SUPPORTING INFORMATION

Influence of Substituents on the Through-Space Shielding of Aromatic Rings

Colin W. Anson[†] *and Dasan M. Thamattoor**

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dmthamat@colby.edu

† Current address: Department of Chemistry, University of Wisconsin- Madison, 1101 University Avenue Madison, WI 53706

Table of Contents

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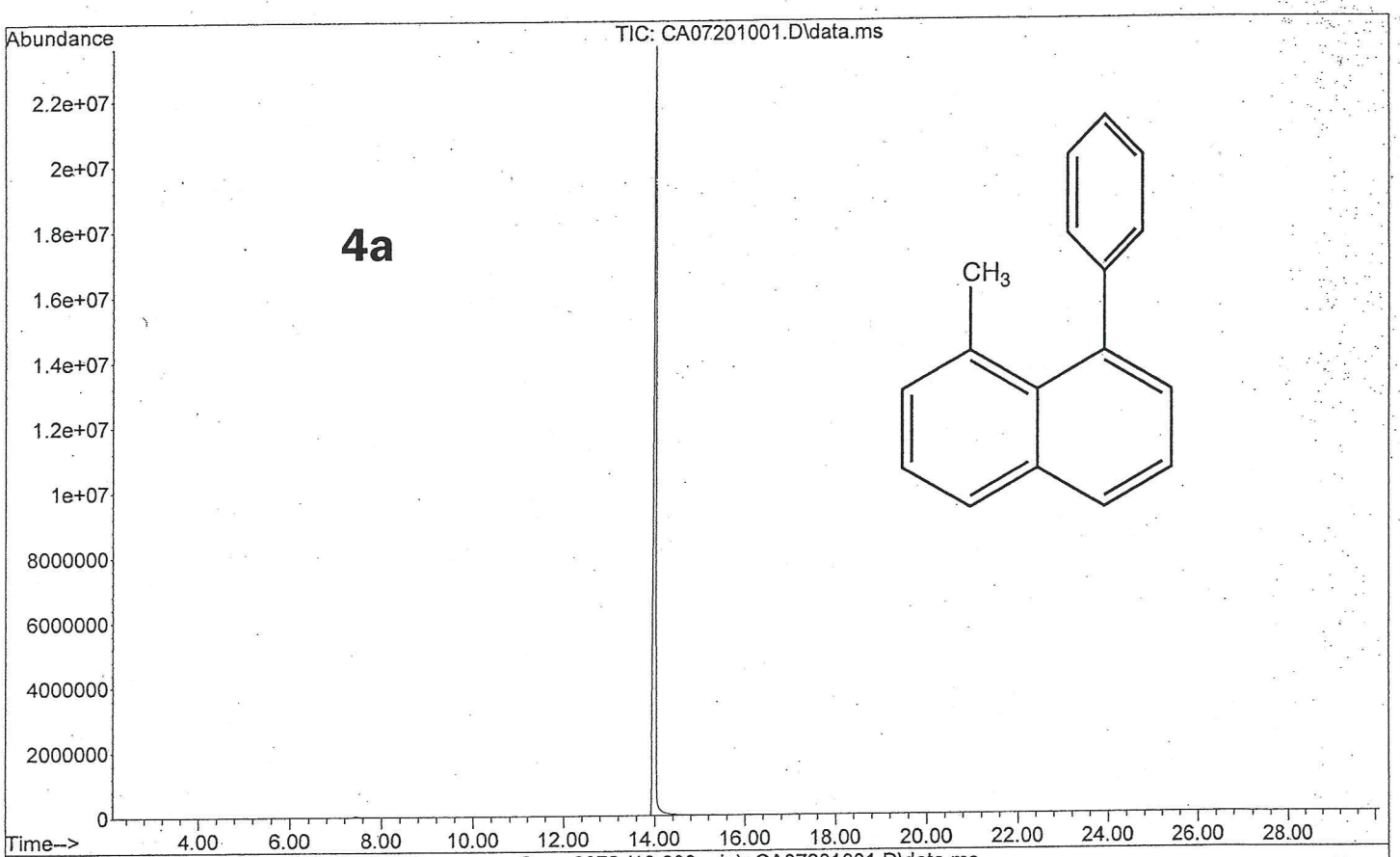

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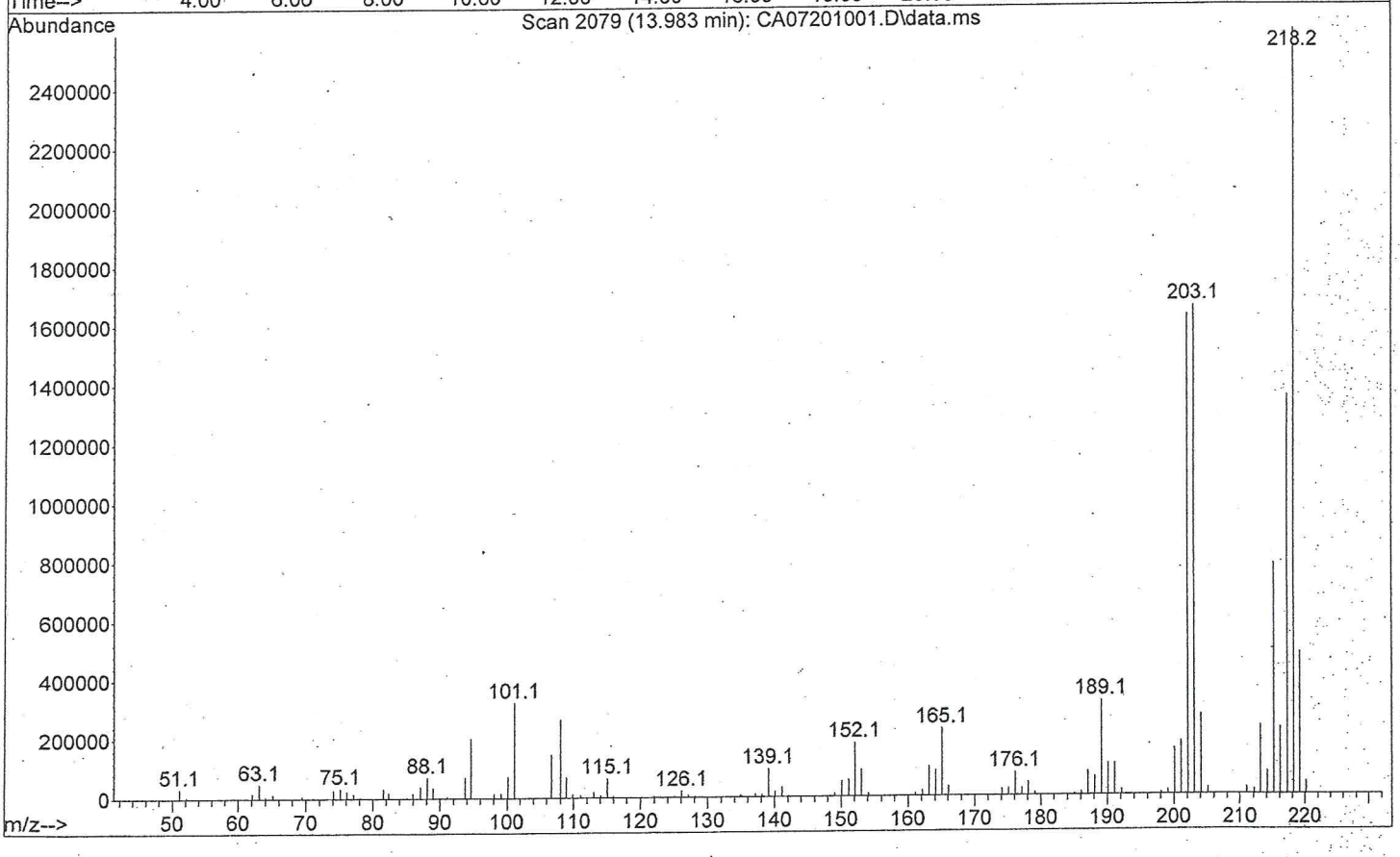

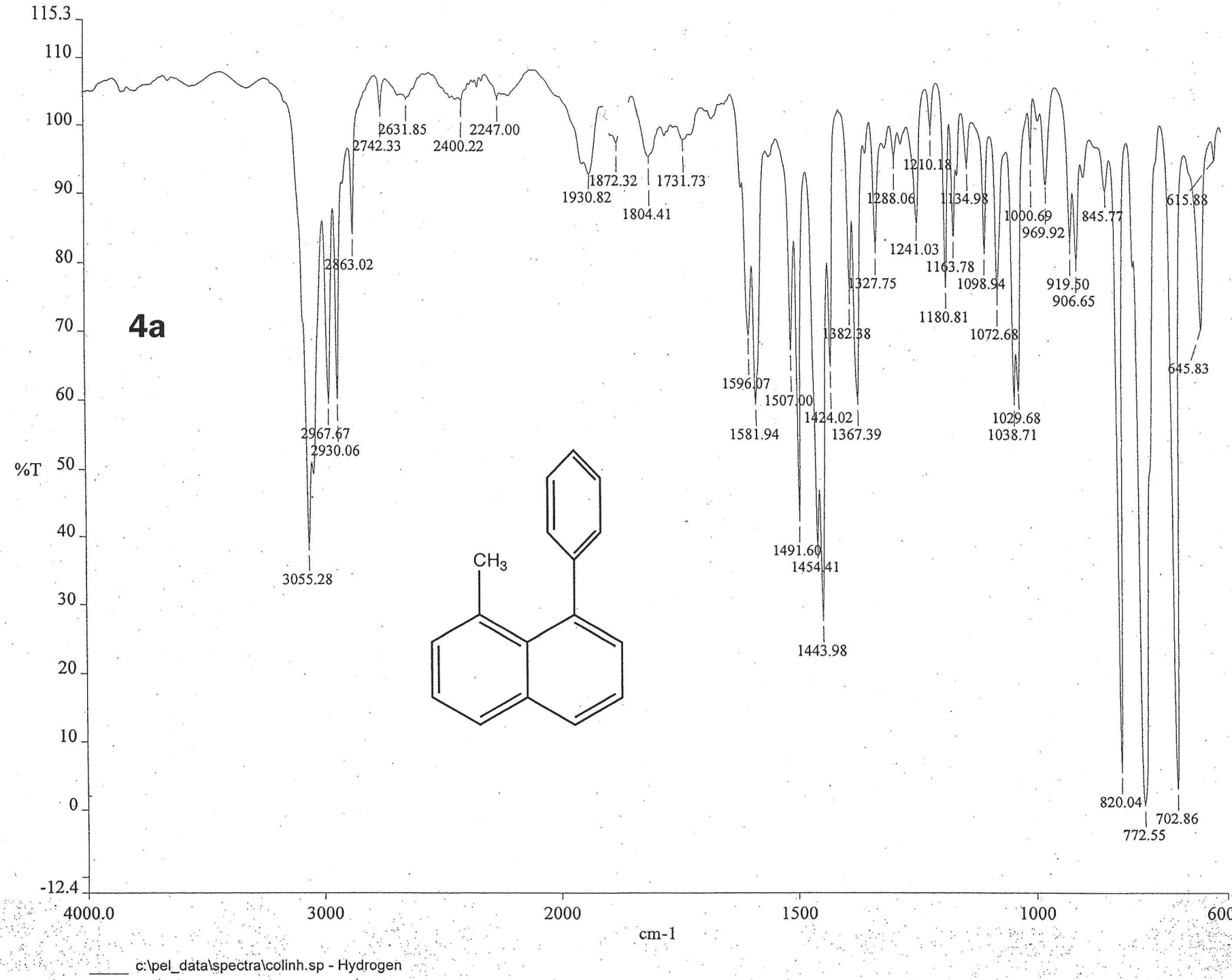
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1581.94
1507.00
1491.60
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1382.38
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1038.71
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1000.69
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CH3
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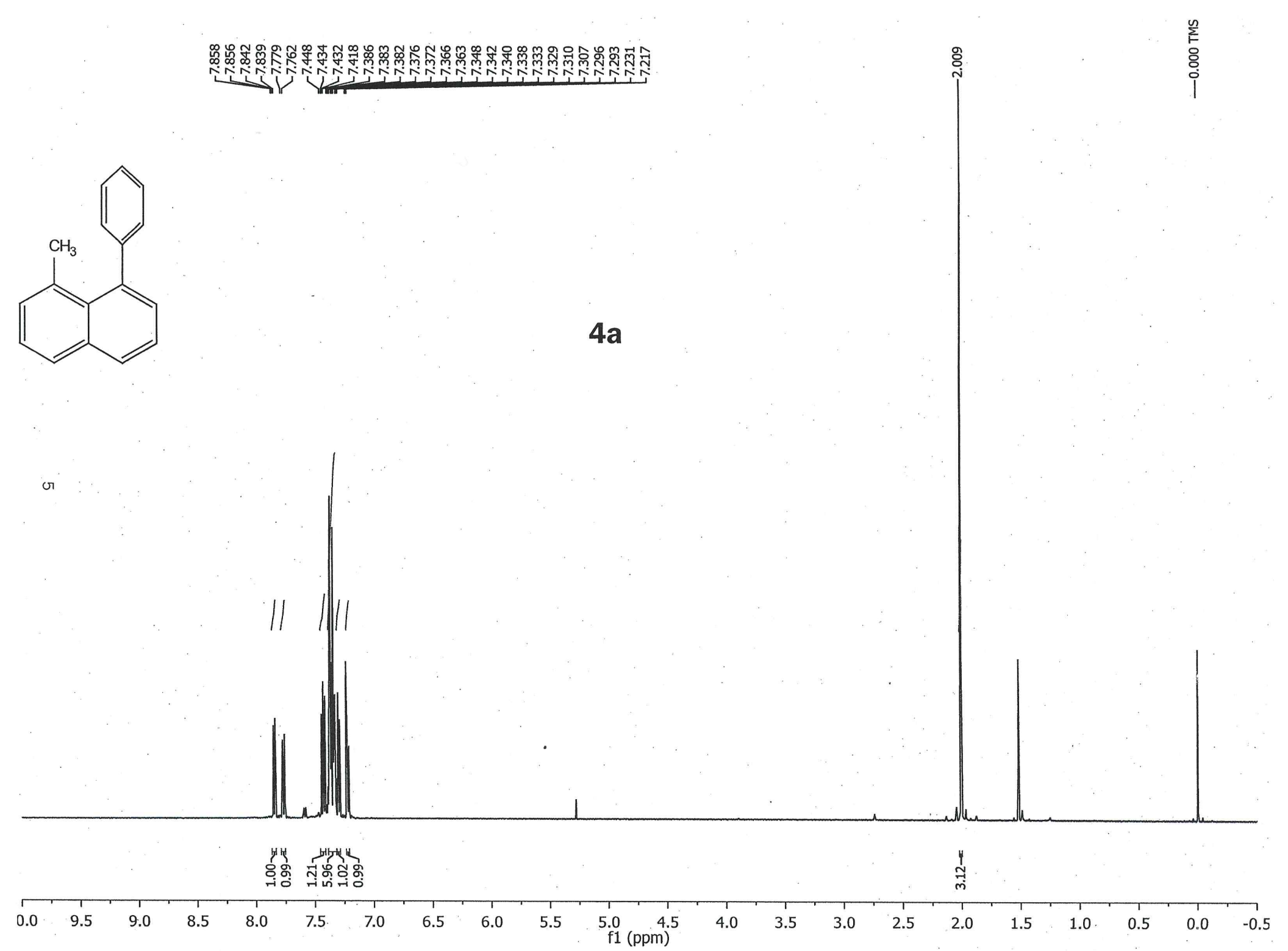
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7.363
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7.342
7.340
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7.310
7.307
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7.217
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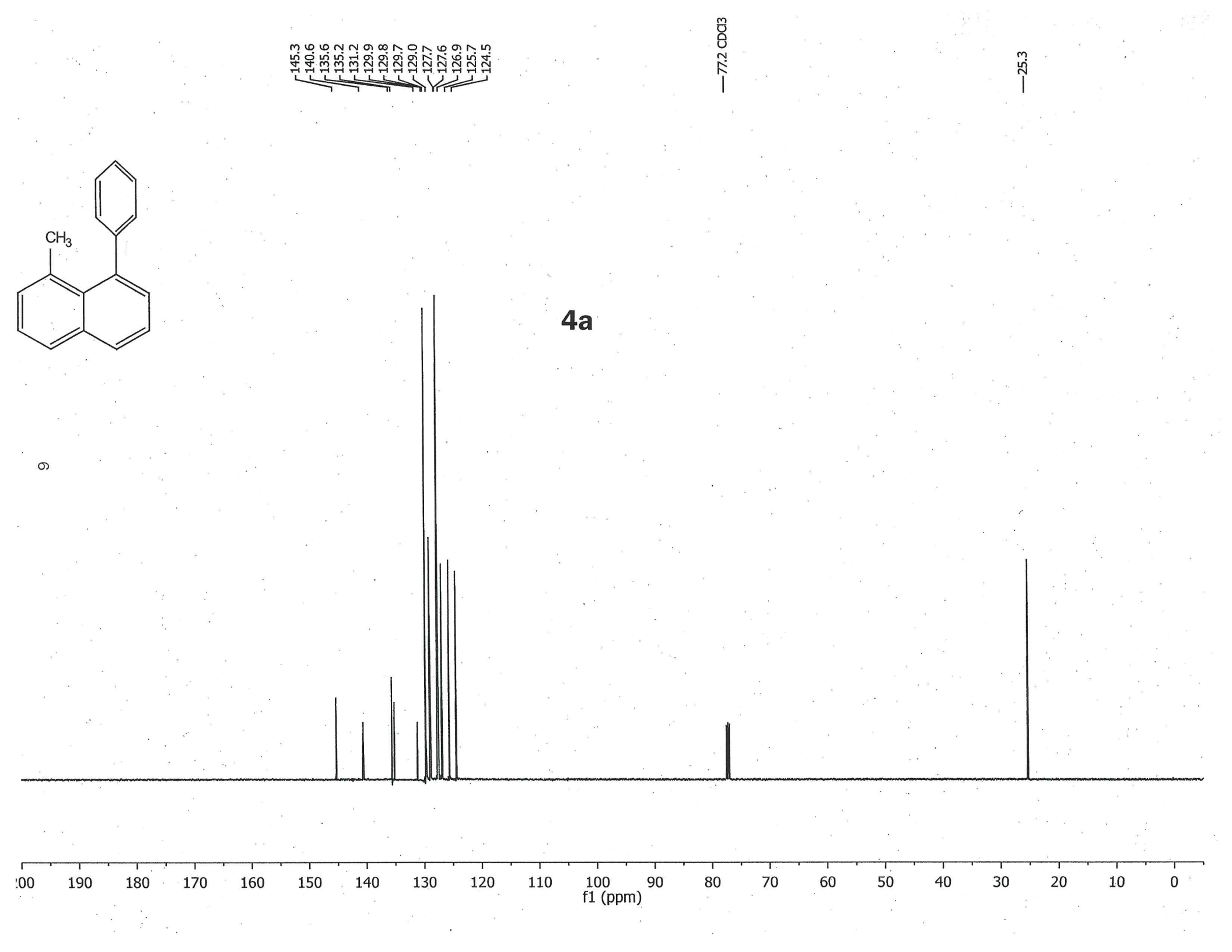
f1 (ppm)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124.5
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CH3
4a
f1 (ppm)

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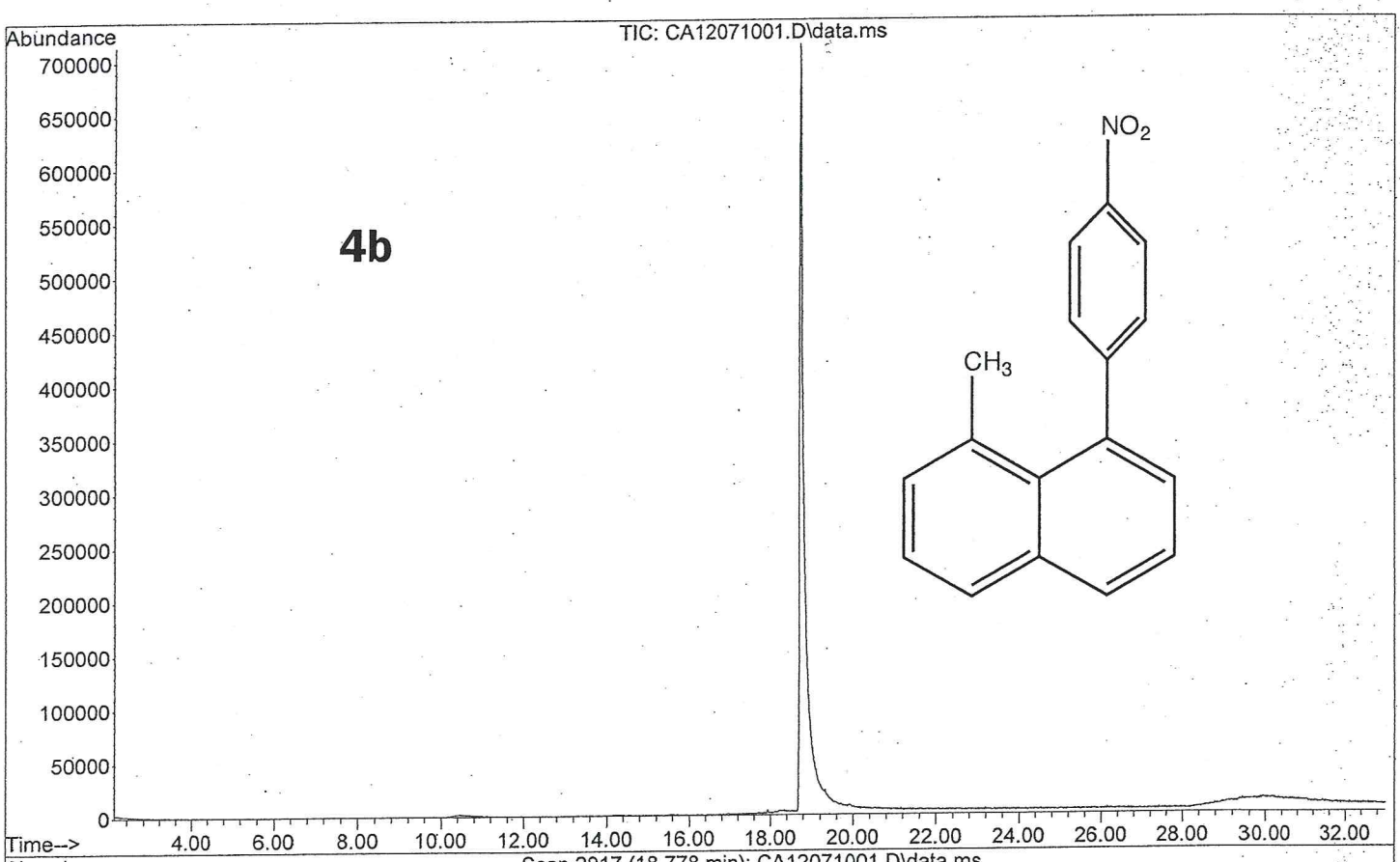

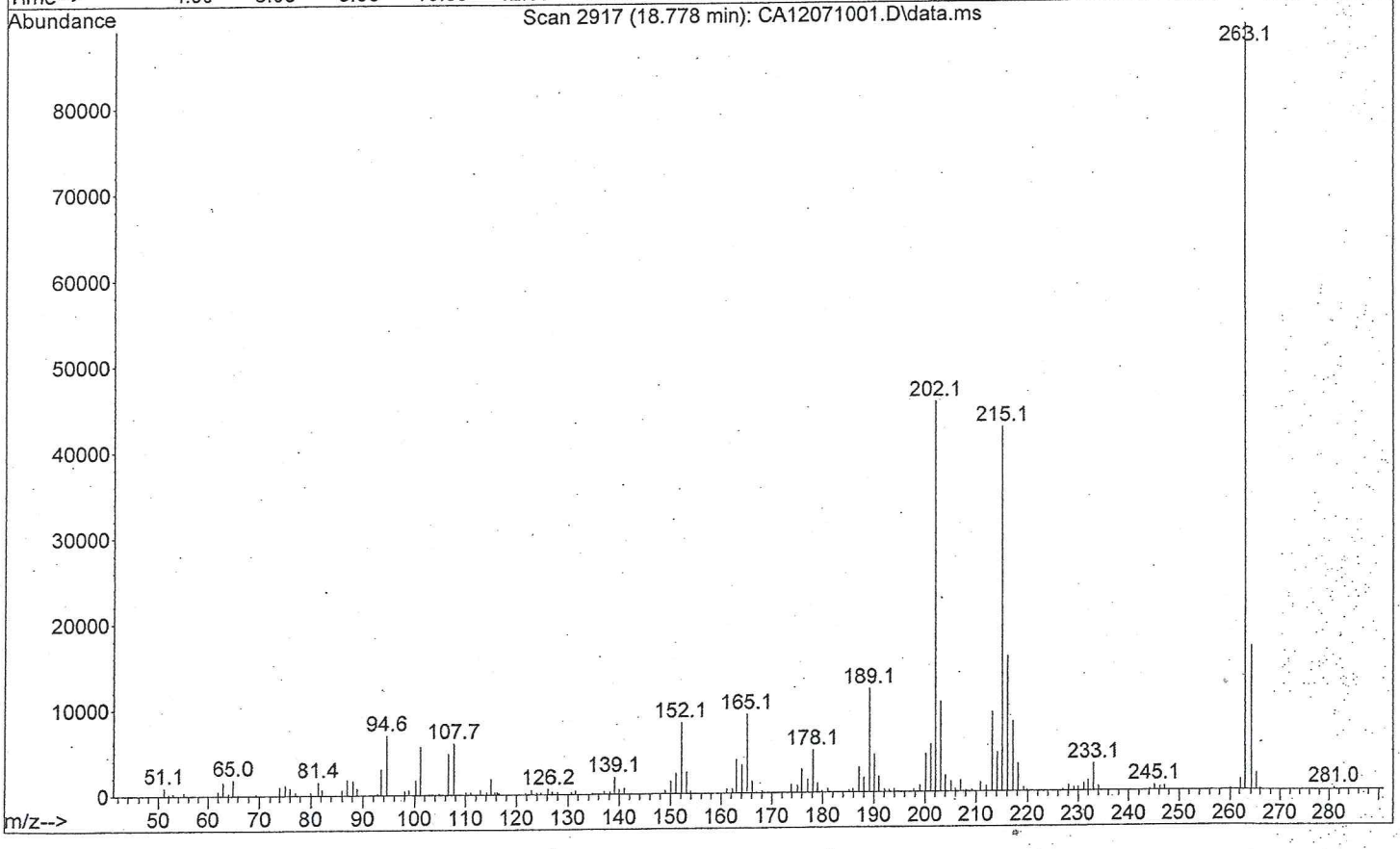

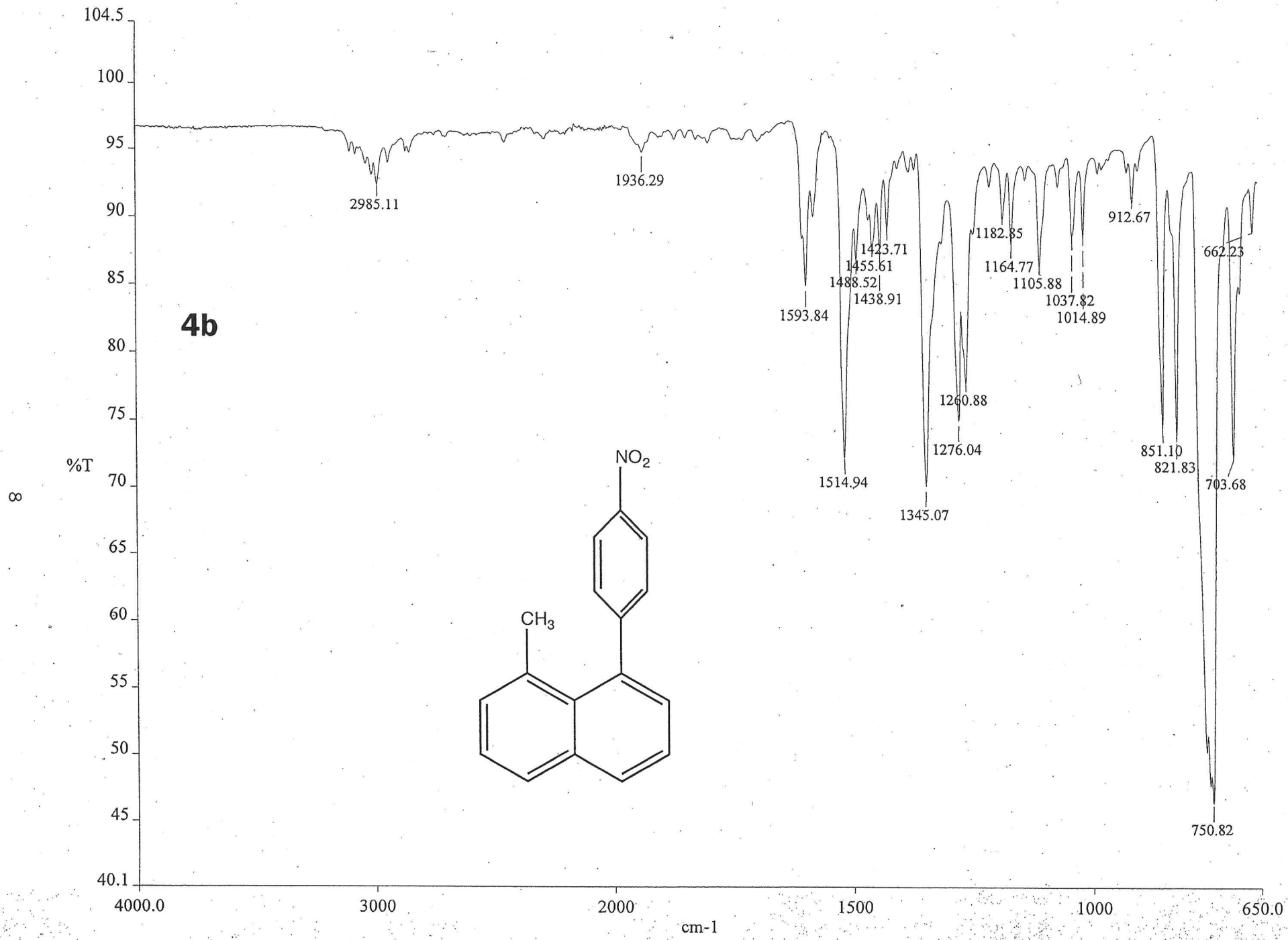
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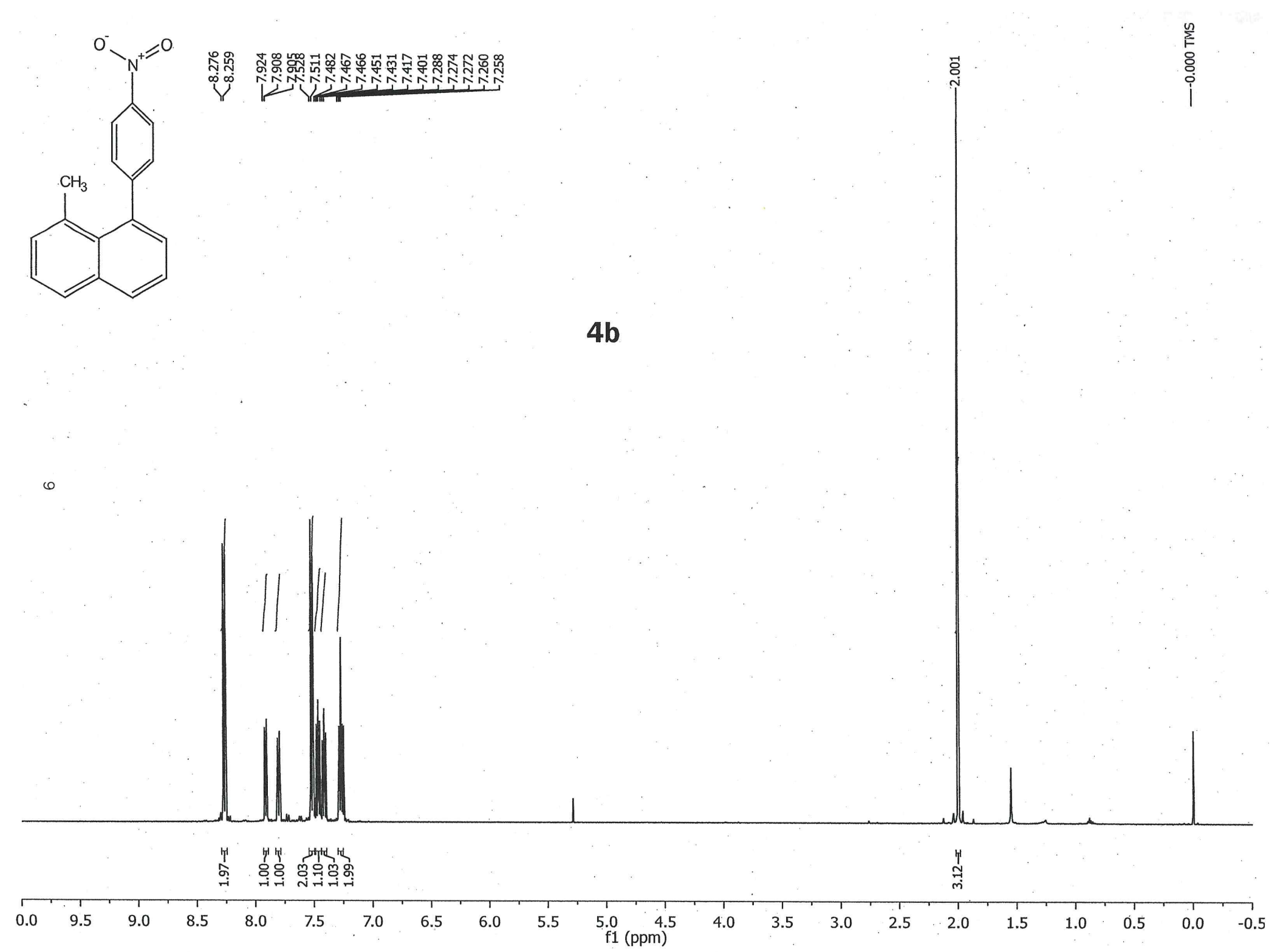
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7.401
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7.274
7.272
7.260
7.258
2.001
-0.000 TMS
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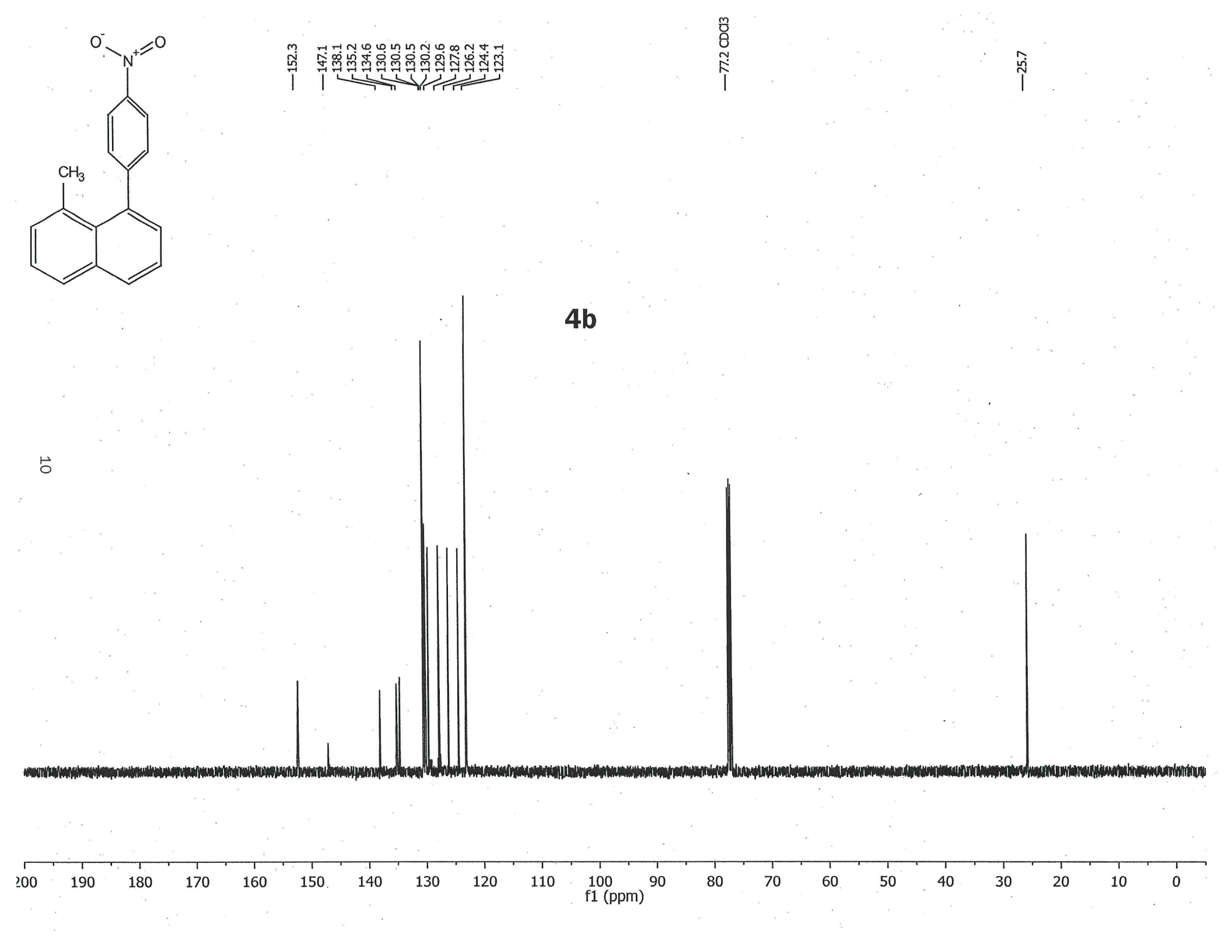
f1 (ppm)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124.4
123.1
77.2 CDCl3
25.7
4b
10
200
190
180
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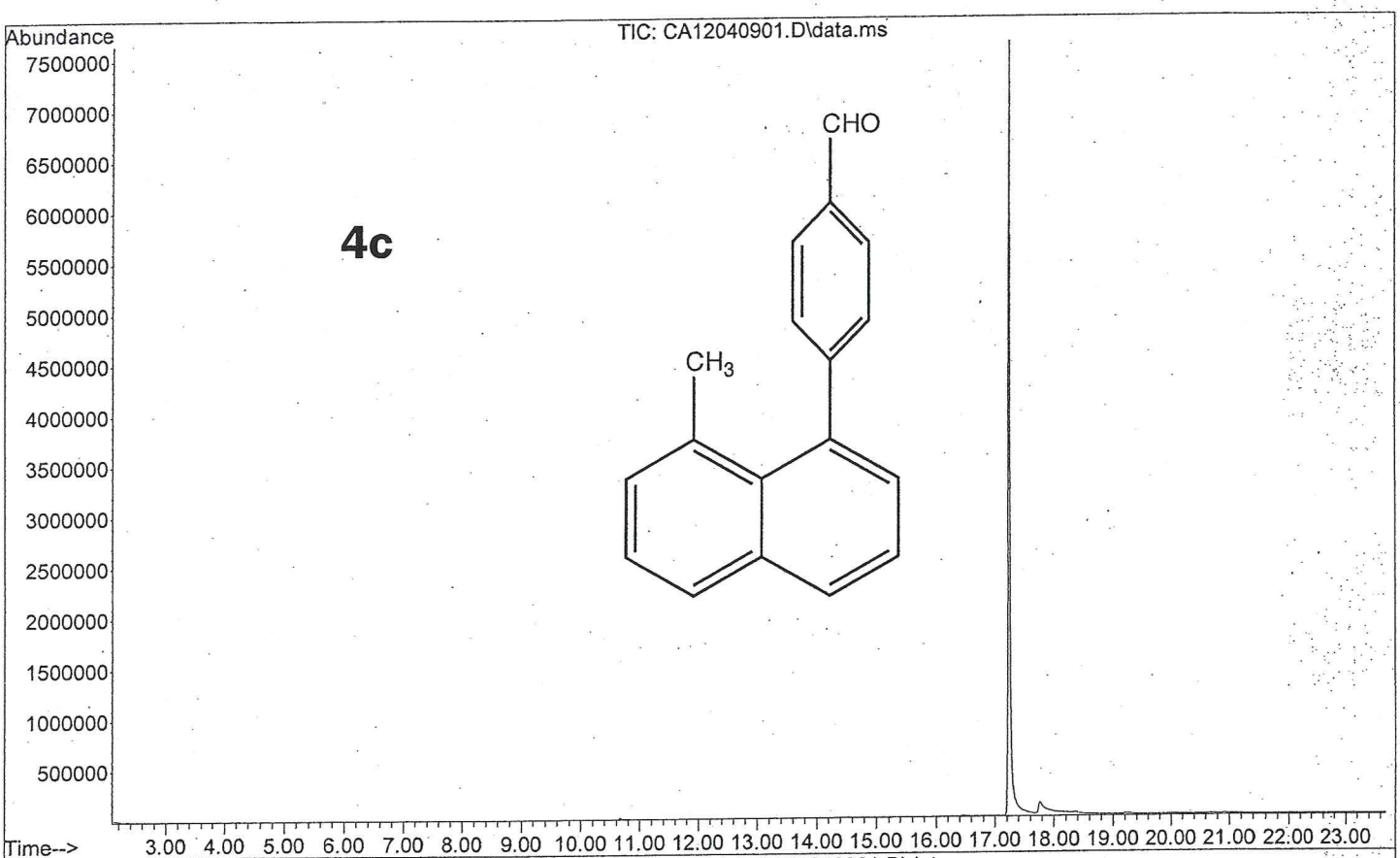

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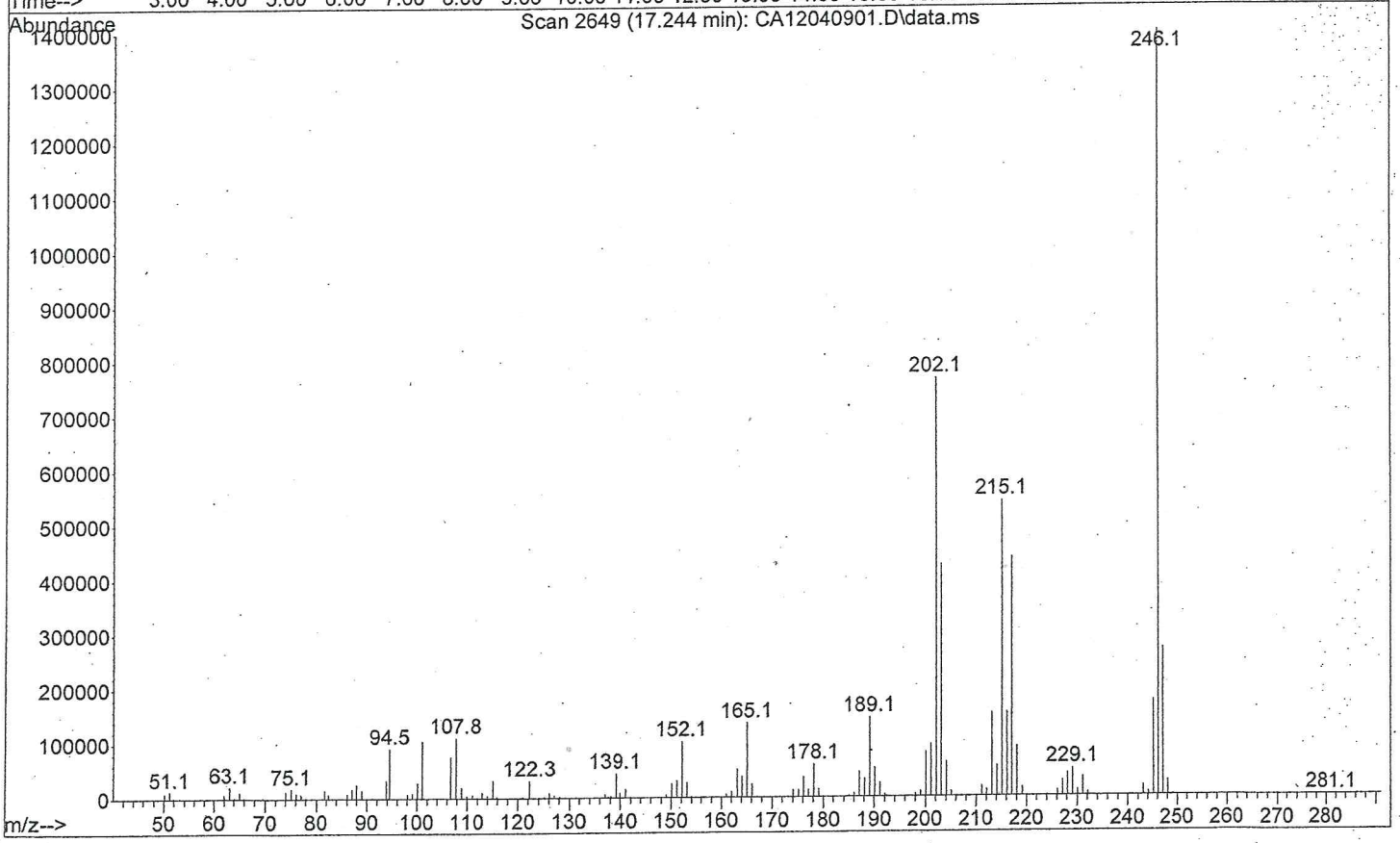

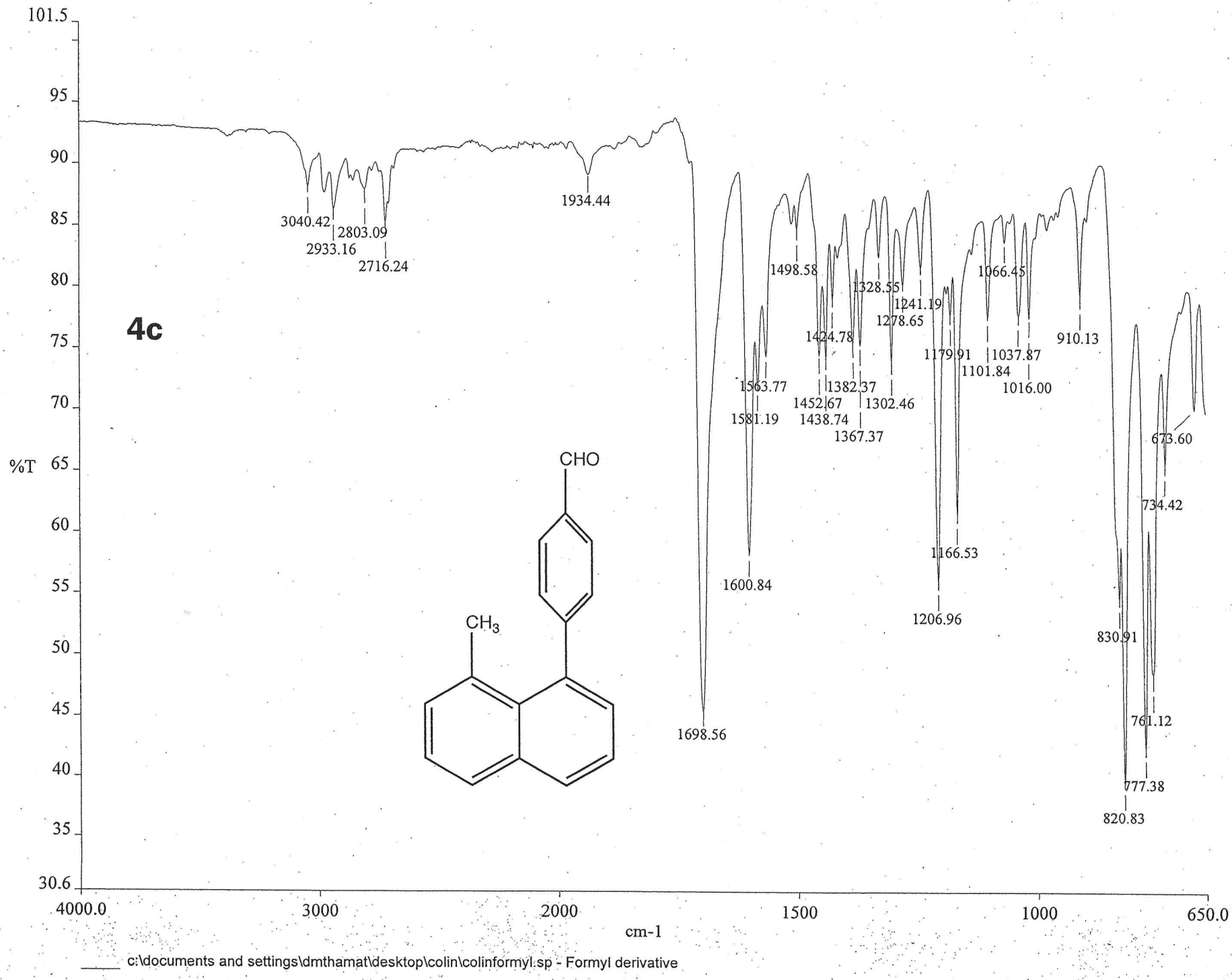
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1367.37
1328.55
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1101.84
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1037.87
1016.00
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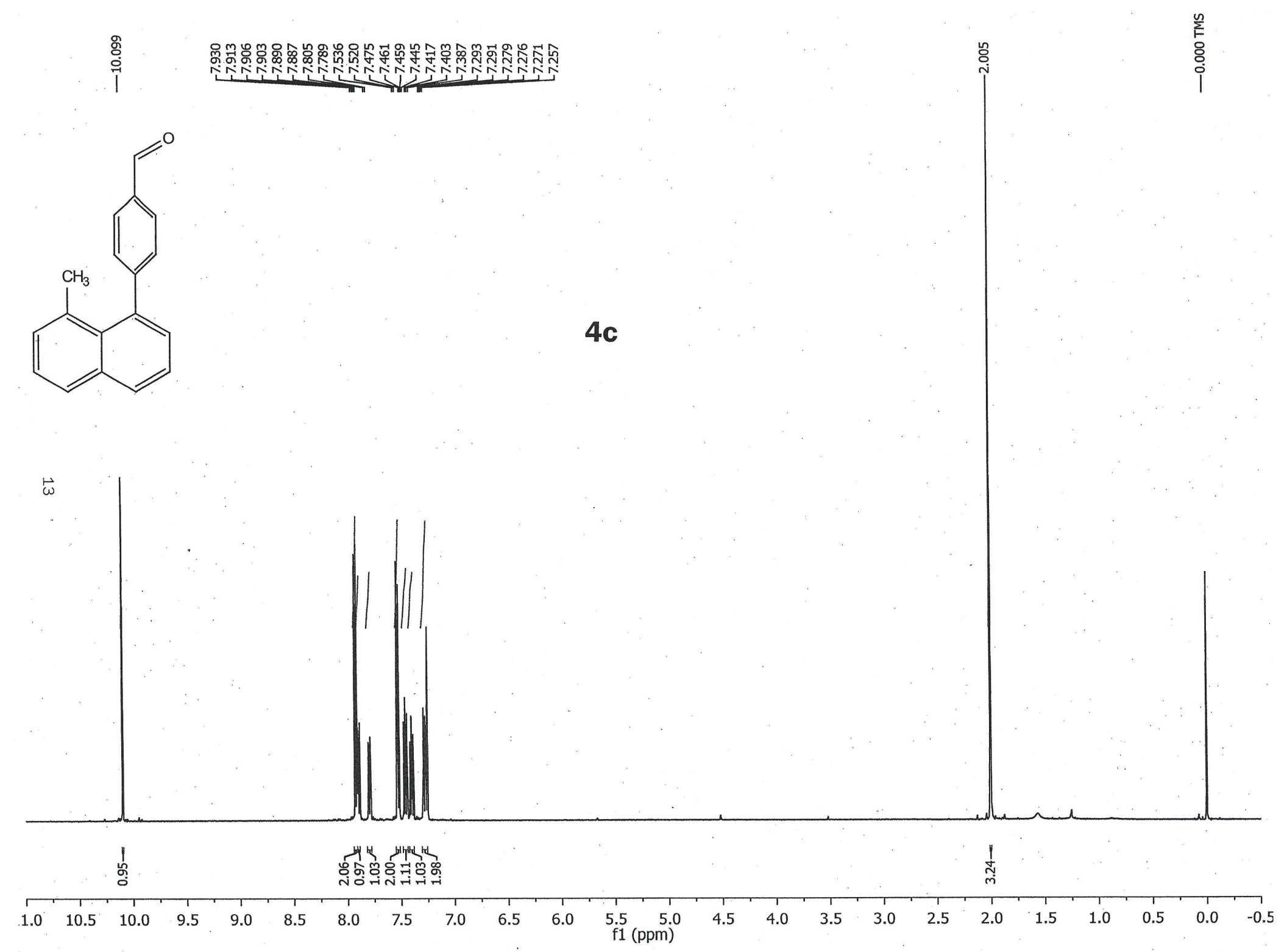
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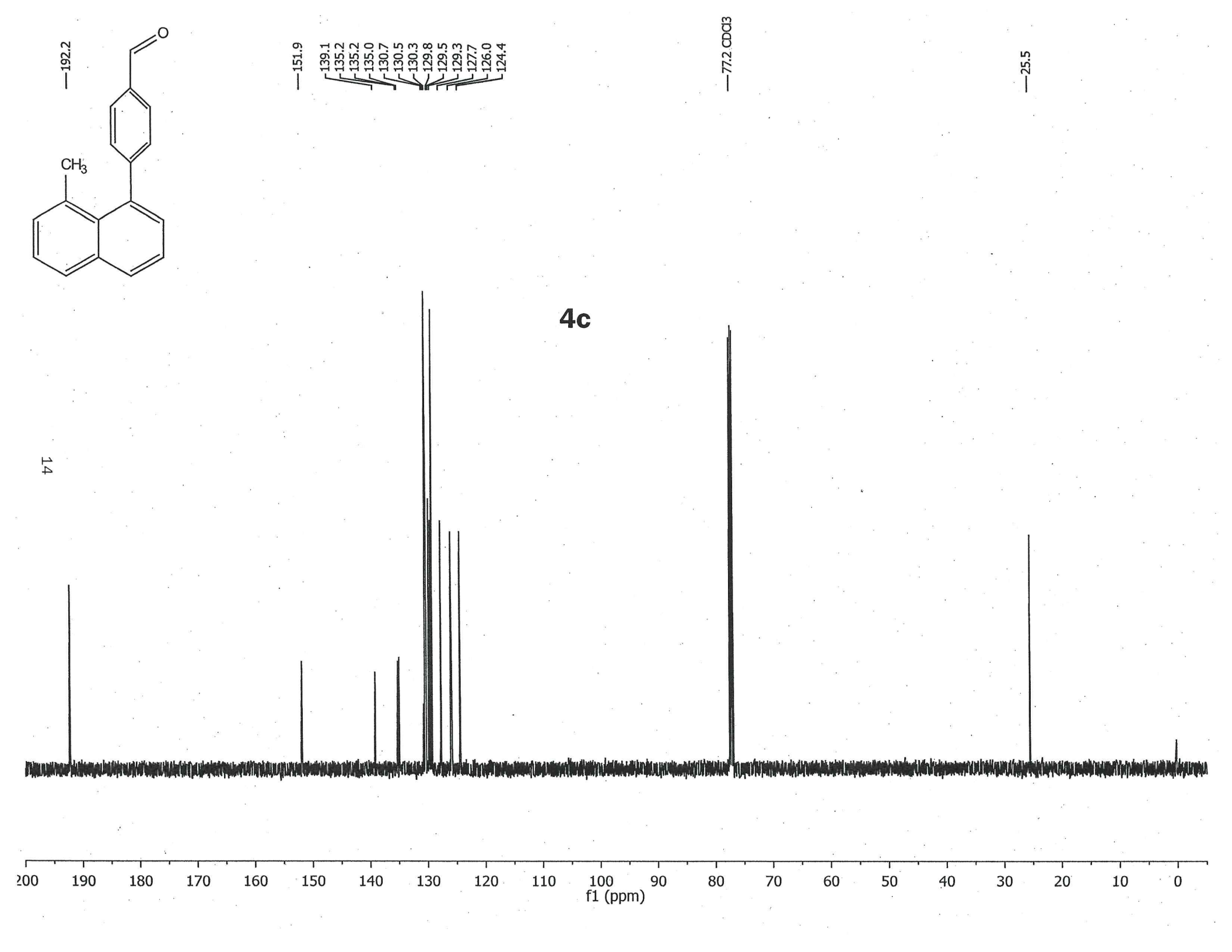
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124.4
77.2 CDCl3
25.5
O
CH3
4c
14
200
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180
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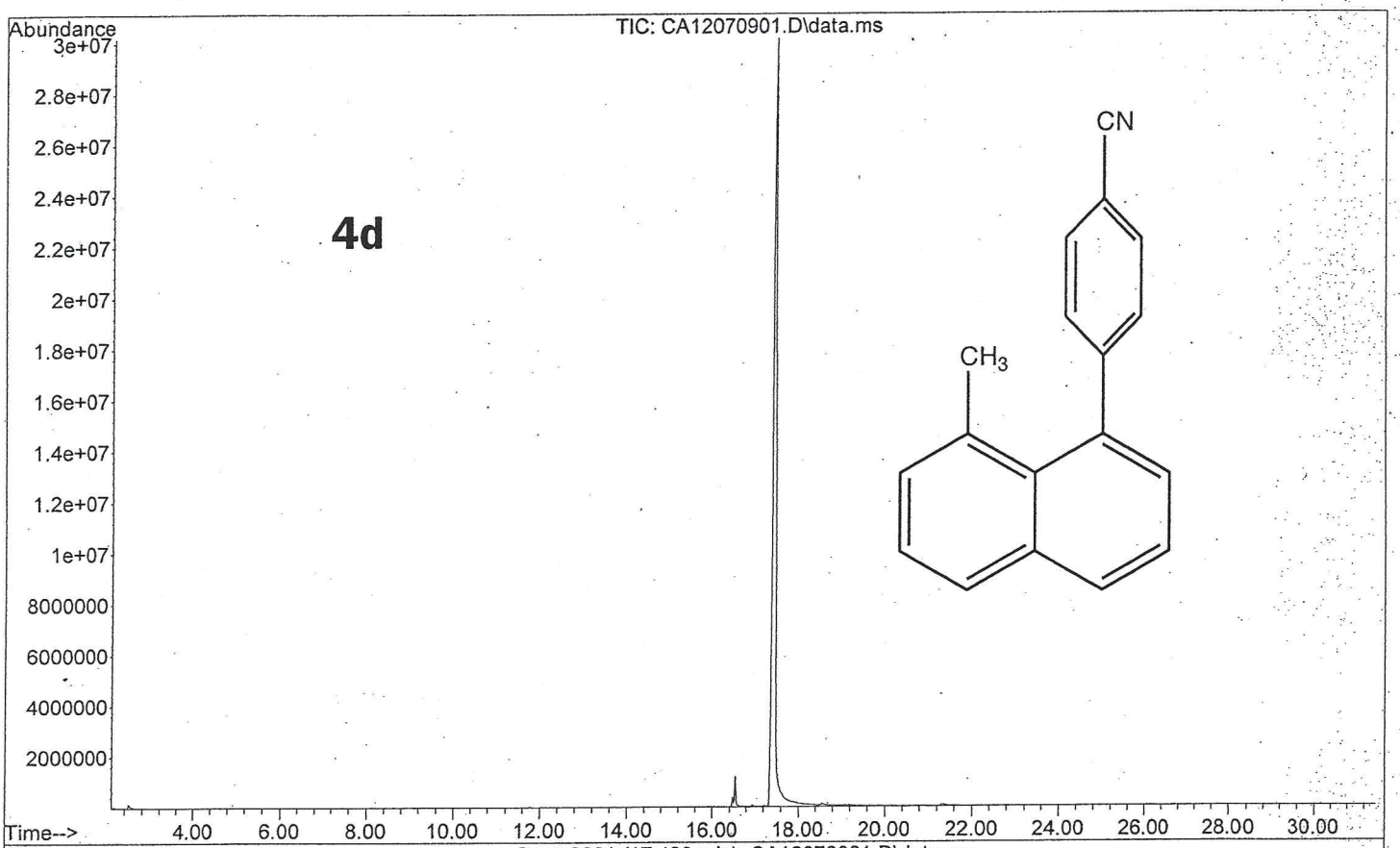

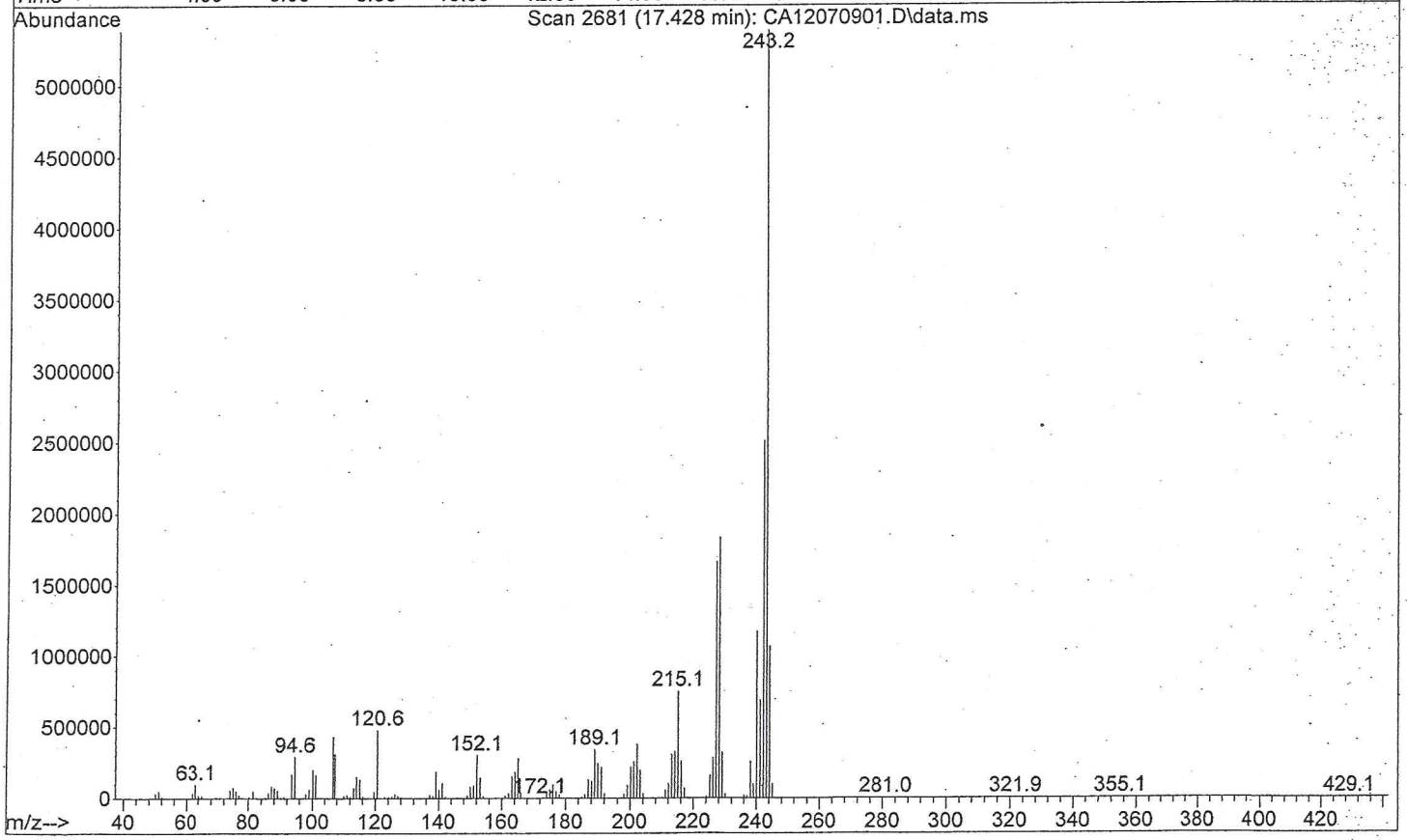

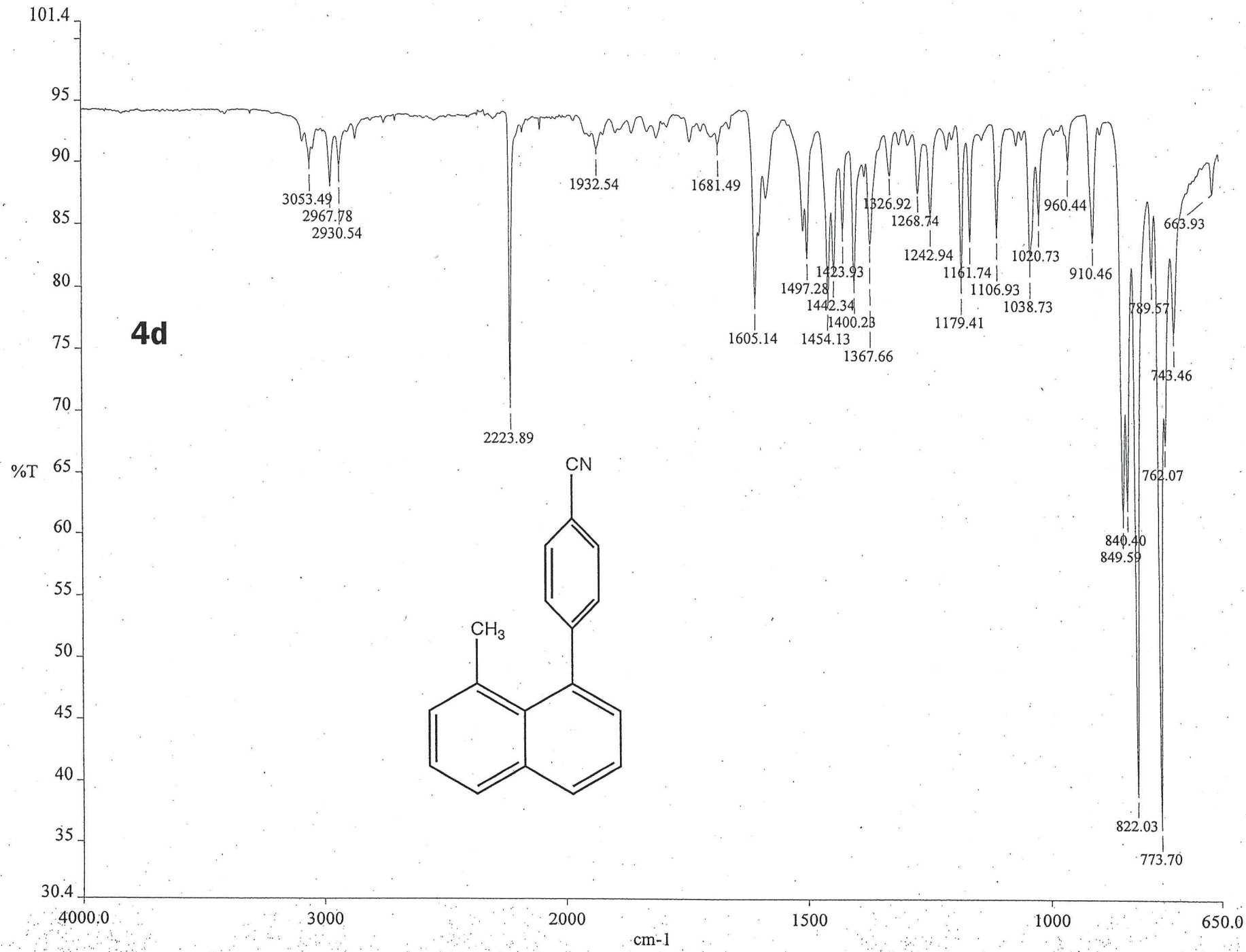
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762.07
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663.93
CN
CH3
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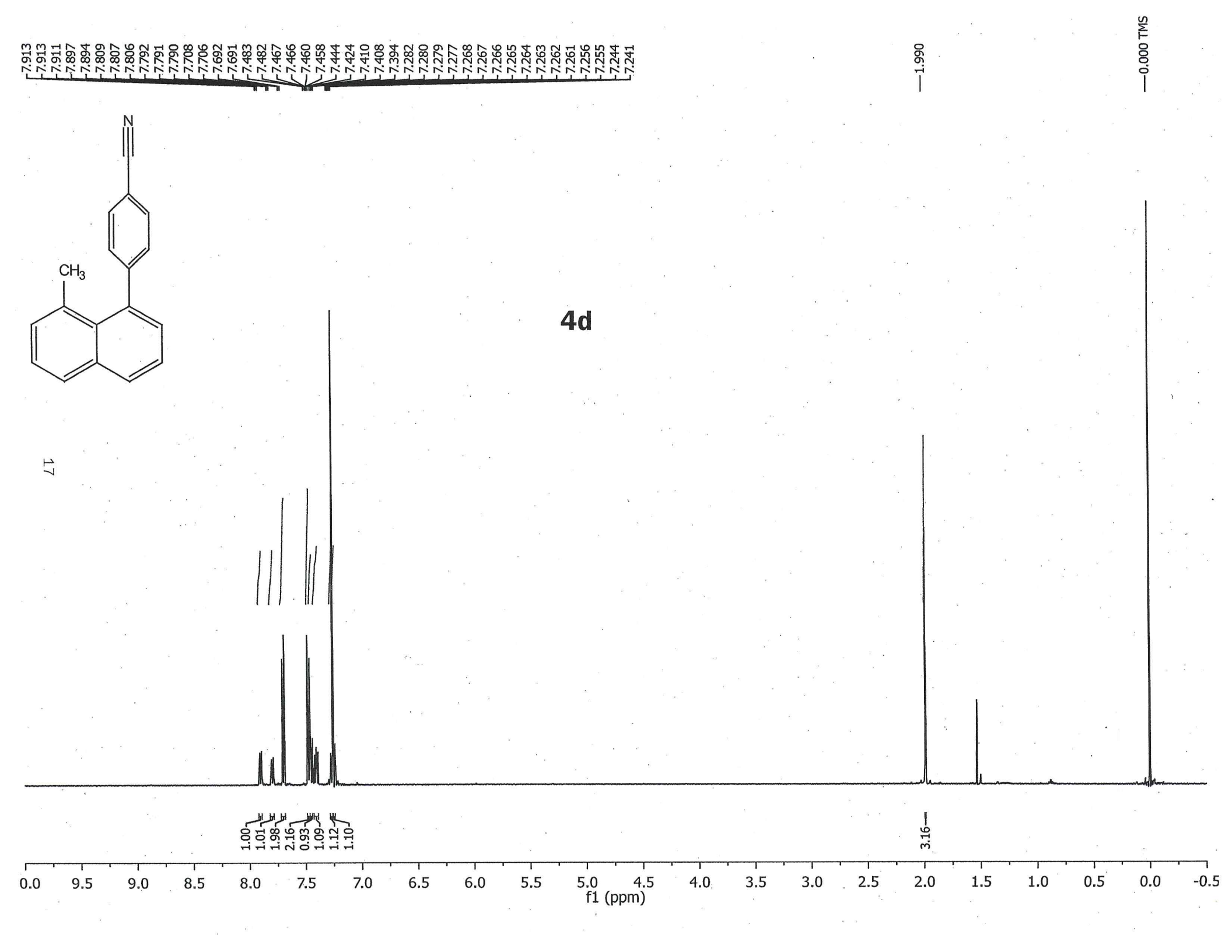
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7.466
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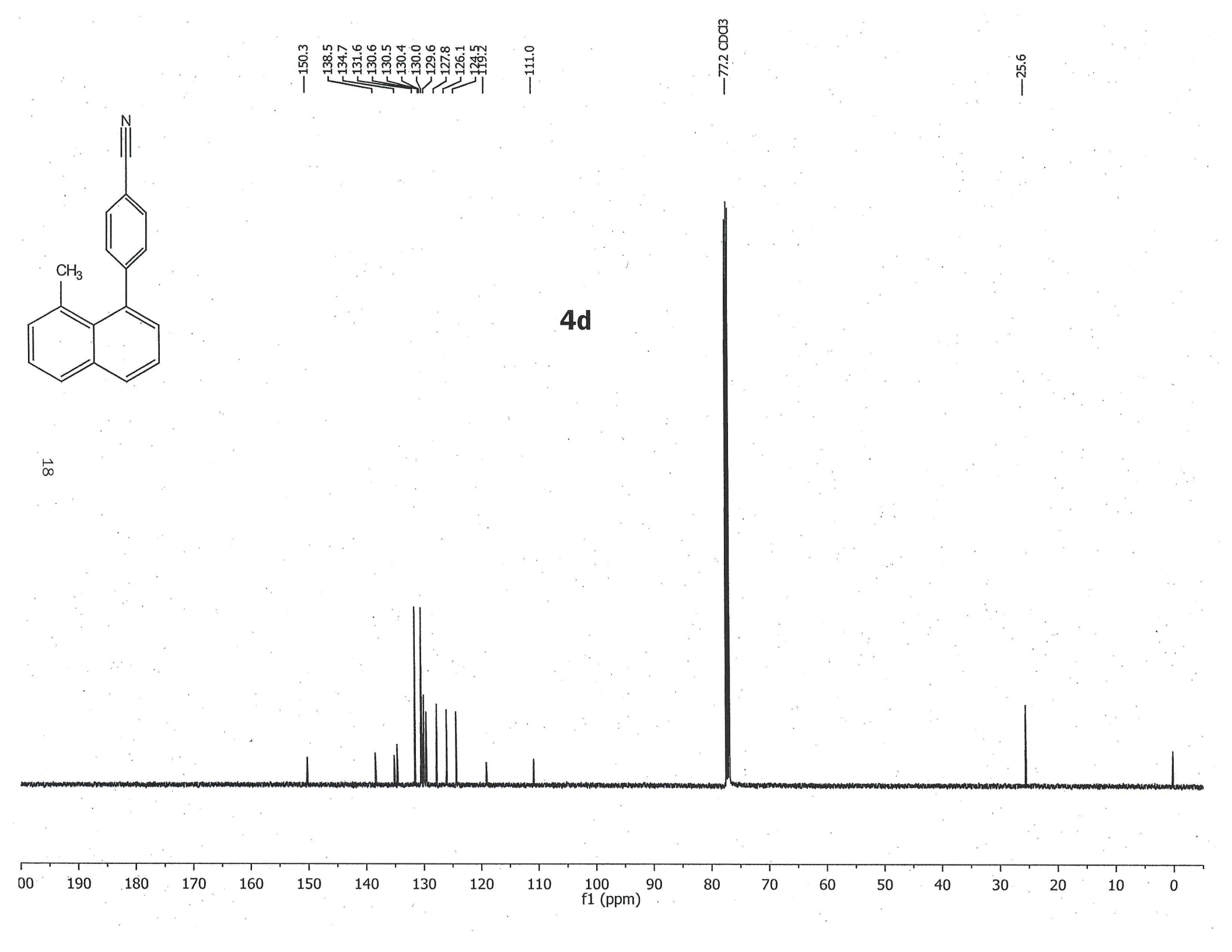
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CH3
4d
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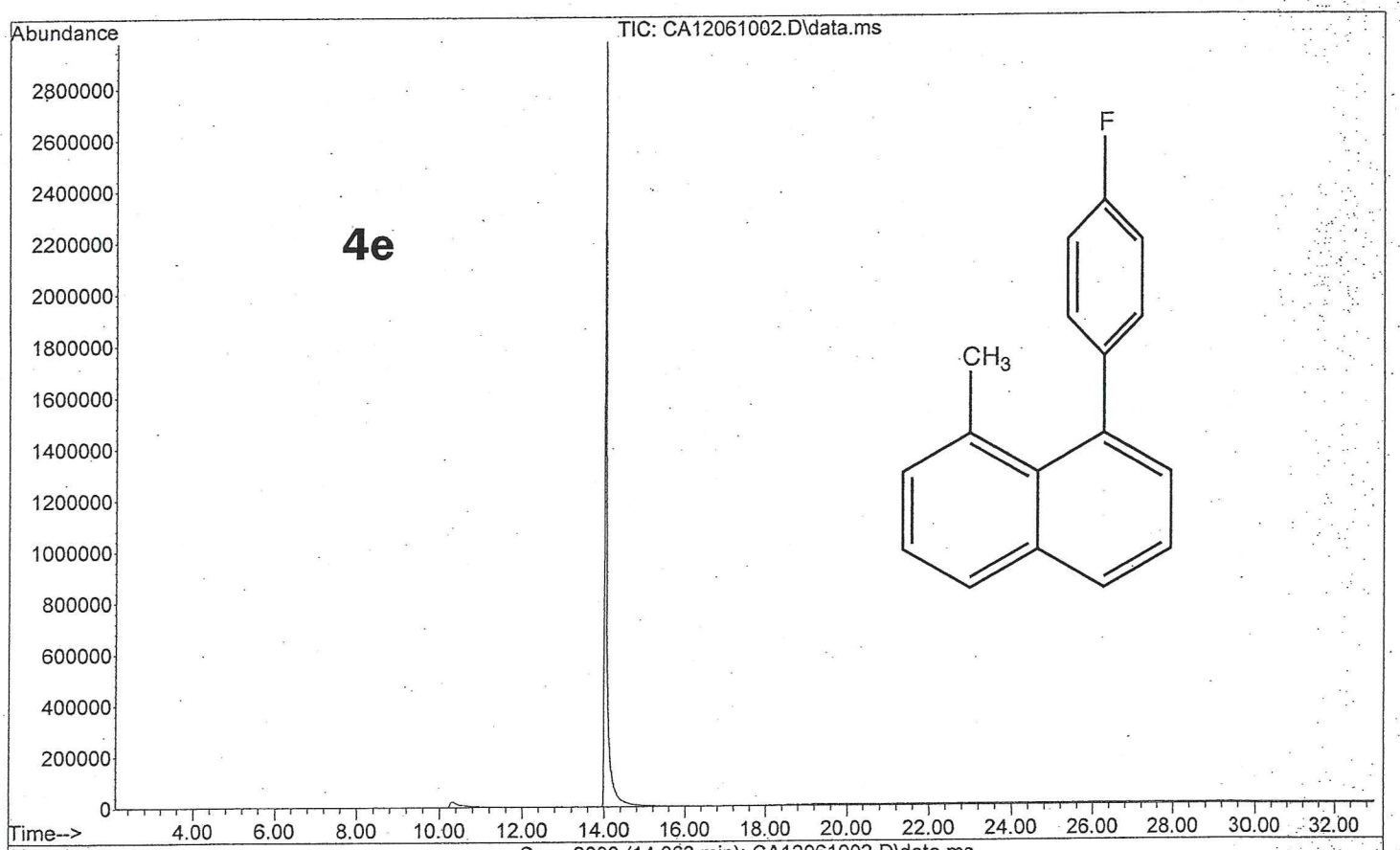

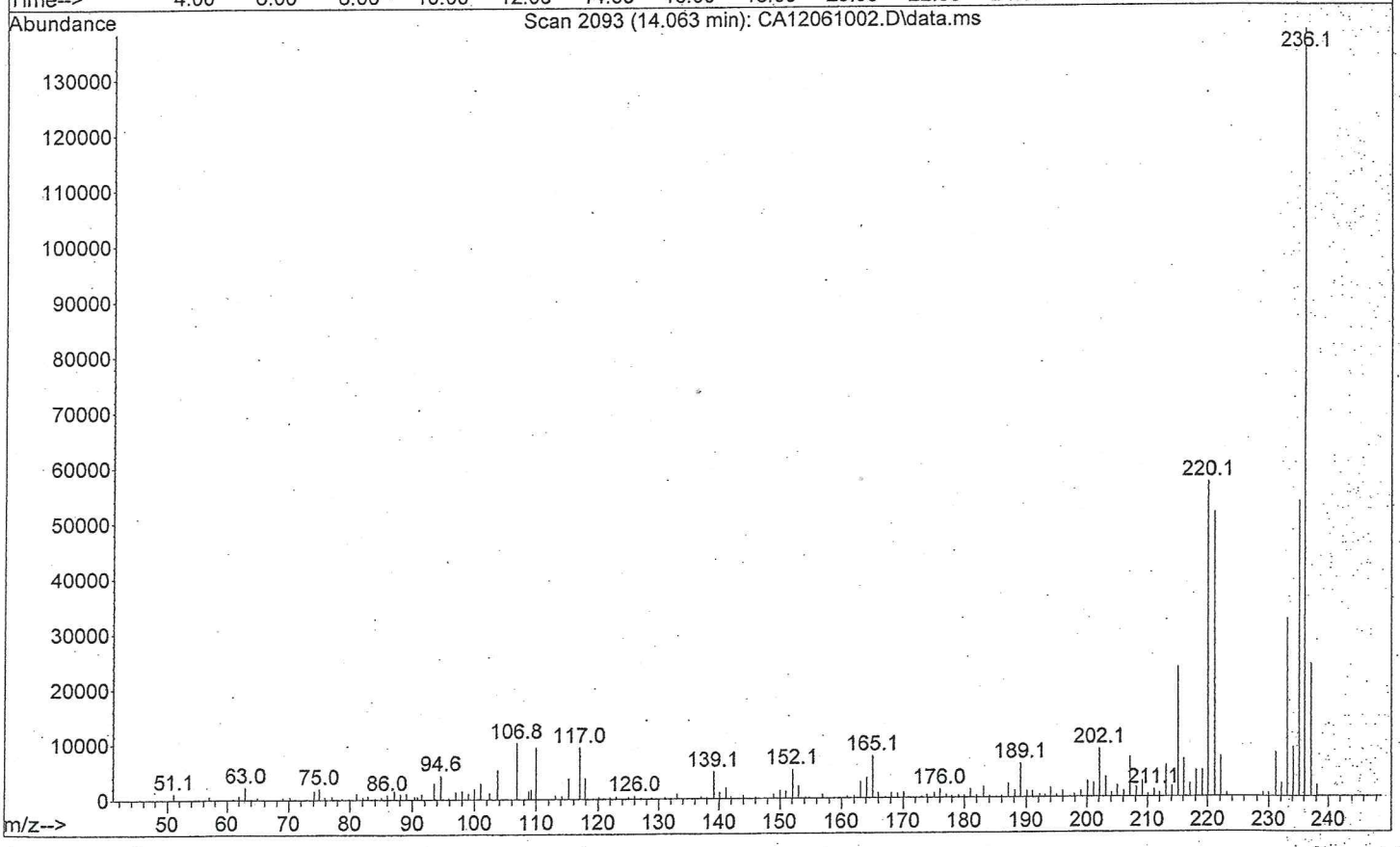

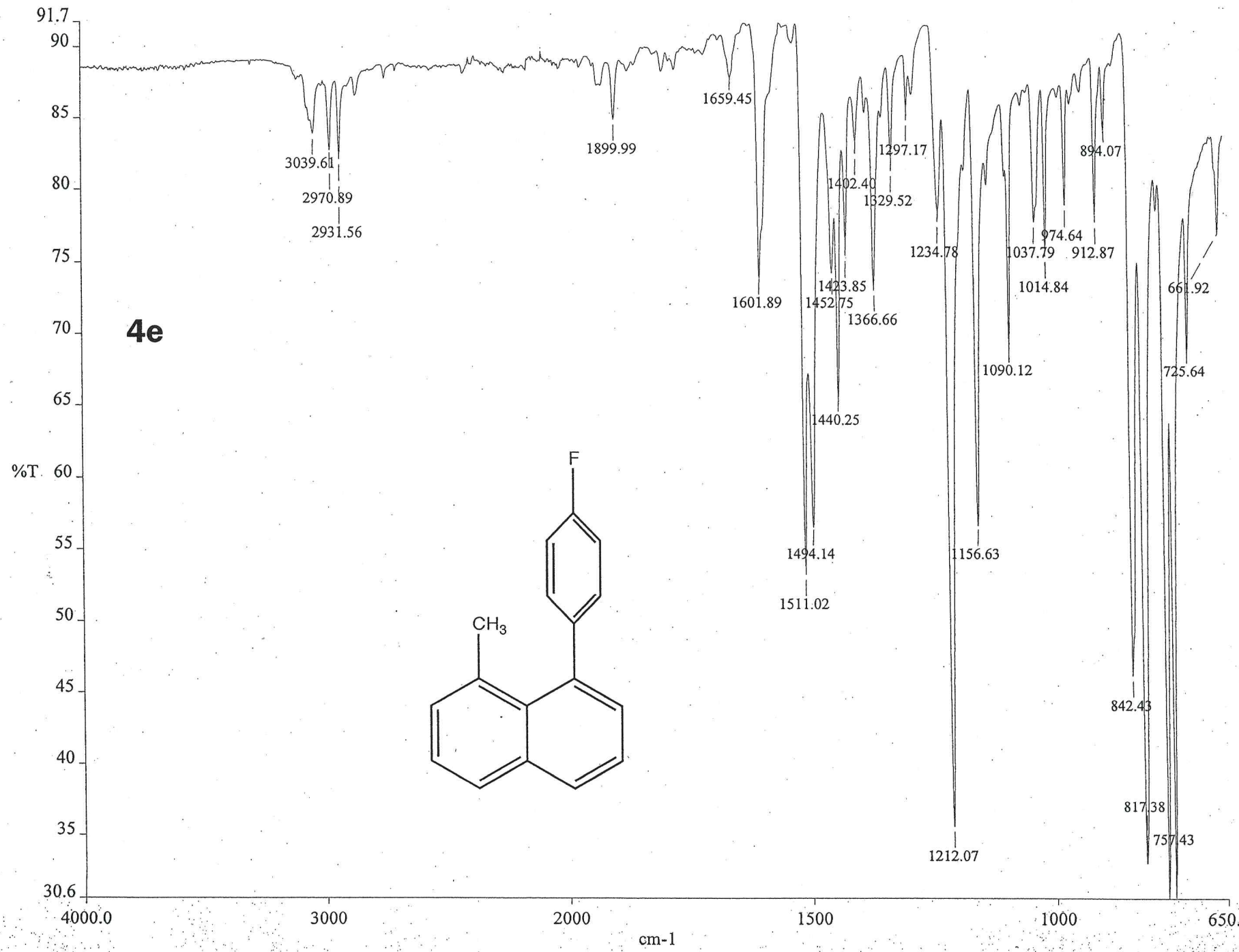
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1402.40
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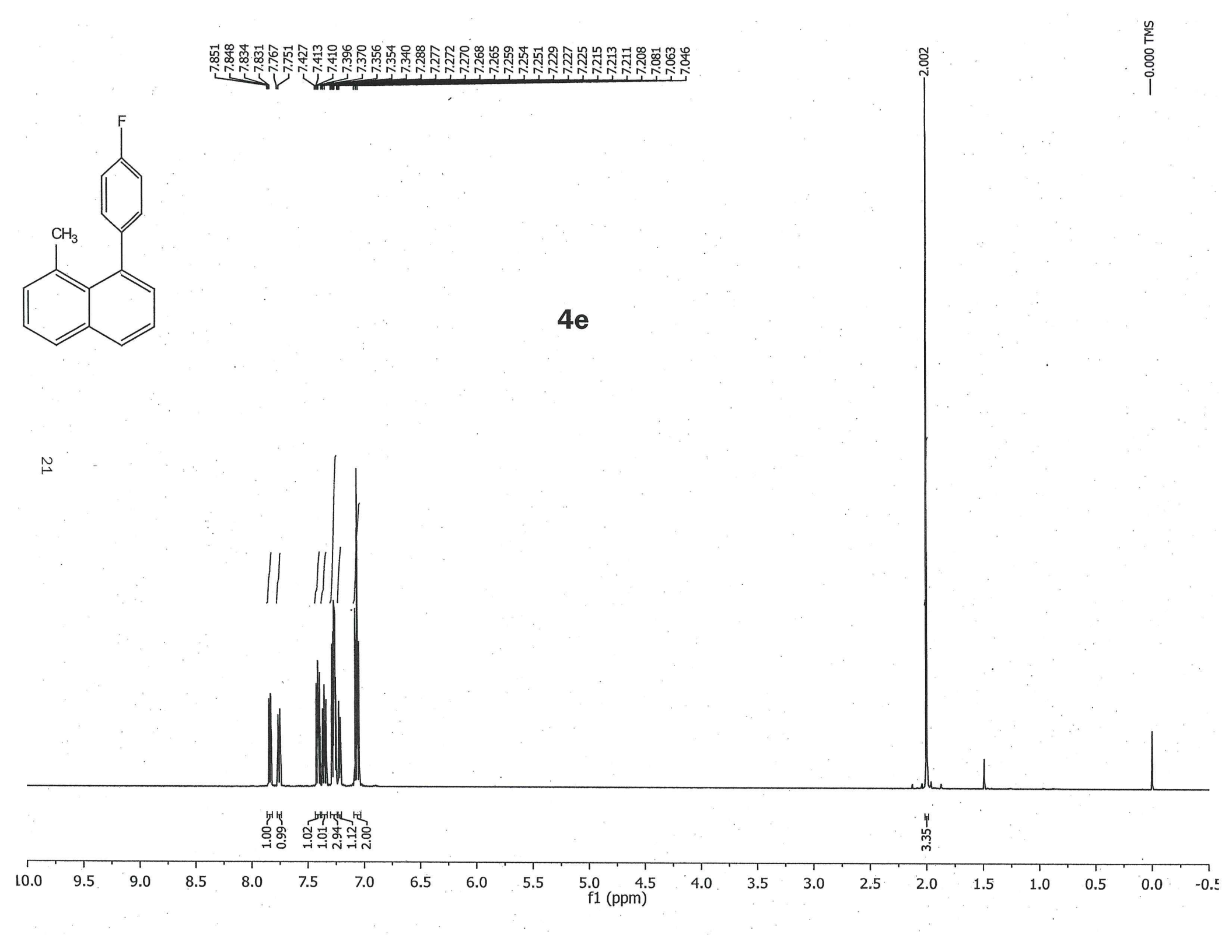
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7.354
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7.229
7.227
7.225
7.215
7.213
7.211
7.208
7.081
7.063
7.046
2.002
0.000 TMS
F
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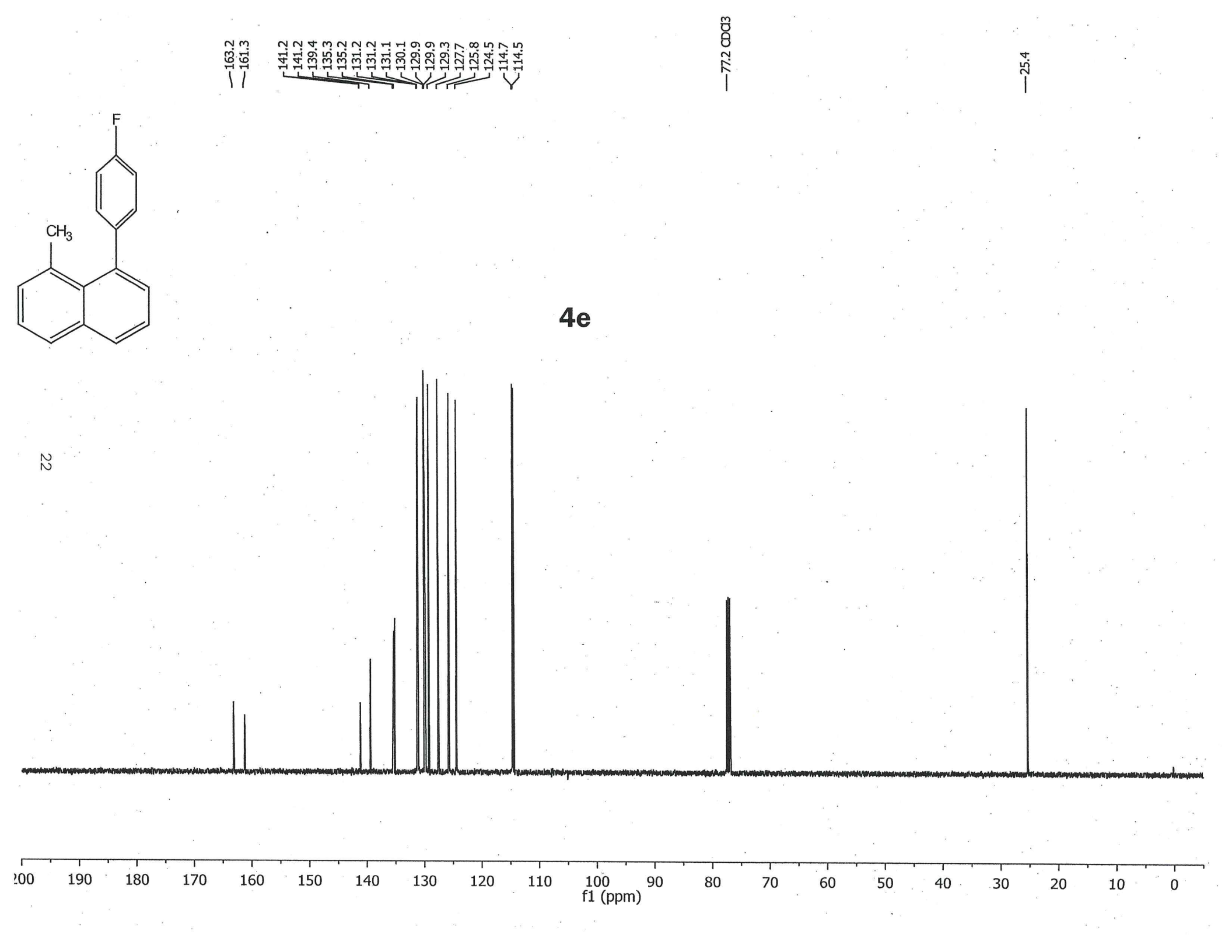
1.12
2.00
3.35
f1 (ppm)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141.2
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129.3
127.7
125.8
124.5
114.7
114.5
77.2 CDCl3
25.4
F
CH3
4e
22
200
190
180
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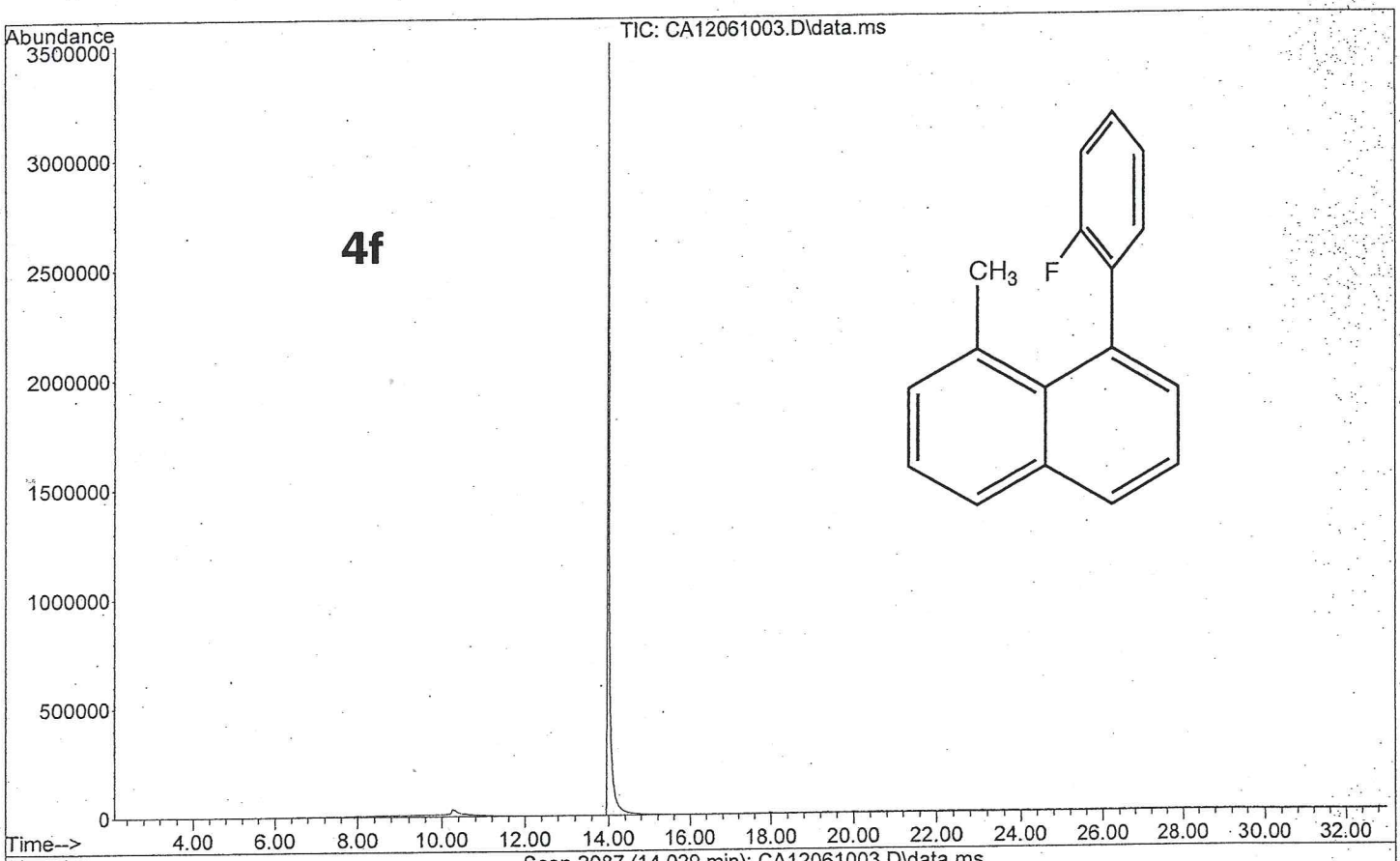

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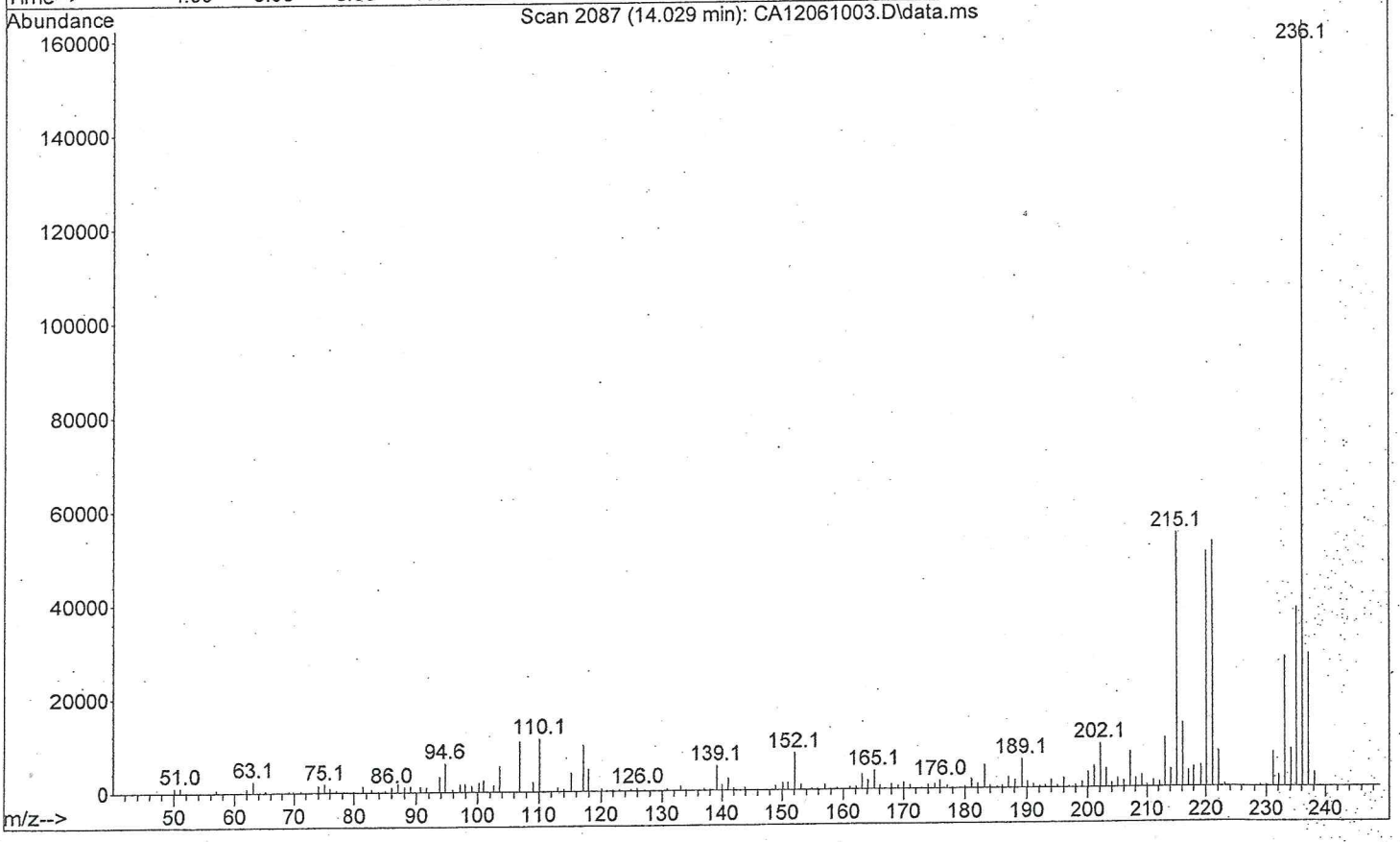

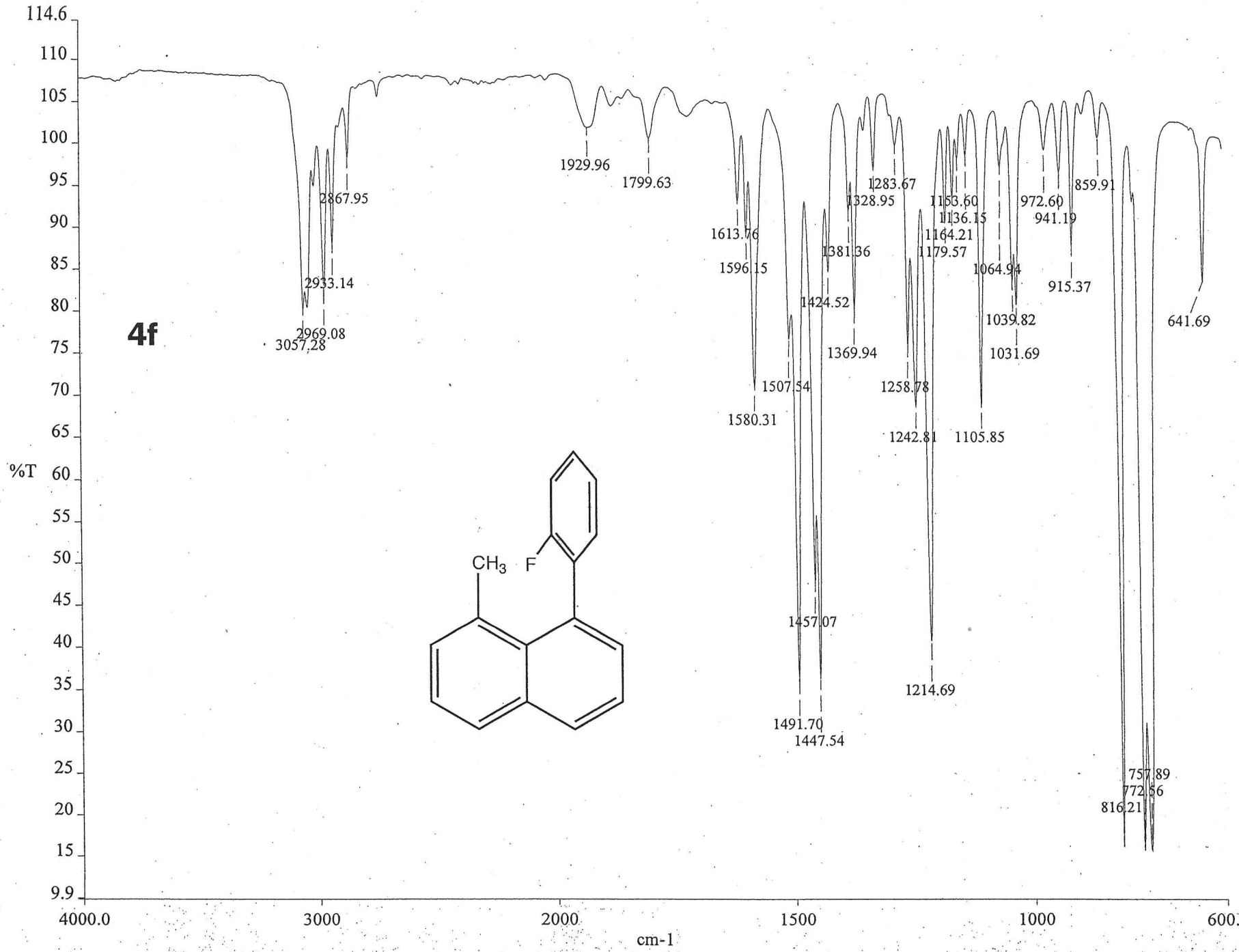
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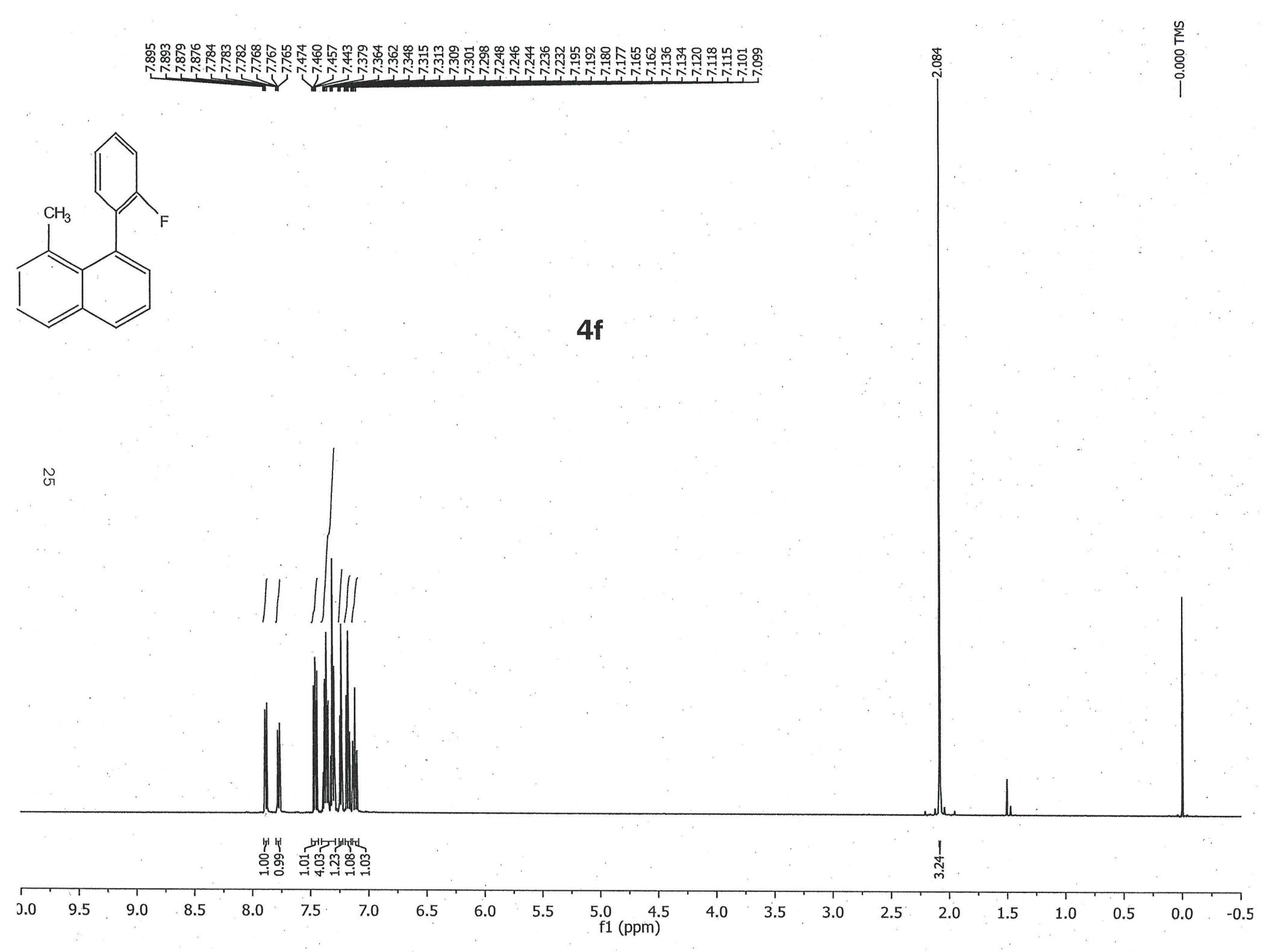
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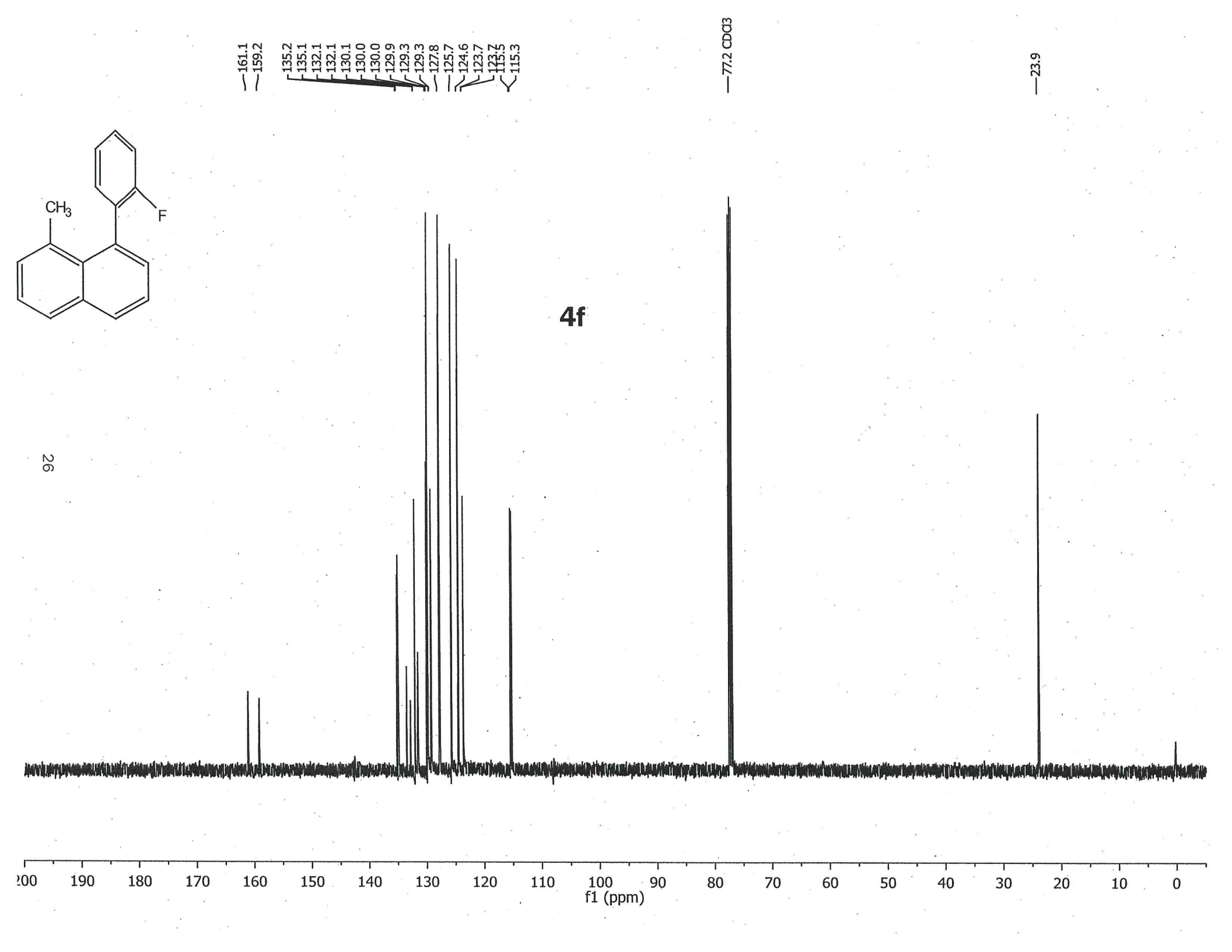
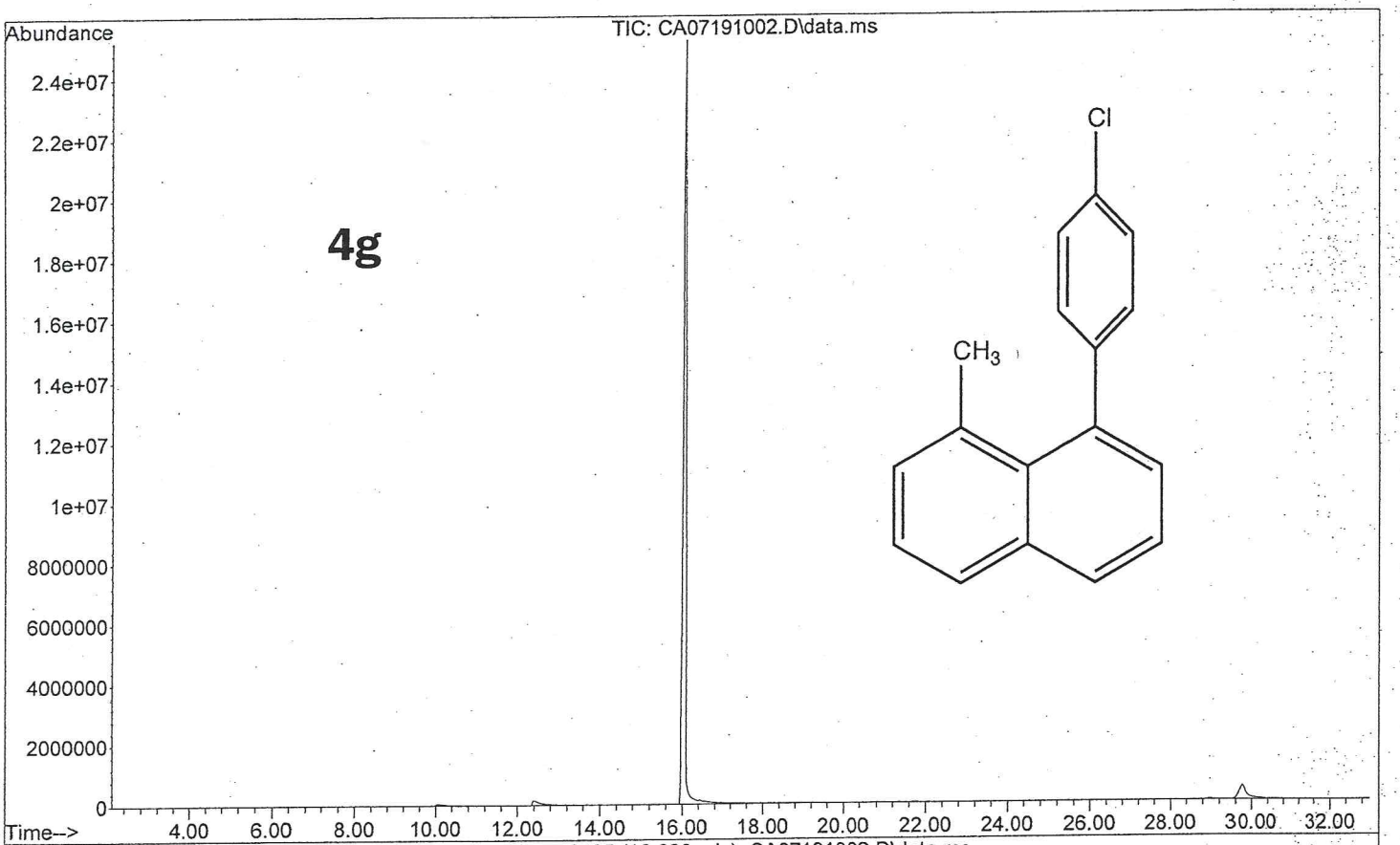
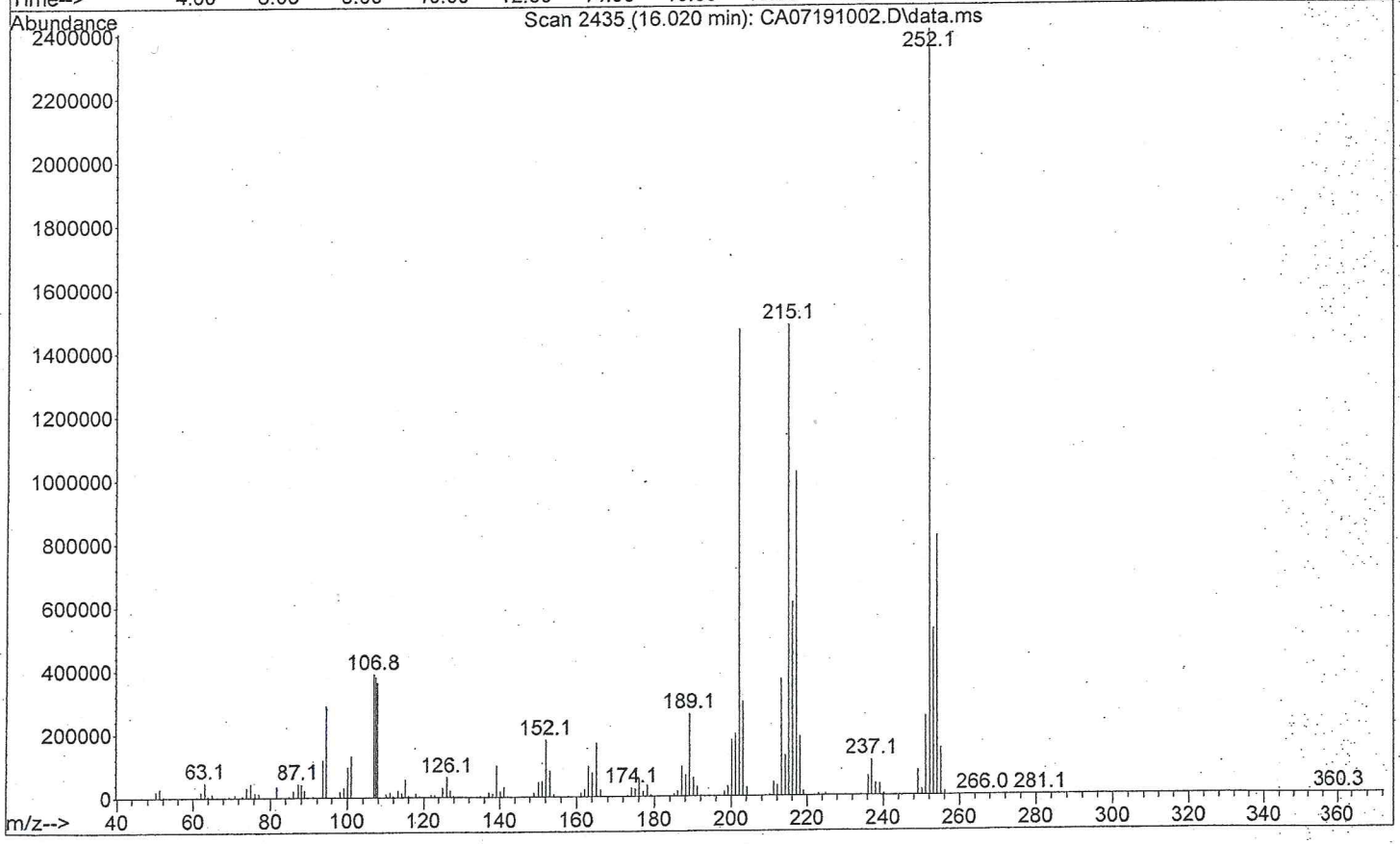
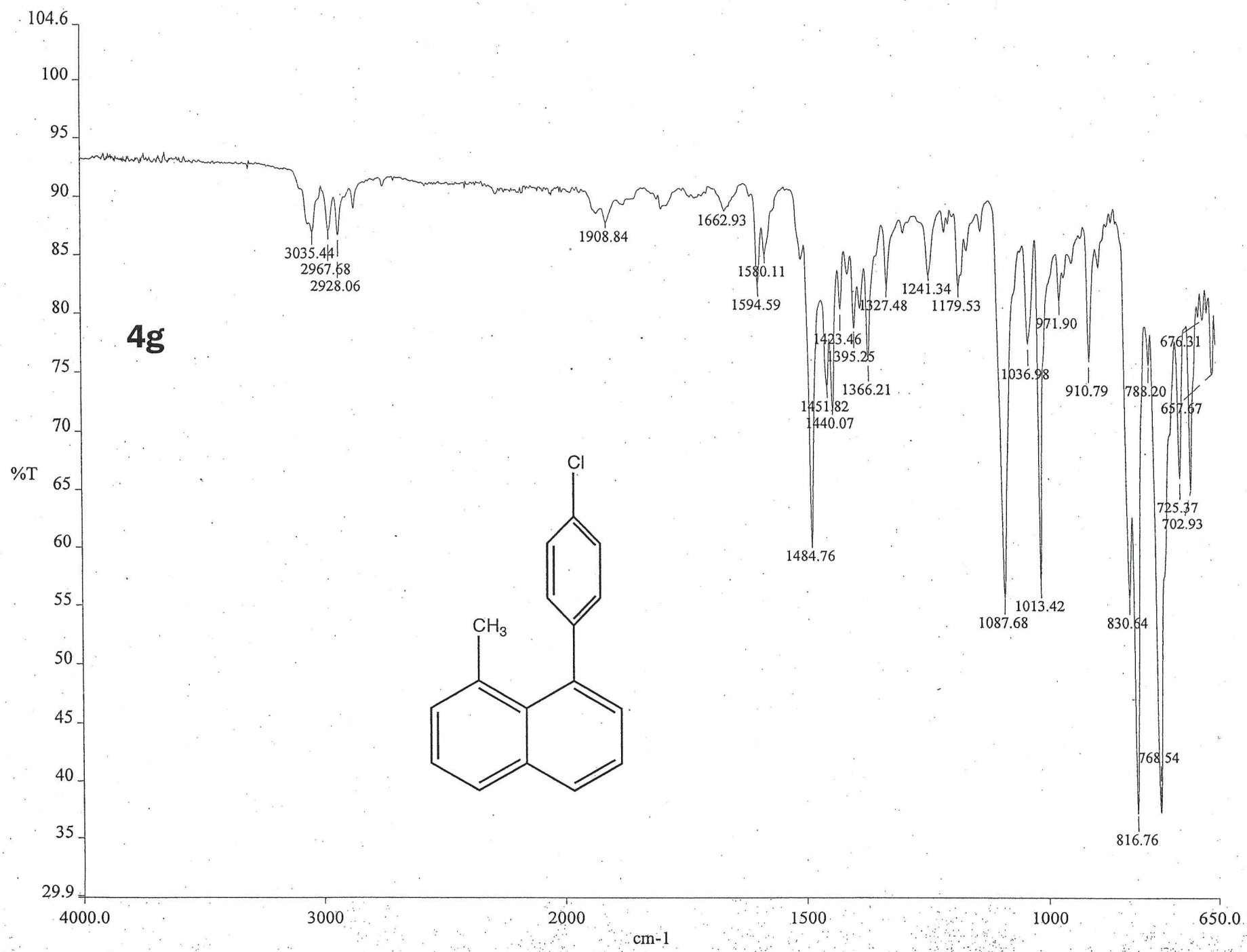
7.474
7.460
7.457
7.443
7.379
7.364
7.362
7.348
7.315
7.313
7.309
7.301
7.298
7.248
7.246
7.244
7.236
7.232
7.195
7.192
7.180
7.177
7.165
7.162
7.136
7.134
7.120
7.118
7.115
7.101
7.099
2.084
0.000 TMS
CH3
F
4f
25
1.00
0.99
1.01
4.03
1.23
1.08
1.03
3.24
f1 (ppm)

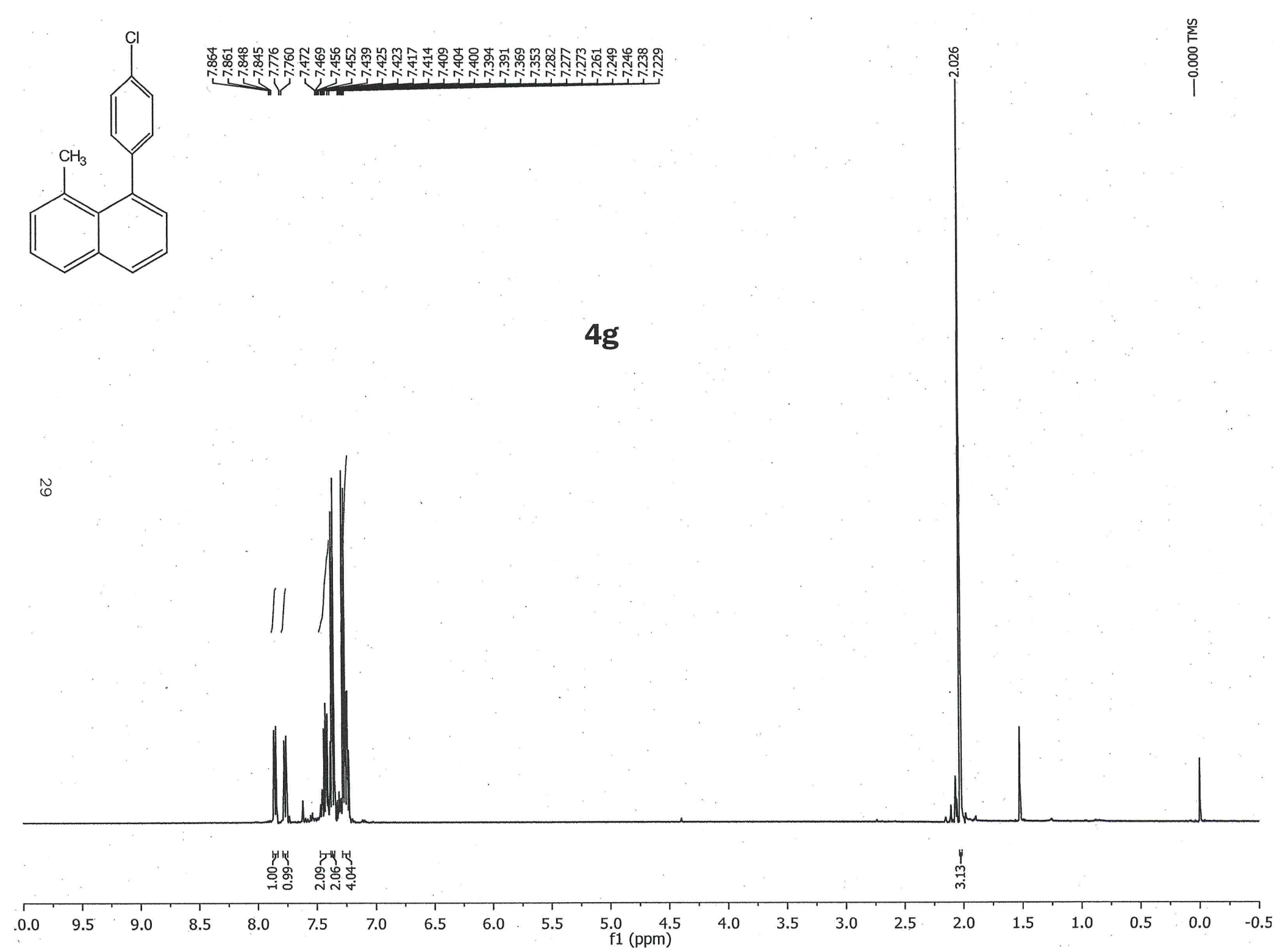

161.1
159.2
135.2
135.1
132.1
132.1
130.1
130.0
130.0
129.9
129.3
129.3
127.8
125.7
124.6
123.7
115.5
115.3
77.2 CDCl3
23.9
CH3
F
4f
26
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

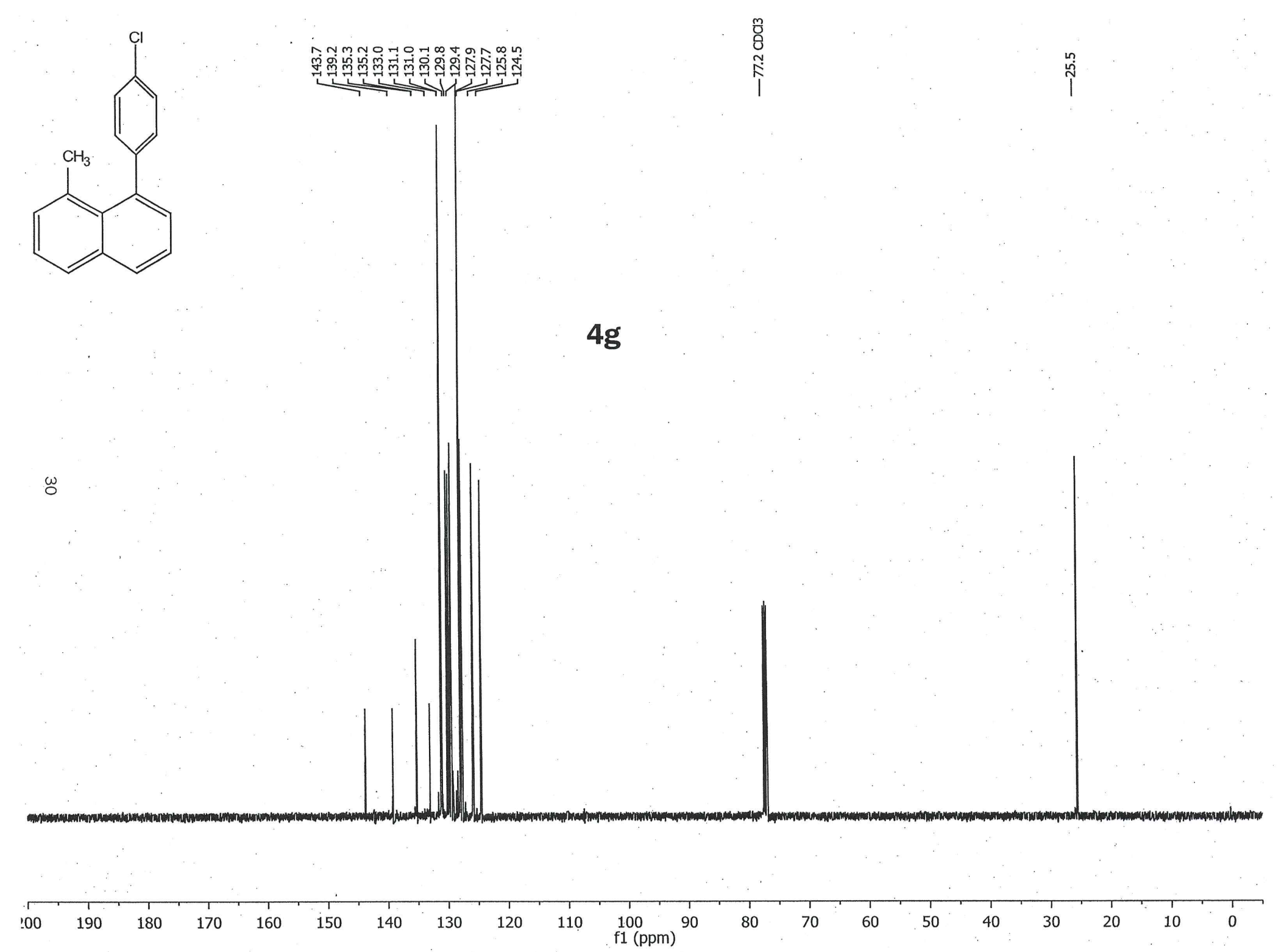
ile :D:\Thamattoor\Colin\CA07191002.D
perator : Colin
cquired : 19 Jul 2010 12:01 using AcqMethod DASMETHOD.M
nstrument : GCMSD 1
ample Name: chloro
isc Info : fr 4
ial Number: 1



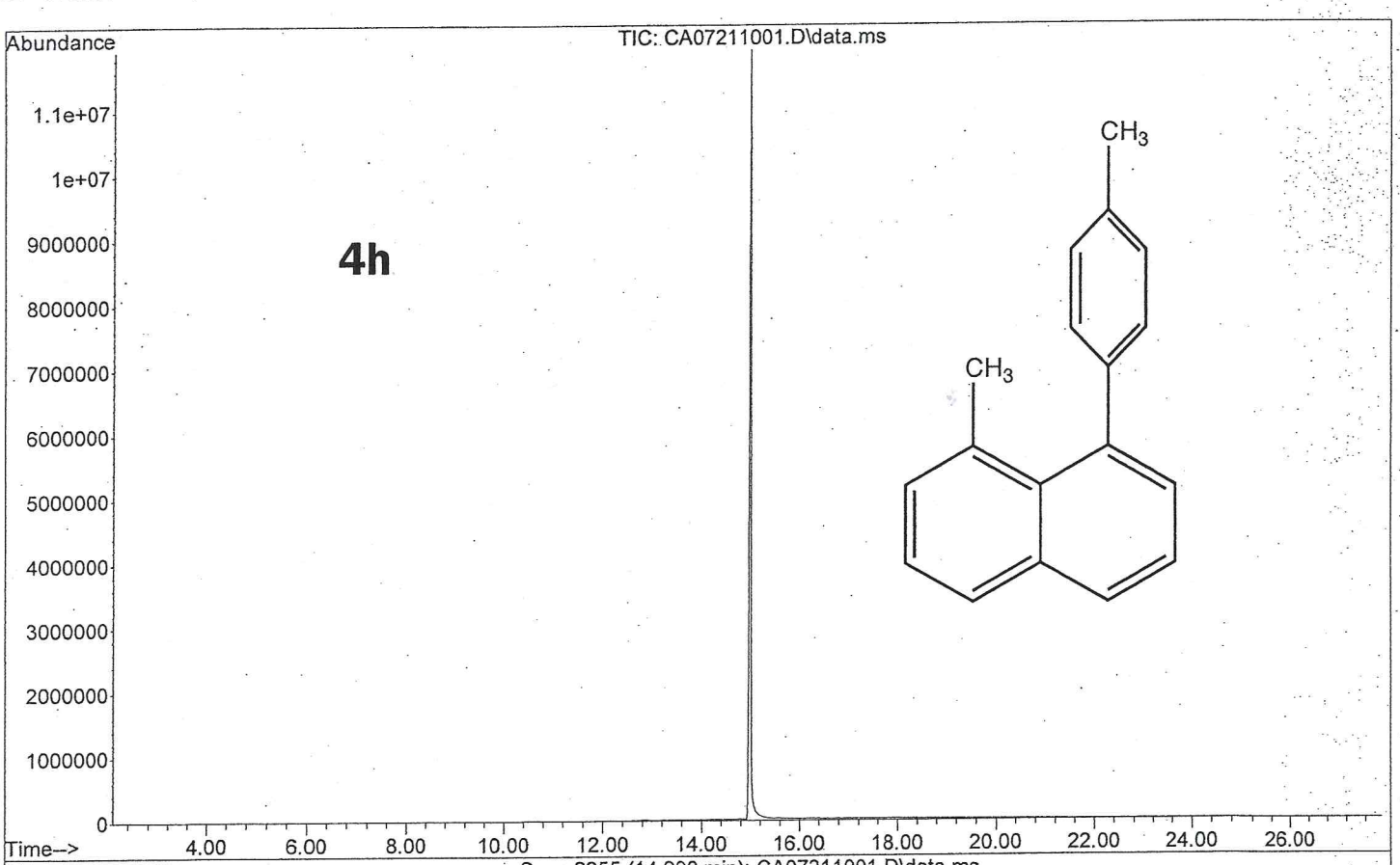


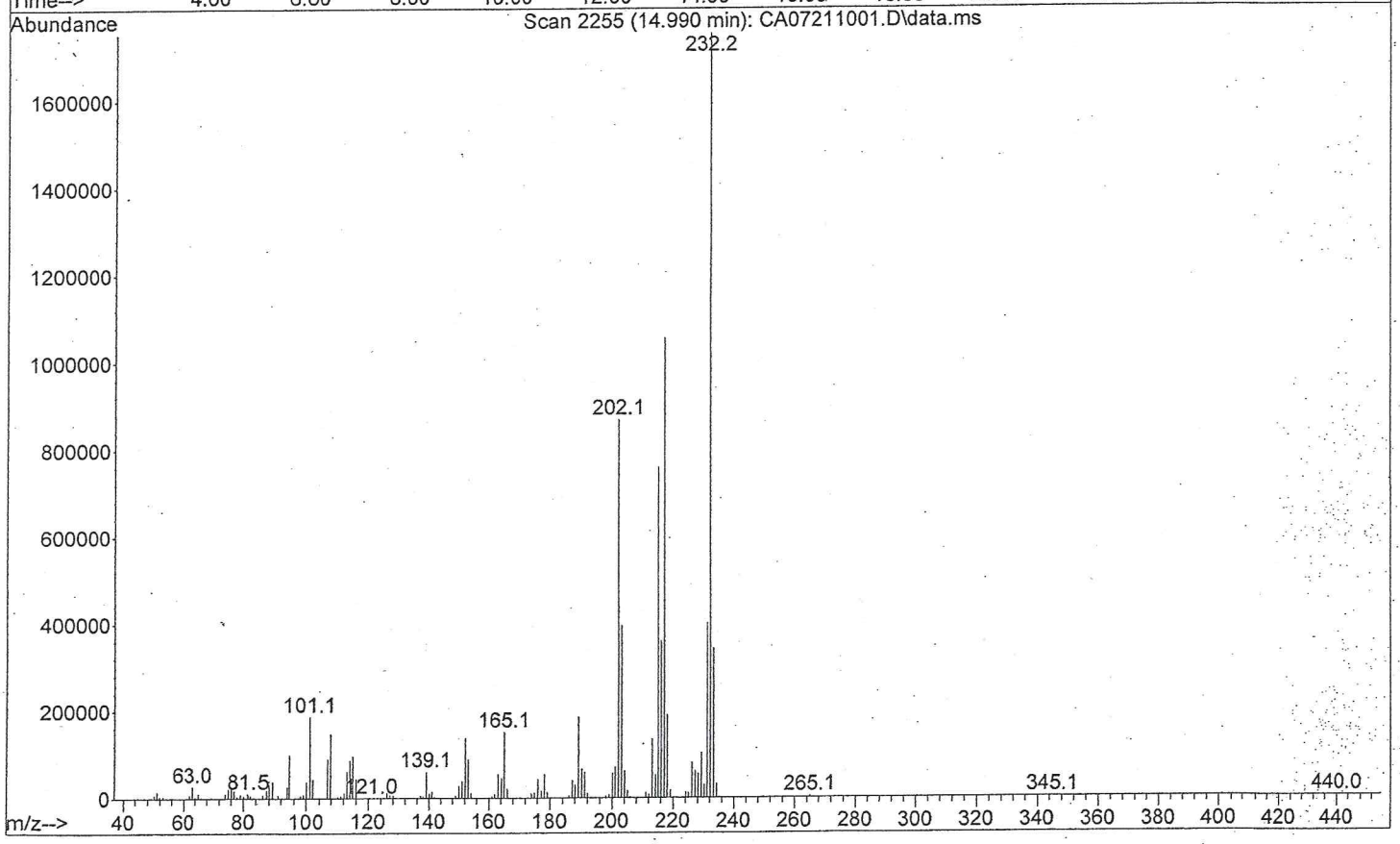

4g
%T
cm-1
104.6
100
95
90
85
80
75
70
65
60
55
50
45
40
35
29.9
4000.0
3000
2000
1500
1000
650.0
3035.44
2967.68
2928.06
1908.84
1662.93
1580.11
1594.59
1423.46
1395.25
1327.48
1241.34
1179.53
971.90
676.31
1036.98
1366.21
910.79
788.20
657.67
1451.82
1440.07
1484.76
725.37
702.93
1087.68
1013.42
830.64
768.54
816.76
Cl
CH3
c:\documents and settings\dmthamat\desktop\colin\colinchloro.sp

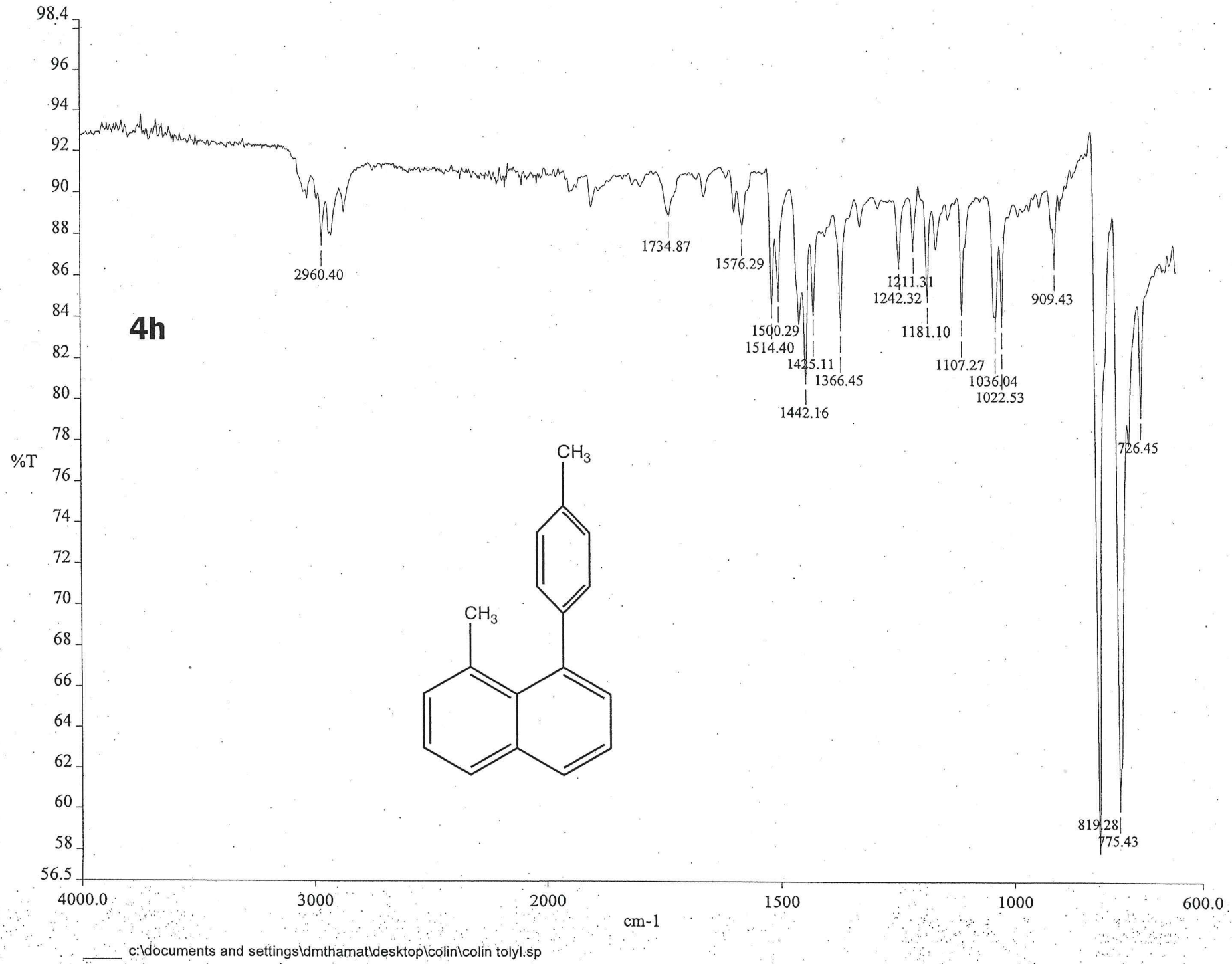

Cl
CH3
7.864
7.861
7.848
7.845
7.776
7.760
7.472
7.469
7.456
7.452
7.439
7.425
7.423
7.417
7.414
7.409
7.404
7.400
7.394
7.391
7.369
7.353
7.282
7.277
7.273
7.261
7.249
7.246
7.238
7.229
2.026
0.000 TMS
4g
29
1.00
0.99
2.09
2.06
4.04
3.13
f1 (ppm)

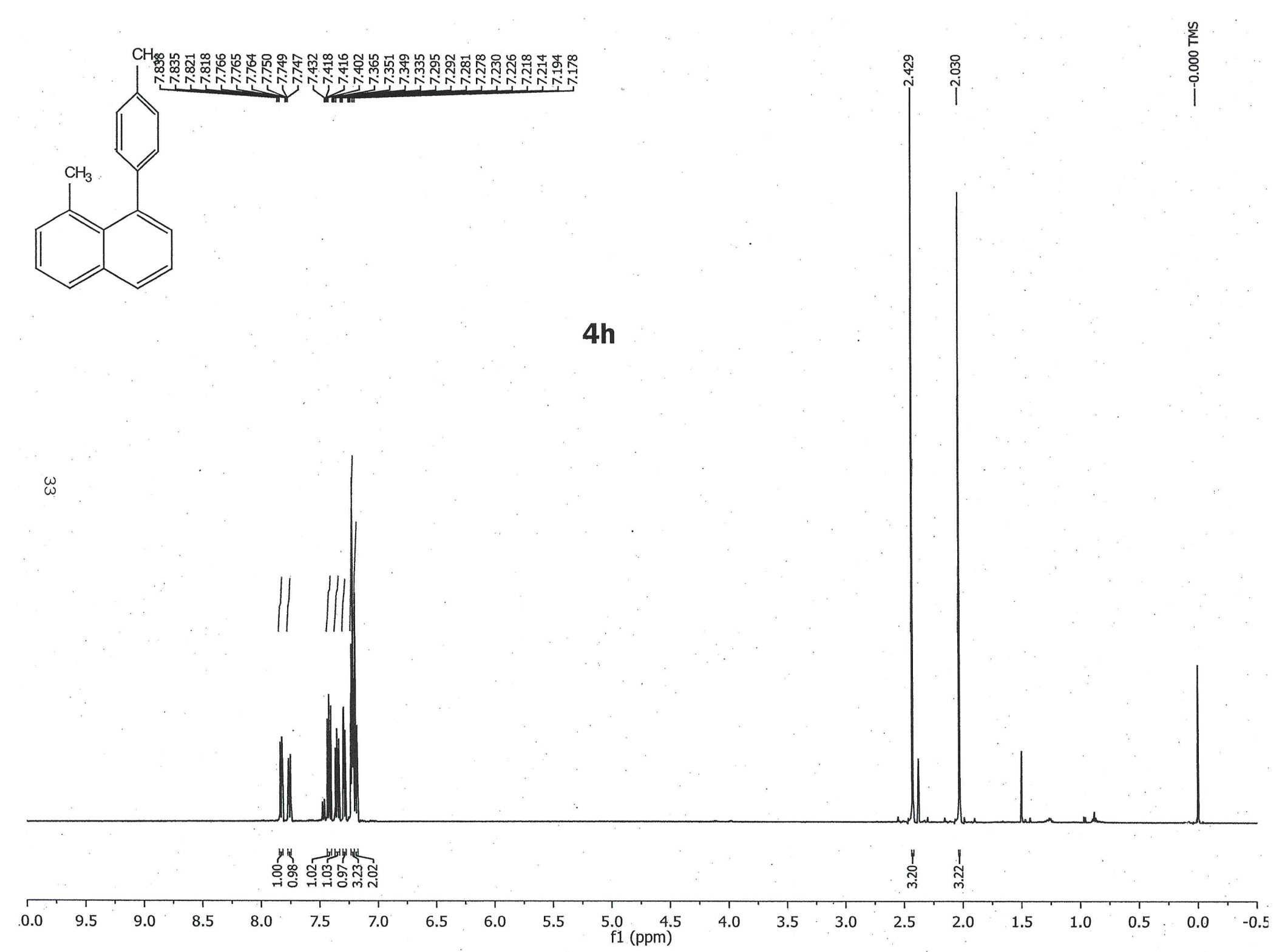

Cl
CH3
143.7
139.2
135.3
135.2
133.0
131.1
131.0
130.1
129.8
129.4
127.9
127.7
125.8
124.5
77.2 CDCl3
25.5
4g
30
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

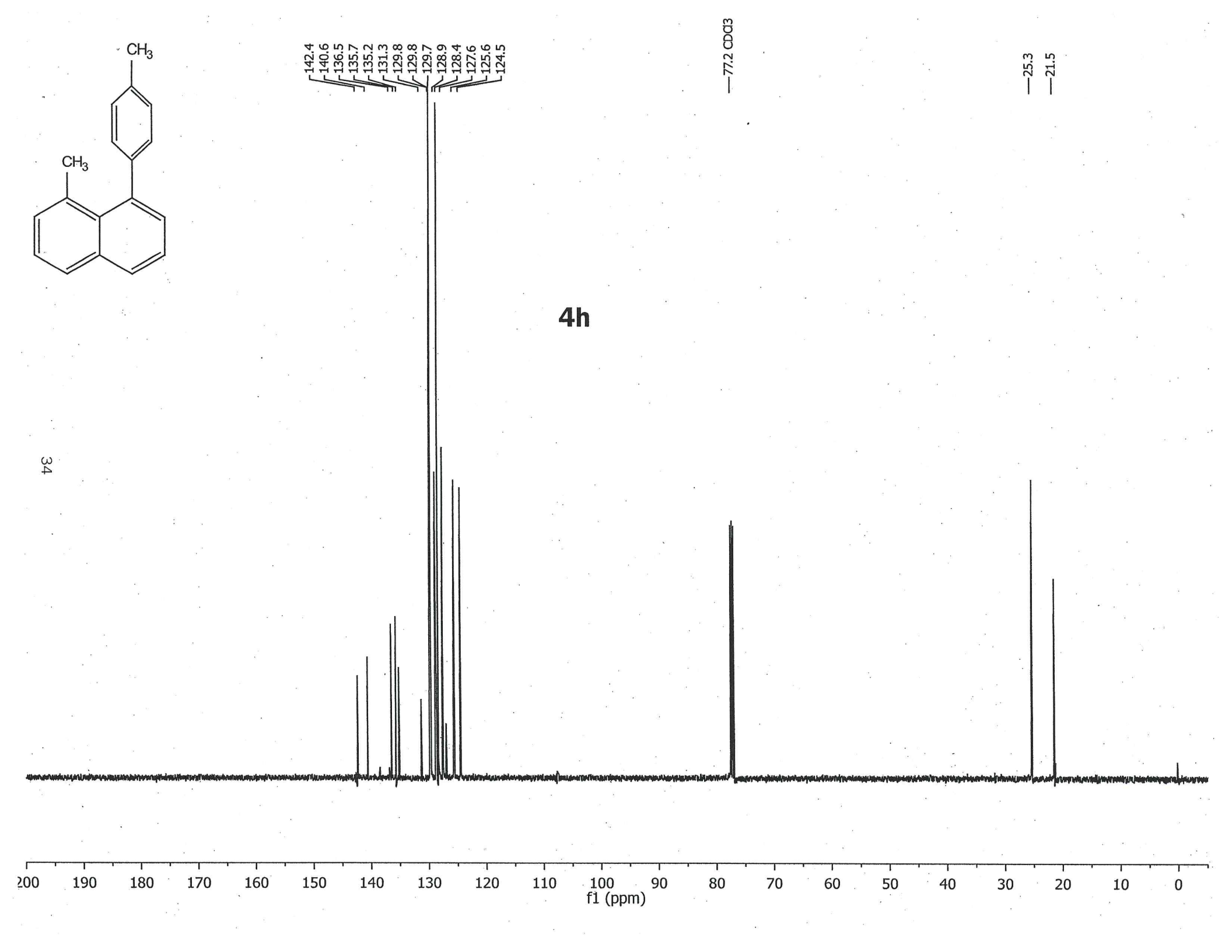
ile :D:\Thamattoor\Colin\CA07211001.D
perator : Eric
cquired : 21 Jul 2010 12:21 using AcqMethod DASMETHOD.M
nstrument : GCMSD 1
ample Name:
isc Info :
ial Number: 1



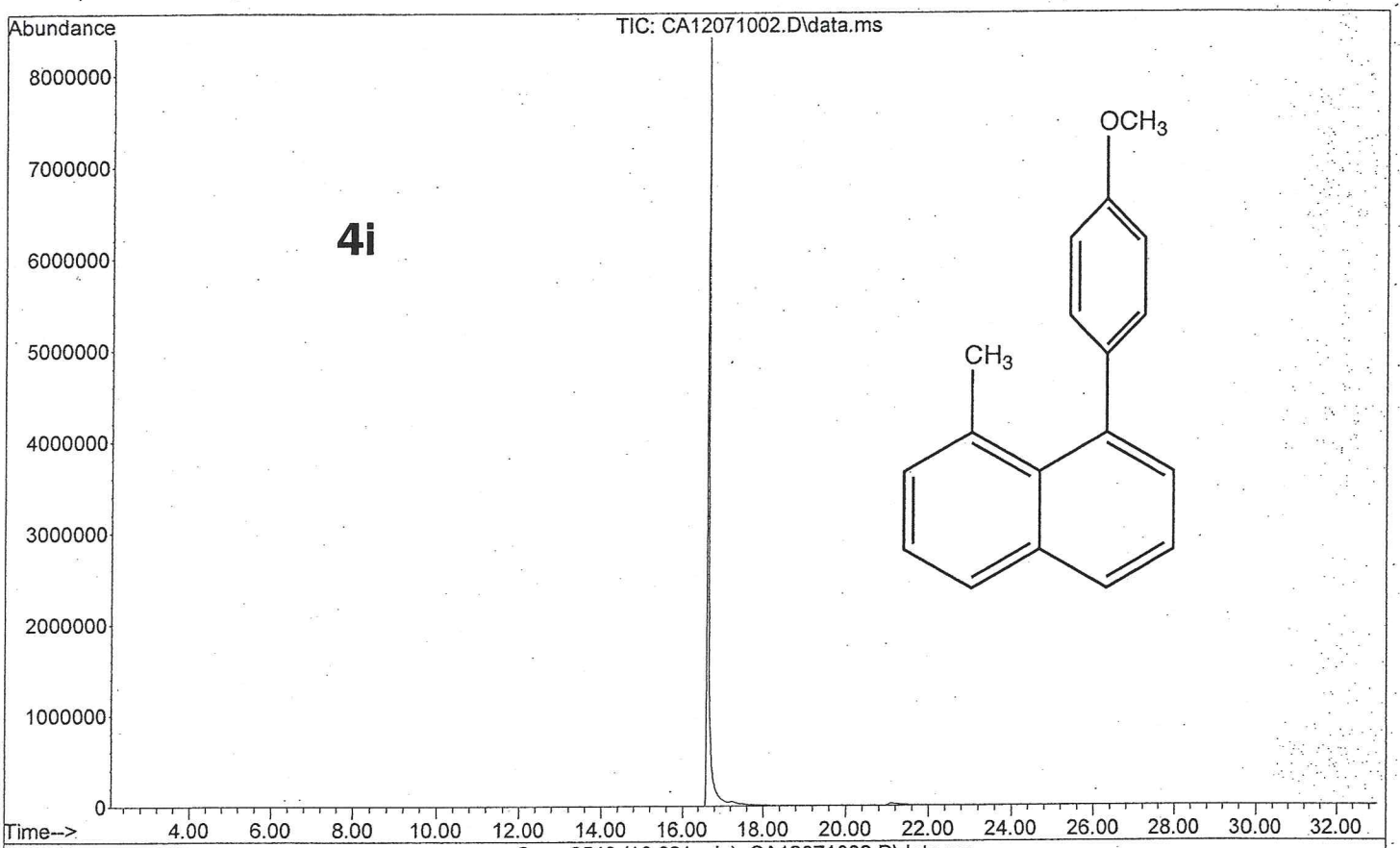


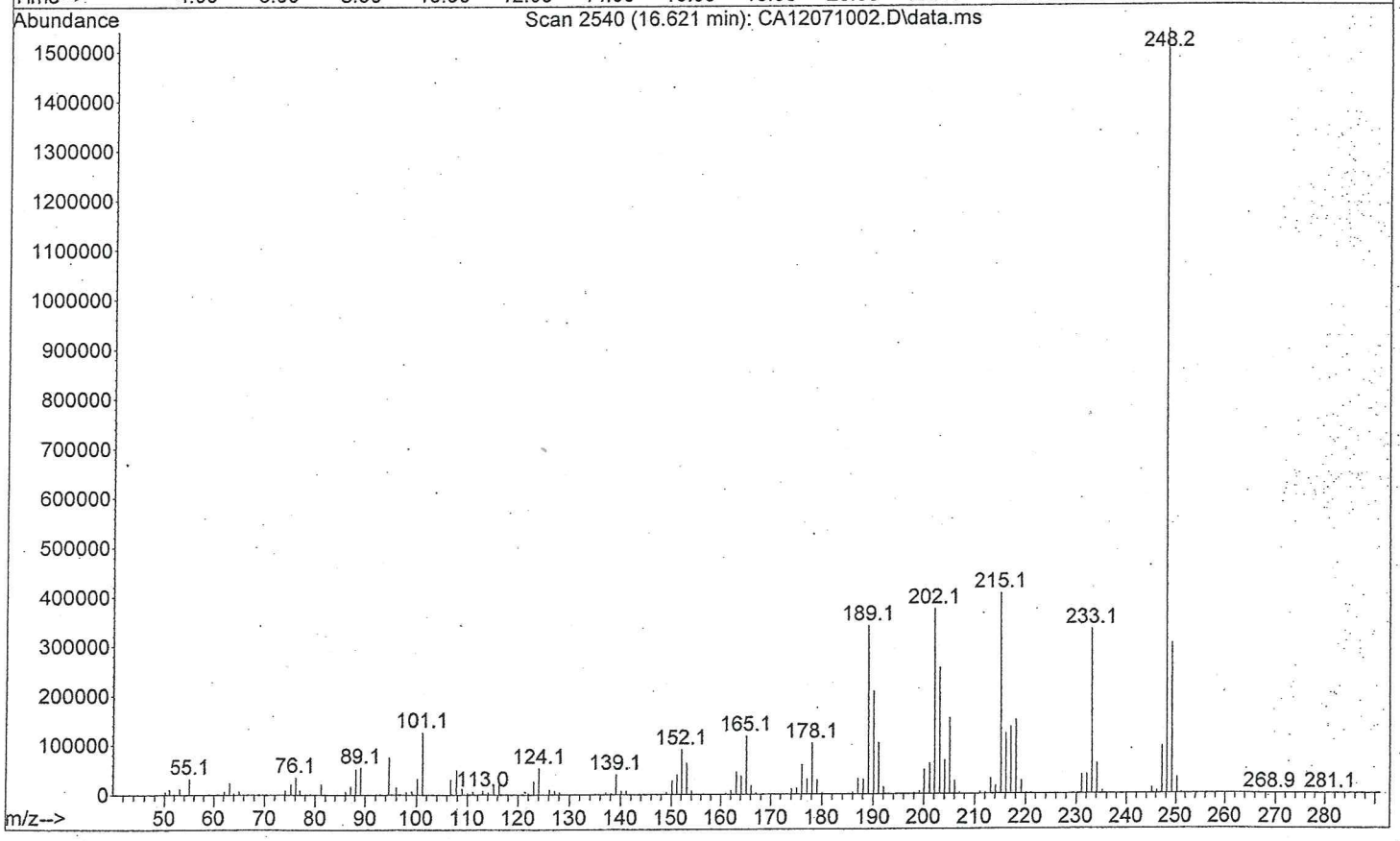

4h
%T
cm-1
2960.40
1734.87
1576.29
1500.29
1514.40
1442.16
1425.11
1366.45
1242.32
1211.31
1181.10
1107.27
1036.04
1022.53
909.43
819.28
775.43
726.45
CH3
CH3
98.4
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
56.5
4000.0
3000
2000
1500
1000
600.0
c:\documents and settings\dmthamat\desktop\colin\colin tolyl.sp

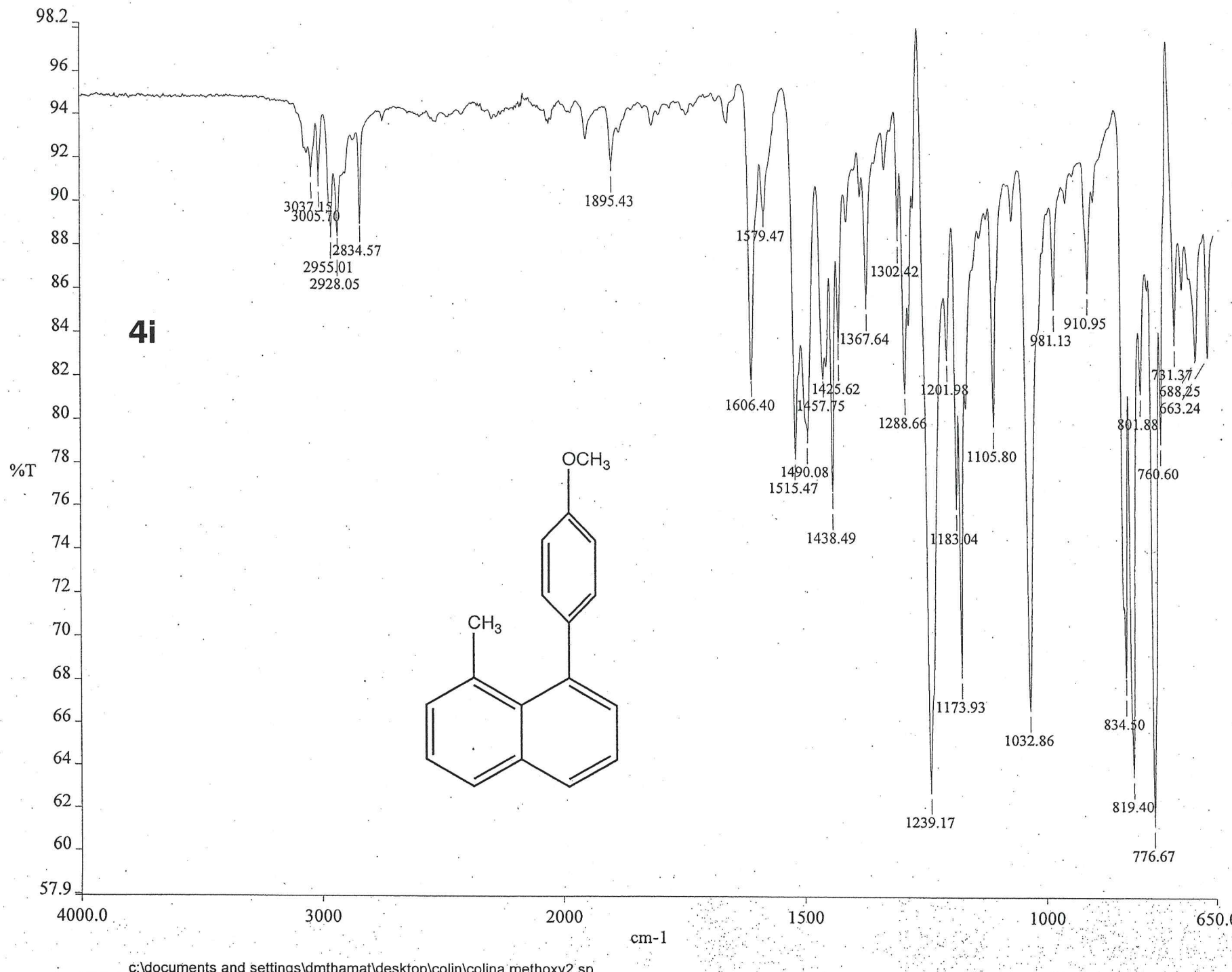

CH3
CH3
7.838
7.835
7.821
7.818
7.766
7.765
7.764
7.750
7.749
7.747
7.432
7.418
7.416
7.402
7.365
7.351
7.349
7.335
7.295
7.292
7.281
7.278
7.230
7.226
7.218
7.214
7.194
7.178
2.429
2.030
0.000 TMS
4h
33
1.00
0.98
1.02
1.03
0.97
3.23
2.02
3.20
3.22
f1 (ppm)


CH3
CH3
142.4
140.6
136.5
135.7
135.2
131.3
129.8
129.8
129.7
128.9
128.4
127.6
125.6
124.5
77.2 CDCl3
25.3
21.5
4h
34
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

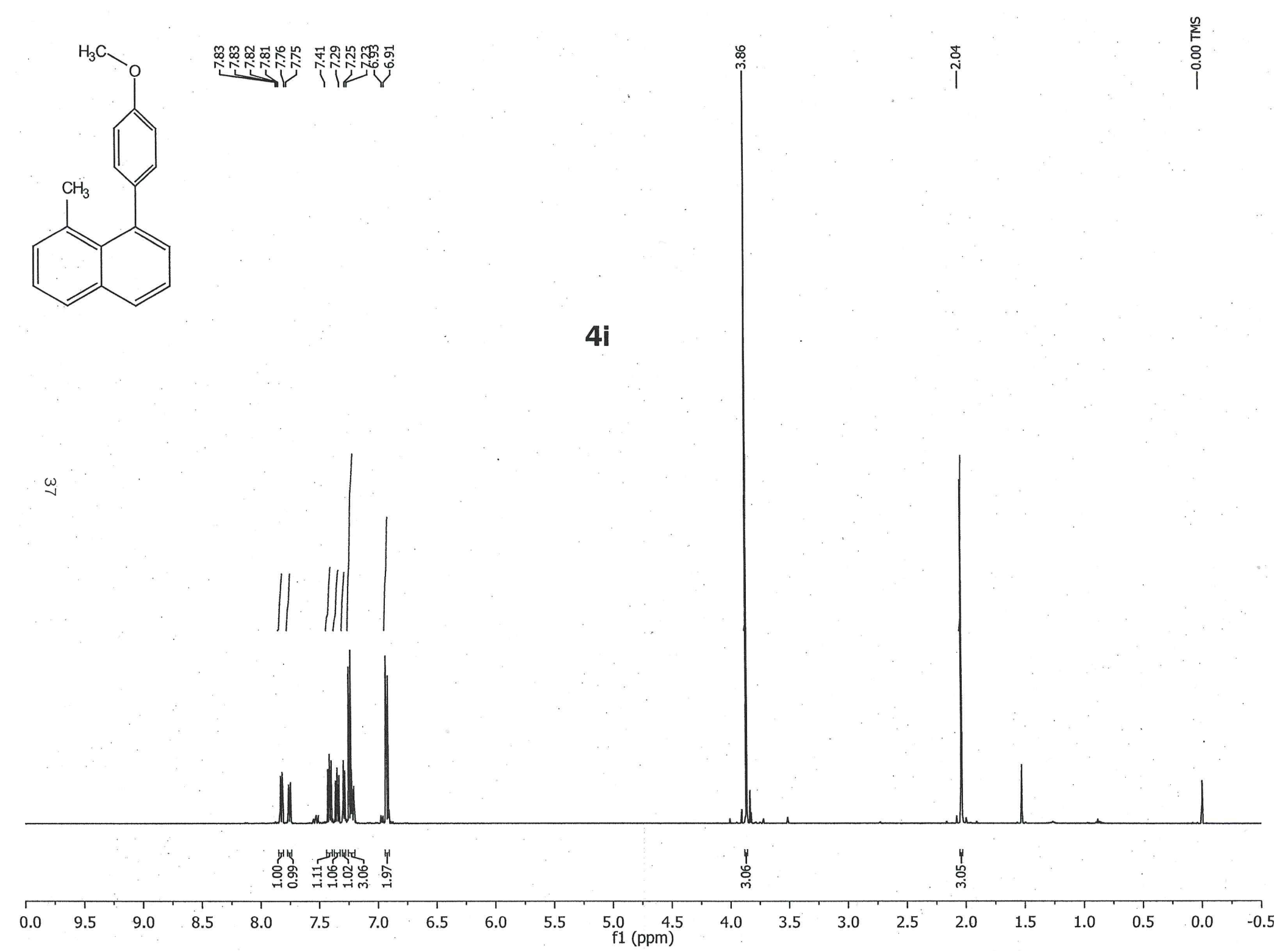
ile :D:\Thamattoor\Colin\Asenior year\CA12071002.D
perator : Colin
cquired : 7 Dec 2010 21:39 using AcqMethod DASMETHOD.M
nstrument : GCMSD 1
ample Name: OMe
isc Info :
tal Number: 1

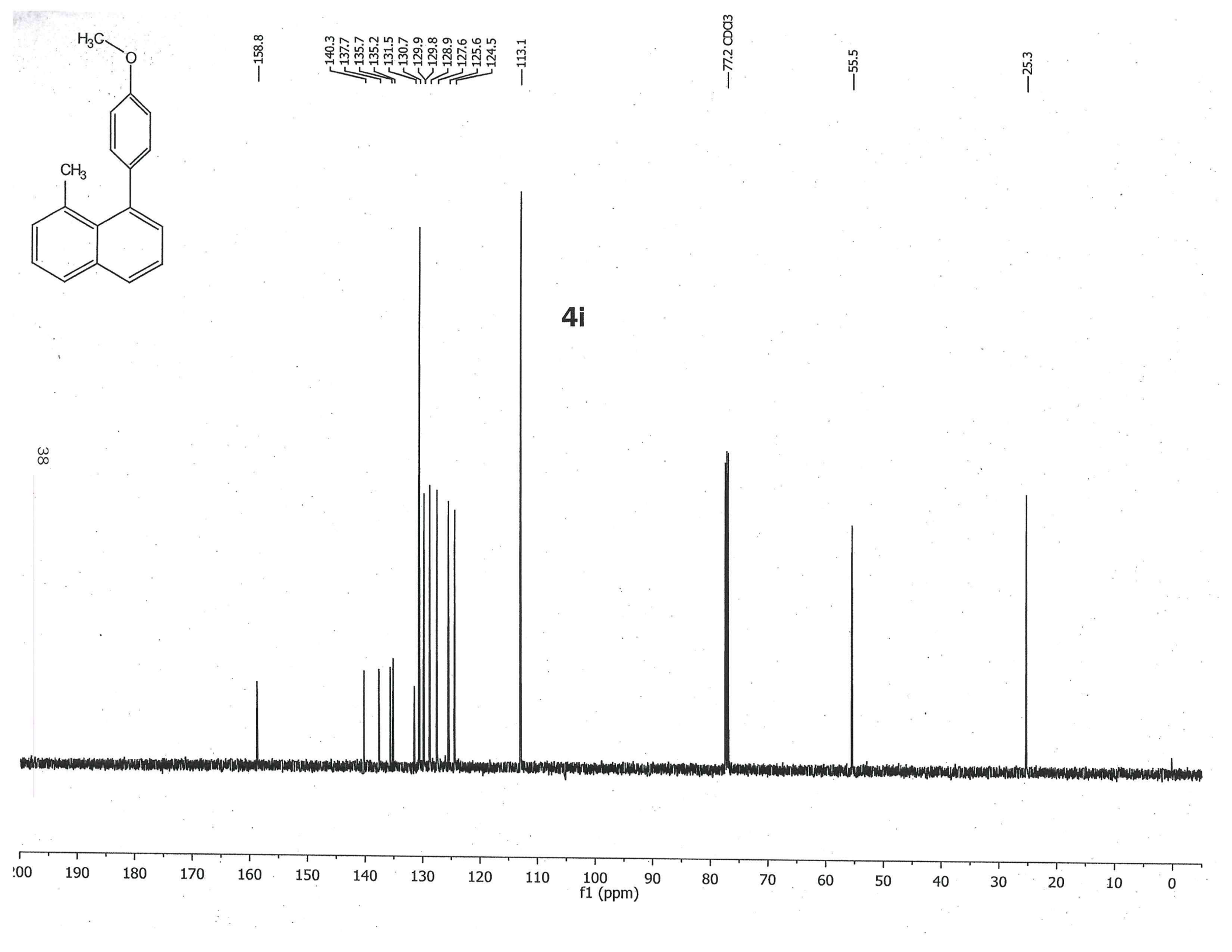




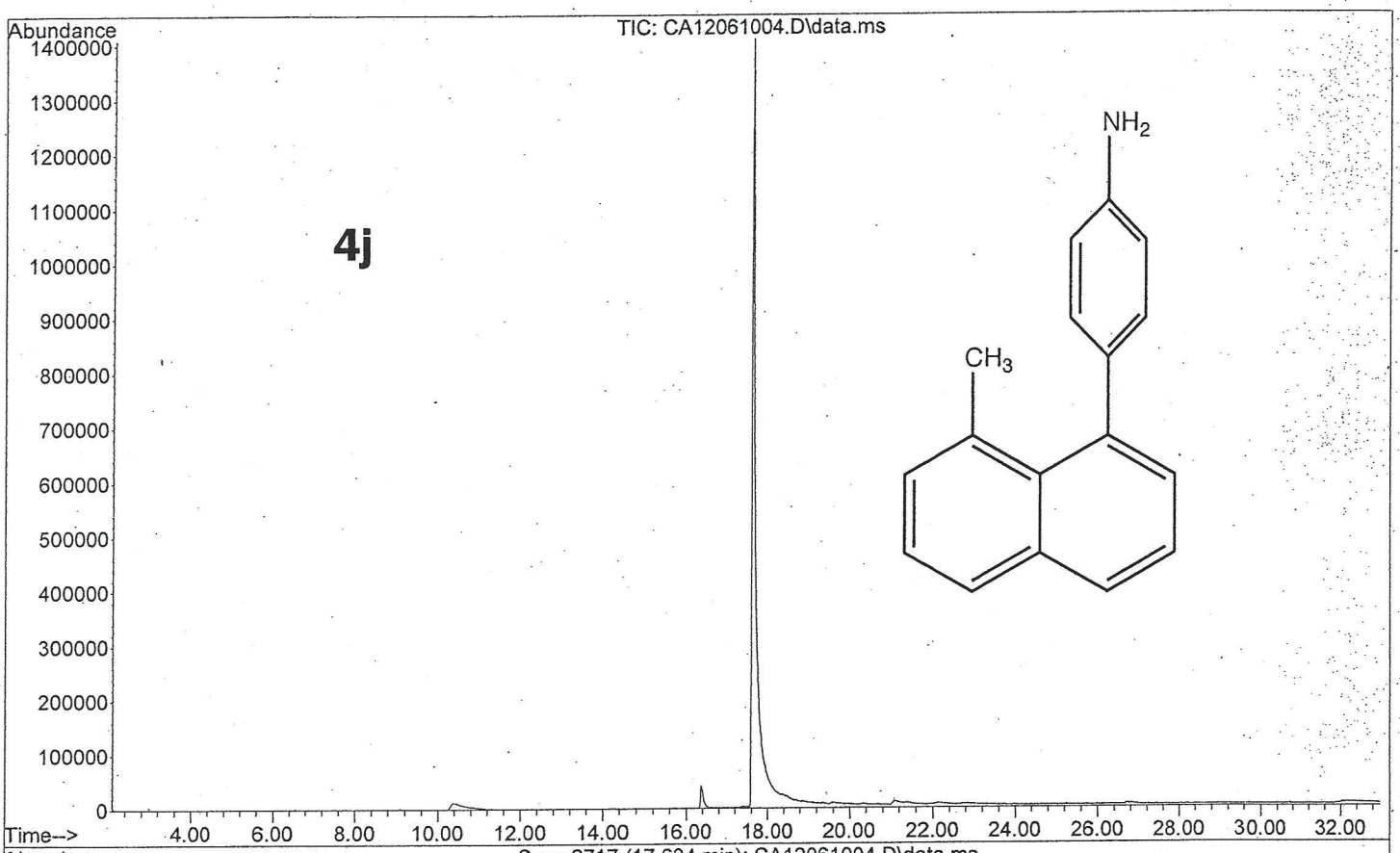


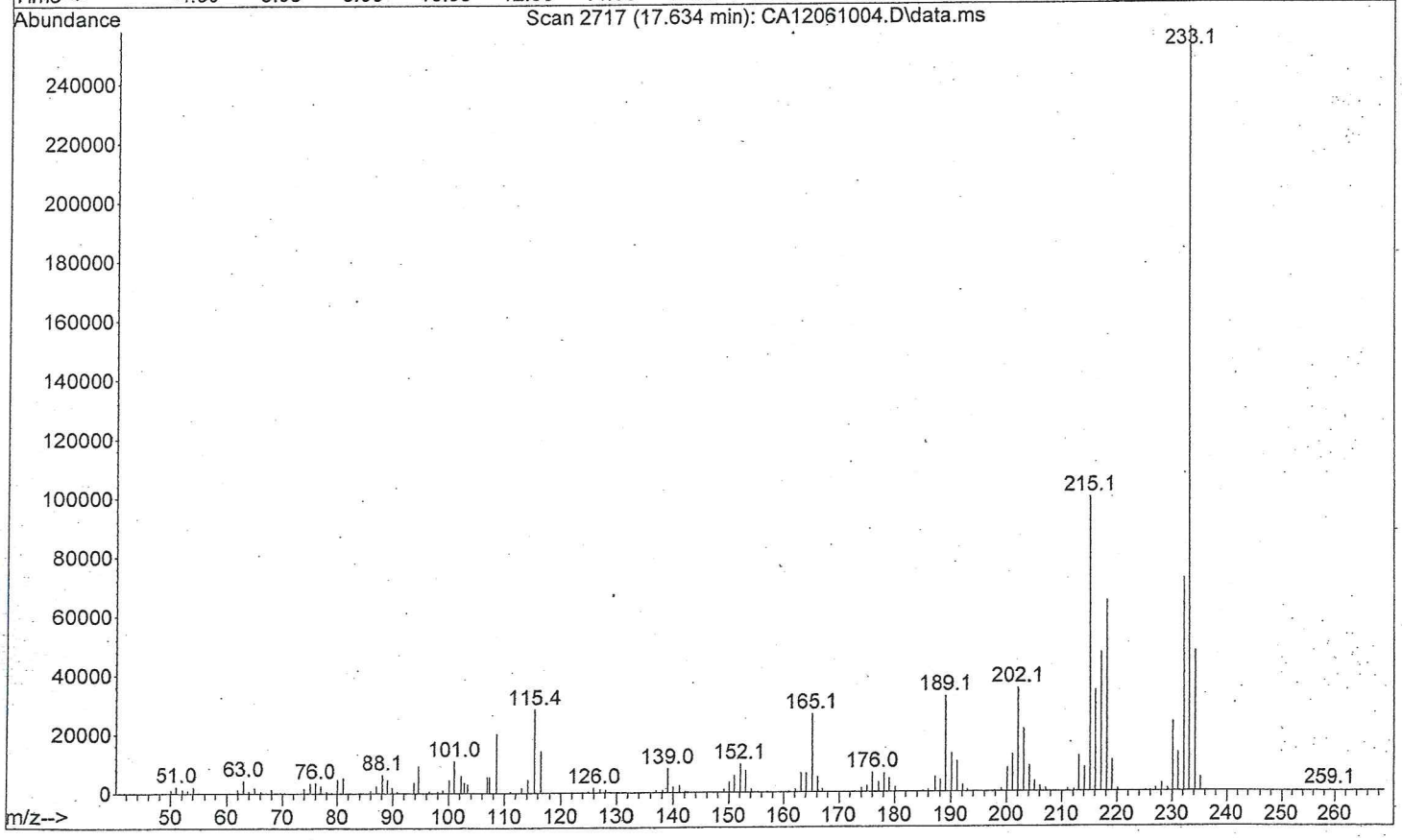
c:\documents and settings\dmthamat\desktop\colin\colina methoxy2.sp

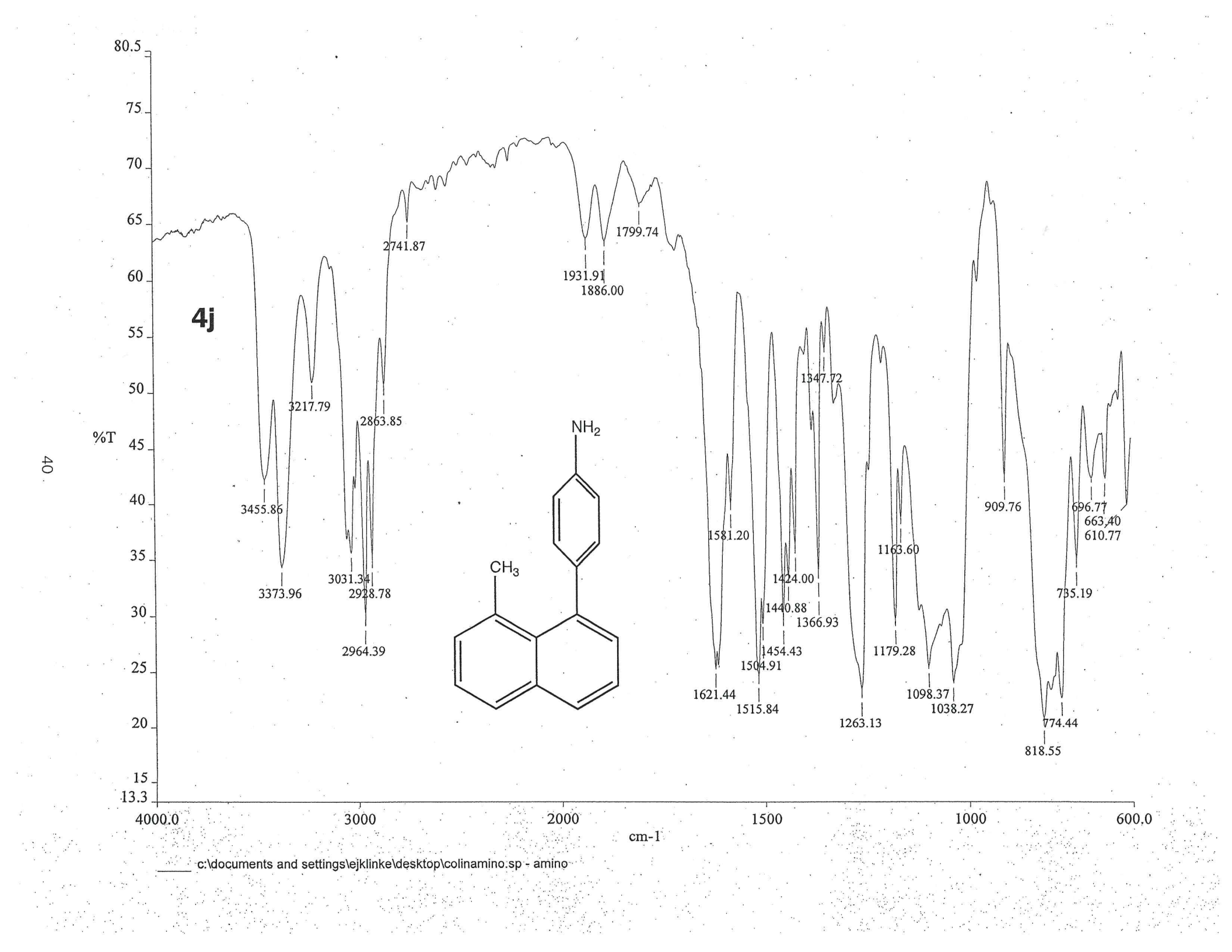

H3C
O
CH3
7.83
7.83
7.82
7.81
7.76
7.75
7.41
7.29
7.25
7.23
6.93
6.91
3.86
2.04
0.00 TMS
4i
37
1.00
0.99
1.11
1.06
1.02
3.06
1.97
3.06
3.05
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

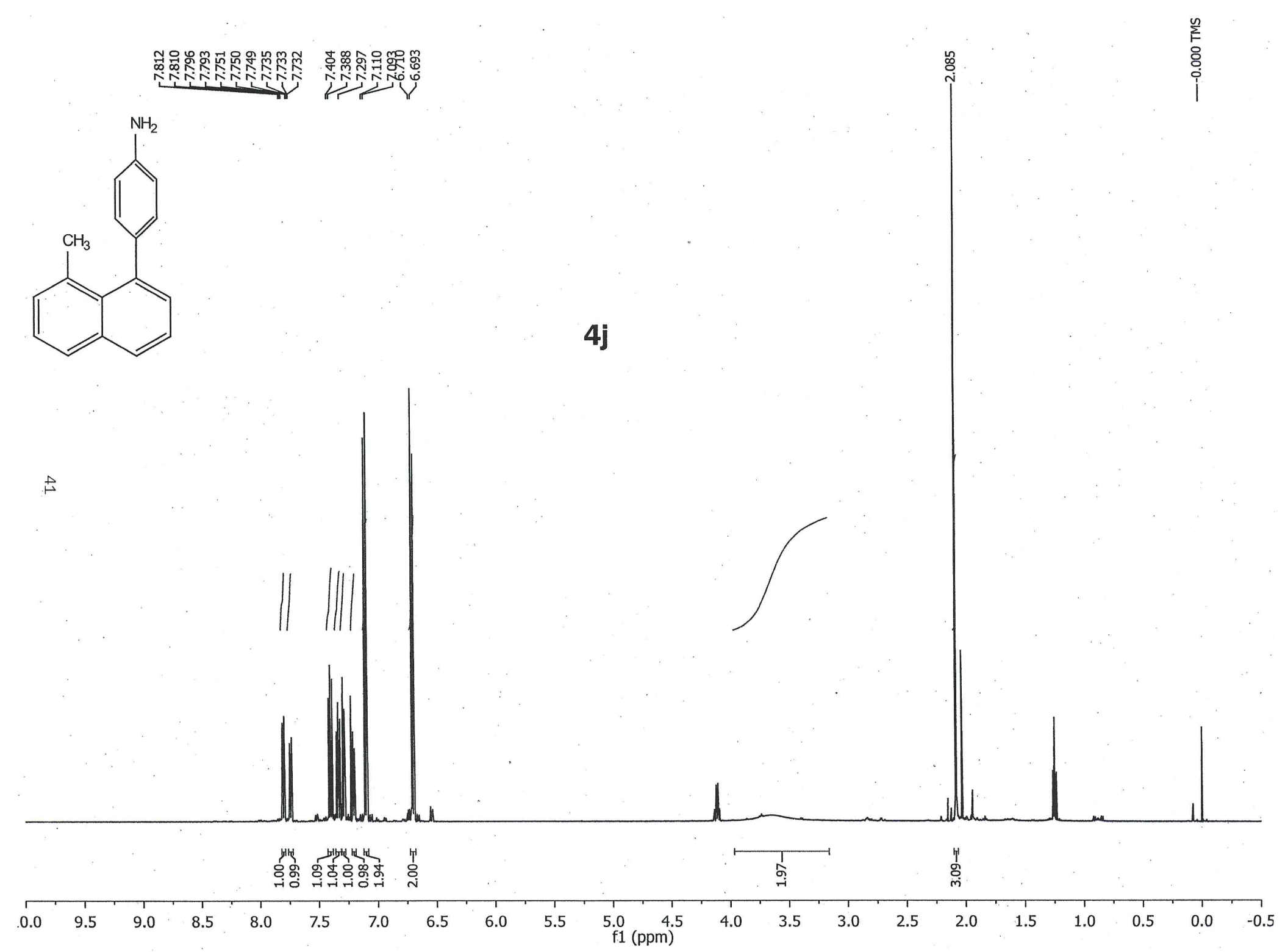

H3C
O
CH3
158.8
140.3
137.7
135.7
135.2
131.5
130.7
129.9
129.8
128.9
127.6
125.6
124.5
113.1
77.2 CDCl3
55.5
25.3
4i
38
f1 (ppm)

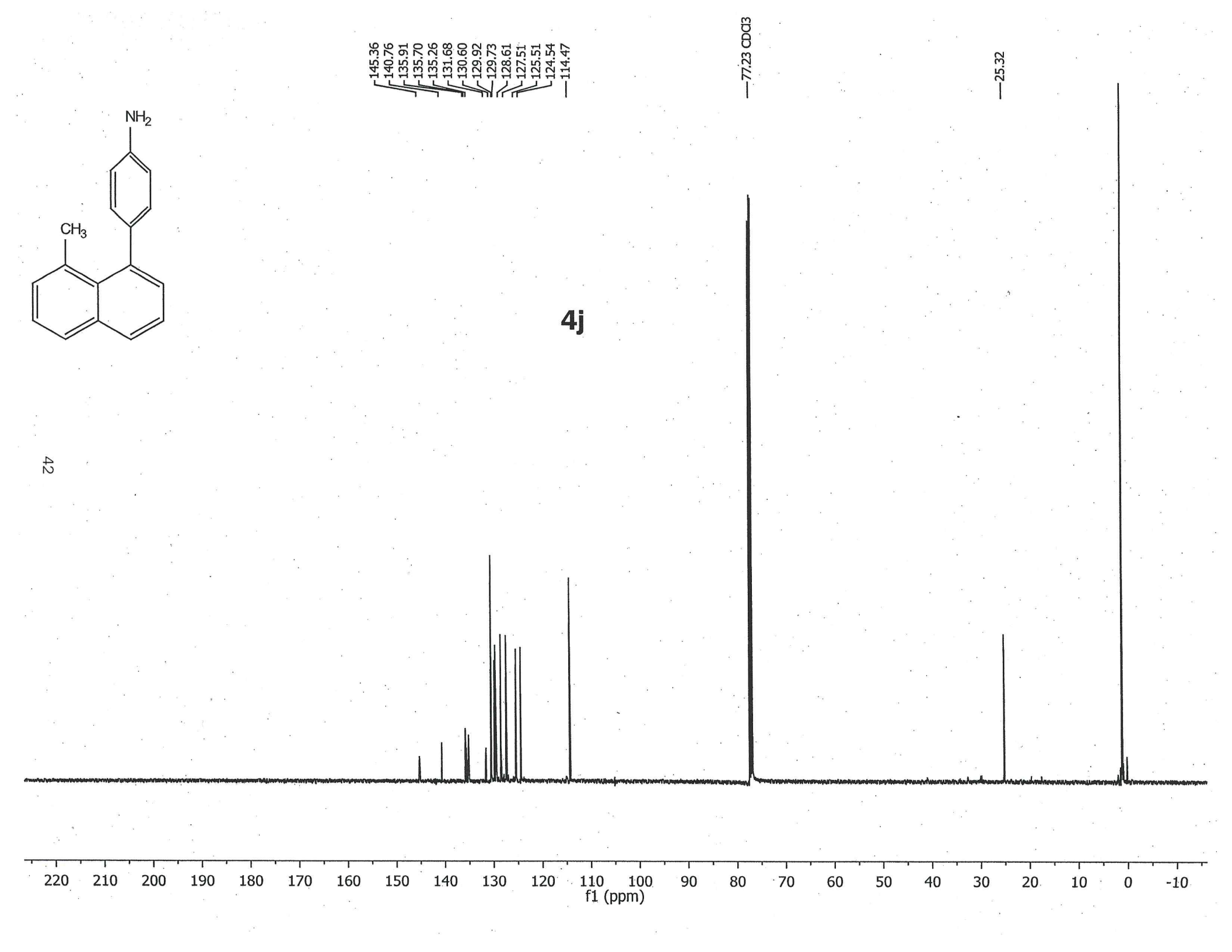
ile :D:\Thamattoor\Colin\Asenior year\CA12061004.D
perator : Colin
cquired : 6 Dec 2010 17:54 using AcqMethod DASMETHOD.M
nstrument : GCMSD 1
ample Name: Amino
isc Info :
ial Number: 1






4j
%T
cm-1
80.5
75
70
65
60
55
50
45
40
35
30
25
20
15
13.3
4000.0
3000
2000
1500
1000
600.0
3455.86
3373.96
3217.79
3031.34
2928.78
2964.39
2863.85
2741.87
1931.91
1886.00
1799.74
1621.44
1581.20
1515.84
1504.91
1454.43
1440.88
1424.00
1366.93
1347.72
1263.13
1179.28
1163.60
1098.37
1038.27
909.76
818.55
774.44
735.19
696.77
663.40
610.77
NH2
CH3
c:\documents and settings\ejklinke\desktop\colinamino.sp - amino


7.812
7.810
7.796
7.793
7.751
7.750
7.749
7.735
7.733
7.732
7.404
7.388
7.297
7.110
7.093
6.710
6.693
2.085
-0.000 TMS
NH2
CH3
4j
1.00
0.99
1.09
1.04
1.00
0.98
1.94
2.00
1.97
3.09
f1 (ppm)


145.36
140.76
135.91
135.70
135.26
131.68
130.60
129.92
129.73
128.61
127.51
125.51
124.54
114.47
77.23 CDCl3
25.32
NH2
CH3
4j
42
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

X-ray data solution and refinement for the structure of 4-(8-Methylnaphthalen-1-yl)benzaldehyde (4c)

From the systematic absences and the observed metric constants and intensity statistics, space group *C*2/*c* was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.[1] All non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and U_{iso} (H) in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints.[2] The structure is disordered, with two orientations of the oxygen and hydrogen atoms of the aldehyde moiety. Atoms O(1) and H(171) comprise the major component of disorder, with atoms O(2) and H(172) as the minor component. Oxygen and aldehyde hydrogen atoms were refined as described above. The occupancy of the major and minor components were constrained to sum to 1.0, and the major component occupancy refined to 0.655(5). The final least-squares refinement converged to $R_1 = 0.0674$ ($I > 2\sigma(I)$, 2413 data) and $wR_2 = 0.1671$ (F^2, 2734 data, 182 parameters). The final CIF is included in the supporting materials; we note that the CheckCIF routine produced an alert A and an Alert B item, related to the disorder of the aldehyde oxygen atoms. Accordingly, the CIF file contains validation reply form items which explain this issue in detail.

1. Betteridge, P. W.; Carruthers, J. R.; Cooper, R. I.; Prout, K.; Watkin, D. J. *J. Appl. Cryst.* **2003**, *36*, 1487.

2. Cooper, R. I.; Thompson, A. L.; Watkin, D. J. *J. Appl. Cryst.* **2010**, *43*, 1100–1107.

1-Methyl-8-phenylnaphthalene (4a)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.206875	-0.361540	0.182000
2	6	0	3.355943	-0.563858	1.270975
3	6	0	2.009677	-0.209519	1.184845
4	6	0	1.487077	0.348232	0.007598
5	6	0	2.355863	0.563700	-1.072330
6	6	0	3.702804	0.205777	-0.989123
7	1	0	5.255573	-0.638579	0.248602
8	1	0	3.742563	-0.991883	2.192380
9	1	0	1.352867	-0.357390	2.038249
10	1	0	1.966156	1.006518	-1.985239
11	1	0	4.358046	0.372544	-1.840257
12	6	0	0.065529	0.817061	-0.047864
13	6	0	-1.092778	-0.043375	-0.044912
14	6	0	-0.099538	2.194241	-0.028910
15	6	0	-1.069450	-1.479338	-0.196281
16	6	0	-2.382347	0.594562	0.081694
17	6	0	-1.369032	2.801627	0.045552
18	1	0	0.788567	2.820147	-0.033027
19	6	0	-2.262477	-2.178937	-0.127386
20	6	0	-3.568182	-0.183898	0.148642
21	6	0	-2.486487	2.009780	0.124618
22	1	0	-1.450752	3.884910	0.066127
23	6	0	-3.510637	-1.550889	0.063610
24	1	0	-2.235362	-3.259516	-0.245311
25	1	0	-4.519967	0.330109	0.259018
26	1	0	-3.476100	2.451686	0.213395
27	1	0	-4.415530	-2.150483	0.114014
28	6	0	0.178048	-2.287340	-0.488822
29	1	0	0.842428	-2.374163	0.376387
30	1	0	-0.106698	-3.300056	-0.791512
31	1	0	0.772882	-1.851548	-1.296255

Zero-point correction=	0.256857
Thermal correction to Energy=	0.269899
Thermal correction to Enthalpy=	0.270843
Thermal correction to Gibbs Free Energy=	0.216809
Sum of electronic and zero-point Energies=	-655.996592
Sum of electronic and thermal Energies=	-655.983551
Sum of electronic and thermal Enthalpies=	-655.982607
Sum of electronic and thermal Free Energies=	-656.036641

4-(8-Methylnaphthalen-1-yl)benzonitrile (4d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.084600	0.585677	1.042134
2	6	0	1.718803	0.844817	1.104078
3	6	0	0.864417	0.490472	0.047580
4	6	0	1.424835	-0.110777	-1.092106
5	6	0	2.788117	-0.371226	-1.169357
6	6	0	3.629687	-0.028291	-0.097048
7	1	0	3.733796	0.855109	1.869168
8	1	0	1.301516	1.319664	1.987305
9	1	0	0.780803	-0.364826	-1.929063
10	1	0	3.211012	-0.831444	-2.056752
11	6	0	5.035869	-0.297272	-0.169193
12	7	0	6.177139	-0.516400	-0.227591
13	6	0	-0.583331	0.862669	0.078061
14	6	0	-1.679473	-0.075040	0.051123
15	6	0	-0.837325	2.226078	0.038242
16	6	0	-1.566041	-1.500871	0.242873
17	6	0	-3.001904	0.472583	-0.137639
18	6	0	-2.141232	2.744514	-0.091397
19	1	0	0.005242	2.911772	0.059738
20	6	0	-2.705050	-2.281711	0.138800
21	6	0	-4.128419	-0.385729	-0.238021
22	6	0	-3.198057	1.877123	-0.205814
23	1	0	-2.294778	3.819190	-0.129727
24	6	0	-3.982164	-1.744136	-0.122668
25	1	0	-2.611585	-3.354595	0.287888
26	1	0	-5.107339	0.059846	-0.396363
27	1	0	-4.210268	2.250347	-0.341015
28	1	0	-4.841383	-2.404811	-0.198254
29	6	0	-0.283290	-2.211884	0.622758
30	1	0	0.413559	-2.315080	-0.215108
31	1	0	0.256834	-1.693280	1.419990
32	1	0	-0.517631	-3.219069	0.980895

Zero-point correction=	0.255431
Thermal correction to Energy=	0.270290
Thermal correction to Enthalpy=	0.271234
Thermal correction to Gibbs Free Energy=	0.212841
Sum of electronic and zero-point Energies=	-748.241799
Sum of electronic and thermal Energies=	-748.226941
Sum of electronic and thermal Enthalpies=	-748.225997
Sum of electronic and thermal Free Energies=	-748.284389

1-(4-Fluorophenyl)-8-methylnaphthalene (4e)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.671036	-0.109317	1.142975
2	6	0	-1.113293	0.442249	-0.021460
3	6	0	-1.964543	0.709014	-1.104331
4	6	0	-3.326632	0.410398	-1.045591
5	6	0	-3.836456	-0.148872	0.119316
6	6	0	-3.029839	-0.411291	1.221082
7	1	0	-1.031508	-0.297736	2.000907
8	1	0	-1.552045	1.147694	-2.008624
9	1	0	-3.989246	0.605907	-1.882470
10	1	0	-3.468810	-0.834802	2.118693
11	6	0	0.326611	0.852031	-0.058214
12	6	0	1.446377	-0.058024	-0.046819
13	6	0	0.550867	2.220648	-0.028495
14	6	0	1.363434	-1.490583	-0.209242
15	6	0	2.760401	0.522653	0.102127
16	6	0	1.844437	2.772011	0.064373
17	1	0	-0.309013	2.884807	-0.037541
18	6	0	2.523884	-2.241590	-0.126588
19	6	0	3.910254	-0.306831	0.182112
20	6	0	2.925167	1.931769	0.154002
21	1	0	1.972789	3.850538	0.092093
22	6	0	3.794877	-1.669544	0.088091
23	1	0	2.452116	-3.319151	-0.252776
24	1	0	4.881613	0.164714	0.309703
25	1	0	3.931683	2.329838	0.258285
26	1	0	4.671941	-2.308169	0.148738
27	6	0	0.087826	-2.243000	-0.529013
28	1	0	-0.592200	-2.313570	0.325622
29	1	0	-0.476588	-1.774758	-1.340185
30	1	0	0.335375	-3.263003	-0.839422
31	9	0	-5.153347	-0.440294	0.186780

Zero-point correction=	0.248640
Thermal correction to Energy=	0.262521
Thermal correction to Enthalpy=	0.263465
Thermal correction to Gibbs Free Energy=	0.207356
Sum of electronic and zero-point Energies=	-755.238052
Sum of electronic and thermal Energies=	-755.224172
Sum of electronic and thermal Enthalpies=	-755.223227
Sum of electronic and thermal Free Energies=	-755.279337

1-(2-Fluorophenyl)-8-methylnaphthalene (4f)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.028505	-0.239575	0.914780
2	6	0	-1.395268	0.384342	-0.163447
3	6	0	-2.200232	0.697778	-1.269639
4	6	0	-3.558426	0.376384	-1.299518
5	6	0	-4.148651	-0.256672	-0.204602
6	6	0	-3.377699	-0.567846	0.916266
7	1	0	-1.739543	1.195628	-2.118445
8	1	0	-4.152947	0.623823	-2.174216
9	1	0	-3.802415	-1.052932	1.789273
10	6	0	0.030919	0.835576	-0.090125
11	6	0	1.190392	-0.022297	-0.124694
12	6	0	0.189743	2.208437	0.029810
13	6	0	1.174019	-1.451665	-0.323305
14	6	0	2.477622	0.615755	0.024902
15	6	0	1.455205	2.815123	0.153509
16	1	0	-0.700355	2.830736	0.053321
17	6	0	2.373747	-2.142927	-0.322255
18	6	0	3.670581	-0.154454	0.022872
19	6	0	2.575987	2.025161	0.163573
20	1	0	1.531211	3.894331	0.252764
21	6	0	3.622491	-1.514363	-0.140290
22	1	0	2.349484	-3.219014	-0.475542
23	1	0	4.619822	0.361078	0.146651
24	1	0	3.564740	2.464445	0.272308
25	1	0	4.532754	-2.107790	-0.144814
26	6	0	-0.079394	-2.269084	-0.552365
27	1	0	-0.680227	-2.355728	0.358123
28	1	0	-0.722390	-1.848624	-1.330021
29	1	0	0.196171	-3.282744	-0.859550
30	9	0	-1.291789	-0.559247	2.003892
31	1	0	-5.205389	-0.508024	-0.217704

Zero-point correction=	0.248754
Thermal correction to Energy=	0.262611
Thermal correction to Enthalpy=	0.263555
Thermal correction to Gibbs Free Energy=	0.207603
Sum of electronic and zero-point Energies=	-755.238158
Sum of electronic and thermal Energies=	-755.224301
Sum of electronic and thermal Enthalpies=	-755.223357
Sum of electronic and thermal Free Energies=	-755.279309

4-(8-methylnaphthalen-1-yl)aniline (4j)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.957643	0.746245	-1.086576
2	6	0	-3.316624	0.447904	-1.025693
3	6	0	-3.867645	-0.147869	0.120325
4	6	0	-3.012343	-0.425851	1.200469
5	6	0	-1.655409	-0.127985	1.125697
6	6	0	-1.093323	0.451695	-0.022145
7	1	0	-1.555221	1.210123	-1.983605
8	1	0	-3.959229	0.674406	-1.874017
9	1	0	-3.419026	-0.875479	2.104049
10	1	0	-1.017230	-0.340368	1.979834
11	7	0	-5.219207	-0.505189	0.165187
12	1	0	-5.609126	-0.575147	1.097248
13	1	0	-5.821354	0.034850	-0.444257
14	6	0	0.346019	0.857549	-0.056519
15	6	0	1.462566	-0.057700	-0.047273
16	6	0	0.581433	2.224717	-0.024269
17	6	0	1.372184	-1.488550	-0.223181
18	6	0	2.779852	0.513334	0.111371
19	6	0	1.878181	2.767735	0.072415
20	1	0	-0.274601	2.893873	-0.031960
21	6	0	2.527154	-2.247820	-0.136845
22	6	0	3.923669	-0.324283	0.195405
23	6	0	2.953768	1.921166	0.167010
24	1	0	2.013388	3.845591	0.102327
25	6	0	3.800012	-1.685692	0.092848
26	1	0	2.449605	-3.323794	-0.273588
27	1	0	4.897321	0.140184	0.332233
28	1	0	3.962282	2.312746	0.277494
29	1	0	4.672528	-2.330474	0.156371
30	6	0	0.095780	-2.229723	-0.565716
31	1	0	0.342182	-3.245286	-0.892146
32	1	0	-0.592192	-2.310710	0.281295
33	1	0	-0.460663	-1.743428	-1.371527

Zero-point correction=	0.273468
Thermal correction to Energy=	0.287969
Thermal correction to Enthalpy=	0.288913
Thermal correction to Gibbs Free Energy=	0.231923
Sum of electronic and zero-point Energies=	-711.333211
Sum of electronic and thermal Energies=	-711.318710
Sum of electronic and thermal Enthalpies=	-711.317766
Sum of electronic and thermal Free Energies=	-711.374756