Organocatalyzed straightforward synthesis of highly fluorescent 3,5-disubstituted 2,6-dicyanoanilines via domino annulation of α-enolicdithioesters with malononitrile

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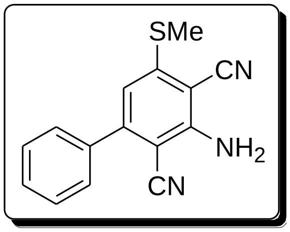
1. Experimental Section

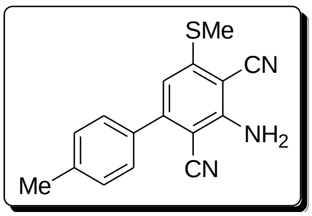
General. Malononitrile purchased from Sigma-Aldrich was used as such without any further purification. α-Enolicdithioesters (Table 2, entries 1-18) were prepared following the known procedure. Thin-layer chromatography (TLC) was performed using silica gel 60 F_{254} precoated plates. Infrared (IR) spectra are measured using KBr, and wavelengths (ν) are reported in cm^{-1}. ^{1}H and ^{13}C NMR spectra were recorded on NMR spectrometer operating at 400, 300, 125, 100, and 75.5 MHz. Chemical shifts (δ) are given in parts per million (ppm) using the residue solvent peaks as reference relative to TMS. '*J*' values are given in Hertz (Hz). High resolution mass spectra (HRMS) were recorded using electrospray ionization (ESI) mass spectrometry. The melting points are uncorrected.

General procedure for the synthesis of the 2,6-dicyanoanilines (3a-r). To a mixture of α-enolicdithioesters (1.0 equiv.) and malononitrile (2.0 equiv.) in ethanol (3 mL), piperidine (0.2 equiv.) was added and the reaction mixture was refluxed for the stipulated period of time (Table 2). After completion of the reaction (monitored by TLC), the ethanol was evaporated and the water (20 mL) was added to the reaction mixture followed by extraction with dichloromethane (2 × 10 mL). The combined organic layer was dried over anhyd. Na_2SO_4 and then evaporated under vacuo. The crude residue was purified by column chromatography over silica gel using ethyl acetate/hexane (1:10) as eluent to afford pure dicyanoaniline derivatives.

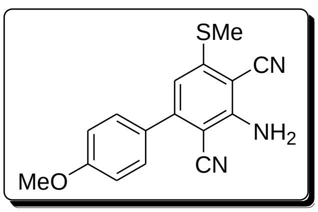
2. Characterisation data of the isolated compounds



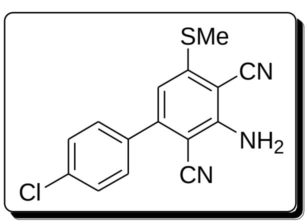
2,6-dicyano-3-phenyl-5-thiomethylaniline (3a). White solid (96% yield), mp 242-243 °C. IR (KBr, cm^{-1}): ν_{max} = 3394, 3343, 3247, 2921, 2852, 2216, 1655, 1544, 1430, 1284, 699. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.50 (m, 5H), 6.56 (s, 1H), 5.24 (br, 2H), 2.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.5, 151.0, 149.8, 137.4, 129.7, 128.9, 128.2, 116.1, 115.9, 114.2, 93.1, 92.5, 15.0.



2,6-dicyano-3-(4'-methylphenyl)-5-thiomethylaniline (3b). White solide (89% yield), mp 210 °C. IR (KBr, cm^{-1}): ν_{max} = 3463, 3371, 3227, 2927, 2212, 1635, 1563, 802. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (d, J = 8 HZ, 2H), 7.33 (d, J = 8 Hz, 2H), 6.56 (s, 1H), 5.25 (br, 2H), 2.58(s, 3H), 2.44(s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.6, 150.8, 149.9, 140.0, 134.6, 129.5, 128.1, 116.1, 114.3, 114.1, 92.8, 92.4, 21.3, 14.9.

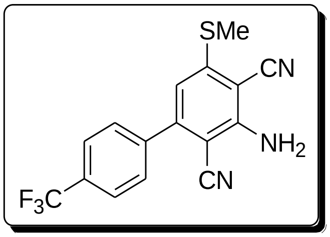


2,6-dicyano-3-(4'-methoxyphenyl)-5-thiomethylaniline (3c). White solid (90% yield), mp 209-210 °C. IR (KBr, cm^{-1}): ν_{max} = 3455, 3335, 3235, 2223, 1644, 1567, 1515, 1281, 1255, 1179, 1028, 826. ^{1}H NMR (300 MHz, CDCl3): δ 7.50 (d, J = 9 Hz, 2H), 7.02 (d, J = 9 Hz, 2H), 6.53 (s, 1H), 5.21 (br, 2H), 3.87 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (75 MHz, CDCl3): δ 160.6, 152.8, 150.4, 149.4, 129.6, 129.5, 116.0, 114.2, 114.1, 113.7, 92.5, 92.1, 55.2, 14.8. HRMS (ESI): calcd for $C_{16}H_{13}N_3OS$ $[M+Na]^+$ 318.0671, found 318.0670.

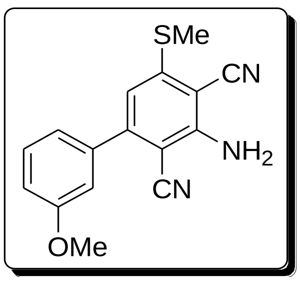


2,6-dicyano-3-(4'-chlorophenyl)-5-thiomethylaniline (3d). White solid (85% yield), mp 245-246 °C. IR (KBr, cm^{-1}): ν_{max} = 3432, 3352, 3259, 2925, 2222, 1647, 1543, 1015, 814. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.54-7.43 (m, 4H), 6.51 (s, 1H), 5.25 (br, 2H), 2.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.5, 151.3, 148.5, 142.5, 136.1, 129.6, 129.2, 117.0, 115.7, 113.9, 93.4, 92.3, 15.0. HRMS (ESI): calcd for $C_{15}H_{10}ClN_3S$ $[M+H]^+$ 300.0356, found 300.0373.

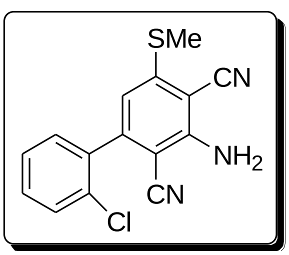
2,6-dicyano-3-(4'-trifluoromethylphenyl)-5-thiomethylaniline(3e). White solid (84% yield), mp 215-216 °C. IR (KBr, cm^{-1}): ν_{max} = 3479, 3348, 3244, 2926, 2223, 1643, 1562, 1545, 1328, 1164. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.78 (d, J = 8.1 Hz, 2H), 7.65 (d, J = 8.1 Hz, 2H), 6.53 (s, 1H), 5.28 (br, 2H), 2.57 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.7, 151.1, 147.7, 140.7, 131.0 (q, J = 32.5 Hz, ArC-CF_3), 128.4, 125.2, 121.5 (q, J = 269.5Hz, CF_3) 115.3, 113.8, 112.8, 92.9, 91.5, 14.4. HRMS (ESI): calcd for $C_{16}H_{10}F_3N_3S$ $[M+NH_4]^+$ 351.0885, found 351.0899.



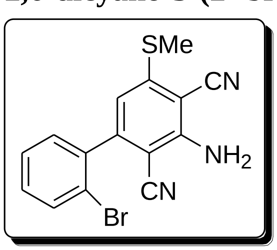
2,6-dicyano-3-(3'-methoxyphenyl)-5-thiomethylaniline (3f). White solid (90% yield), mp 200-201 °C. IR (KBr, cm^{-1}): ν_{max} = 3462, 3359, 3239, 3084, 2938, 2214, 1636, 1562, 1455, 1292, 1238, 1057, 885, 791. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.43-7.38 (m, 1H), 7.10-7.01 (m, 3H), 6.56 (s, 1H), 5.23 (br, 2H), 3.86 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.7, 152.5, 151.0, 149.6, 138.7, 130.0, 120.5, 115.9, 115.2, 114.2 114.1, 114.0, 93.1, 92.5, 55.4, 15.0. HRMS (ESI): calcd for $C_{16}H_{13}N_3OS$ $[M+NH_4]^+$ 313.1117, found 313.1126.



2,6-dicyano-3-(2'-chlorophenyl)-5-thiomethylaniline (3g). White solid (90% yield), mp 179-180 °C. IR (KBr, cm^{-1}): ν_{max} = 3471, 3357, 3238, 2923, 2214, 1632, 1563, 1544, 1480, 1288, 960, 762. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.54-7.51 (m, 1H), 7.42-7.26 (m, 3H), 6.51 (s, 1H), 5.22 (br, 2H), 2.54 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.0, 150.8, 147.2, 136.3, 132.4, 130.6, 130.3, 130.2, 127.0, 114.9, 114.8, 113.8, 96.1, 93.8, 14.9.

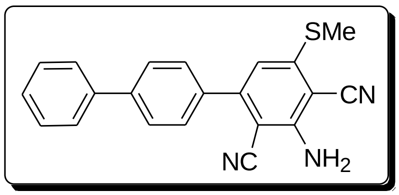


2,6-dicyano-3-(2'-bromophenyl)-5-thiomethylaniline(3h). White solid (88% yield), mp 173 °C. IR (KBr, cm^{-1}): ν_{max} = 3466, 3357, 3239, 2922, 2212, 1632, 1545, 1287, 766. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.72 (d, J = 7.8 Hz, 1H), 7.45-7.29 (m, 3H), 6.48 (s, 1H), 5.29 (br, 2H), 2.53 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.0, 150.9 148.8, 138.2, 133.3, 130.8, 130.2, 127.6,

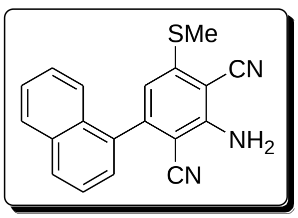


121.9, 115.0, 114.7, 114.0, 93.9, 93.5, 14.9.

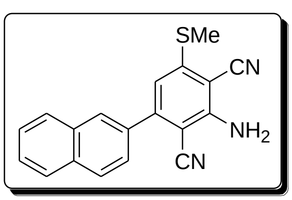
3-Biphenyl-2,6-dicyano-5-thiomethylaniline (3i). White solid (92% yield), mp 179-180 °C. IR (KBr, cm^{-1}): ν_{max} = 3467, 3358, 3239, 3058, 2922, 2212, 1631, 1287, 766. ^1H NMR (300 MHz, $CDCl_3$): δ 7.72-7.70 (m, 2H), 7.64-7.60 (m, 1H), 7.49 – 7.40 (m, 2H), 7.35-7.29 (m, 4H), 6.49 (s, 1H), 5.24 (br, 2H), 2.54 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 151.9, 151.0, 148.8, 138.2, 133.3, 130.8, 130.2, 128.9, 127.6, 127.1, 121.9, 115.0, 114.8, 114.0, 94.0, 93.5, 14.9.



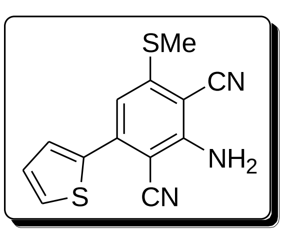
2,6-dicyano-3-(1'-naphthyl)-5-thiomethylaniline (3j). White solid (93% yield), mp 156-157 °C. IR (KBr, cm^{-1}): ν_{max} = 3452, 3334, 3236, 2224, 2210, 1645, 1564, 1548, 1289, 815, 743. ^1H NMR (300 MHz, $CDCl_3$): δ 7.97-7.92 (m, 2H), 7.57-7.45 (m, 5H), 6.61 (s, 1H), 5.25 (br, 2H), 2.49 (s, 3H), ^{13}C NMR (100 MHz, DMSO): δ 153.5, 151.6, 149.4, 136.0, 133.5, 130.7, 129.7, 128.8, 127.4, 127.2, 126.8, 125.8, 125.3, 116.0, 114.9, 114.3, 94.1, 92.2 14.5. HRMS (ESI): calcd for $C_{19}H_{13}N_3S$ $[M+Na]^+$ 338.0722, found 338.0731.



2,6-dicyano-3-(2'-naphthyl)-5-thiomethylaniline(3k). White solid (92% yield), mp 240-241 °C. IR (KBr, cm^{-1}): ν_{max} = 3453, 3335, 2225, 2205, 1643, 1562, 1126. ^1H NMR (300 MHz, $CDCl_3$): δ 7.99-7.89 (m, J = 7.42 Hz, 4H), 7.60-7.53 (m, 3H), 6.65 (s, 1H), 5.25 (br, 2H), 2.57 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.6, 151.0, 149.8, 134.7, 133.5, 132.9, 128.7, 128.4, 128.0, 127.7, 127.3, 126.9, 125.4, 116.0, 114.4, 112.4, 92.9, 92.6, 15.0. HRMS (ESI): calcd for $C_{19}H_{13}N_3S$ $[M+Na]^+$ 338.0722, found 338.0726.

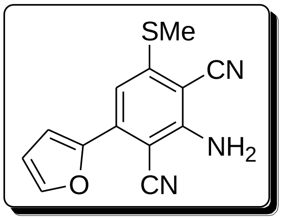


2,6-dicyano-3-(2'-thienyl)-5-thiomethylaniline(3l). White solid (80% yield), mp 225-226 °C. IR (KBr, cm^{-1}): ν_{max} = 3461, 3370, 3101, 2930, 2211, 1420, 1624, 1556, 1290, 817, 725. ^1H NMR (300 MHz, $CDCl_3$): δ 7.69 (d, J = 3.3 Hz, 1H), 7.51 (d, J = 5.1 Hz, 1H), 7.19 (dd, J = 4.8, 3.75 Hz, 1H), 6.67 (s, 1H), 5.24 (br, 2H), 2.59 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.8, 151.1,

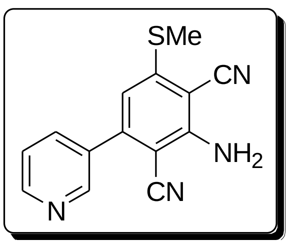


141.5, 138.5, 128.8, 128.6, 128.5, 116.2, 114.2, 113.5, 92.8, 90.8, 14.9. HRMS (ESI): calcd for $C_{13}H_9N_3S_2$ $[M+H]^+$ 272.0311, found 272.0312.

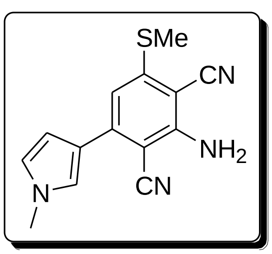
2,6-dicyano-3-(2'-furyl)-5-thiomethylaniline(3m). White solid (86% yield), mp 250-252 °C. IR (KBr, cm^{-1}): ν_{max} = 3411, 3345, 3248, 2924, 2853, 2212, 1651, 1578, 1551, 1485, 1462, 1296, 1029, 965, 885, 748. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.60 (d, J = 1.2 Hz, 1H), 7.45 (dd, J = 3.6, 3.3 Hz, 1H), 7.02 (d, J = 2.7 Hz, 1H), 6.60 (s, 1H), 5.21 (br, 2H), 2.62 (s, 3H). ^{13}C NMR (100 MHz, DMSO): δ 154.3, 151.7, 149.0, 146.0, 136.6, 116.8, 113.6, 114.9, 113.6, 113.3, 108.8, 94.8, 91.3, 14.4.



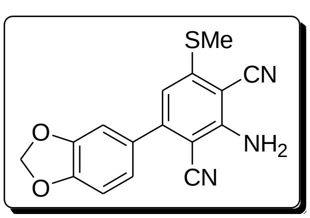
2,6-dicyano-3-(3'-pyridyl)-5-thiomethylaniline(3n). White solid (90% yield), mp 262-263 °C. IR (KBr, cm^{-1}): ν_{max} = 3386, 3257, 3138, 2924, 2854, 2215, 1668, 1591, 1551, 1412, 1102, 1028, 806, 711. ^{1}H NMR (300 MHz, DMSO): δ 8.77 (s, 1H), 8.69 (d, J = 4.8 Hz, 1H), 8.04 (d, J = 7.8 Hz, 1H)), 7.57-7.53 (m, 1H), 6.83 (br, NH_2, 2H), 6.64 (s, 1H), 2.61 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.8, 151.2, 150.0, 148.2, 145.7, 135.3, 133.1, 122.9, 115.3, 113.7, 112.7, 93.4, 91.6, 14.4. HRMS (ESI): calcd for $C_{14}H_{10}N_4S$ $[M+H]^+$ 267.0699, found 267.0700.



2,6-dicyano-3-(3'-N-methylpyrrolo)-5-thiomethylaniline (3o). White solid (70% yield), mp 231-232 °C. IR (KBr, cm^{-1}): ν_{max} = 3450, 3352, 3245, 2928, 2199, 1645, 1568, 1539. ^{1}H NMR (300 MHz, DMSO): δ 7.47 (s, 1H), 6.85 (s, 1H), 6.61 (br, NH_2, 1H), 6.47 (s, 2H), 3.62 (s, 3H), 2.59 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.9, 144.9, 143.7, 123.8, 123.2, 122.6, 120.5, 117.4, 112.2, 108.4, 95.3, 94.4, 36.6, 15.0.

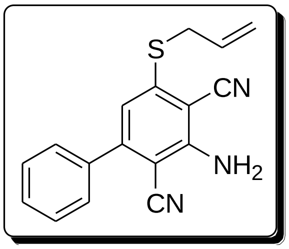


2,6-dicyano-3-(3',4'-methylenedioxyphenyl)-5-thiomethylaniline(3p). White solid (83% yield), mp 238-239 °C. IR (KBr, cm^{-1}): ν_{max} = 3449, 3358, 3254, 2929, 2222, 2209, 1655, 1503, 1564, 1459, 1291, 1247, 1037, 823. ^{1}H NMR



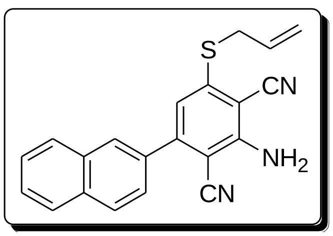
(300 MHz, CDCl3): δ 7.01-6.90 (m, 3H), 6.51 (s, 1H), 6.05 (s, 2H), 5.21 (br, 2H), 2.56 (s, 3H). 13C NMR (75 MHz, CDCl3): δ 153.2, 150.6, 149.0, 148.1, 147.3, 131.1, 122.7, 122.6, 122.4, 115.9, 114.2, 101.3, 94.5, 93.9, 91.3, 13.8.

2,6-dicyano-3-phenyl-5-thioallylaniline (3q). White solid (85% yield), mp 238-239 °C. IR



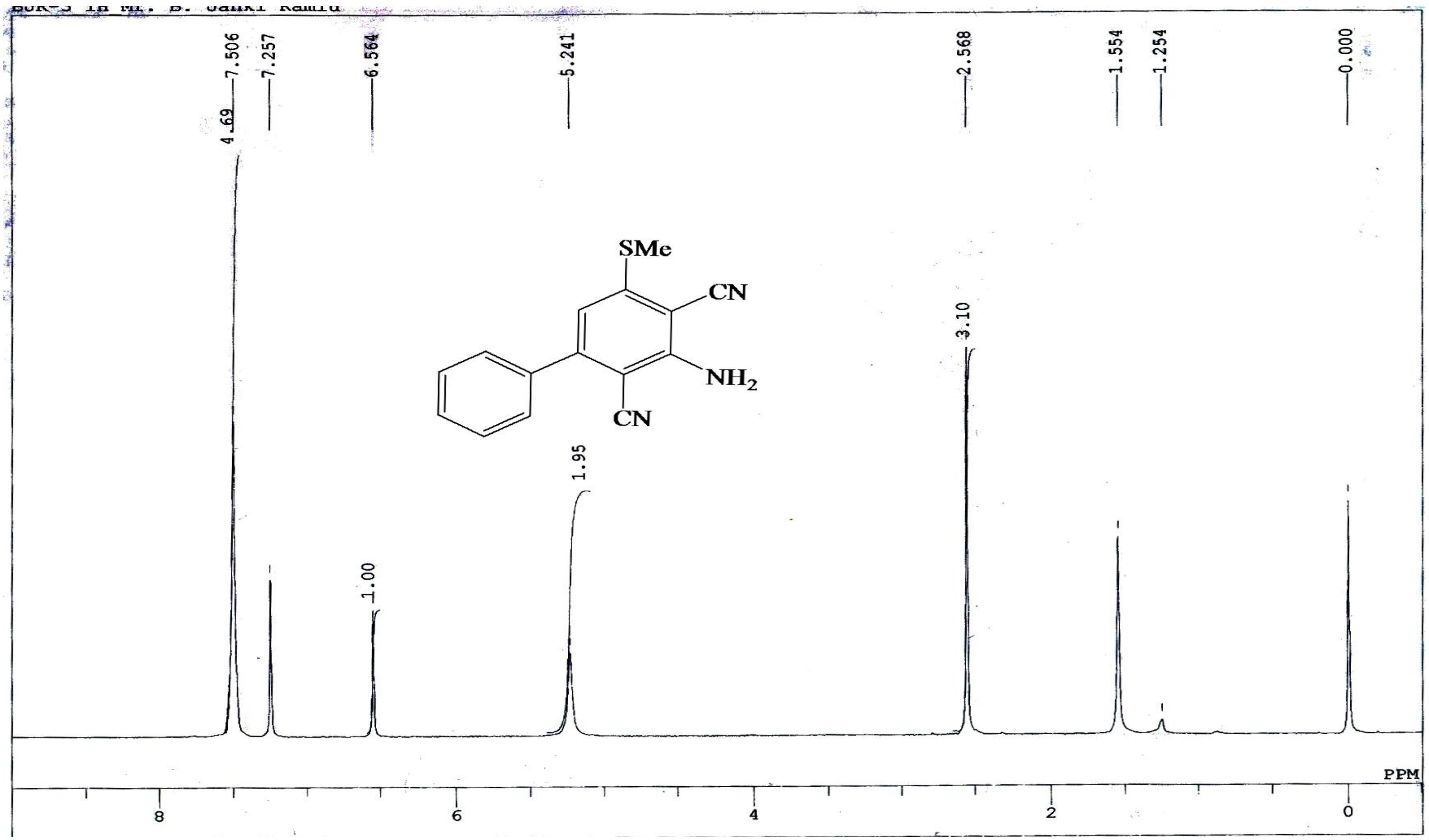
(KBr, cm^{-1}): ν_{max} = 3477, 3362, 3232, 2952, 2212, 1639, 1560, 692. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.48 (m, 5H), 6.65 (s, 1H), 5.91-5.82 (m, 1H), 5.33-5.21 (m, NH_2, $=CH_2$, 4H), 3.70 (d, J = 6.6, 2H), ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.7, 149.5, 148.7, 137.3, 131.4, 129.7, 128.9, 128.2, 119.6, 116.4, 115.9, 114.3, 94.3, 92.9, 35.3. . HRMS (ESI): calcd for $C_{17}H_{13}N_3S$ $[M+H]^+$ 292.0903, found 292.0903.

2,6-dicyano-3-(2'-naphthyl)-5-thioallylaniline (3r). White solid (87% yield), mp 187-189 °C.

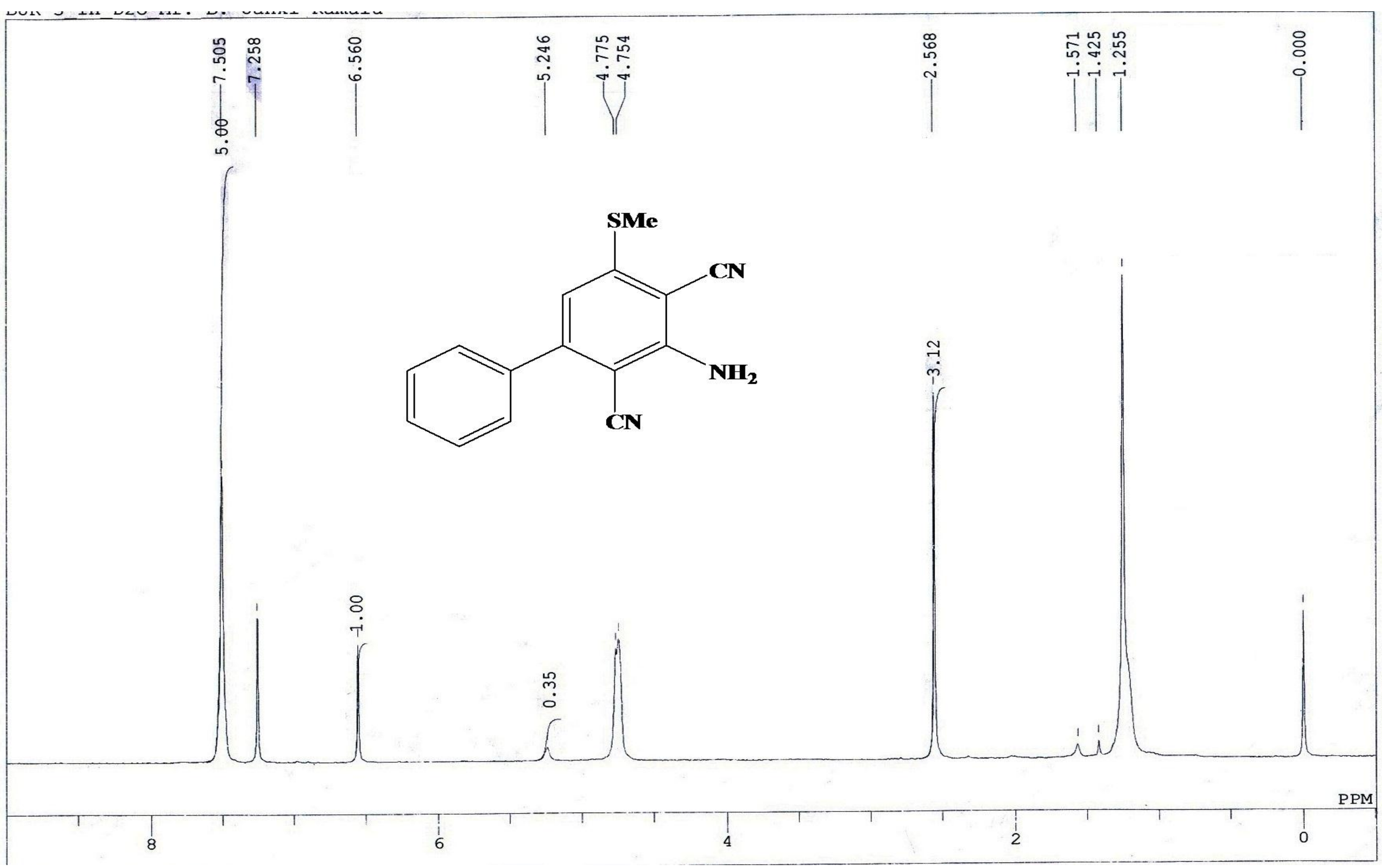


IR (KBr, cm^{-1}): ν_{max} = 3458, 3424, 3354, 3249, 3056, 2210, 1650, 1563, 1542, 813. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.98 – 7.90 (m, 4H), 7.58 (d, J = 6.3, 3H), 6.75 (s, 1H), 5.96 – 5.84 (m, 1H), 5.35 – 5.23 (m, NH_2, $=CH_2$, 4H), 3.73 (d, J = 6.6, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.8, 149.5, 148.6, 134.7, 133.6, 133.0, 131.6, 128.7, 128.5, 128.1, 127.7, 127.3, 126.9, 125.3, 119.5, 117.0, 115.8, 114.3, 94.7, 93.3, 35.5.

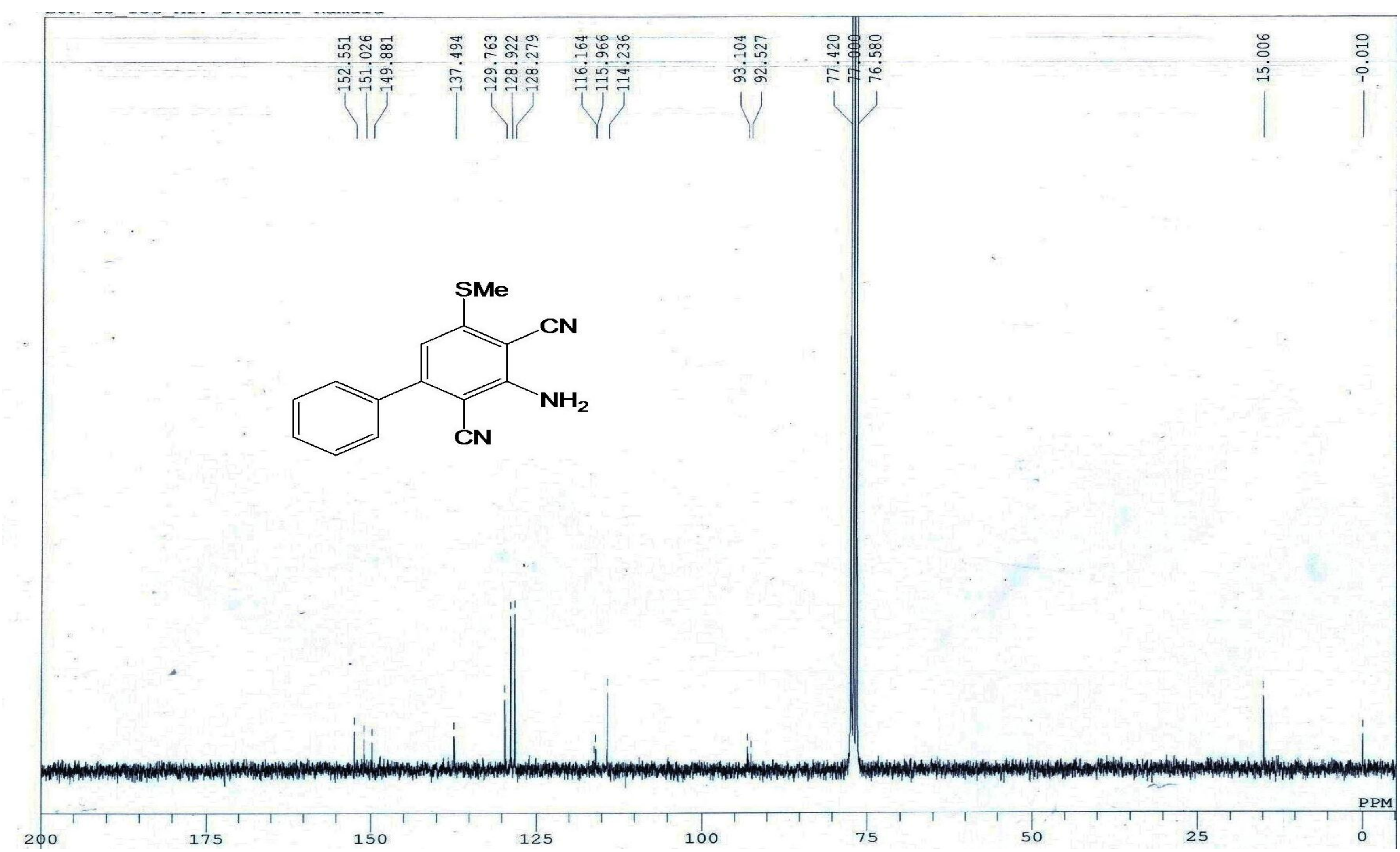
^{1}H NMR SPECTRUM OF 3a



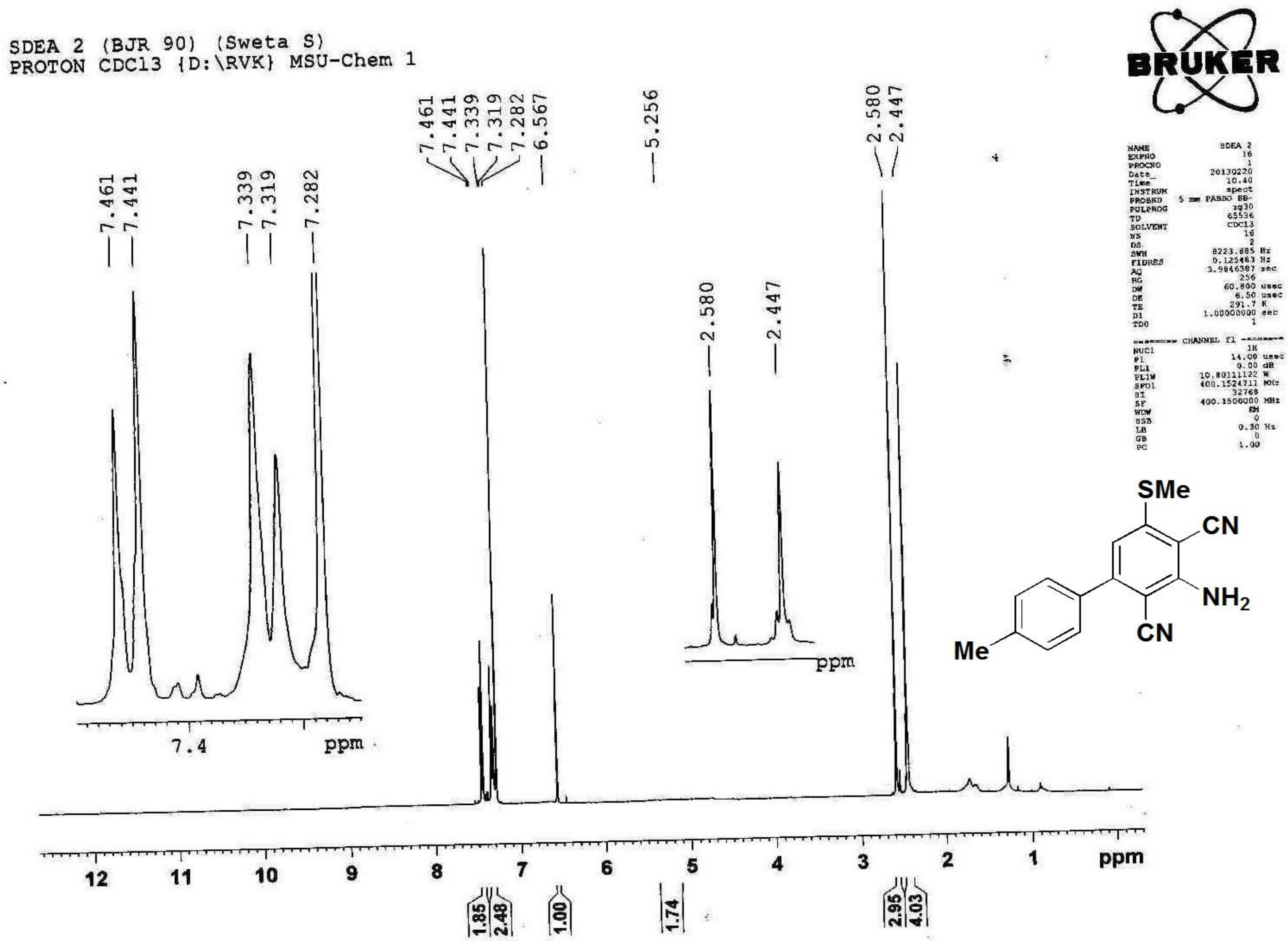
D_2O EXACHANGE NMR SPECTRUM OF 3a



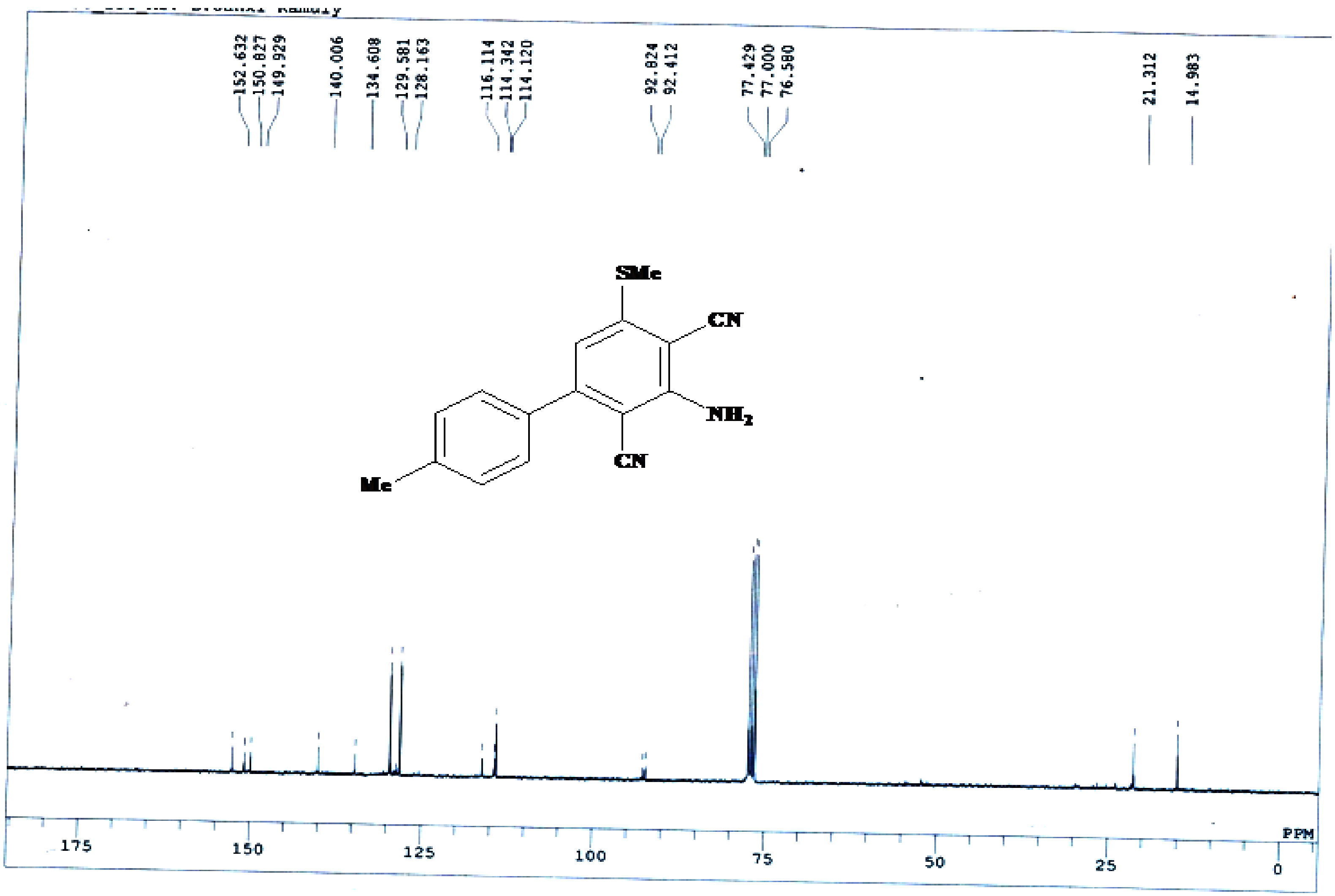
^{13}C NMR SPECTRUM OF 3a



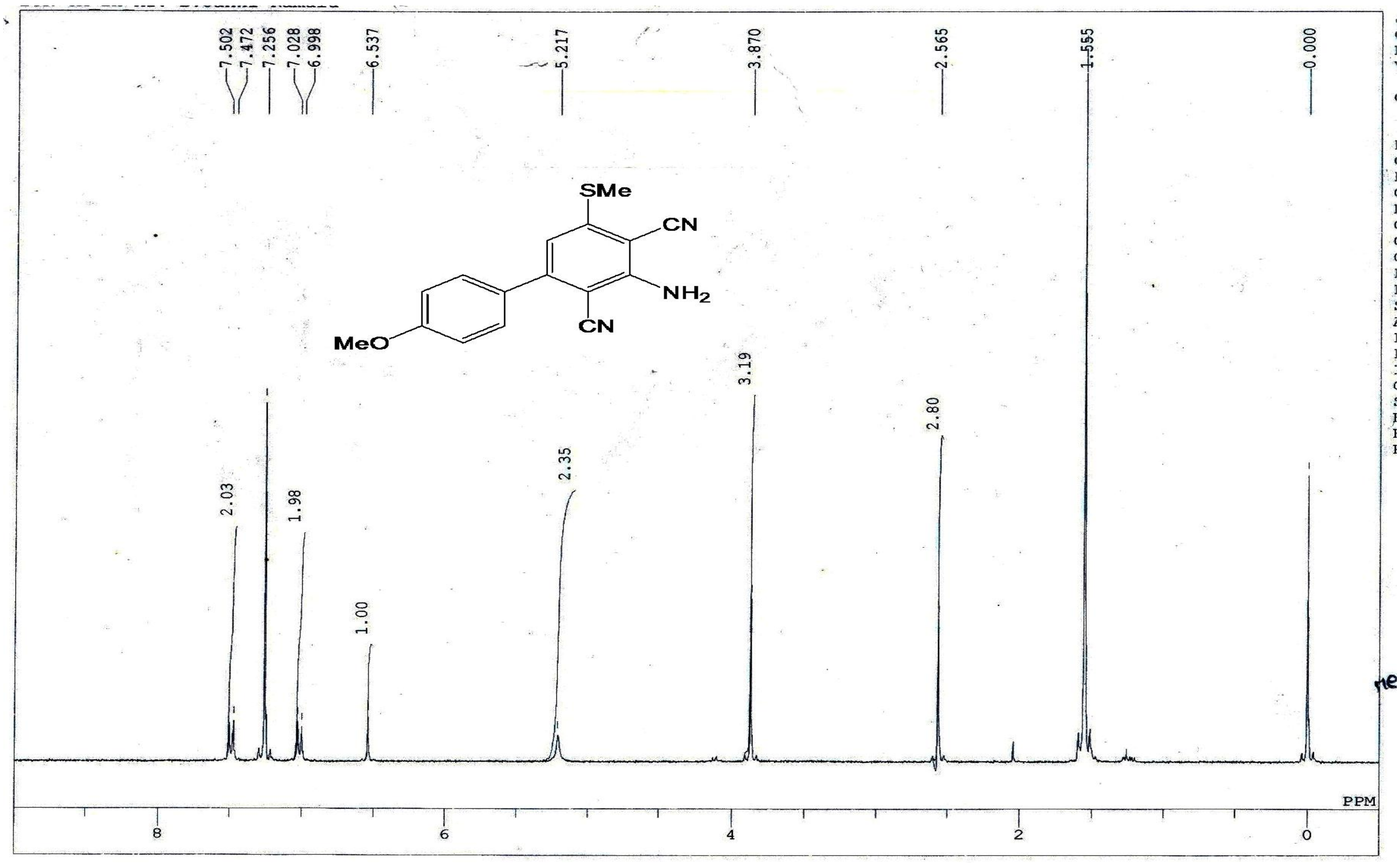
^{1}H NMR SPECTRUM OF 3b



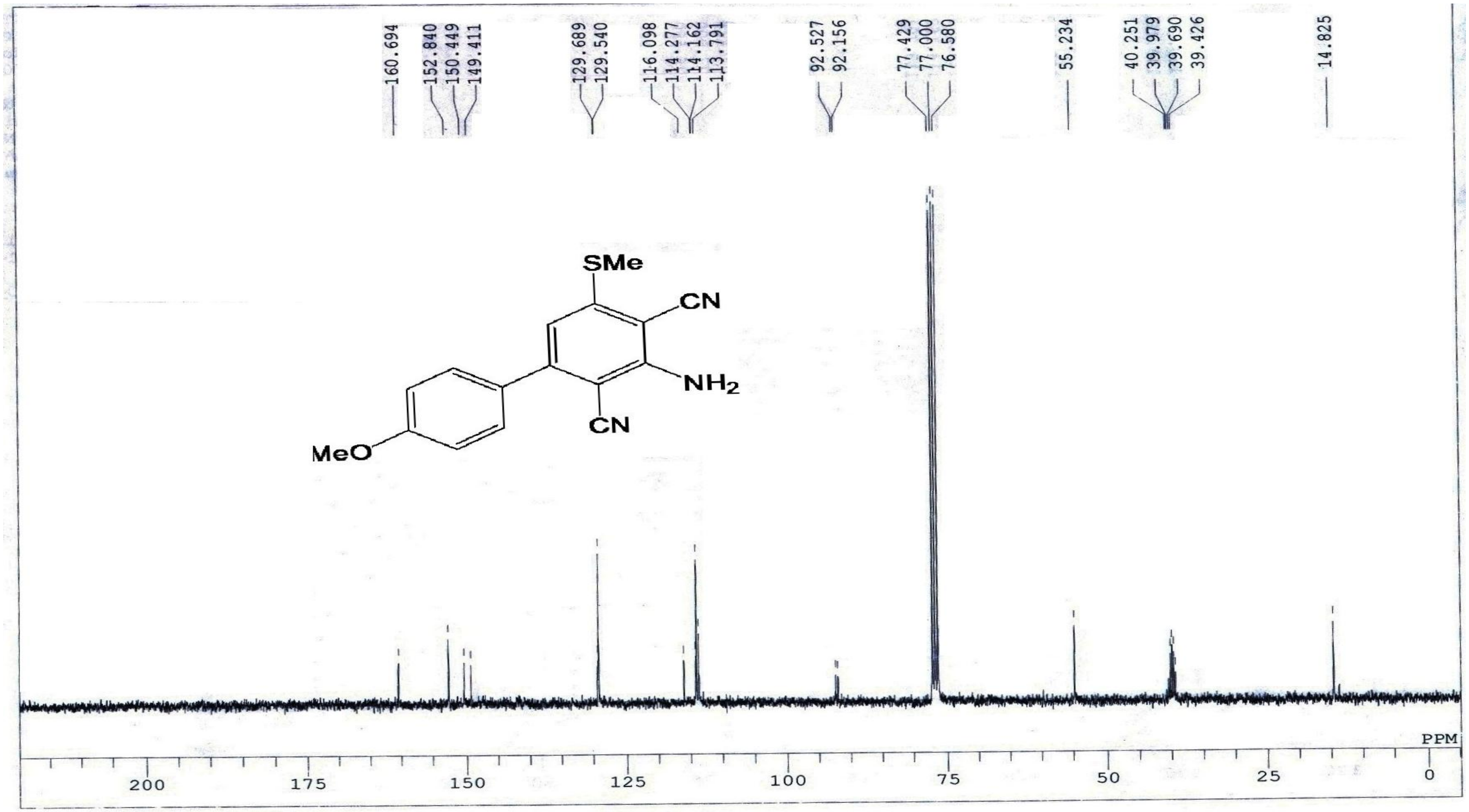
[13]C NMR SPECTRUM OF 3b



[1]H NMR SPECTRUM OF 3c

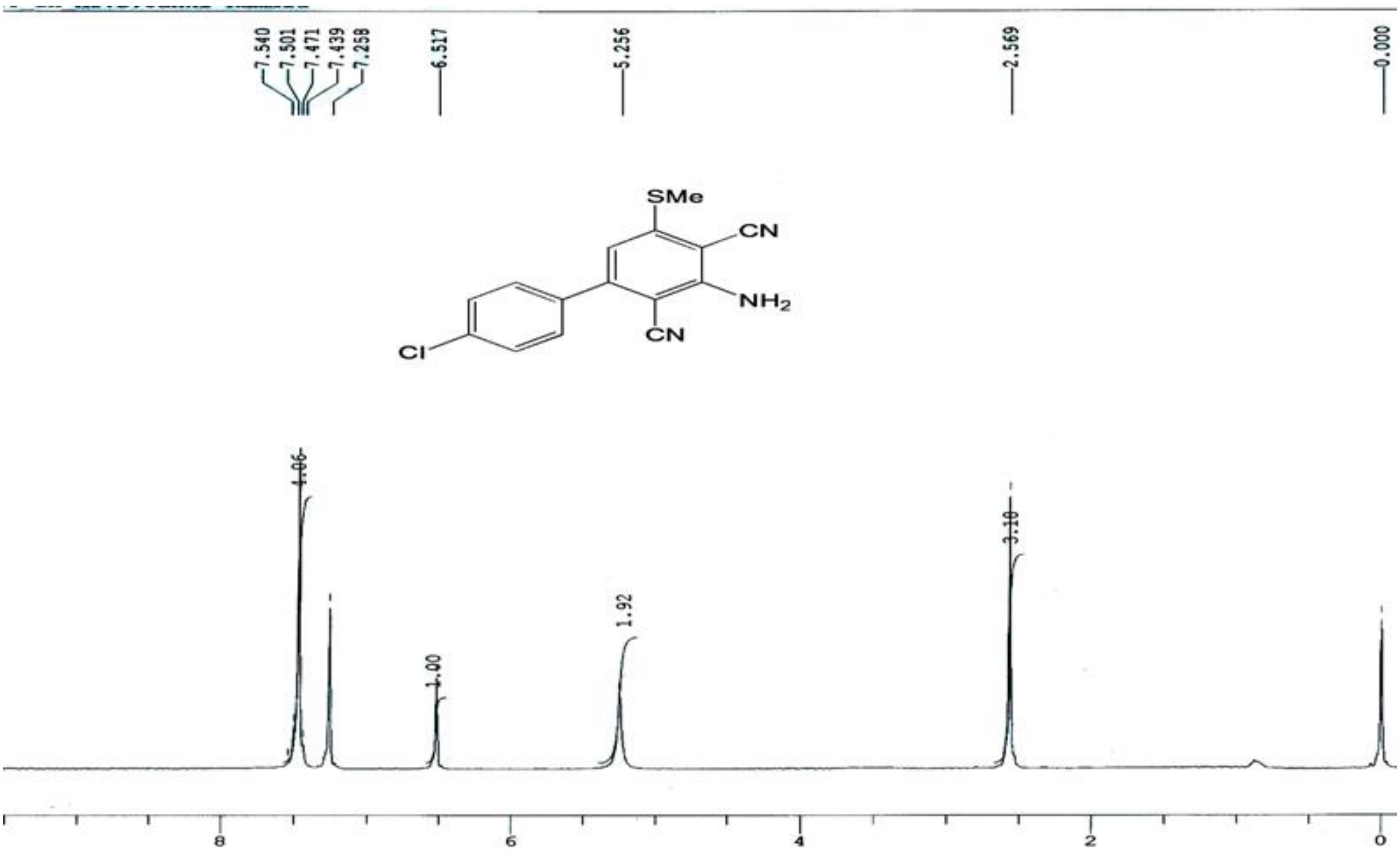


^{13}C NMR SPECTRUM OF 3c

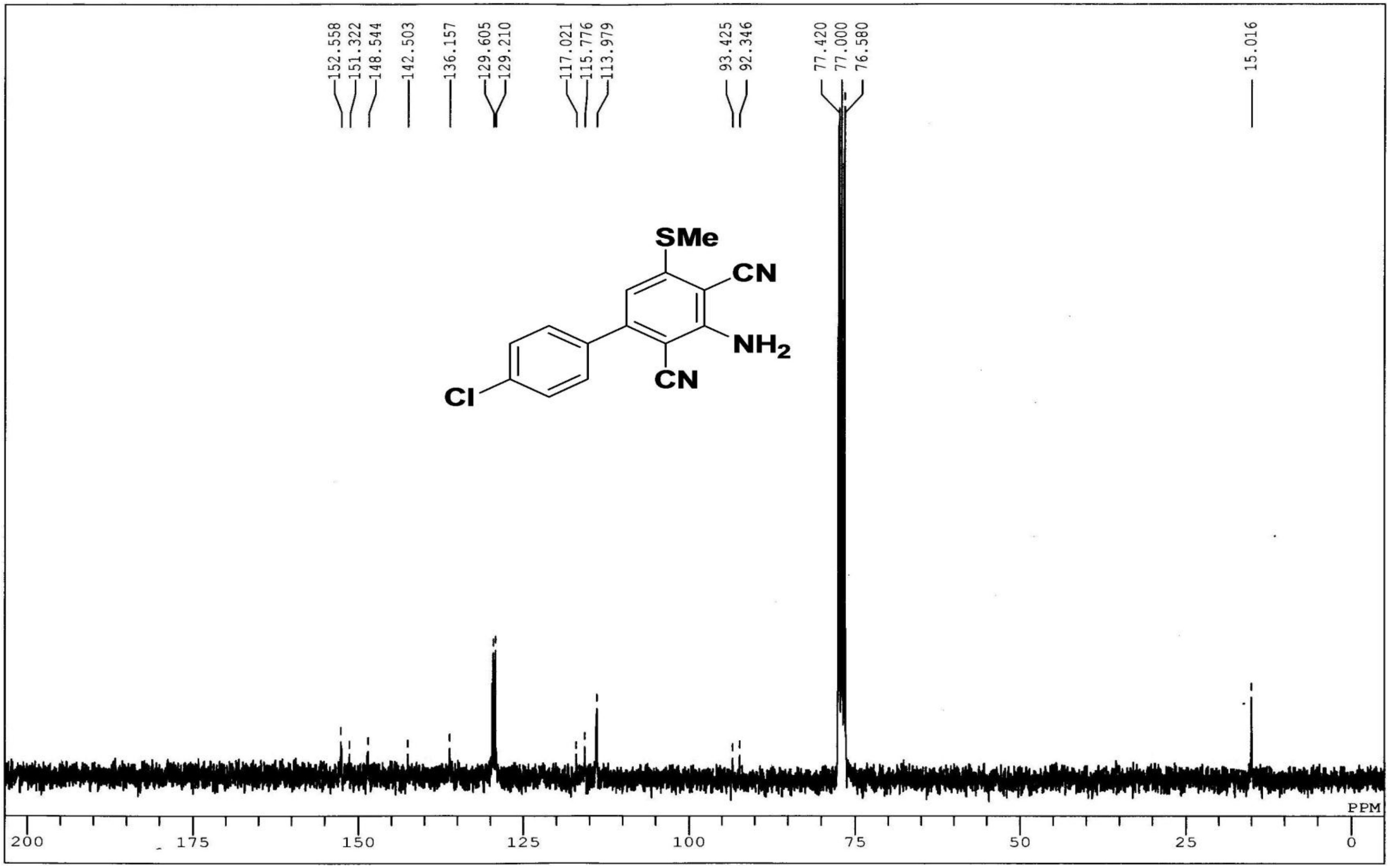


Electronic Supplementary Material (ESI) for RSC Advances

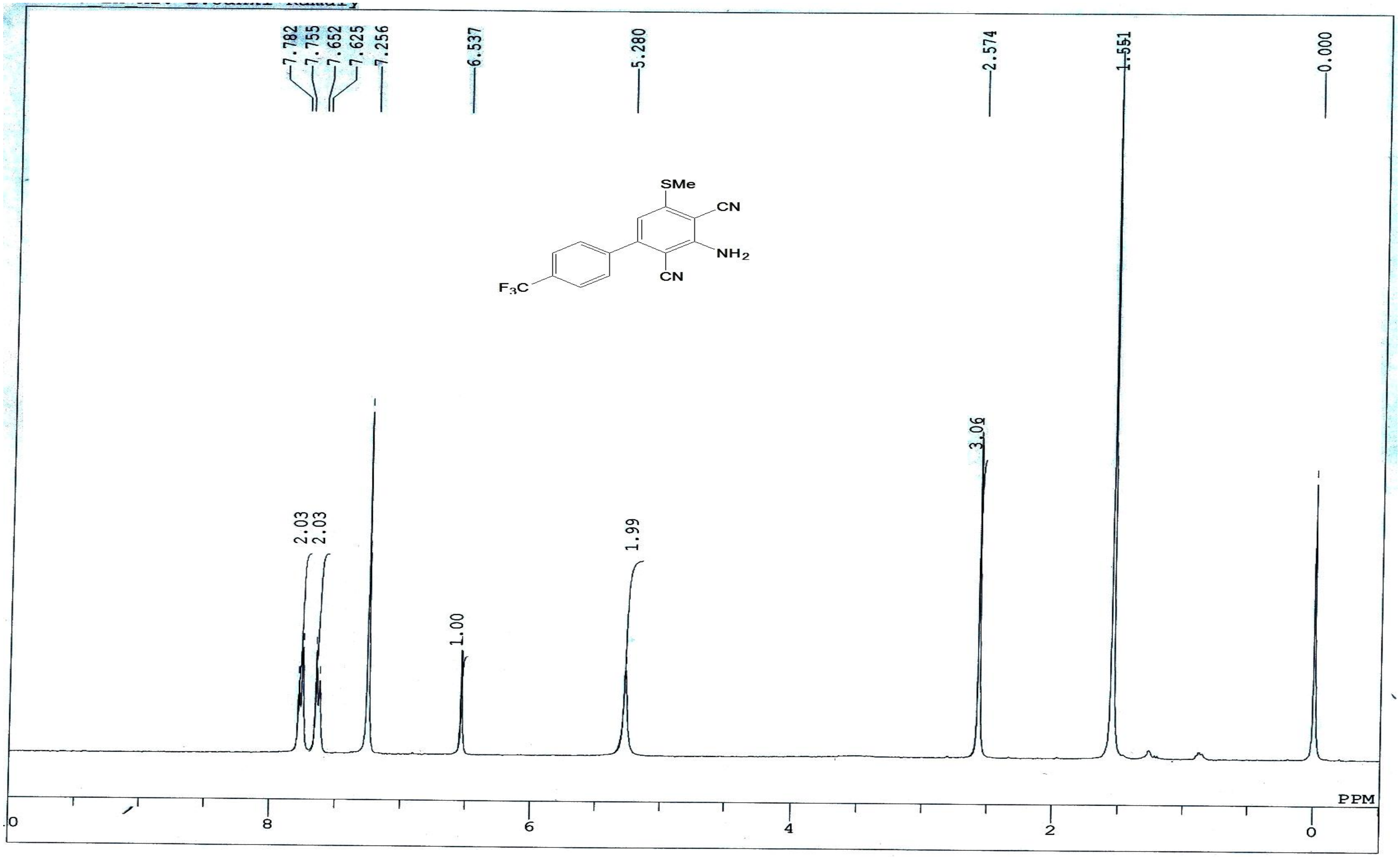
^{1}H NMR SPECTRUM OF 3d



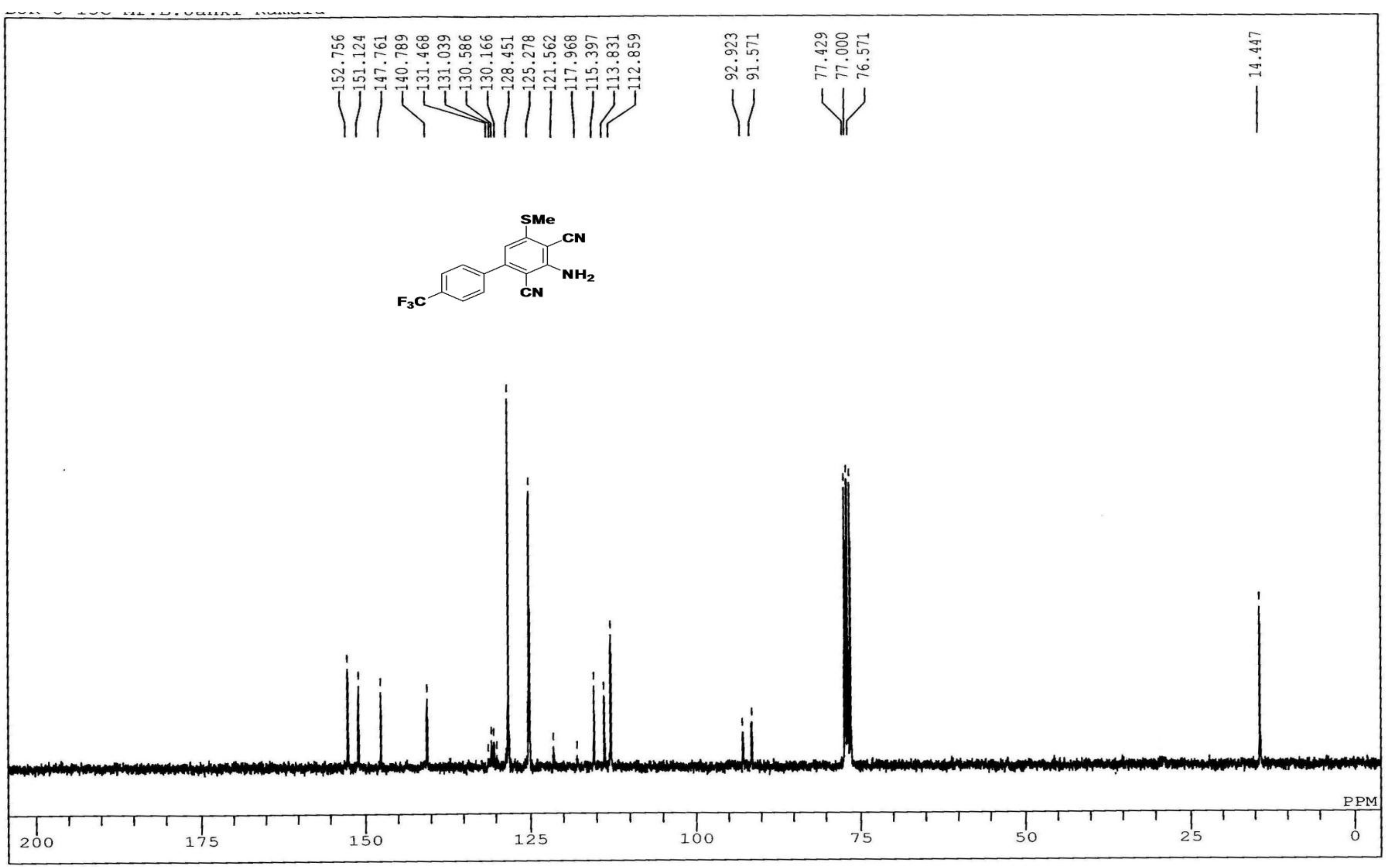
^{13}C NMR SPECTRUM OF 3d



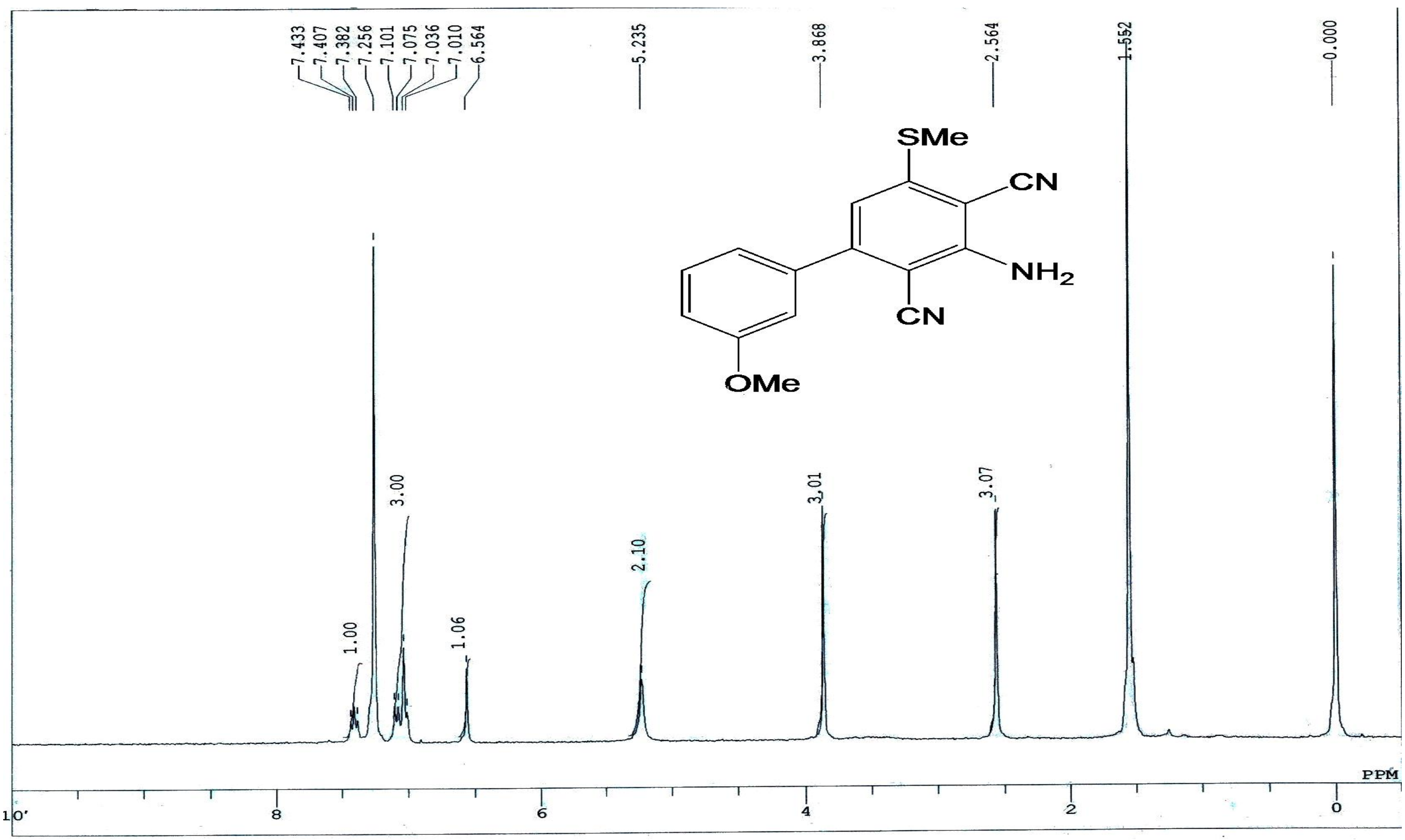
^{1}H NMR SPECTRUM OF 3e



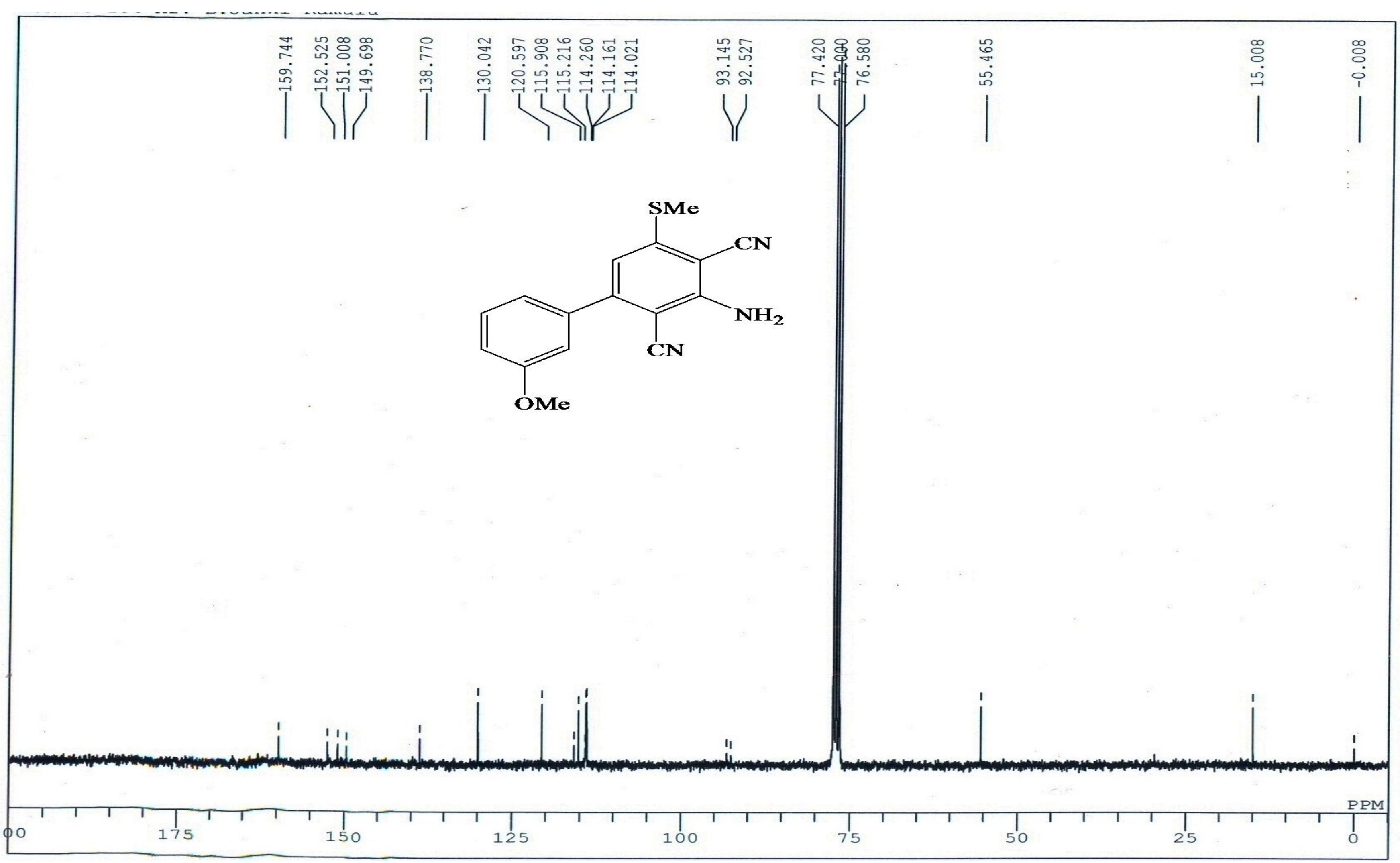
^{13}C NMR SPECTRUM OF 3e



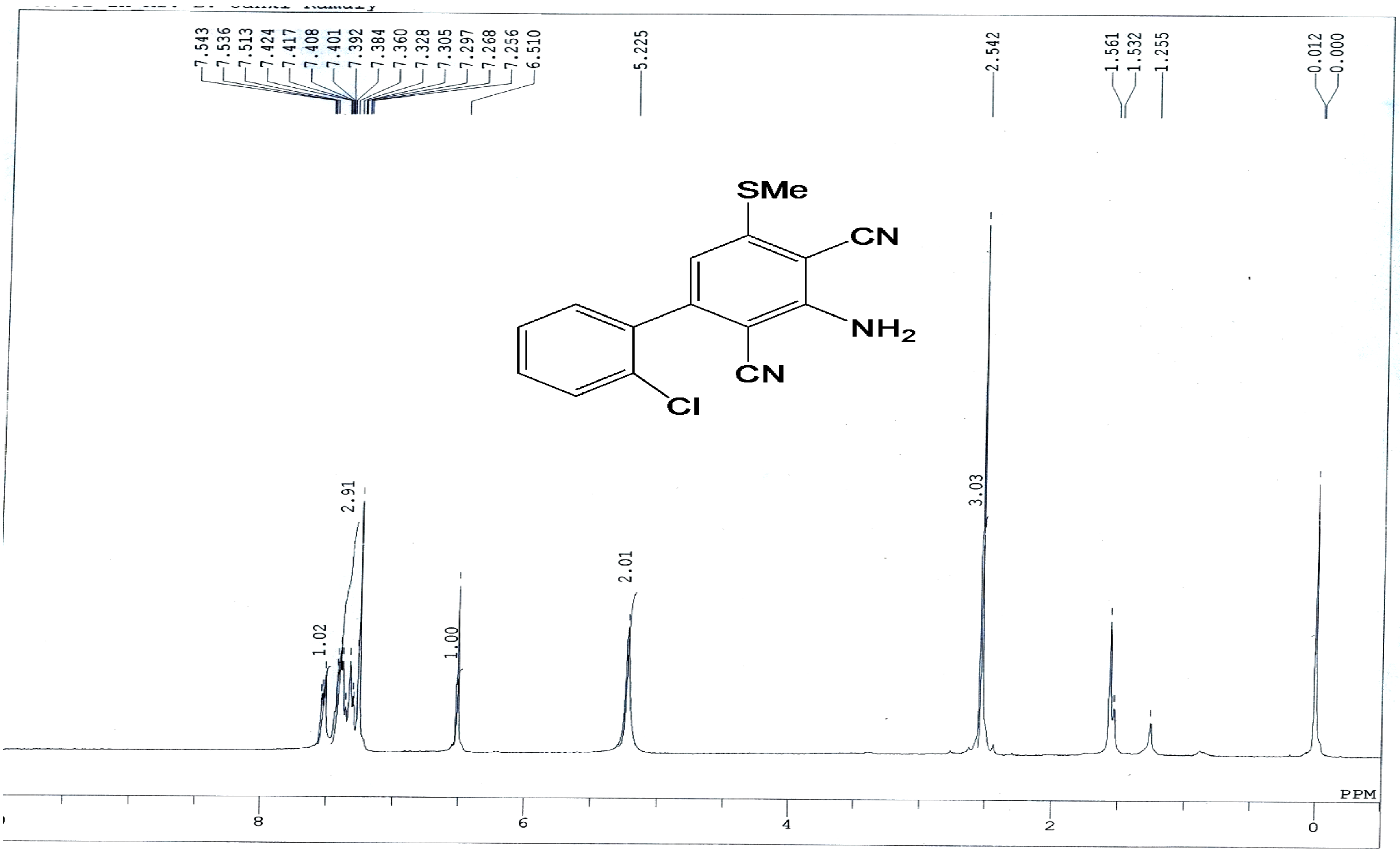
[1]H NMR SPECTRUM OF 3f



^{13}C NMR SPECTRUM OF 3f

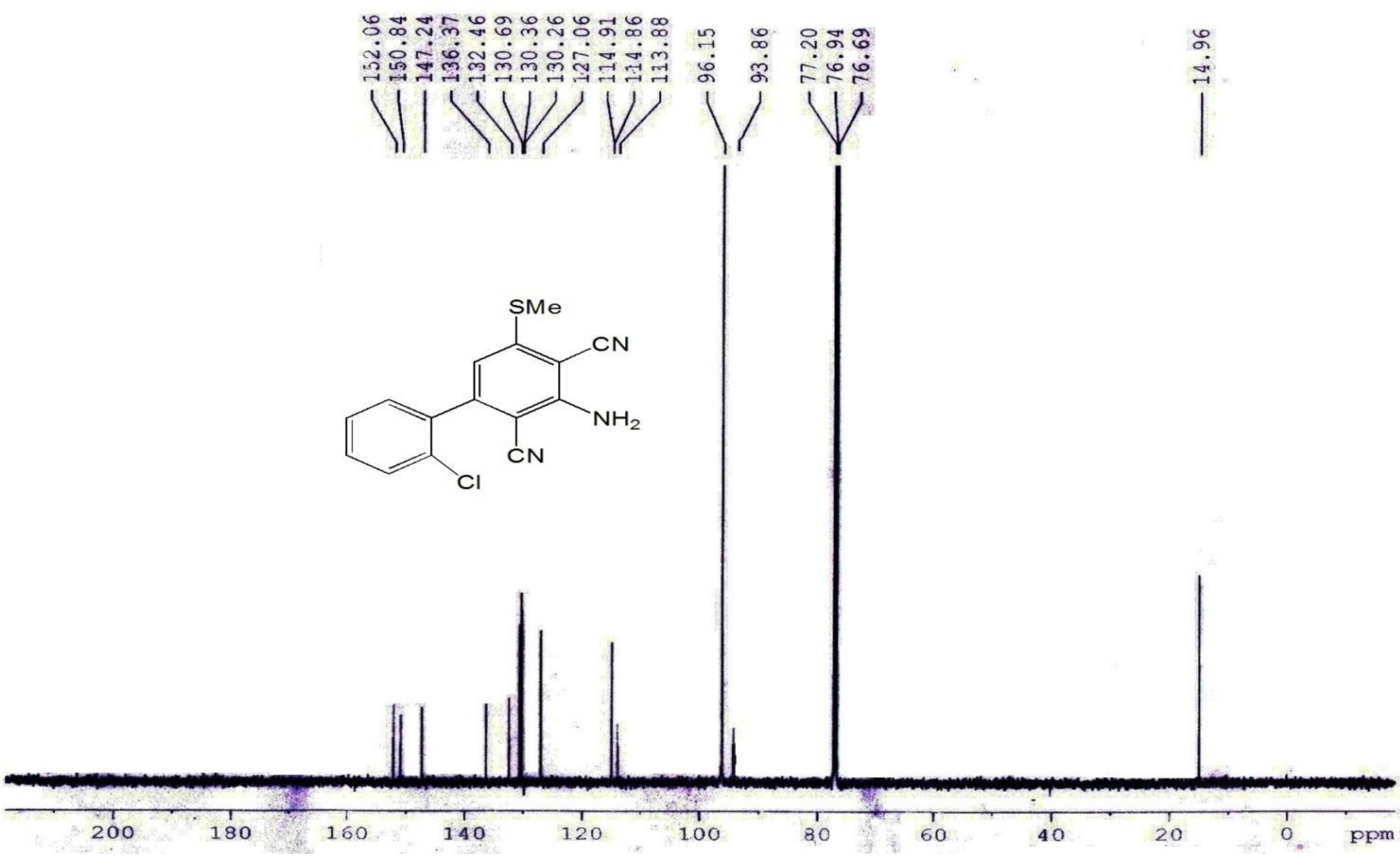


^{1}H NMR SPECTRUM OF 3g

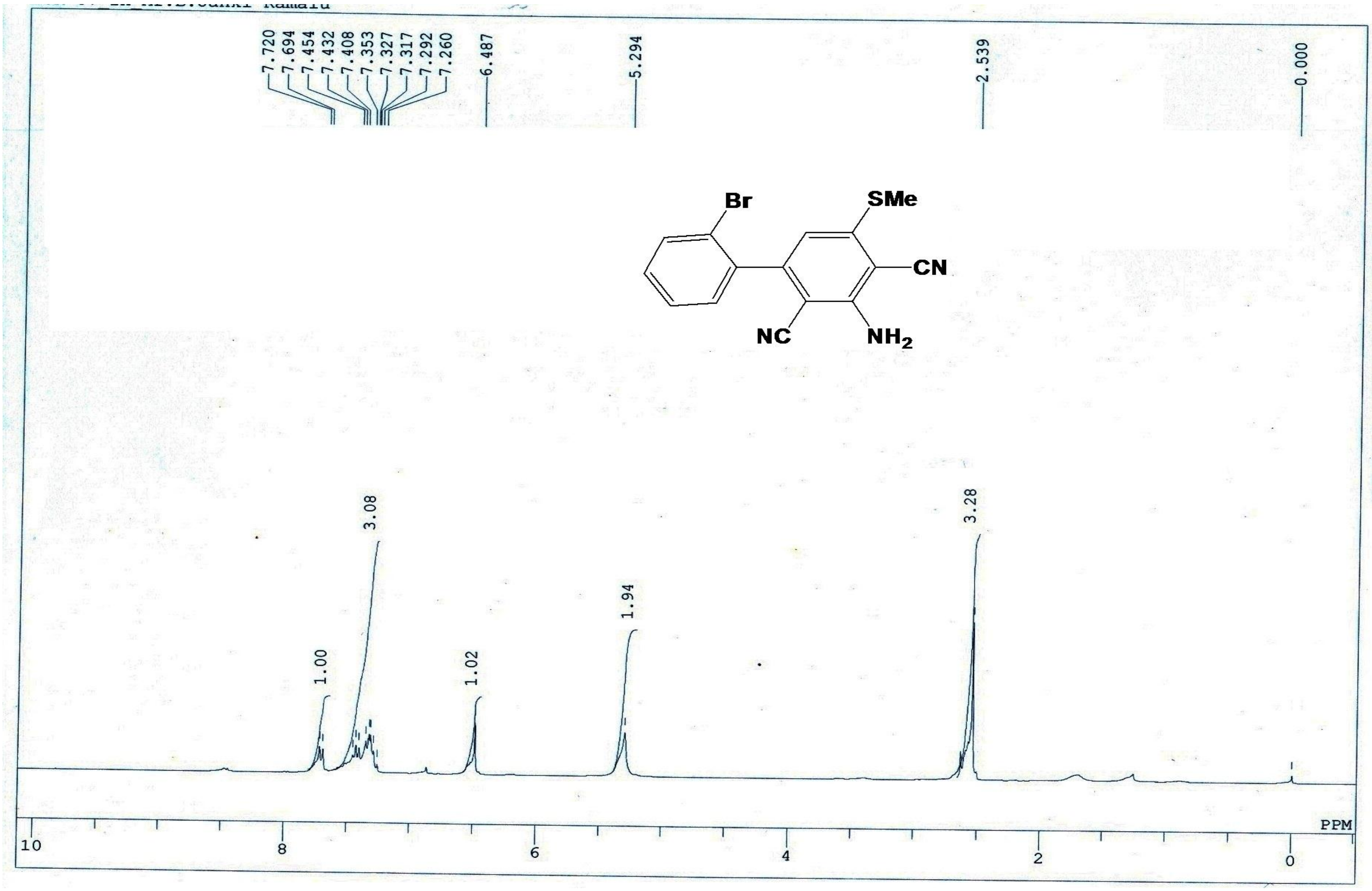


Electronic Supplementary Material (ESI) for RSC Advances

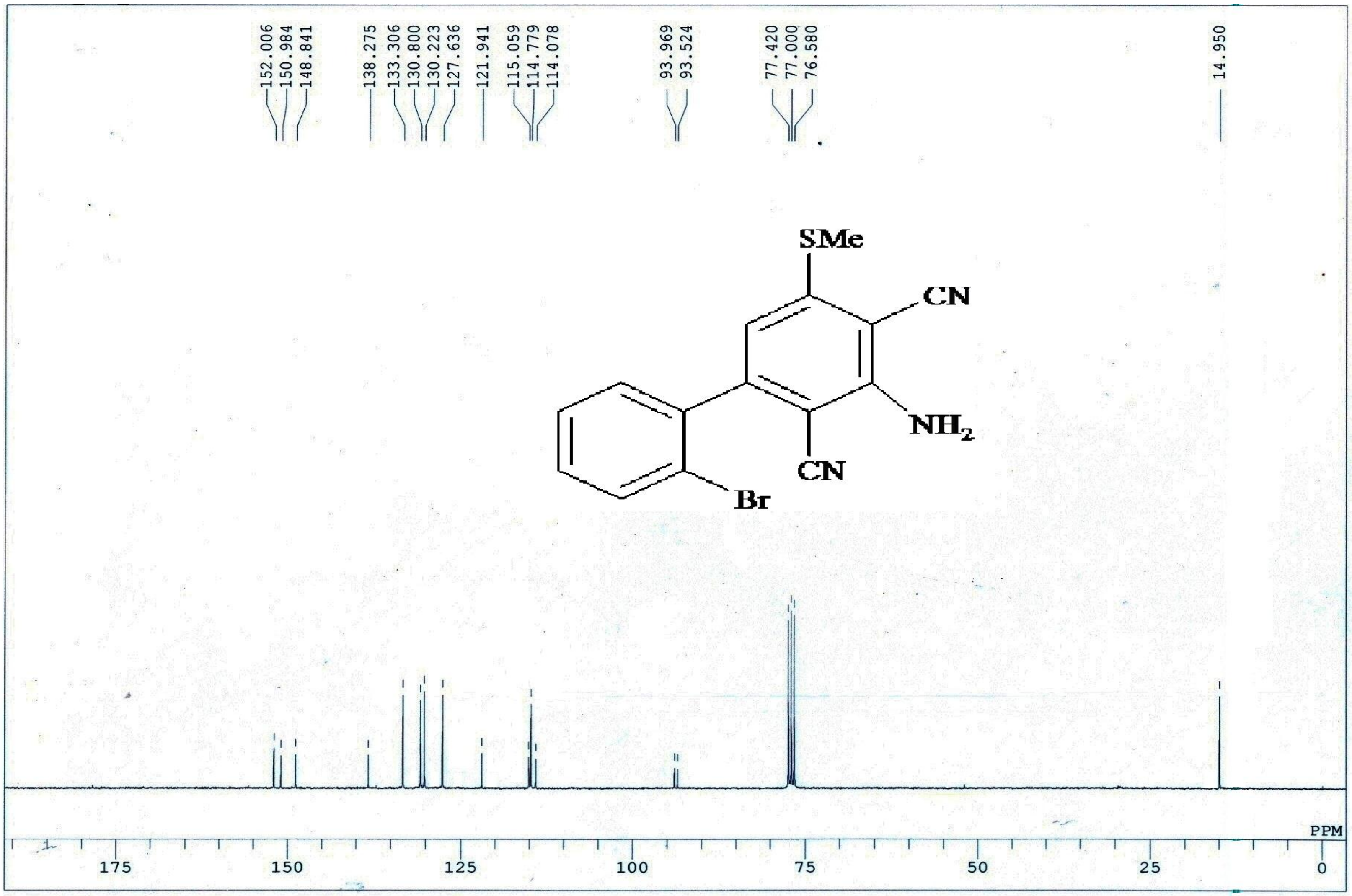
^{13}C NMR SPECTRUM OF 3g



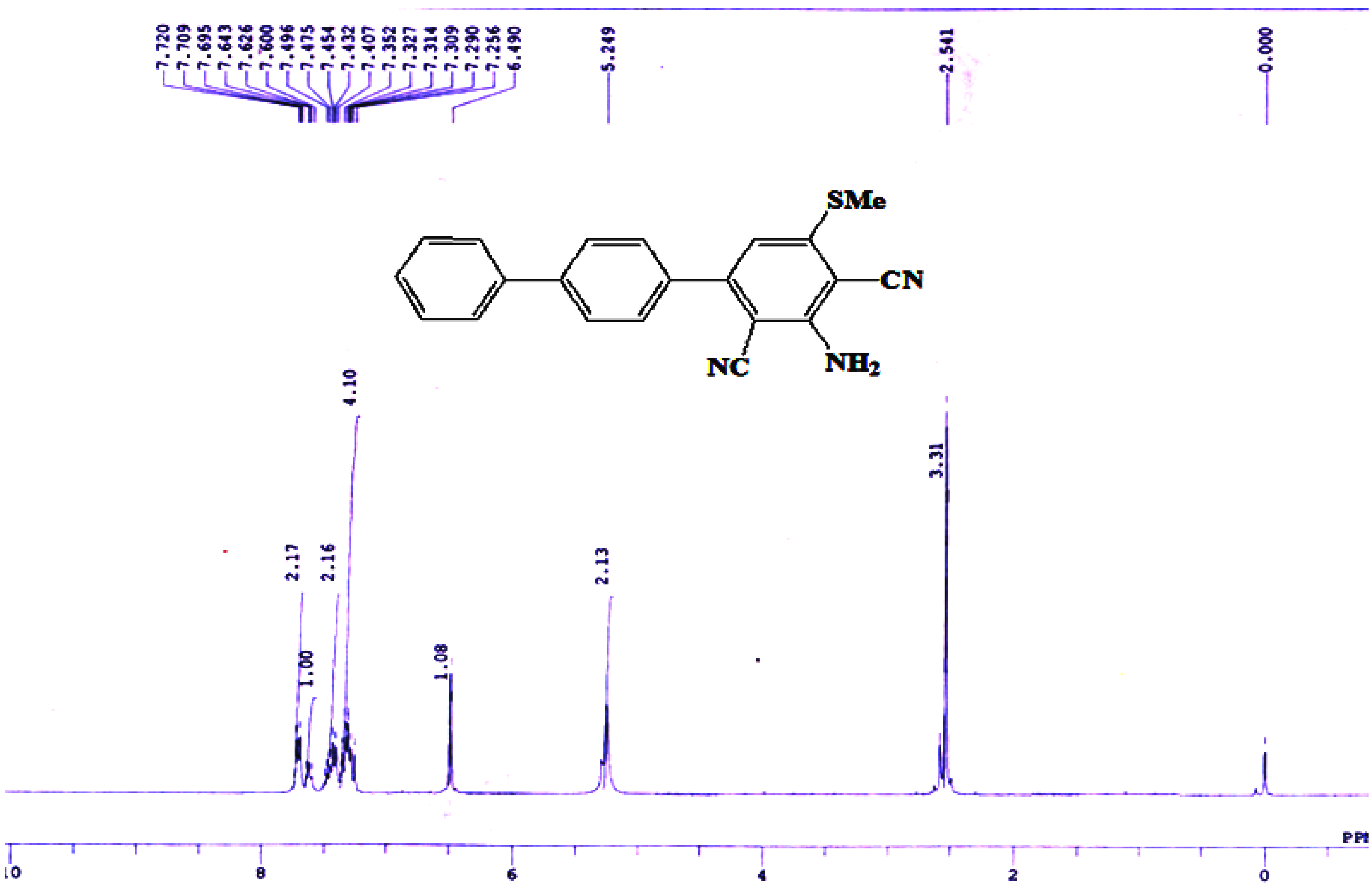
^{1}H NMR SPECTRUM OF 3h



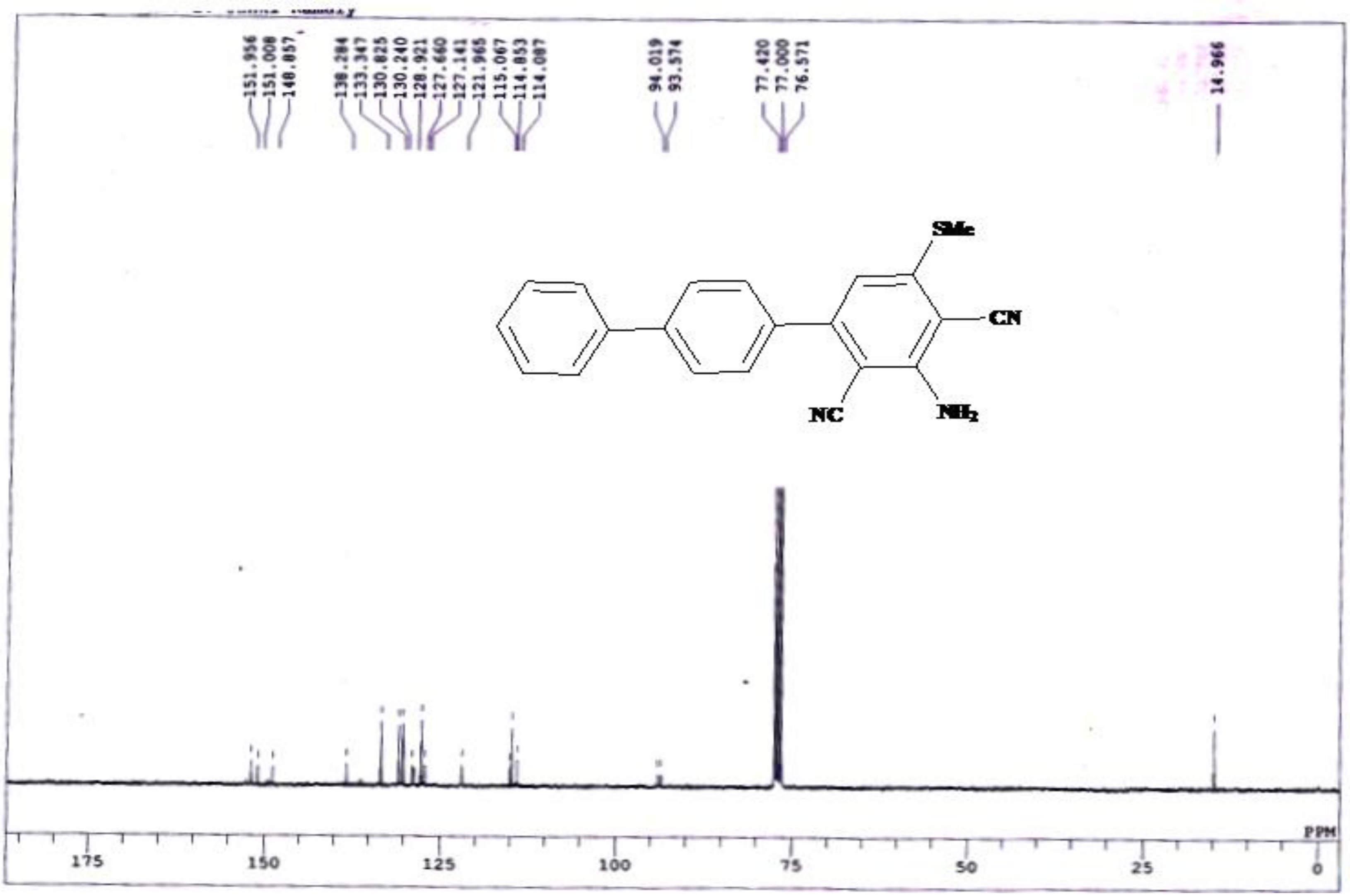
^{13}C NMR SPECTRUM OF 3h



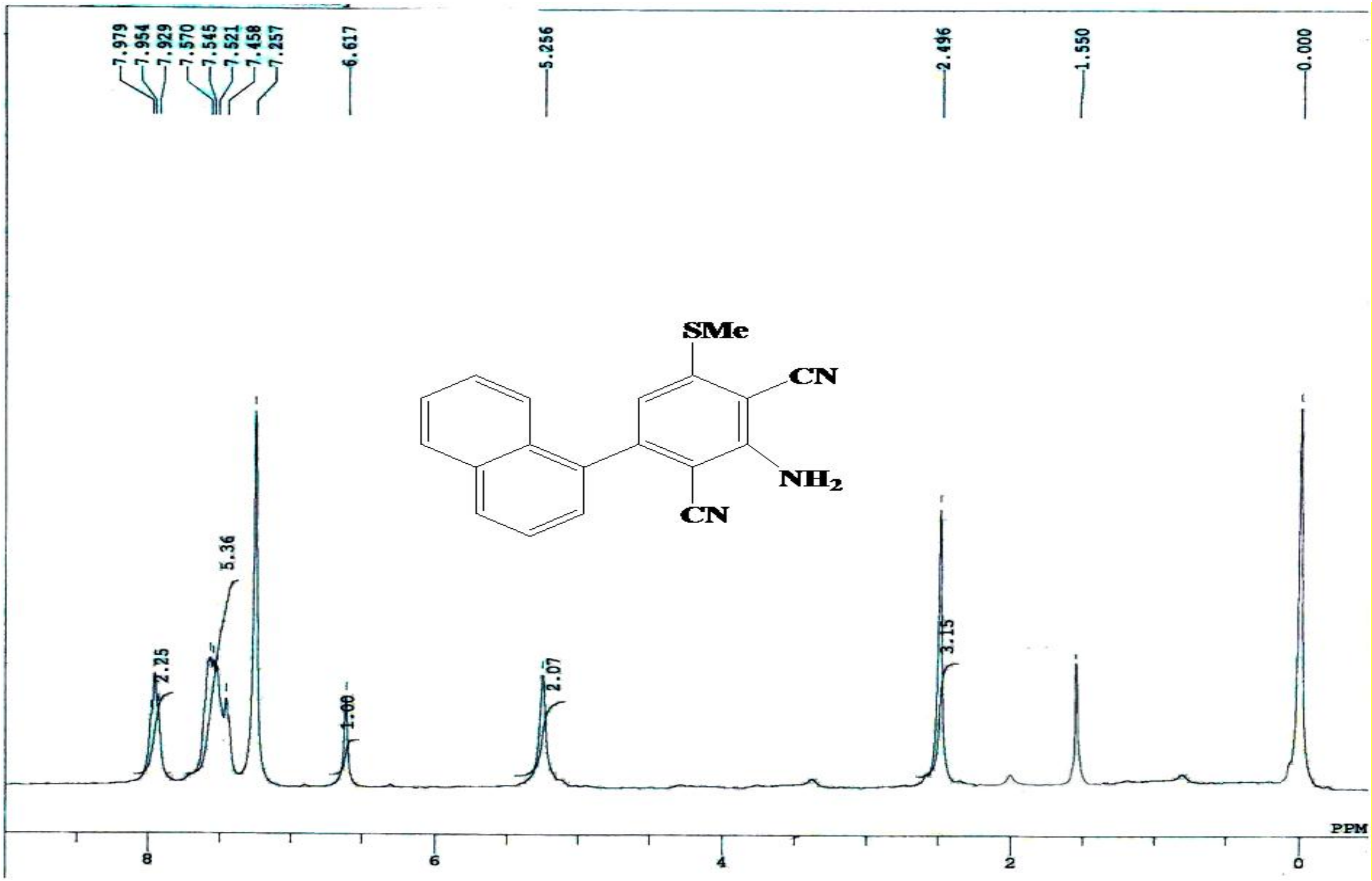
^{1}H NMR SPECTRUM OF 3i



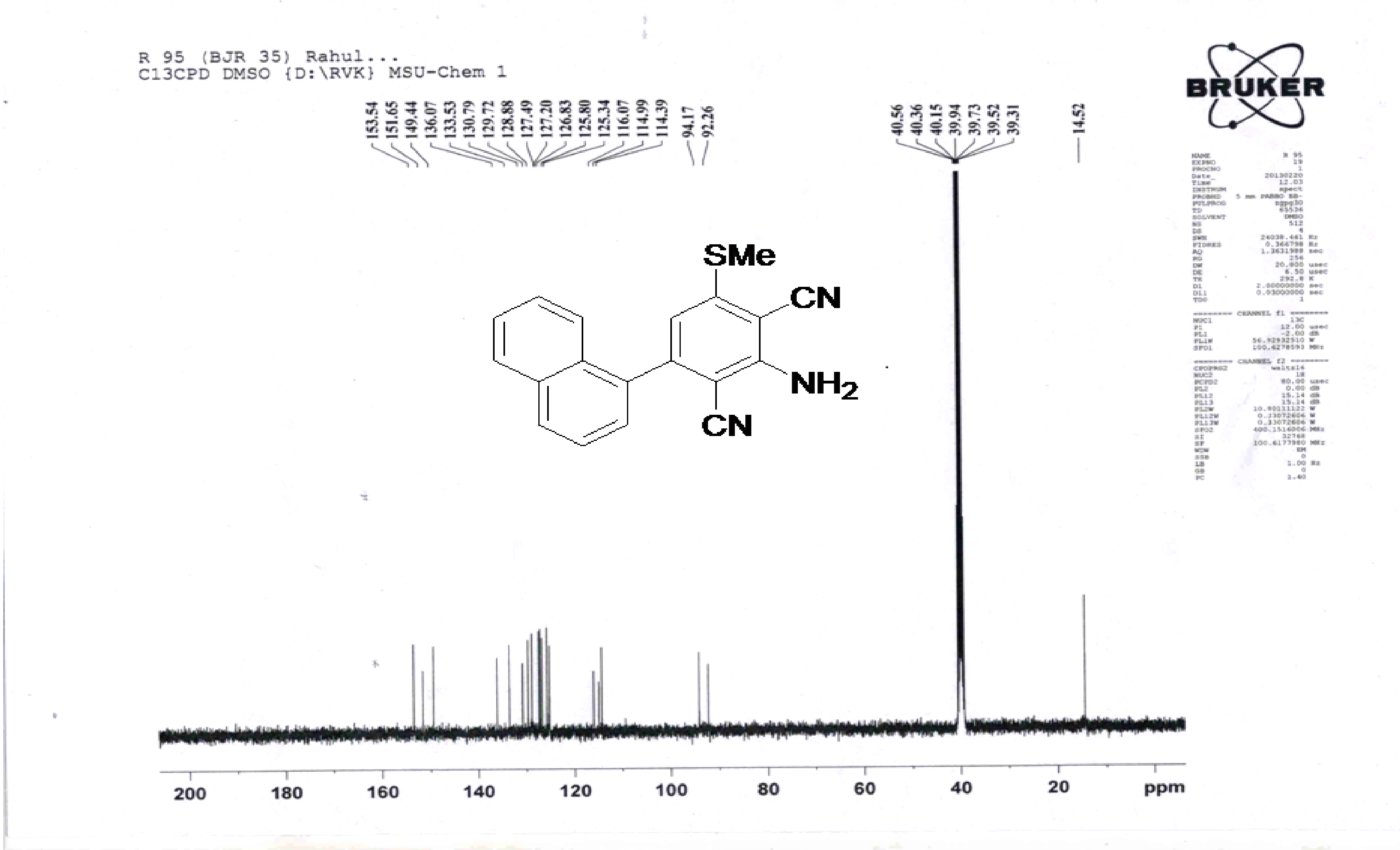
^{13}C NMR SPECTRUM OF 3i



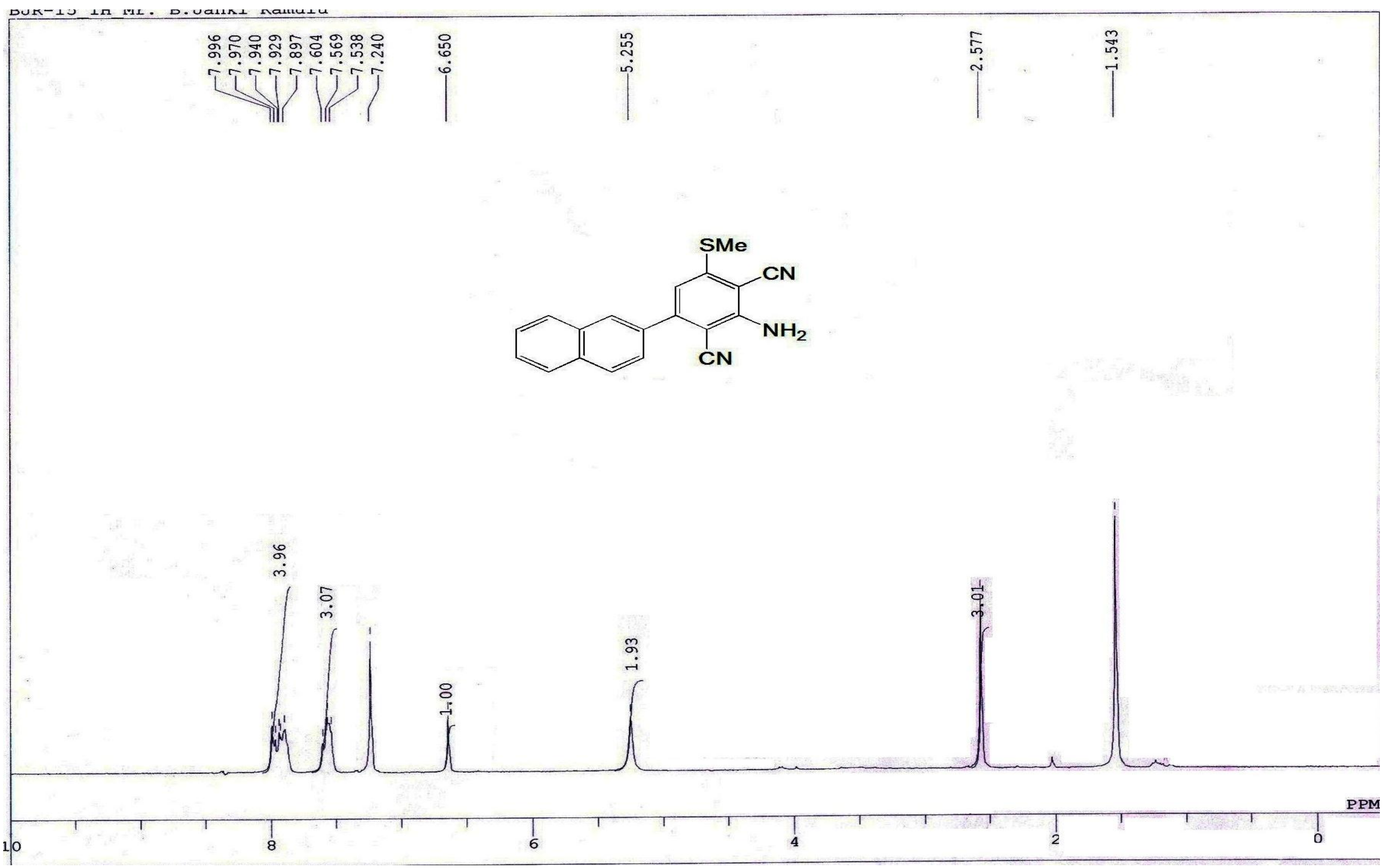
[1]H NMR SPECTRUM OF 3j



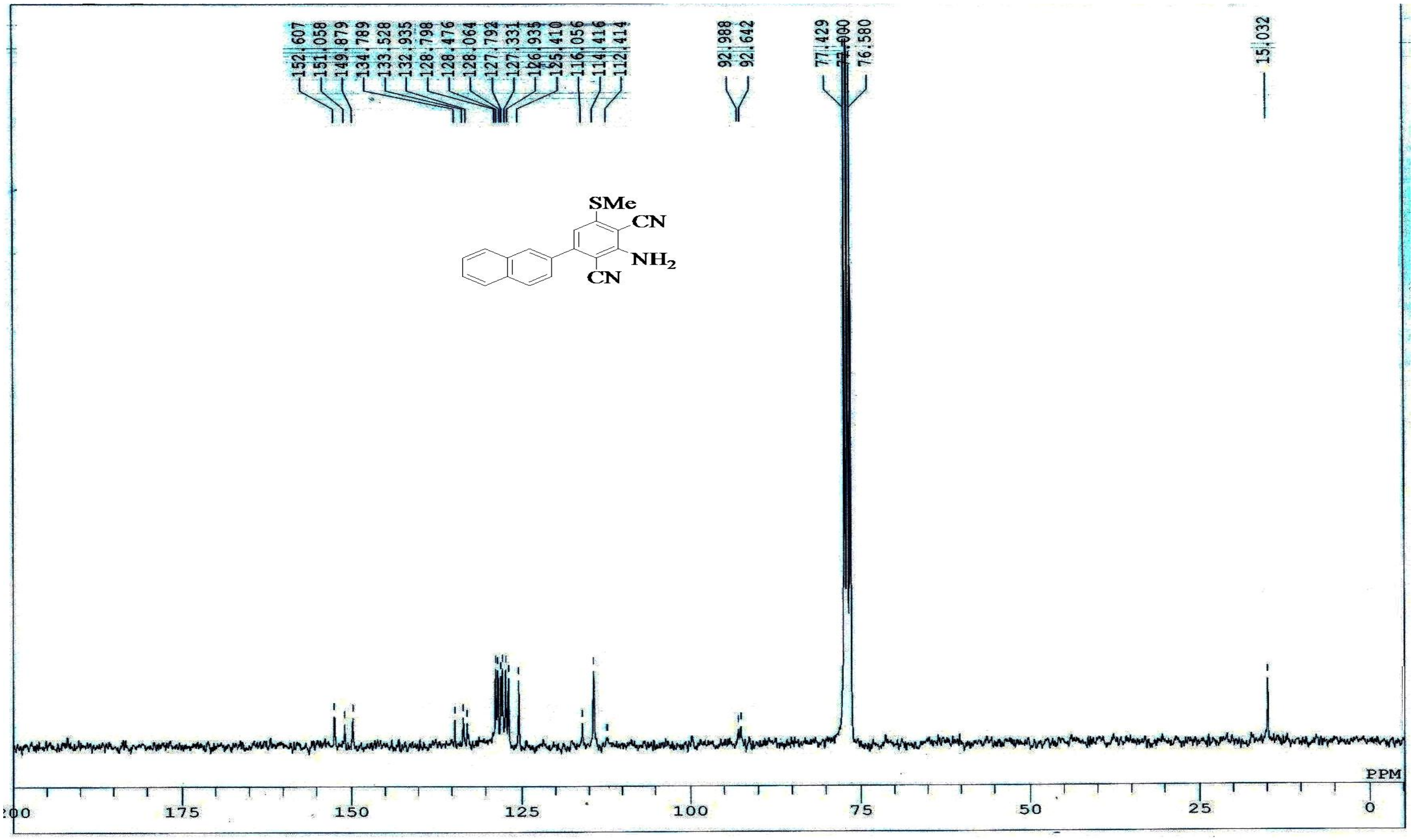
^{13}C NMR SPECTRUM OF 3j



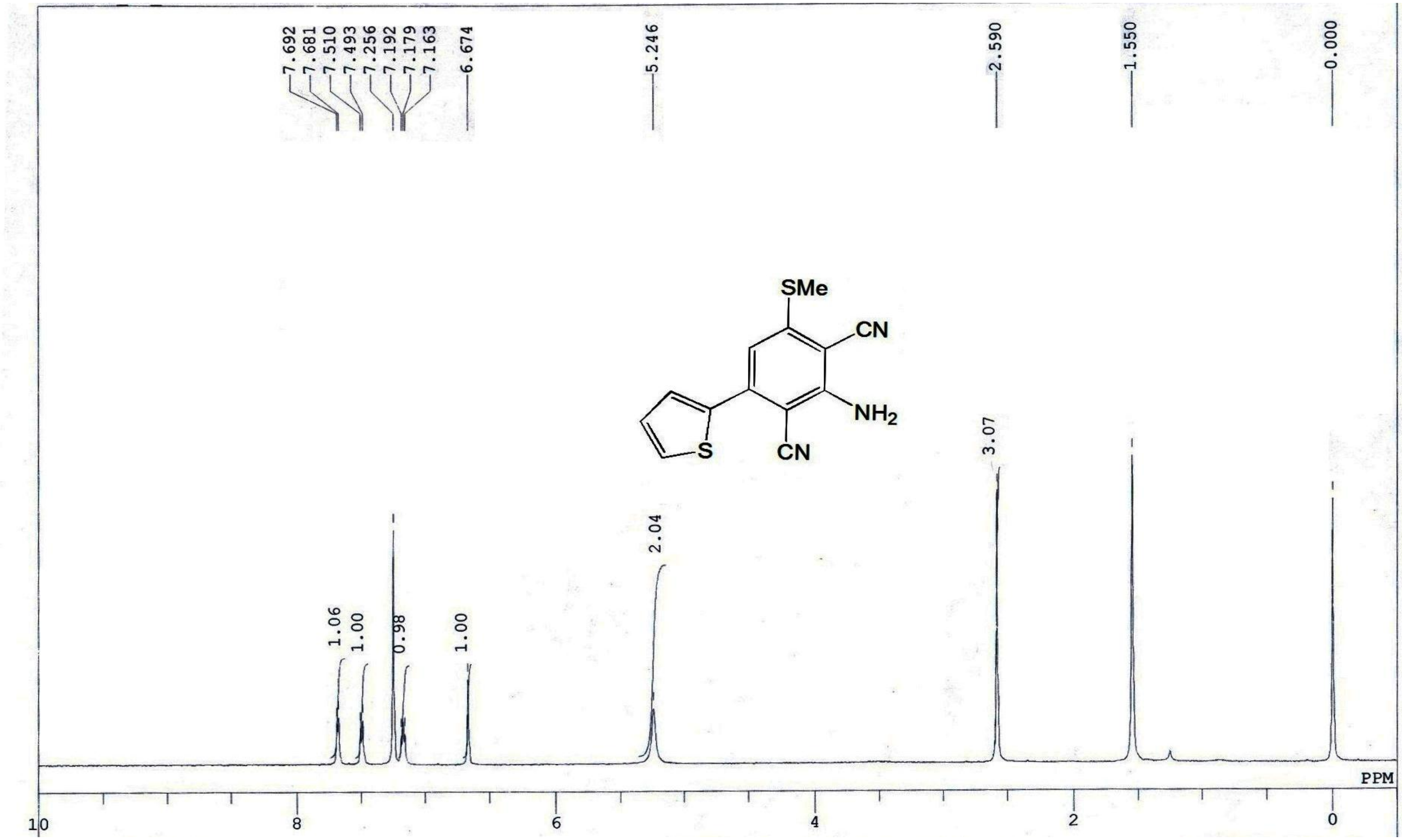
[1]H NMR SPECTRUM OF 3k



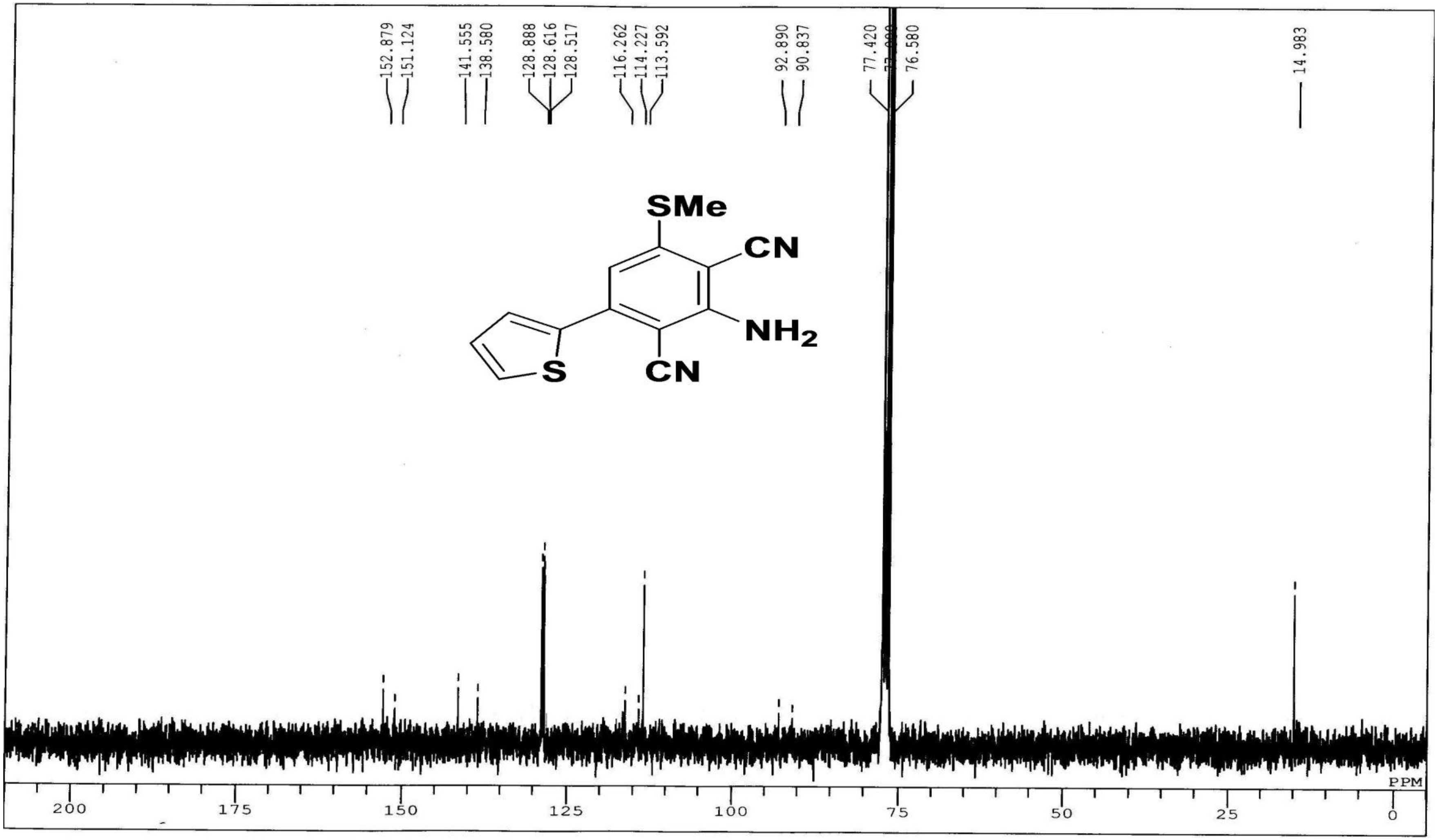
^{13}C NMR SPECTRUM OF 3k



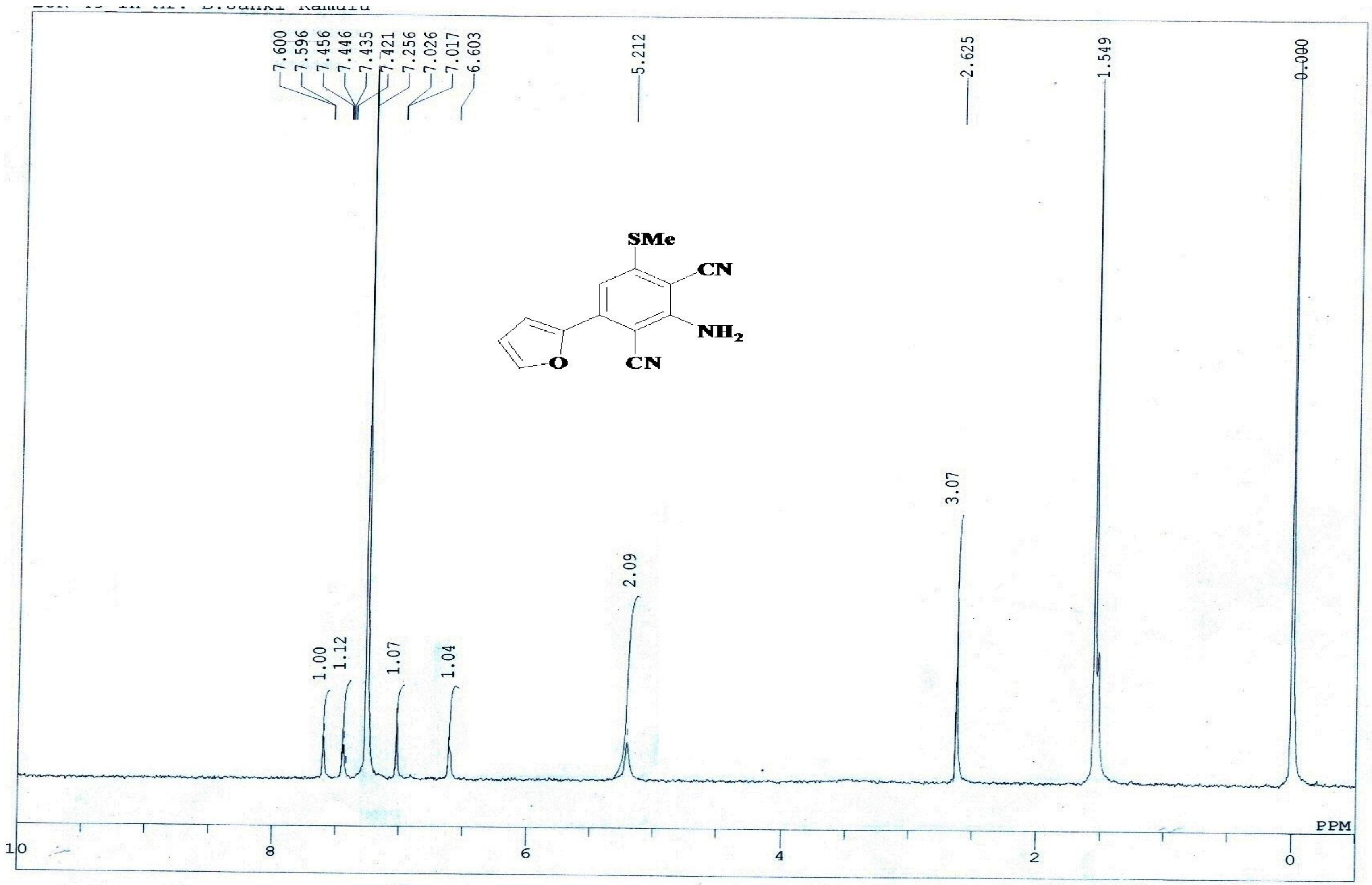
^{1}H NMR SPECTRUM OF 3l



^{13}C NMR SPECTRUM OF 3l



[1]HNMRSPECTRUM OF 3m



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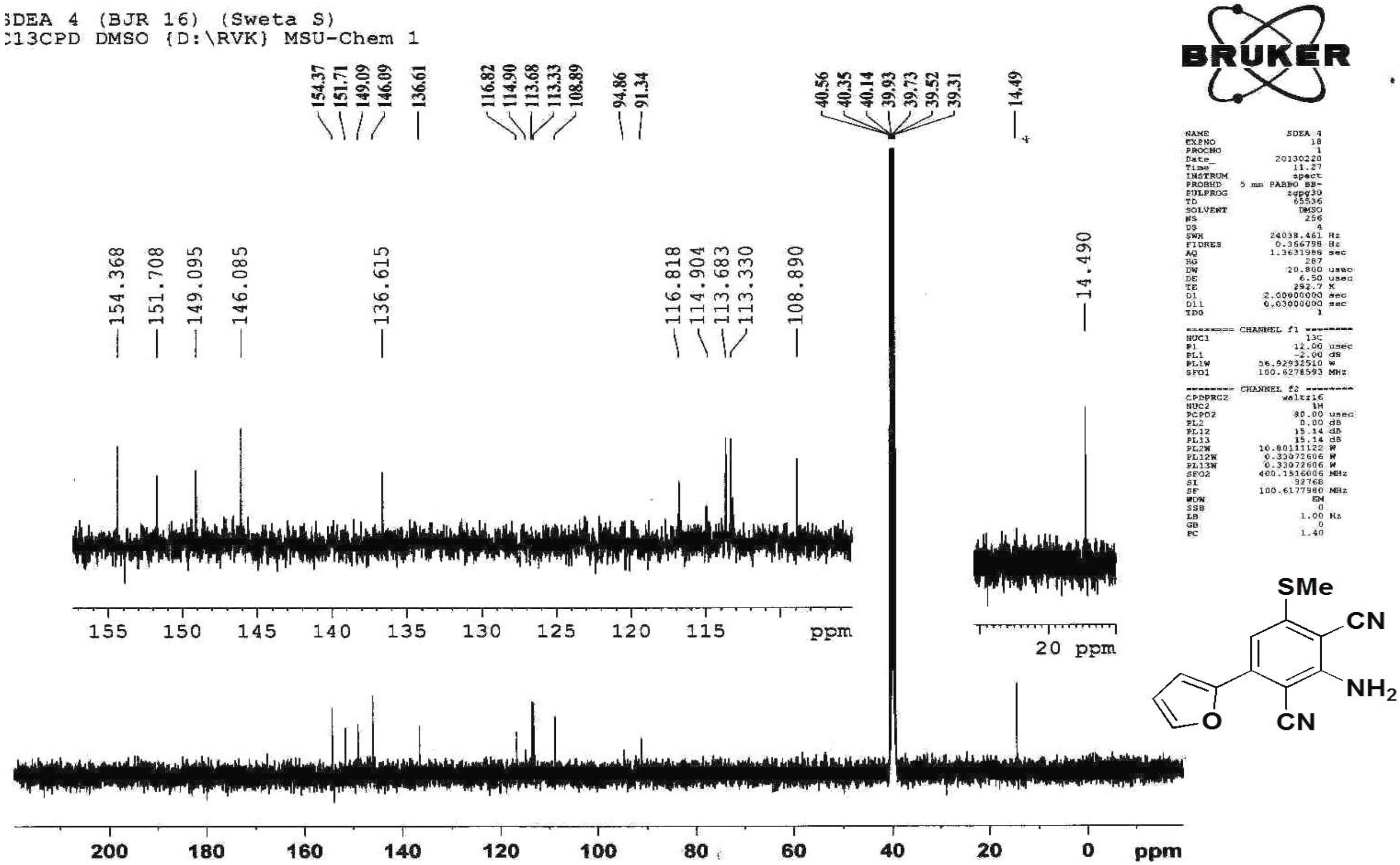
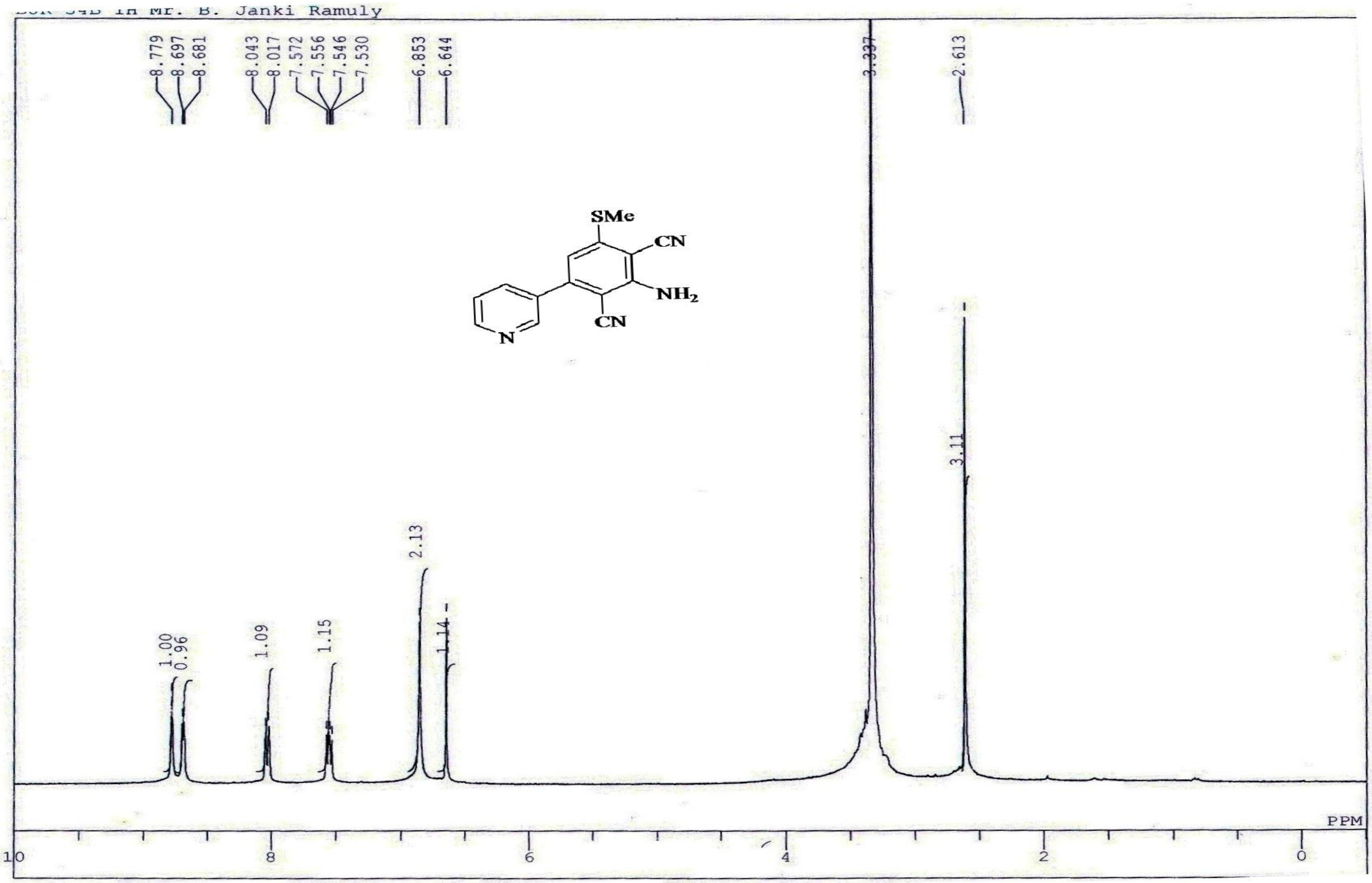
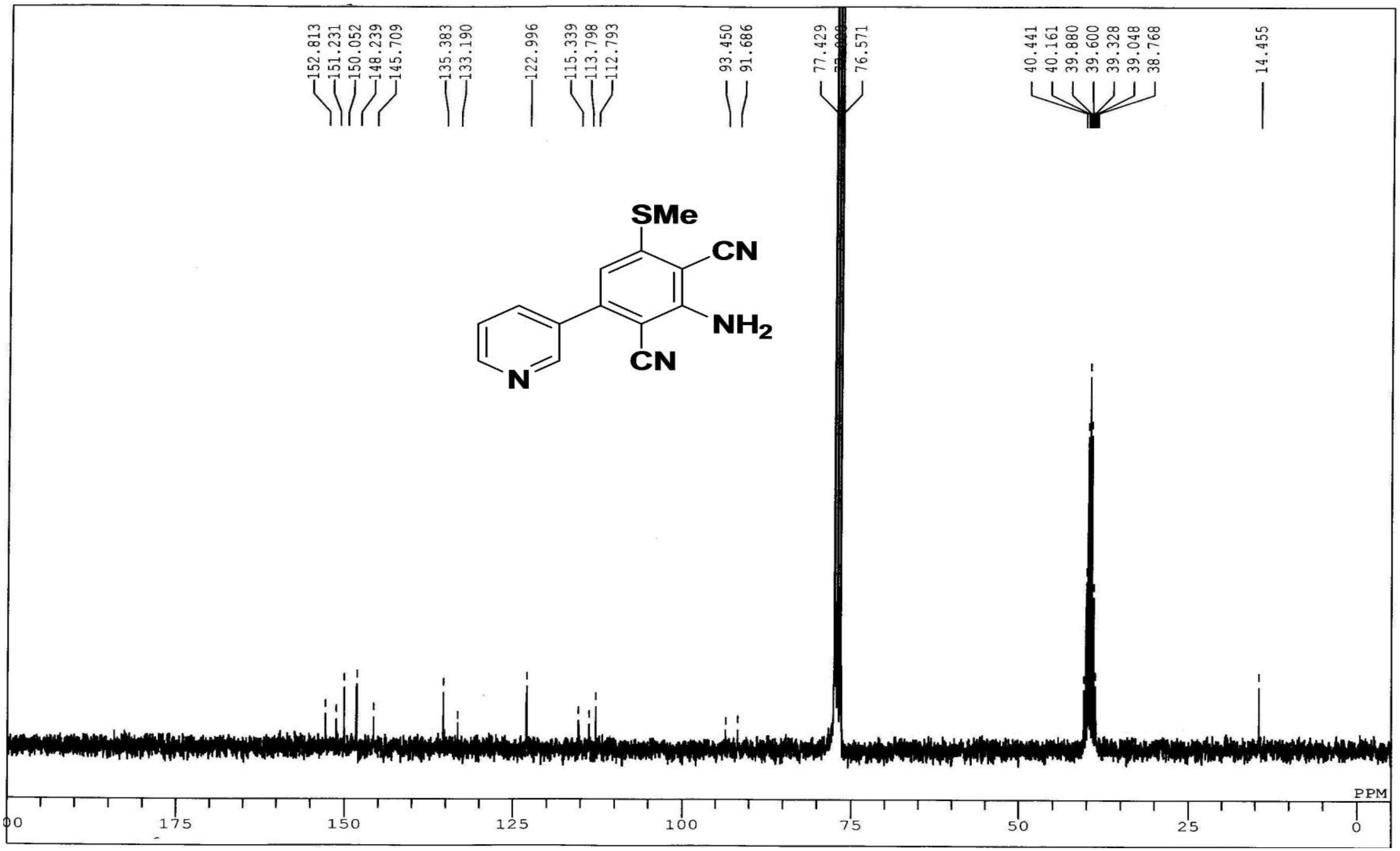
^{13}C NMR SPECTRUM OF 3m



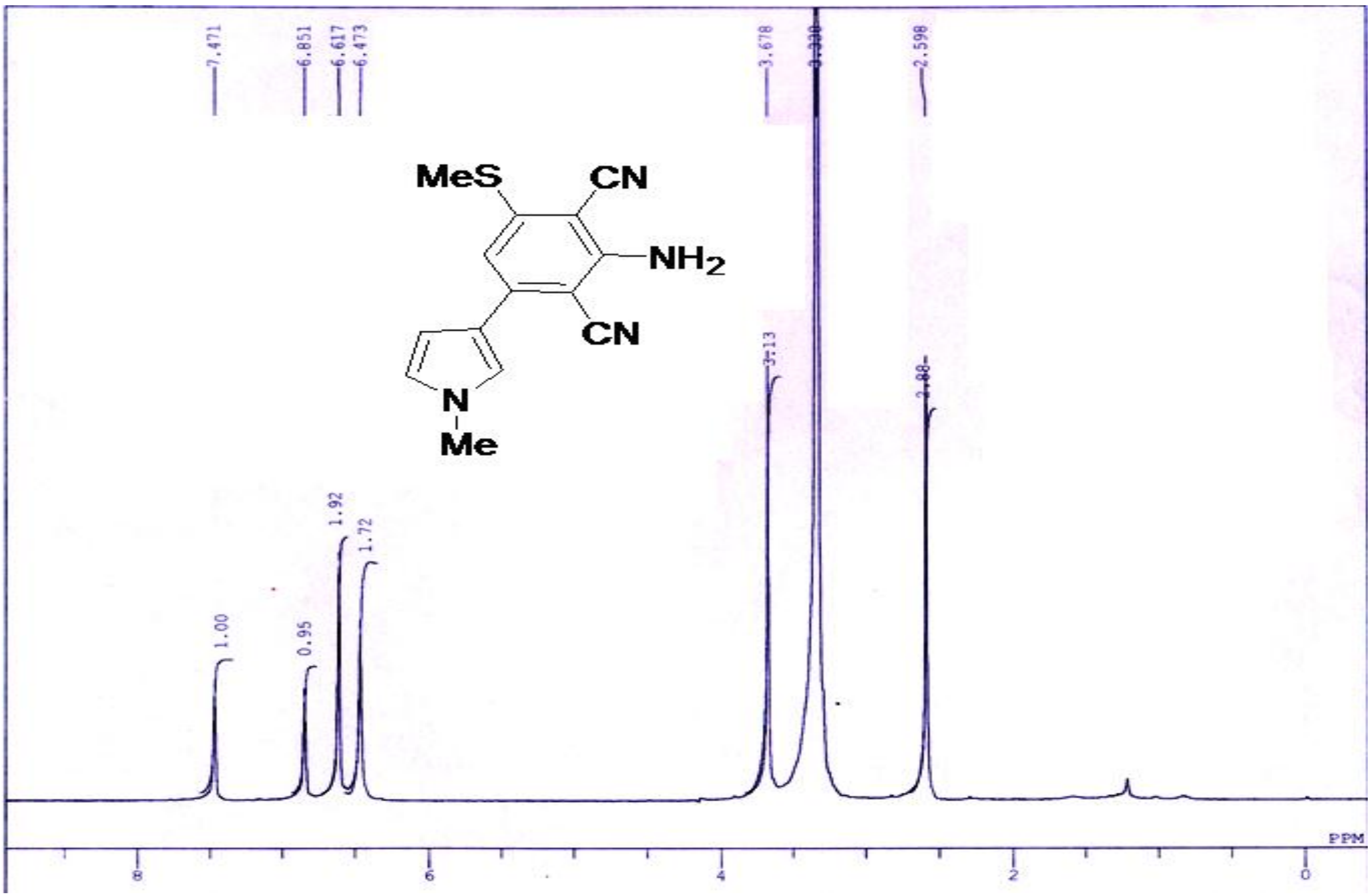
[1]H NMR SPECTRUM OF 3n



^{13}C NMR SPECTRUM OF 3n



[1]H NMR SPECTRUM OF 3o



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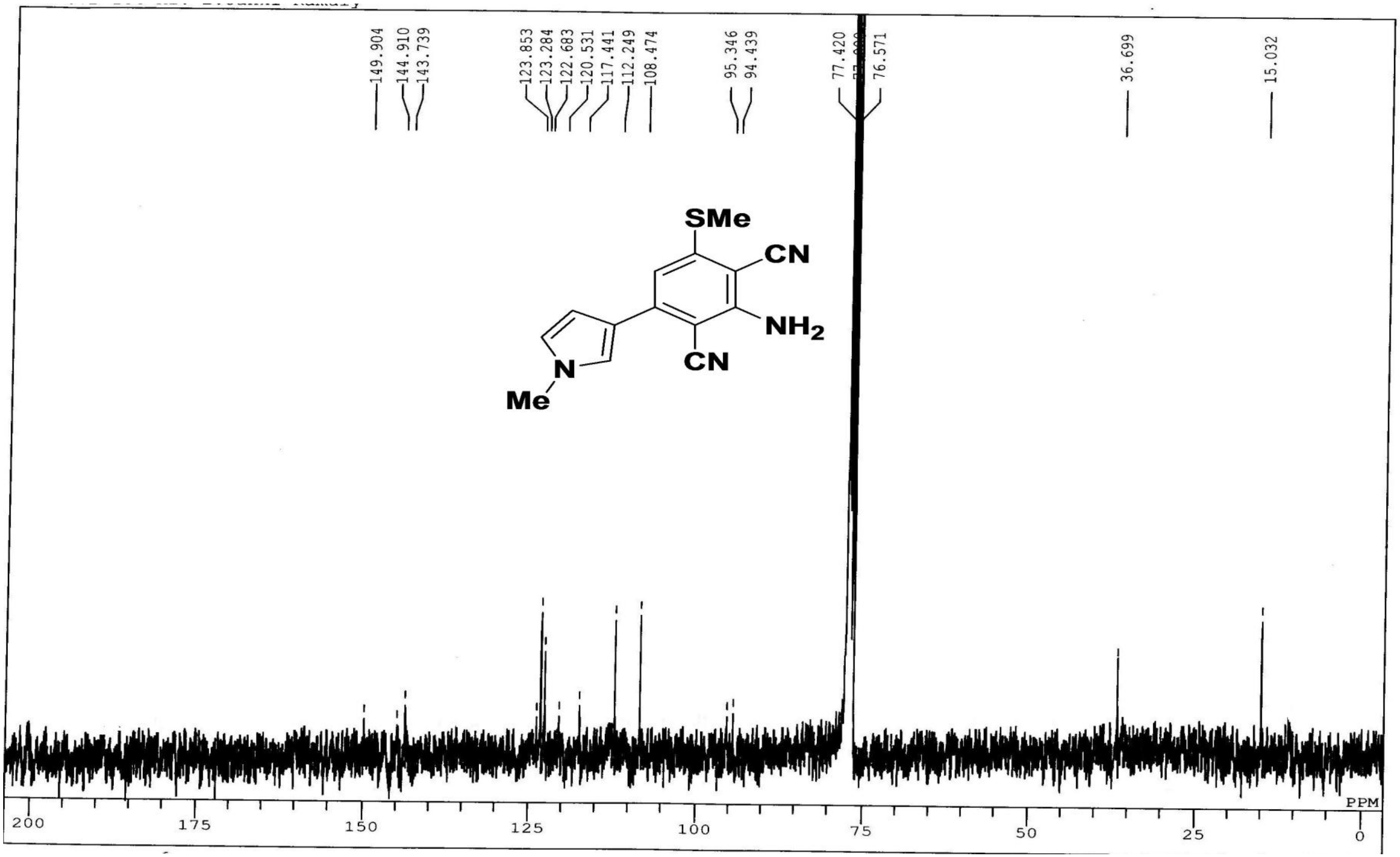
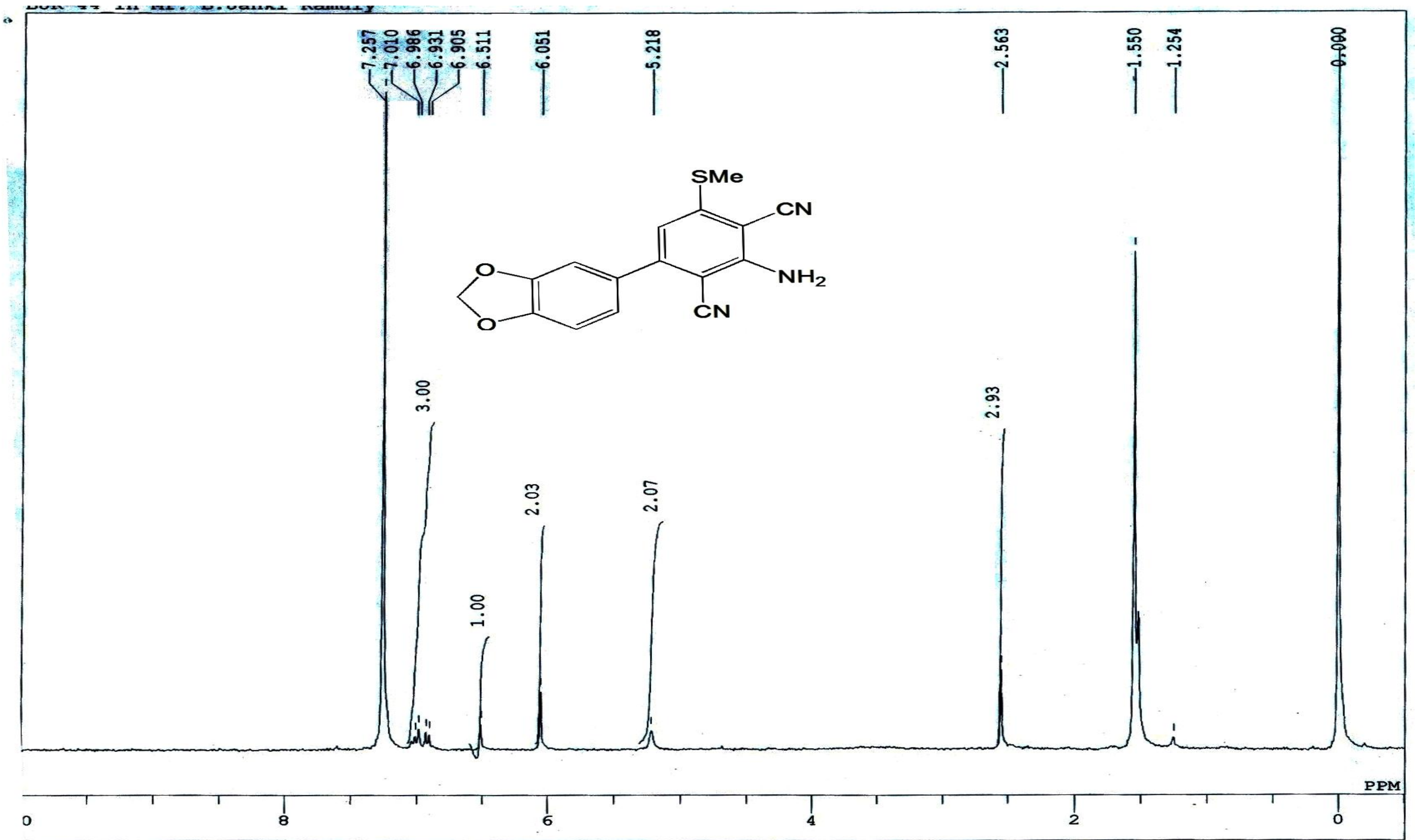
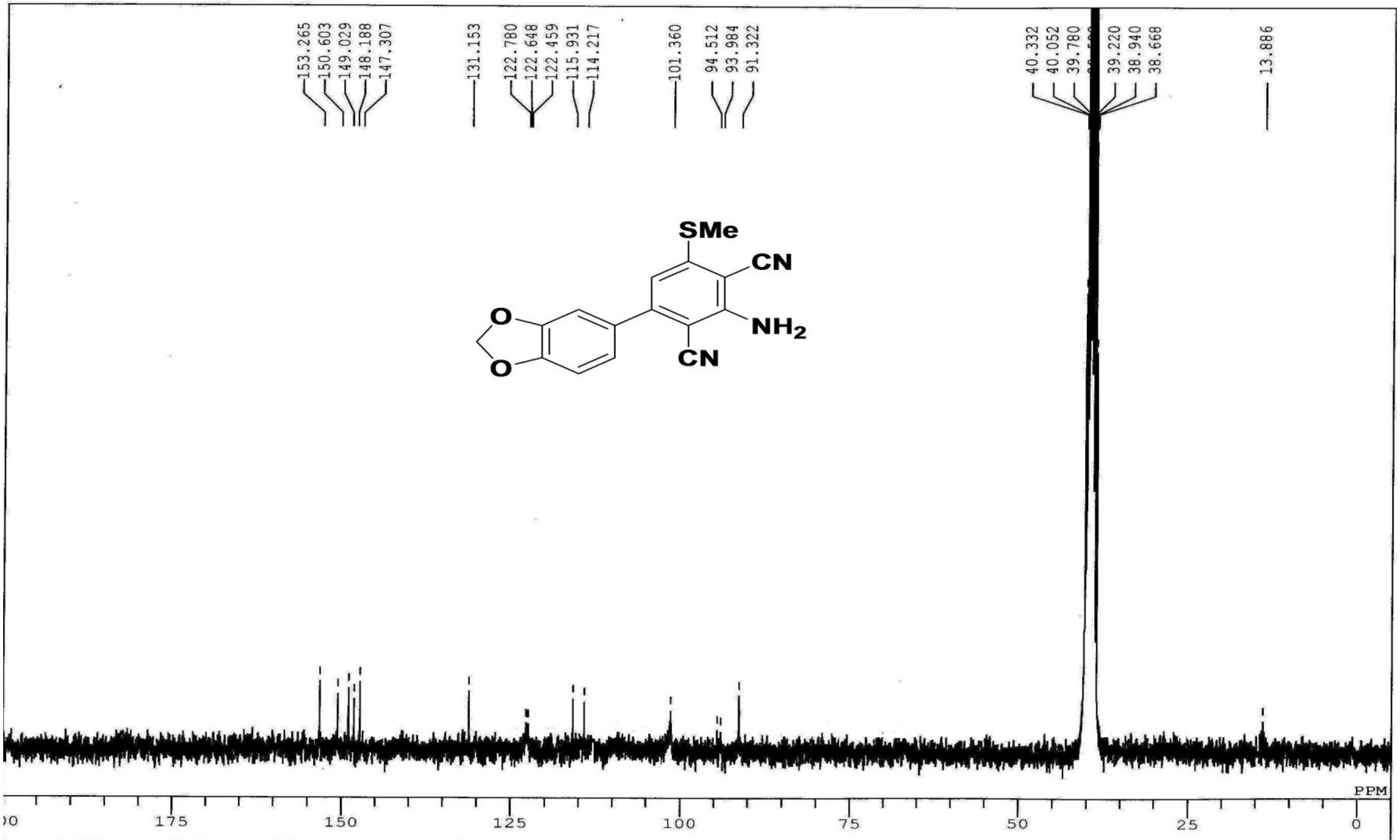
^{13}C NMR SPECTRUM OF 3o



^{1}H NMR SPECTRUM OF 3p



^{13}C NMR SPECTRUM OF 3p



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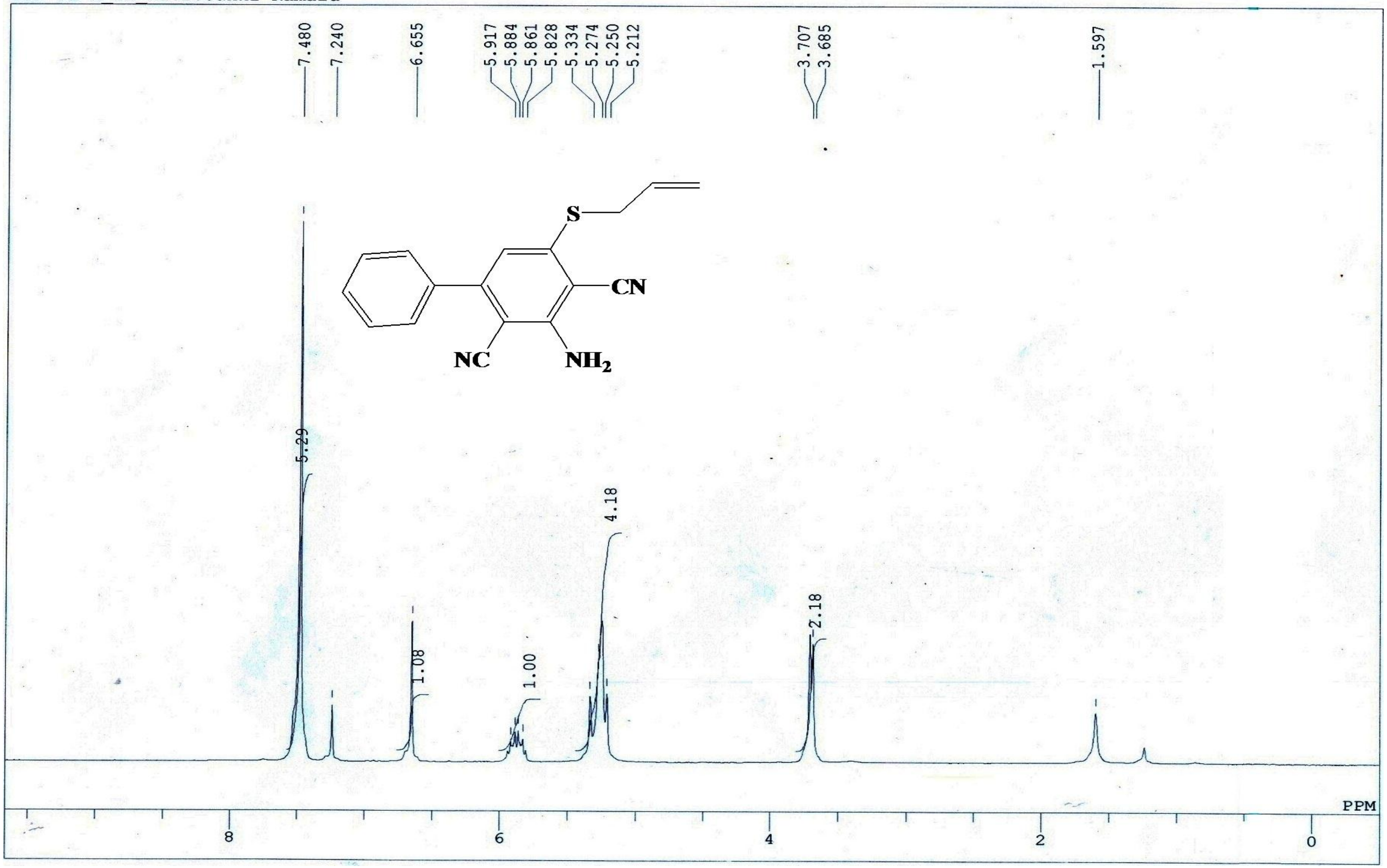
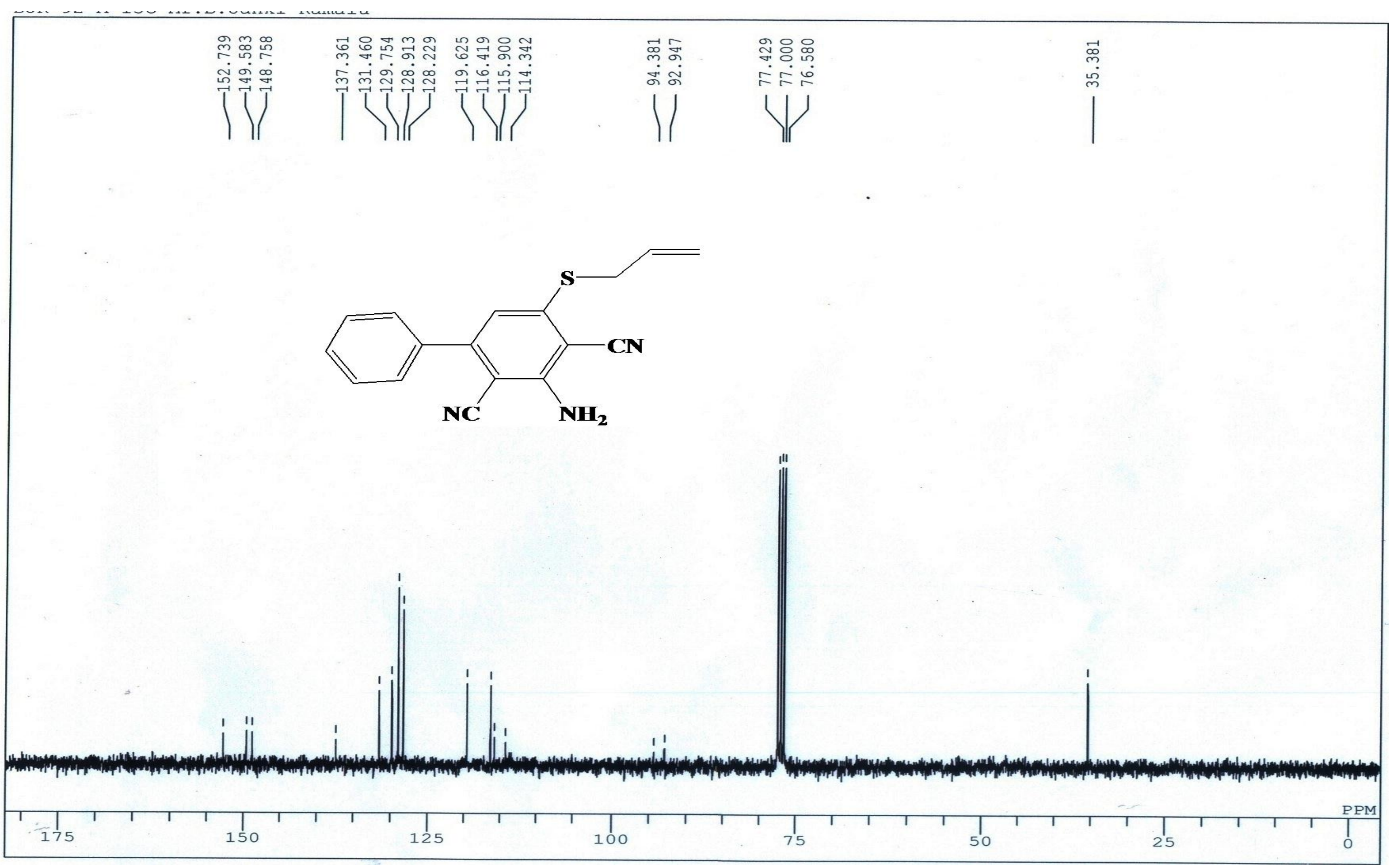
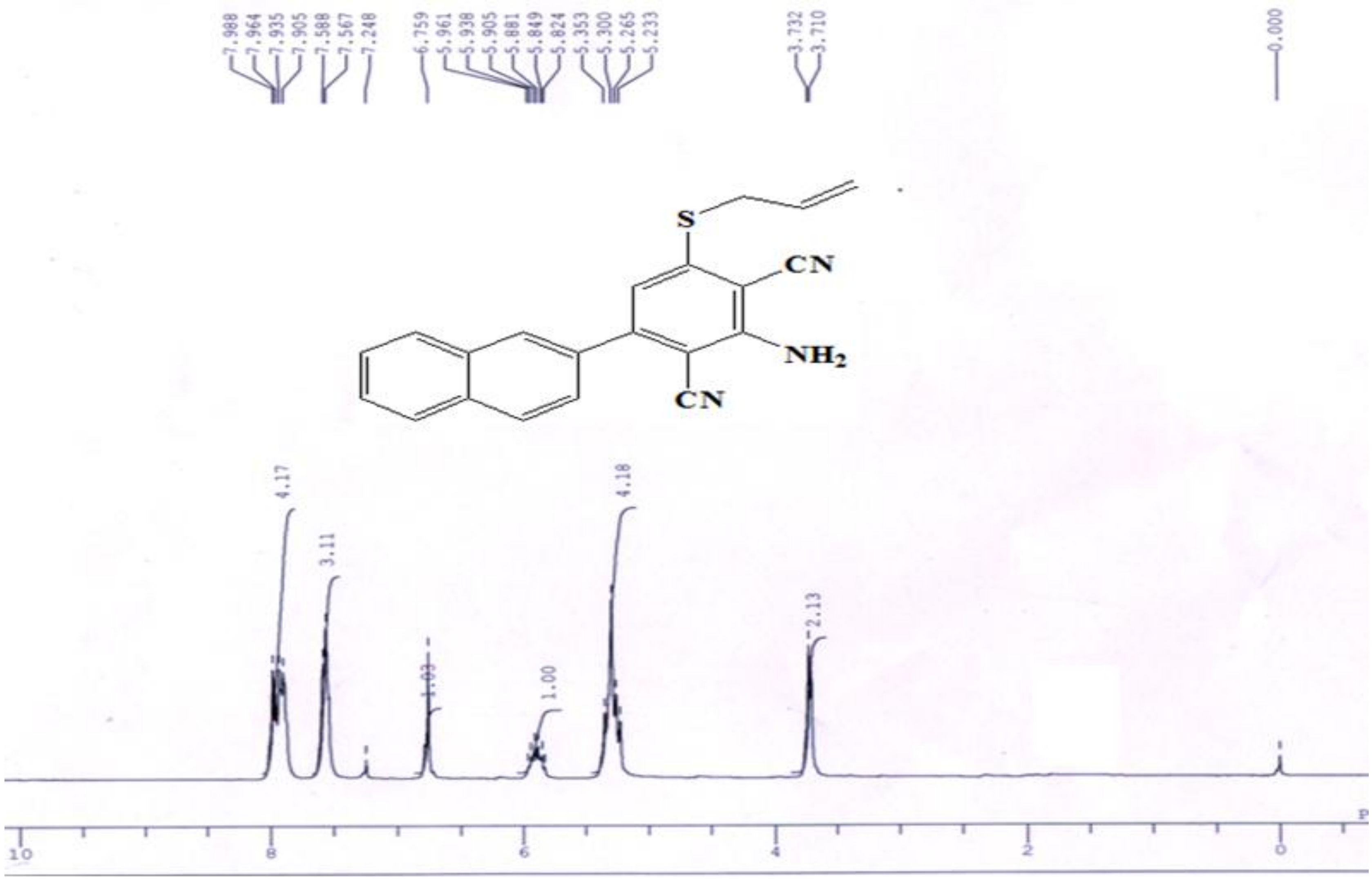
^{1}H NMR SPECTRUM OF 3q



^{13}C NMR SPECTRUM OF 3q

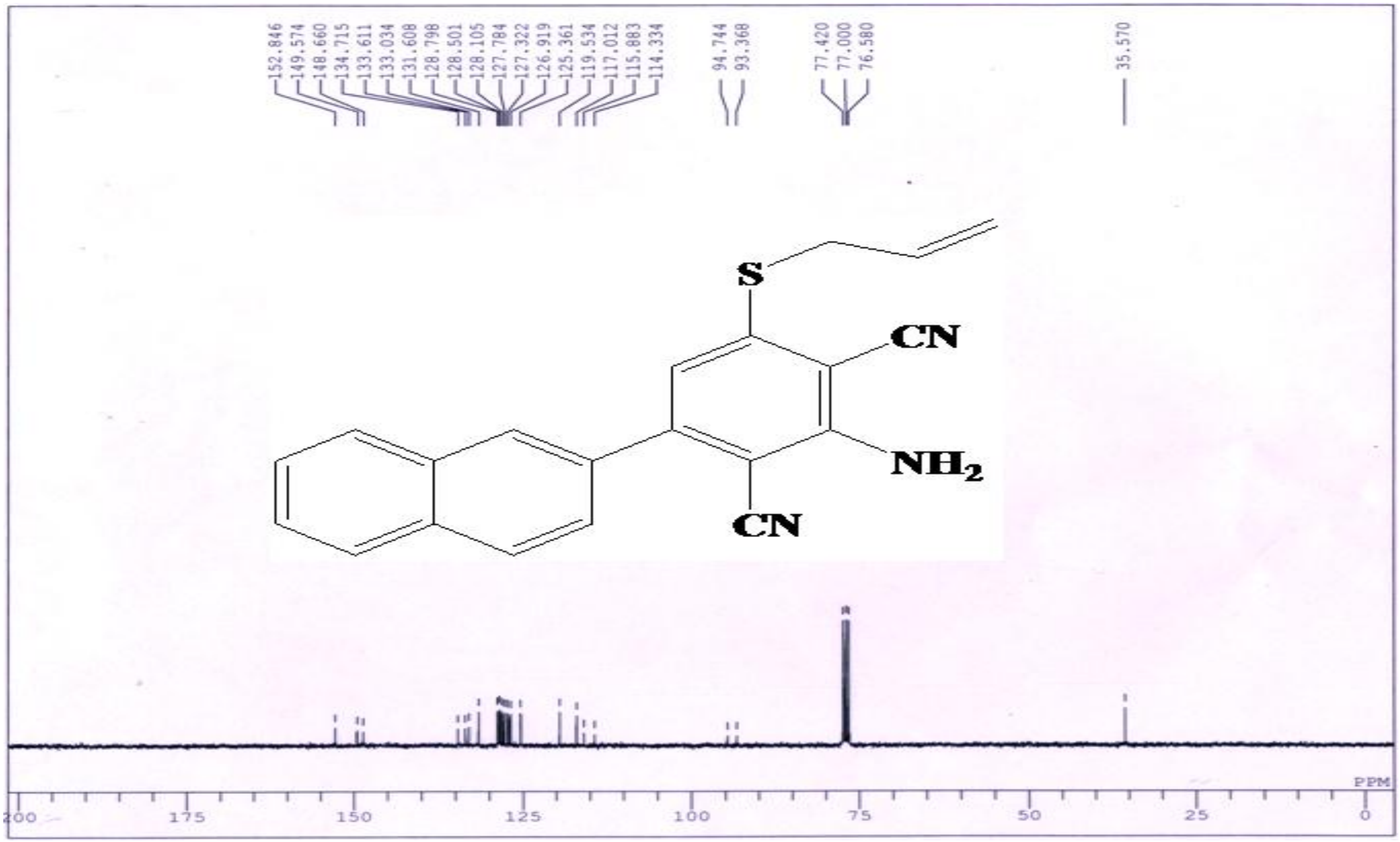


[1]H NMR SPECTRUM OF 3r



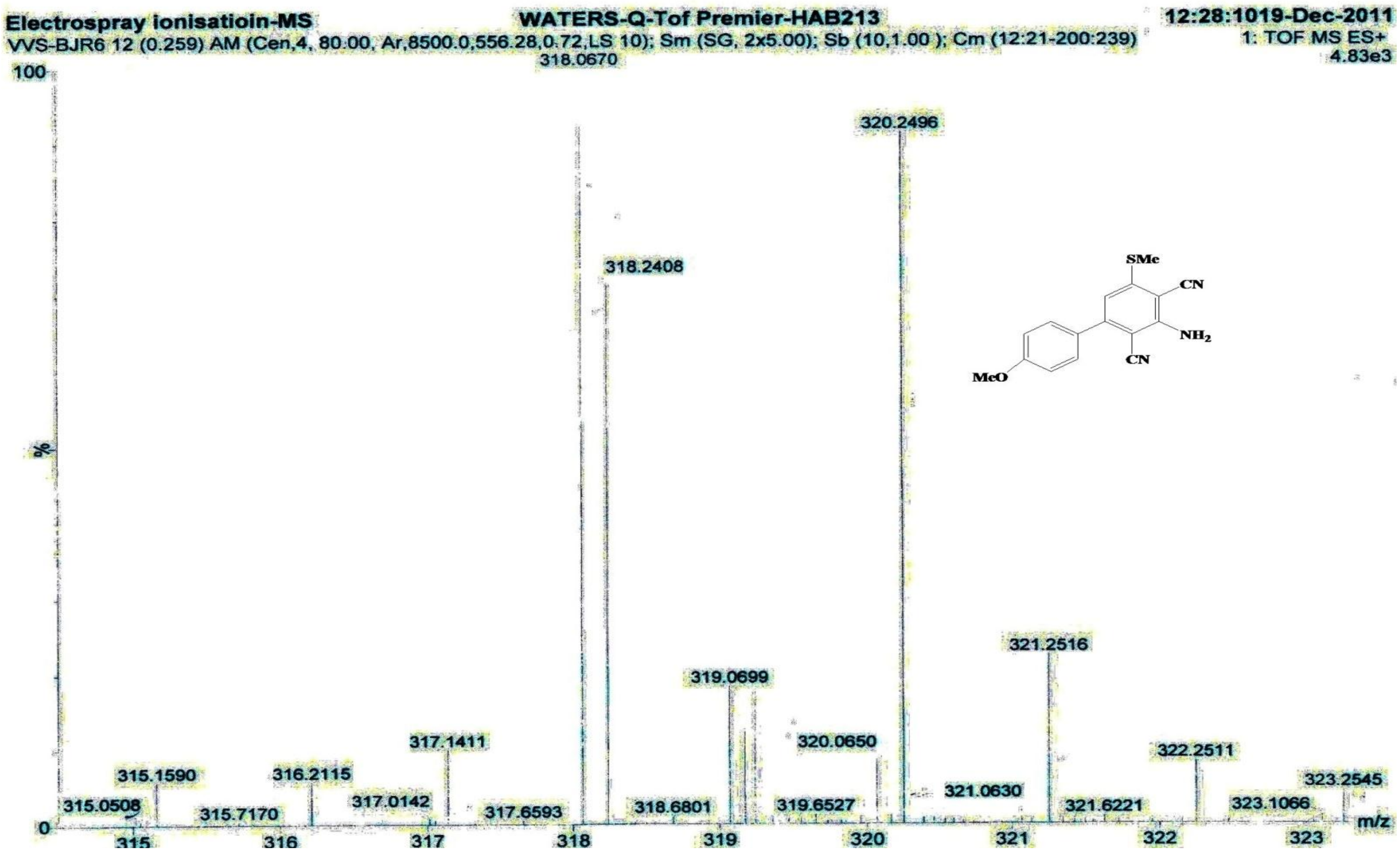
Electronic Supplementary Material (ESI) for RSC Advances

^{13}C NMR SPECTRUM OF 3r

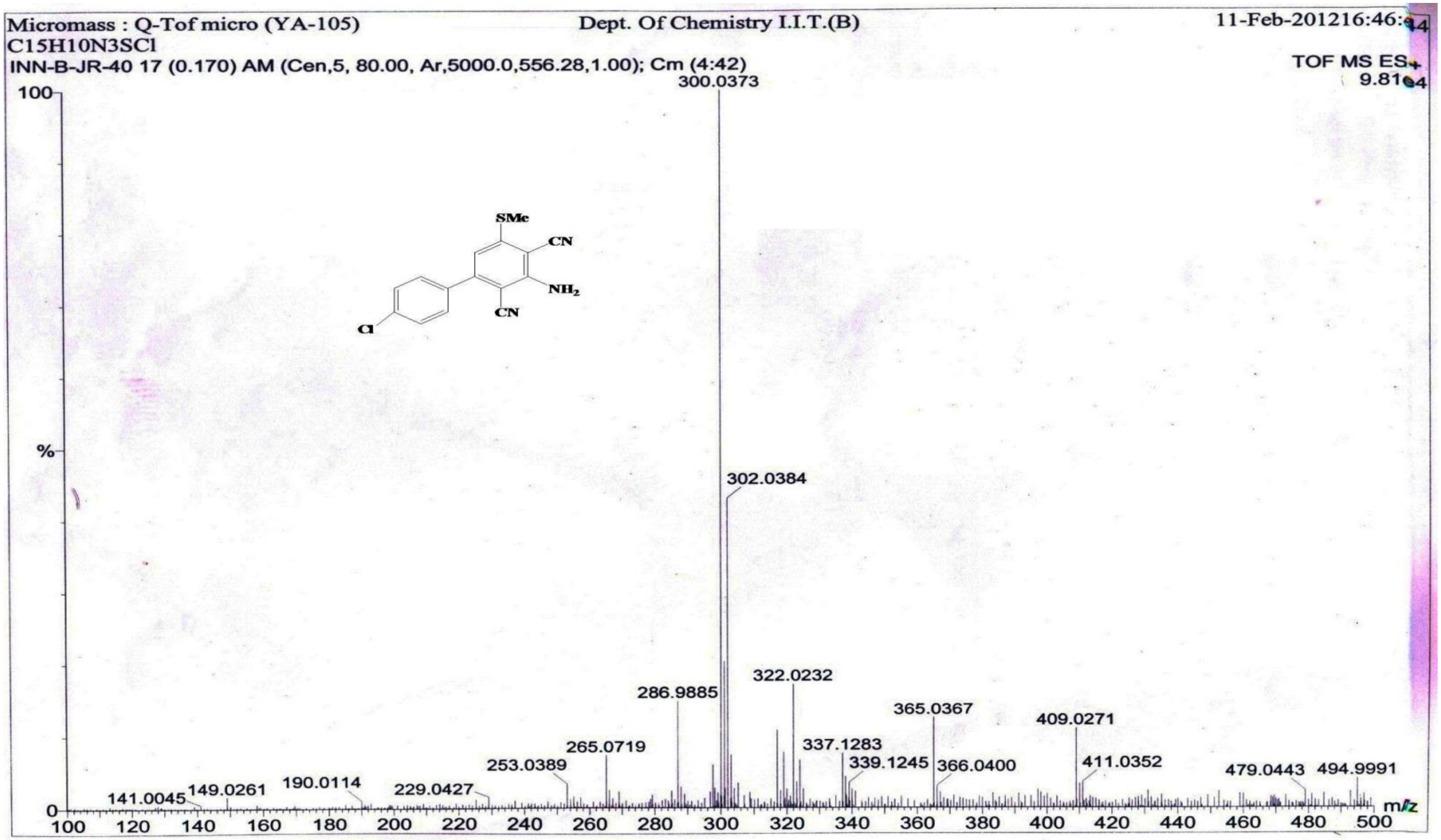


Electronic Supplementary Material (ESI) for RSC Advances

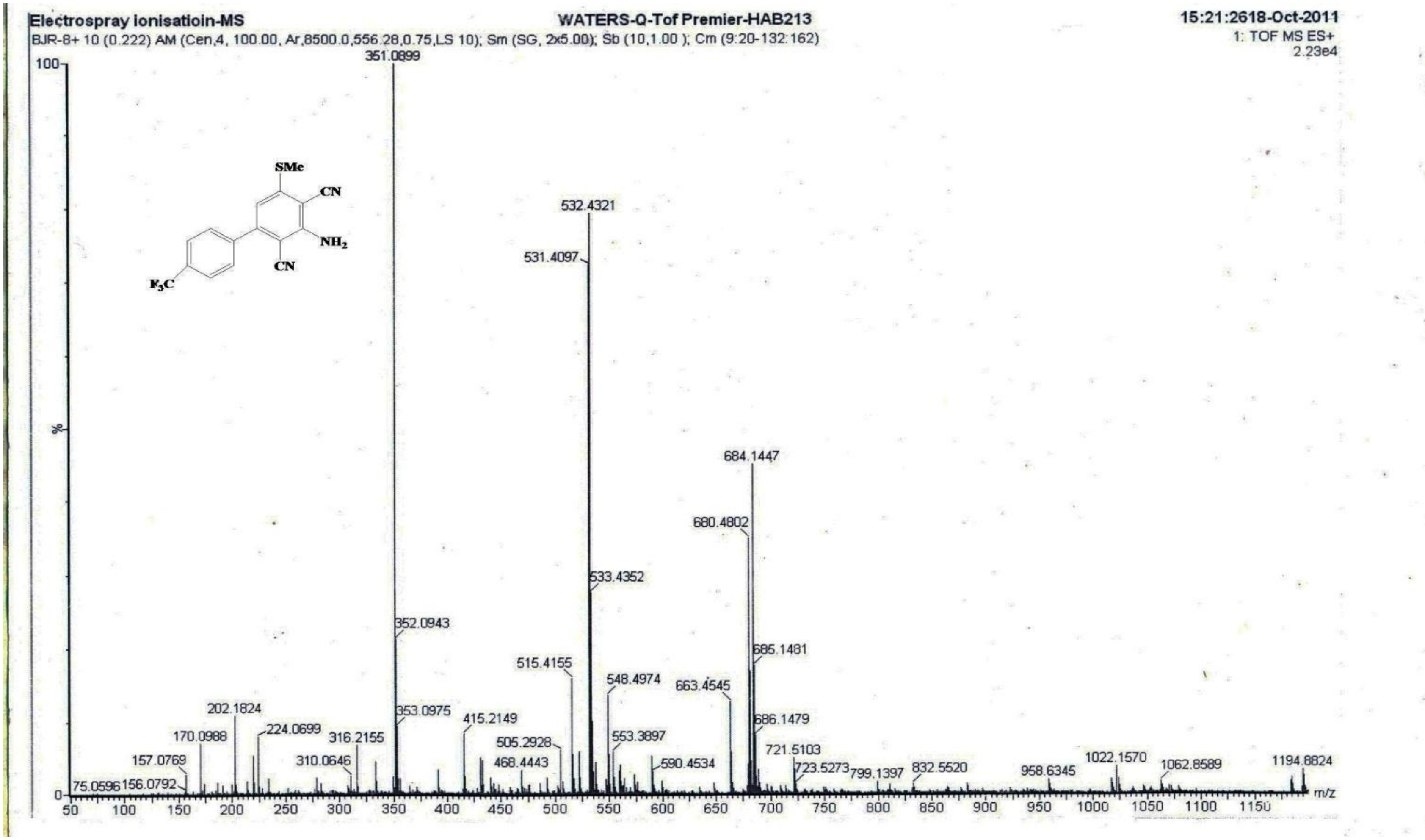
HRMS OF 3c



HRMS OF 3d


Micromass : Q-Tof micro (YA-105)
Dept. Of Chemistry I.I.T.(B)
11-Feb-201216:46:44
C15H10N3SCl
INN-B-JR-40 17 (0.170) AM (Cen,5, 80.00, Ar,5000.0,556.28,1.00); Cm (4:42)
TOF MS ES+
9.81e4
300.0373
302.0384
322.0232
286.9885
365.0367
409.0271
265.0719
337.1283
339.1245
366.0400
411.0352
253.0389
479.0443
494.9991
190.0114
229.0427
149.0261
141.0045
SMe
CN
NH2
CN
Cl
100
%
0
m/z

HRMS OF 3e


Electrospray ionisatioin-MS
WATERS-Q-Tof Premier-HAB213
15:21:2618-Oct-2011
BJR-8+ 10 (0.222) AM (Cen,4, 100.00, Ar,8500.0,556.28,0.75,LS 10); Sm (SG, 2x5.00); Sb (10,1.00); Cm (9:20-132:162)
1: TOF MS ES+
2.23e4
SMe
CN
NH2
CN
F3C
351.0899
532.4321
531.4097
684.1447
680.4802
533.4352
352.0943
685.1481
515.4155
548.4974
663.4545
202.1824
353.0975
415.2149
686.1479
170.0988
224.0699
316.2155
505.2928
553.3897
721.5103
157.0769
310.0646
468.4443
590.4534
723.5273
799.1397
832.5520
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1062.8589
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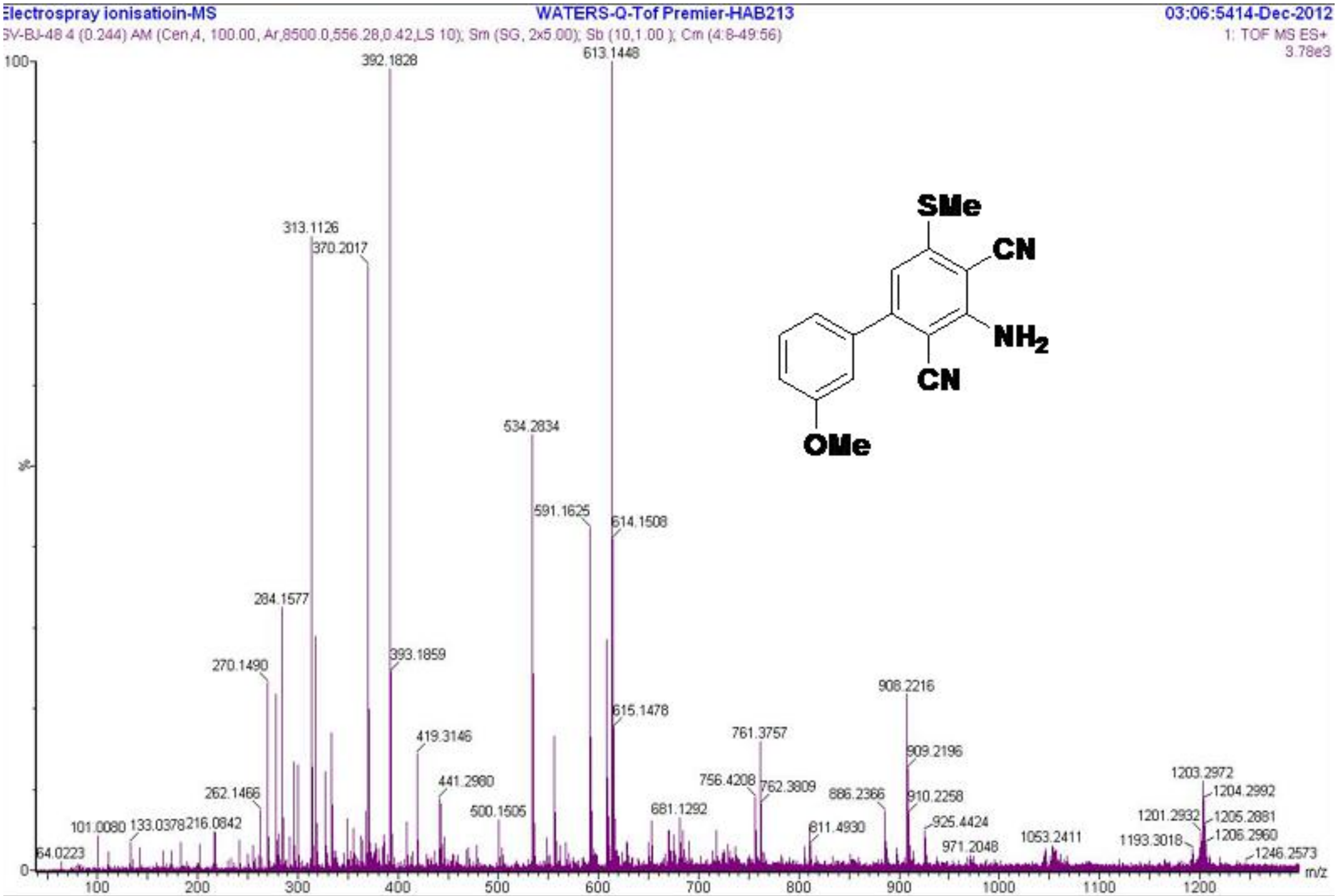
75.0596
156.0792
100
%
0
m/z

HRMS OF 3f


Electrospray ionisatioin-MS
WATERS-Q-Tof Premier-HAB213
03:06:5414-Dec-2012
1: TOF MS ES+
3.78e3
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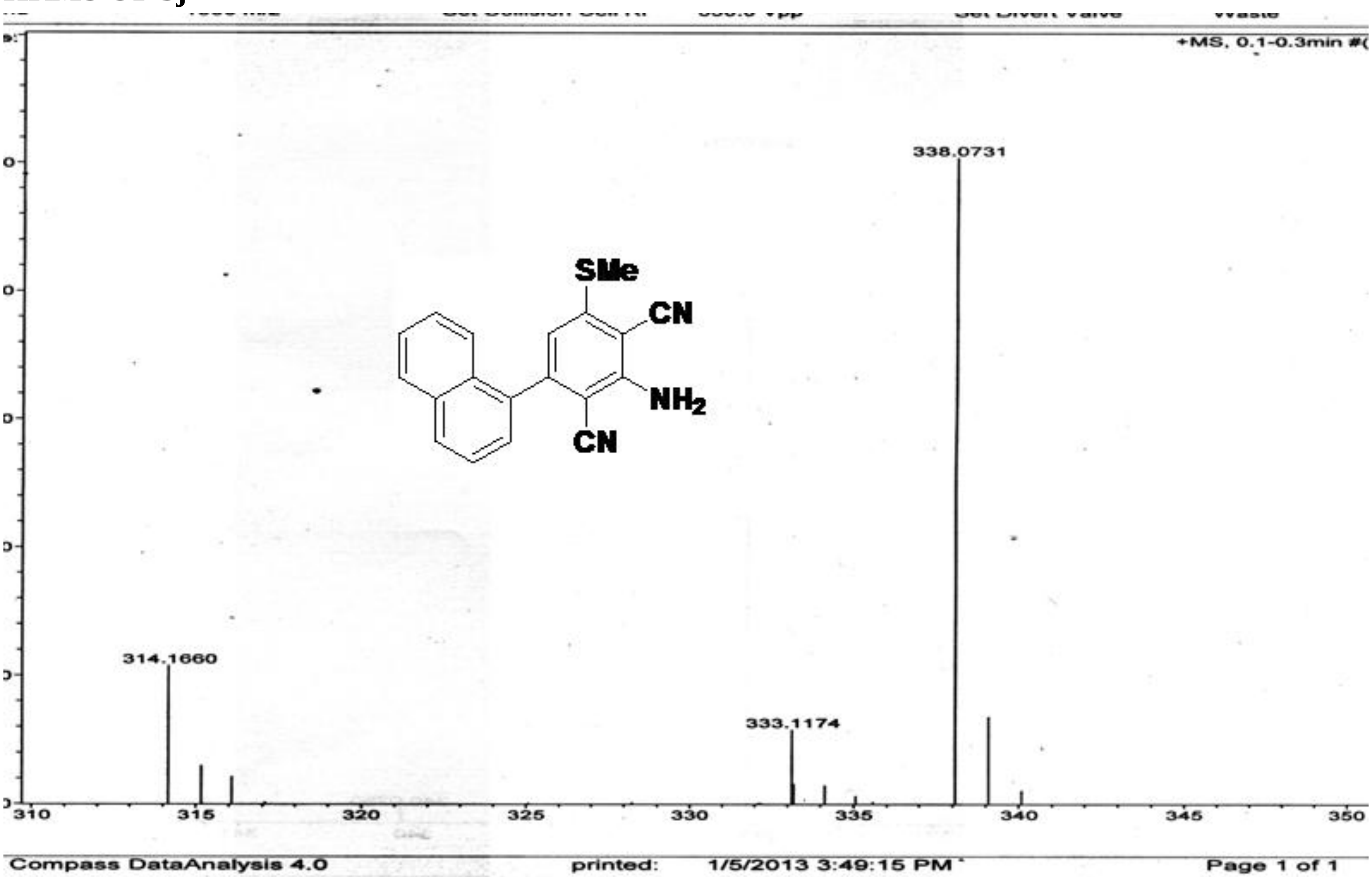
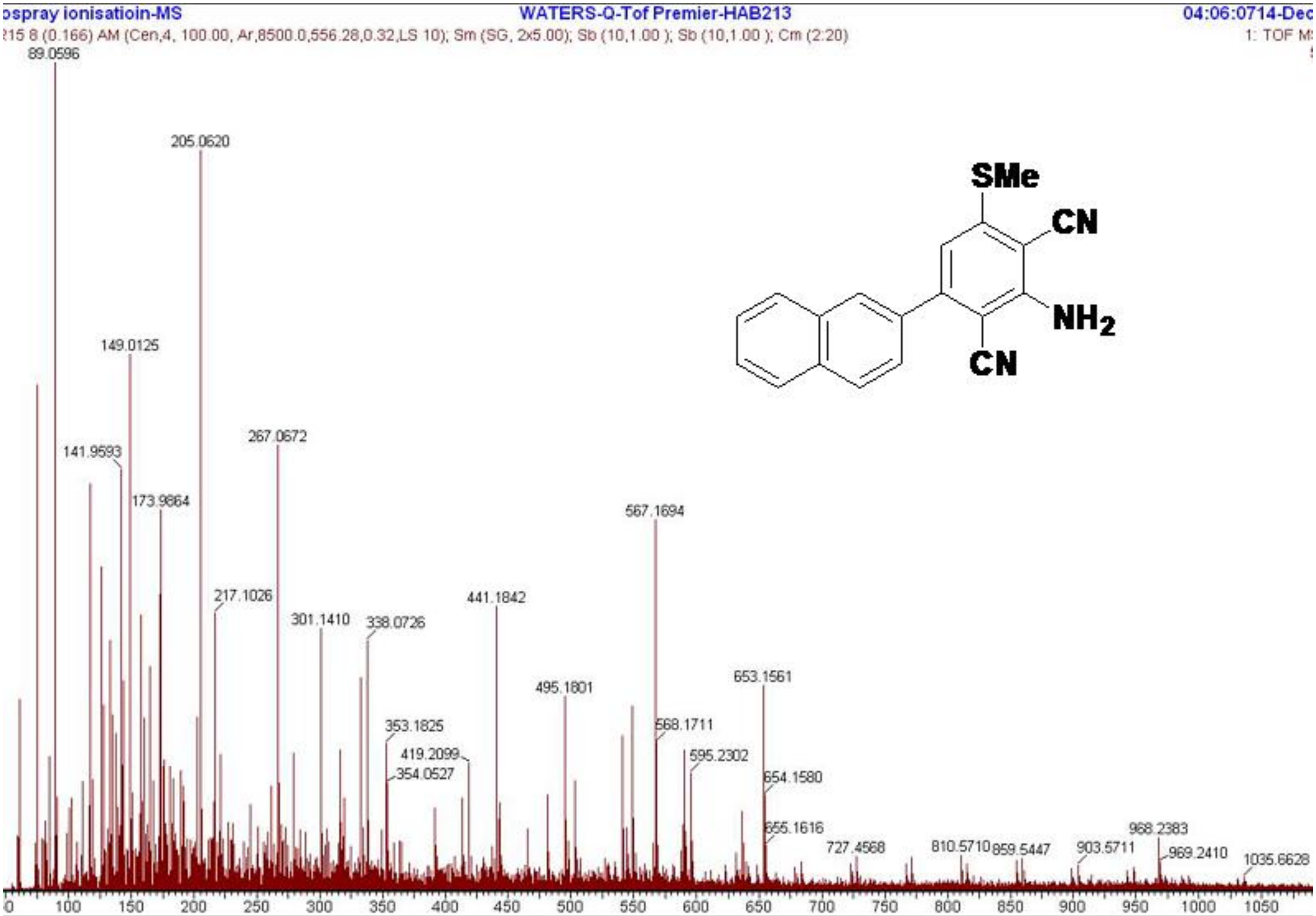
613.1448
313.1126
370.2017
534.2834
591.1625
614.1508
284.1577
393.1859
270.1490
908.2216
615.1478
761.3757
419.3146
909.2196
441.2980
756.4208
762.3809
886.2366
910.2258
1203.2972
1204.2992
262.1466
500.1505
681.1292
1201.2932
1205.2881
101.0080
133.0378
216.0842
811.4930
925.4424
1053.2411
1193.3018
1206.2960
64.0223
971.2048
1246.2573
m/z
SMe
CN
NH2
CN
OMe

HRMS OF 3j

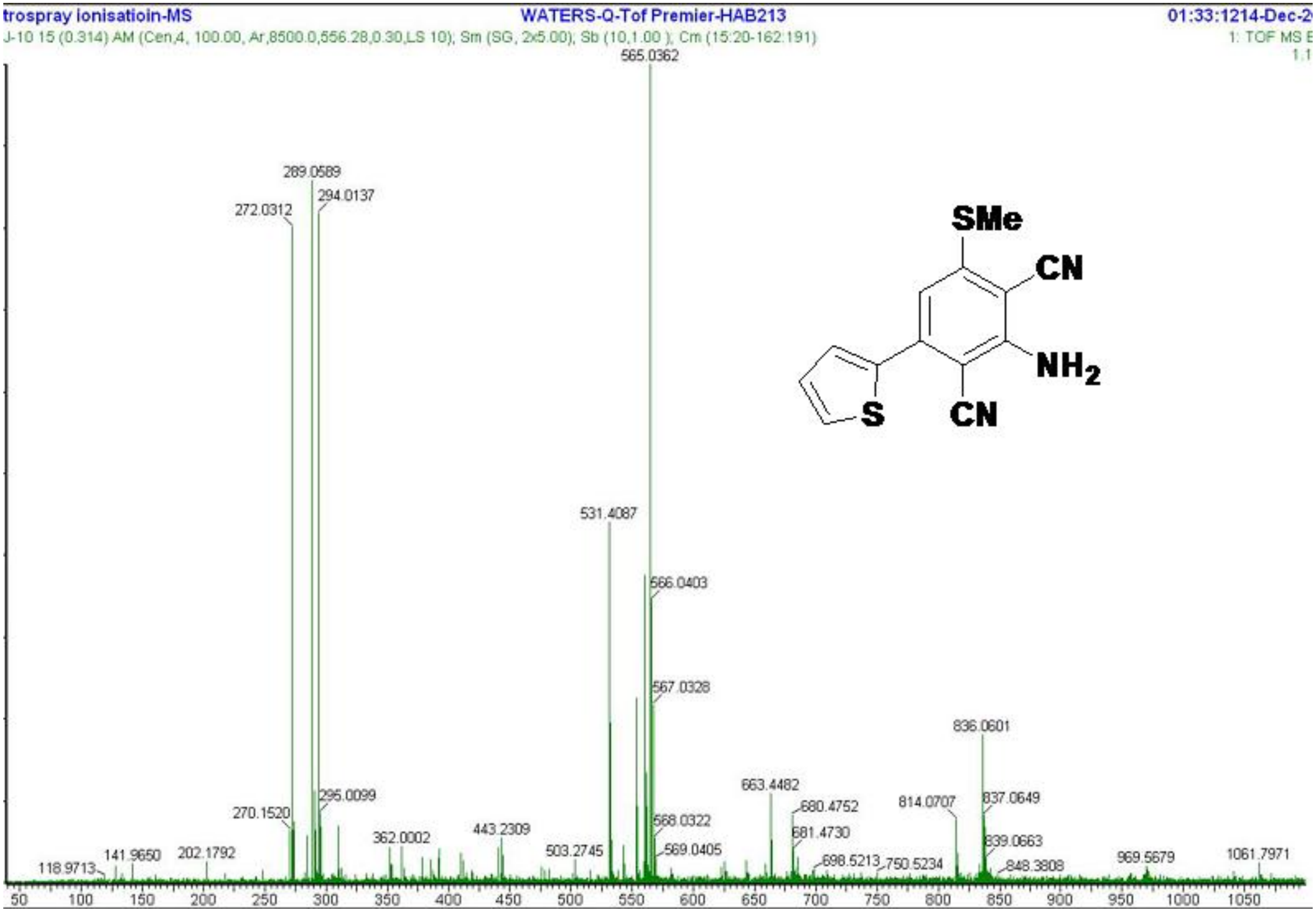

+MS, 0.1-0.3min #(
338.0731
314.1660
333.1174
SMe
CN
NH2
CN
310
315
320
325
330
335
340
345
350
Compass DataAnalysis 4.0
printed:
1/5/2013 3:49:15 PM
Page 1 of 1

Electronic Supplementary Material (ESI) for RSC Advances

HRMS OF 3k



HRMS OF 3l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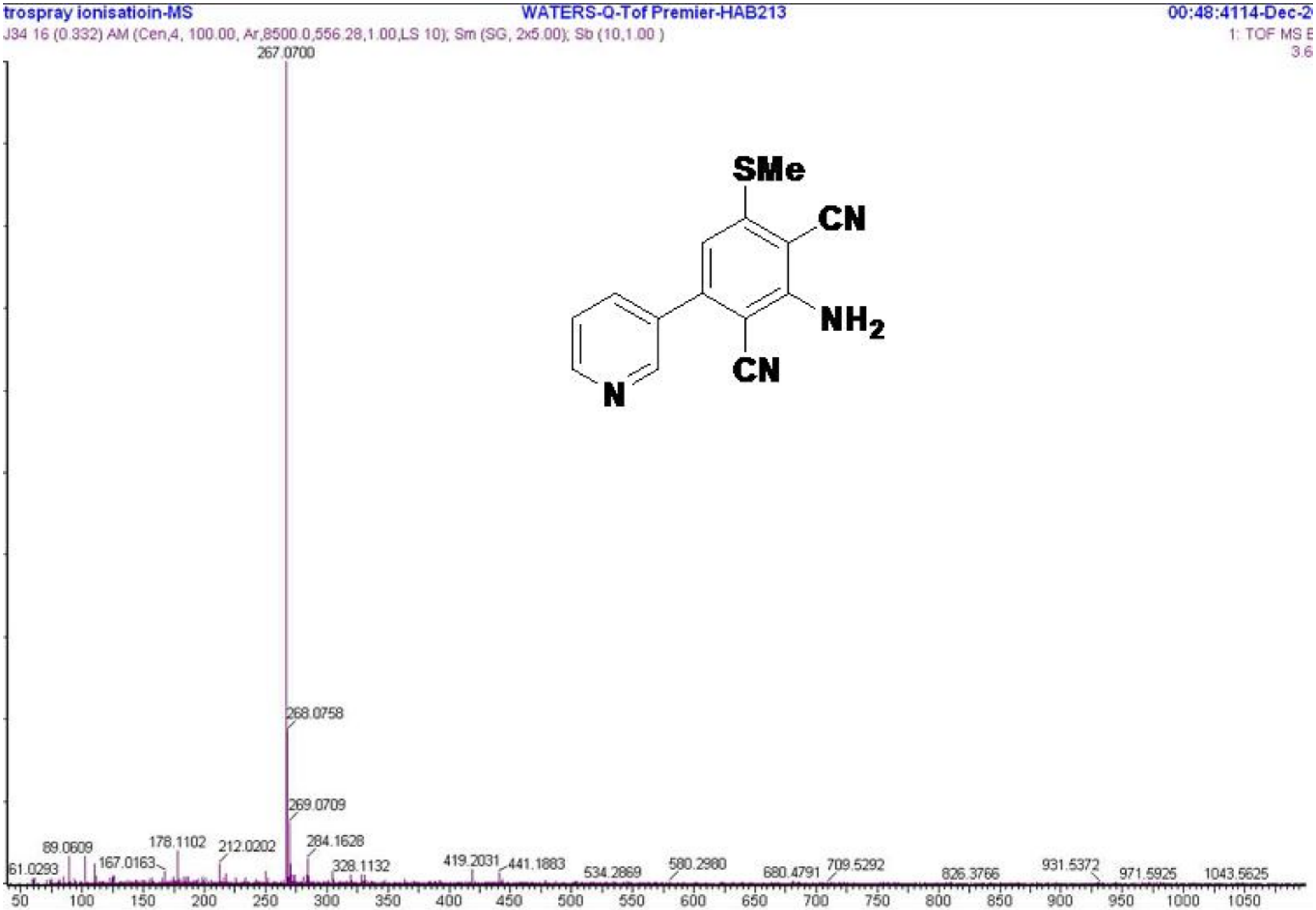
01:33:1214-Dec-2
J-10 15 (0.314) AM (Cen,4, 100.00, Ar,8500.0,556.28,0.30,LS 10); Sm (SG, 2x5.00); Sb (10,1.00); Cm (15:20-162:191)
1: TOF MS E
565.0362
289.0589
294.0137
272.0312
531.4087
566.0403
567.0328
836.0601
663.4482
295.0099
270.1520
680.4752
814.0707
837.0649
568.0322
681.4730
443.2309
362.0002
839.0663
503.2745
569.0405
141.9650
202.1792
698.5213
750.5234
848.3808
969.5679
1061.7971
118.9713
SMe
CN
NH2
S
CN

HRMS OF 3n


trospray ionisatioin-MS
WATERS-Q-Tof Premier-HAB213
00:48:4114-Dec-2
J34 16 (0.332) AM (Cen,4, 100.00, Ar,8500.0,556.28,1.00,LS 10); Sm (SG, 2x5.00); Sb (10,1.00)
1: TOF MS E
3.6
267.0700
268.0758
269.0709
284.1628
328.1132
212.0202
178.1102
167.0163
89.0609
61.0293
419.2031
441.1883
534.2869
580.2980
680.4791
709.5292
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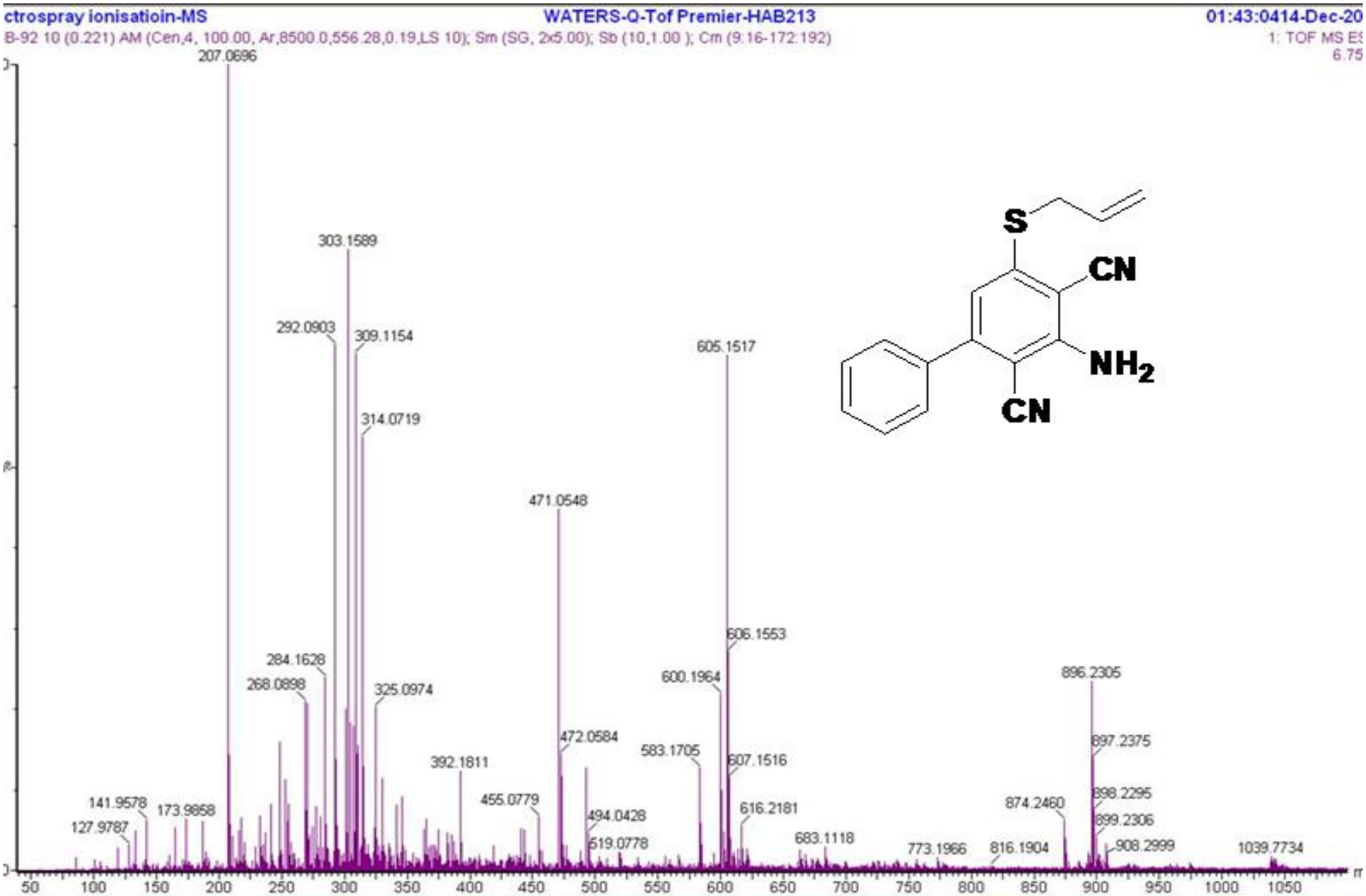
931.5372
971.5925
1043.5625
SMe
CN
NH2
CN
N

HRMS OF 3q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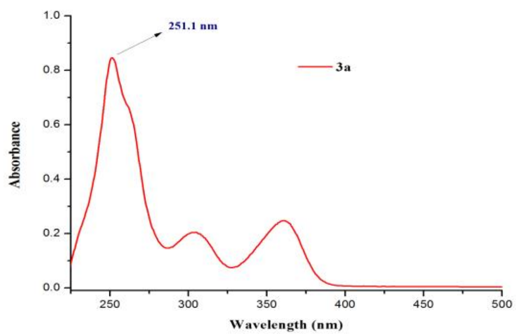
01:43:0414-Dec-20
B-92 10 (0.221) AM (Cen,4, 100.00, Ar,8500.0,556.28,0.19,LS 10); Sm (SG, 2x5.00); Sb (10,1.00); Cm (9:16-172:192)
1: TOF MS ES
6.75
207.0696
303.1589
292.0903
309.1154
314.0719
605.1517
471.0548
606.1553
284.1628
268.0898
325.0974
600.1964
896.2305
472.0584
583.1705
897.2375
392.1811
607.1516
141.9578
173.9858
455.0779
898.2295
127.9787
494.0428
616.2181
874.2460
899.2306
519.0778
683.1118
908.2999
773.1966
816.1904
1039.7734
S
CN
NH2
CN
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050

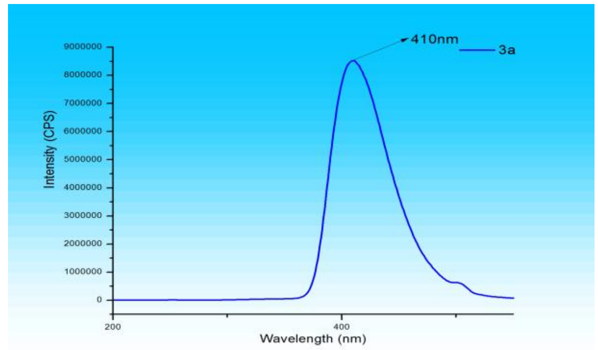
Optical Spectra: **UV-**absorption spectra were recorded in UV–visible spectrophotometer. Fluorescence spectra were recorded in spectrofluorophotometer. The concentration of compounds for UV-visible and fluorescence were 5×10^{-4} mol/L. All spectra were recorded at room temperature. For the determination of fluorescence quantum yields following equation was used

$$\Phi_s = [(A_r I_s n_s^2) / (A_s I_r n_r^2)]\, \Phi_r$$

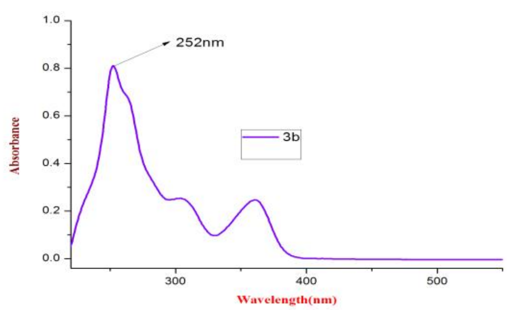
where the subscript *s* refers to the sample and the subscript *r* refers to the reference standard; Φ is quantum yield, *A* is the absorbance at the excitation wavelength, *I* is the emission intensity height, and *n* is the index of refraction (at the sodium D line) of the solvent containing the sample and the reference standard. The reference standard chosen was anthracene ($\Phi_{ref} = 0.27 \pm 0.03$ in ethanol) because its fluorescence emission is in the same range as our samples. The indices of refraction for the solvents used were taken from the commercial source and distilled by reported method.

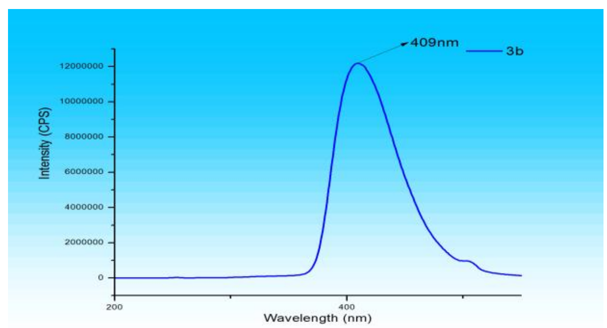
Compound 3a: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



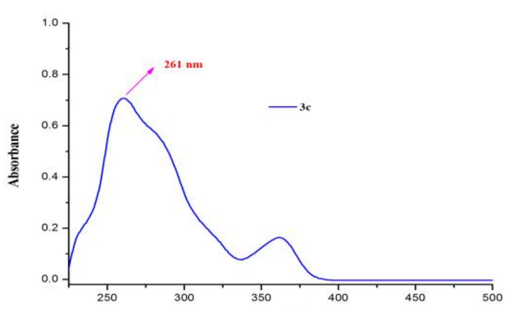


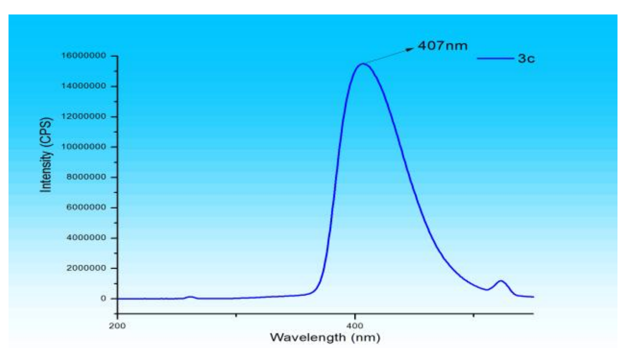
Compound 3b: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



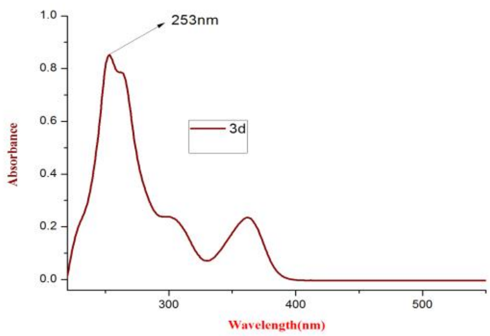


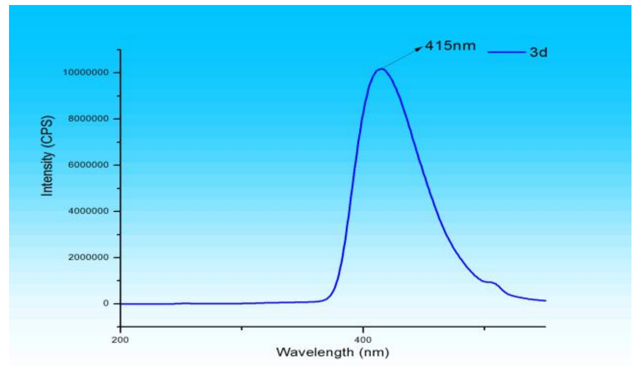
Compound 3c: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



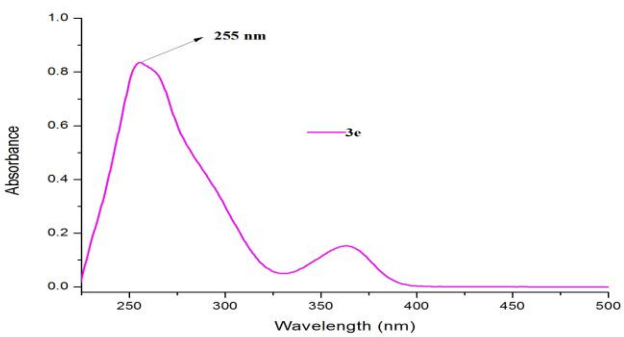


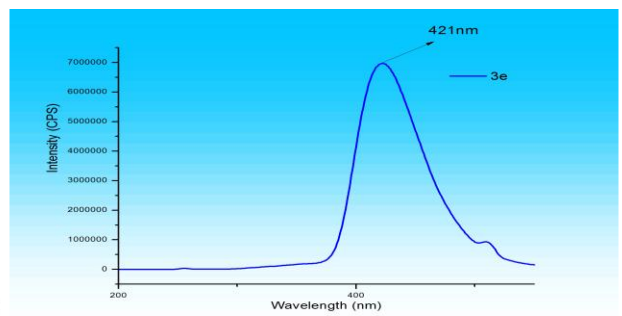
Compound 3d: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



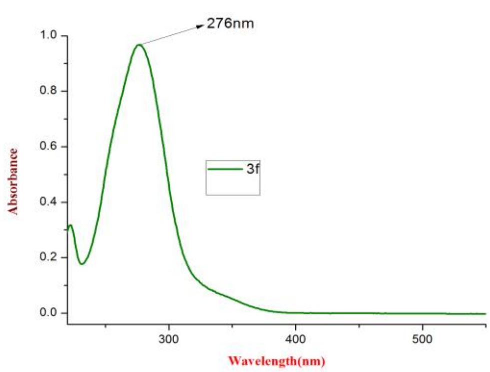


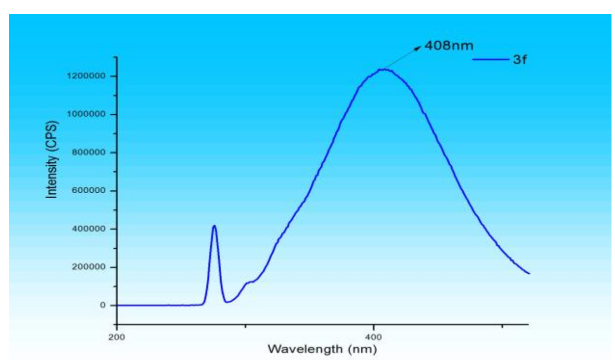
Compound 3e: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



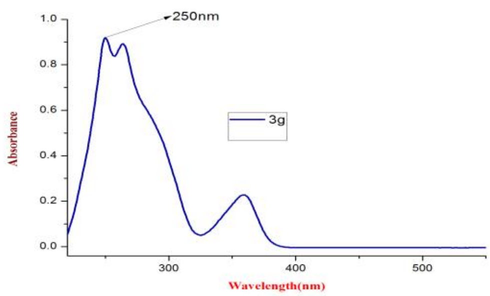


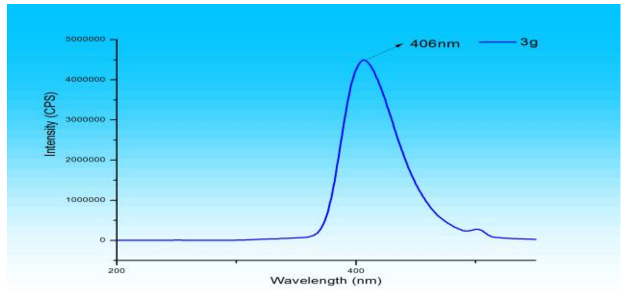
Compound 3f: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



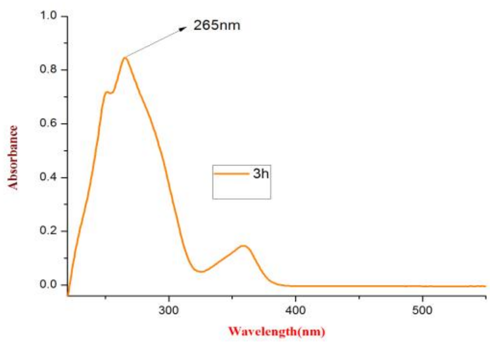


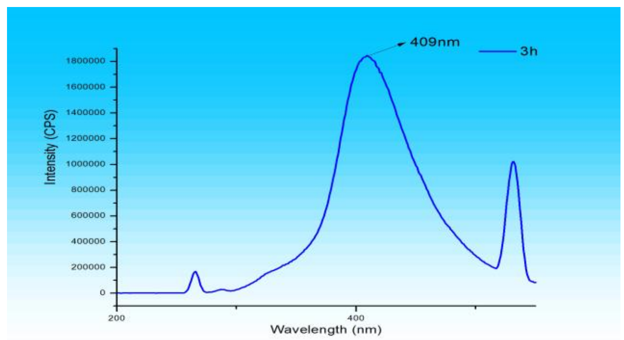
Compound 3g: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



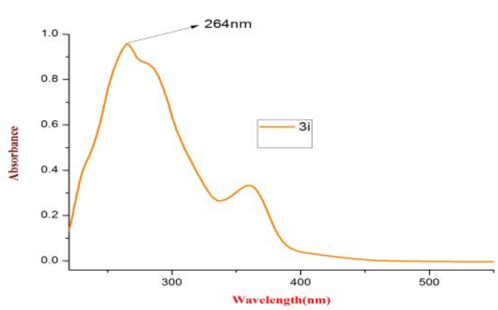


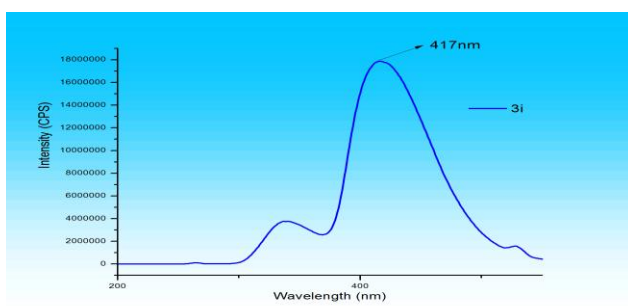
Compound 3h: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



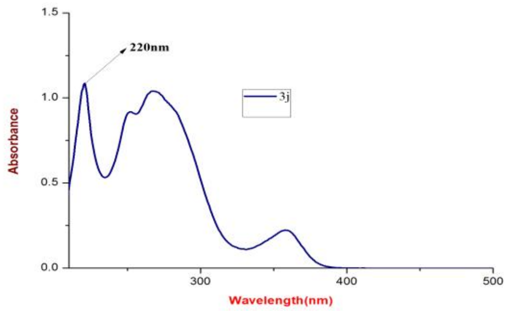


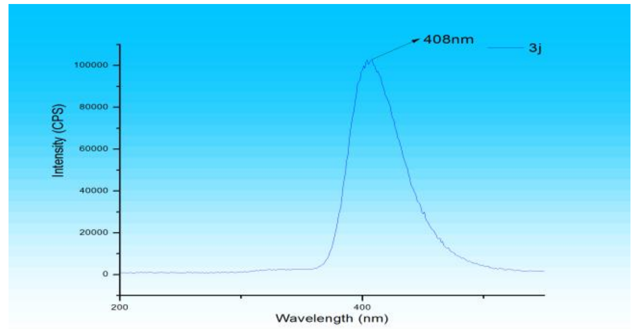
Compound 3i: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



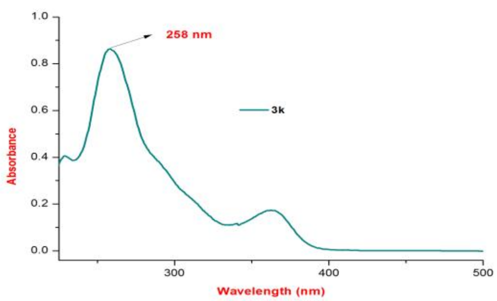


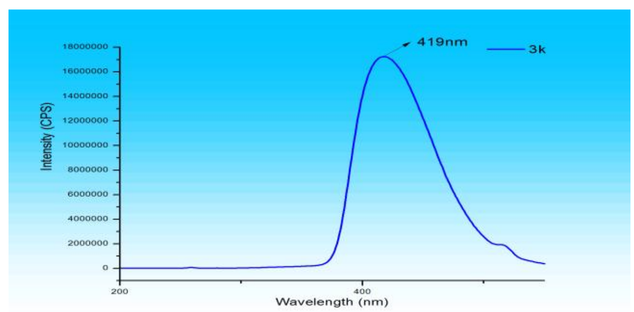
Compound 3j: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



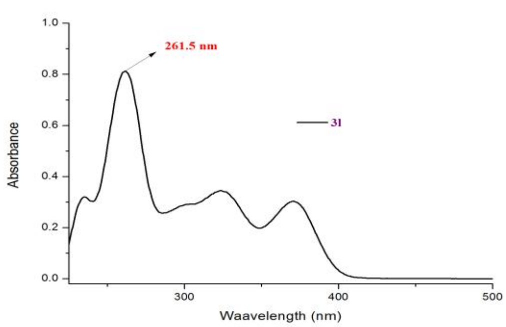


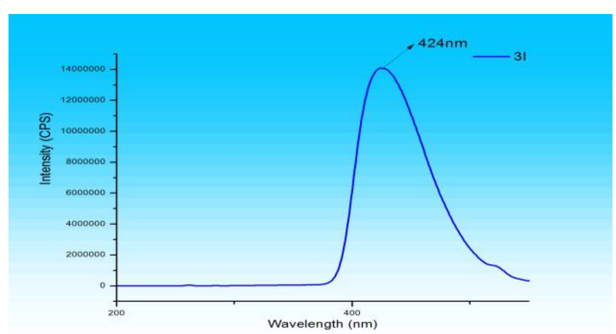
Compound 3k: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)





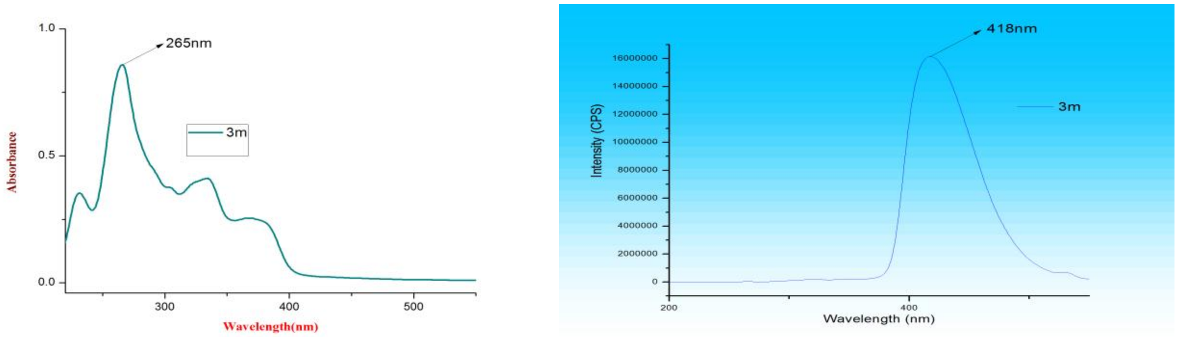
Compound 3l: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



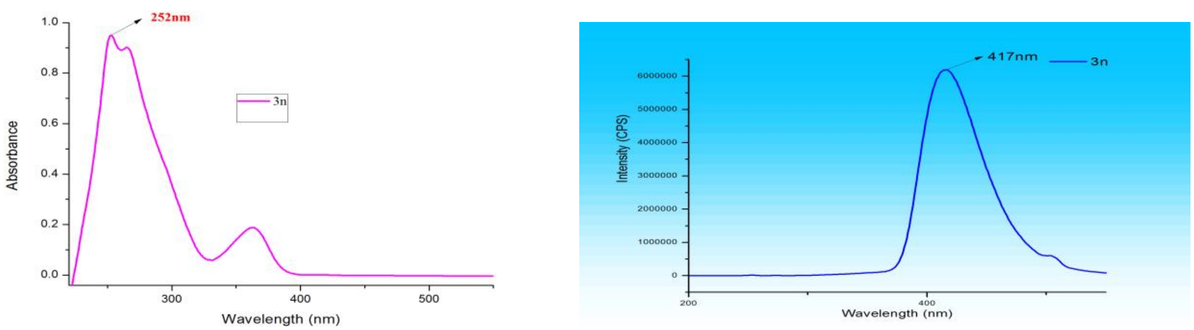


Electronic Supplementary Material (ESI) for RSC Advances

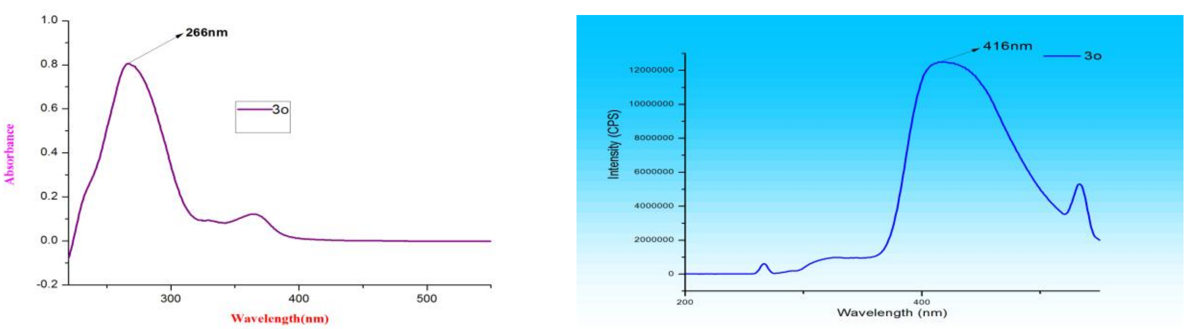
Compound 3m: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



Compound 3n: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)

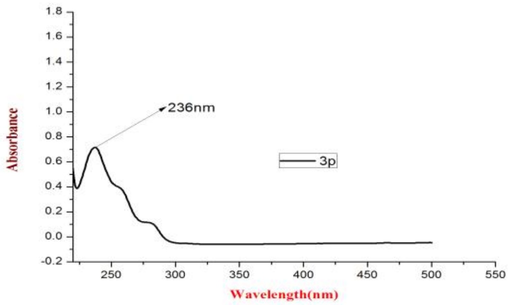


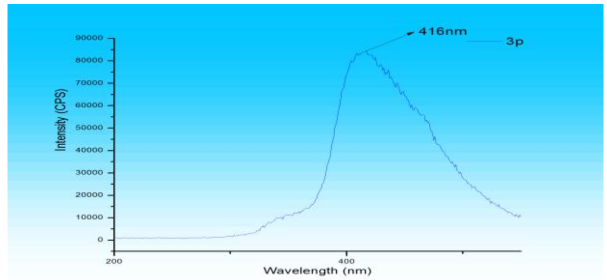
Compound 3o: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)



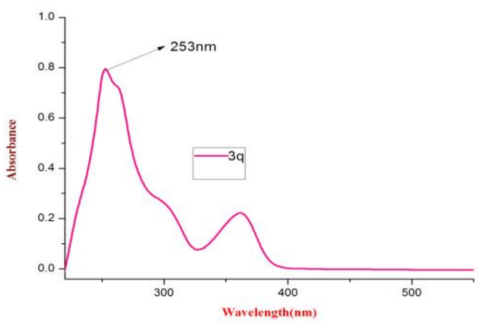
Electronic Supplementary Material (ESI) for RSC Advances

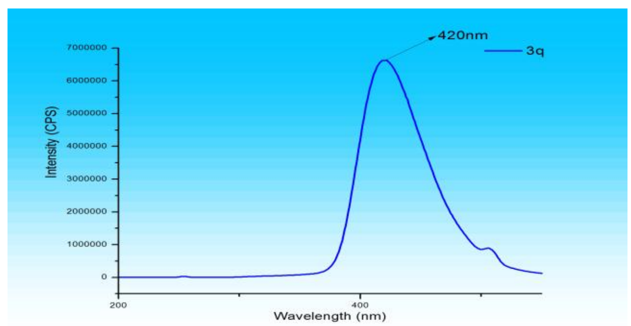
Compound 3p: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)





Compound 3q: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)





Compound 3r: UV-Vis spectrum (Left) & Fluorescence spectrum (Right)