Supporting Documents

Organoiodine (III) mediated intramolecular oxidative cyclization of 1-(3-arylisoquinolin-1-yl)-2-(arylmethylene)hydrazines to 5-aryl-3-(aryl)-[1,2,4]triazolo[3,4-*a*] isoquinolines

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*5-Phenyl-3-(thiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline, (**4a**)*

Brown solid, mp 195.1 °C, IR (KBr-ν cm^{-1}): 3061,1724, 1636, 1522, 1451, 1374, 1294, 1224, 1150, 844, 777, 762, 705, 538, 491. ^{1}H NMR (400 MHz, DMSO-D_6, 25 °C) δ ppm: 8.66 (d, *J* = 5.04 Hz, 1H), 7.99 (d, *J* = 7.12 Hz, 1H), 7.79 (m, 2H), 7.51 (d, *J* = 5.08 Hz, 1H), 7.34-7.15 (m, 6H), 6.66 (m, 1H), 6.50 (d, *J* = 3.60 Hz,1H); ^{13}CNMR (100 MHz DMSO-D_6) δ ppm: 149.93, 143.71, 135.21, 133.32, 131.43, 130.83, 130.54, 129.49, 129.32, 128.97, 128.89, 128.17, 128.07, 127.84, 127.24, 123.38, 120.69, 117.36. Calcd for $C_{20}H_{13}N_3S$, HRMS (EI) 327.0830; found, 327.1192 (M^+).

*5-Phenyl-3-(4-cyanophenyl)-[1,2,4]triazolo[3,4- a]isoquinoline, (**4b**)*

Brown solid, mp 282.5 °C, IR (KBr-ν cm^{-1}): 3050, 3026, 2919, 2831, 2372, 2333, 2227, 1522, 1468, 1452, 1381, 836, 767, 710, 561. ^{1}H NMR (400 MHz, DMSO-D_6, 25 °C) δ ppm: 8.68 (d, *J* = 5.80 Hz, 1H), 7.99 (d, *J* = 4.24 Hz, 1H), 7.80 (d, *J* = 5.08 Hz, 2H), 7.53 (d, *J* = 8.12 Hz, 2H), 7.36-7.08 (m, 8H); ^{13}CNMR(100MHz, DMSO-D_6) δ ppm: 149.50, 147.57, 134.49, 133.26, 132.67, 130.97, 130.40, 130.22, 130.14, 129.08, 129.02, 128.88, 127.70, 127.39, 122.95, 120.18, 118.45, 116.40, 110.88. Calcd for $C_{23}H_{14}N_4$, HRMS (EI) calcd., 346.1218; found, 346.1686 (M^+).

*5-Phenyl-3-(4-methoxyphenyl)-[1,2,4]triazolo[3,4-a]isoquinoline, (**4c**)*

Brown solid, mp 155.6- 155.9 °C, IR (KBr-ν cm^{-1}): 3428, 2838, 1636, 1609, 1530, 1468, 1453.18, 1438, 1374, 1301, 1249, 1170, 1023, 830, 763, 699, 551. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.64 (d, *J* = 5.88 Hz, 1H), 7.97 (d, *J* = 6.60 Hz,1H), 7.77 (d, *J* = 5.92 Hz, 2H), 7.26 (s,1H), 7.22-7.18 (m, 3H), 7.10-7.03 (m, 4H), 6.59 (d, *J* = 6.92 Hz, 2H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, DMSO-

D_6) δ ppm: 159.80, 149.50, 149.32, 135.39, 133.24, 131.18, 130.59, 130.52, 129.41, 129.34, 129.00, 127.92, 127.79, 123.31, 121.23, 120.92, 116.81, 113.29, 55.66. Calcd., for $C_{23}H_{17}N_3O$, HRMS (EI) calcd., 351.1371; found, 351.1692 (M+).

*5-Phenyl-3-(benzo[b]thiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline, (**4d**)*

Brown solid, mp 267.6-267.8 °C, IR (KBr-ν cm^{-1}): 3054, 1637, 1524, 1444, 1374, 1331, 830, 749, 699, 569. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.67 (d, *J* = 3.72 Hz, 1H), 8.01 (d, *J* = 4.95 Hz, 1H), 7.90-7.80 (m, 3H), 7.47-7.26 (m, 6H), 7.06 (d, *J* = 6.96 Hz, 3H), 6.73 (s, 1H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 150.22, 143.80, 139.80, 139.11, 135.16, 133.45, 130.97, 130.65, 129.59, 129.44, 129.10, 128.50, 128.41, 128.01, 127.89, 125.67, 125.01, 124.44, 123.48, 122.39, 120. 64, 117.53. Calcd., for $C_{24}H_{15}N_3S$, HRMS (EI) calcd., 377.0986; found, 378.1164(M+).

*5-Phenyl-3-(4-chlorophenyl)-[1,2,4]triazolo[3,4-a]isoquinoline, (4**e**)*

Brown solid, mp 265.0 -265.7 °C, IR (KBr-ν cm^{-1}): 3061, 1641, 1527, 1459, 1011, 829, 760, 768, 694, 552. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.66 (d, *J* = 7.64 Hz, 1H), 7.99-7.96 (m, 1H), 7.79 (d, *J* = 8.00 Hz, 2H), 7.29-7.07 (m, 10H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 149.75, 148.42, 135.13, 133.92, 133.19, 131.55, 130.76, 130.61, 129.57, 129.43, 129.16, 128.08, 127.97, 127.84, 127.70, 123.38, 120.78, 116.84. Calcd., for $C_{22}H_{14}ClN_3$, HRMS

(EI) calcd., 355.0876; found, 355.1037 (M+).

*5-Phenyl-3-(2-trifluoromethylphenyl)-[1,2,4]triazolo[3,4-a]isoquinoline, (**4f**)*

Brown solid, mp 244.5 -244.8 °C, IR (KBr-ν cm^{-1}): 3432, 3039, 1643, 1527, 1457, 1311, 1106, 1032, 764, 699, 555. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.67 (d, *J* = 4.92 Hz, 1H), 7.96 (d, *J* =2.91 Hz, 1H),7.80 (t, *J* =3.72 Hz, 2H), 7.55-7.40 (m, 4H), 7.23 (s, 1H), 7.13-7.04 (m, 4H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 149.38, 145.72, 134.97, 133.97, 132.29, 131.86, 130.94, 130.60, 130.50, 129.60, 129.36, 128.68, 128.38, 128.02, 127.87, 127.03, 126.23, 126.18, 125.32, 123.46, 120.62, 116.85. Calcd., for $C_{23}H_{14}N_3F_3$, HRMS (EI) calcd., 389.1139; found, 390.1674(M+).

*5-(4-Chlorophenyl)-3-(furan-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline, (**4g**)*

Brown solid, mp 248.0-248.2 °C, IR (KBr-ν cm^{-1}): 3056, 2922, 1640, 1527, 1489, 1390, 1089, 816, 767. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.66 (t, *J* = 4.92 Hz, 1H), 7.98 (d, *J* =7.56 Hz, 1H), 7.80 (d, *J* =7.64 Hz, 2H),7.41-7.28 (m, 6H), 6.62 (d, *J* = 4.40 Hz, 1H), 6.39 (s, 1H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 149.75, 145.05, 140.81, 140.71, 134.07, 133.85, 132.11, 131.06, 130.52, 130.33, 129.76, 128.25, 128.02, 123.53, 120.58, 117.47, 114.32, 111.56. Calcd., for $C_{20}H_{12}ClN_3O$, HRMS (EI) calcd., 345.0669; found, 346.1236 (M+).

*5-(4-Chlorophenyl)-3-(4-N,N-dimethylaminophenyl)-[1,2,4]triazolo[3,4- a]isoquinoline, (**4h**)*

Brown solid, mp 260.3-260.6 °C, IR (KBr-ν cm^{-1}): 3054, 2800, 1611, 1481, 1454, 1353, 1310, 1089, 1016, 817, 763, 556. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.64 (t, *J* = 8.0 Hz, 1H), 7.98-7.96 (m, 1H), 7.78 (d, *J* = 4.40 Hz, 2H), 7.27 (s, 1H), 7.19 (d, *J* = 6.40 Hz, 2H), 7.09 (d, *J* = 4.40 Hz, 2 H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.39 (d, *J* = 8.8 Hz, 2H), 2.88 (s, 6H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 150.99, 133.61, 131.23, 130.68, 130.50, 130.33, 129.41, 127.81, 127.66, 123.26, 116.66, 115.76, 111.41, 40.10. Calcd., for $C_{24}H_{19}ClN_4$, HRMS (EI) calcd., 398.1298; found, 399.1703 (M+).

*5-(4-Chlorophenyl)-3-(1H-Indol-3-yl)-[1,2,4]triazolo[3,4-a]isoquinoline, (**4i**)*

Brown solid, mp 142.7-142.9 °C, IR (KBr-ν cm^{-1}): 3054, 2936, 1641, 1598, 1527, 1459, 829, 760, 694. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 11.31 (s, 1H), 8.66 (d, *J* = 3.63 Hz,1H), 7.96 (t, *J* =4.59 Hz, 1H), 7.84-7.76 (m, 2H),7.66 (t, *J* = 7.92 Hz, 1H), 7.30 (t, *J* = 8.28 Hz, 3H), 7.24 (d, *J* = 7.68 Hz, 2H), 7.17 (d, *J* = 8.25 Hz, 1H), 7.06 (t, *J* = 7.5 Hz, 1H) 7.00 (s, 1H), 6.96 (t, *J* = 7.38 Hz, 1H), 6.88 (t, *J* = 9.00 Hz, 2H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 149.26, 144.72, 135.75, 135.56, 134.47, 133.48, 131.65, 130.61, 130.49, 130.35, 130.32, 129.43, 127.92, 127.84, 126.98, 126.78, 123.77, 123.23, 122.05, 121.16, 119.93, 119.84, 117.03, 111.70, 103.34. Calcd., for $C_{24}H_{15}ClN_4$, HRMS (EI) calcd., 394.8557; found, 395.1314 (M+).

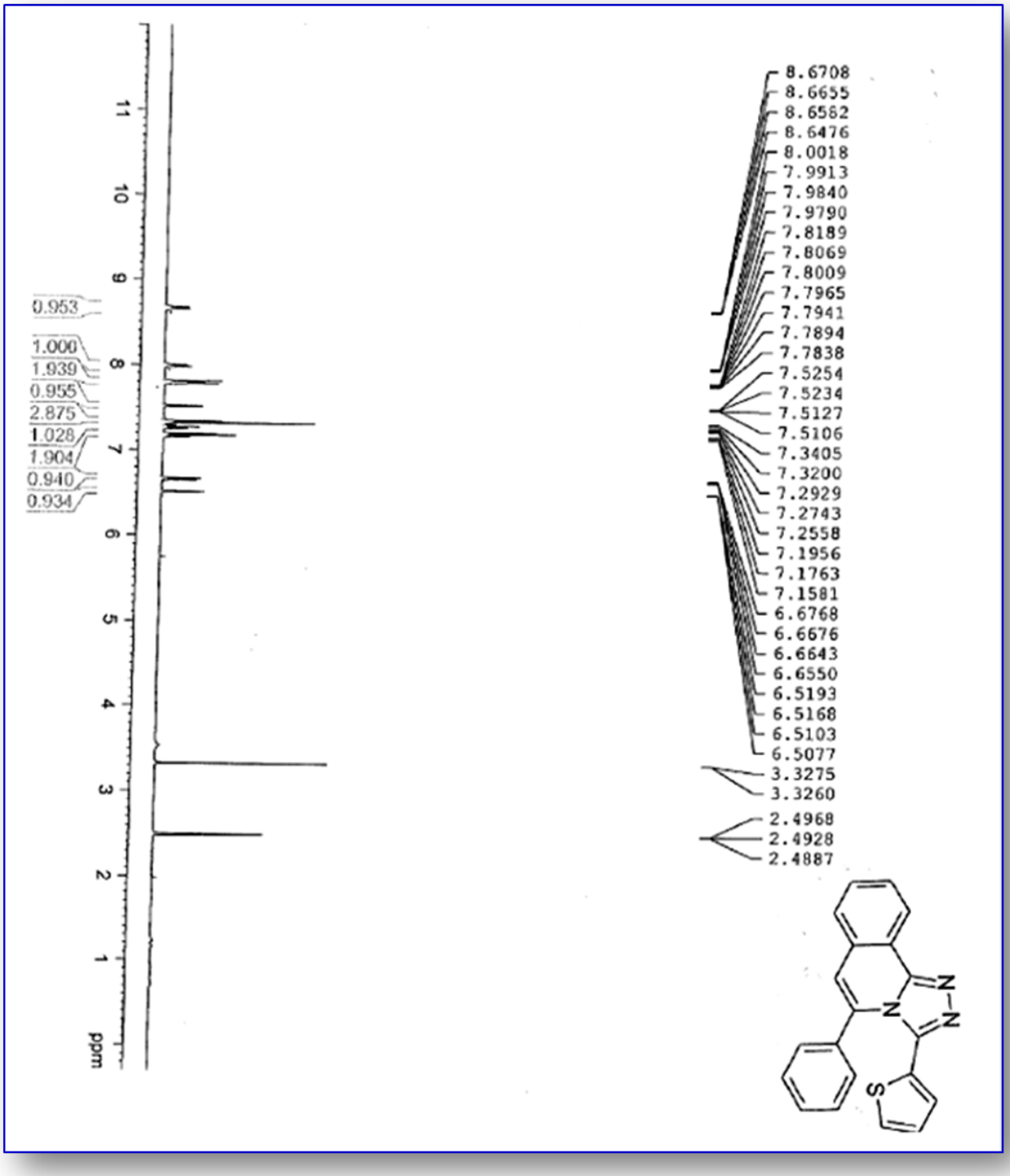
*5-(5-(4-Chlorophenyl)-[1,2,4]triazolo[3,4-a]isoquinolin-3-yl)-2,4-dimethylthiazole, (**4j**)* Brown solid, mp 142.7-143.0 °C, IR (KBr-ν cm^{-1}): 3853, 3423, 3035, 2923, 1639, 1324, 1174, 1085, 1011, 831, 761

503. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.67-8.65 (d, *J* = 5.84 Hz,1H), 8.00-7.97 (m, 1H), 7.83-7.79 (m, 2H) 7.42-7.40 (m, 2H), 7.33 (s, 1H), 7.29-7.27 (d, *J* = 6.68 Hz, 2H), 2.49 (s, 3H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 167.36, 153.10, 149.59, 140.22, 134.02, 133.39, 130.84, 130.55, 130.11, 129.30, 127.54, 127.30, 122.98, 120.47, 117.42, 117.00, 18.48, 15.92. Calcd., for $C_{21}H_{15}ClN_4S$, HRMS (EI) calcd., 390.8886; found, 391.12 (M+).

*5-(4-Chlorophenyl)-3-p-tolyl-[1,2,4]triazolo[3,4-a]isoquinoline, (**4k**)*

Brown solid, mp 247.7 -247.9 °C, IR (KBr-ν cm^{-1}): 3033, 1642, 1525, 1455, 1399, 1314, 1087, 1011, 919, 815, 758, 723, 557. ^{1}H NMR (400 MHz, DMSO- D_6, 25 °C) δ ppm: 8.65 (d *J* = 5.88 Hz, 1H), 7.96 (d, *J* =5.79 Hz, 1H), 7.78 (d, *J* = 5.88 Hz, 2H), 7.28 (s, 1H), 7.21 (d, *J* = 8.43 Hz, 2H), 7.08 (d, *J* = 8.46 Hz, 2H), 6.99 (d, *J* = 8.04 Hz, 2H), 6.91 (d, *J* = 7.89 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, DMSO- D_6) δ ppm: 149.31, 138.75, 134.17, 134.02, 132.00, 131.29, 130.68, 130.44, 129.94, 129.51, 128.31, 127.87, 127.82, 126.03, 123.35, 120.99, 116.79, 21.30. Calcd., for $C_{23}H_{16}ClN_3$, HRMS (EI) calcd., 369.8462; found, 370.1642 (M+).

4a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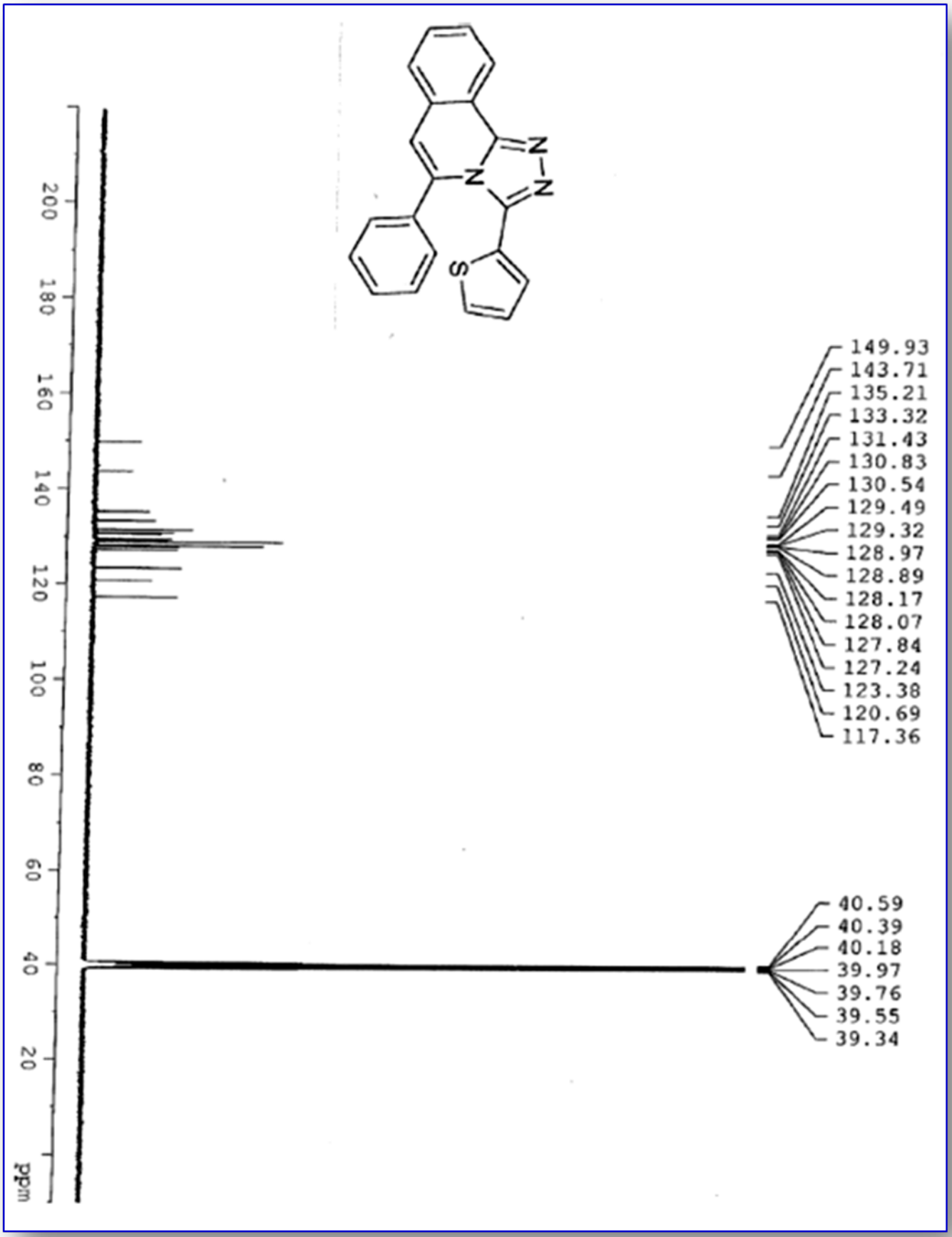
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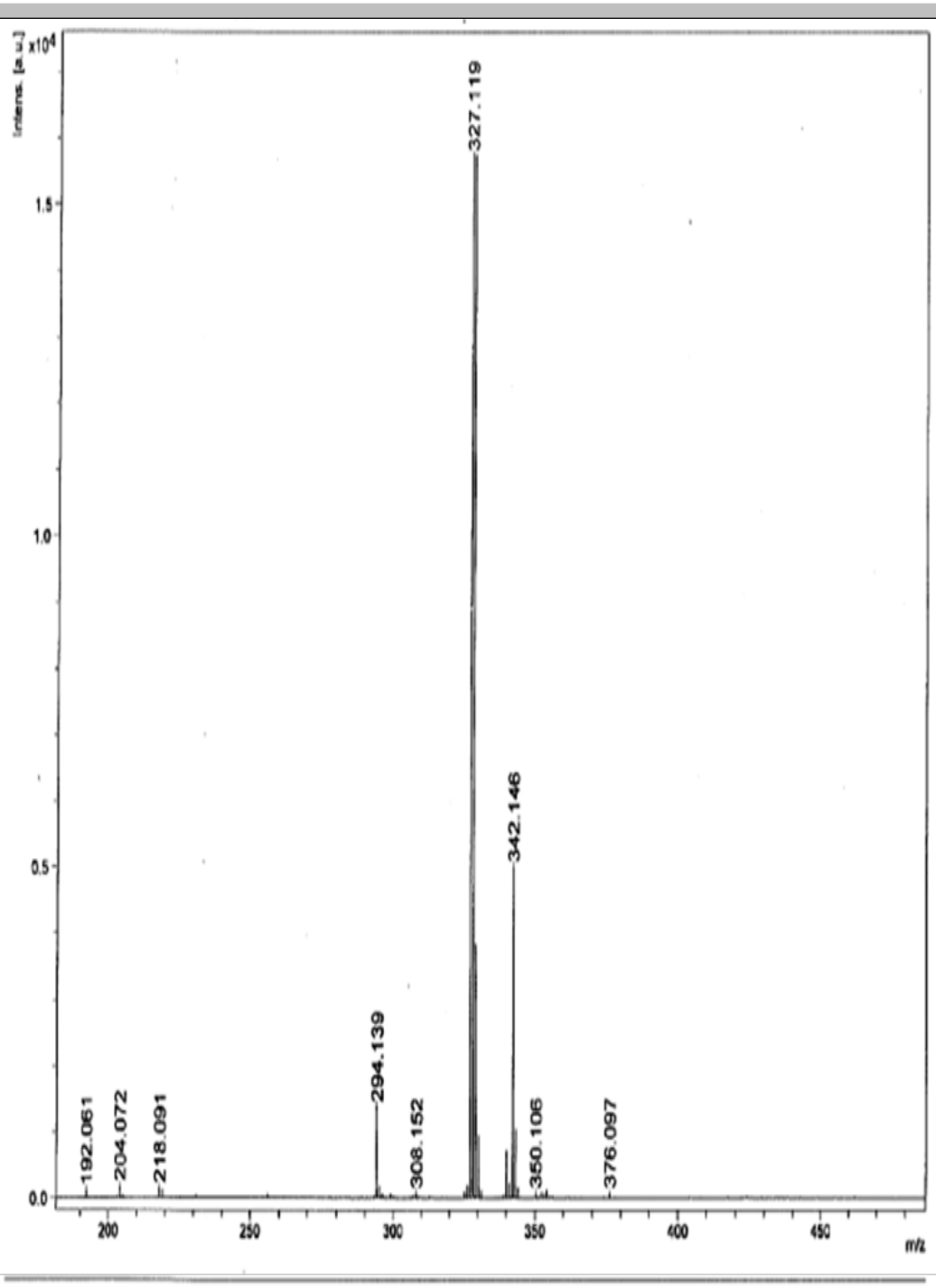
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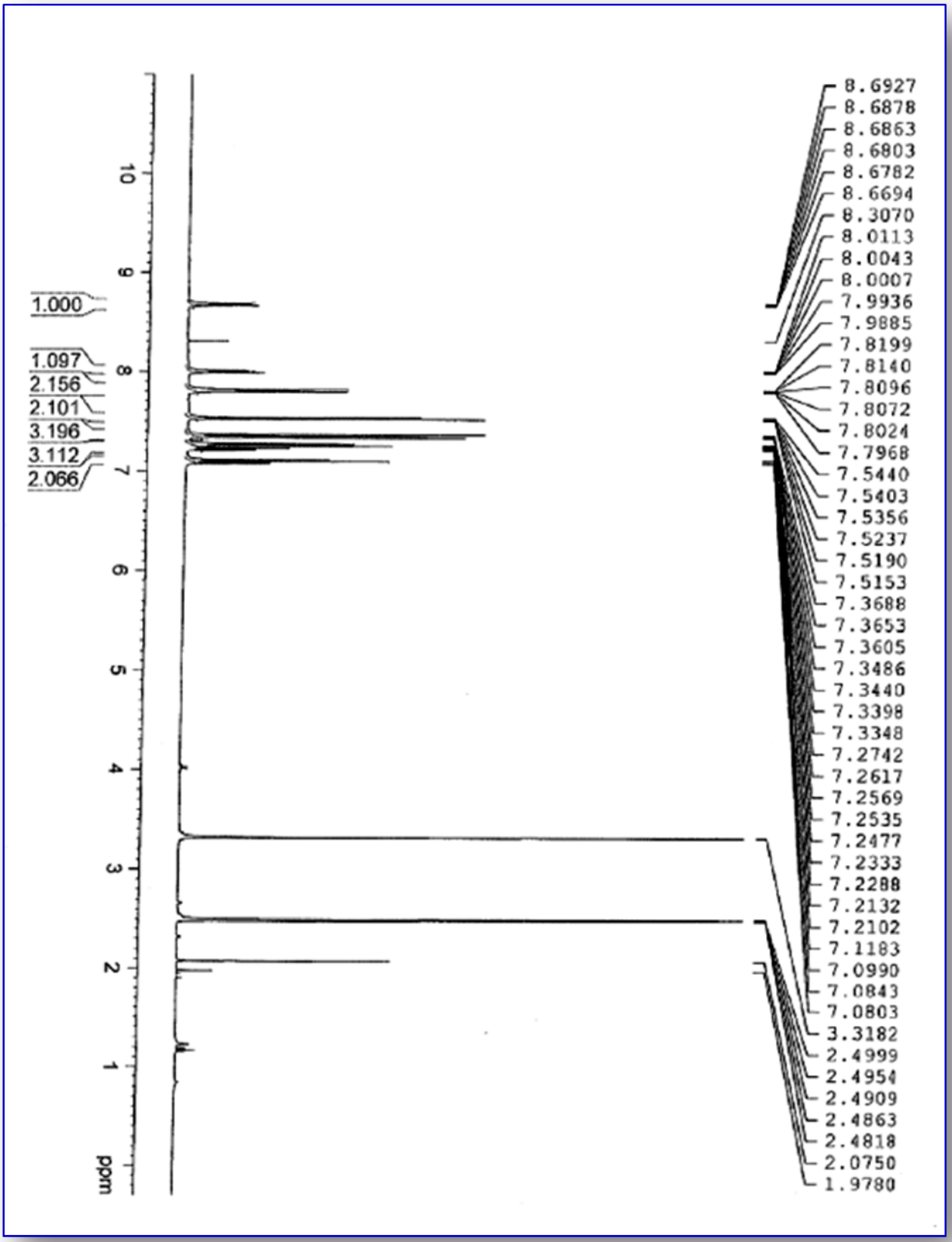
m/z

4b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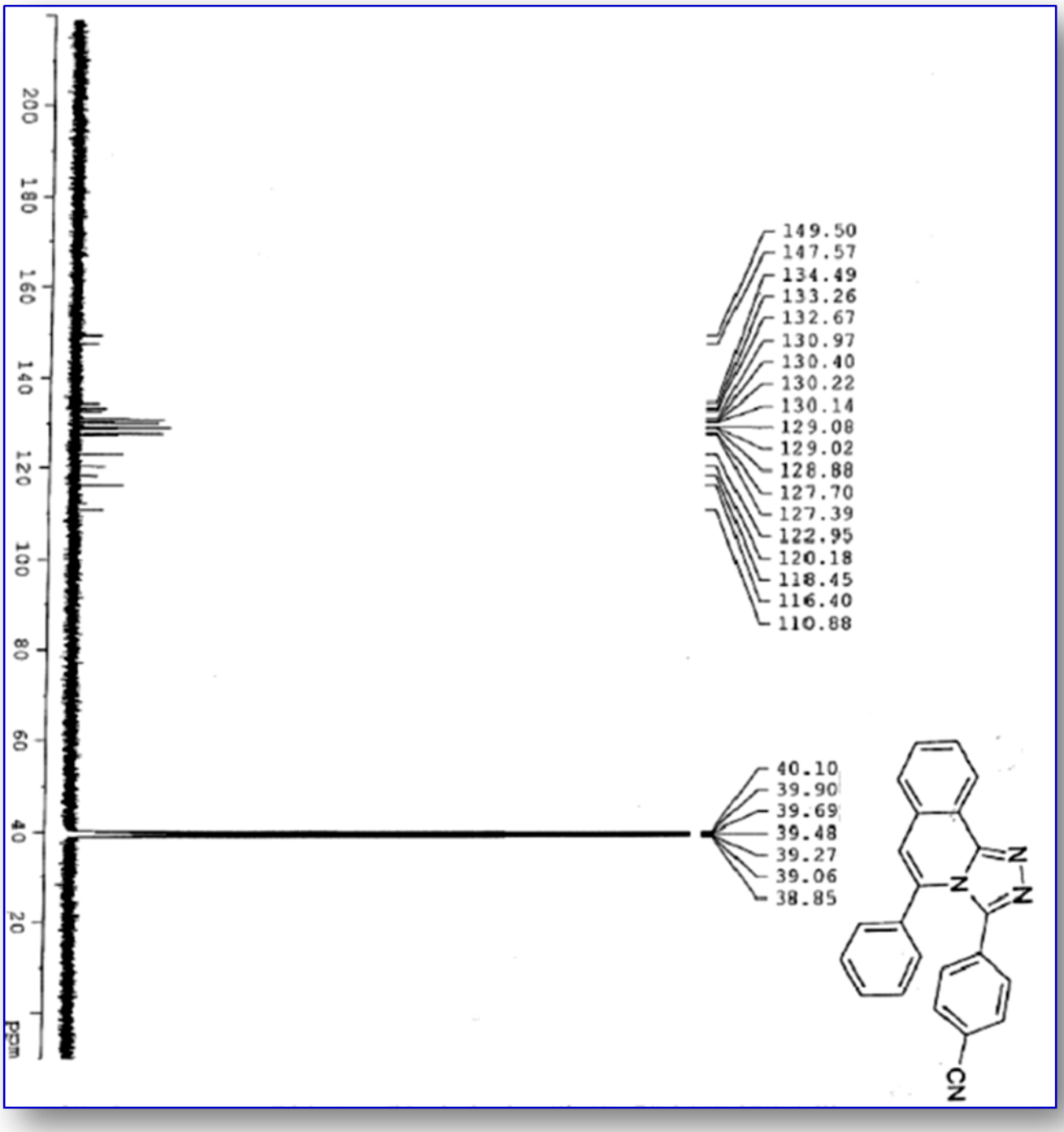
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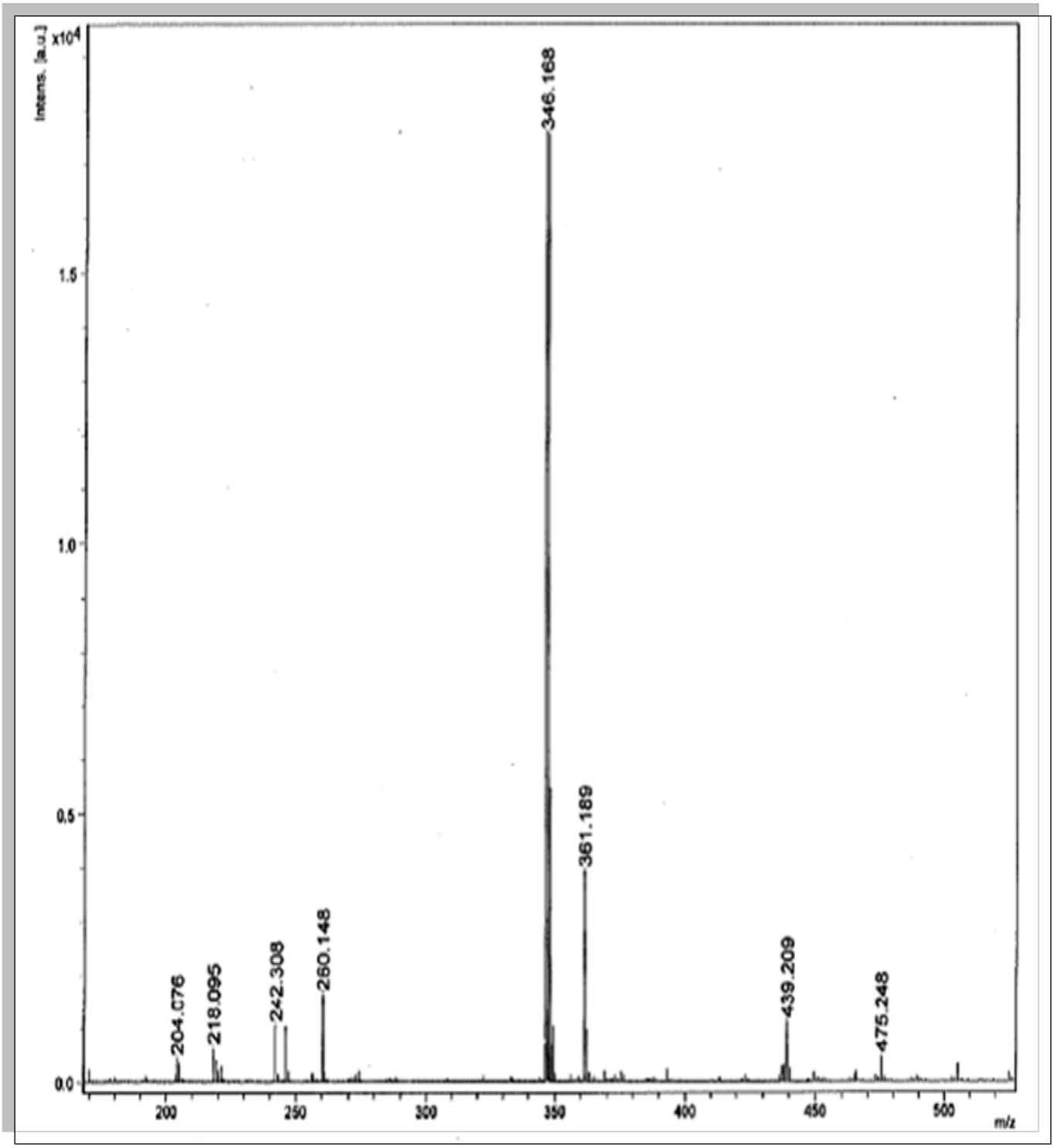
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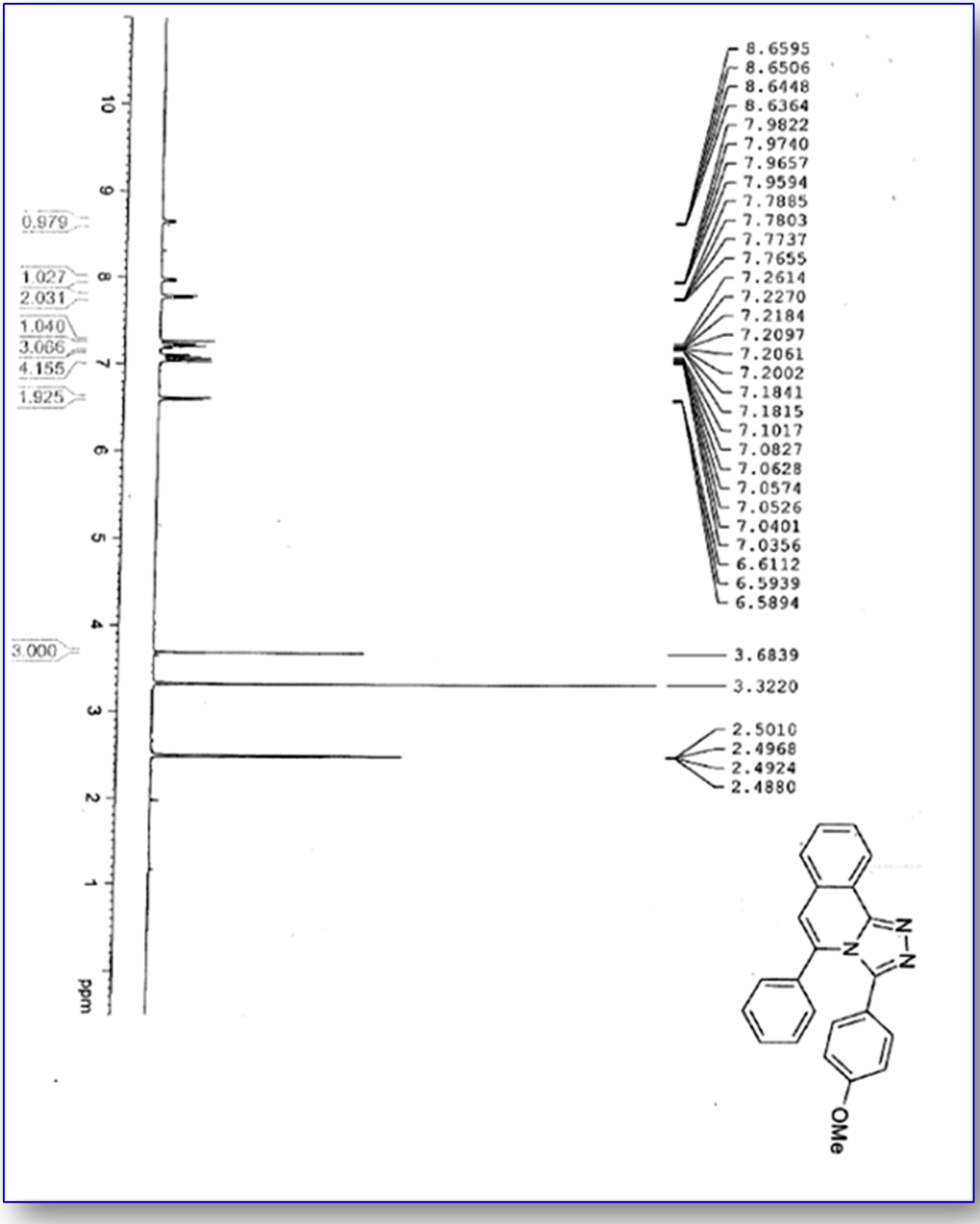
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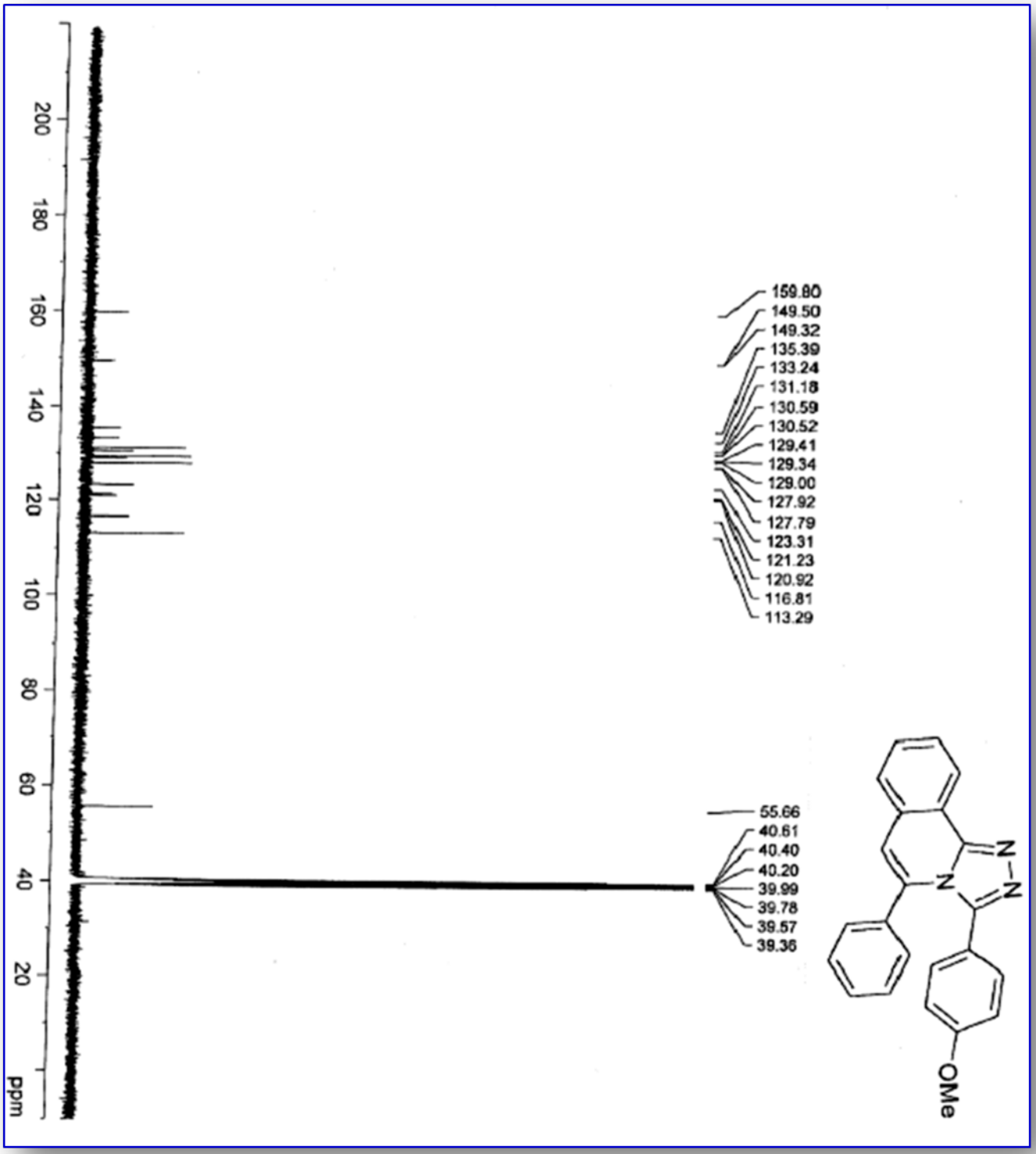
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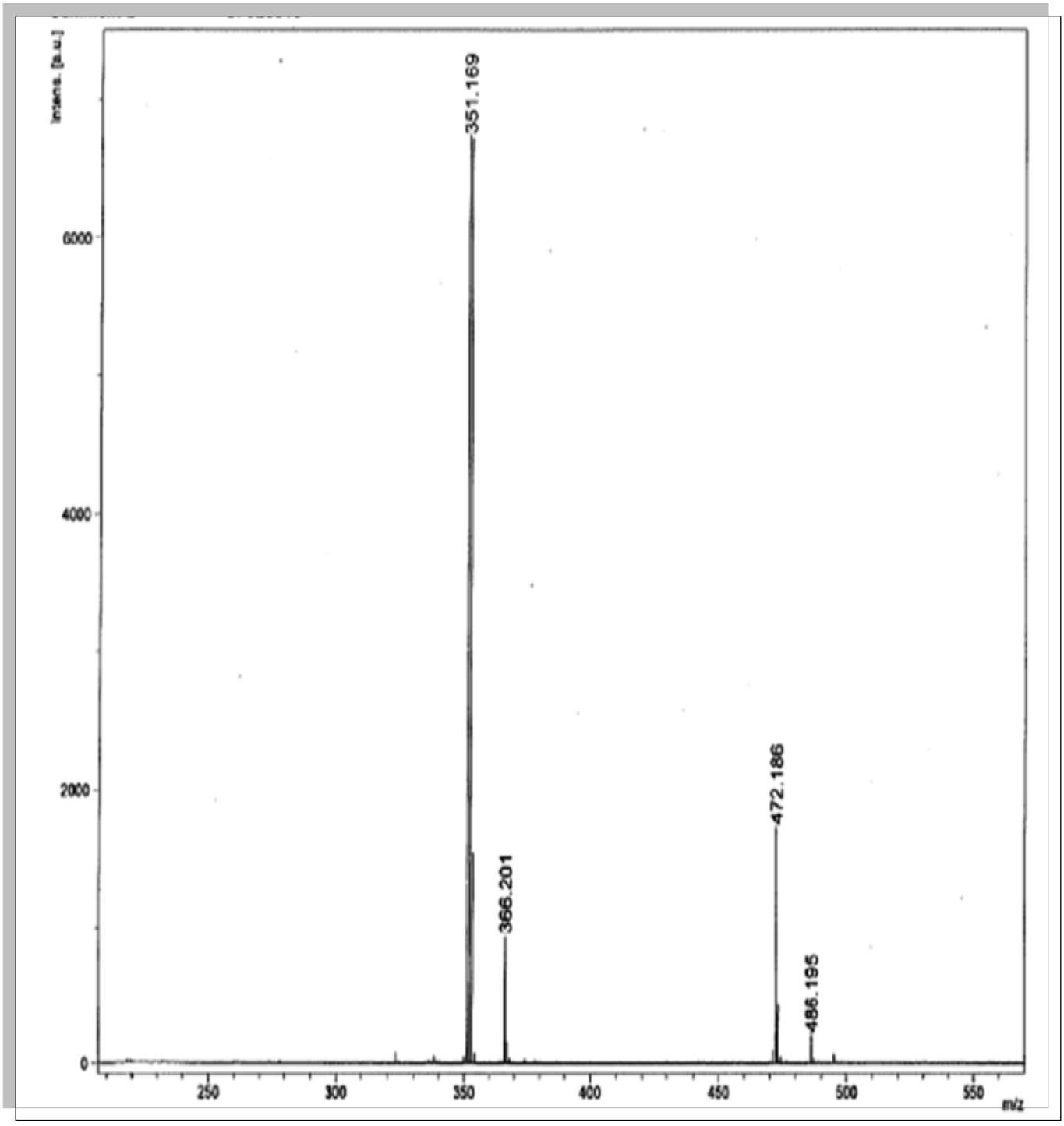
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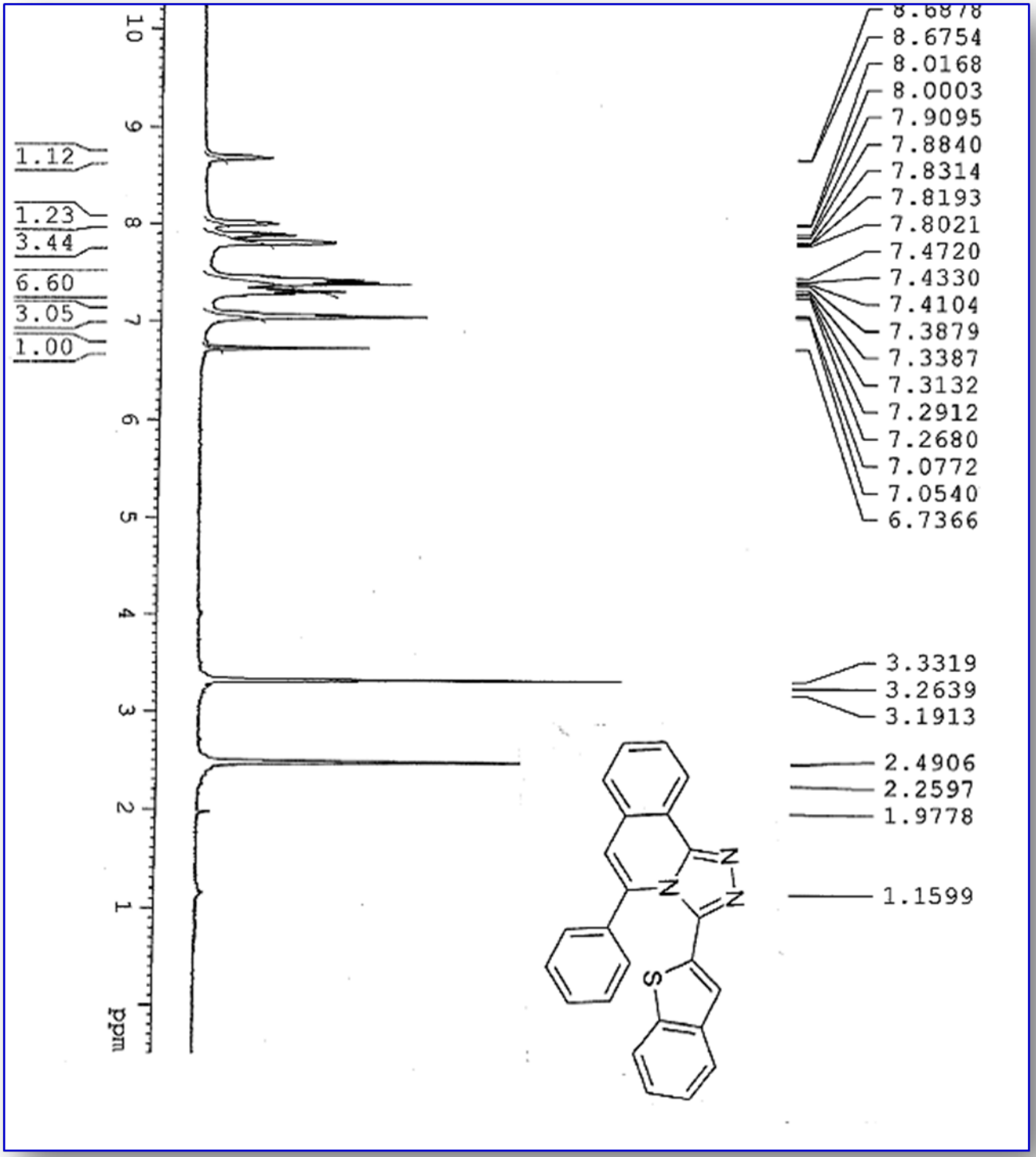
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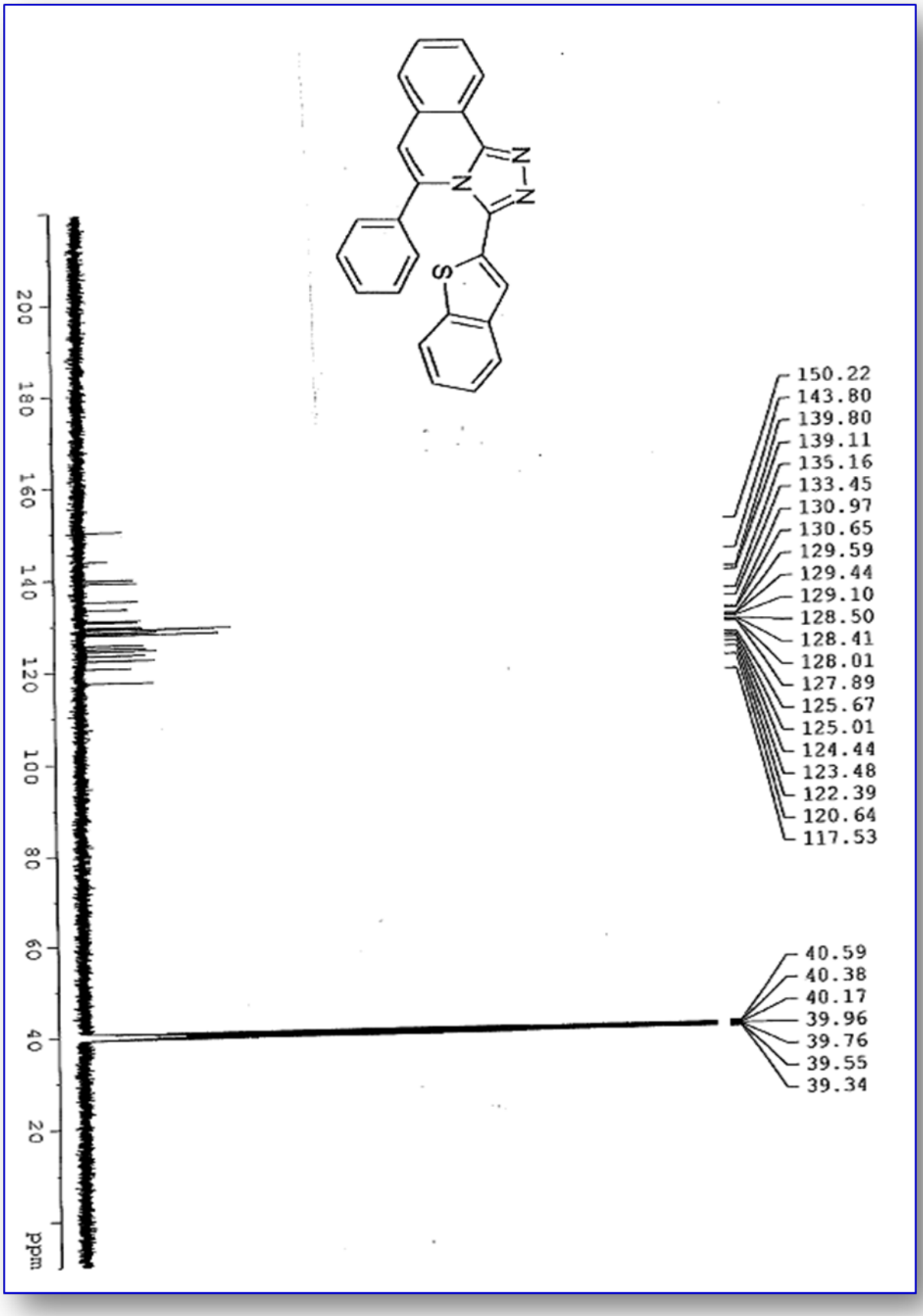
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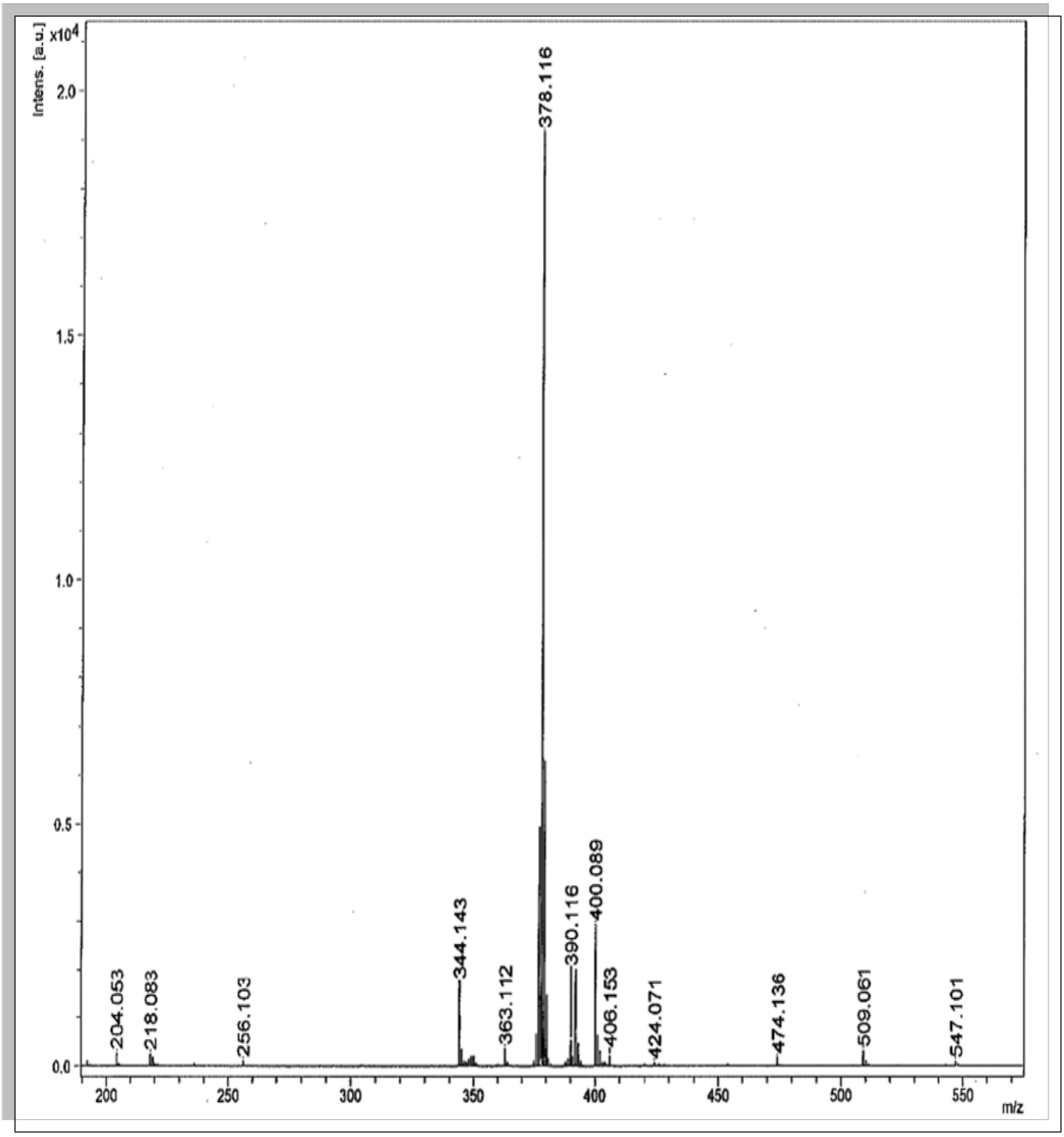
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424.071
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509.061
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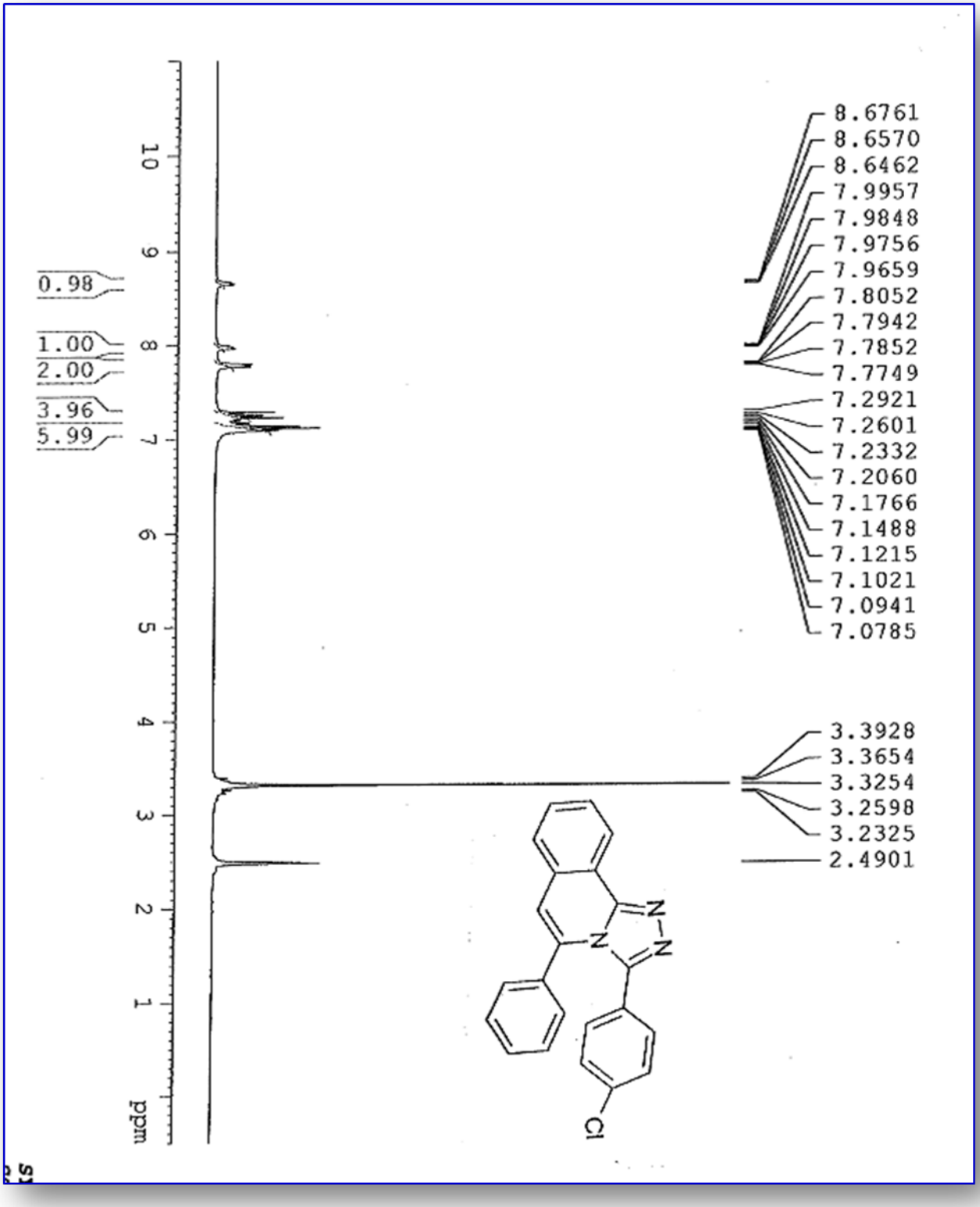
200
250
300
350
400
450
500
550
m/z

4e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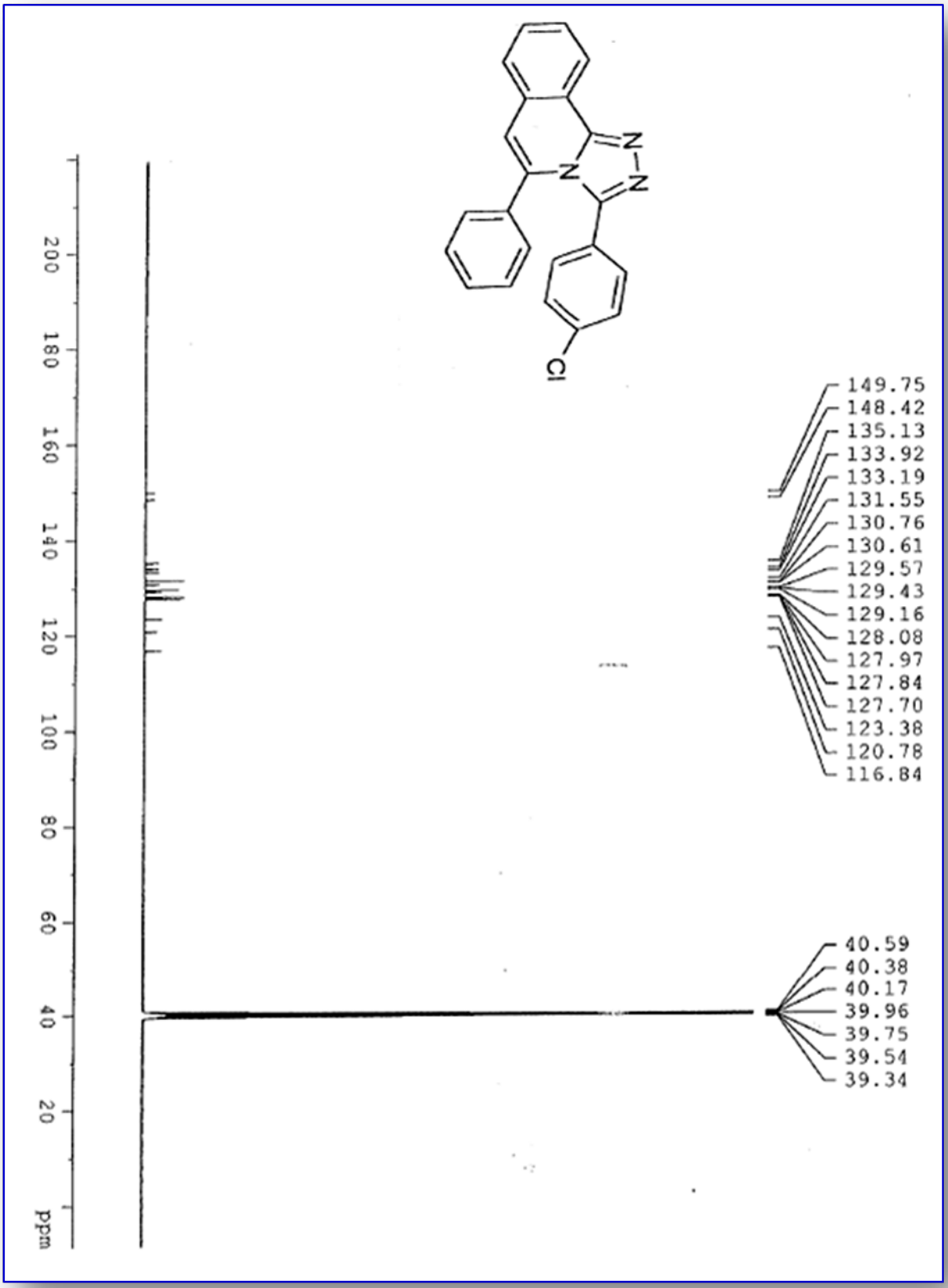
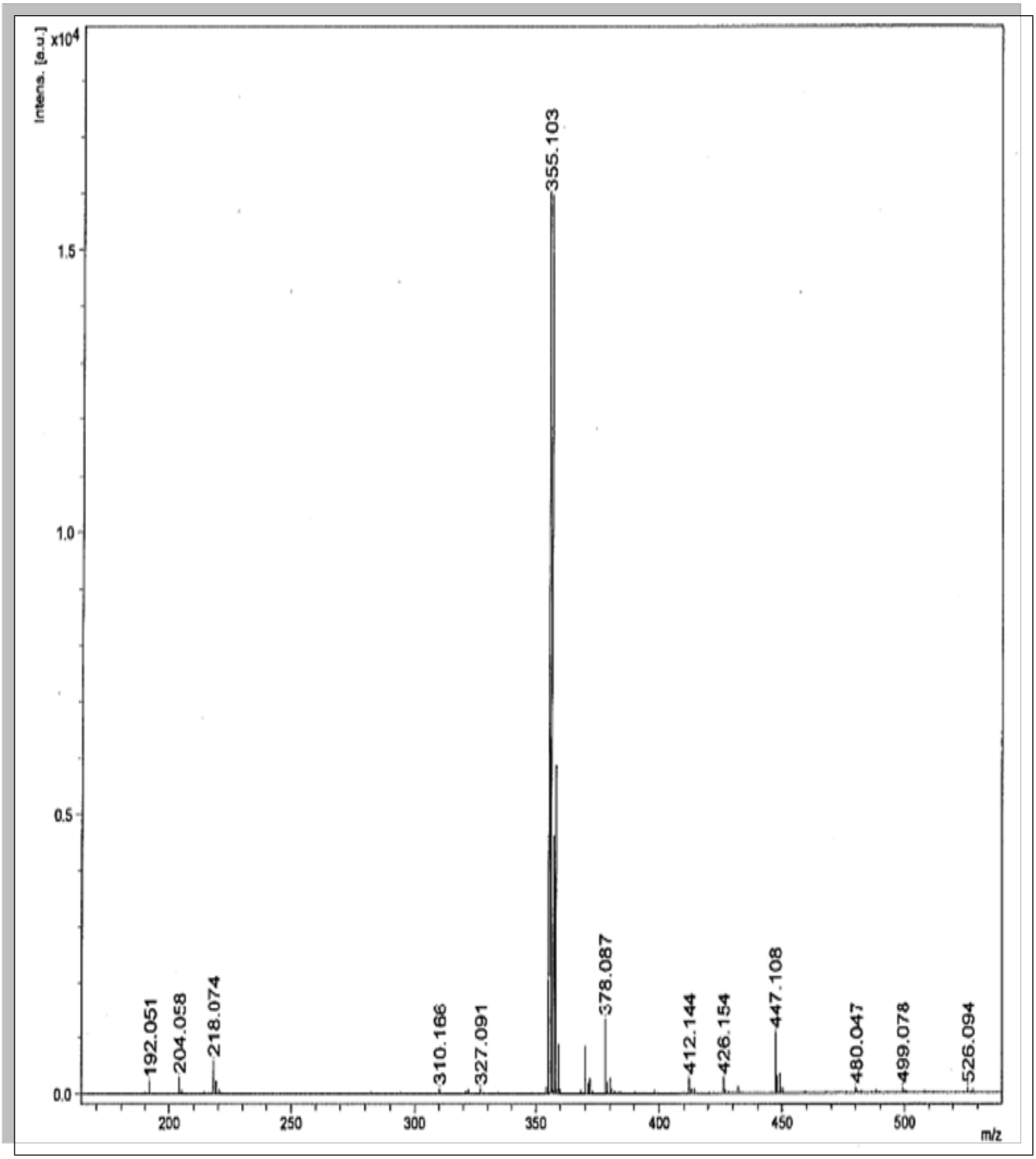
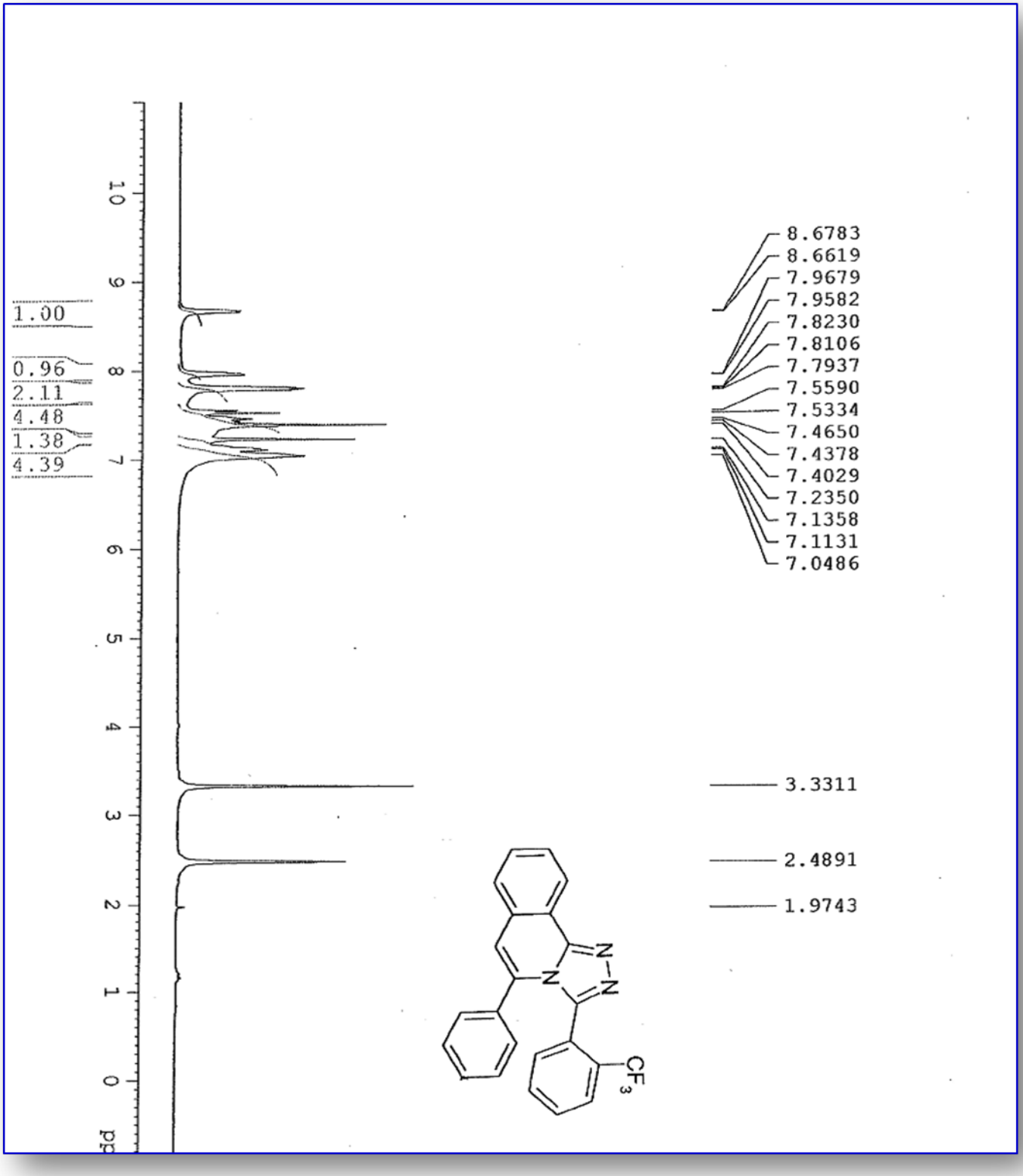
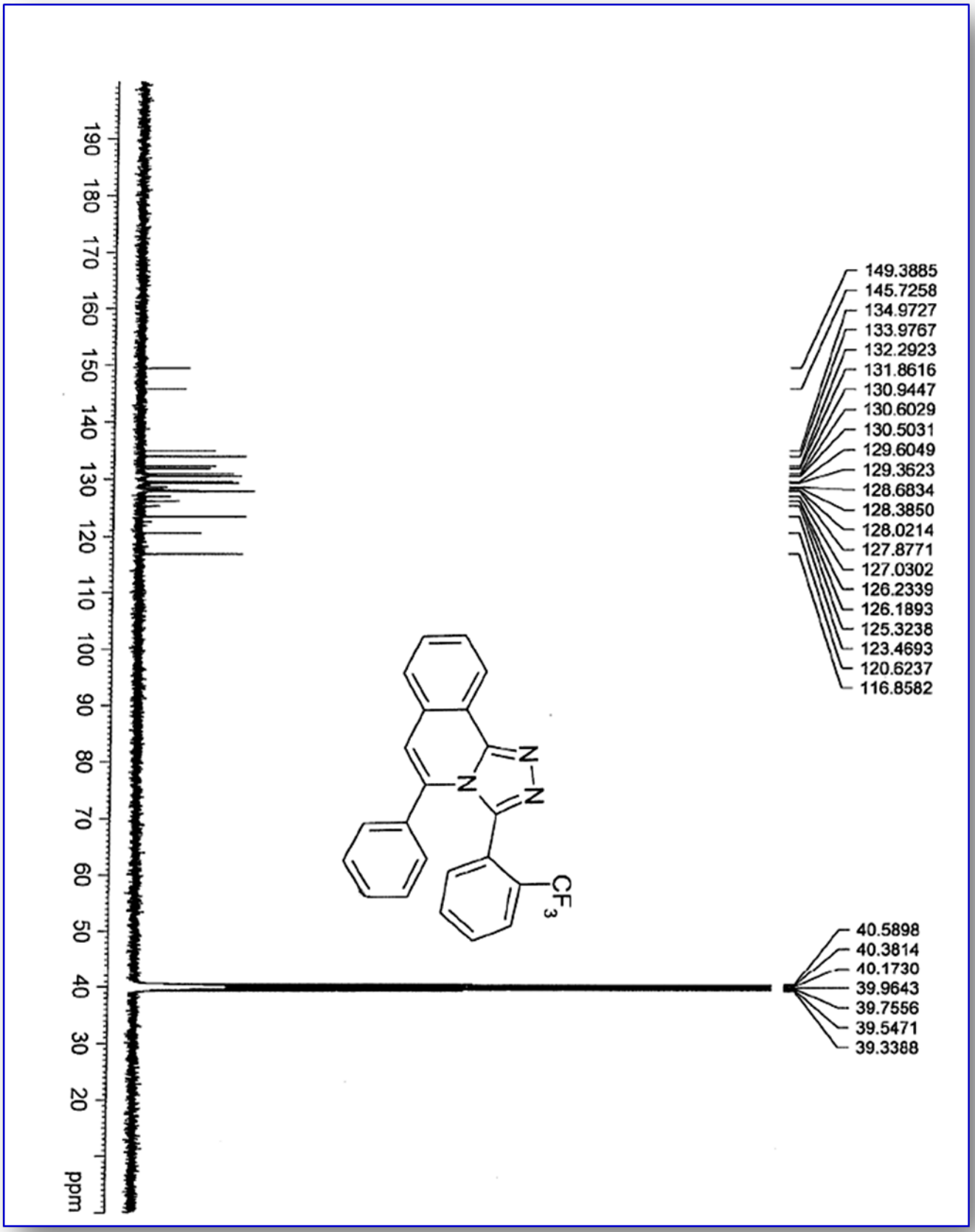
8.6570
8.6462
7.9957
7.9848
7.9756
7.9659
7.8052
7.7942
7.7852
7.7749
7.2921
7.2601
7.2332
7.2060
7.1766
7.1488
7.1215
7.1021
7.0941
7.0785
3.3928
3.3654
3.3254
3.2598
3.2325
2.4901
0.98
1.00
2.00
3.96
5.99
ppm
Cl

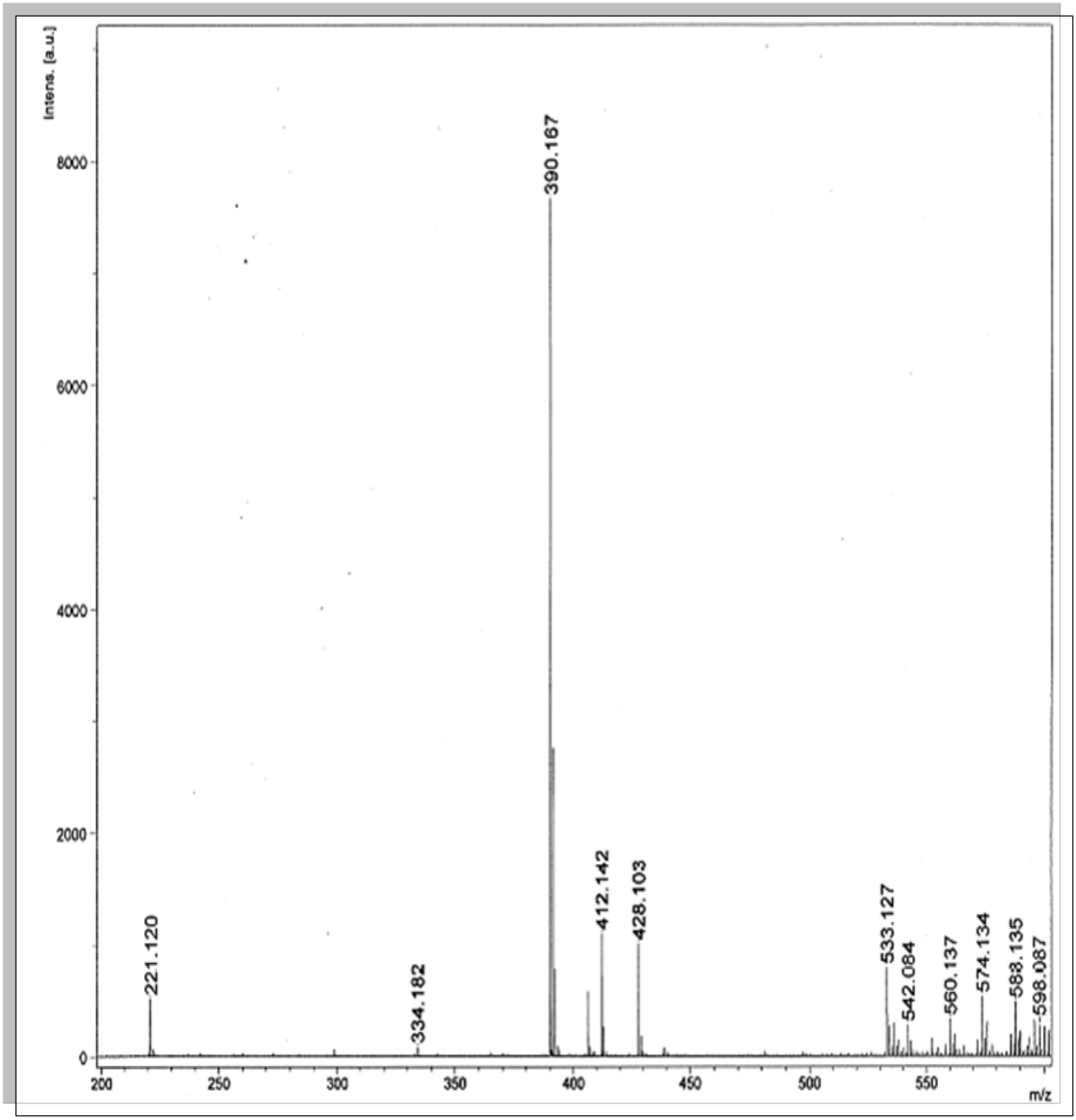

N
N
N
Cl
149.75
148.42
135.13
133.92
133.19
131.55
130.76
130.61
129.57
129.43
129.16
128.08
127.97
127.84
127.70
123.38
120.78
116.84
40.59
40.38
40.17
39.96
39.75
39.54
39.34
200
180
160
140
120
100
80
60
40
20
ppm


Intens. [a.u.]
x10^4
1.5
1.0
0.5
0.0
355.103
192.051
204.058
218.074
310.166
327.091
378.087
412.144
426.154
447.108
480.047
499.078
526.094
200
250
300
350
400
450
500
m/z

4f


8.6783
8.6619
7.9679
7.9582
7.8230
7.8106
7.7937
7.5590
7.5334
7.4650
7.4378
7.4029
7.2350
7.1358
7.1131
7.0486
3.3311
2.4891
1.9743
1.00
0.96
2.11
4.48
1.38
4.39
CF3


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
149.3885
145.7258
134.9727
133.9767
132.2923
131.8616
130.9447
130.6029
130.5031
129.6049
129.3623
128.6834
128.3850
128.0214
127.8771
127.0302
126.2339
126.1893
125.3238
123.4693
120.6237
116.8582
40.5898
40.3814
40.1730
39.9643
39.7556
39.5471
39.3388
N
N
N
CF3


Intens. [a.u.]
8000
6000
4000
2000
0
200
250
300
350
400
450
500
550
m/z
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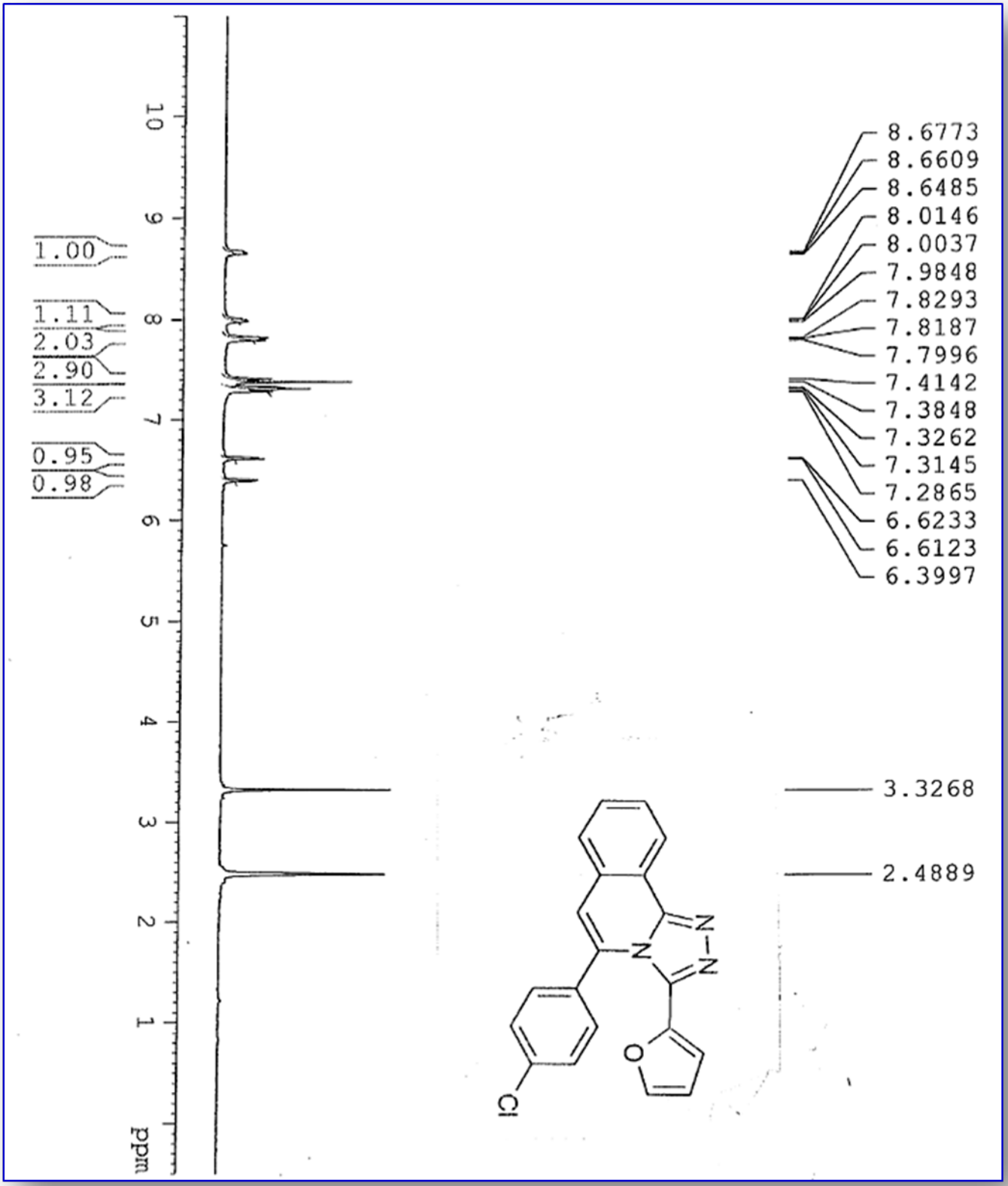
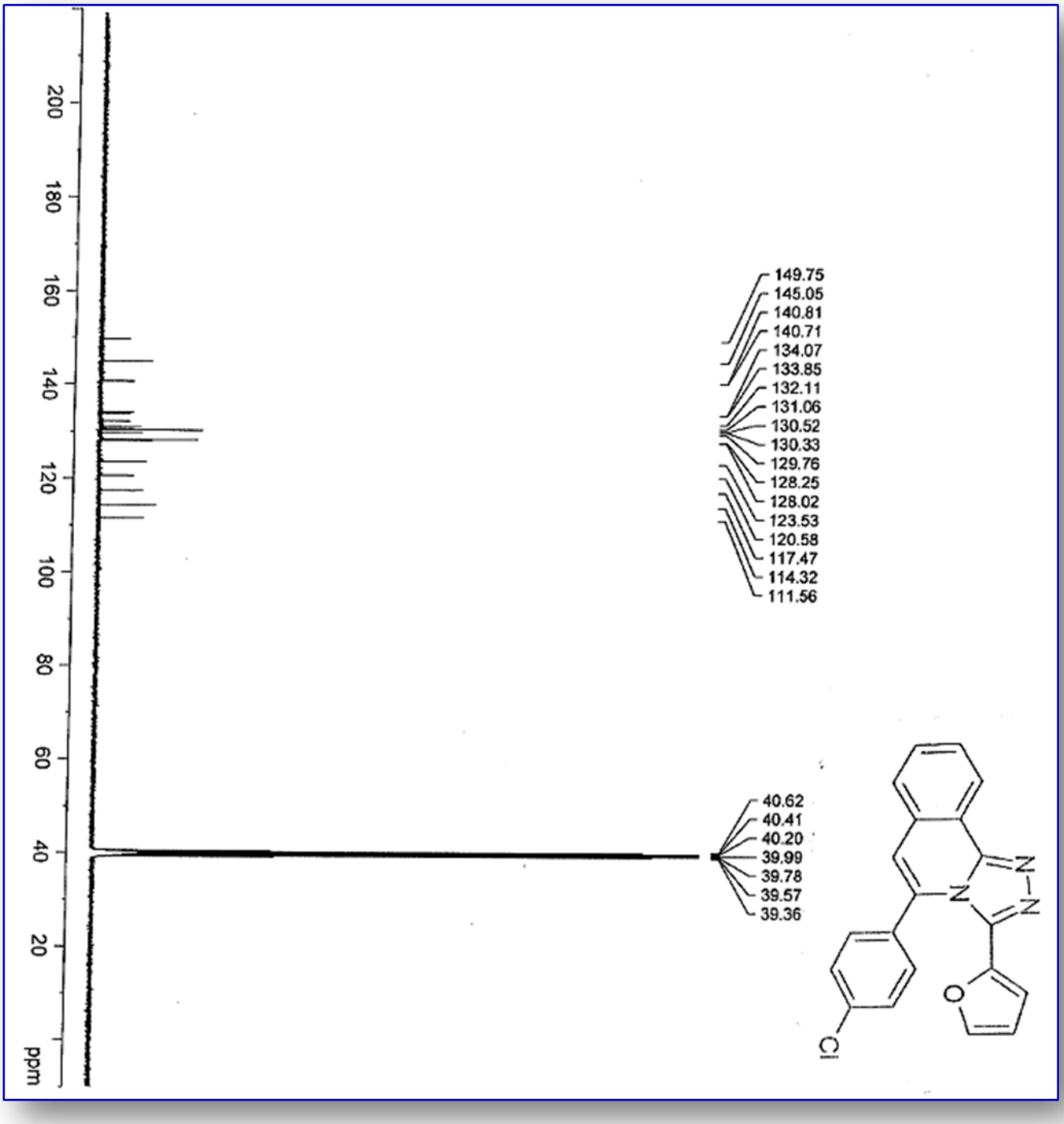
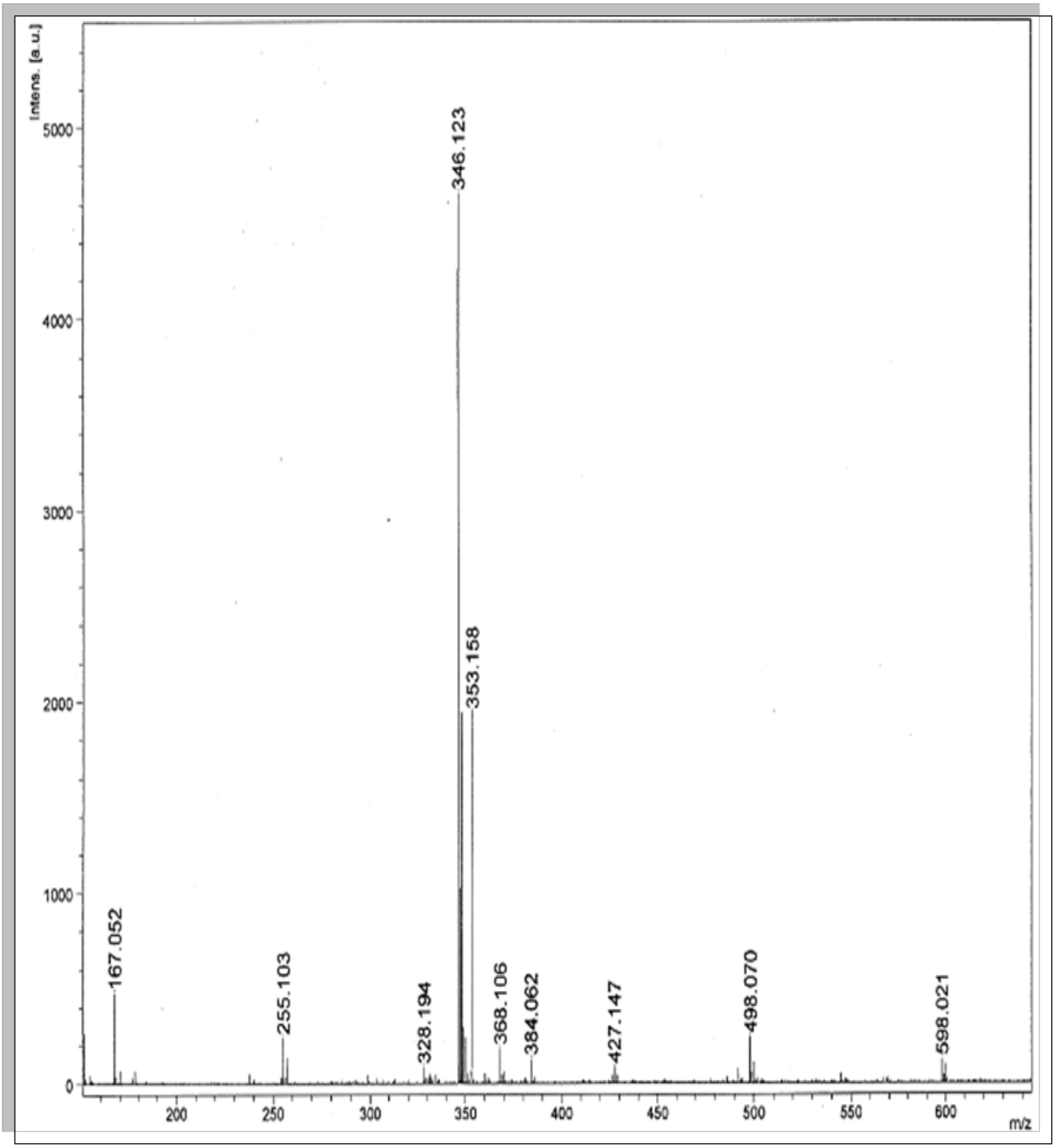
334.182
390.167
412.142
428.103
533.127
542.084
560.137
574.134
588.135
598.087

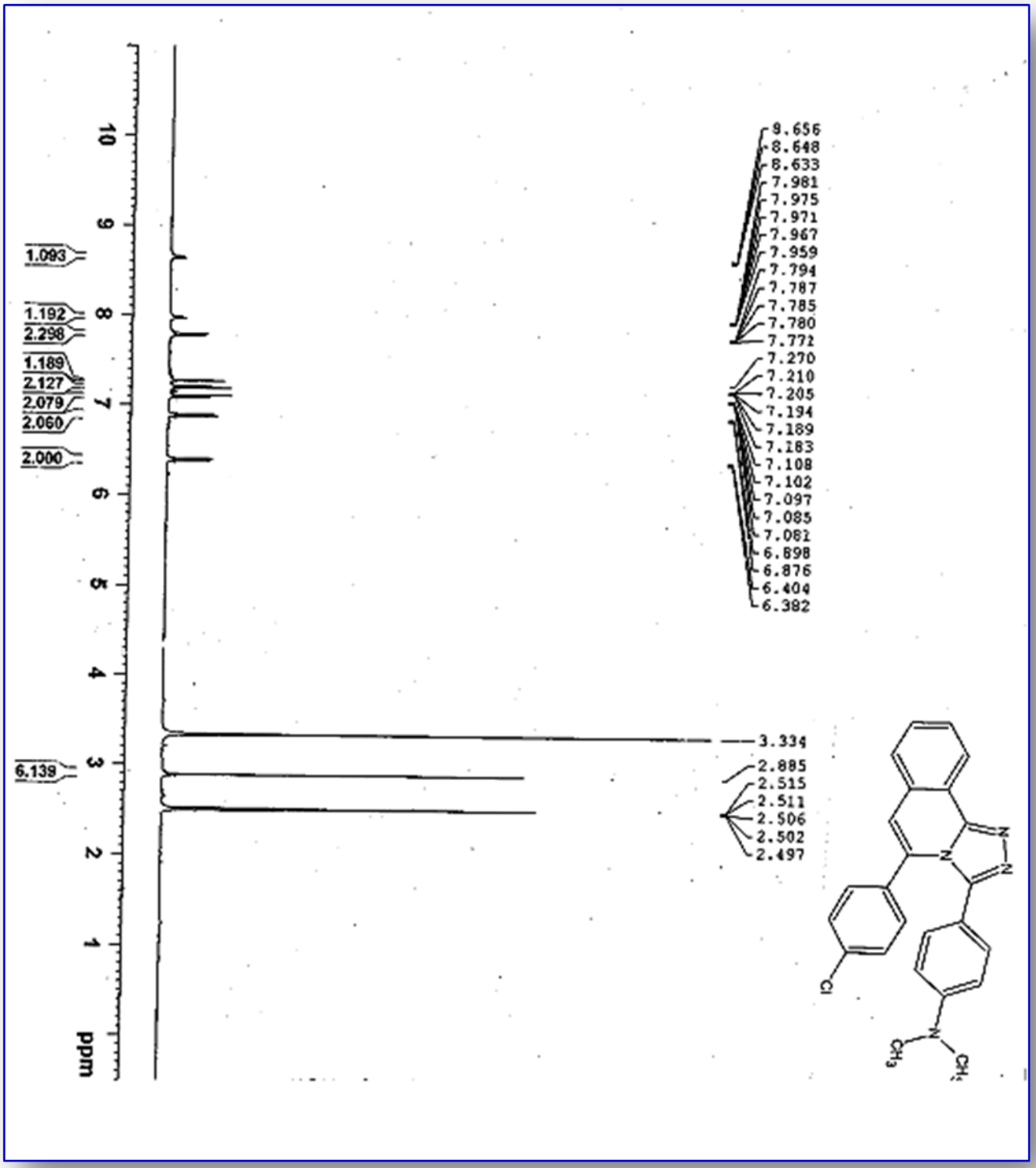
4g

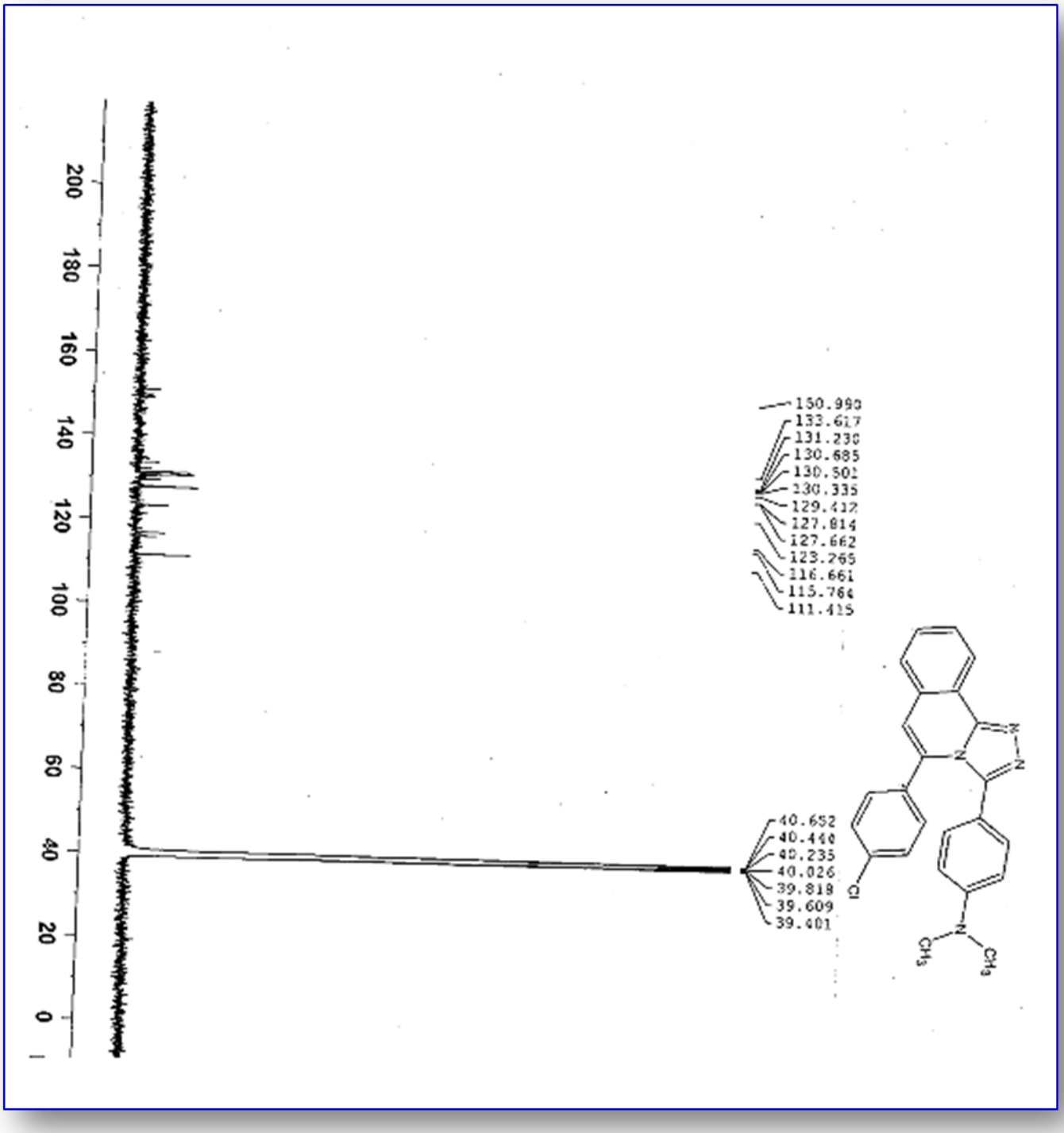

8.6773
8.6609
8.6485
8.0146
8.0037
7.9848
7.8293
7.8187
7.7996
7.4142
7.3848
7.3262
7.3145
7.2865
6.6233
6.6123
6.3997
3.3268
2.4889
1.00
1.11
2.03
2.90
3.12
0.95
0.98
ppm
N
N
N
O
Cl

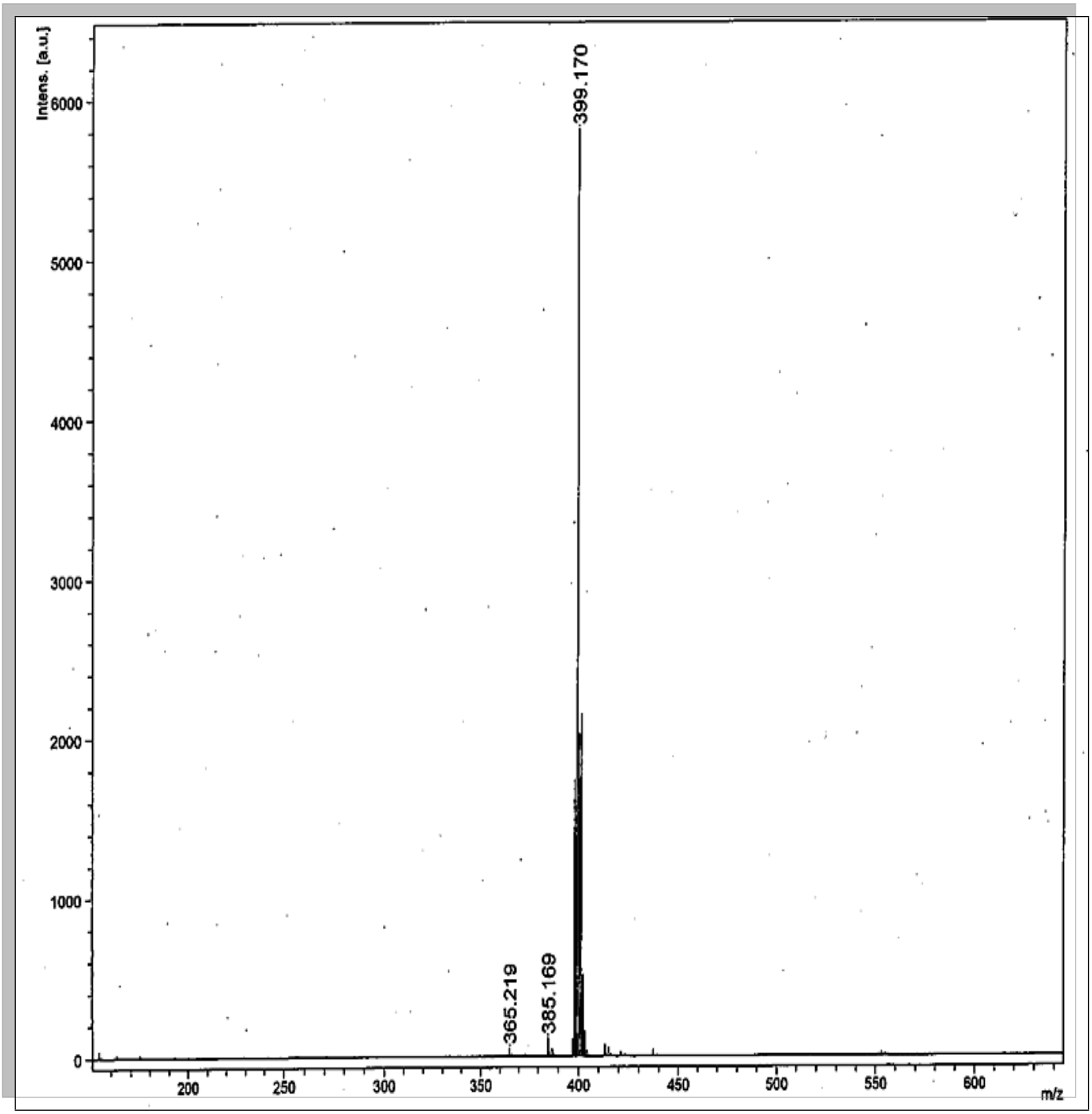

200
180
160
140
120
100
80
60
40
20
ppm
149.75
145.05
140.81
140.71
134.07
133.85
132.11
131.06
130.52
130.33
129.76
128.25
128.02
123.53
120.58
117.47
114.32
111.56
40.62
40.41
40.20
39.99
39.78
39.57
39.36
N
N
N
O
Cl


Intens. [a.u.]
5000
4000
3000
2000
1000
0
346.123
353.158
167.052
255.103
328.194
368.106
384.062
427.147
498.070
598.021
200
250
300
350
400
450
500
550
600
m/z

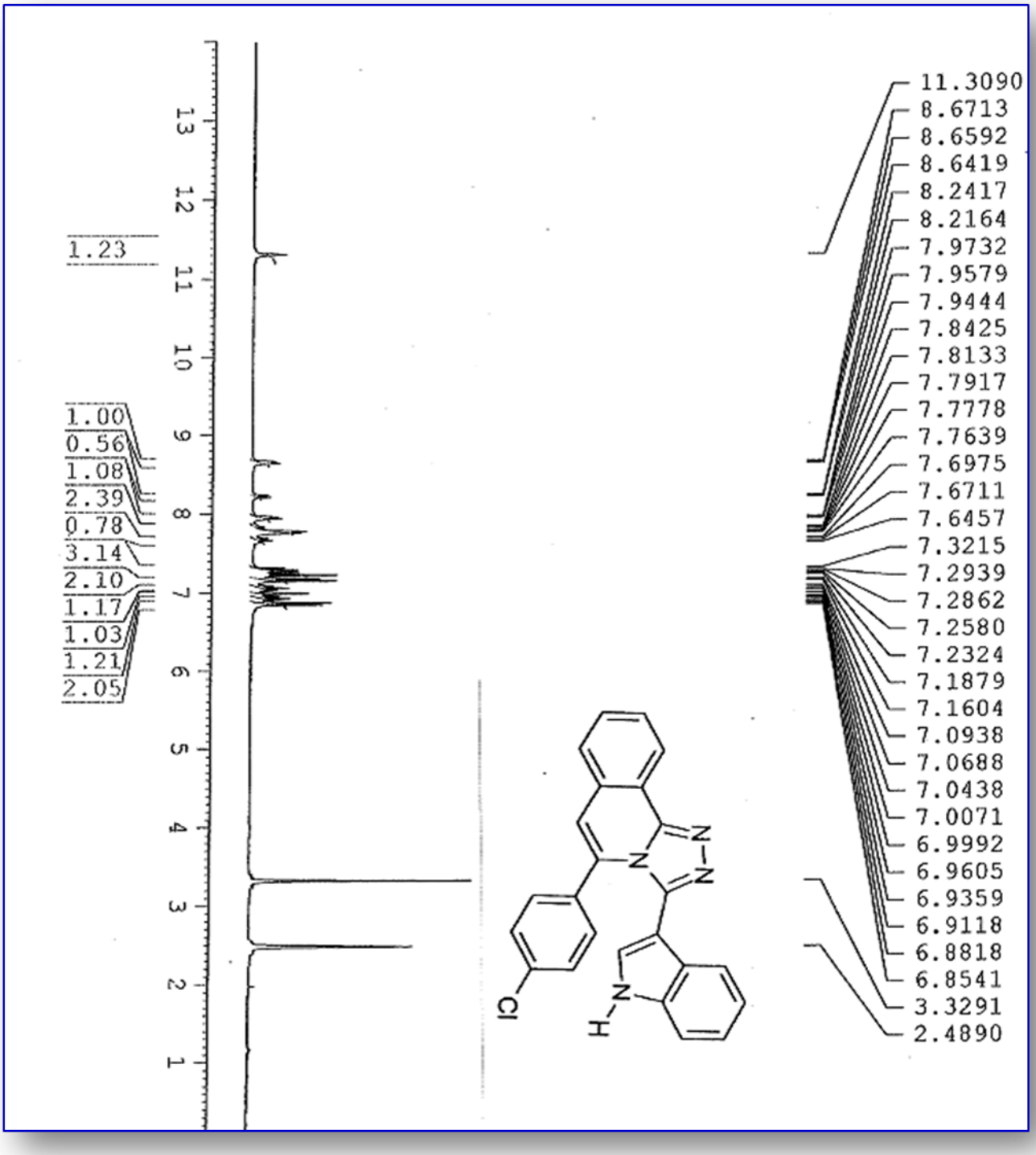
4h

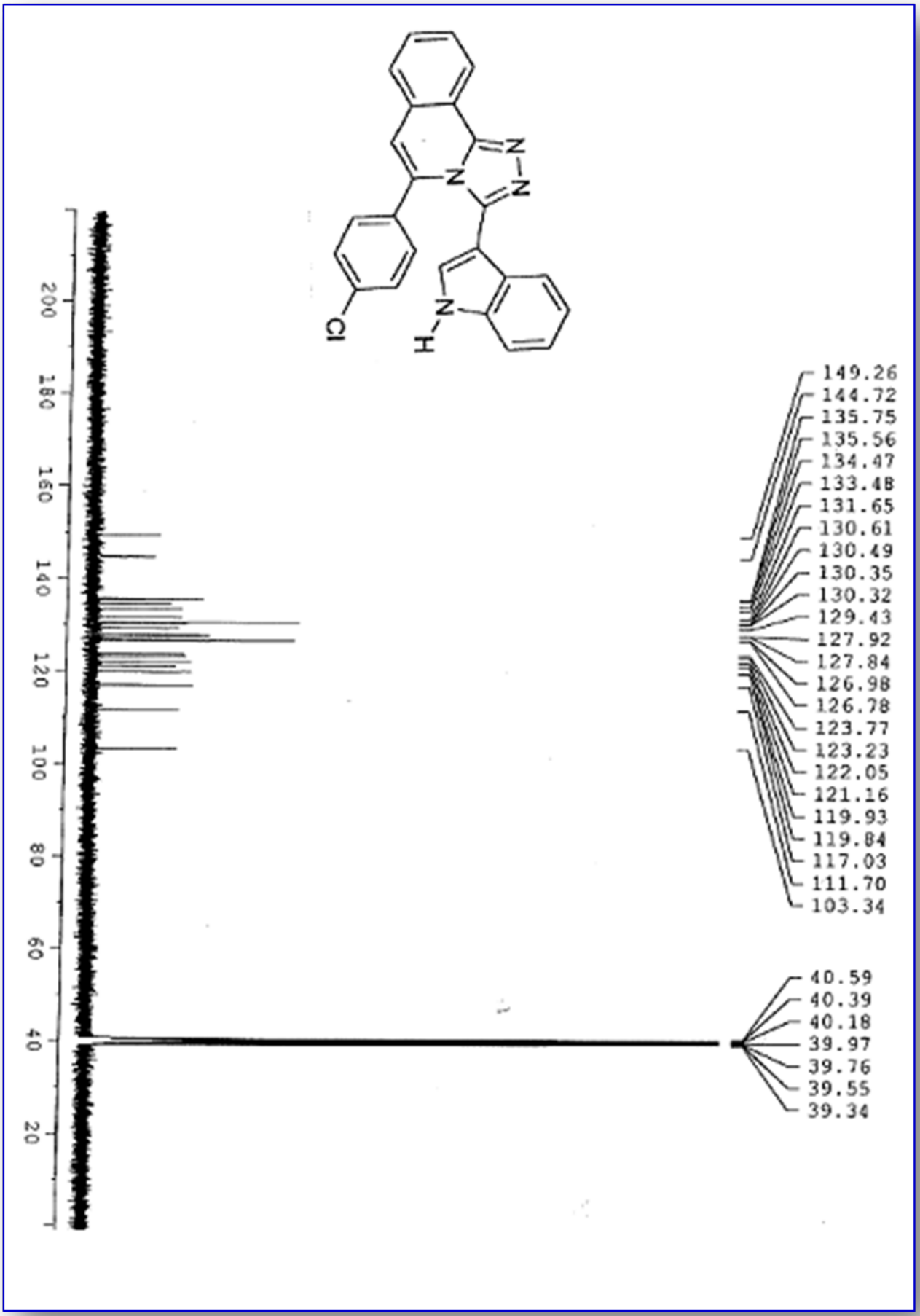

9.656
8.648
8.633
7.981
7.975
7.971
7.967
7.959
7.794
7.787
7.785
7.780
7.772
7.270
7.210
7.205
7.194
7.189
7.183
7.108
7.102
7.097
7.085
7.081
6.898
6.876
6.404
6.382
3.334
2.885
2.515
2.511
2.506
2.502
2.497
1.093
1.192
2.298
1.189
2.127
2.079
2.060
2.000
6.139
ppm
Cl
N
CH3
CH3

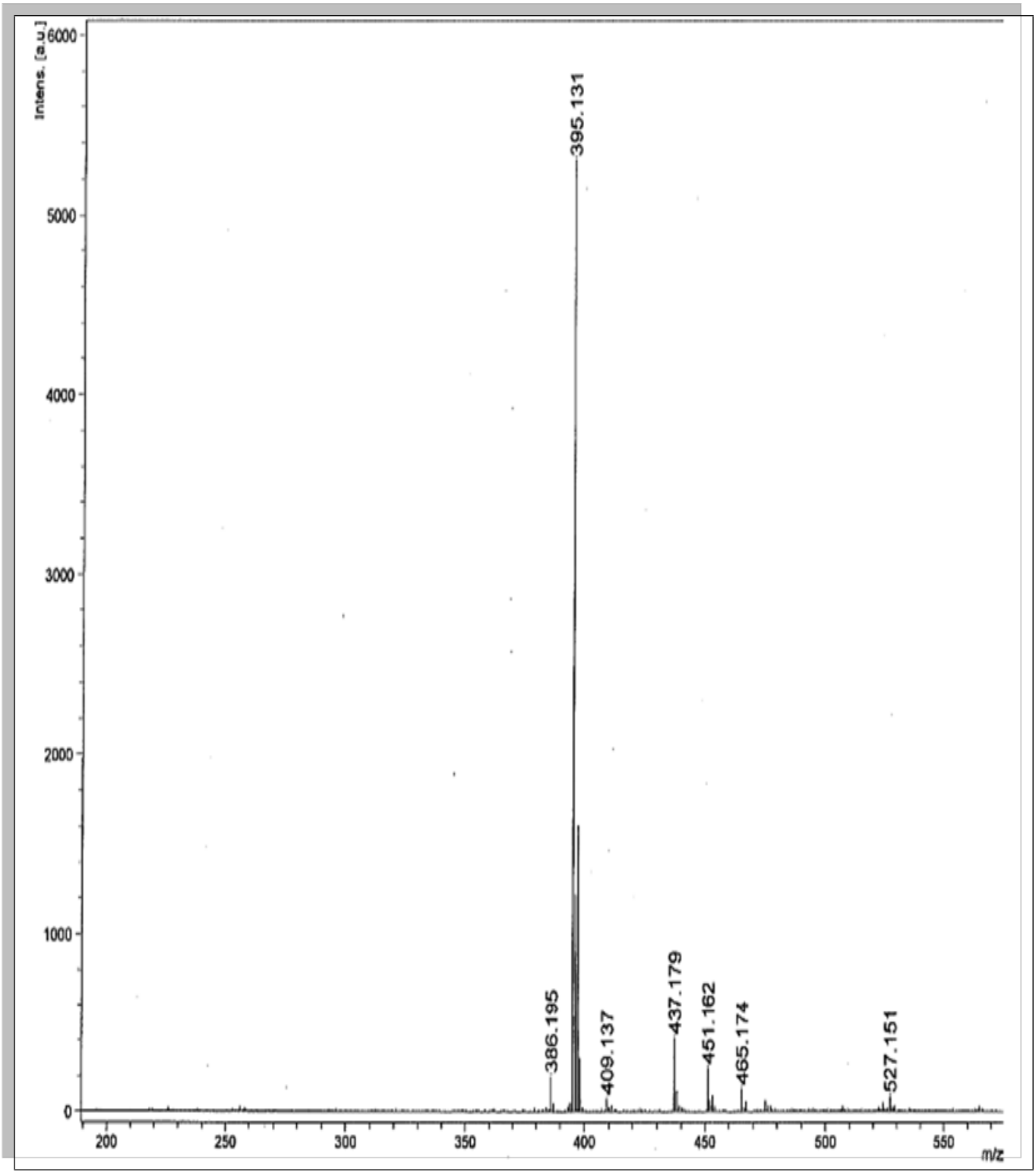

200
180
160
140
120
100
80
60
40
20
0
150.990
133.617
131.230
130.685
130.501
130.335
129.412
127.814
127.662
123.265
116.661
115.764
111.415
40.652
40.440
40.235
40.026
39.818
39.609
39.401
Cl
N
N
N
N
CH3
CH3


Intens. [a.u.]
6000
5000
4000
3000
2000
1000
0
399.170
385.169
365.219
200
250
300
350
400
450
500
550
600
m/z

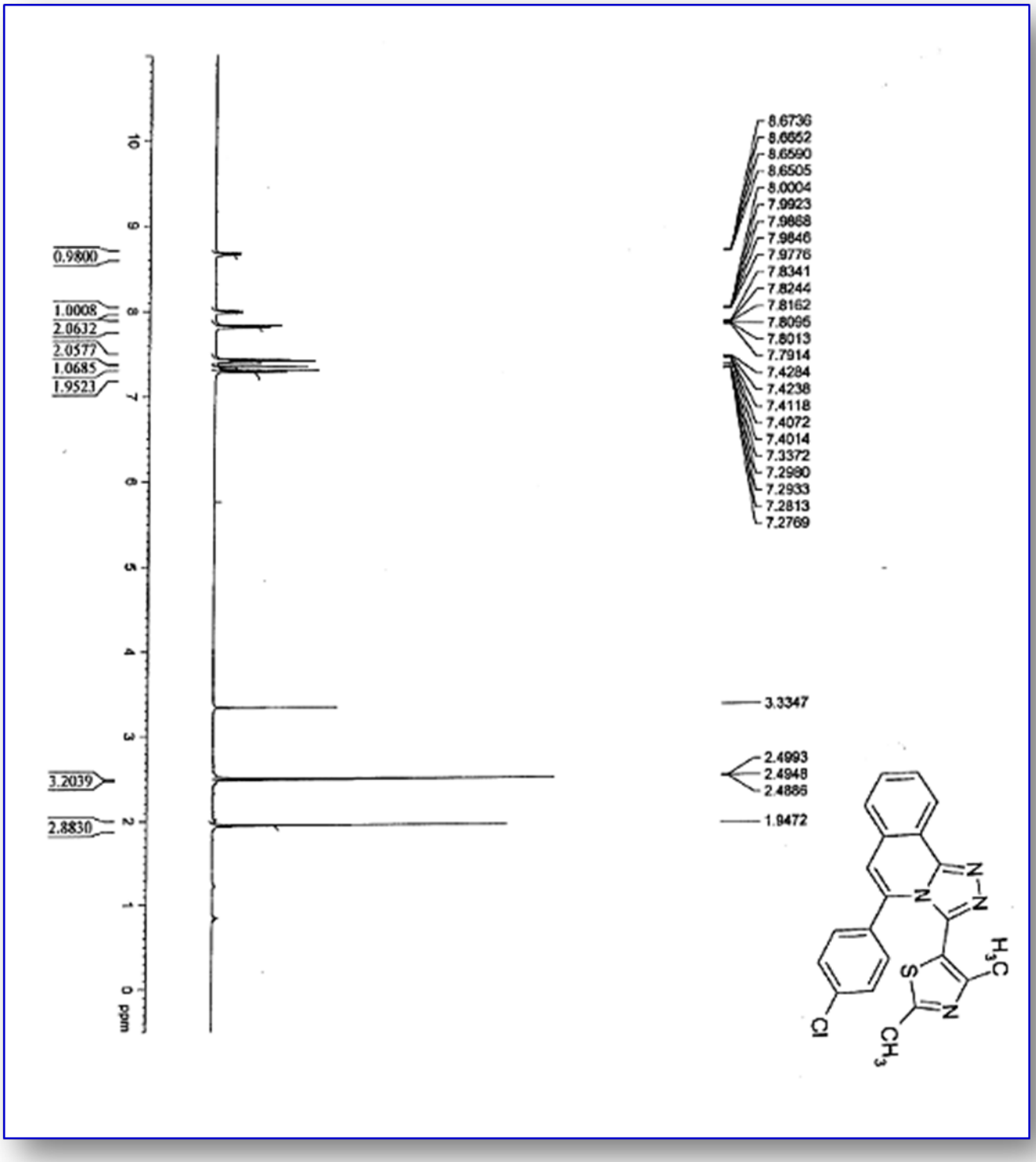
4i

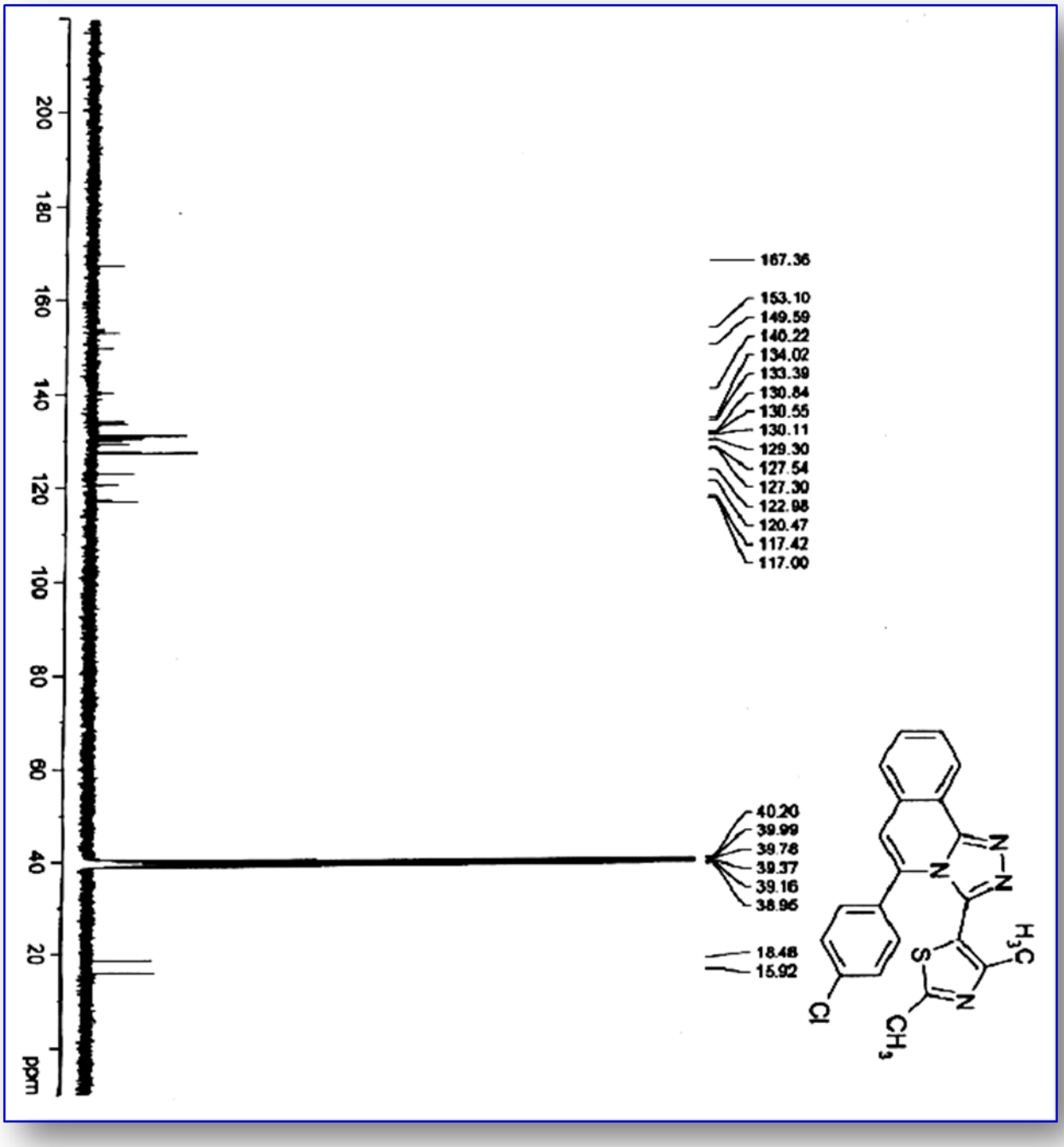

11.3090
8.6713
8.6592
8.6419
8.2417
8.2164
7.9732
7.9579
7.9444
7.8425
7.8133
7.7917
7.7778
7.7639
7.6975
7.6711
7.6457
7.3215
7.2939
7.2862
7.2580
7.2324
7.1879
7.1604
7.0938
7.0688
7.0438
7.0071
6.9992
6.9605
6.9359
6.9118
6.8818
6.8541
3.3291
2.4890
1.23
1.00
0.56
1.08
2.39
0.78
3.14
2.10
1.17
1.03
1.21
2.05
13 12 11 10 9 8 7 6 5 4 3 2 1
N
N
N
H
Cl

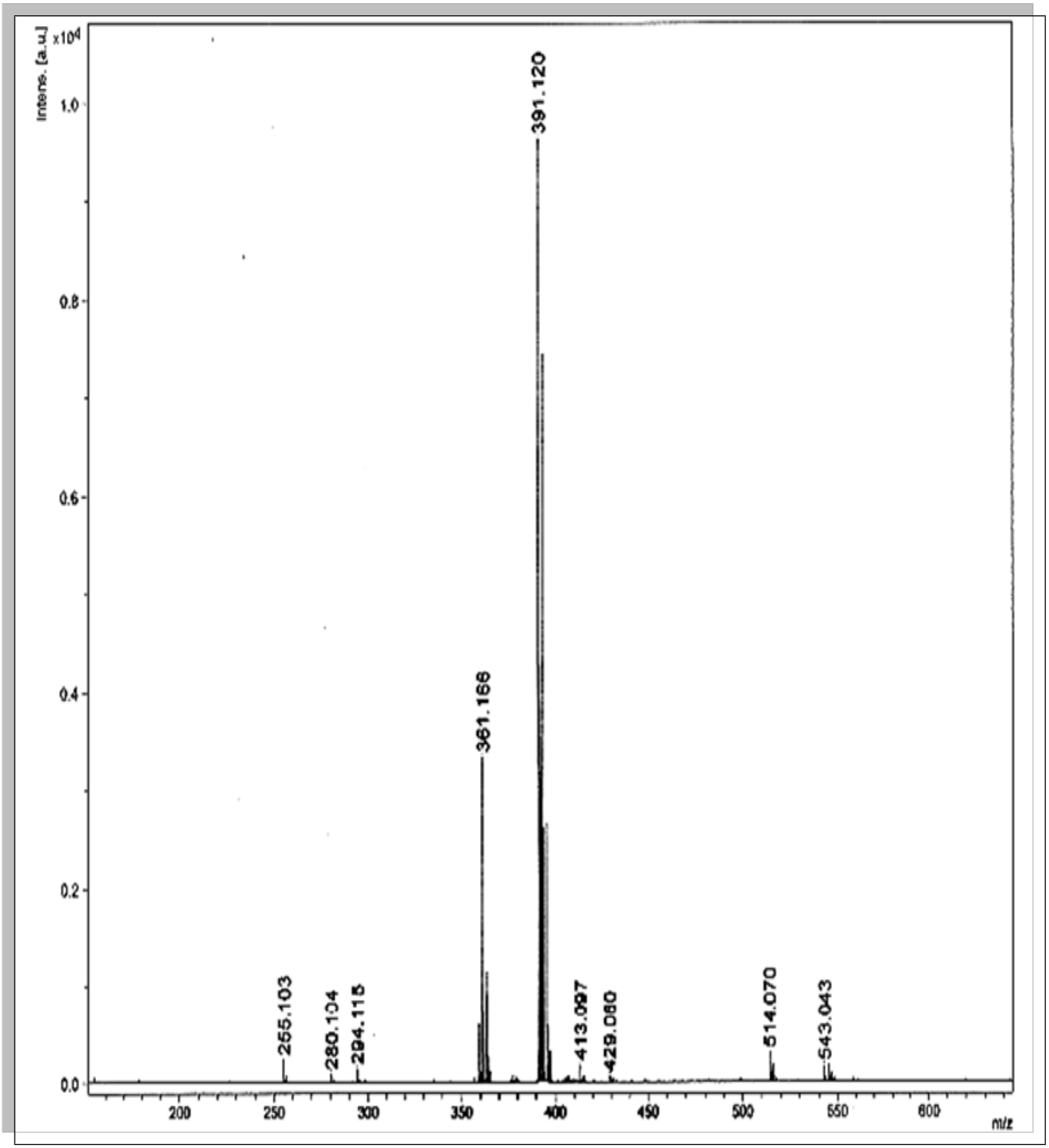

N
N
N
Cl
H
200
180
160
140
120
100
80
60
40
20
149.26
144.72
135.75
135.56
134.47
133.48
131.65
130.61
130.49
130.35
130.32
129.43
127.92
127.84
126.98
126.78
123.77
123.23
122.05
121.16
119.93
119.84
117.03
111.70
103.34
40.59
40.39
40.18
39.97
39.76
39.55
39.34


Intens. [a.u.]
6000
5000
4000
3000
2000
1000
0
395.131
386.195
409.137
437.179
451.162
465.174
527.151
200
250
300
350
400
450
500
550
m/z

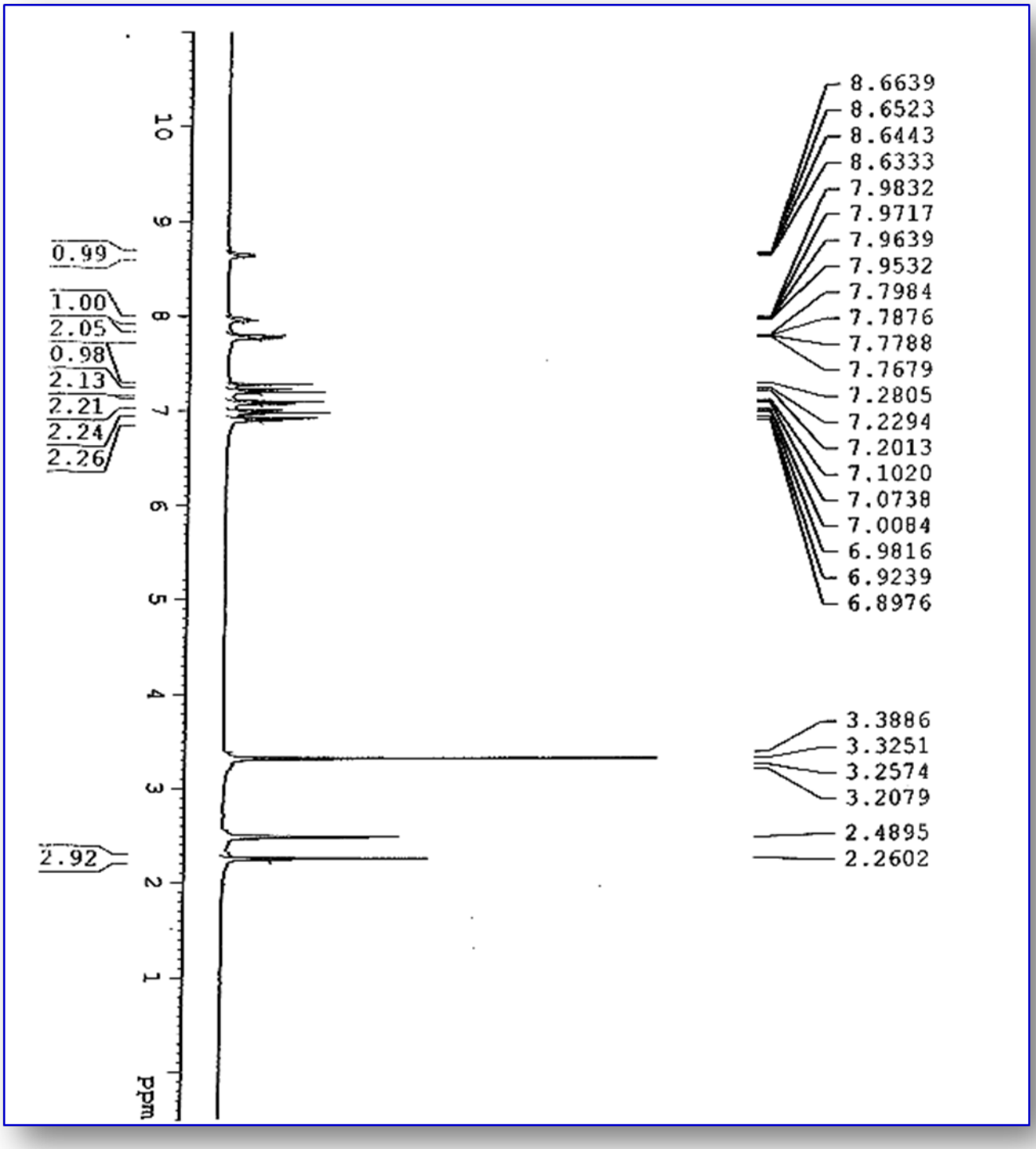
4j

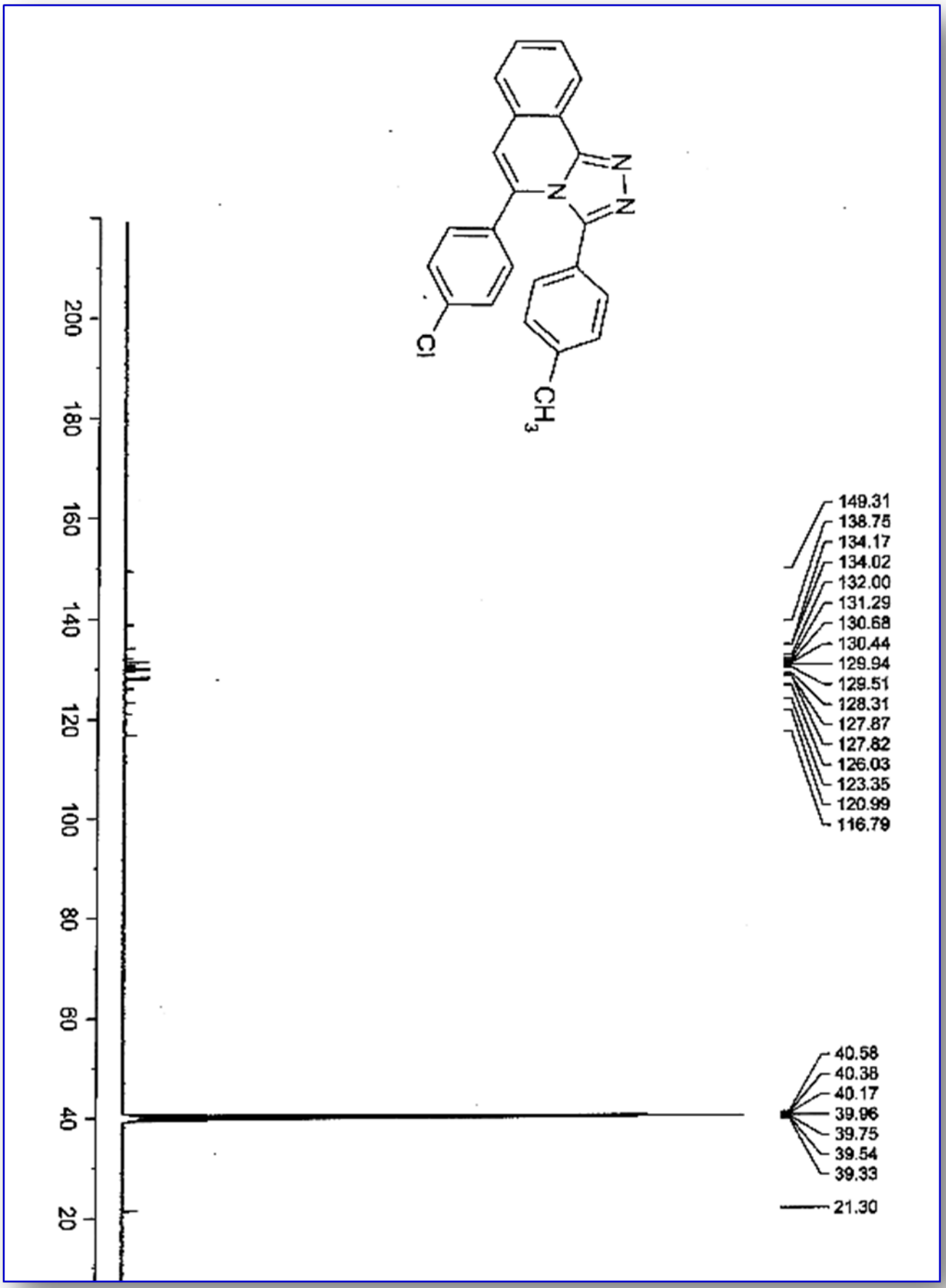

0.9800
1.0008
2.0632
2.0577
1.0685
1.9523
3.2039
2.8830
10
9
8
7
6
5
4
3
2
1
0 ppm
8.6736
8.6652
8.6590
8.6505
8.0004
7.9923
7.9868
7.9846
7.9776
7.8341
7.8244
7.8162
7.8095
7.8013
7.7914
7.4284
7.4238
7.4118
7.4072
7.4014
7.3372
7.2990
7.2933
7.2813
7.2769
3.3347
2.4993
2.4948
2.4886
1.9472
N
N
N
S
N
H3C
CH3
Cl

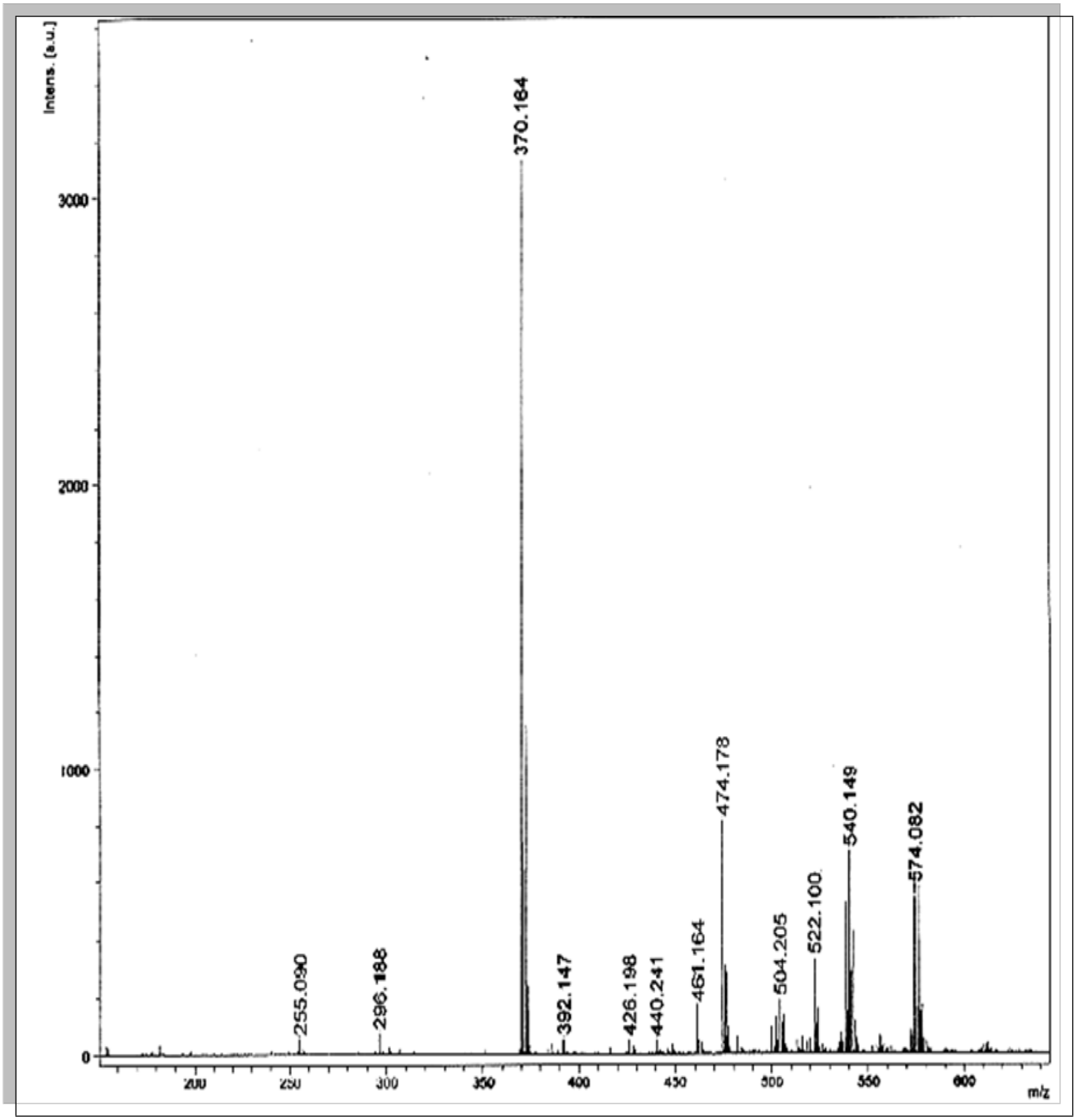

167.36
153.10
149.59
140.22
134.02
133.39
130.84
130.55
130.11
129.30
127.54
127.30
122.98
120.47
117.42
117.00
40.20
39.99
39.78
39.37
39.16
38.95
18.48
15.92
200
180
160
140
120
100
80
60
40
20
ppm
N
N
N
S
Cl
H3C
CH3


Intens. [a.u.]
x10^4
1.0
0.8
0.6
0.4
0.2
0.0
391.120
361.166
255.103
280.104
294.115
413.097
429.080
514.070
543.043
200
250
300
350
400
450
500
550
600
m/z

4k


8.6639
8.6523
8.6443
8.6333
7.9832
7.9717
7.9639
7.9532
7.7984
7.7876
7.7788
7.7679
7.2805
7.2294
7.2013
7.1020
7.0738
7.0084
6.9816
6.9239
6.8976
3.3886
3.3251
3.2574
3.2079
2.4895
2.2602
0.99
1.00
2.05
0.98
2.13
2.21
2.24
2.26
2.92
10
9
8
7
6
5
4
3
2
1
ppm


Cl
CH3
N
N
N
200
180
160
140
120
100
80
60
40
20
149.31
138.75
134.17
134.02
132.00
131.29
130.68
130.44
129.94
129.51
128.31
127.87
127.82
126.03
123.35
120.99
116.79
40.58
40.38
40.17
39.96
39.75
39.54
39.33
21.30


Intens. (a.u.)
3000
2000
1000
0
370.184
255.090
296.188
392.147
426.198
440.241
461.164
474.178
504.205
522.100
540.149
574.082
200
250
300
350
400
450
500
550
600
m/z