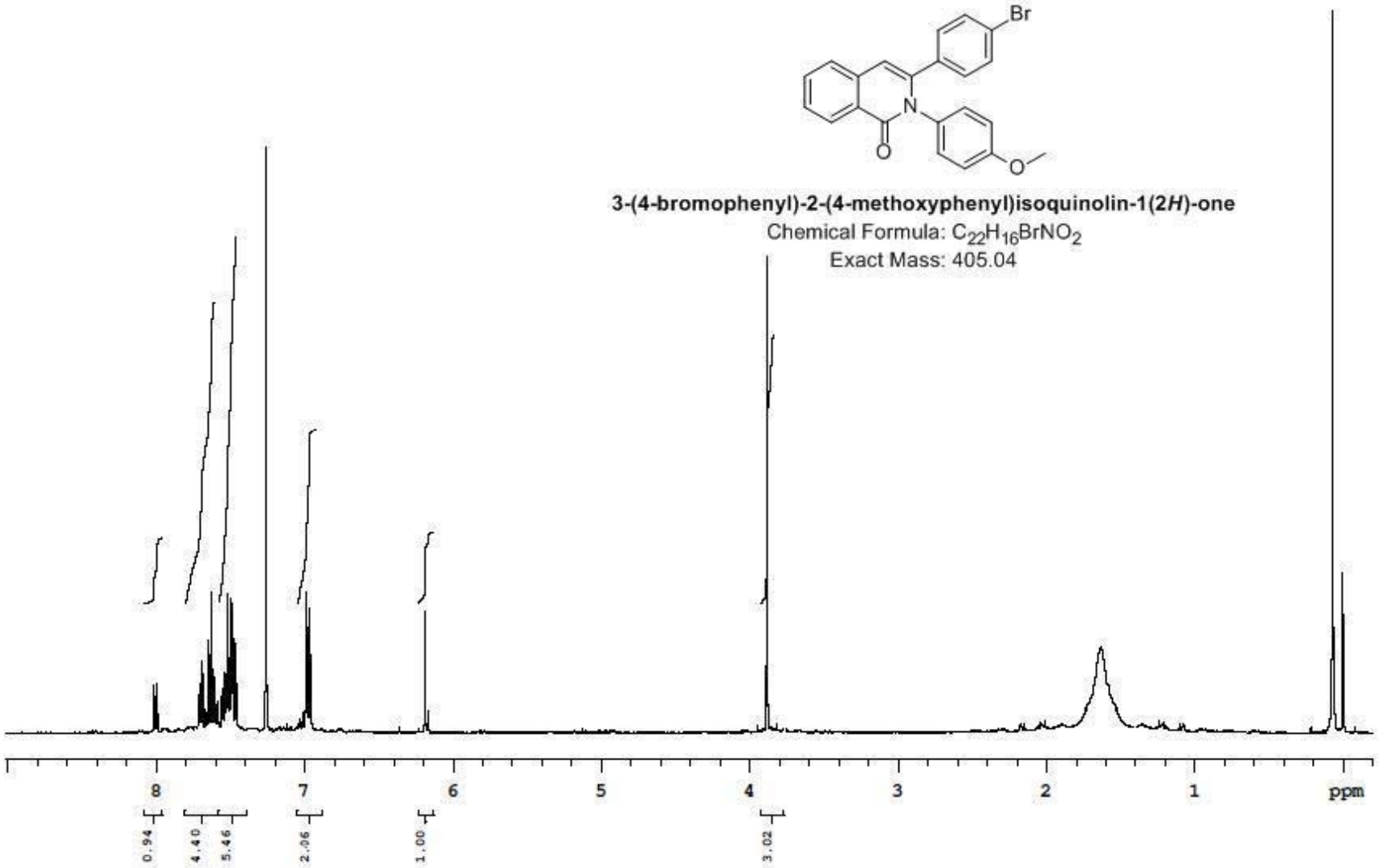
1: TOF MS ES+
1.01e+004

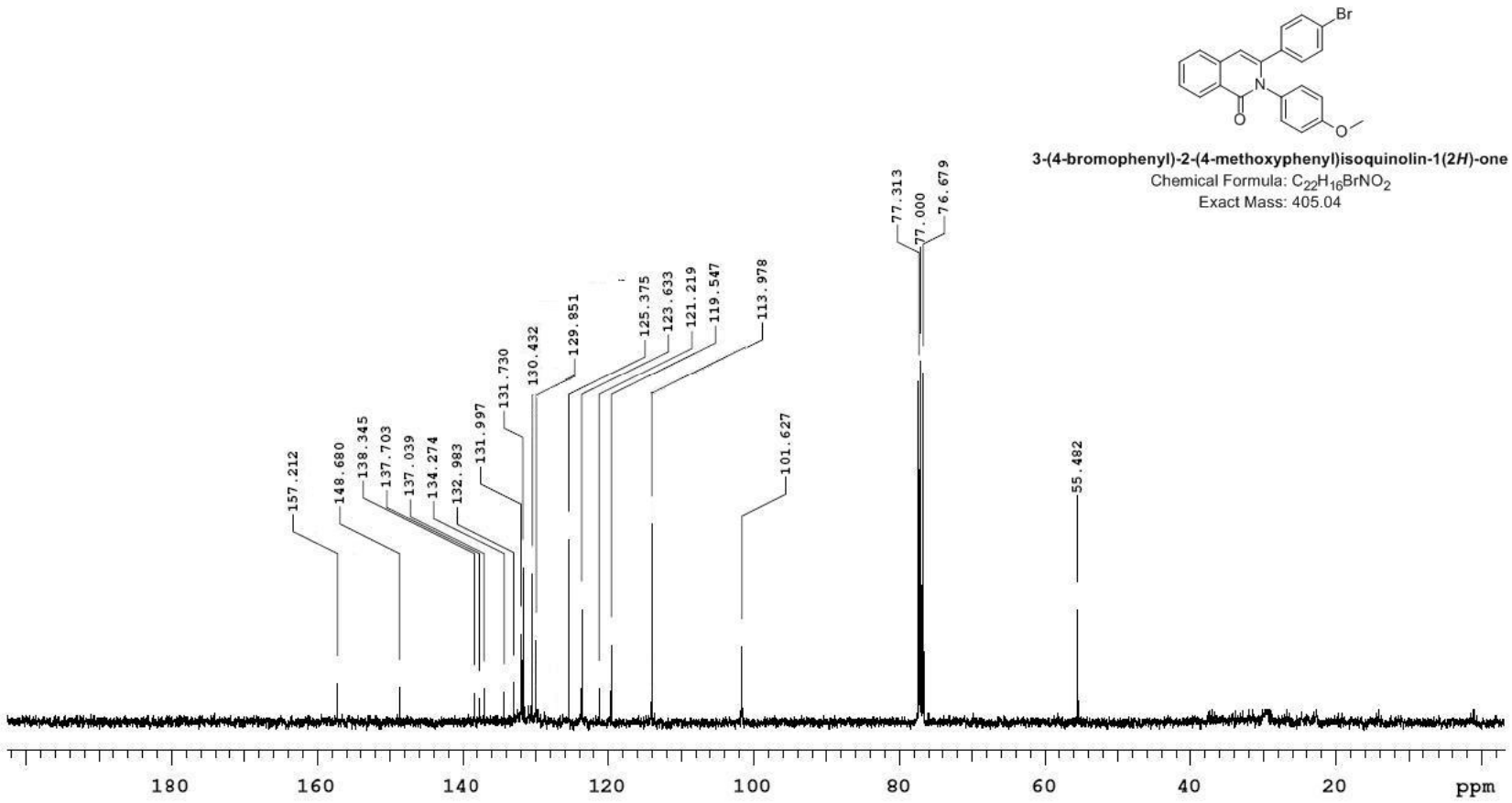


Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
336.1967	336.1964	0.3	0.9	10.5	6.0	C22 H26 N O2



3-hexyl-2-(4-methoxyphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{22}H_{25}NO_2$
Exact Mass: 335.19


Br
N
O
O
3-(4-bromophenyl)-2-(4-methoxyphenyl)isoquinolin-1(2H)-one
Chemical Formula: C22H16BrNO2
Exact Mass: 405.04
8
7
6
5
4
3
2
1
ppm
0.94
4.40
5.46
2.06
1.00
3.02


Br
N
O
O
3-(4-bromophenyl)-2-(4-methoxyphenyl)isoquinolin-1(2H)-one
Chemical Formula: C22H16BrNO2
Exact Mass: 405.04
157.212
148.680
138.345
137.703
137.039
134.274
132.983
131.997
131.730
130.432
129.851
125.375
123.633
121.219
119.547
113.978
101.627
77.313
77.000
76.679
55.482
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

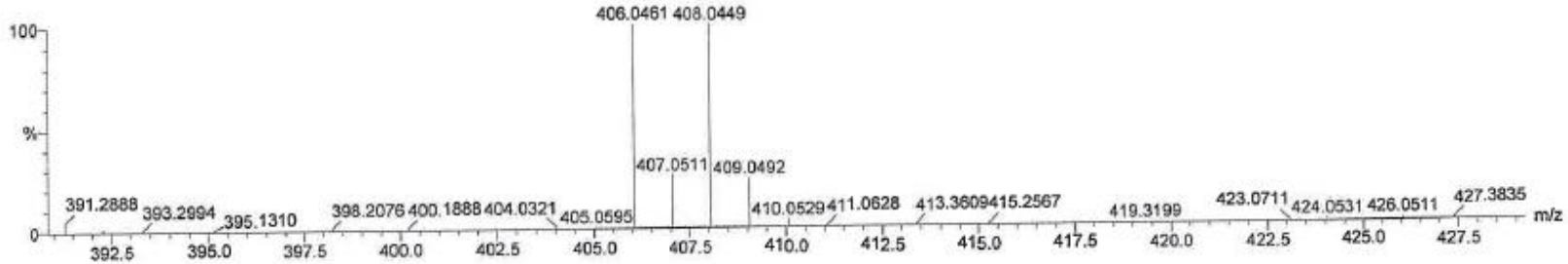
Single Mass Analysis

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

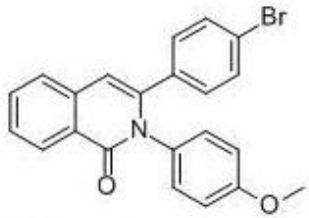
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-3 O: 0-2 Br: 0-1

B036/CVIG1/035
131202005 9 (0.338) Cm (9:10)

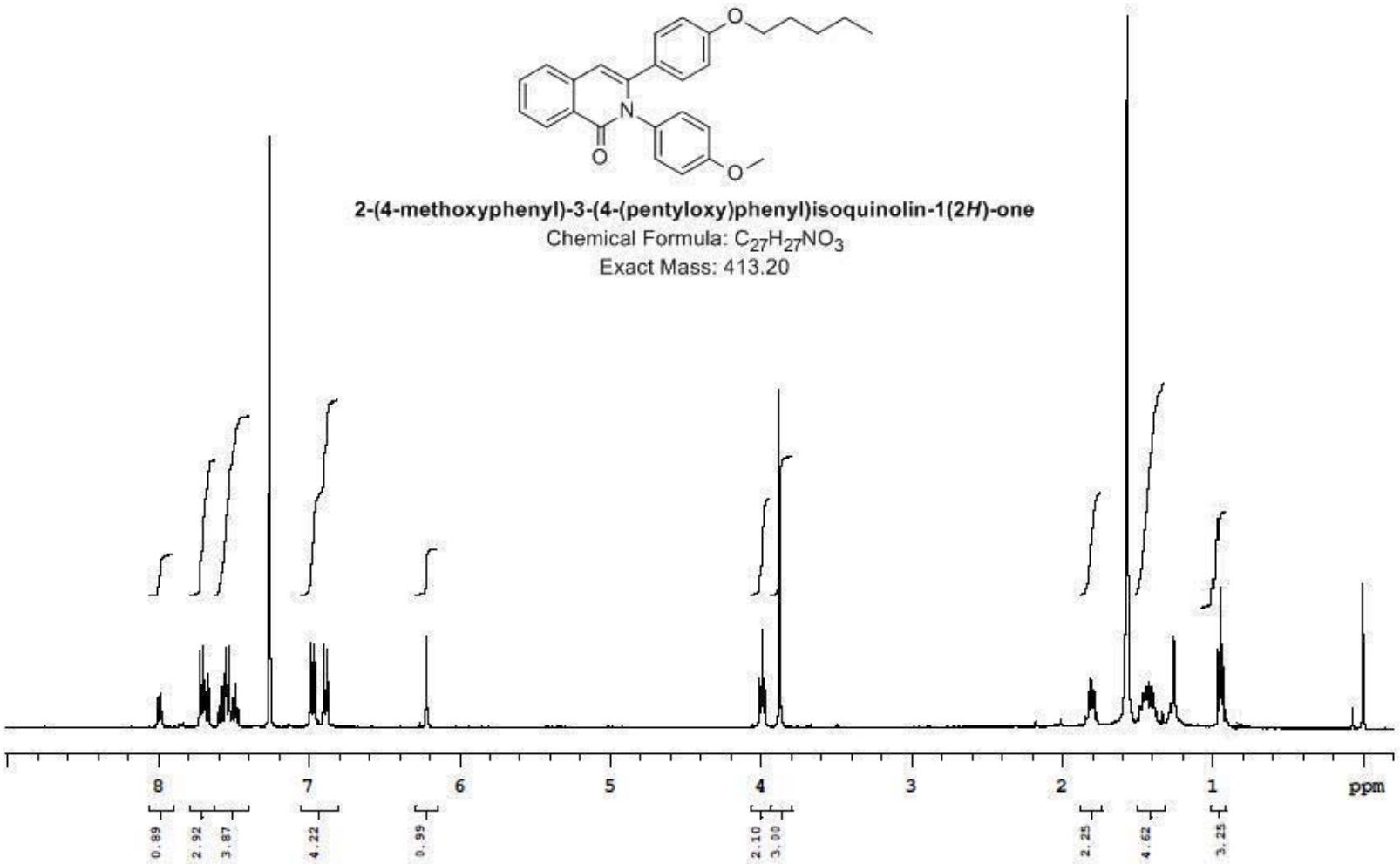
1: TOF MS ES+
6.25e+003



Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
406.0461	406.0443	1.8	4.4	14.5	2.4	C22 H17 N O2 Br



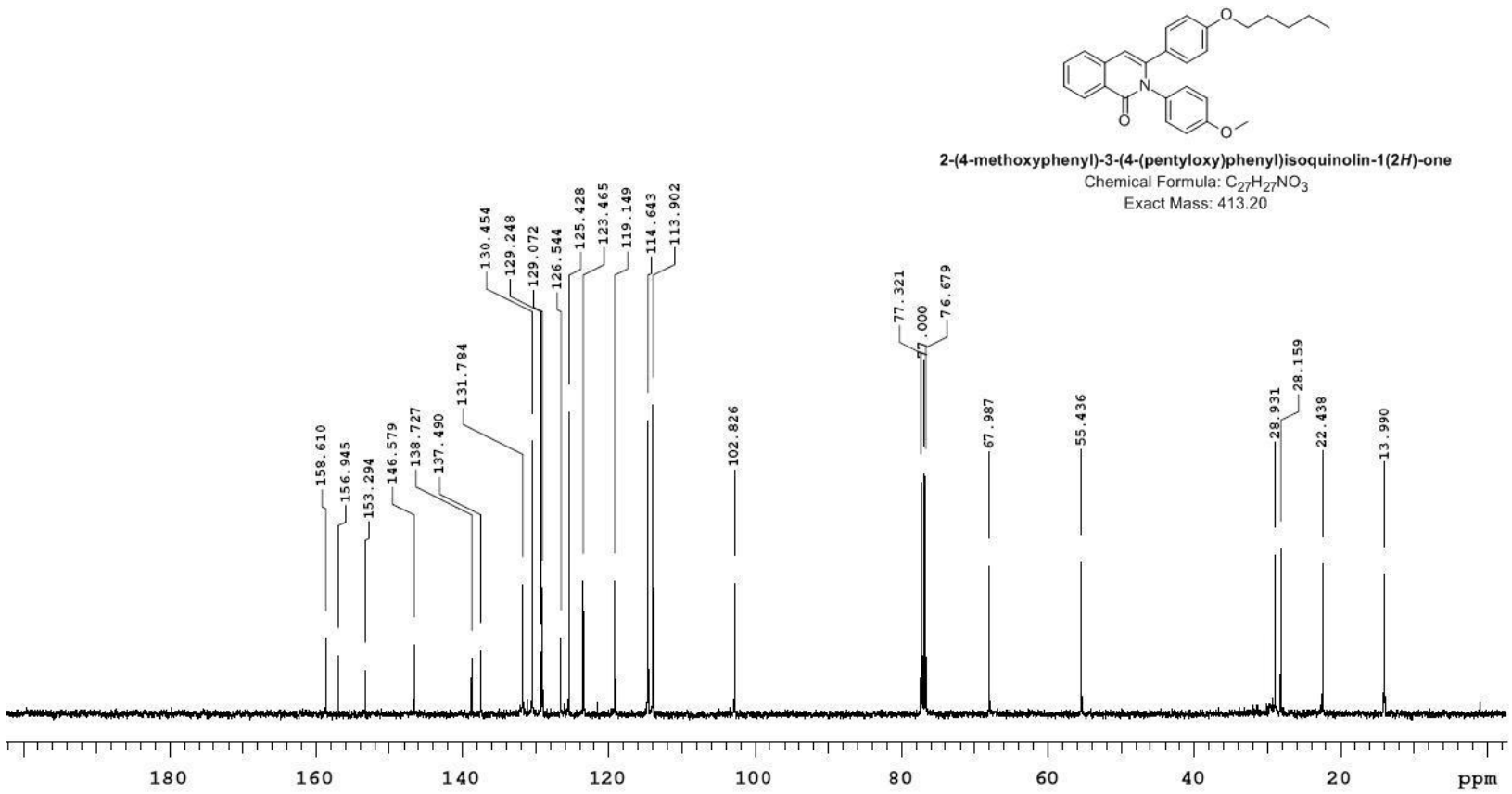
3-(4-bromophenyl)-2-(4-methoxyphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{22}H_{16}BrNO_2$
Exact Mass: 405.04



2-(4-methoxyphenyl)-3-(4-(pentyloxy)phenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{27}H_{27}NO_3$

Exact Mass: 413.20


2-(4-methoxyphenyl)-3-(4-(pentyloxy)phenyl)isoquinolin-1(2H)-one
Chemical Formula: C27H27NO3
Exact Mass: 413.20
158.610
156.945
153.294
146.579
138.727
137.490
131.784
130.454
129.248
129.072
126.544
125.428
123.465
119.149
114.643
113.902
102.826
77.321
77.000
76.679
67.987
55.436
28.931
28.159
22.438
13.990
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

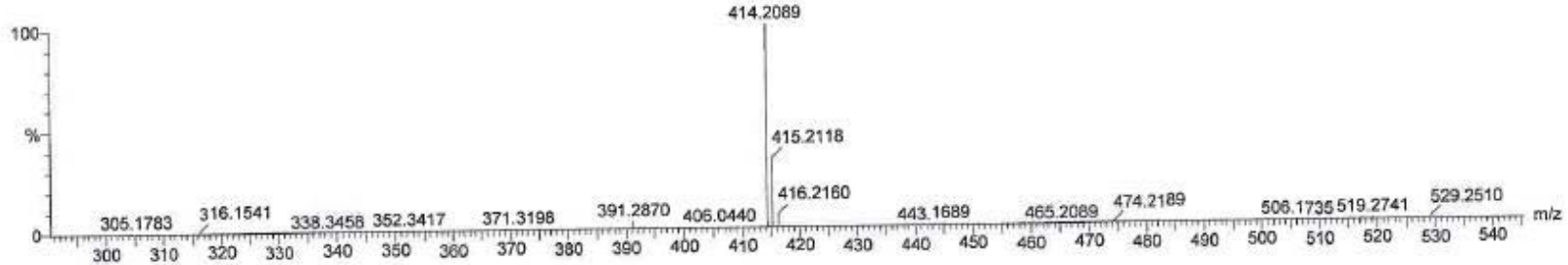
Single Mass Analysis

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

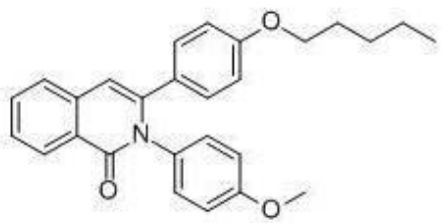
Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-2 O: 0-3

B036/CVIG1/036
131202006 9 (0.337) Cm (9)

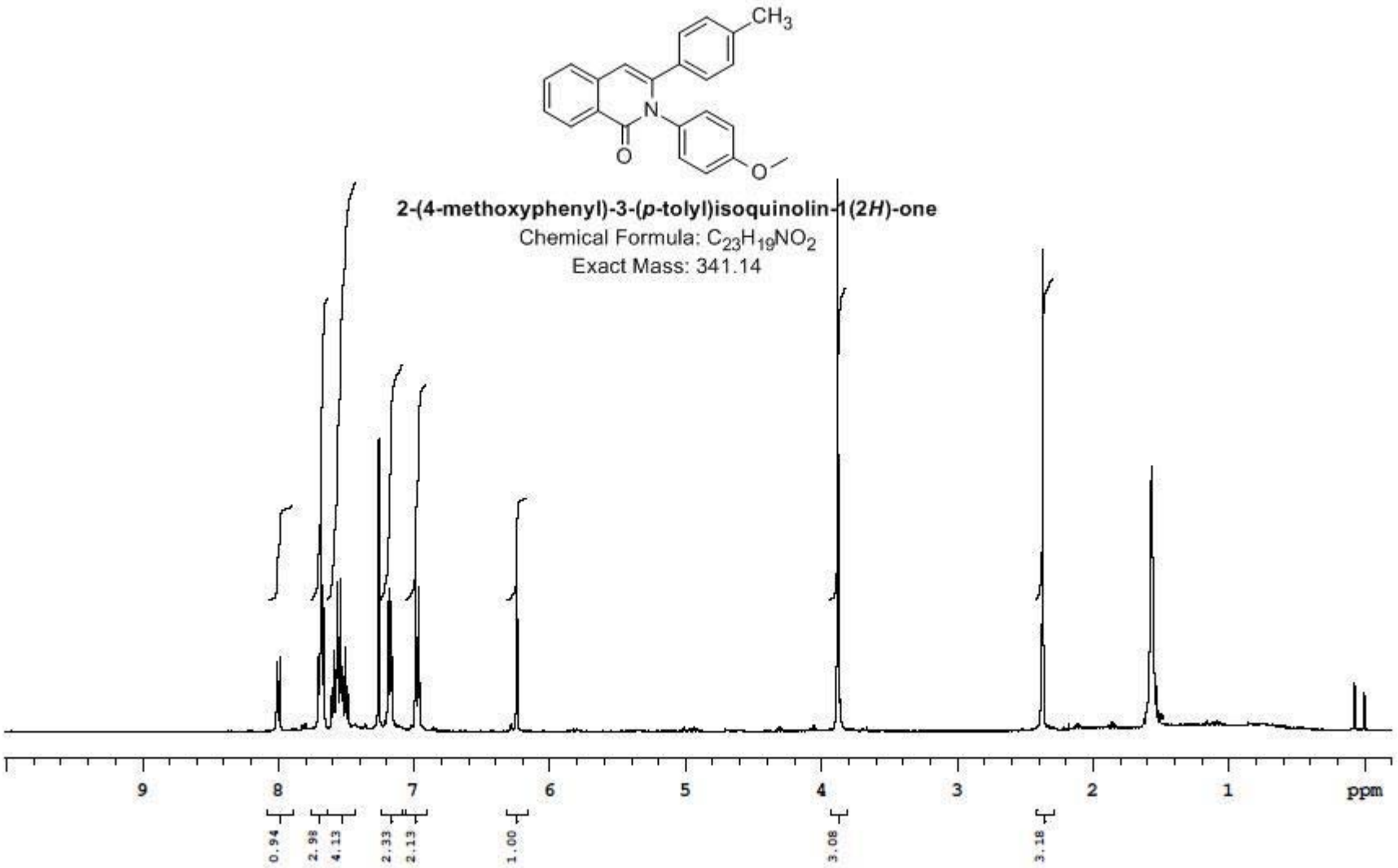
1: TOF MS ES+
9.86e+003

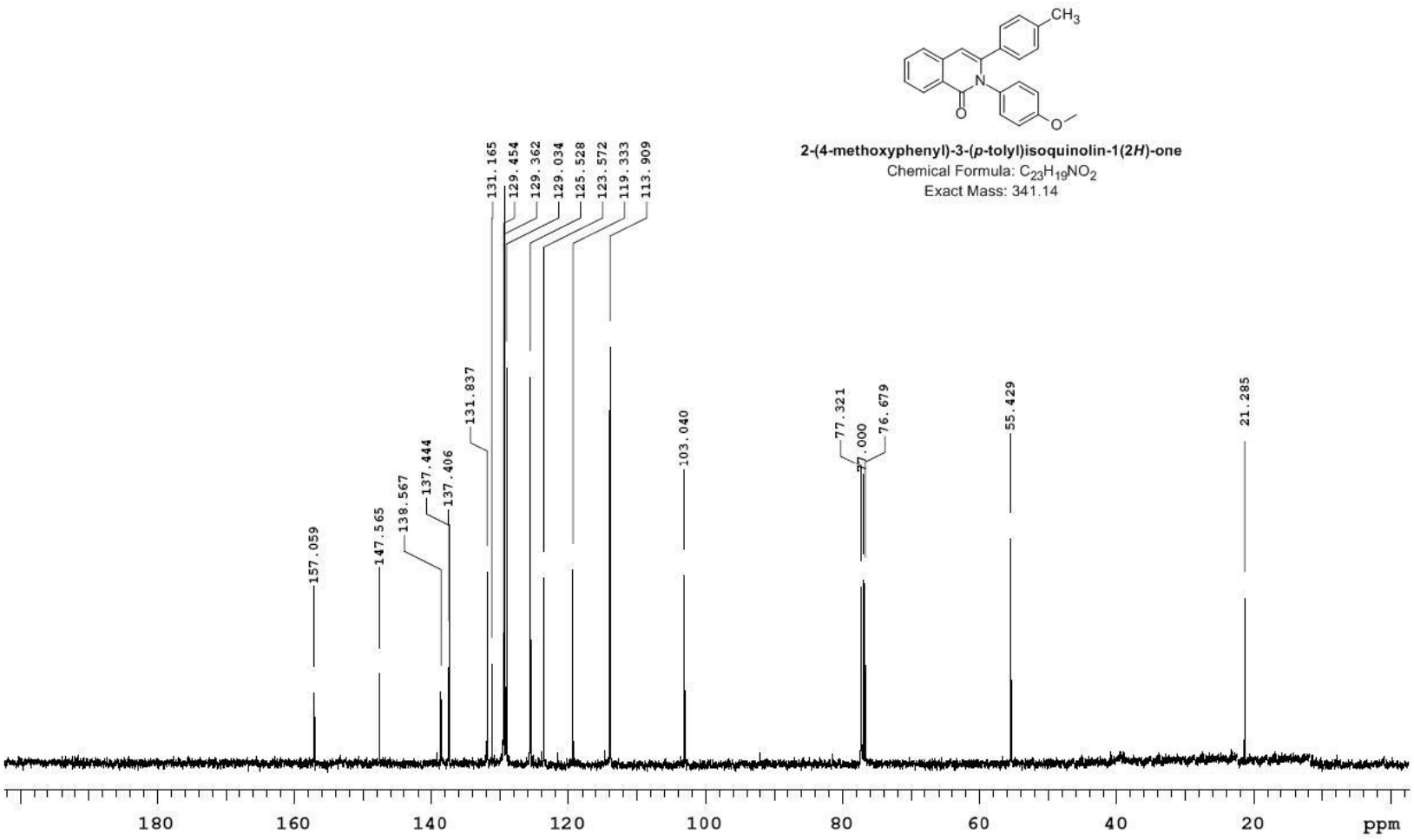


Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
414.2089	414.2069	2.0	4.8	14.5	15.4	C27 H28 N O3



2-(4-methoxyphenyl)-3-(4-(pentyloxy)phenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{27}H_{27}NO_3$
Exact Mass: 413.20


CH3
N
O
O
2-(4-methoxyphenyl)-3-(p-tolyl)isoquinolin-1(2H)-one
Chemical Formula: C23H19NO2
Exact Mass: 341.14
9
8
7
6
5
4
3
2
1
ppm
0.94
2.98
4.13
2.33
2.13
1.00
3.08
3.18


CH3
N
O
O
2-(4-methoxyphenyl)-3-(p-tolyl)isoquinolin-1(2H)-one
Chemical Formula: C23H19NO2
Exact Mass: 341.14
157.059
147.565
138.567
137.444
137.406
131.837
131.165
129.454
129.362
129.034
125.528
123.572
119.333
113.909
103.040
77.321
77.000
76.679
55.429
21.285
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

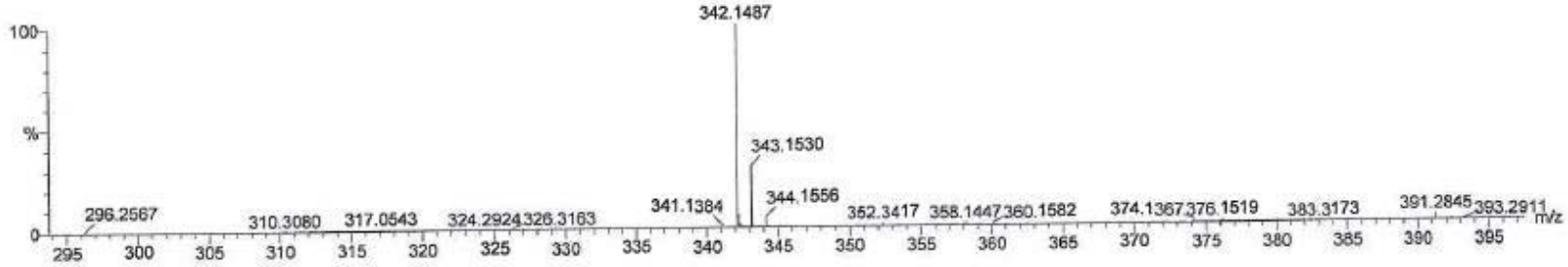
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

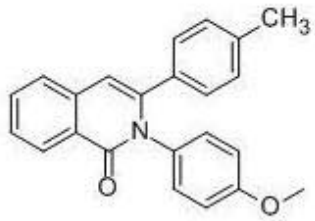
Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-2 O: 0-2

B036/CVIG1/037
131129005 9 (0.337) Cm (9:10-1)

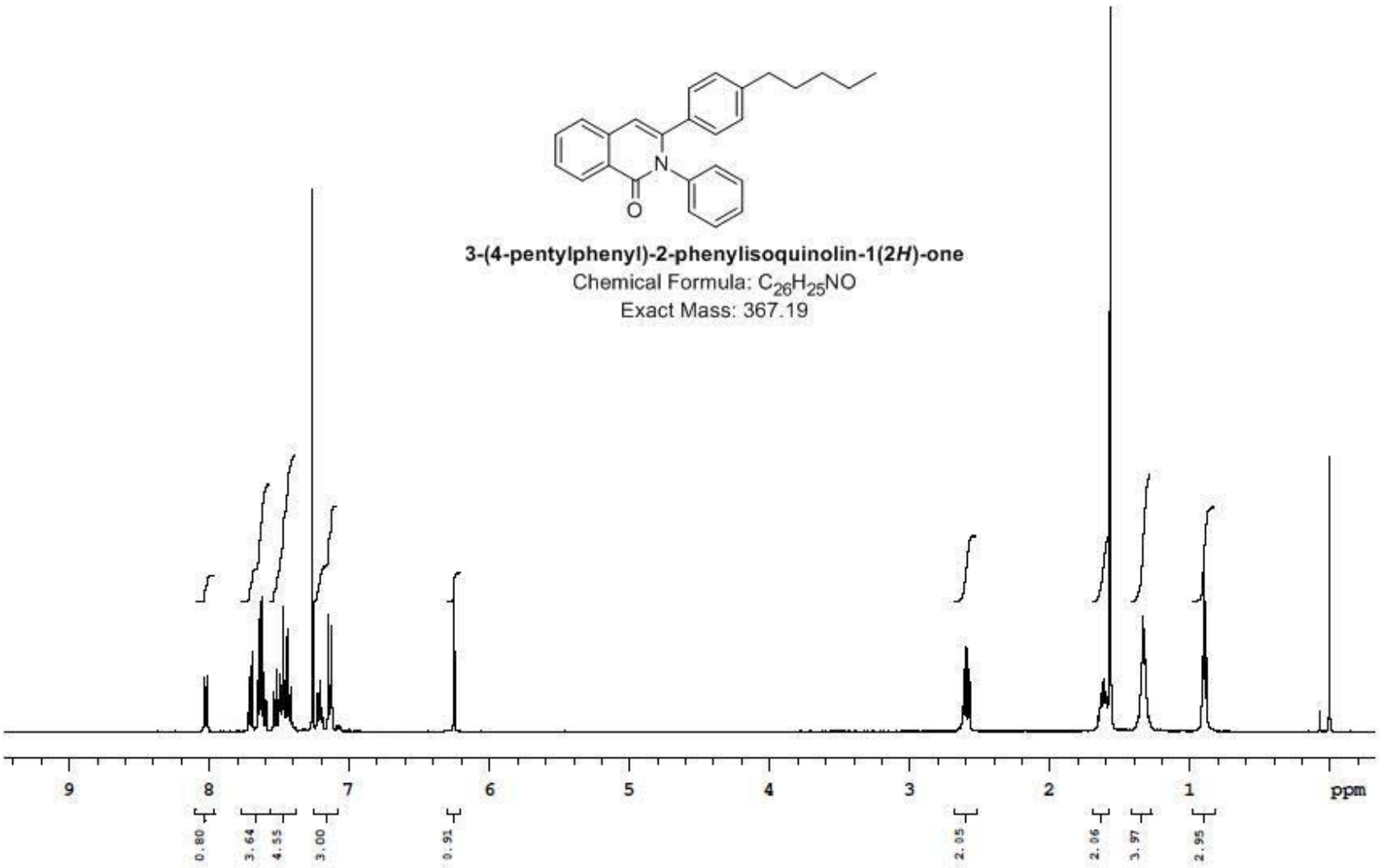
1: TOF MS ES+
1.34e+004



Minimum:		5.0	50.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
342.1487	342.1494	-0.7	-2.0	14.5	40.3	C23 H20 N O2



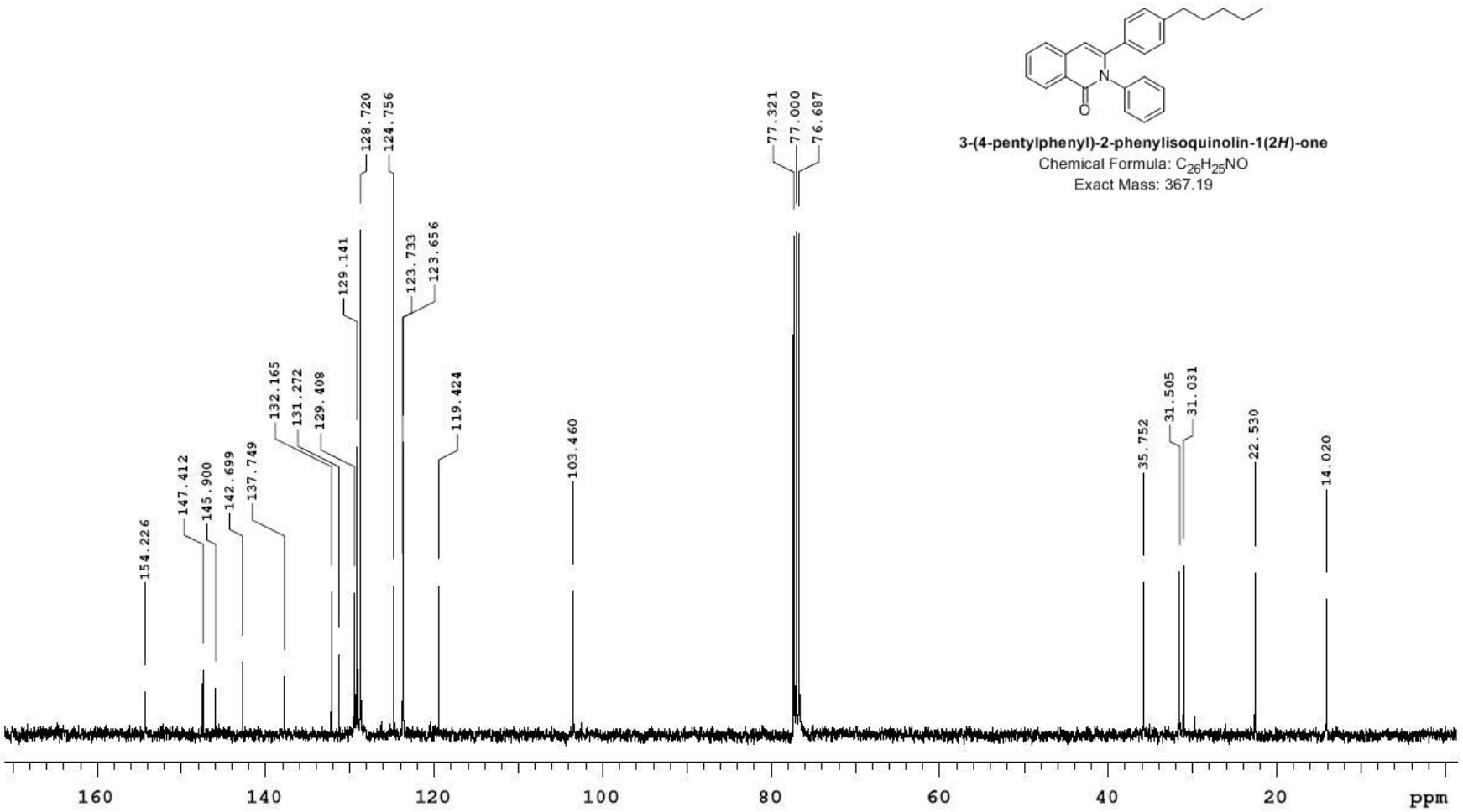
2-(4-methoxyphenyl)-3-(*p*-tolyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{23}H_{19}NO_2$
Exact Mass: 341.14



3-(4-pentylphenyl)-2-phenylisoquinolin-1(2*H*)-one

Chemical Formula: $C_{26}H_{25}NO$

Exact Mass: 367.19



3-(4-pentylphenyl)-2-phenylisoquinolin-1(2*H*)-one

Chemical Formula: $C_{26}H_{25}NO$

Exact Mass: 367.19

Elemental Composition Report

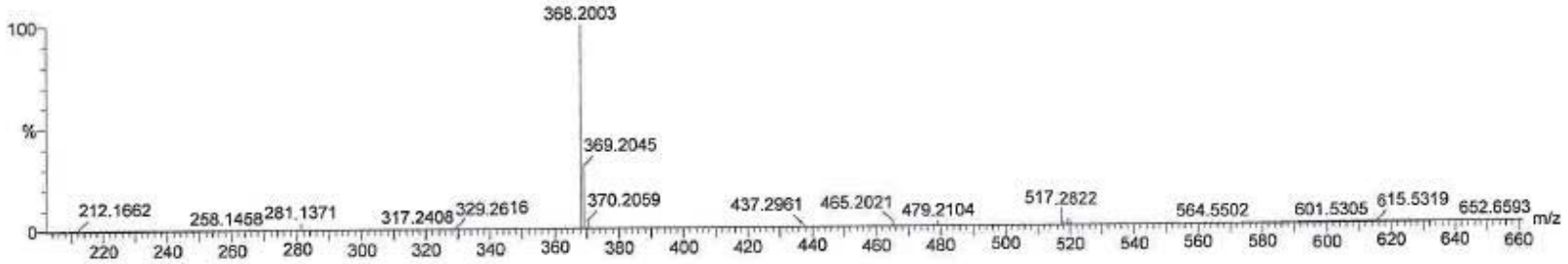
Single Mass Analysis

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

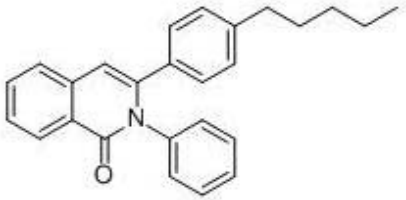
Monoisotopic Mass, Even Electron Ions
113 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-1 O: 0-13

B036/CABA1/002
131205008 17 (0.619) Cm (13:17-20:28)

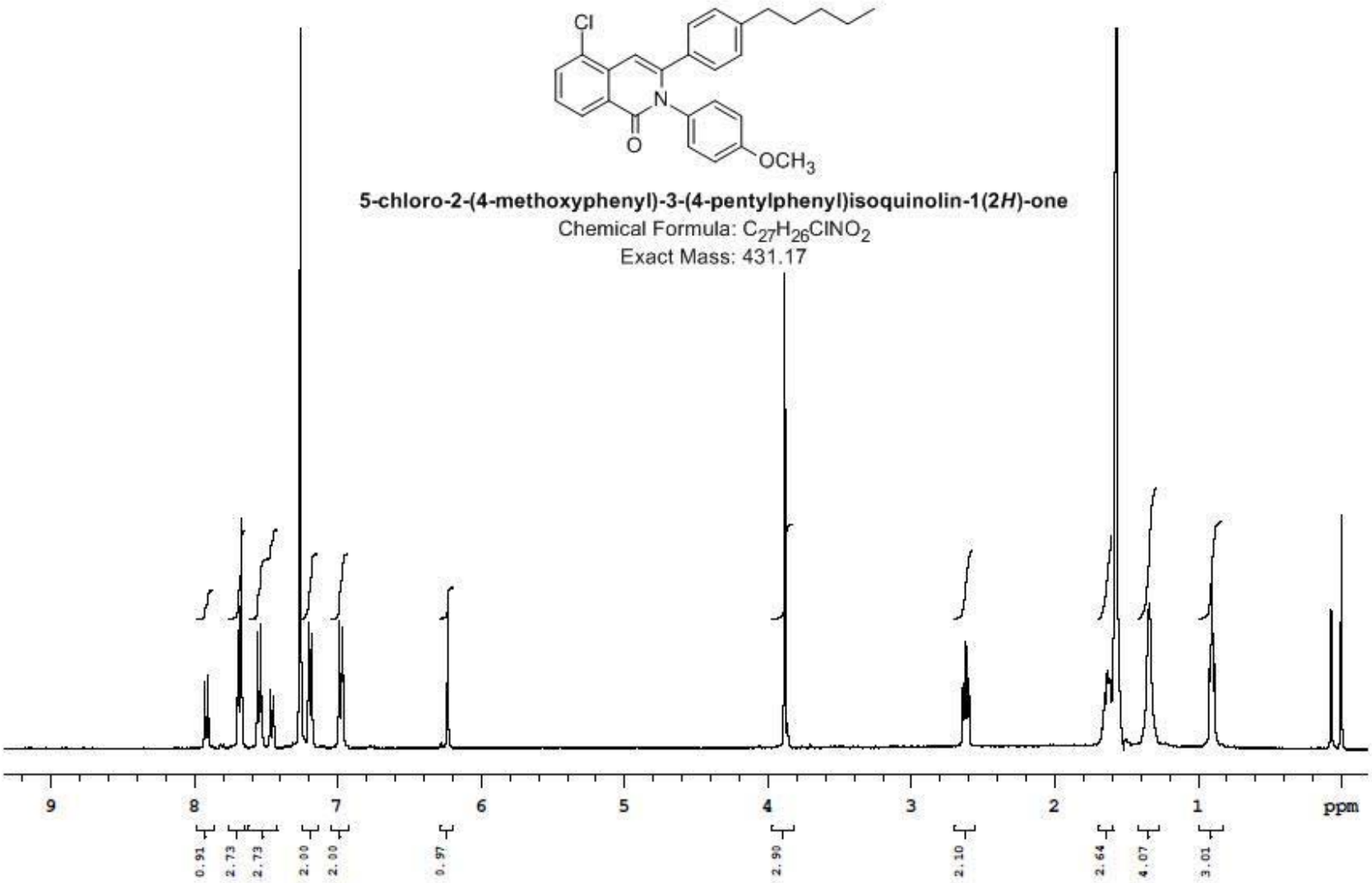
1: TOF MS ES+
7.07e+003



Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
368.2003	368.2014	-1.1	-3.0	14.5	8.5	C26 H26 N O



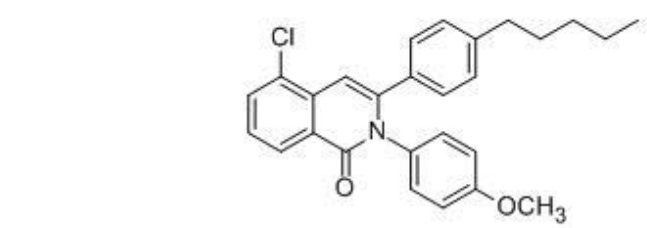
3-(4-pentylphenyl)-2-phenylisoquinolin-1(2*H*)-one
Chemical Formula: $C_{26}H_{25}NO$
Exact Mass: 367.19



5-chloro-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{27}H_{26}ClNO_2$

Exact Mass: 431.17



5-chloro-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{27}H_{26}ClNO_2$

Exact Mass: 431.17

Elemental Composition Report

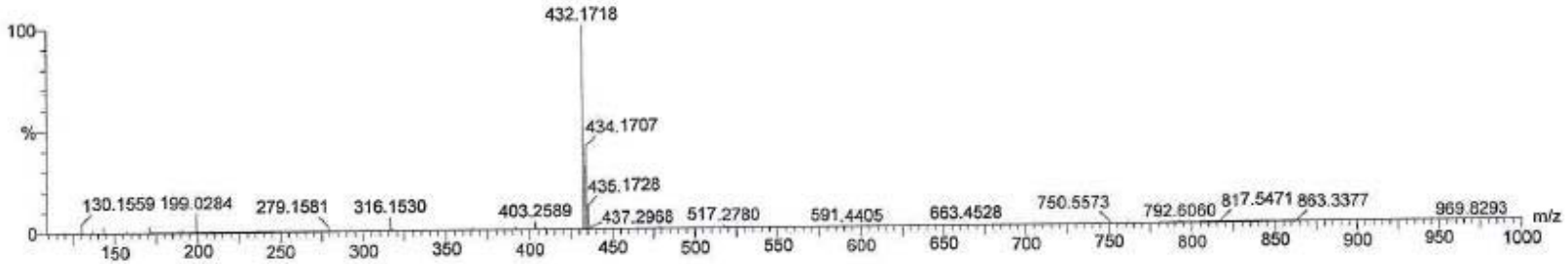
Single Mass Analysis

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

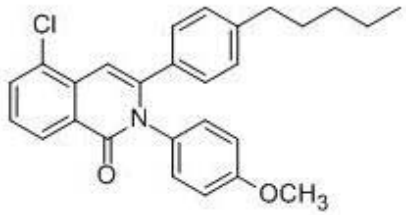
Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-1 O: 0-2 Cl: 0-1

B036/CCMB1/002
131205007 9 (0.338) Cm (9:11-19:20)

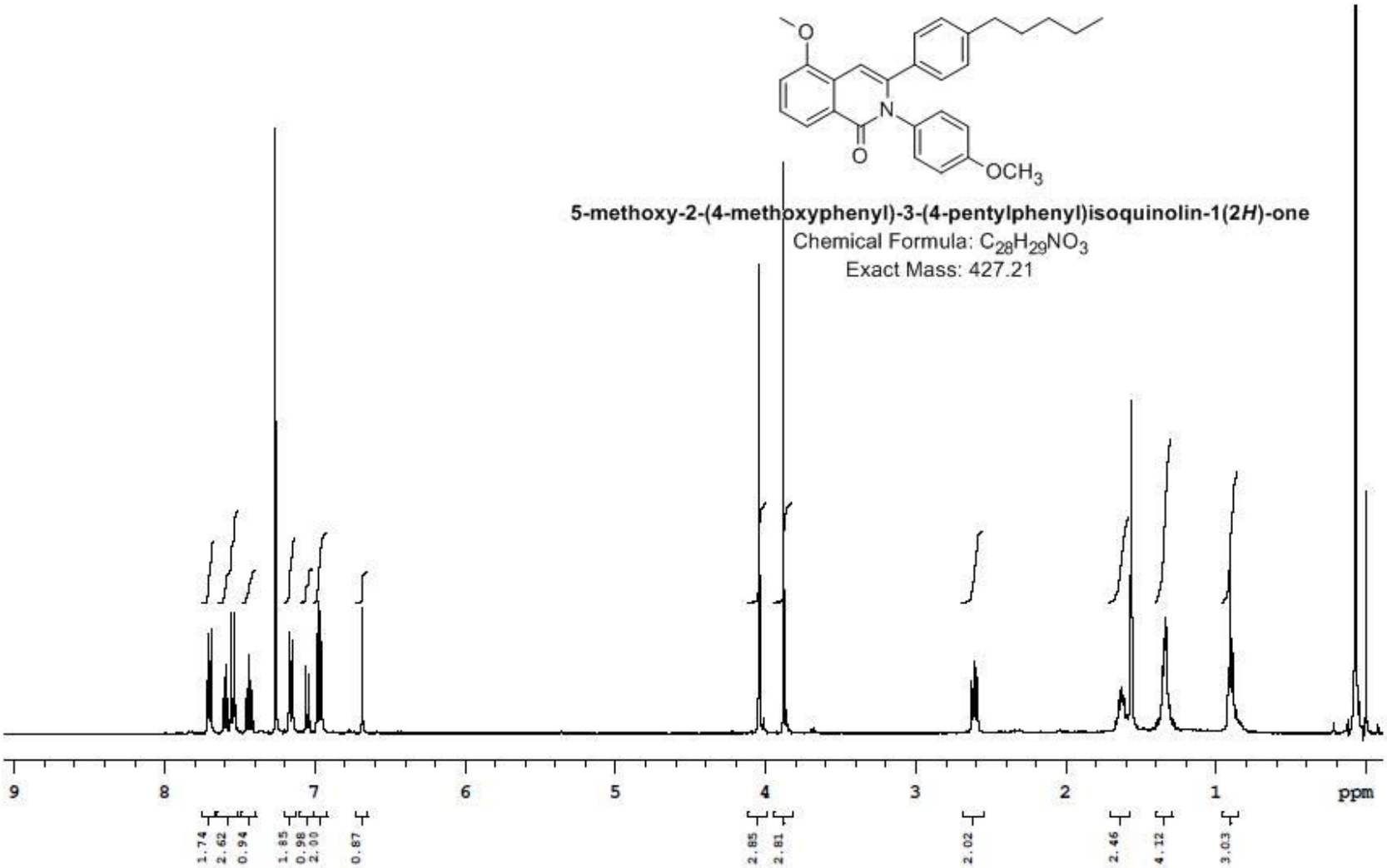
1: TOF MS ES+
6.11e+004

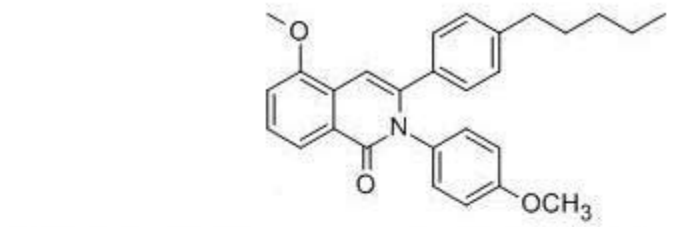


Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
432.1718	432.1730	-1.2	-2.8	14.5	72.2	C27 H27 N O2 Cl



5-chloro-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{27}H_{26}ClNO_2$
Exact Mass: 431.17


O
N
O
OCH3
5-methoxy-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2H)-one
Chemical Formula: C28H29NO3
Exact Mass: 427.21
9
8
7
6
5
4
3
2
1
ppm
1.74
2.62
0.94
1.85
0.98
2.00
0.87
2.85
2.81
2.02
2.46
4.12
3.03



5-methoxy-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{28}H_{29}NO_3$

Exact Mass: 427.21

Elemental Composition Report

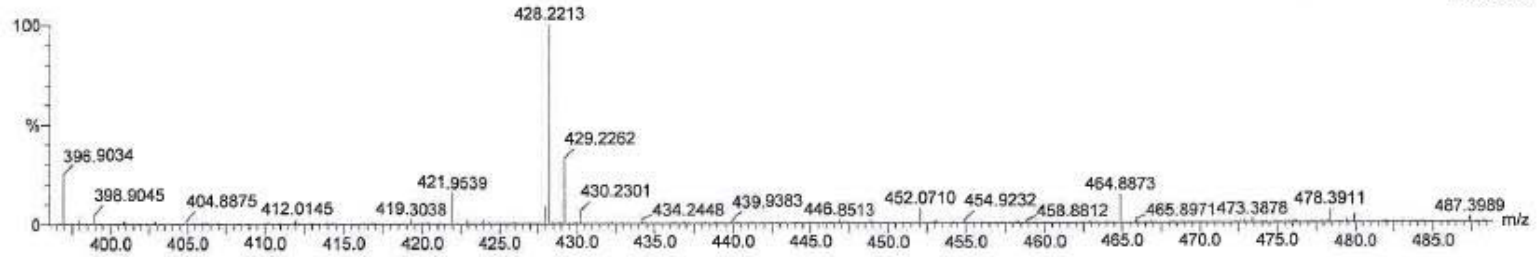
Single Mass Analysis

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

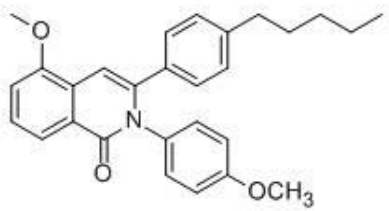
Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-32 N: 0-1 O: 0-5

B036/CMBA2/002P
131227001 21 (0.705) Cm (21:24-35)

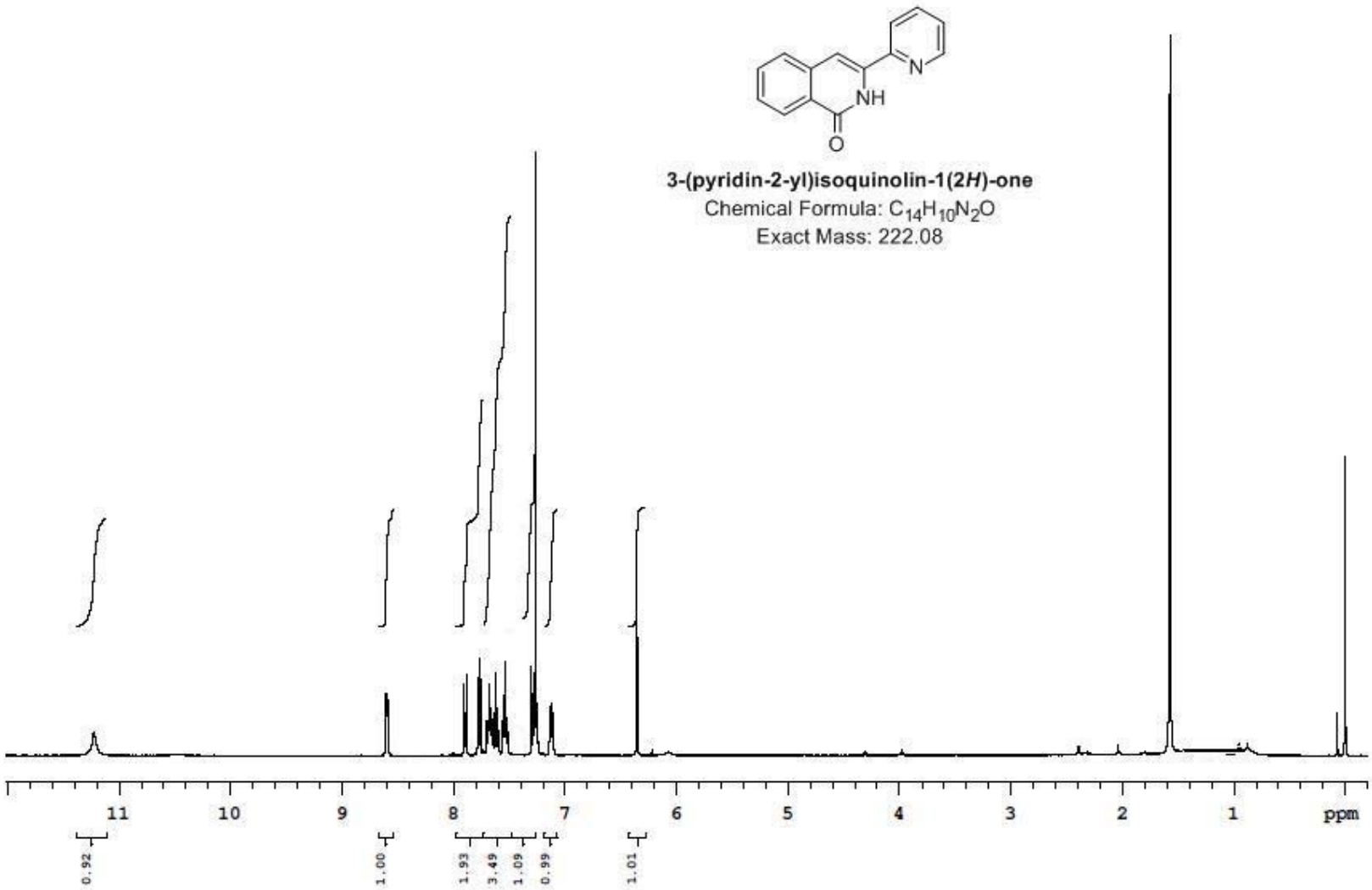
1: TOF MS ES+
2.55e+003

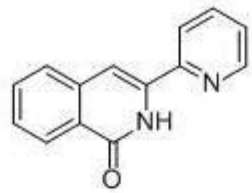


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.2213	428.2226	-1.3	-3.0	14.5	0.2	C28 H30 N O3



5-methoxy-2-(4-methoxyphenyl)-3-(4-pentylphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{28}H_{29}NO_3$
Exact Mass: 427.21

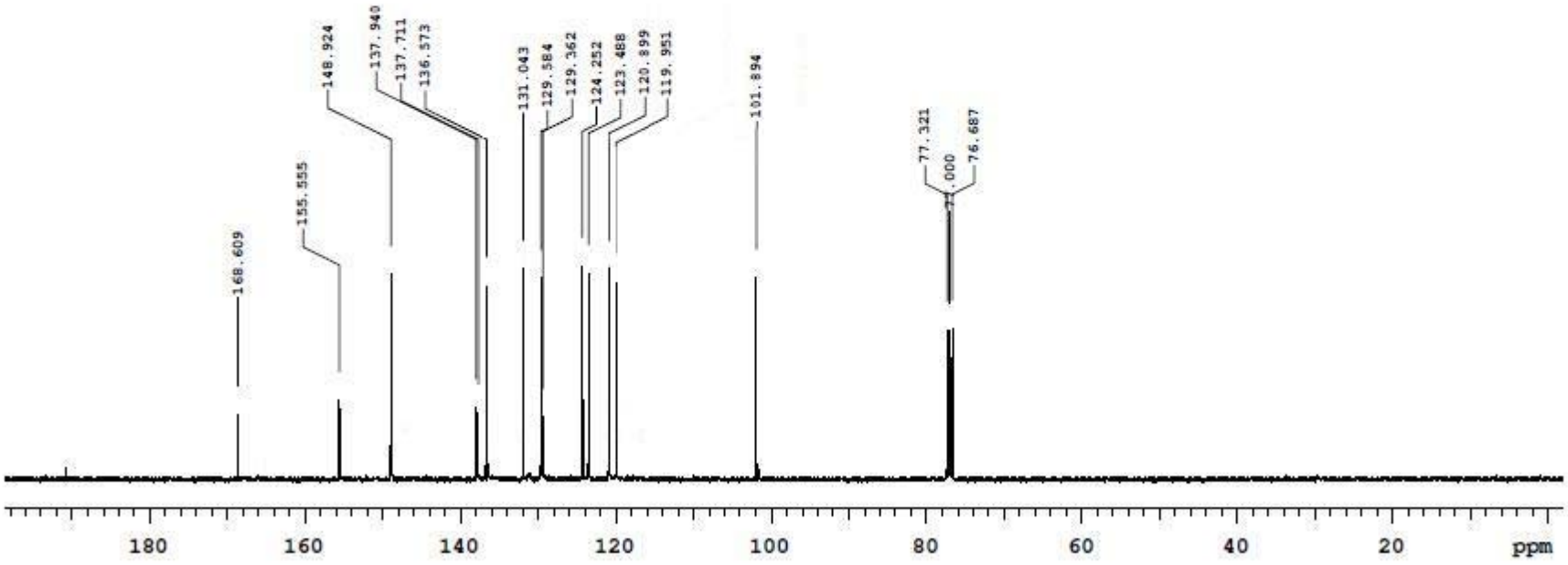

N
NH
O
3-(pyridin-2-yl)isoquinolin-1(2H)-one
Chemical Formula: C14H10N2O
Exact Mass: 222.08
11
10
9
8
7
6
5
4
3
2
1
ppm
0.92
1.00
1.93
3.49
1.09
0.99
1.01



3-(pyridin-2-yl)isoquinolin-1(2*H*)-one

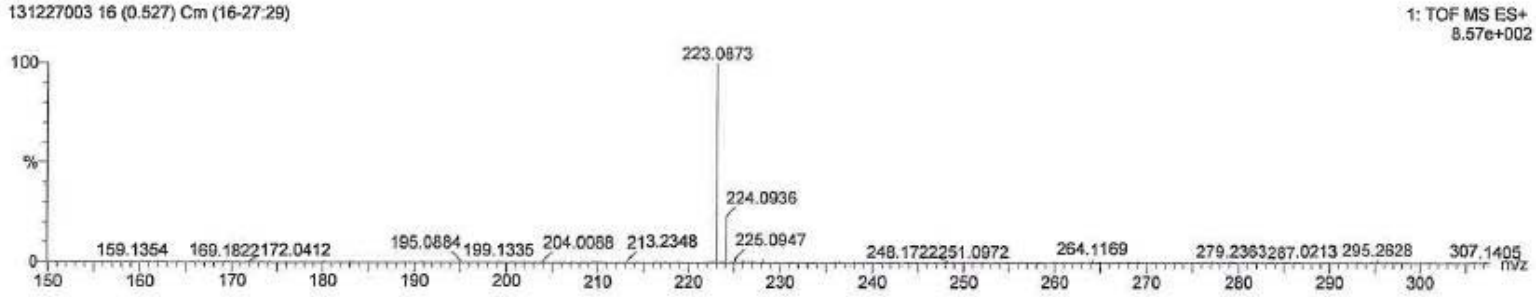
Chemical Formula: $C_{14}H_{10}N_2O$

Exact Mass: 222.08

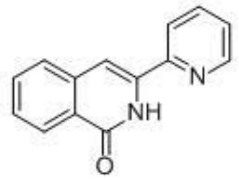


Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

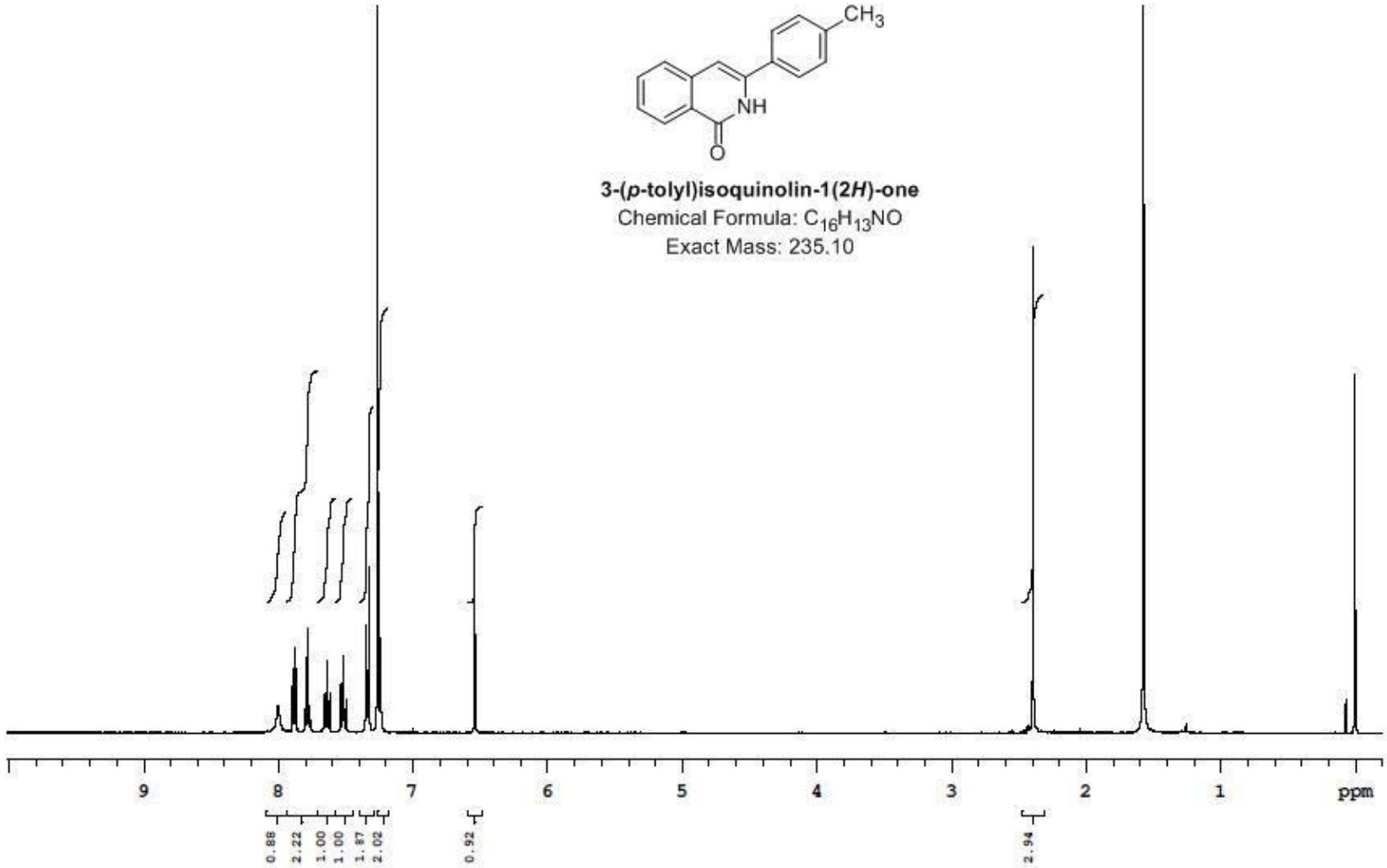
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-28 H: 0-25 N: 0-3 O: 0-3
B036/CGA3/004
131227003 16 (0.527) Cm (16-27:29)

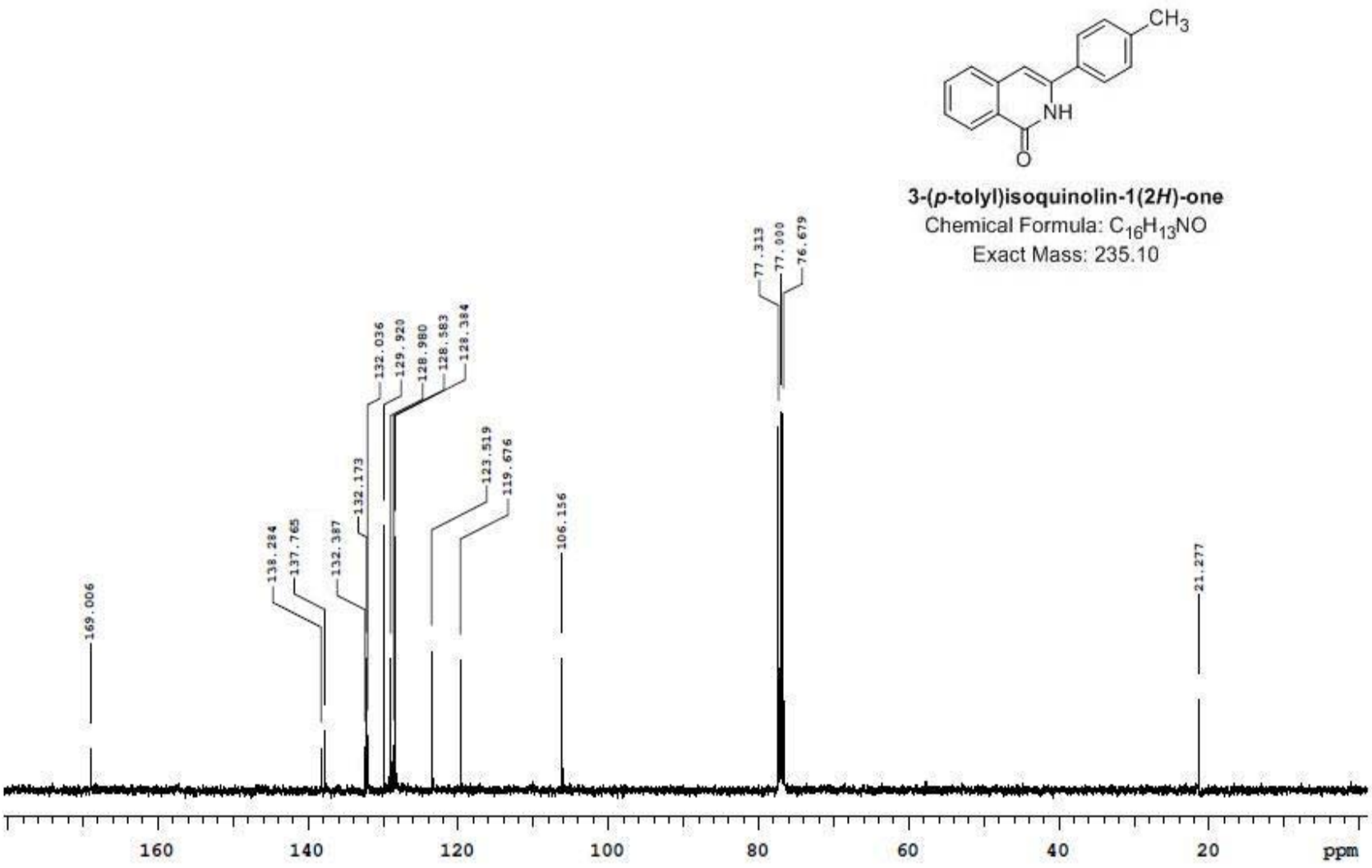


Minimum:				-5.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
223.0873	223.0871	0.2	0.9	10.5	7.1	C14 H11 N2 O



3-(pyridin-2-yl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{14}H_{10}N_2O$
Exact Mass: 222.08


CH3
NH
O
3-(p-tolyl)isoquinolin-1(2H)-one
Chemical Formula: C16H13NO
Exact Mass: 235.10
9
8
7
6
5
4
3
2
1
ppm
0.88
2.22
1.00
1.00
1.87
2.02
0.92
2.94

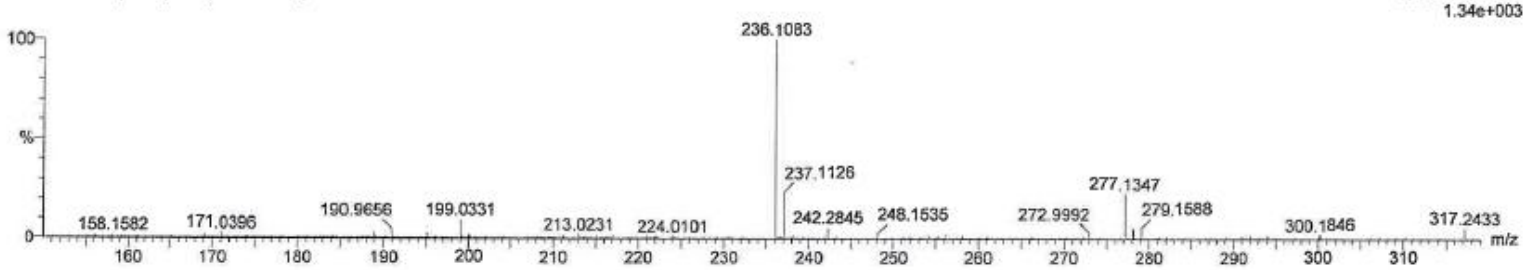

CH3
NH
O
3-(p-tolyl)isoquinolin-1(2H)-one
Chemical Formula: C16H13NO
Exact Mass: 235.10
169.006
138.284
137.765
132.387
132.173
132.036
129.920
128.980
128.583
128.384
123.519
119.676
106.156
77.313
77.000
76.679
21.277
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

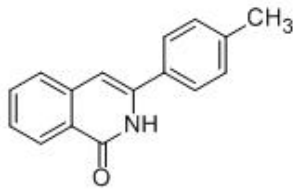
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-28 H: 0-25 N: 0-3 O: 0-3
B036/CGA1/005
131227004 15 (0.507) Cm (14:15-27:28)

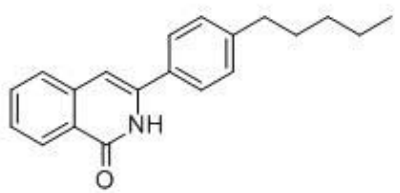
1: TOF MS ES+
1.34e+003



Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
236.1083	236.1075	0.8	3.4	10.5	6.0	C16 H14 N O



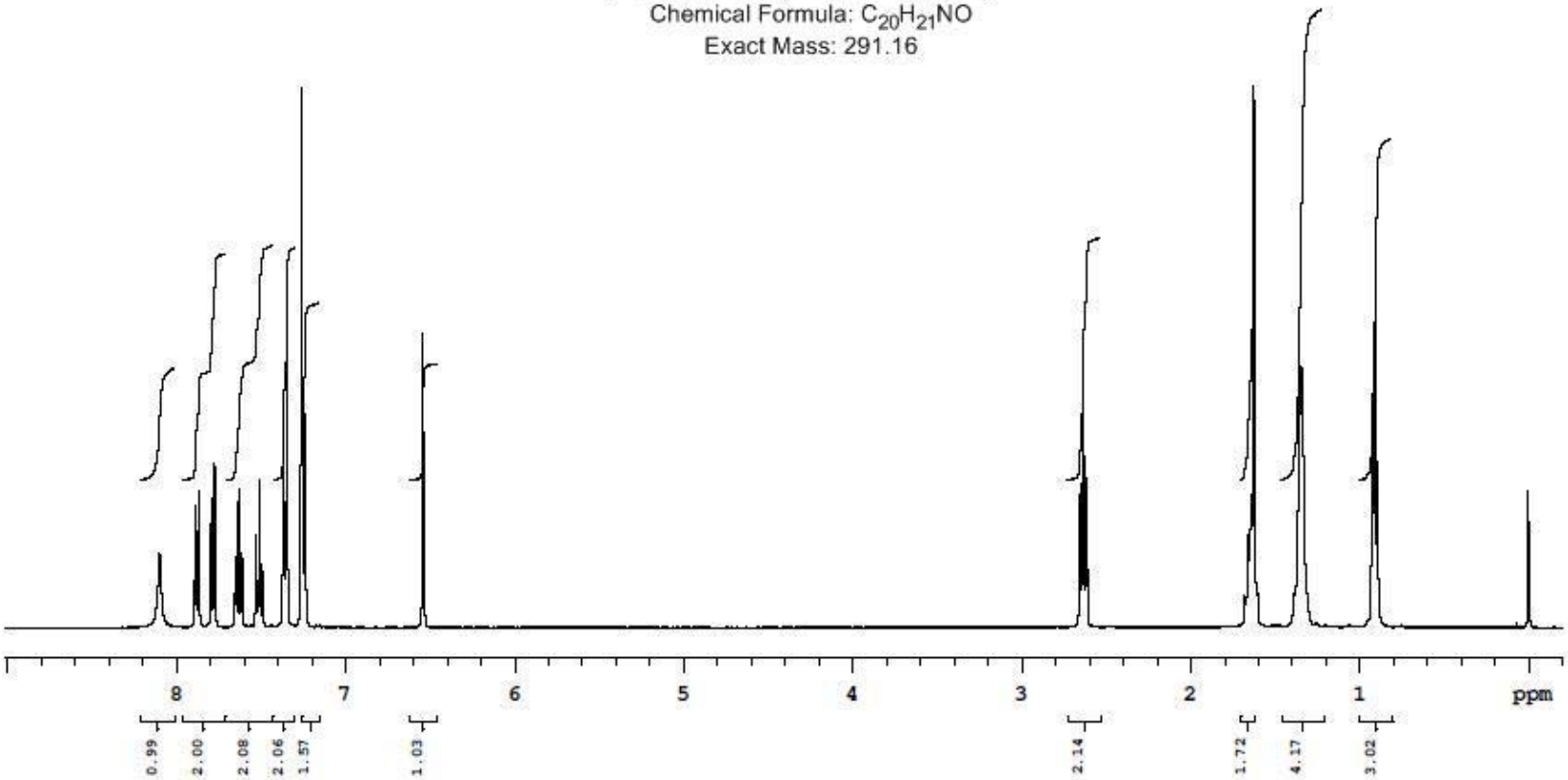
3-(*p*-tolyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{16}H_{13}NO$
Exact Mass: 235.10

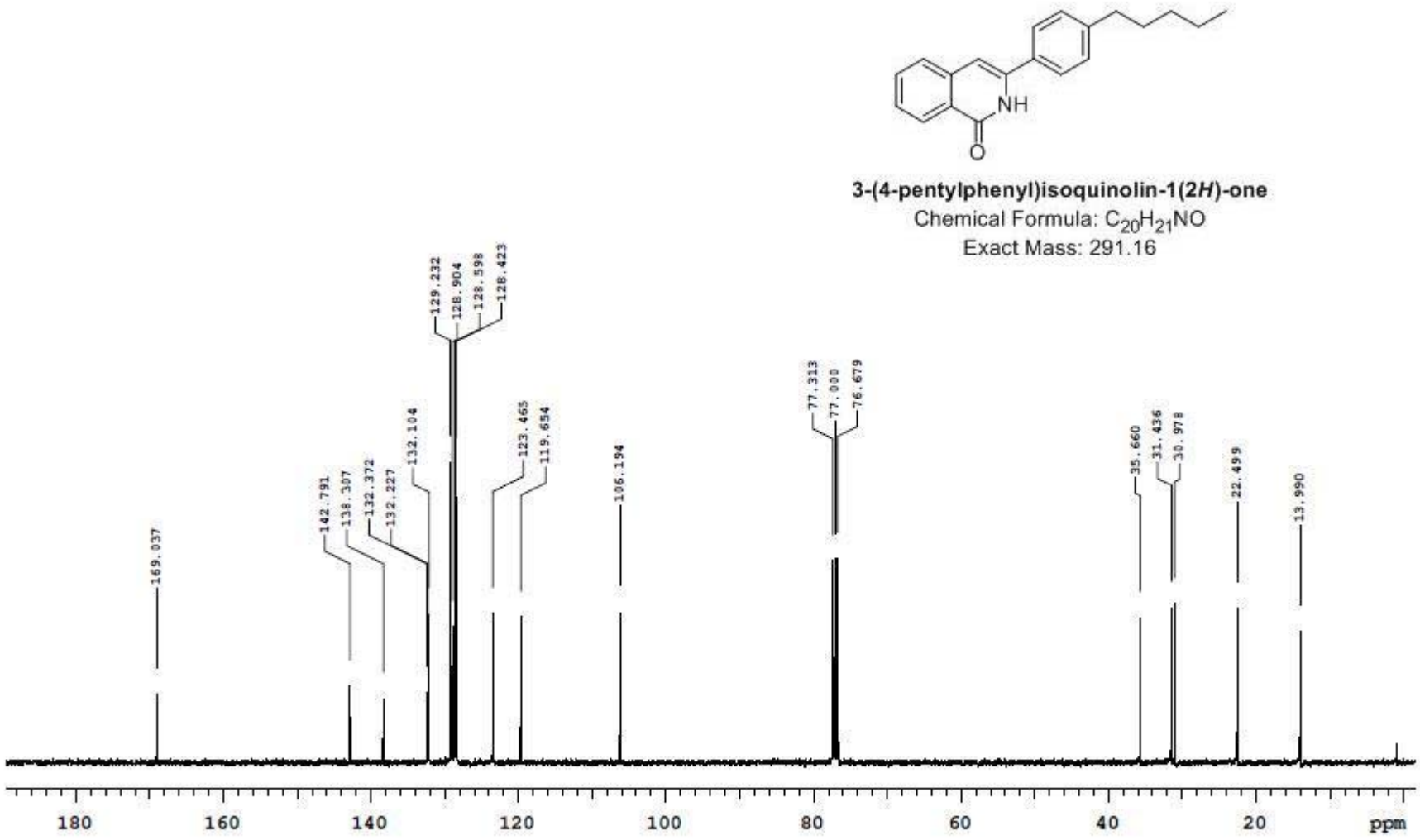


3-(4-pentylphenyl)isoquinolin-1(2*H*)-one

Chemical Formula: $C_{20}H_{21}NO$

Exact Mass: 291.16




NH
O
3-(4-pentylphenyl)isoquinolin-1(2H)-one
Chemical Formula: C20H21NO
Exact Mass: 291.16
169.037
142.791
138.307
132.372
132.227
132.104
129.232
128.904
128.598
128.423
123.465
119.654
106.194
77.313
77.000
76.679
35.660
31.436
30.978
22.499
13.990
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

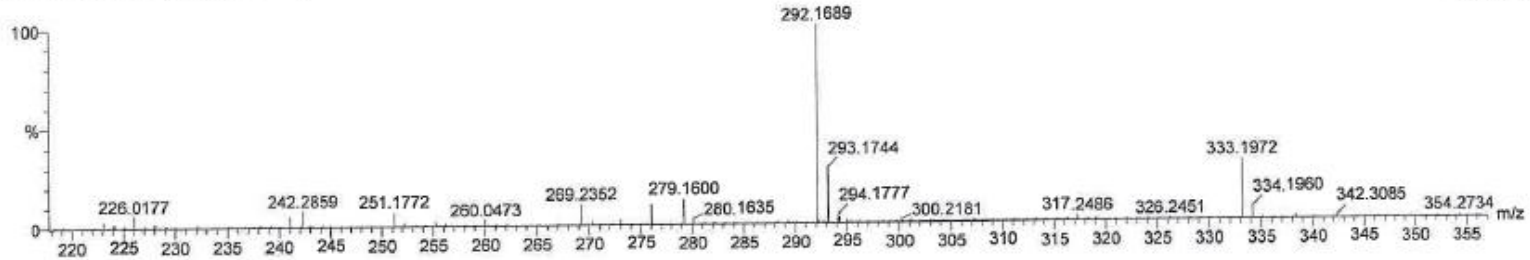
Single Mass Analysis

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

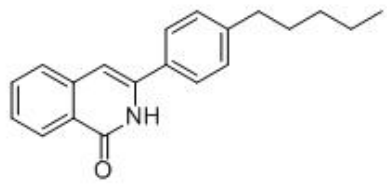
Monoisotopic Mass, Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-28 H: 0-25 N: 0-3 O: 0-3

B036/CGA1/006
131227005 14 (0.461) Cm (14:16-27:28)

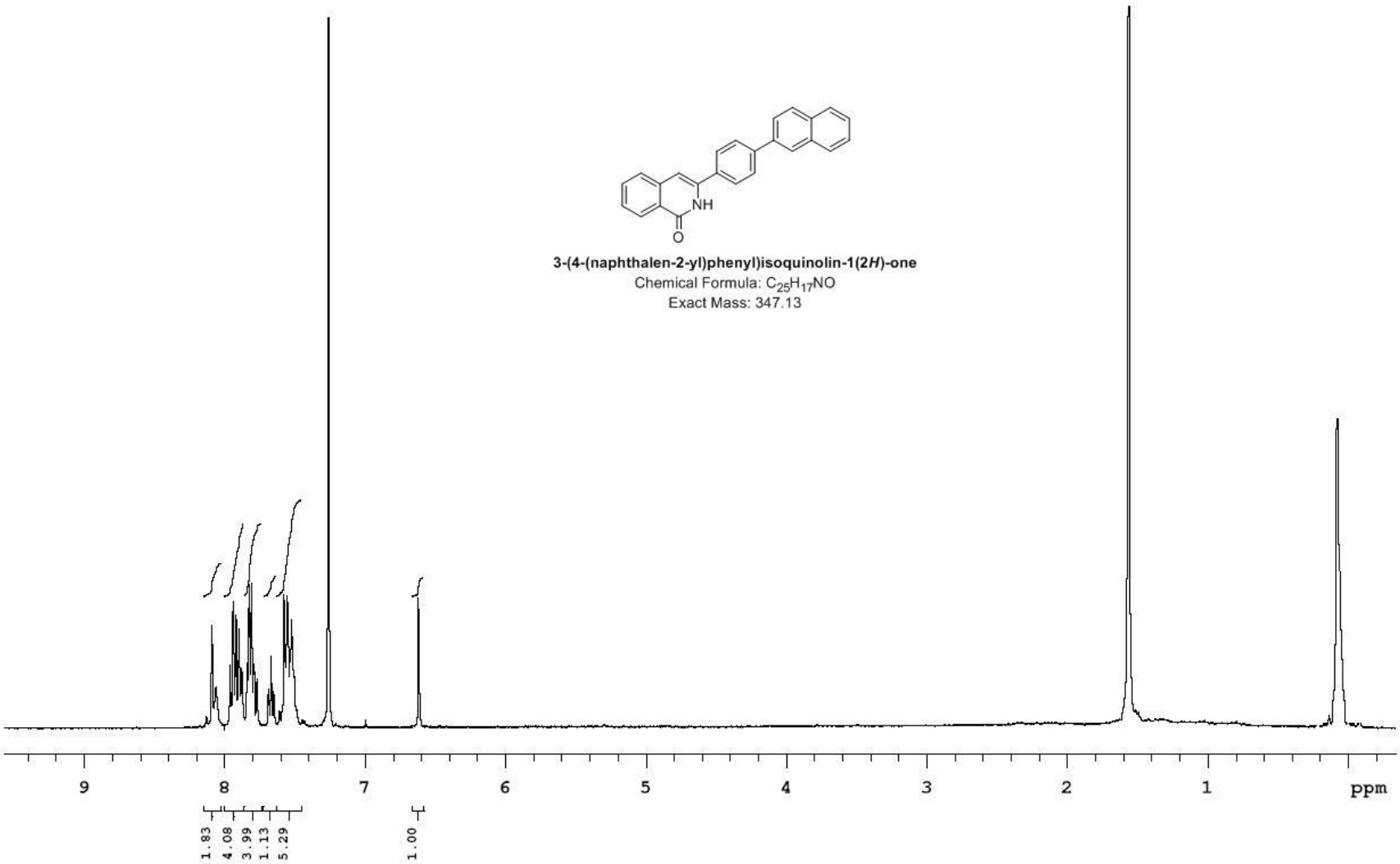
1: TOF MS ES+
1.72e+003

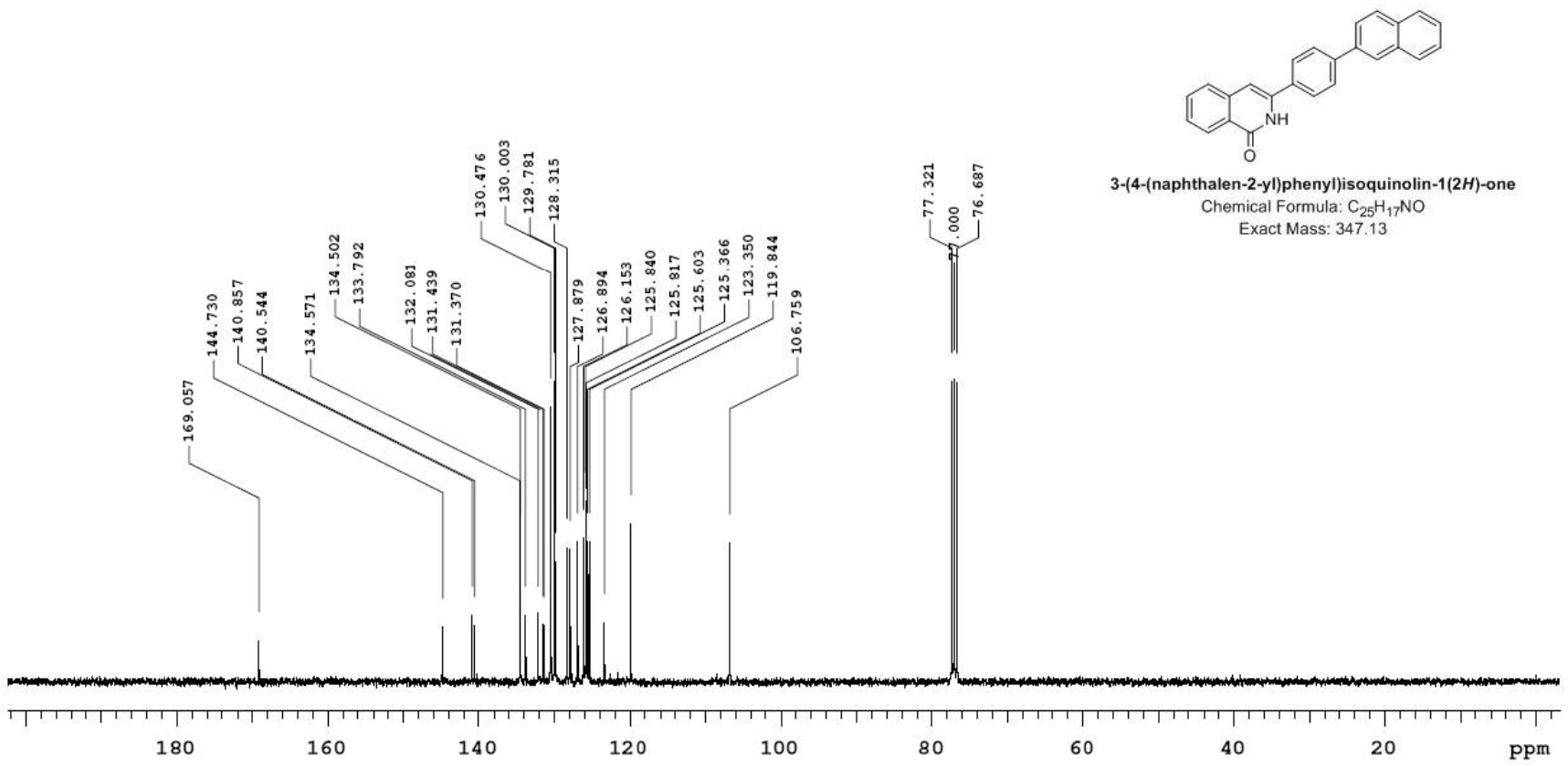


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.1689	292.1701	-1.2	-4.1	10.5	6.4	C20 H22 N O



3-(4-pentylphenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{20}H_{21}NO$
Exact Mass: 291.16


NH
O
3-(4-(naphthalen-2-yl)phenyl)isoquinolin-1(2H)-one
Chemical Formula: C25H17NO
Exact Mass: 347.13
9
8
7
6
5
4
3
2
1
ppm
1.83
4.08
3.99
1.13
5.29
1.00


169.057
144.730
140.857
140.544
134.571
134.502
133.792
132.081
131.439
131.370
130.476
130.003
129.781
128.315
127.879
126.894
126.153
125.840
125.817
125.603
125.366
123.350
119.844
106.759
77.321
77.000
76.687
NH
O
3-(4-(naphthalen-2-yl)phenyl)isoquinolin-1(2H)-one
Chemical Formula: C25H17NO
Exact Mass: 347.13
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

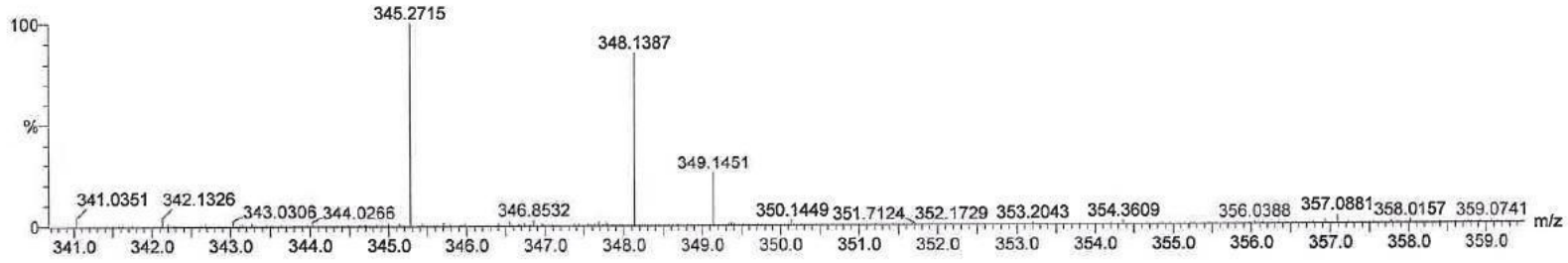
Single Mass Analysis

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

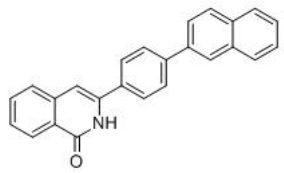
Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-27 H: 0-19 N: 0-1 O: 0-2

B036/CGAT1/009
140121006 22 (0.599) Cm (20:22-38:40)

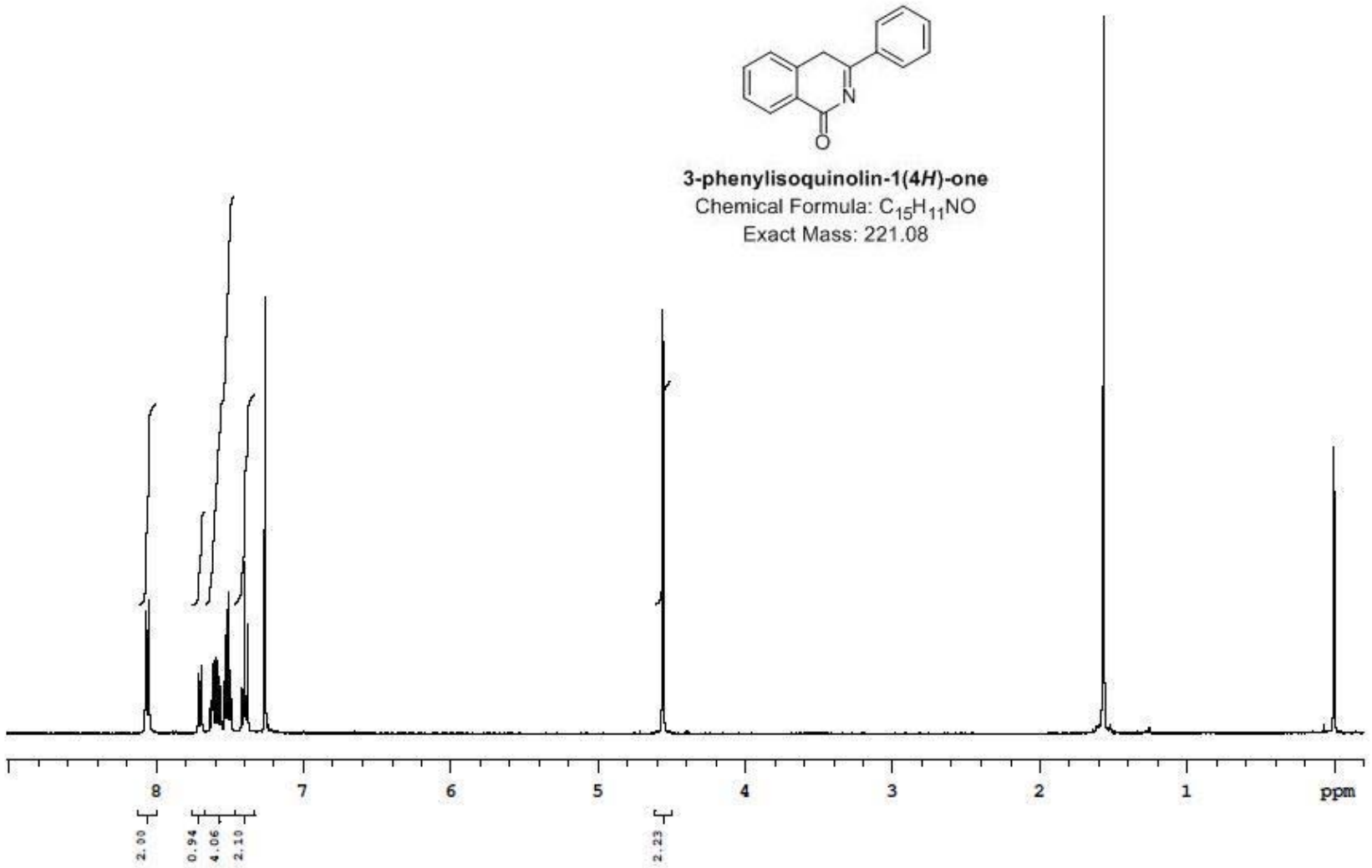
1: TOF MS ES+
1.69e+003

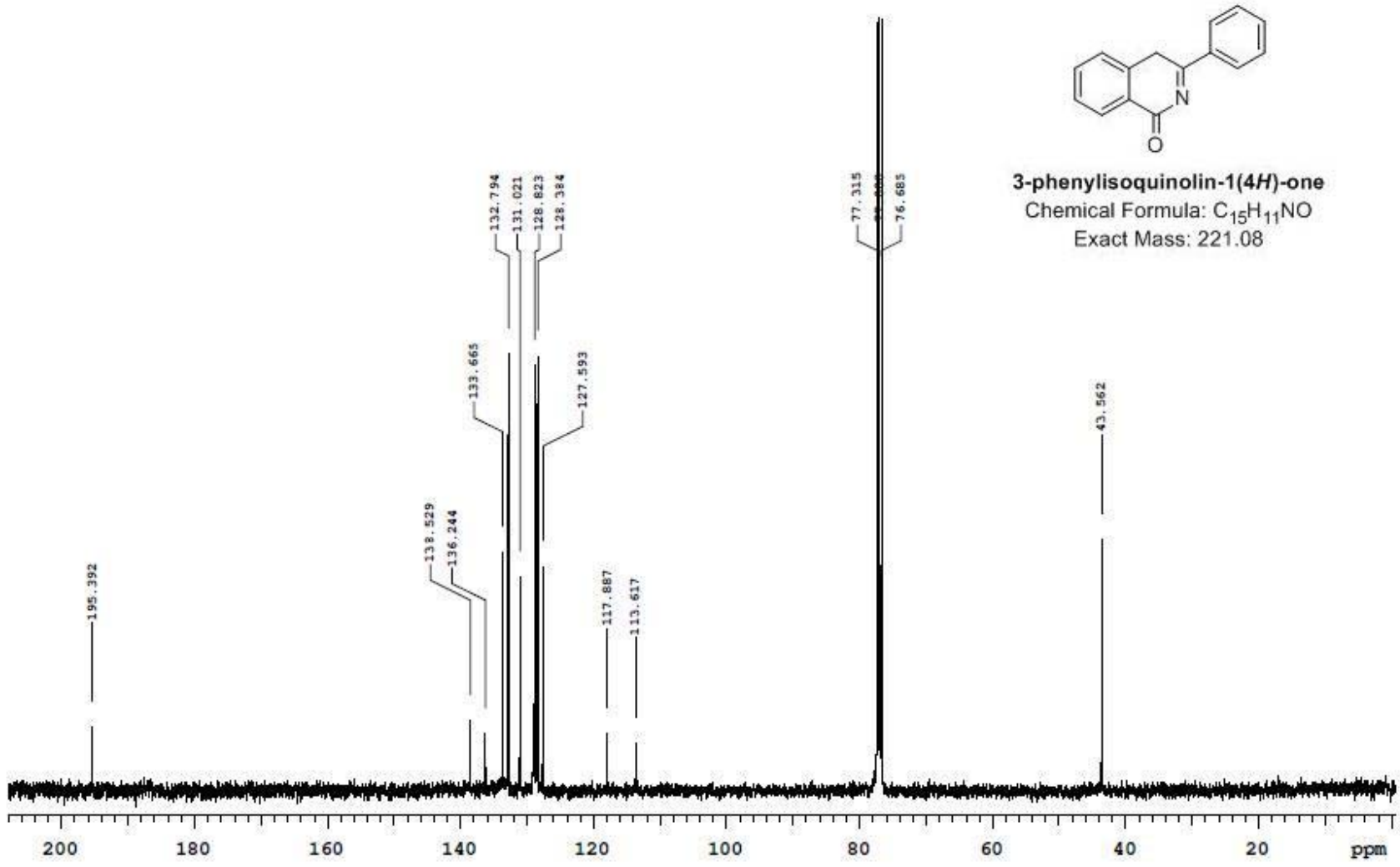


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.1387	348.1388	-0.1	-0.3	17.5	0.9	C25 H18 N O



3-(4-(naphthalen-2-yl)phenyl)isoquinolin-1(2*H*)-one
Chemical Formula: $C_{25}H_{17}NO$
Exact Mass: 347.13


N
O
3-phenylisoquinolin-1(4H)-one
Chemical Formula: C15H11NO
Exact Mass: 221.08
8
7
6
5
4
3
2
1
ppm
2.00
0.94
4.06
2.10
2.23


195.392
138.529
136.244
133.665
132.794
131.021
128.823
128.384
127.593
117.887
113.617
77.315
76.685
43.562
200
180
160
140
120
100
80
60
40
20
ppm
N
O
3-phenylisoquinolin-1(4H)-one
Chemical Formula: C15H11NO
Exact Mass: 221.08

Elemental Composition Report

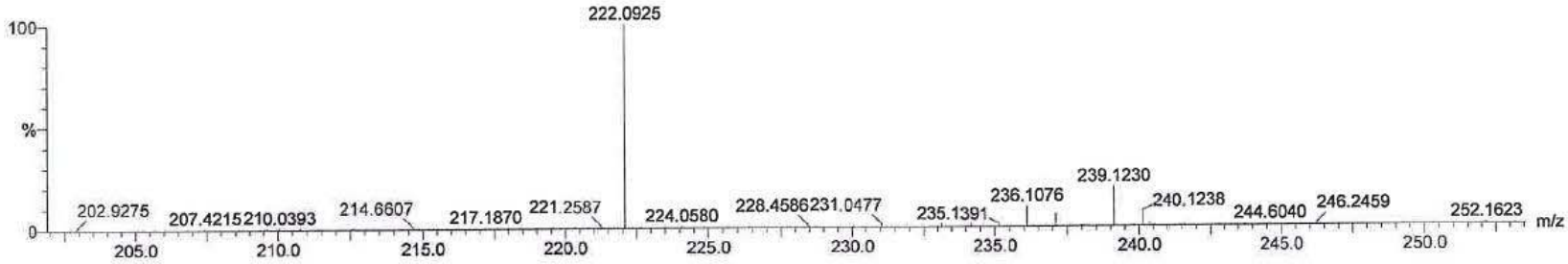
Single Mass Analysis

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

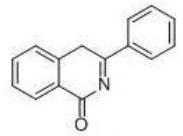
Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-3

B036/CAMIDE/001
131203002 12 (0.420) Cm (12:14-21:30)

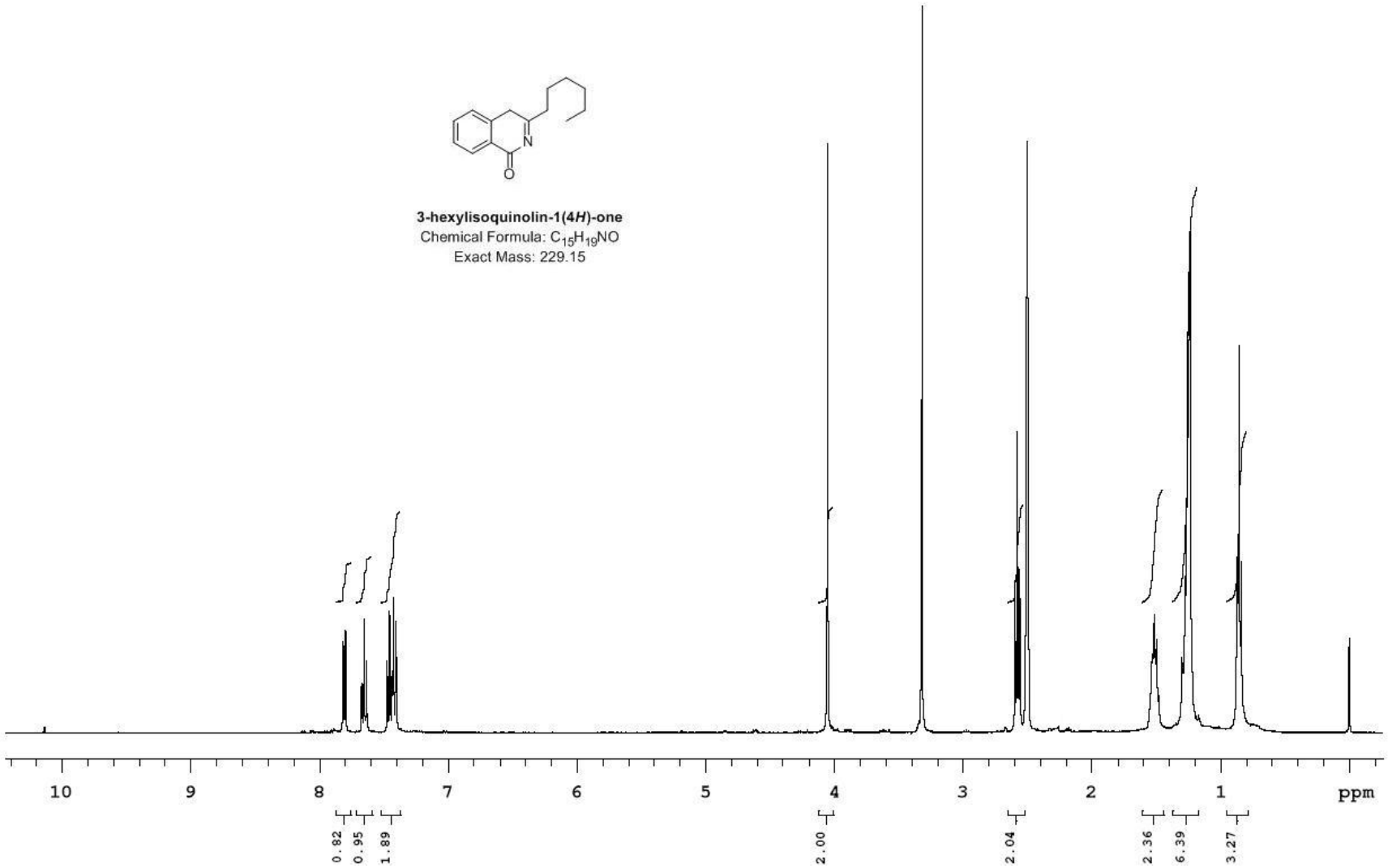
1: TOF MS ES+
4.00e+002

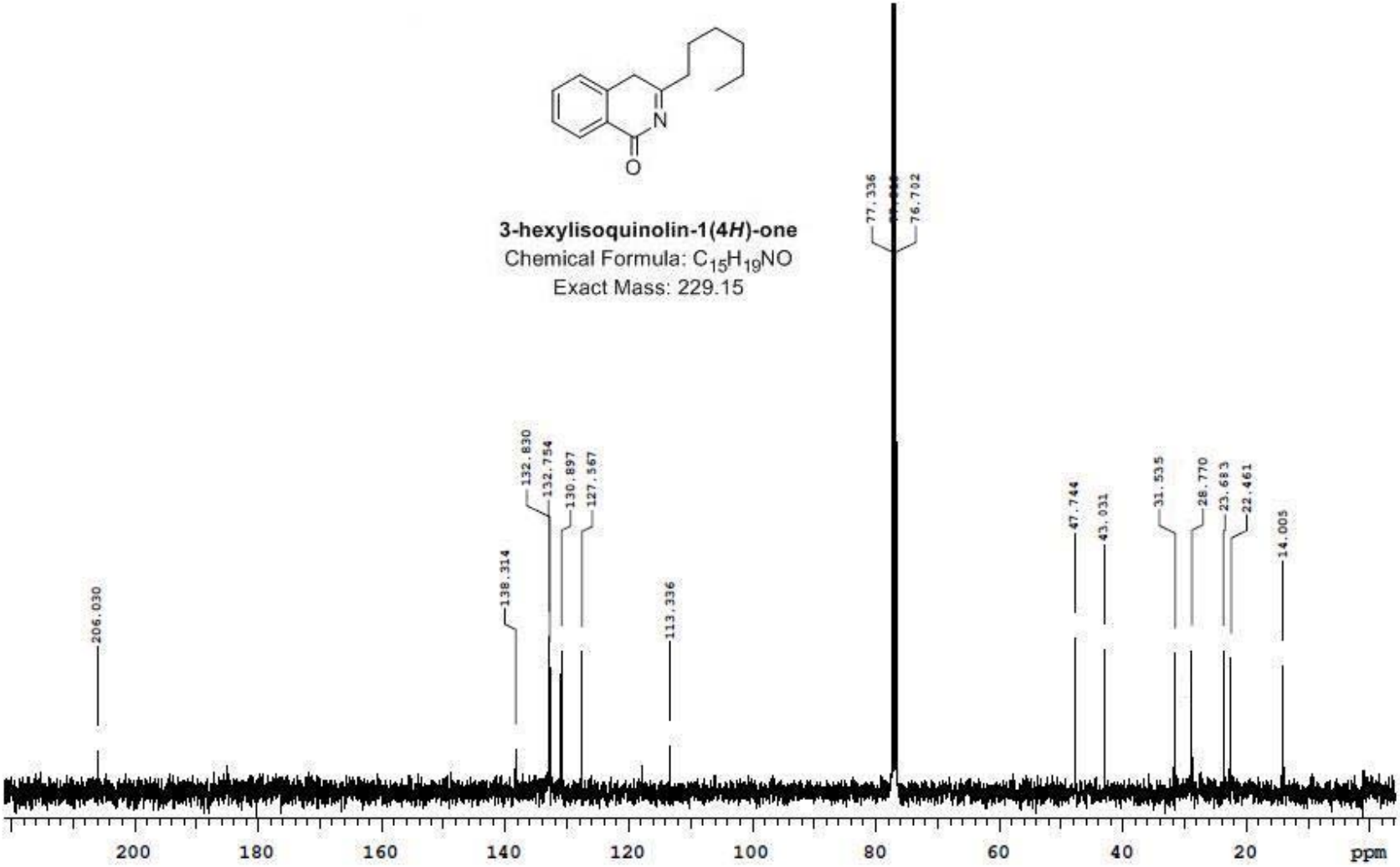


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
222.0925	222.0919	0.6	2.7	10.5	n/a	C15 H12 N O



3-phenylisoquinolin-1(4*H*)-one
Chemical Formula: $C_{15}H_{11}NO$
Exact Mass: 221.08


N
O
3-hexylisoquinolin-1(4H)-one
Chemical Formula: C15H19NO
Exact Mass: 229.15
10
9
8
7
6
5
4
3
2
1
ppm
0.82
0.95
1.89
2.00
2.04
2.36
6.39
3.27


3-hexylisoquinolin-1(4H)-one
Chemical Formula: C15H19NO
Exact Mass: 229.15
206.030
138.314
132.830
132.754
130.897
127.567
113.336
77.336
76.702
47.744
43.031
31.535
28.770
23.683
22.461
14.005
200
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

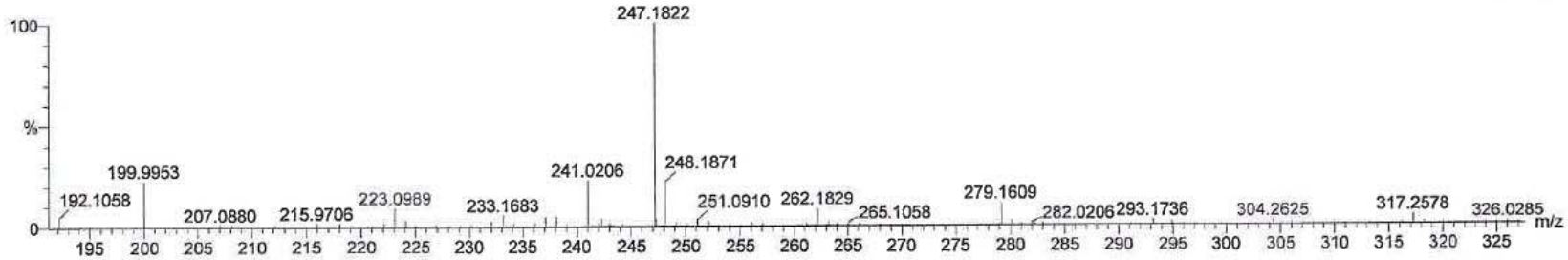
Single Mass Analysis

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

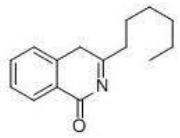
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-2 O: 0-2

B036/CGAJ1/003/NP
140206001 17 (0.545) Cm (17:23-1:3)

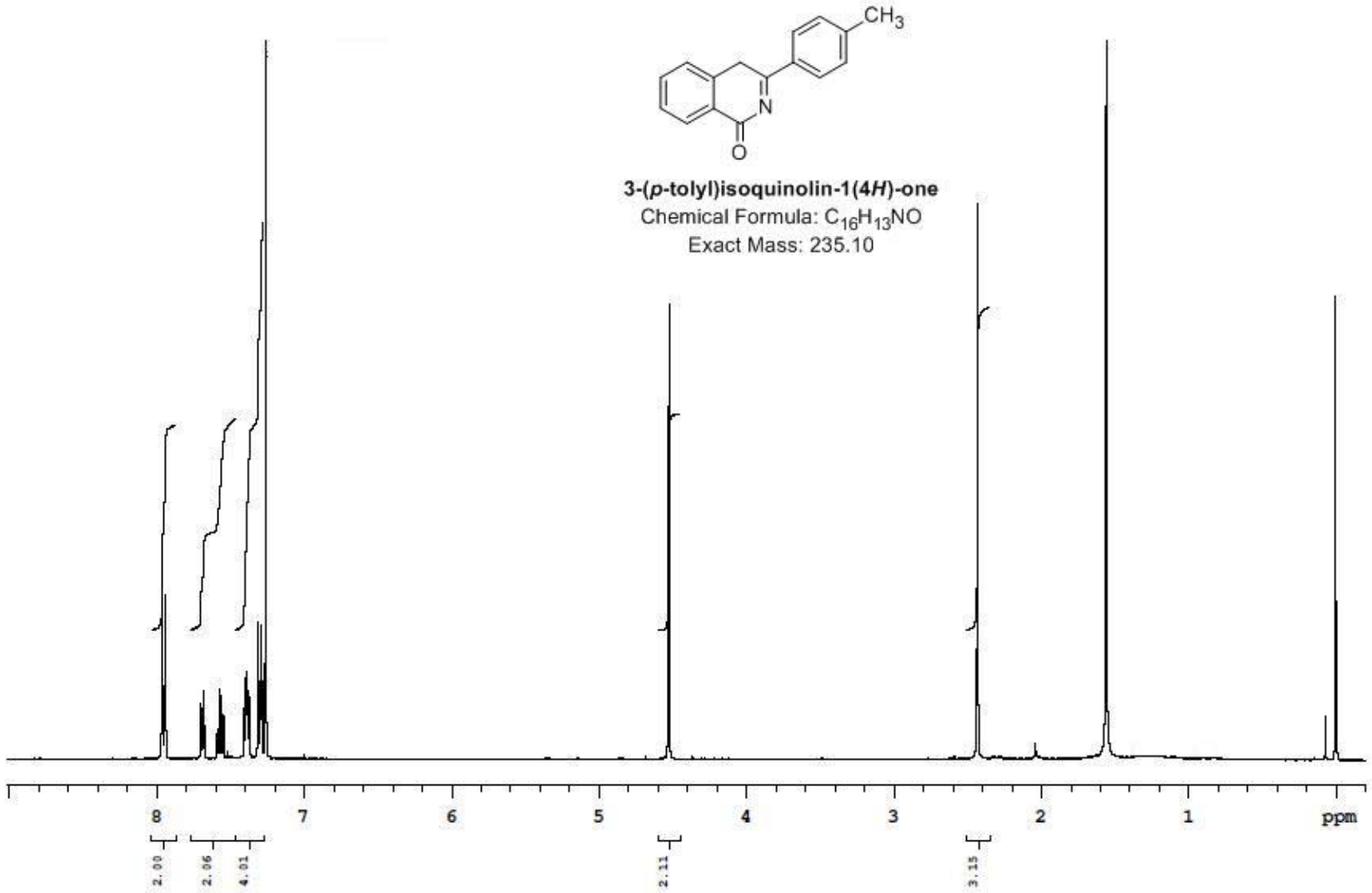
1: TOF MS ES+
1.64e+004

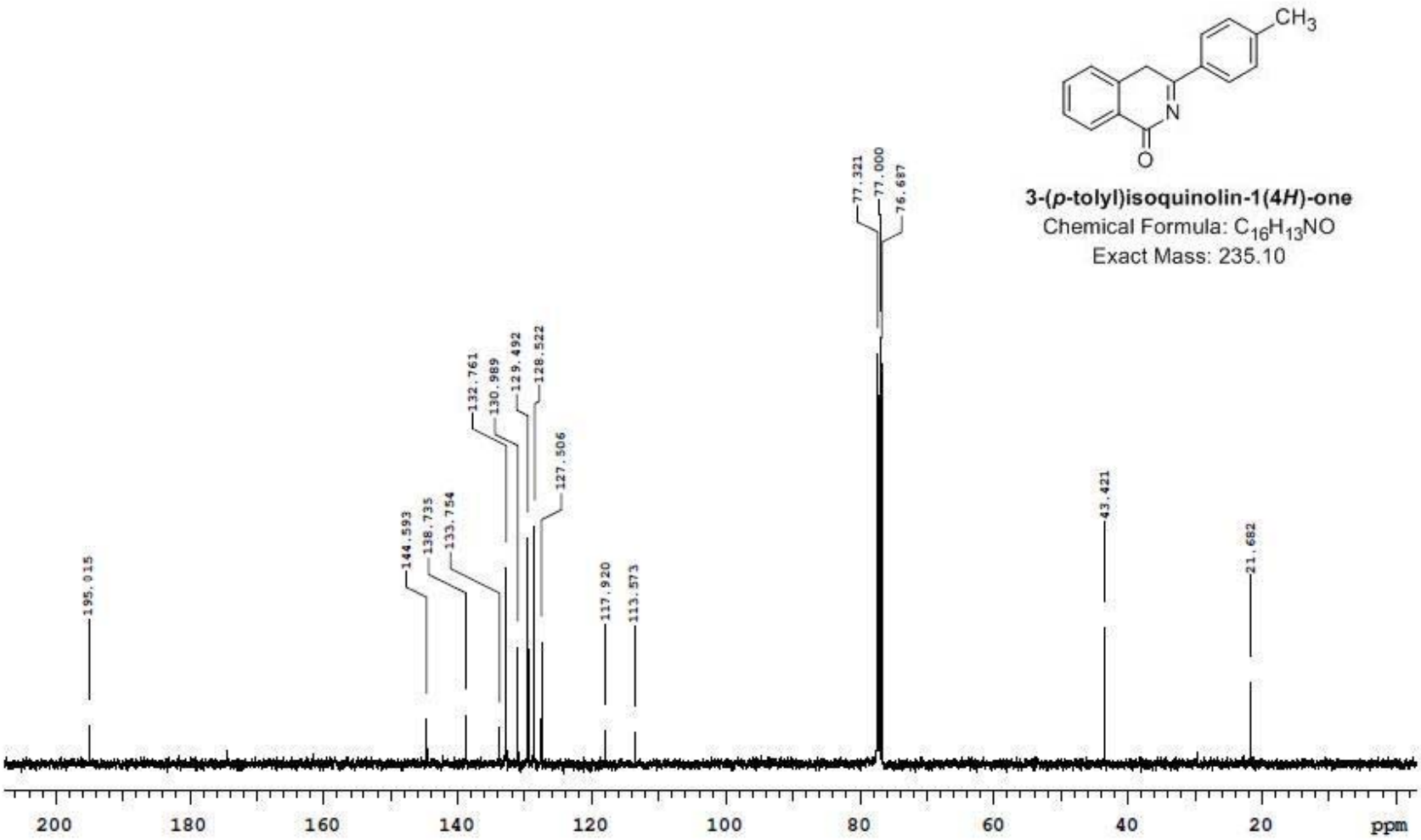


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
247.1822	247.1810	1.2	4.9	5.5	61.3	C15 H23 N2 O



3-hexylisoquinolin-1(4*H*)-one
Chemical Formula: $C_{15}H_{19}NO$
Exact Mass: 229.15


CH3
N
O
3-(p-tolyl)isoquinolin-1(4H)-one
Chemical Formula: C16H13NO
Exact Mass: 235.10
8
7
6
5
4
3
2
1
ppm
2.00
2.06
4.01
2.11
3.15


CH3
N
O
3-(p-tolyl)isoquinolin-1(4H)-one
Chemical Formula: C16H13NO
Exact Mass: 235.10
195.015
144.593
138.735
133.754
132.761
130.989
129.492
128.522
127.506
117.920
113.573
77.321
77.000
76.687
43.421
21.682
200
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

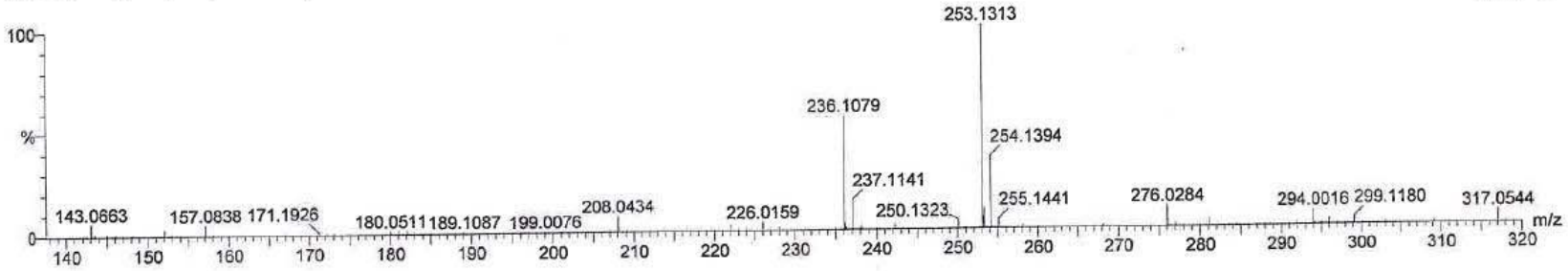
Single Mass Analysis

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

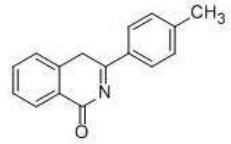
Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-1 O: 0-1

B036/CGAJ1/005/NP
140206002 11 (0.345) Cm (11:16-20:32)

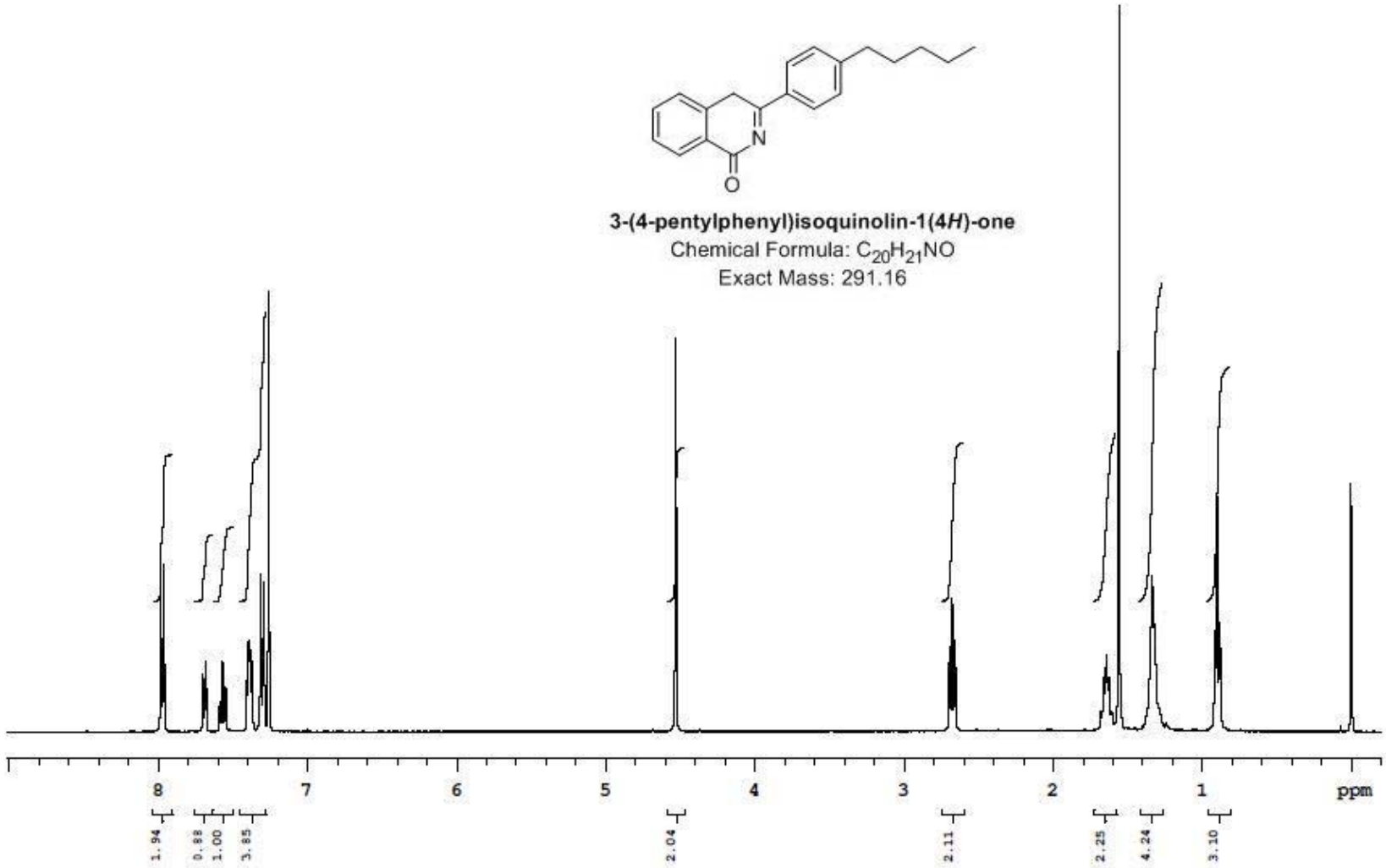
1: TOF MS ES+
3.06e+004



Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
236.1079	236.1075	0.4	1.7	10.5	186.2	C16 H14 N O



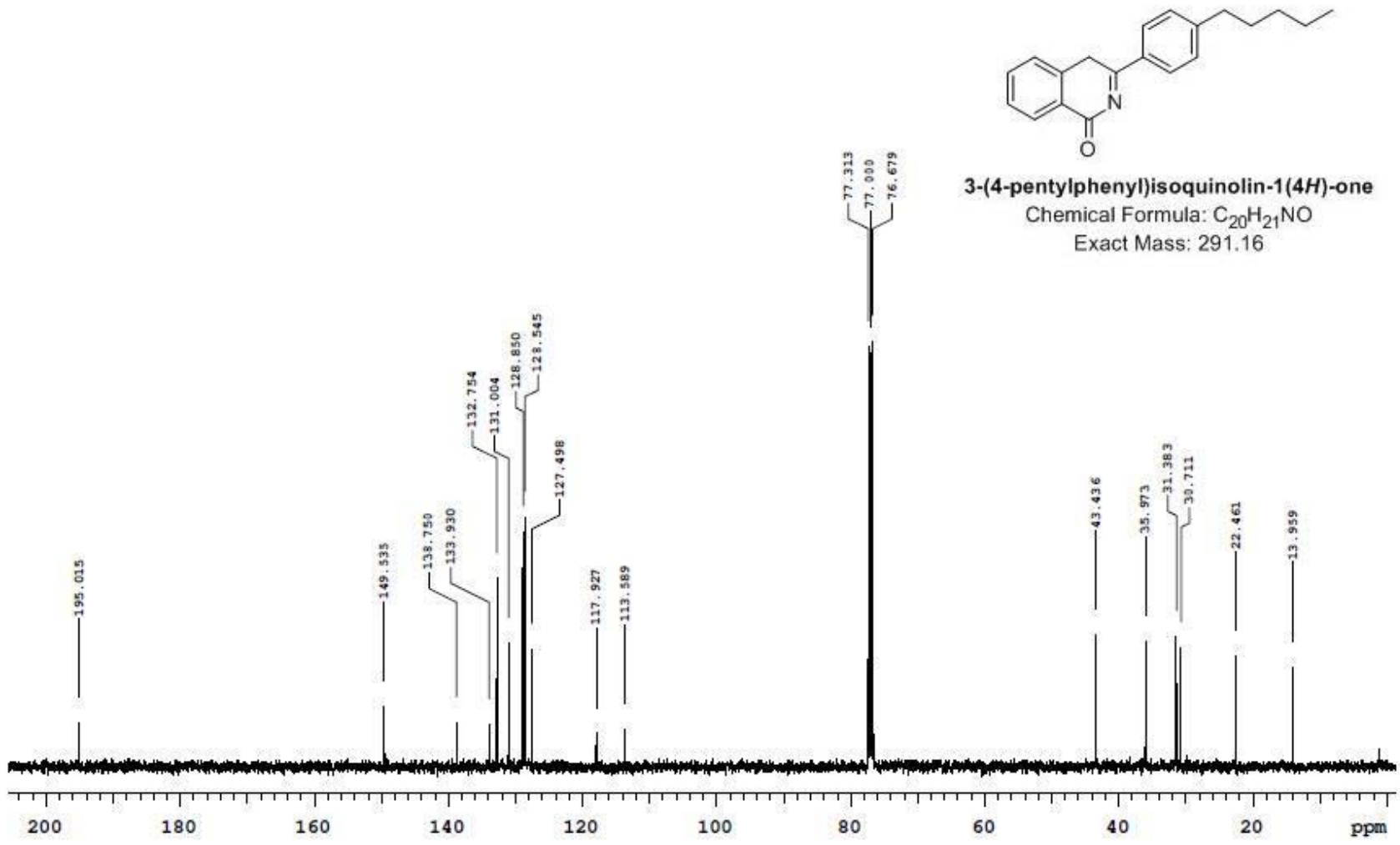
3-(*p*-tolyl)isoquinolin-1(4*H*)-one
Chemical Formula: $C_{16}H_{13}NO$
Exact Mass: 235.10



3-(4-pentylphenyl)isoquinolin-1(4*H*)-one

Chemical Formula: $C_{20}H_{21}NO$

Exact Mass: 291.16


3-(4-pentylphenyl)isoquinolin-1(4H)-one
Chemical Formula: C20H21NO
Exact Mass: 291.16
195.015
149.535
138.750
133.930
132.754
131.004
128.850
128.545
127.498
117.927
113.589
77.313
77.000
76.679
43.436
35.973
31.383
30.711
22.461
13.959
200
180
160
140
120
100
80
60
40
20
ppm

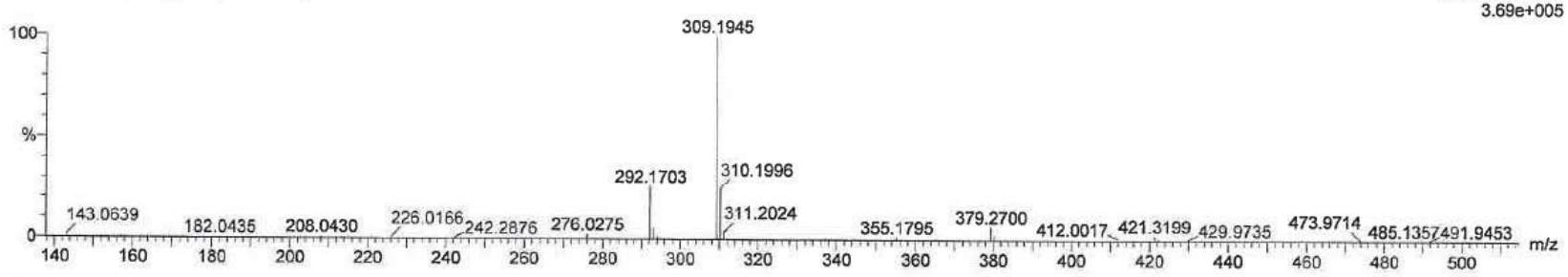
Elemental Composition Report

Single Mass Analysis

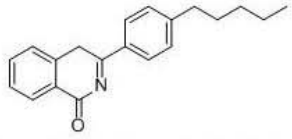
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-1 O: 0-1
B036/CGAJ1/006/NP
140206003 10 (0.322) Cm (9:11-33:36)

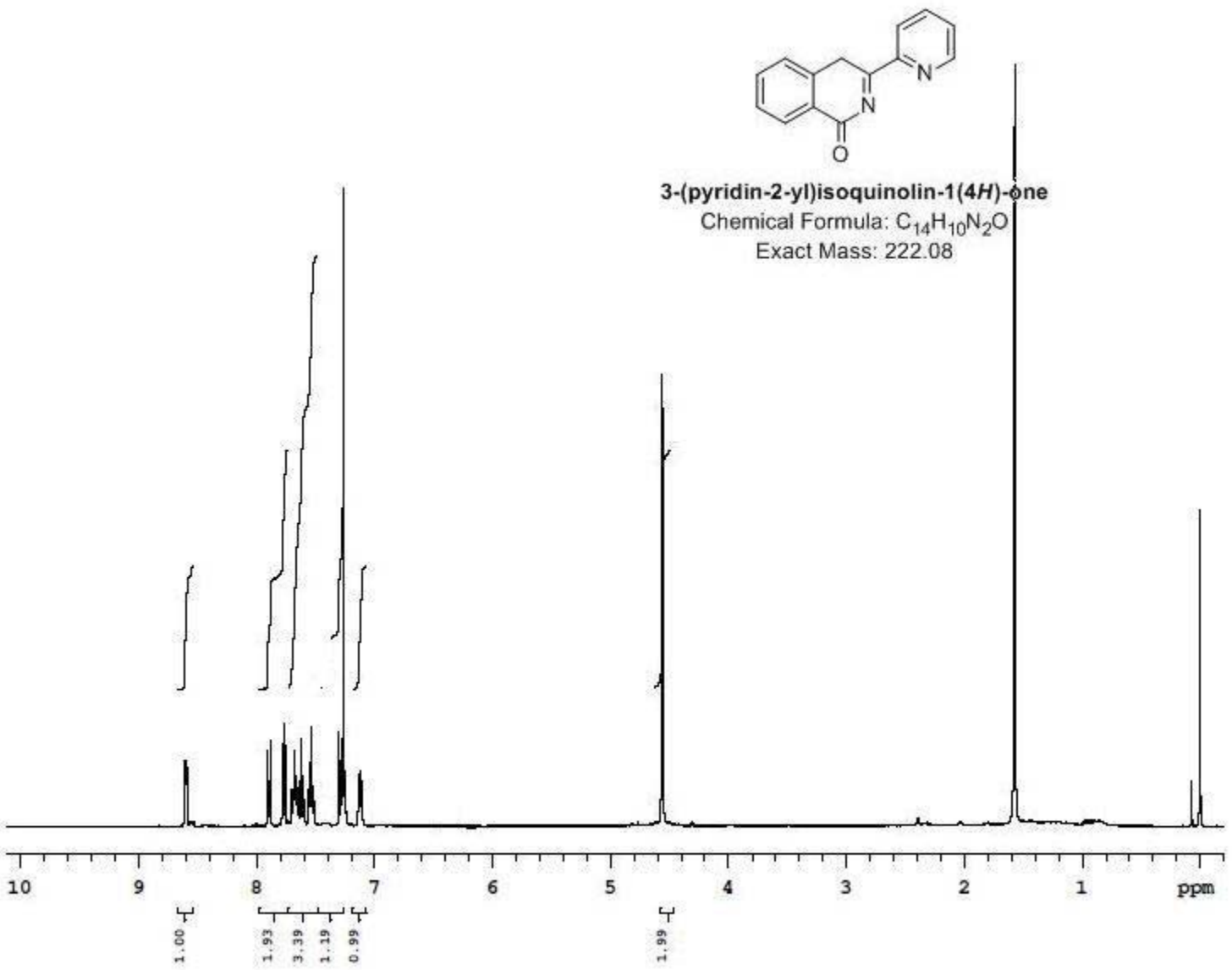
1: TOF MS ES+
3.69e+005

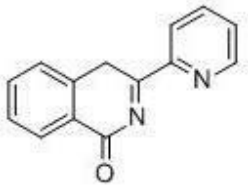


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.1703	292.1701	0.2	0.7	10.5	30.3	C20 H22 N O



3-(4-pentylphenyl)isoquinolin-1(4*H*)-one
Chemical Formula: $C_{20}H_{21}NO$
Exact Mass: 291.16

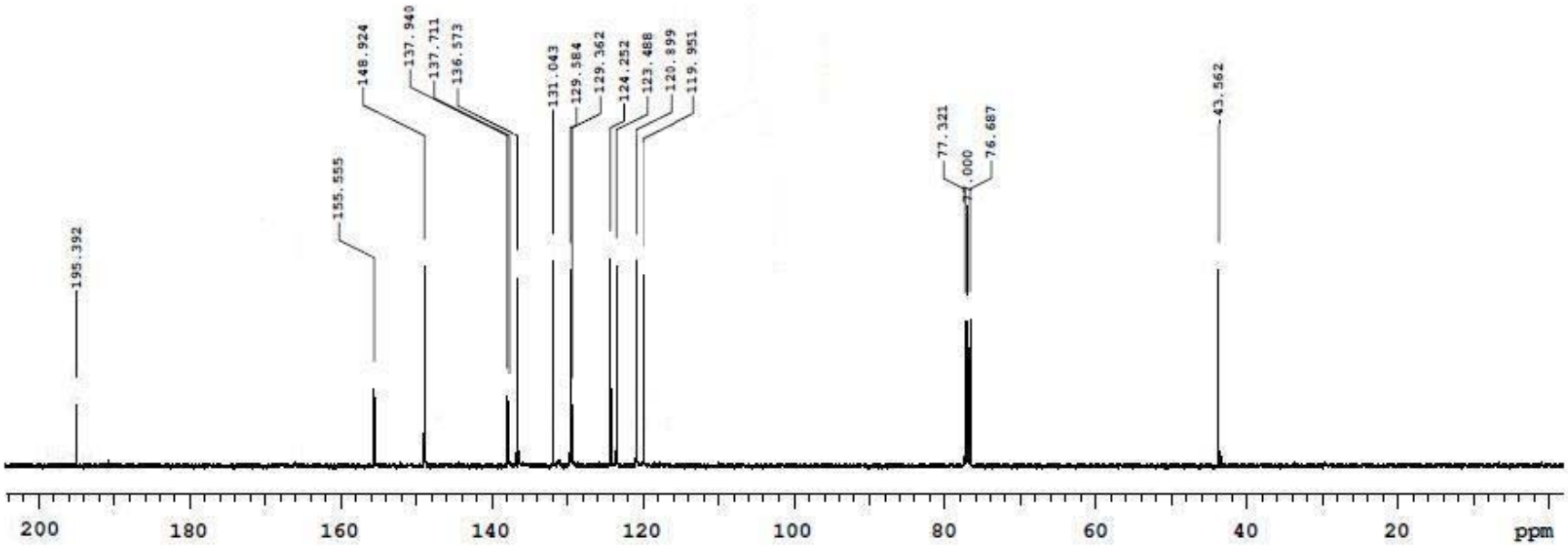

N
N
O
3-(pyridin-2-yl)isoquinolin-1(4H)-one
Chemical Formula: C14H10N2O
Exact Mass: 222.08
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.93
3.39
1.19
0.99
1.99



3-(pyridin-2-yl)isoquinolin-1(4*H*)-one

Chemical Formula: $C_{14}H_{10}N_2O$

Exact Mass: 222.08



Elemental Composition Report

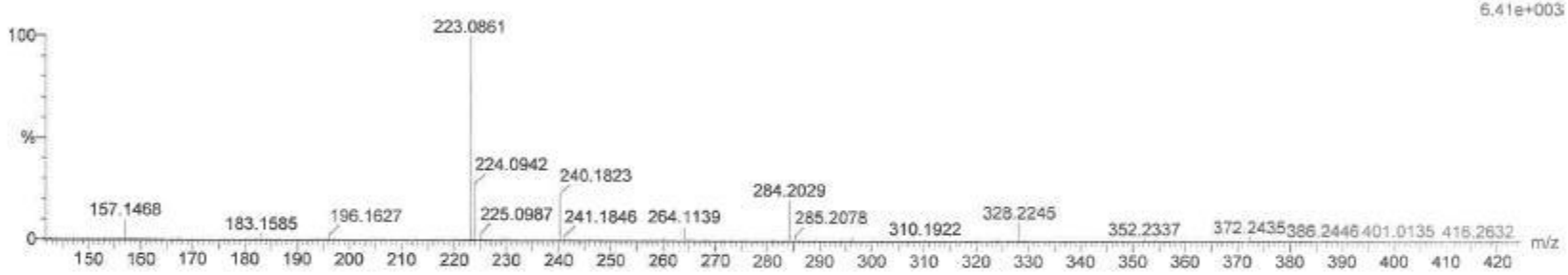
Single Mass Analysis

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

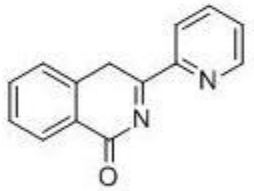
Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-15 N: 0-3 O: 0-2

8036/CGAJ1/012
140227006 12 (0.369) Cm (8:12-17:24)

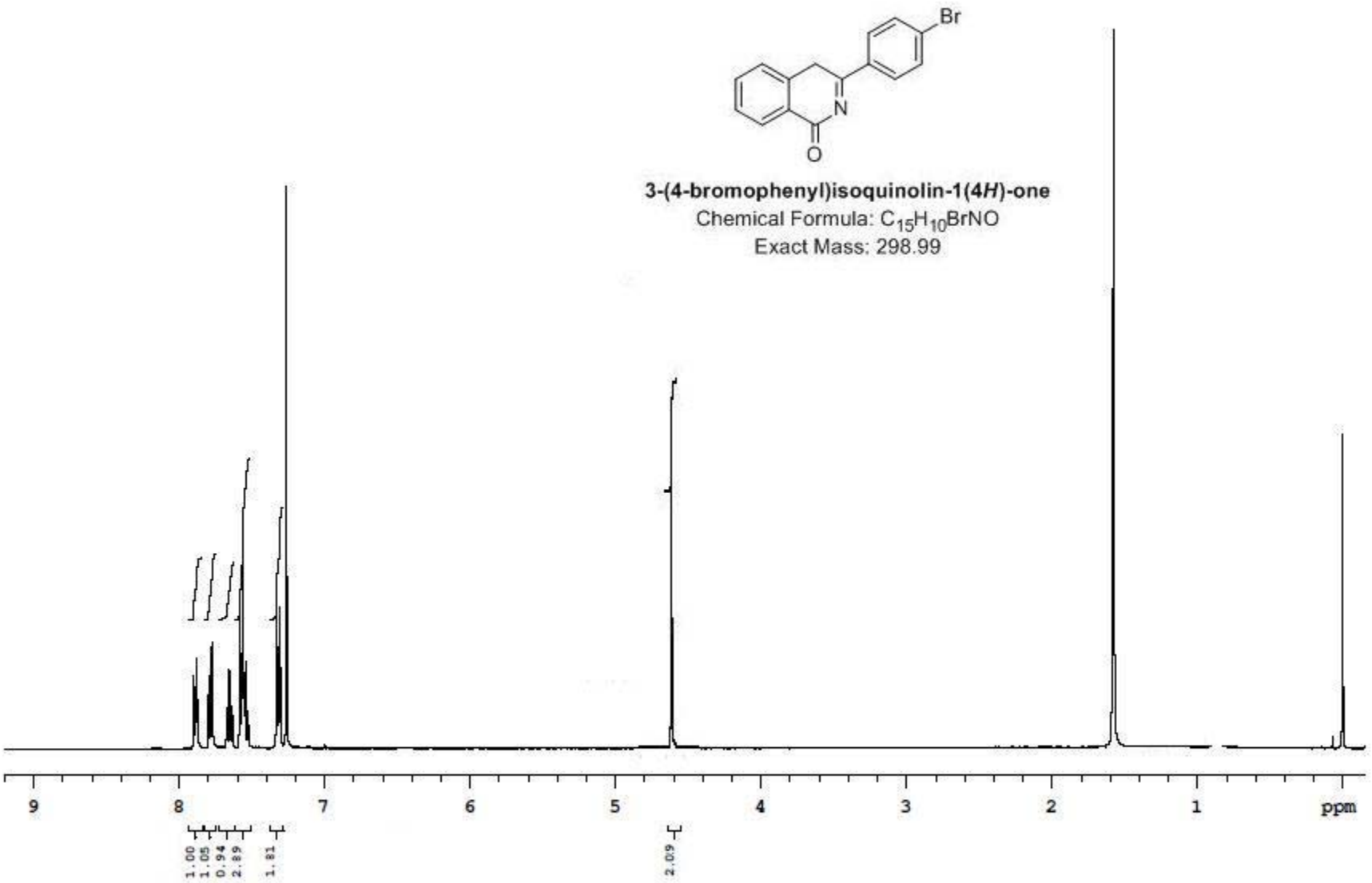
1: TOF MS ES+
6.41e+003

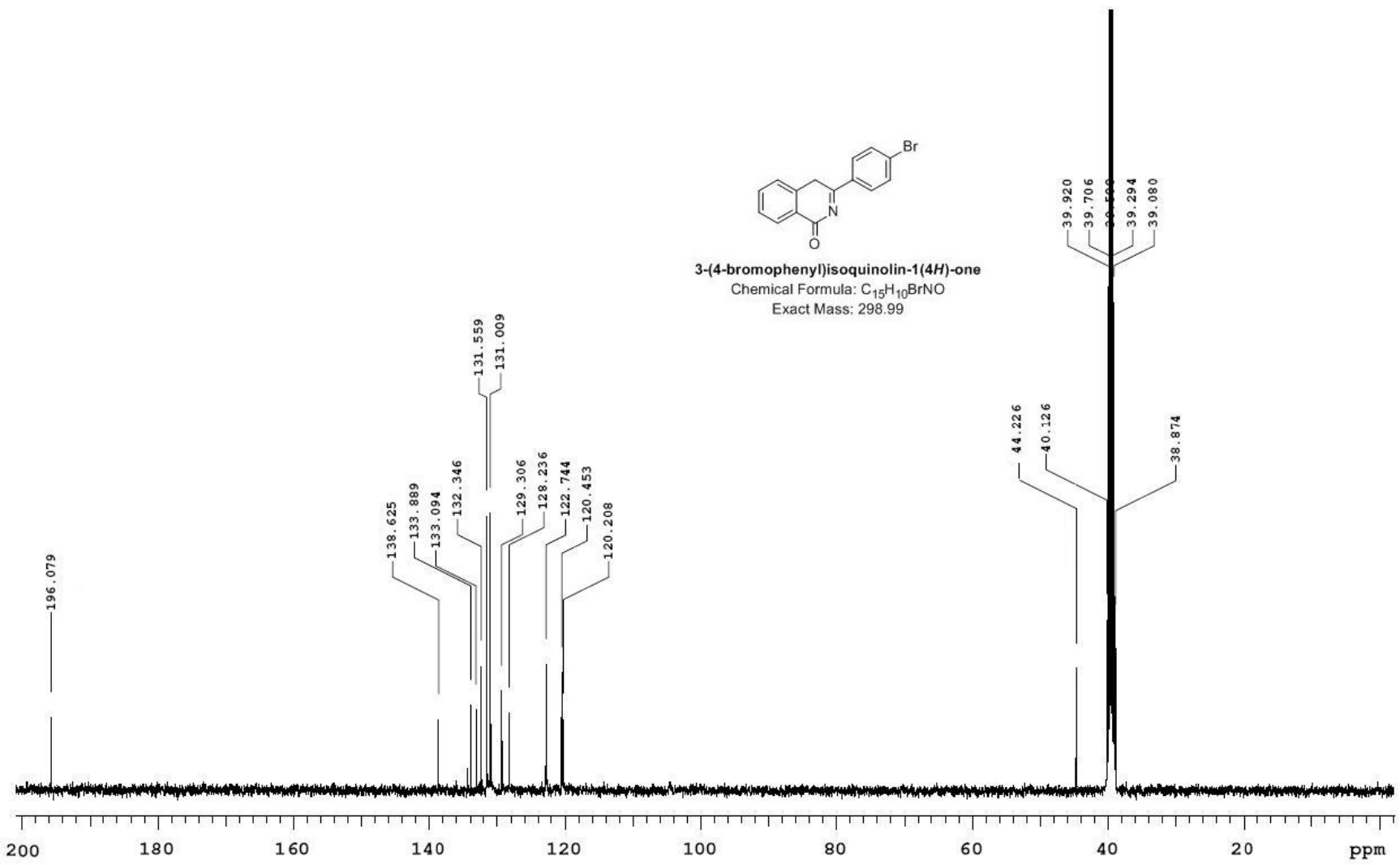


Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
223.0861	223.0871	-1.0	-4.5	10.5	159.2	C14 H11 N2 O



3-(pyridin-2-yl)isoquinolin-1(4*H*)-one
Chemical Formula: $C_{14}H_{10}N_2O$
Exact Mass: 222.08


Br
N
O
3-(4-bromophenyl)isoquinolin-1(4H)-one
Chemical Formula: C15H10BrNO
Exact Mass: 298.99
9
8
7
6
5
4
3
2
1
ppm
1.00
1.05
0.94
2.89
1.81
2.09


Br
N
O
3-(4-bromophenyl)isoquinolin-1(4H)-one
Chemical Formula: C15H10BrNO
Exact Mass: 298.99
196.079
138.625
133.889
133.094
132.346
131.559
131.009
129.306
128.236
122.744
120.453
120.208
44.226
40.126
39.920
39.706
39.294
39.080
38.874
200
180
160
140
120
100
80
60
40
20
ppm

Elemental Composition Report

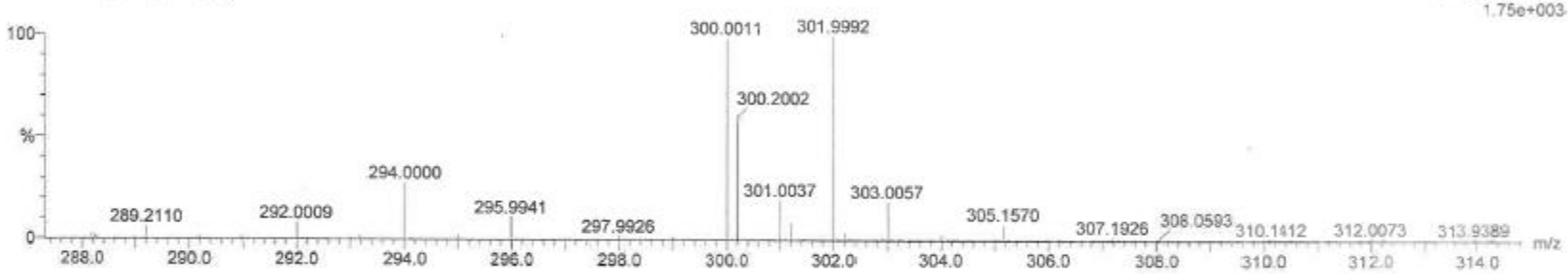
Single Mass Analysis

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

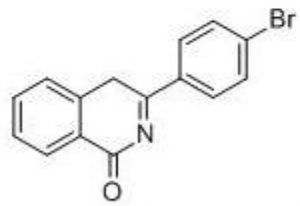
Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-15 N: 0-3 O: 0-2 Br: 0-1

B036/CGAJ1/014
140227011 7 (0.221) Cm (7:8)

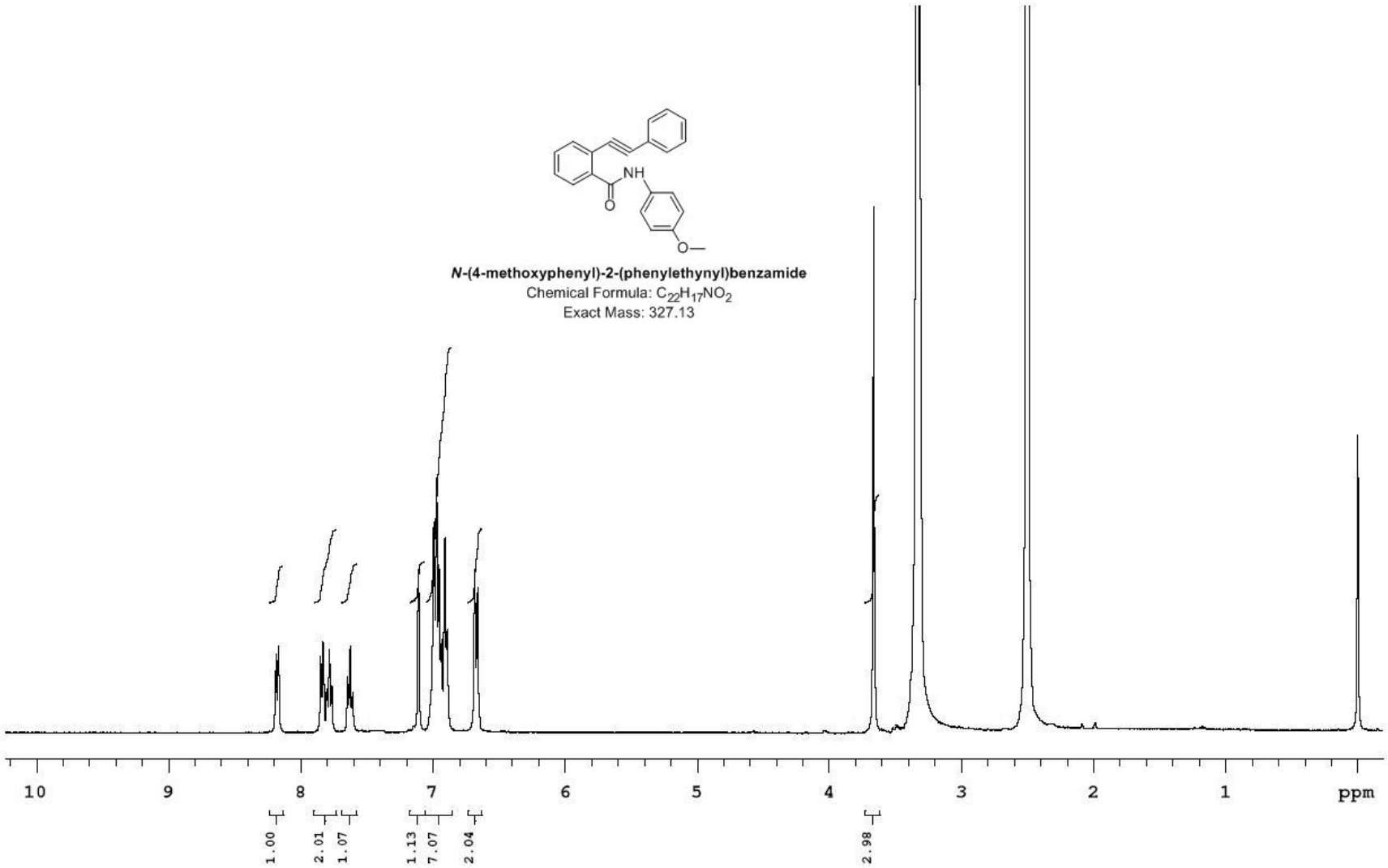
1 TOF MS ES+
1.75e+003



Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
300.0011	300.0024	-1.3	-4.3	10.5	3.0	C15 H11 N O Br



3-(4-bromophenyl)isoquinolin-1(4*H*)-one
Chemical Formula: $C_{15}H_{10}BrNO$
Exact Mass: 298.99


NH
O
O—
***N*-(4-methoxyphenyl)-2-(phenylethynyl)benzamide**
Chemical Formula: $C_{22}H_{17}NO_2$
Exact Mass: 327.13
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.01
1.07
1.13
7.07
2.04
2.98

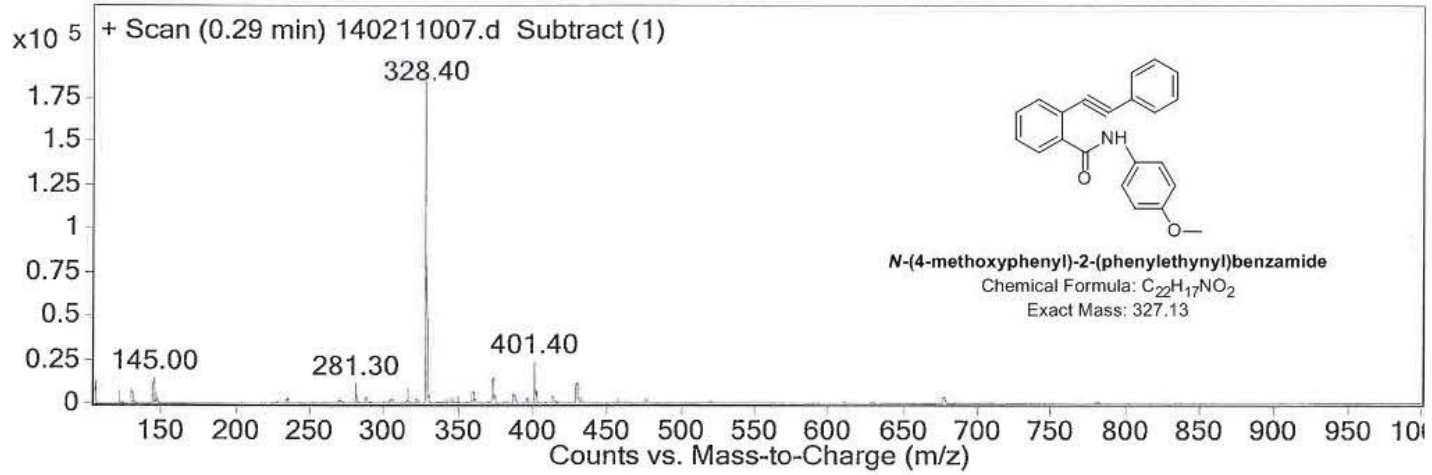
CPS,MIYAPUR

Mass Analysis Report

Data Filename	140211007.d	**Sample Name**	B036/CGAJ1/009/Methoxy(114020668)
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.M	**IRM Calibration Status**	Success
DA Method	CACH8.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



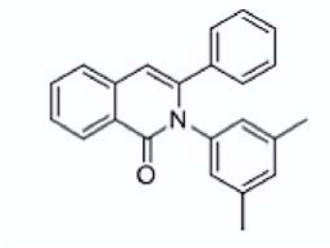
--- End Of Report ---

B Singh
11/02/2014

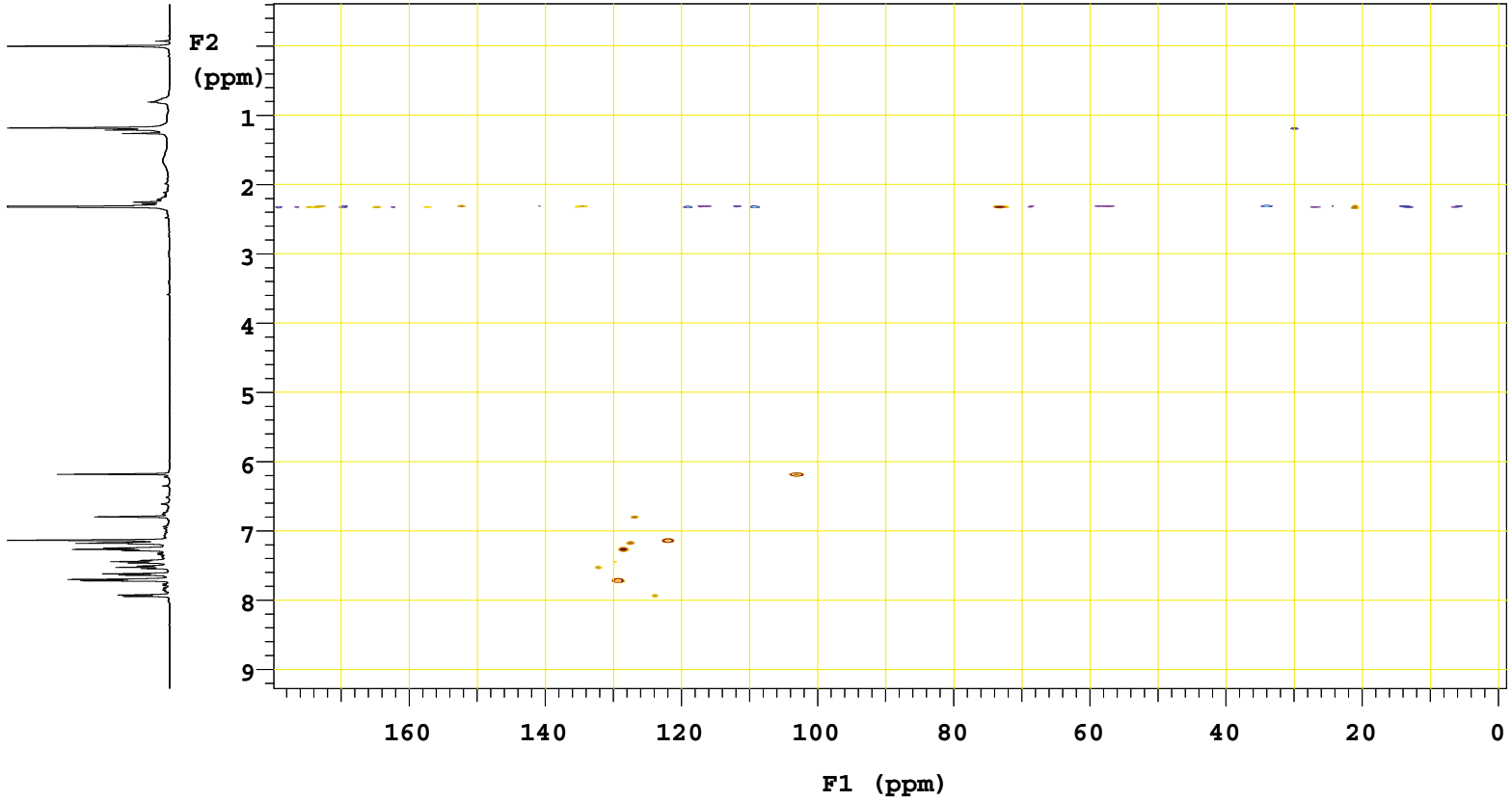
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3

NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

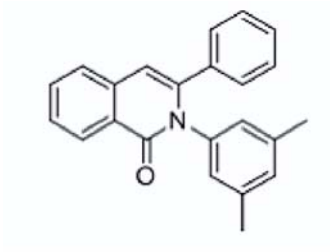


NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



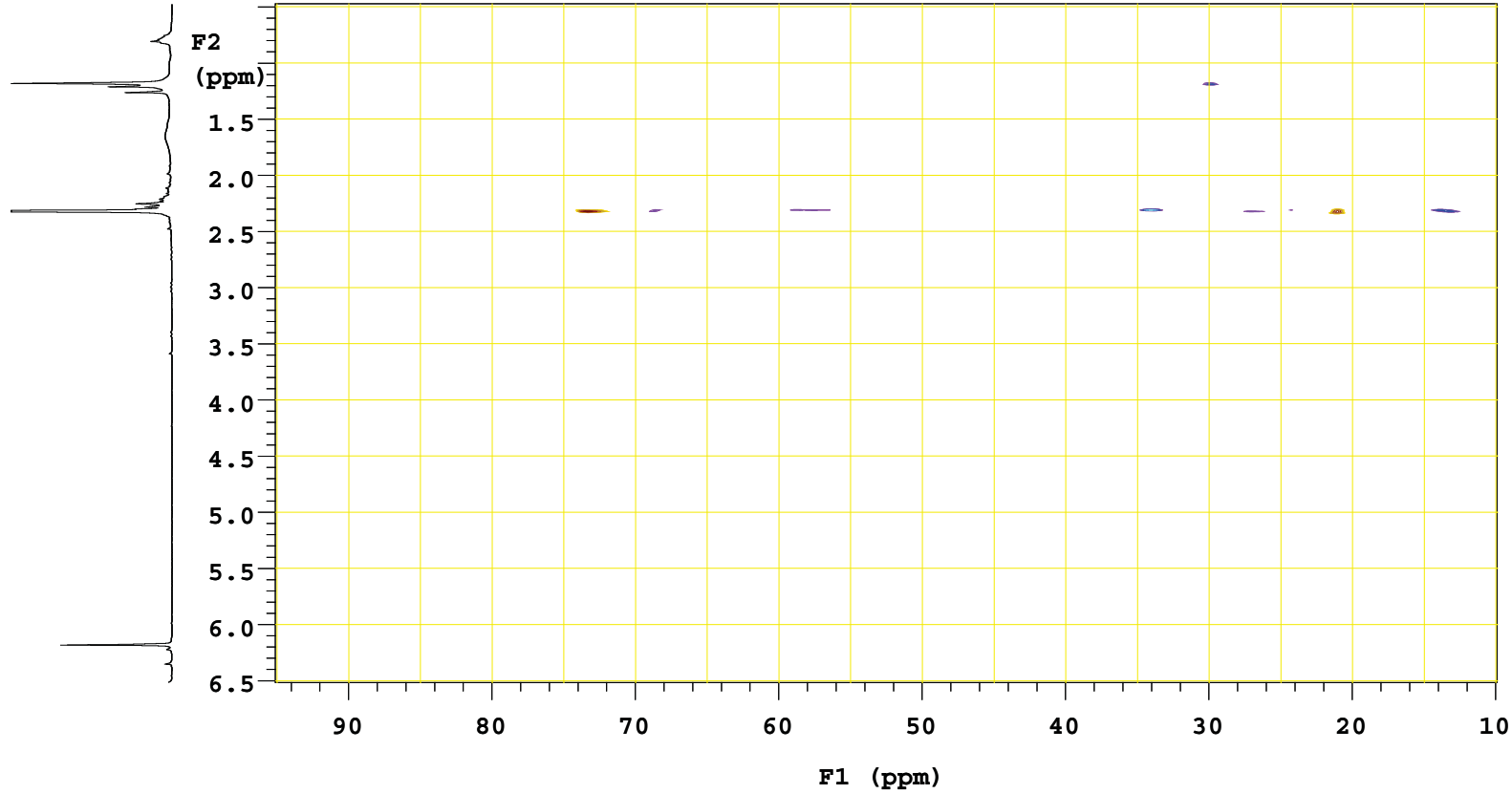
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3



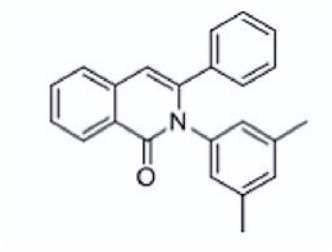
NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



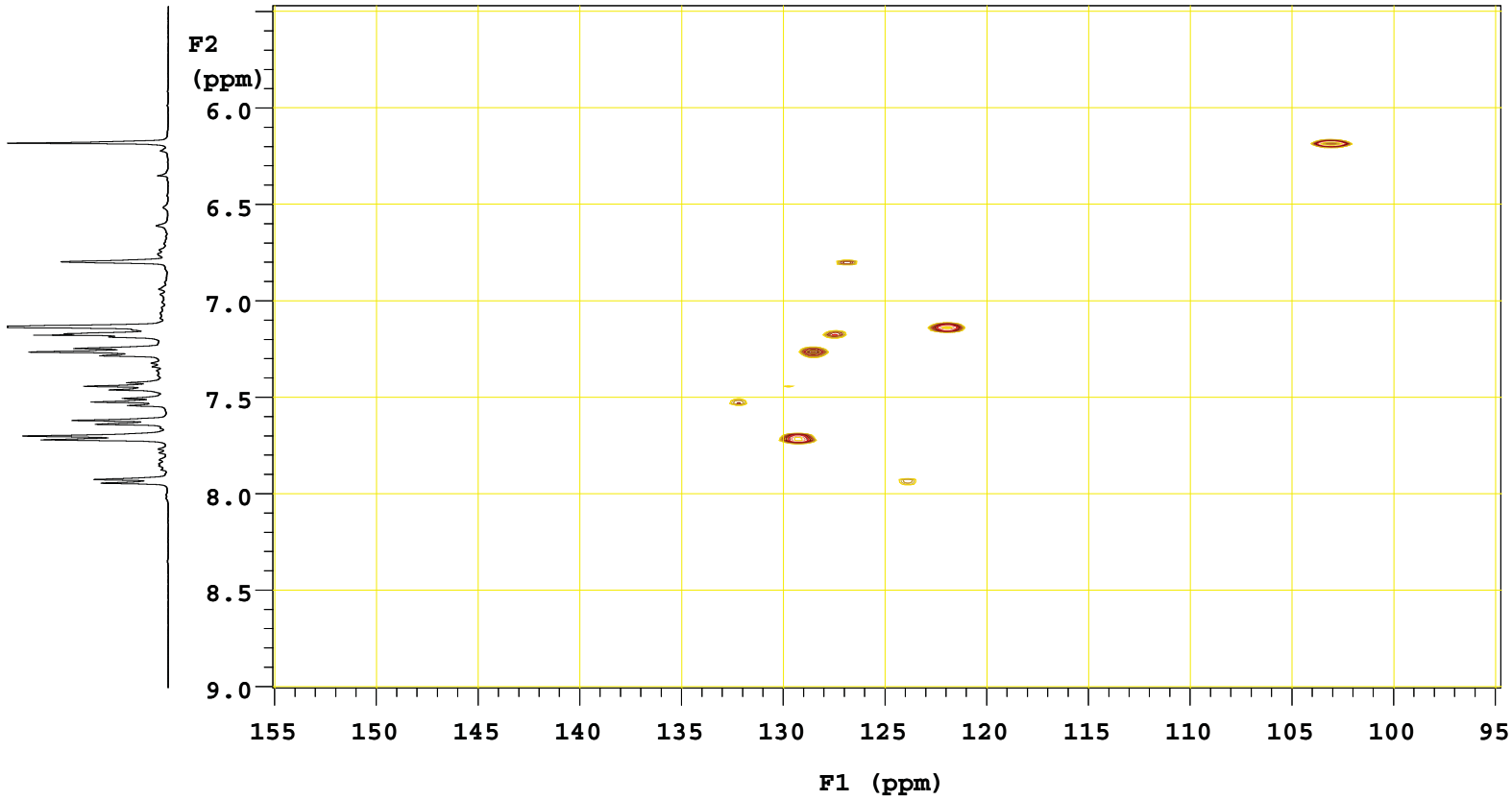
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3



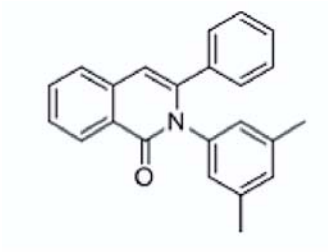
NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



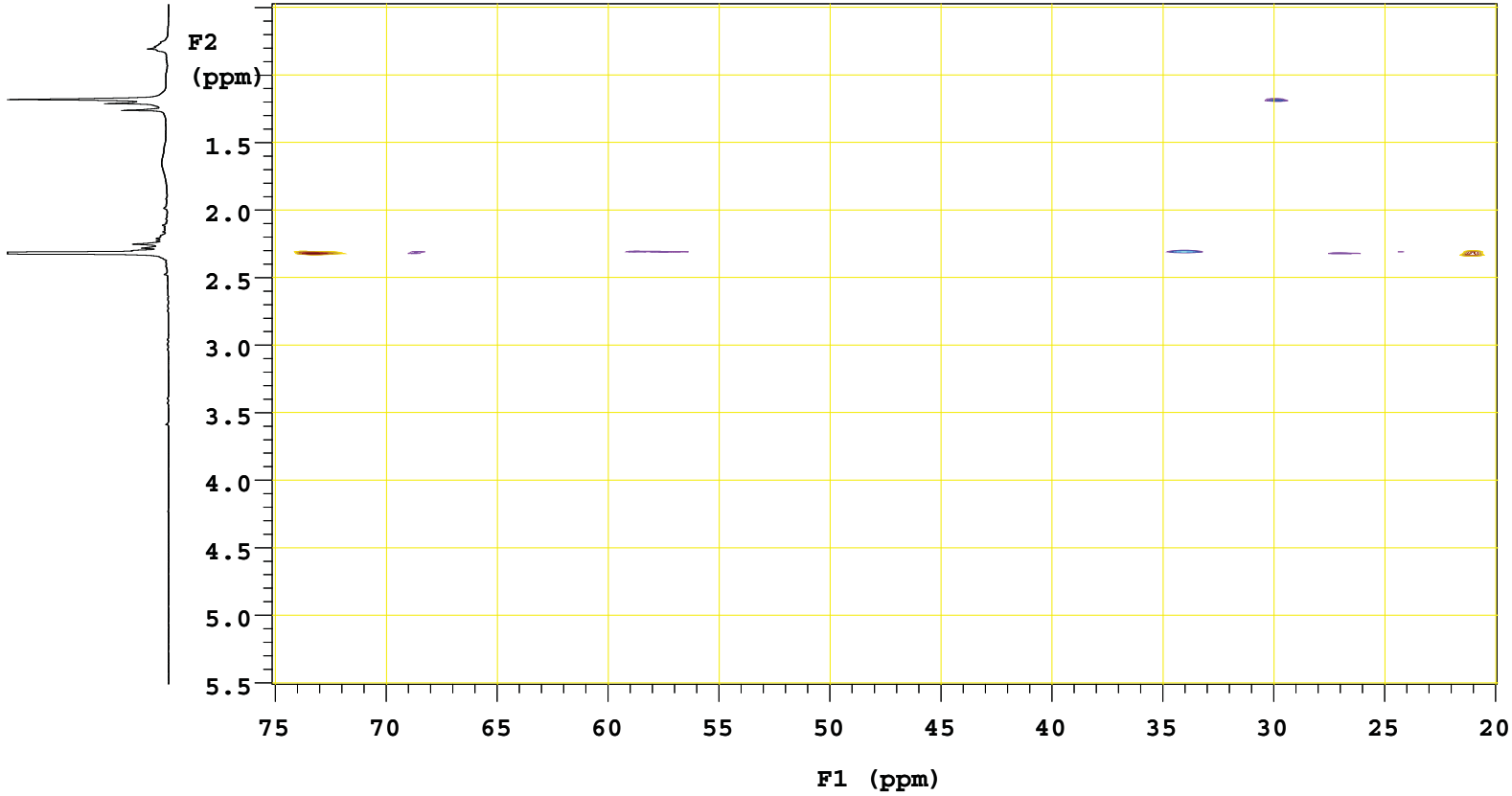
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3

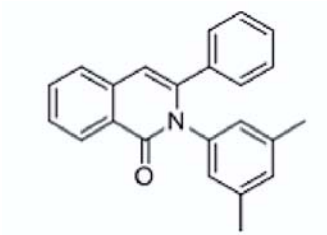


NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



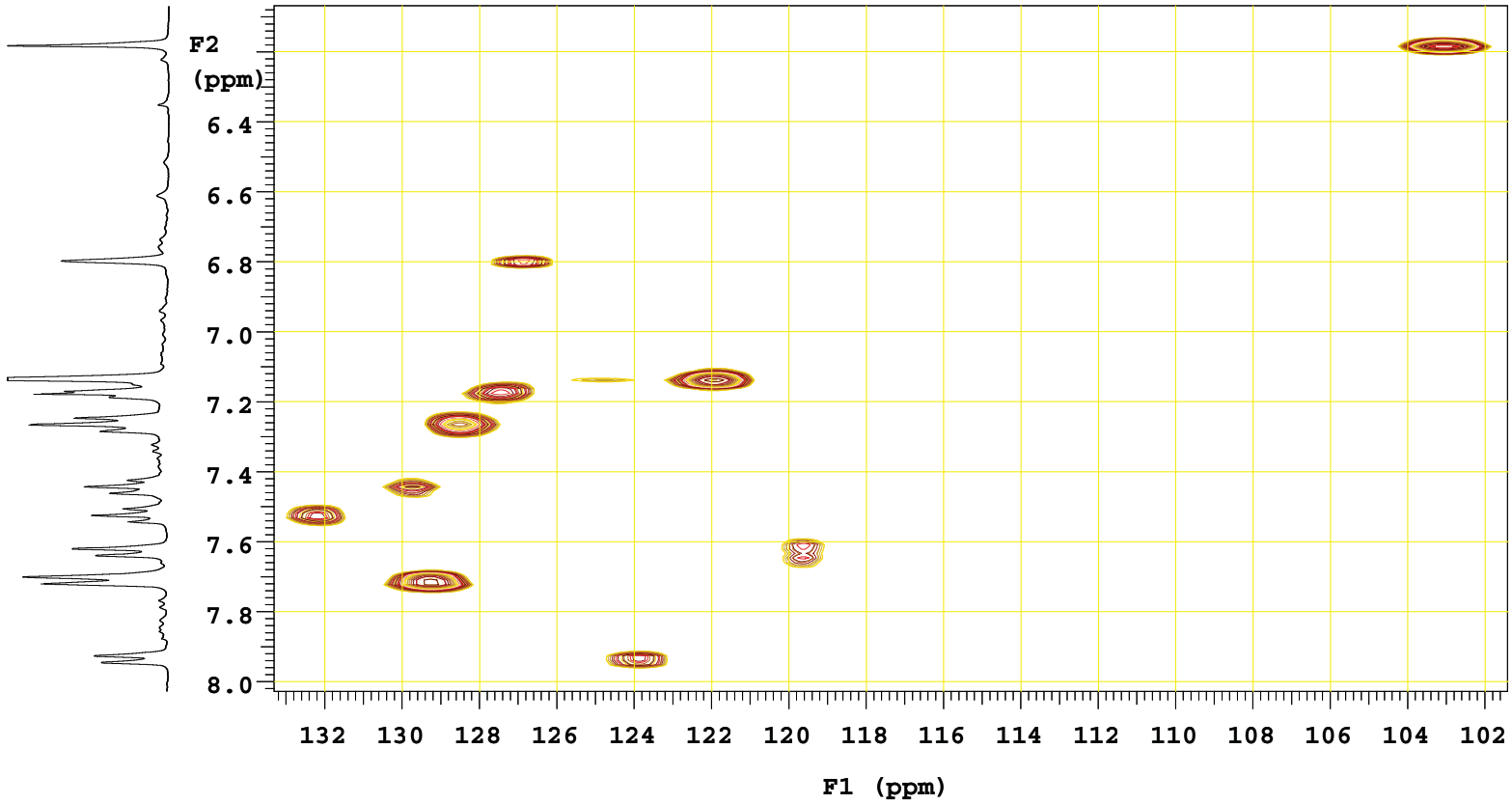
Compound **3a**



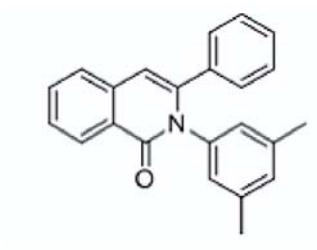
TDC-010 B036-CDMA1-015 in CDCl3

NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



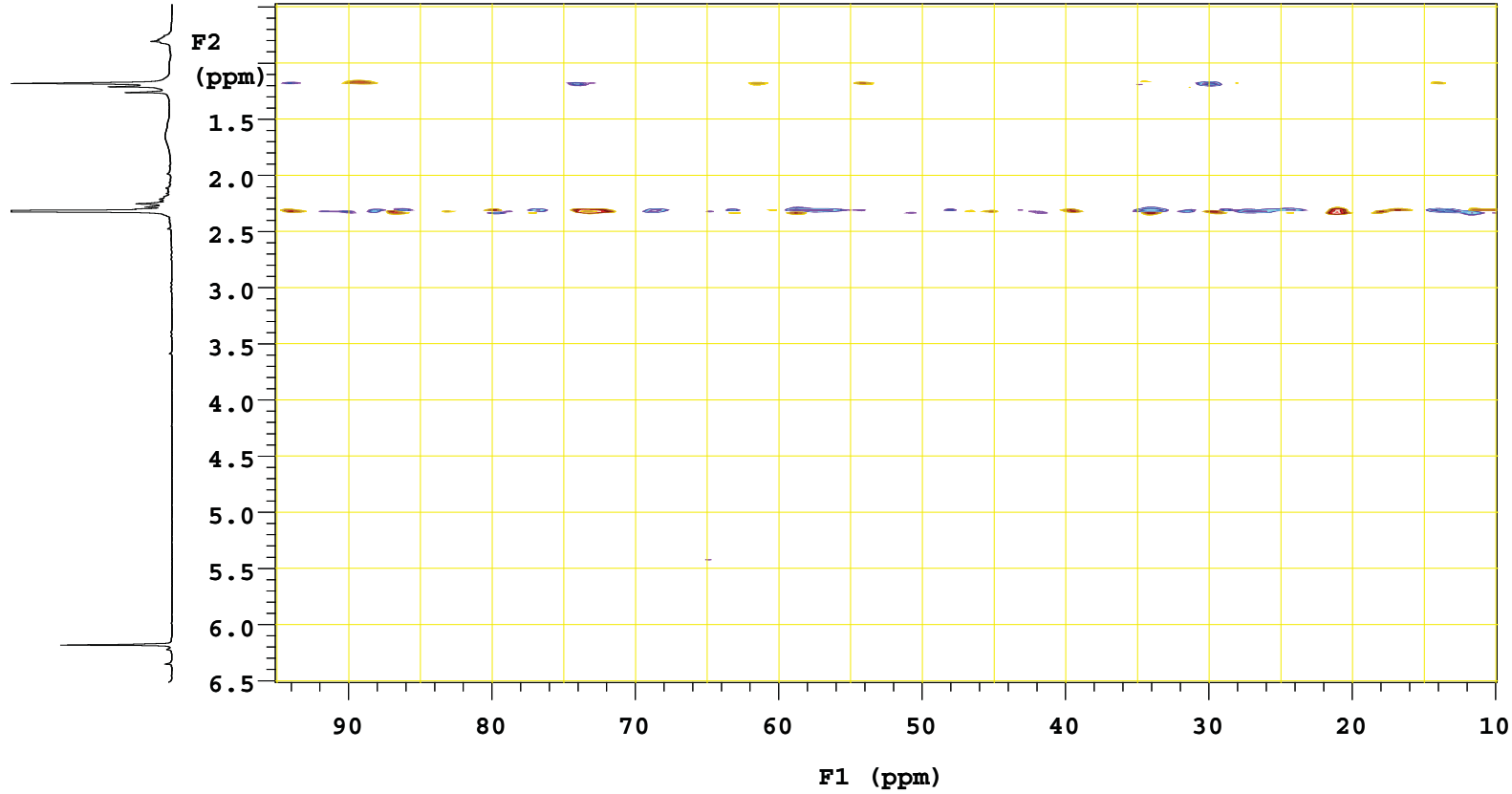
Compound **3a**



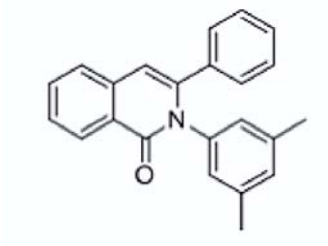
TDC-010 B036-CDMA1-015 in CDCl3

NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



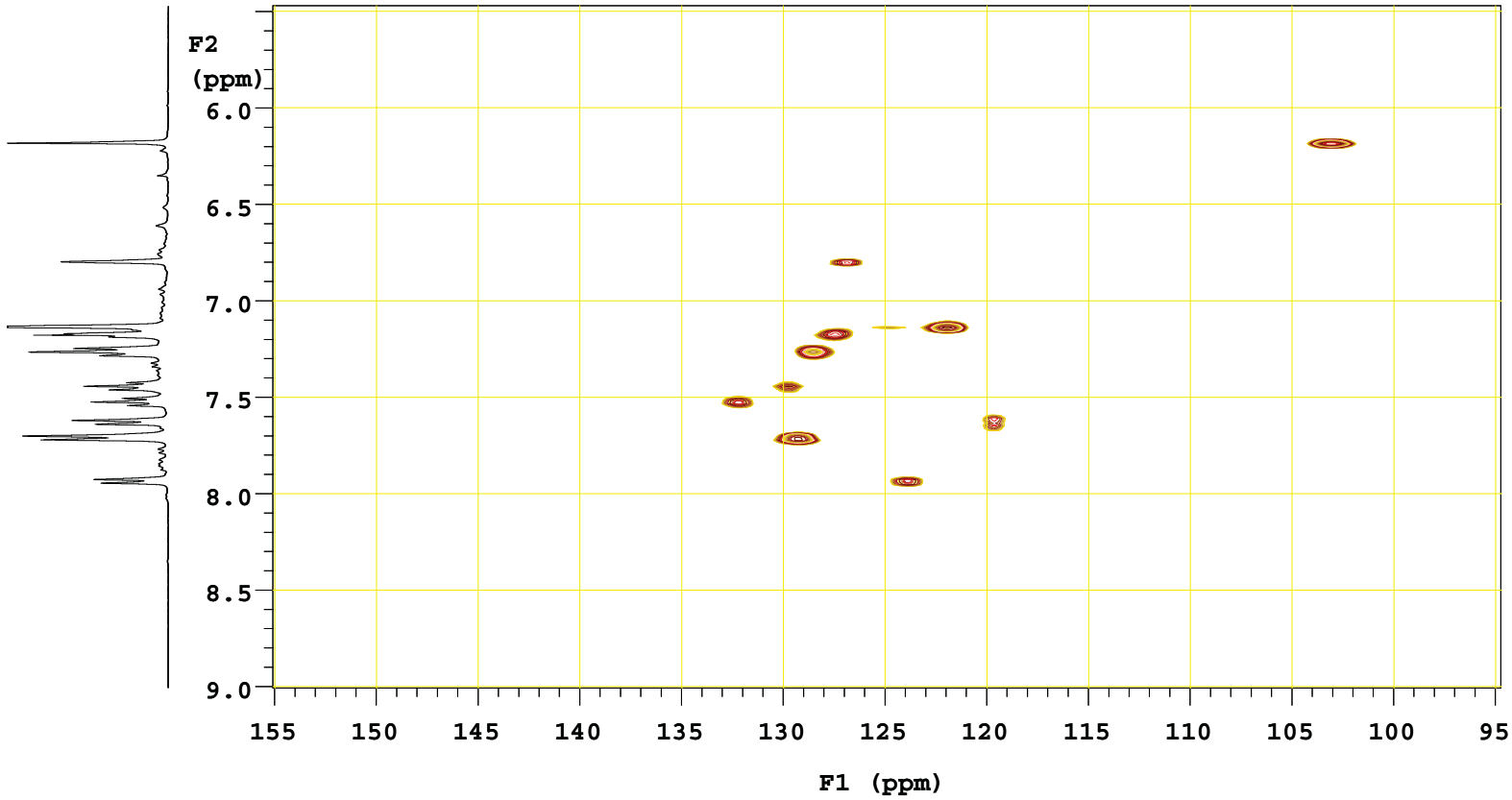
Compound **3a**



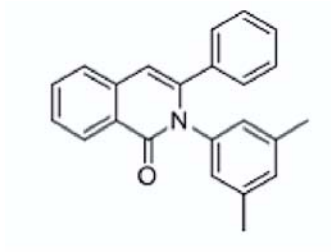
TDC-010 B036-CDMA1-015 in CDCl3

NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



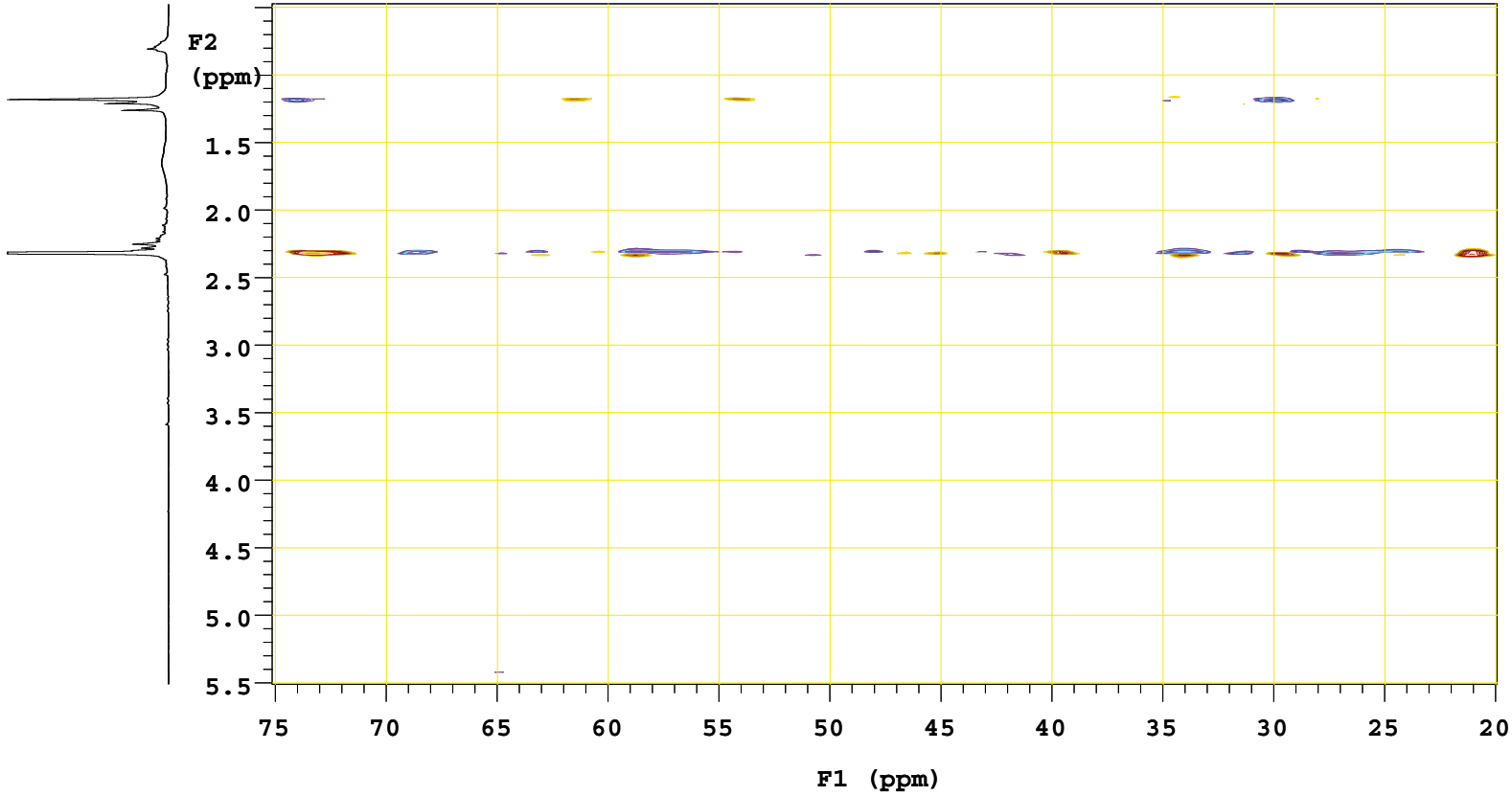
Compound **3a**



TDC-010 B036-CDMA1-015 in CDCl3

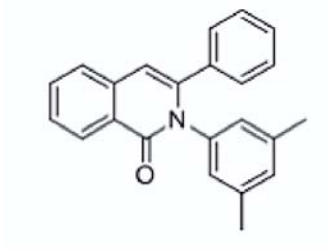
NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



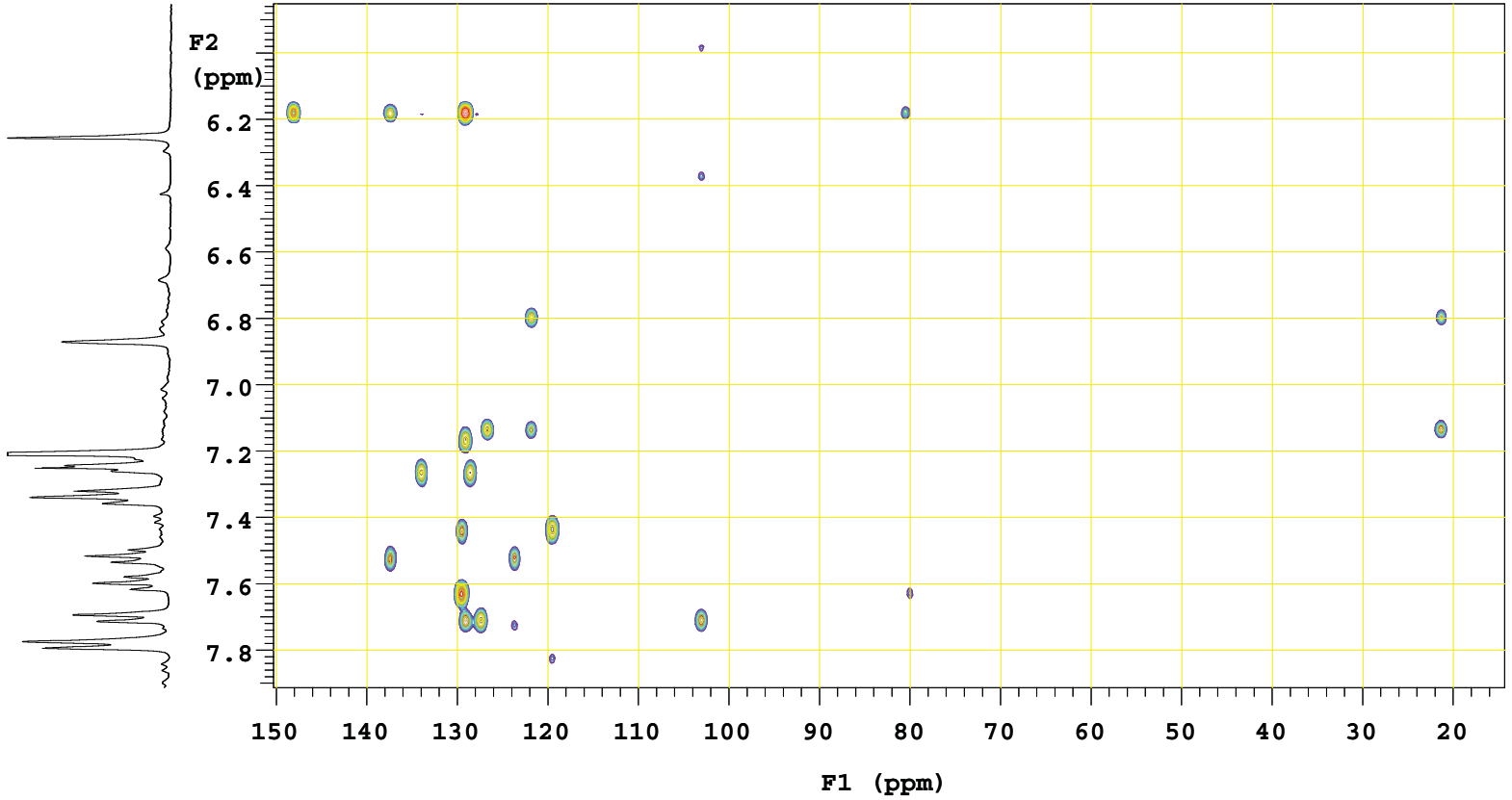
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3



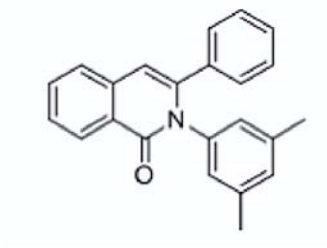
NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC



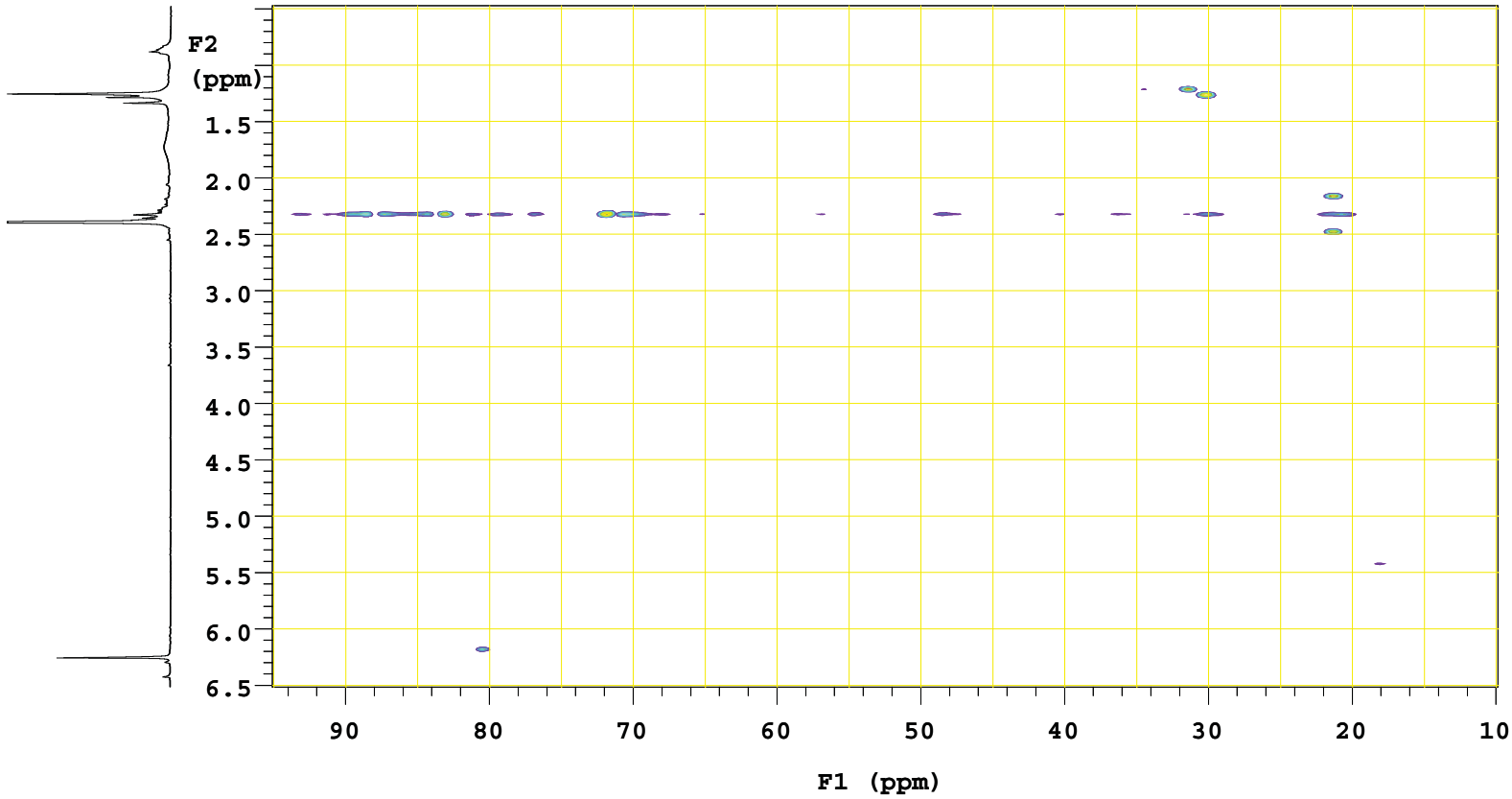
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3



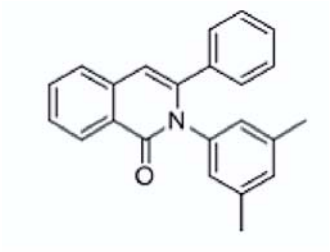
NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC



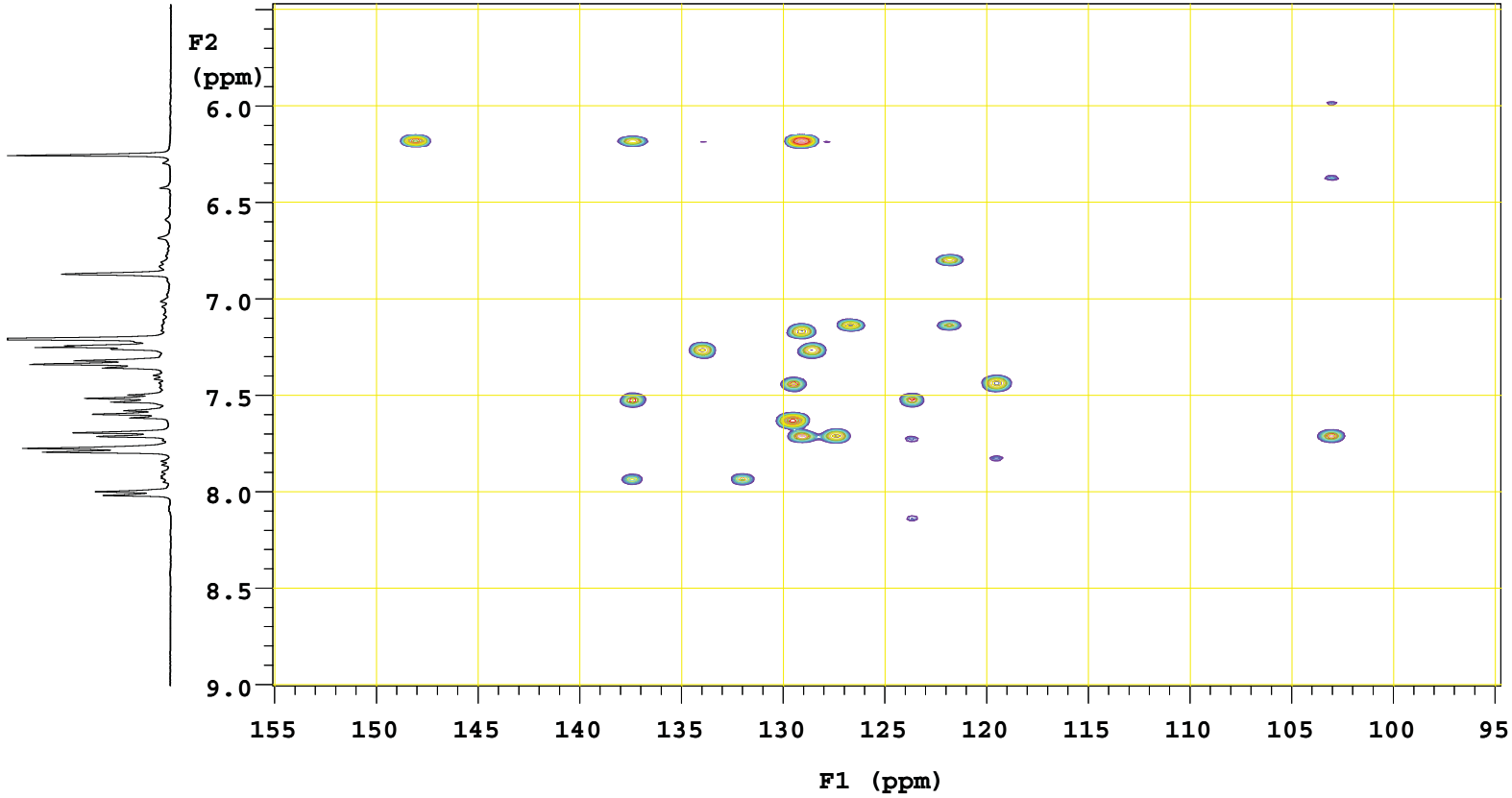
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3



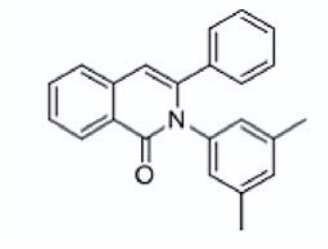
NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC



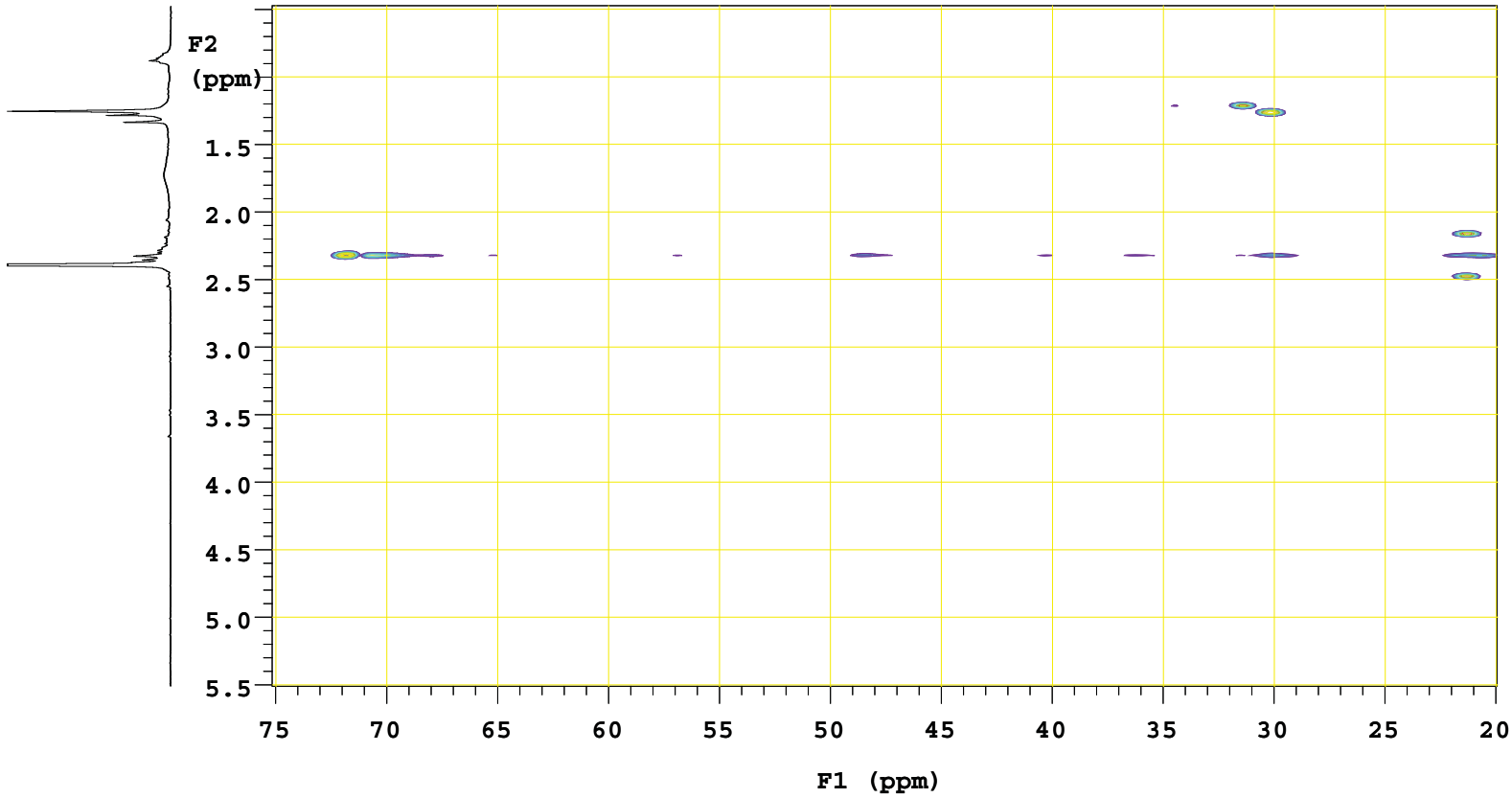
Compound **3a**

TDC-010 B036-CDMA1-015 in CDCl3

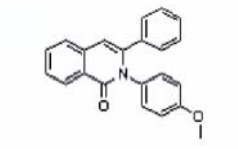


NMR-400MHz
AR.No: ME0414/618
Analyst: Ganesh
Date:04th April.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC



Compound **3i**

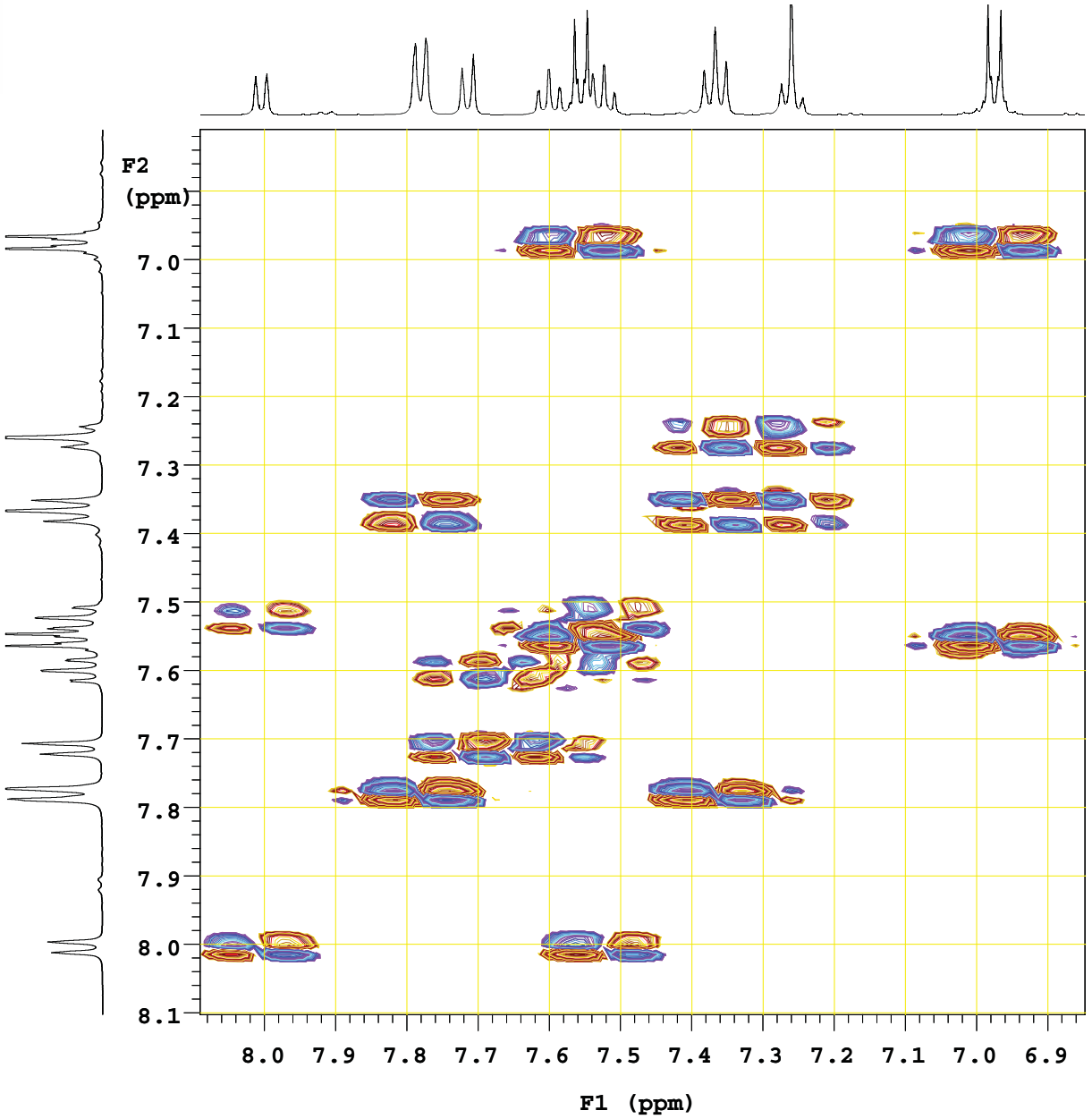


B036-CVIG1-032 in CDCl3
TDC-010

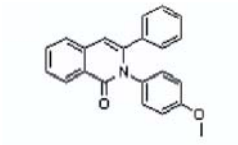
AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

exp2 gDQCOSY

SAMPLE		FLAGS	
date	Apr 8 2014	hs	nn
solvent	CDCl3	sspul	y
sample		hsglvl	4237
ACQUISITION		SPECIAL	
sw	6419.5	temp	25.0
at	0.160	gain	24
np	2048	spin	not used
fb	not used	F2 PROCESSING	
ss	32	sb	-0.120
d1	1.000	sbs	-0.080
nt	16	lsfid	-20
2D ACQUISITION		fn	2048
sw1	6419.5	F1 PROCESSING	
ni	256	sb1	-0.025
TRANSMITTER		sbs1	-0.025
tn	H1	proc1	lp
sfrq	499.626	fn1	2048
tof	100.3	DISPLAY	
tpwr	57	sp	3402.5
pw	7.375	wp	645.7
GRADIENTS		sp1	3421.3
gzlvl1	3177.5	wp1	620.6
gt1	0.002500	rf1	4249.5
gzlvl2	6355	rfp	3627.3
gt2	0.002500	rfl1	4249.5
gstab	0.000500	rfp1	3627.3
DECOUPLER		PLOT	
dn	C13	wc	139.3
dm	nnn	sc	10.0
		wc2	139.3
		sc2	0
		vs	171
		th	2
		ai cdc ph	



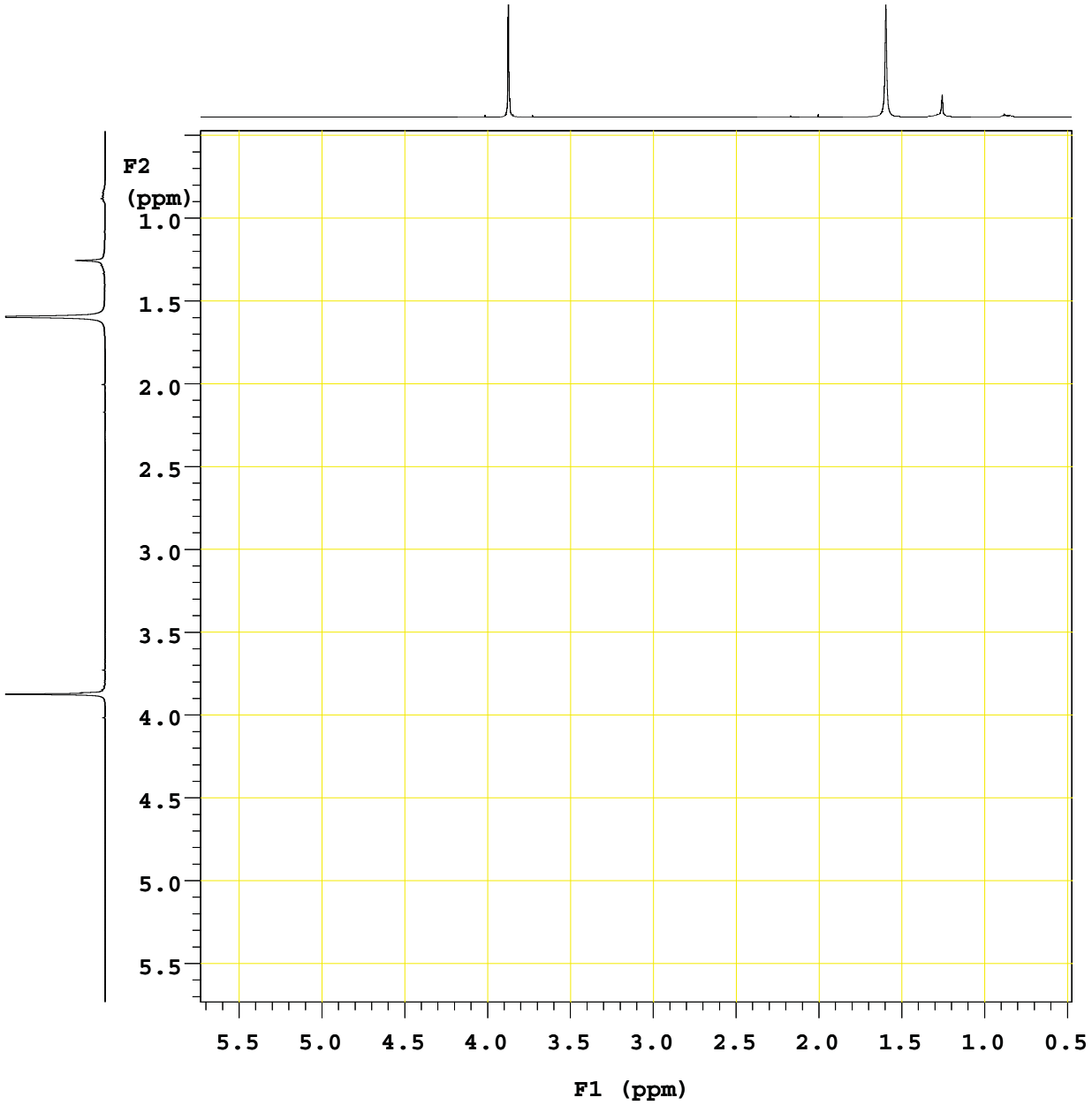
Compound **3i**



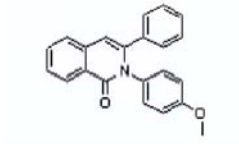
B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gDQCOSY



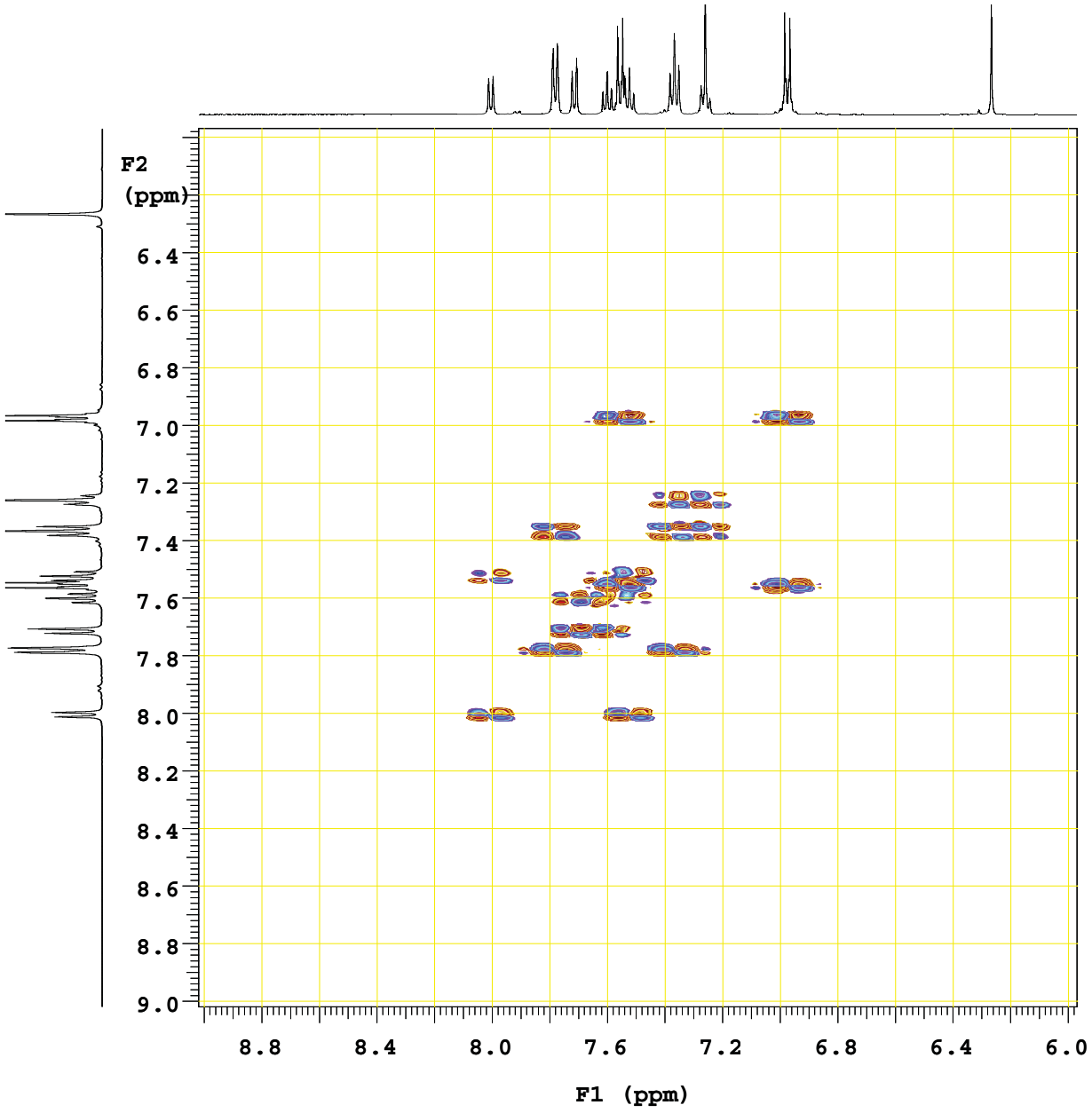
Compound **3i**



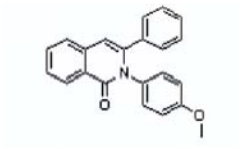
B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gDQCOSY



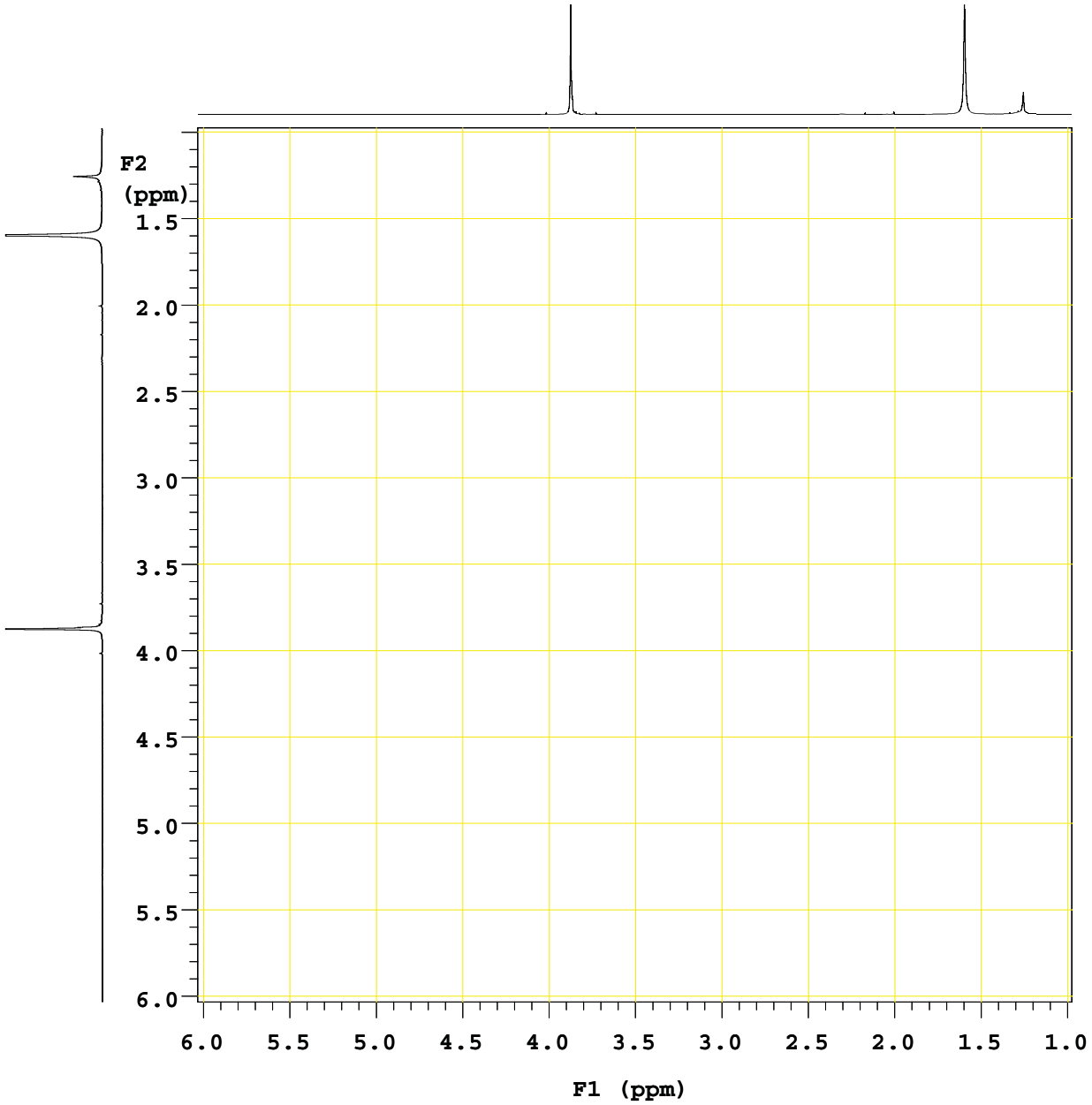
Compound **3i**



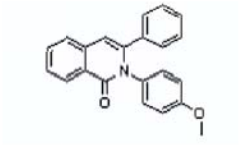
B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gDQCOSY



Compound **3i**

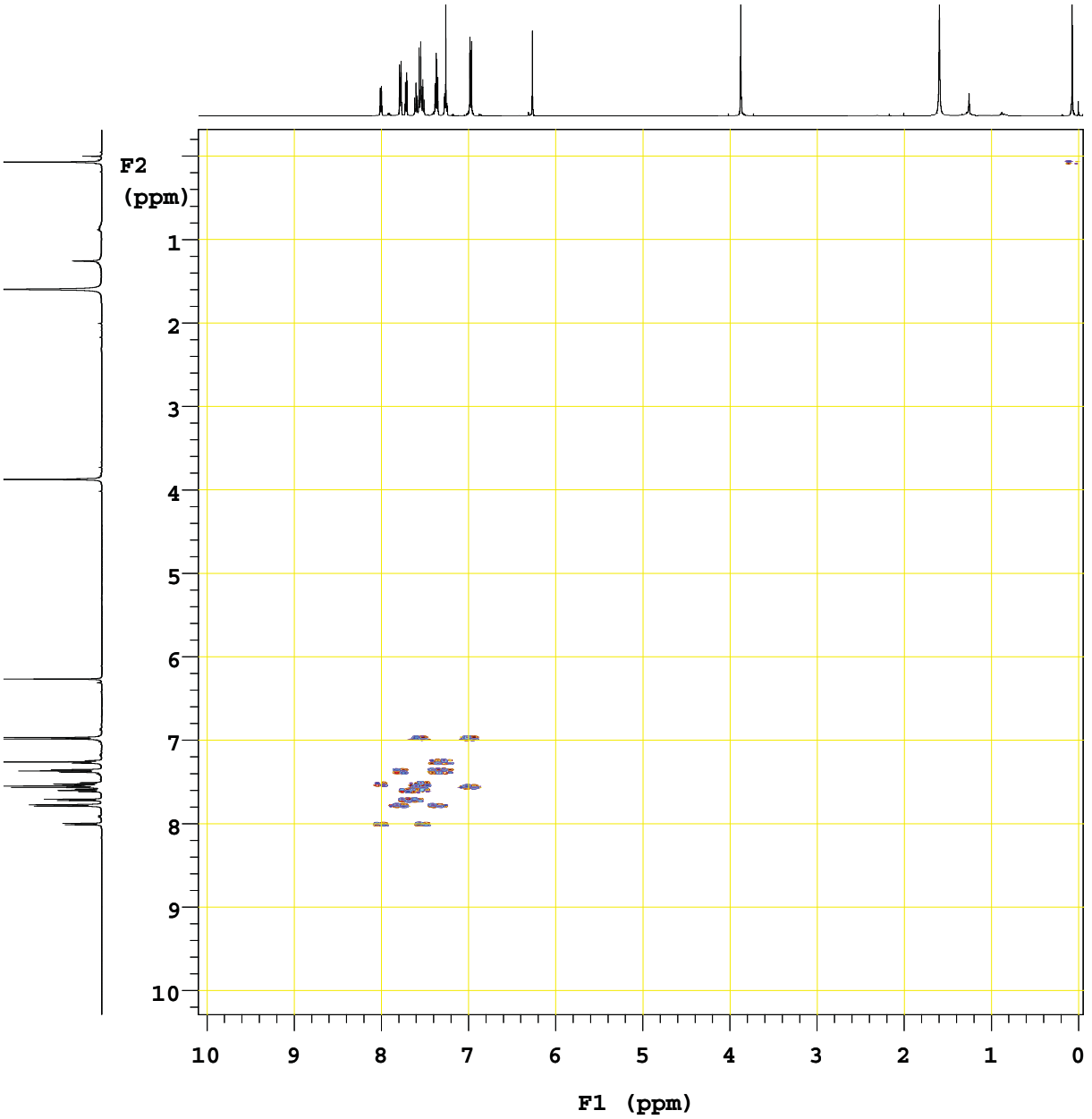


B036-CVIG1-032 in CDCl3
TDC-010

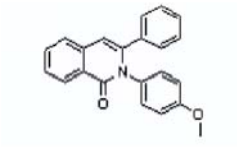
AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

exp2 gDQCOSY

SAMPLE		FLAGS	
date	Apr 8 2014	hs	nn
solvent	CDCl3	sspul	y
sample		hsglvl	4237
ACQUISITION		SPECIAL	
sw	6419.5	temp	25.0
at	0.160	gain	24
np	2048	spin	not used
fb	not used	F2 PROCESSING	
ss	32	sb	-0.120
d1	1.000	sbs	-0.080
nt	16	lsfid	-20
2D ACQUISITION		fn	2048
sw1	6419.5	F1 PROCESSING	
ni	256	sb1	-0.025
TRANSMITTER		sbs1	-0.025
tn	H1	proc1	lp
sfrq	499.626	fn1	2048
tof	100.3	DISPLAY	
tpwr	57	sp	-158.4
pw	7.375	wp	5297.4
GRADIENTS		sp1	-26.7
gzlvl1	3177.5	wp1	5071.7
gt1	0.002500	rf1	4249.5
gzlvl2	6355	rfp	3627.3
gt2	0.002500	rfl1	4249.5
gstab	0.000500	rfp1	3627.3
DECOUPLER		PLOT	
dn	C13	wc	139.3
dm	nnn	sc	10.0
		wc2	139.3
		sc2	0
		vs	171
		th	2
		ai cdc ph	



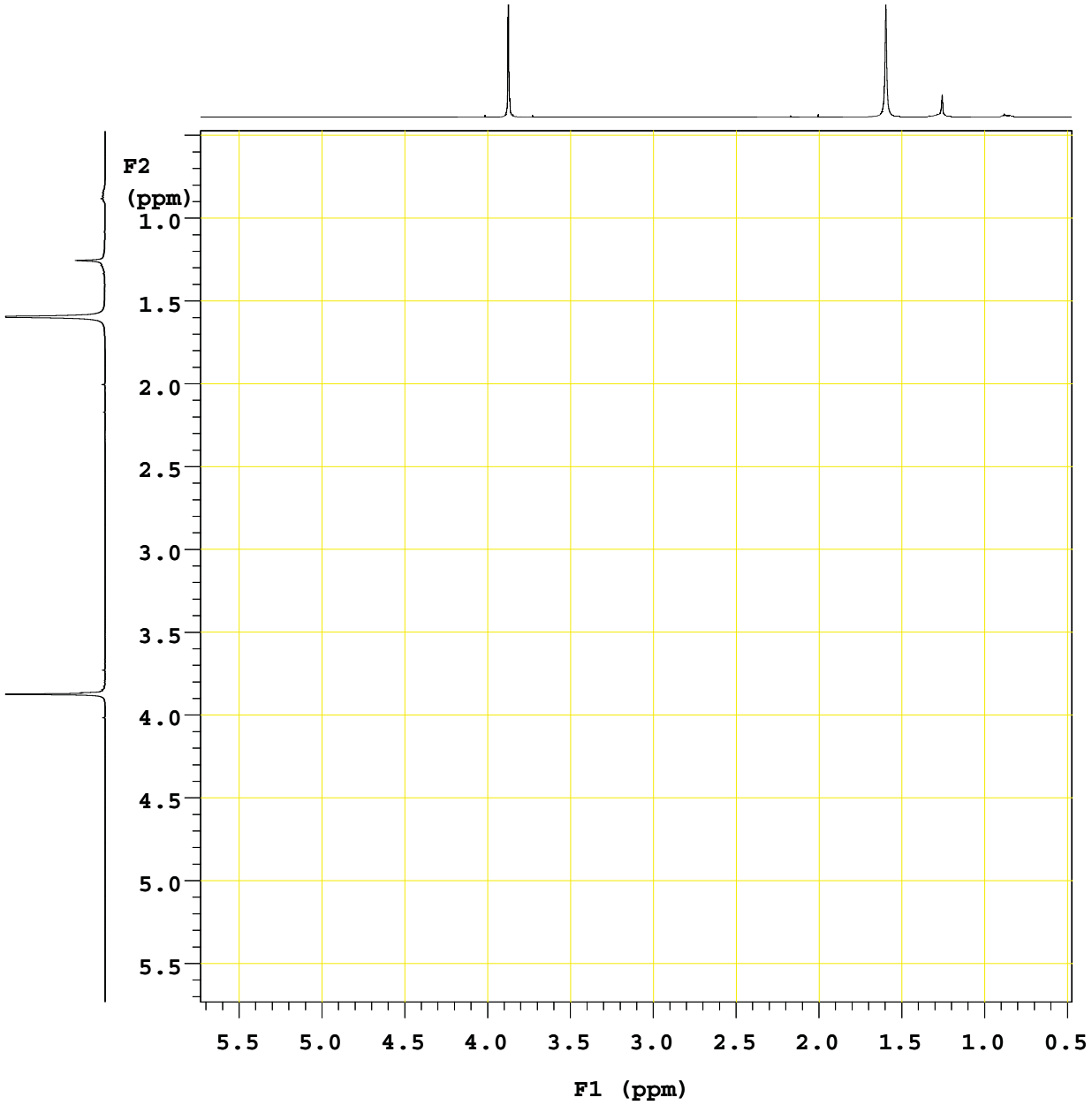
Compound **3i**



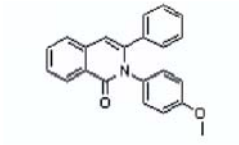
B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gDQCOSY



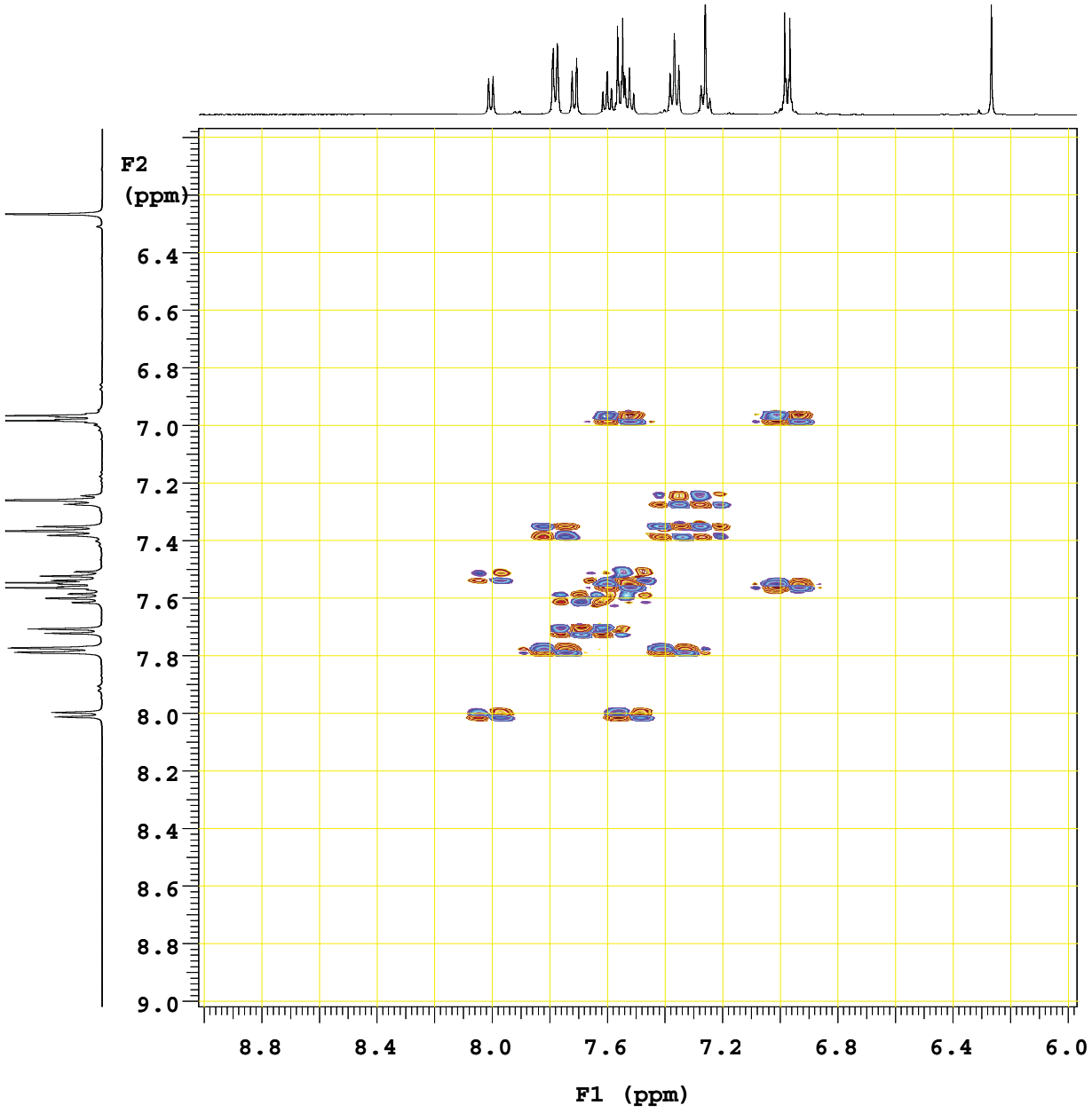
Compound **3i**



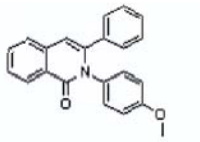
B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gDQCOSY



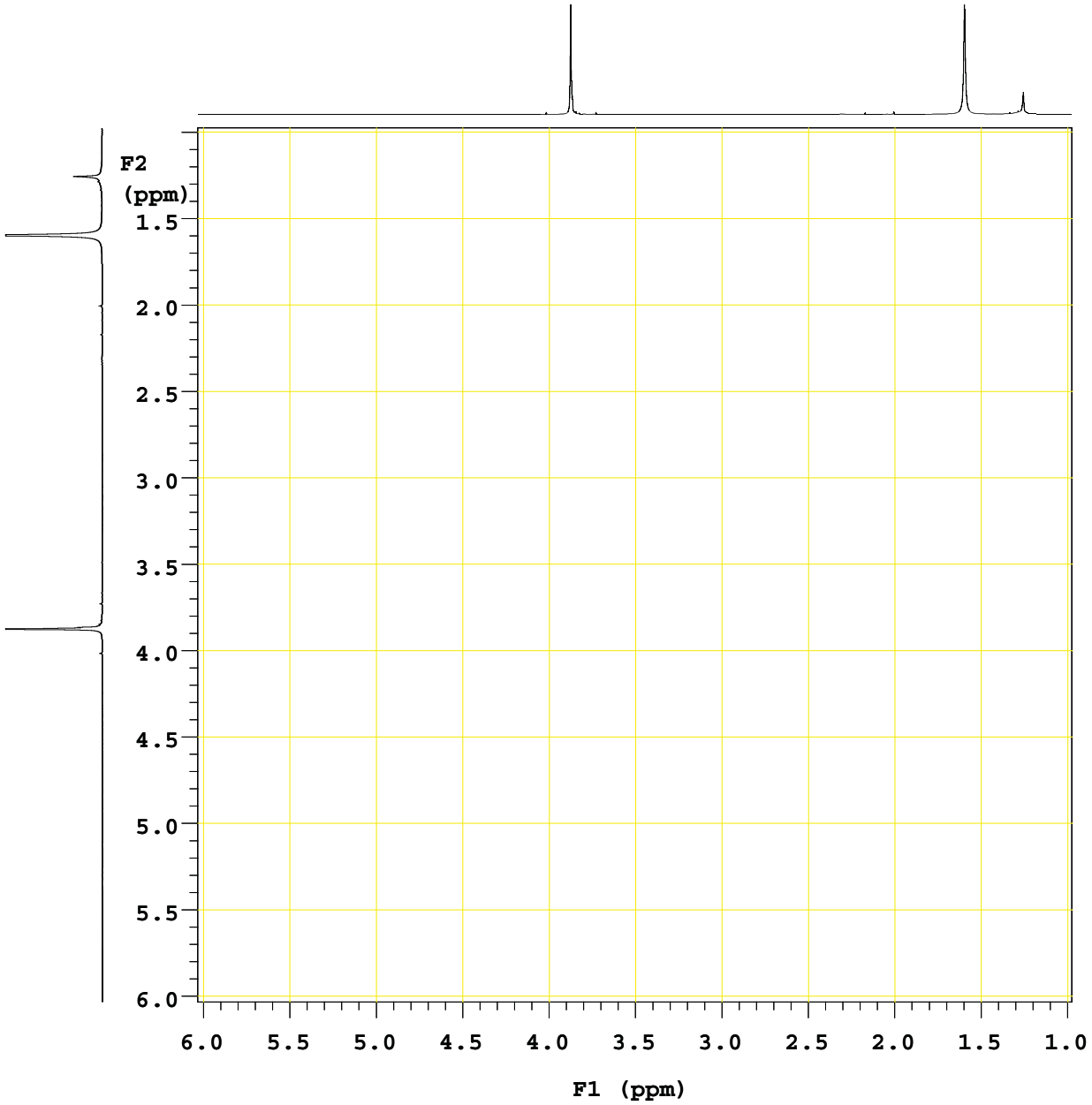
Compound **3i**



B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/35
Date:08th April.2014
Analyst: Haribabu.R

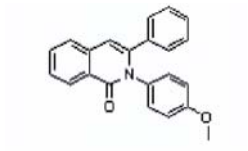
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gDQCOSY



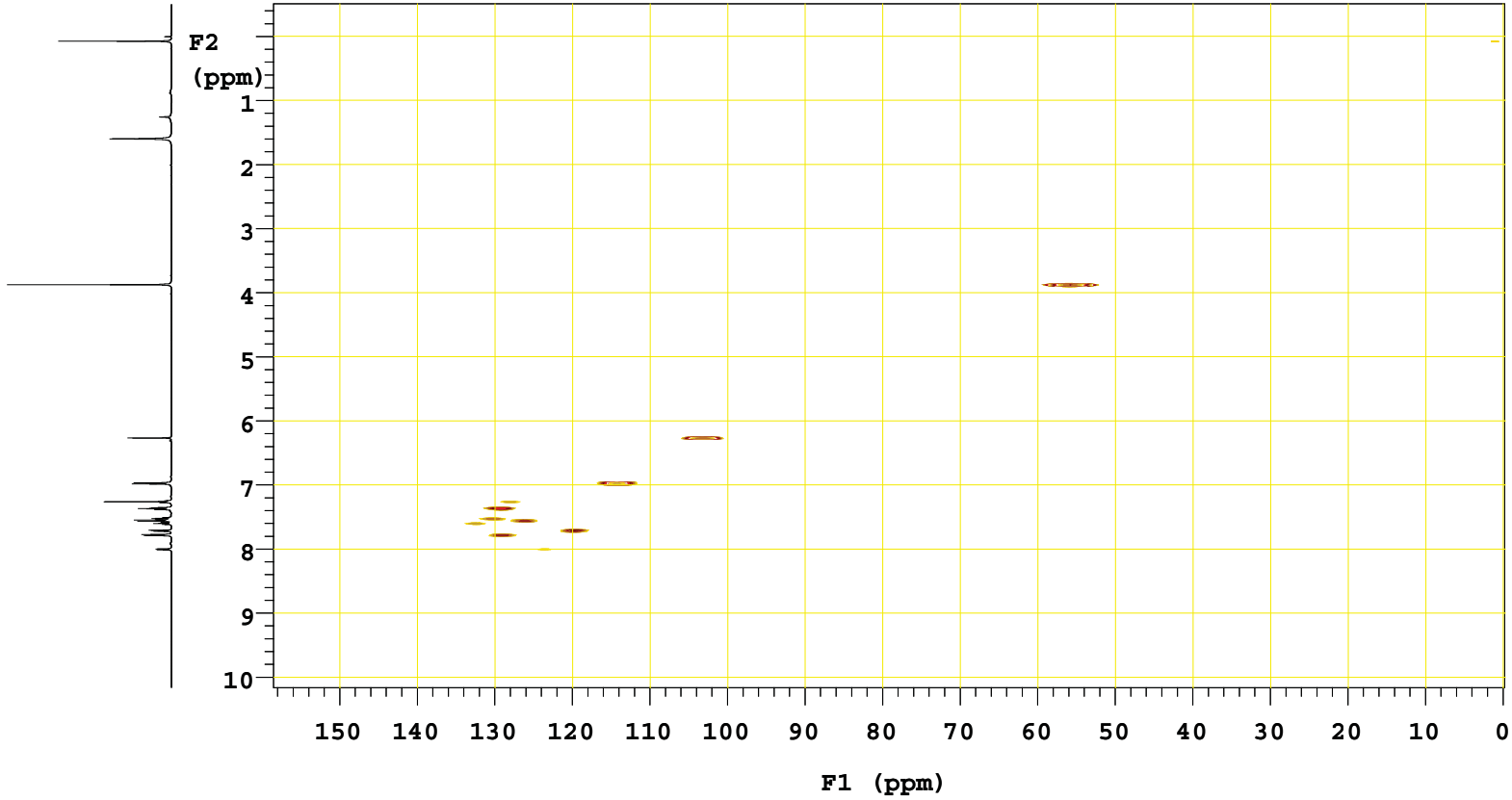
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



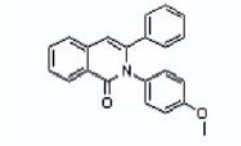
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



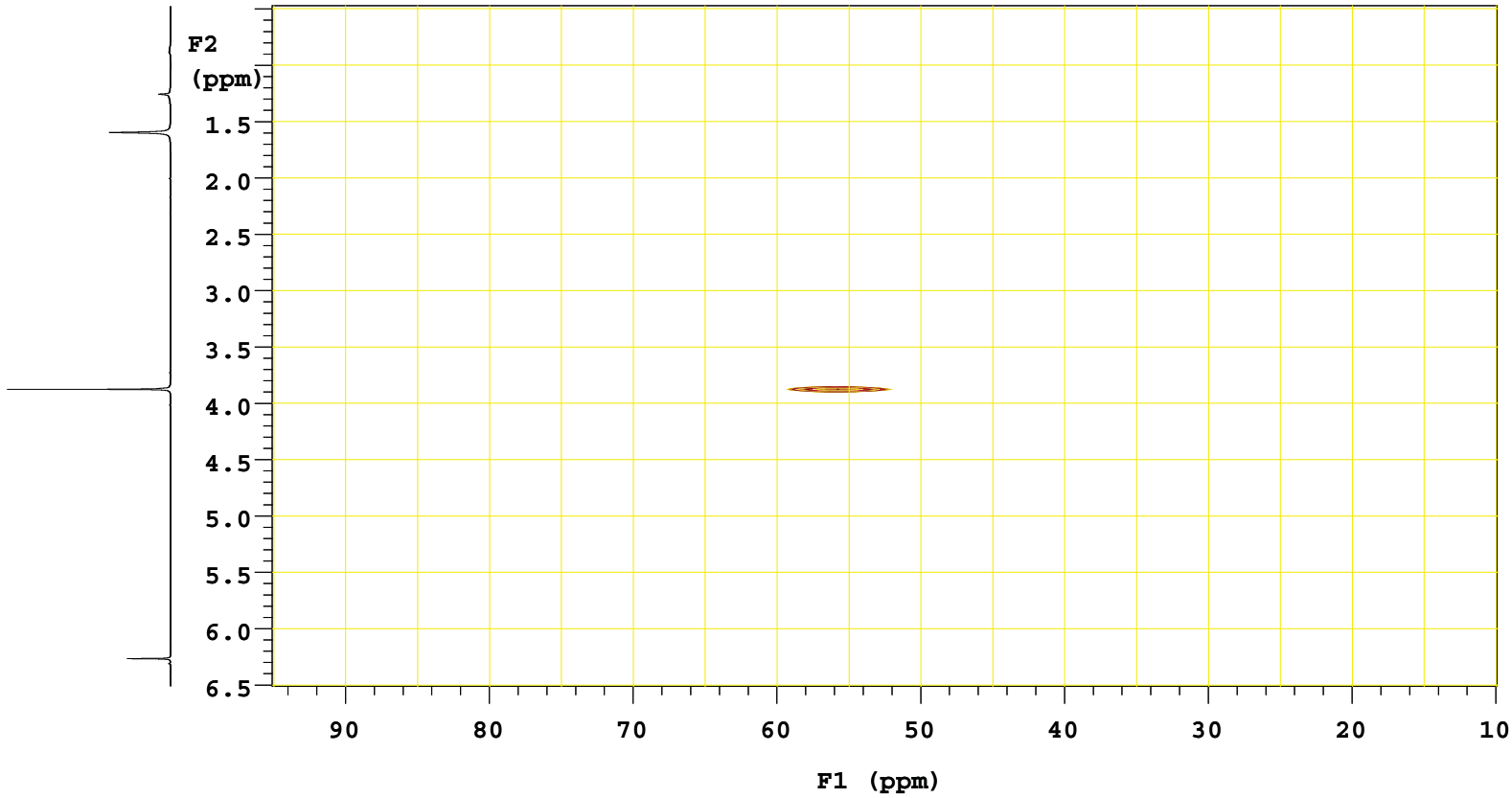
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



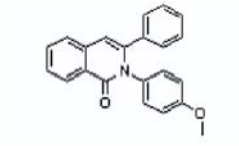
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



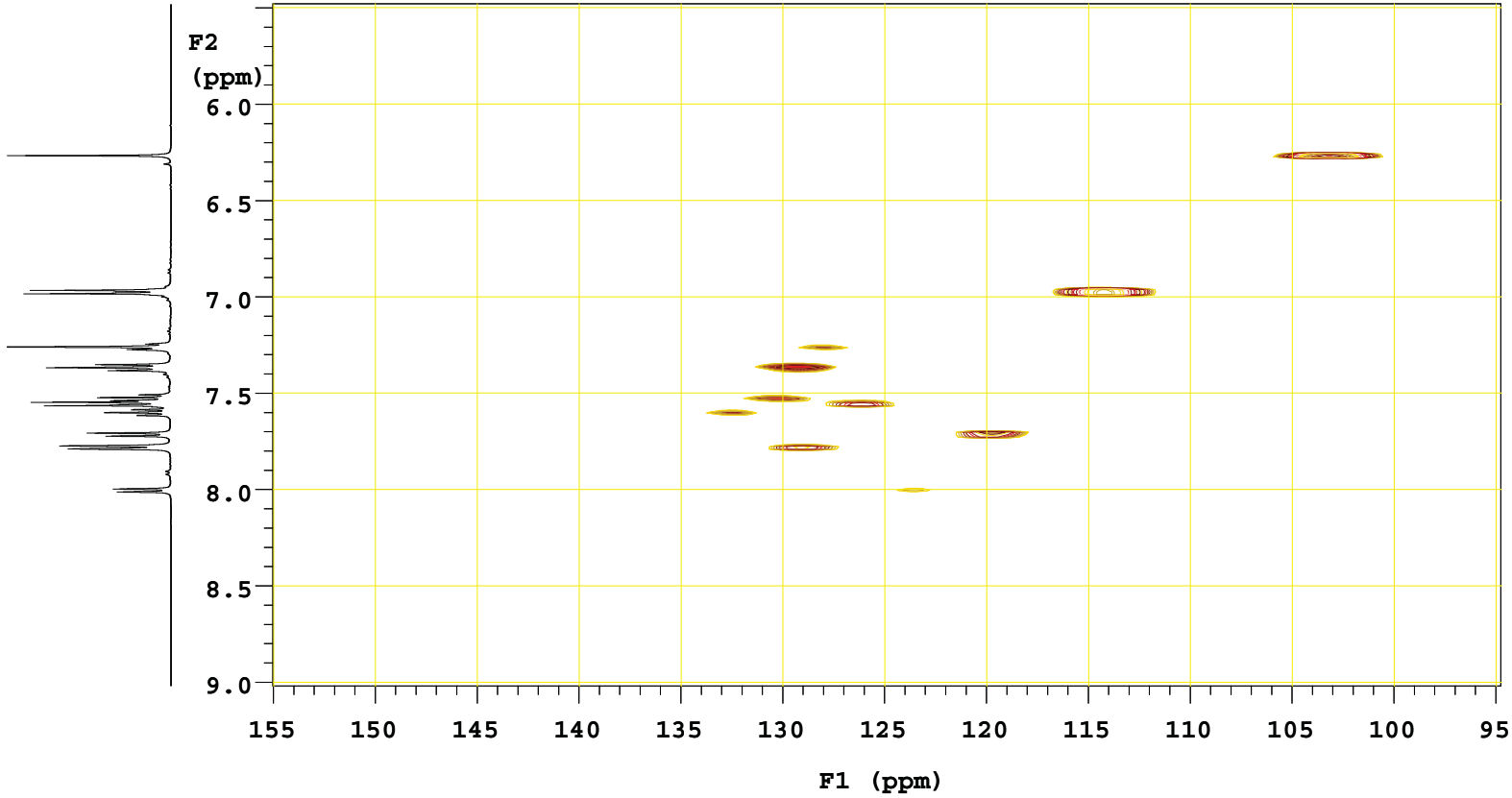
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



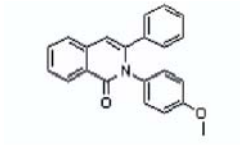
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



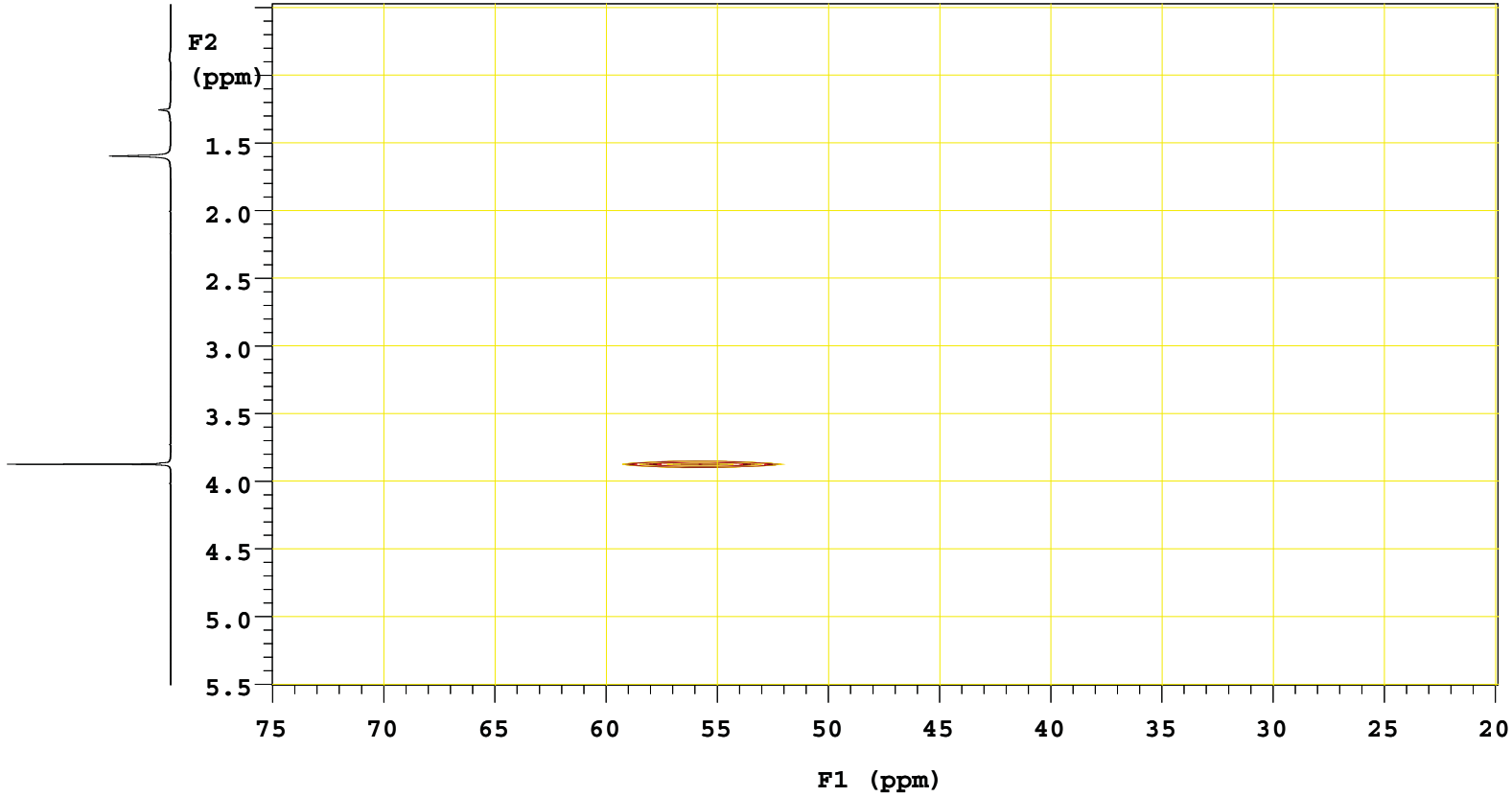
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



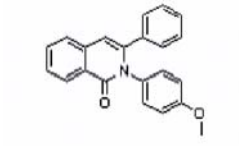
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



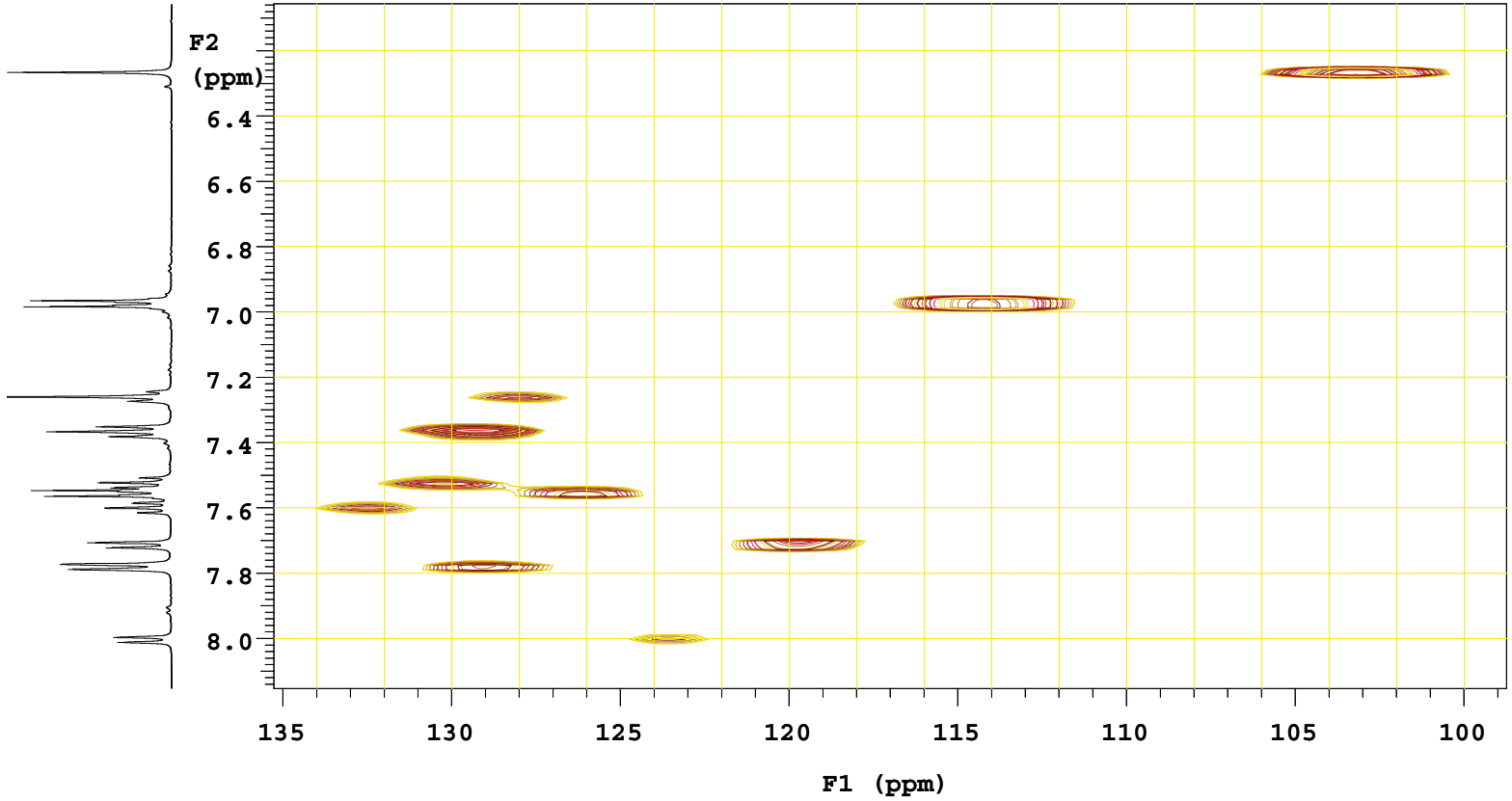
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



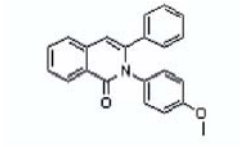
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



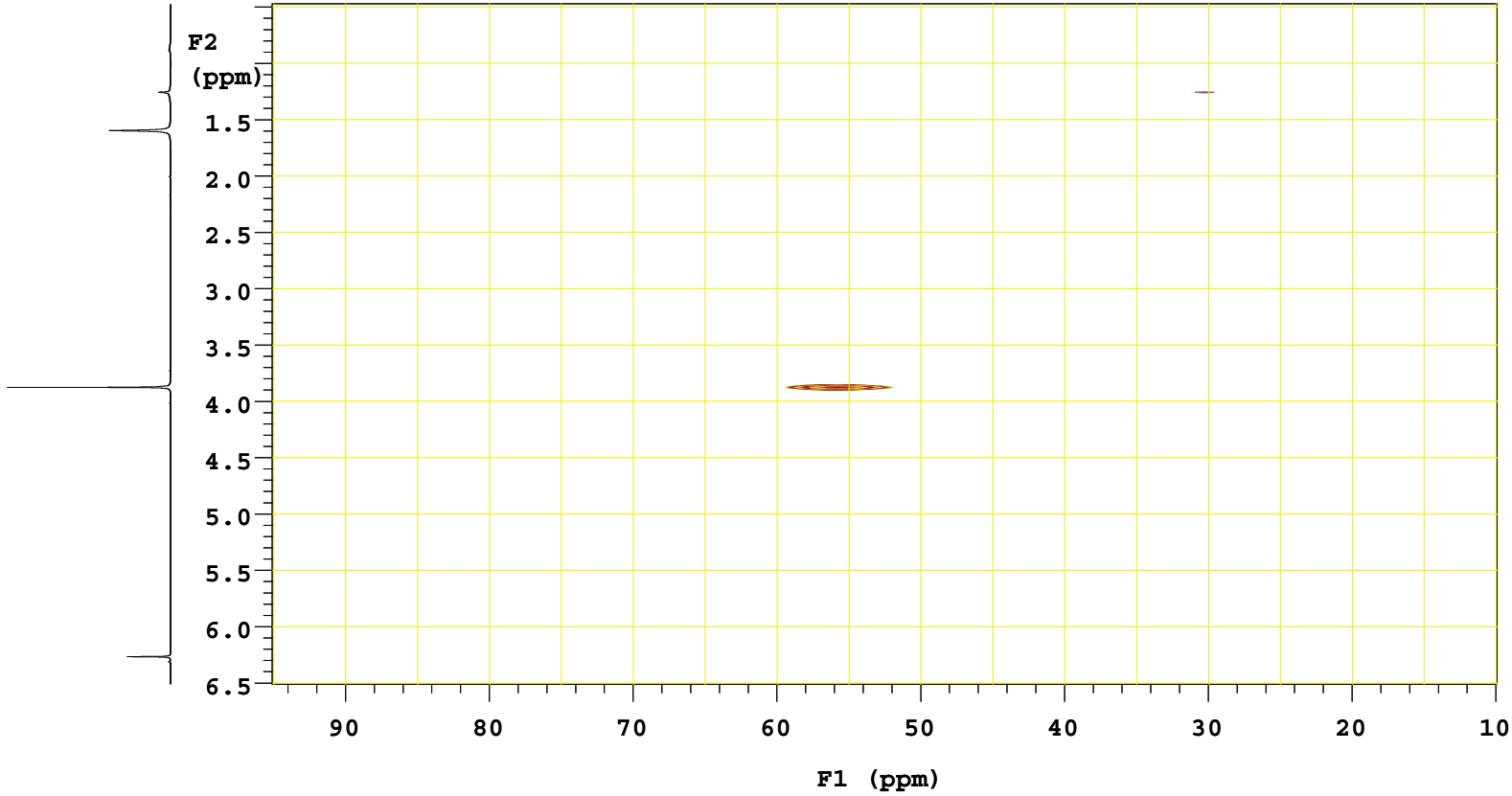
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



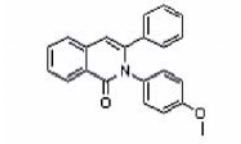
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



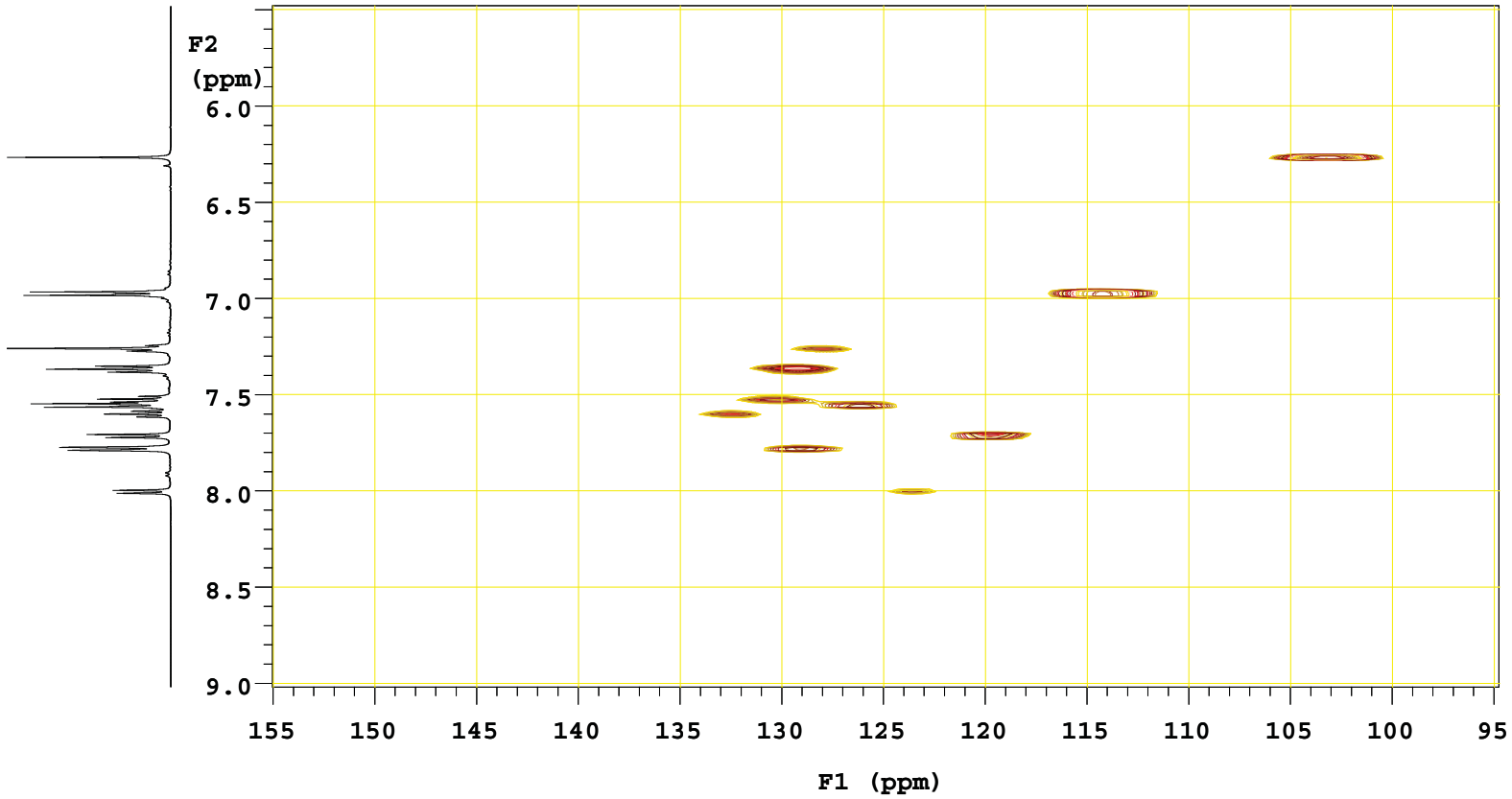
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



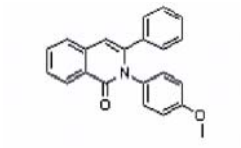
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



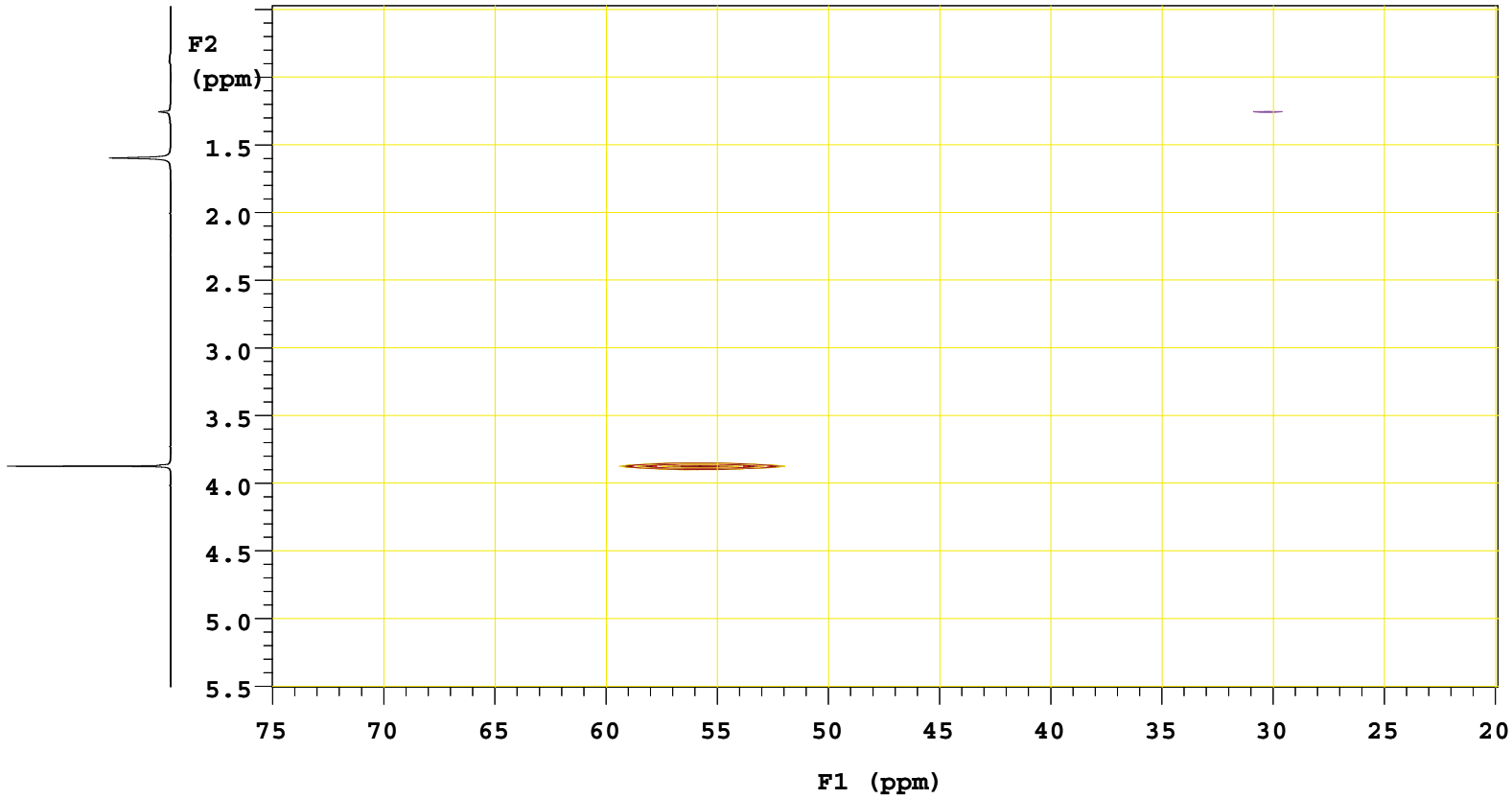
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/33
Date:08th April.2014
Analyst: Haribabu.R



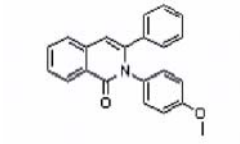
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



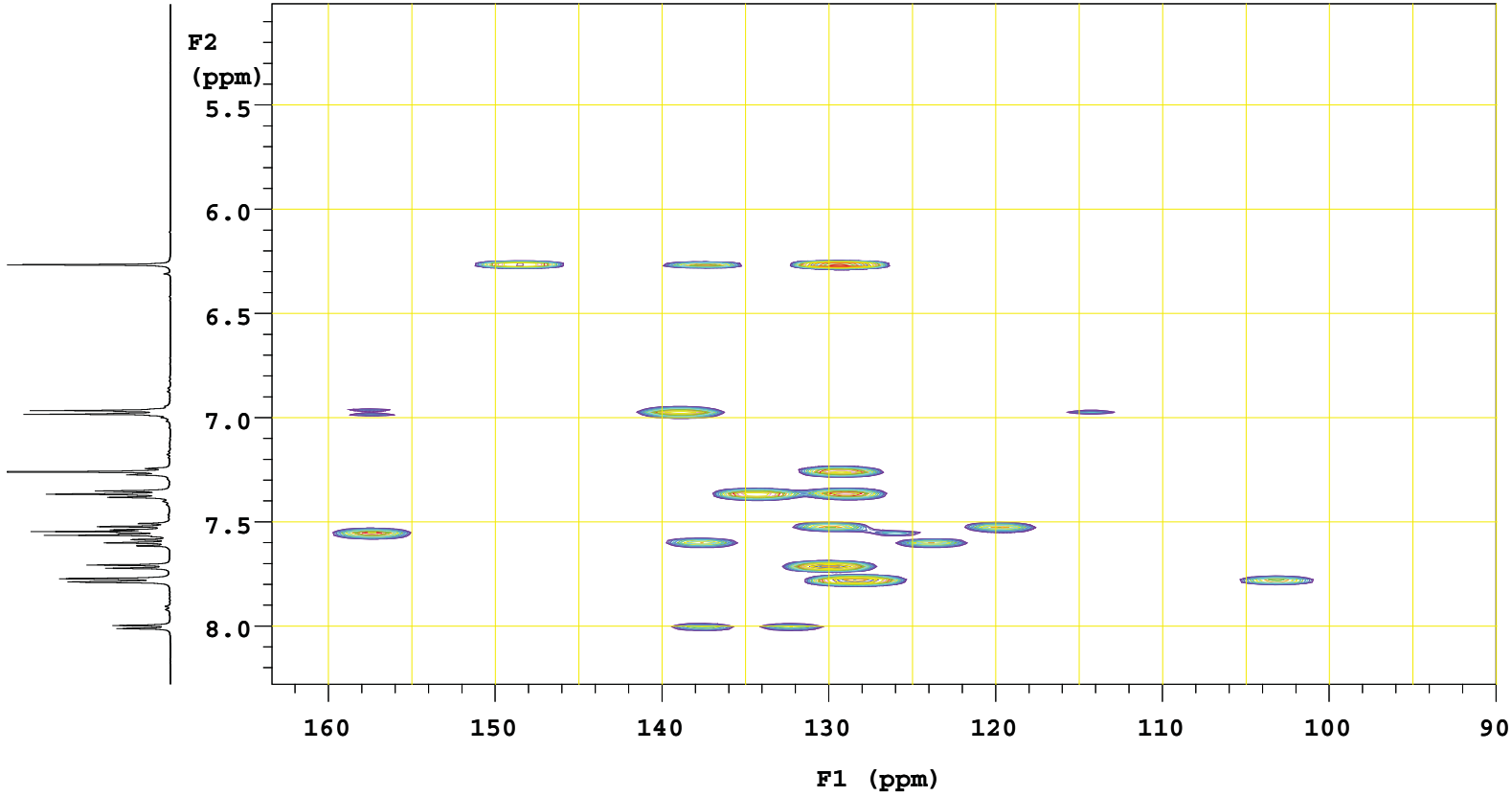
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/34
Date:08th April.2014
Analyst: Haribabu.R



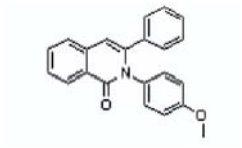
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHMBC



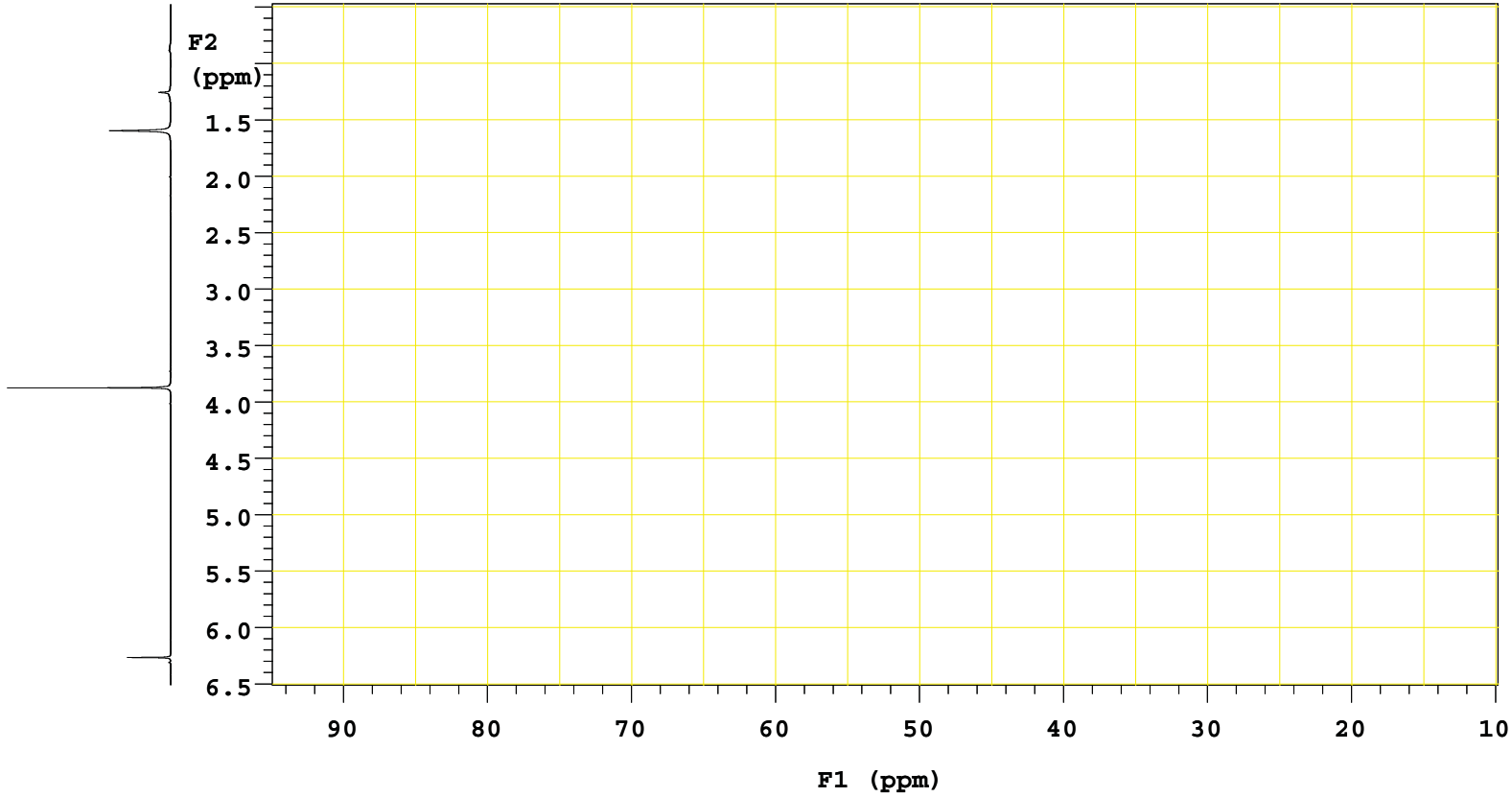
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/34
Date:08th April.2014
Analyst: Haribabu.R



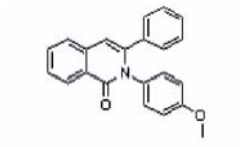
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHMBC



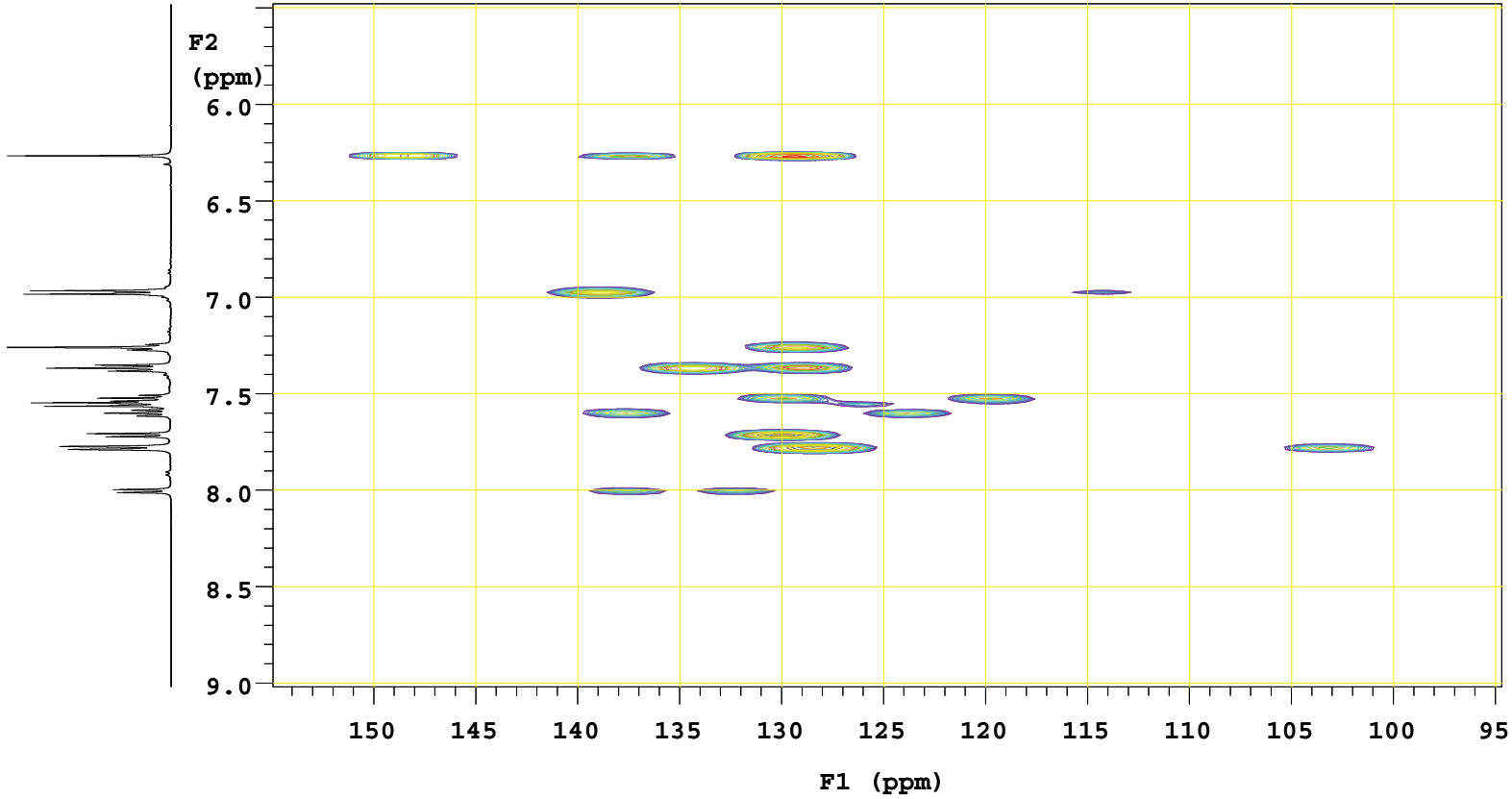
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/34
Date:08th April.2014
Analyst: Haribabu.R



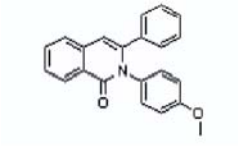
NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHMBC



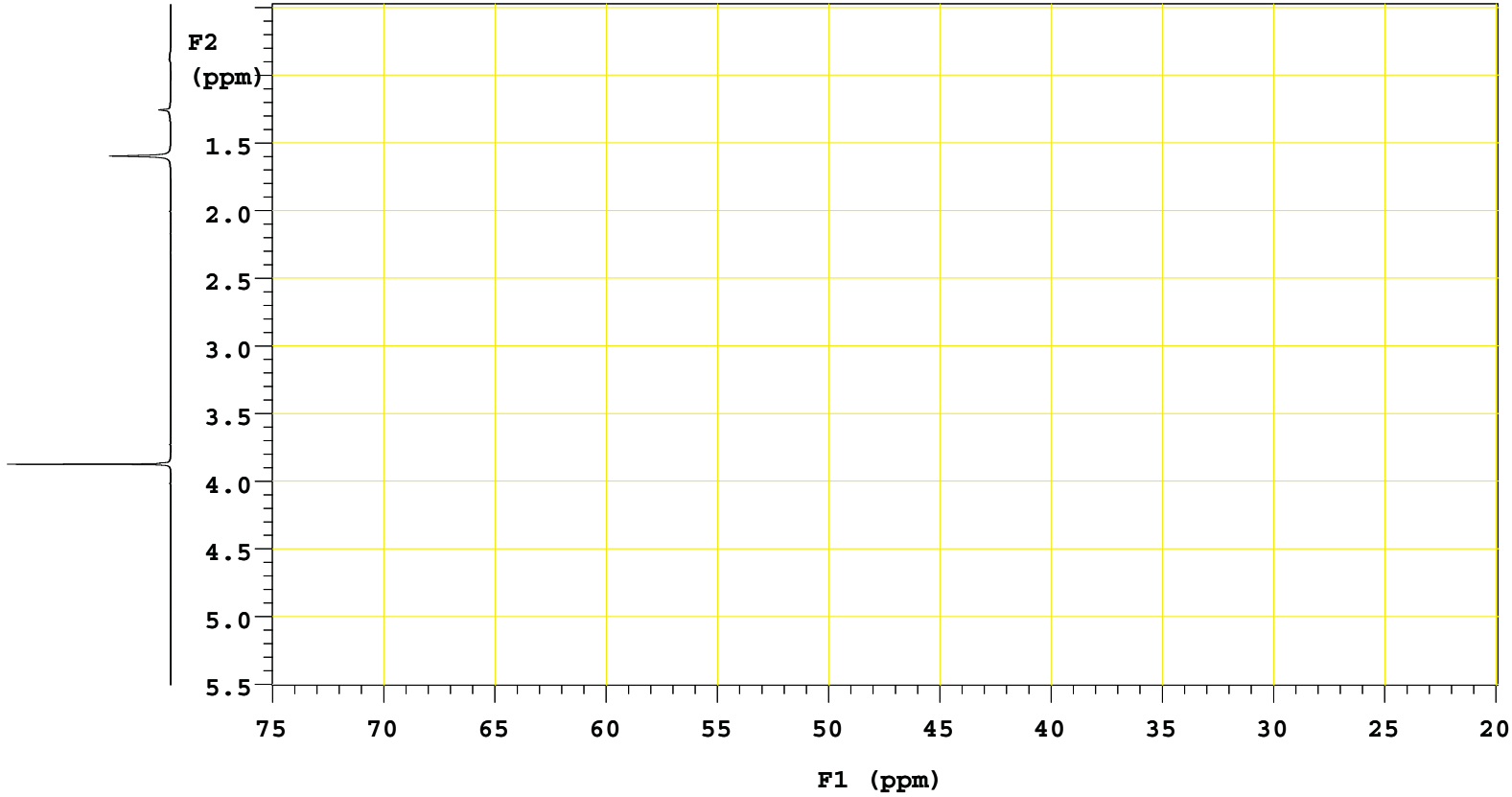
Compound **3i**

B036-CVIG1-032 in CDCl3
TDC-010

AR.No:IN0414/34
Date:08th April.2014
Analyst: Haribabu.R

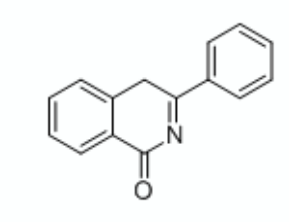


NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHMBC



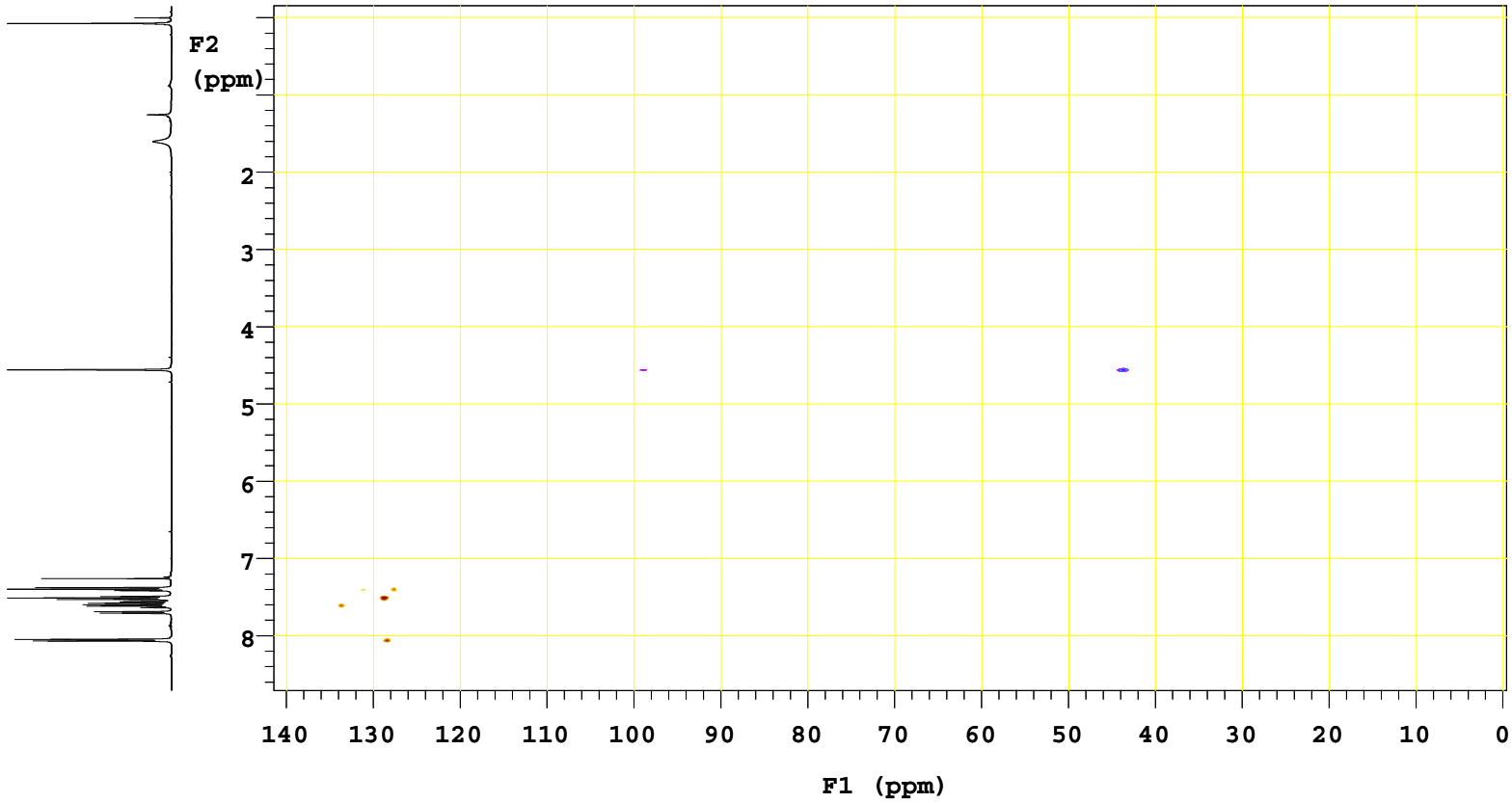
Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3



NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

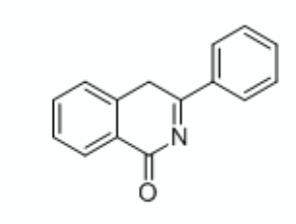
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



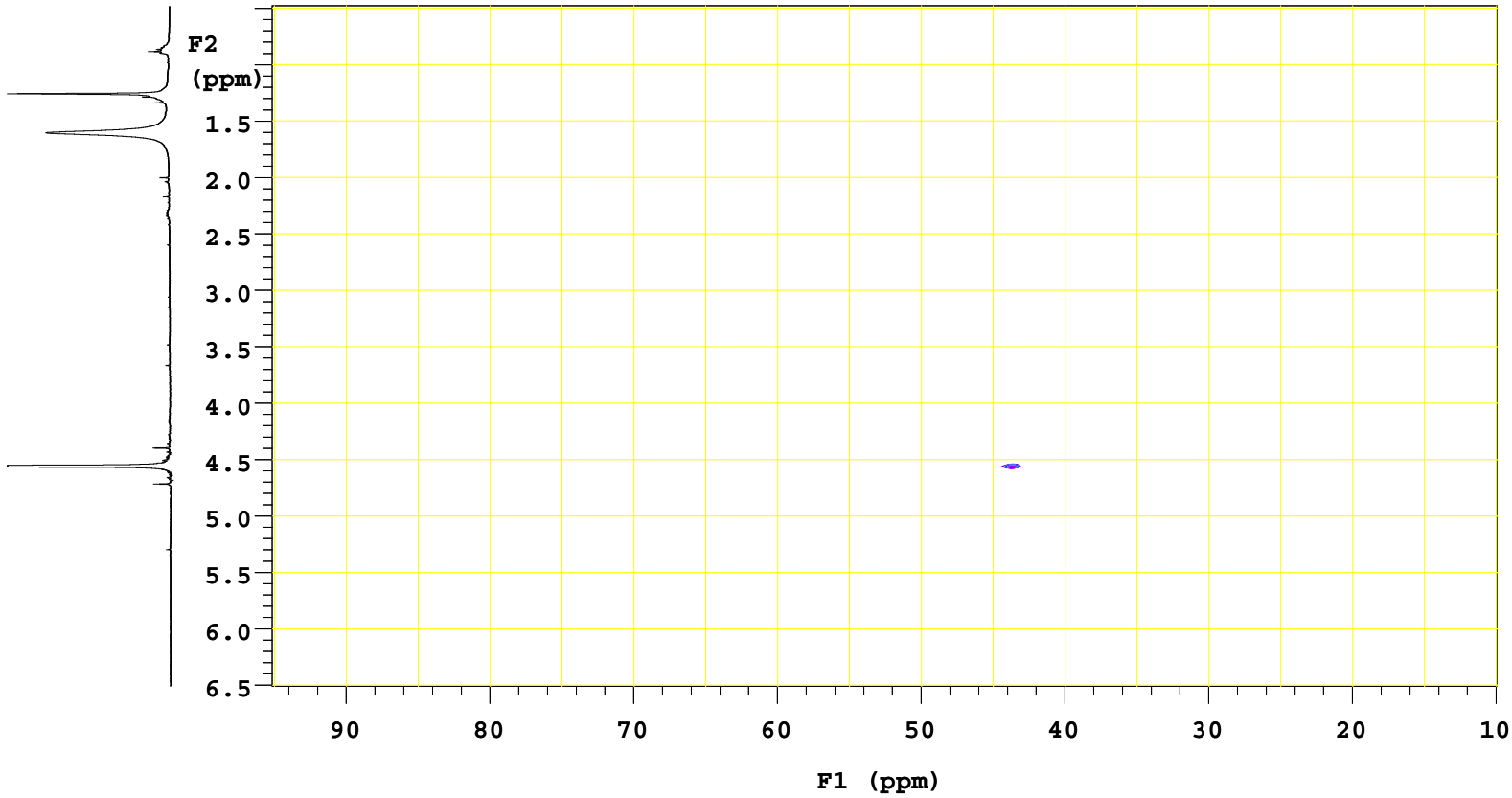
Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

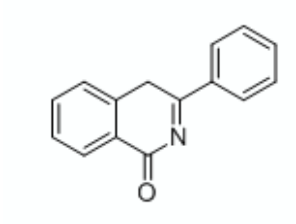


NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



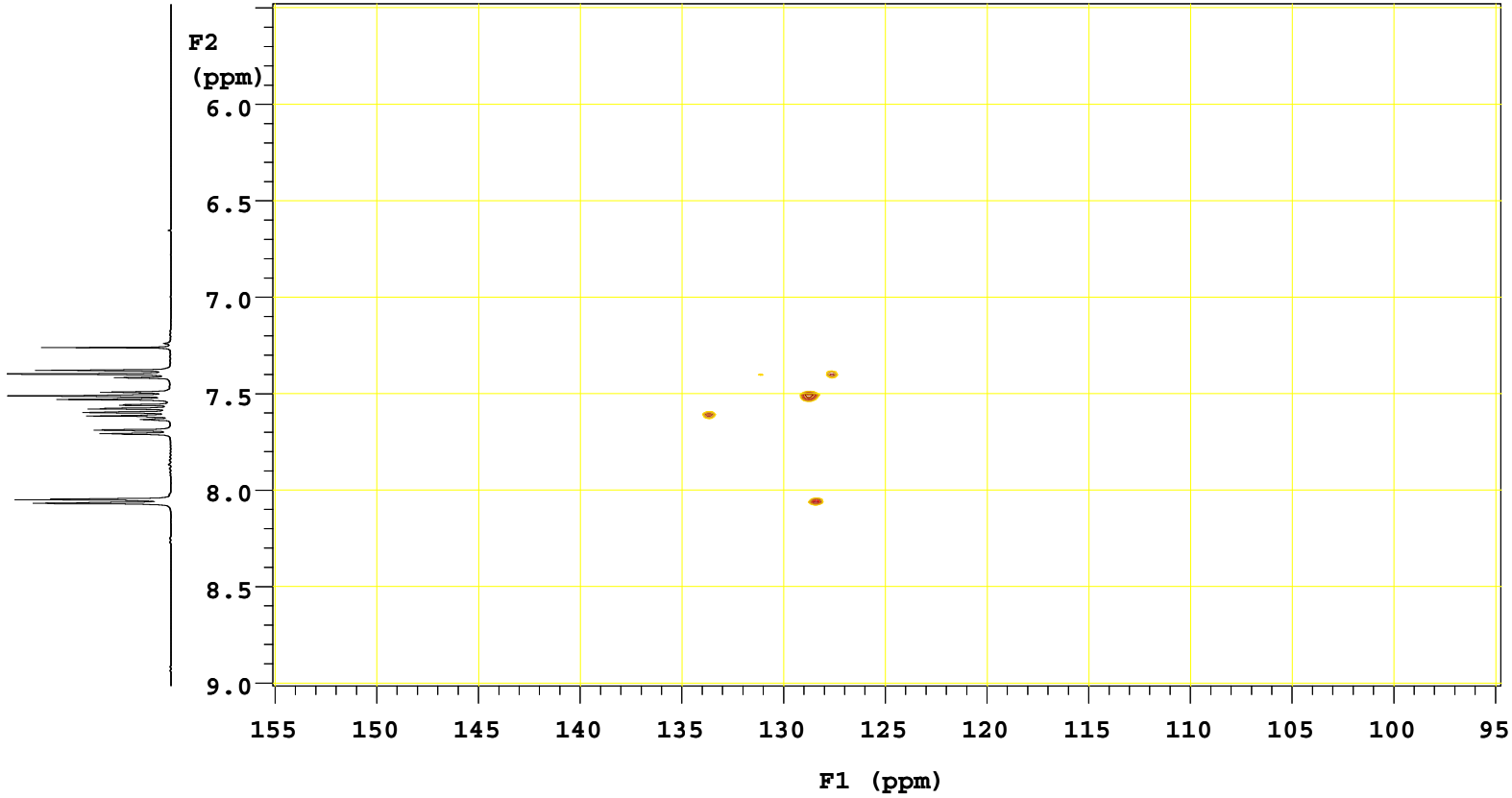
Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3



NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

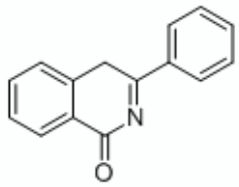
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



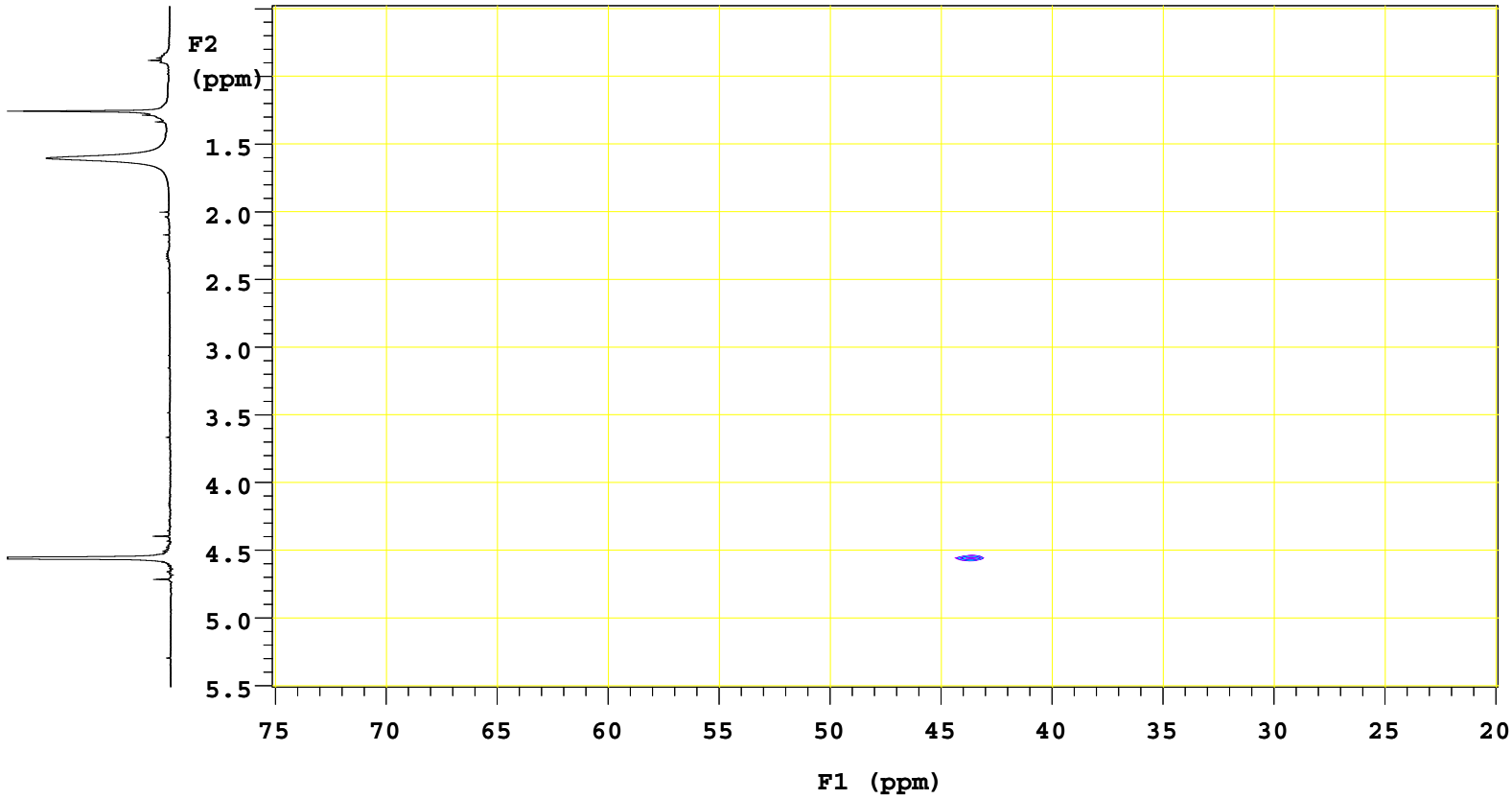
Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3

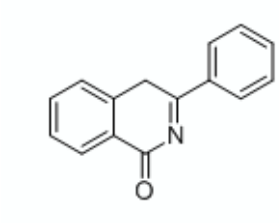
NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014



NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



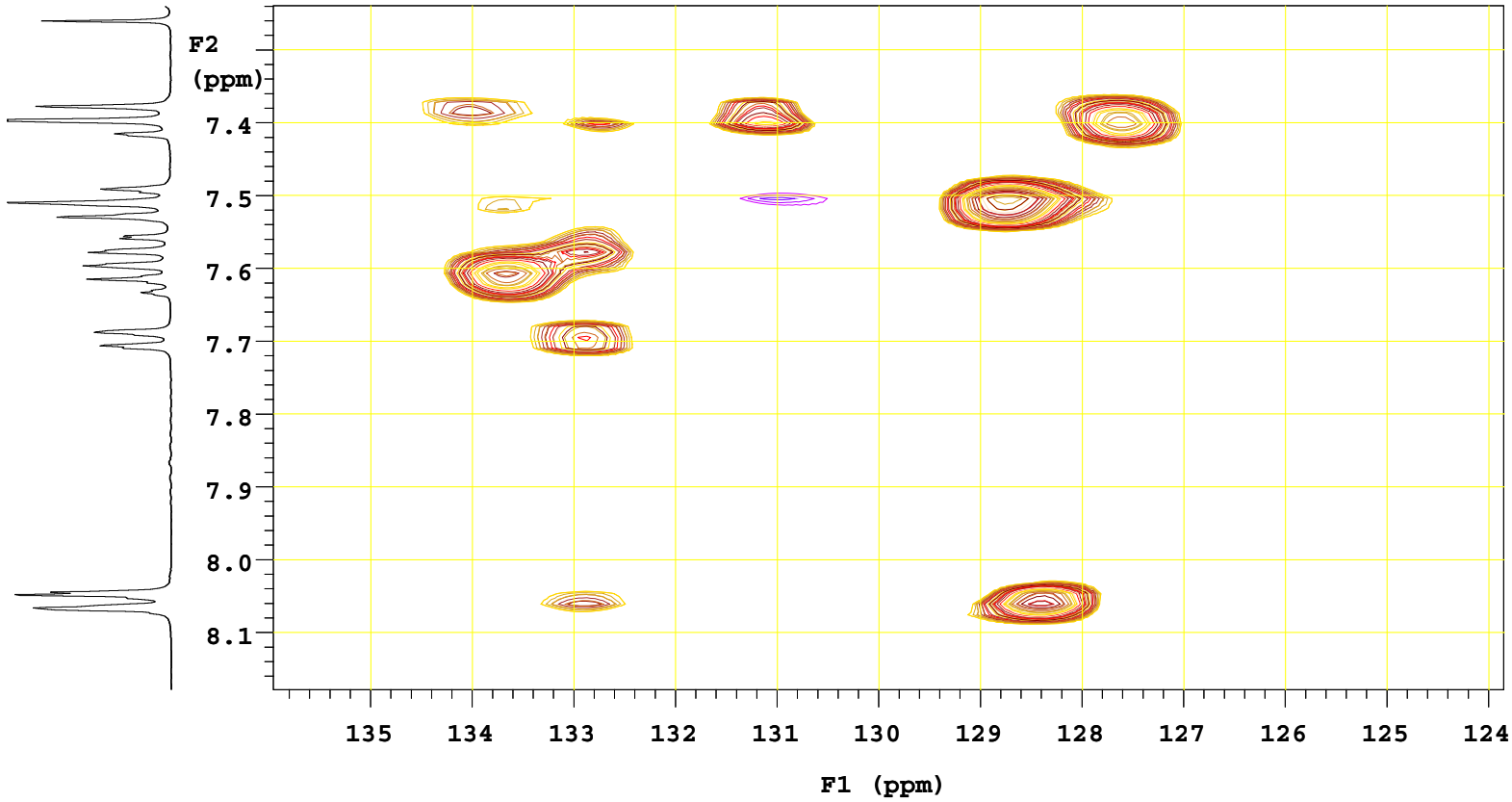
Compound **4a**



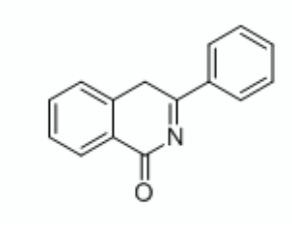
TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



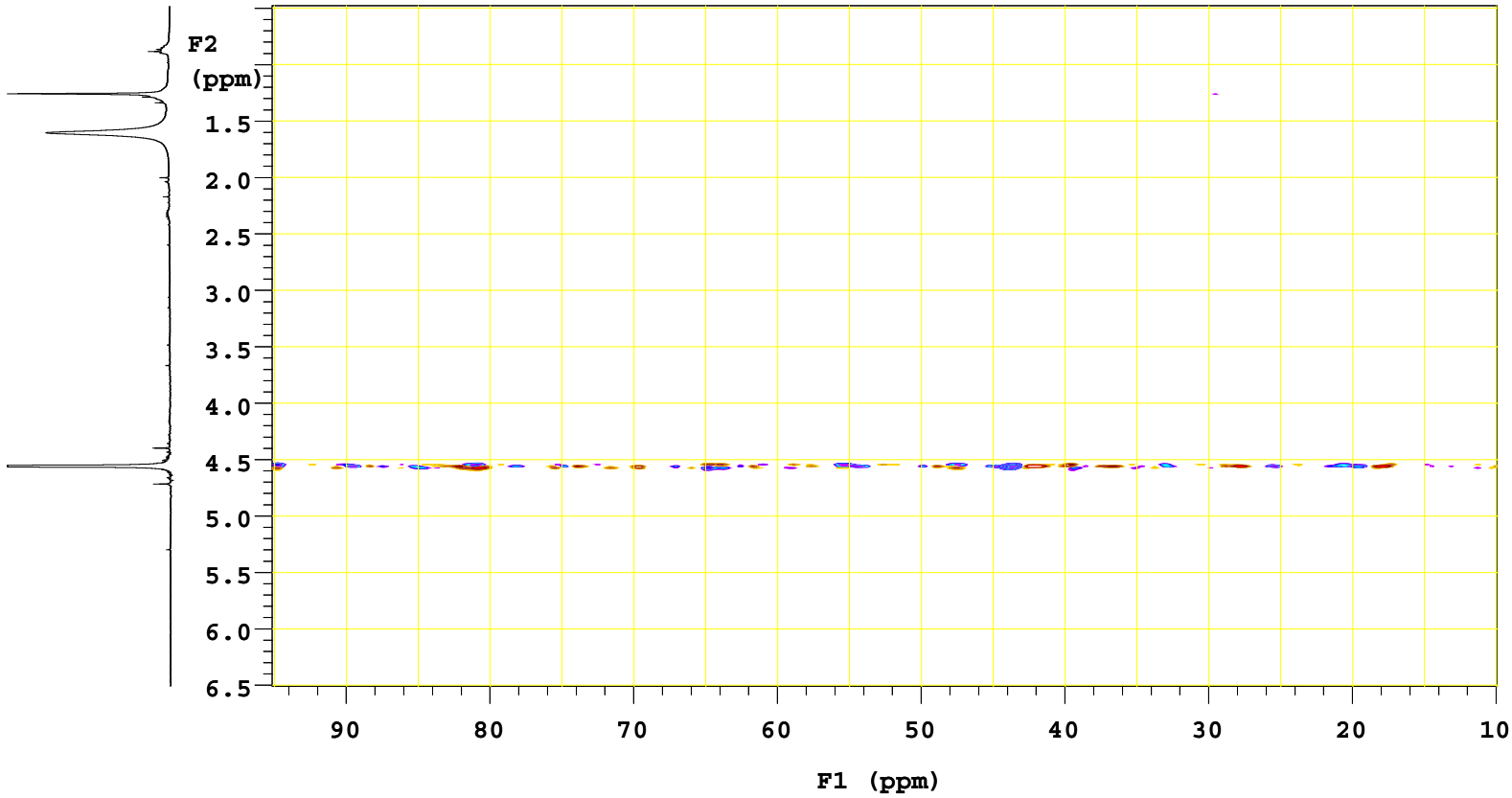
Compound **4a**



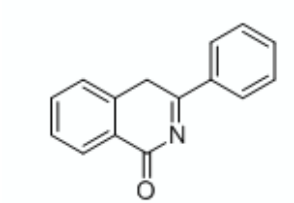
TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



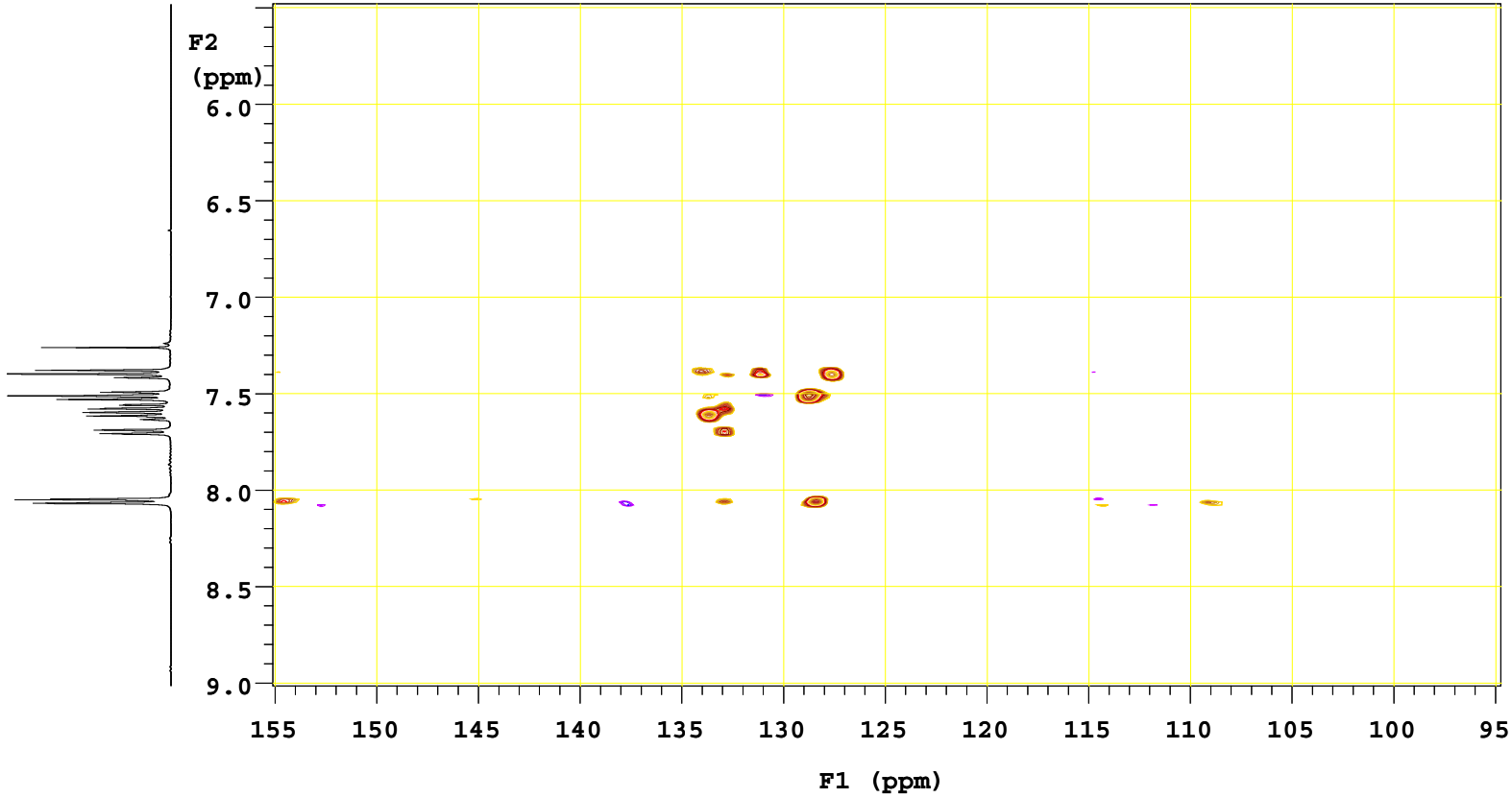
Compound **4a**



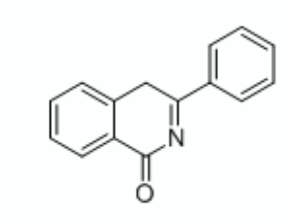
TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



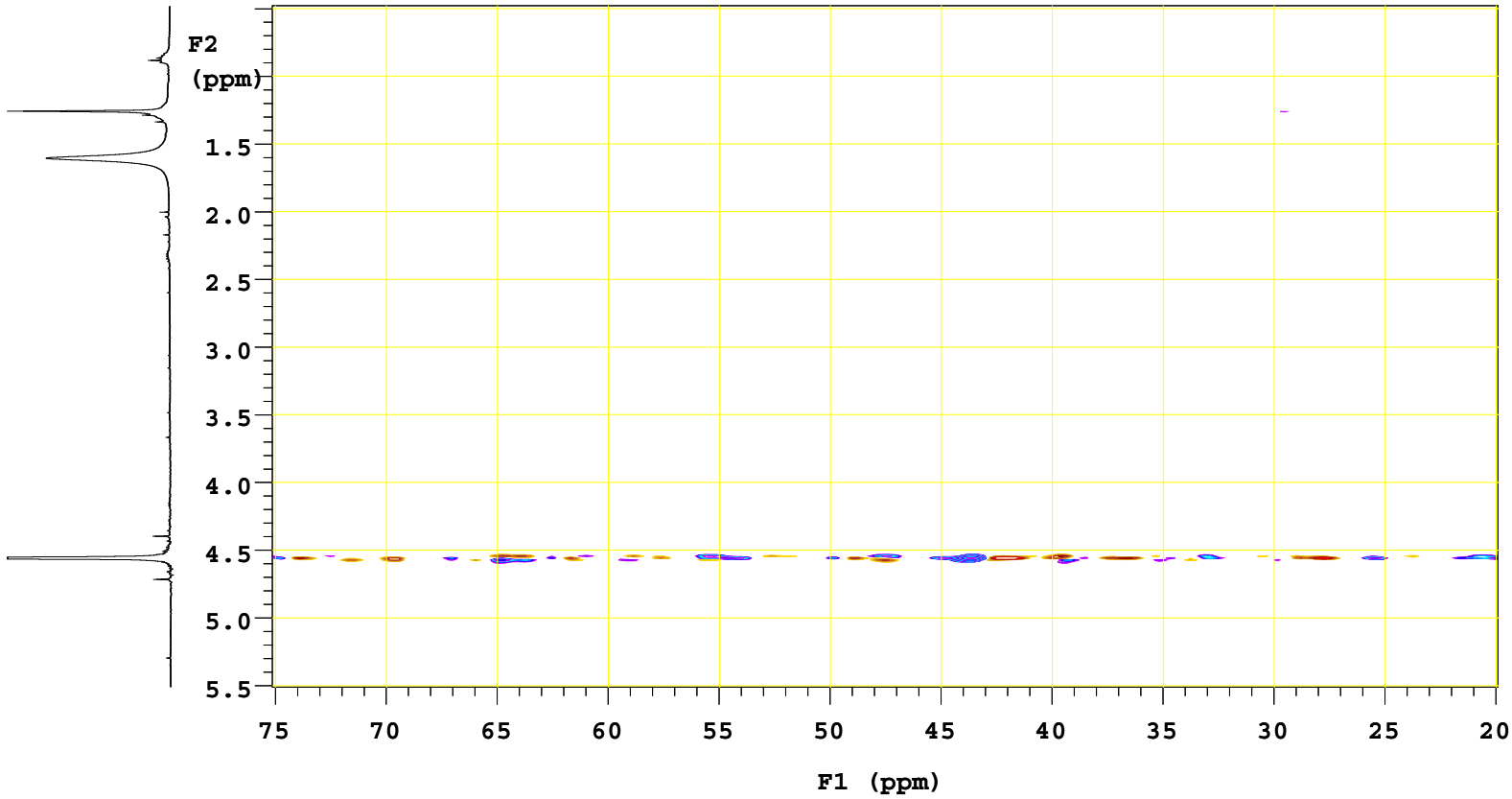
Compound **4a**



TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

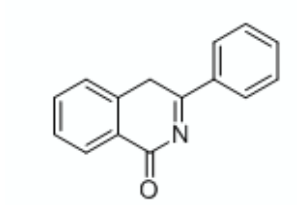
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHSQC



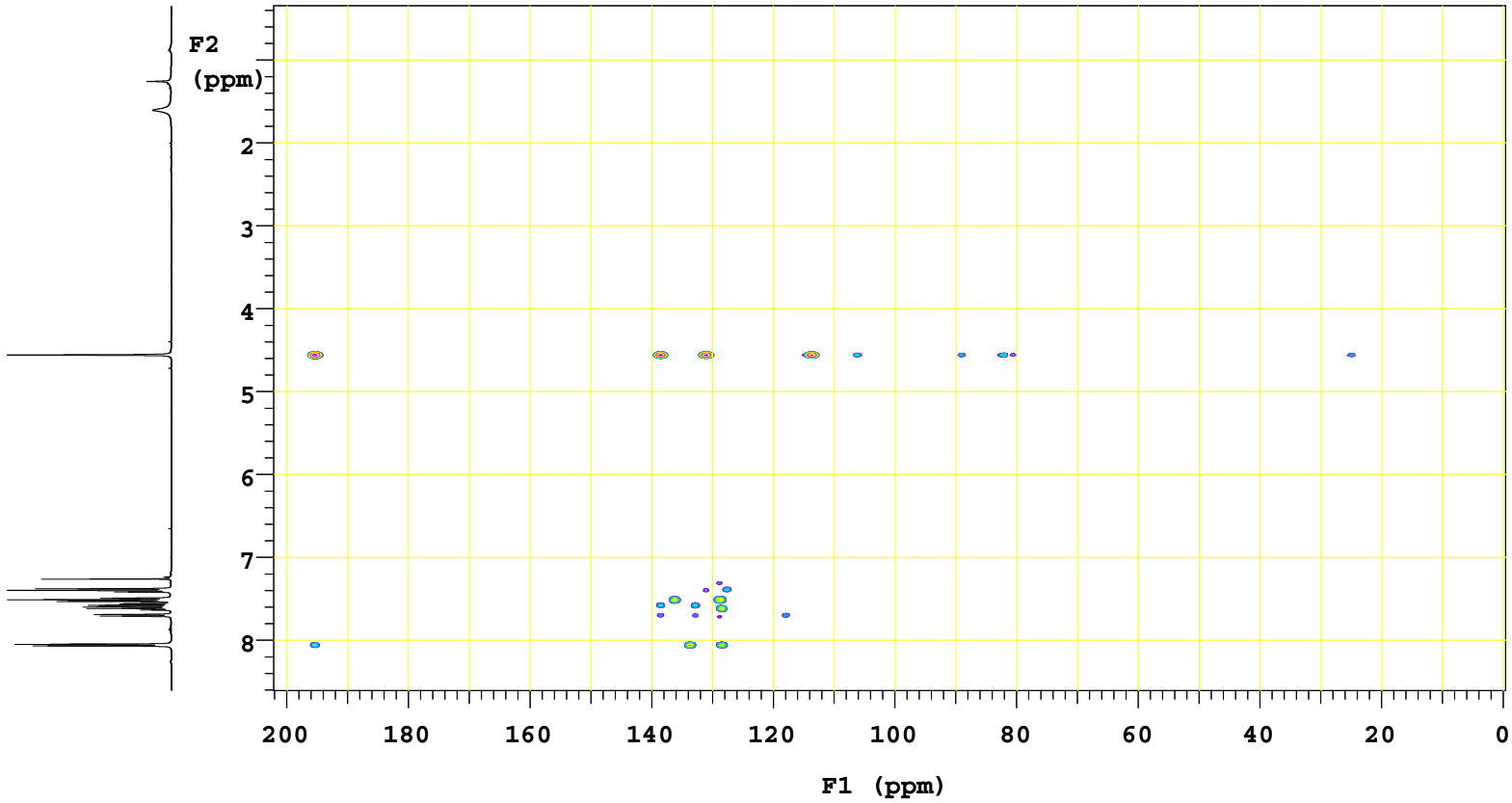
Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014



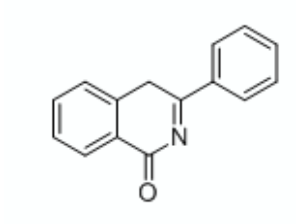
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC



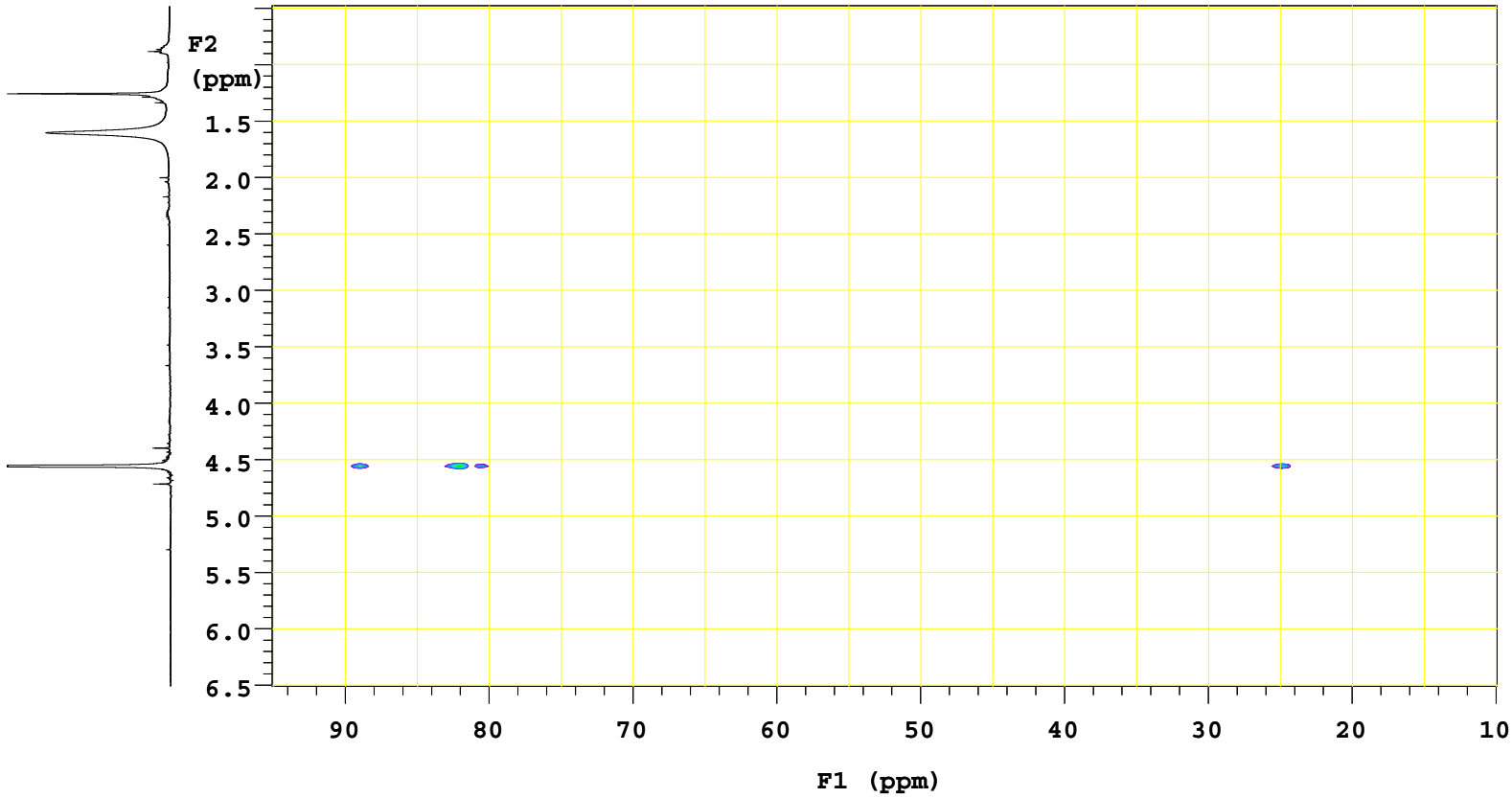
Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014



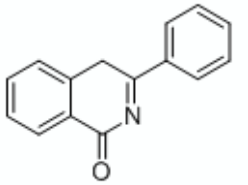
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC



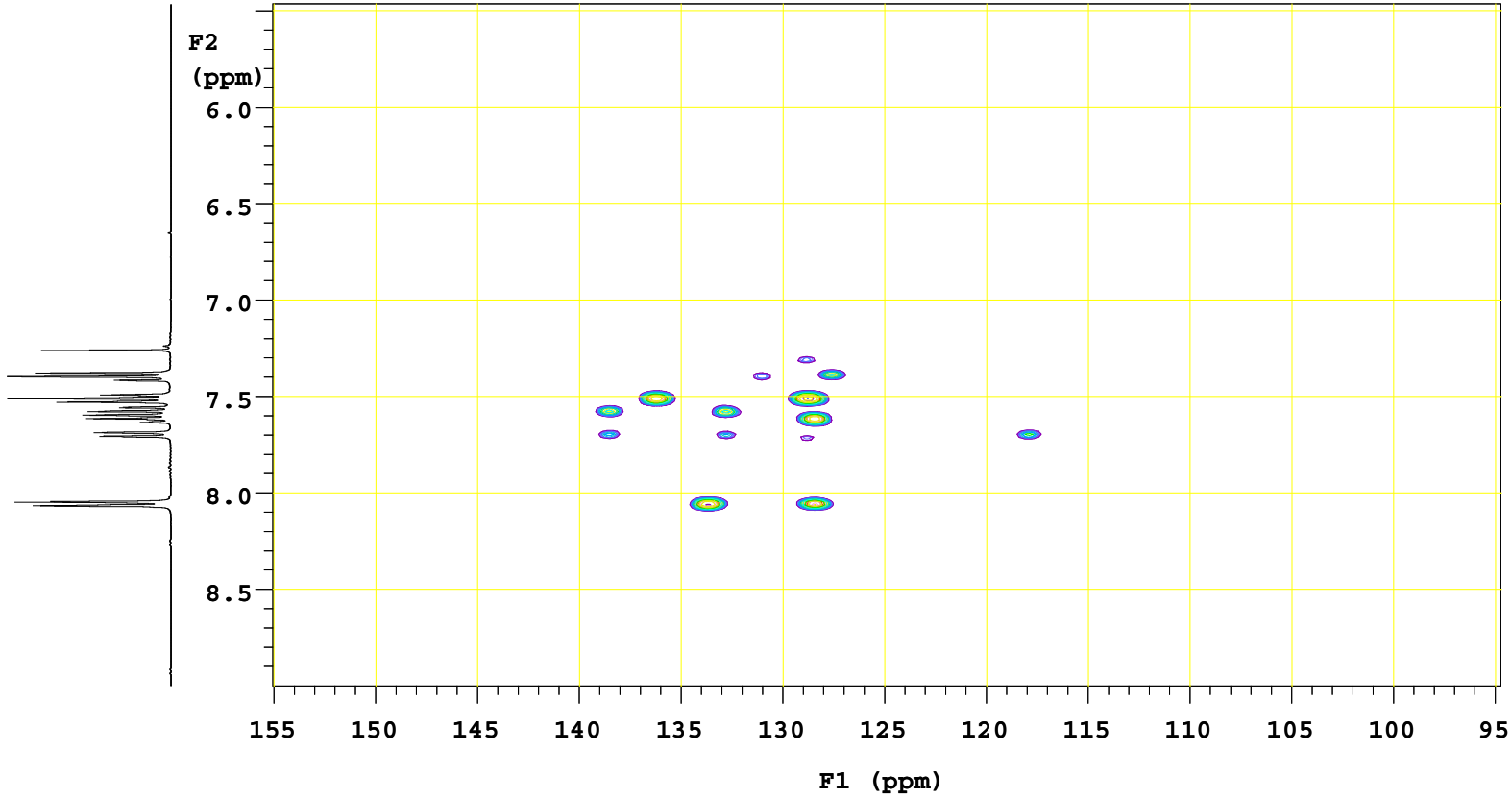
Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3

NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

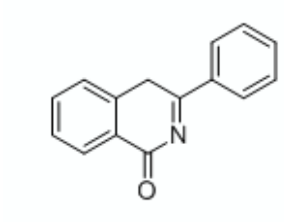


NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC



Compound **4a**

TDC-010 B036/CSBA1/002 in CDCl3



NMR-400MHz
AR.No: ME0314/2680
Analyst: Haribabu
Date:28th March.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : gHMBC