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Supplementary Information

A Multicomponent Quadruple/Double Quadruple Domino Reaction: Highly Efficient Synthesis of Polyheterocyclic Architectures

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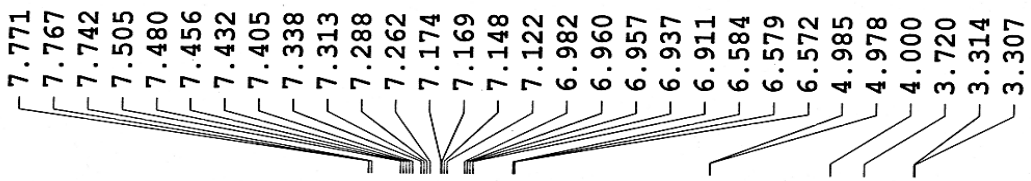
Table of Contents **Page**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7.174
7.169
7.148
7.122
6.982
6.960
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6.572
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4.978
4.000
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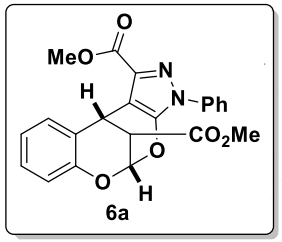
3.314
3.307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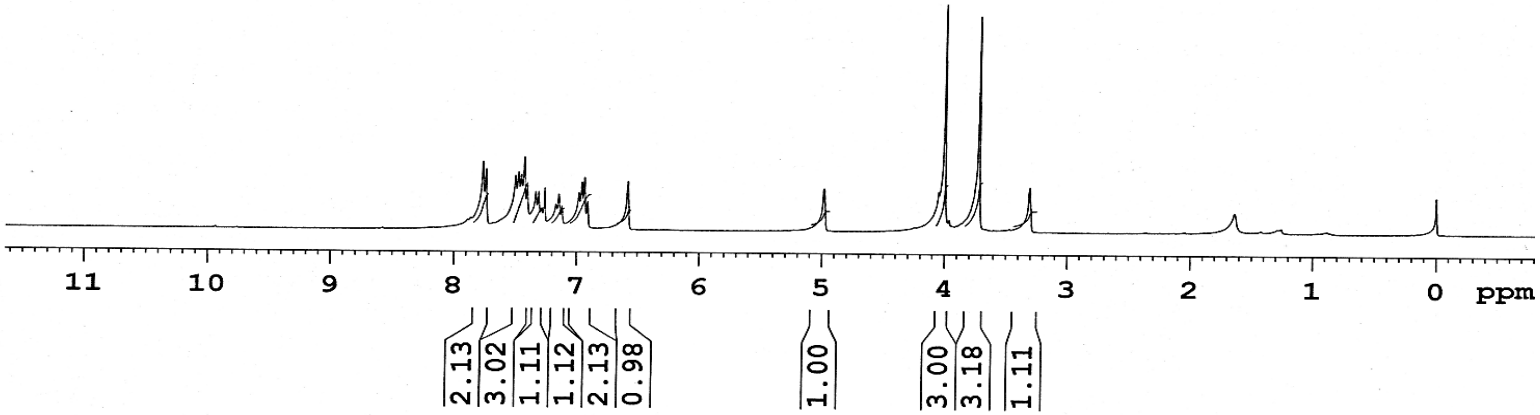
N
Ph
H
CO2Me
O
O
H
6a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7
6
5
4
3
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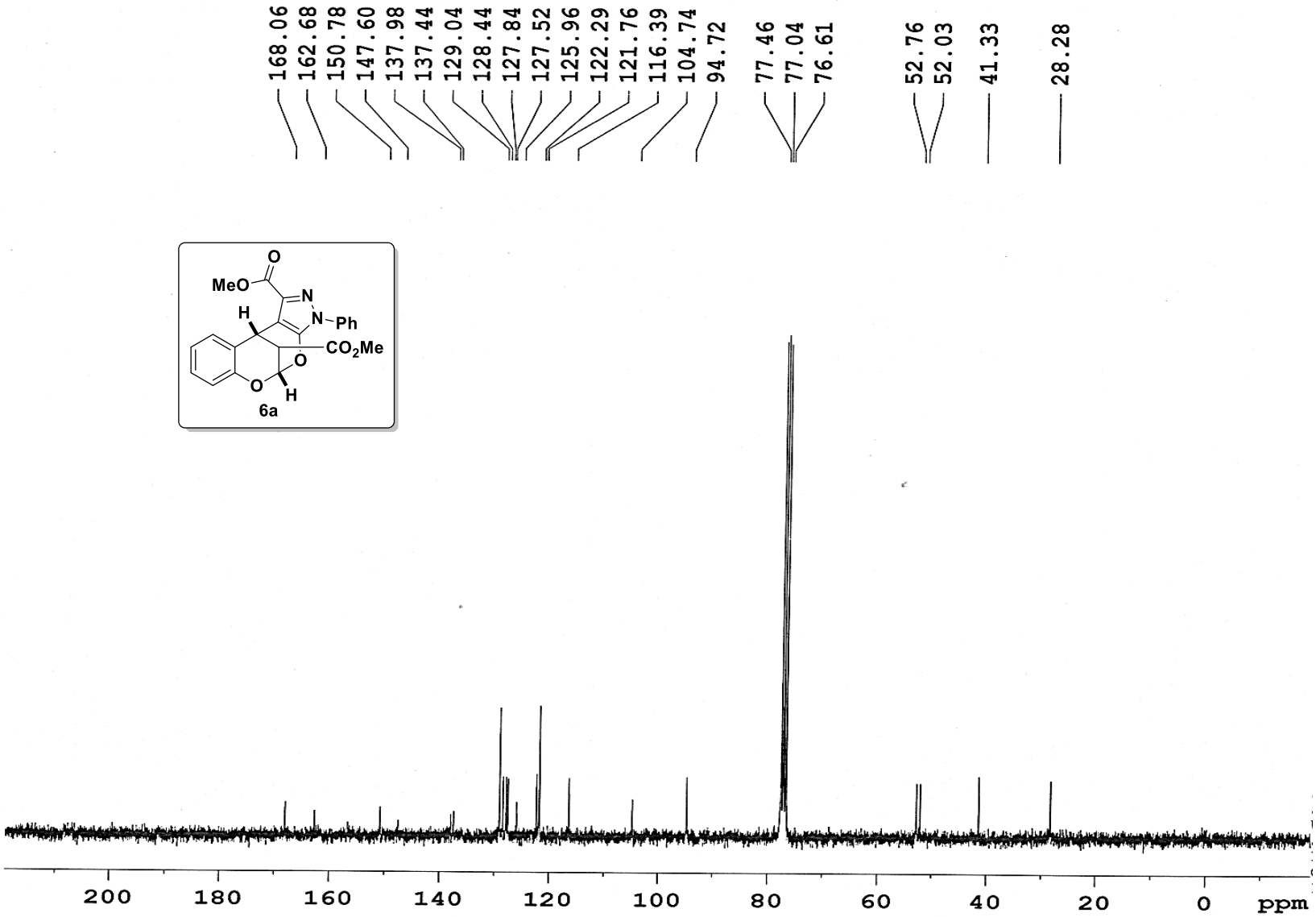
1.12
2.13
0.98
1.00
3.00
3.18
1.11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128.44
127.84
127.52
125.96
122.29
121.76
116.39
104.74
94.72
77.46
77.04
76.61
52.76
52.03
41.33
28.28
MeO
O
N
N
Ph
H
CO2Me
O
O
H
6a
200
180
160
140
120
100
80
60
40
20
0
ppm

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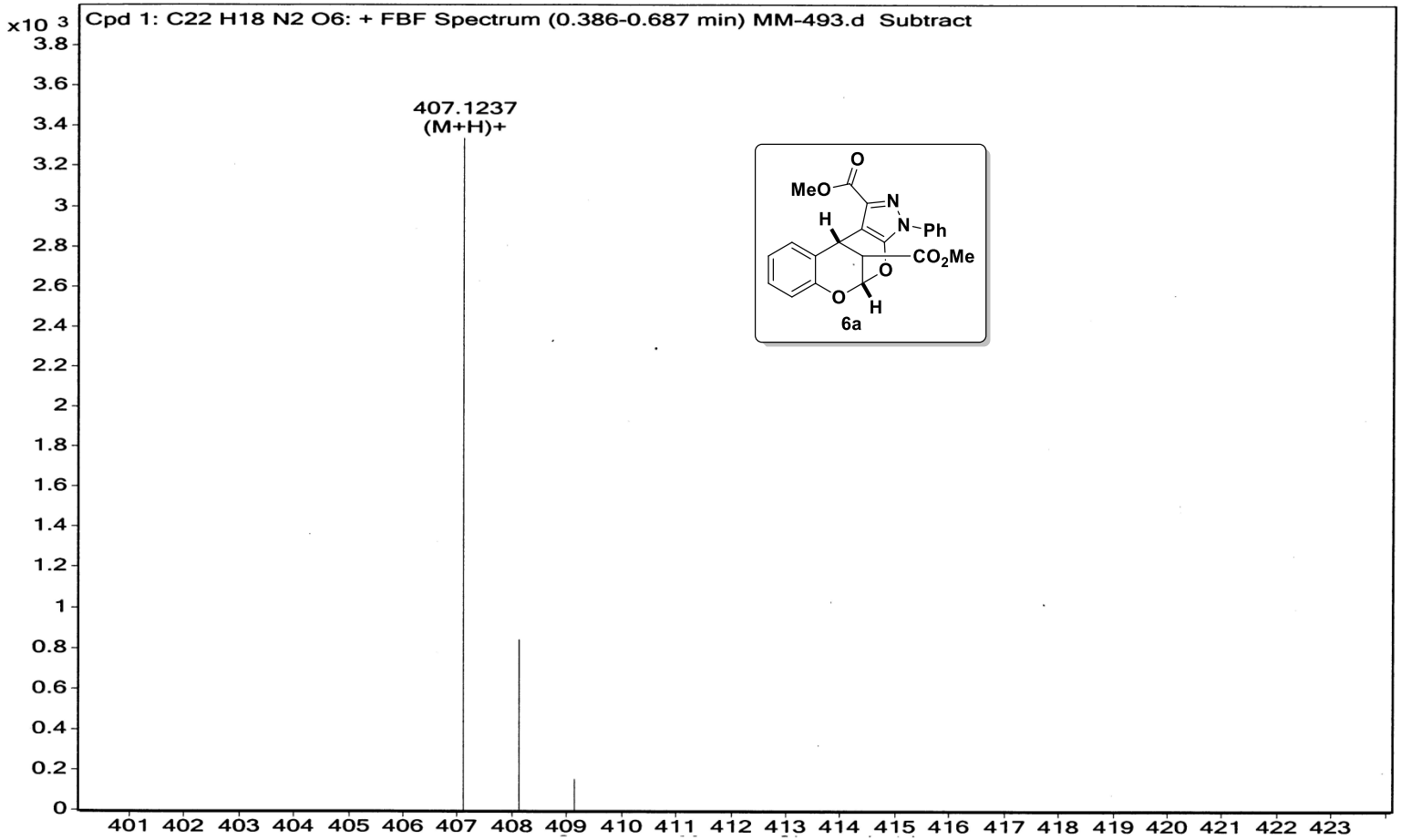

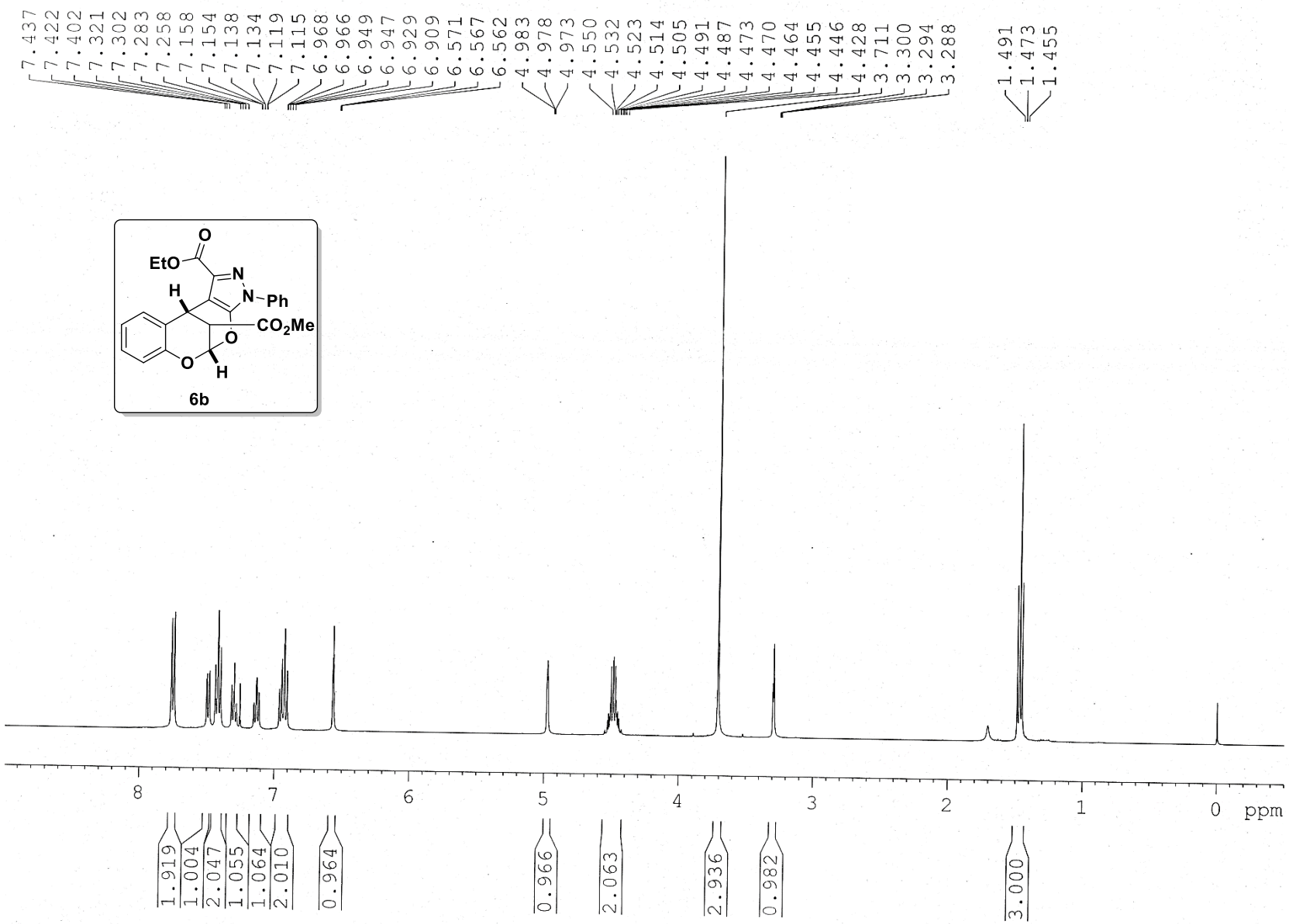
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7.258
7.158
7.154
7.138
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7.119
7.115
6.968
6.966
6.949
6.947
6.929
6.909
6.571
6.567
6.562
4.983
4.978
4.973
4.550
4.532
4.523
4.514
4.505
4.491
4.487
4.473
4.470
4.464
4.455
4.446
4.428
3.711
3.300
3.294
3.288
1.491
1.473
1.455
EtO
O
N
N-Ph
H
CO2Me
O
O
H
6b
8
7
6
5
4
3
2
1
0
ppm
1.919
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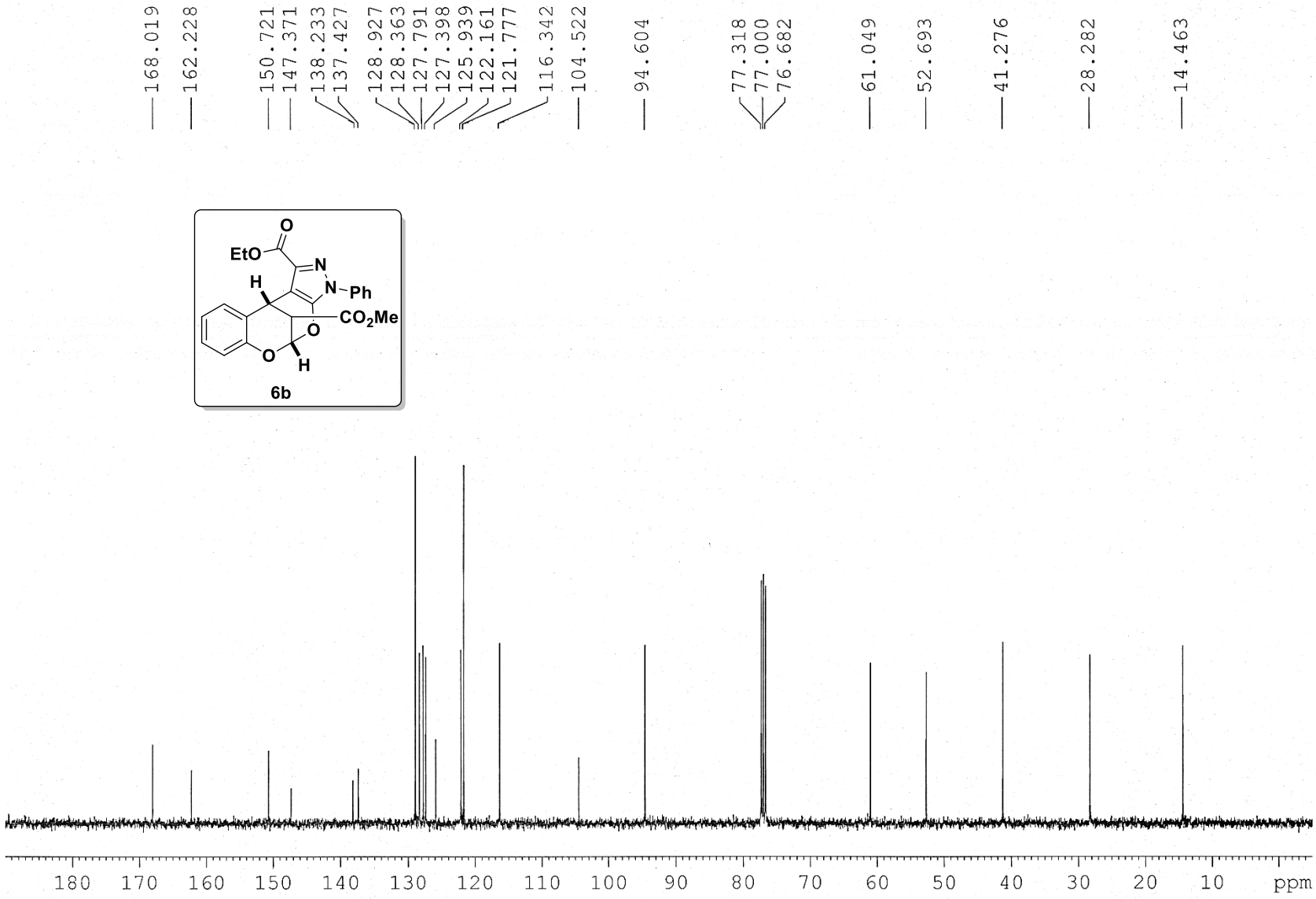
0.982
3.000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150.721
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137.427
128.927
128.363
127.791
127.398
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122.161
121.777
116.342
104.522
94.604
77.318
77.000
76.682
61.049
52.693
41.276
28.282
14.463
EtO
O
N
N
Ph
H
CO2Me
O
O
H
6b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

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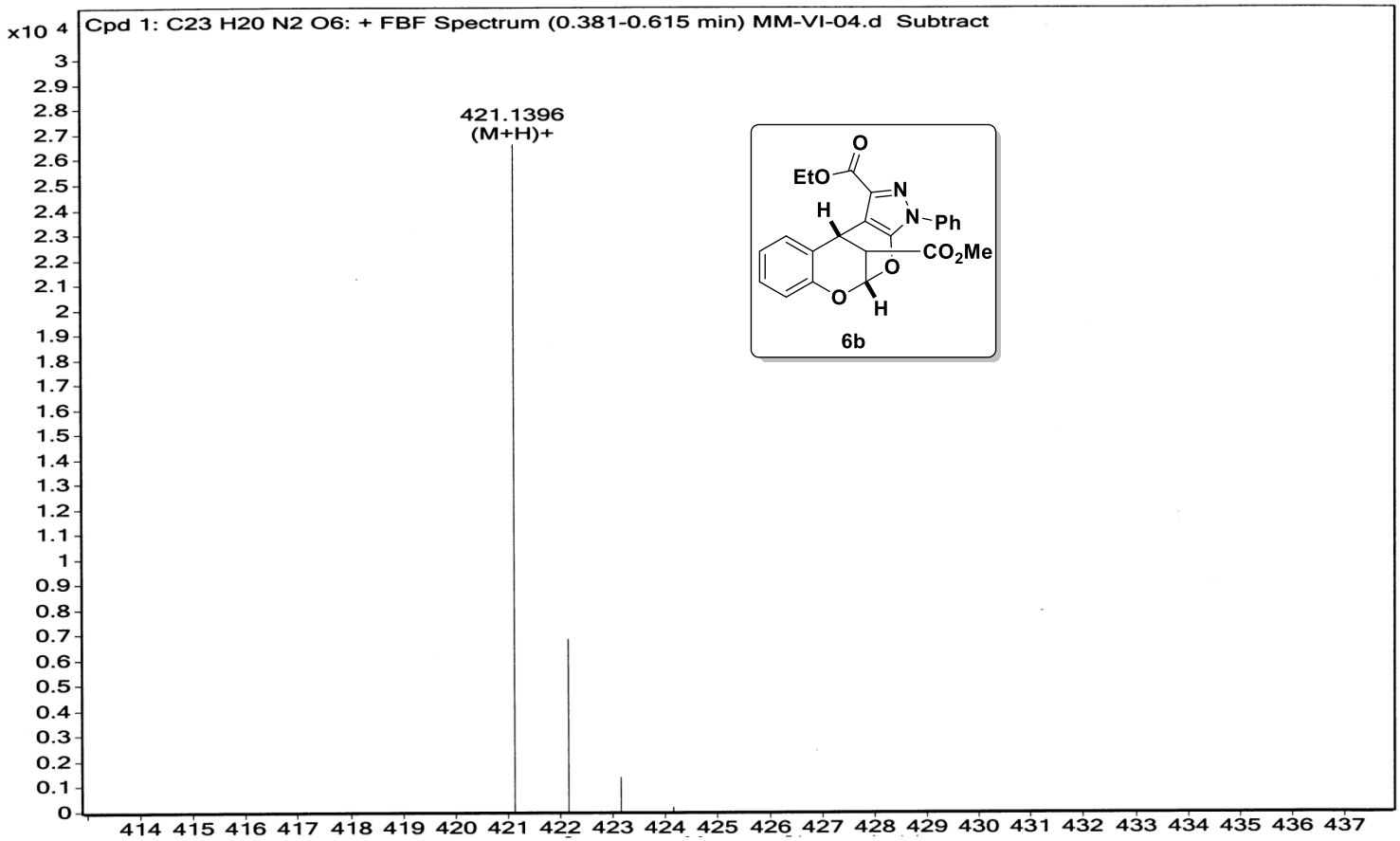

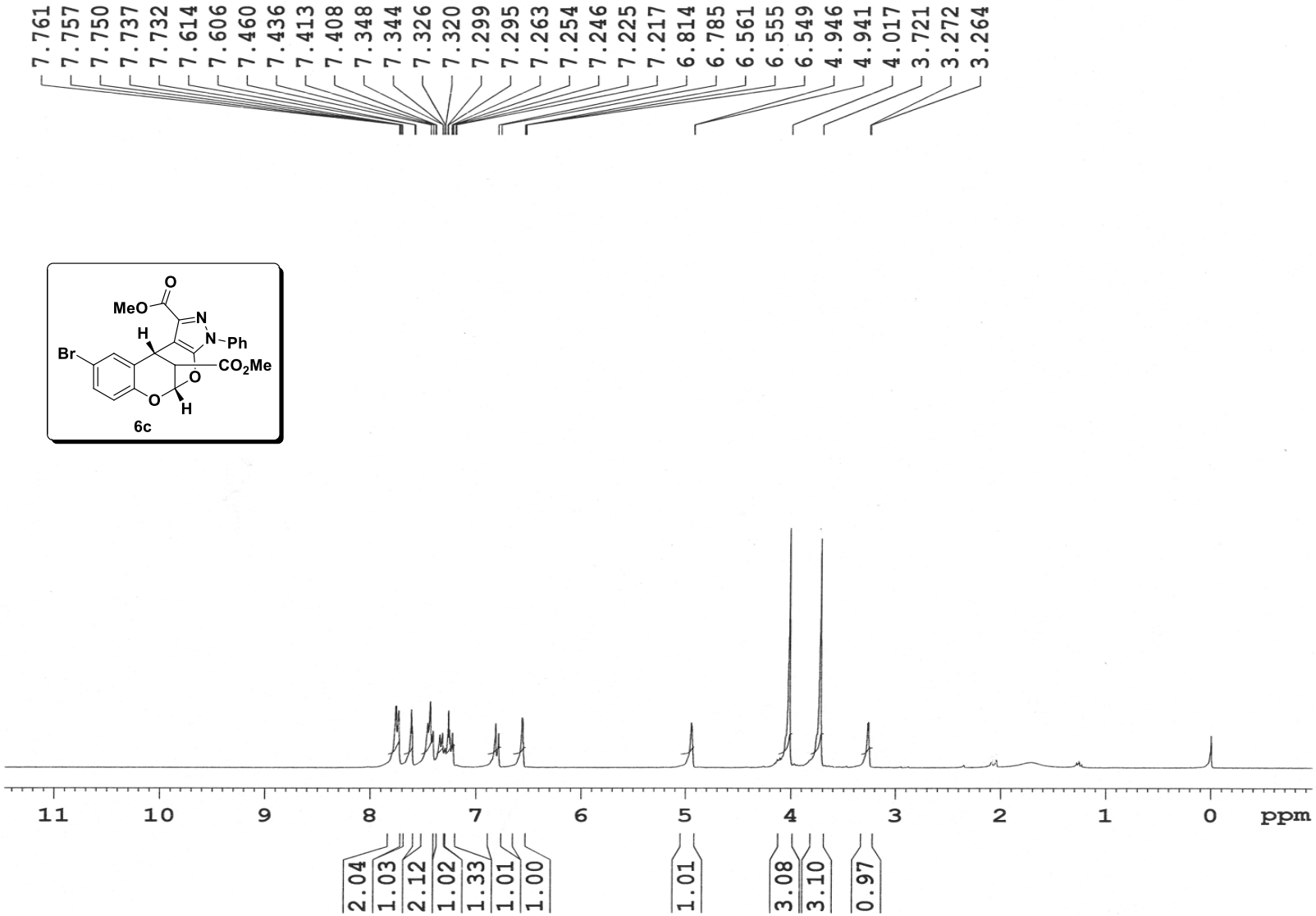
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7.460
7.436
7.413
7.408
7.348
7.344
7.326
7.320
7.299
7.295
7.263
7.254
7.246
7.225
7.217
6.814
6.785
6.561
6.555
6.549
4.946
4.941
4.017
3.721
3.272
3.264
MeO
O
N
N
Ph
H
Br
CO2Me
O
O
H
6c
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
1.03
2.12
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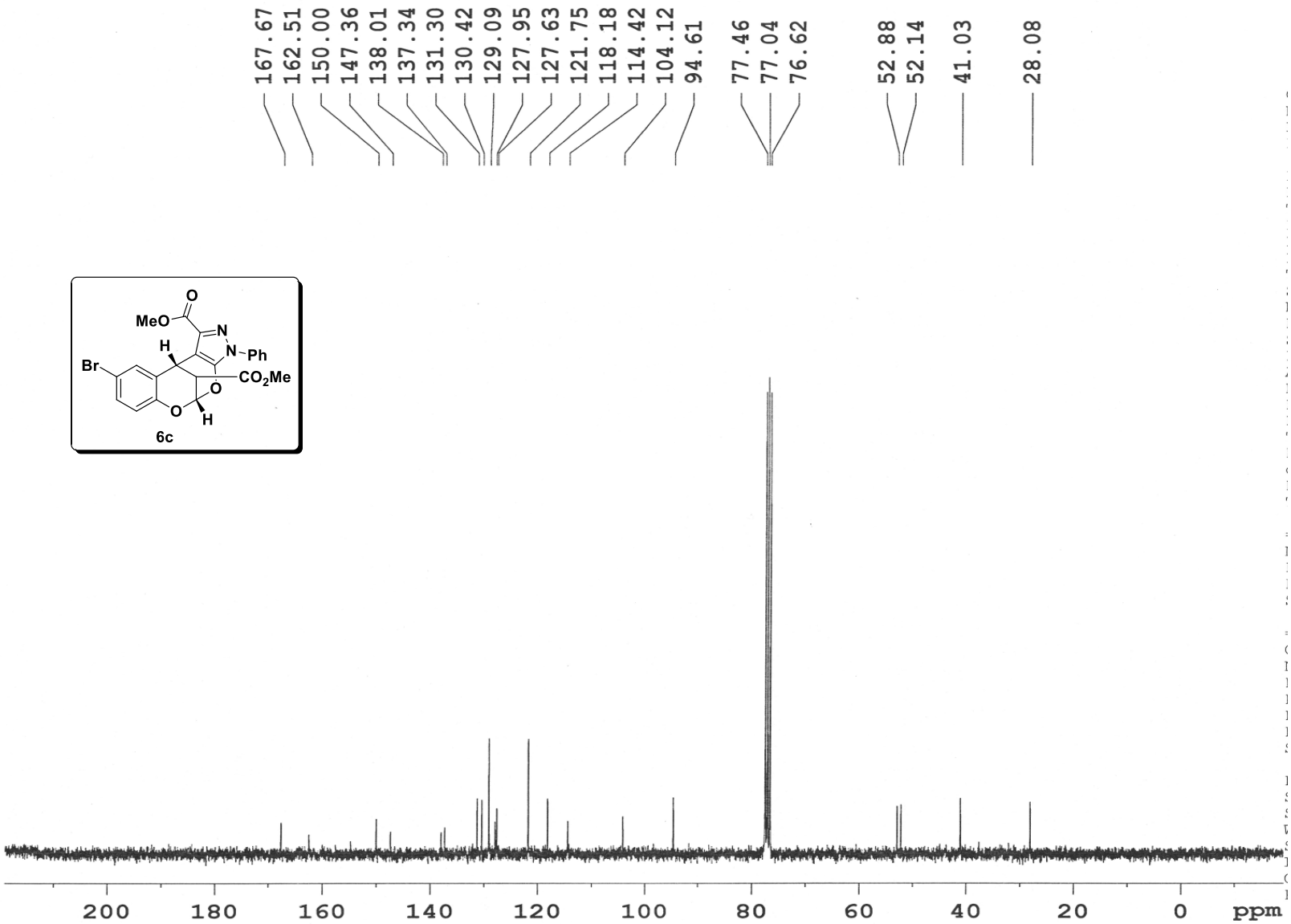
1.00
1.01
3.08
3.10
0.97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118.18
114.42
104.12
94.61
77.46
77.04
76.62
52.88
52.14
41.03
28.08
MeO
O
N
N
Ph
H
Br
CO2Me
O
O
H
6c
200
180
160
140
120
100
80
60
40
20
0
ppm

Sample Name	PVK-JS-V1-94	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
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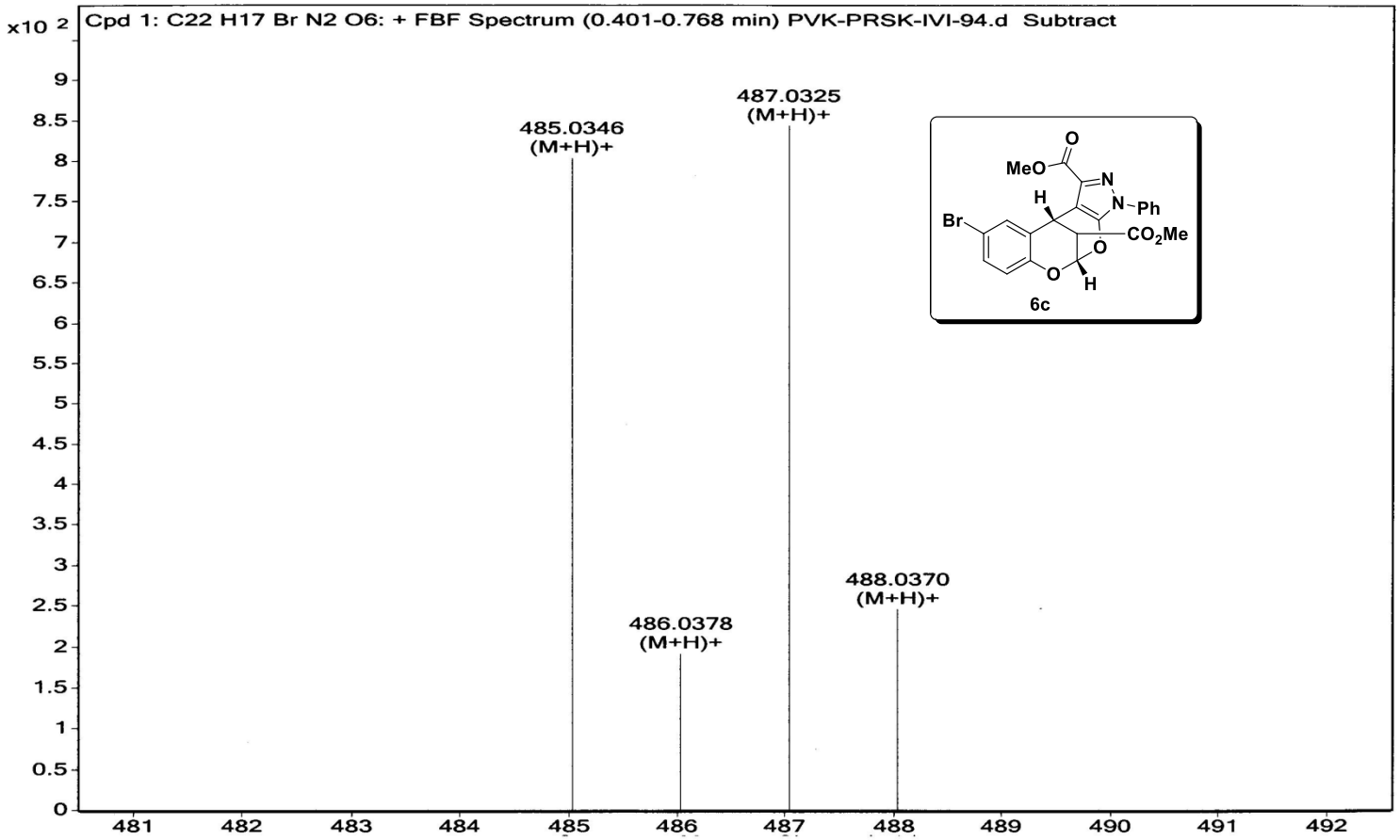

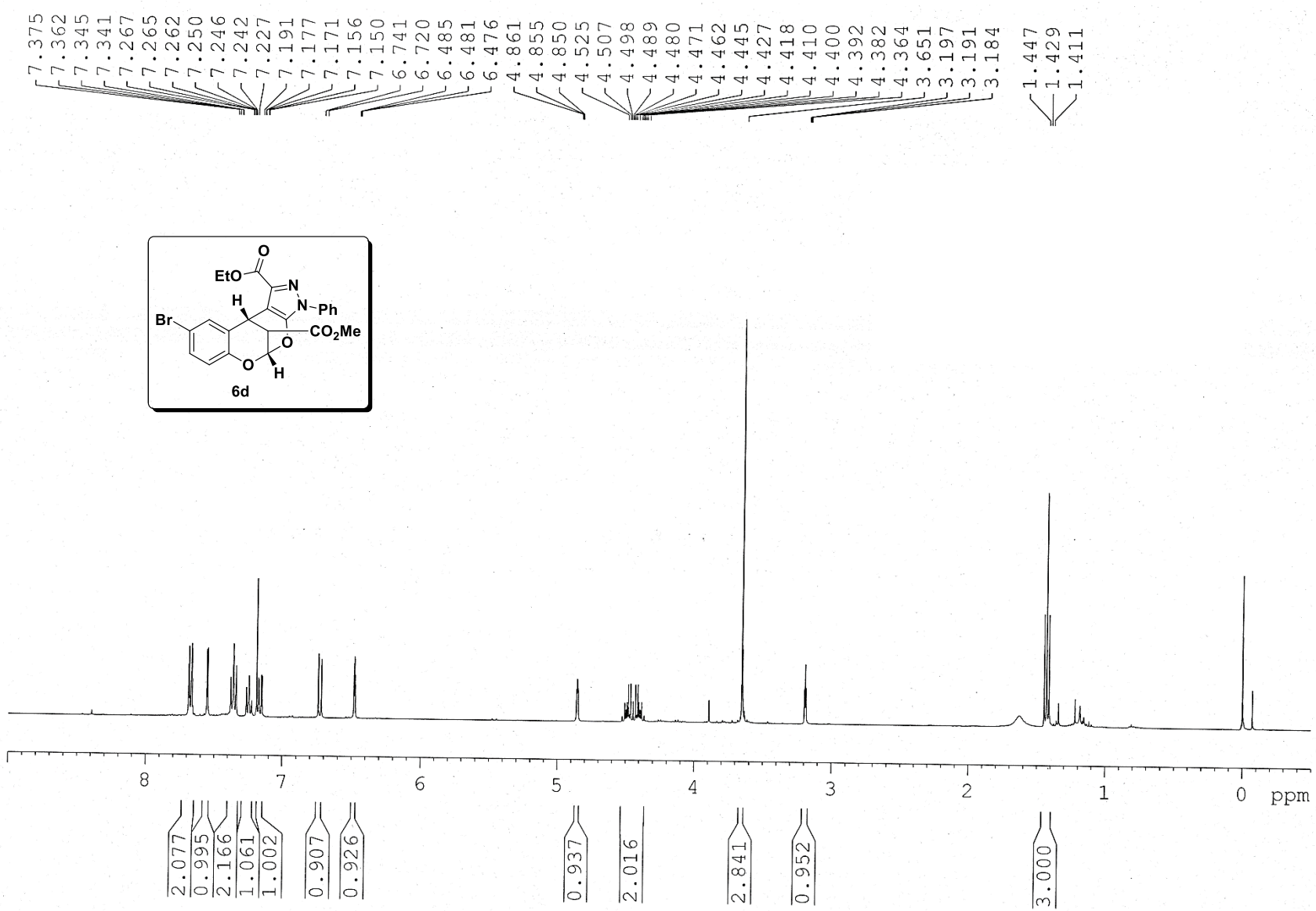
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7.262
7.250
7.246
7.242
7.227
7.191
7.177
7.171
7.156
7.150
6.741
6.720
6.485
6.481
6.476
4.861
4.855
4.850
4.525
4.507
4.498
4.489
4.480
4.471
4.462
4.445
4.427
4.418
4.410
4.400
4.392
4.382
4.364
3.651
3.197
3.191
3.184
1.447
1.429
1.411
O
EtO
N
N
Ph
H
Br
CO2Me
O
O
H
6d
8
7
6
5
4
3
2
1
0
ppm
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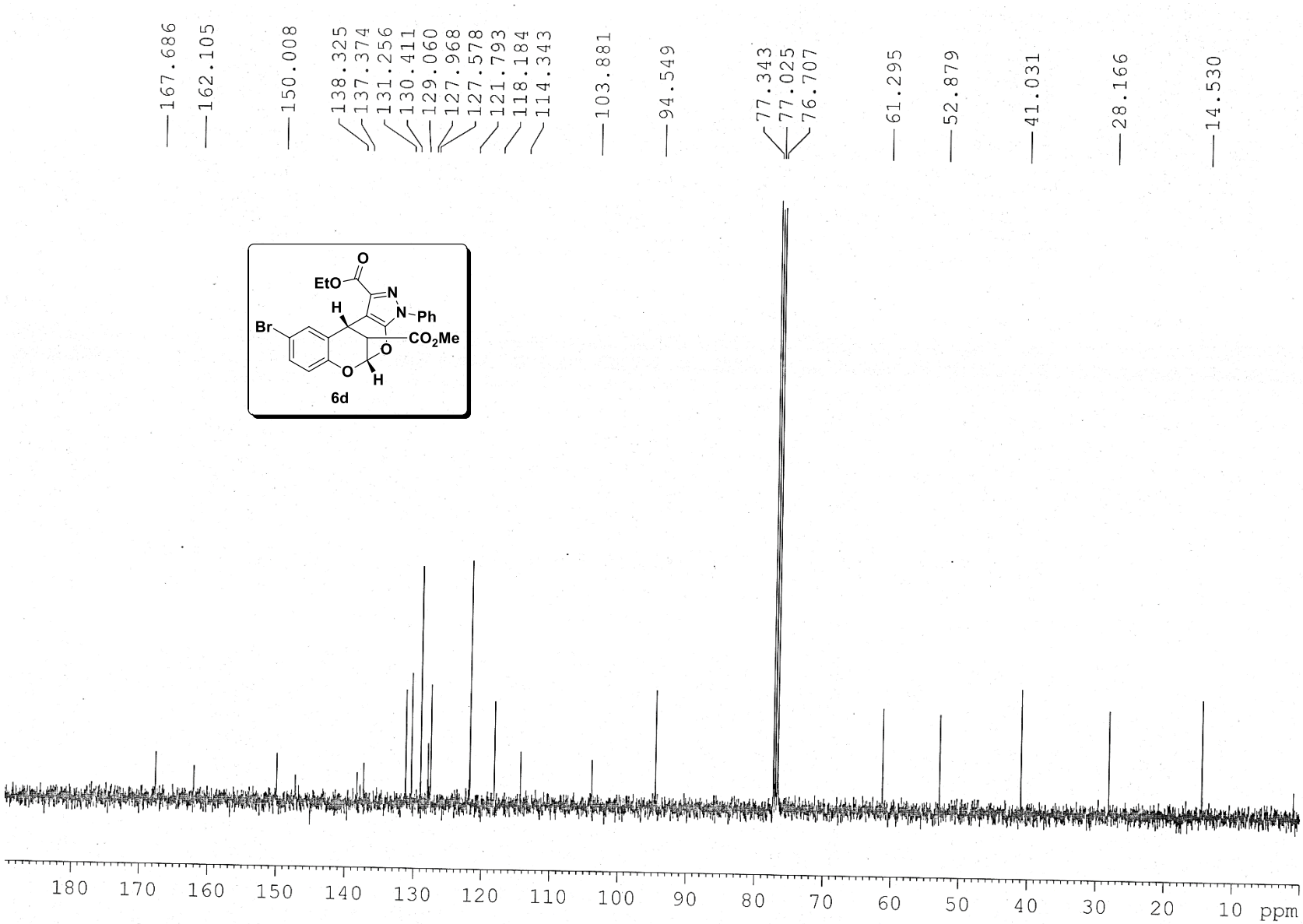
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129.060
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127.578
121.793
118.184
114.343
103.881
94.549
77.343
77.025
76.707
61.295
52.879
41.031
28.166
14.530
EtO
O
N
N
Ph
H
Br
CO2Me
O
O
H
6d
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Sample Name	MM-VI-05	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
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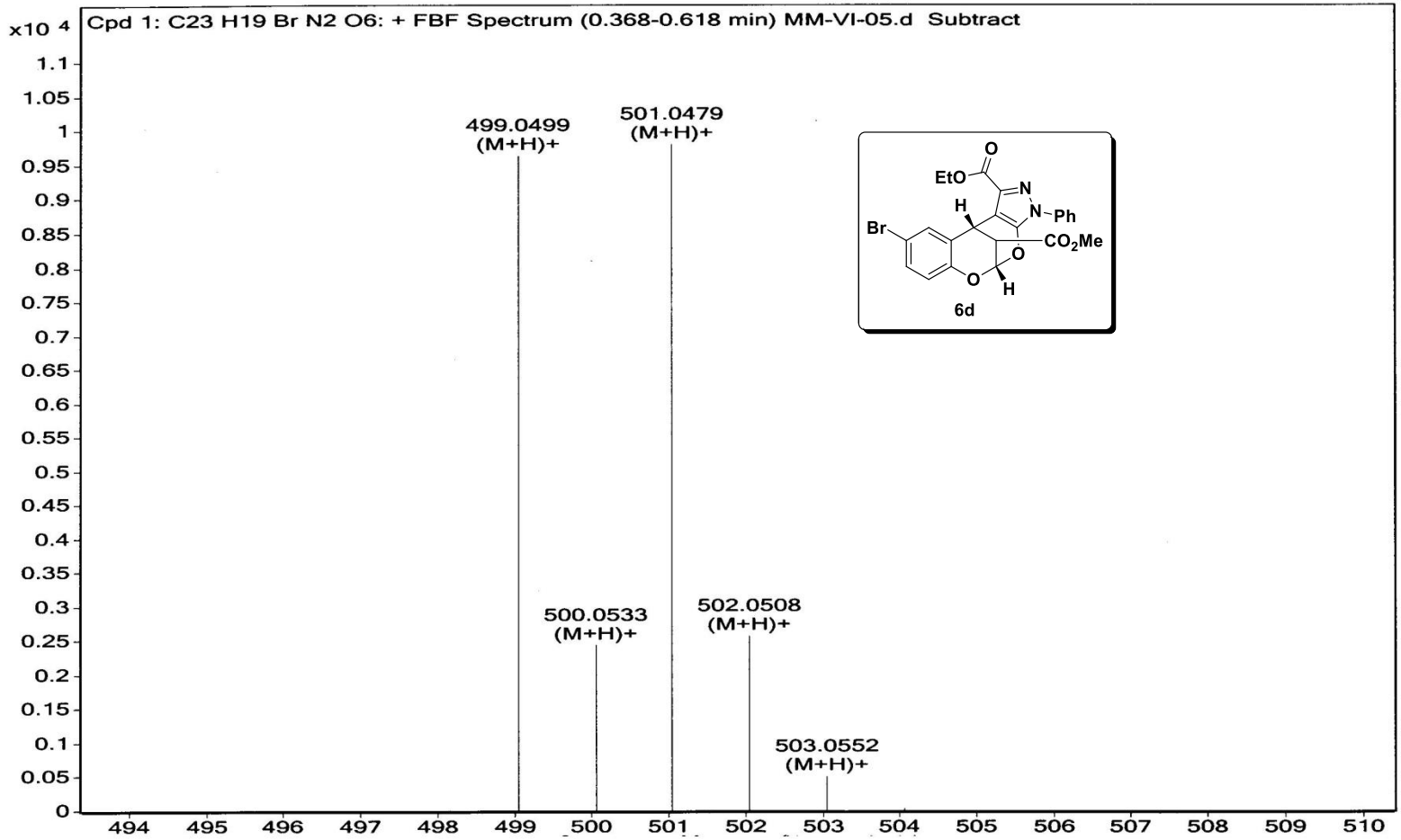

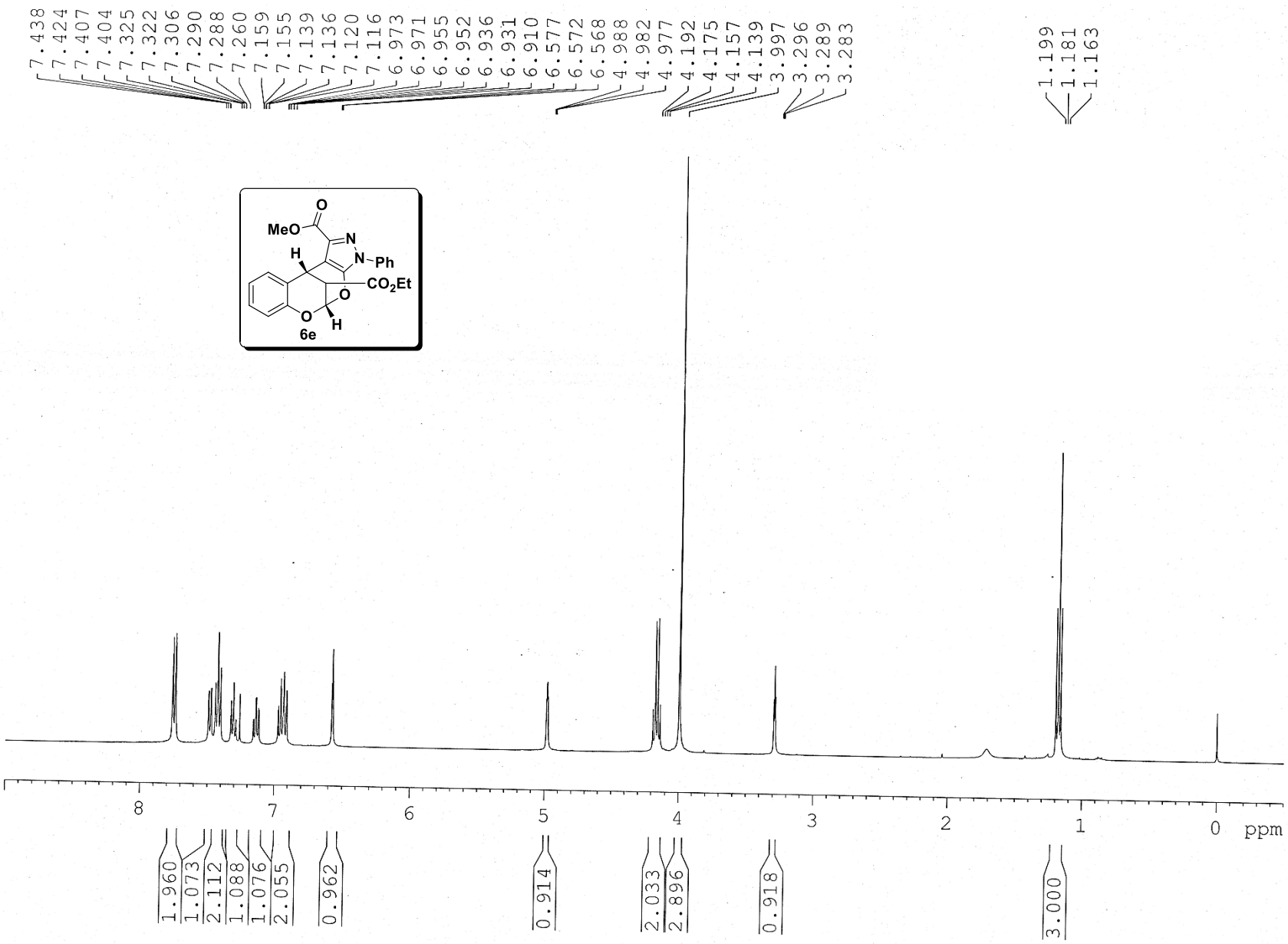
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7.404
7.325
7.322
7.306
7.290
7.288
7.260
7.159
7.155
7.139
7.136
7.120
7.116
6.973
6.971
6.955
6.952
6.936
6.931
6.910
6.577
6.572
6.568
4.988
4.982
4.977
4.192
4.175
4.157
4.139
3.997
3.296
3.289
3.283
1.199
1.181
1.163
MeO
O
N
N
Ph
H
CO2Et
O
O
H
6e
8
7
6
5
4
3
2
1
0
ppm
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0.914
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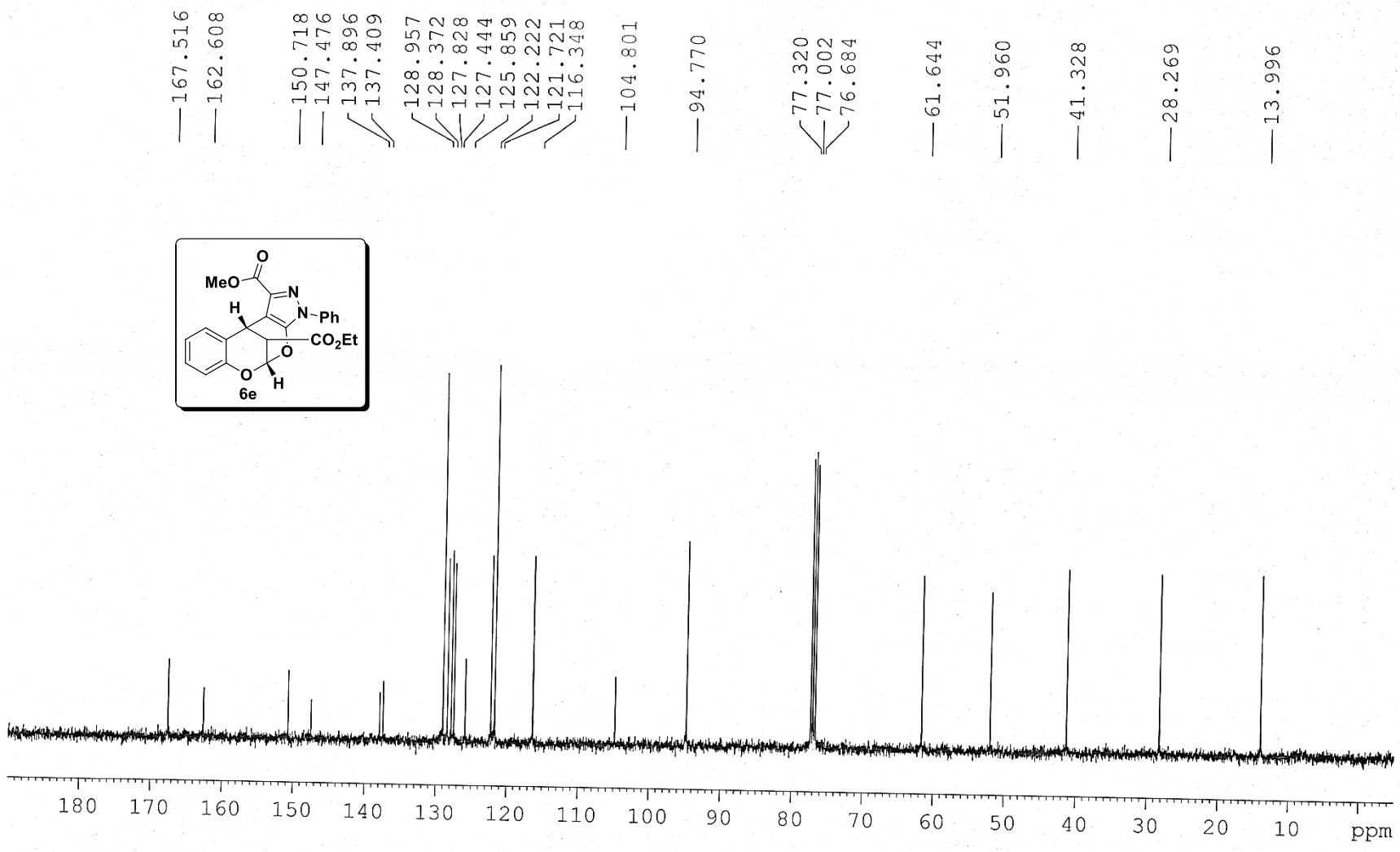
0.918
3.000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137.409
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128.372
127.828
127.444
125.859
122.222
121.721
116.348
104.801
94.770
77.320
77.002
76.684
61.644
51.960
41.328
28.269
13.996
MeO
O
N
N
Ph
H
CO2Et
O
O
H
6e
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Sample Name	PVK-JS-V1-10	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
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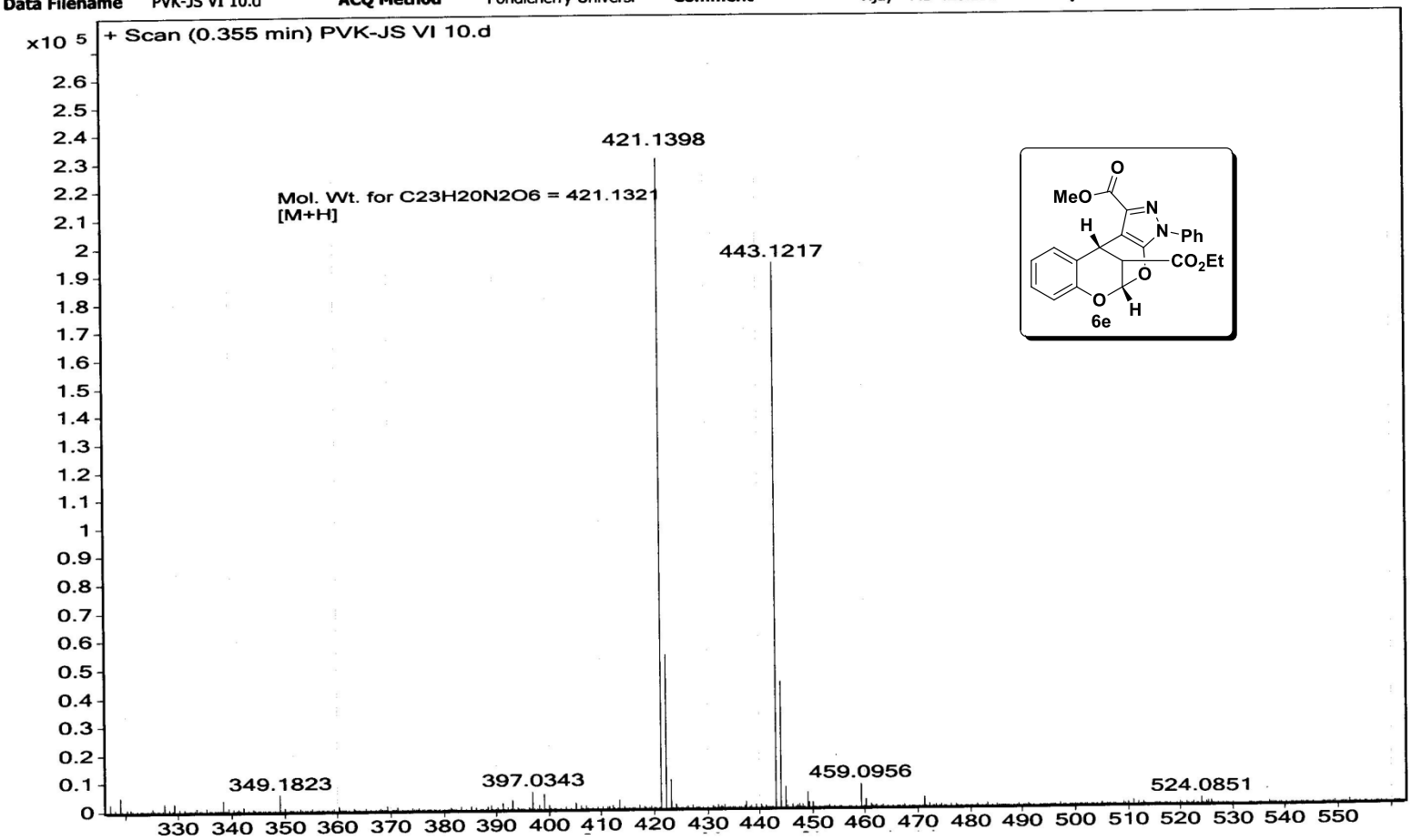

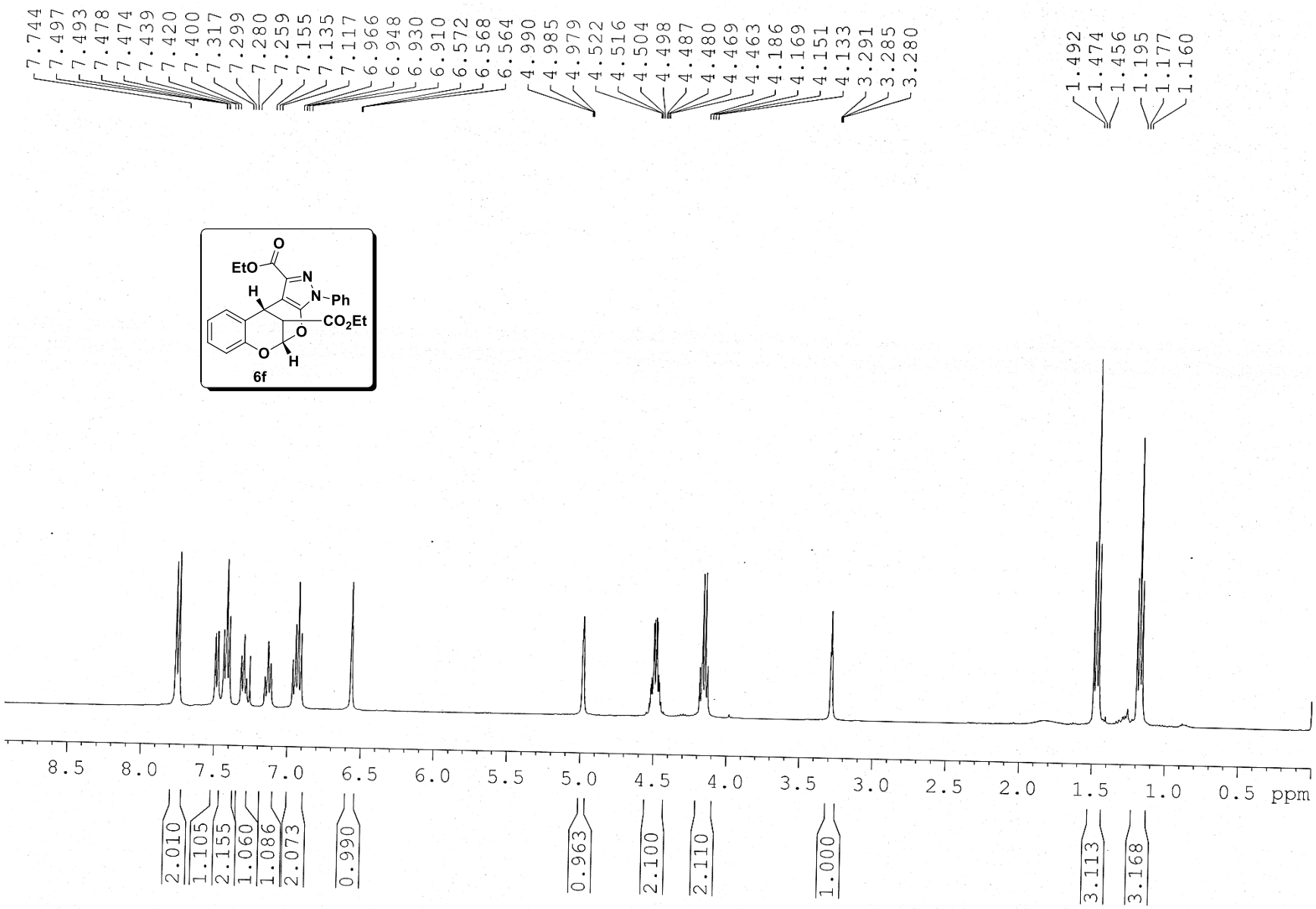
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7.493
7.478
7.474
7.439
7.420
7.400
7.317
7.299
7.280
7.259
7.155
7.135
7.117
6.966
6.948
6.930
6.910
6.572
6.568
6.564
4.990
4.985
4.979
4.522
4.516
4.504
4.498
4.487
4.480
4.469
4.463
4.186
4.169
4.151
4.133
3.291
3.285
3.280
1.492
1.474
1.456
1.195
1.177
1.160
EtO
O
N
N-Ph
H
CO2Et
O
O
H
6f
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.010
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0.963
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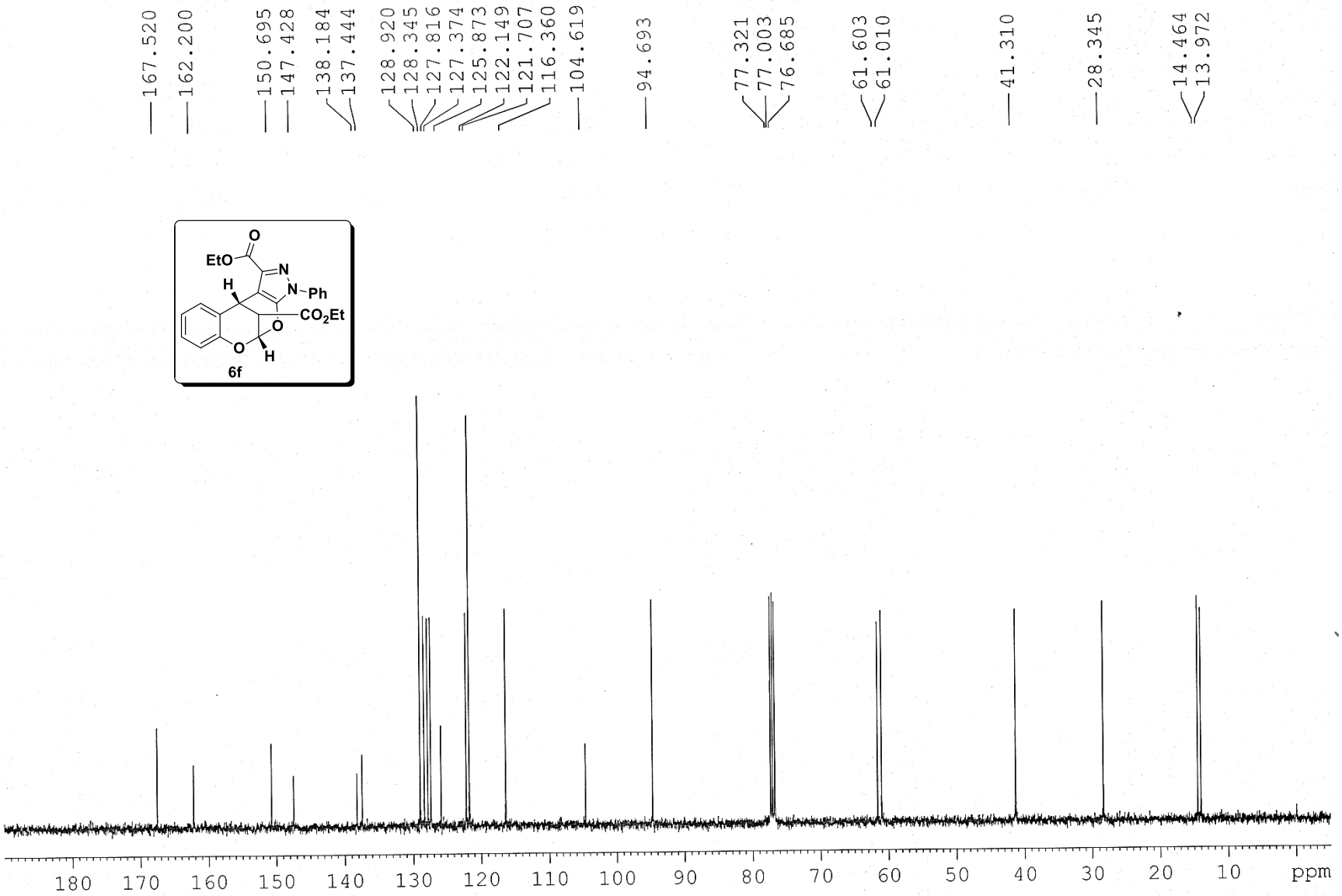
2.110
1.000
3.113
3.168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147.428
138.184
137.444
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128.345
127.816
127.374
125.873
122.149
121.707
116.360
104.619
94.693
77.321
77.003
76.685
61.603
61.010
41.310
28.345
14.464
13.972
EtO
O
N
N
Ph
H
CO2Et
O
O
H
6f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Sample Name	PVK-JS-V1-09	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
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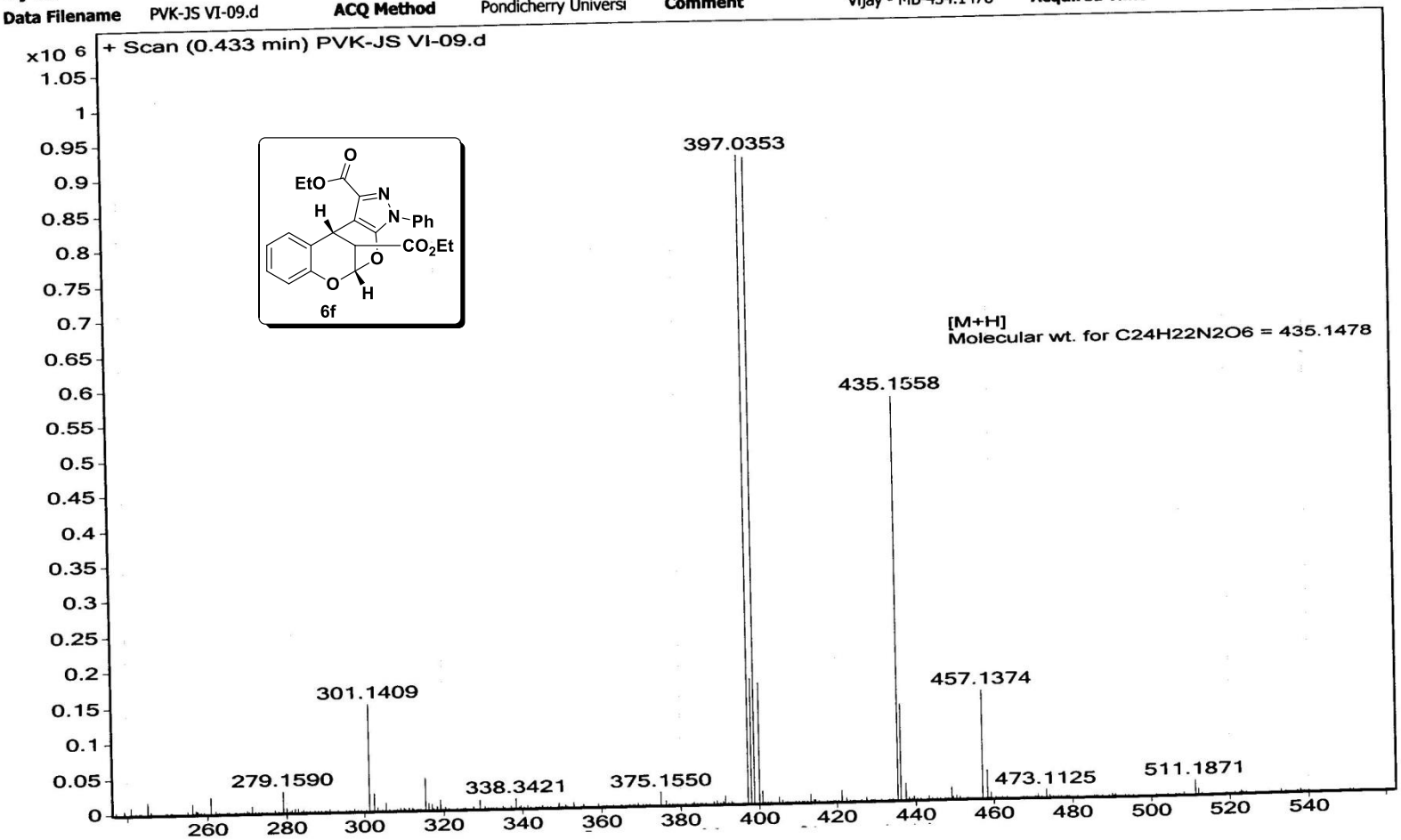

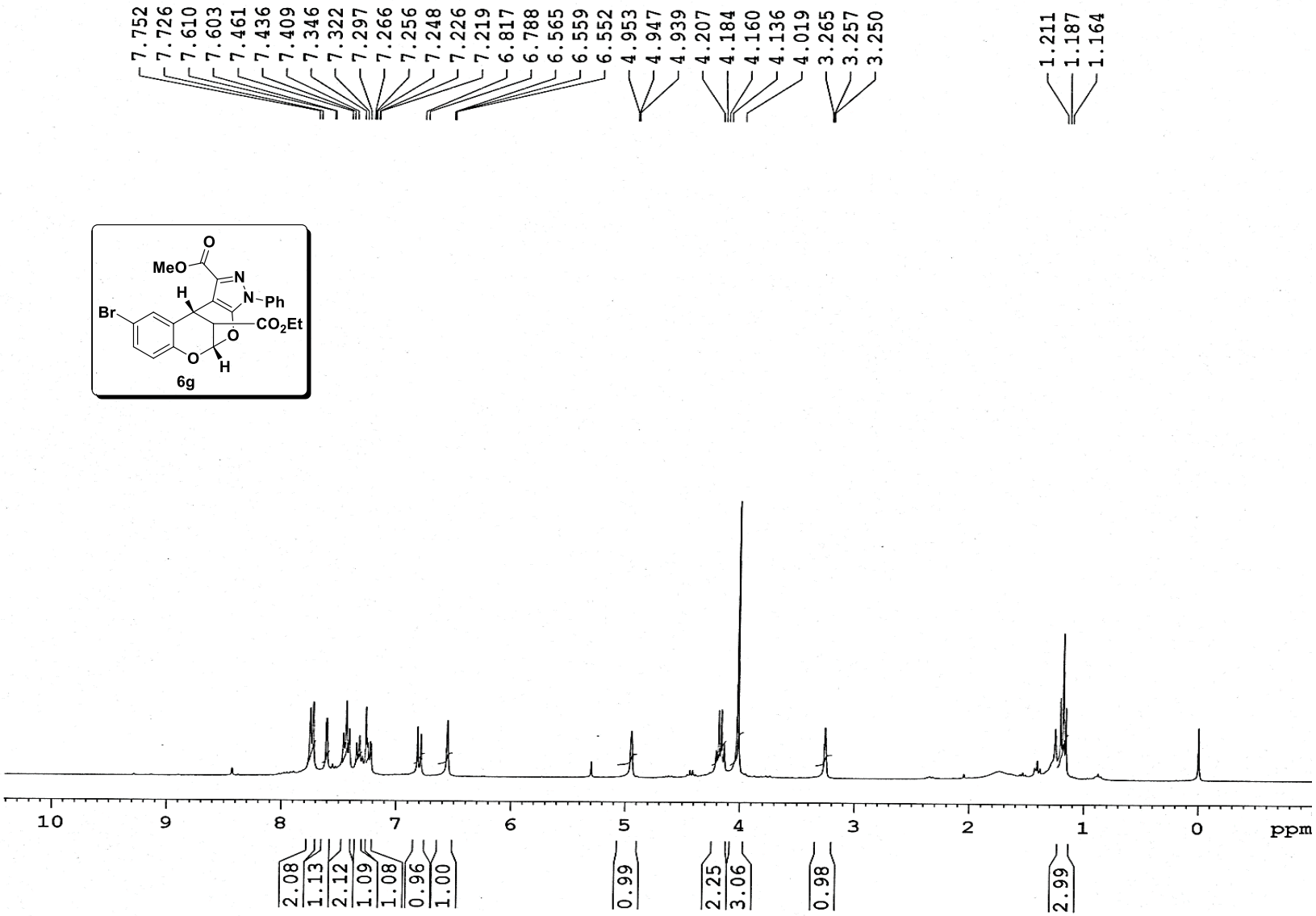
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7.248
7.226
7.219
6.817
6.788
6.565
6.559
6.552
4.953
4.947
4.939
4.207
4.184
4.160
4.136
4.019
3.265
3.257
3.250
1.211
1.187
1.164
MeO
O
N
N
Ph
H
Br
CO2Et
O
O
H
6g
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.08
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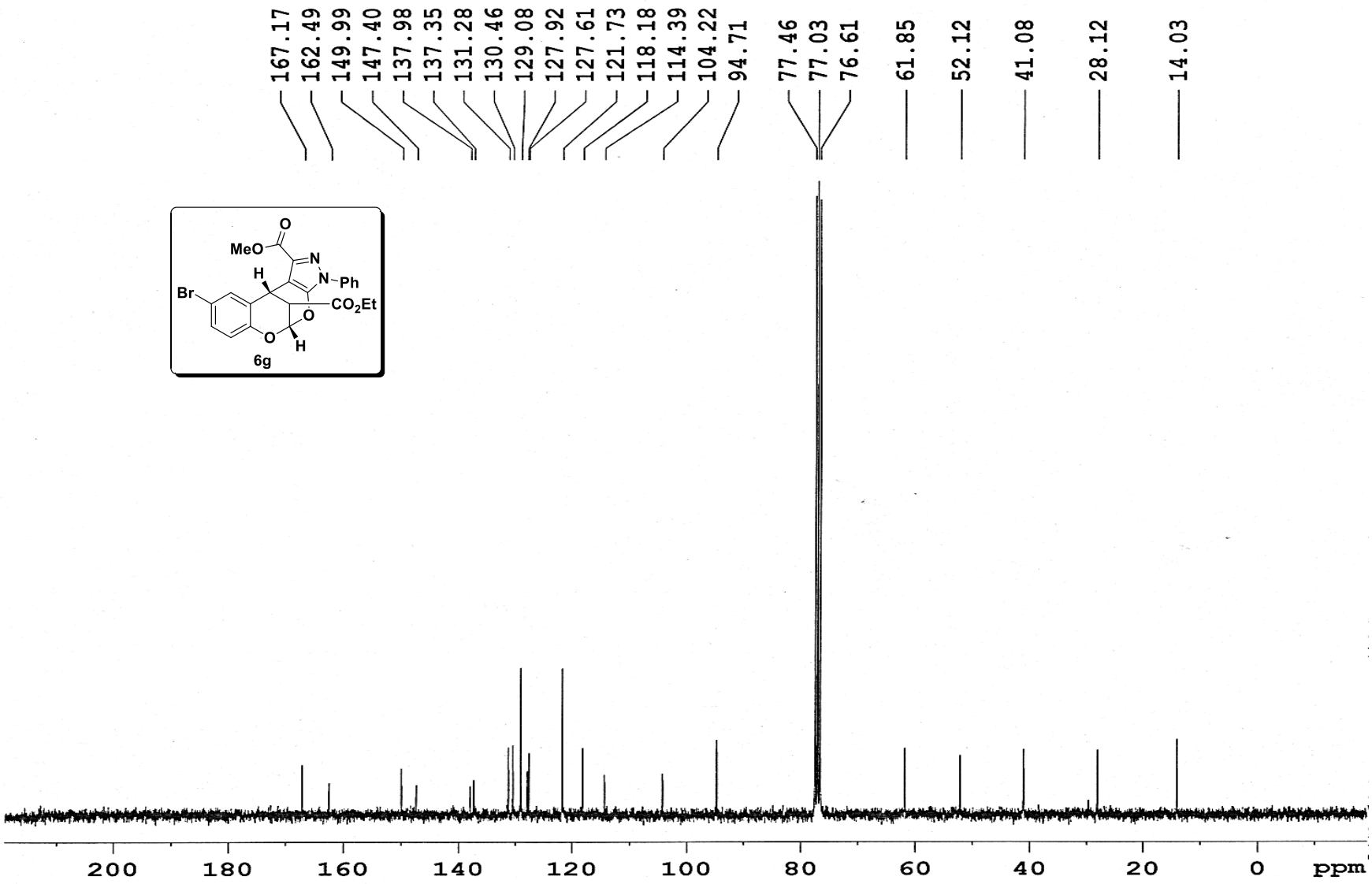
2.25
3.06
0.98
2.99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137.35
131.28
130.46
129.08
127.92
127.61
121.73
118.18
114.39
104.22
94.71
77.46
77.03
76.61
61.85
52.12
41.08
28.12
14.03
MeO
O
N
N-Ph
H
Br
CO2Et
O
O
H
6g
200
180
160
140
120
100
80
60
40
20
0
ppm

Sample Name	PVK-PRSK-IV-105	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
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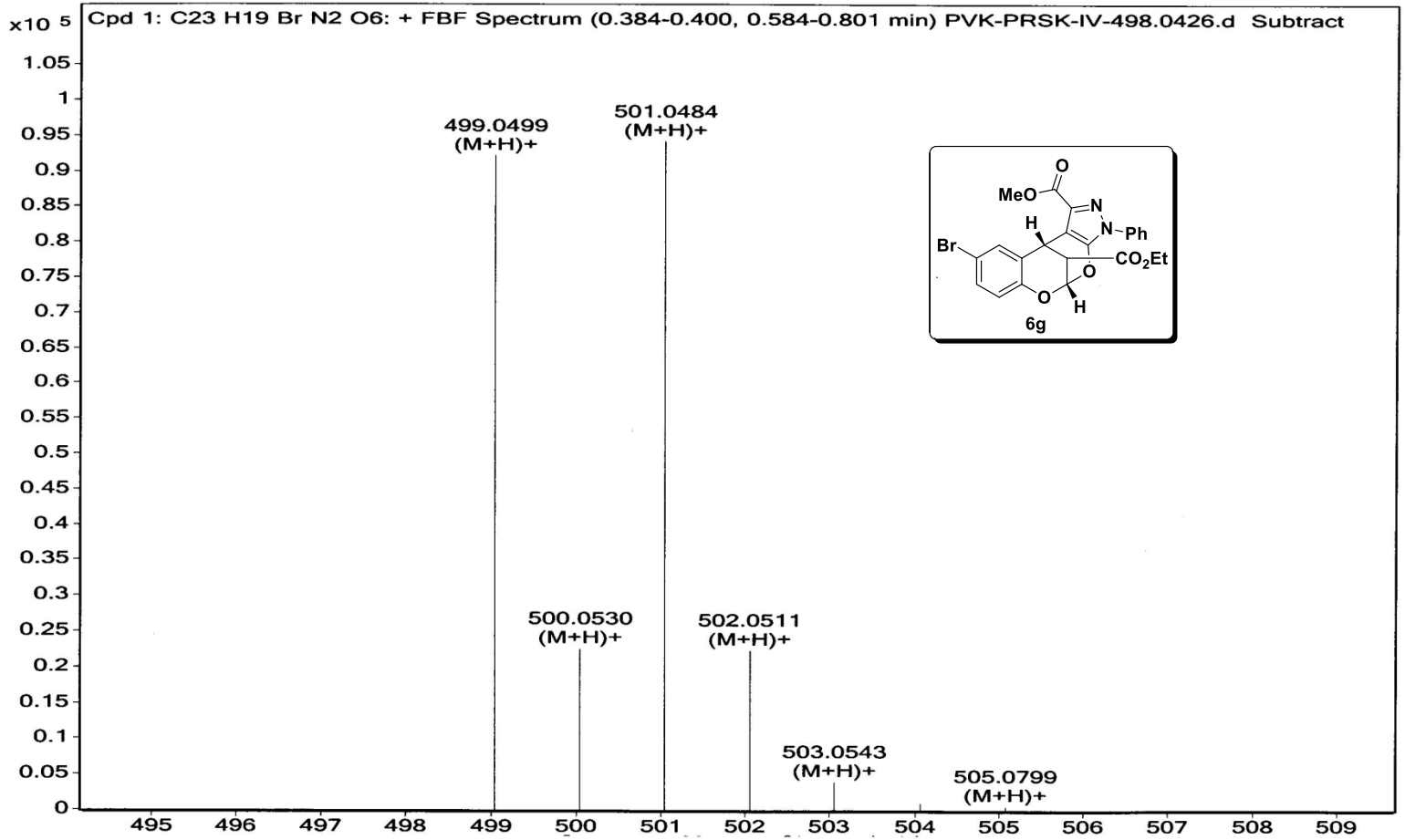

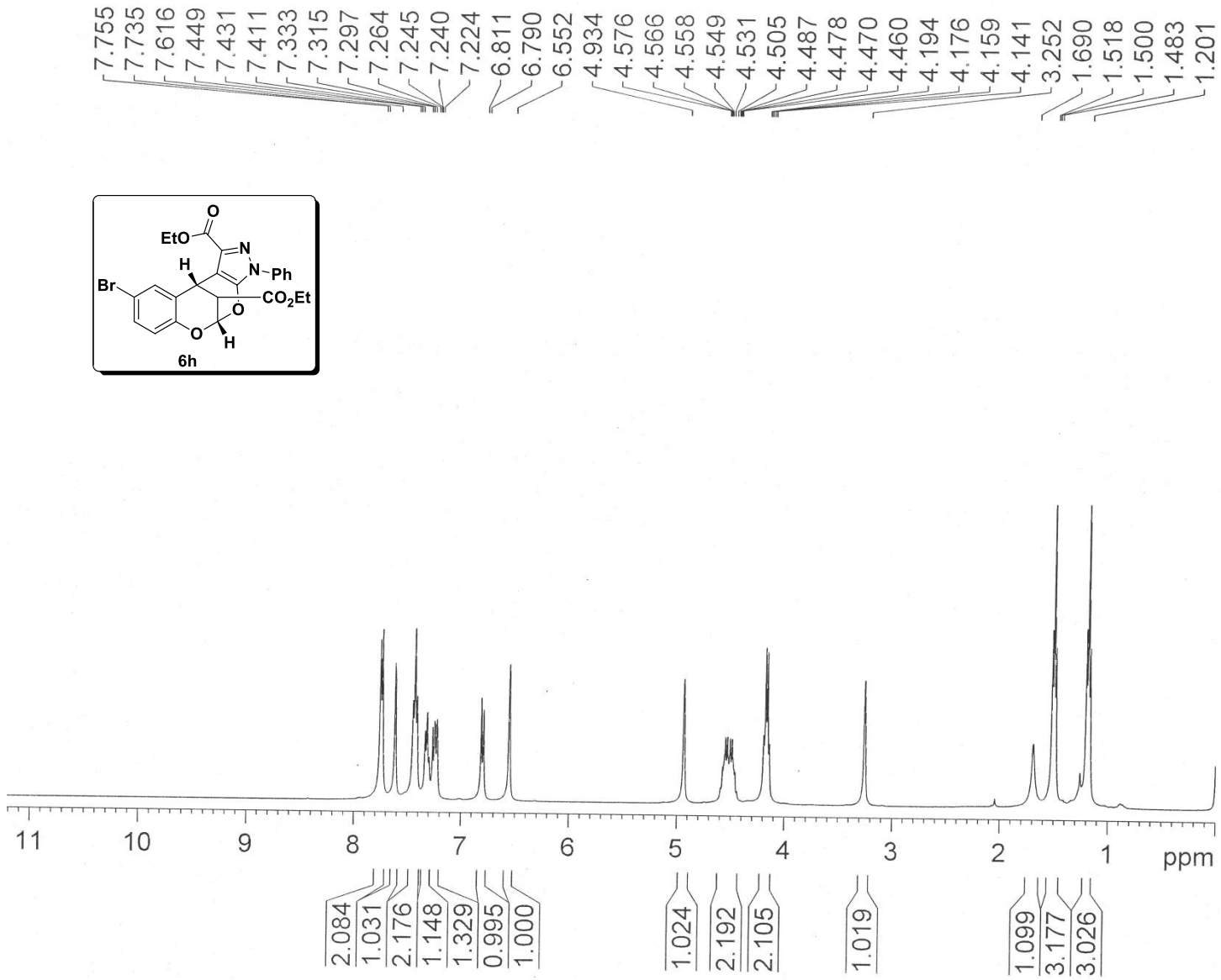
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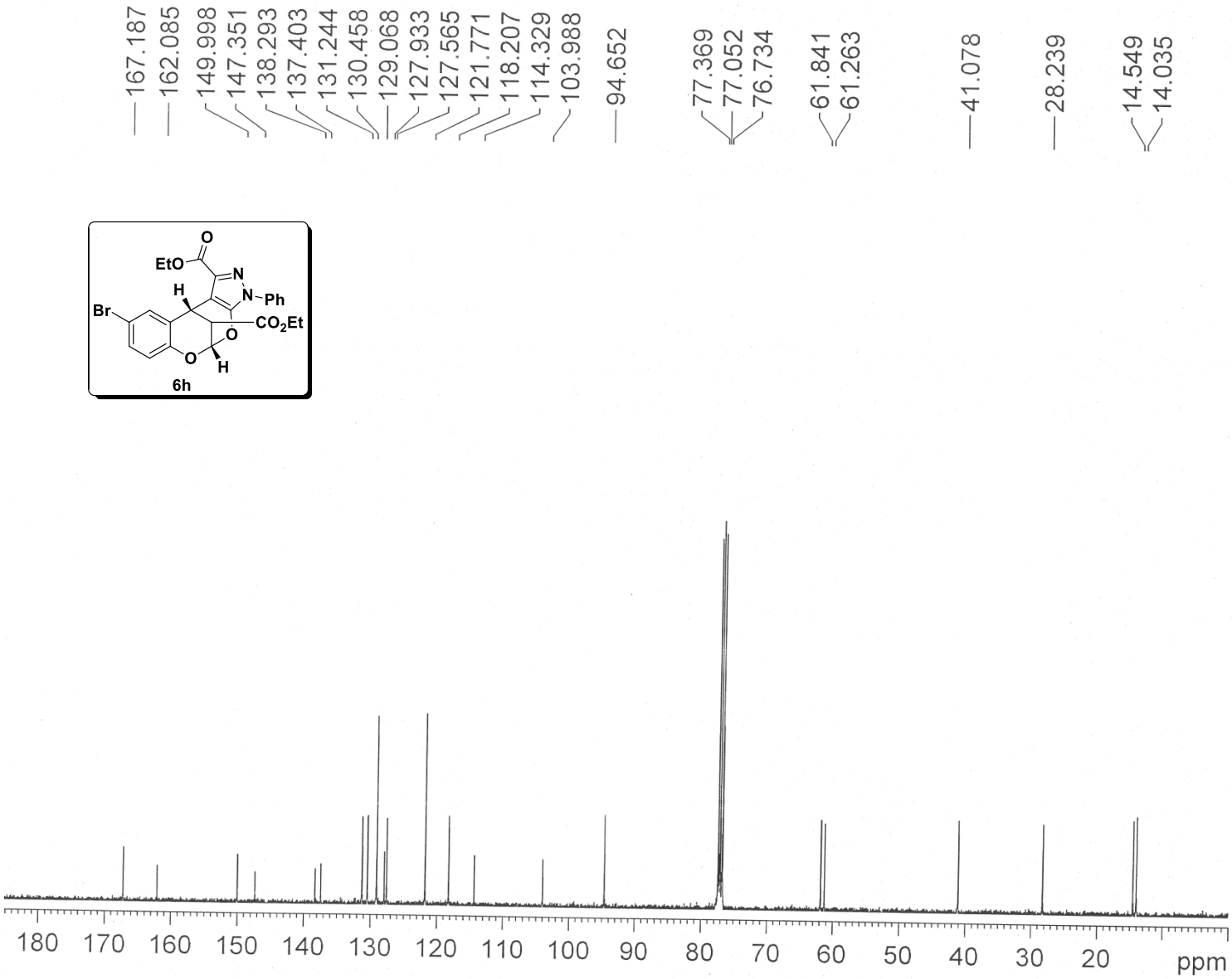
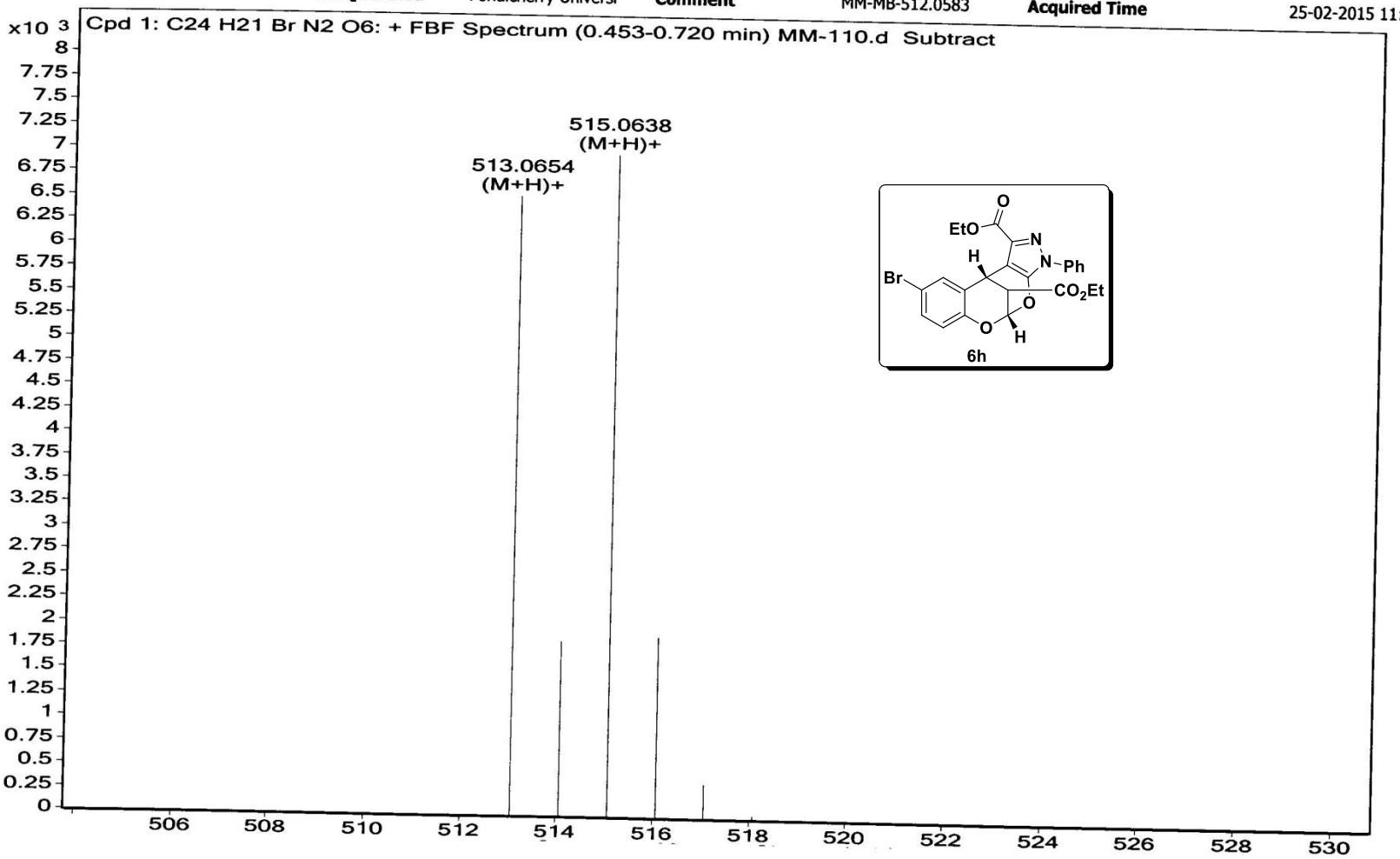
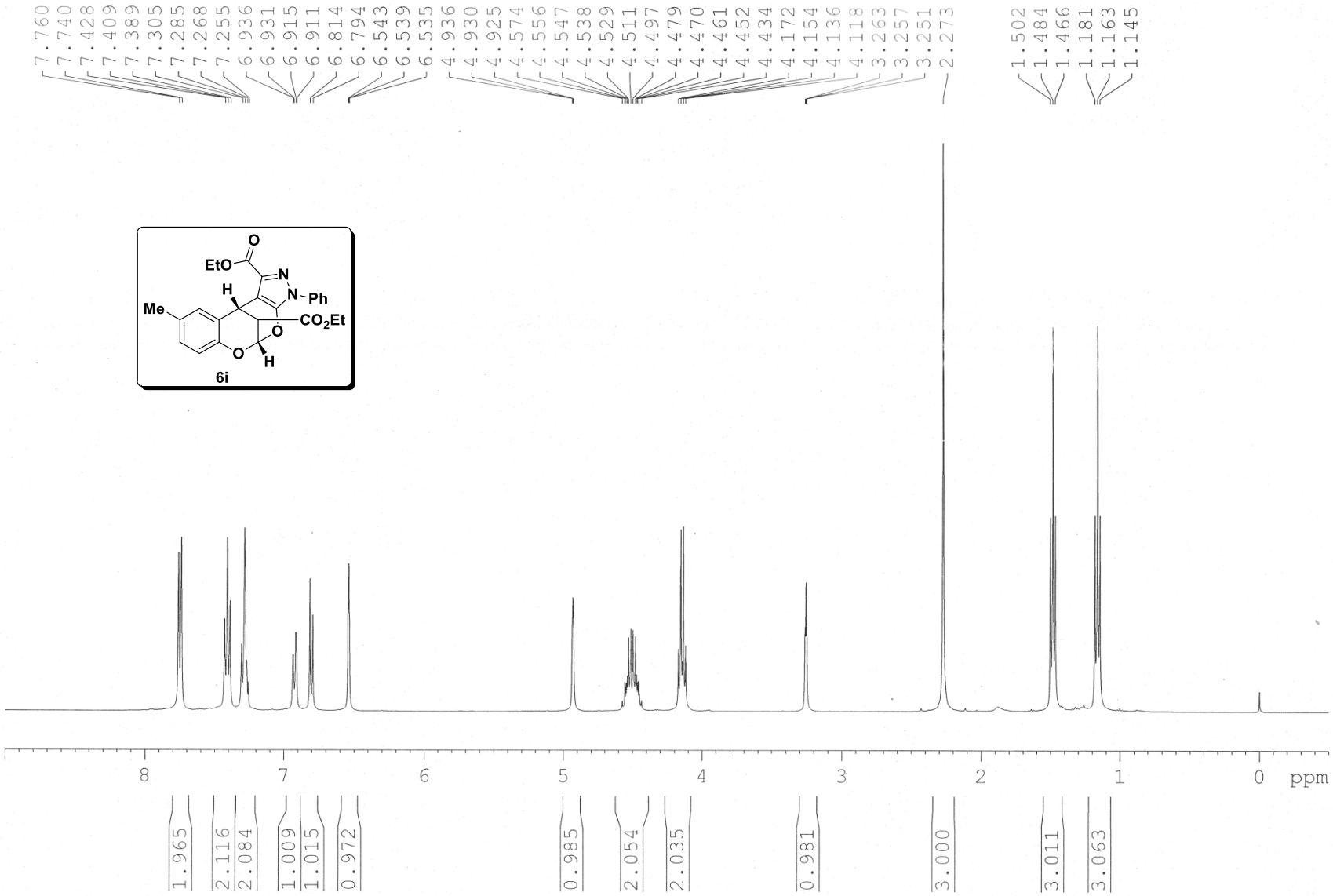
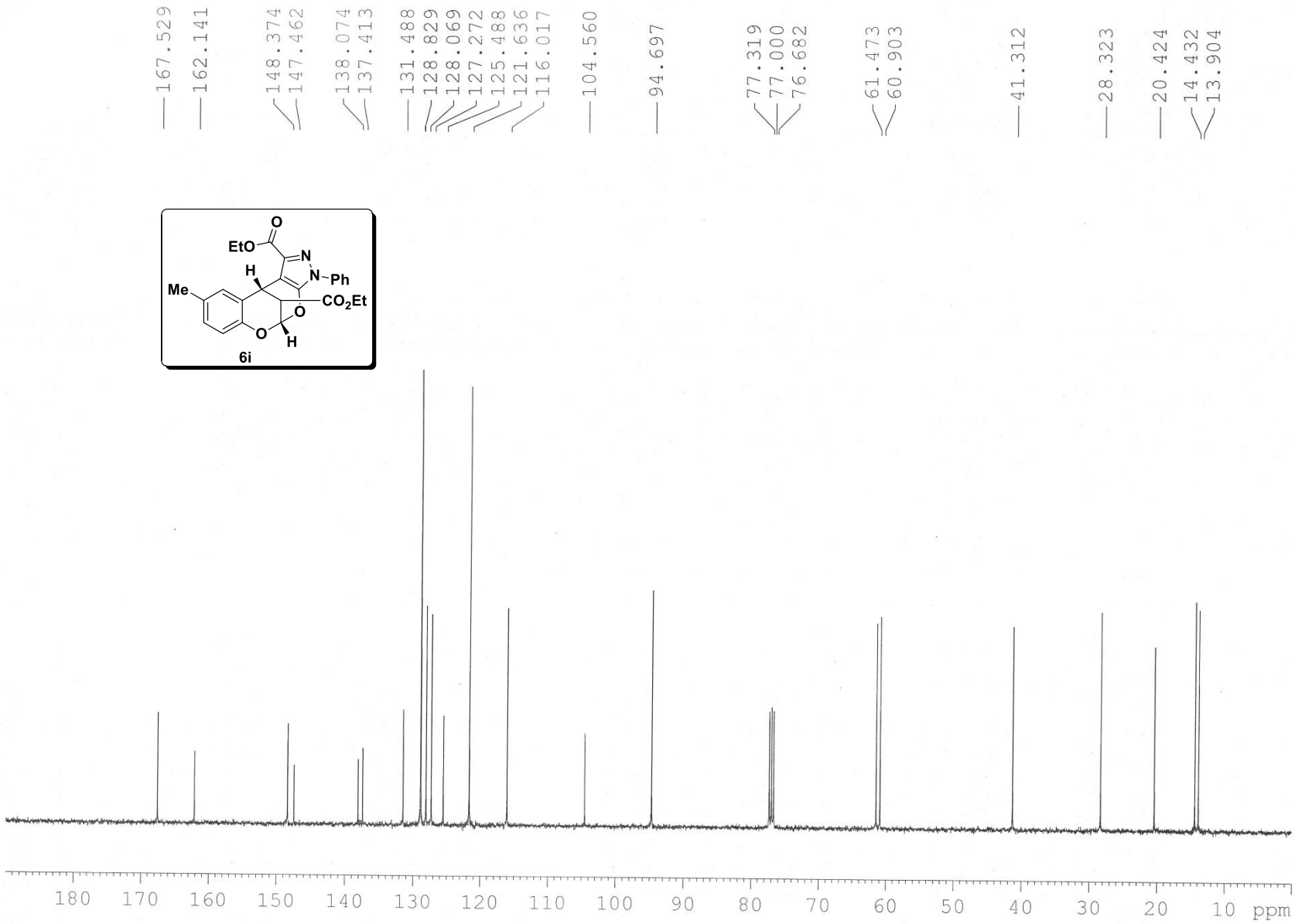
7.297
7.264
7.245
7.240
7.224
6.811
6.790
6.552
4.934
4.576
4.566
4.558
4.549
4.531
4.505
4.487
4.478
4.470
4.460
4.194
4.176
4.159
4.141
3.252
1.690
1.518
1.500
1.483
1.201
EtO
O
N
N
Ph
H
Br
CO2Et
O
O
H
6h
11
10
9
8
7
6
5
4
3
2
1
ppm
2.084
1.031
2.176
1.148
1.329
0.995
1.000
1.024
2.192
2.105
1.019
1.099
3.177
3.026


167.187
162.085
149.998
147.351
138.293
137.403
131.244
130.458
129.068
127.933
127.565
121.771
118.207
114.329
103.988
94.652
77.369
77.052
76.734
61.841
61.263
41.078
28.239
14.549
14.035
EtO
O
N
N
Ph
H
Br
CO2Et
O
O
H
6h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

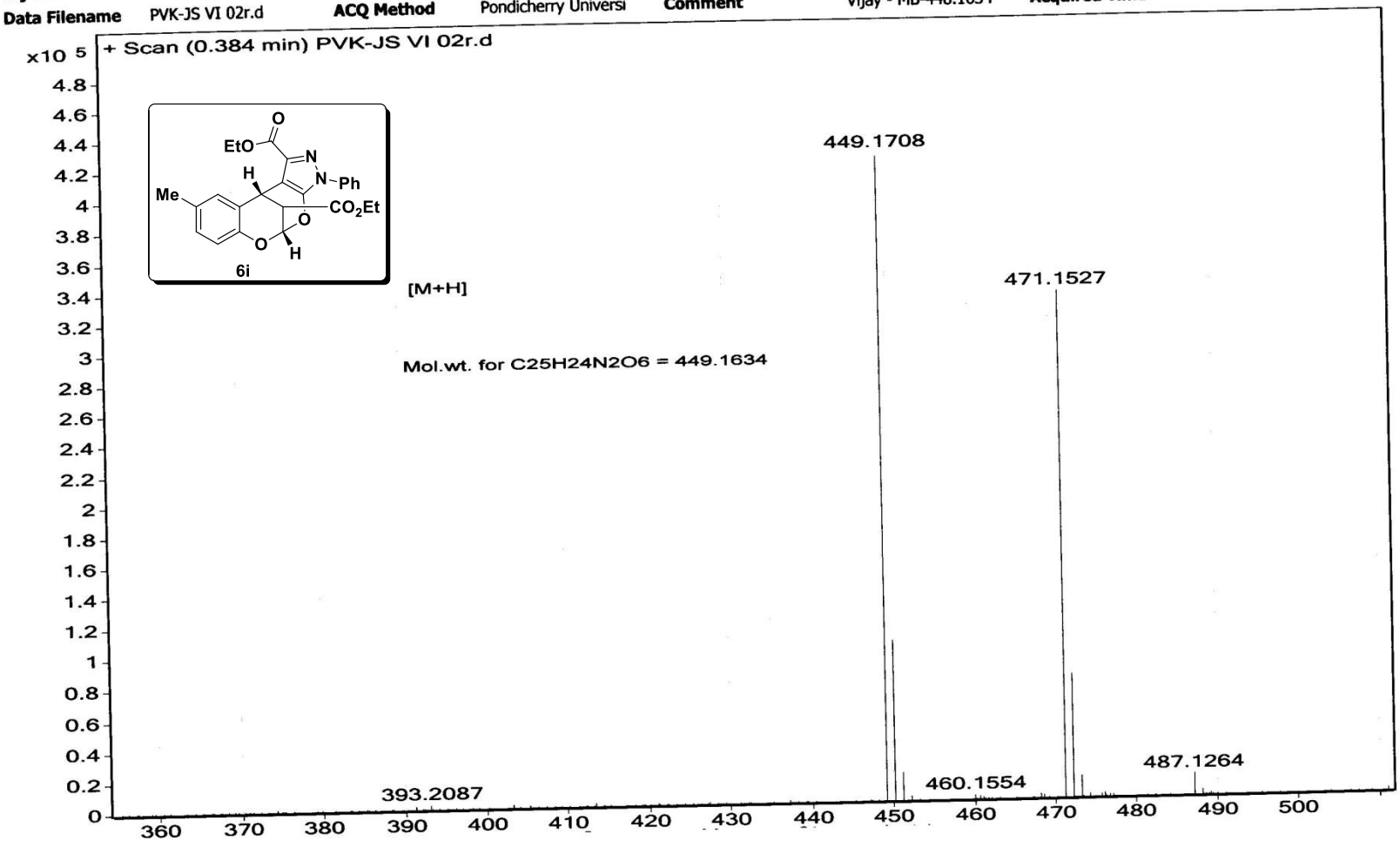
Sample Name	MM-110	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-110.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-512.0583	**Acquired Time**	25-02-2015 11:44:27

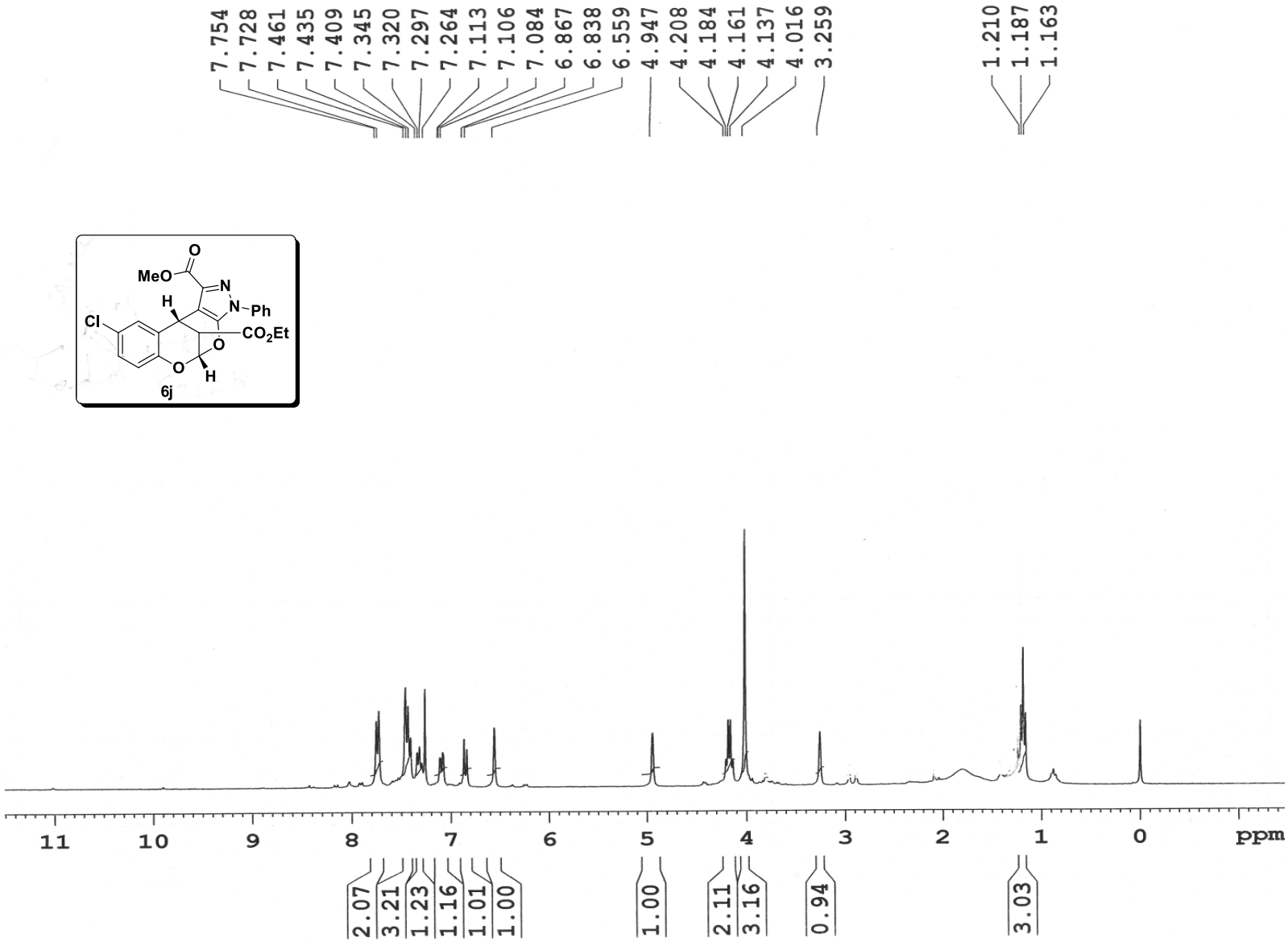


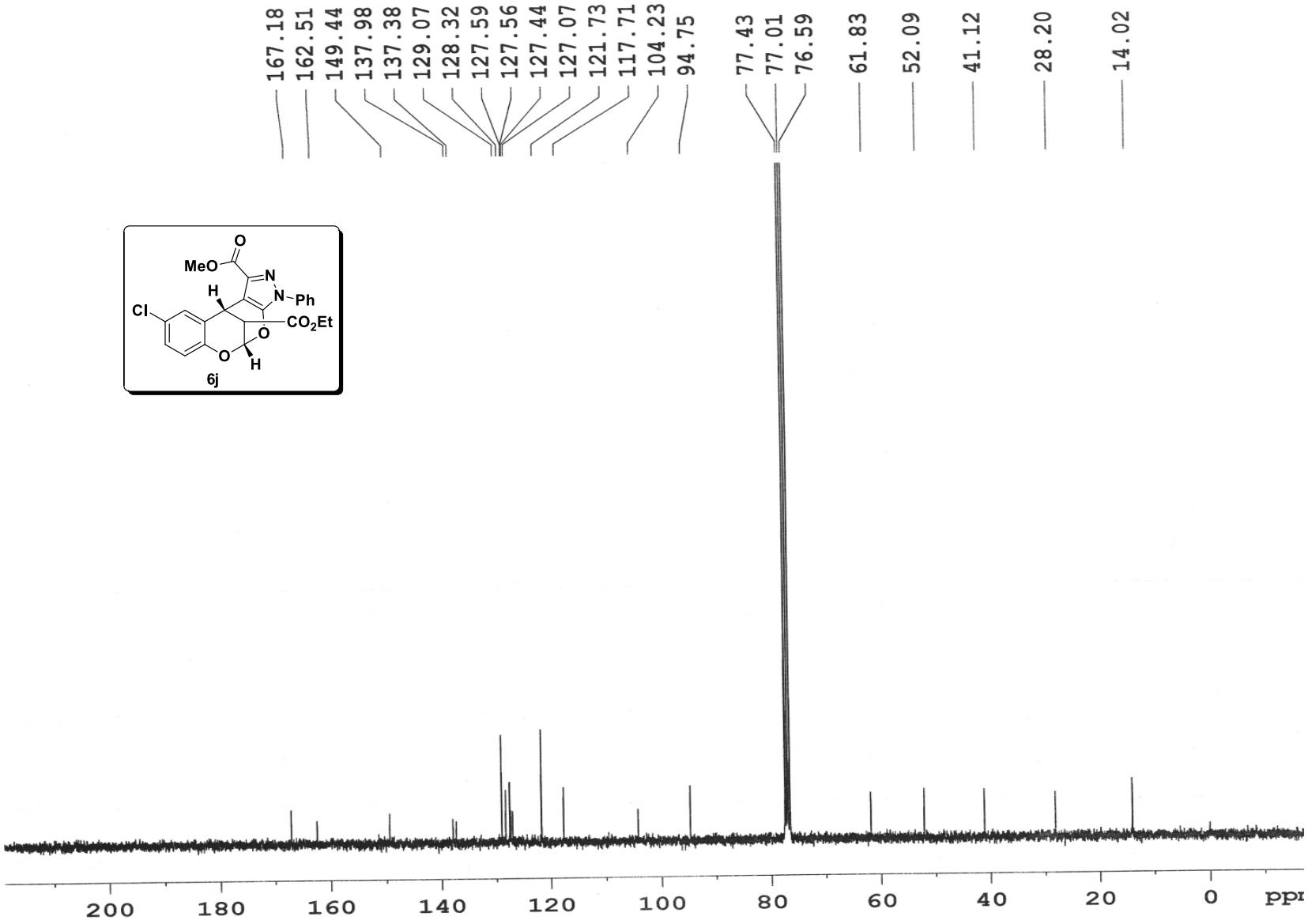

7.760
7.740
7.428
7.409
7.389
7.305
7.285
7.268
7.255
6.936
6.931
6.915
6.911
6.814
6.794
6.543
6.539
6.535
4.936
4.930
4.925
4.574
4.556
4.547
4.538
4.529
4.511
4.497
4.479
4.470
4.461
4.452
4.434
4.172
4.154
4.136
4.118
3.263
3.257
3.251
2.273
1.502
1.484
1.466
1.181
1.163
1.145
EtO
O
N
N
Ph
H
Me
CO2Et
O
O
H
6i
8
7
6
5
4
3
2
1
0
ppm
1.965
2.116
2.084
1.009
1.015
0.972
0.985
2.054
2.035
0.981
3.000
3.011
3.063


167.529
162.141
148.374
147.462
138.074
137.413
131.488
128.829
128.069
127.272
125.488
121.636
116.017
104.560
94.697
77.319
77.000
76.682
61.473
60.903
41.312
28.323
20.424
14.432
13.904
EtO
O
N
N-Ph
H
Me
CO2Et
O
O
H
6i
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

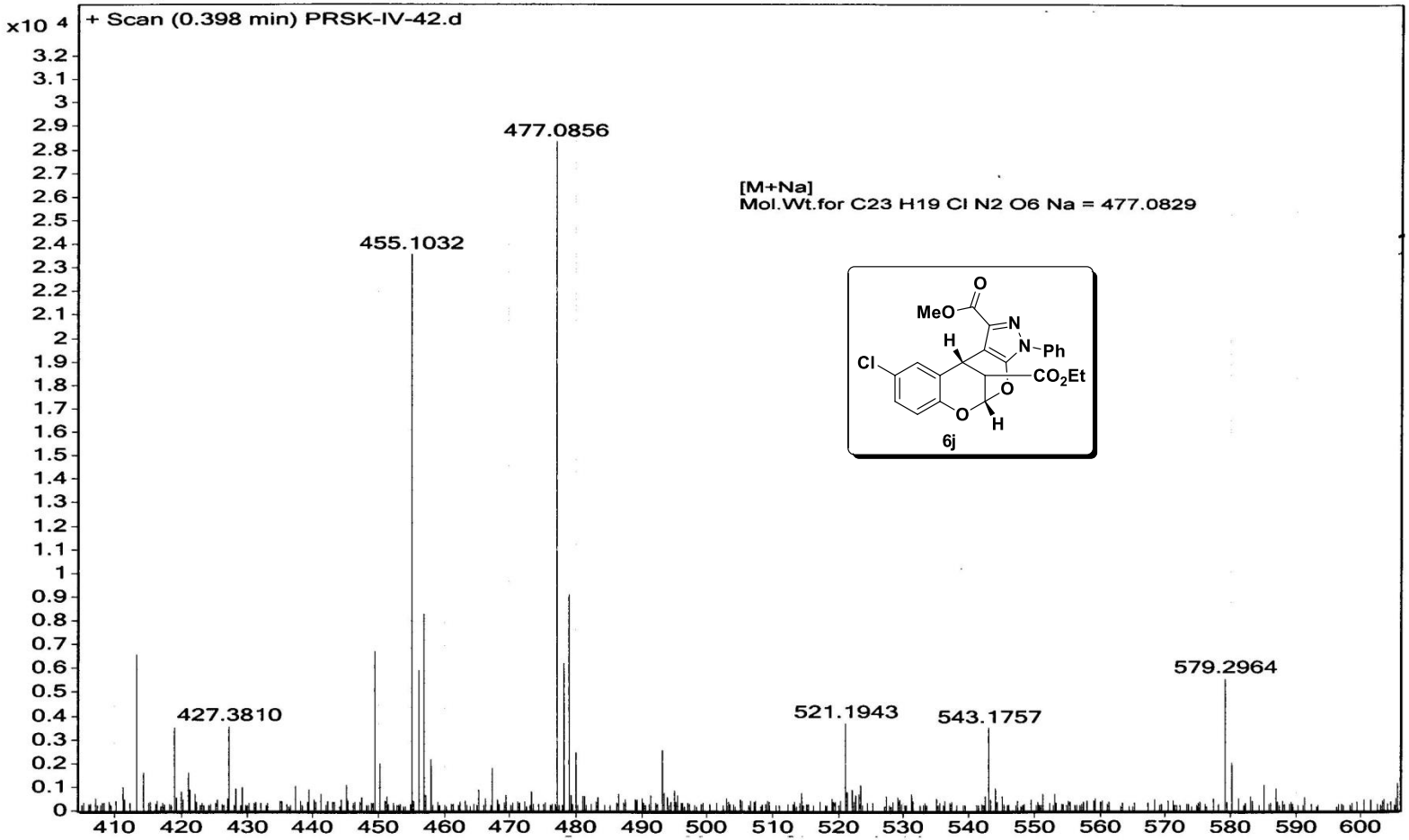
Sample Name	PVK-JS-V1-02	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-JS VI 02r.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay - MB-448.1634	**Acquired Time**	10-09-2014 16:08:26

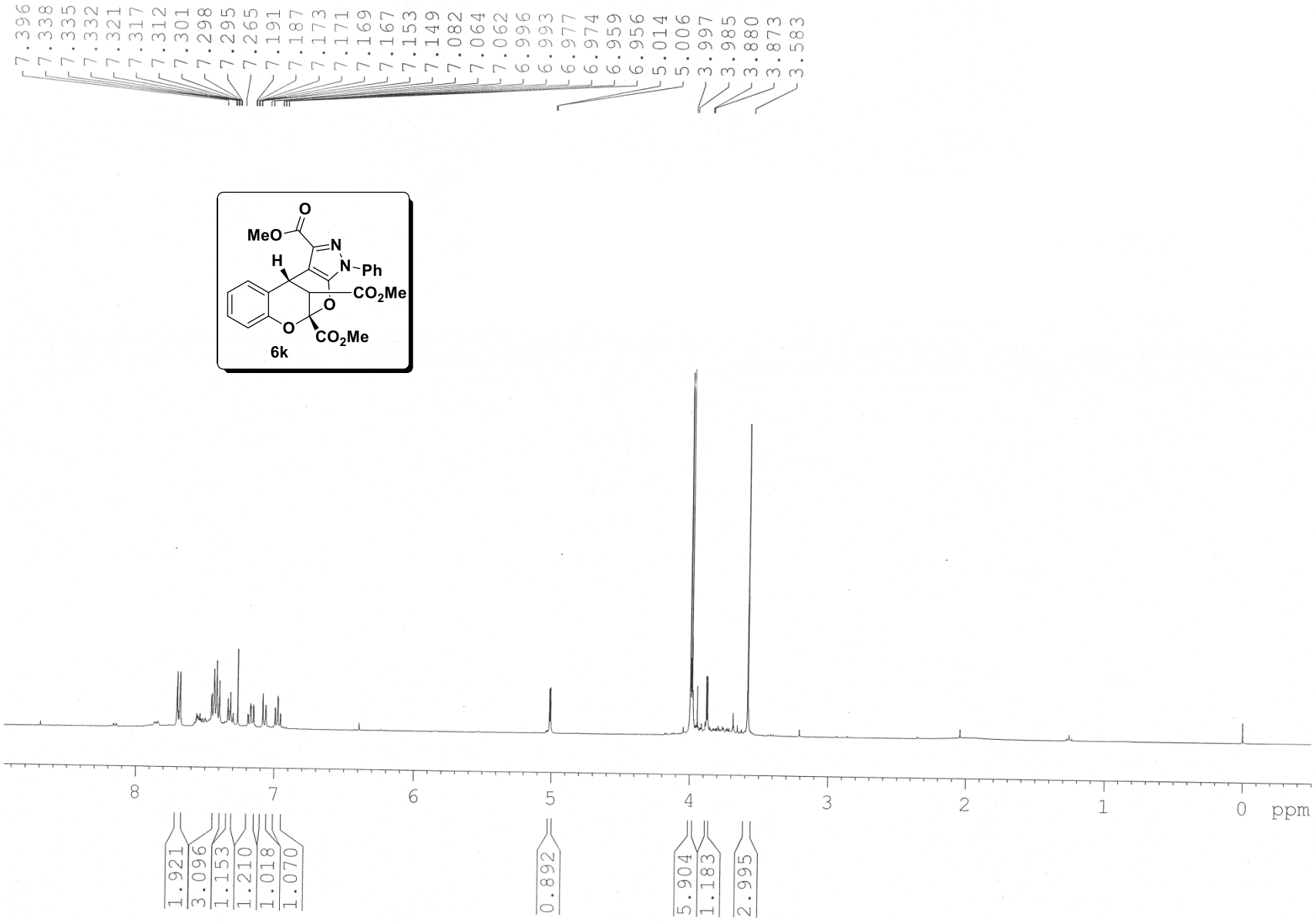


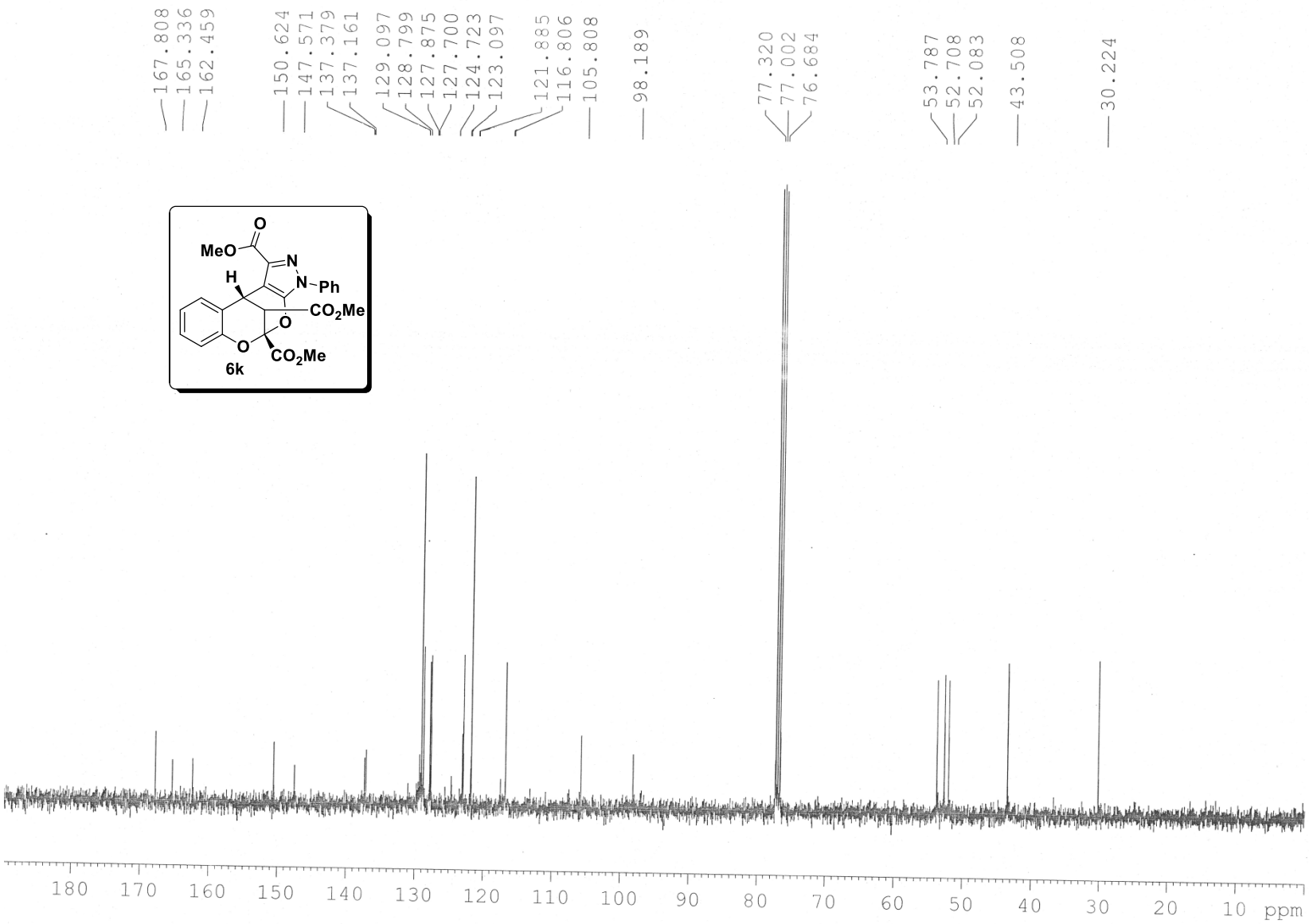

7.754
7.728
7.461
7.435
7.409
7.345
7.320
7.297
7.264
7.113
7.106
7.084
6.867
6.838
6.559
4.947
4.208
4.184
4.161
4.137
4.016
3.259
1.210
1.187
1.163
MeO
O
N
N
Ph
H
Cl
CO2Et
O
O
H
6j
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
3.21
1.23
1.16
1.01
1.00
1.00
2.11
3.16
0.94
3.03


167.18
162.51
149.44
137.98
137.38
129.07
128.32
127.59
127.56
127.44
127.07
121.73
117.71
104.23
94.75
77.43
77.01
76.59
61.83
52.09
41.12
28.20
14.02
MeO
O
N
N
Ph
H
Cl
CO2Et
O
O
H
6j
200
180
160
140
120
100
80
60
40
20
0
ppm

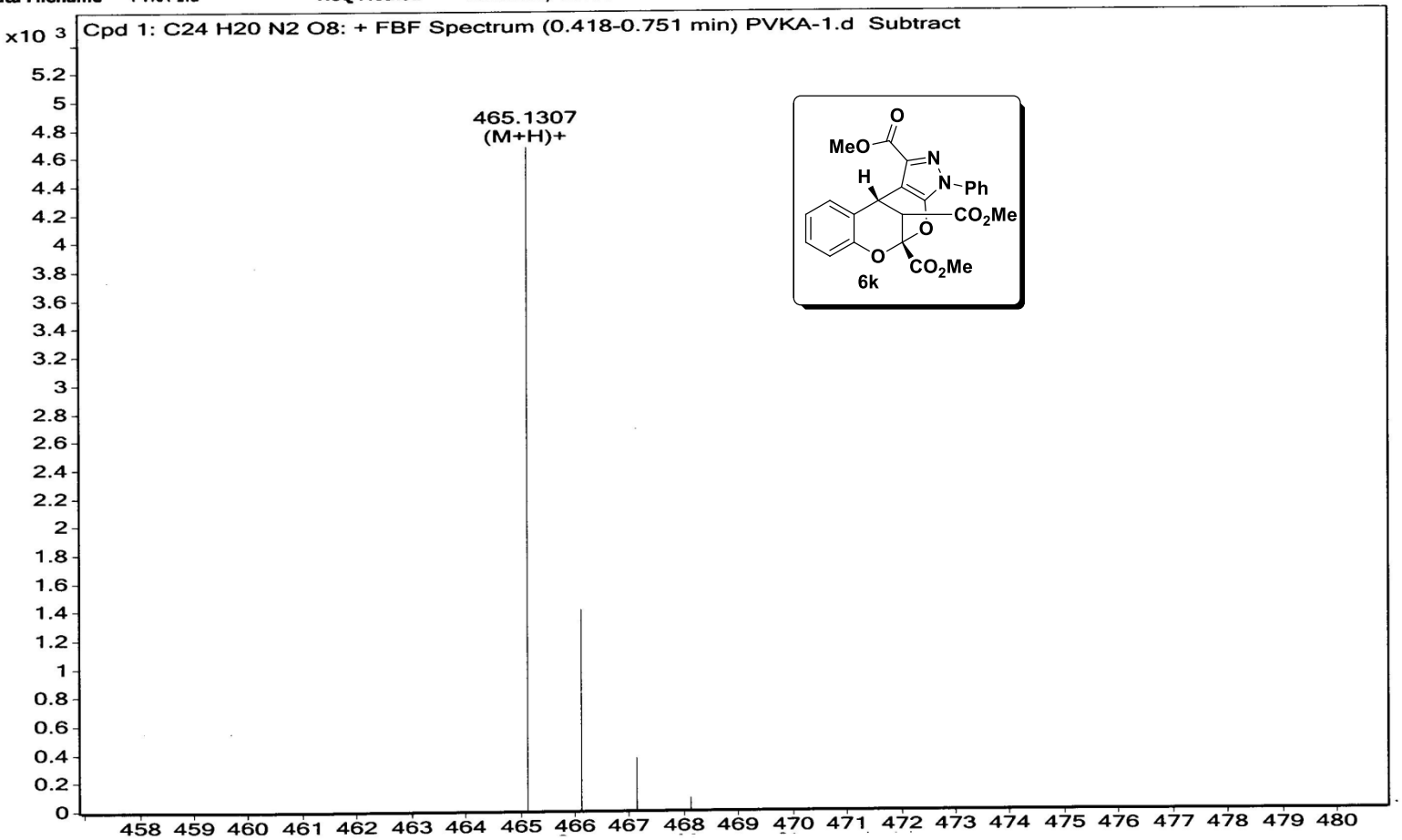
Sample Name	PRSK-IV-42	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-IV-42.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay-MB-454.0932	**Acquired Time**	16-09-2014 11:18:07

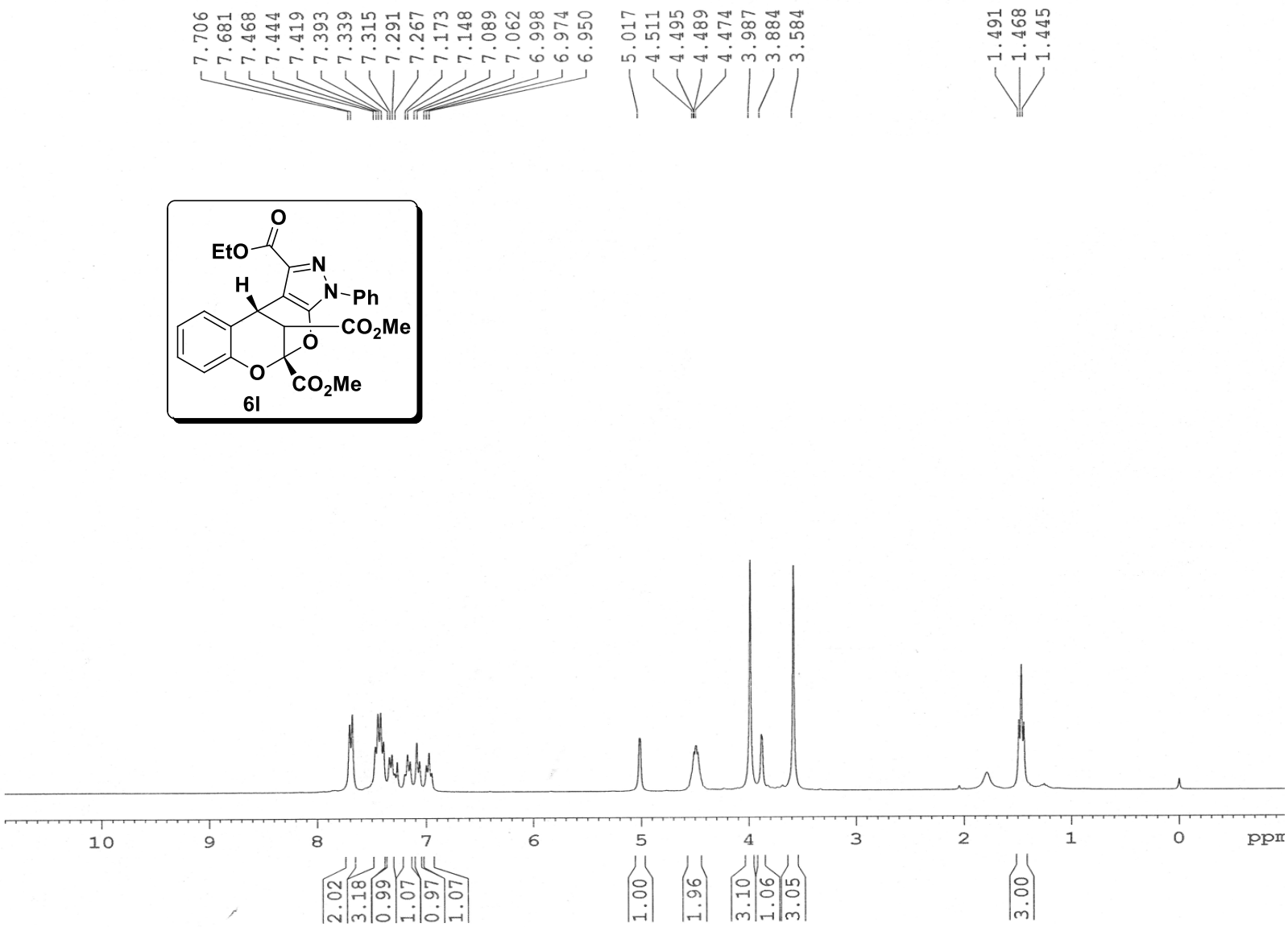


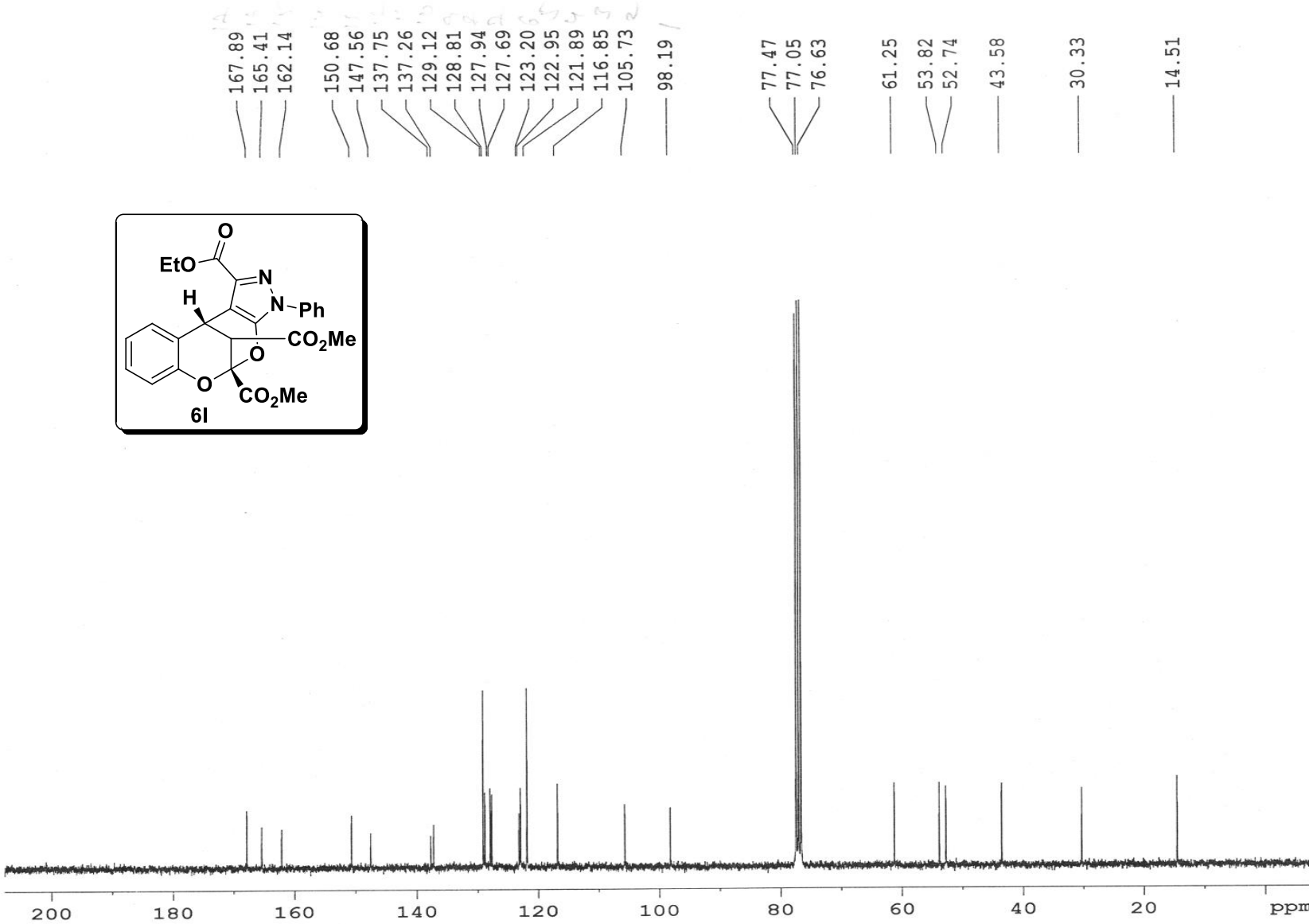

7.396
7.338
7.335
7.332
7.321
7.317
7.312
7.301
7.298
7.295
7.265
7.191
7.187
7.173
7.171
7.169
7.167
7.153
7.149
7.082
7.064
7.062
6.996
6.993
6.977
6.974
6.959
6.956
5.014
5.006
3.997
3.985
3.880
3.873
3.583
MeO
O
N
N
Ph
H
CO2Me
O
O
CO2Me
6k
8
7
6
5
4
3
2
1
0
ppm
1.921
3.096
1.153
1.210
1.018
1.070
0.892
5.904
1.183
2.995


167.808
165.336
162.459
150.624
147.571
137.379
137.161
129.097
128.799
127.875
127.700
124.723
123.097
121.885
116.806
105.808
98.189
77.320
77.002
76.684
53.787
52.708
52.083
43.508
30.224
MeO
O
N
N-Ph
H
CO2Me
O
O
CO2Me
6k
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

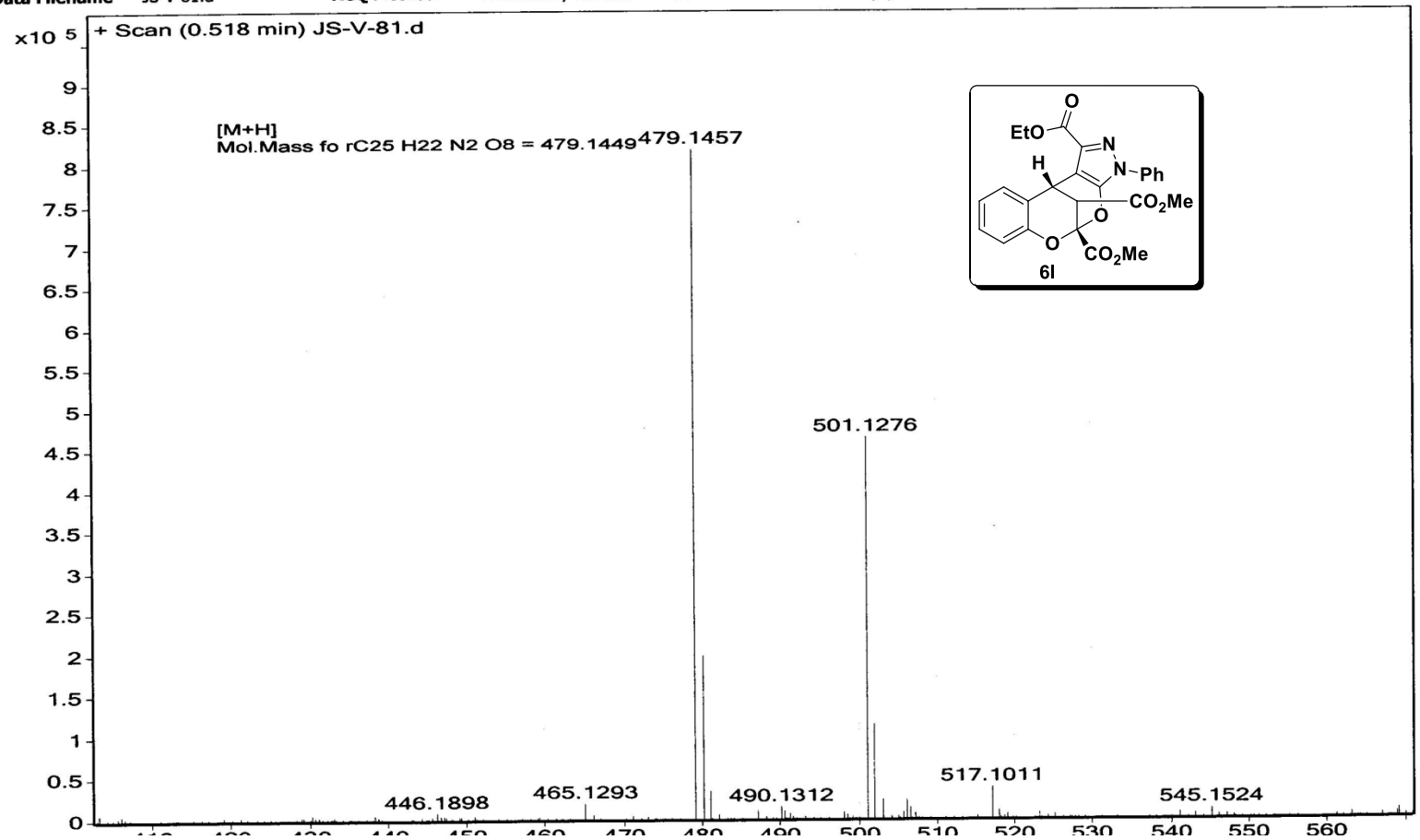
Sample Name	PVKA-1	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVKA-1.d	**ACQ Method**	Pondicherry Universi	**Comment**	MS-MB-464.1220	**Acquired Time**	16-03-2015 14:51:40

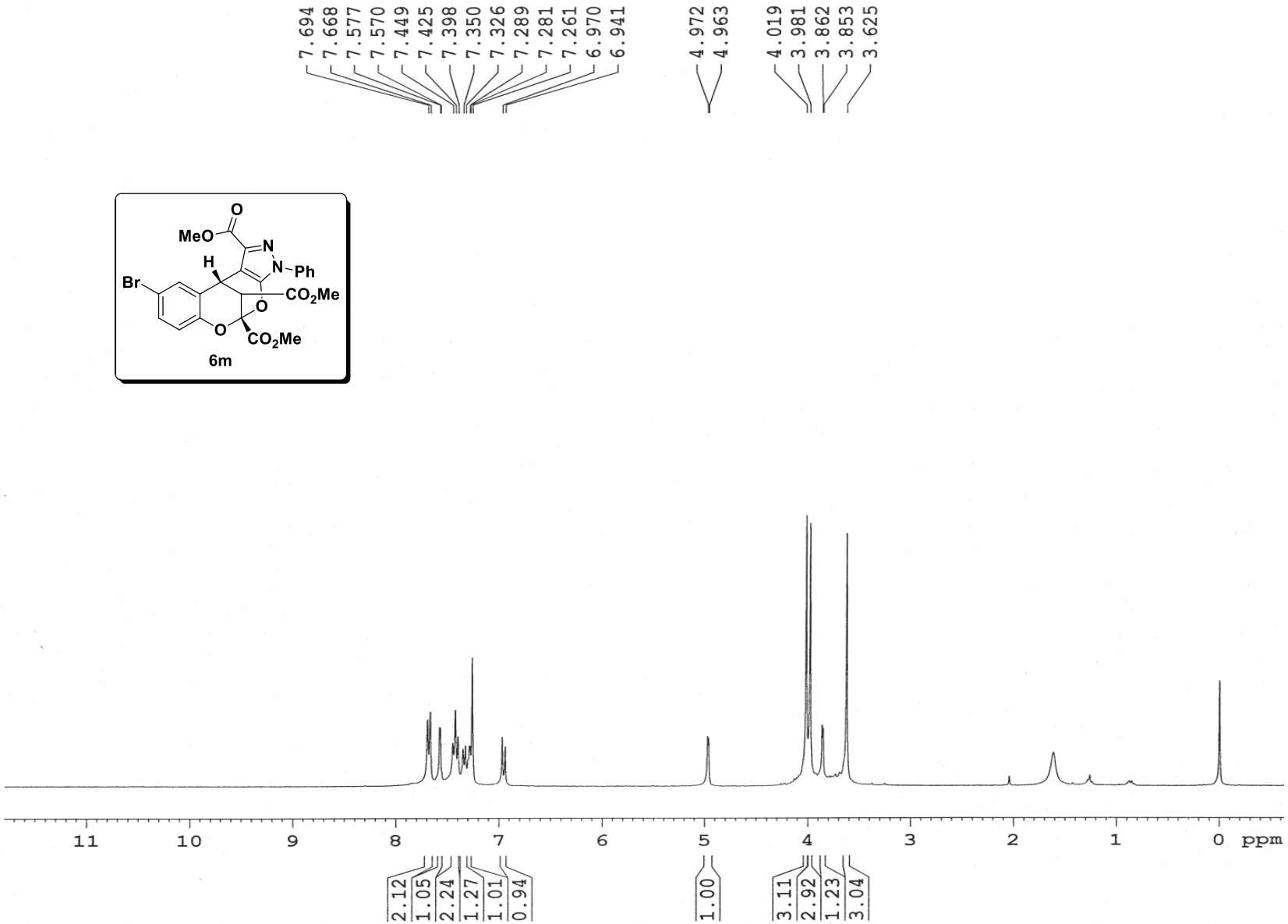


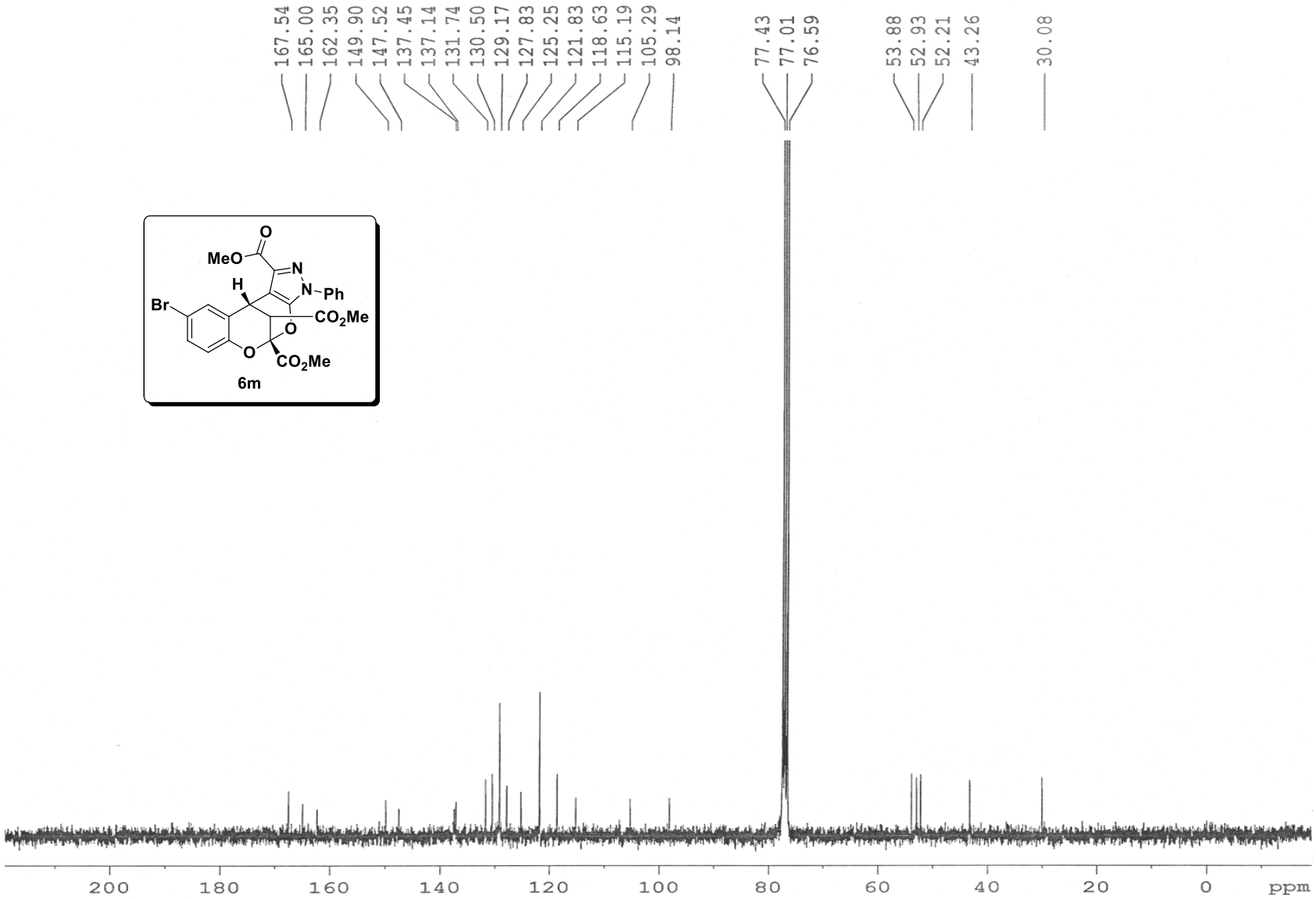

7.706
7.681
7.468
7.444
7.419
7.393
7.339
7.315
7.291
7.267
7.173
7.148
7.089
7.062
6.998
6.974
6.950
5.017
4.511
4.495
4.489
4.474
3.987
3.884
3.584
1.491
1.468
1.445
EtO
O
N
N
Ph
H
CO2Me
O
O
CO2Me
6l
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
3.18
0.99
1.07
0.97
1.07
1.00
1.96
3.10
1.06
3.05
3.00


167.89
165.41
162.14
150.68
147.56
137.75
137.26
129.12
128.81
127.94
127.69
123.20
122.95
121.89
116.85
105.73
98.19
77.47
77.05
76.63
61.25
53.82
52.74
43.58
30.33
14.51
EtO
O
N
N
Ph
H
CO2Me
O
O
CO2Me
6l
200
180
160
140
120
100
80
60
40
20
ppm

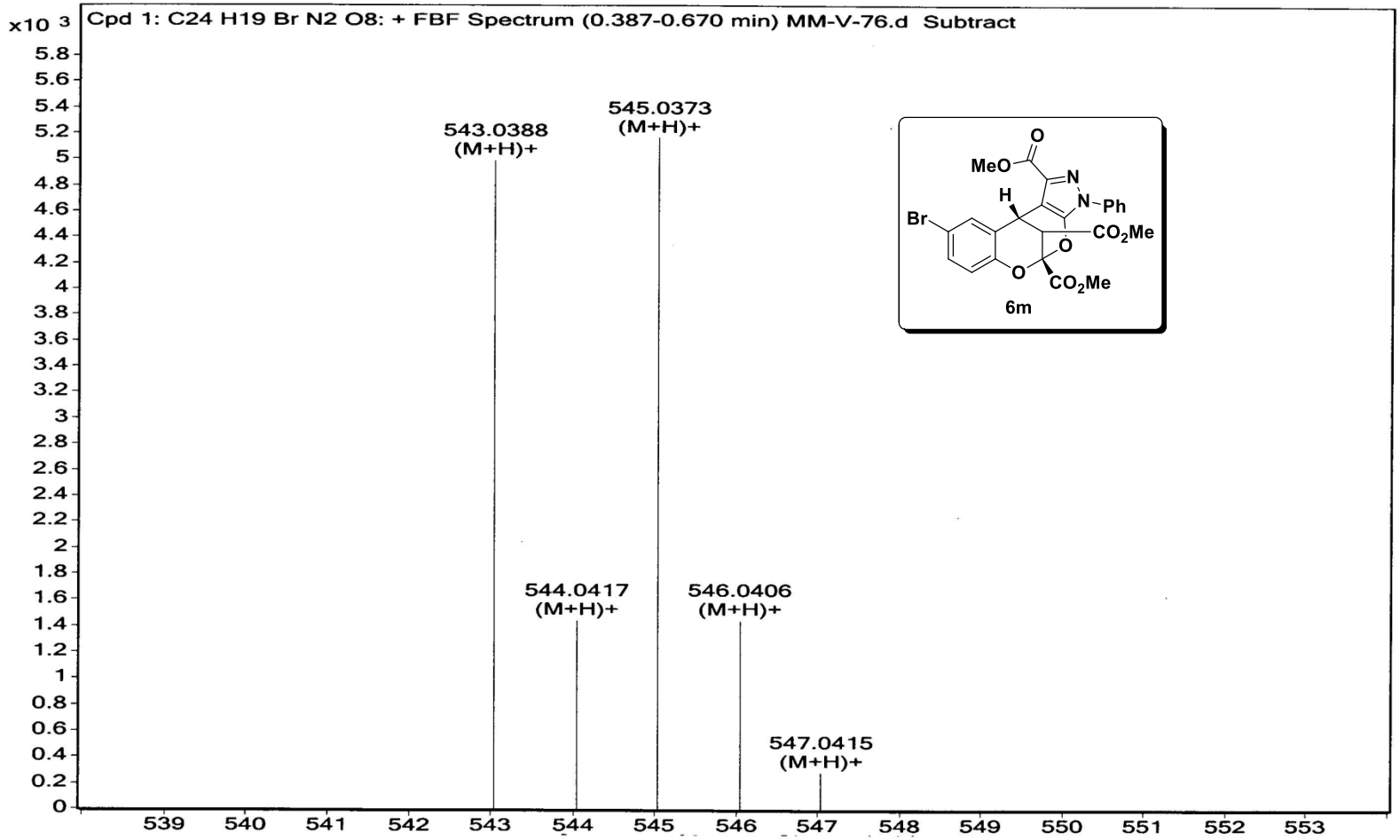
Sample Name	JS-V-81	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	JS-V-81.d	**ACQ Method**	Pondicherry Universi	**Comment**	vijay-MB-478.1376	**Acquired Time**	24-09-2014 16:08:39

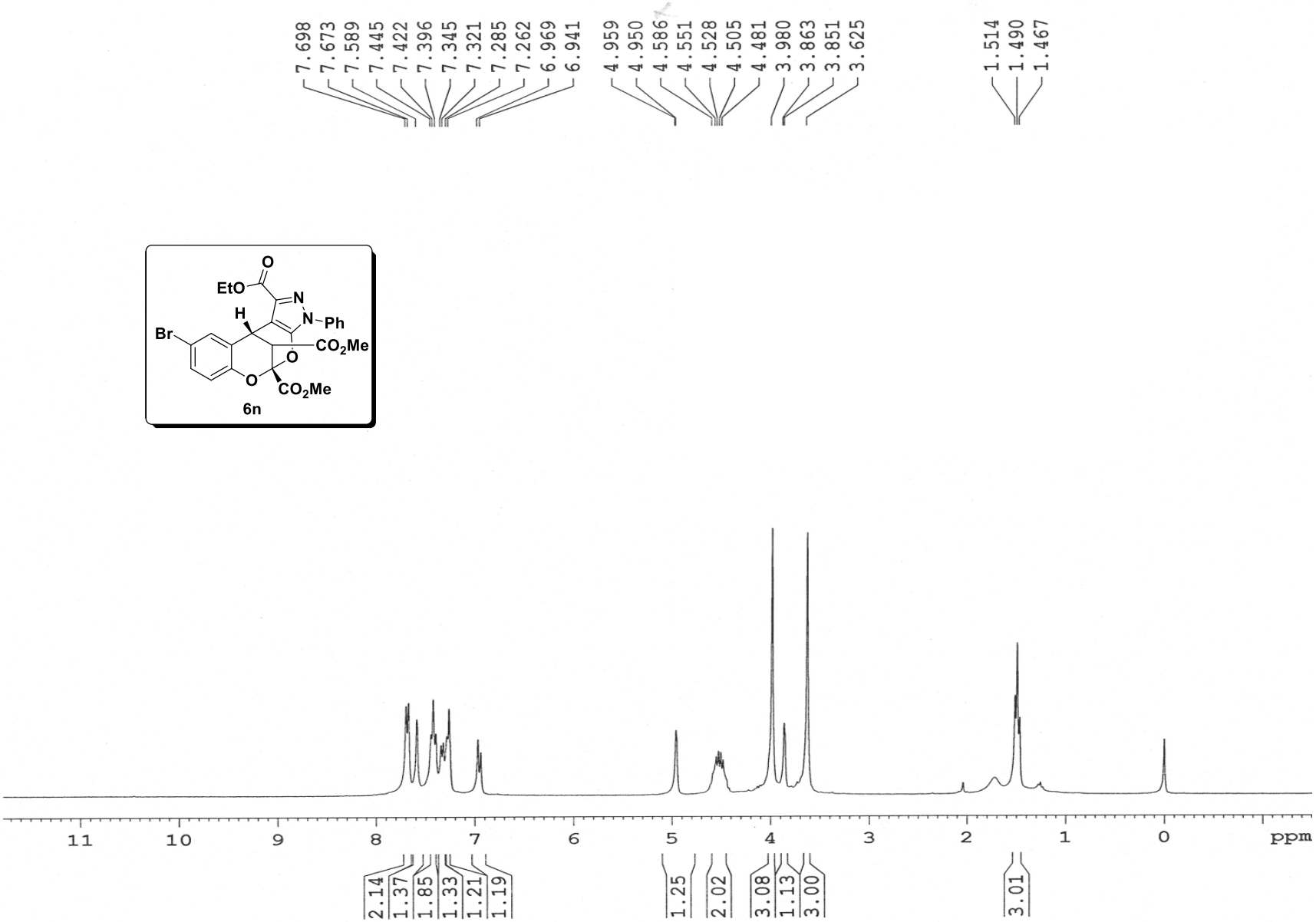


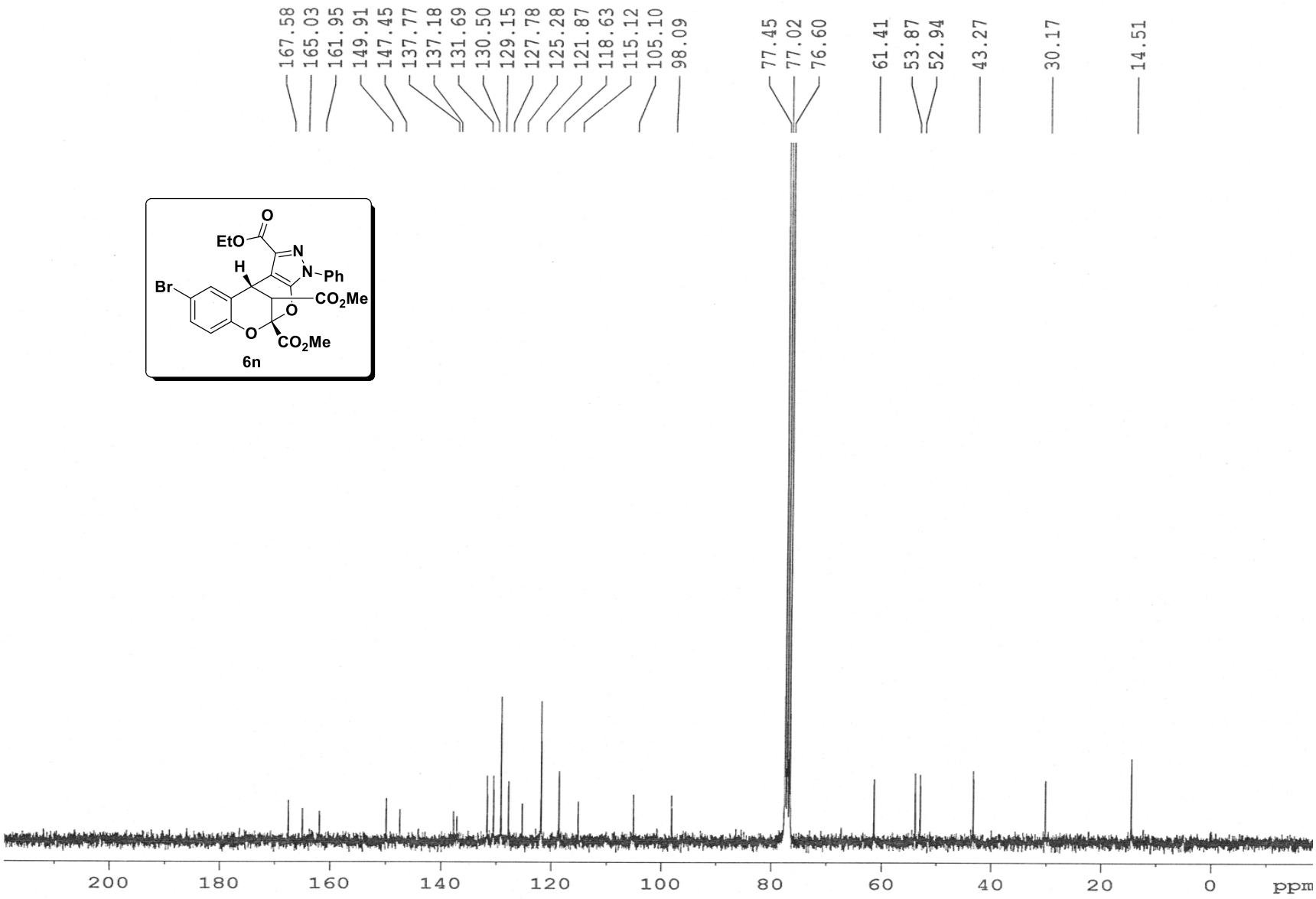

7.694
7.668
7.577
7.570
7.449
7.425
7.398
7.350
7.326
7.289
7.281
7.261
6.970
6.941
4.972
4.963
4.019
3.981
3.862
3.853
3.625
MeO
O
N
N
Ph
H
Br
CO2Me
O
O
CO2Me
6m
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
1.05
2.24
1.27
1.01
0.94
1.00
3.11
2.92
1.23
3.04


167.54
165.00
162.35
149.90
147.52
137.45
137.14
131.74
130.50
129.17
127.83
125.25
121.83
118.63
115.19
105.29
98.14
77.43
77.01
76.59
53.88
52.93
52.21
43.26
30.08
MeO
O
N
N-Ph
H
Br
CO2Me
O
O
CO2Me
6m
200
180
160
140
120
100
80
60
40
20
0
ppm

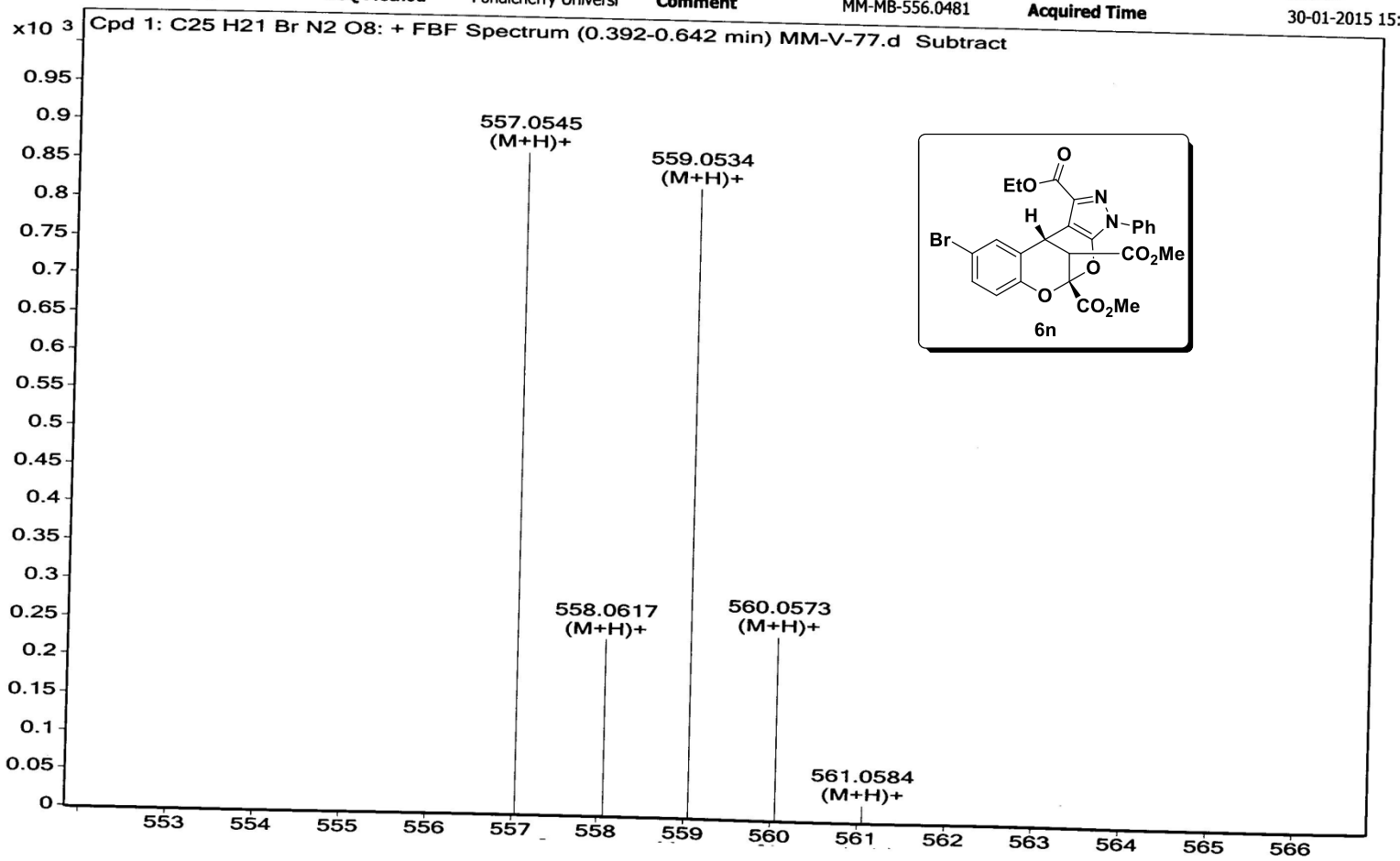
Sample Name	MM-V-76	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-V-76.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-542.0325	**Acquired Time**	30-01-2015 14:52:34

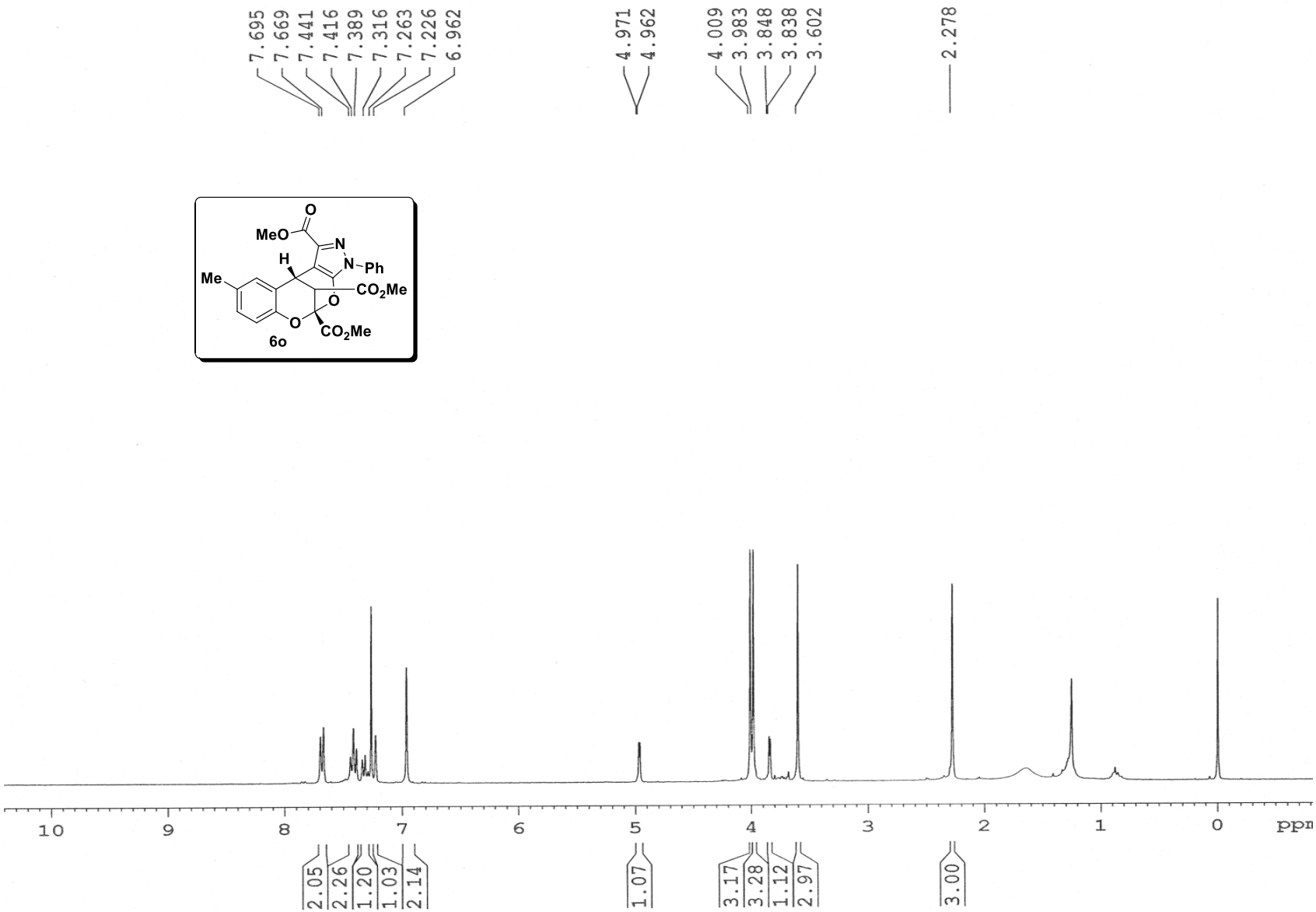


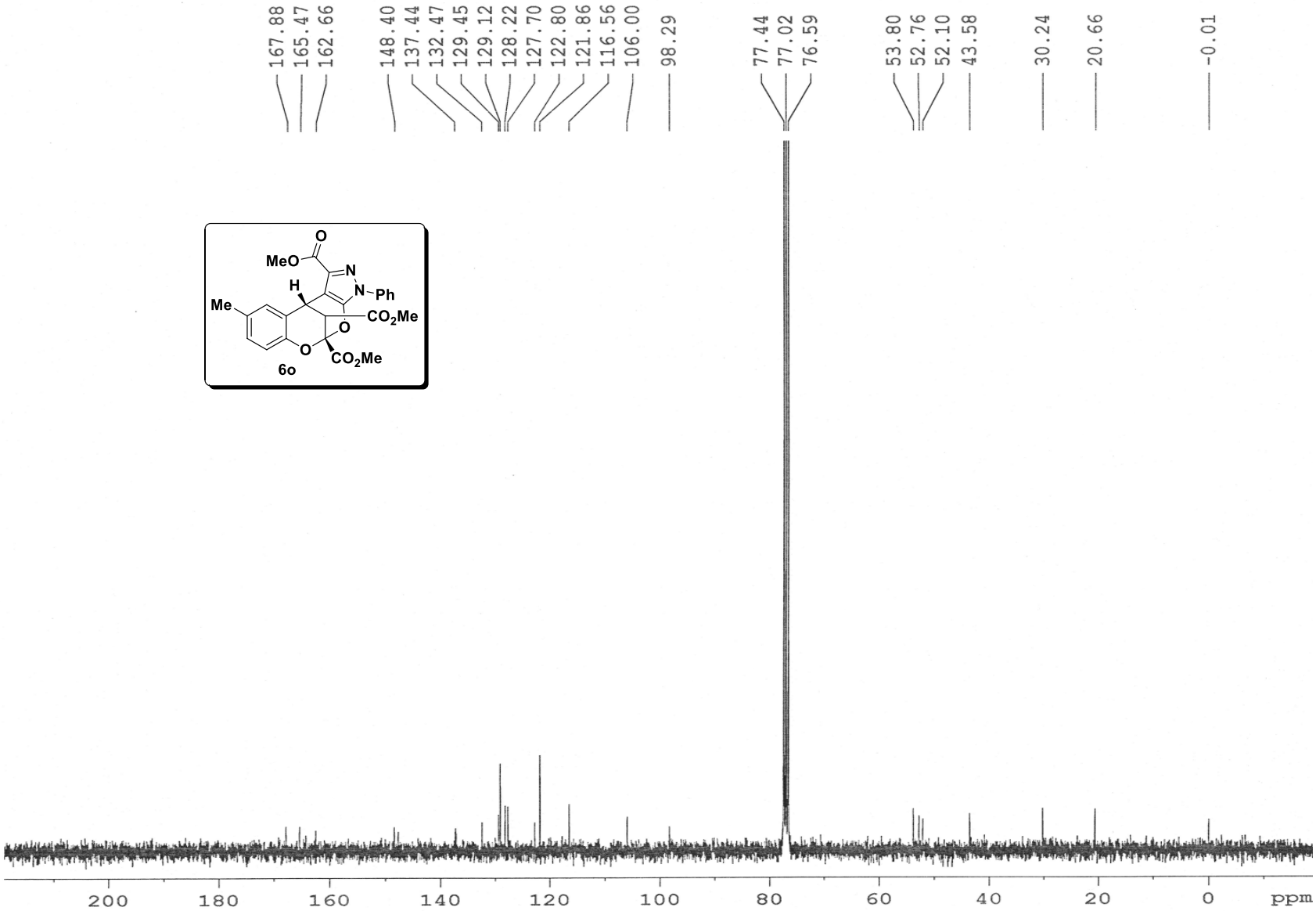

7.698
7.673
7.589
7.445
7.422
7.396
7.345
7.321
7.285
7.262
6.969
6.941
4.959
4.950
4.586
4.551
4.528
4.505
4.481
3.980
3.863
3.851
3.625
1.514
1.490
1.467
EtO
O
N
N
Ph
H
Br
CO2Me
O
O
CO2Me
6n
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.14
1.37
1.85
1.33
1.21
1.19
1.25
2.02
3.08
1.13
3.00
3.01


167.58
165.03
161.95
149.91
147.45
137.77
137.18
131.69
130.50
129.15
127.78
125.28
121.87
118.63
115.12
105.10
98.09
77.45
77.02
76.60
61.41
53.87
52.94
43.27
30.17
14.51
EtO
O
N
N
Ph
H
Br
CO2Me
O
O
CO2Me
6n
200
180
160
140
120
100
80
60
40
20
0
ppm

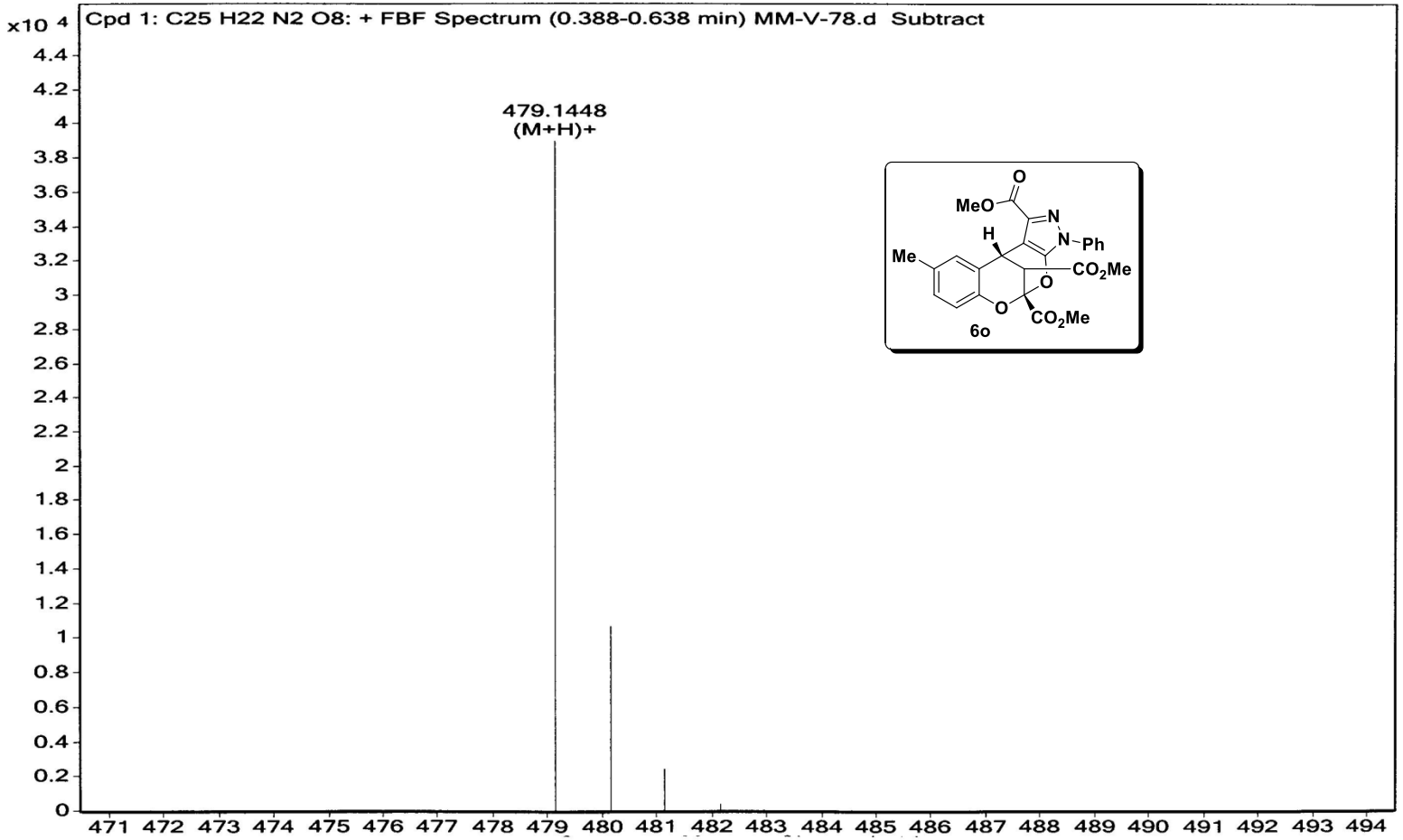
Sample Name	MM-V-77	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-V-77.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-556.0481	**Acquired Time**	30-01-2015 15:10:37

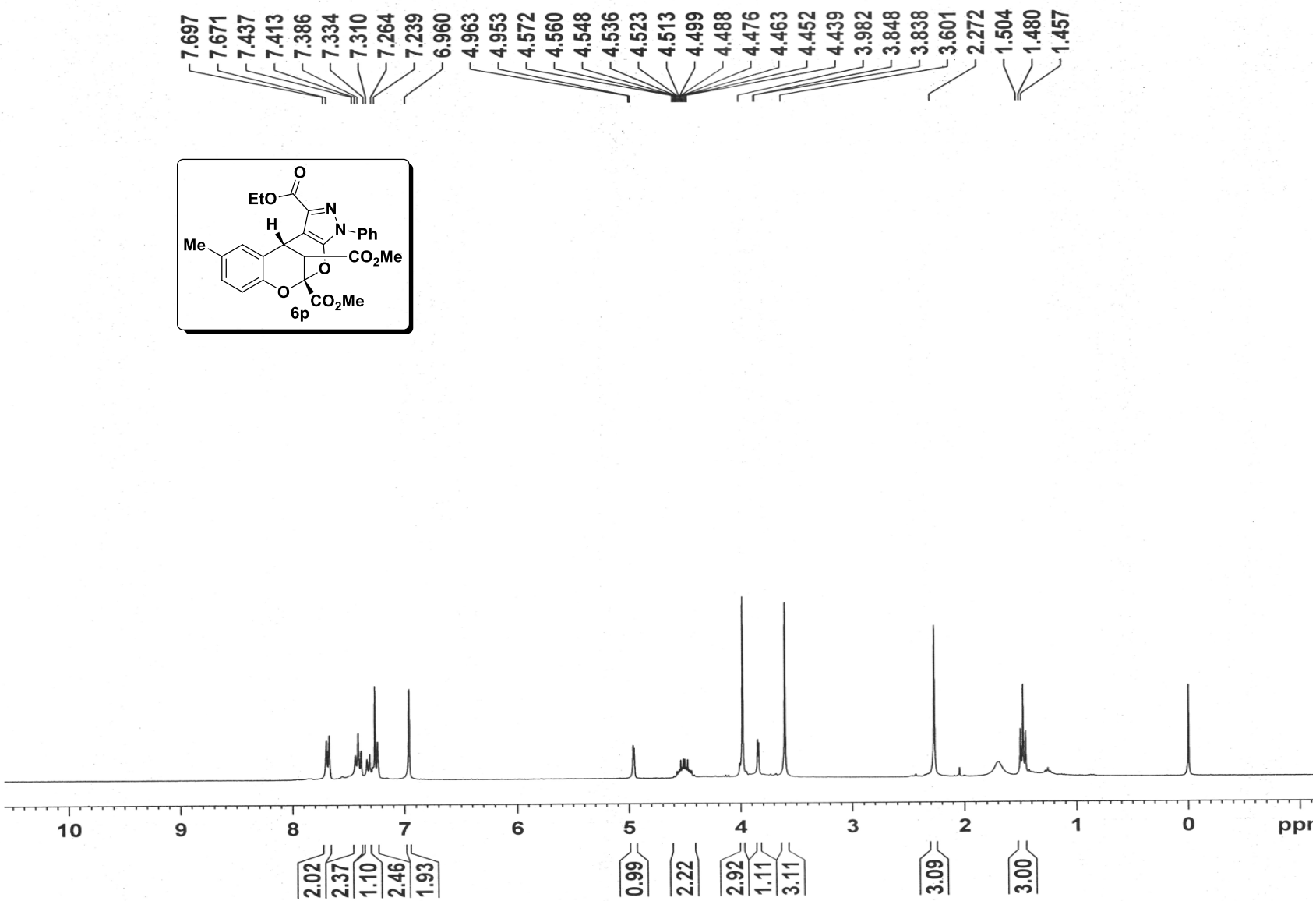


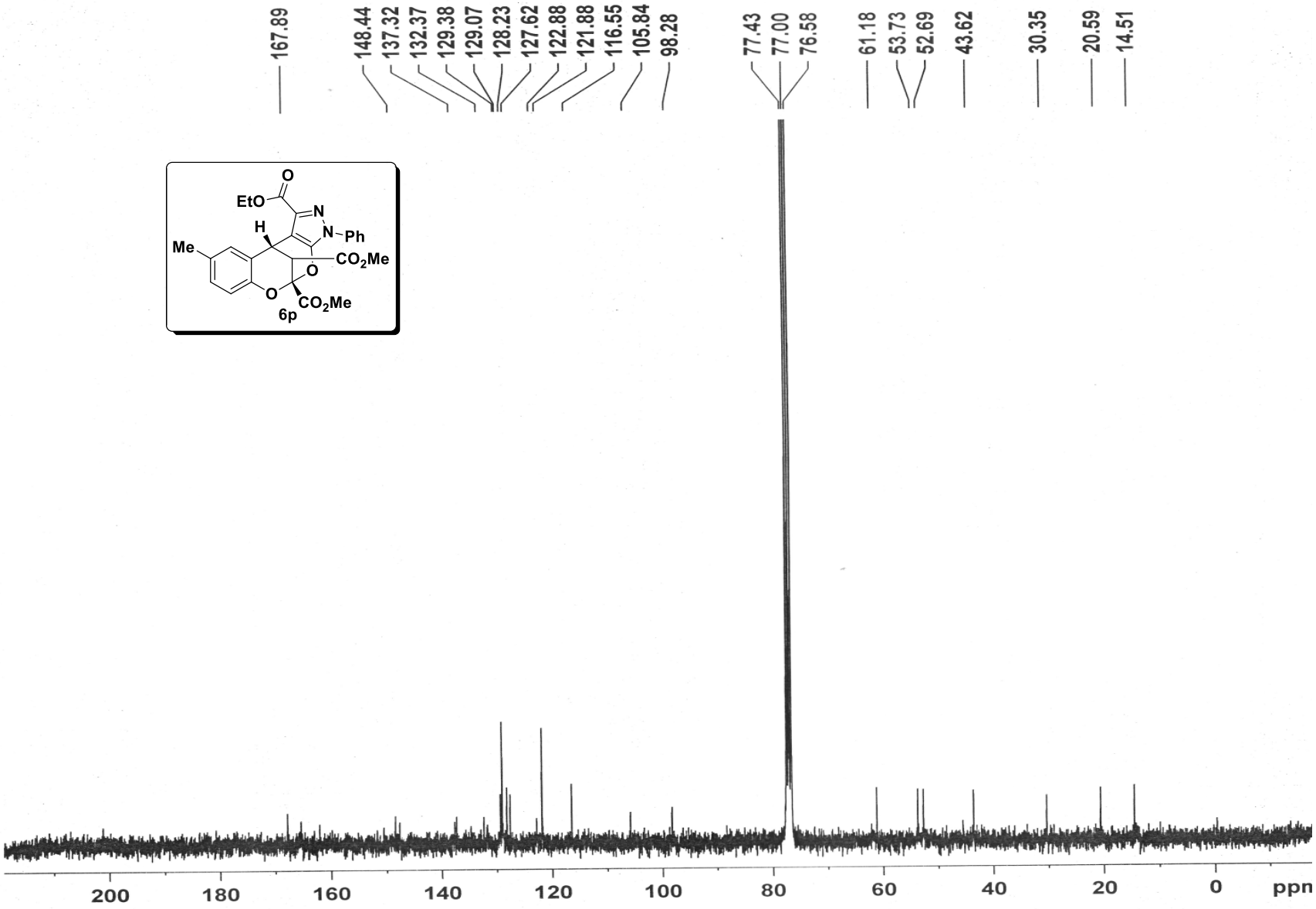

7.695
7.669
7.441
7.416
7.389
7.316
7.263
7.226
6.962
4.971
4.962
4.009
3.983
3.848
3.838
3.602
2.278
MeO
O
N
N
Ph
H
Me
CO2Me
O
O
CO2Me
6o
10
9
8
7
6
5
4
3
2
1
0
ppm
2.05
2.26
1.20
1.03
2.14
1.07
3.17
3.28
1.12
2.97
3.00


167.88
165.47
162.66
148.40
137.44
132.47
129.45
129.12
128.22
127.70
122.80
121.86
116.56
106.00
98.29
77.44
77.02
76.59
53.80
52.76
52.10
43.58
30.24
20.66
-0.01
MeO
O
N
N
Ph
H
Me
CO2Me
O
O
CO2Me
6o
200
180
160
140
120
100
80
60
40
20
0
ppm

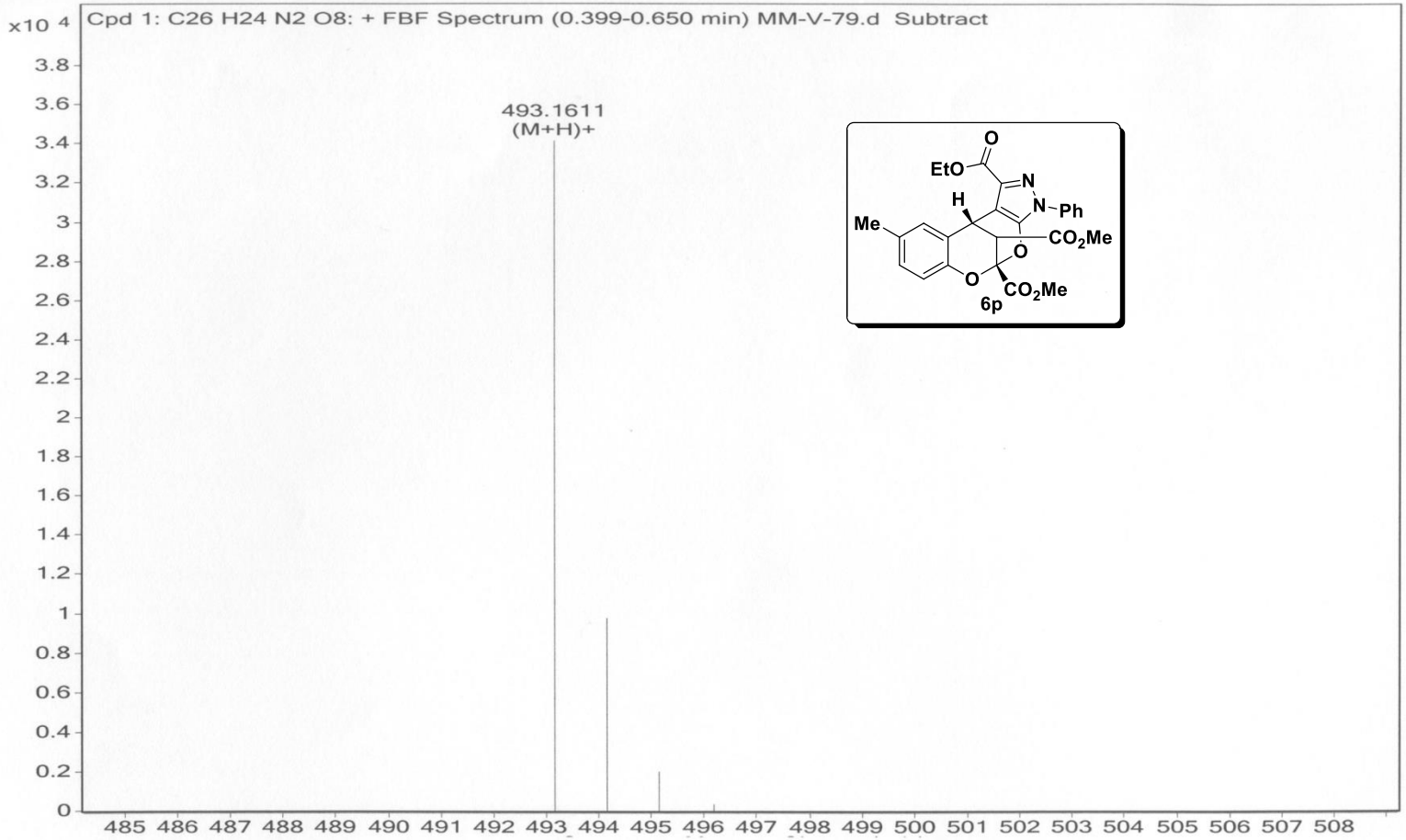
Sample Name	MM-V-78	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-V-78.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-478.1376	**Acquired Time**	30-01-2015 15:15:19

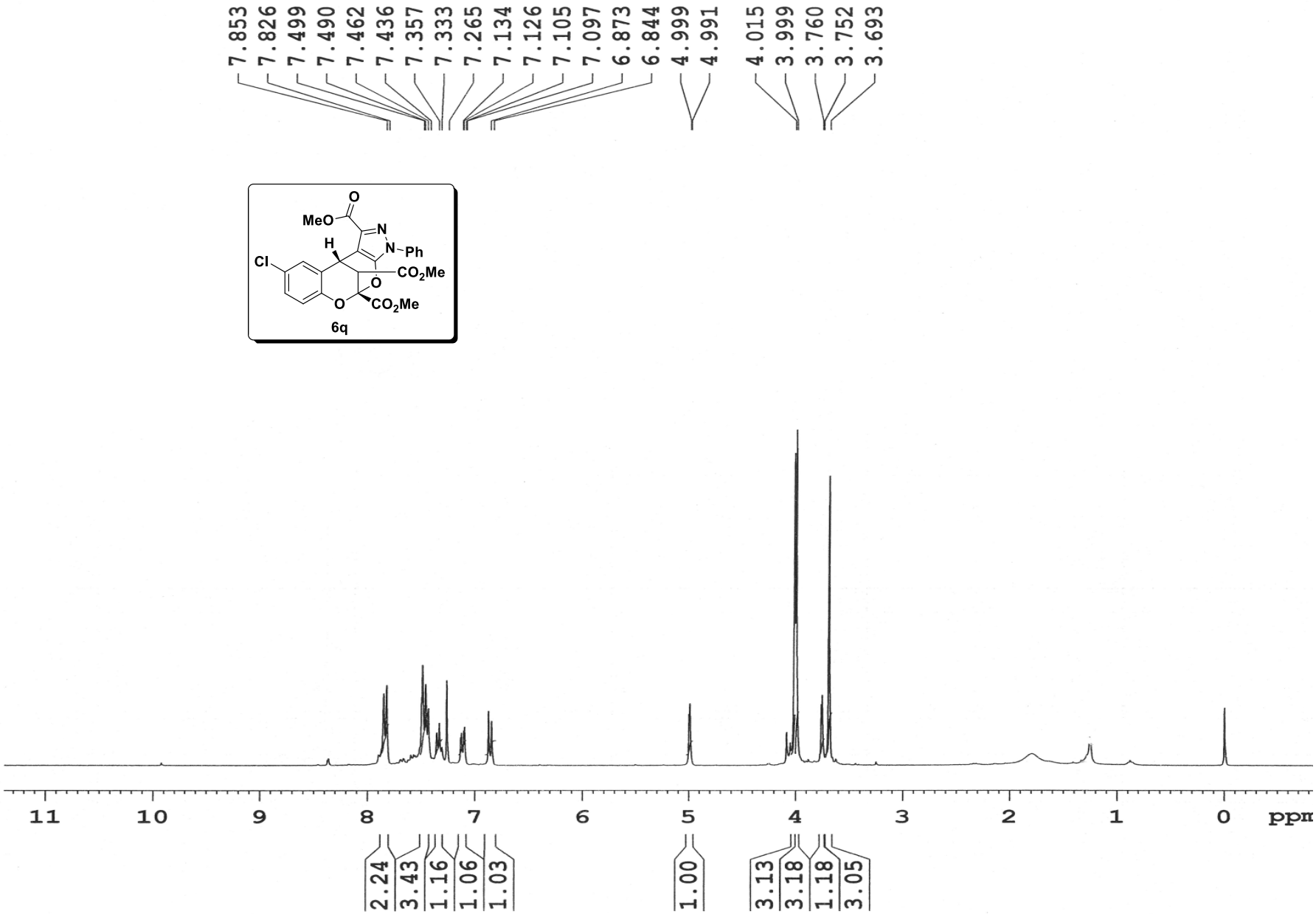


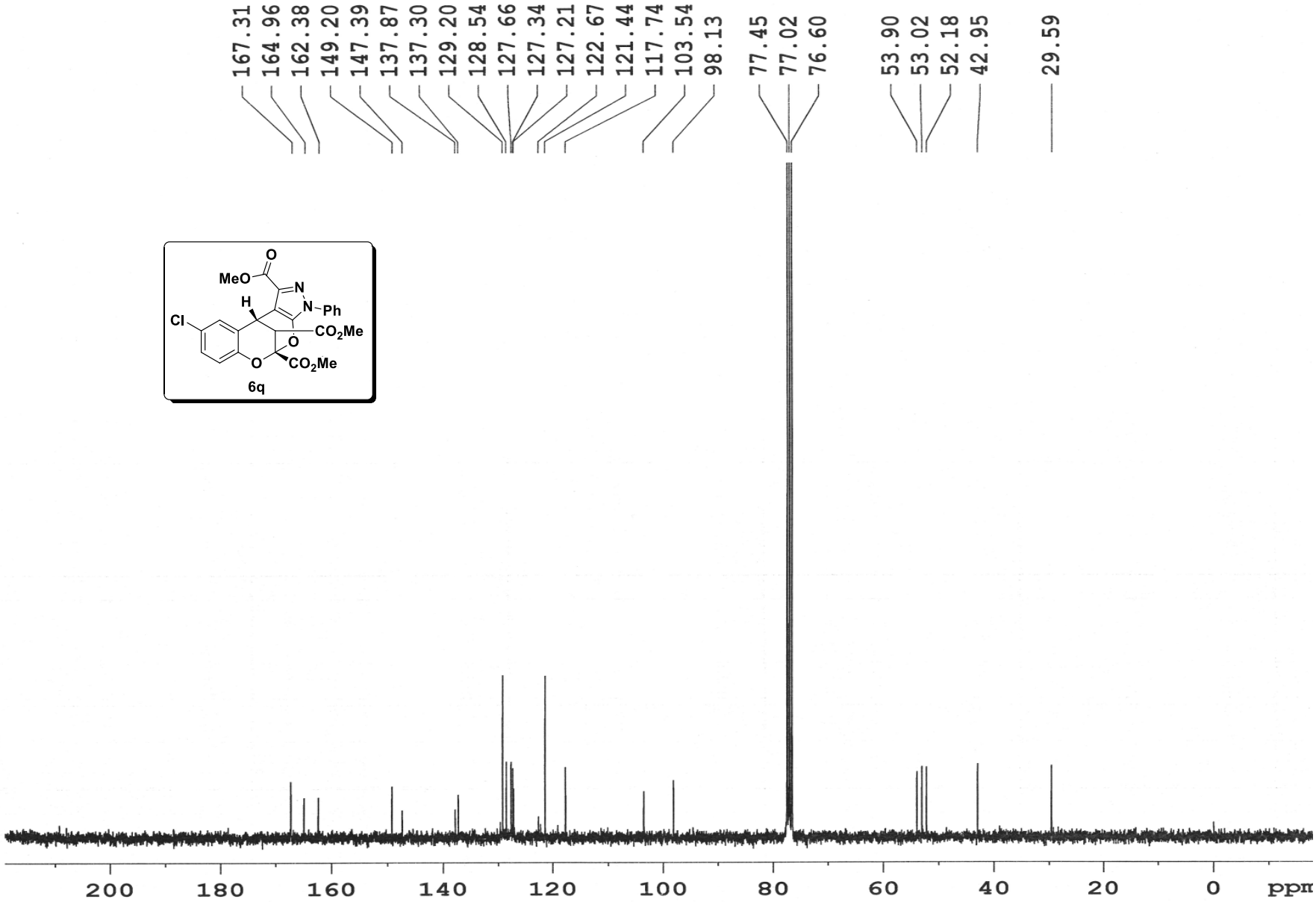

7.697
7.671
7.437
7.413
7.386
7.334
7.310
7.264
7.239
6.960
4.963
4.953
4.572
4.560
4.548
4.536
4.523
4.513
4.499
4.488
4.476
4.463
4.452
4.439
3.982
3.848
3.838
3.601
2.272
1.504
1.480
1.457
EtO
O
N
N
Ph
H
Me
CO2Me
O
O
CO2Me
6p
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
2.37
1.10
2.46
1.93
0.99
2.22
2.92
1.11
3.11
3.09
3.00


167.89
148.44
137.32
132.37
129.38
129.07
128.23
127.62
122.88
121.88
116.55
105.84
98.28
77.43
77.00
76.58
61.18
53.73
52.69
43.62
30.35
20.59
14.51
EtO
O
N
N
Ph
H
Me
CO2Me
O
O
CO2Me
6p
200
180
160
140
120
100
80
60
40
20
0
ppm

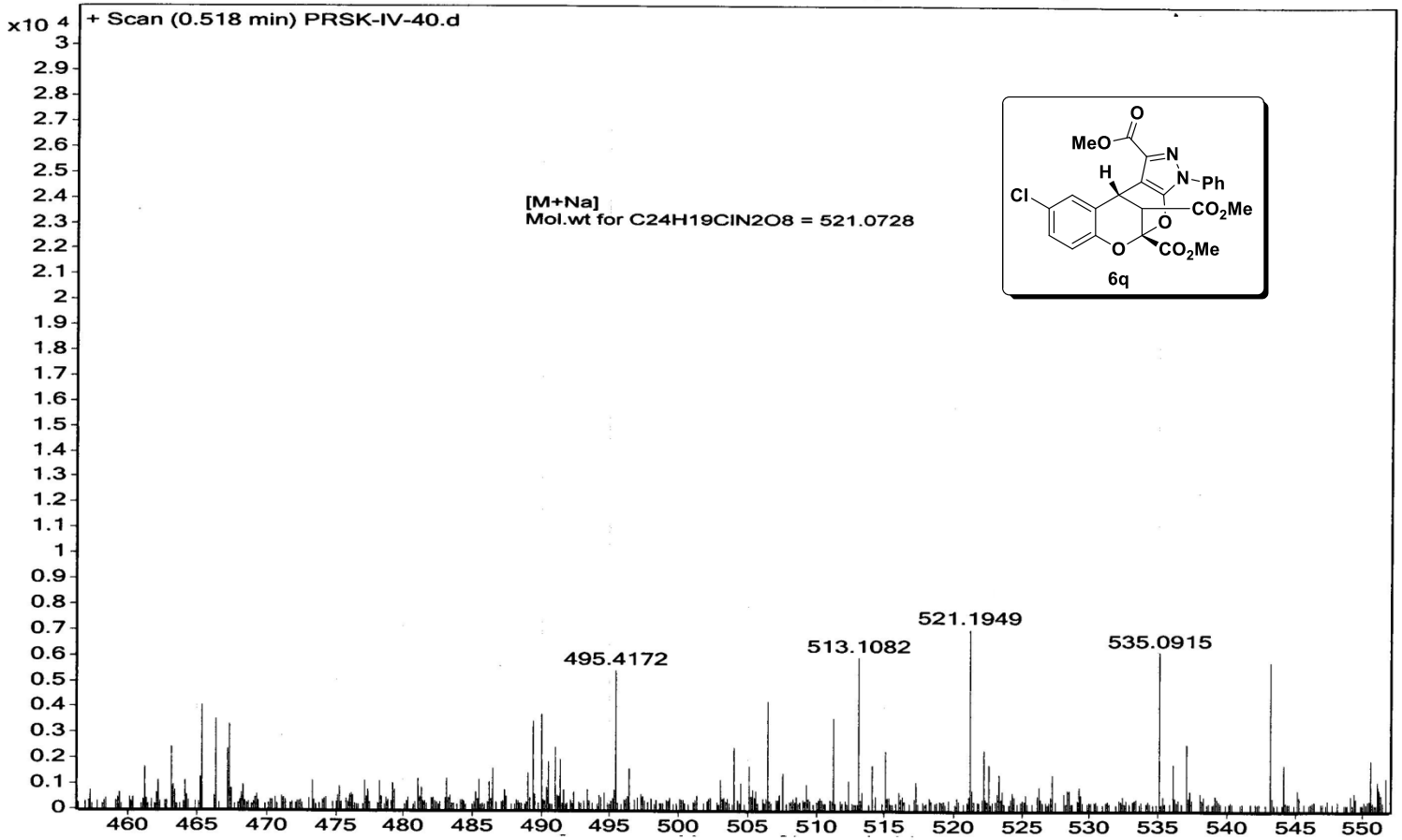
Sample Name	MM-V-79	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-V-79.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-492.1533	**Acquired Time**	02-02-2015 16:04:48

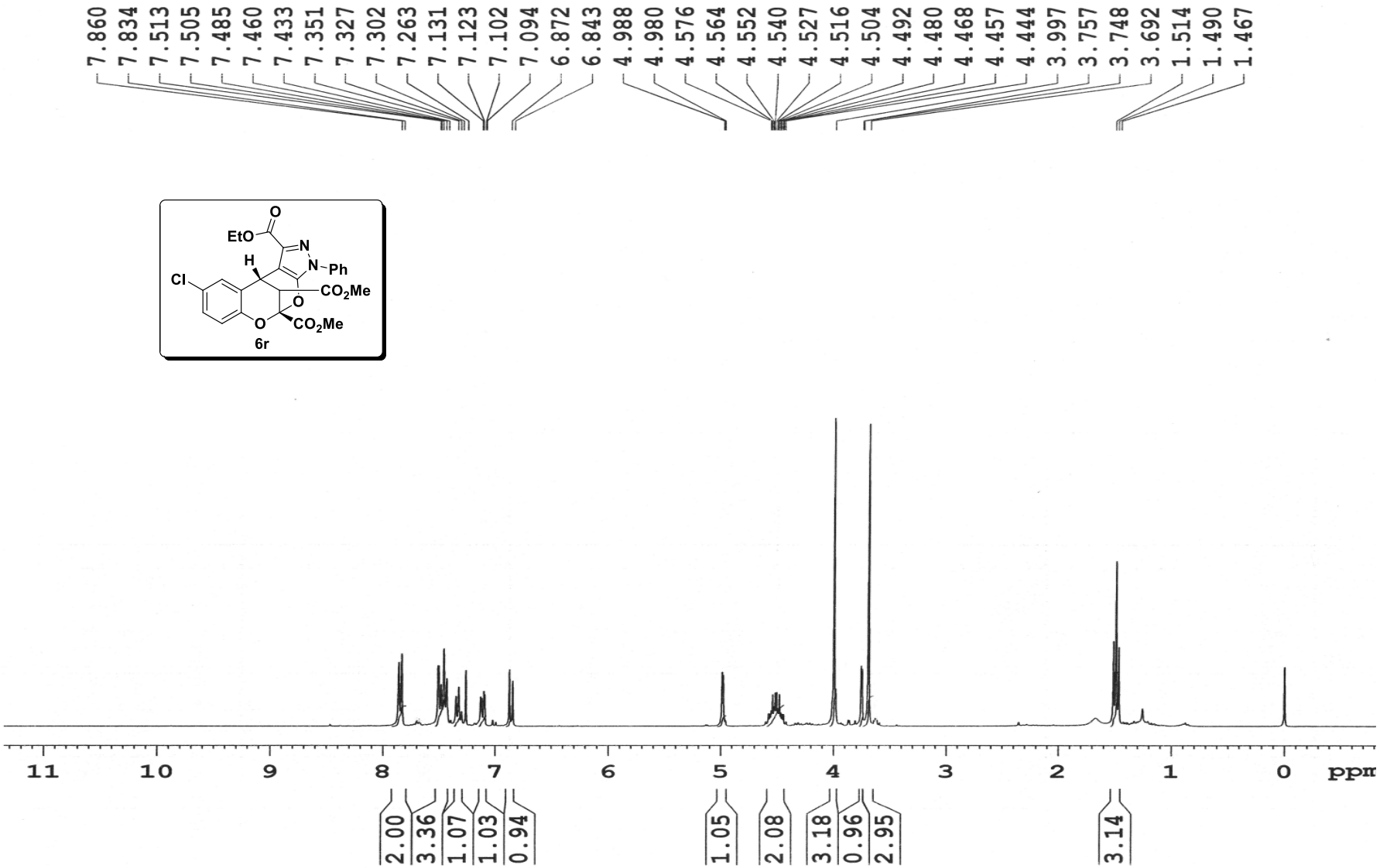


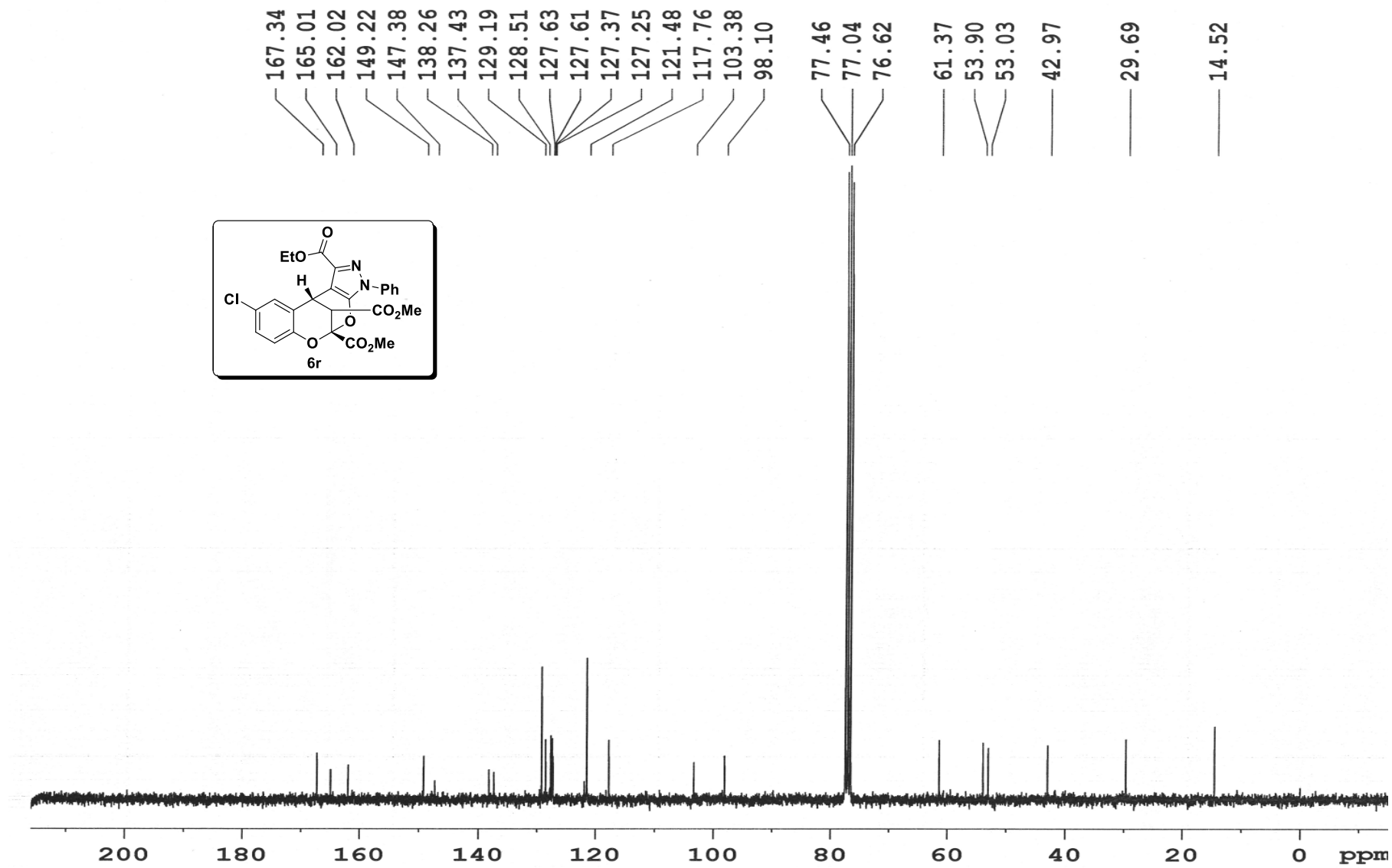

7.853
7.826
7.499
7.490
7.462
7.436
7.357
7.333
7.265
7.134
7.126
7.105
7.097
6.873
6.844
4.999
4.991
4.015
3.999
3.760
3.752
3.693
MeO
O
N
N
Ph
H
Cl
CO2Me
O
O
CO2Me
6q
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.24
3.43
1.16
1.06
1.03
1.00
3.13
3.18
1.18
3.05


167.31
164.96
162.38
149.20
147.39
137.87
137.30
129.20
128.54
127.66
127.34
127.21
122.67
121.44
117.74
103.54
98.13
77.45
77.02
76.60
53.90
53.02
52.18
42.95
29.59
MeO
O
N
N
Ph
H
Cl
CO2Me
O
O
CO2Me
6q
200
180
160
140
120
100
80
60
40
20
0
ppm

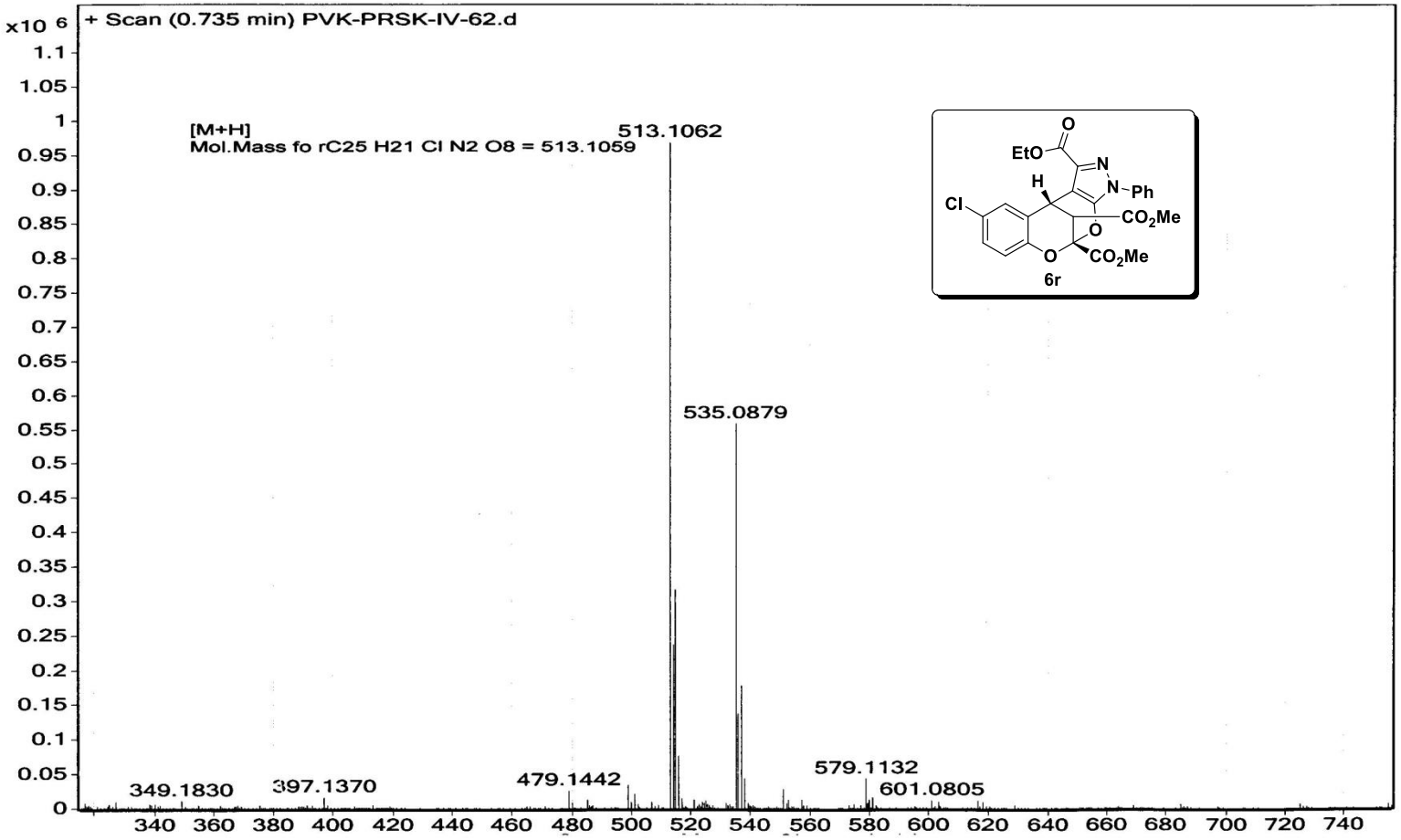
Sample Name	PRSK-IV-40	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-IV-40.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay-MB-498.0830	**Acquired Time**	16-09-2014 11:15:19

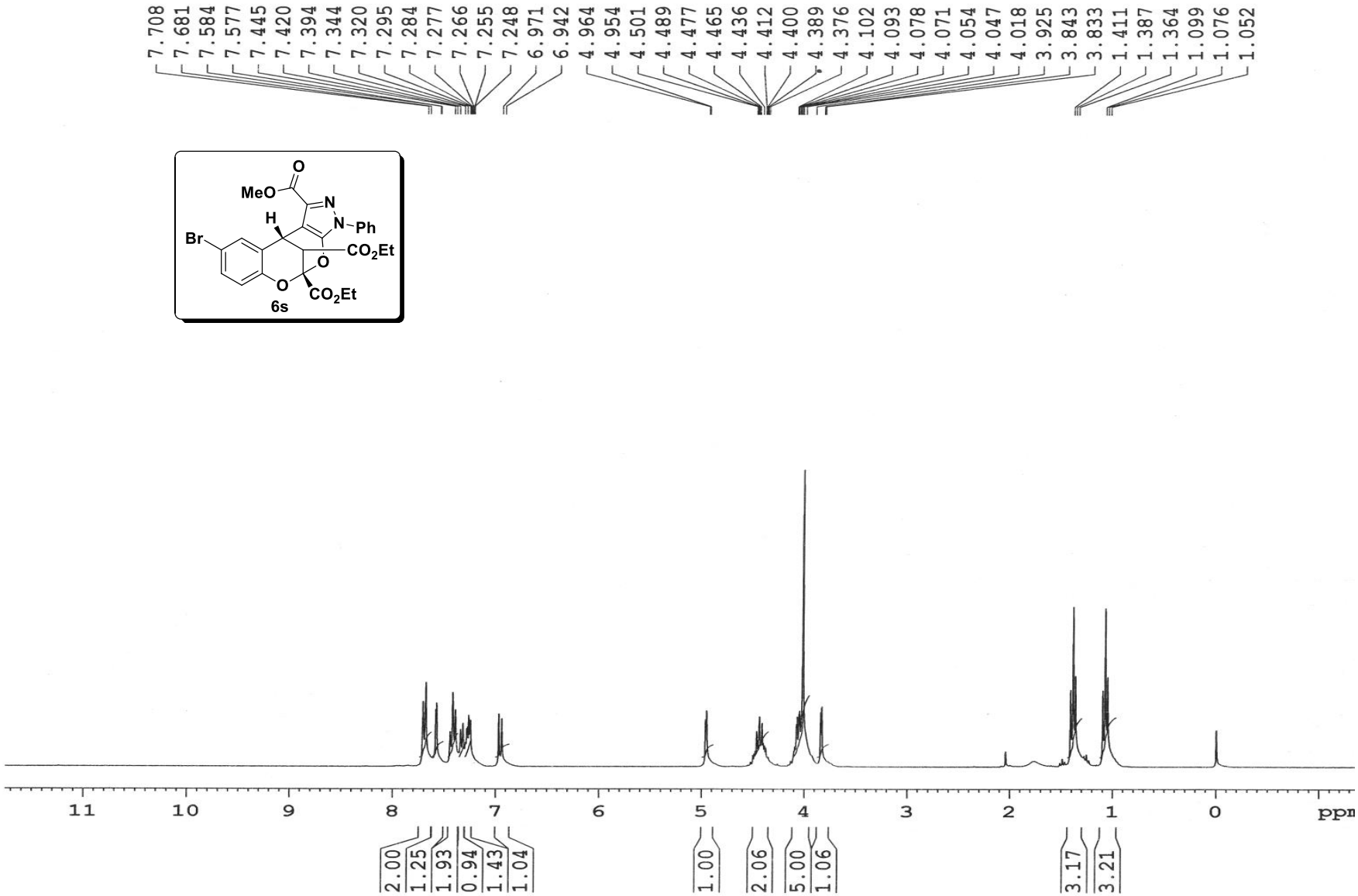


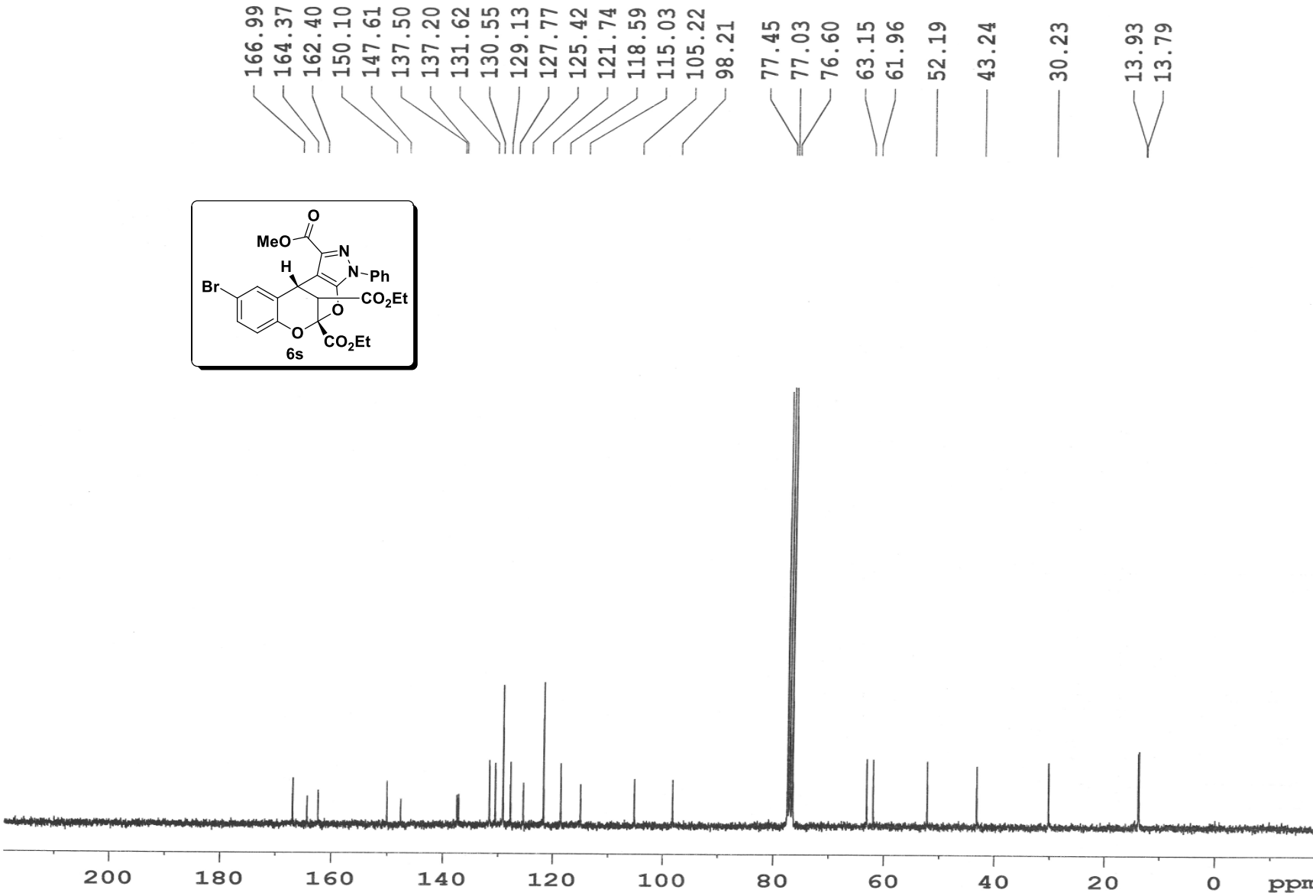

7.860
7.834
7.513
7.505
7.485
7.460
7.433
7.351
7.327
7.302
7.263
7.131
7.123
7.102
7.094
6.872
6.843
4.988
4.980
4.576
4.564
4.552
4.540
4.527
4.516
4.504
4.492
4.480
4.468
4.457
4.444
3.997
3.757
3.748
3.692
1.514
1.490
1.467
EtO
O
N
N
Ph
H
Cl
CO2Me
O
O
CO2Me
6r
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.36
1.07
1.03
0.94
1.05
2.08
3.18
0.96
2.95
3.14


167.34
165.01
162.02
149.22
147.38
138.26
137.43
129.19
128.51
127.63
127.61
127.37
127.25
121.48
117.76
103.38
98.10
77.46
77.04
76.62
61.37
53.90
53.03
42.97
29.69
14.52
O
EtO
N
N
Ph
H
Cl
CO2Me
O
O
CO2Me
6r
200
180
160
140
120
100
80
60
40
20
0
ppm

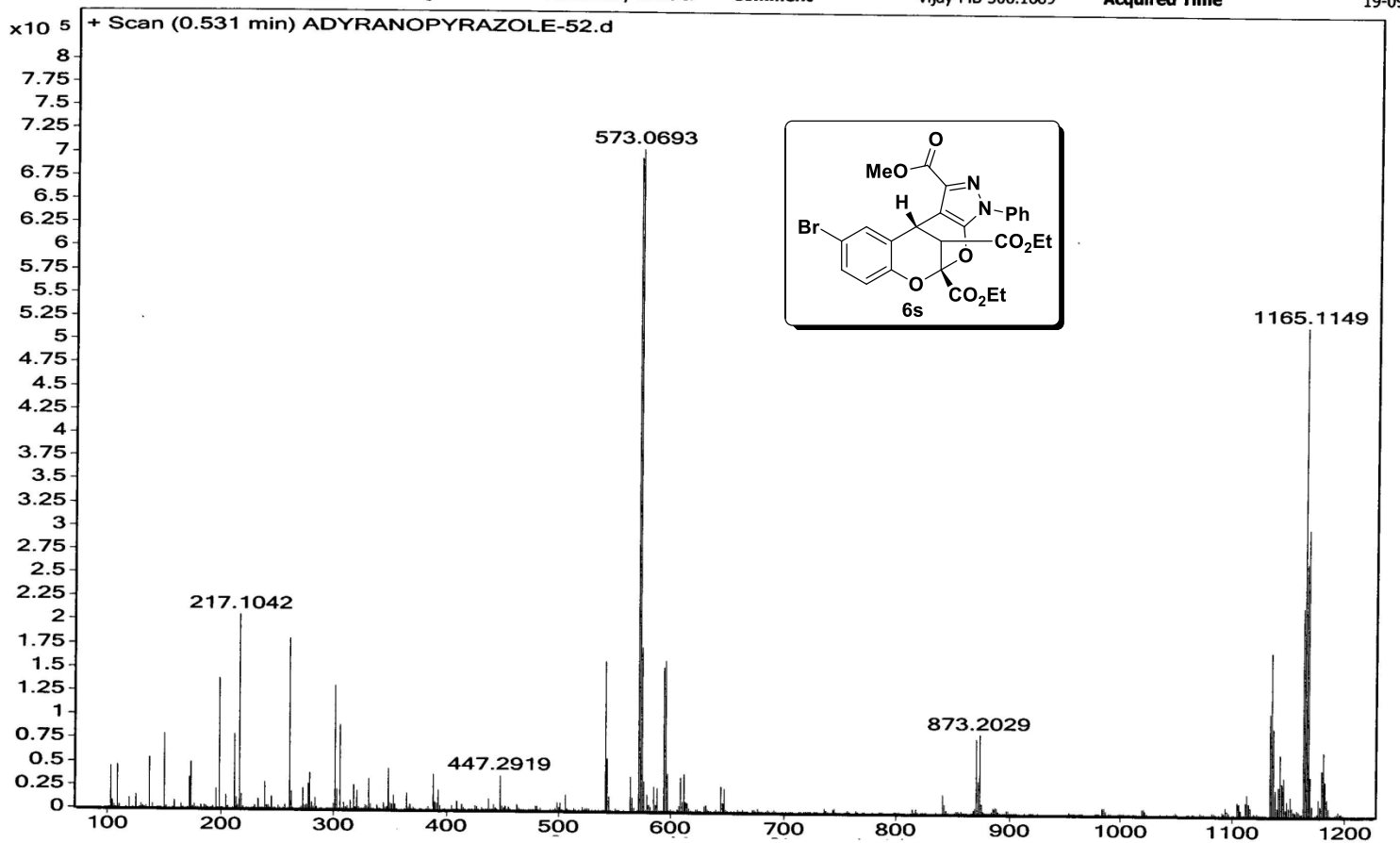
Sample Name	PVK-PRSK-IV-62	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-PRSK-IV-62.d	**ACQ Method**	Pondicherry Universi	**Comment**	PV-MB-512.0986	**Acquired Time**	15-09-2014 10:55:56

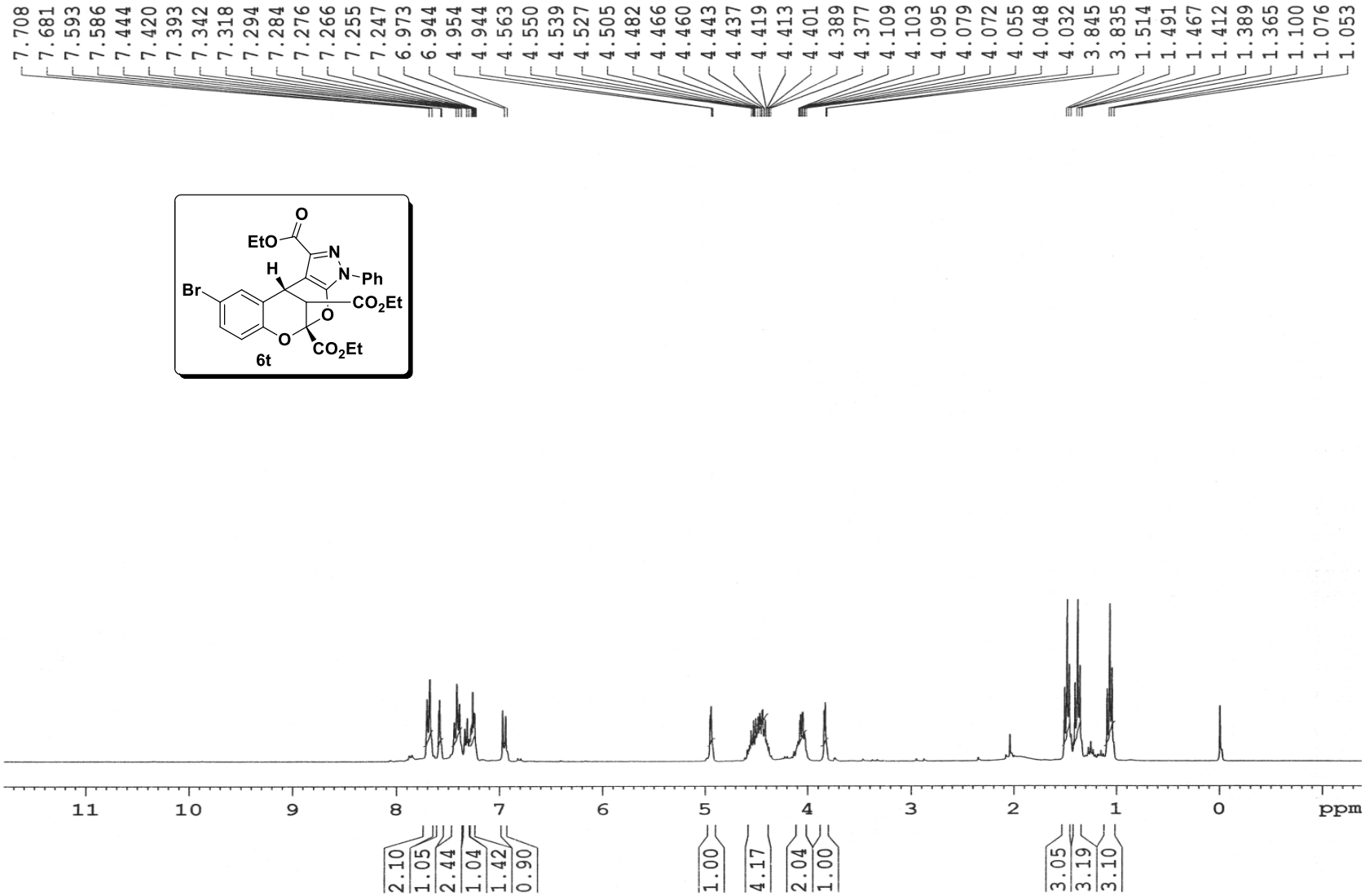


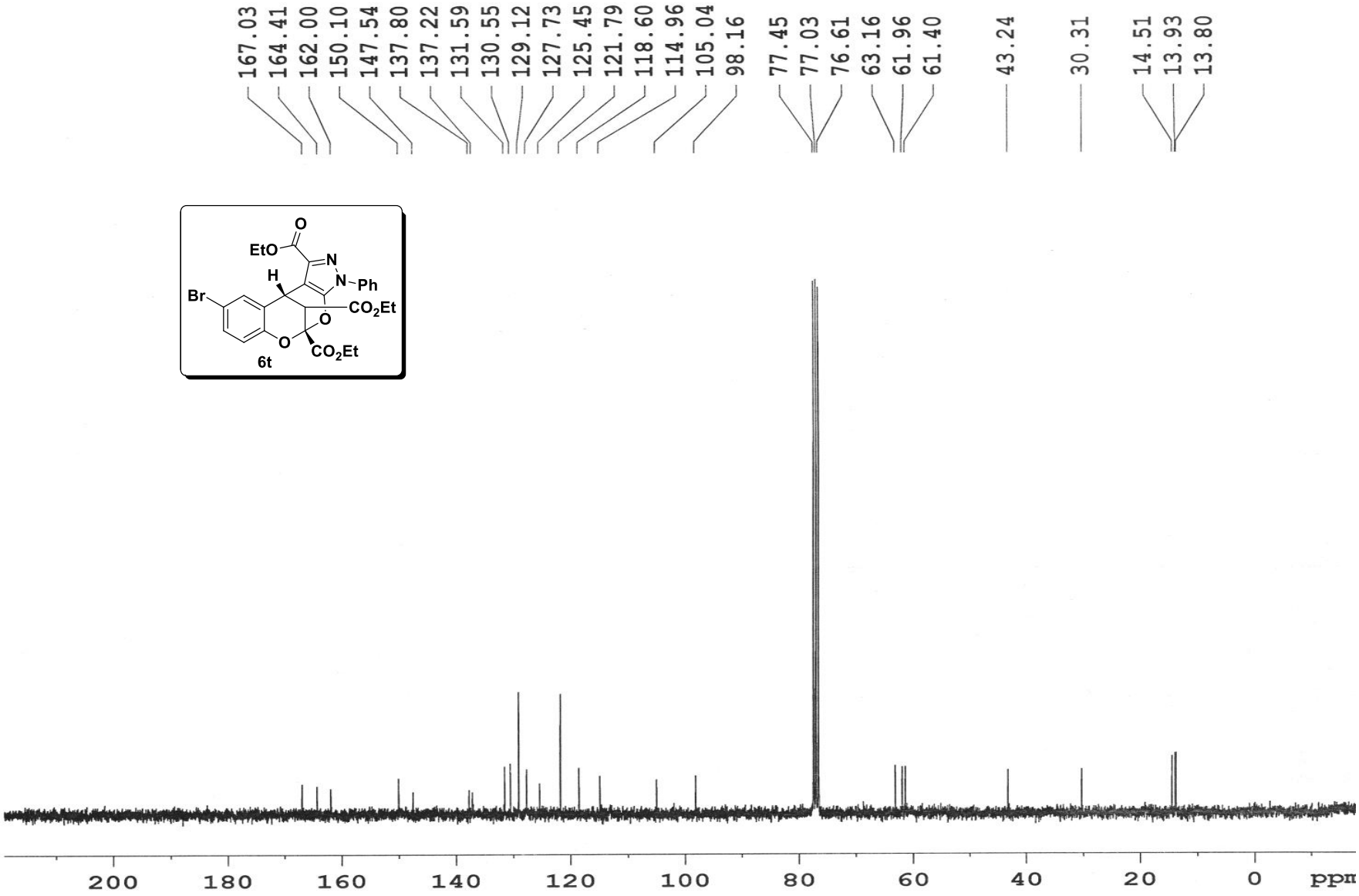

7.708
7.681
7.584
7.577
7.445
7.420
7.394
7.344
7.320
7.295
7.284
7.277
7.266
7.255
7.248
6.971
6.942
4.964
4.954
4.501
4.489
4.477
4.465
4.436
4.412
4.400
4.389
4.376
4.102
4.093
4.078
4.071
4.054
4.047
4.018
3.925
3.843
3.833
1.411
1.387
1.364
1.099
1.076
1.052
MeO
O
N
N
Ph
H
Br
CO2Et
O
O
CO2Et
6s
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.25
1.93
0.94
1.43
1.04
1.00
2.06
5.00
1.06
3.17
3.21


166.99
164.37
162.40
150.10
147.61
137.50
137.20
131.62
130.55
129.13
127.77
125.42
121.74
118.59
115.03
105.22
98.21
77.45
77.03
76.60
63.15
61.96
52.19
43.24
30.23
13.93
13.79
MeO
O
N
N
Ph
H
Br
CO2Et
O
O
CO2Et
6s
200
180
160
140
120
100
80
60
40
20
0
ppm

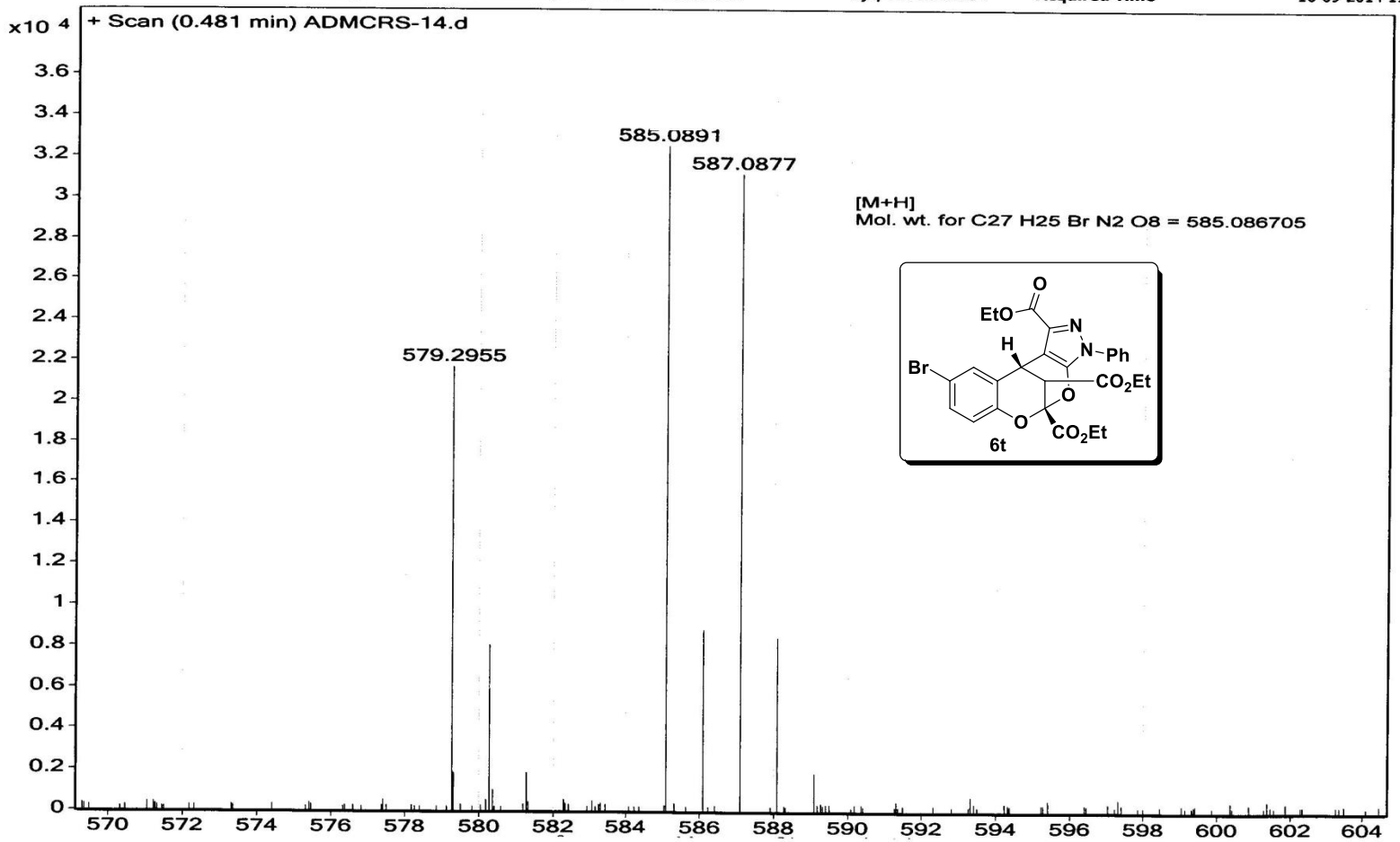
Sample Name	AD-PYRANOPYRAZOLE-52	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	ADYRANOPYRAZOLE-52.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay-MB-506.1689	**Acquired Time**	19-09-2014 10:58:33

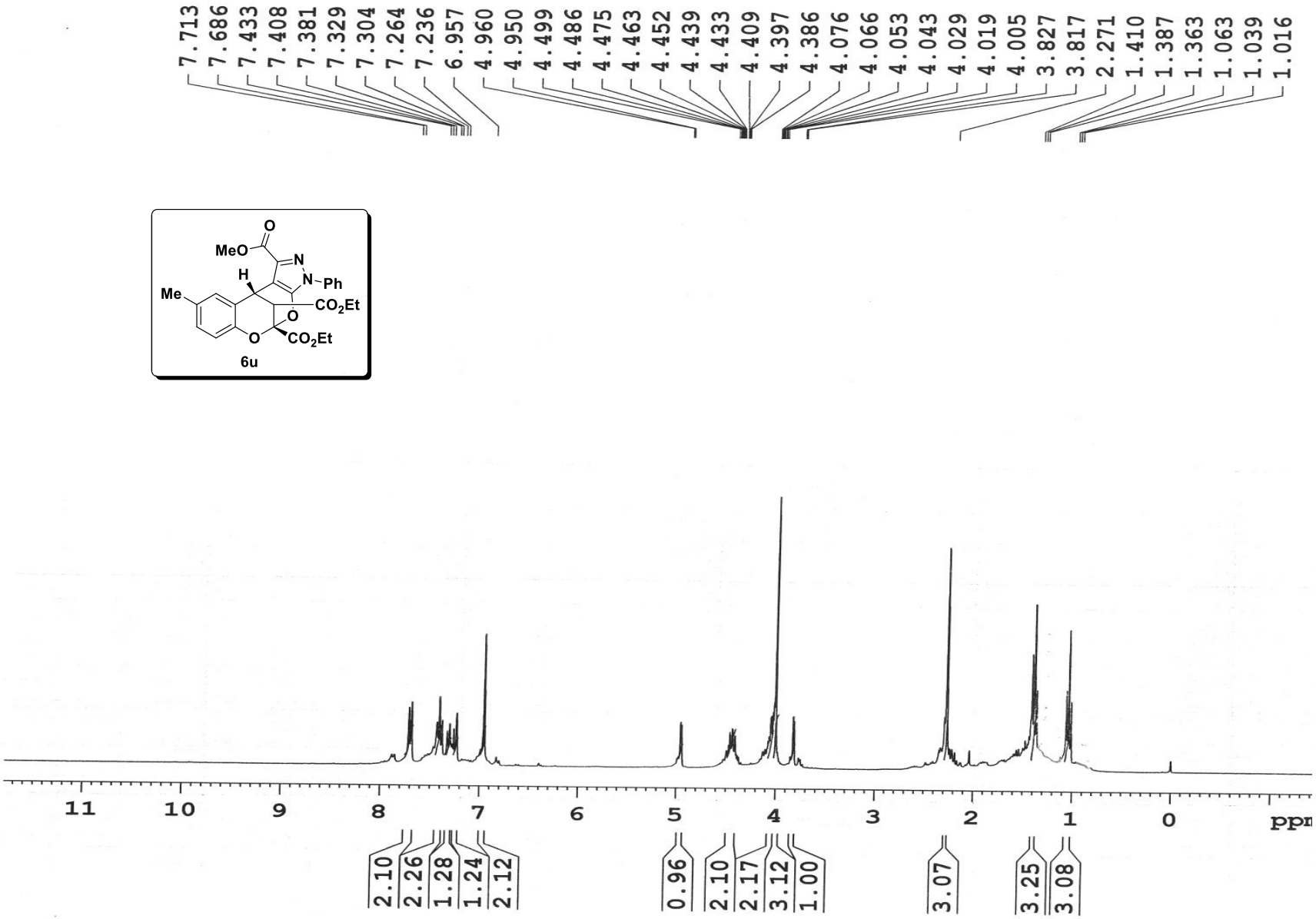


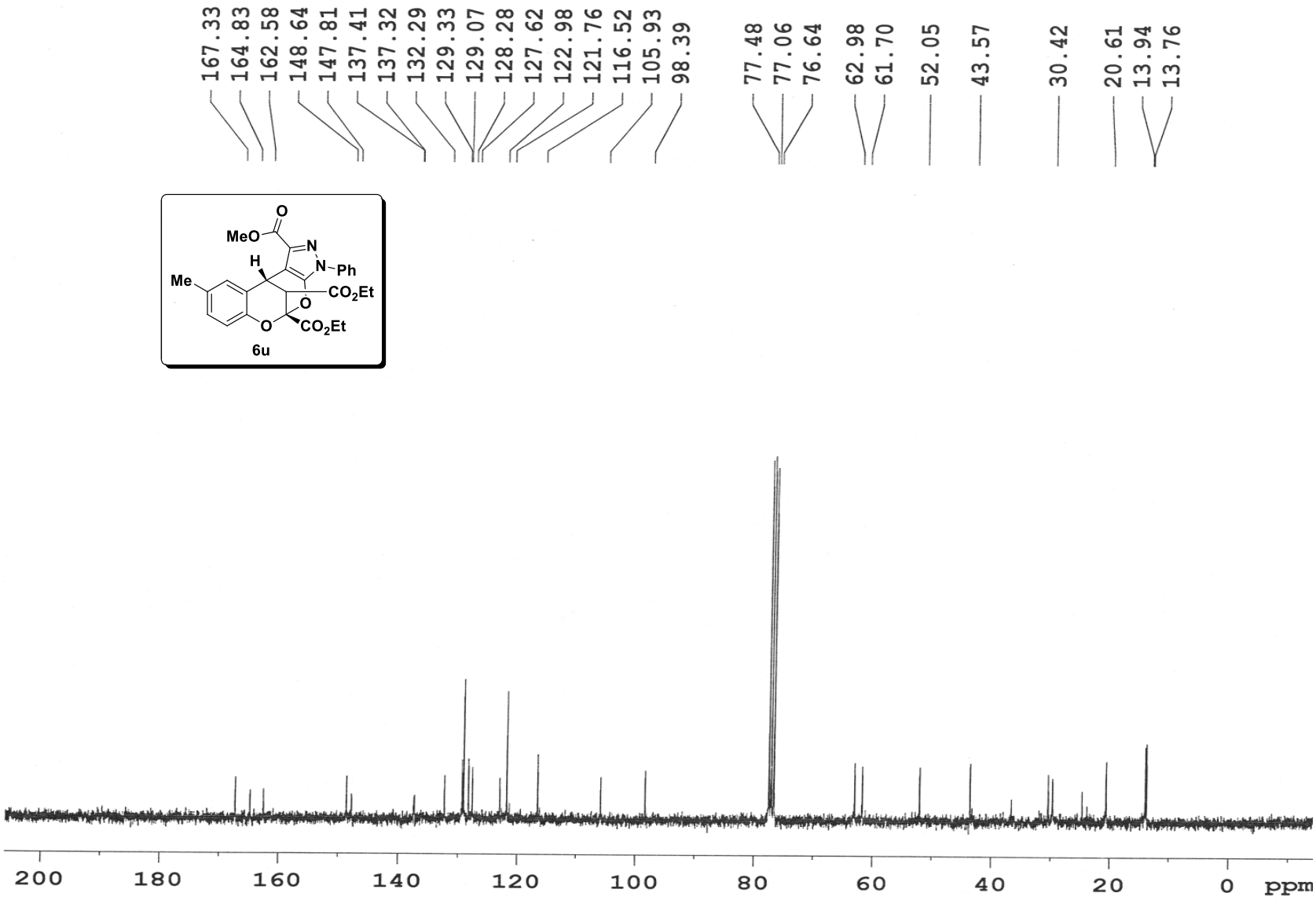

7.708
7.681
7.593
7.586
7.444
7.420
7.393
7.342
7.318
7.294
7.284
7.276
7.266
7.255
7.247
6.973
6.944
4.954
4.944
4.563
4.550
4.539
4.527
4.505
4.482
4.466
4.460
4.443
4.437
4.419
4.413
4.401
4.389
4.377
4.109
4.103
4.095
4.079
4.072
4.055
4.048
4.032
3.845
3.835
1.514
1.491
1.467
1.412
1.389
1.365
1.100
1.076
1.053
EtO
O
N
N
Ph
H
Br
CO2Et
O
O
CO2Et
6t
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.10
1.05
2.44
1.04
1.42
0.90
1.00
4.17
2.04
1.00
3.05
3.19
3.10


167.03
164.41
162.00
150.10
147.54
137.80
137.22
131.59
130.55
129.12
127.73
125.45
121.79
118.60
114.96
105.04
98.16
77.45
77.03
76.61
63.16
61.96
61.40
43.24
30.31
14.51
13.93
13.80
EtO
O
N
N
Ph
H
Br
CO2Et
O
O
CO2Et
6t
200
180
160
140
120
100
80
60
40
20
0
ppm

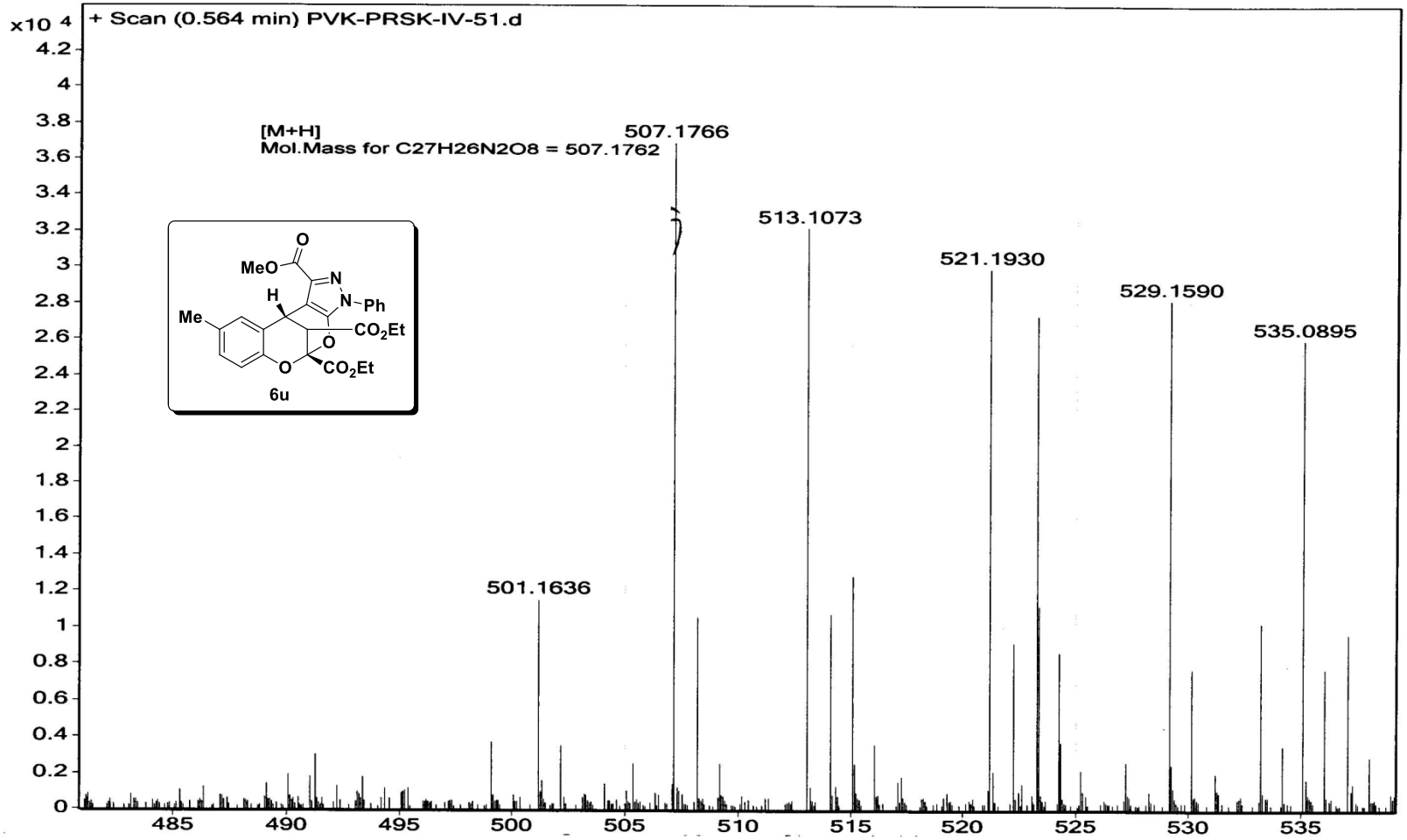
Sample Name	ADMCRS-14	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	ADMCRS-14.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay-MB-584.0794	**Acquired Time**	16-09-2014 11:21:29

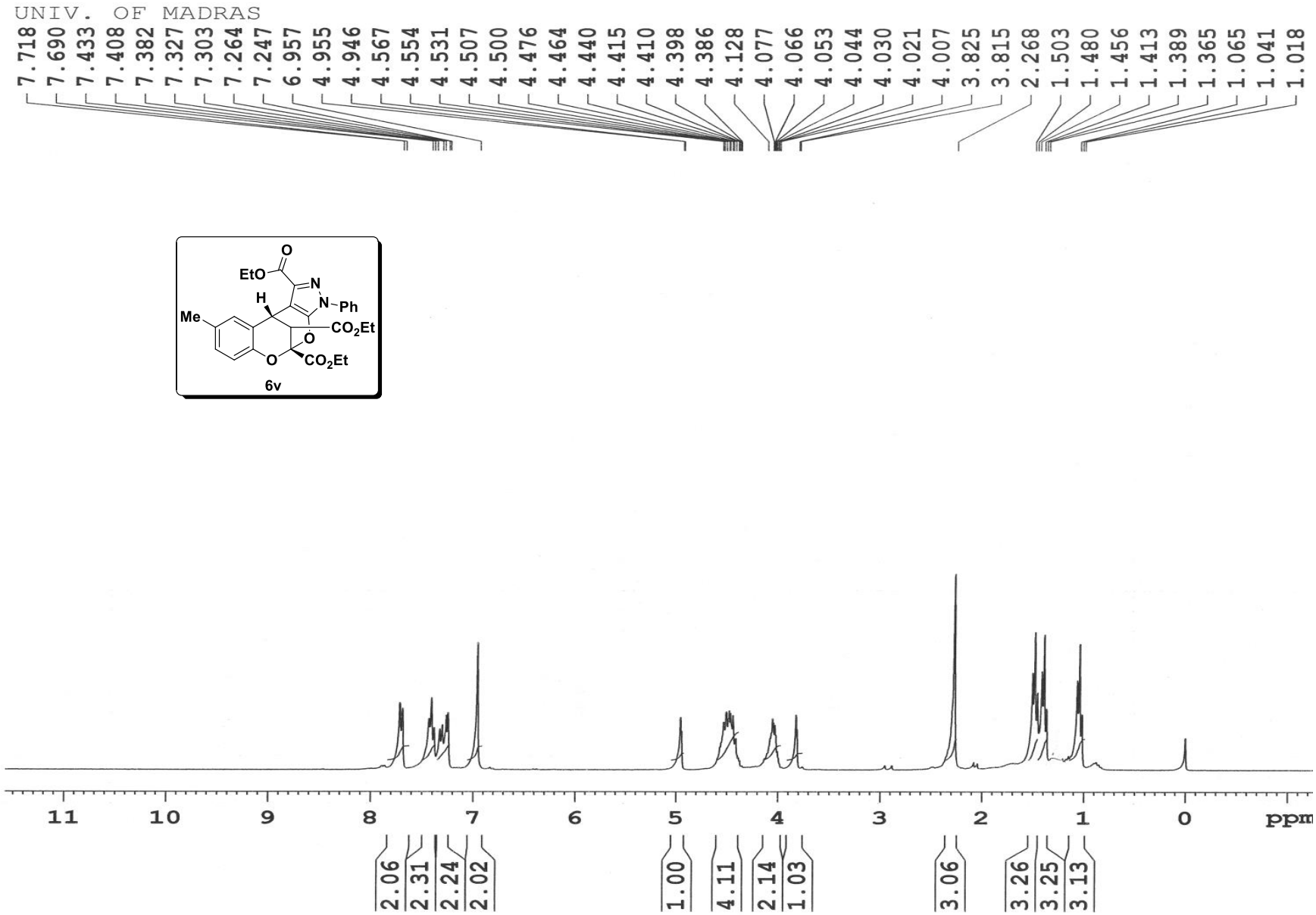


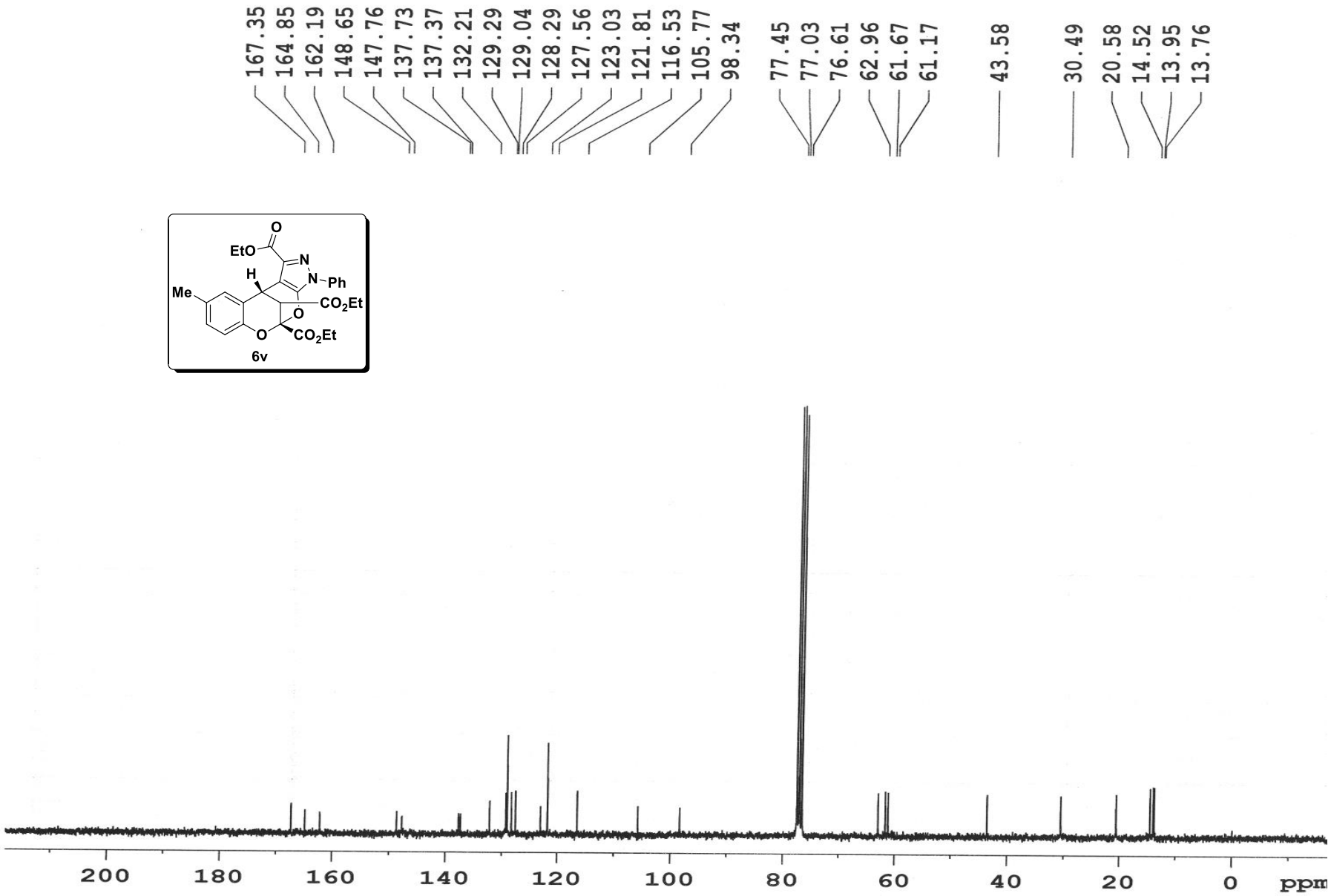

7.713
7.686
7.433
7.408
7.381
7.329
7.304
7.264
7.236
6.957
4.960
4.950
4.499
4.486
4.475
4.463
4.452
4.439
4.433
4.409
4.397
4.386
4.076
4.066
4.053
4.043
4.029
4.019
4.005
3.827
3.817
2.271
1.410
1.387
1.363
1.063
1.039
1.016
MeO
O
N
N-Ph
H
Me
CO2Et
O
O
CO2Et
6u
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.10
2.26
1.28
1.24
2.12
0.96
2.10
2.17
3.12
1.00
3.07
3.25
3.08


167.33
164.83
162.58
148.64
147.81
137.41
137.32
132.29
129.33
129.07
128.28
127.62
122.98
121.76
116.52
105.93
98.39
77.48
77.06
76.64
62.98
61.70
52.05
43.57
30.42
20.61
13.94
13.76
MeO
O
N
N
Ph
H
Me
CO2Et
O
O
CO2Et
6u
200
180
160
140
120
100
80
60
40
20
0
ppm

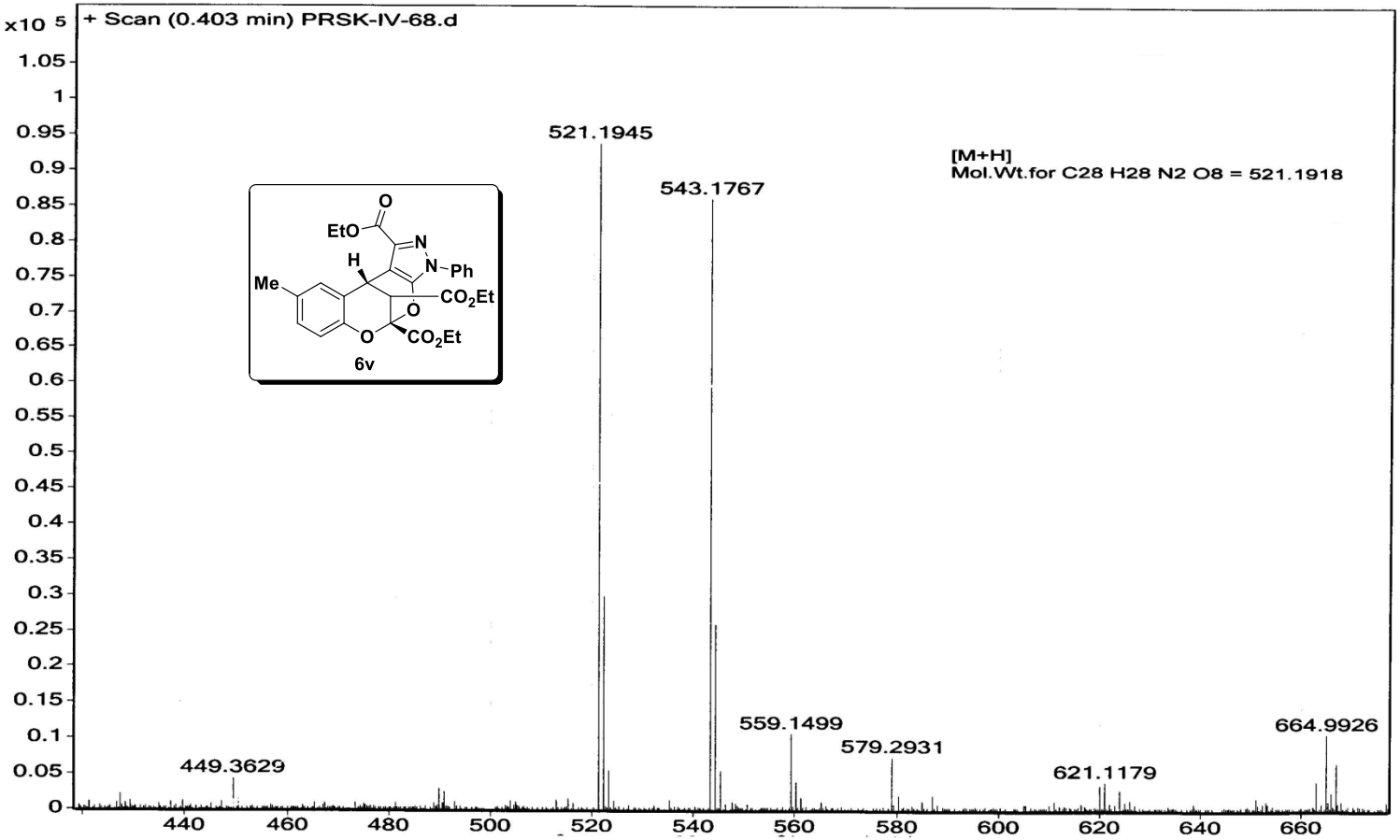
Sample Name	PVK-PRSK-IV-51	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-PRSK-IV-51.d	**ACQ Method**	Pondicherry Universi	**Comment**	PV-MB-506.1689	**Acquired Time**	15-09-2014 10:59:02

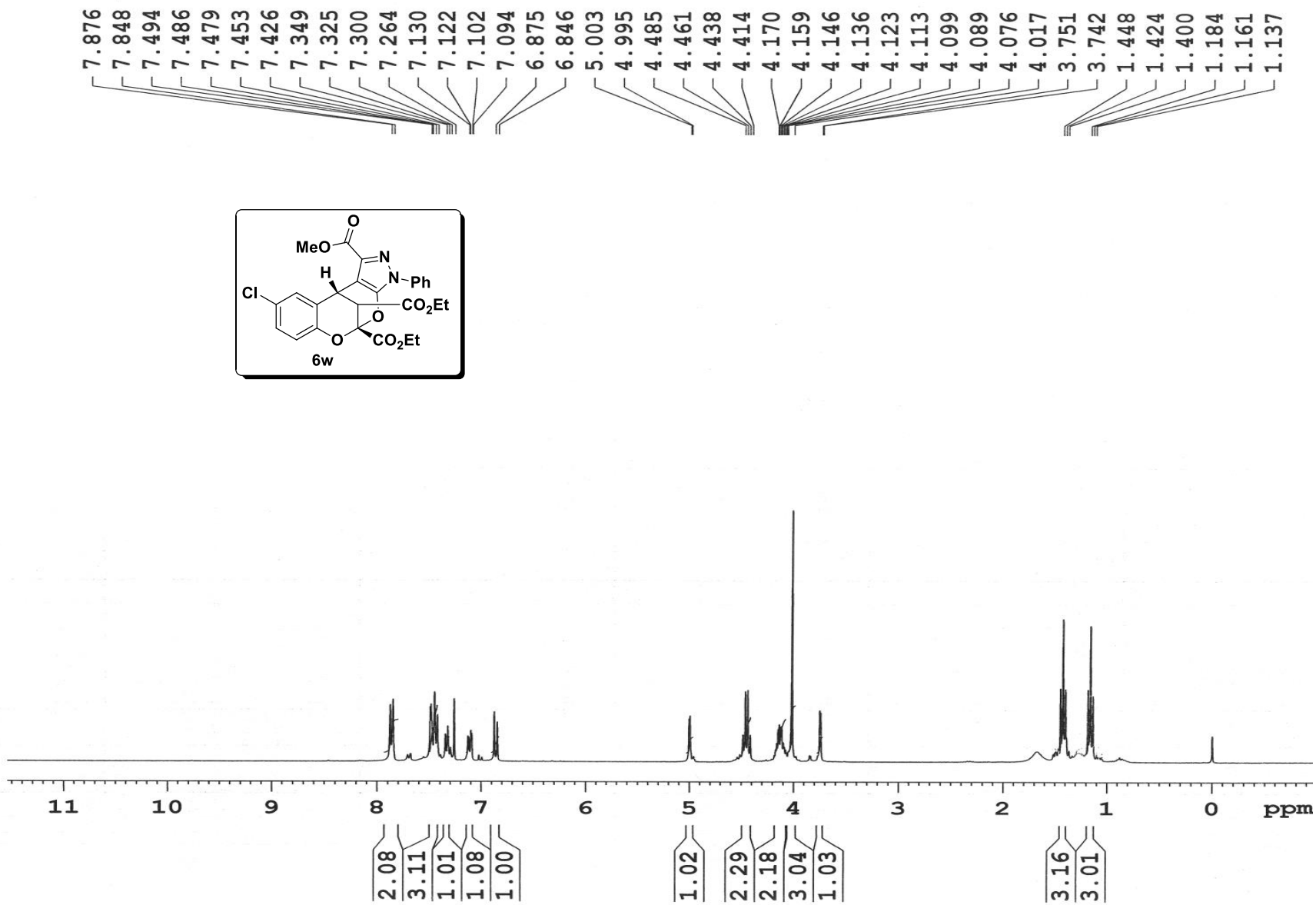


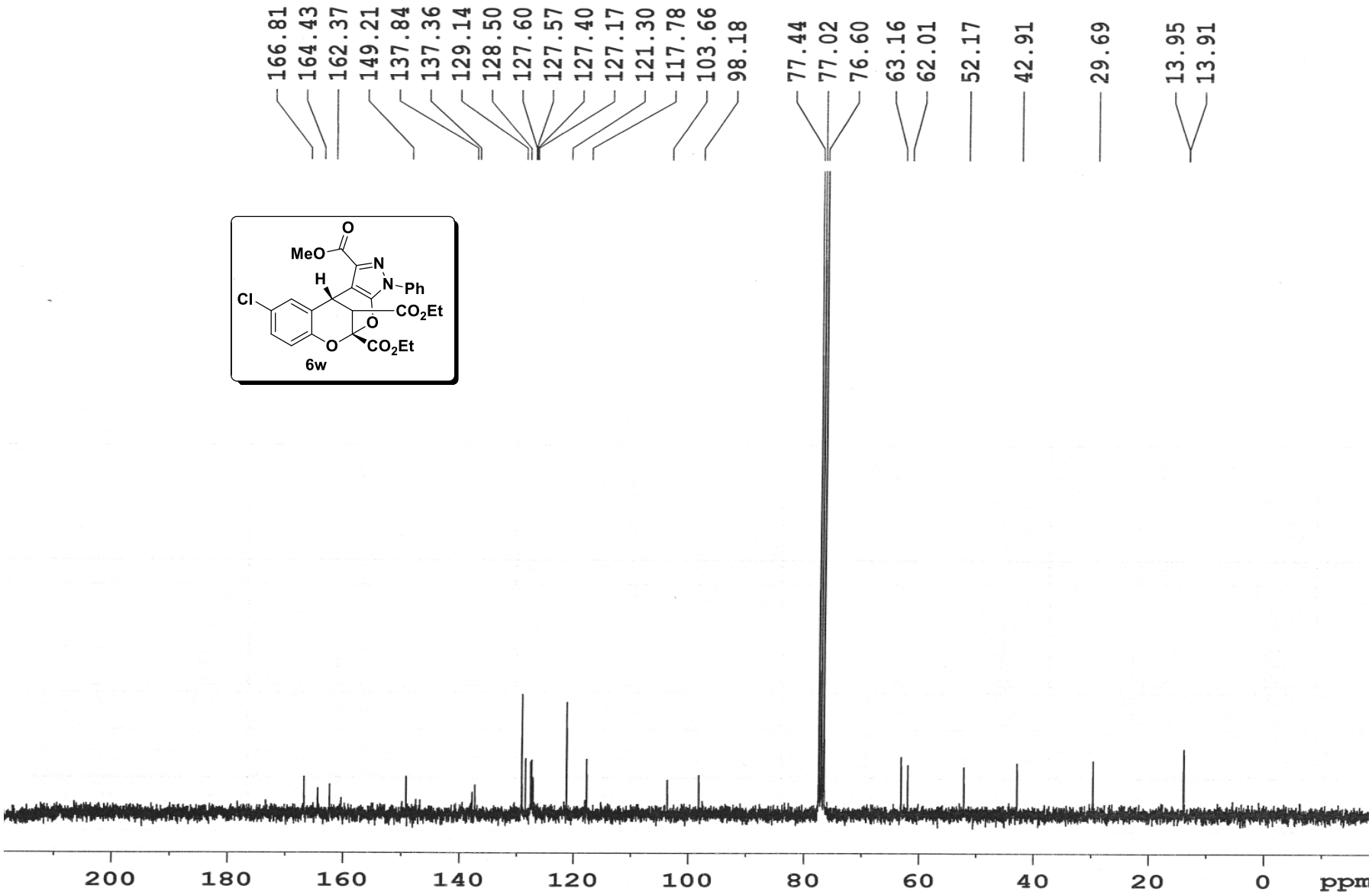

UNIV. OF MADRAS
7.718 7.690 7.433 7.408 7.382 7.327 7.303 7.264 7.247 6.957 4.955 4.946 4.567 4.554 4.531 4.507 4.500 4.476 4.464 4.440 4.415 4.410 4.398 4.386 4.128 4.077 4.066 4.053 4.044 4.030 4.021 4.007 3.825 3.815 2.268 1.503 1.480 1.456 1.413 1.389 1.365 1.065 1.041 1.018
EtO
O
N
N
Ph
H
Me
CO2Et
O
O
CO2Et
6v
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.06 2.31 2.24 2.02 1.00 4.11 2.14 1.03 3.06 3.26 3.25 3.13


167.35
164.85
162.19
148.65
147.76
137.73
137.37
132.21
129.29
129.04
128.29
127.56
123.03
121.81
116.53
105.77
98.34
77.45
77.03
76.61
62.96
61.67
61.17
43.58
30.49
20.58
14.52
13.95
13.76
EtO
O
N
N
Ph
H
Me
CO2Et
O
O
CO2Et
6v
200
180
160
140
120
100
80
60
40
20
0
ppm

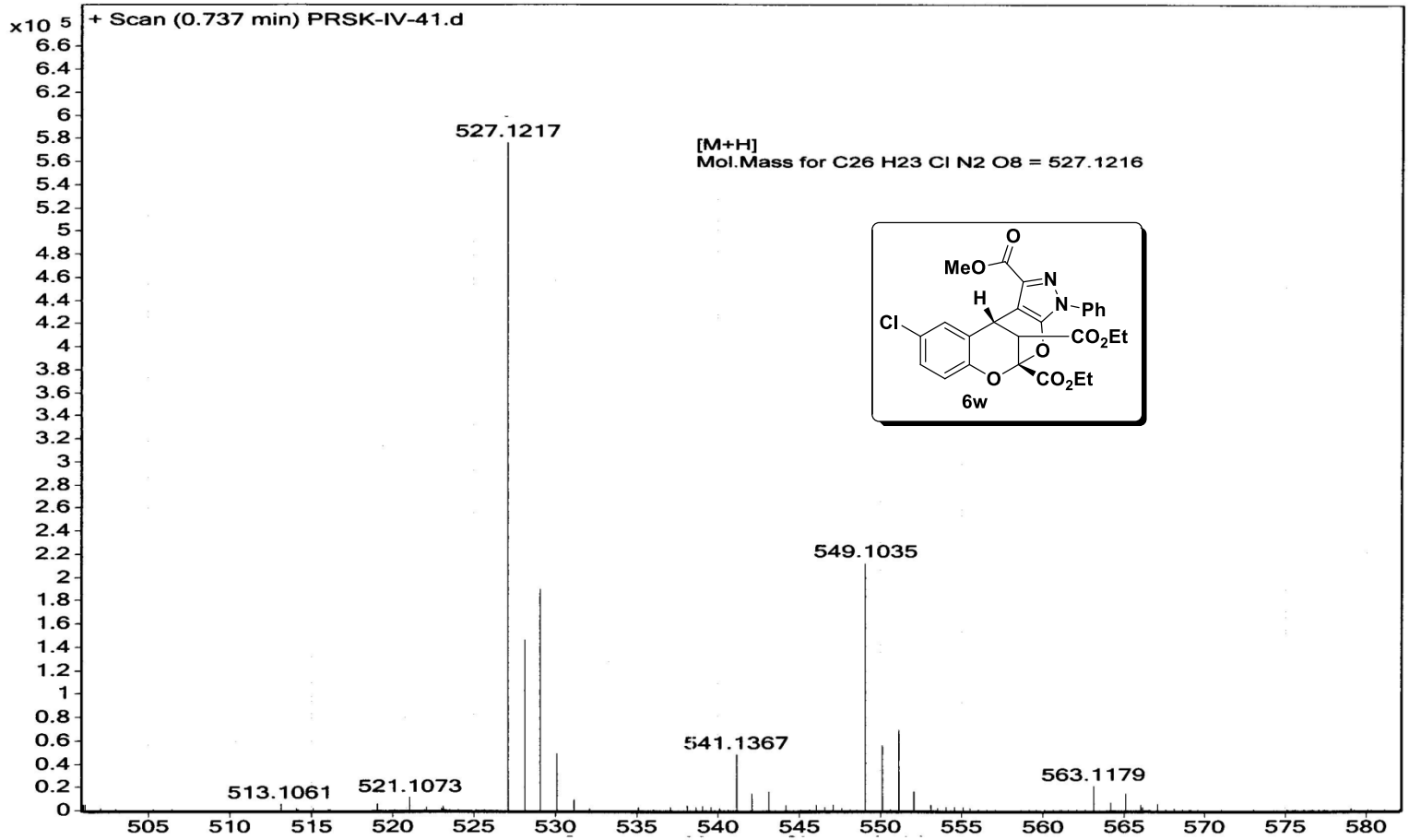
Sample Name	PRSK-IV-68	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-IV-68.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay-MB-520.1846	**Acquired Time**	16-09-2014 11:08:59

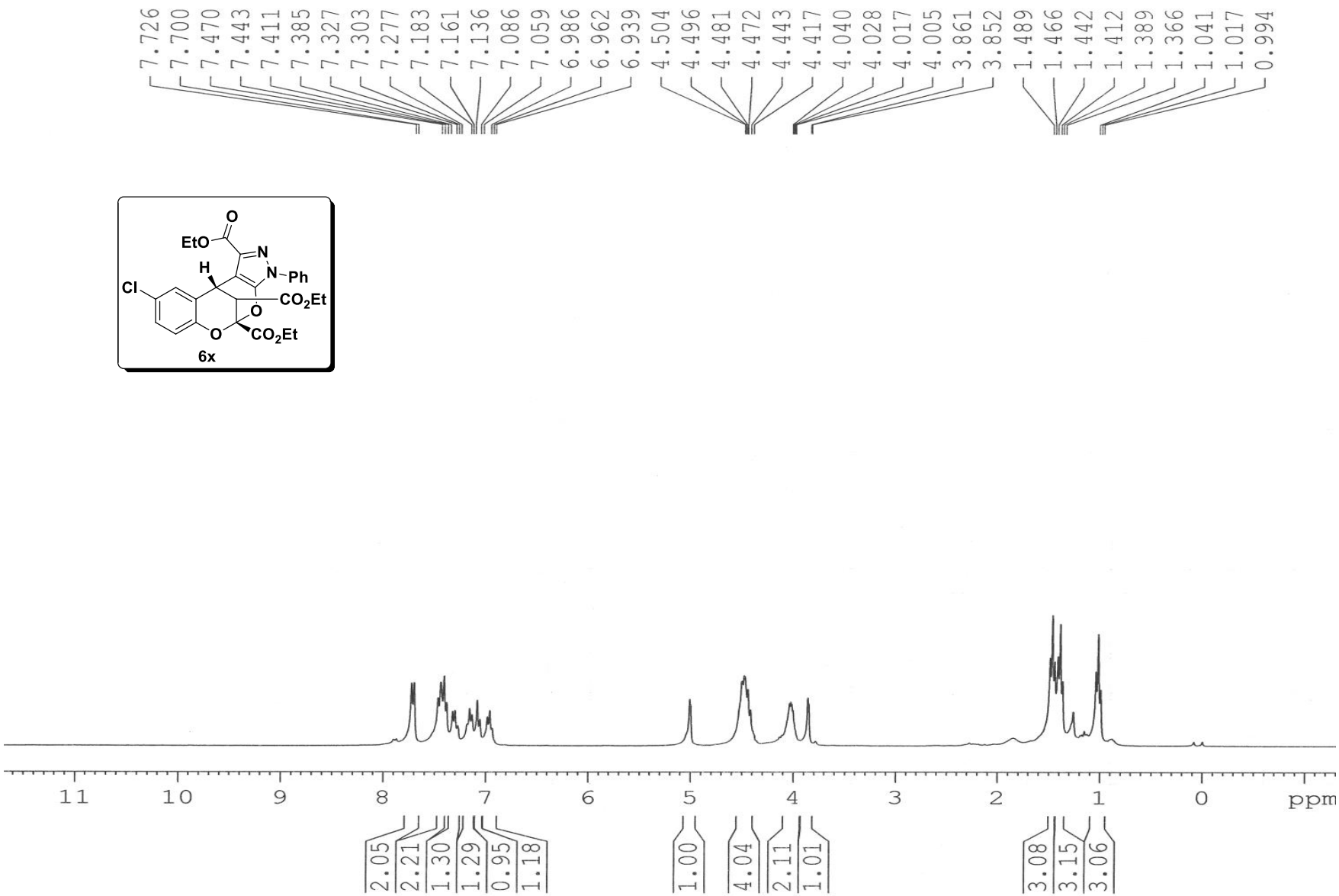


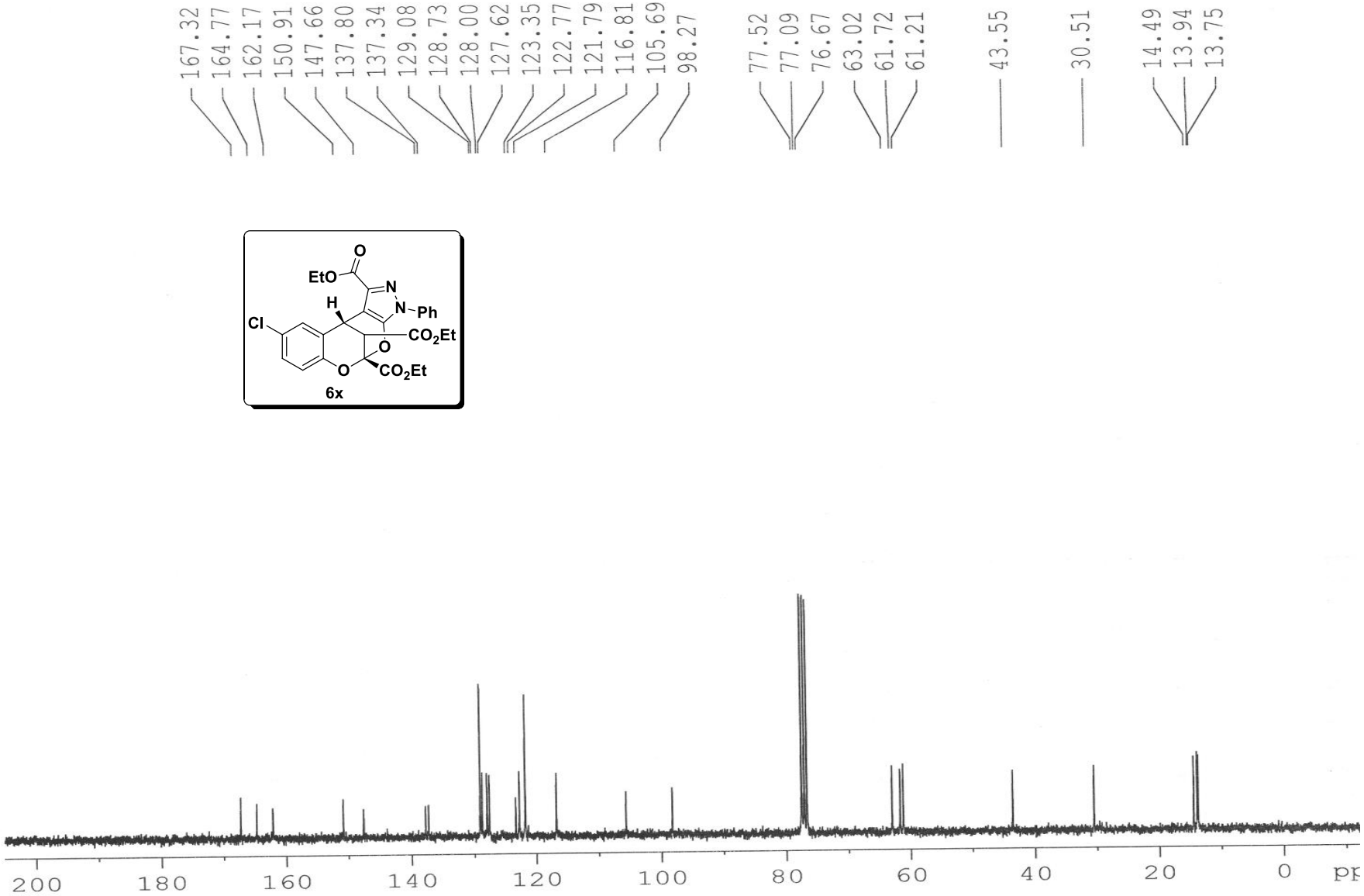

7.876
7.848
7.494
7.486
7.479
7.453
7.426
7.349
7.325
7.300
7.264
7.130
7.122
7.102
7.094
6.875
6.846
5.003
4.995
4.485
4.461
4.438
4.414
4.170
4.159
4.146
4.136
4.123
4.113
4.099
4.089
4.076
4.017
3.751
3.742
1.448
1.424
1.400
1.184
1.161
1.137
MeO
O
N
N-Ph
H
Cl
CO2Et
O
O
CO2Et
6w
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.08
3.11
1.01
1.08
1.00
1.02
2.29
2.18
3.04
1.03
3.16
3.01


166.81
164.43
162.37
149.21
137.84
137.36
129.14
128.50
127.60
127.57
127.40
127.17
121.30
117.78
103.66
98.18
77.44
77.02
76.60
63.16
62.01
52.17
42.91
29.69
13.95
13.91
MeO
O
N
N
Ph
H
Cl
CO2Et
O
O
CO2Et
6w
200
180
160
140
120
100
80
60
40
20
0
ppm

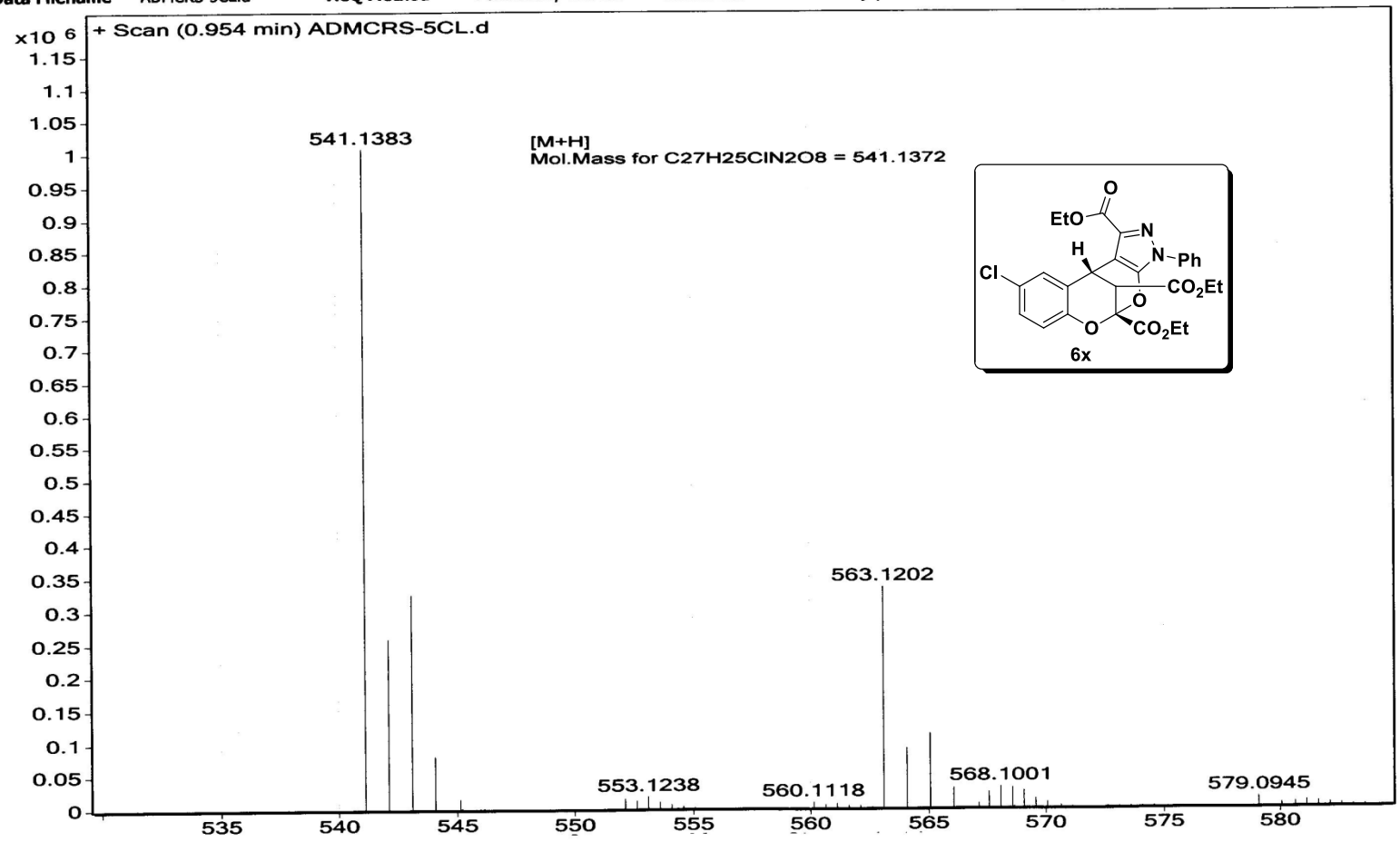
Sample Name	PRSK-IV-41	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-IV-41.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay-MB-526.1143	**Acquired Time**	19-09-2014 11:05:08

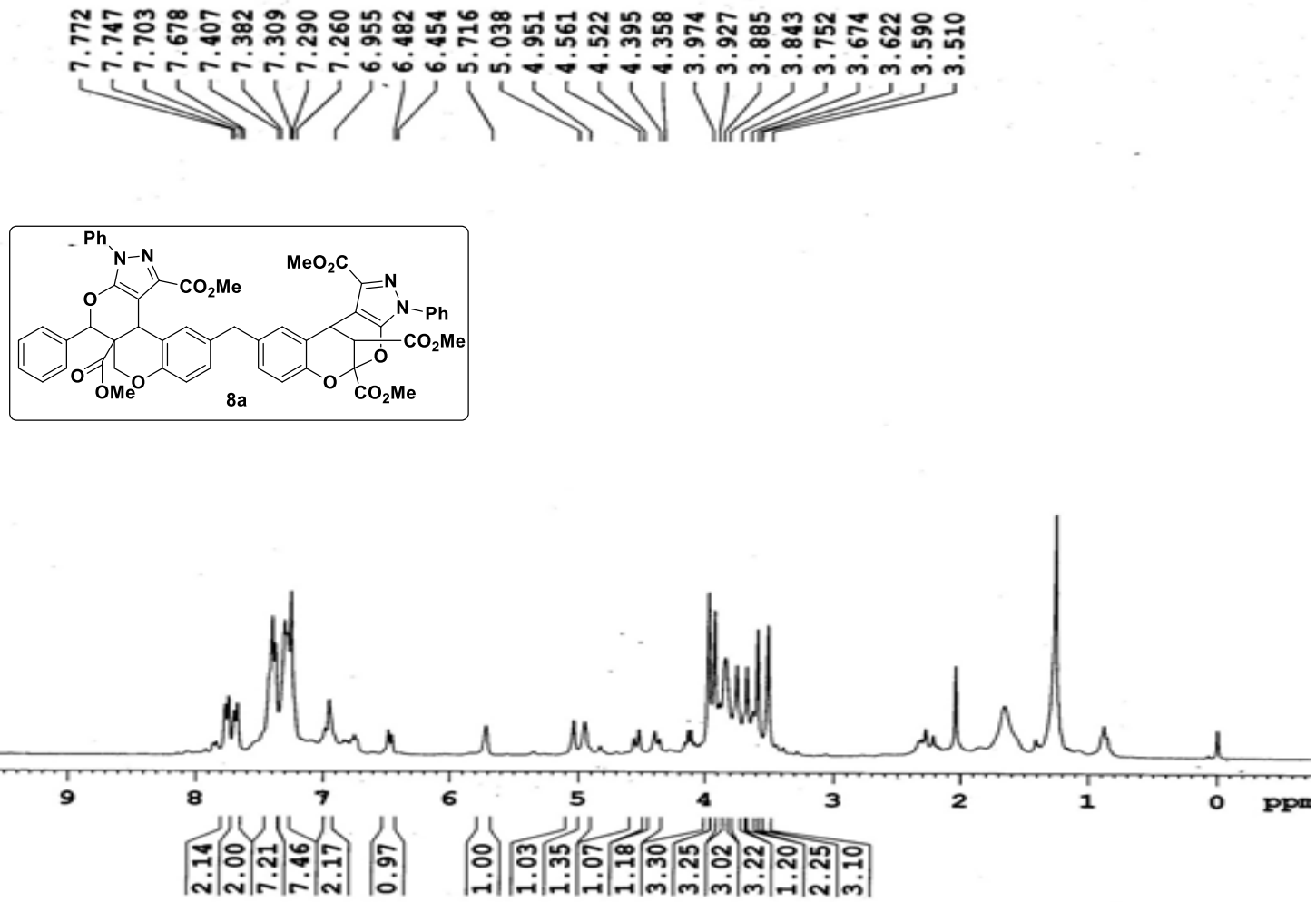


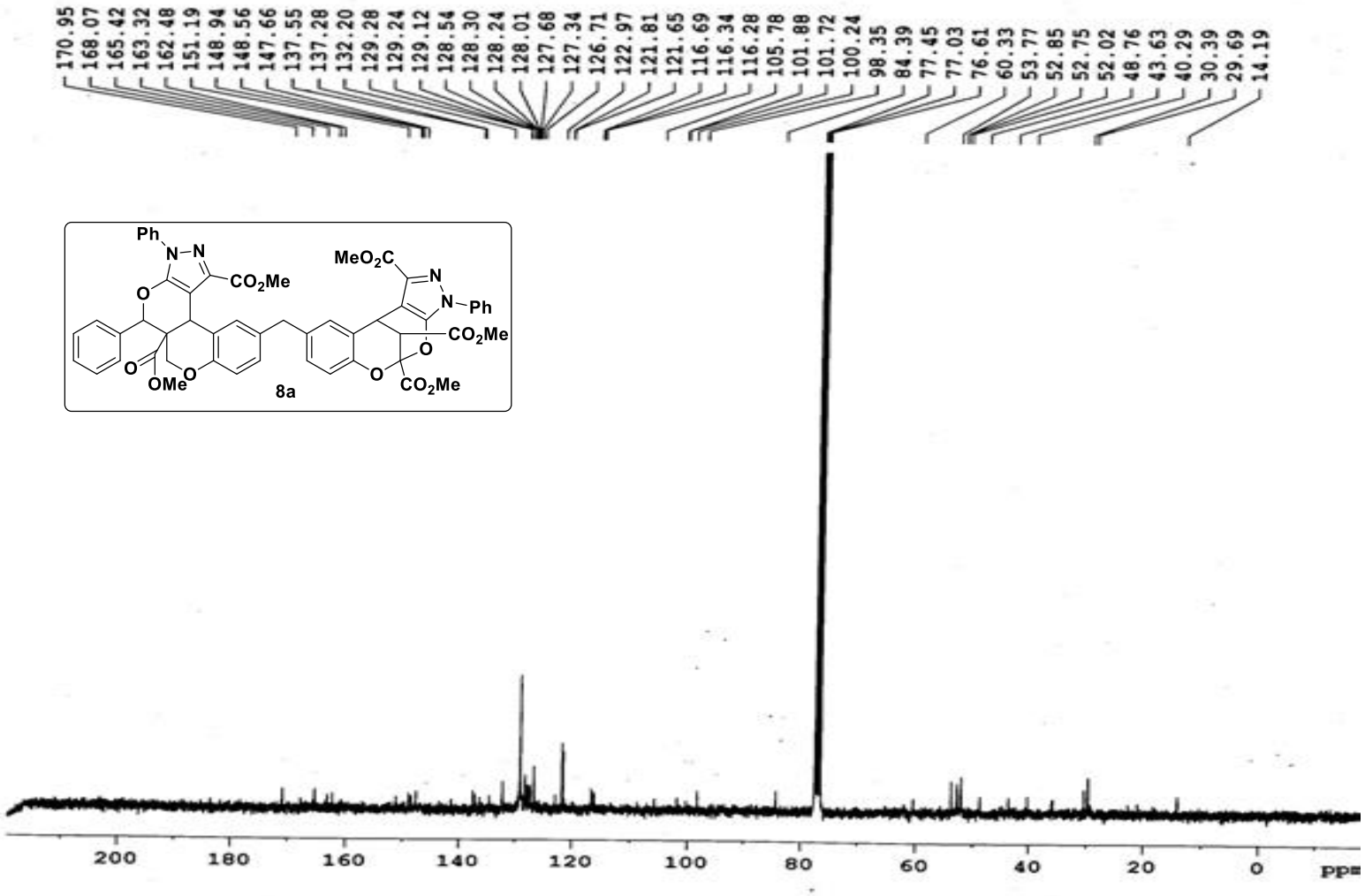

7.726
7.700
7.470
7.443
7.411
7.385
7.327
7.303
7.277
7.183
7.161
7.136
7.086
7.059
6.986
6.962
6.939
4.504
4.496
4.481
4.472
4.443
4.417
4.040
4.028
4.017
4.005
3.861
3.852
1.489
1.466
1.442
1.412
1.389
1.366
1.041
1.017
0.994
EtO
O
N
N
Ph
H
Cl
CO2Et
O
O
CO2Et
6x
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.05
2.21
1.30
1.29
0.95
1.18
1.00
4.04
2.11
1.01
3.08
3.15
3.06


167.32
164.77
162.17
150.91
147.66
137.80
137.34
129.08
128.73
128.00
127.62
123.35
122.77
121.79
116.81
105.69
98.27
77.52
77.09
76.67
63.02
61.72
61.21
43.55
30.51
14.49
13.94
13.75
EtO
O
N
N
Ph
H
Cl
CO2Et
O
O
CO2Et
6x
200
180
160
140
120
100
80
60
40
20
0
pp

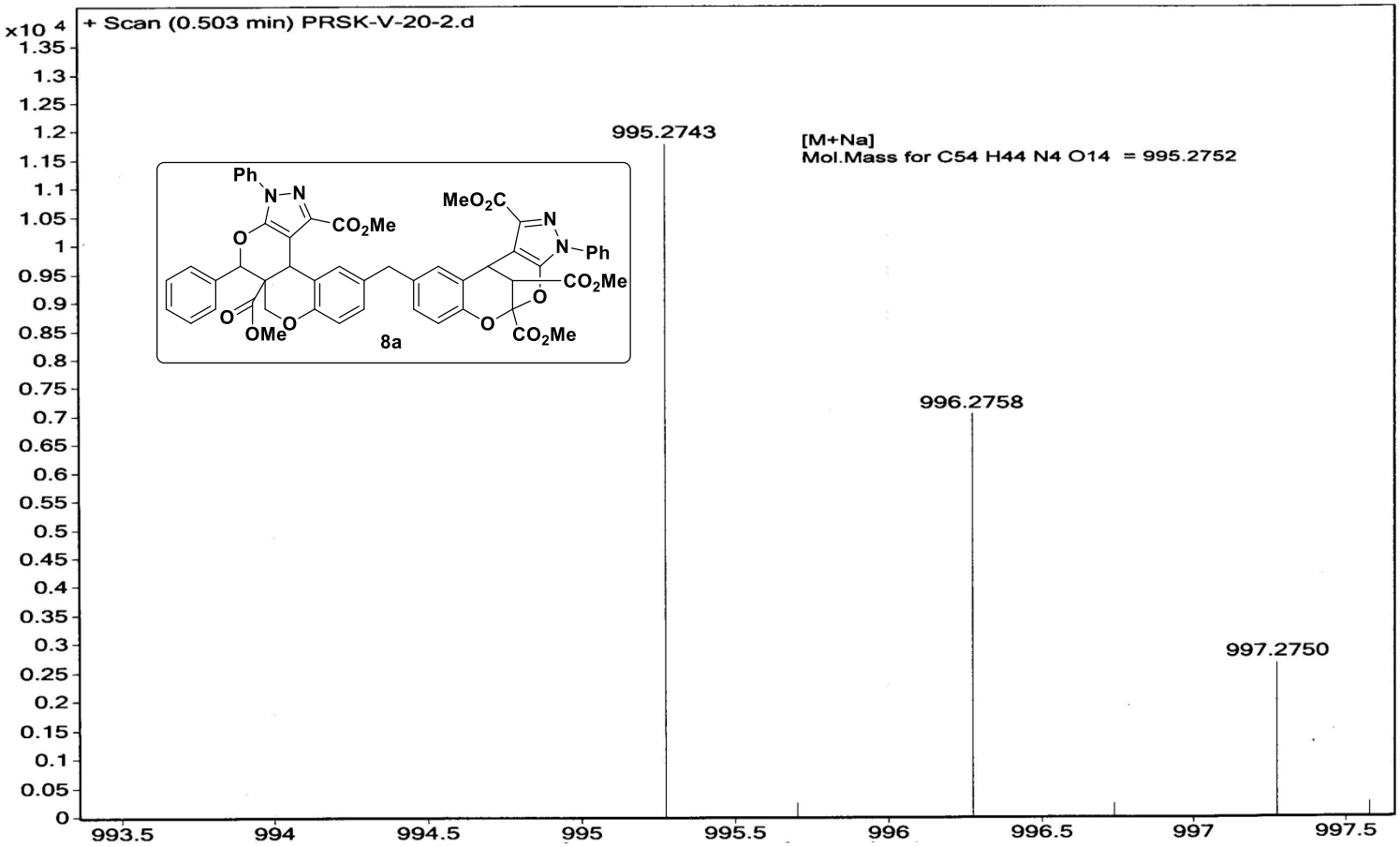
Sample Name	ADMCRS-5CL	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	ADMCRS-5CL.d	**ACQ Method**	Pondicherry Universi	**Comment**	Vijay-MB-540.1299	**Acquired Time**	19-09-2014 10:55:10

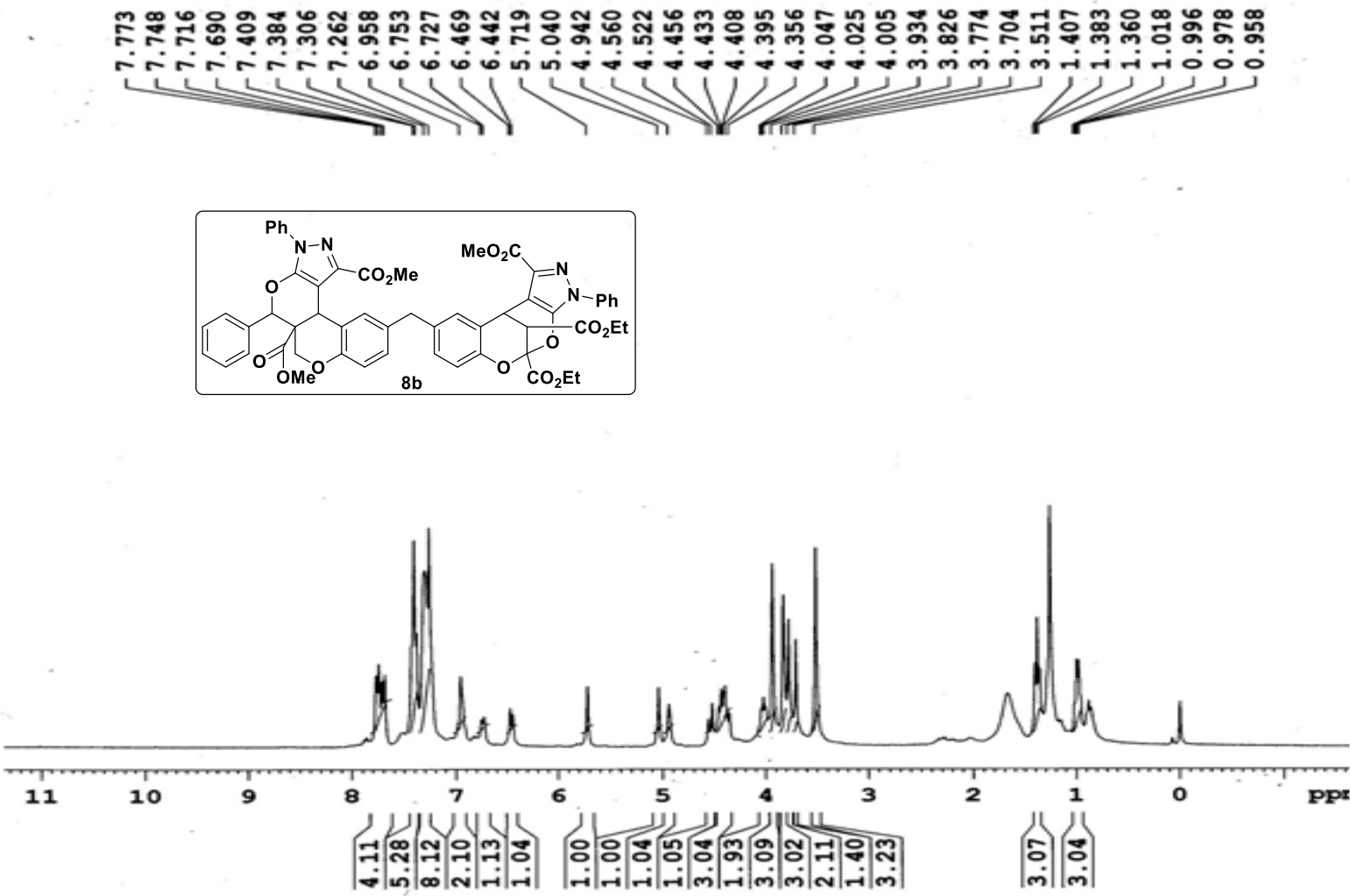


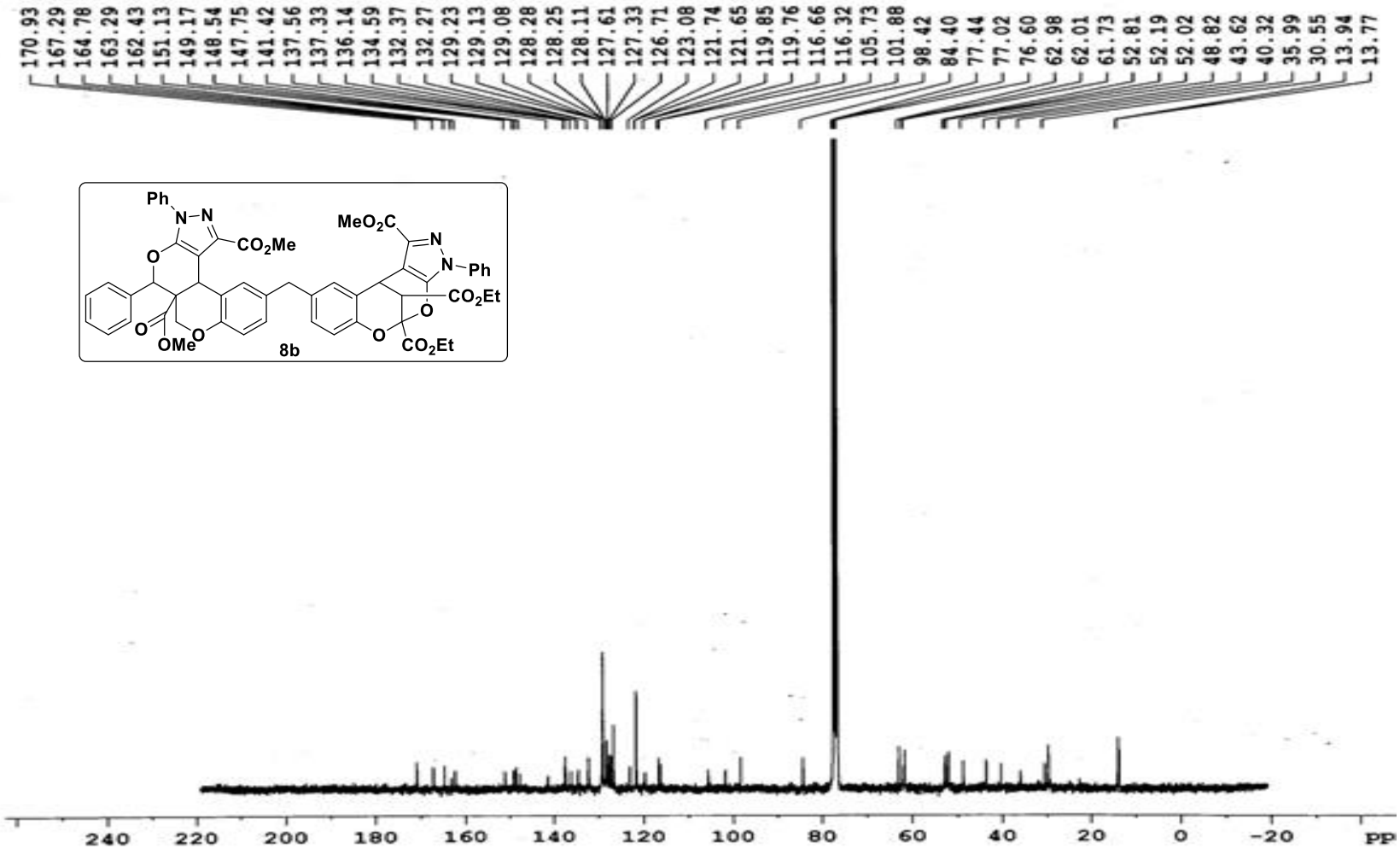

7.772
7.747
7.703
7.678
7.407
7.382
7.309
7.290
7.260
6.955
6.482
6.454
5.716
5.038
4.951
4.561
4.522
4.395
4.358
3.974
3.927
3.885
3.843
3.752
3.674
3.622
3.590
3.510
Ph
N–N
CO2Me
O
O
OMe
O
MeO2C
N
N–Ph
CO2Me
O
O
CO2Me
8a
10
9
8
7
6
5
4
3
2
1
0
ppm
2.14
2.00
7.21
7.46
2.17
0.97
1.00
1.03
1.35
1.07
1.18
3.30
3.25
3.02
3.22
1.20
2.25
3.10


170.95
168.07
165.42
163.32
162.48
151.19
148.94
148.56
147.66
137.55
137.28
132.20
129.28
129.24
129.12
128.54
128.30
128.24
128.01
127.68
127.34
126.71
122.97
121.81
121.65
116.69
116.34
116.28
105.78
101.88
101.72
100.24
98.35
84.39
77.45
77.03
76.61
60.33
53.77
52.85
52.75
52.02
48.76
43.63
40.29
30.39
29.69
14.19
Ph
N–N
CO2Me
O
O
OMe
O
MeO2C
N
N–Ph
CO2Me
O
O
CO2Me
8a
200
180
160
140
120
100
80
60
40
20
0
ppm

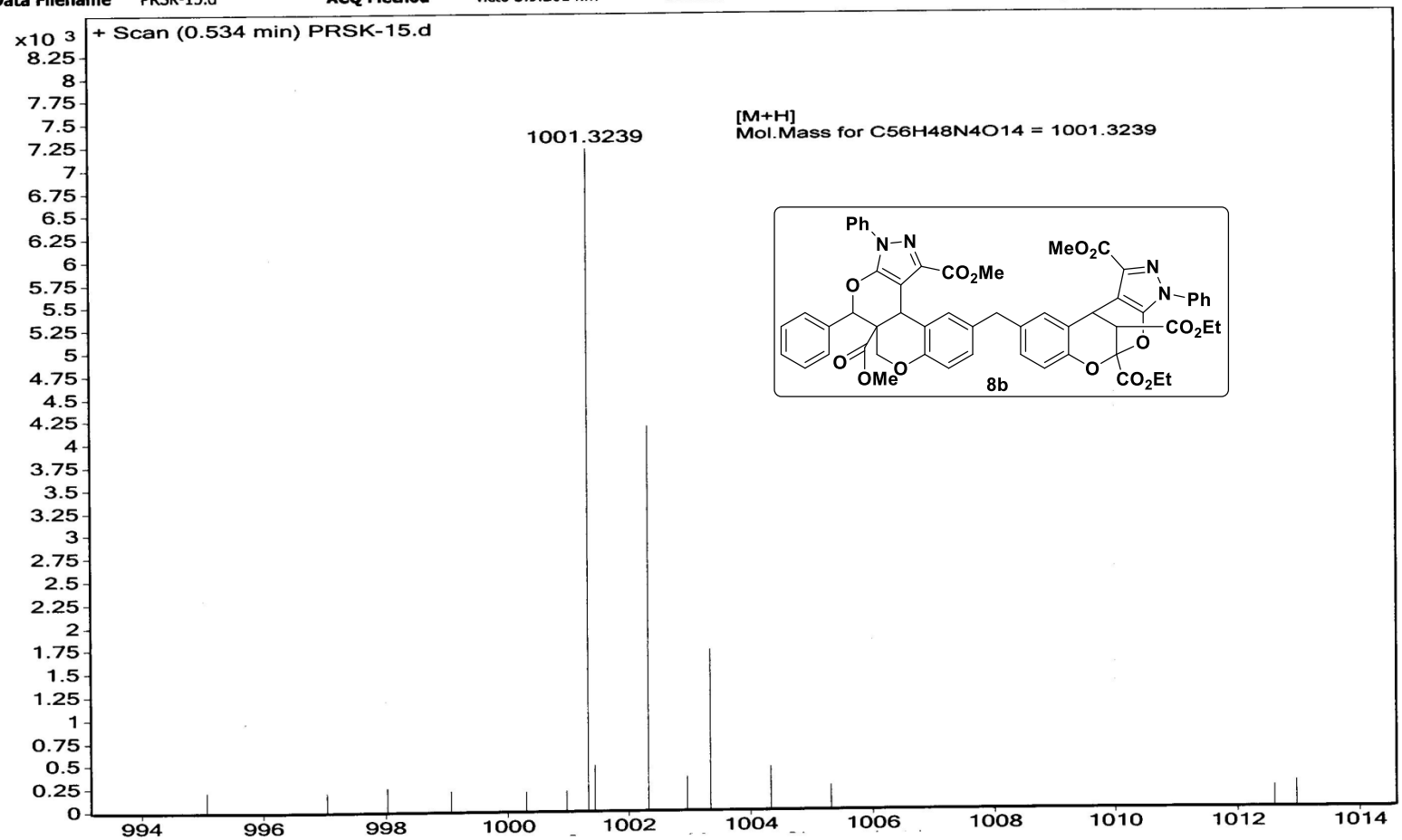
Sample Name	PRSK-V-20-2	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-V-20-2.d	**ACQ Method**	victo 3.9.2014.m	**Comment**	MB-ACN	**Acquired Time**	05-09-2014 12:40:57

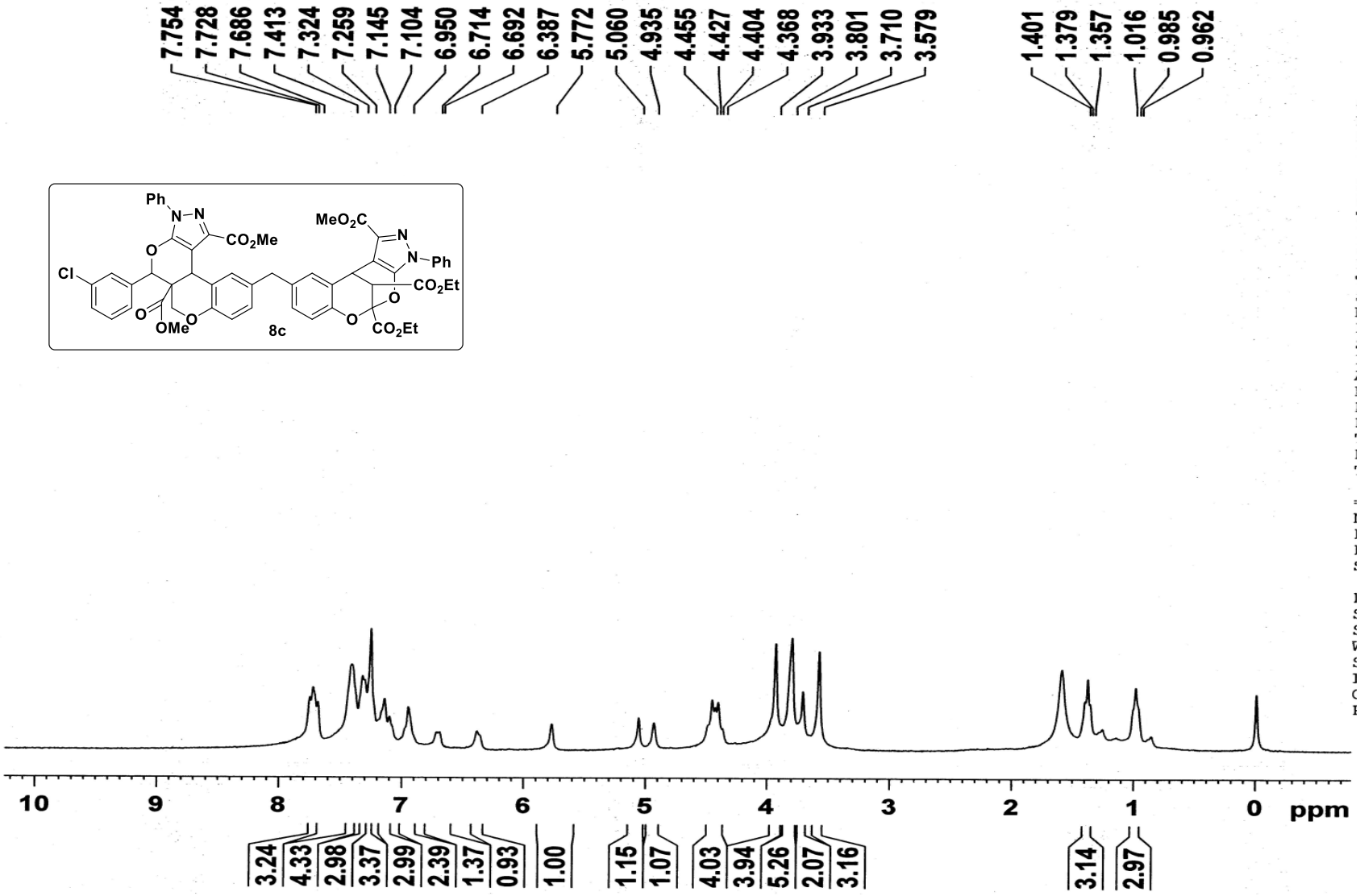


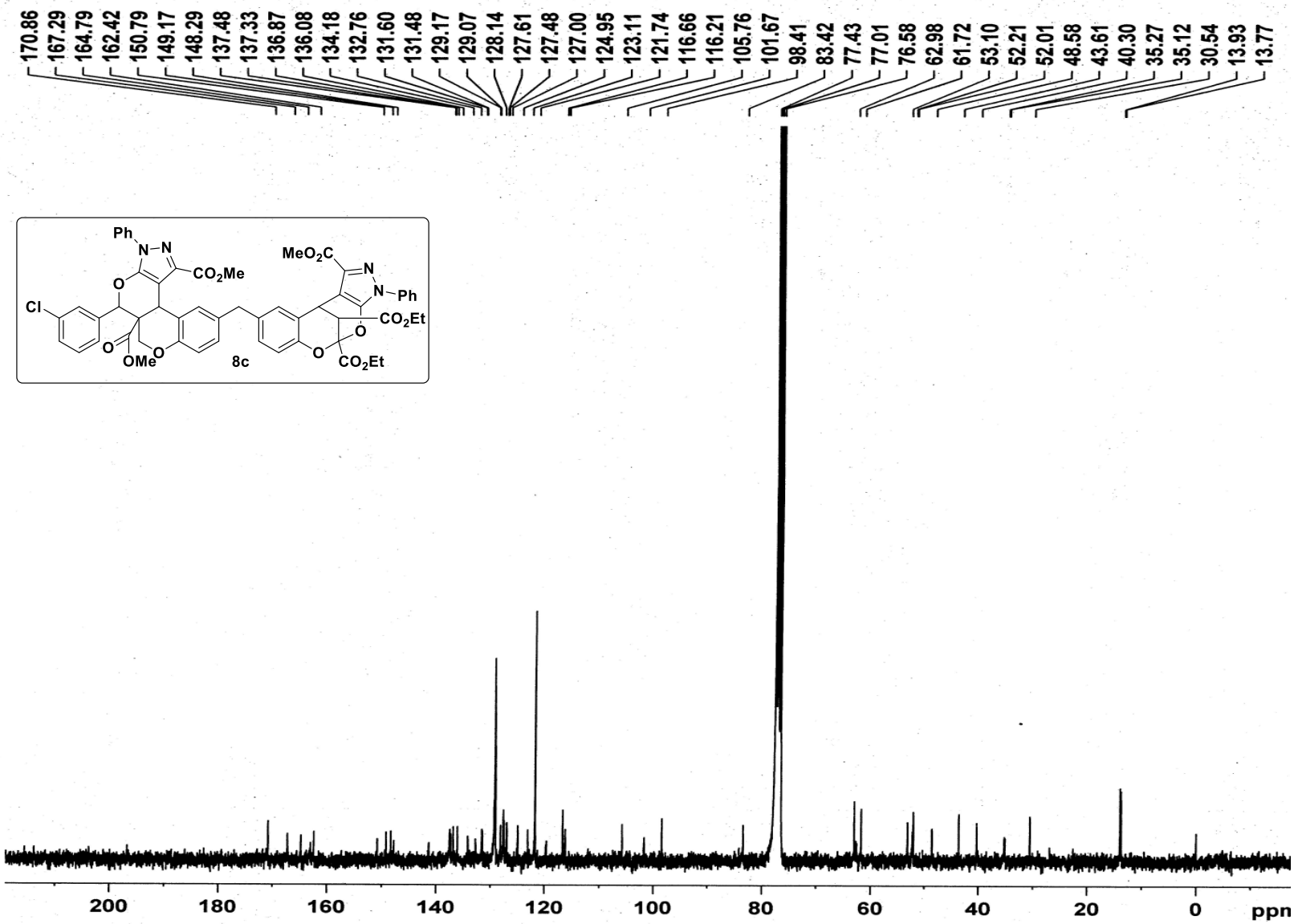

7.773
7.748
7.716
7.690
7.409
7.384
7.306
7.262
6.958
6.753
6.727
6.469
6.442
5.719
5.040
4.942
4.560
4.522
4.456
4.433
4.408
4.395
4.356
4.047
4.025
4.005
3.934
3.826
3.774
3.704
3.511
1.407
1.383
1.360
1.018
0.996
0.978
0.958
Ph
N–N
CO2Me
O
O
OMe
O
MeO2C
N
N–Ph
CO2Et
O
O
CO2Et
8b
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.11
5.28
8.12
2.10
1.13
1.04
1.00
1.00
1.04
1.05
3.04
1.93
3.09
3.02
2.11
1.40
3.23
3.07
3.04


170.93
167.29
164.78
163.29
162.43
151.13
149.17
148.54
147.75
141.42
137.56
137.33
136.14
134.59
132.37
132.27
129.23
129.13
129.08
128.28
128.25
128.11
127.61
127.33
126.71
123.08
121.74
121.65
119.85
119.76
116.66
116.32
105.73
101.88
98.42
84.40
77.44
77.02
76.60
62.98
62.01
61.73
52.81
52.19
52.02
48.82
43.62
40.32
35.99
30.55
13.94
13.77
Ph
N–N
CO2Me
O
O
OMe
O
MeO2C
N
N–Ph
CO2Et
O
O
CO2Et
8b
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
pp

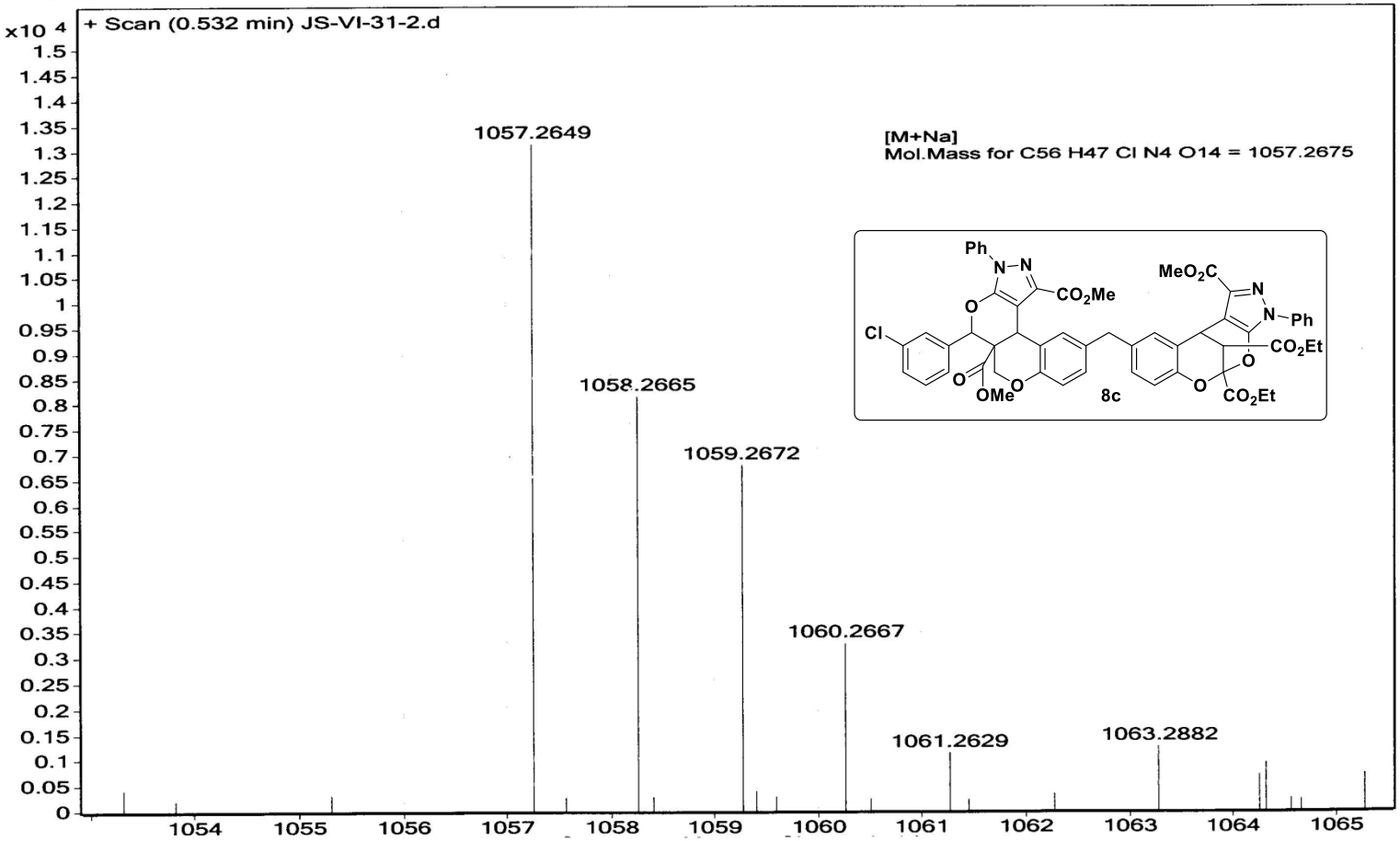
Sample Name	PRSK-15	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-15.d	**ACQ Method**	victo 3.9.2014.m	**Comment**	HSP-	**Acquired Time**	05-09-2014 12:04:37

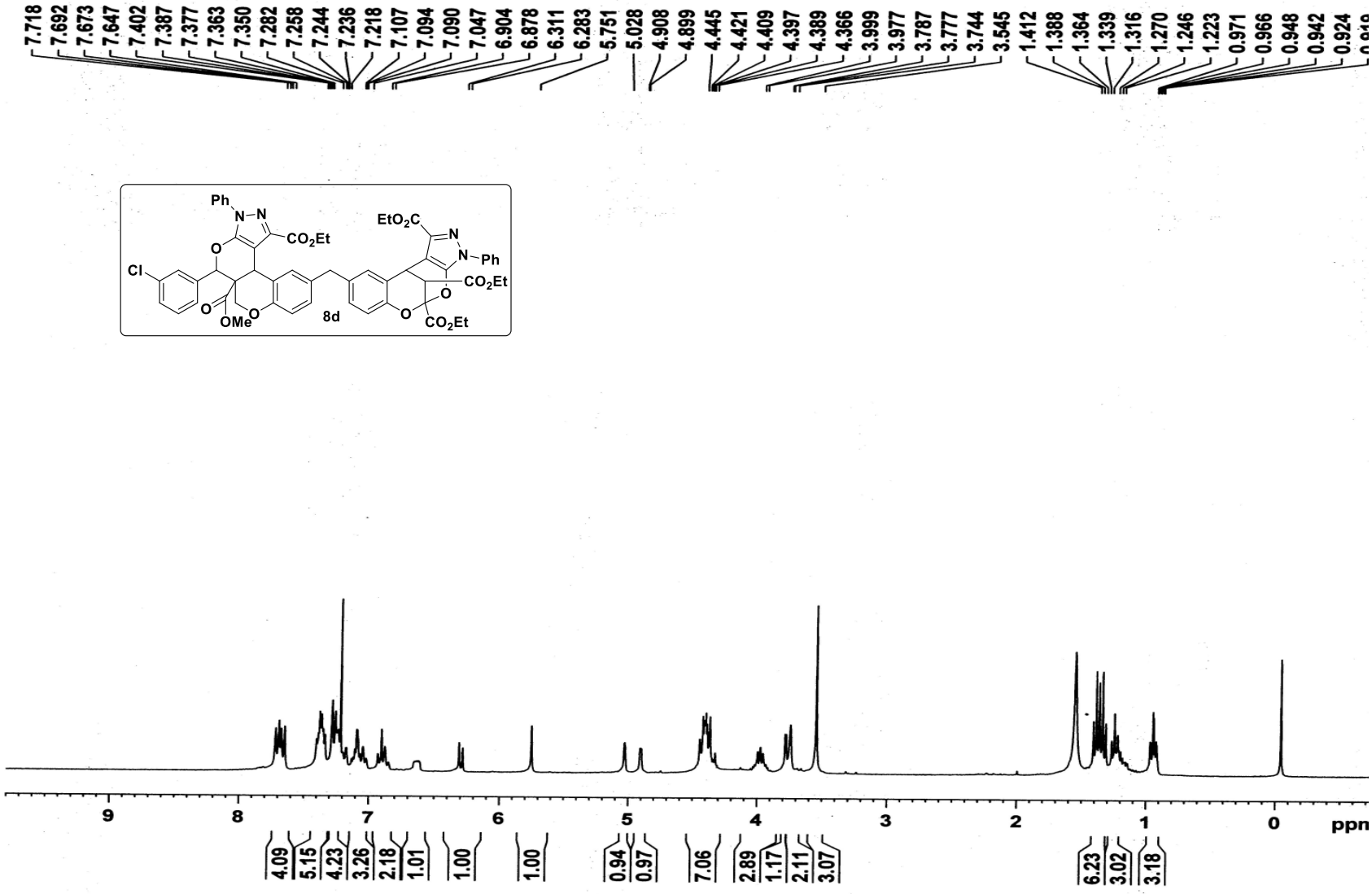


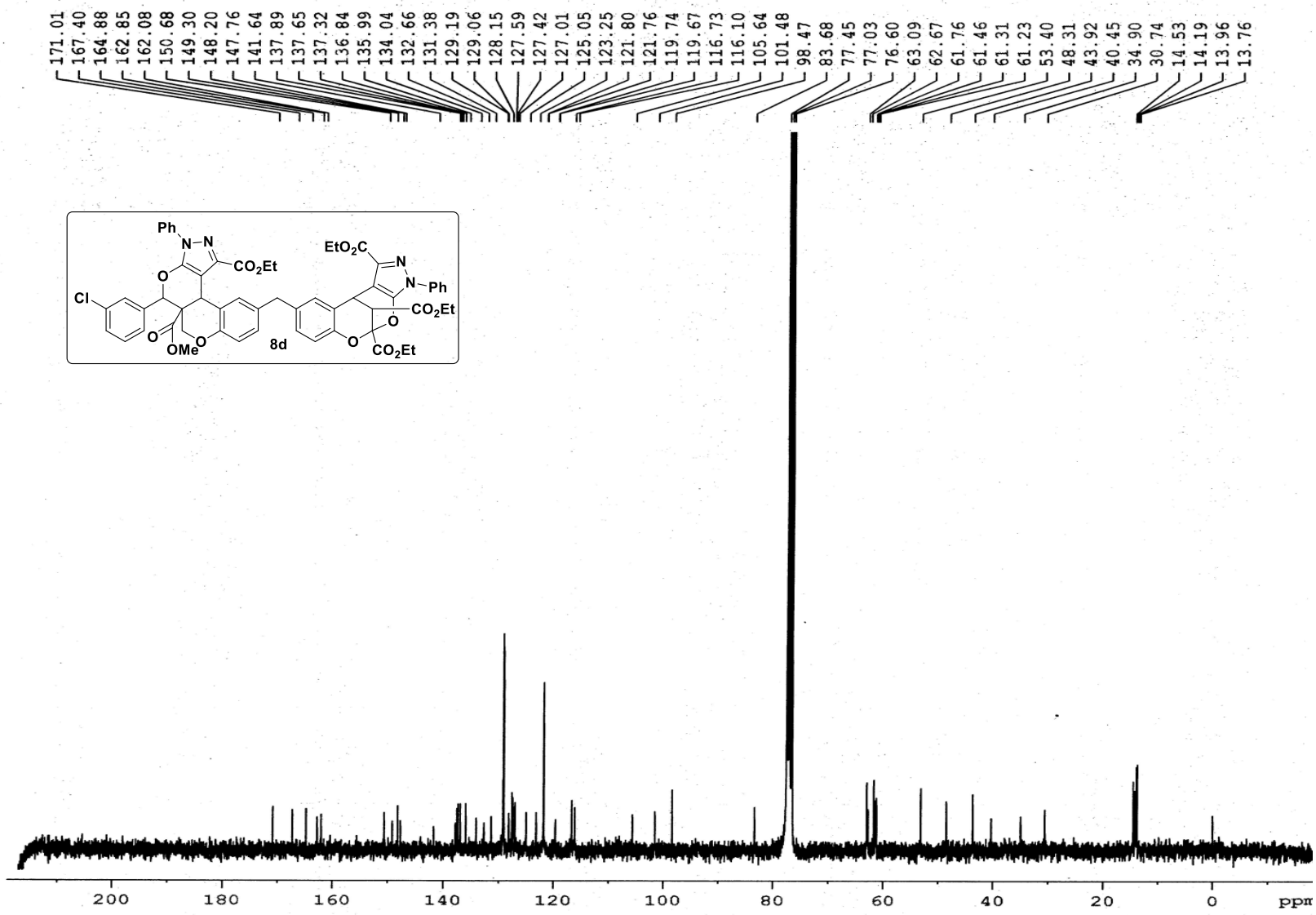

7.754
7.728
7.686
7.413
7.324
7.259
7.145
7.104
6.950
6.714
6.692
6.387
5.772
5.060
4.935
4.455
4.427
4.404
4.368
3.933
3.801
3.710
3.579
1.401
1.379
1.357
1.016
0.985
0.962
Ph
N–N
CO2Me
MeO2C
N
N–Ph
CO2Et
Cl
O
OMe
8c
CO2Et
10
9
8
7
6
5
4
3
2
1
0
ppm
3.24
4.33
2.98
3.37
2.99
2.39
1.37
0.93
1.00
1.15
1.07
4.03
3.94
5.26
2.07
3.16
3.14
2.97


170.86
167.29
164.79
162.42
150.79
149.17
148.29
137.48
137.33
136.87
136.08
134.18
132.76
131.60
131.48
129.17
129.07
128.14
127.61
127.48
127.00
124.95
123.11
121.74
116.66
116.21
105.76
101.67
98.41
83.42
77.43
77.01
76.58
62.98
61.72
53.10
52.21
52.01
48.58
43.61
40.30
35.27
35.12
30.54
13.93
13.77
Ph
N–N
CO2Me
O
Cl
O
OMe
O
8c
MeO2C
N
N–Ph
CO2Et
O
O
CO2Et
200
180
160
140
120
100
80
60
40
20
0
ppm

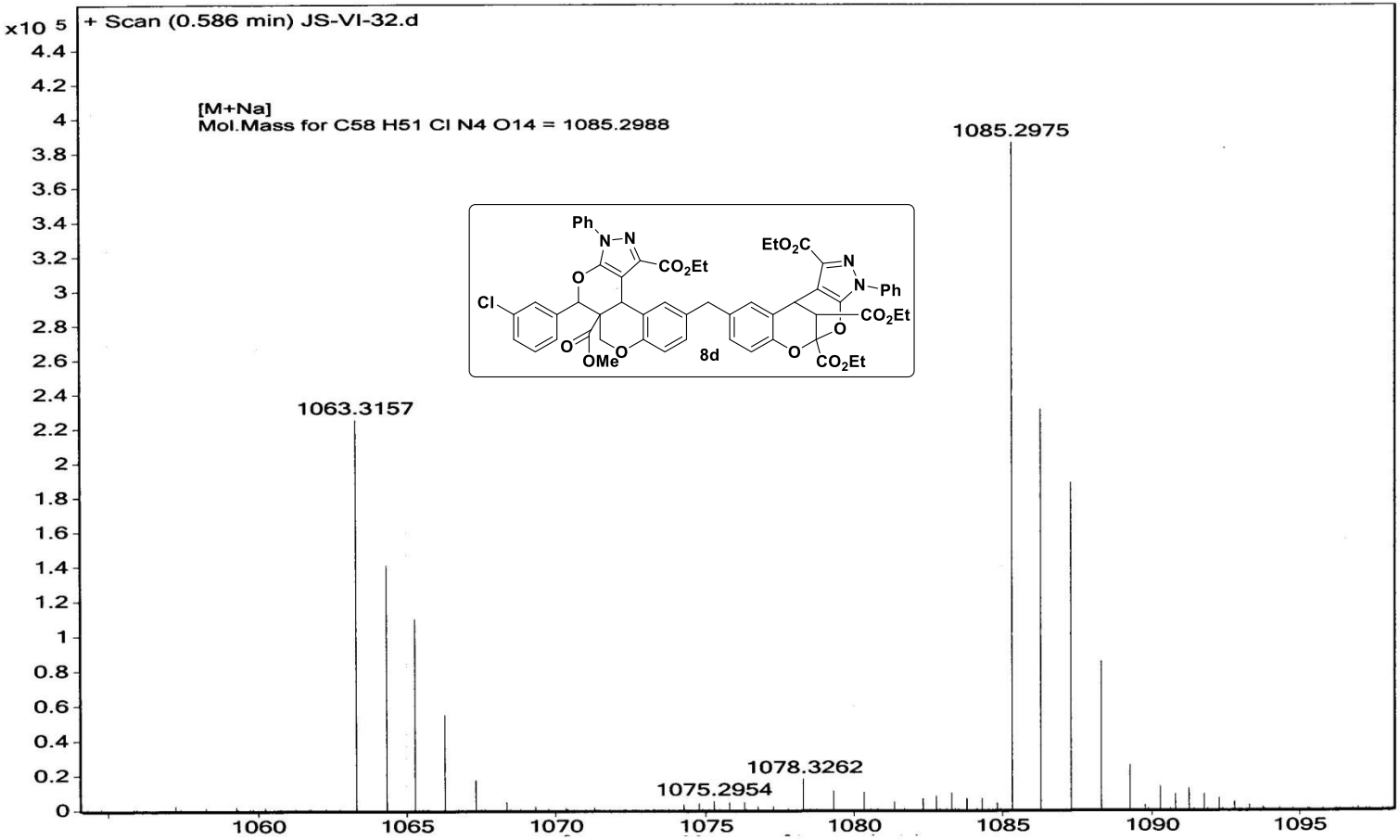
Sample Name	JS-VI-31-2	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	JS-VI-31-2.d	**ACQ Method**	victo 3.9.2014.m	**Comment**	MB-ACN	**Acquired Time**	05-09-2014 12:18:57

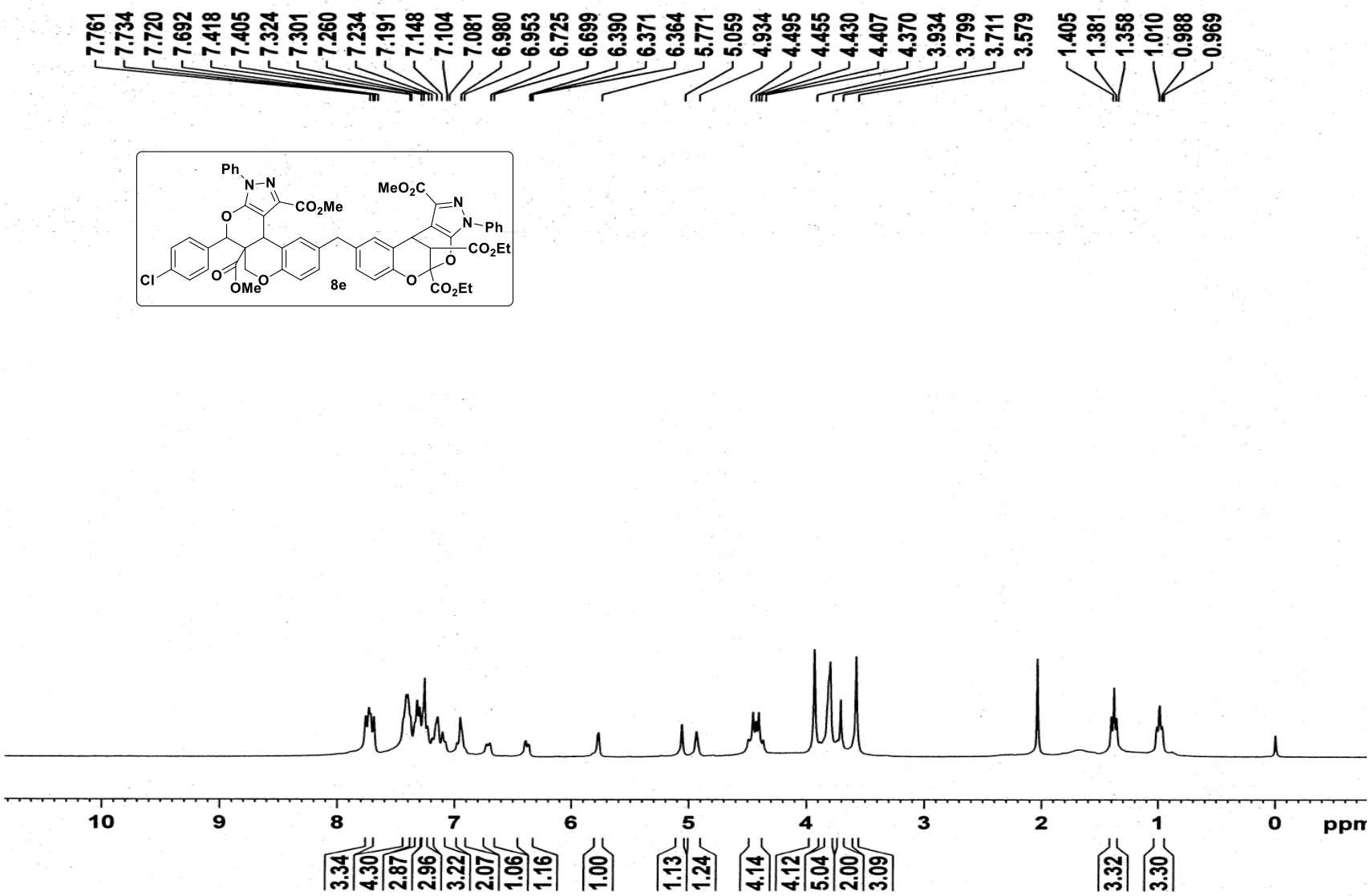


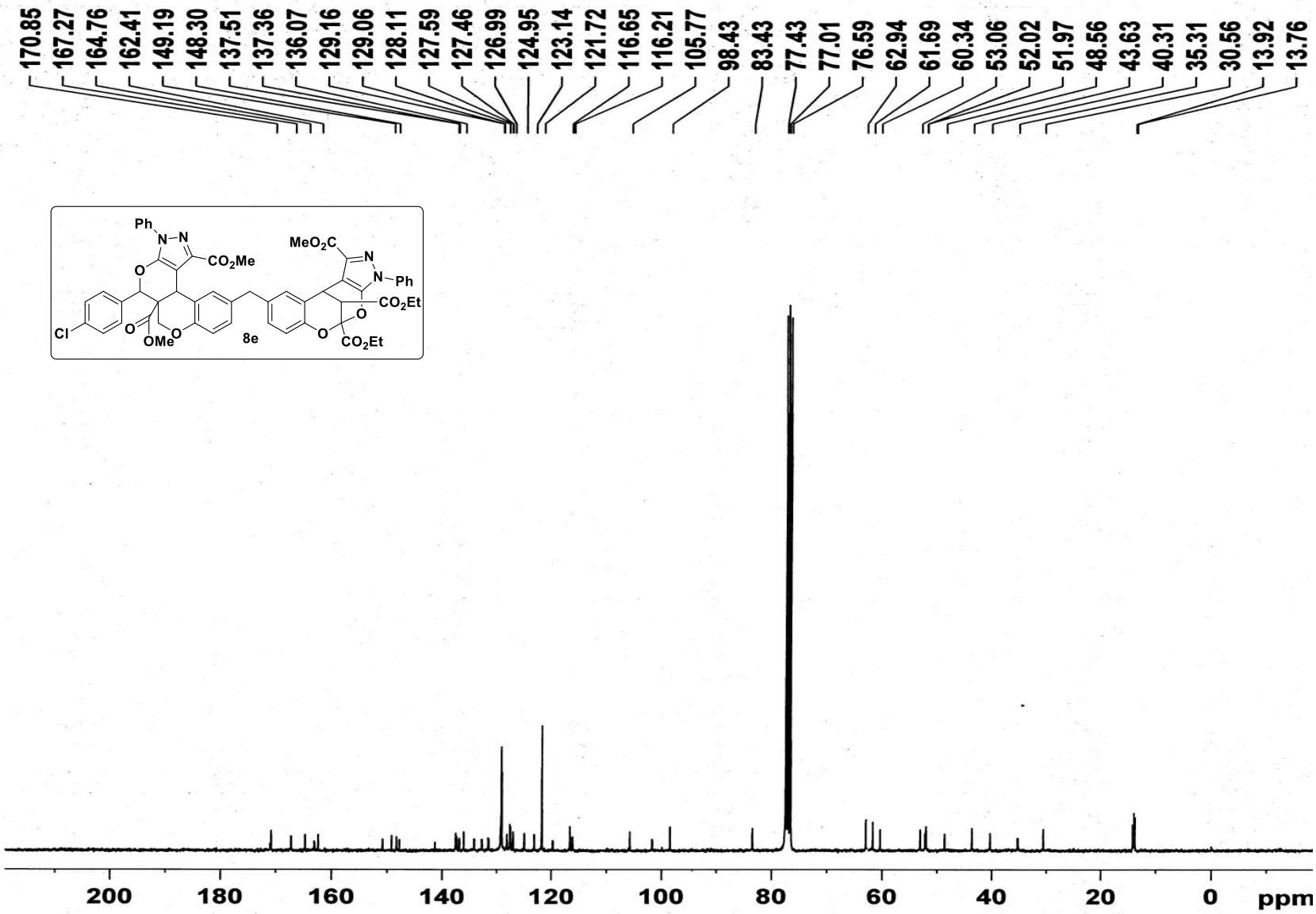

7.718
7.692
7.673
7.647
7.402
7.387
7.377
7.363
7.350
7.282
7.258
7.244
7.236
7.218
7.107
7.094
7.090
7.047
6.904
6.878
6.311
6.283
5.751
5.028
4.908
4.899
4.445
4.421
4.409
4.397
4.389
4.366
3.999
3.977
3.787
3.777
3.744
3.545
1.412
1.388
1.364
1.339
1.316
1.270
1.246
1.223
0.971
0.966
0.948
0.942
0.924
Ph
N–N
CO2Et
O
Cl
O
OMe
O
8d
EtO2C
N
N–Ph
CO2Et
O
O
CO2Et
9
8
7
6
5
4
3
2
1
0
ppm
4.09
5.15
4.23
3.26
2.18
1.01
1.00
1.00
0.94
0.97
7.06
2.89
1.17
2.11
3.07
6.23
3.02
3.18


171.01
167.40
164.88
162.85
162.08
150.68
149.30
148.20
147.76
141.64
137.89
137.65
137.32
136.84
135.99
134.04
132.66
131.38
129.19
129.06
128.15
127.59
127.42
127.01
125.05
123.25
121.80
121.76
119.74
119.67
116.73
116.10
105.64
101.48
98.47
83.68
77.45
77.03
76.60
63.09
62.67
61.76
61.46
61.31
61.23
53.40
48.31
43.92
40.45
34.90
30.74
14.53
14.19
13.96
13.76
Ph
N–N
CO2Et
O
Cl
O
OMe
O
8d
EtO2C
N
N–Ph
CO2Et
O
O
CO2Et
200
180
160
140
120
100
80
60
40
20
0
ppm

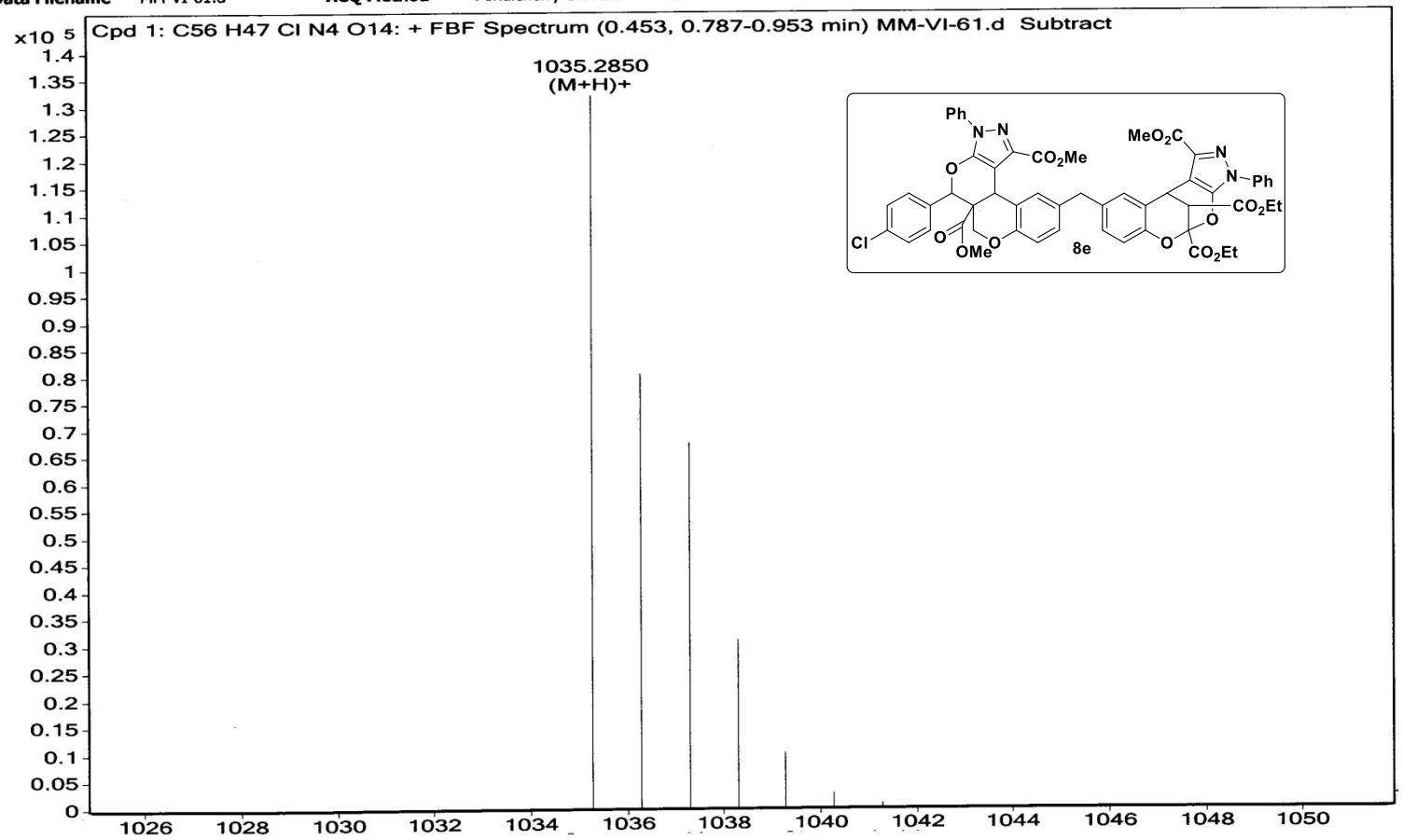
Sample Name	JS-VI-32	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	JS-VI-32.d	**ACQ Method**	victo 3.9.2014.m	**Comment**	MB-ACN	**Acquired Time**	05-09-2014 12:50:04

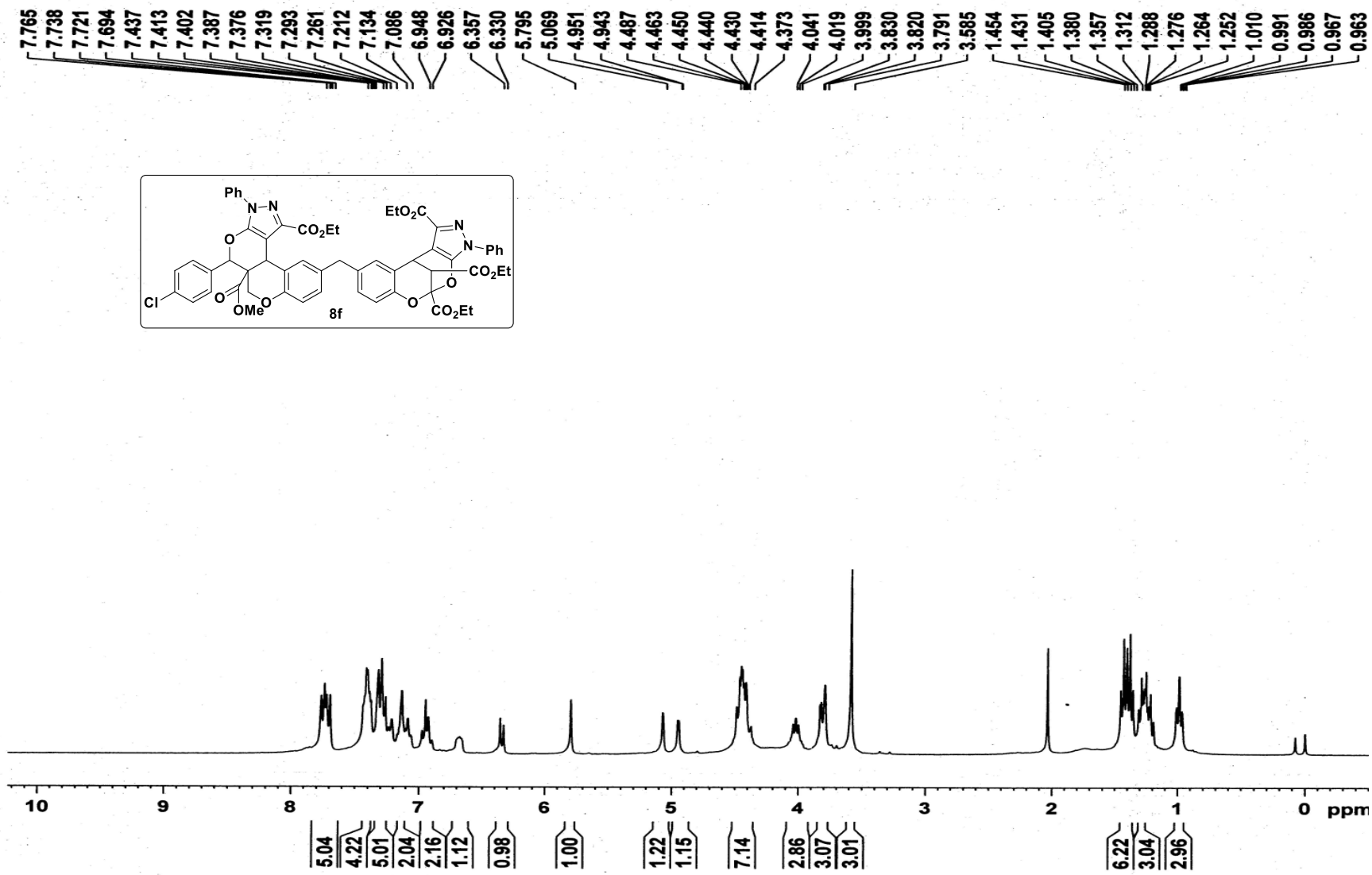


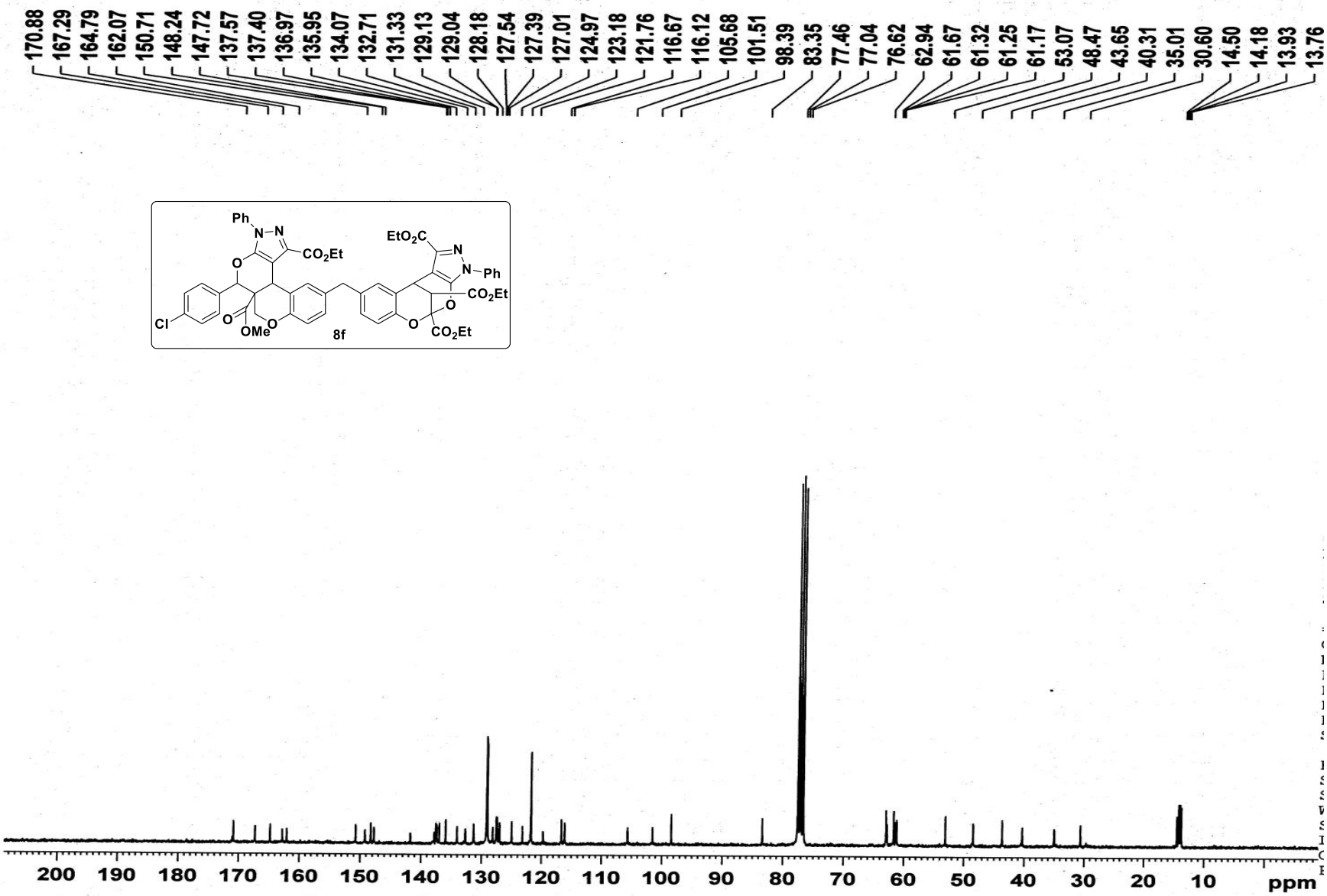

7.761
7.734
7.720
7.692
7.418
7.405
7.324
7.301
7.260
7.234
7.191
7.148
7.104
7.081
6.980
6.953
6.725
6.699
6.390
6.371
6.364
5.771
5.059
4.934
4.495
4.455
4.430
4.407
4.370
3.934
3.799
3.711
3.579
1.405
1.381
1.358
1.010
0.988
0.969
Ph
N–N
CO2Me
MeO2C
N
N–Ph
CO2Et
O
Cl
OMe
8e
CO2Et
10
9
8
7
6
5
4
3
2
1
0
ppm
3.34
4.30
2.87
2.96
3.22
2.07
1.06
1.16
1.00
1.13
1.24
4.14
4.12
5.04
2.00
3.09
3.32
3.30


170.85
167.27
164.76
162.41
149.19
148.30
137.51
137.36
136.07
129.16
129.06
128.11
127.59
127.46
126.99
124.95
123.14
121.72
116.65
116.21
105.77
98.43
83.43
77.43
77.01
76.59
62.94
61.69
60.34
53.06
52.02
51.97
48.56
43.63
40.31
35.31
30.56
13.92
13.76
Ph
N–N
CO2Me
O
Cl
O
OMe
O
8e
MeO2C
N
N–Ph
CO2Et
O
O
CO2Et
200
180
160
140
120
100
80
60
40
20
0
ppm

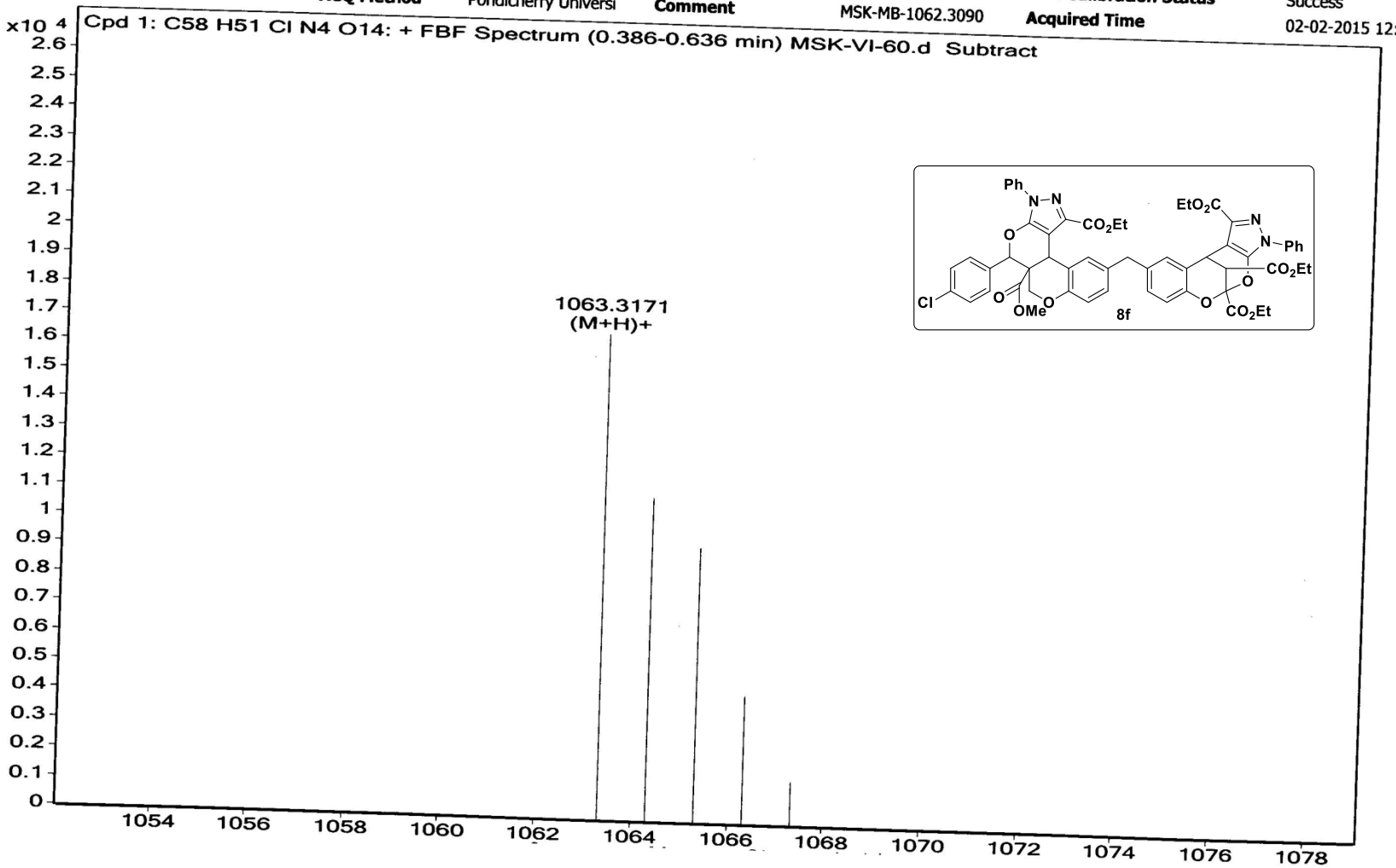
Sample Name	MM-VI-61	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-VI-61.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-1034.2777	**Acquired Time**	05-03-2015 10:57:09

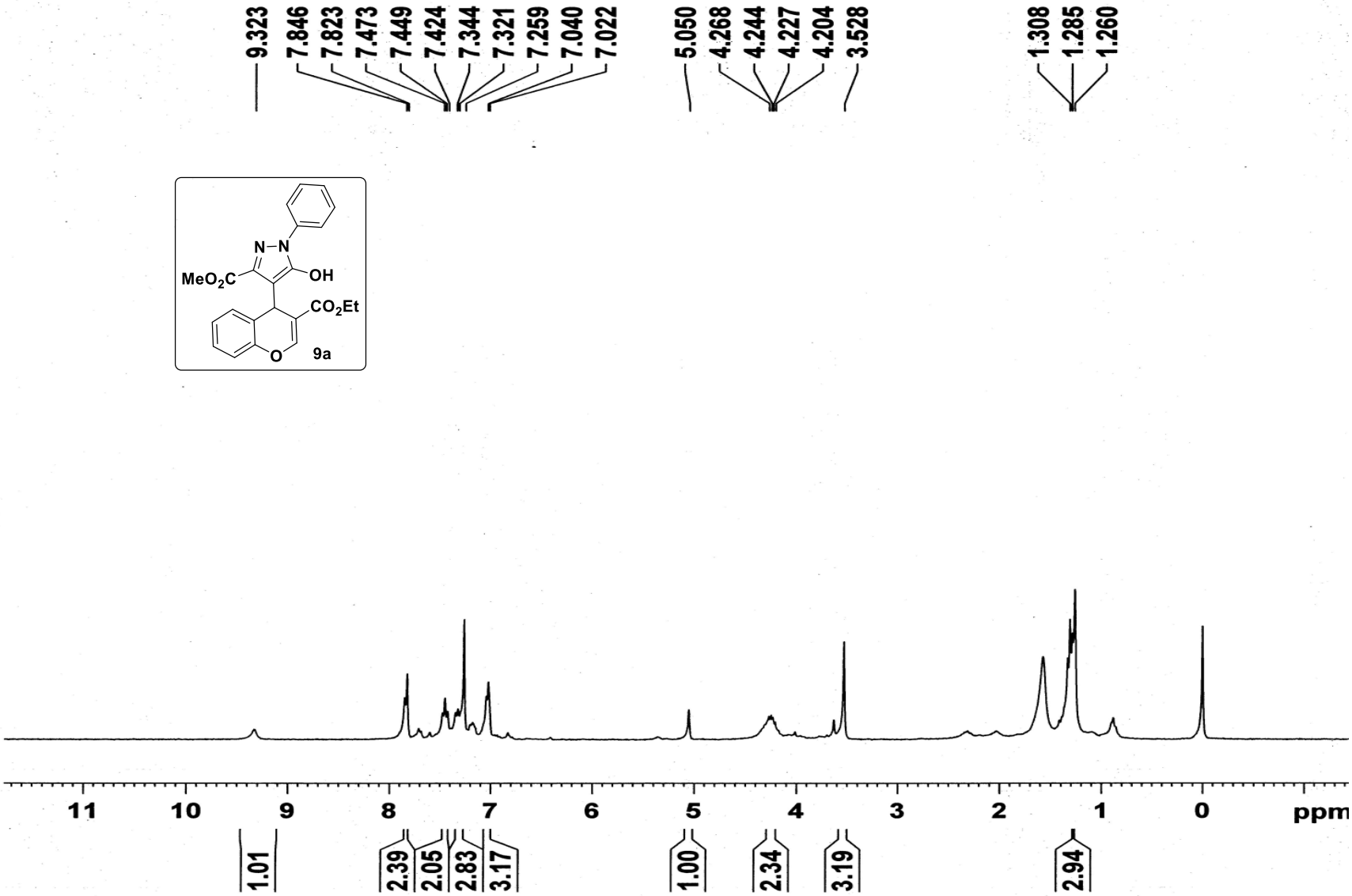


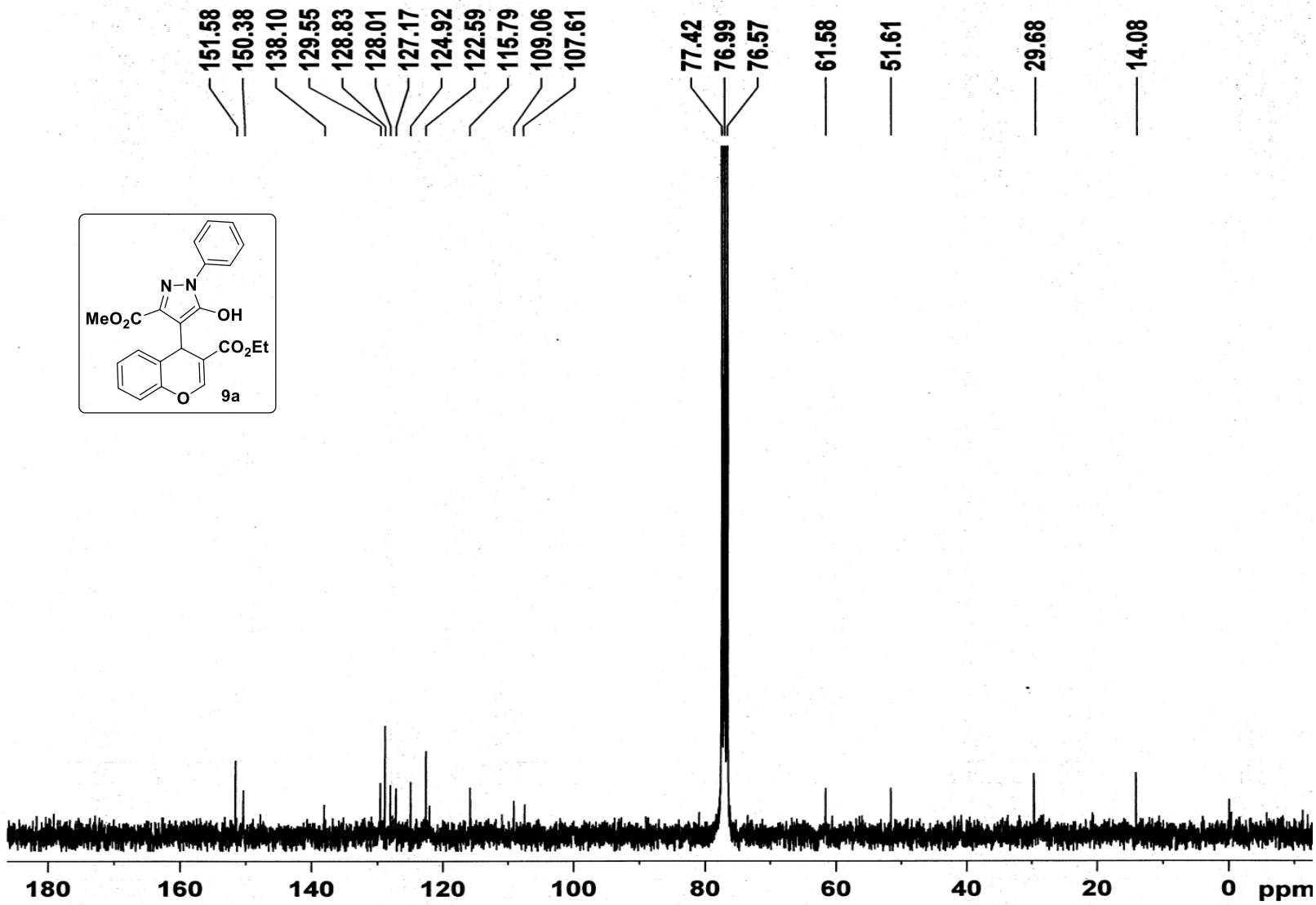

7.765
7.738
7.721
7.694
7.437
7.413
7.402
7.387
7.376
7.319
7.293
7.261
7.212
7.134
7.086
6.948
6.926
6.357
6.330
5.795
5.069
4.951
4.943
4.487
4.463
4.450
4.440
4.430
4.414
4.373
4.041
4.019
3.999
3.830
3.820
3.791
3.585
1.454
1.431
1.405
1.380
1.357
1.312
1.288
1.276
1.264
1.252
1.010
0.991
0.986
0.967
0.963
Ph
N–N
CO2Et
O
Cl
O
OMe
O
EtO2C
N
N–Ph
CO2Et
O
O
CO2Et
8f
10
9
8
7
6
5
4
3
2
1
0
ppm
5.04
4.22
5.01
2.04
2.16
1.12
0.98
1.00
1.22
1.15
7.14
2.86
3.07
3.01
6.22
3.04
2.96


170.88
167.29
164.79
162.07
150.71
148.24
147.72
137.57
137.40
136.97
135.95
134.07
132.71
131.33
129.13
129.04
128.18
127.54
127.39
127.01
124.97
123.18
121.76
116.67
116.12
105.68
101.51
98.39
83.35
77.46
77.04
76.62
62.94
61.67
61.32
61.25
61.17
53.07
48.47
43.65
40.31
35.01
30.60
14.50
14.18
13.93
13.76
Ph
N–N
CO2Et
O
Cl
O
OMe
O
8f
EtO2C
N
N–Ph
CO2Et
O
O
CO2Et
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

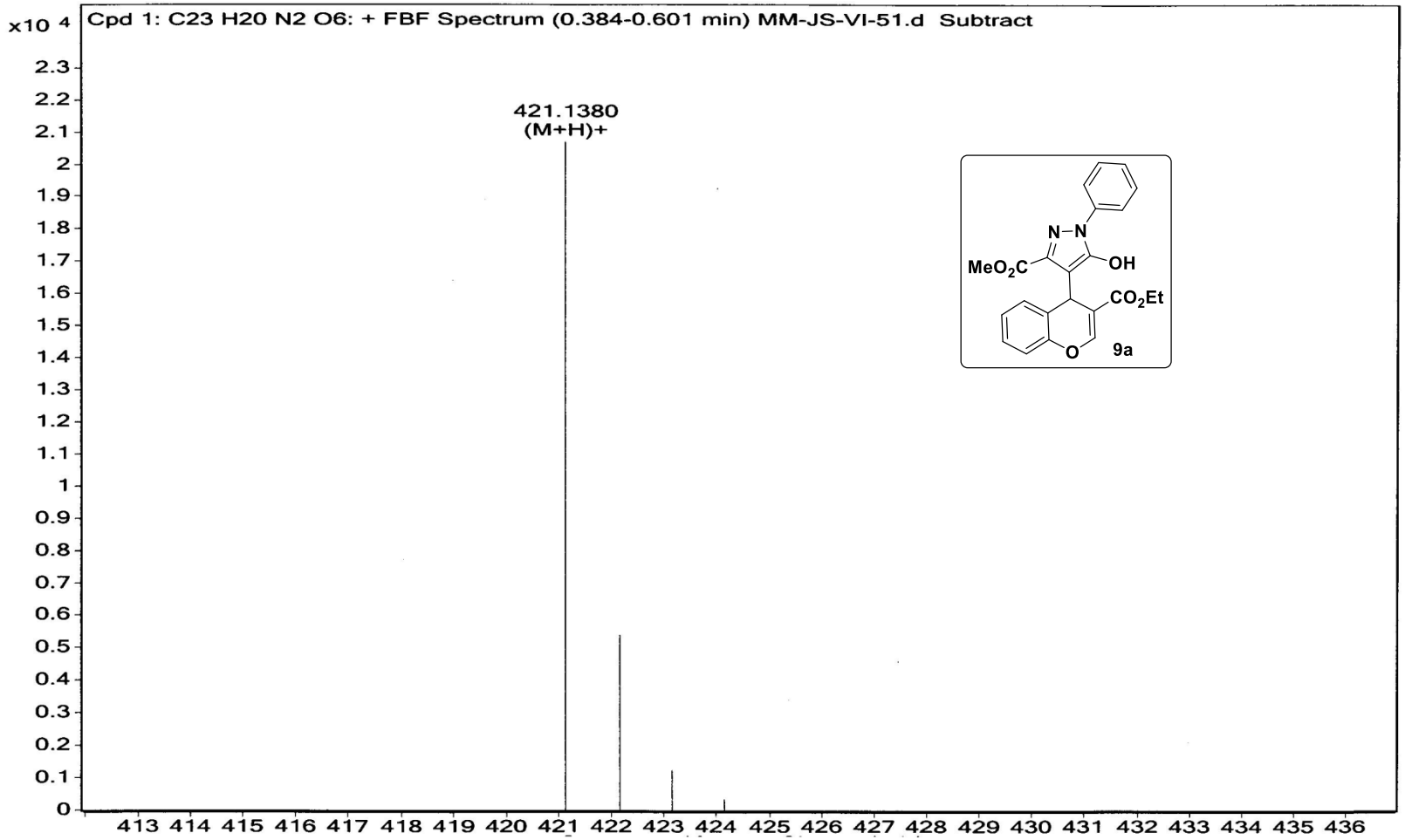
Sample Name	MSK-VI-60	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MSK-VI-60.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-1062.3090	**Acquired Time**	02-02-2015 12:29:49

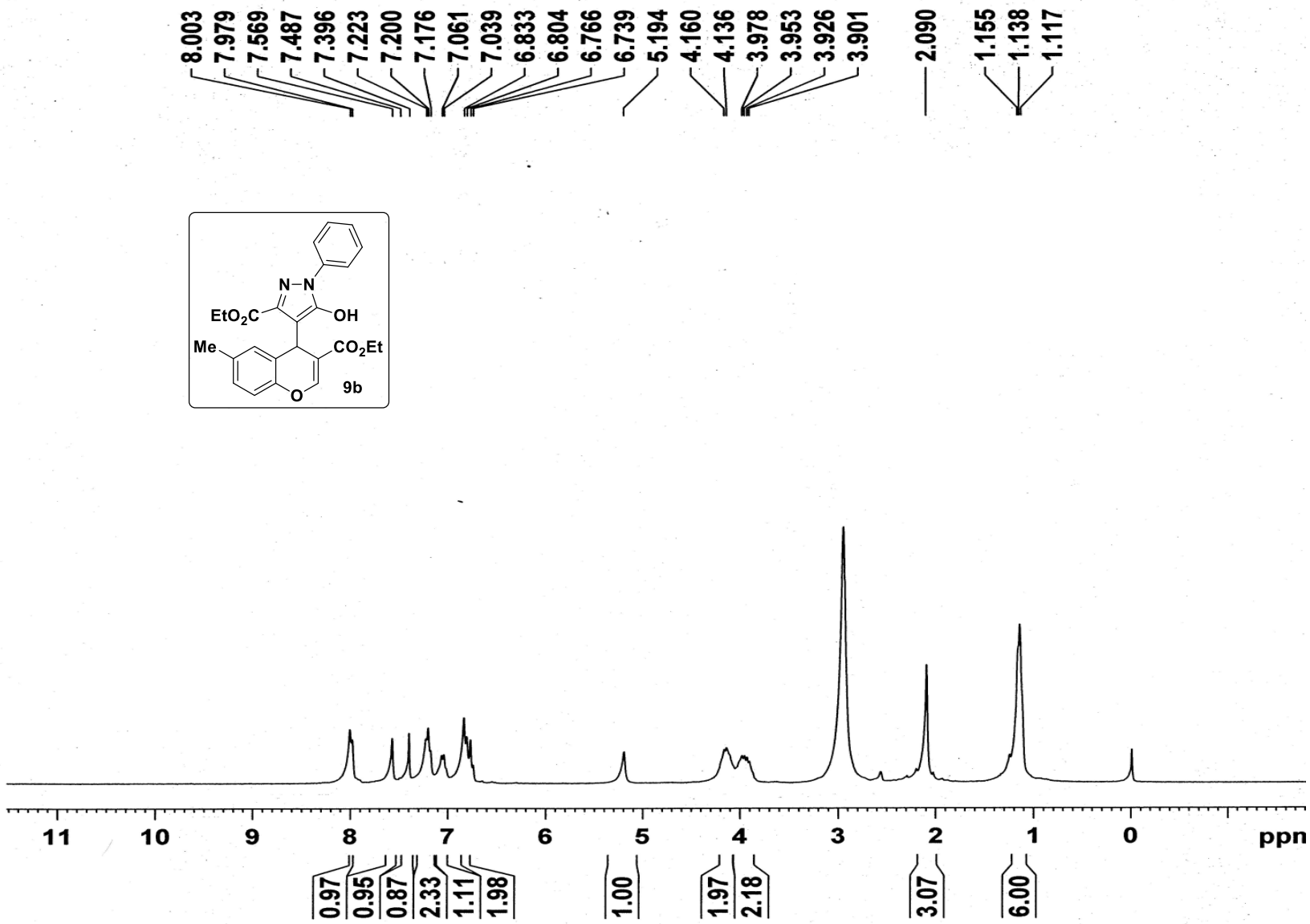


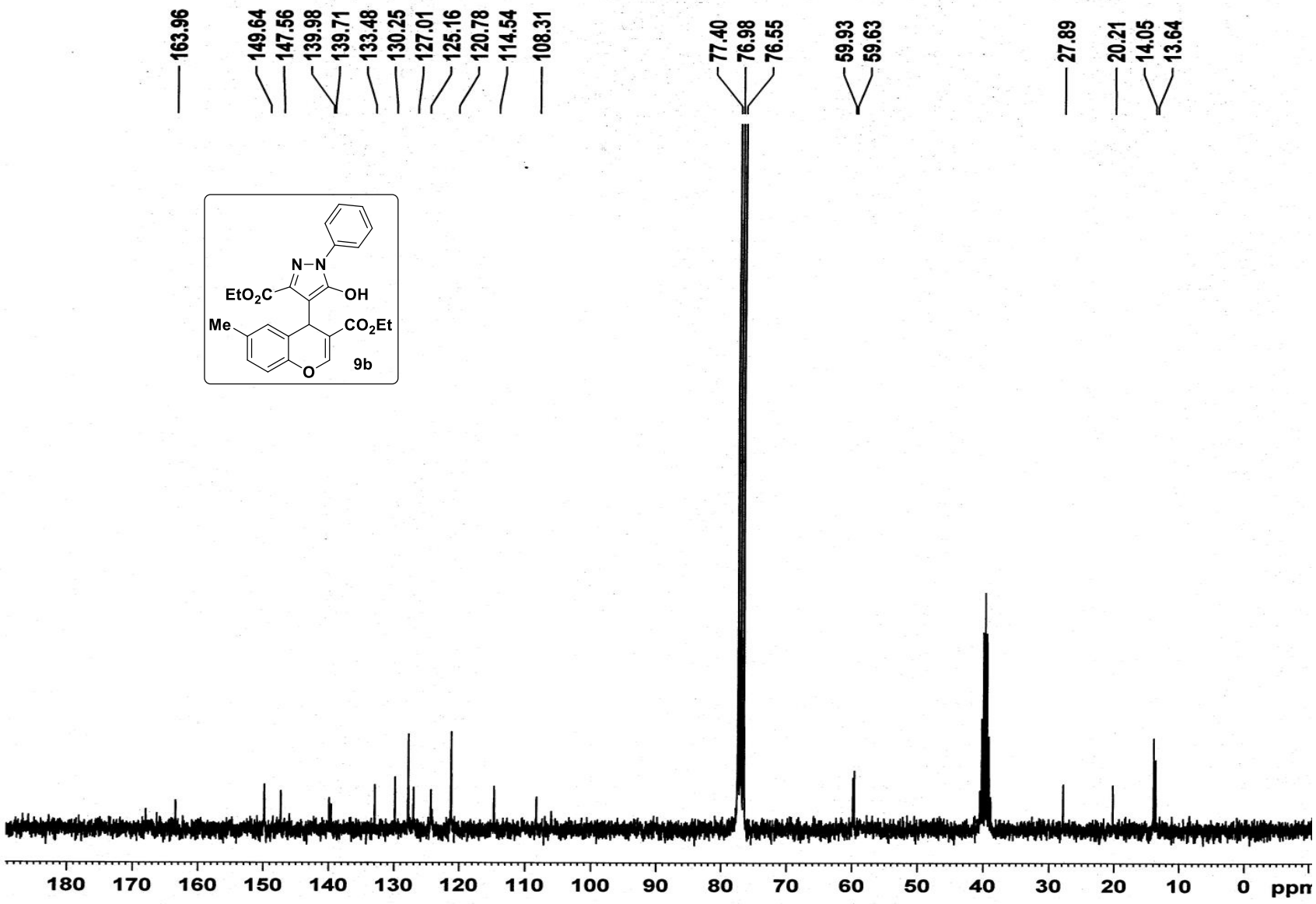

9.323
7.846
7.823
7.473
7.449
7.424
7.344
7.321
7.259
7.040
7.022
5.050
4.268
4.244
4.227
4.204
3.528
1.308
1.285
1.260
N–N
MeO2C
OH
CO2Et
O
9a
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
2.39
2.05
2.83
3.17
1.00
2.34
3.19
2.94


151.58
150.38
138.10
129.55
128.83
128.01
127.17
124.92
122.59
115.79
109.06
107.61
77.42
76.99
76.57
61.58
51.61
29.68
14.08
N–N
MeO2C
OH
CO2Et
O
9a
180
160
140
120
100
80
60
40
20
0
ppm

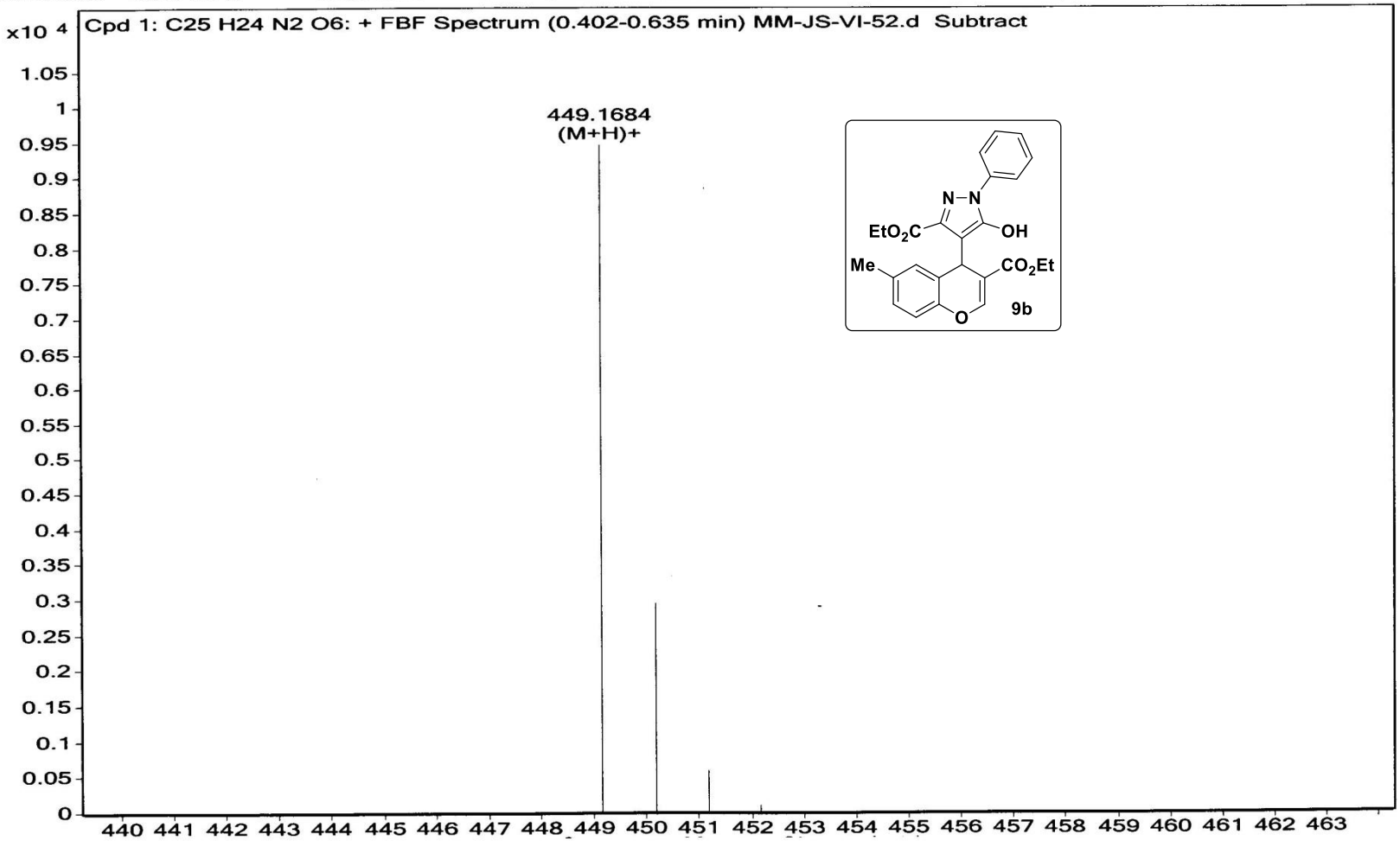
Sa... Name	MM-JS-VI-51	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-JS-VI-51.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-420.1321	**Acquired Time**	26-02-2015 10:36:31

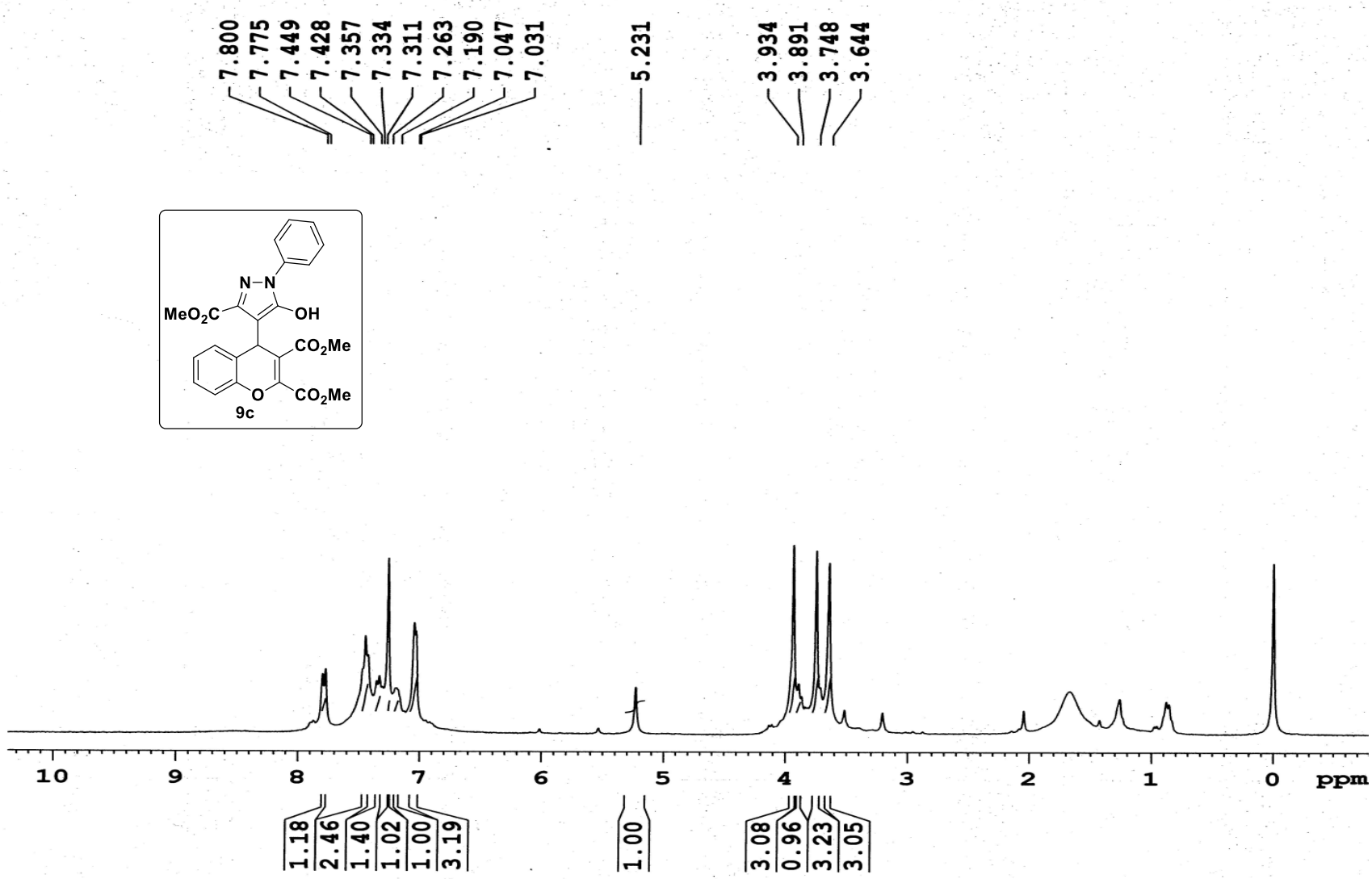


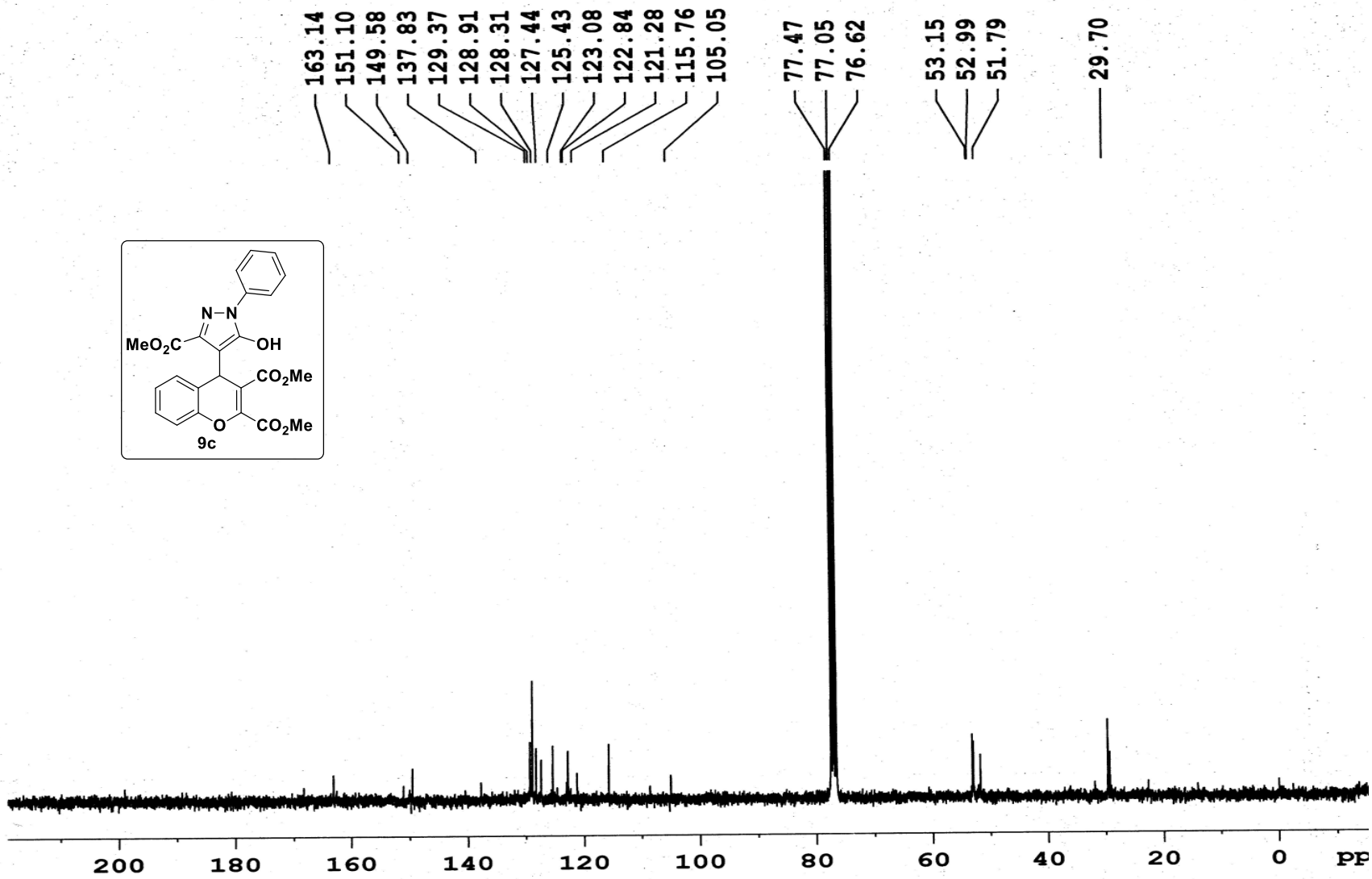

8.003
7.979
7.569
7.487
7.396
7.223
7.200
7.176
7.061
7.039
6.833
6.804
6.766
6.739
5.194
4.160
4.136
3.978
3.953
3.926
3.901
2.090
1.155
1.138
1.117
N–N
EtO2C
OH
Me
CO2Et
O
9b
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
0.95
0.87
2.33
1.11
1.98
1.00
1.97
2.18
3.07
6.00


163.96
149.64
147.56
139.98
139.71
133.48
130.25
127.01
125.16
120.78
114.54
108.31
77.40
76.98
76.55
59.93
59.63
27.89
20.21
14.05
13.64
N–N
EtO2C
OH
Me
CO2Et
O
9b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

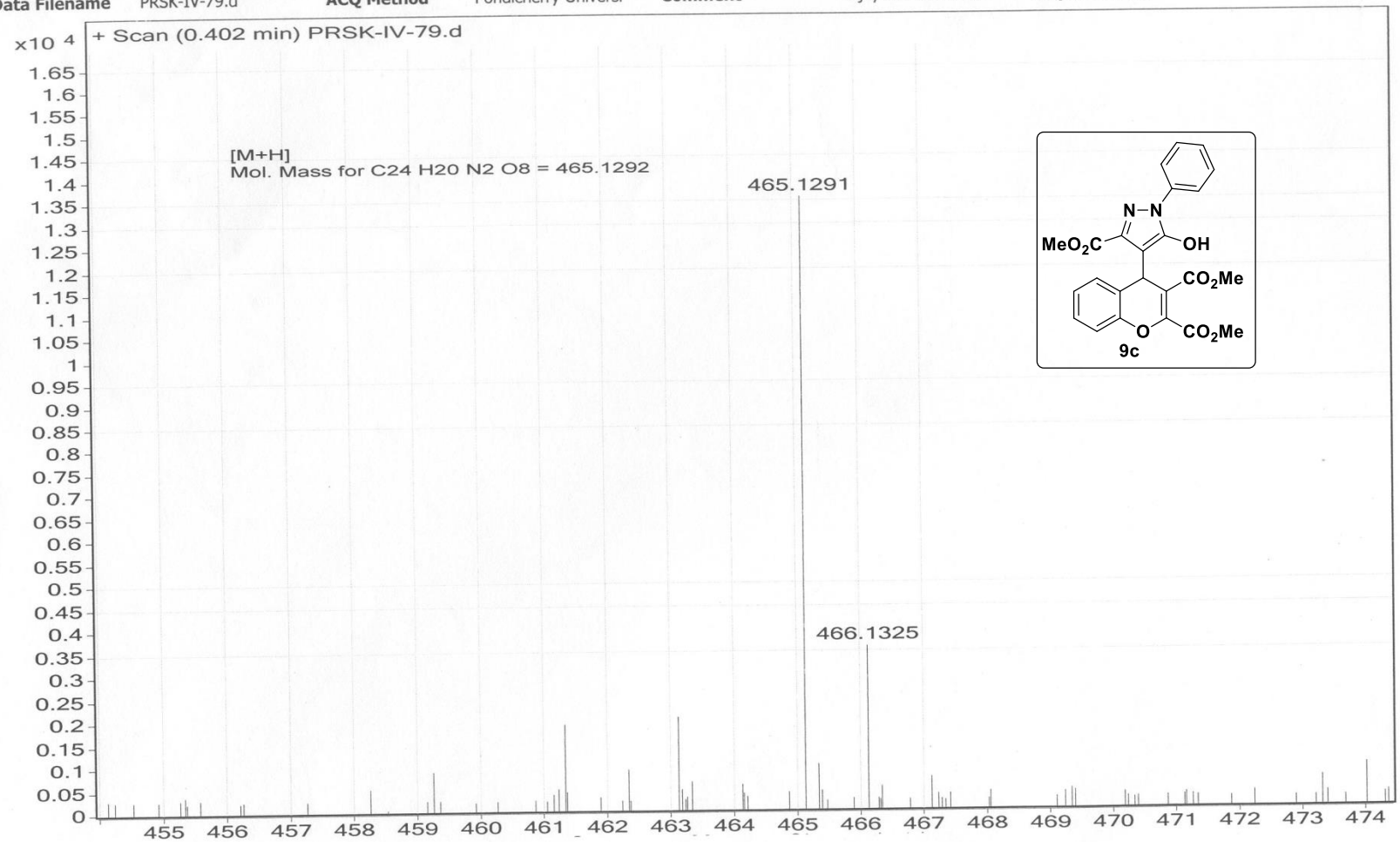
Sample Name	MM-JS-VI-52	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-JS-VI-52.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-448.1634	**Acquired Time**	26-02-2015 10:59:13

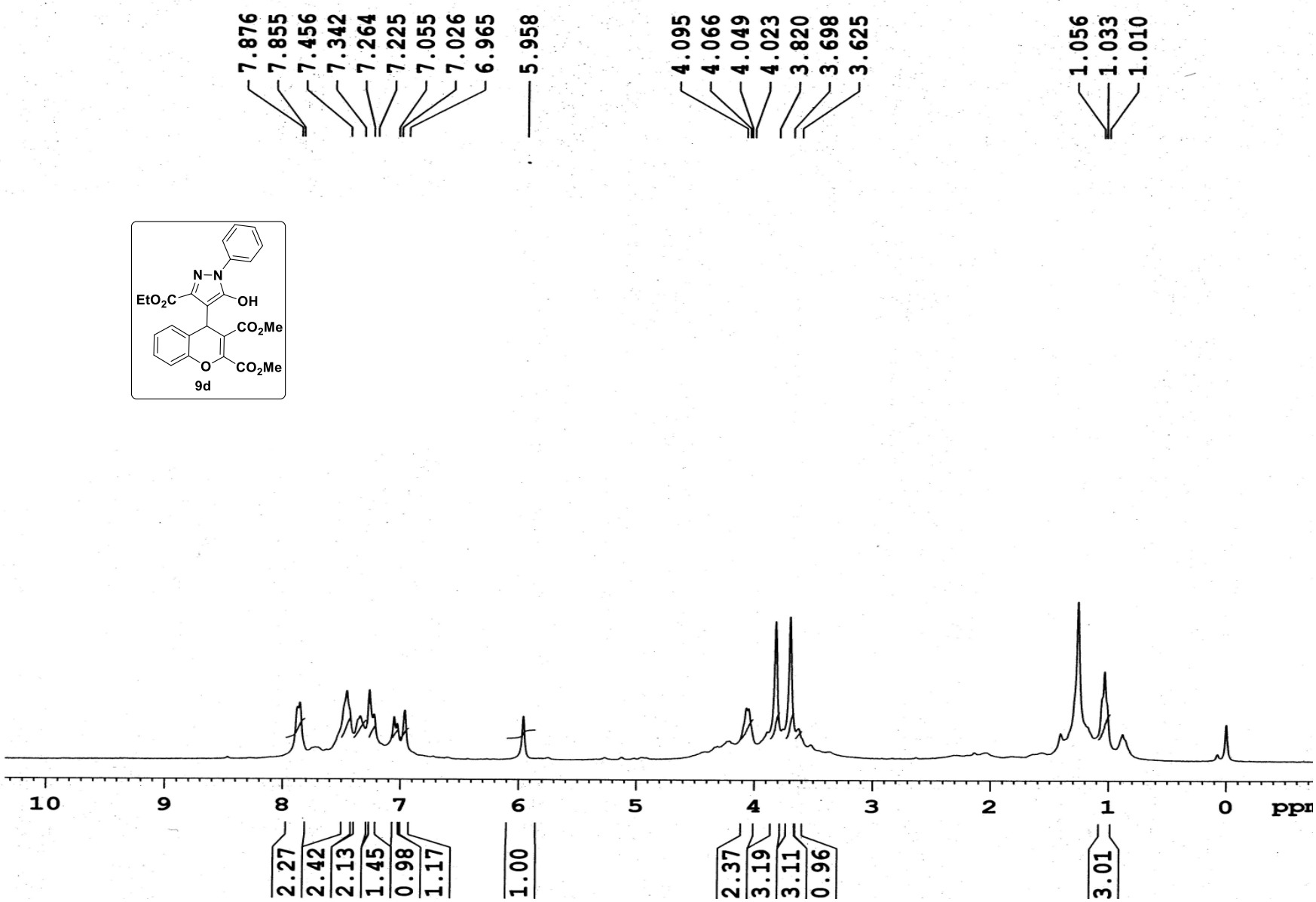


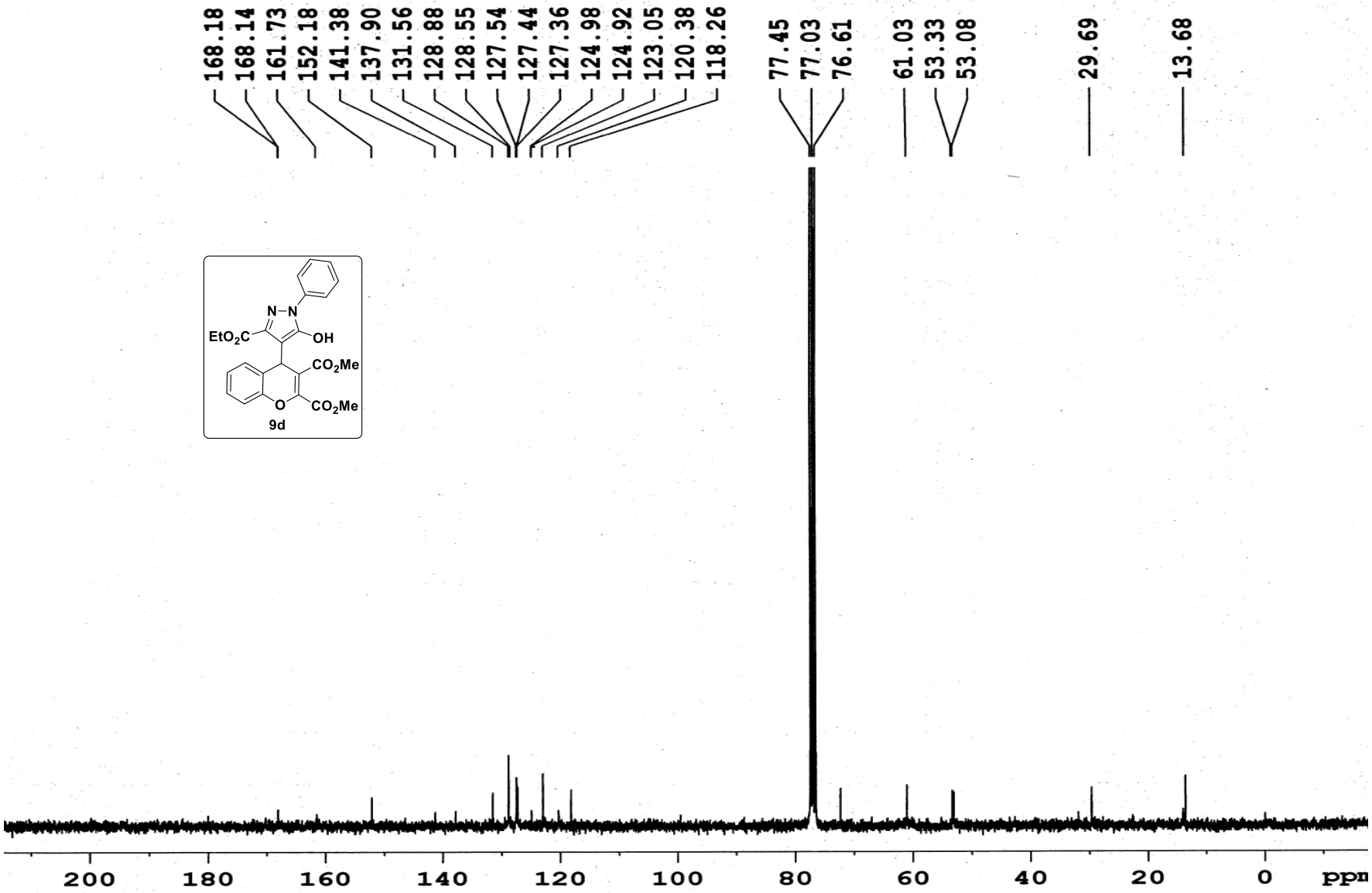

7.800
7.775
7.449
7.428
7.357
7.334
7.311
7.263
7.190
7.047
7.031
5.231
3.934
3.891
3.748
3.644
N–N
MeO2C
OH
CO2Me
CO2Me
O
9c
10
9
8
7
6
5
4
3
2
1
0
ppm
1.18
2.46
1.40
1.02
1.00
3.19
1.00
3.08
0.96
3.23
3.05


163.14
151.10
149.58
137.83
129.37
128.91
128.31
127.44
125.43
123.08
122.84
121.28
115.76
105.05
77.47
77.05
76.62
53.15
52.99
51.79
29.70
N–N
MeO2C
OH
CO2Me
CO2Me
O
9c
200
180
160
140
120
100
80
60
40
20
0
PP

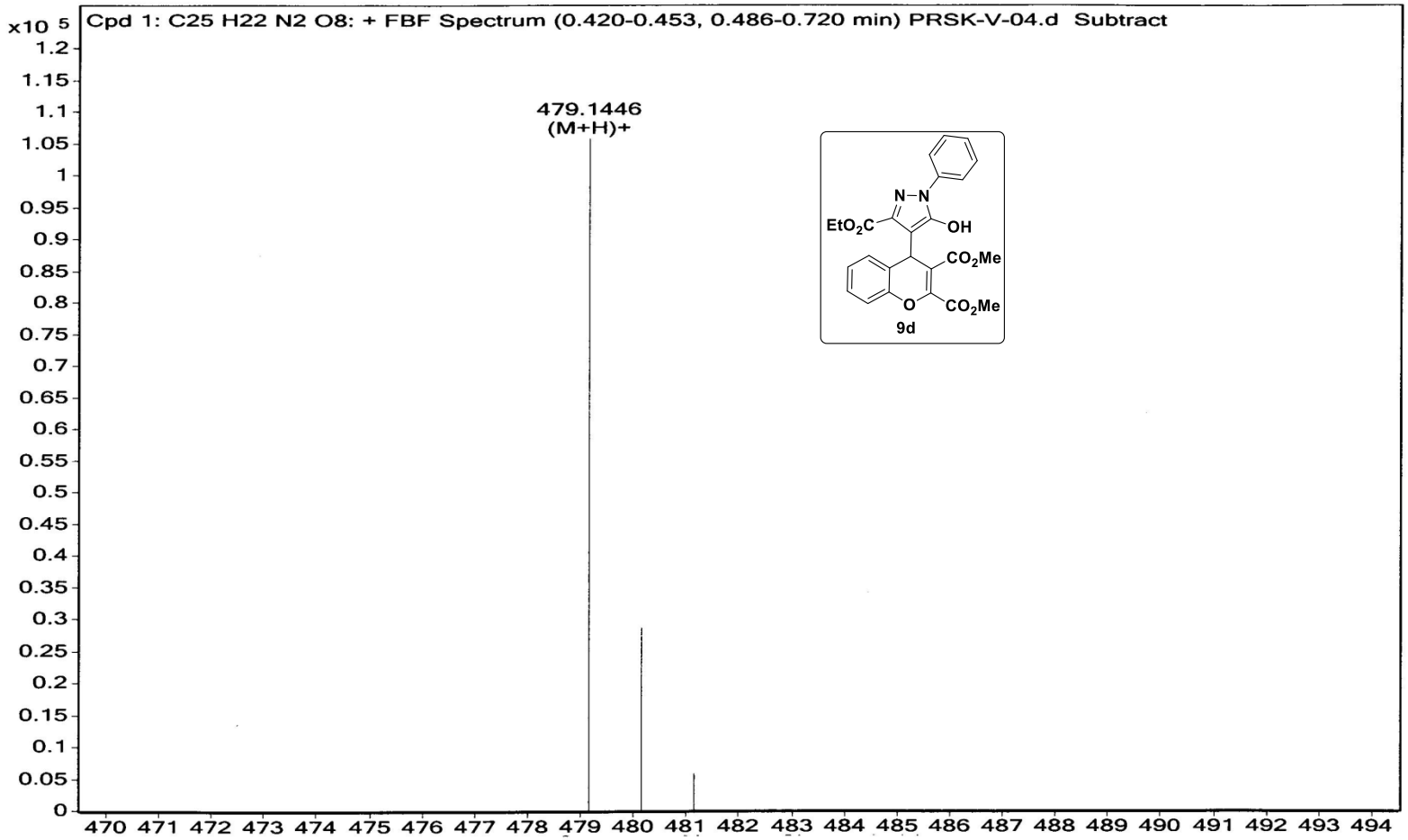
Sample Name	PRSK-IV-79	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-IV-79.d	**ACQ Method**	Pondicherry Universi	**Comment**	vijay-MB-464.1220	**Acquired Time**	24-09-2014 16:05:12

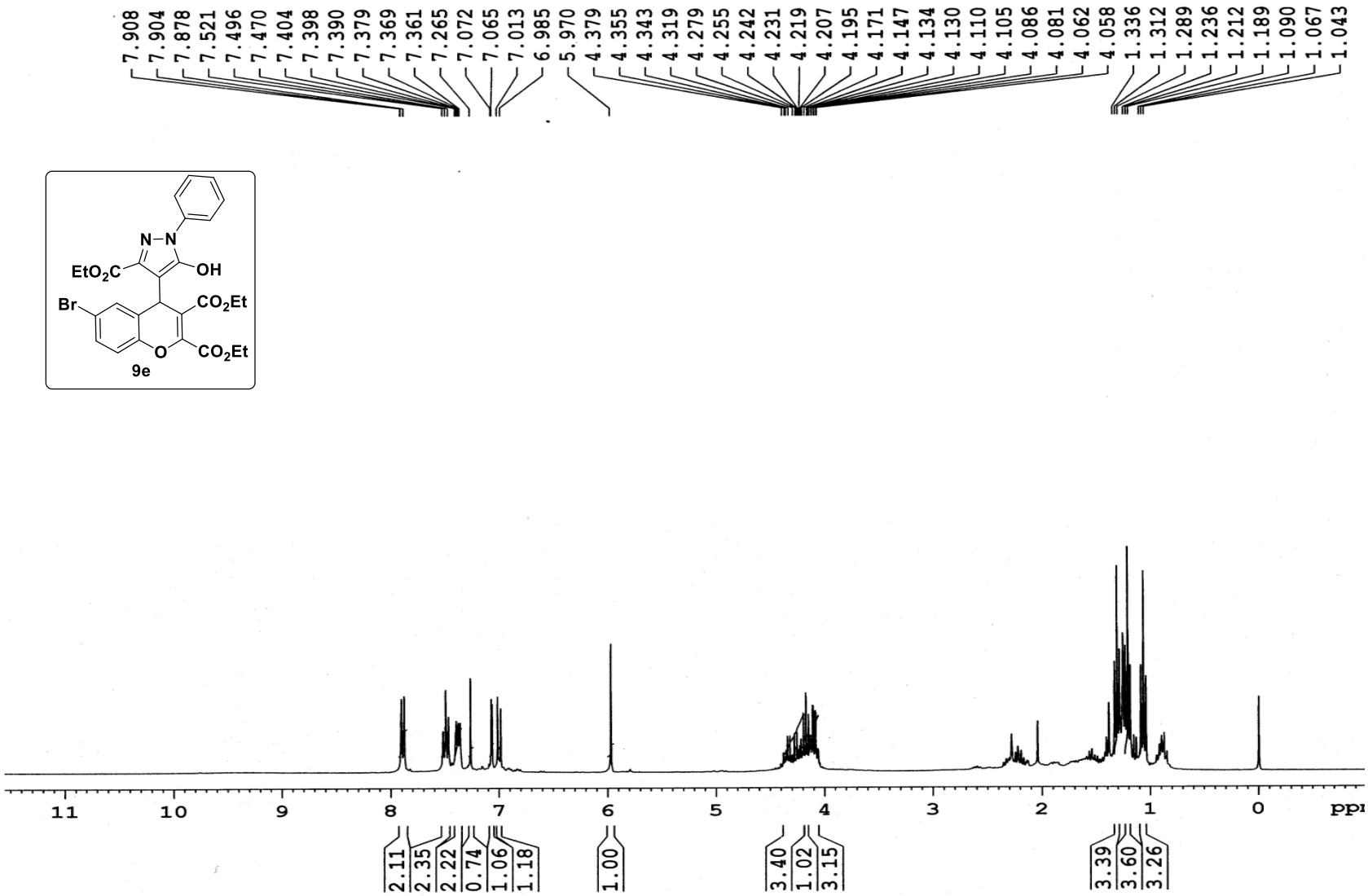


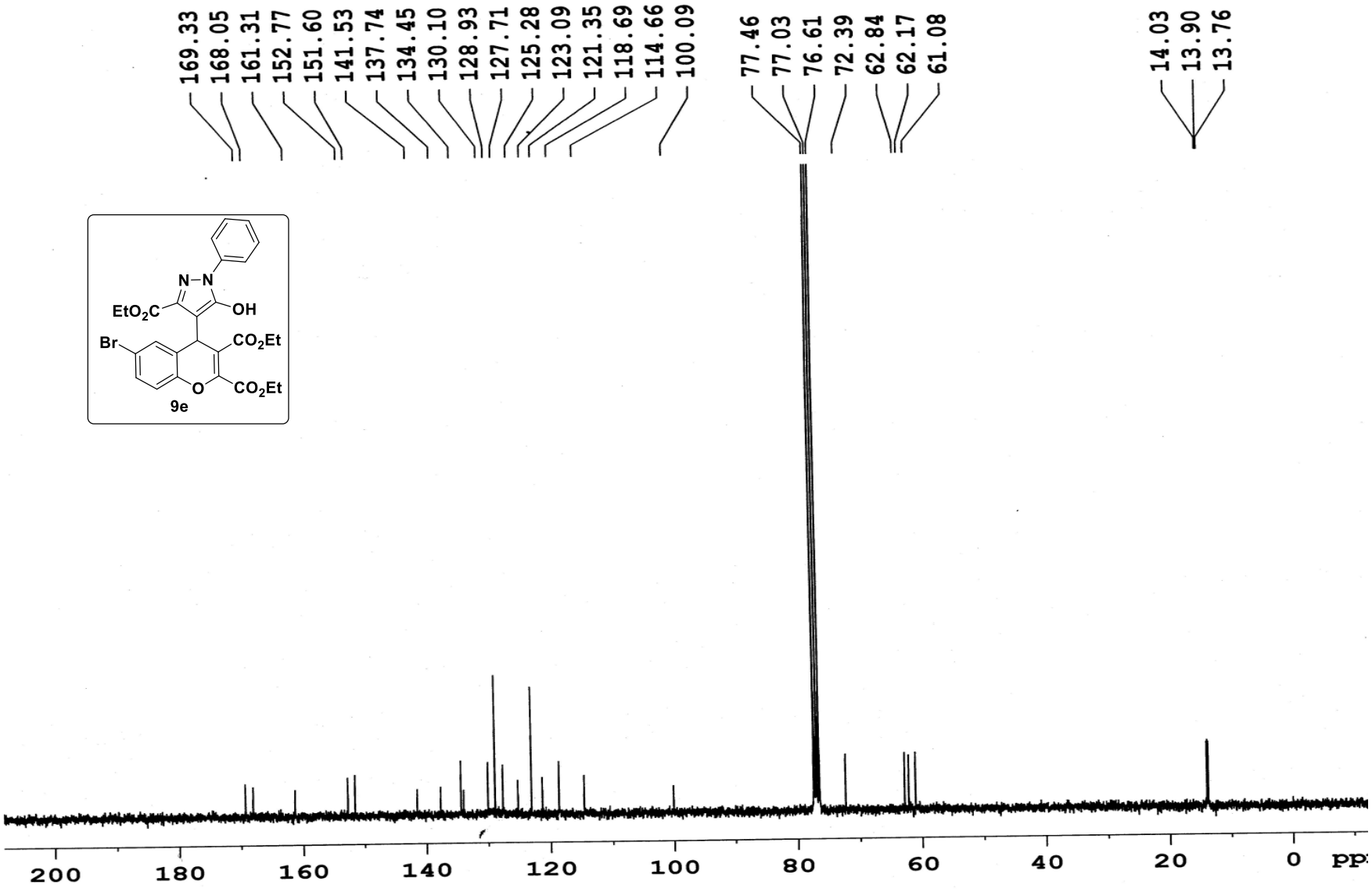

7.876
7.855
7.456
7.342
7.264
7.225
7.055
7.026
6.965
5.958
4.095
4.066
4.049
4.023
3.820
3.698
3.625
1.056
1.033
1.010
N–N
EtO2C
OH
CO2Me
CO2Me
O
9d
10
9
8
7
6
5
4
3
2
1
0
ppm
2.27
2.42
2.13
1.45
0.98
1.17
1.00
2.37
3.19
3.11
0.96
3.01


168.18
168.14
161.73
152.18
141.38
137.90
131.56
128.88
128.55
127.54
127.44
127.36
124.98
124.92
123.05
120.38
118.26
77.45
77.03
76.61
61.03
53.33
53.08
29.69
13.68
EtO2C
N–N
OH
CO2Me
CO2Me
O
9d
200
180
160
140
120
100
80
60
40
20
0
ppm

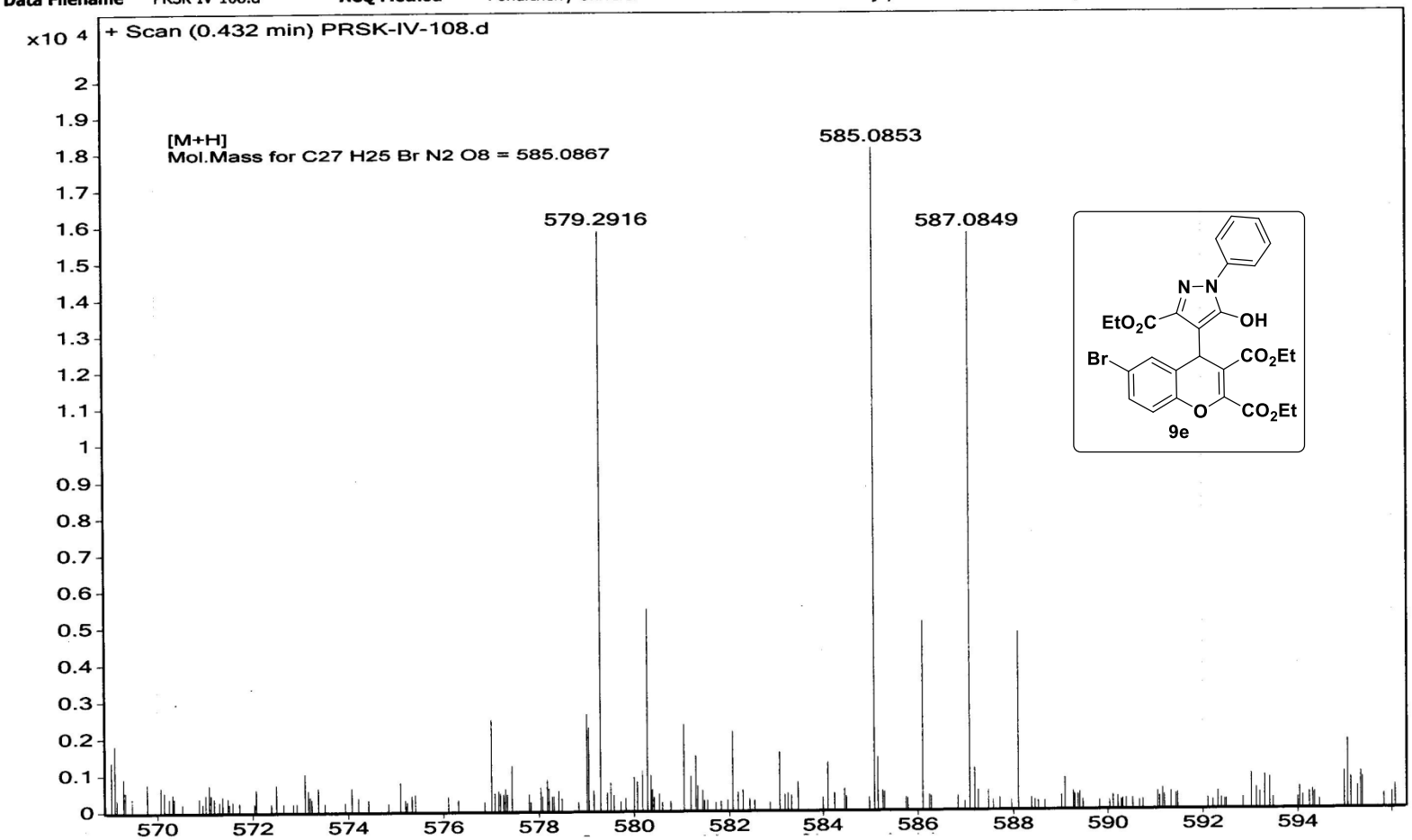
Sample Name	PRSK-V-04	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-V-04.d	**ACQ Method**	Pondicherry Universi	**Comment**	PV-MB-478.1376	**Acquired Time**	13-04-2015 11:33:08




7.908
7.904
7.878
7.521
7.496
7.470
7.404
7.398
7.390
7.379
7.369
7.361
7.265
7.072
7.065
7.013
6.985
5.970
4.379
4.355
4.343
4.319
4.279
4.255
4.242
4.231
4.219
4.207
4.195
4.171
4.147
4.134
4.130
4.110
4.105
4.086
4.081
4.062
4.058
1.336
1.312
1.289
1.236
1.212
1.189
1.090
1.067
1.043
N–N
EtO2C
OH
Br
CO2Et
O
CO2Et
9e
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.11
2.35
2.22
0.74
1.06
1.18
1.00
3.40
1.02
3.15
3.39
3.60
3.26


169.33
168.05
161.31
152.77
151.60
141.53
137.74
134.45
130.10
128.93
127.71
125.28
123.09
121.35
118.69
114.66
100.09
77.46
77.03
76.61
72.39
62.84
62.17
61.08
14.03
13.90
13.76
N–N
EtO2C
OH
Br
CO2Et
O
CO2Et
9e
200
180
160
140
120
100
80
60
40
20
0
ppm

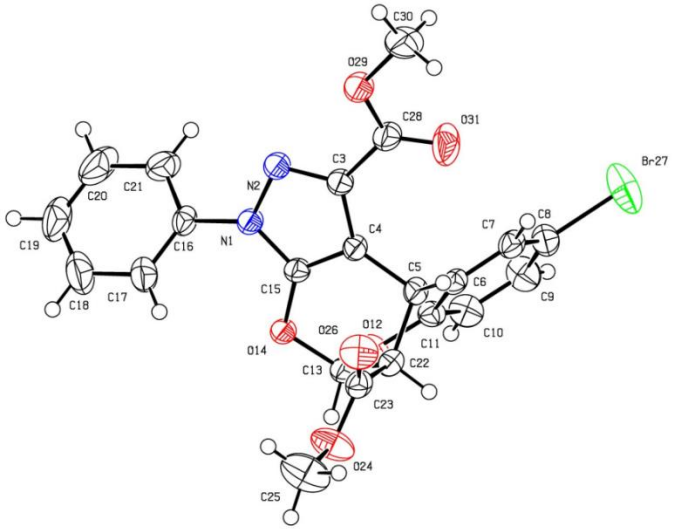
Sample Name	PRSK-IV-108	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PRSK-IV-108.d	**ACQ Method**	Pondicherry Universi	**Comment**	vijay-MB-584.0794	**Acquired Time**	24-09-2014 16:12:21



Compund 6c

Table 1 Crystal data and structure refinement for Compund 6c.

Identification code	Compund 6c
Empirical formula	$C_{22}H_{17}BrN_2O_6$
Formula weight	485.29
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.0079(7)
b/Å	10.6912(11)
c/Å	12.9965(11)
α/°	79.773(8)
β/°	82.666(7)
γ/°	69.817(8)
Volume/Å^3	1025.11(16)
Z	2
ρ_{calc}g/cm^3	1.572
μ/mm^{-1}	2.048
F(000)	492.0
Crystal size/mm^3	0.35 × 0.24 × 0.22
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.08 to 58.28
Index ranges	$-10 \leq h \leq 10$, $-14 \leq k \leq 14$, $-17 \leq l \leq 16$
Reflections collected	9637
Independent reflections	4659 [R_{int} = 0.0427, R_{sigma} = 0.0741]
Data/restraints/parameters	4659/0/282
Goodness-of-fit on F^2	0.995
Final R indexes [I>=2σ (I)]	R_1 = 0.0491, wR_2 = 0.0872

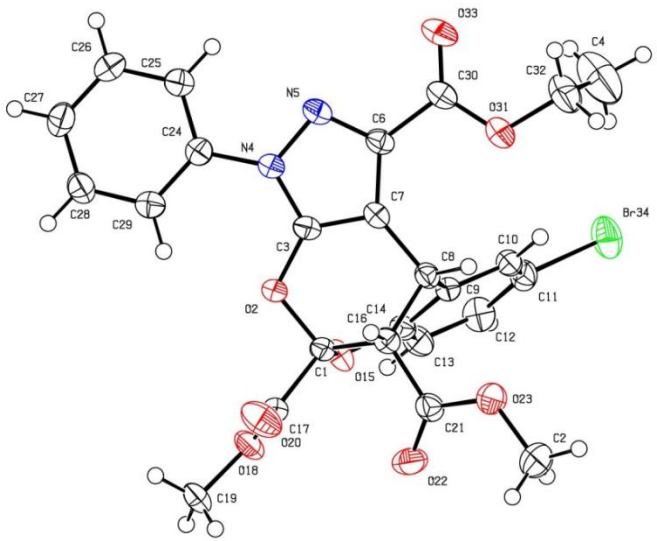


Final R indexes [all data] $R_1 = 0.1010$, $wR_2 = 0.1046$
Largest diff. peak/hole / e Å^{-3} 0.36/-0.39

Compound 6n

Table 1 Crystal data and structure refinement for Compound 6n.

Identification code	Compound 6n
Empirical formula	$C_{25}H_{21}BrN_2O_8$
Formula weight	557.35
Temperature/K	298.0
Crystal system	monoclinic
Space group	$P2_1/a$
a/Å	8.5538(5)
b/Å	28.5184(14)
c/Å	9.9217(5)
α/°	90.00
β/°	104.085(5)
γ/°	90.00
Volume/Å^3	2347.5(2)
Z	4
ρ_{calc}g/cm^3	1.577
μ/mm^{-1}	1.806
F(000)	1136.0
Crystal size/mm^3	0.5 × 0.4 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.4 to 58.42
Index ranges	$-10 \leq h \leq 10$, $-37 \leq k \leq 32$, $-13 \leq l \leq 12$
Reflections collected	12825
Independent reflections	5425 [$R_{int} = 0.0357$, $R_{sigma} = 0.0546$]



Data/restraints/parameters	5425/0/328
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0463, wR_2 = 0.0808
Final R indexes [all data]	R_1 = 0.0835, wR_2 = 0.0930
Largest diff. peak/hole / e $Å^{-3}$	0.32/-0.48