

Supporting information

A Ligand-free Copper(1) catalysed intramolecular N-arylation of diazoaminobenzenes in PEG-water : an expeditious protocol towards regiospecific 1-aryl benzotriazoles

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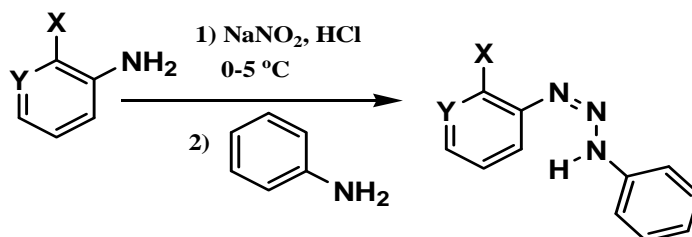
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1. Materials and Methods

All solvents were dried by standard methods. Unless otherwise specified, chemicals were purchased from commercial suppliers and used without further purification. Some of 2-halo anilines were prepared using some reported methods^{1,2}. Column chromatography was performed on silica gel (60-120 mesh). TLC was done on glass sheets pre-coated with silica gel (with binder, 300 mesh, Merck). The ¹H- and ¹³C-NMR spectra were taken in CDCl₃ with TMS as an internal reference. The chemical shifts were reported as δ values (ppm) relative to TMS. IR spectra were recorded in KBr pellets. Compounds **2a**³, **2b**³, **2c**³, **2m**⁴, **2n**⁵, **2r**⁶, **2s**⁶ are known in the literature and thus spectroscopic data elemental analysis data and ¹³C NMR spectra are not given (only ¹H NMR are given).

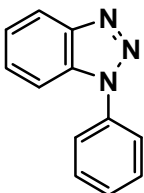
2. Synthesis of diazoaminobenzenes

Diazoaminobenzenes were prepared using a reported procedure¹ with some modification. In a 20 mL Erlenmeyer flask, 2-halo aniline (7 mmol), concentrated hydrochloric acid (1 mL) and 4 mL of water were stirred for 10 min. After adding 2 g of crushed ice into it, 7 mmol of sodium nitrite in 1 mL of cold water was added dropwise for 5 min. maintaining 0-5 °C of temperature with constant stirring. It was then allowed to stand for another 15 min. 7 mmol of aniline or substituted aniline was then added into it with constant stirring maintaining 0-5 °C of temperature. After 5 min, 1 g of crystalline sodium acetate in 2 mL of cold water was added drop wise for five min with constant stirring. A yellow precipitate begins to form immediately. It was stirred for another 45 min. maintaining a temperature not above 20 °C. The precipitate was filtered and recrystallized from petroleum ether (boiling range 60-80 °C).



3. Analytical data of compounds

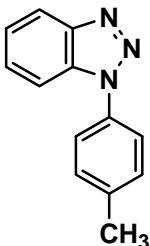
Compound 2a:



Characteristic: Pale yellow solid (Reaction time 2.5 h, isolated yield 92 %)

$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 7.42 (1H, t, $J = 7.6$ Hz), 7.68 - 7.46 (4H, m), 7.74 (1H, d, $J = 8.3$ Hz), 7.76 (2H, d, $J = 7.6$ Hz), 8.14 (1H, d, $J = 8.3$ Hz).

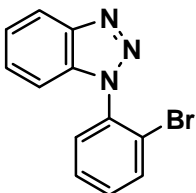
Compound 2b:



Characteristic: Pale yellow crystalline solid (Reaction time 2.5 h, isolated yield 92 %)

$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 2.42 (3H, s), 7.42 - 7.32 (3H, m), 7.49 (1H, t, $J = 7.6$ Hz), 7.62 (2H, d, $J = 7.6$ Hz), 7.68 (1H, d, $J = 8.3$ Hz) 8.11 (1H, d, $J = 8.3$ Hz).

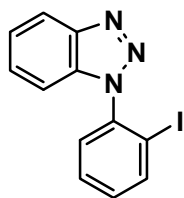
Compound 2c:



Characteristic: light red crystalline solid (Reaction time 3.0 h, isolated yield 90 %)

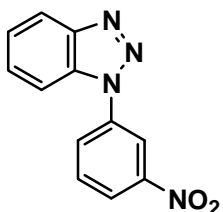
$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 7.37 (1H, d, $J = 8.1$ Hz), 7.60 - 7.40 (5H, m), 7.84 (1H, d, $J = 8.1$ Hz), 8.16 (1H, d, $J = 8.1$ Hz).

Compound 2d:



Characteristic: White crystalline solid (Reaction time 2.5 h, isolated yield 92 %)

Compound 2e:



Characteristic: Yellow crystalline solid (Reaction time 3 h, isolated yield 89 %)

Melting point: 180 – 182 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 7.52 (1H, t, J=7.8Hz), 7.67 (1H, t, J=8.1Hz), 7.85 (2H, t, J=8.4 Hz), 8.21 (1H, d, J=8.1 Hz), 8.25 (1H, dd, J=8.1 and 0.6 Hz), 8.38 (1H, d, J=7.8 Hz), 8.72 (1H, s).

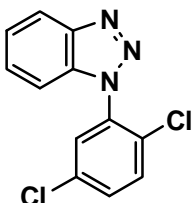
¹³C NMR (75 MHz, CDCl₃): δ 109.8, 117.0, 120.8, 122.9, 125.0, 128.0, 129.4, 131.0, 131.8, 138.0, 146.7, 149.0.

EI-MS (m/z): 240 (M⁺), 209, 208, 207, 191, 133.

IR (KBr, cm⁻¹): 740, 1049, 1089, 1182, 1242, 1346, 1529, 2374, 2866, 2922, 3090 cm⁻¹.

Elemental Analysis calculated for C₁₂H₈N₄O₂ : C 60.00, H 3.36, N 23.32; Found: C 59.92, H 3.38, N 23.38 %.

Compound 2f:



Characteristic: White solid (Reaction time 3 h, isolated yield 90 %)

Melting point: 110 – 112 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 7.40 (1H, d, J=8.1 Hz), 7.46 (1H, dt, J=7.5 and 1.5 Hz), 7.62-7.49 (4H, m), 8.17 (1H, d, J=8.4Hz).

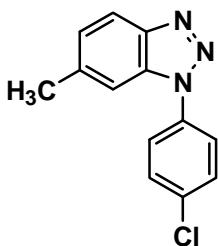
¹³C NMR (75 MHz, CDCl₃): δ 110.3, 120.3, 124.4, 128.4, 129.2, 129.3, 131.2, 131.7, 133.4, 133.6, 134.9, 145.6.

EI-MS (m/z): 263 (M⁺), 237, 235, 202, 200, 164.

IR (KBr, cm⁻¹): 733, 811, 998, 1038, 1101, 1287, 1422, 1481, 1580, 2280, 2372, 3090 cm⁻¹.

Elemental Analysis calculated for C₁₂H₇N₃Cl₂ : C 54.57, H 2.67, N 15.91; Found: C 54.50, H 2.70, N 15.95 %.

Compound 2g:



Characteristic: White solid (Reaction time 2.5 h, isolated yield 92 %)

Melting point: 128 – 130 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 2.33 (3H, s), 7.05 (1H, d, J= 7.2Hz), 7.26 (1H, s), 7.36 (2H, d, J= 9.0 Hz), 7.51 (2H, d, J=8.7Hz), 7.79 (1H, d, J= 8.7Hz).

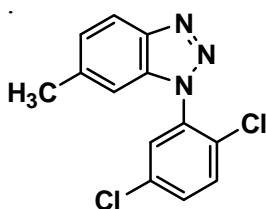
^{13}C NMR (75 MHz, CDCl_3): δ 22.1, 109.3, 119.8, 124.0, 126.7, 130.0, 134.2, 135.6, 139.3.

EI-MS (m/z): 243 (M^+), 216, 214, 180.

IR (KBr, cm^{-1}): 810, 1063, 1499, 1613, 2373, 2917, 3063 cm^{-1} .

Elemental Analysis calculated for $\text{C}_{13}\text{H}_{10}\text{N}_3\text{Cl}$: C 64.07, H 4.14, N 17.24; Found: C 64.05, H 4.13, N 17.27 %.

Compound 2h:



Characteristic: White solid (Reaction time 3 h, isolated yield 91 %)

Melting point: 132 °C (EtOAc)

^1H NMR (300 MHz, CDCl_3): δ 2.53 (3H, s), 7.36-7.22 (2H, m), 7.62-7.50 (3H, m), 8.09 (1H, s).

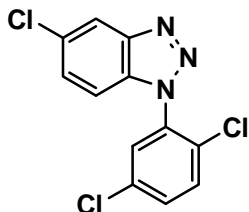
^{13}C NMR (75 MHz, CDCl_3): δ 22.0, 109.5, 119.7, 126.6, 129.2, 129.5, 131.1, 131.7, 133.5, 135.2, 139.4.

EI-MS (m/z): 277 (M^+), 250, 248, 216, 214.

IR (KBr, cm^{-1}): 800, 1041, 1482, 1581, 2373, 2924, 3077 cm^{-1} .

Elemental Analysis calculated for $\text{C}_{13}\text{H}_{10}\text{N}_3\text{Cl}_2$: C 56.14, H 3.26, N 15.11; Found: C 56.07, H 3.28, N 15.16 %.

Compound 2i:



Characteristic: White solid (Reaction time 6 h, isolated yield 91 %)

Melting point: 154 - 156 °C (EtOAc)

^1H NMR (300 MHz, CDCl_3): δ 7.34 (1H, d, J = 8.7 Hz), 7.63-7.50 (4H, m), 8.15 (1H, d, J = 1.2Hz).

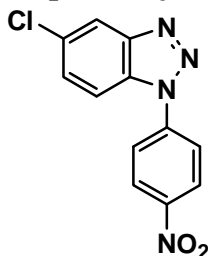
^{13}C NMR (75 MHz, CDCl_3): δ 111.4, 119.7, 129.2, 129.2, 129.4, 130.5, 131.5, 131.8, 132.2, 133.8, 134.5, 146.3.

EI-MS (m/z): 297 (M^+), 269, 234, 198, 164.

IR (KBr, cm^{-1}): 816, 1045, 1102, 1210, 1290, 1422, 1479, 1579, 1736, 2373, 3091 cm^{-1} .

Elemental Analysis calculated for $\text{C}_{12}\text{H}_6\text{N}_3\text{Cl}_3$: C 48.28, H 2.03, N 14.07; Found: C 48.20, H 2.08, N 14.10 %.

Compound 2j:



Characteristic: Yellow solid (Reaction time 6.5 h, isolated yield 84 %)

Melting point: 182 -184 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 7.62 (1H, dd, J= 8.7 and 1.5 Hz), 7.78 (1H, d, J=8.7 Hz), 8.05 (2H, d, J= 9.0 Hz), 8.18 (1H, br.d, J=0.9 Hz), 8.52 (2H, d, J= 9.0 Hz).

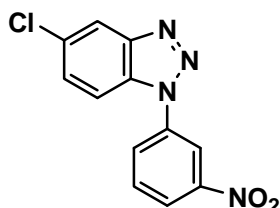
¹³C NMR (75 MHz, CDCl₃): δ 111.0, 120.3, 122.4, 125.7, 130.1, 130.4, 131.1, 141.5, 147.2, 147.6.

EI-MS (m/z): 274 (M⁺), 229, 207, 202, 200, 165, 164.

IR (KBr, cm⁻¹): 816, 1045, 1102, 1210, 1290, 1422, 1479, 1579, 1736, 2373, 3091 cm⁻¹.

Elemental Analysis calculated for C₁₂H₇N₄O₂Cl : C 52.47, H 2.57, N 20.40; Found: C 52.39, H 2.61, N 20.44 %.

Compound 2k:



Characteristic: Yellow solid (Reaction time 6 h, isolated yield 84 %)

Melting point: 184 – 186 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 7.62 (1H, dd, J=9.0 and 1.8 Hz), 7.76 (1H, d, J= 8.7 Hz), 7.86 (1H, t, J= 8.4 Hz), 8.18 (1H, br.t, J= 0.9 Hz), 8.21 (1H, td, J= 8.1 and 1.2 Hz), 8.40 (1H, td, J= 8.4 and 1.2 Hz), 8.68 (1H, t, J= 1.8 Hz).

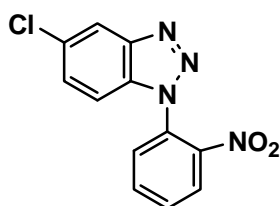
¹³C NMR (75 MHz, CDCl₃): δ 110.8, 117.1, 120.2, 123.3, 128.0, 130.0, 130.5, 130.9, 131.2, 137.6, 147.4, 149.1.

EI-MS (m/z): 274 (M⁺), 229, 202, 200, 199, 174, 165, 164.

IR (KBr, cm⁻¹): 810, 1062, 1349, 1535, 2375, 3093 cm⁻¹.

Elemental Analysis calculated for C₁₂H₇N₄O₂Cl : C 52.47, H 2.57, N 20.40; Found: C 52.39, H 2.60, N 20.45 %.

Compound 2l:



Characteristic: Yellow solid (Reaction time 6 h, isolated yield 82 %)

Melting point: 152 – 154 °C (EtOAc)

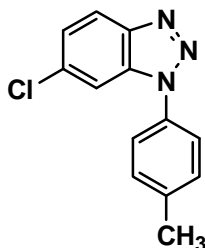
¹H NMR (300 MHz, CDCl₃): δ 7.39 (1H, d, J= 8.4 Hz), 7.46 (1H, d, J= 7.5 Hz), 7.61-7.49 (4H, m), 8.15 (1H, d, J= 8.4 Hz).

¹³C NMR (75 MHz, CDCl₃): δ 110.3, 120.1, 124.3, 128.3, 129.0, 129.2, 131.1, 131.6, 133.3, 133.4, 134.8, 145.7.

EI-MS (m/z): 274 (M⁺), 246, 229, 200, 174, 164.

IR (KBr, cm^{-1}): 732, 998, 1038, 1099, 1286, 1422, 1480, 1581, 1903, 3090 cm^{-1} .
Elemental Analysis calculated for $\text{C}_{12}\text{H}_7\text{N}_4\text{O}_2\text{Cl}$: C 52.47, H 2.57, N 20.40; Found: C 52.38, H 2.61, N 20.45 %

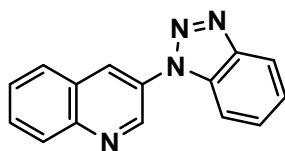
Compound 2m: (Reaction time 2.5 h, isolated yield 92 %)



Characteristic: Pale yellow crystalline solid

^1H NMR (300 MHz, CDCl_3): δ 2.48 (3H, s), 7.40 (3H, two doublets merged together as a triplet, $J = 8.3$ and 8.6 Hz), 7.61 (2H, d, $J = 8.3$ Hz), 7.71 (1H, d, $J = 1.5$ Hz), 8.05 (1H, d, $J = 8.6$ Hz).

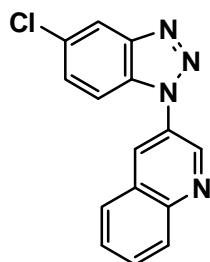
Compound 2n: (Reaction time 3 h, isolated yield 82 %)



Characteristic: White solid

^1H NMR (300 MHz, CDCl_3): δ 7.49 (1H, t, $J = 7.6$ Hz), 7.62 (1H, t, $J = 7.7$ Hz), 7.68 (1H, t, $J = 7.7$ Hz), 7.82 (2H, br.d, $J = 8.2$ Hz), 7.97 (1H, d, $J = 8.0$ Hz), 8.19 (1H, d, $J = 8.5$ Hz), 8.24 (1H, d, $J = 8.5$ Hz), 8.54 (1H, d, $J = 1.8$ Hz), 9.41 (1H, s).

Compound 2o:



Characteristic: White solid (Reaction time 6.5 h, isolated yield 88 %)

Melting point: 186 – 188 $^{\circ}\text{C}$ (EtOAc)

^1H NMR (300 MHz, CDCl_3): δ 7.76 (1H, d, $J = 9.0$ Hz), 7.78 – 7.67 (2H, m), 7.87 (1H, dt, $J = 1.2$ and 8.4 Hz), 7.99 (1H, d, $J = 8.1$ Hz), 8.19 (1H, d, $J = 1.5$ Hz), 8.25 (1H, d, $J = 8.4$ Hz), 8.53 (1H, d, $J = 2.1$ Hz), 9.37 (1H, d, $J = 2.7$ Hz).

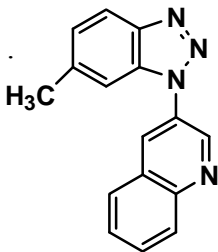
^{13}C NMR (75 MHz, CDCl_3): δ 110.8, 120.0, 127.5, 128.1, 128.3, 128.5, 129.7, 129.8, 130.2, 130.7, 130.8, 131.1, 144.7, 147.2, 147.8.

EI-MS (m/z): 280 (M^+), 252, 217, 190.

IR (KBr, cm^{-1}): 743, 812, 865, 1073, 1202, 1280, 1480, 1598, 2362, 3091 cm^{-1} .

Elemental Analysis calculated for $C_{15}H_9N_4Cl$: C 64.18, H 3.23, N 19.96; Found: C 64.10, H 3.28, N 19.99 %.

Compound 2p:



Characteristic: White solid (Reaction time 3 h, isolated yield 90 %)

Melting point: 122- 124 °C (EtOAc)

1H NMR (300 MHz, $CDCl_3$): δ 2.57 (3H, s), 7.29 (1H, d, $J = 7.2$ Hz), 7.58 (1H, s), 7.67 (1H, t, $J = 7.8$ Hz), 7.82 (1H, t, $J = 7.8$ Hz), 7.97 (1H, d, $J = 8.1$ Hz), 8.04 (1H, d, $J = 8.7$ Hz), 8.22 (1H, d, $J = 8.7$ Hz), 8.50 (1H, d, $J = 1.2$ Hz), 9.39 (1H, s).

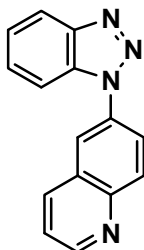
^{13}C NMR (75 MHz, $CDCl_3$): δ 22.0, 109.0, 119.9, 126.9, 127.5, 128.0, 129.5, 130.3, 130.6, 132.7, 139.7, 144.9, 145.1, 147.4.

EI-MS (m/z): 260 (M^+), 244, 223, 209, 192.

IR (KBr, cm^{-1}): 1056, 1286, 1470, 1498, 1605, 2376, 2917, 3054 cm^{-1} .

Elemental Analysis calculated for $C_{16}H_{12}N_4$: C 73.83, H 4.65, N 21.52; Found: C 73.78, H 4.66, N 21.56 %.

Compound 2q:



Characteristic: White solid (Reaction time 3 h, isolated yield 75 %)

Melting point: 226 – 228 °C (EtOAc)

1H NMR (300 MHz, $CDCl_3$): δ 7.30 – 7.23 (1H, m), 7.56 (1H, dt, $J = 1.5$ and 7.5 Hz), 7.63 (1H, dd, $J = 1.4$ and 7.5 Hz), 7.75- 7.66 (4H, m), 7.84 (1H, d, $J = 9.4$ Hz), 8.04 (1H, dd, $J = 1.5$ and 8.0 Hz), 8.86 (1H, d, $J = 3.0$ Hz).

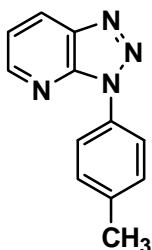
^{13}C NMR (75 MHz, $CDCl_3$): δ 120.2, 120.4, 121.6, 125.1, 128.8, 129.4, 130.3, 130.6, 132.1, 133.9, 138.6, 141.5, 142.7, 148.6, 149.8.

EI-MS (m/z): 246 (M^+), 225, 205, 168, 156.

IR (KBr, cm^{-1}): 769, 1058, 1097, 1312, 1356, 1409, 1445, 1494, 1588, 2373, 3055 cm^{-1} .

Elemental Analysis calculated for $C_{15}H_{10}N_4$: C 73.16, H 4.09, N 22.75; Found: C 73.11, H 4.11, N 22.78 %.

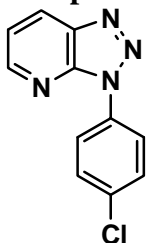
Compound 2r: (Reaction time 6 h, isolated yield 86 %)



Characteristic: Pale yellow crystalline solid

$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 2.42 (3H, s), 7.40 – 7.35 (3H, m), 8.09 (2H, d, $J = 8.4$ Hz), 8.41 (1H, dd, $J = 8.4$ and 1.5 Hz), 8.71 (1H, dd, $J = 4.5$ and 1.5 Hz).

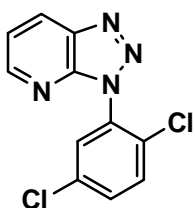
Compound 2s: (Reaction time 6 h, isolated yield 88 %)



Characteristic: Pale white crystalline solid

$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 7.43 – 7.38 (1H, m), 7.52 (2H, d, $J = 9.0$ Hz), 8.27 (2H, d, $J = 9.0$ Hz), 8.43 (1H, d, $J = 8.1$ Hz), 8.73 (1H, d, $J = 4.2$ Hz).

Compound 2t:



Characteristic: White crystalline solid (Reaction time 6 h, isolated yield 88 %)

Melting point: 146-148 °C (EtOAc)

$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 7.44-7.39 (1H, m), 7.51-7.47 (1H, m), 7.61-7.55 (2H, m), 8.46 (1H, d, $J = 8.4$ Hz), 8.70 (1H, d, $J = 4.5$ Hz).

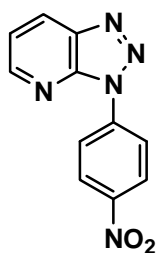
$^{13}\text{C NMR}$ (75 MHz, CDCl_3): δ 120.3, 129.1, 129.2, 130.0, 131.4, 131.6, 133.3, 133.5, 136.5, 146.2, 151.2.

EI-MS (m/z): 264 (M^+), 238, 236, 201, 174, 166.

IR (KBr, cm^{-1}): 786, 1049, 1248, 1407, 1495, 1565, 2345, 3044 cm^{-1} .

Elemental Analysis calculated for $\text{C}_{11}\text{H}_6\text{N}_4\text{Cl}_2$: C 49.84, H 2.28, N 21.13; Found: C 49.80, H 2.30, N 21.15 %.

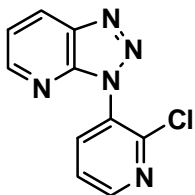
Compound 2u:



Characteristic: yellow crystalline solid (Reaction time 6.5 h, isolated yield 75 %)

Melting point: 178 – 180 °C (EtOAc)

Compound 2v:



Characteristic: White crystalline solid (Reaction time 6.5 h, isolated yield 84 %)

Melting point: 152 - 154 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 7.56-7.44 (2H, m), 7.99 (1H, dd, J = 8.1 and 1.5 Hz), 8.51 (1H, dd, J = 8.5 and 1.5 Hz), 8.80 – 8.63 (2H, m).

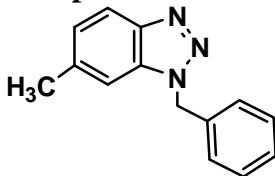
¹³C NMR (75 MHz, CDCl₃): δ 120.5, 123.1, 129.2, 130.1, 136.7, 137.6, 146.3, 148.6, 151.0, 151.4.

EI-MS (m/z): 231 (M⁺), 205, 203, 176, 168.

IR (KBr, cm⁻¹): 773, 811, 1046, 1237, 1406, 1479, 1588, 2374, 3070 cm⁻¹.

Elemental Analysis calculated for C₁₀H₆N₅Cl: C 51.85, H 2.61, N 30.23; Found: C 51.80, H 2.63, N 30.26 %.

Compound 2w:



Characteristic: Off white solid (Reaction time 3 h, isolated yield 85%)

Melting point: 126 - 128 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 2.40 (3H, s), 5.74 (2H, s), 7.13 – 7.09 (2H, m), 7.31 – 7.26 (5H, m), 7.88 (1H, d, J = 8.4 Hz).

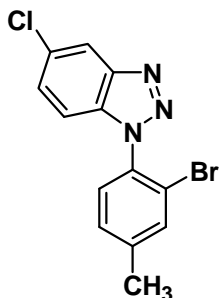
¹³C NMR (75 MHz, CDCl₃): δ 22.0, 52.0, 108.9, 119.3, 126.4, 127.5, 128.4, 129.0, 133.3, 134.9, 138.2, 144.7.

EI-MS (m/z): 223 (M⁺), 208, 162.

IR (KBr, cm⁻¹): 708, 1221, 1450, 1618, 2375, 2921, 3032 cm⁻¹.

Elemental Analysis calculated for C₁₄H₁₃N₃: C 75.31, H 5.87, N 18.82; Found: C 75.18, H 5.95, N 18.87 %

Compound 2x:



Characteristic: White solid (Reaction time 3 h, isolated yield 92 %)

Melting point: 140 - 142 °C (EtOAc)

¹H NMR (300 MHz, CDCl₃): δ 2.53 (3H, s), 7.18 (1H, s), 7.27 (1H, d, J= 8.4 Hz), 7.62 – 7.49 (3H, m), 8.03 (1H, d, J= 8.4 Hz).

¹³C NMR (75 MHz, CDCl₃): δ 21.9, 109.4, 119.5, 126.6, 129.0, 129.3, 131.0, 131.6, 133.4, 134.0, 134.9, 139.3.

EI-MS (m/z): 322 (M⁺+1), 290, 266, 207, 166.

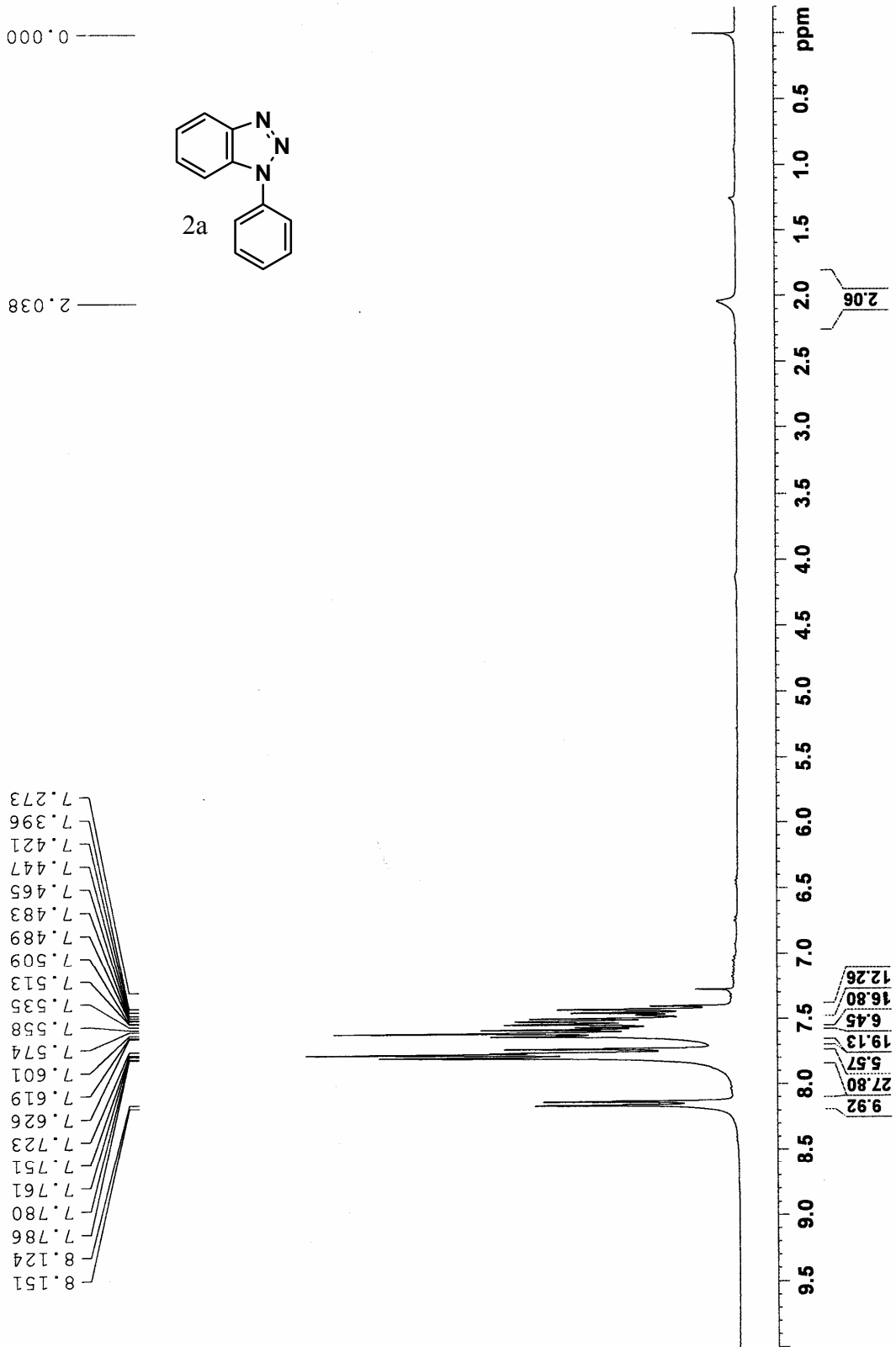
IR (KBr, cm⁻¹): 799, 1040, 1481, 1580, 2340, 3075 cm⁻¹.

Elemental Analysis calculated for C₁₃H₉N₃BrCl : C 48.40, H 2.81, N 13.03; Found: C 48.36, H 2.82, N 13.06 %

4. References

- 1) Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A.R. *Vogel's Textbook of Practical Organic Chemistry*; Pearson Education, Fifth Edition, Third Indian reprint, 2005.
- 2) Xiao, W. J.; Alper, H. *J. Org. Chem.* **1999**, *64*, 9646
- 3) V. Zimmermann and S. Bräse, *J. Comb. Chem.* 2007, **9**, 1114.
- 4) D. D. M. Casoni, A. Mangini, R. Passerini and C. Zauli, *Gazzetta Chimica Italiana* 1958, **88**, 977
- 5) I. P. Beletskaya, D. V. Davydov and M. Moreno-Manas, *Tetrahedron Letters* 1998, **39**, 5617
- 6) R. L. Clark, A. A. Pessolano, T. Ying Shen, D. P. Jacobus, H. Jones, V. J. Lotti and L. M. Flataker, *Journal of Medicinal Chemistry* 1978, **21**, 965

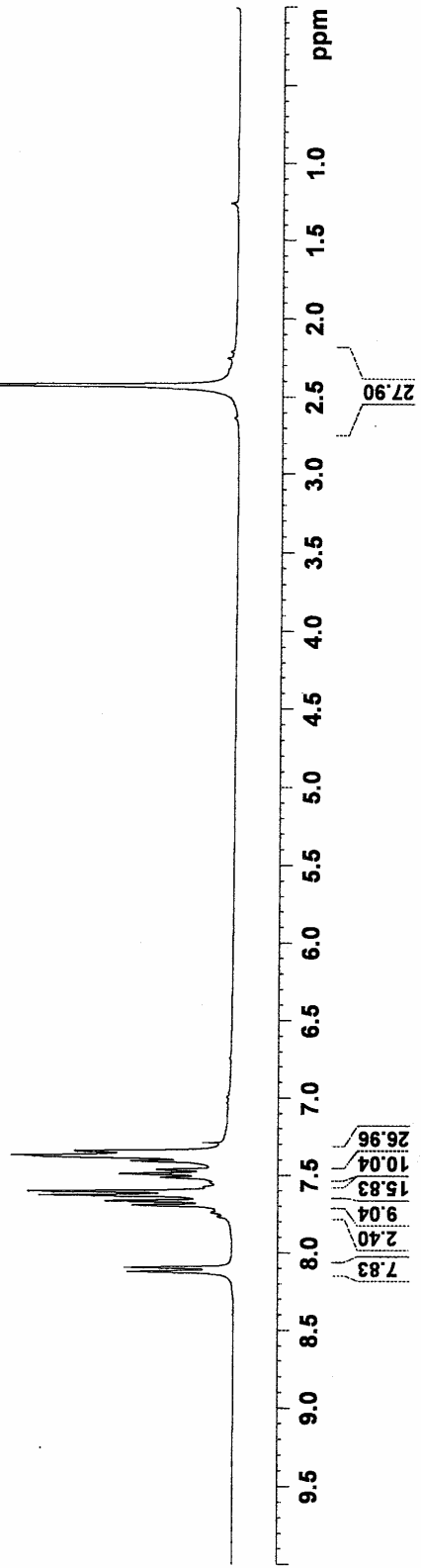
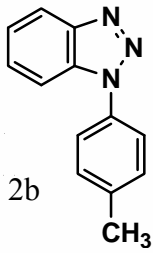
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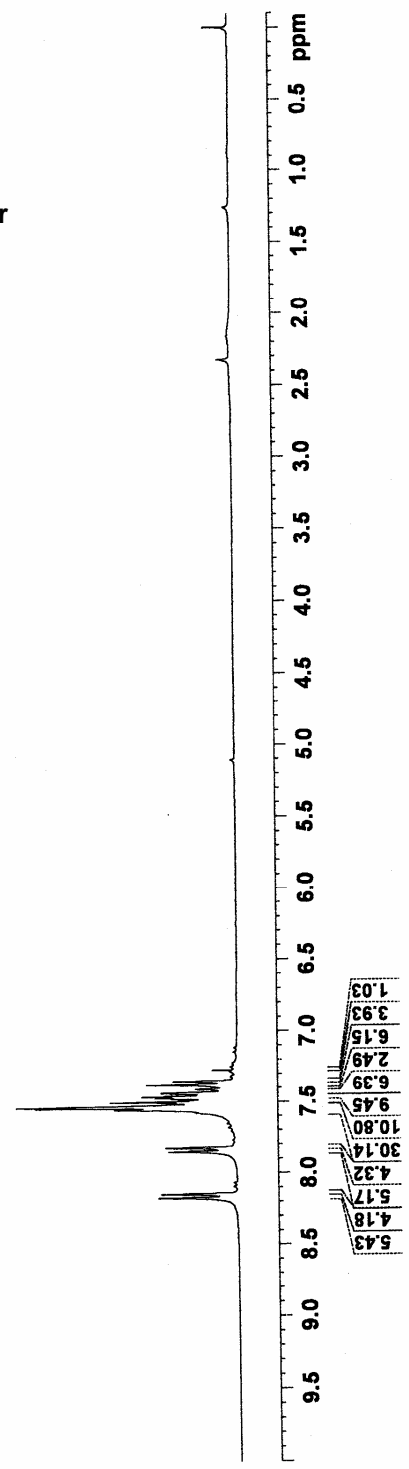
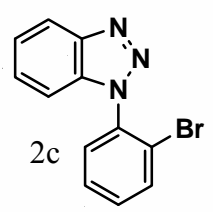
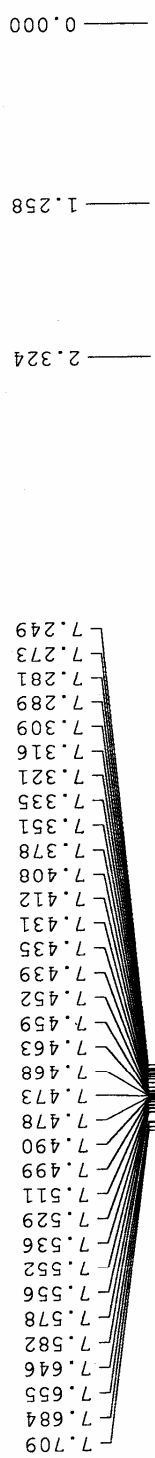
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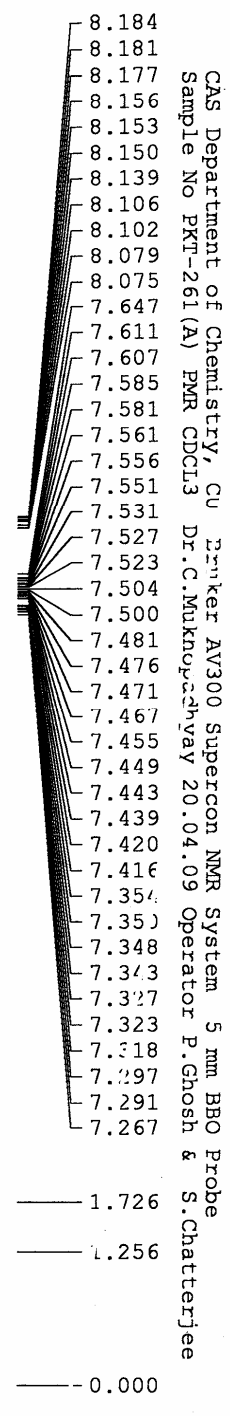
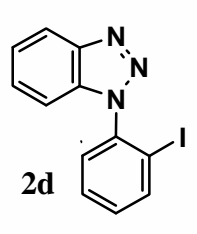
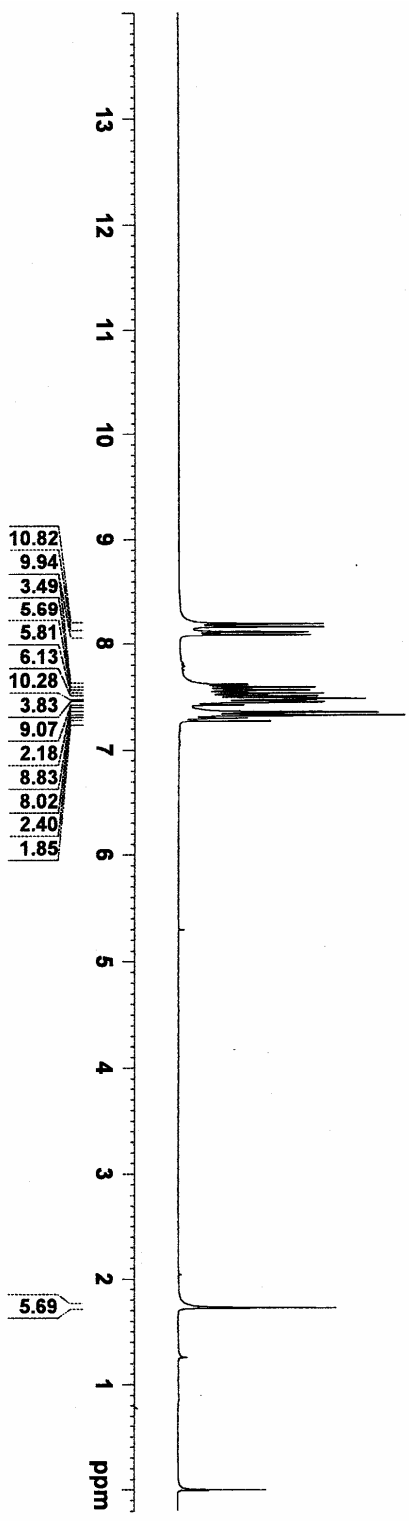
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 7.597
 7.570
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 7.343
 7.288

2.423

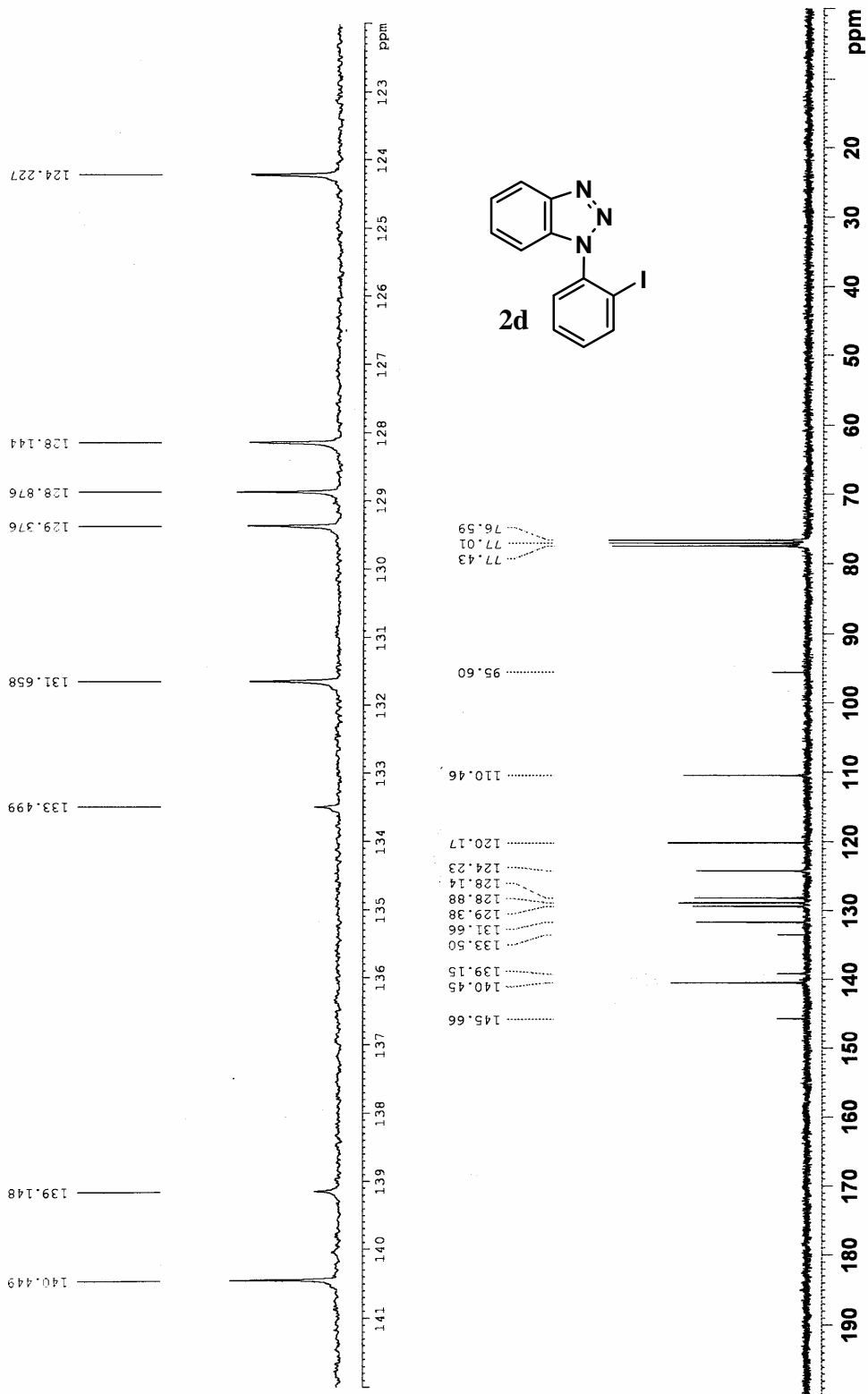


CAS Department of Chemistry, CU Bruker AV300 Supercon NMR System 5 mm BBO Probe
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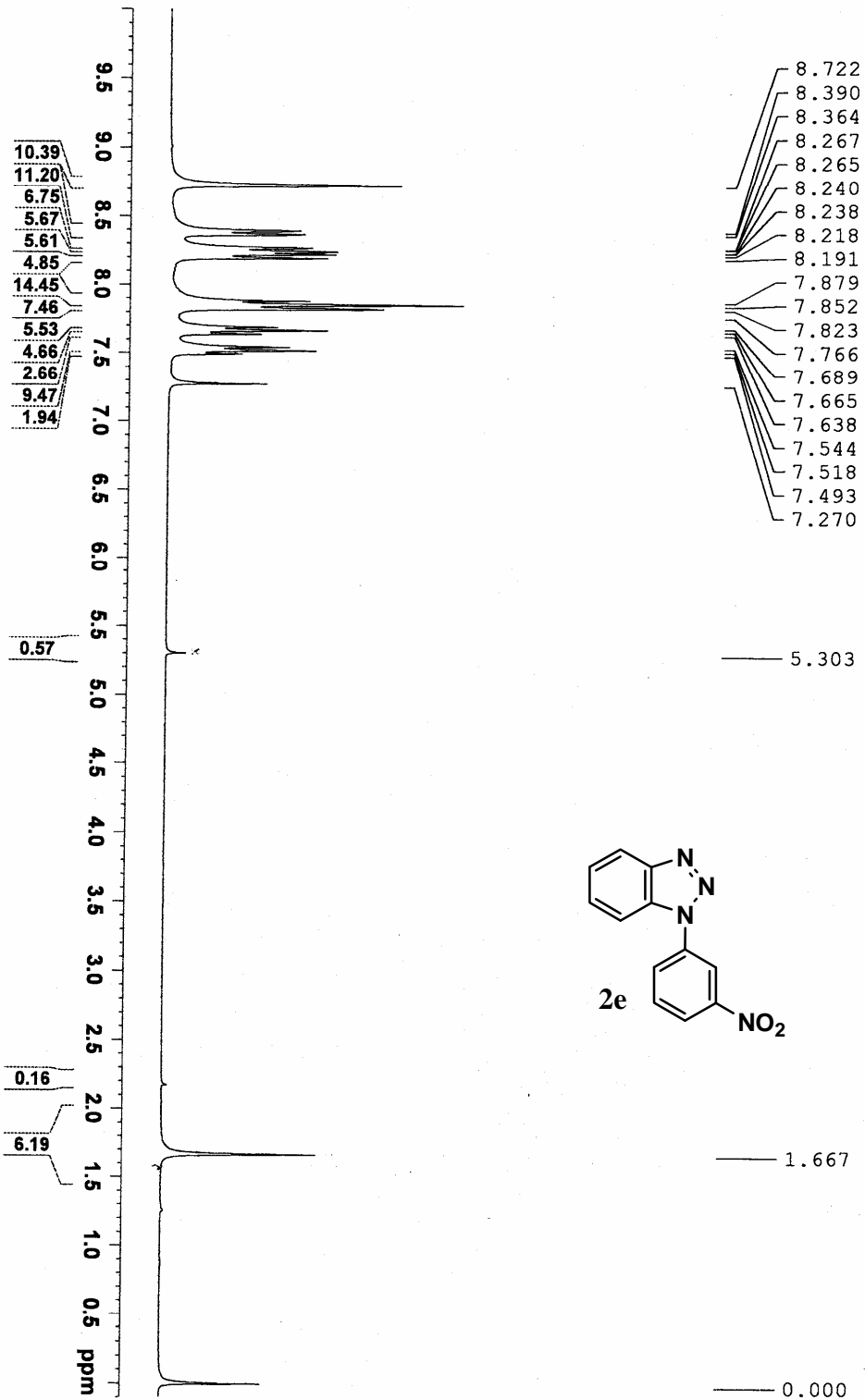




CAS Department of Chemistry, CU Bruker AV300 Supercon NMR System 5 mm BBO Probe
Sample No PKT-261(A) CMR CDCL3 Dr.C.Mukhopadhyay 22.04.09 Operator P.Ghosh & S.Chatterjee

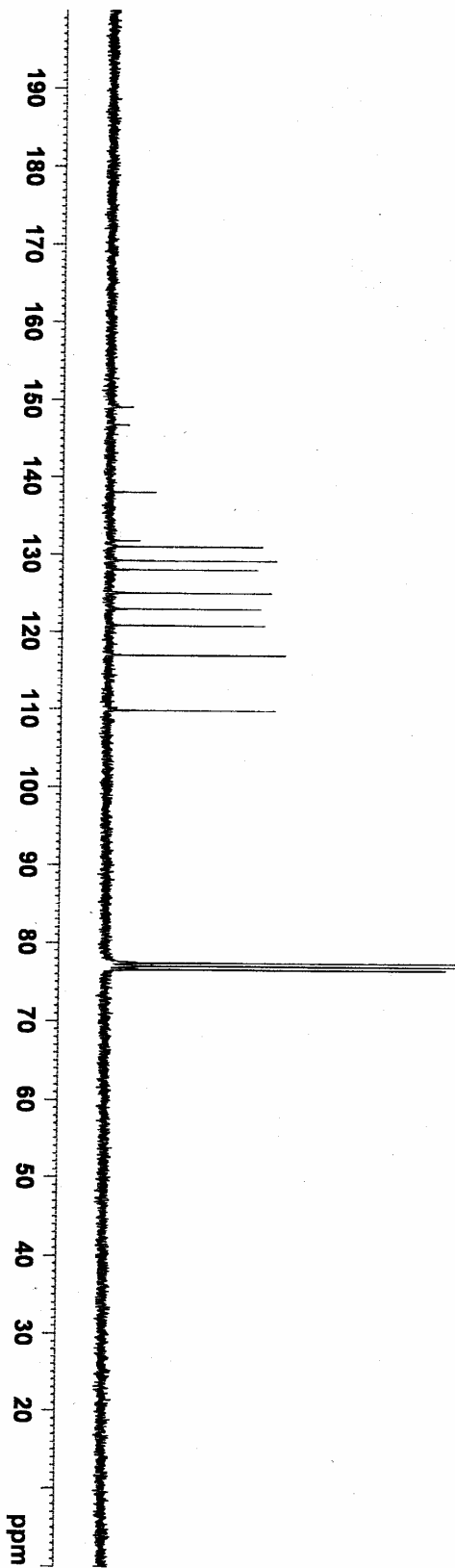
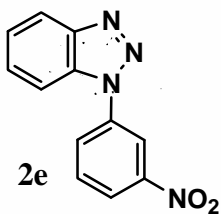


CAS Department of Chemistry, CU Bruker AV300 Supercon NMR System 5 mm BBO Probe
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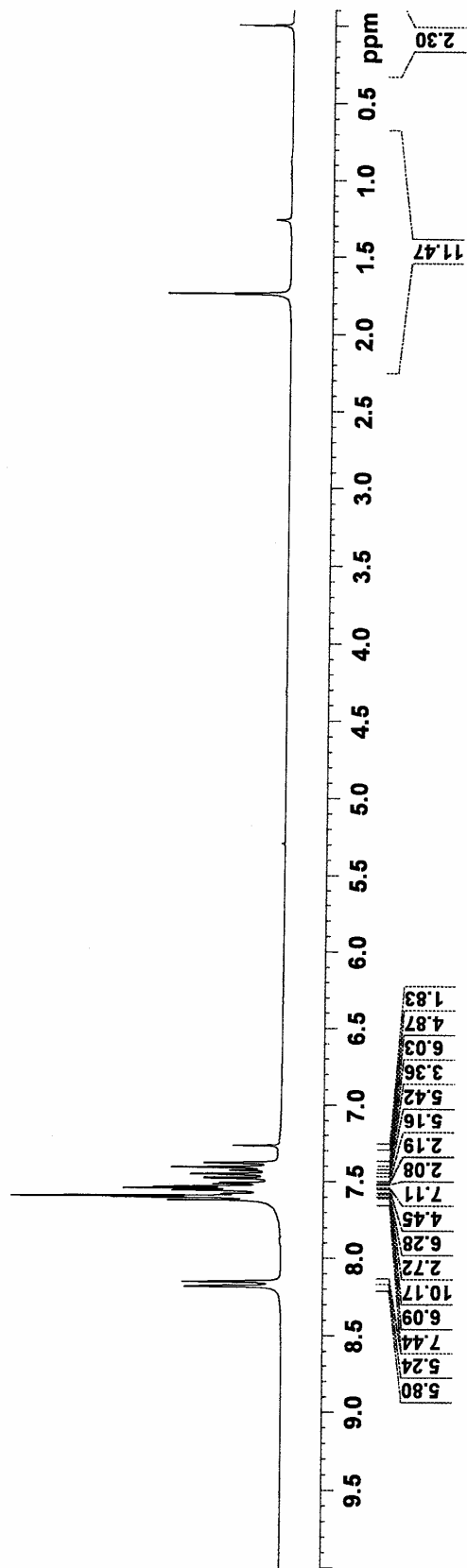
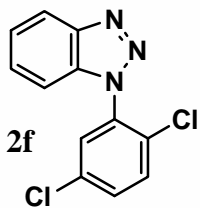
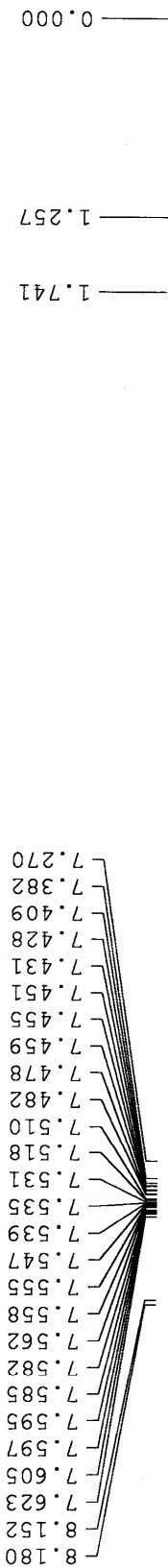


CAS Department of Chemistry, CU Bruker AV300 Supercon NMR System 5 mm BBO Probe
Sample No PKT-252(A) CMR CDCl₃ Dr.C.Mukhopadhyay 25.03.09 Operator P.Ghosh & S.Chatterjee

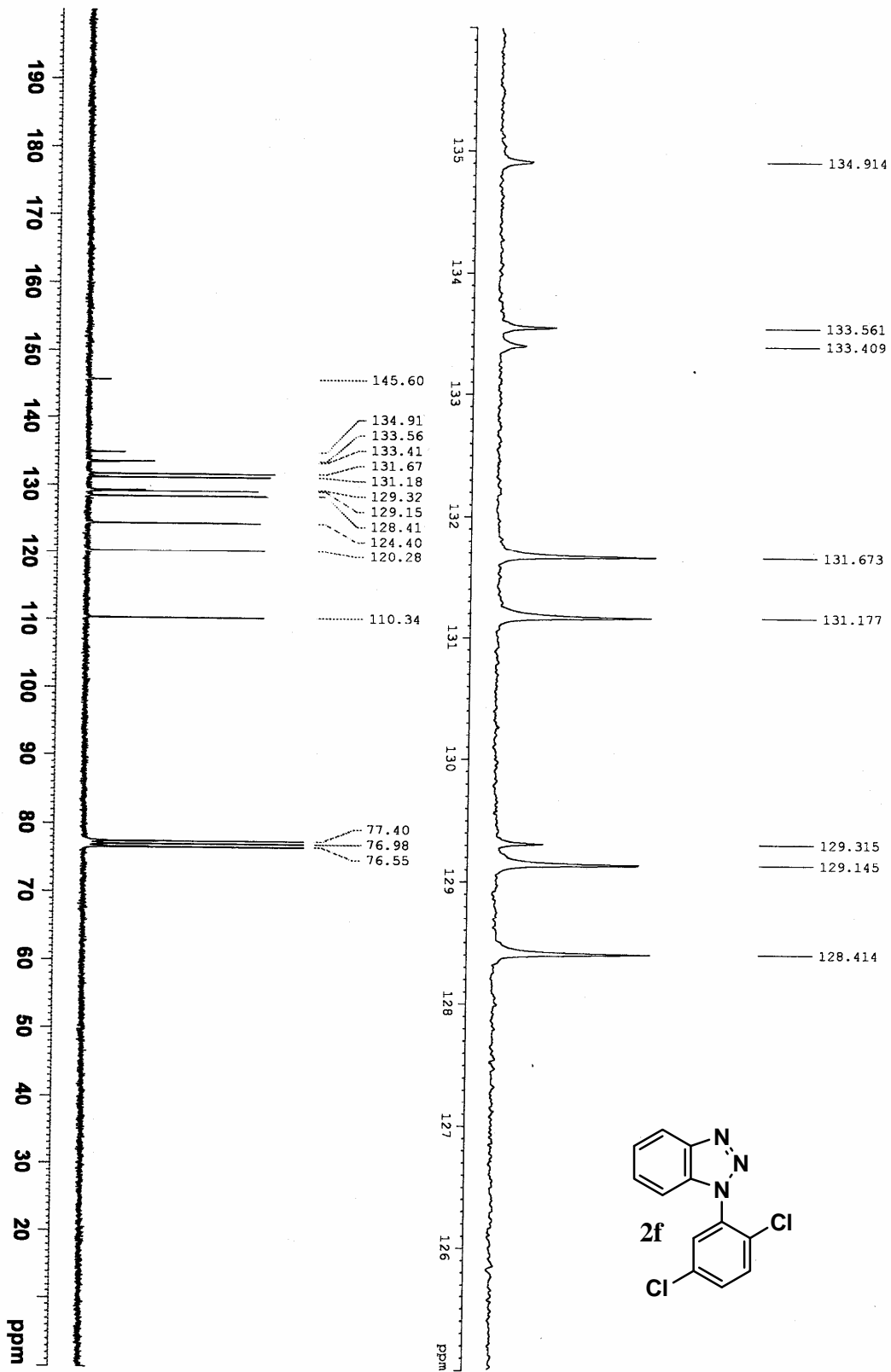
| | | |
|--------|--------|-------|
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| 146.72 | 131.76 | 76.98 |
| | 130.89 | 76.55 |
| | 129.14 | |
| | 127.83 | |
| | 124.07 | |
| | 122.89 | |
| | 120.79 | |
| | 117.01 | |
| | 109.83 | |



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
 Sample no PKT-279 (A) PMR CDCl3 Dr.C.Mukhopadhyay 17.06.09 Operator P.Ghosh & S.Chatterjee



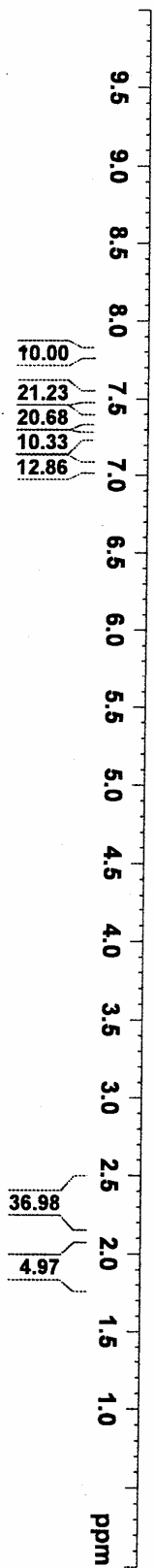
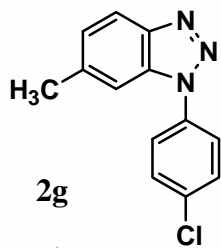
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Sample no PKT-279(A) CMR CDCL3 Dr.C.Mukhopadhyay 16.06.09 Operator P.Ghosh & S.Chatterjee



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
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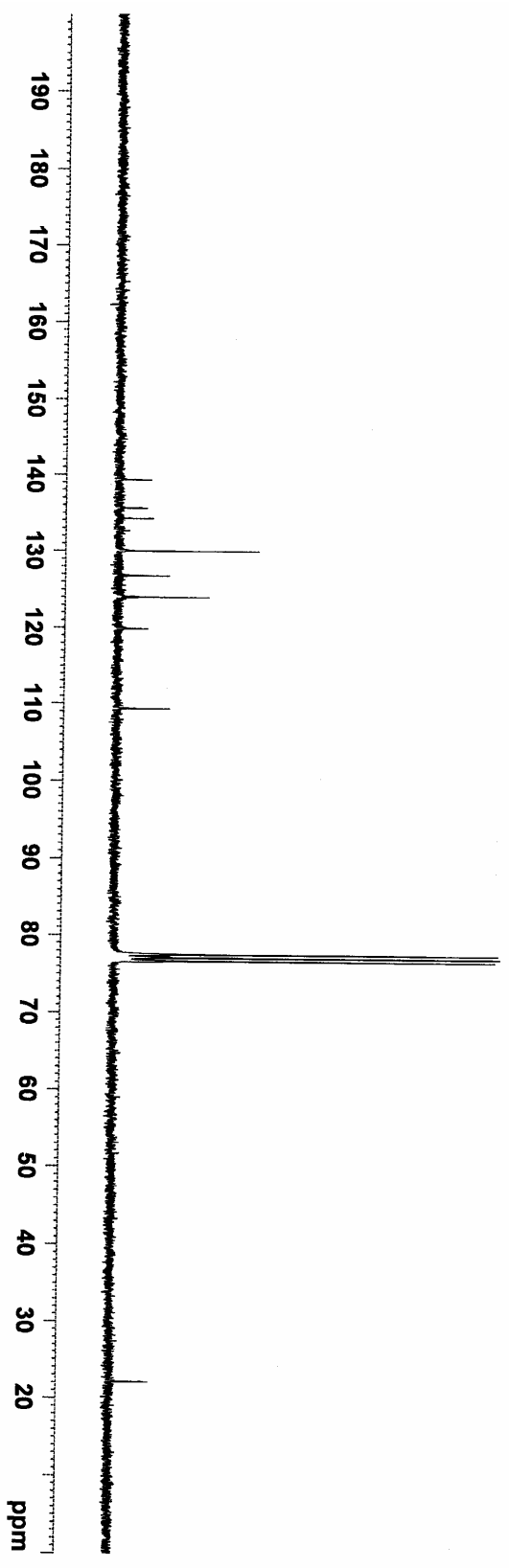
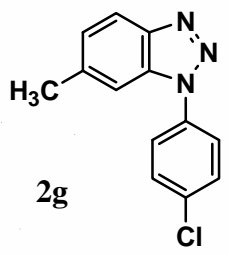
- 7.806
- 7.777
- 7.525
- 7.496
- 7.377
- 7.347
- 7.312
- 7.258
- 7.062
- 7.042
- 7.038

- 2.403
- 2.331
- 1.915

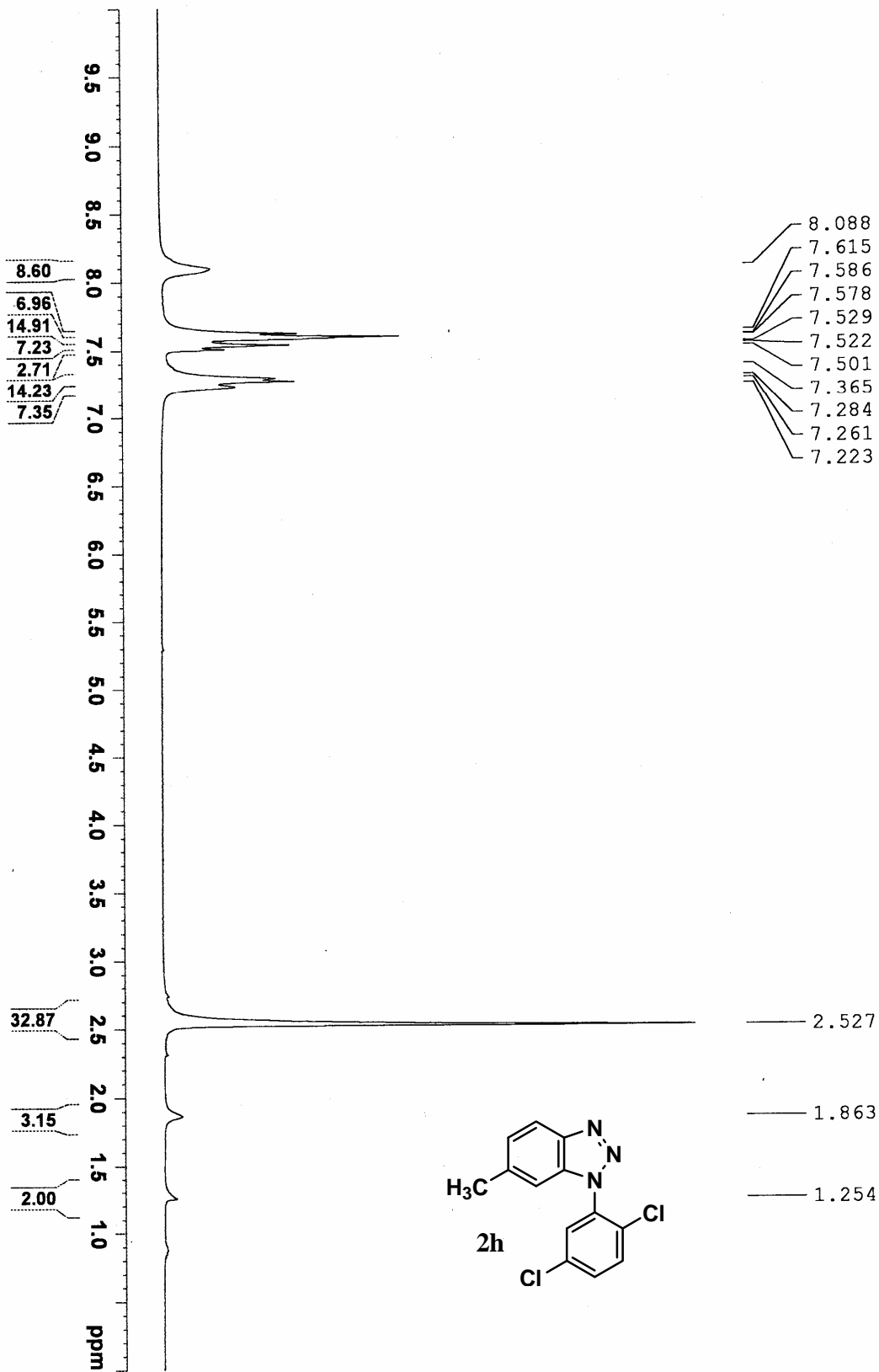


CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-340(A) CMR CDCl3 Dr. C.Mukhopadhyay 04.02.10 Operator P.Ghosh & S.Chatterjee

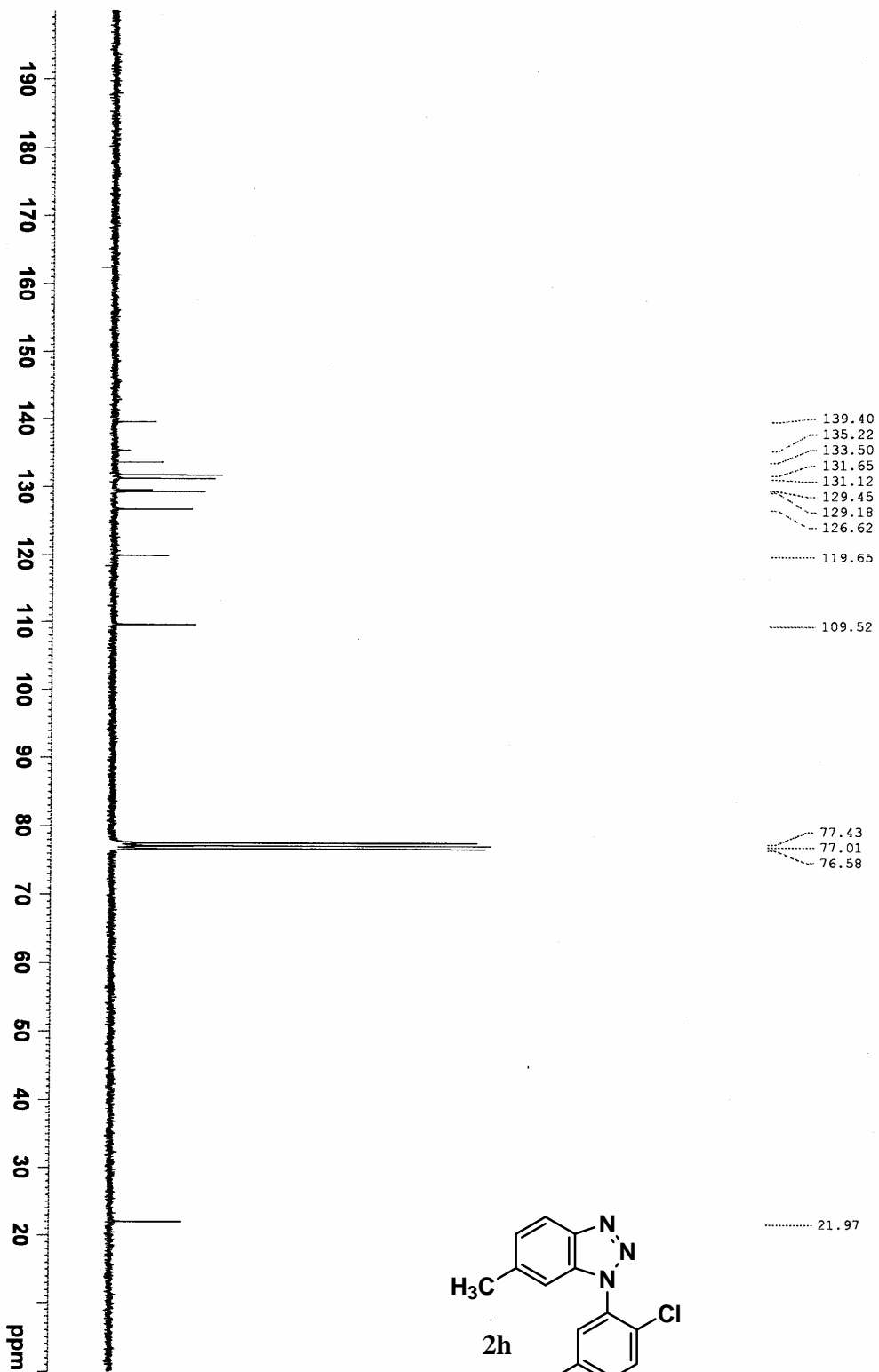
- 139.29
- 135.60
- 134.24
- 129.97
- 126.74
- 123.95
- 119.82
- 109.28
- 77.40
- 76.98
- 76.55
- 22.05



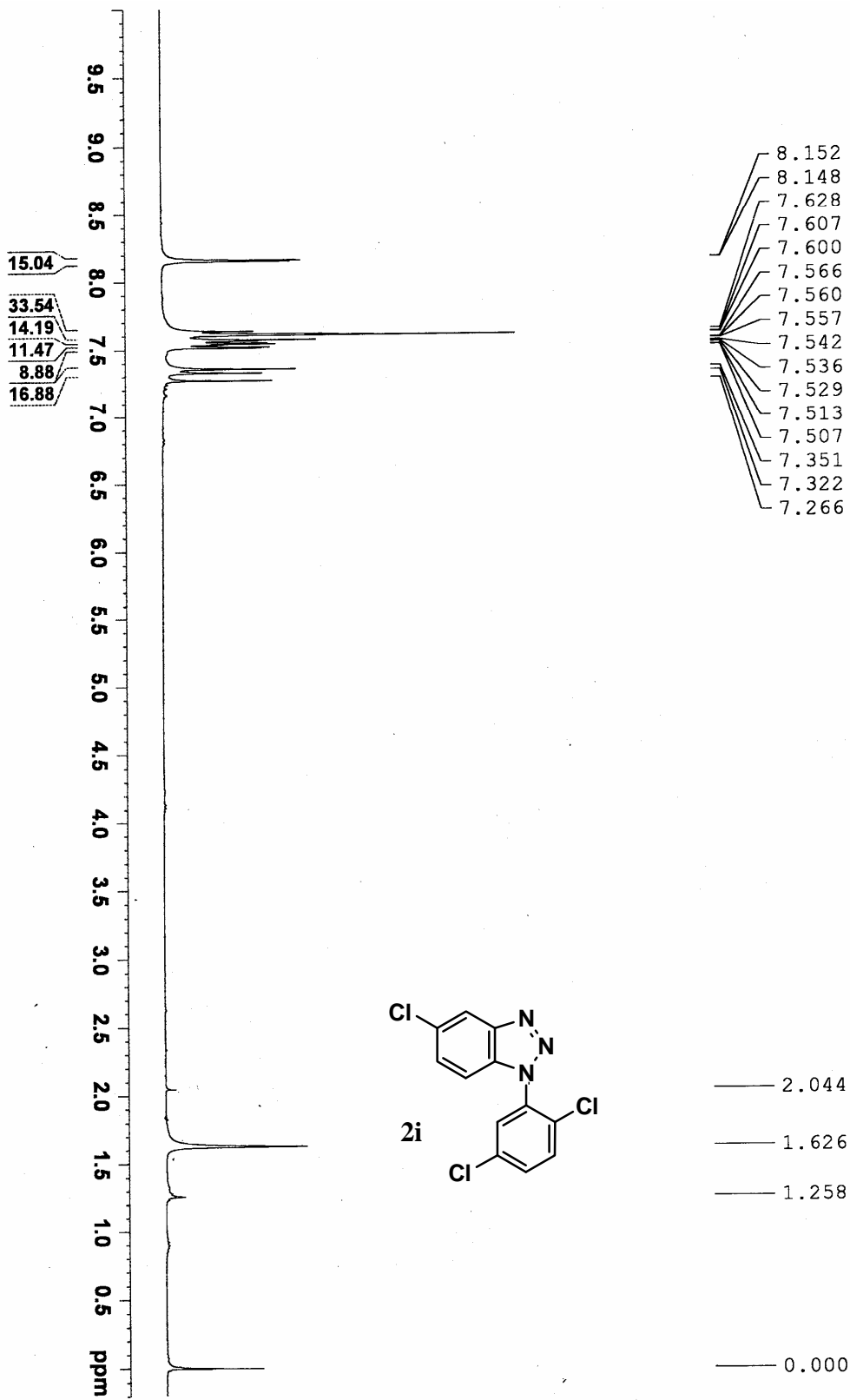
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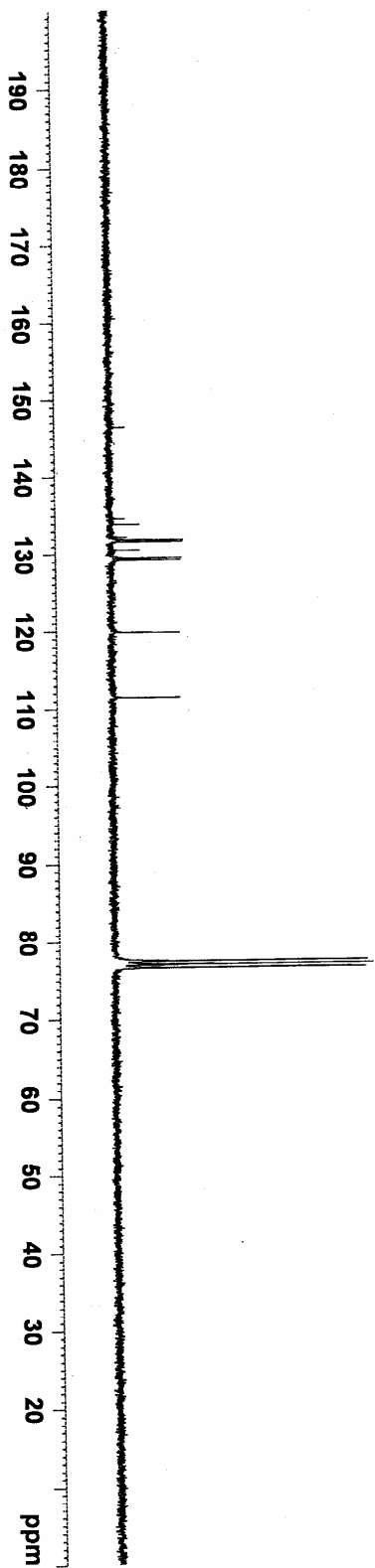
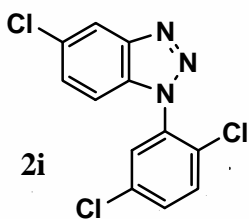
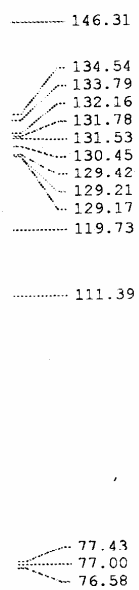
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Sample no PKT-339(A) CMR CDCI3 Dr. C.Mukhopadhyay 01.02.10 Operator P.Ghosh & S.Chatterjee



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-267(A) PMR CDCl₃ Dr.C.Mukhopadhyay 07.05.09 Operator P.Ghosh & S.Chatterjee



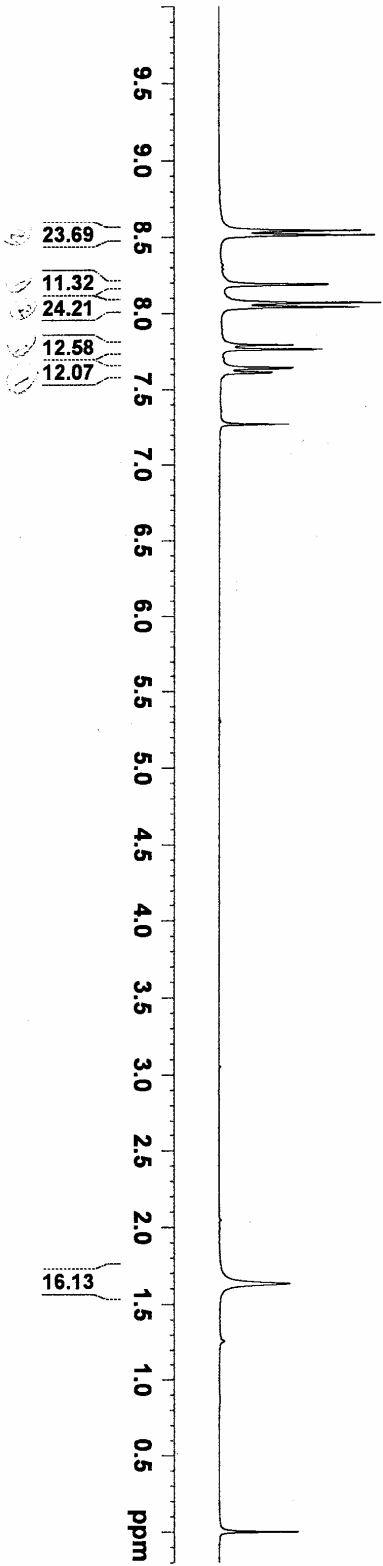
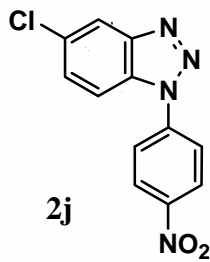
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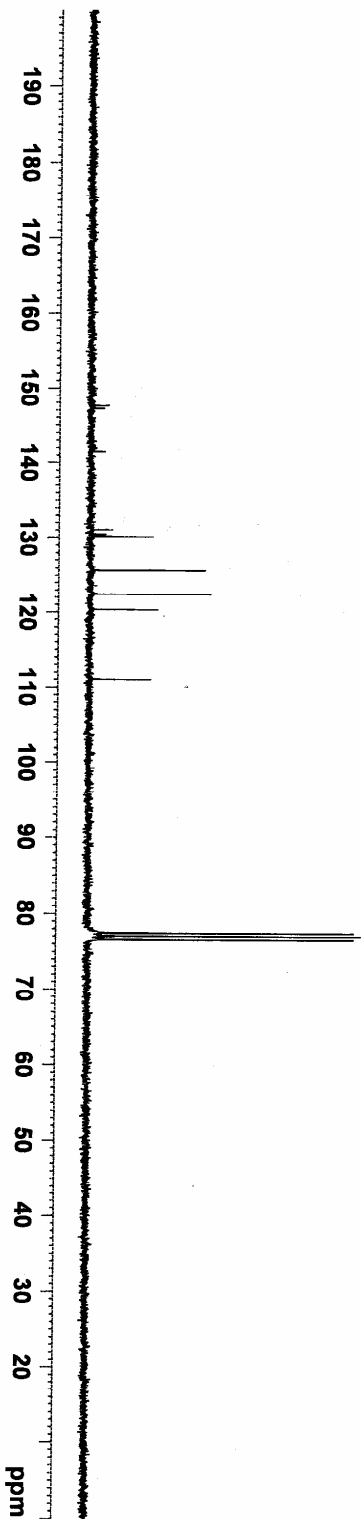
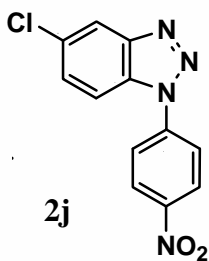
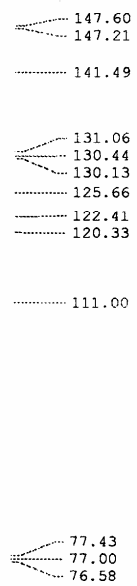
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Sample no PKI-275(A) PMR CDCl3 Dr.C.Mukhopadhyay 05.06.09 Operator P.Ghosh& S.Chatterjee

8.536
8.506
8.314
8.285
8.185
8.182
8.065
8.035
7.790
7.761
7.697
7.640
7.635
7.611
7.606
7.268

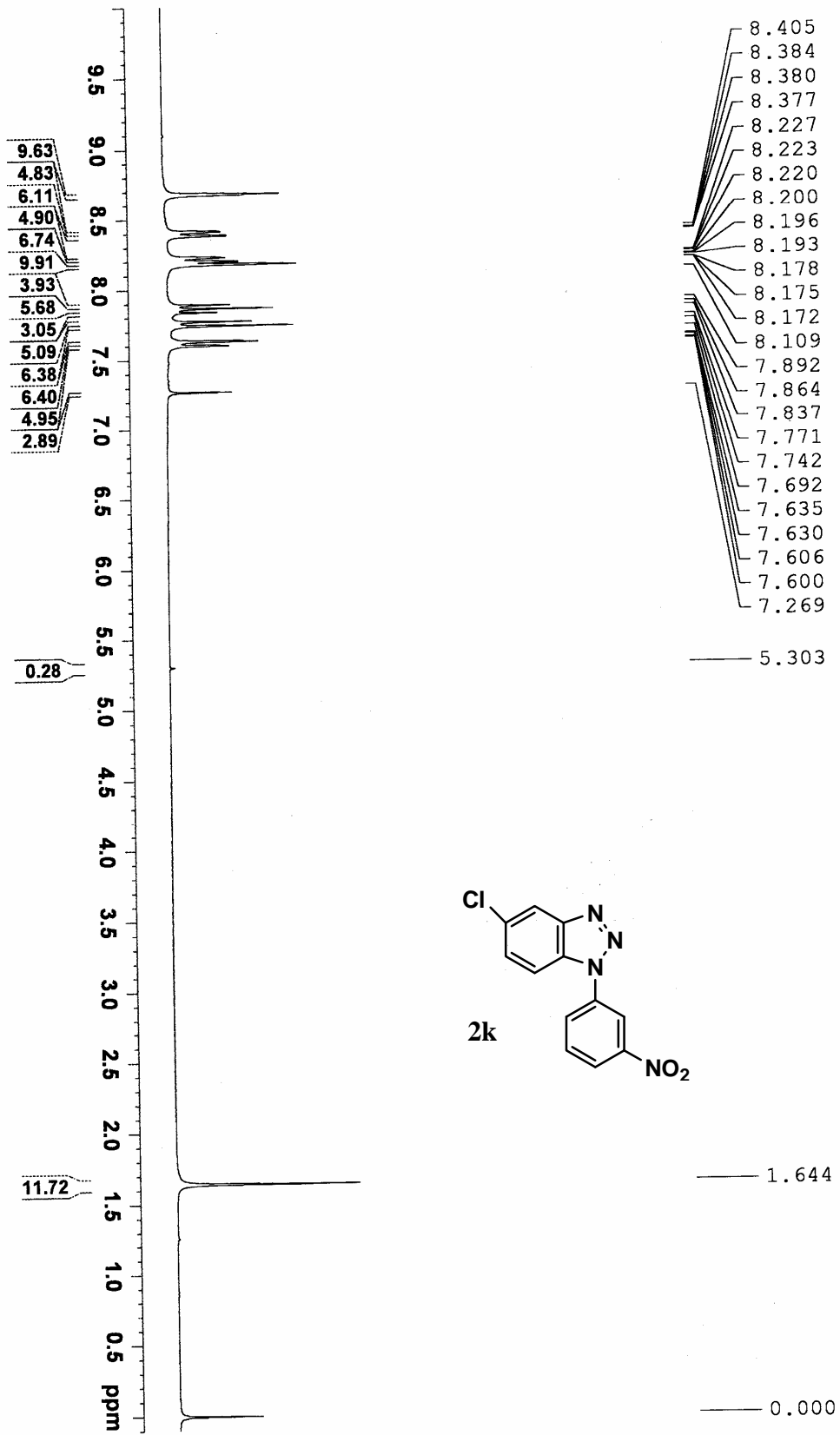
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1.254
0.000



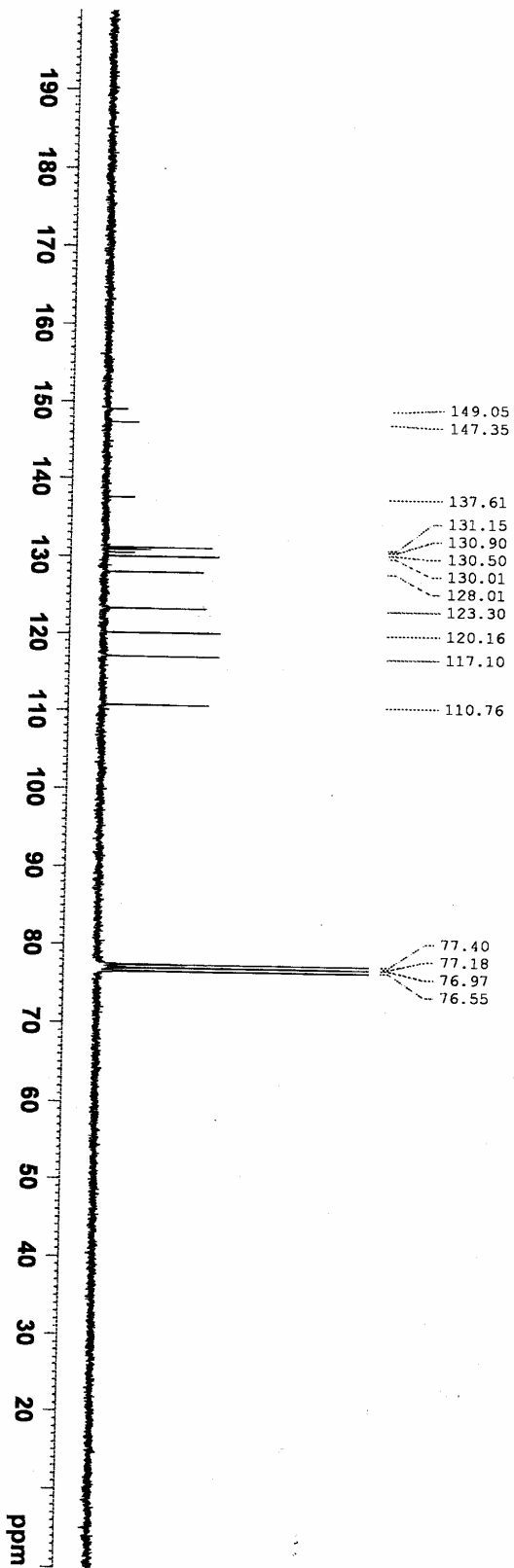
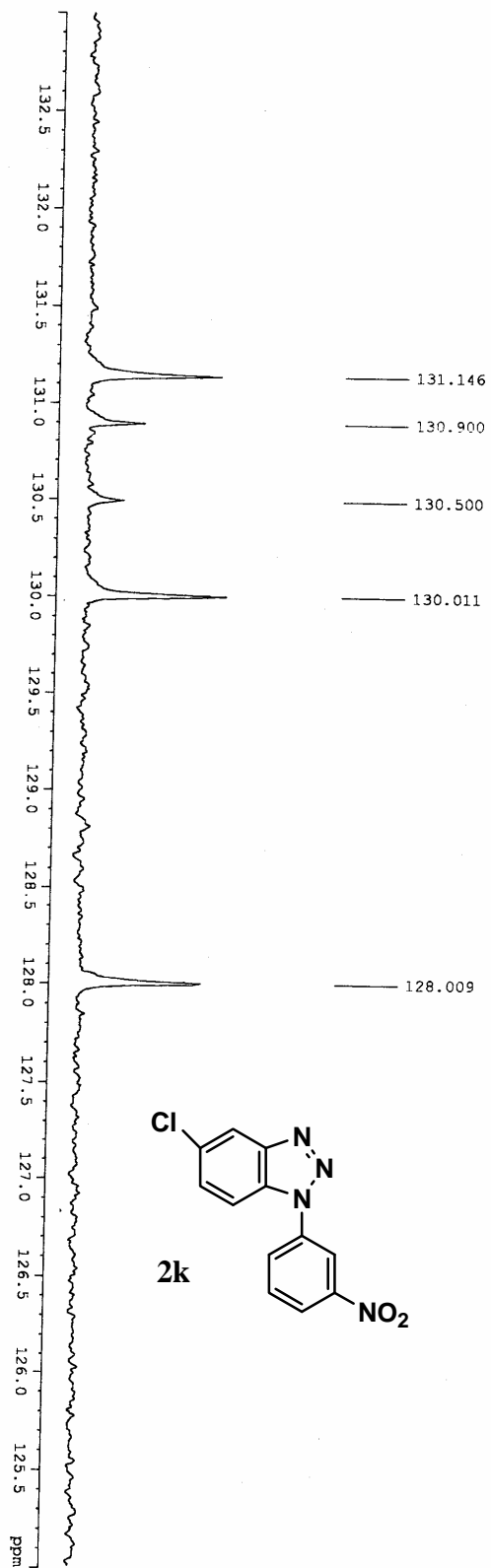
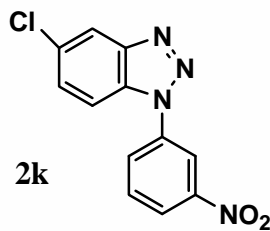
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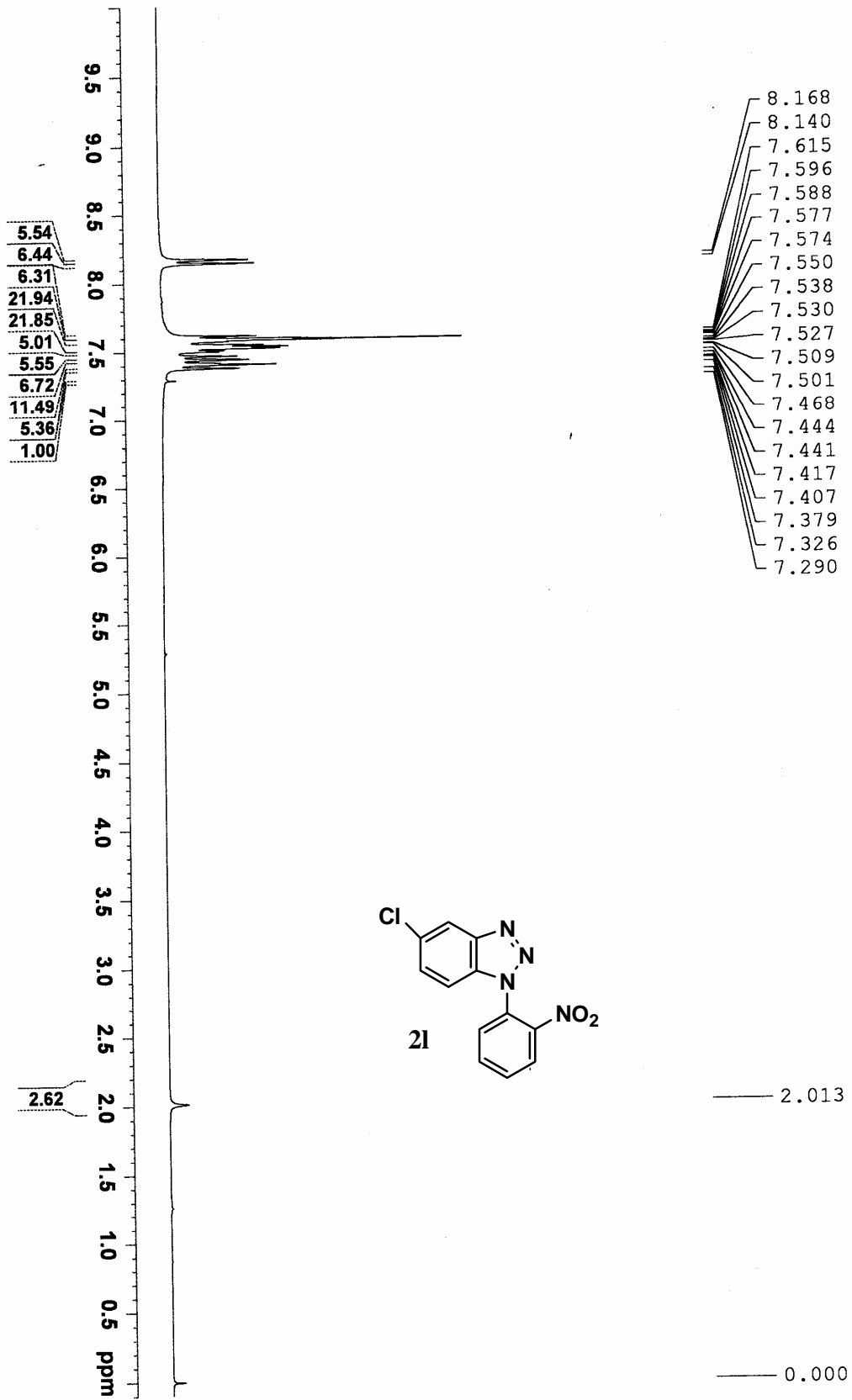
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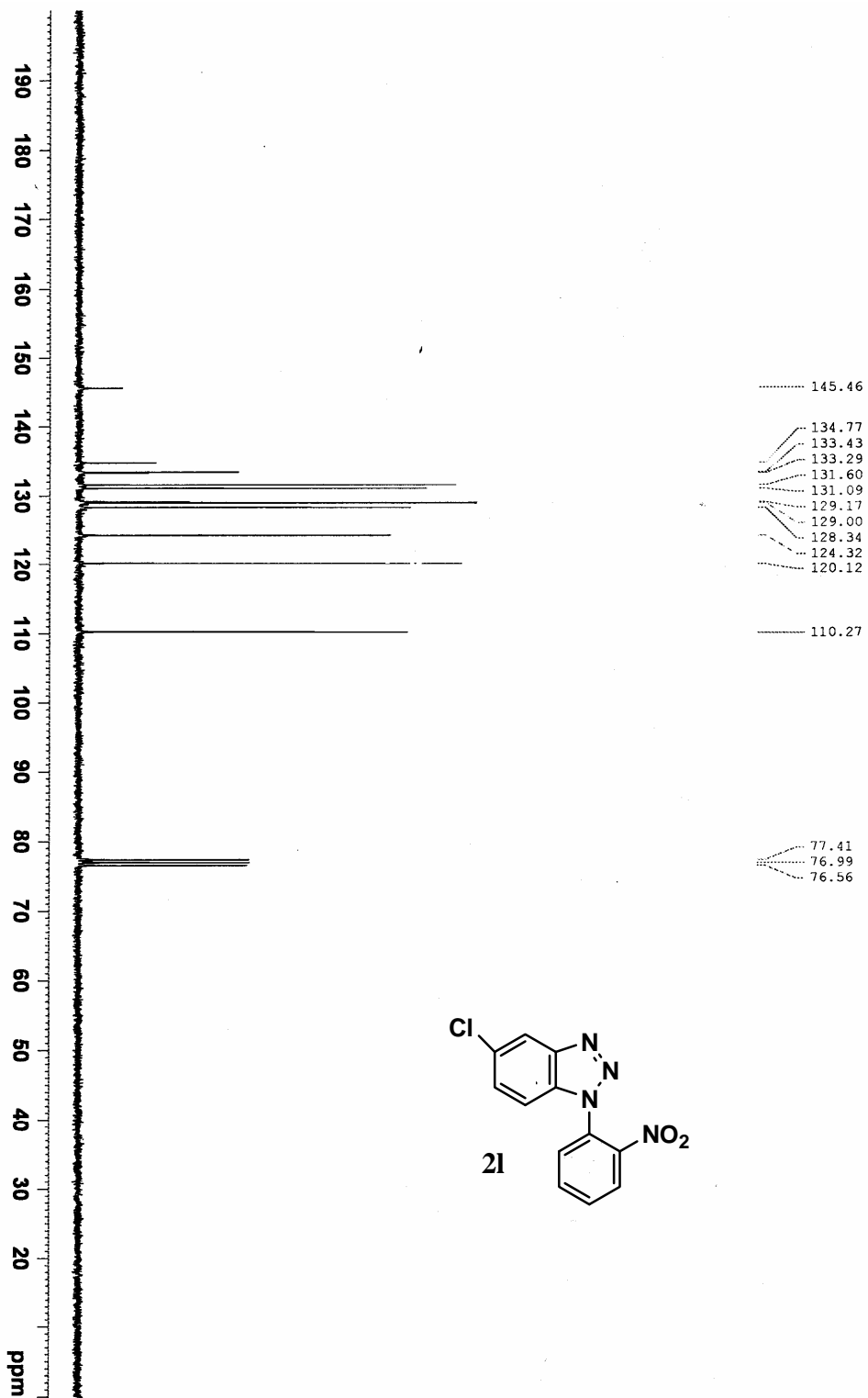
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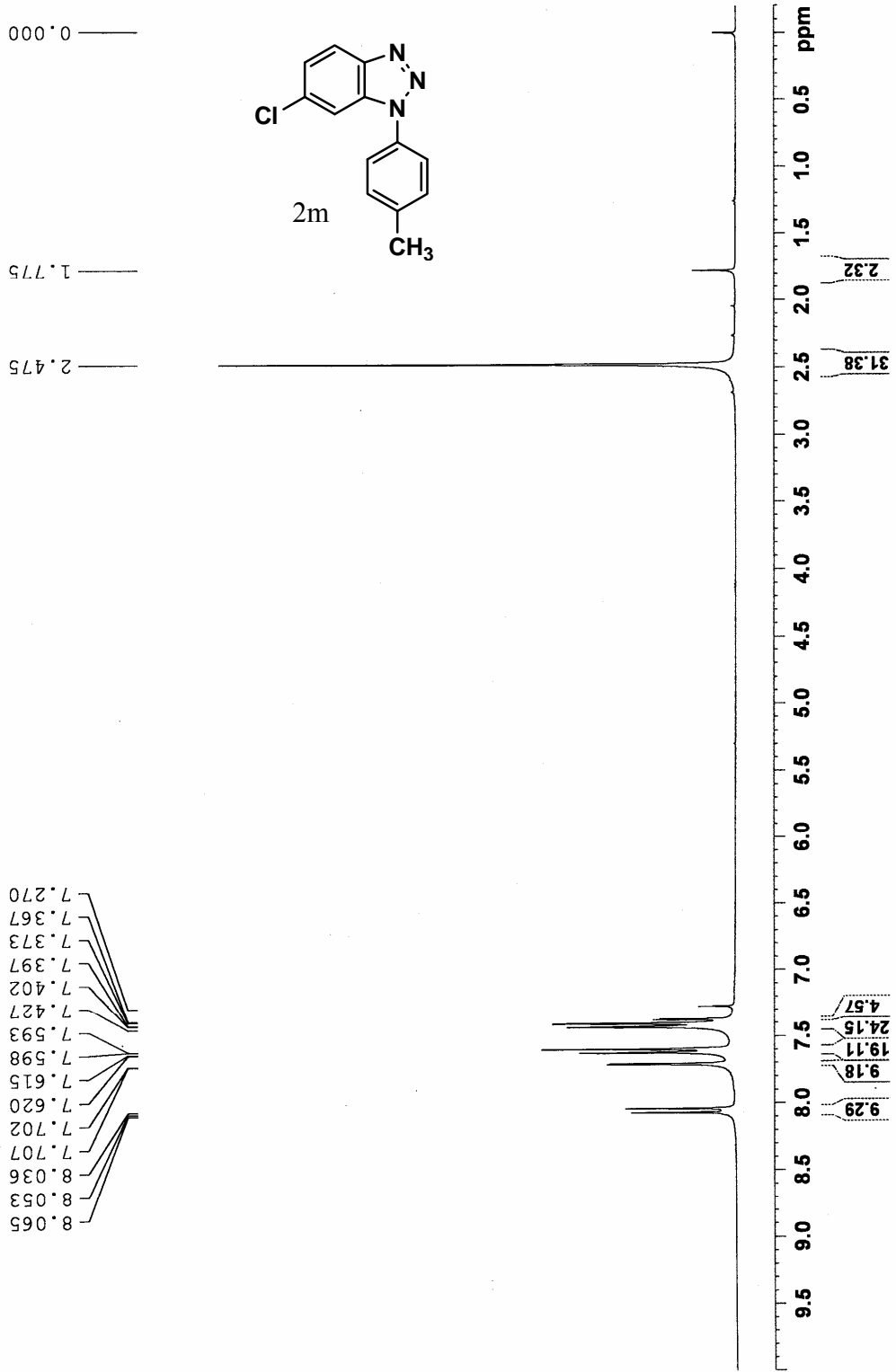
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CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
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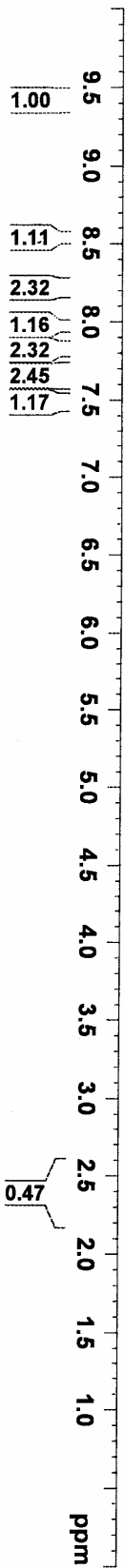
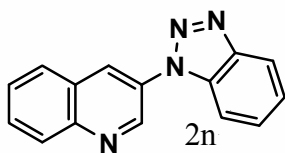
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Sample no PKT-337(A) FMR CDCL3 Dr.C.Mukhopadhyay 19.01.10 Operator P.Ghosh & S.Chatterjee



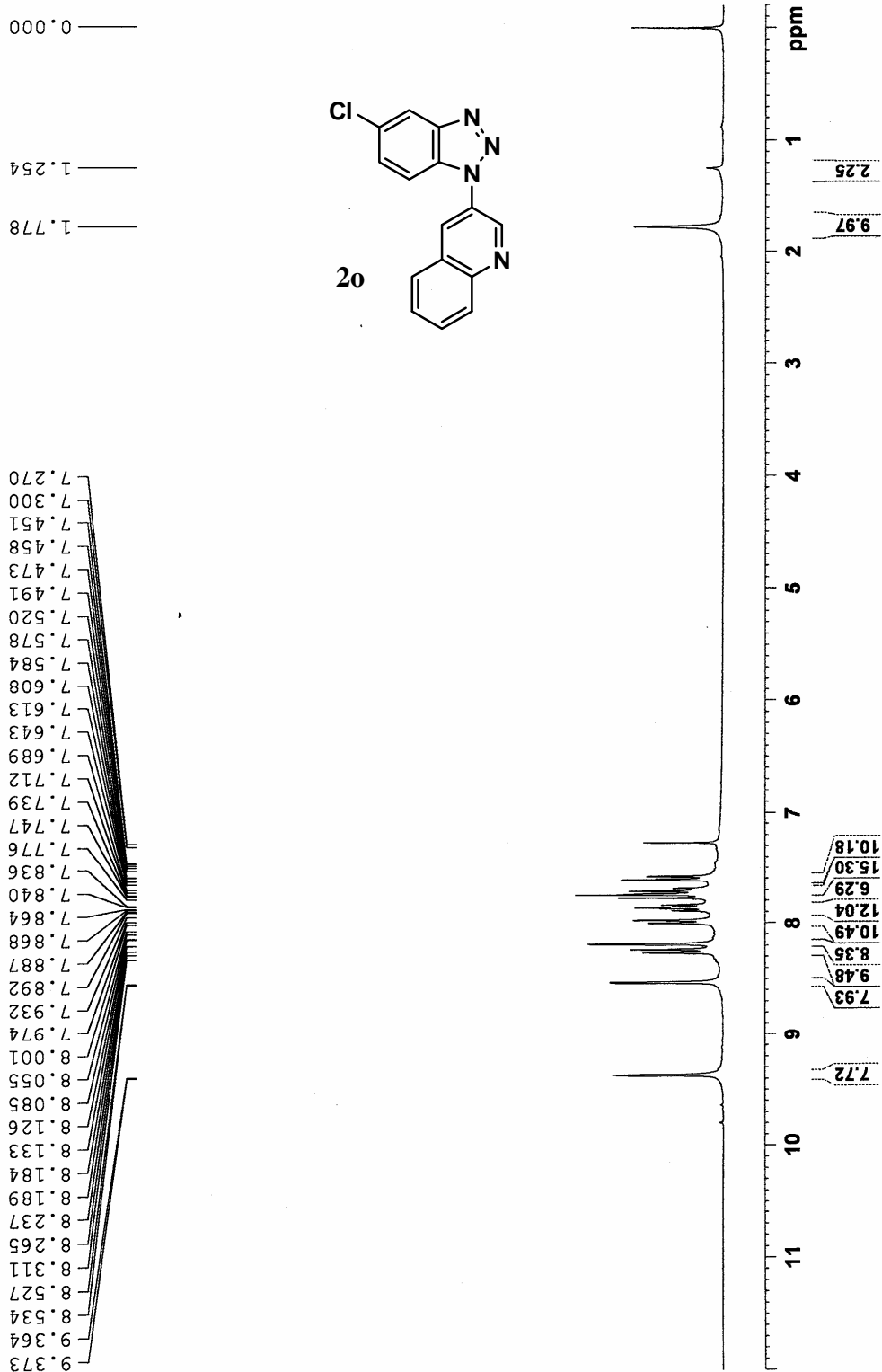
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Sample no PKT-363(A) PMR CDCL3 Dr.C.Mukhopadhyay 06.05.10 Operator P.Ghosh & S.Chatterjee

9.410
8.539
8.533
8.246
8.217
8.204
8.176
8.078
7.981
7.954
7.853
7.849
7.831
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7.259

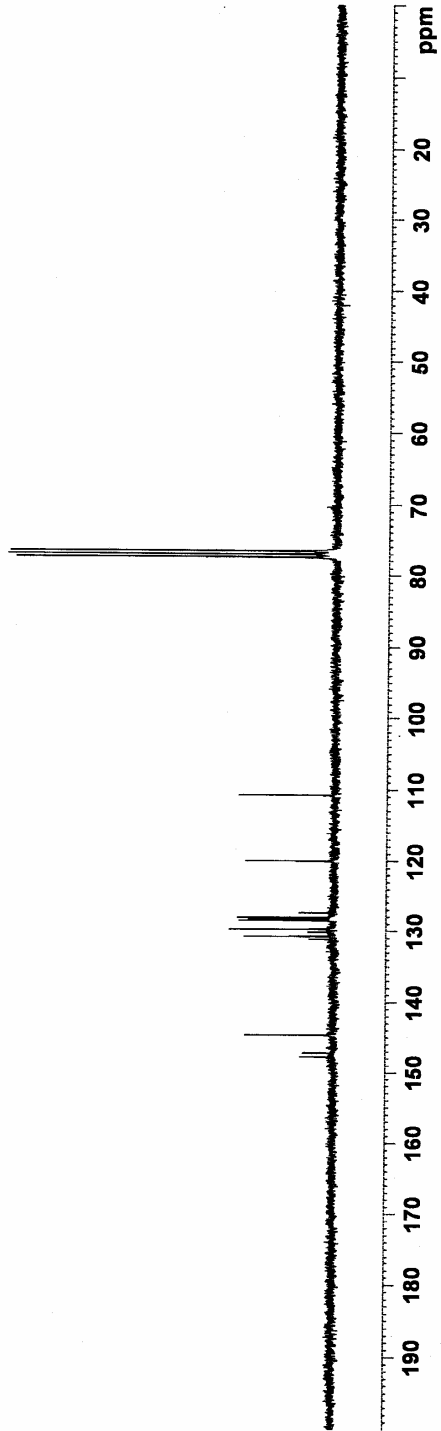
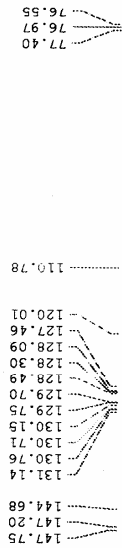
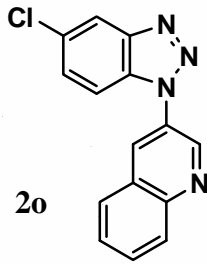
2.368



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
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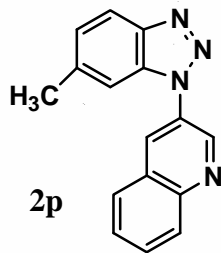


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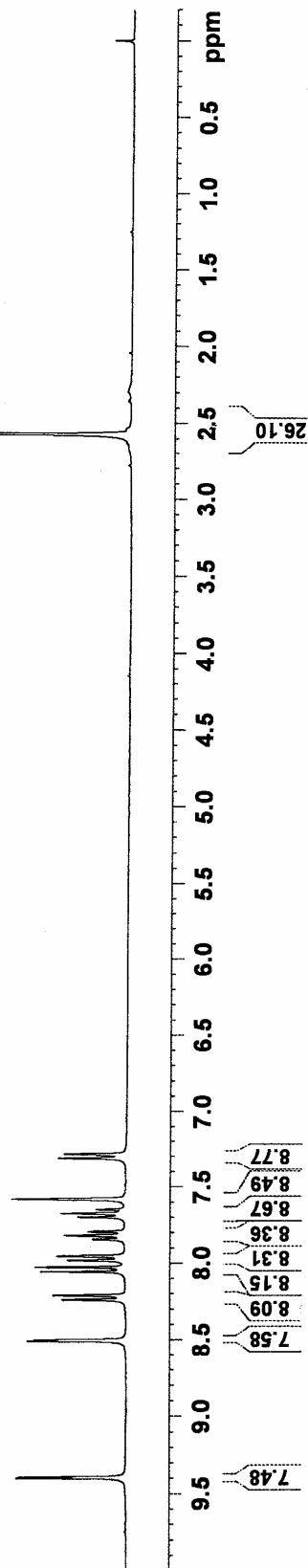


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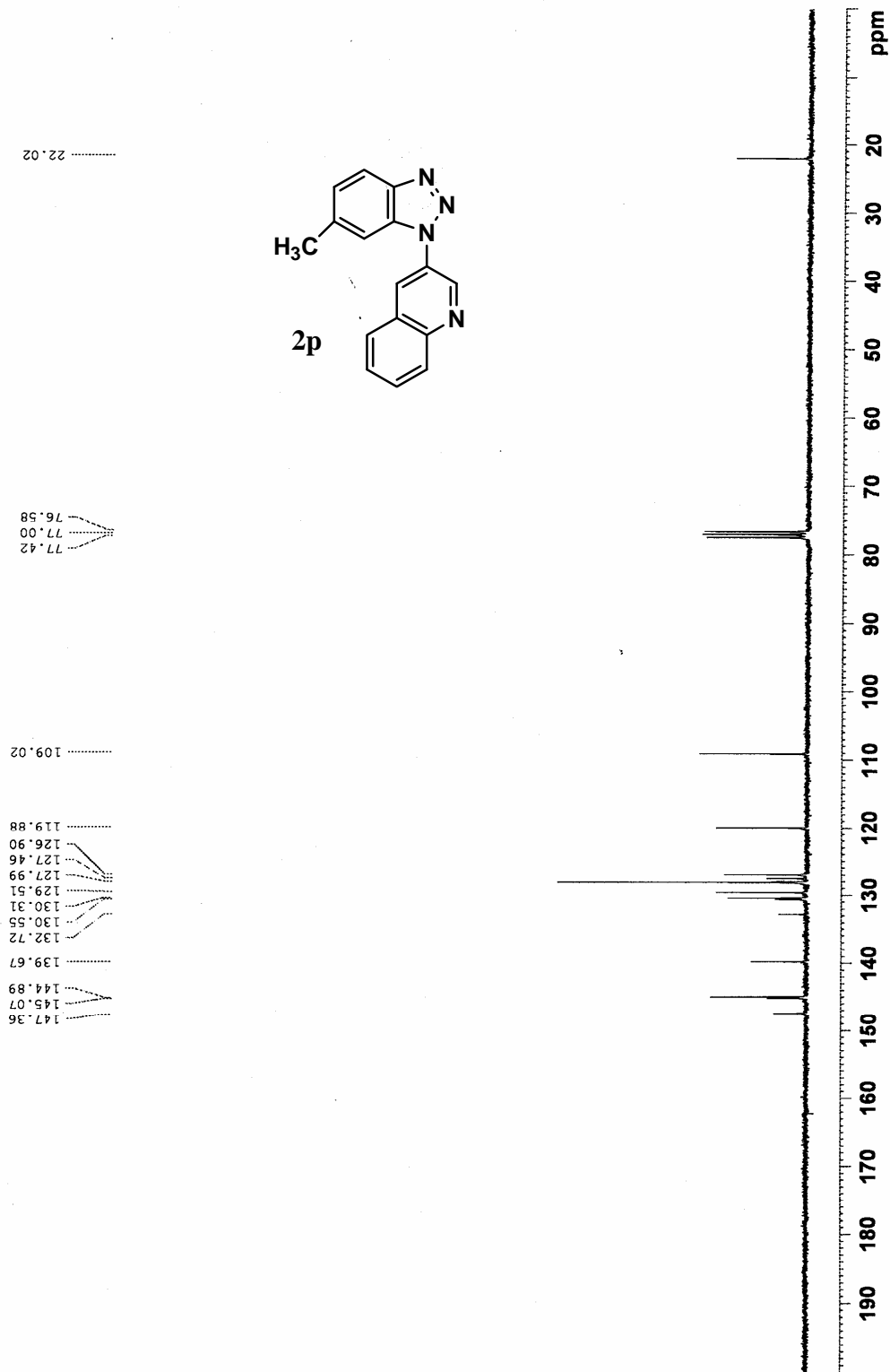
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8.207
8.052
8.023
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7.840
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7.645
7.577
7.311
7.310
7.292
7.291
7.283



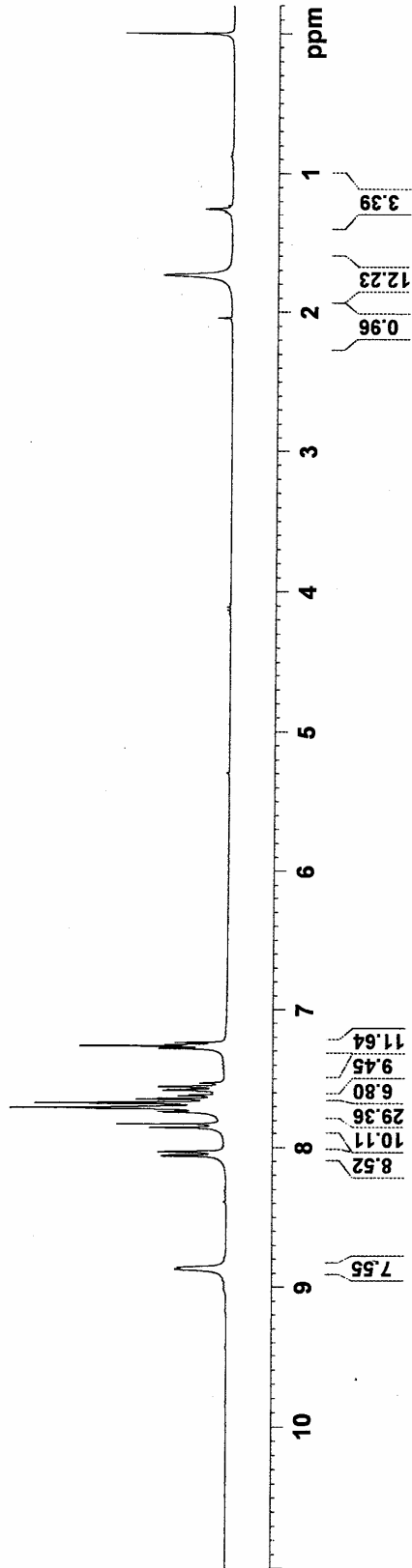
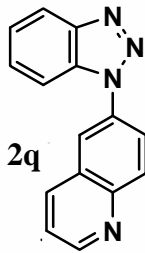
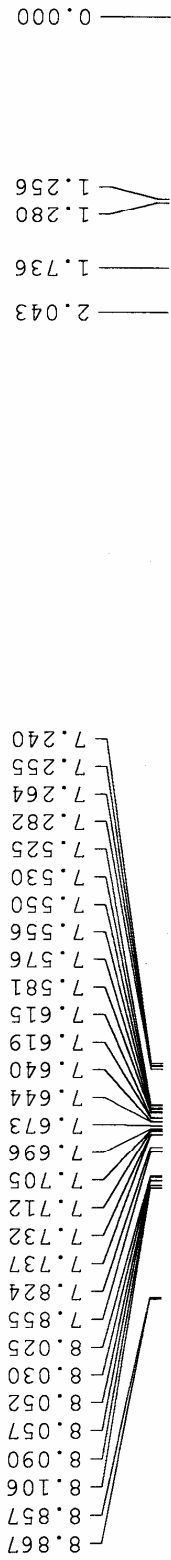
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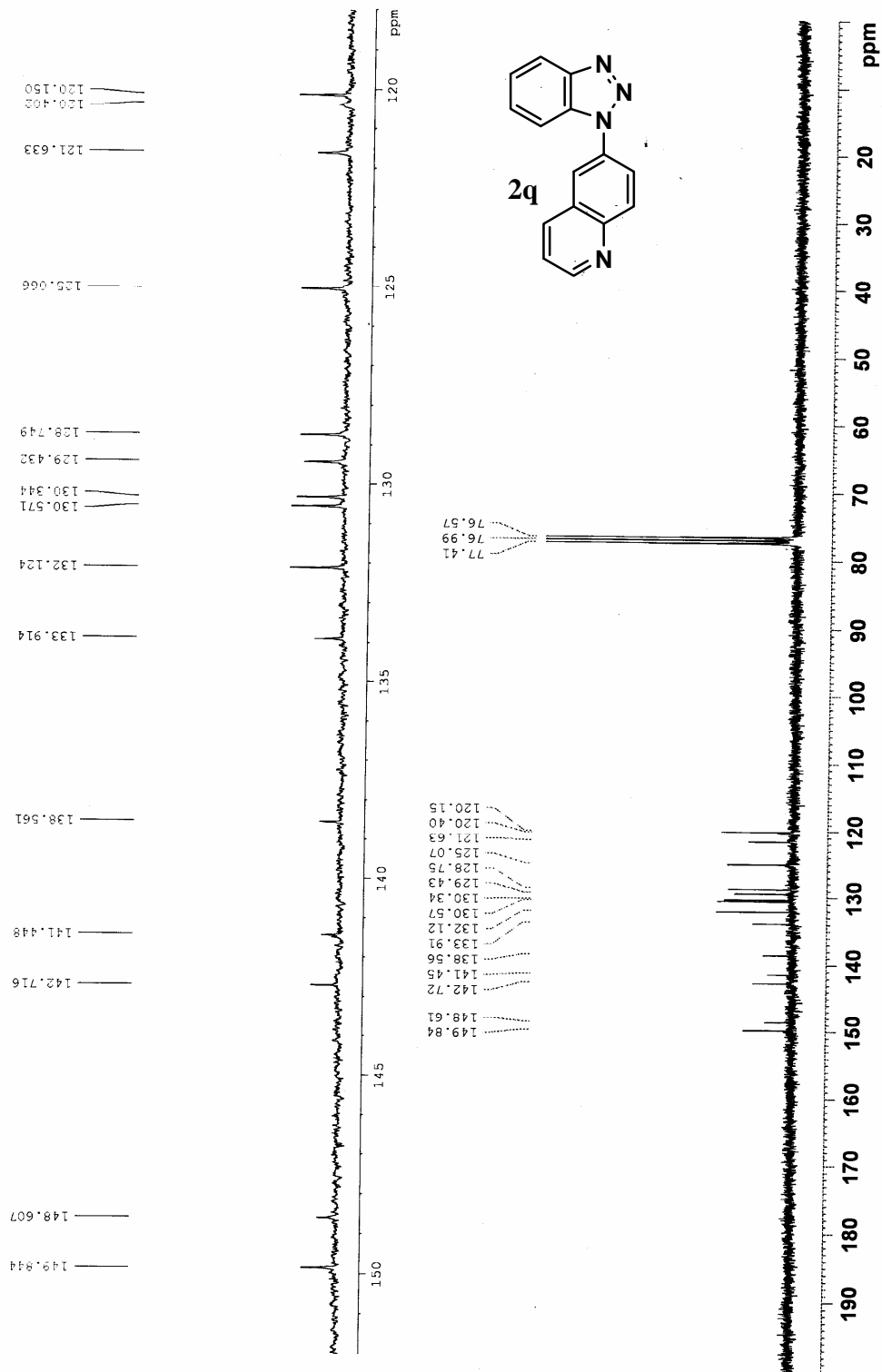
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Sample no PKT-334(A) CMR CDCl3 Dr. C.Mukhopadhyay 12.01.10 Operator P.Ghosh & S.Chatterjee



CAS Department of Chemistry, CU Bruker AV300 Supercon NMR System 5 mm BBO Probe
 Sample No PKT-262 (A) PMR CDCL3 Dr.C.Mukhopadhyay 21.04.09 Operator P.Ghosh & S.Chatterjee



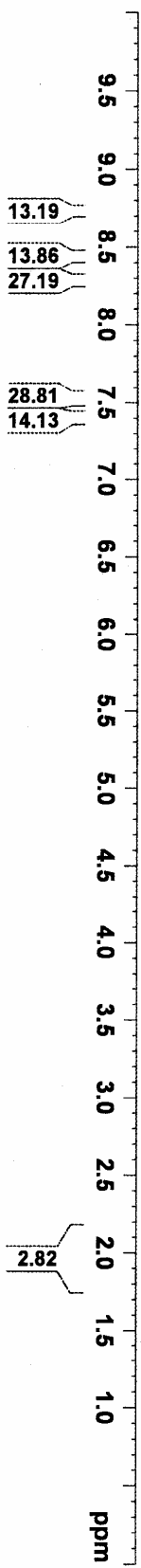
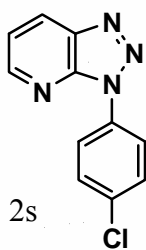
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Sample no PKT-262(A) CMR CDCL3 Dr.C.Mukhopadhyay 29.04.09 Operator P.Ghosh & S.Chatterjee



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-365(A) PMR CDCl3 Dr.C.Mukhopadhyay 06.05.10 Operator P.Ghosh & S.Chatterjee

8.736
8.722
8.448
8.421
8.288
8.263
8.259
7.538
7.513
7.508
7.428
7.412
7.404
7.400
7.389
7.385
7.264
7.260

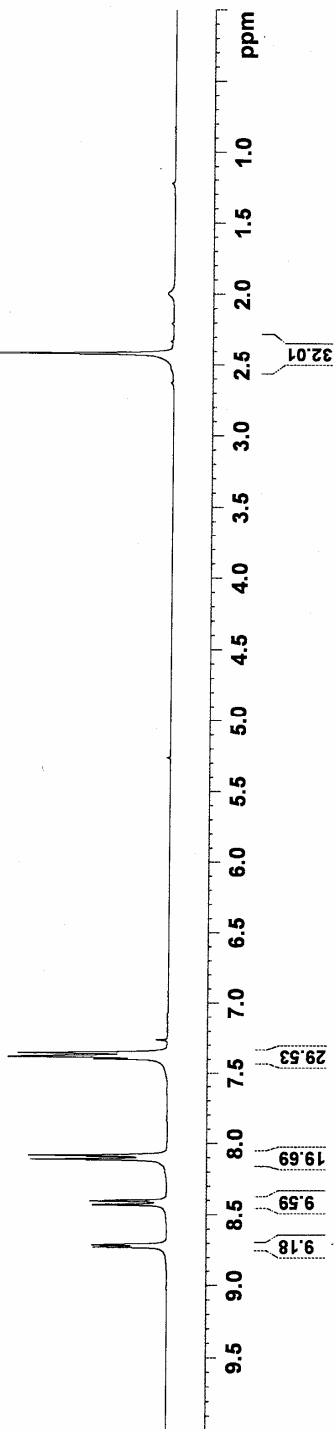
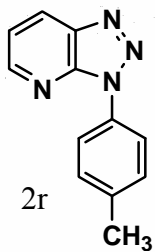
1.975



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
 Sample no PKT-366(A) PMR CDCL3 Dr.C.Mukhopadhyay 06.05.10 Operator P.Ghosh & S.Chatterjee

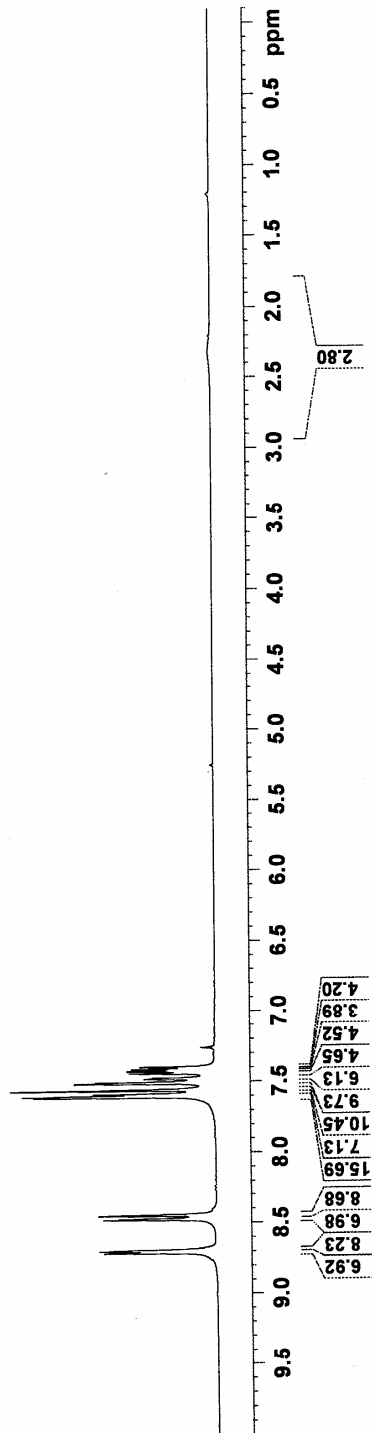
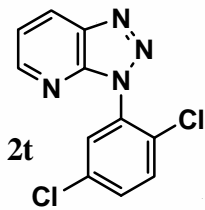
8.724
8.719
8.709
8.704
8.430
8.425
8.402
8.397
8.108
8.080
7.396
7.381
7.379
7.369
7.353
7.260

2.416



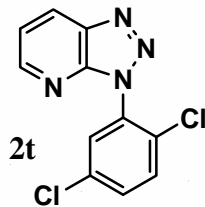
CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-355(A) PMR CDCl3 Dr.C.Mukhopadhyay 26.03.10 Operator P.Ghosh & S.Chatterjee

8.707
8.692
8.476
8.448
7.606
7.598
7.586
7.557
7.510
7.505
7.502
7.481
7.473
7.440
7.425
7.412
7.397
7.259



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-355(A) CMR CDCL3 Dr.C.Mukhopadhyay 01.04.10 Operator P.Ghosh & S.Chatterjee

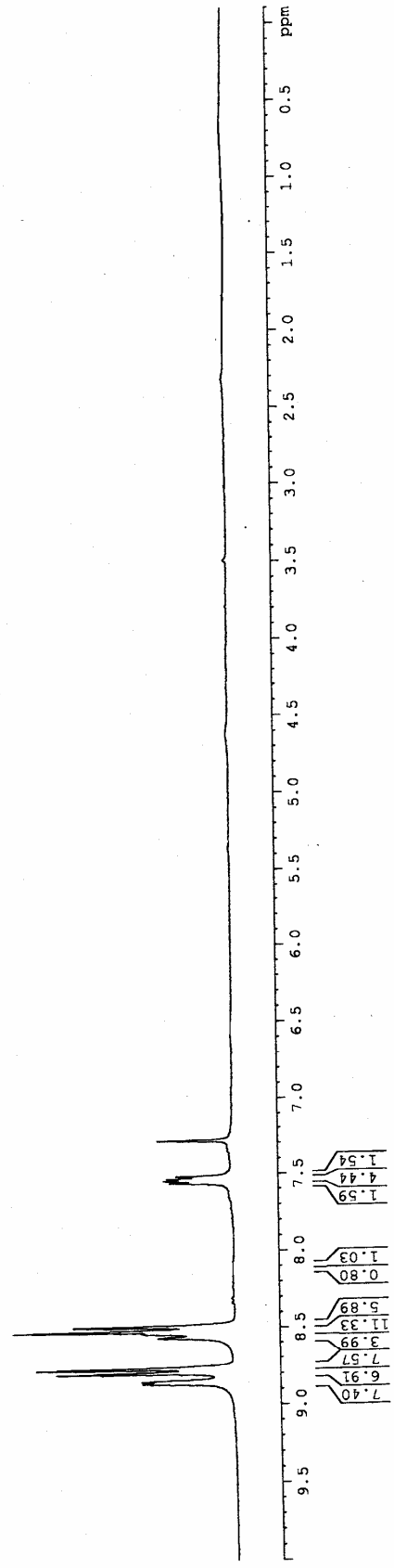
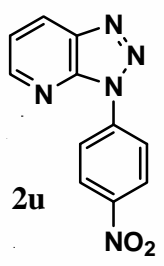
162.21
151.23
146.16
136.50
133.48
133.30
131.59
131.43
130.02
129.22
129.05
120.27
118.04
77.43
77.01
76.58



CAS Department of Chemistry, CU Bruker AV300 Supercon NMR System 5mm BBO probe
 Sample no PKT-356(A) CDCL3 PMR Dr. C.Mukhopadhyay 05.04.10 Operator P.Ghosh & S.Chatterjee

8.861
8.848
8.791
8.762
8.562
8.532
8.515
8.485

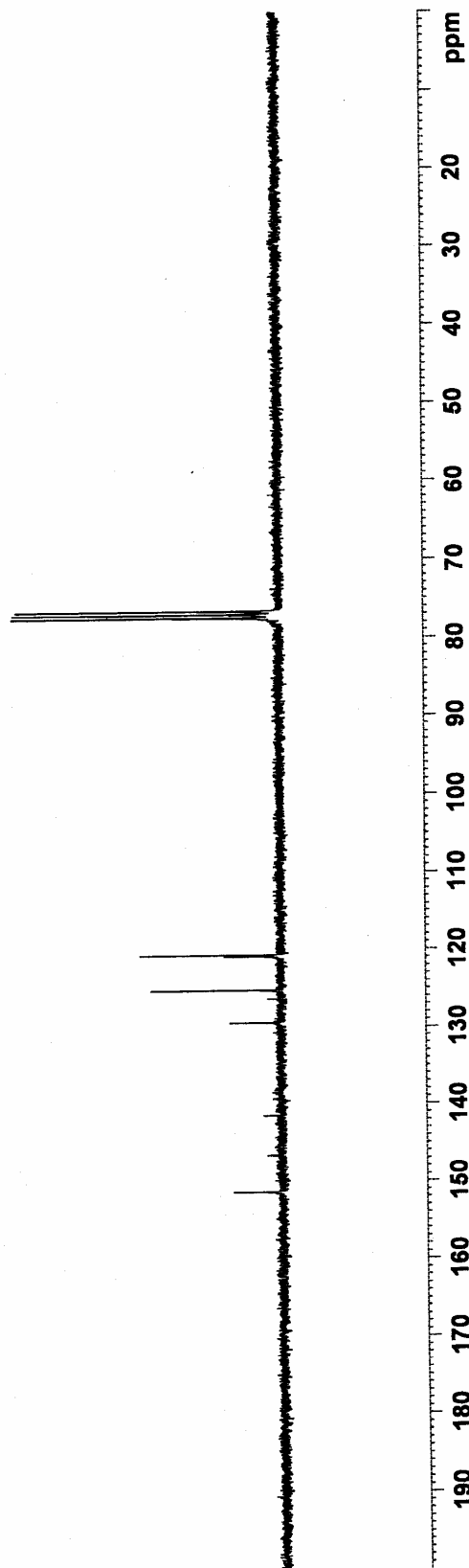
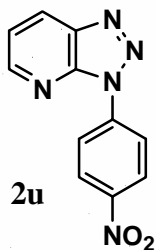
7.559
7.544
7.532
7.517
7.330
7.282



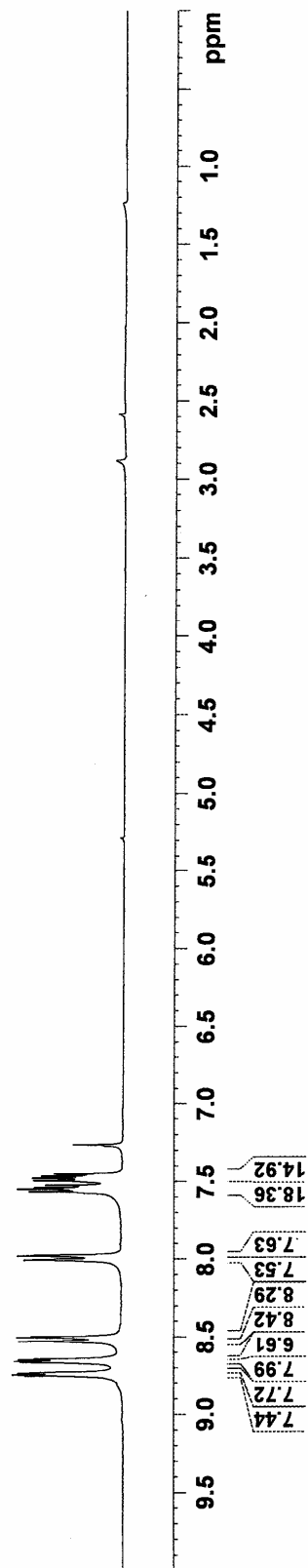
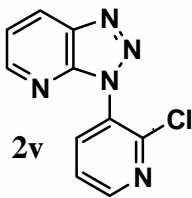
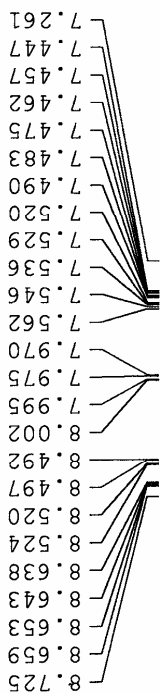
CAS Department of Chemistry, CU Bruker AV300 Supercon NMR System 5 mm BBO Probe
Sample No PKT-356(A) CMR CDCl3 Dr.C.Mukhopadhyay 08.04.10 Operator P.Ghosh & S.Chatterjee

151.26
146.56
141.38
129.40
126.33
125.19
120.86
120.67

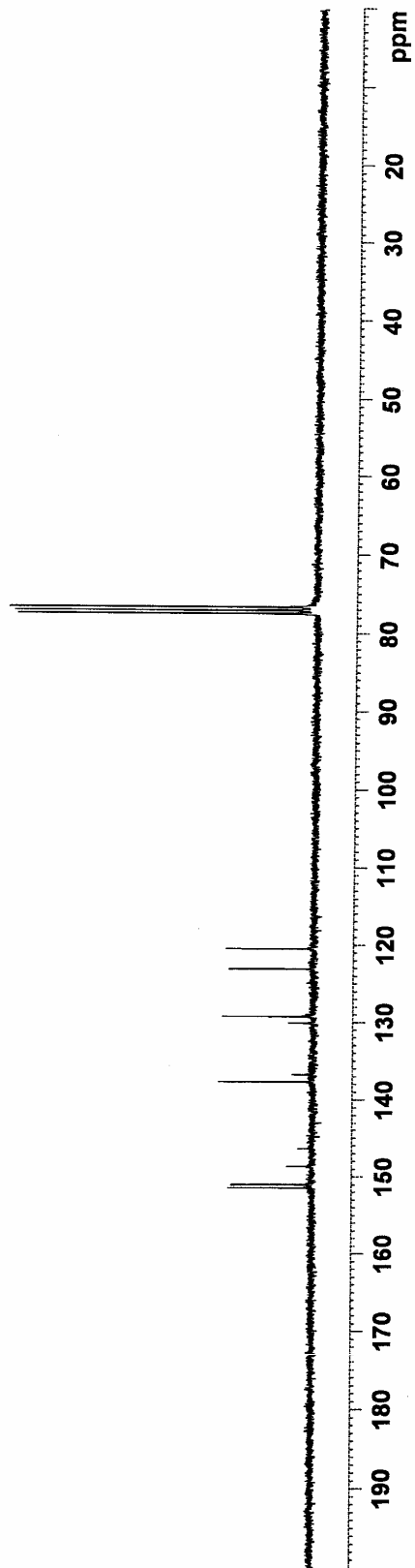
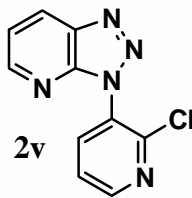
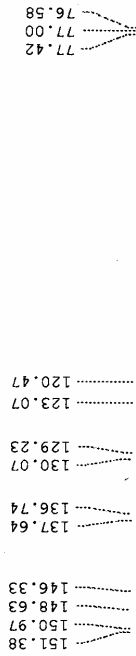
77.42
77.00
76.58



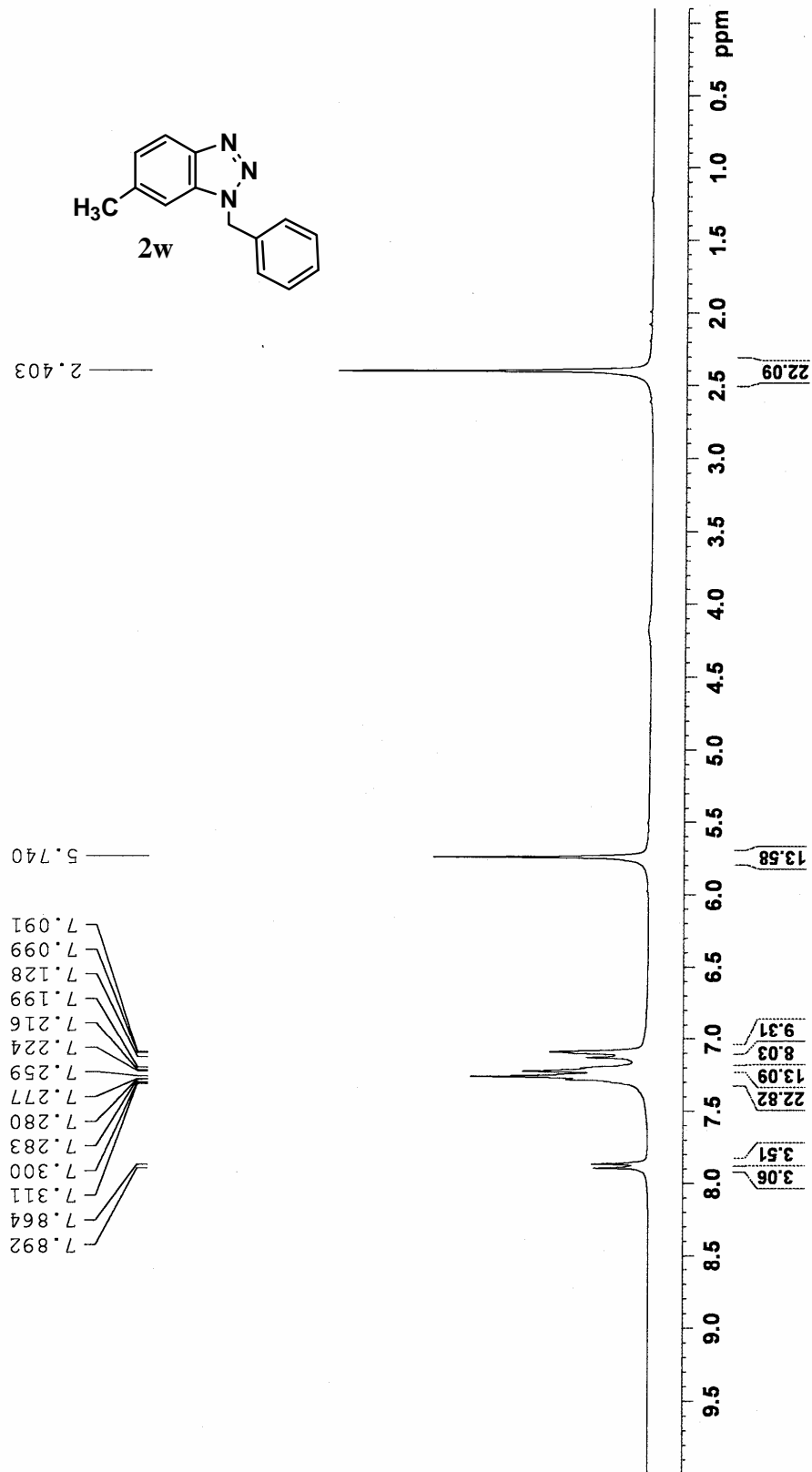
CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
 Sample no PKT-350(A) PMR CDCL3 Dr.C.Mukhopadhyay 10.03.10 Operator P.Ghosh & S.Chatterjee



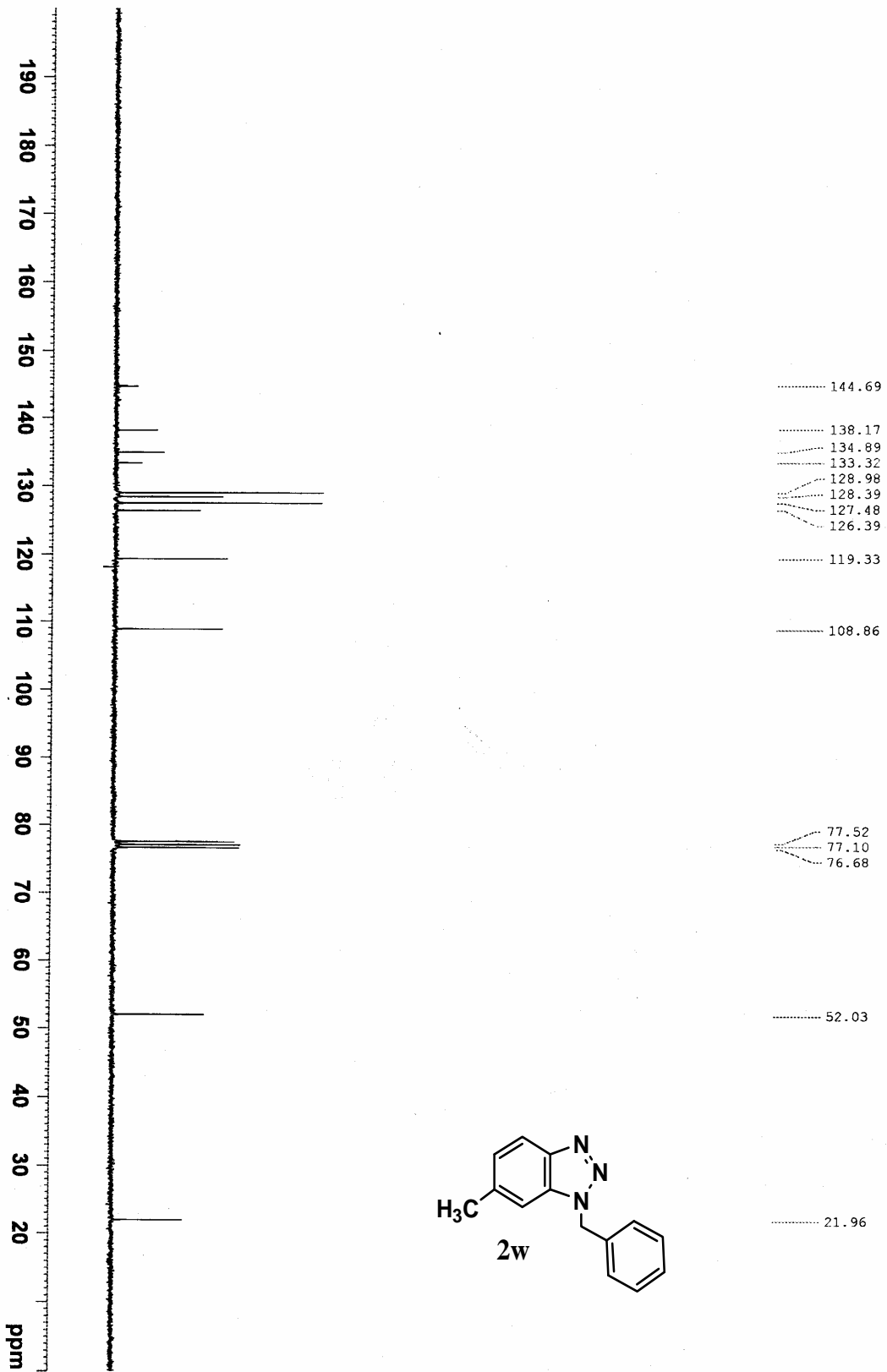
CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-350(A) CMR CDCL3 Dr.C.Mukhopadhyay 16.03.10 Operator P.Ghosh & S.Chatterjee



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-382(A) PMR CDCL3 Dr. C.Mukhopadhyay 08.07.10 Operator P.Ghosh & S.Chatterjee

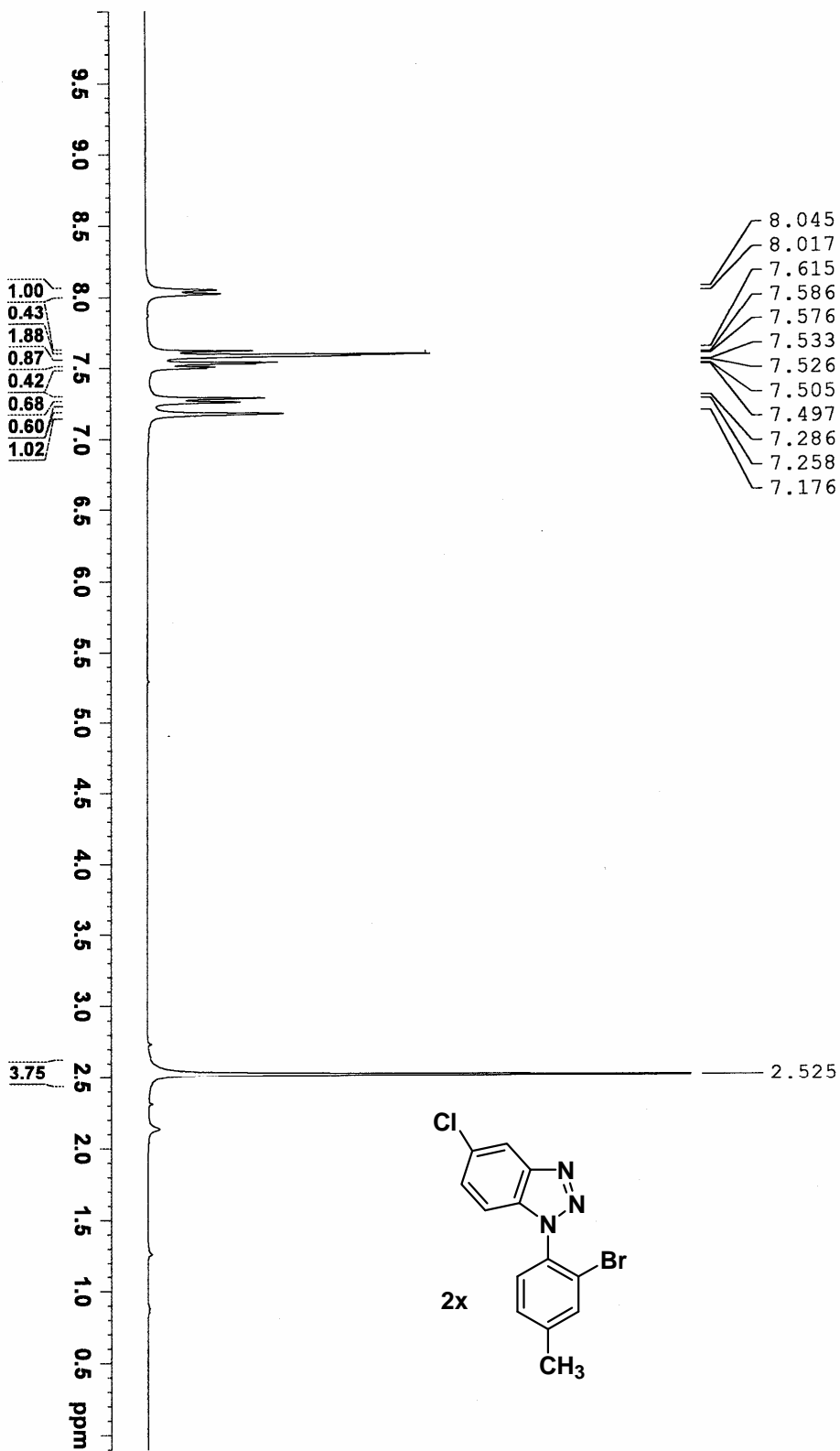


CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-382 (A) CMR CDCl3 Dr. C. Mukhopadhyay 12.07.10 Operator P. Ghosh & S. Chatterjee



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-354 (A) PMR CDCl3 Dr.C.Mukhopadhyay 25.03.10 Operator P.Ghosh & S.Chatterjee

- 8.045
- 8.017
- 7.615
- 7.586
- 7.576
- 7.533
- 7.526
- 7.505
- 7.497
- 7.286
- 7.258
- 7.176



CAS DEPT OF CHEMISTRY CU Bruker AV 300 Supercon NMR System 5mmBBO Probe
Sample no PKT-354 (A) CMR CDCL3 Dr.C.Mukhopadhyay 29.03.10 Operator P.Ghosh & S.Chatterjee

