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Supplementary Material

General

MS spectra and high resolution mass spectra were obtained on a Varian MAT 711 mass spectrometer (EI). The temperature of operation is stated at the described compound.

IR spectra were recorded on a Nicolet 750 FT infrared spectrometer. The solvent is stated at the described compound.

7-Carbomethoxy-9-cyano-8-methyl-pyrido[1,2-a]indole (5a).

IR (KBr, cm^{-1}) 3323 (m), 2953 (m), 2924 (vs), 2854 (s), 2223 (m), 1732 (s), 1603 (m), 1459 (s), 1317 (s), 1244 (s), 1201 (m), 744 (w).

MS (110°C); m/z (rel intensity) 264 (18, M^+), 204 (12), 182 (30), 181 (16), 156 (10), 155 (28), 149 (12), 97 (10), 85 (18), 71 (38), 57 (100), 55 (42).

High resolution MS calcd for $C_{16}H_{12}N_2O_2$ (M^+) 264.0898, found 264.0898.

7-Carbomethoxy-9-cyano-1,8-dimethyl-pyrido[1,2-a]indole (5b).

IR ($CHCl_3$, cm^{-1}) 3019 (s), 2977 (m), 2953 (s), 2189 (m), 1731 (s), 1668 (s), 1605 (vs), 1440 (s), 1262 (s), 1161 (s), 1106 (m).

MS (150°C) m/z (rel intensity) 278 (26, M^+), 277 (19, M^+-H), 218 (6, M^+-$COCH_3$), 168 (28), 95 (31), 83 (31), 55 (100).

High resolution MS calcd for $C_{17}H_{14}N_2O_2$ (M^+) 278.1044, found 278.1055

7-Carbomethoxy-9-cyano-10-(2-ethoxy ethyl)-8-methyl-pyrido[1,2-a]indole (5c).

IR (CCl_4, cm^{-1}) 2868 (m), 2222 (w, CN), 1729 (vs, CO), 1605 (s), 1465 (m), 1329 (m), 1264 (vs), 1111 (m).

MS (135°C) m/z (rel intensity) 336 (18, M^+), 322 (12), 277 (100, M^+-COOCH3), 217 (18), 149 (20), 55 (12).

High resolution MS calcd for $C_{20}H_{20}N_2O_3$ (M^+) 336.1743, found 336.1743

6-Dimethylamino-7,9-dicyano-7,8,10-trimethyl-6,7-dihydro-pyrido[1,2-a]indole (6b).

IR (CCl_4, cm^{-1}) 2927 (m), 2230 (w, CN), 1456 (s), 1436 (s), 1338 (vs), 1216 (m), 1062 (m), 1044 (m), 1016 (m).

MS (110°C) m/z (rel intensity) 304 (56, M^+) 260 (60, M^+-$N(CH_3)_2$), 245 (100), 119 (28), 117 (28), 57 (22), 55 (20).

High resolution MS calcd for $C_{19}H_{20}N_4$ (M^+) 330.1844, found 330.1844

***cis*-6-(1-Pyrrolidinyl)-7,8,10-trimethyl-7,9-dicyano-6,7-dihydro-pyrido[1,2-a]indole (7b).**

IR (CCl_4, cm^{-1}) 2974 (w), 2230 (w, CN), 1734 (w), 1457 (m), 1337 (s), 1216 (vs), 1128 (m).

MS (160°C) m/z (rel intensity) 330 (26, M^+), 2612 (100, M^+-C_4H_7N), 245 (46), 149 (16), 73 (72), 70 (30), 57 (56).

High resolution MS calcd for $C_{21}H_{22}N_4$ (M^+) 330.1844, found 330.1844.

***trans*-6-(1-Pyrrolidinyl)-7,8,10-trimethyl-7,9-dicyano-6,7-dihydro-pyrido[1,2-a]indole (*trans*-7b).**

IR (CCl_4, cm^{-1}) 2975 (m), 2935 (m), 2229 (w, CN), 1734 (w), 1457 (s), 1338 (vs), 1216 (s), 908 (m).

MS (140°C) m/z (rel intensity) 330 (24, M^+), 261 (100, M^+-C_4H_7N), 245 (50), 149 (24), 69 (28), 57 (50), 55 (42).

High resolution MS calcd for $C_{21}H_{22}N_4$ (M^+) 330.1844, found 330.1844

Spiro[γ-butyrolactone-2,7′-(6-dimethylamino-8,10-dimethyl-9-cyano)-pyrido[1,2-a]indole] (8b).

IR (CCl_4, cm^{-1}) 2924 (m), 2228 (w, CN), 1788 (vs), 1457 (s), 1437 (s), 1339 (s), 1216 (vs), 1142 (vs), 1032 (vs).

MS (140°C) m/z (rel intensity) 335 (M^+, 28), 291 (22), 247 (100), 149 (20), 71 (24), 57 (42), 55 (34).

High resolution MS calcd for $C_{20}H_{21}N_3O_2$ (M^+) 335.1633, found 335.1633.

4a,6-Dicyano-5,7-dimethyl-indolo[1,2-a]-1,2,3,4,4a,12a-hexahydro-1,8-naphthyridine (9b).

IR (CCl_4, cm^{-1}) 2957 (w), 2927 (m), 2231 (m, CN), 2201 (w, CN), 1456 (vs), 1328 (s), 1264 (s), 1147 (w).

MS (130°C) m/z (rel intensity) 302 (100, M^+), 244 (24), 208 (36), 196 (36), 149 (39), 56 (68).

High resolution MS calcd for $C_{19}H_{18}N_4$ (M^+) 302.1531, found 302.1531.

7-(2-Ethoxyethyl)-4a,6-dicyano-5-methyl-indolo[1,2a]-1,2,3,4,4a,12a-hexahydro -1,8-naphthyridine (9c).

IR (CCl_4, cm^{-1}) 2976 (m), 2871 (m), 2230 (w, CN), 2201 (w, CN), 1457 (m), 1376 (m), 1129 (vs), 1112 (vs).

MS (130°C) m/z (rel intensity) 360 (36, M^+), 301 (100, M^+-$CH_2OC_2H_5$), 254 (14), 195 (76), 149 (22), 57 (26).

High resolution MS calcd for $C_{22}H_{24}N_4O$ (M^+) 360.1950, found 360.1950.

4a-Carbomethoxy-6-cyano-5,7-dimethyl-indolo[1,2-a]1,2,3,4,4a,12a-hexahydro-1,8-naphthyridine (10b).

IR (CCl_4, cm^{-1}) 2955 (m), 2228 (w, CN), 1736 (vs, CO), 1457 (m), 1434 (m), 1236 (vs), 1112 (m).

MS (140°C) m/z (rel intensity) 335 (100, M^+), 276 (58, M^+-$COOCH_3$), 261 (22), 233 (20), 149 (28), 57 (46).

High resolution MS calcd for $C_{20}H_{21}N_3O_2$ (M^+) 335.1633, found 335.1634.

4a-Carbomethoxy-6-cyano-1,5,7-trimethyl-indolo[1,2-a]-1,2,3,4,4a,12a-hexahydro-1,8-naphthyridine (11b).

IR (CCl_4, cm^{-1}) 2955 (m), 2854 (w), 2789 (m), 2227 (w, CN), 1737 (vs, CO), 1457 (m), 1230 (vs), 1130 (s).

MS (80°C) m/z (rel intensity) 349 (100, M^+), 290 (18, M^+-$COOCH_3$), 233 (20), 196 (88), 181 (38), 130 (24), 70 (62), 57 (30).

High resolution MS calcd for $C_{21}H_{23}N_3O_2$ (M^+) 349.1790 found 349.1790

5-Methoxycarbonyl-2,2-dicyano-1,3-dihydro-pyrido[3,2,1-jk]carbazole (12e).

IR (CCl_4, cm^{-1}) 2929 (s), 2855 (m), 1729 (vs), 1465 (s), 1437 (s), 1263 (vs), 1102 (s).

MS (160°C) m/z (rel intensity) 315 (100, M^+), 287 (10), 256 (12, M^+-$COOCH_3$), 237 (12), 85 (12), 69 (14), 57 (26), 55 (24).

High resolution MS calcd for $C_{19}H_{13}N_3O_2$ (M^+) 315.1007, found 315.1007

Spiro[γ-butyrolactone-2,5′-6-dimethylamino-1,2,3,3a-tetrahydro-3-acetyl-pyrido[3,2,1-lm]β-carboline] (13d).

IR (CCl_4, cm^{-1}) 2941 (m), 2793 (w), 1780 (vs), 1672 (vs), 1448 (s), 1399 (vs), 1218 (s), 1145 (s), 1029 (s), 909 (m).

MS (145°C) m/z (rel intensity) 365 (16, M^+), 322 (100, M^+-$COCH_3$), 278 (78), 235 (28), 149 (16), 69 (24), 57 (50), 55 (48).

High resolution MS calcd for $C_{21}H_{23}N_3O_3$ (M^+) 365.1739, found 365.1739

1-Cyano-2-methyl-4-carbomethoxy-9H-carbazole (14a).

IR (CCl_4, cm^{-1}) 3457 (w), 2957 (m), 2936 (w), 2146 (w), 1744 (vs), 1728 (m), 1456 (s), 1436 (s), 1305 (m), 1249 (s), 1164 (s).

MS (140°C) m/z (rel intensity) 264 (100, M^+), 249 (7, M^+-CH_3), 233 (85, M^+-OCH_3), 205 (44, M^+-$COOCH_3$), 204 (42), 177 (18), 151 (11).

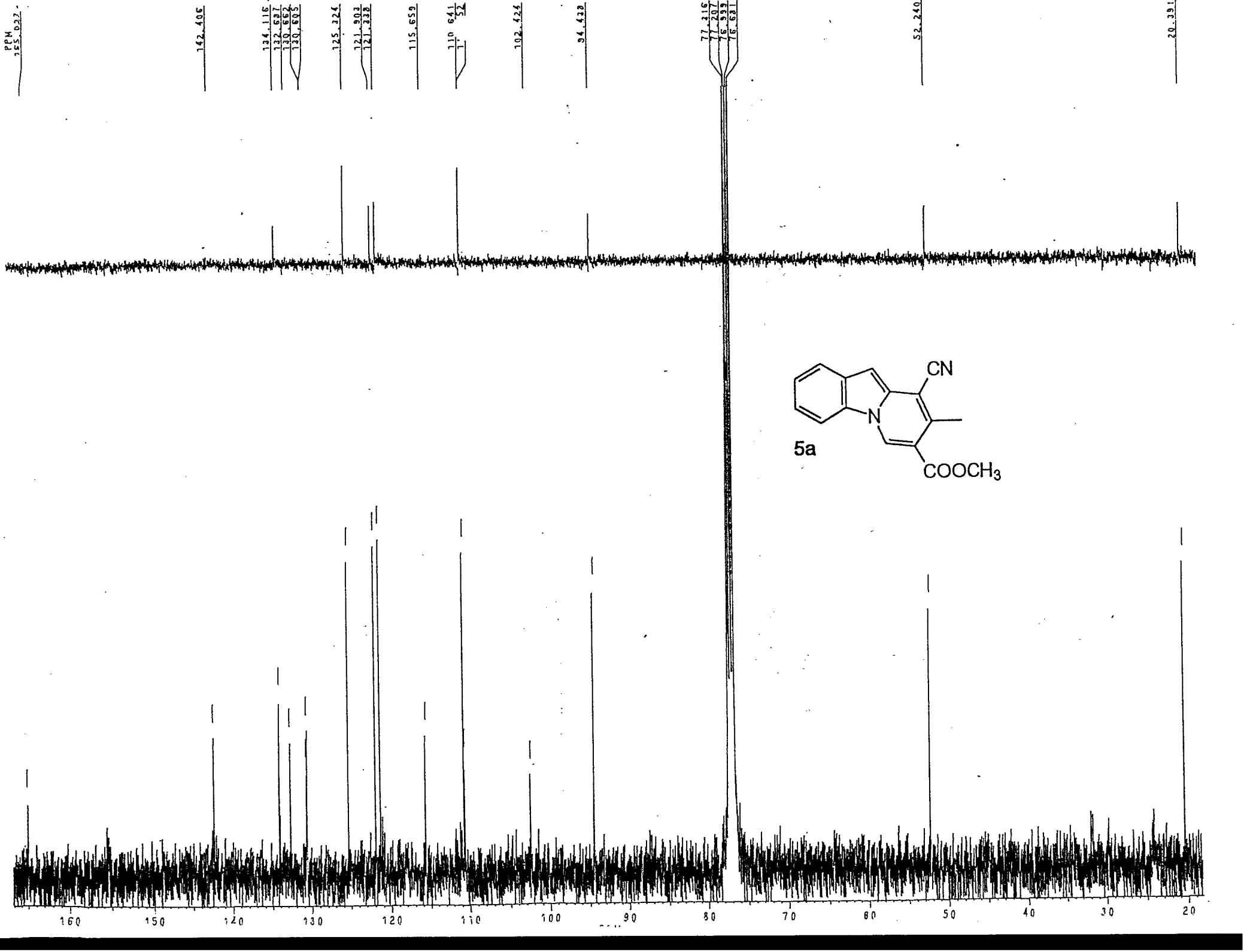
High resolution MS calcd for $C_{16}H_{12}N_2O_2$ (M^+) 264.0898, found 264.0898

2,3-Dimethyl-1,4-dicyano-9H-carbazole (15a).

IR ($CHCl_3$, cm^{-1}) 3447 (m), 3025 (m), 3014 (s), 2223 (s), 1601 (s), 1459 (s), 1420 (s), 1304 (s), 908 (vs).

MS (170°C) m/z (rel intensity) 245 (100, M^+), 244 (28, M^+-H), 230 (26, M^+-CH_3), 207 (10), 99 (18), 73 (20), 71 (21), 57 (62), 55 (38).

High resolution MS calcd for $C_{16}H_{11}N_3$ (M^+) 245.0953, found 245.0953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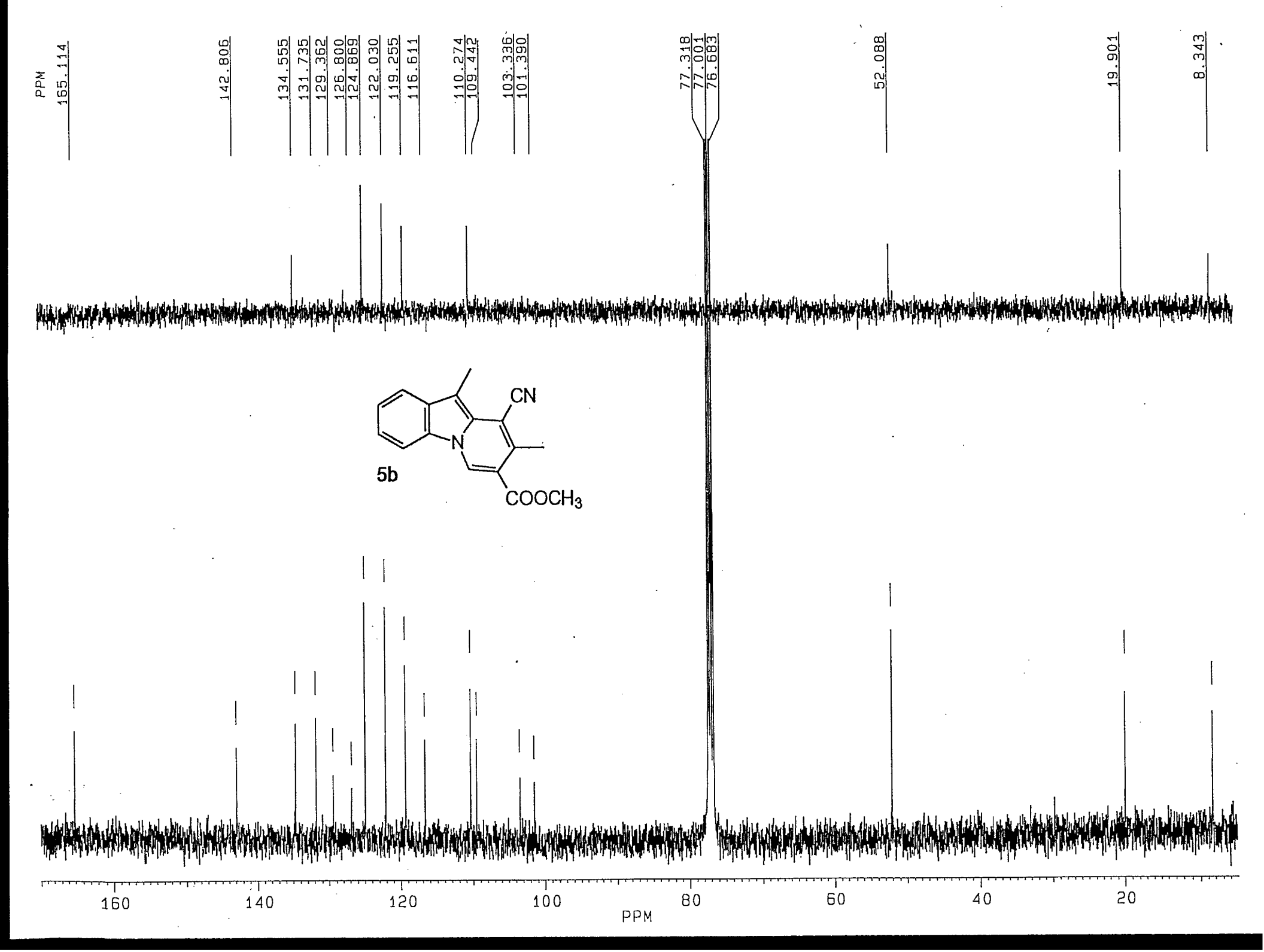
50
40
30
20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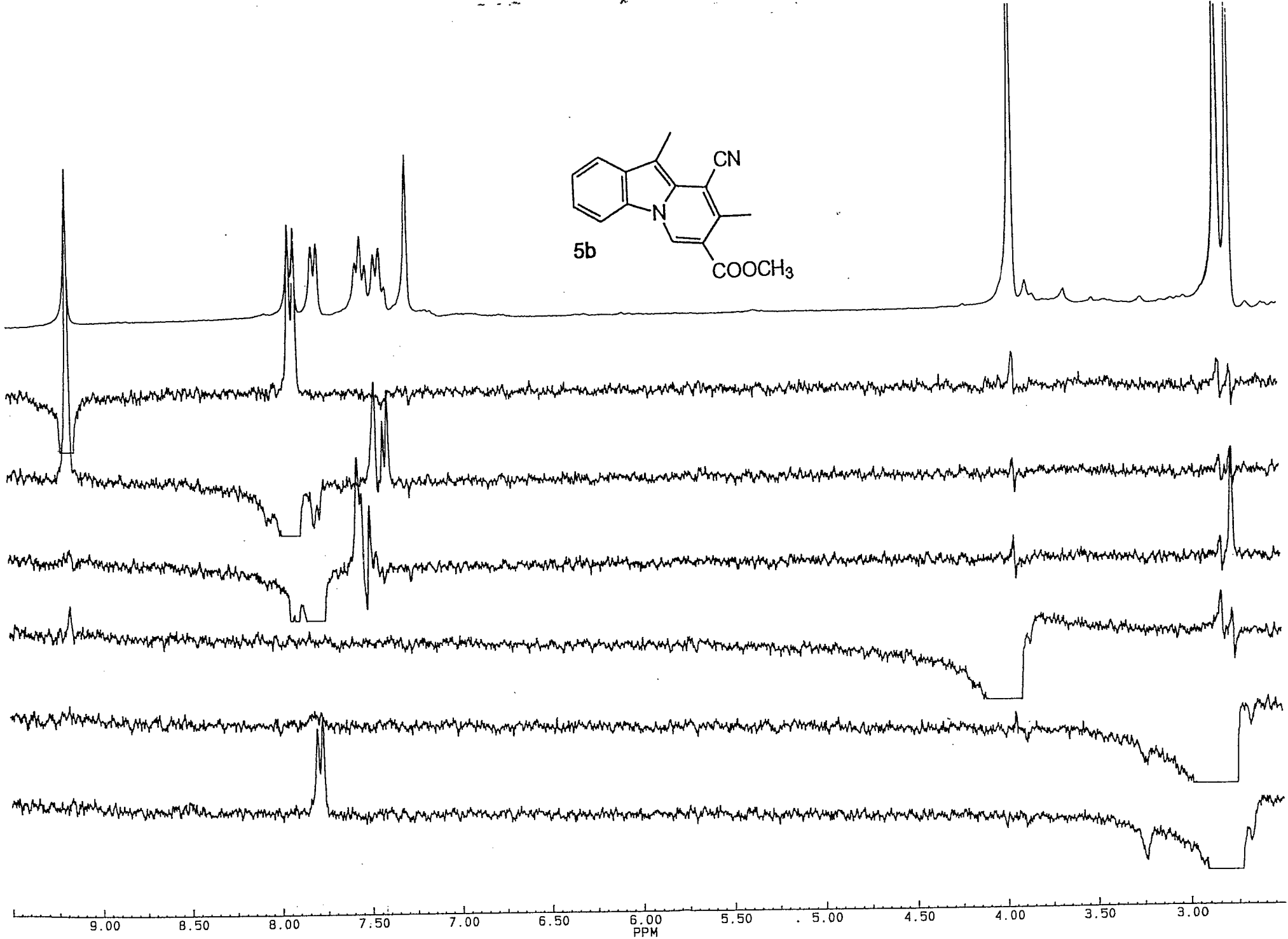
40
20
PPM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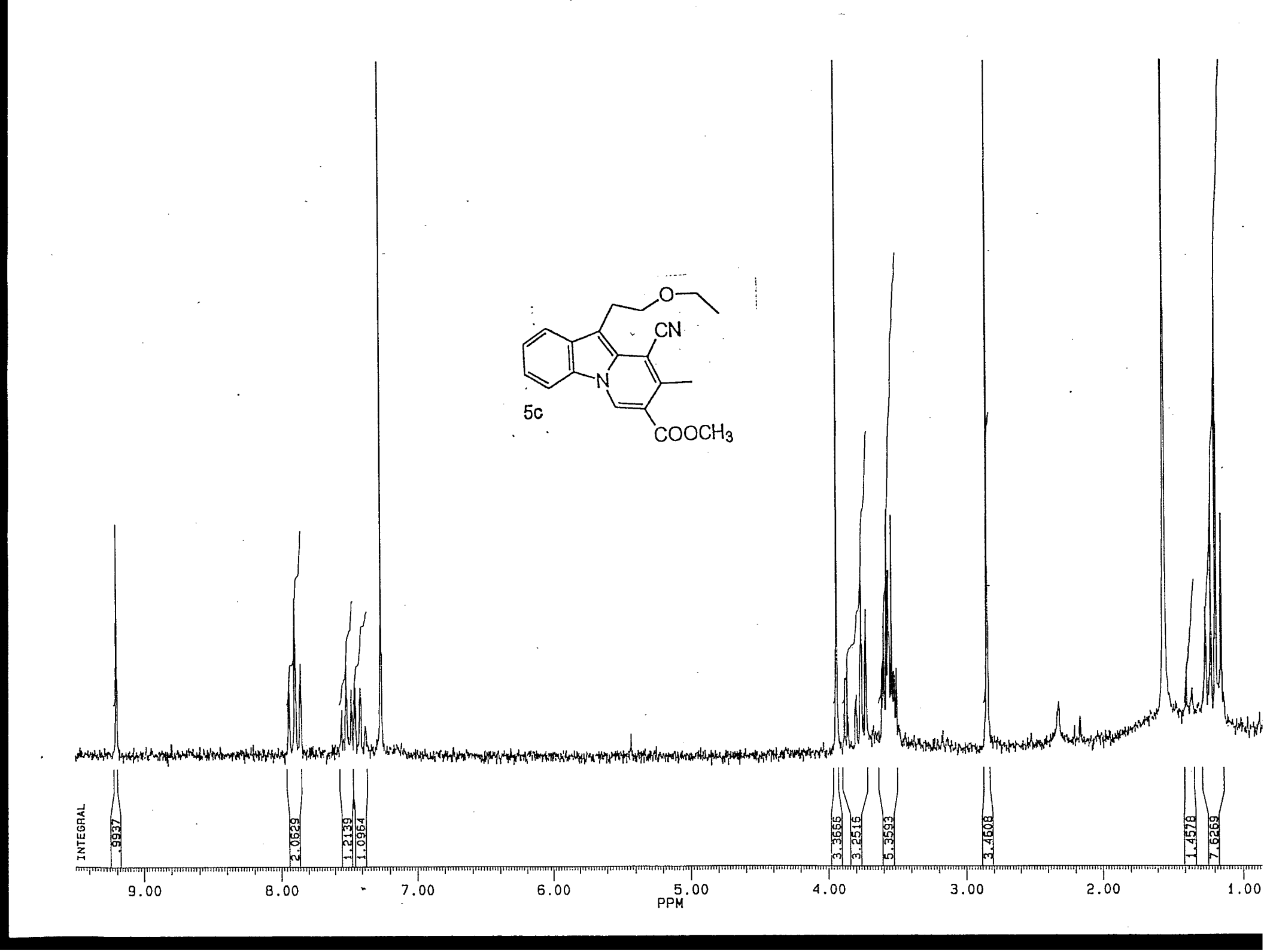
3.00
PPM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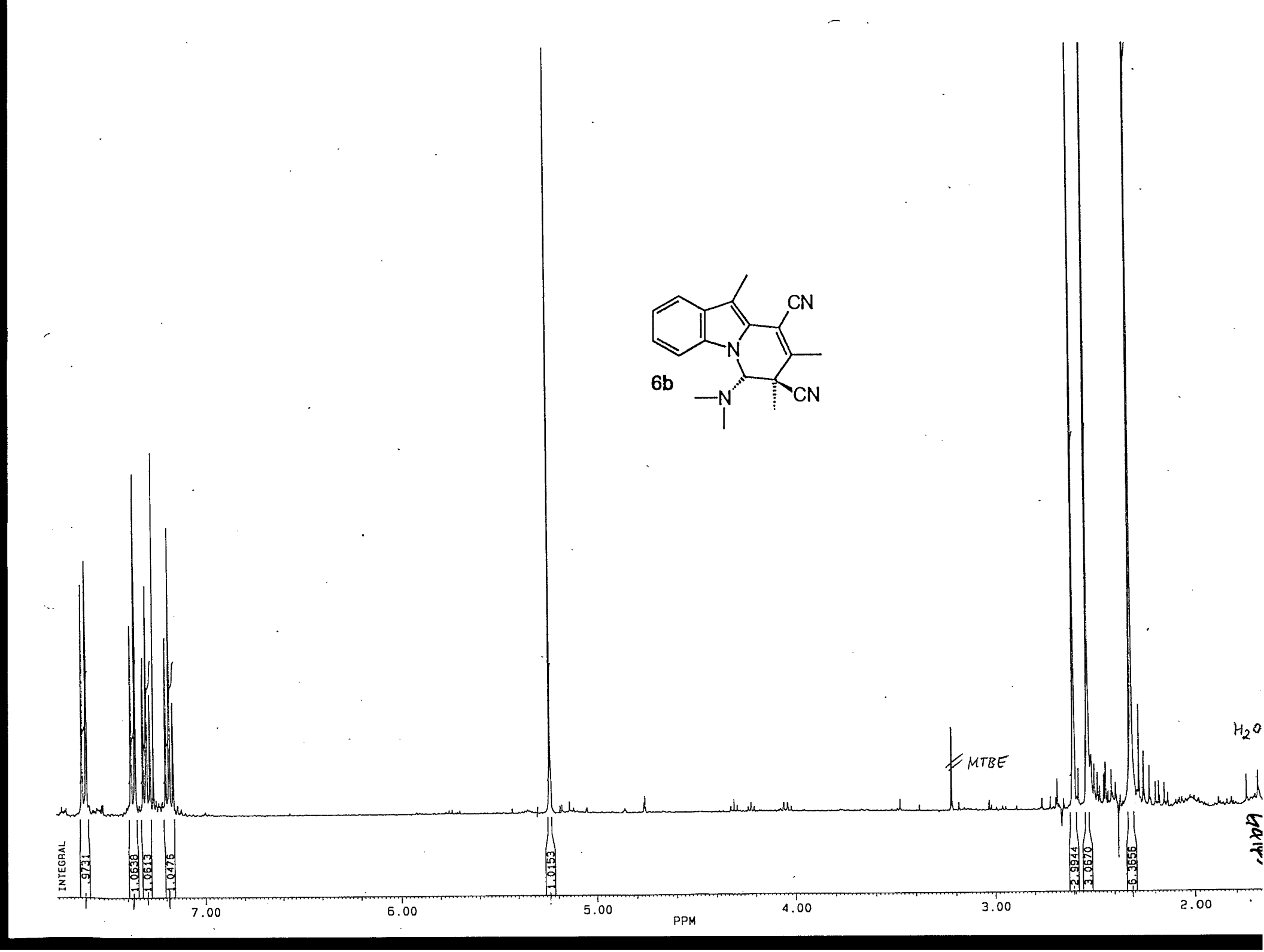
2.00
1.00
PPM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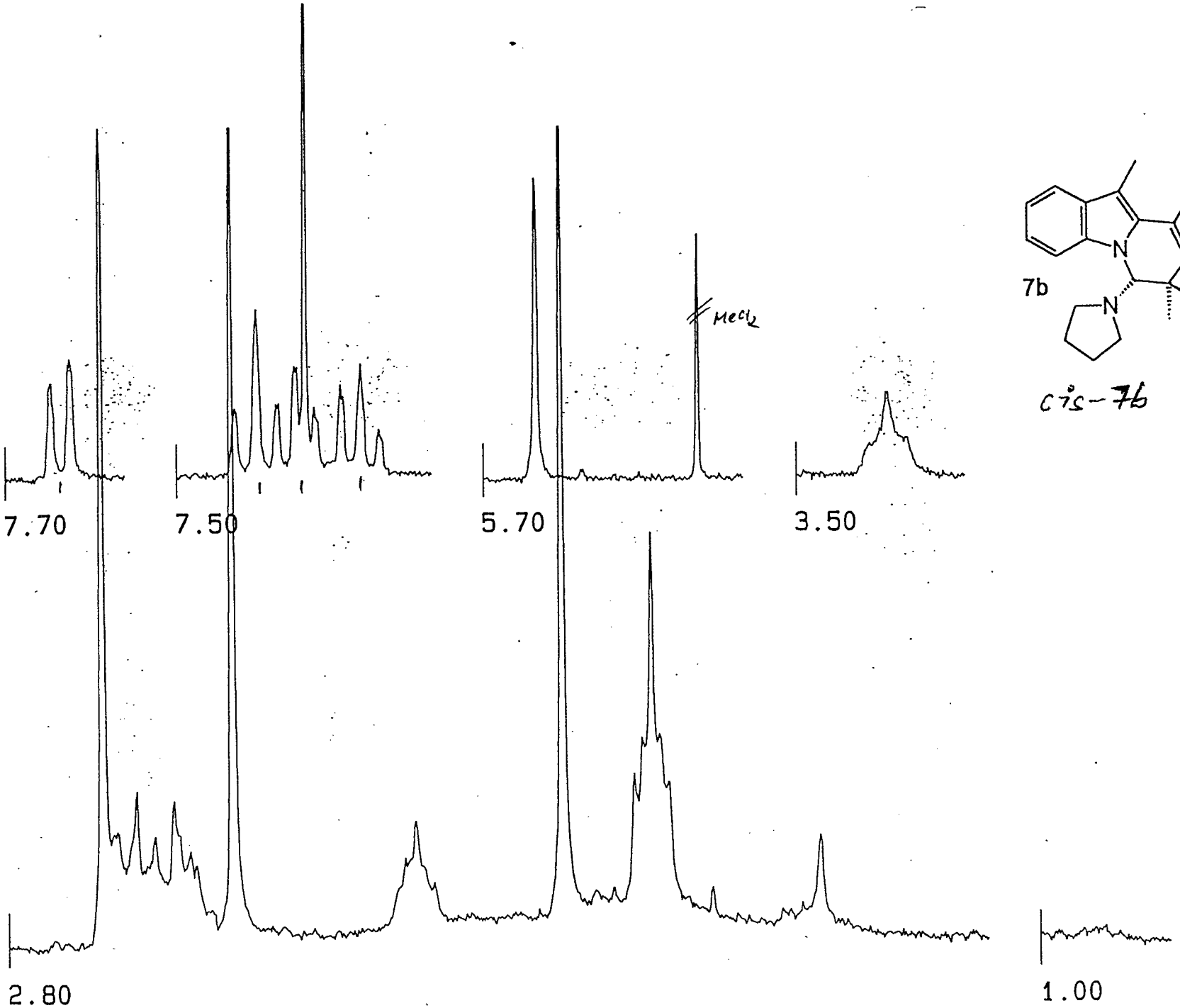
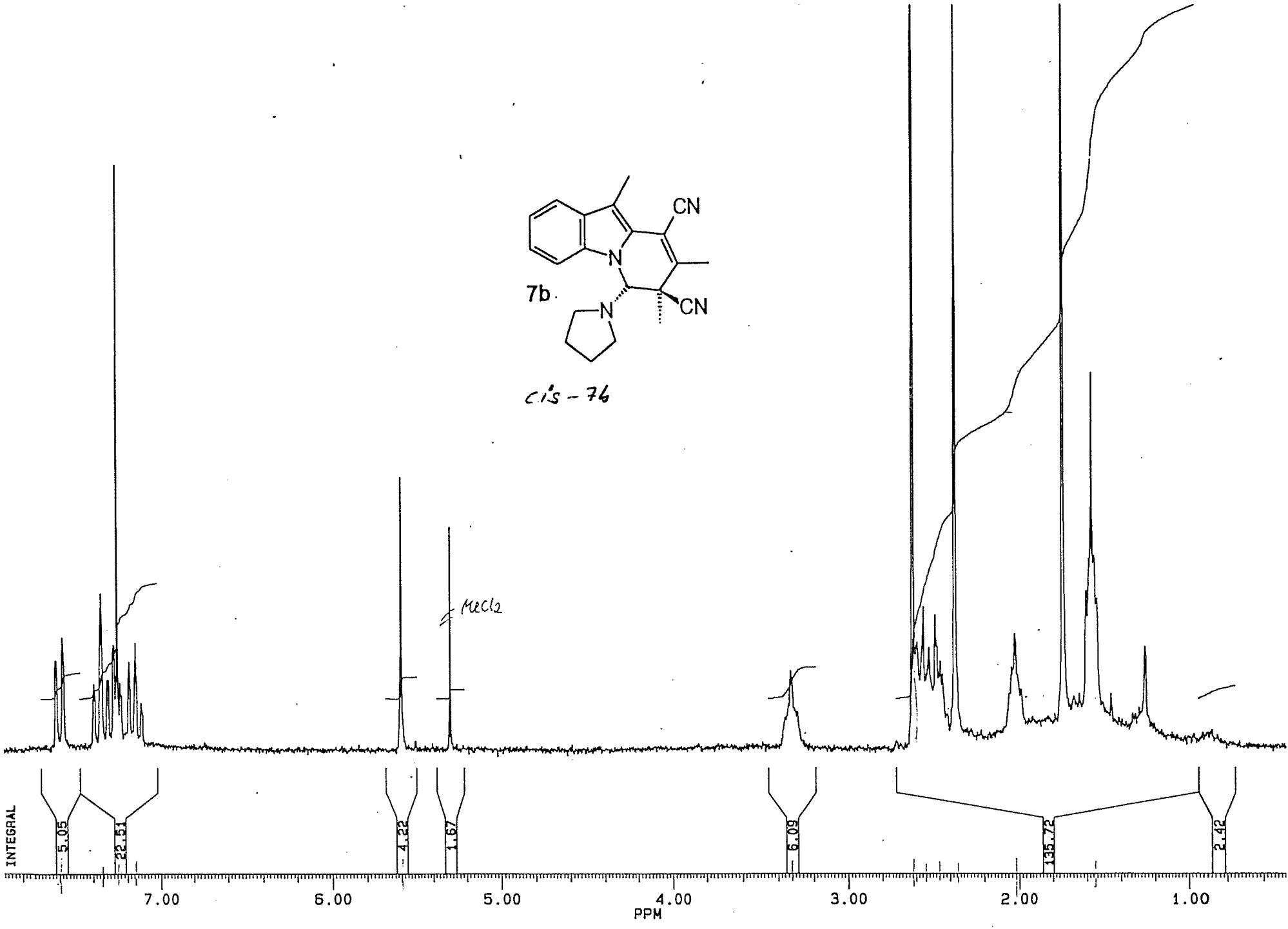
PPM



cis-7b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7b
N
CN
cis - 7b
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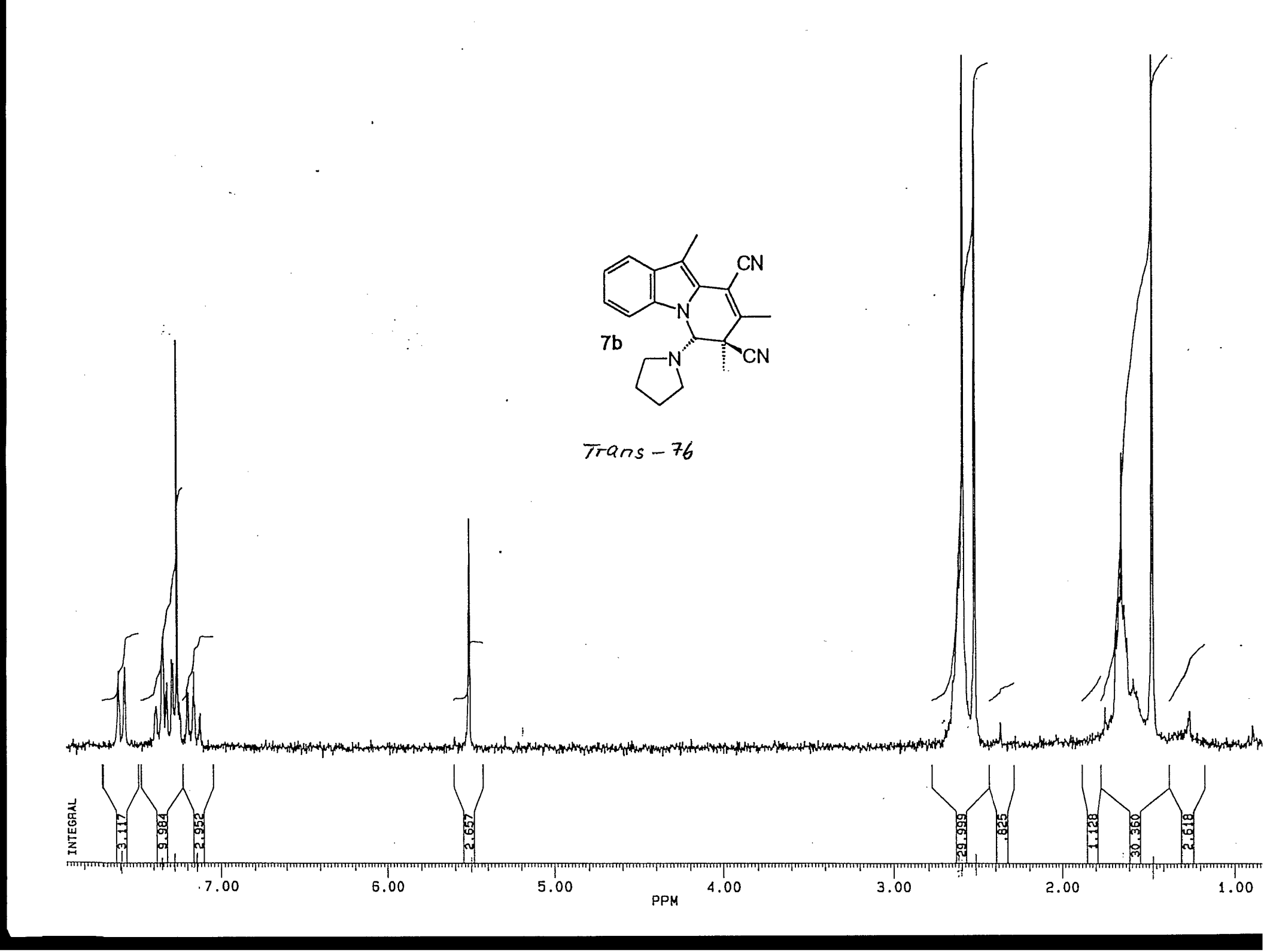
5.00
4.00
3.00
2.00
1.00
PPM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7b
N
CN
Trans – 7b
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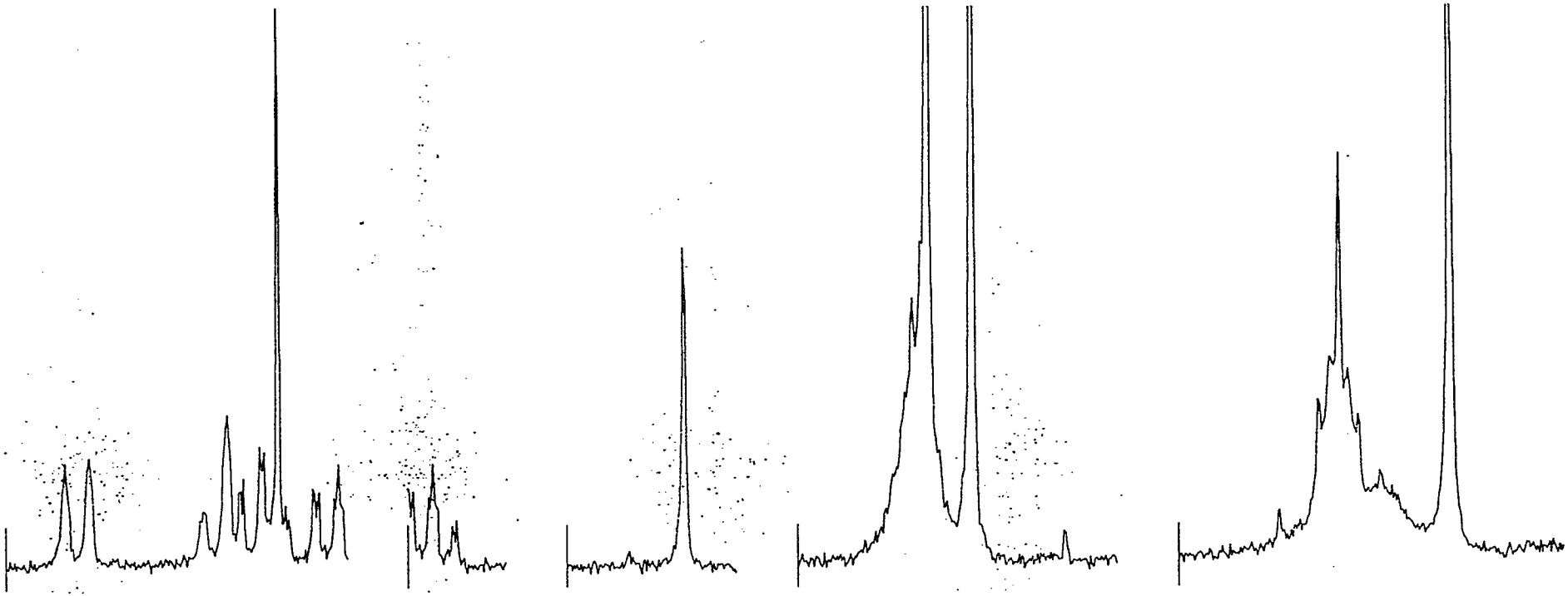
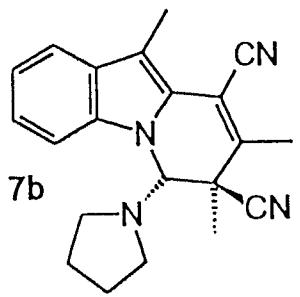
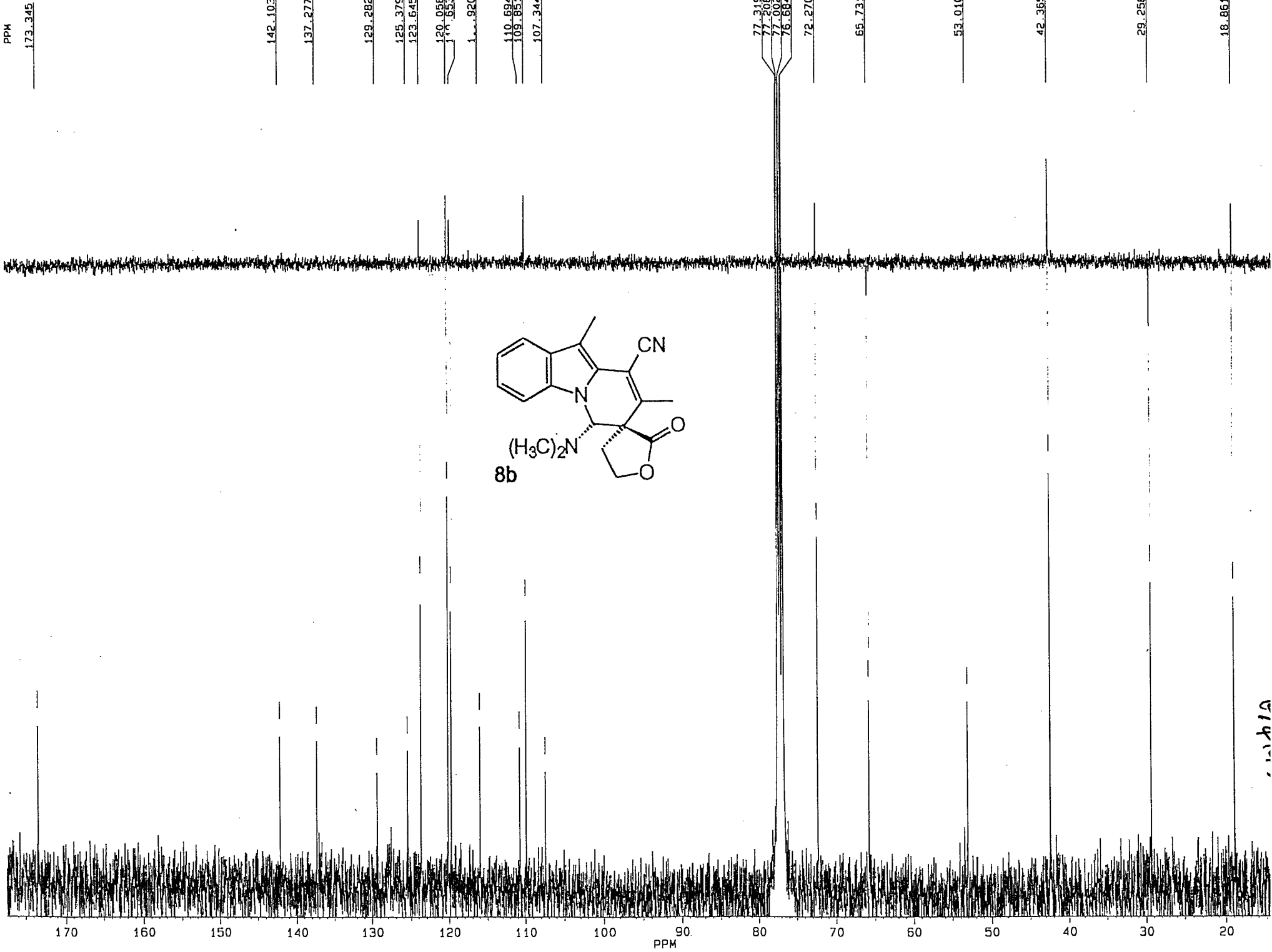
2.00
1.00
PPM





trans-7b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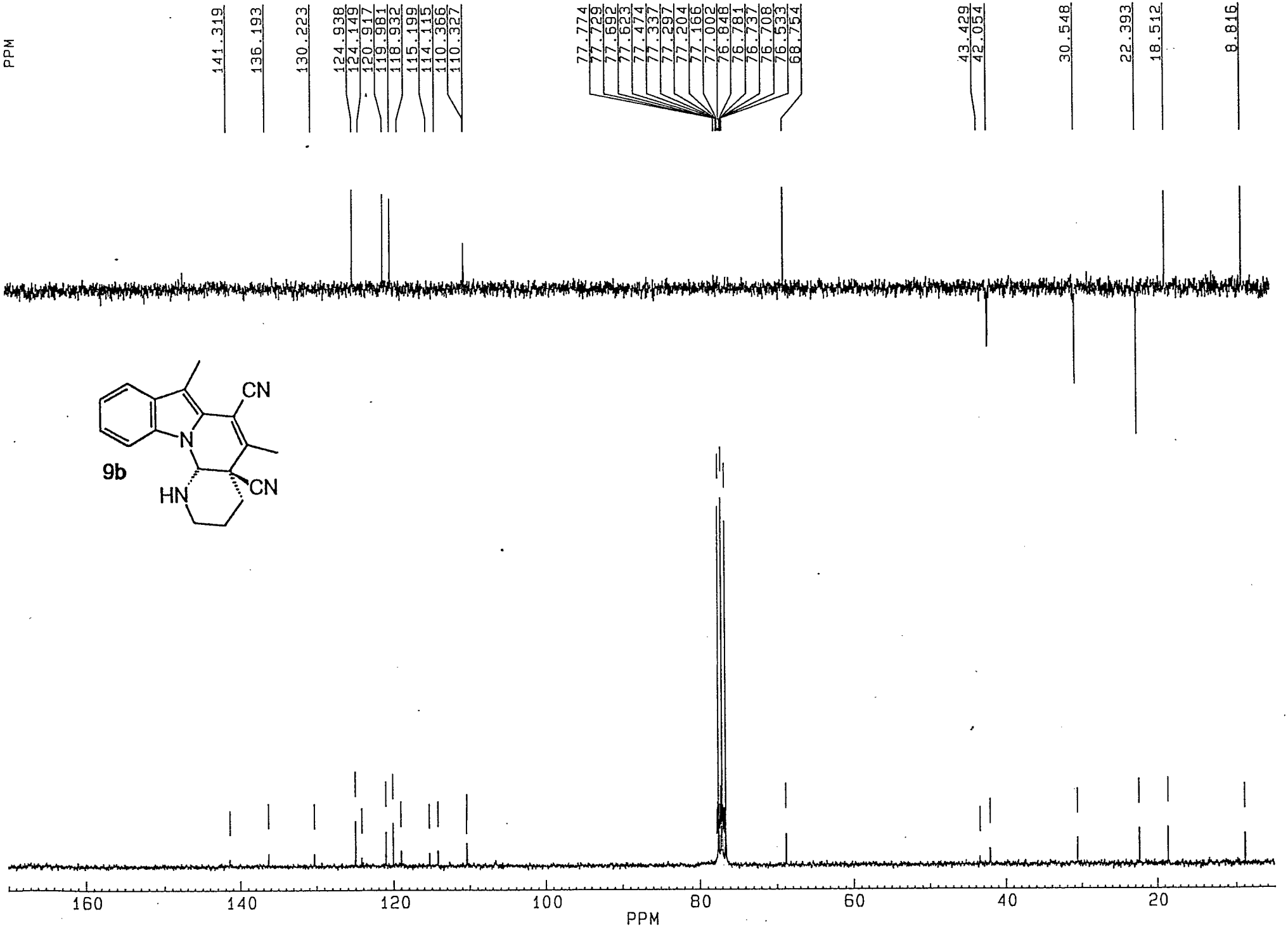
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77.729
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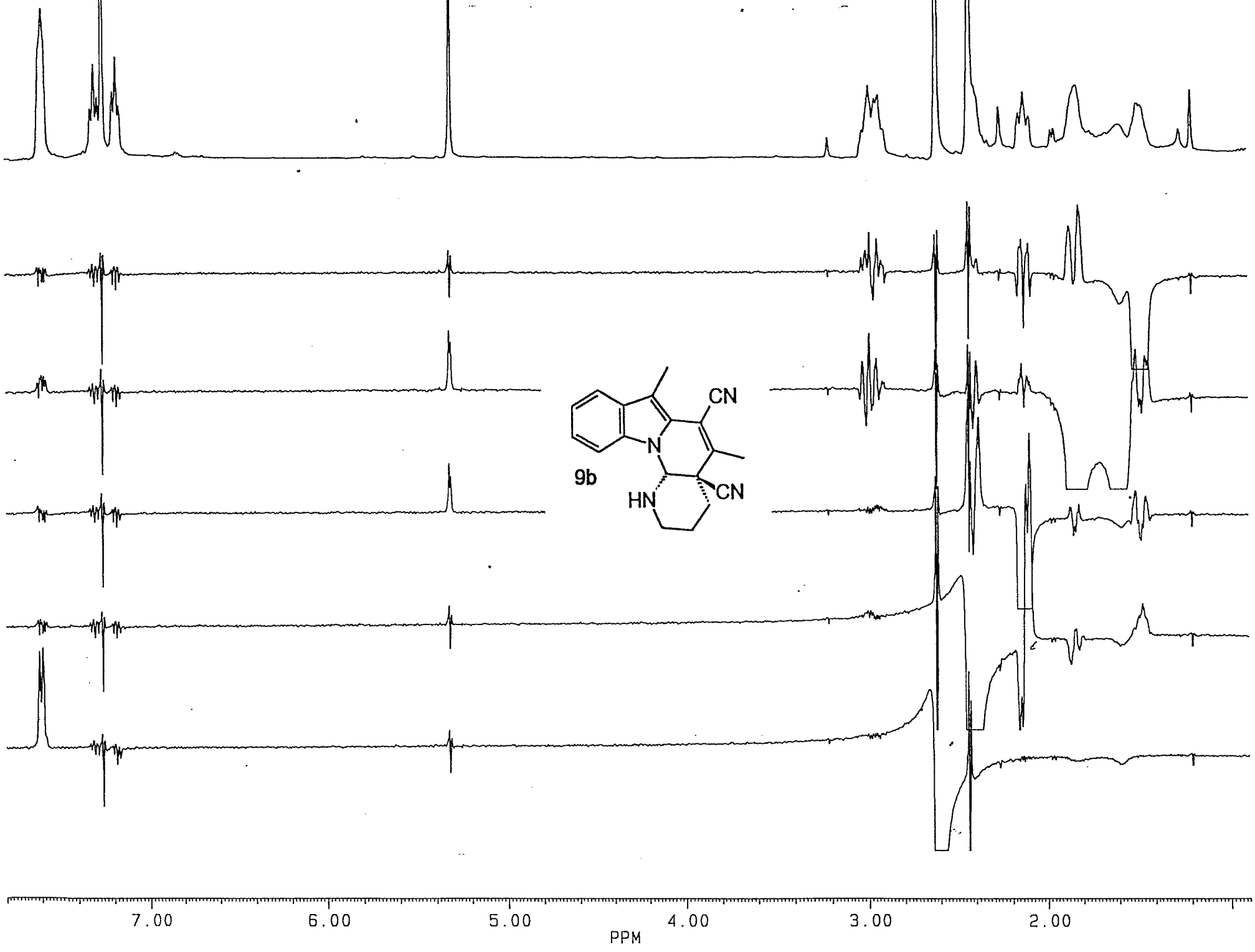
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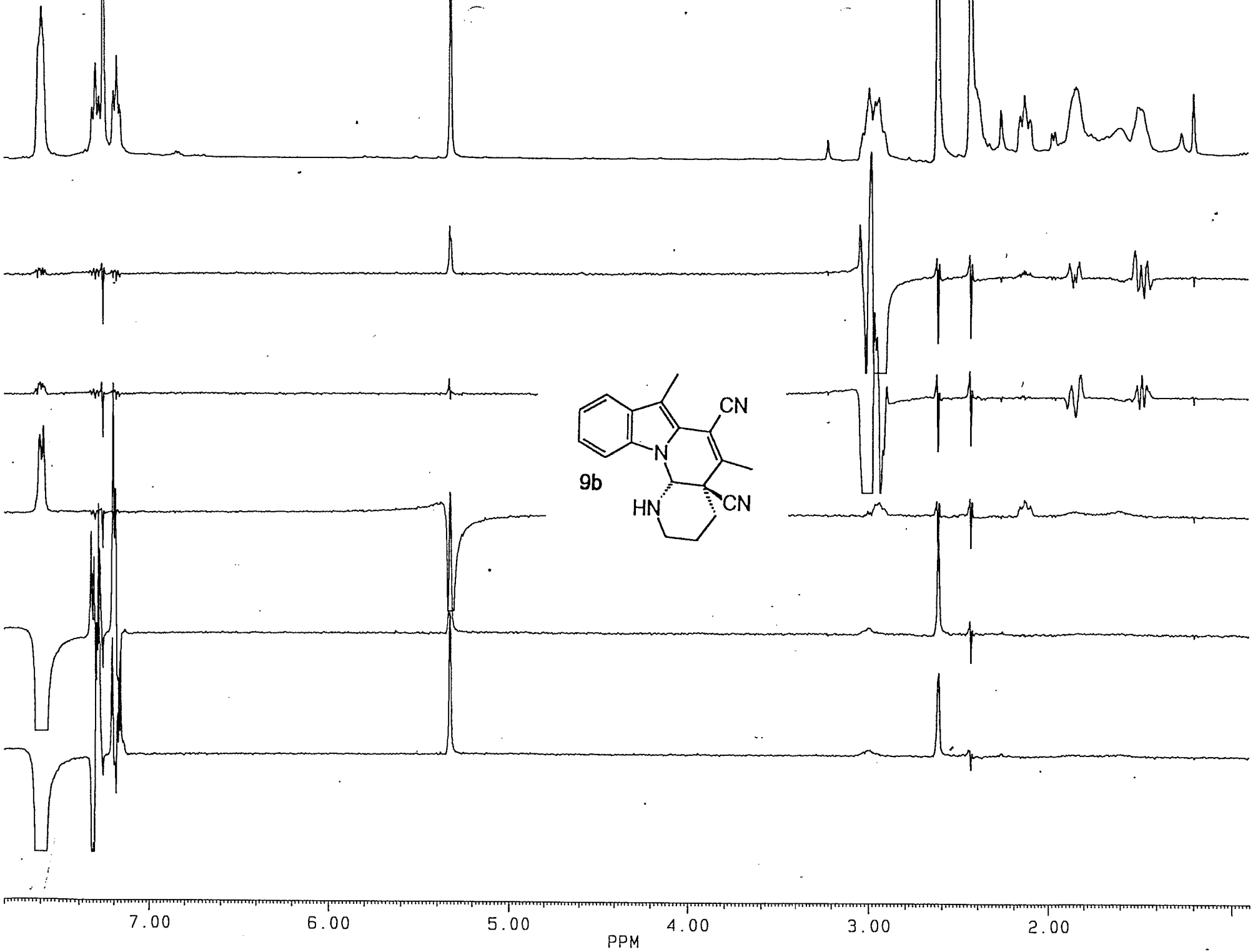
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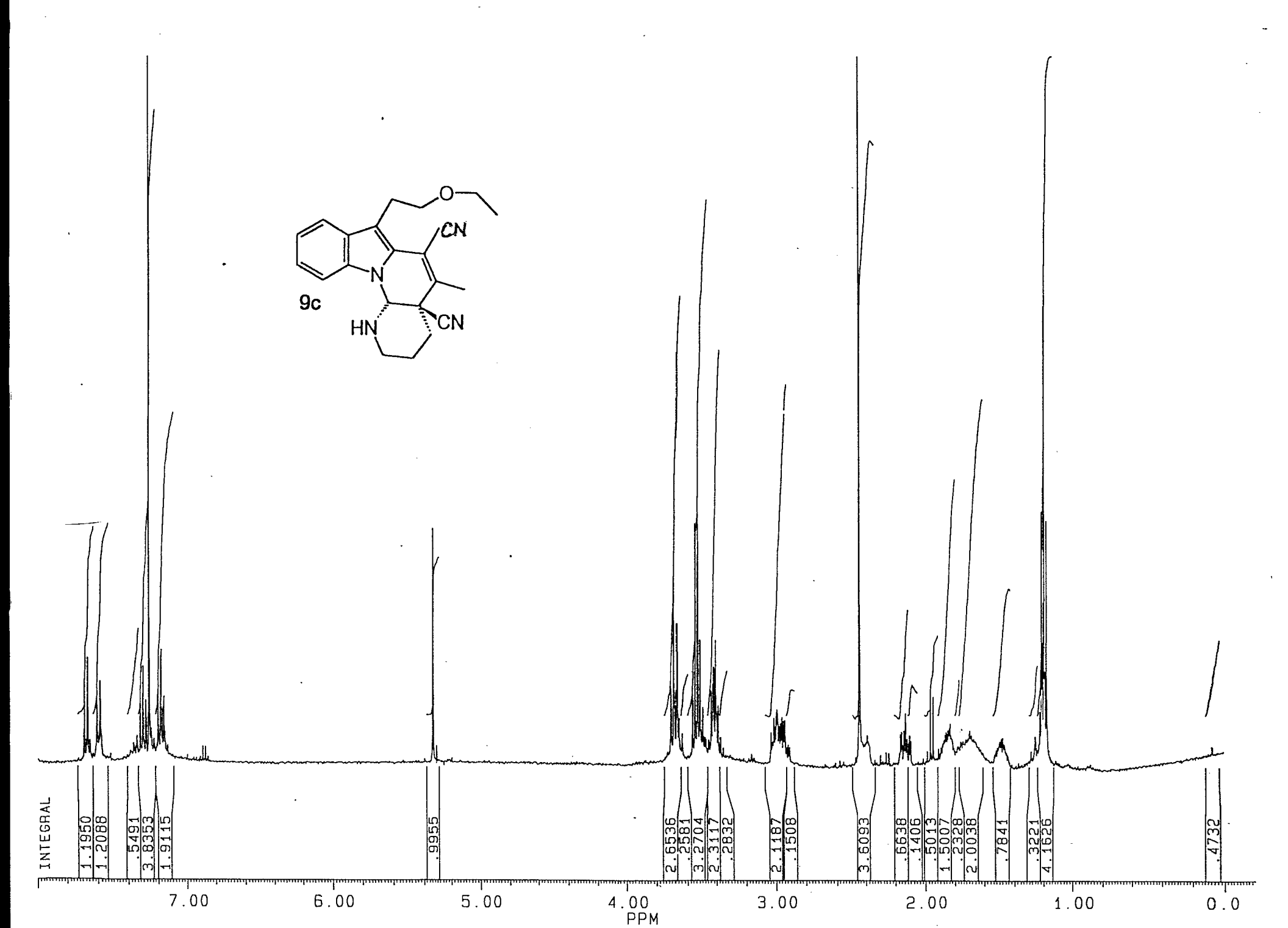
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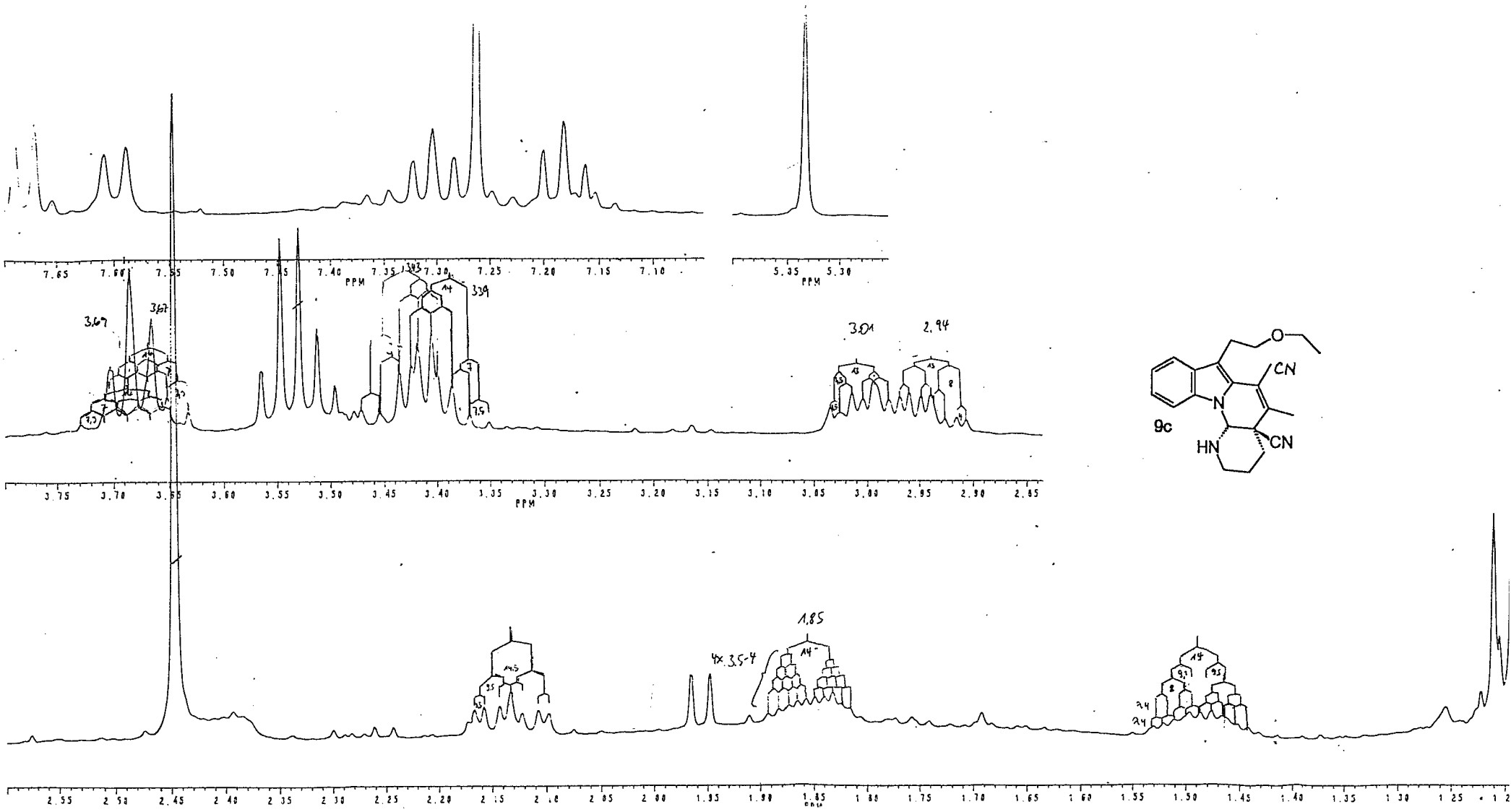
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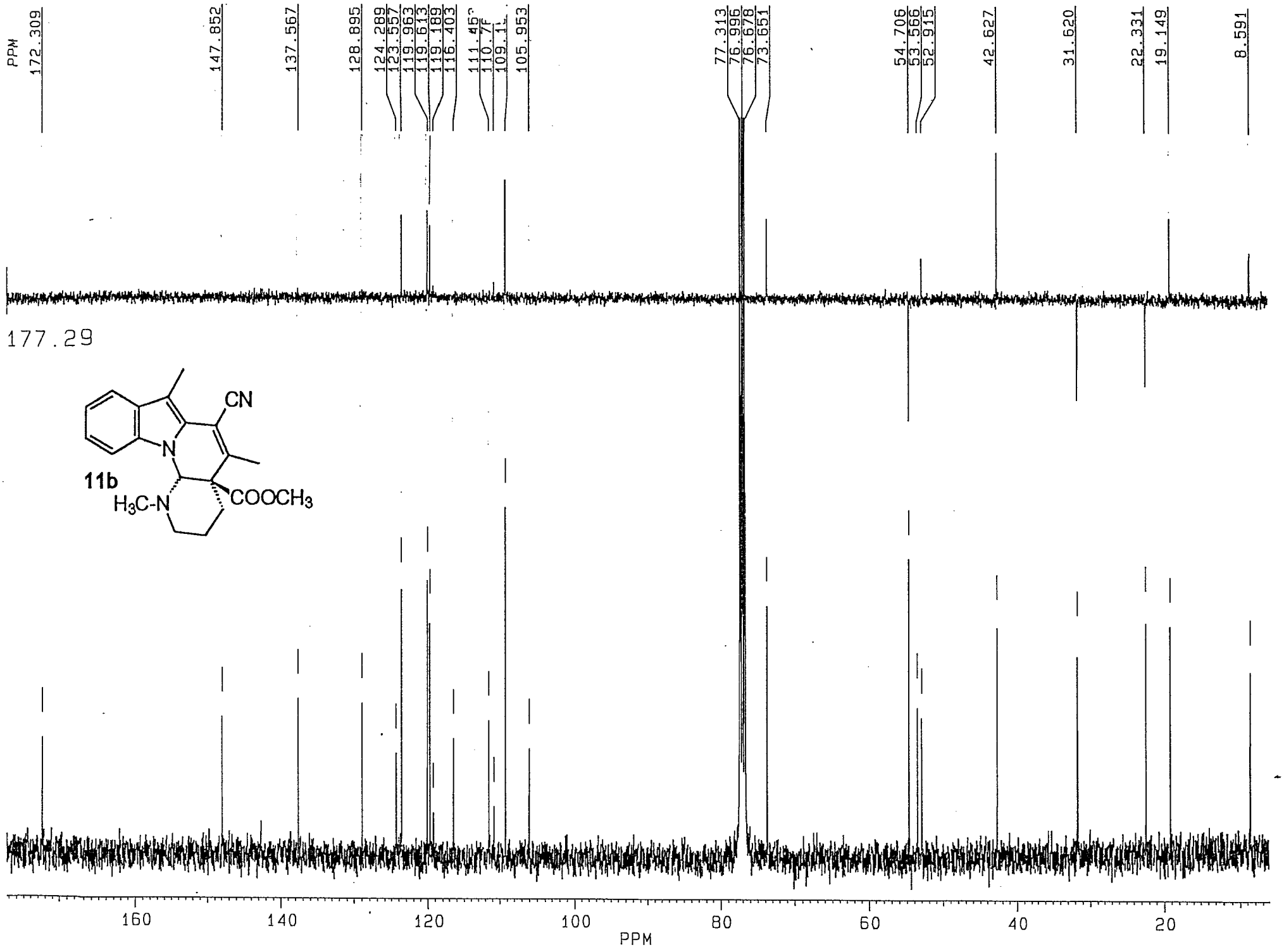
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109.1
105.953
77.313
76.996
76.678
73.651
54.706
53.566
52.915
42.627
31.620
22.331
19.149
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60
40
20
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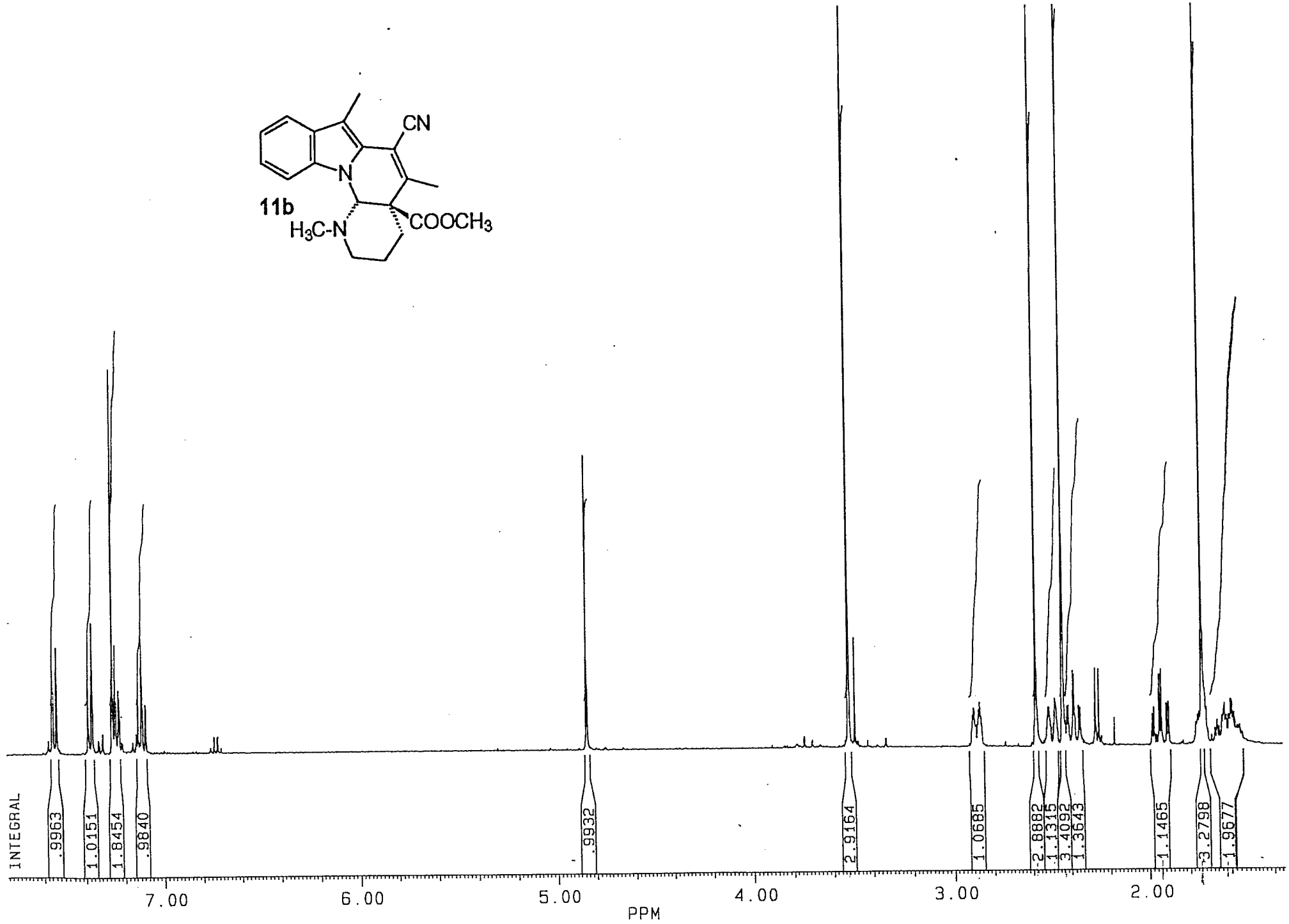
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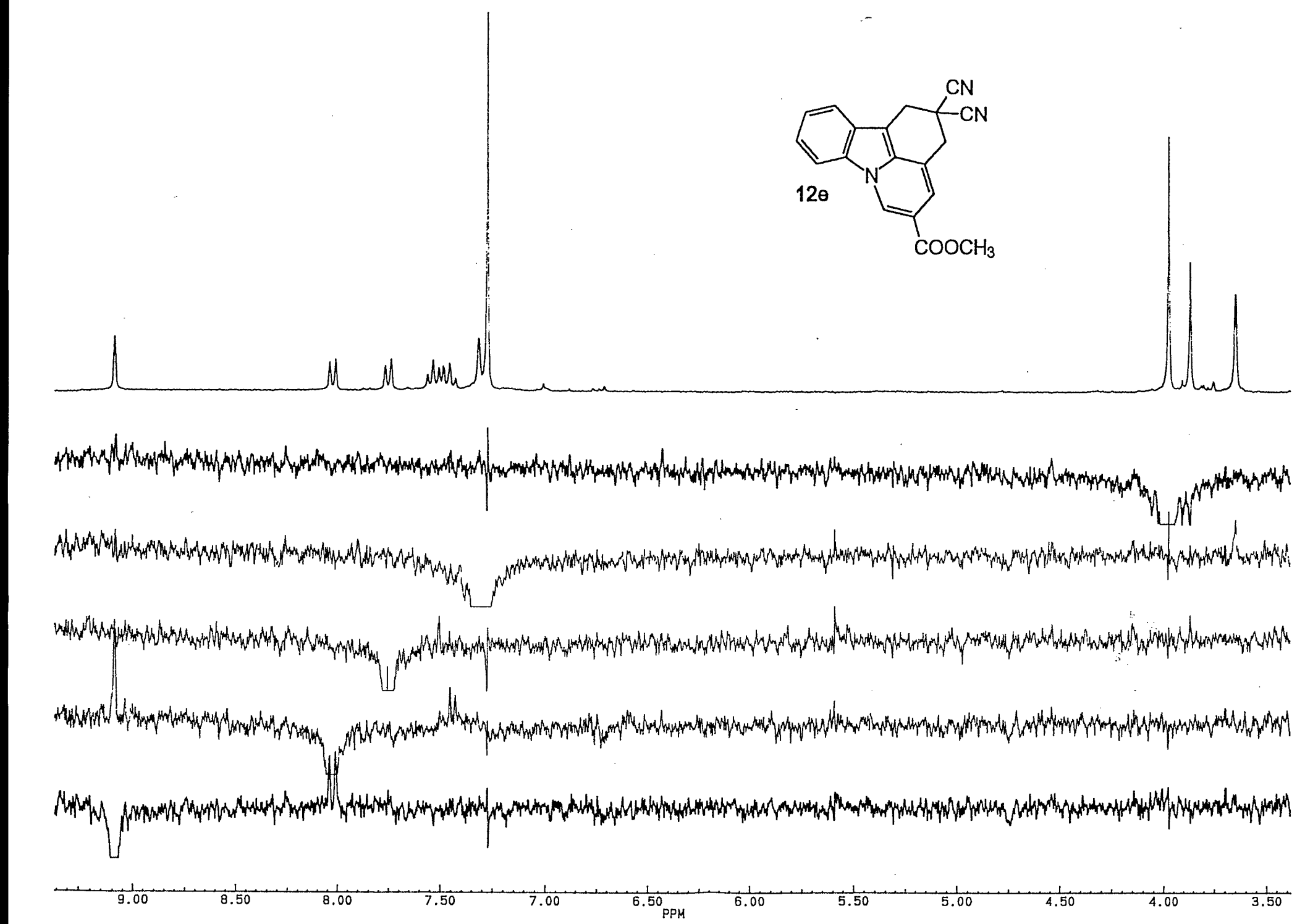
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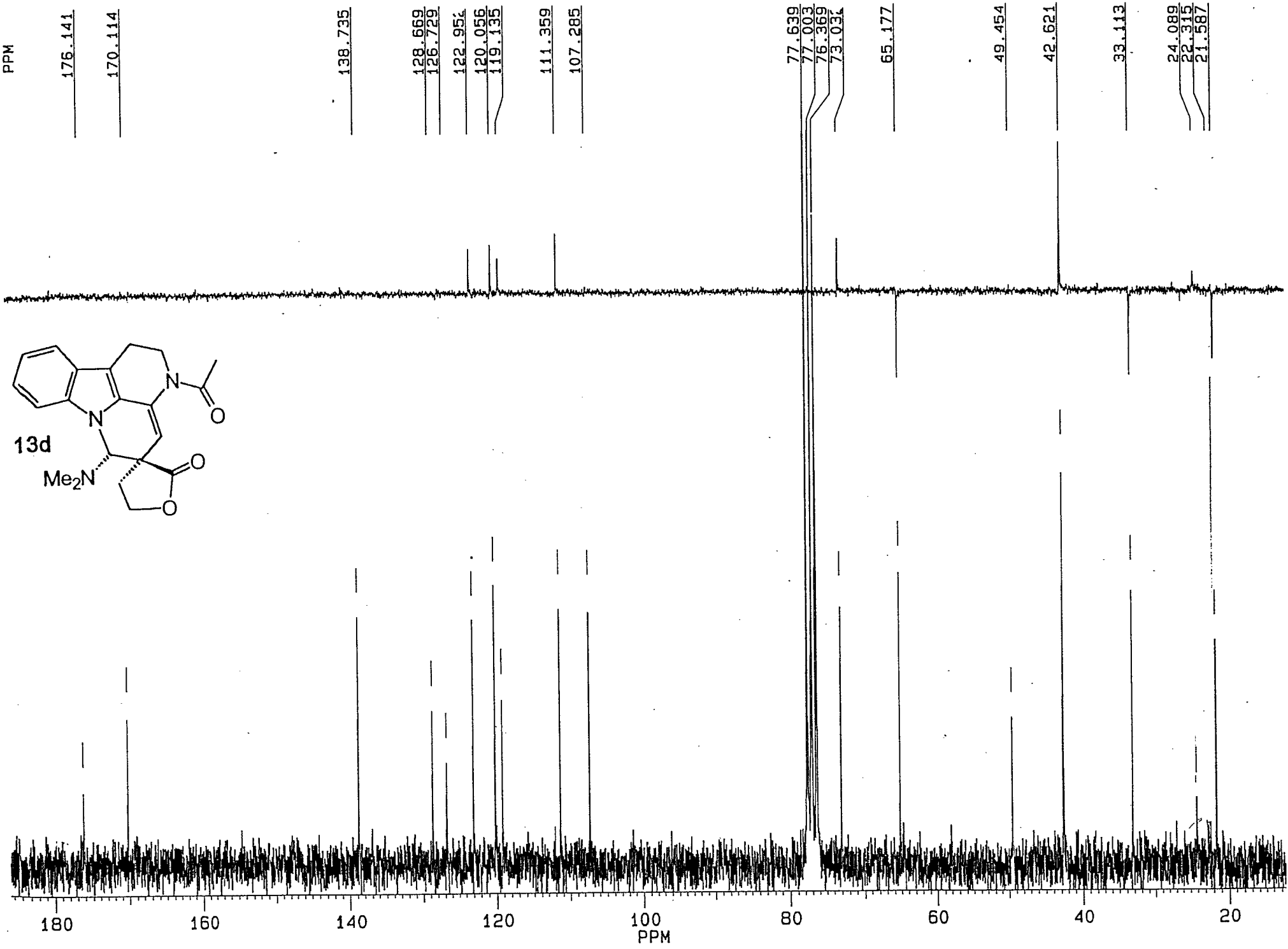
3.50
PPM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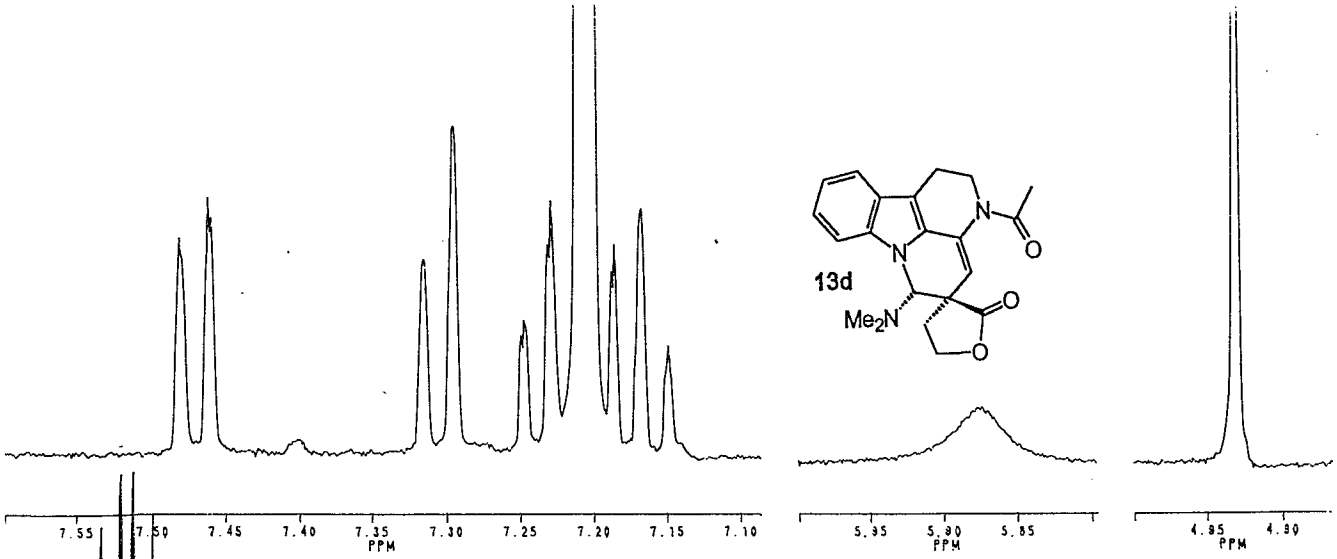
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7.10
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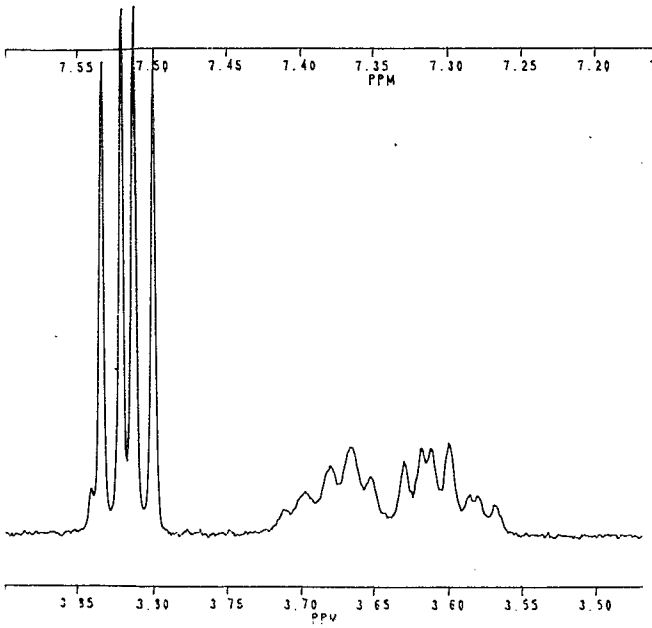
5.90
5.85
PPM

13d

4.95
4.90
PPM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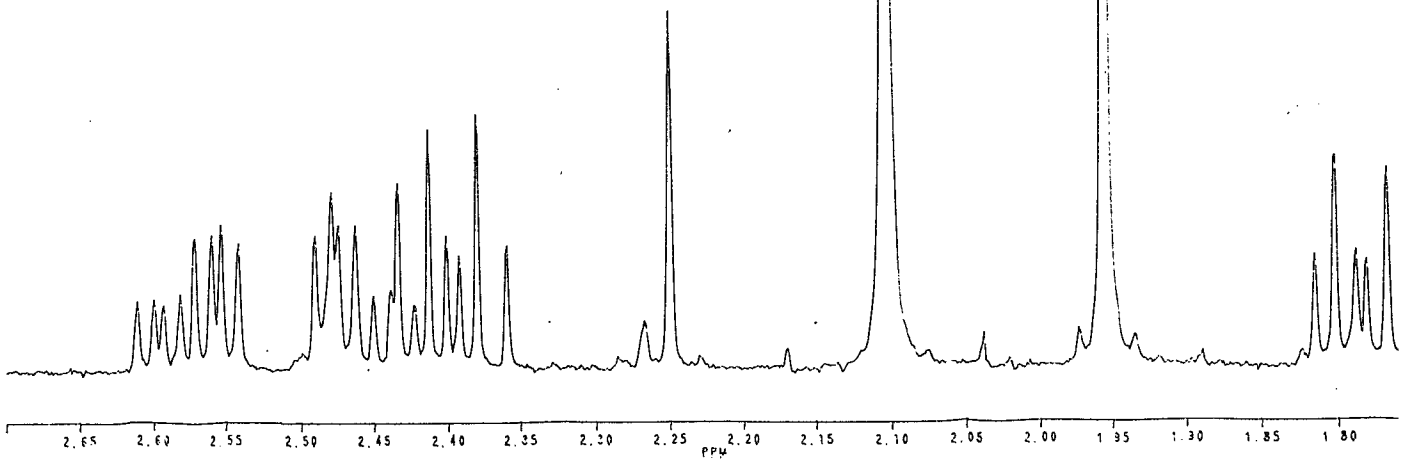
PPM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2.00
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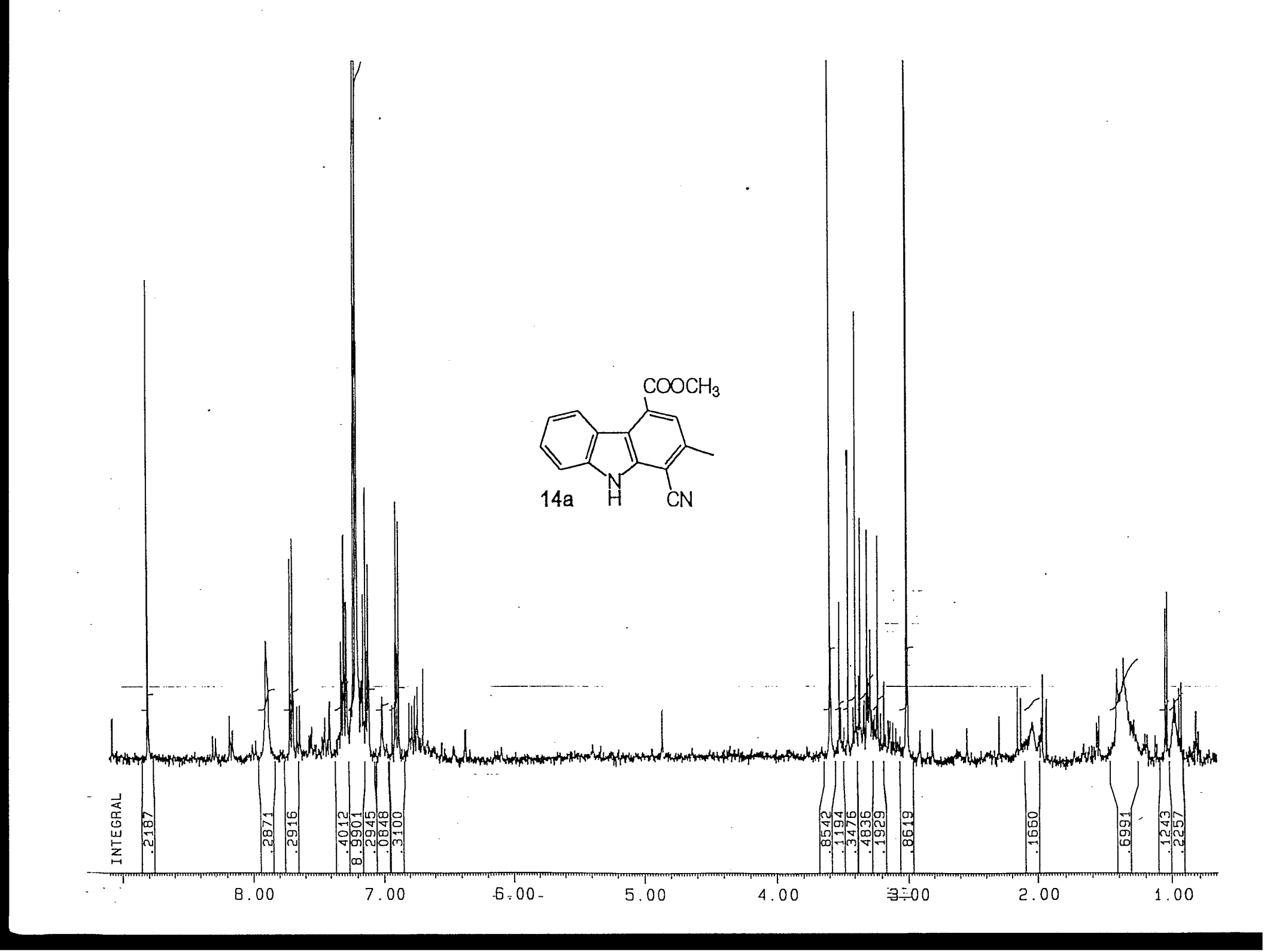
1.85
1.80
PPM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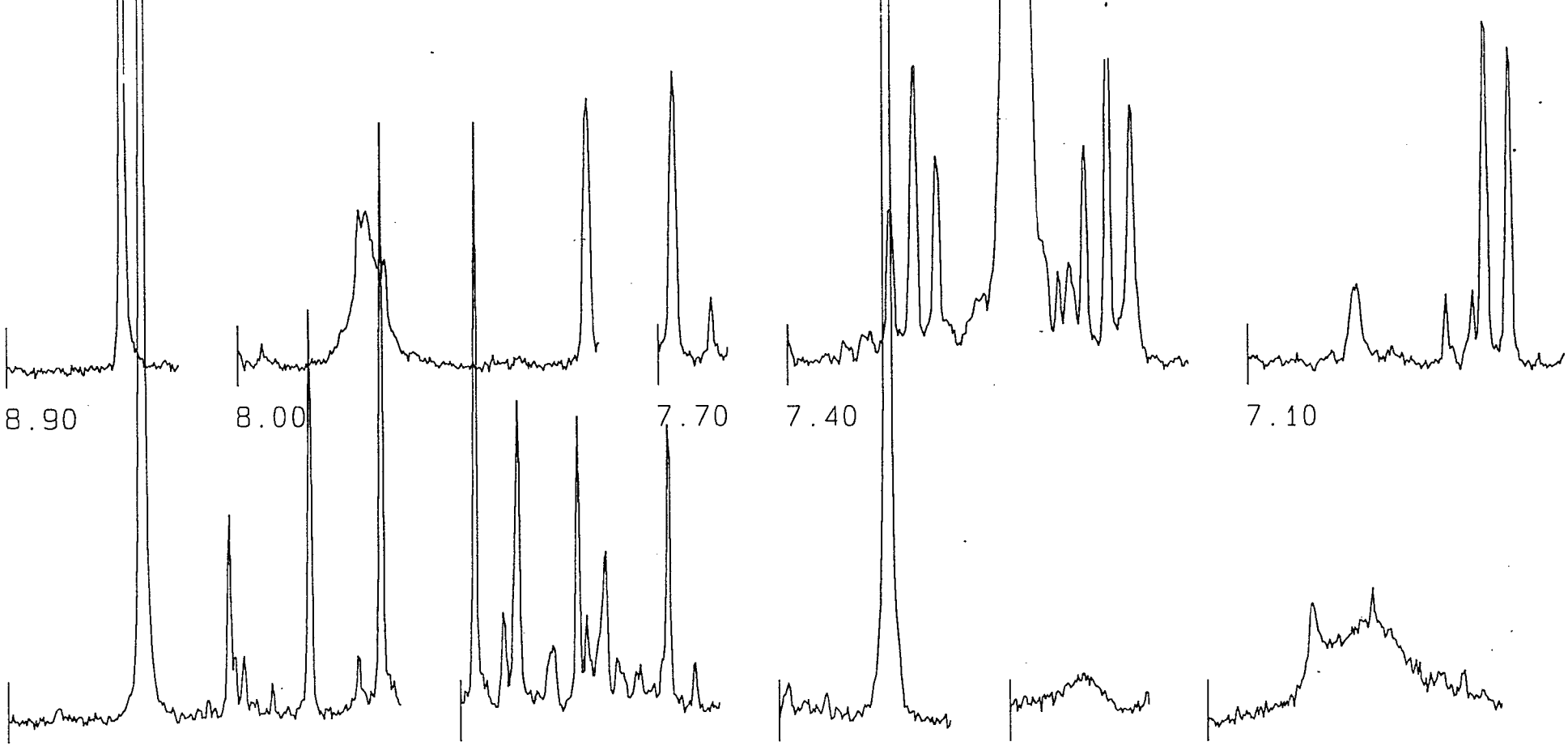
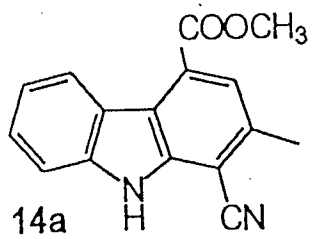
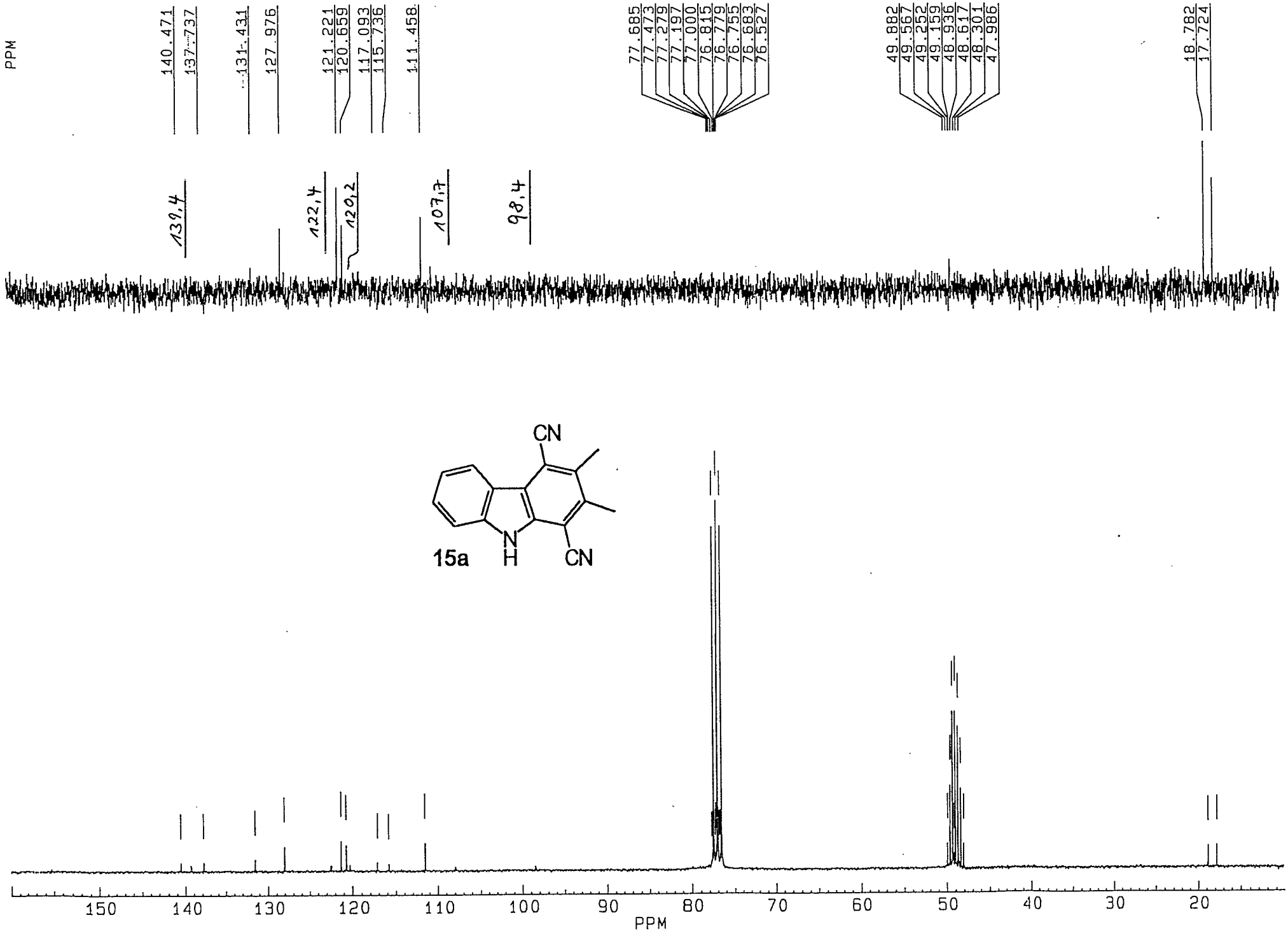




14a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