

Supporting Information

4-Alkylated Silver–N-Heterocyclic Carbene (NHC) Complexes with Cytotoxic Effects in Leukemia Cells

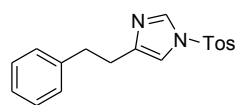
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Hans-René Bjørsvik*^[a]

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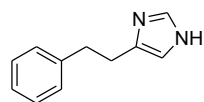
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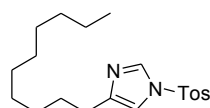
Synthesis of additional derivatives.



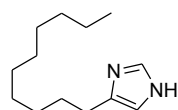
N-tosyl-4-(2-phenylethyl)imidazole 15 [NEW]. Isolated as pale crystals in a yield of 98%. $R_f = 0.58$ [EtOAc: Hx (4:6)]. $^1\text{H-NMR}$ (CDCl_3): δ 7.94 (s, 1H), 7.77 (d, 2H, $J = 8.5$ Hz), 7.34 (d, 2H, $J = 8.3$ Hz), 7.19 (m, 3H), 7.11 (d, 2H, $J = 7.5$ Hz), 6.89 (s, 1H), 2.91 (m, 2H), 2.82 (m, 2H), 2.45 (s, 3H). $^{13}\text{C-NMR}$ (CDCl_3): δ 146.1, 144.8, 141.3, 136.3, 135.3, 130.5, 128.5, 128.4, 127.4, 126.1, 113.4, 35.0, 30.2, 21.9. HRMS (DART): m/z $[\text{MH}]^+$ calcd. for $\text{C}_{18}\text{H}_{19}\text{N}_2\text{O}_2\text{S}$: 327.11617, found 327.11499



4-(5)-(2-phenylethyl)-1H-imidazole 16 [NEW]. Isolated in high purity (100%, based on GC) as a tan oil in a yield of 86%. $^1\text{H-NMR}$ (CDCl_3): δ 9.90 (1H, s, br), 7.55 (1H, s), 7.25 (2H, m), 7.14 (m, 3H), 6.76 (s, 1H), 2.93 (s, 4H). $^{13}\text{C-NMR}$ (CDCl_3): δ 141.7, 136.7, 134.5, 128.7, 126.2, 117.7, 36.1, 29.2. HRMS (DART): m/z $[\text{MH}]^+$ calcd. for $\text{C}_{11}\text{H}_{13}\text{N}_2$: 173.10787, found: 173.10765.

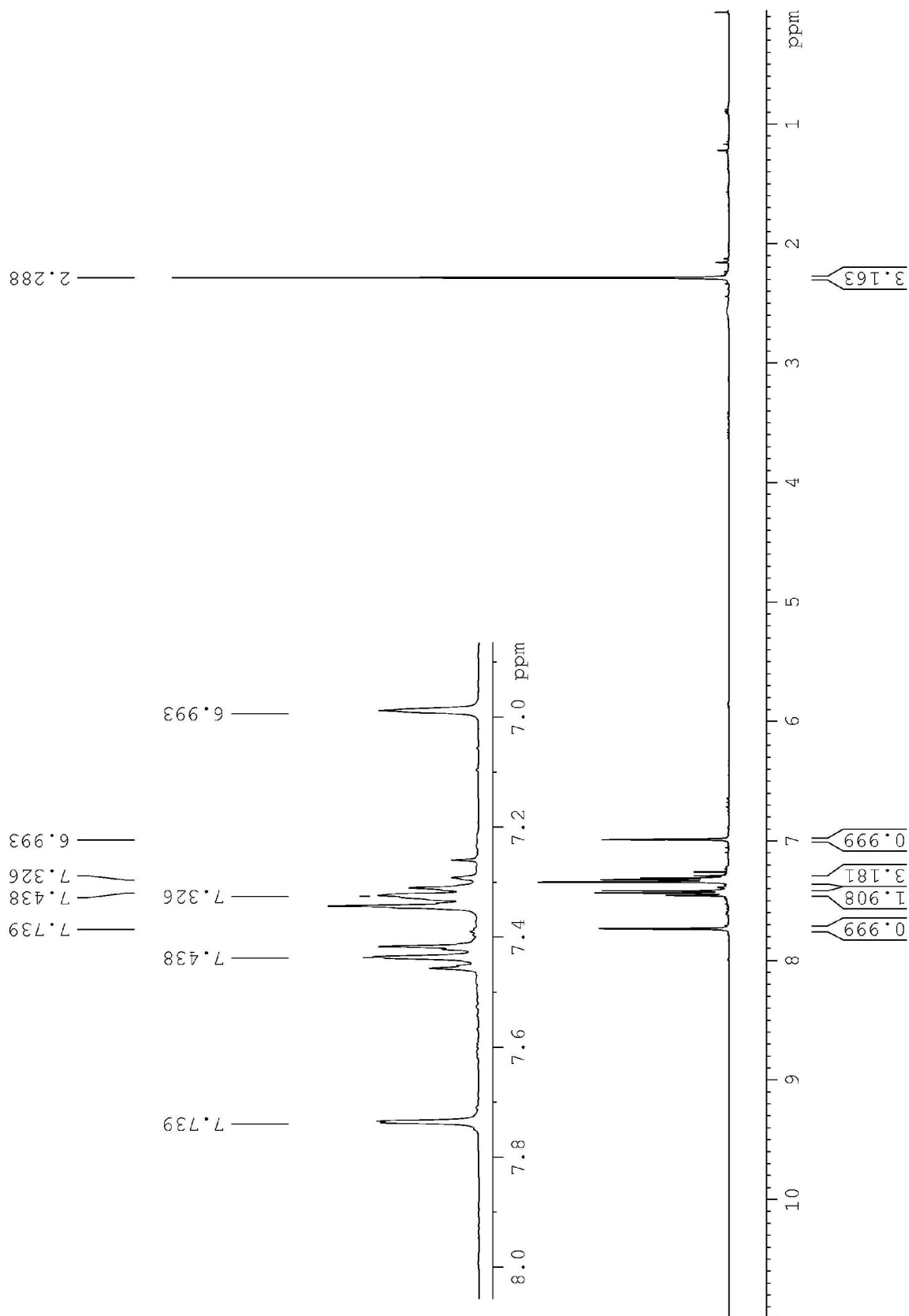


N-tosyl-4-decylimidazole 17 [NEW]. Isolated as tan crystals in the yield of 98%. $^1\text{H-NMR}$ (CDCl_3): δ 7.91 (s, 1H), 7.80 (d, 2H, $J = 8.5$ Hz), 6.96 (s, 1H), 2.49 (t, 2H, $J = 7.7$ Hz), 2.43 (s, 3H), 1.58 (m, 2H), 1.25 (m, 16H), 0.87 (t, 3H, $J = 7.0$ Hz). $^{13}\text{C-NMR}$ (CDCl_3): δ 146.1, 136.2, 135.4, 130.5, 127.4, 127.4, 112.8, 32.0, 29.71, 29.66, 29.5, 29.44, 29.37, 28.7, 28.3, 22.8, 21.8, 14.3. HRMS (DART): m/z $[\text{MH}]^+$ calcd. for $\text{C}_{20}\text{H}_{31}\text{N}_2\text{O}_2\text{S}$: 363.21062, found 363.21053.

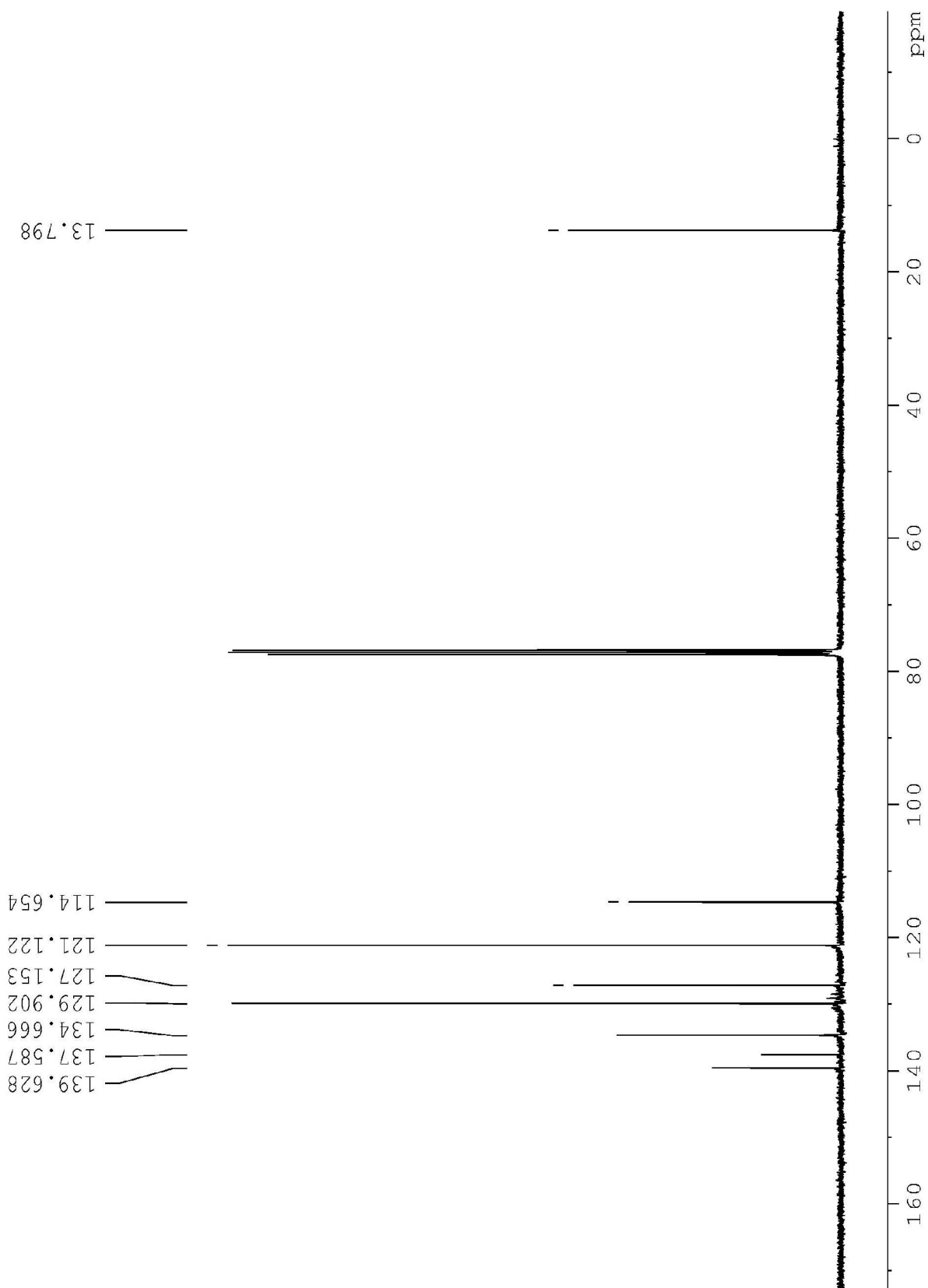


4-(5)-decyl-1H-imidazole 18 [NEW]. Isolated as a yellow oil that was prone to crystallization in a yield of 58%. $^1\text{H-NMR}$ (CDCl_3): δ 9.00 (1H, br, s), 7.00 (1H, s), 3.63 (2H, s, br), 1.49 (1H, m), 1.67 (2H, m), 1.26 (15H, m), 0.86 (3H, t). $^{13}\text{C-NMR}$ (CDCl_3): δ 134.4, 133.1, 114.5, 31.9, 29.57, 29.53, 29.3, 29.2, 29.0, 28.4, 24.6, 22.7, 14.1. HRMS (ESI): m/z $[\text{MH}]^+$ calcd. for $\text{C}_{13}\text{H}_{25}\text{N}_2$: 209.20177, found: 209.20123.

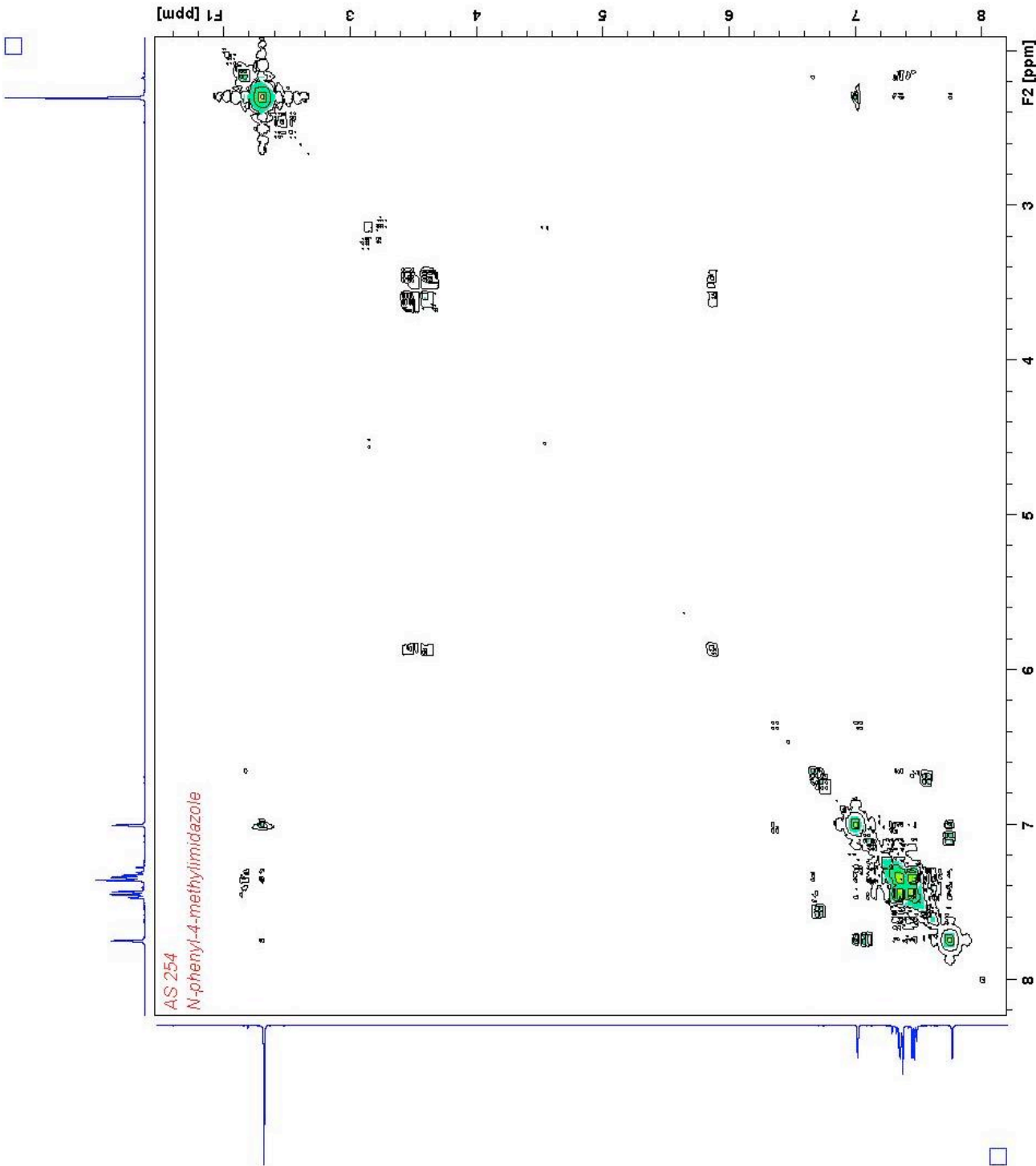
¹H-NMR of *N*-phenyl-4-methylimidazole (3)



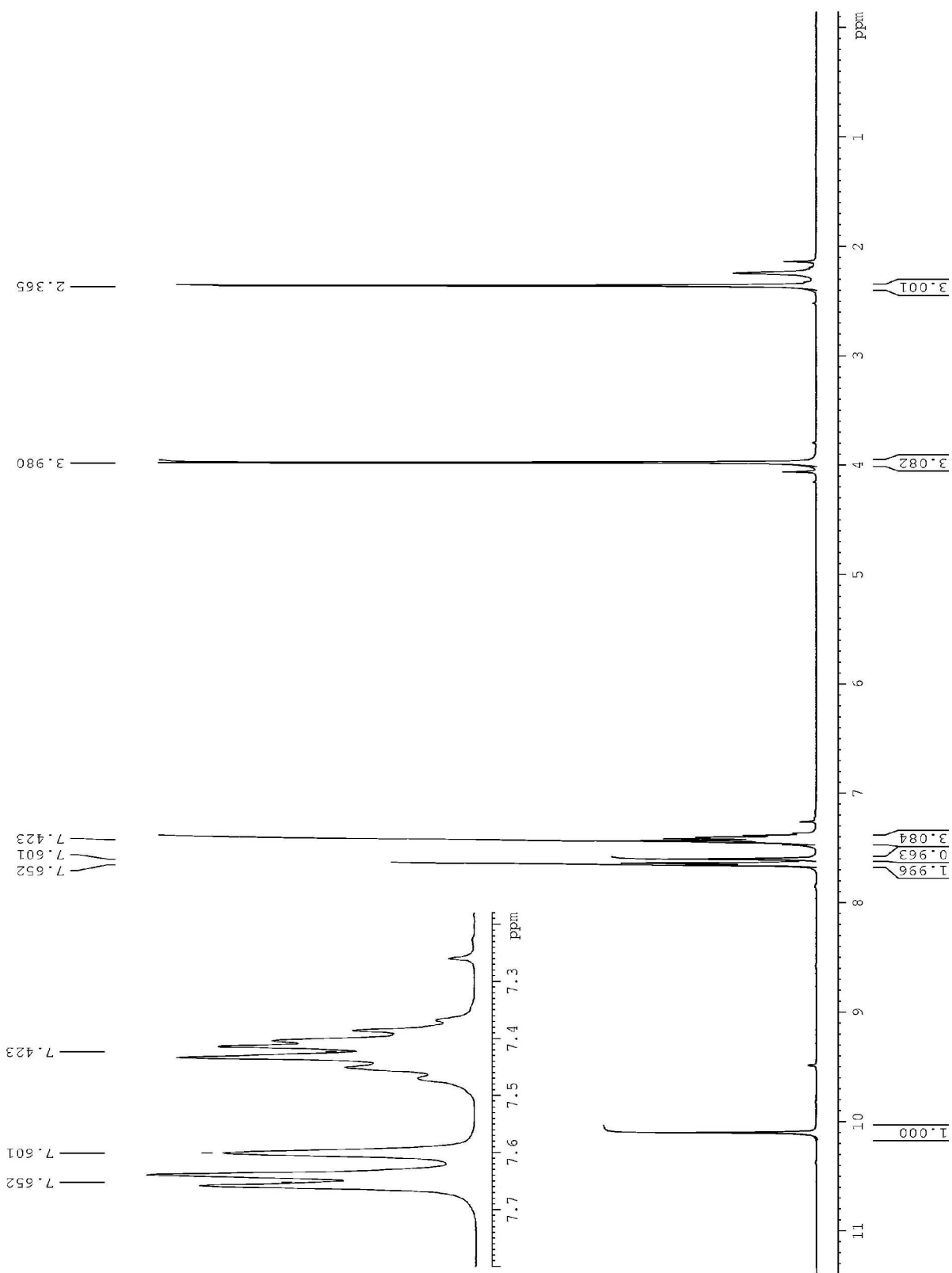
¹³C-NMR of *N*-phenyl-4-methylimidazole (3)



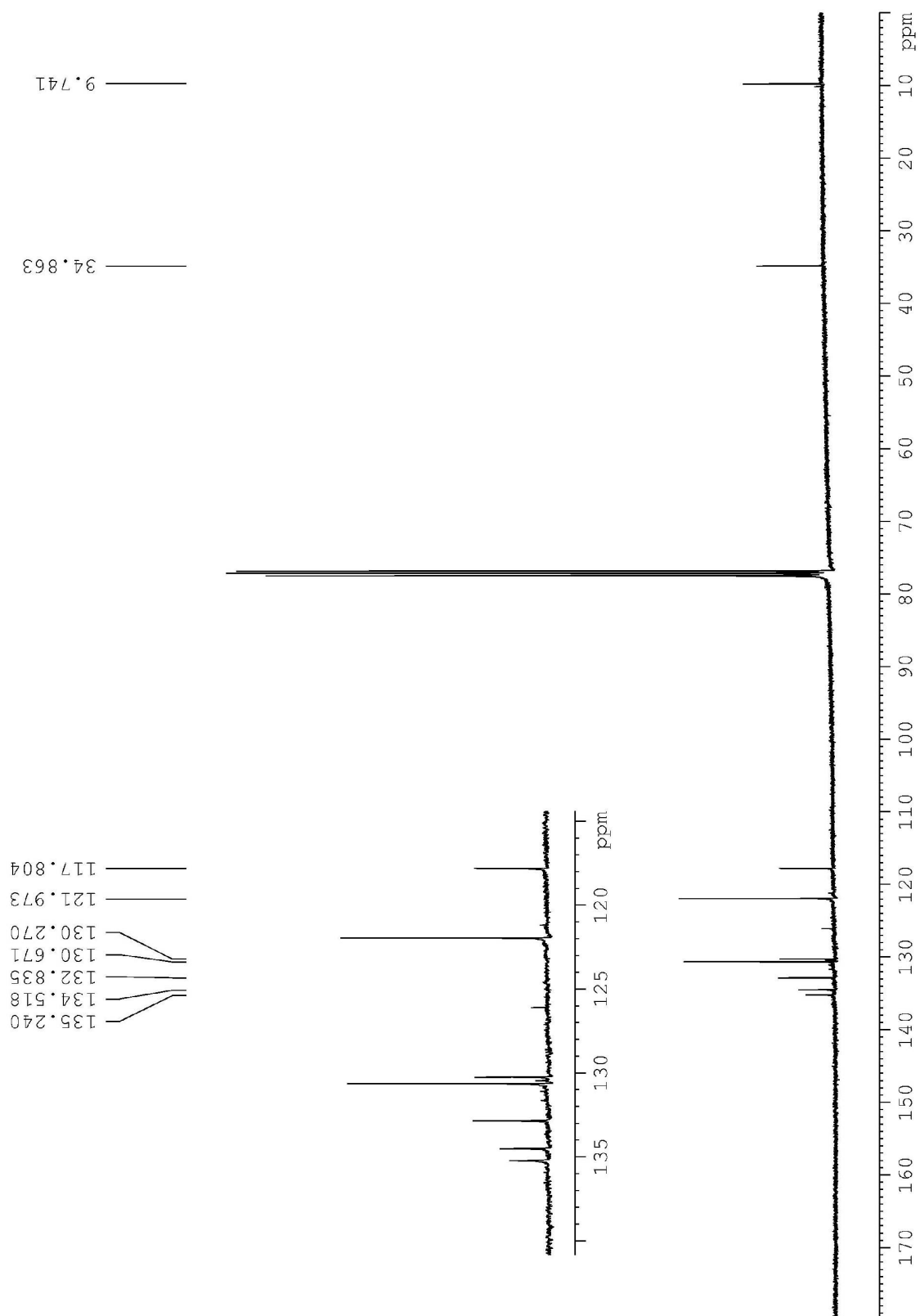
COSY 2D-NMR spectrum of N-phenyl-4-methylimidazole (3)



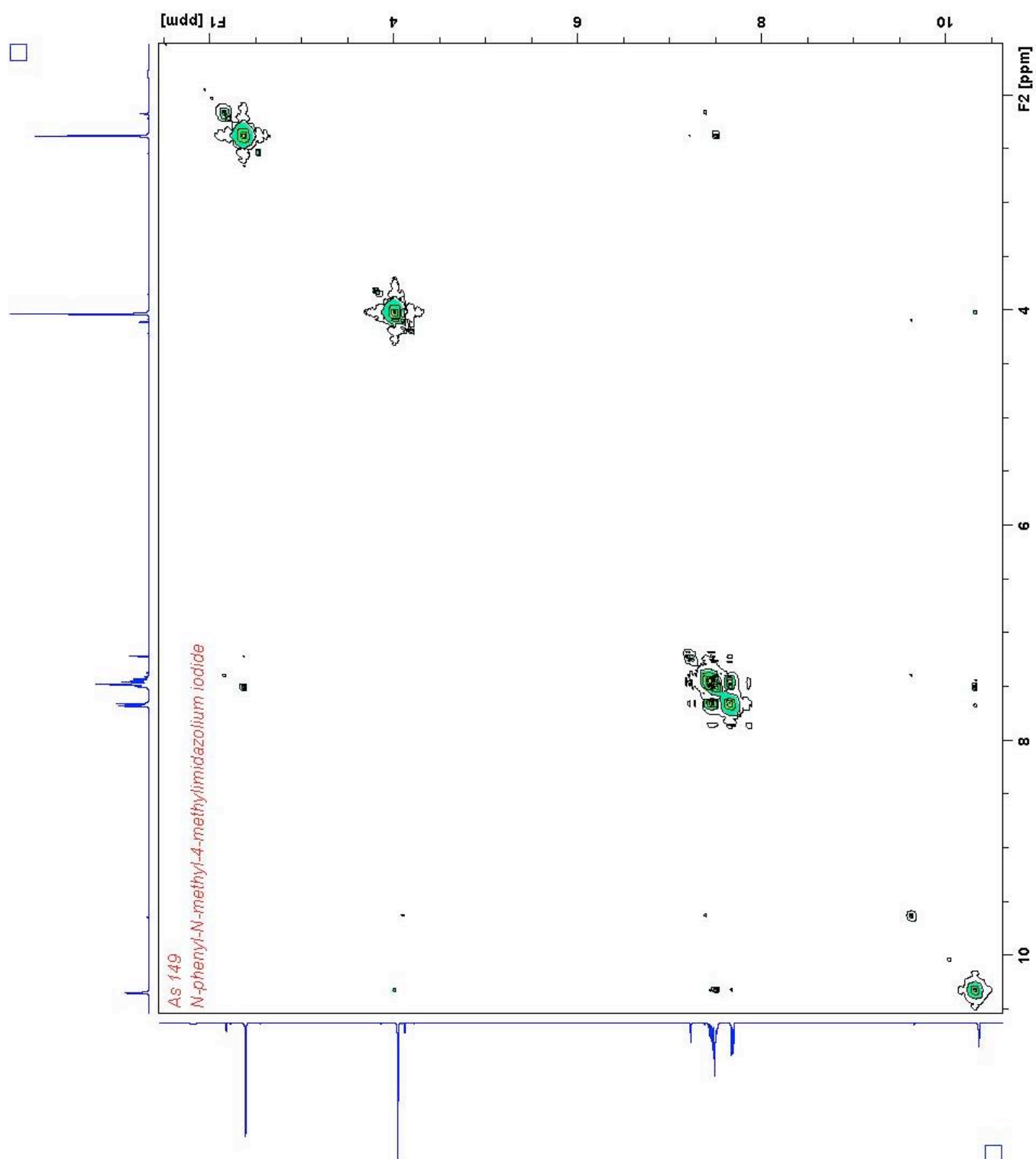
¹H-NMR spectrum of *N*-1-phenyl-*N*-3-methyl-4-methylimidazolium iodide (4)



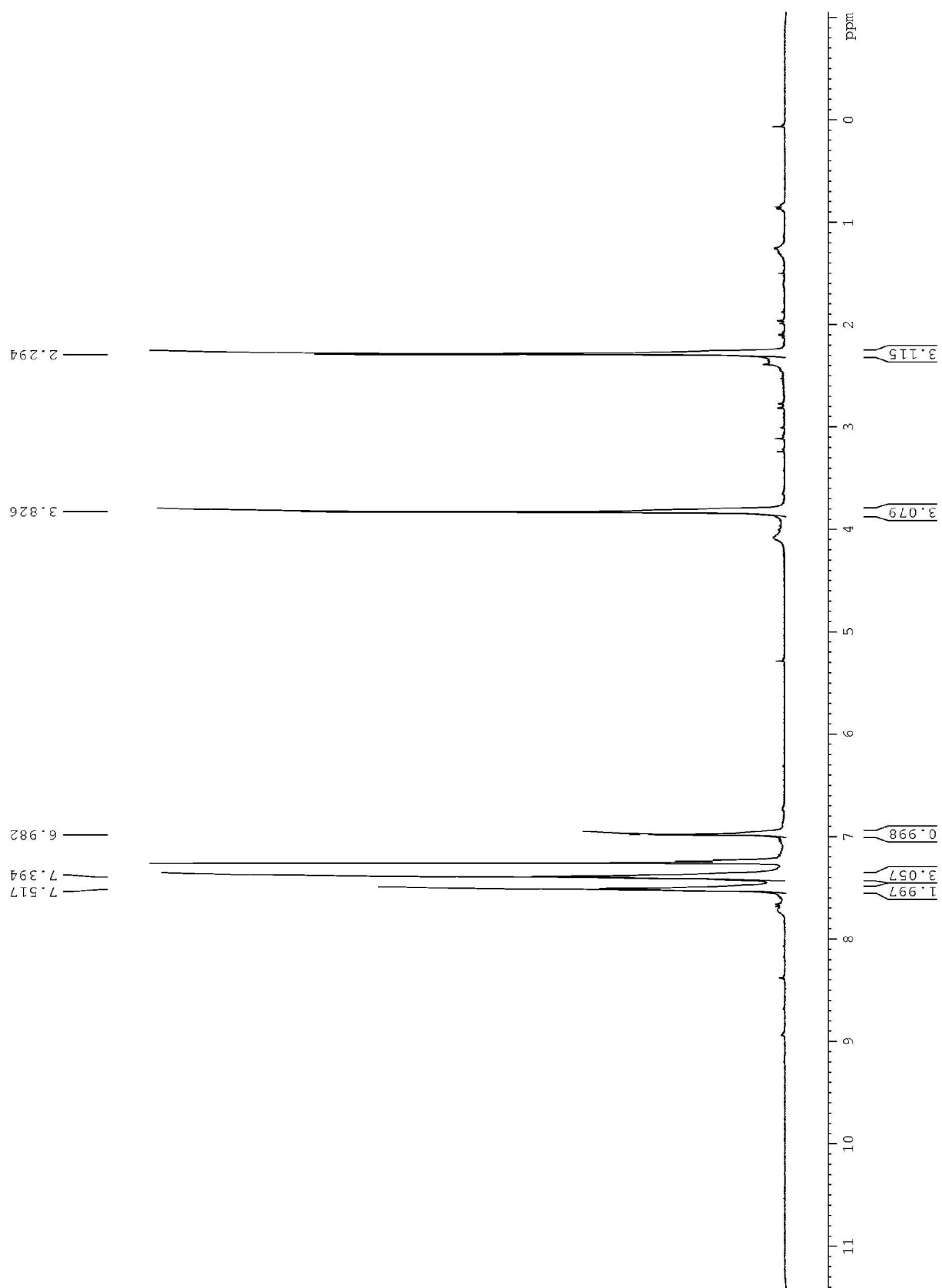
¹³C-NMR spectrum of *N*-1-phenyl-*N*-3-methyl-4-methylimidazolium iodide (4)



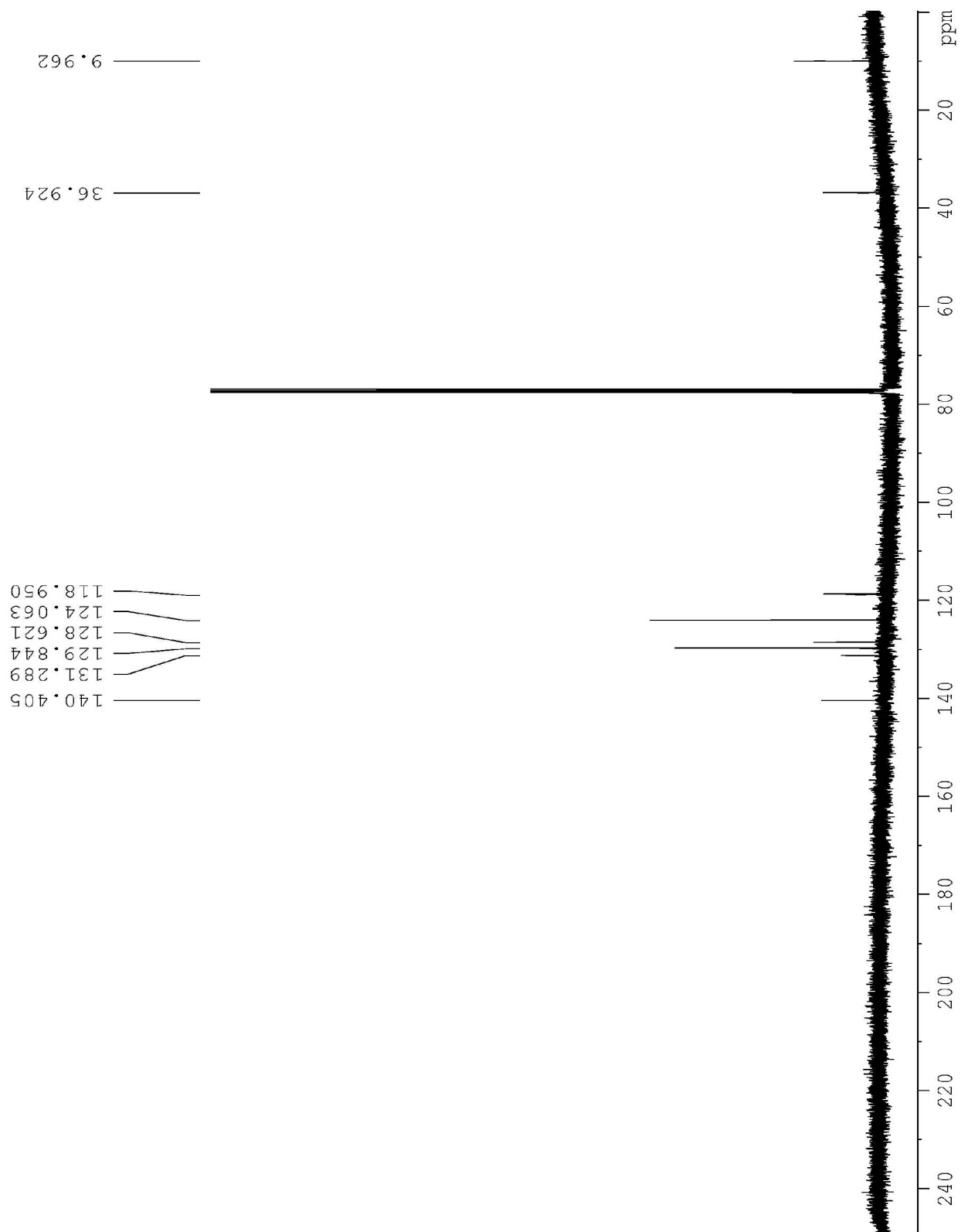
2D-COSY NMR spectrum of *N*-1-phenyl-*N*-3-methyl-4-methylimidazolium iodide
(4)



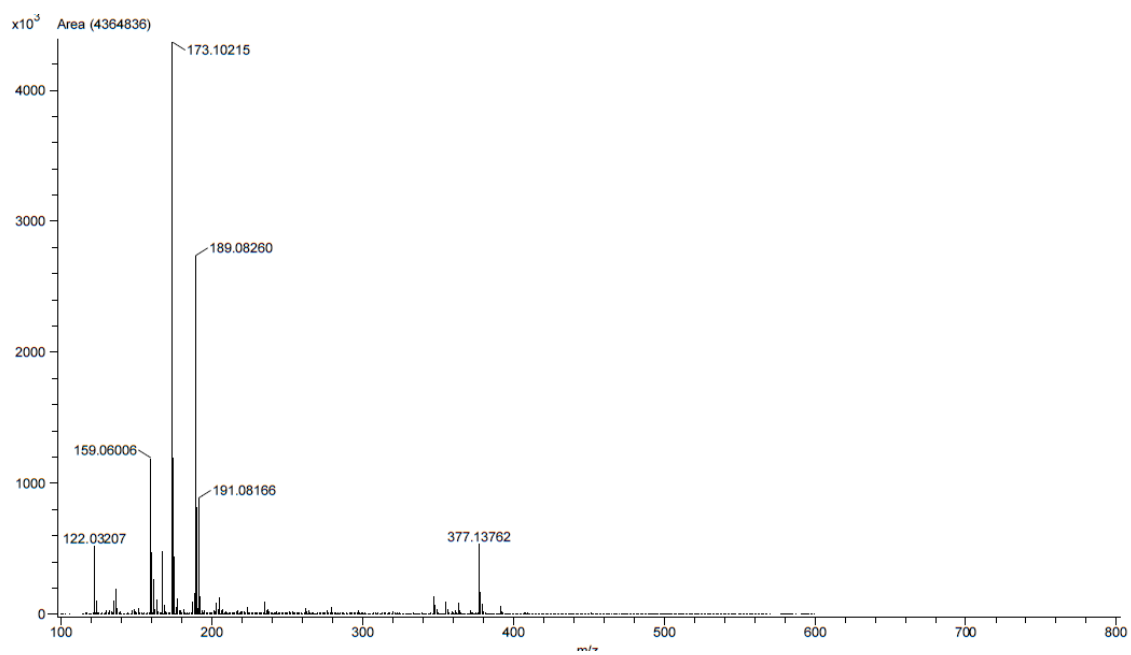
¹H-NMR spectrum of NHC-1



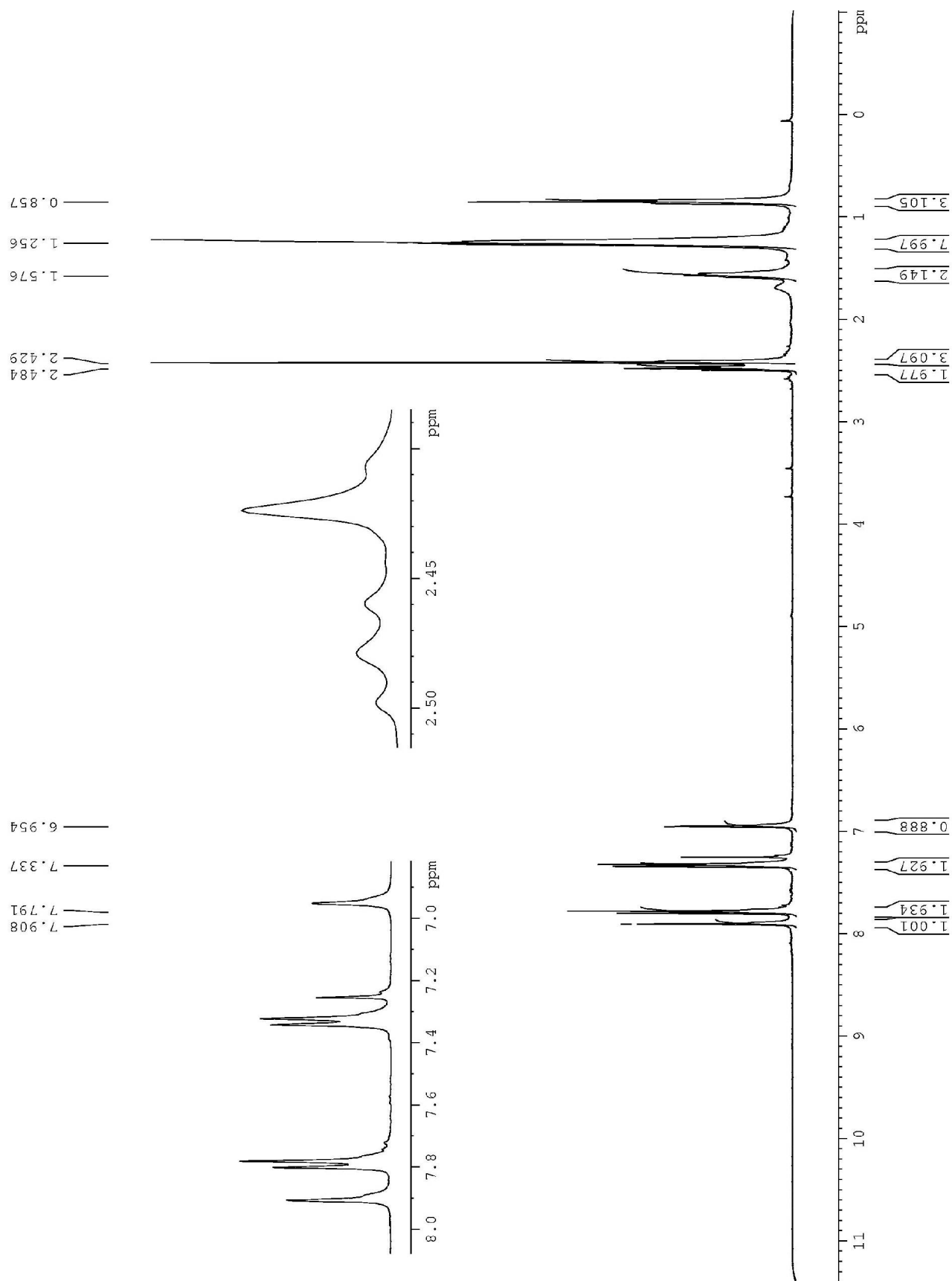
¹³C-NMR spectrum of NHC-1



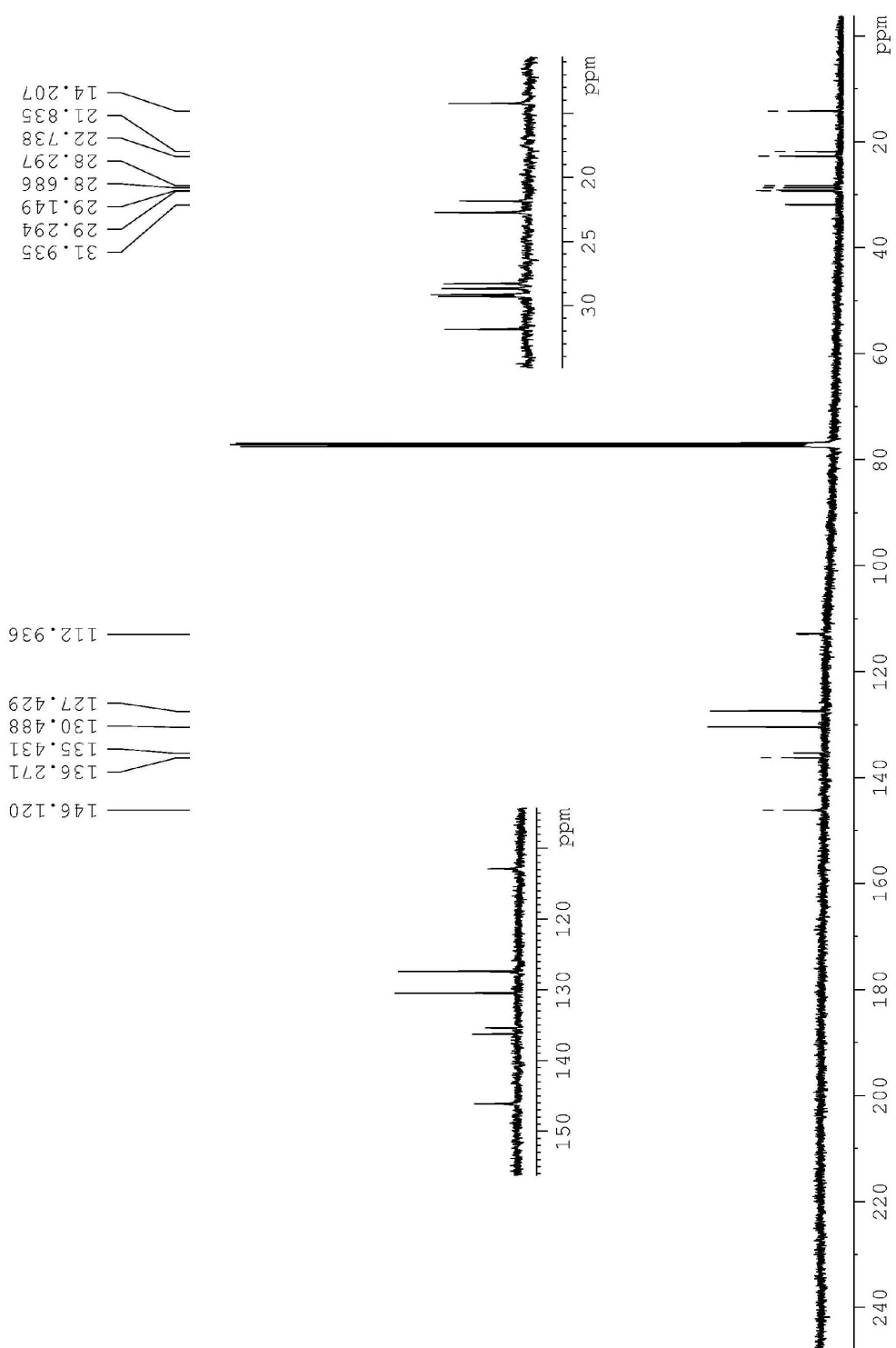
HRMS spectrum of NHC-1



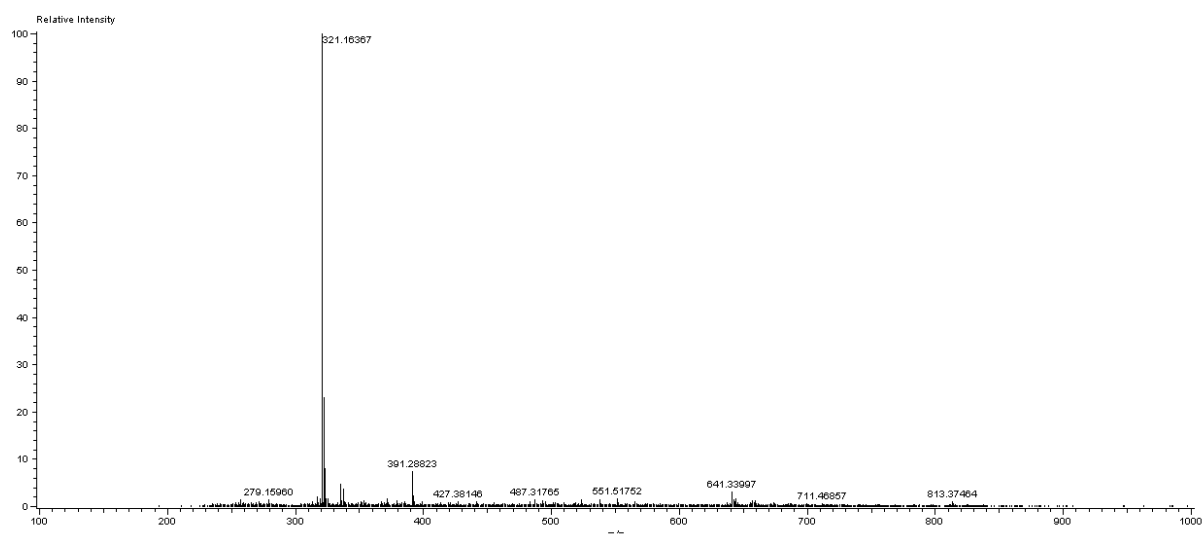
¹H-NMR spectrum of *N*-tosyl-4-heptylimidazole (11)



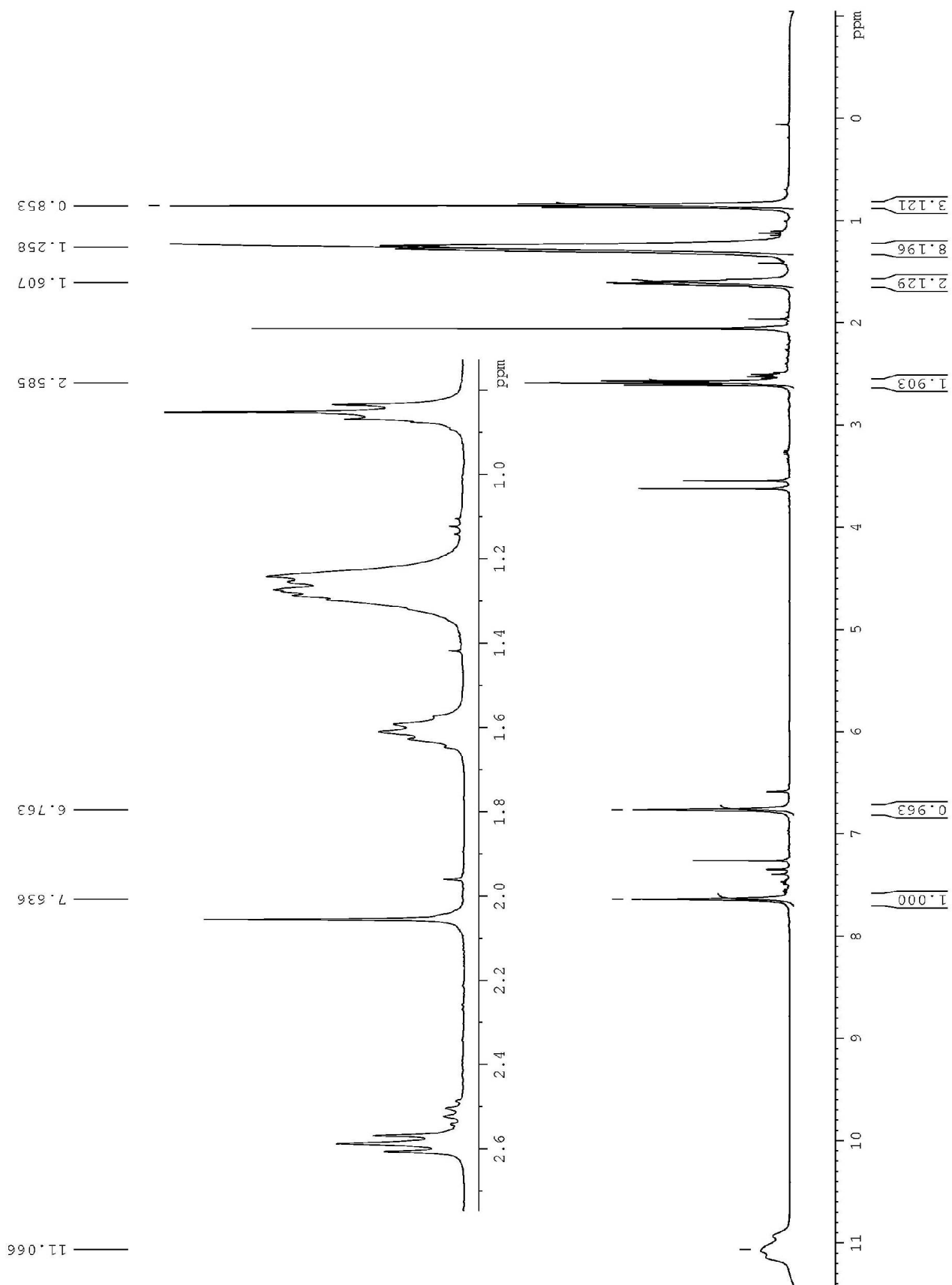
¹³C-NMR spectrum of *N*-tosyl-4-heptylimidazole (11)



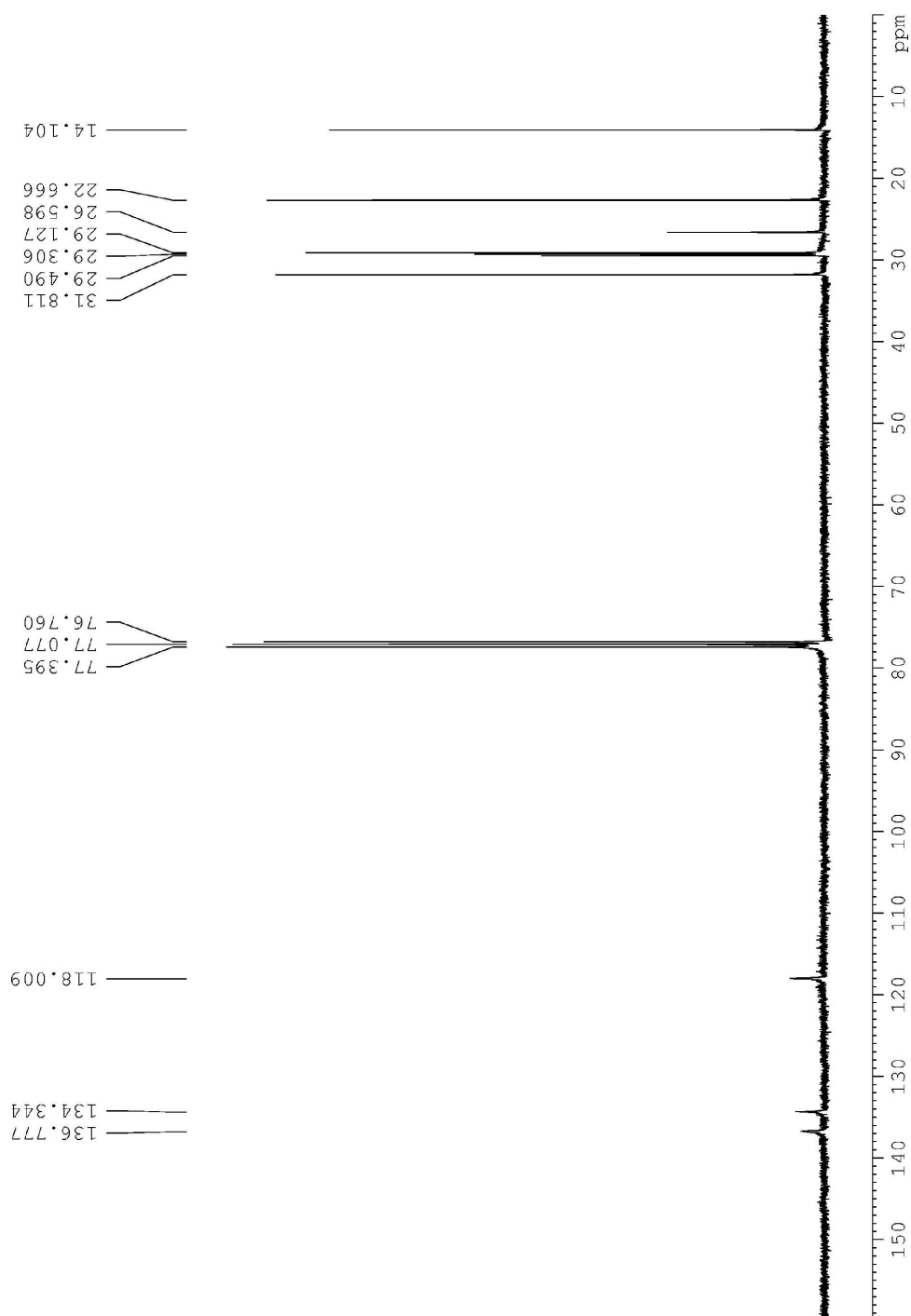
HRMS spectrum of *N*-tosyl-4-heptylimidazole (11)



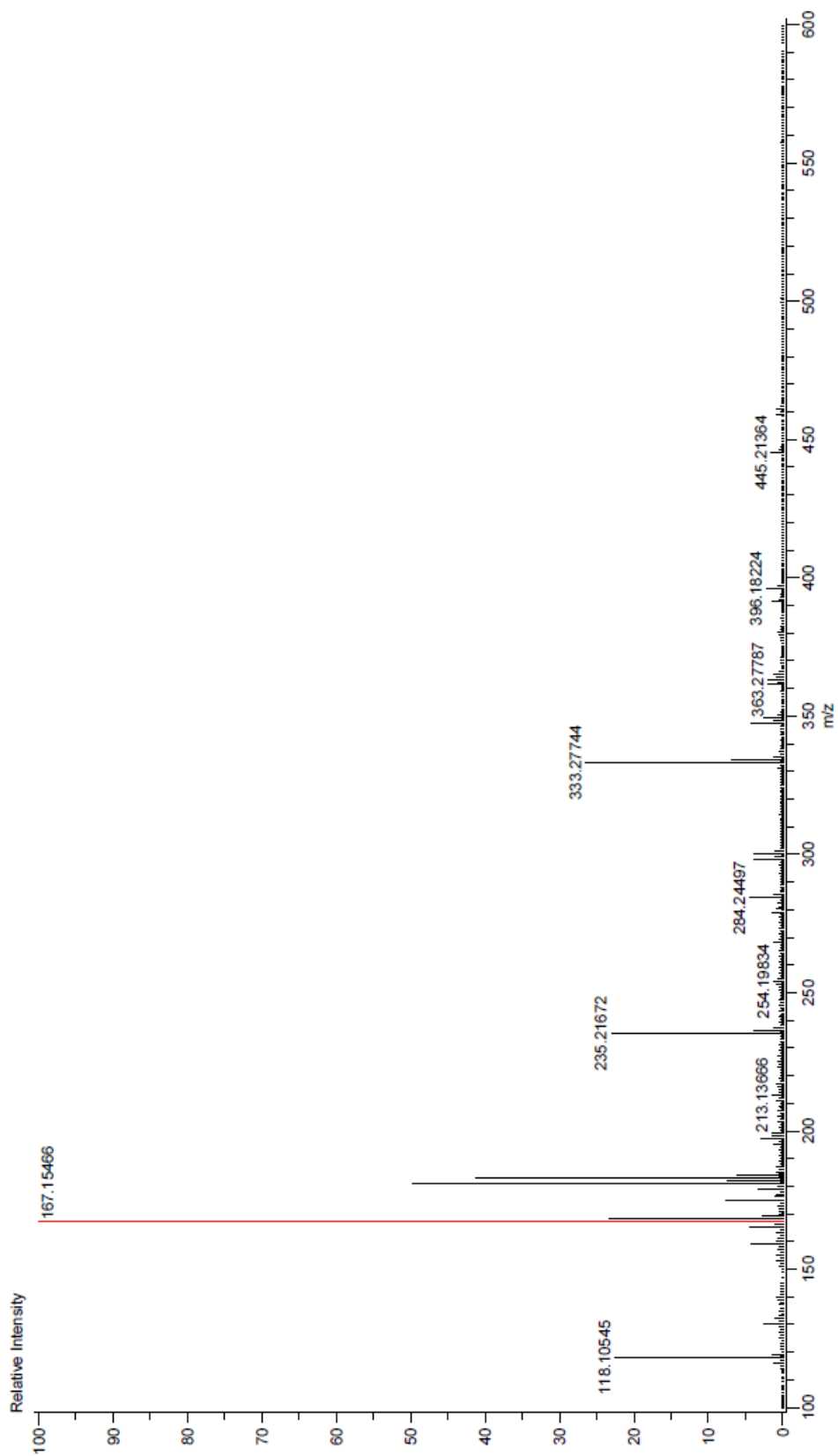
¹H-NMR spectrum of 4-(5)-heptyl-1H-imidazole (12)



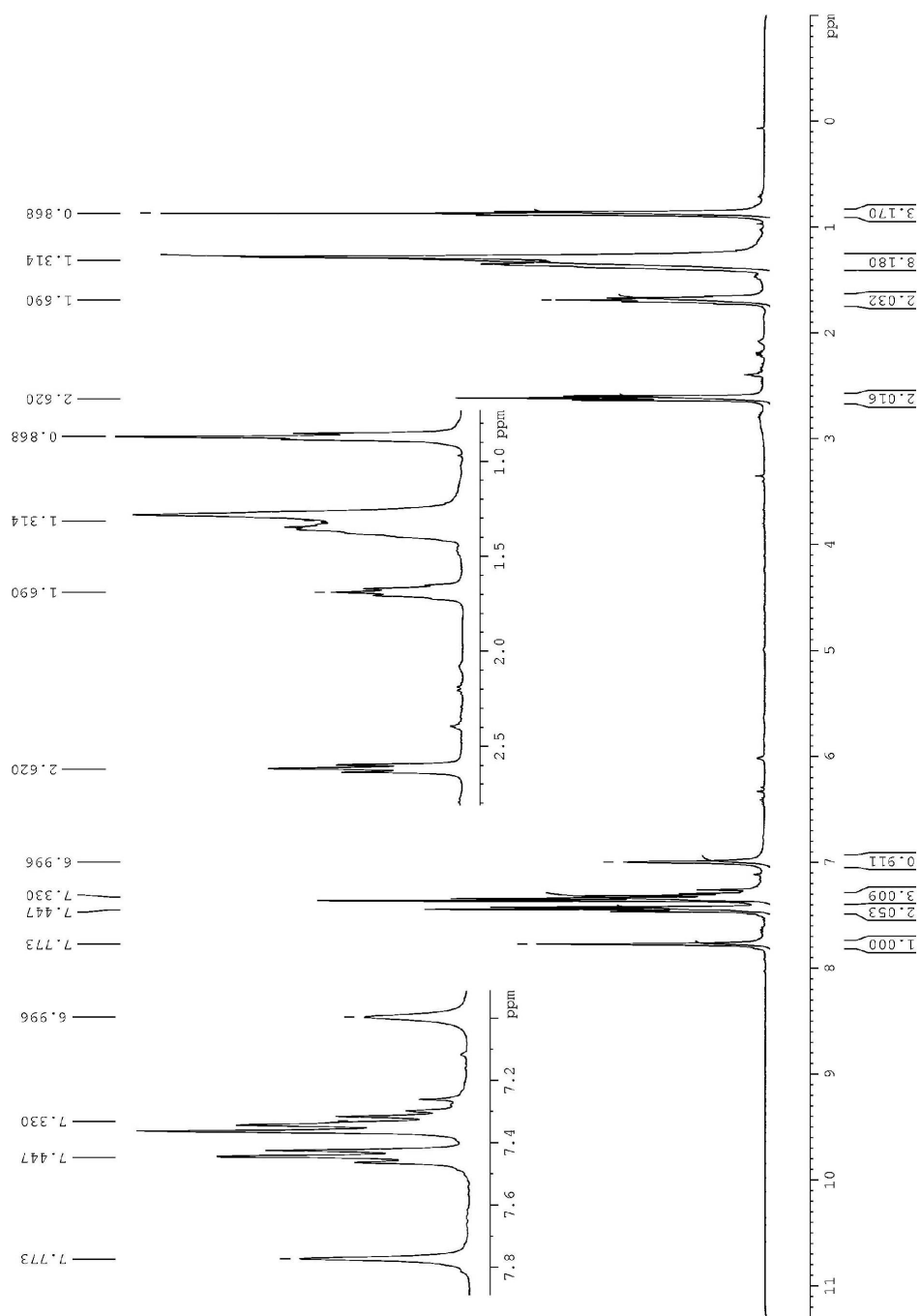
¹³C-NMR spectrum of 4-(5)-heptyl-1H-imidazole (12)



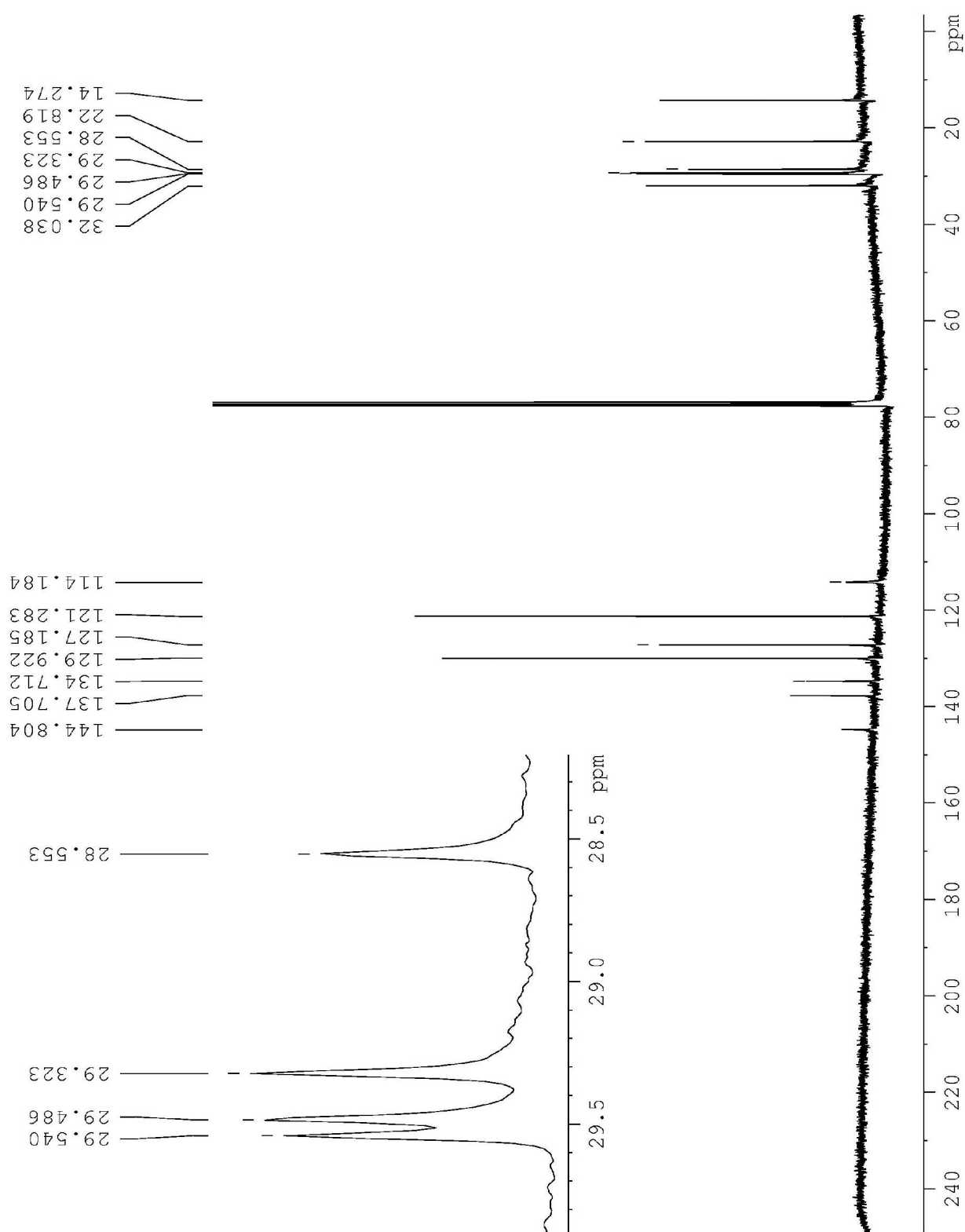
HRMS spectrum of 4-(5)-heptyl-1H-imidazole (12)



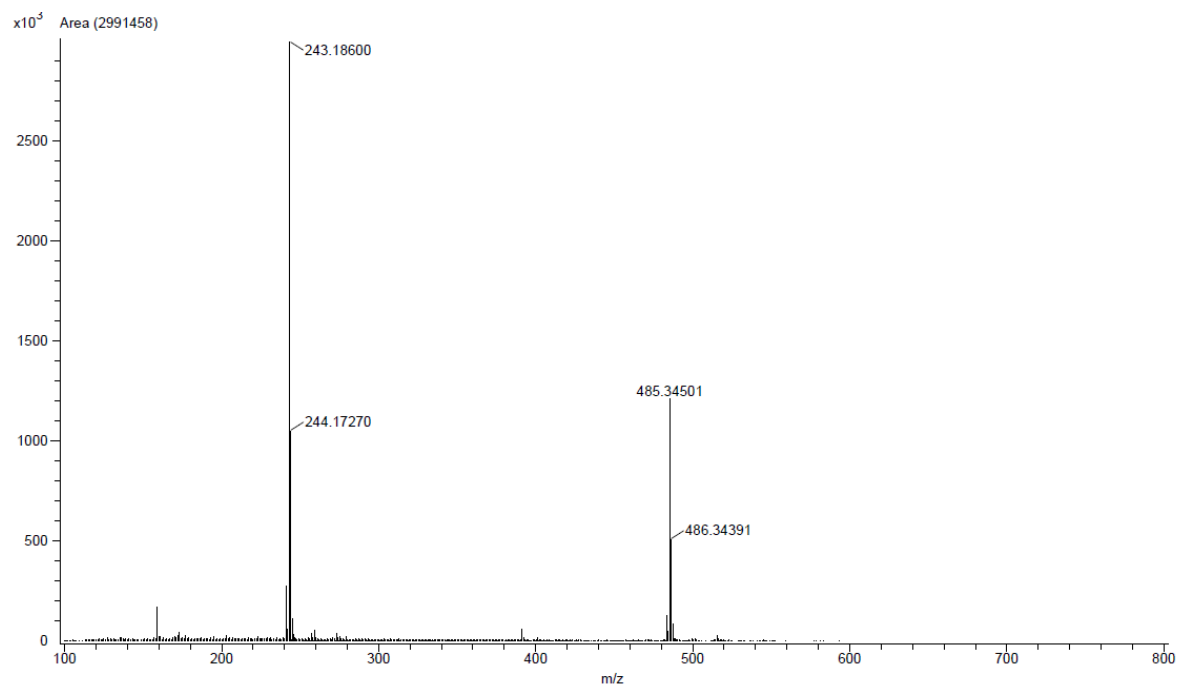
¹H-NMR spectrum of *N*-phenyl-4-heptylimidazole (13)



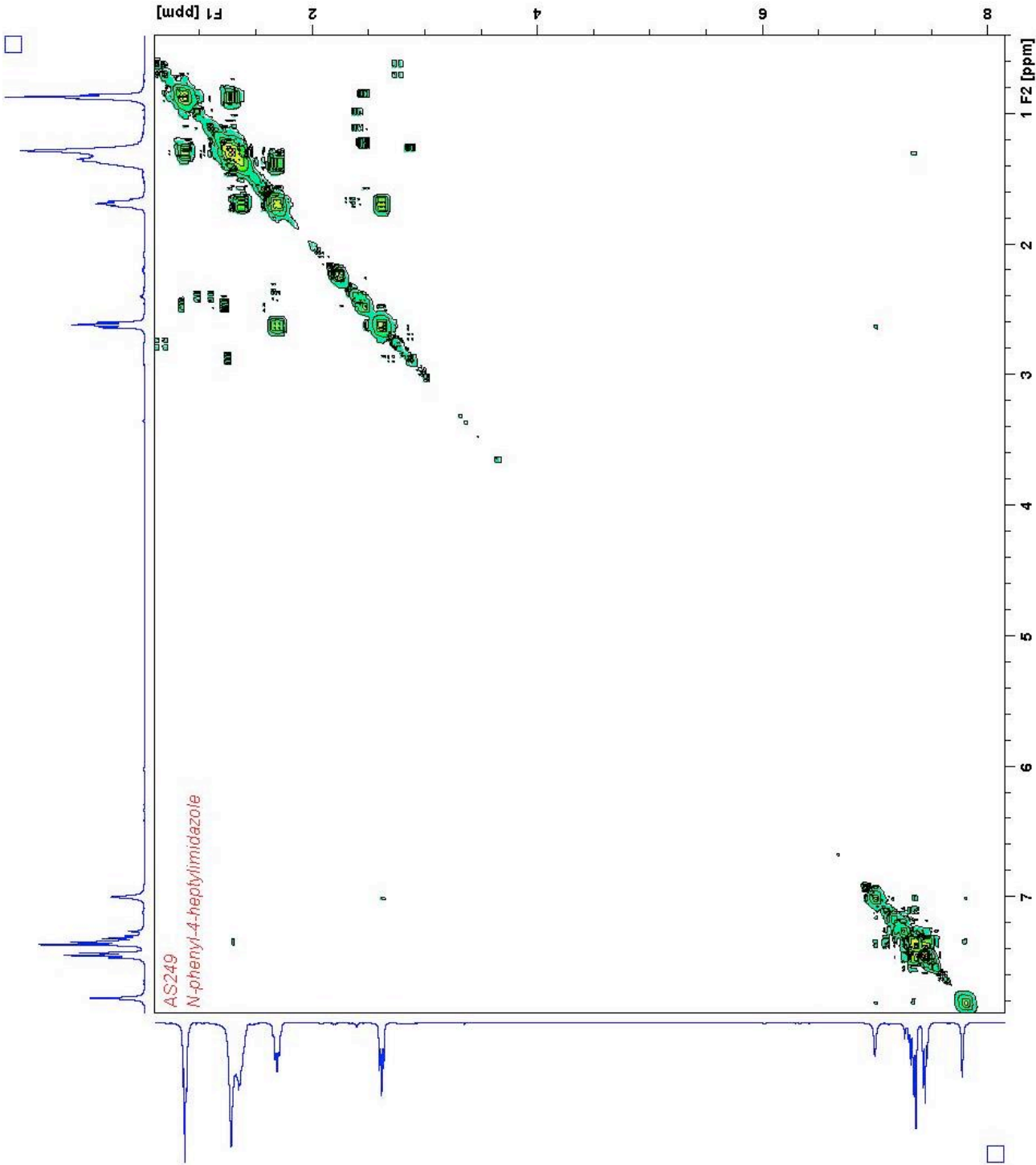
¹³C-NMR spectrum of *N*-phenyl-4-heptylimidazole (13)



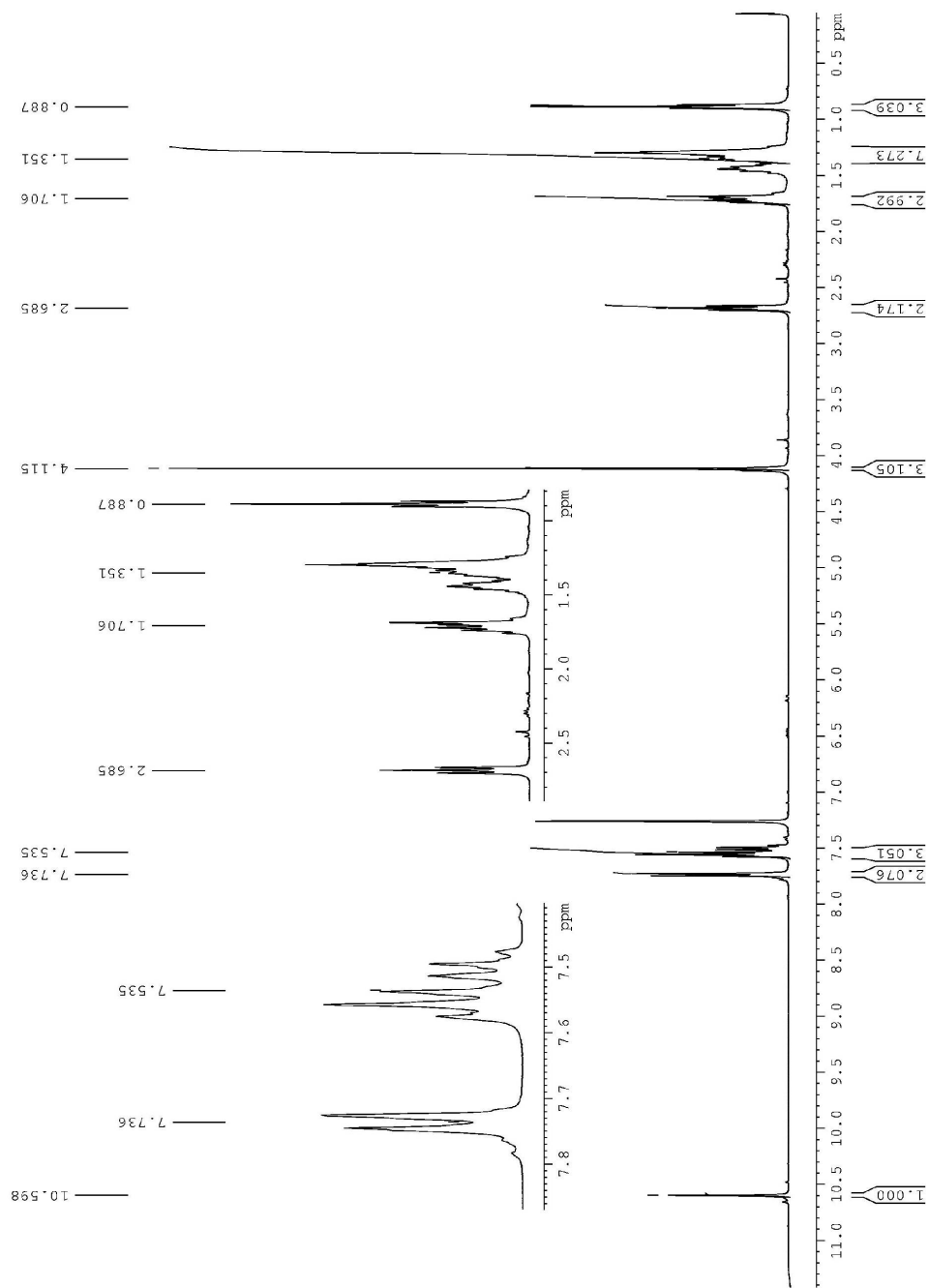
HRMS spectrum of *N*-phenyl-4-heptylimidazole (13)



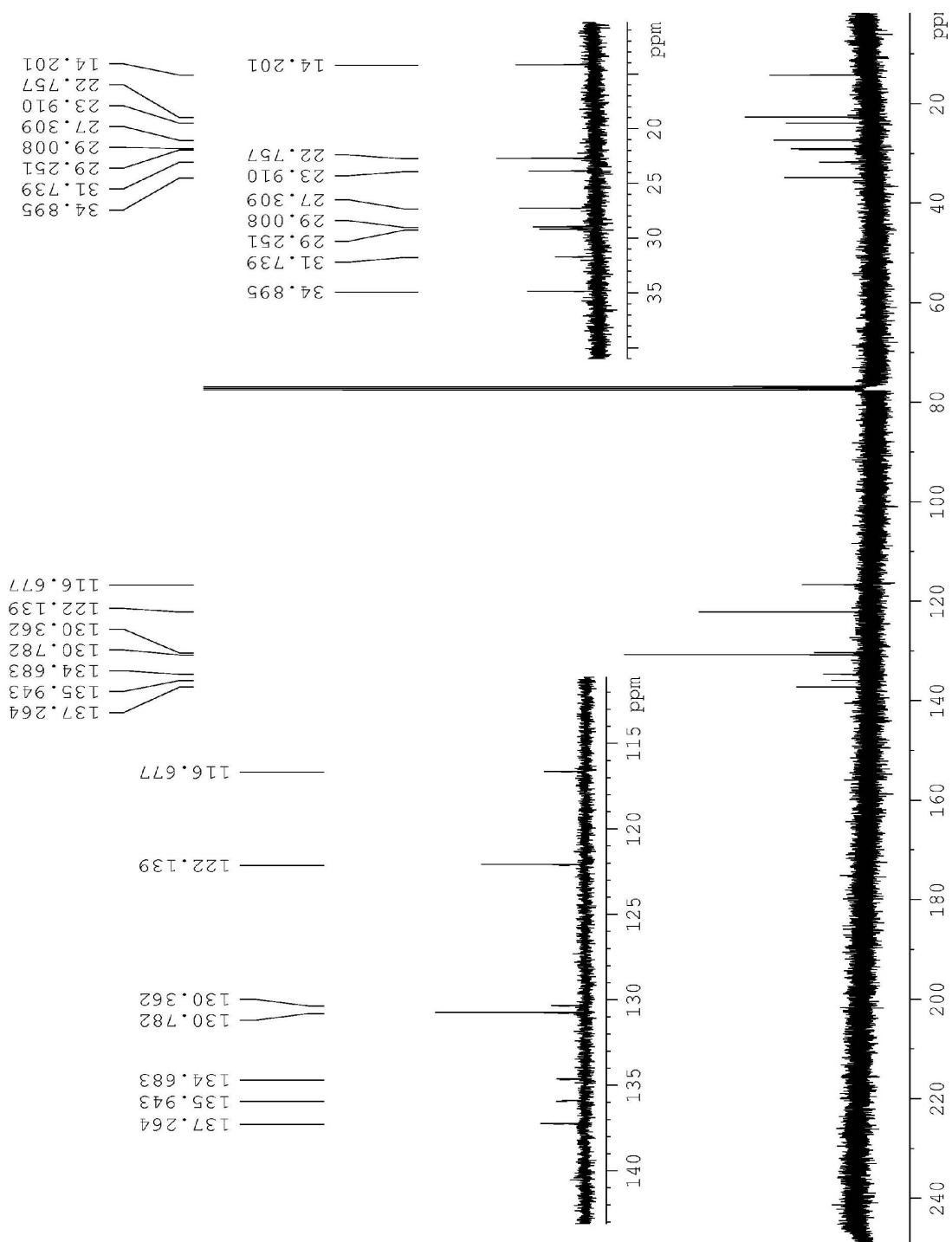
COSY 2D-NMR spectrum of *N*-phenyl-4-heptylimidazole (13)



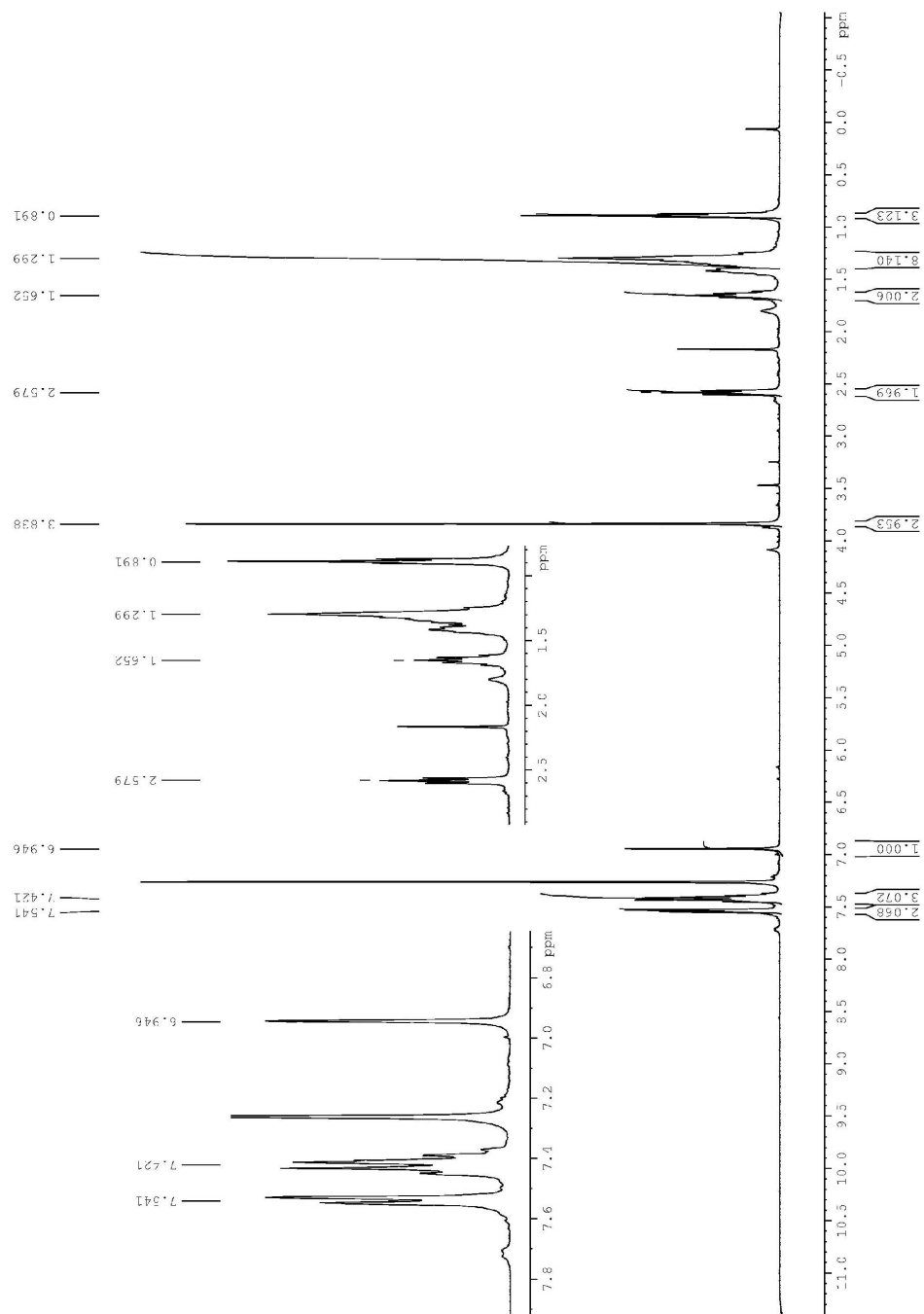
¹H-NMR spectrum of *N*-1-phenyl-*N*-3-methyl-4-heptylimidazolium iodide (14)



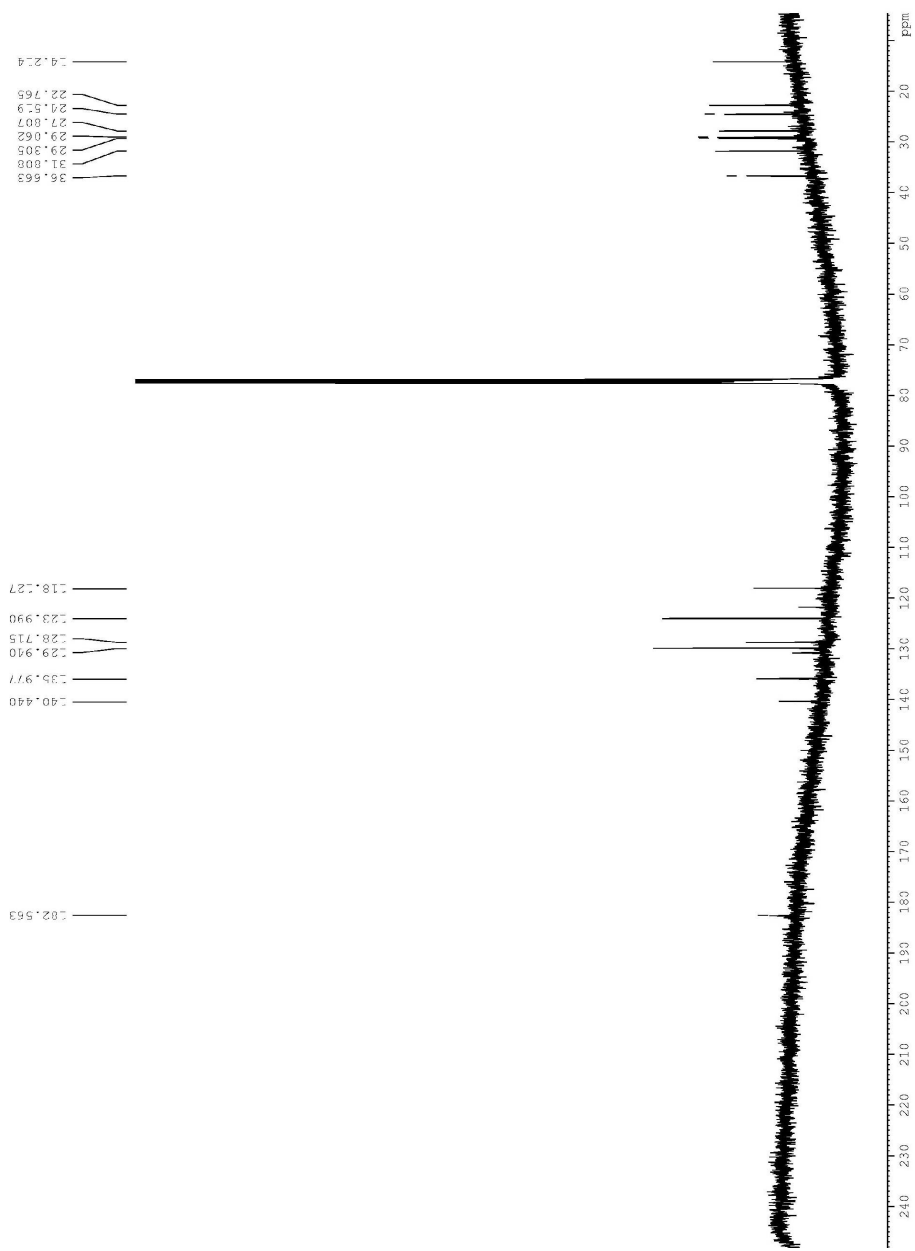
¹³C-NMR spectrum of *N*-1-phenyl-*N*-3-methyl-4-heptylimidazolium iodide (14)



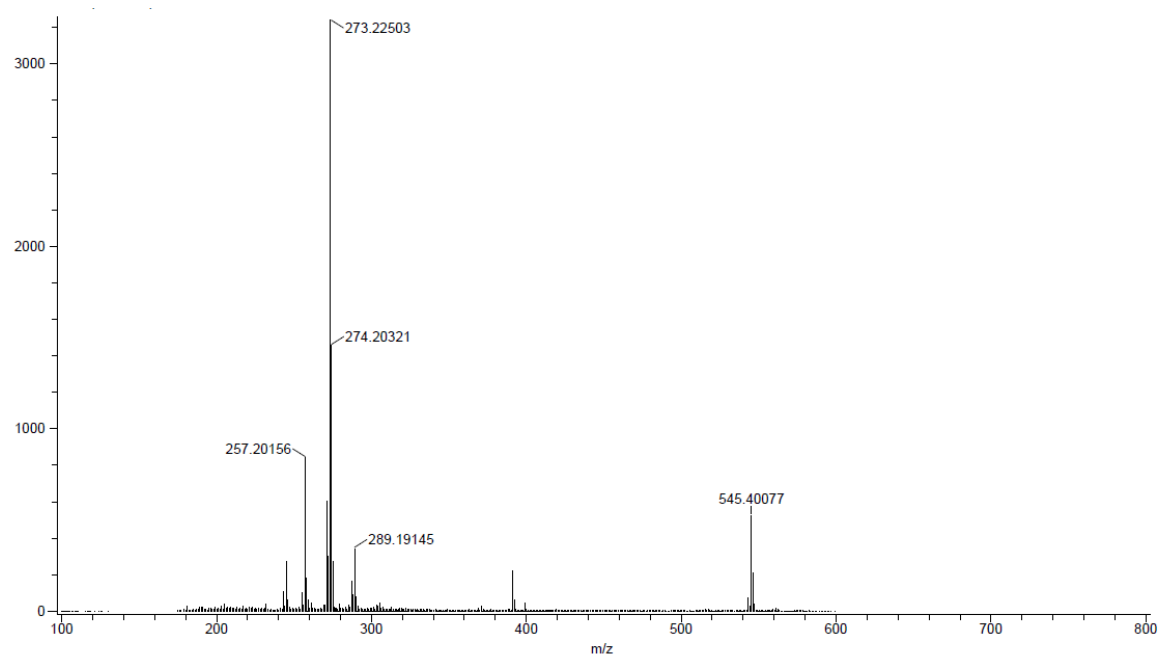
¹H-NMR spectrum of NHC-2



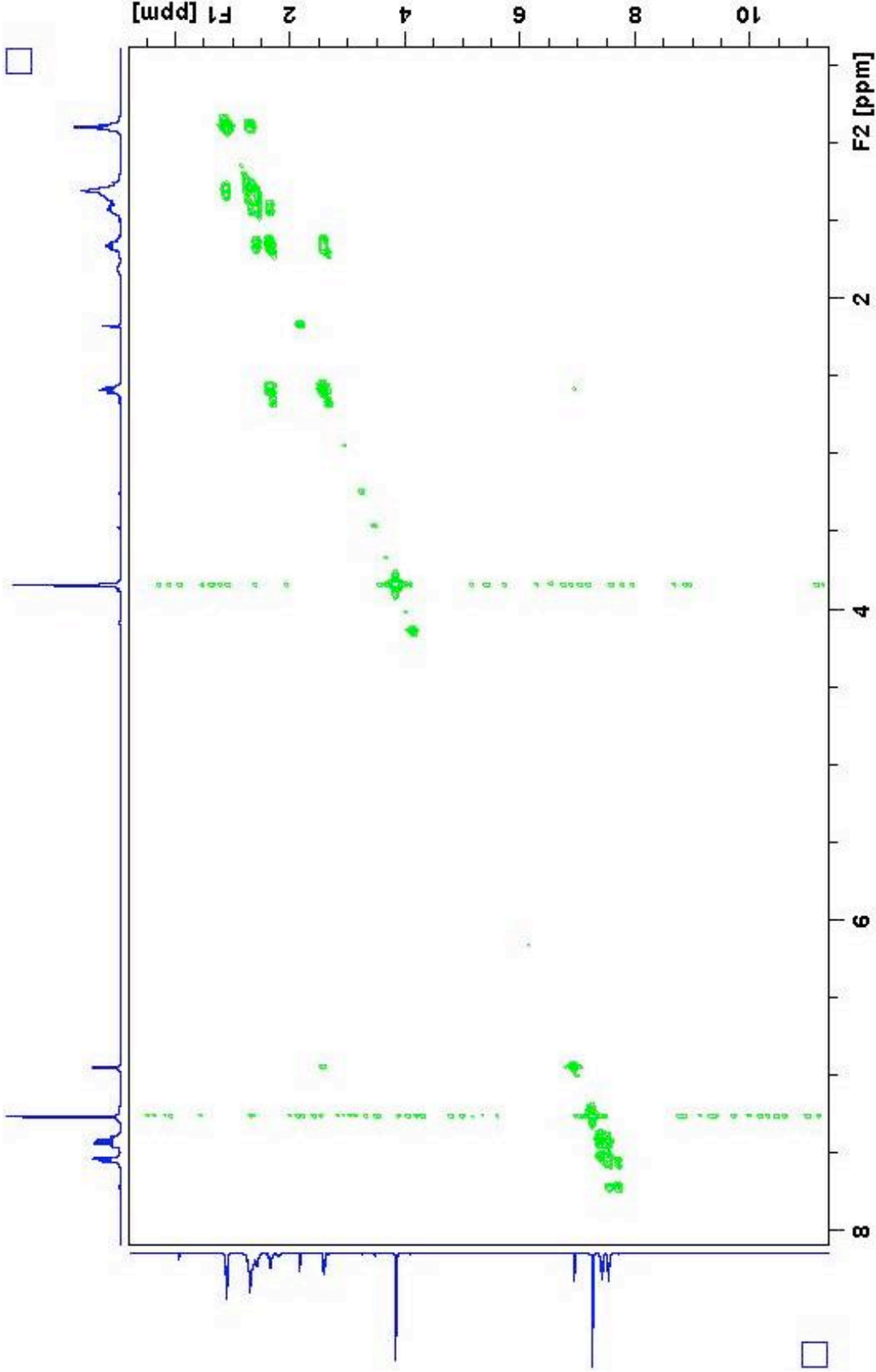
¹³C-NMR spectrum of NHC-2



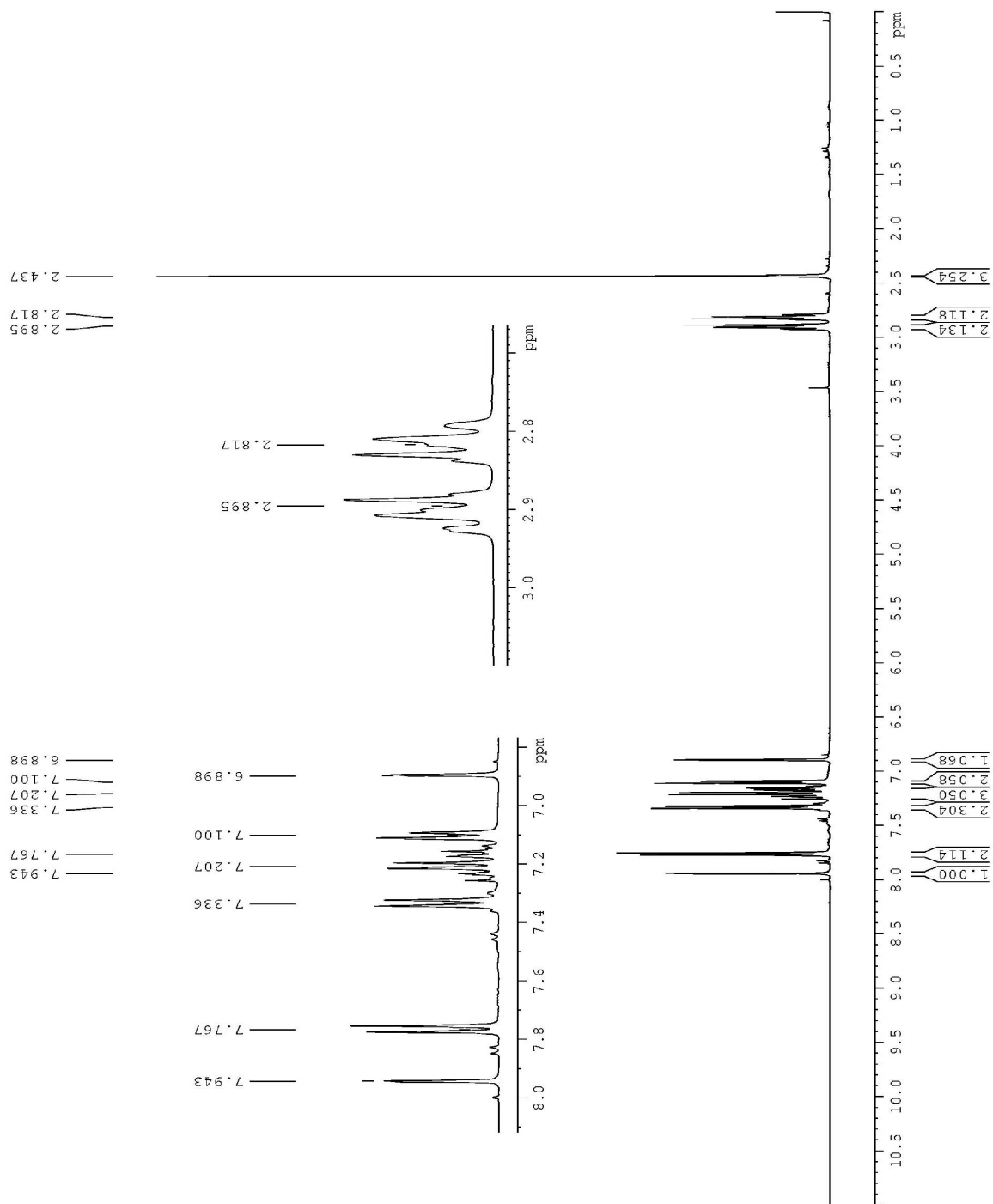
HRMS spectrum of NHC-2



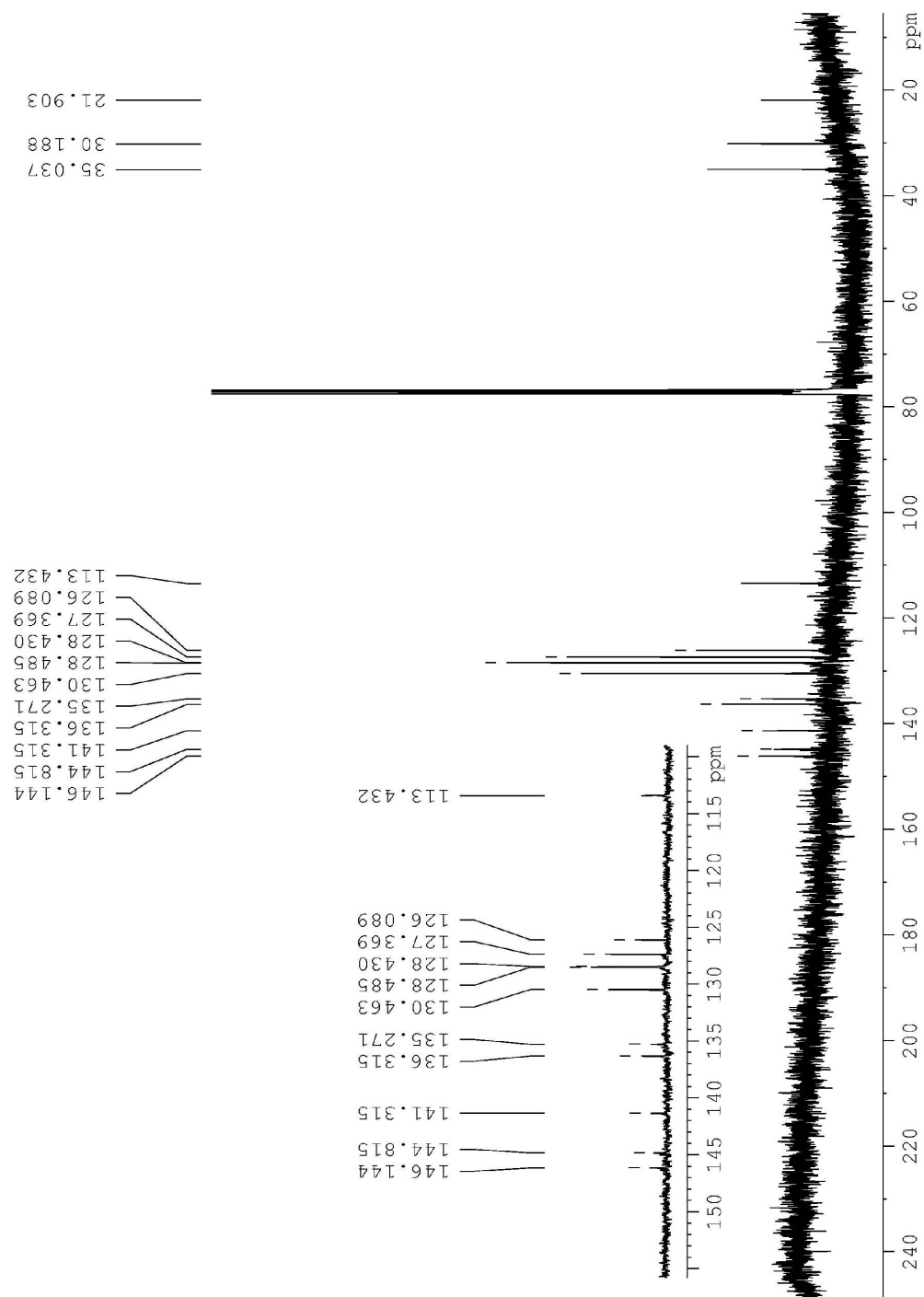
2D COSY-NMR spectrum NHC-2



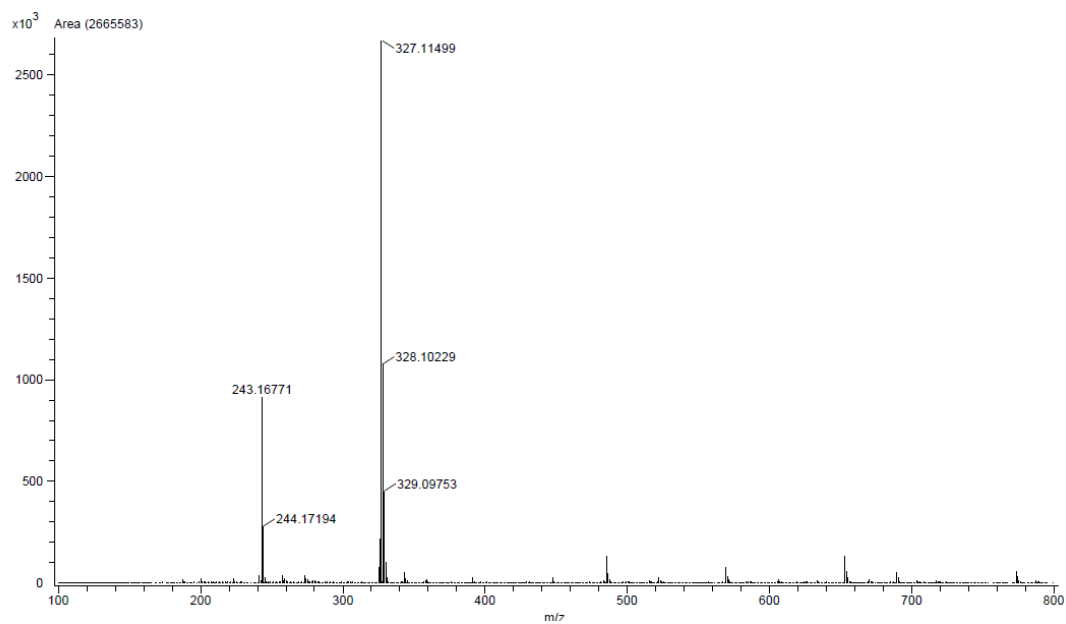
¹H-NMR spectrum of *N*-tosyl-4-(2-phenylethyl)imidazole (15)



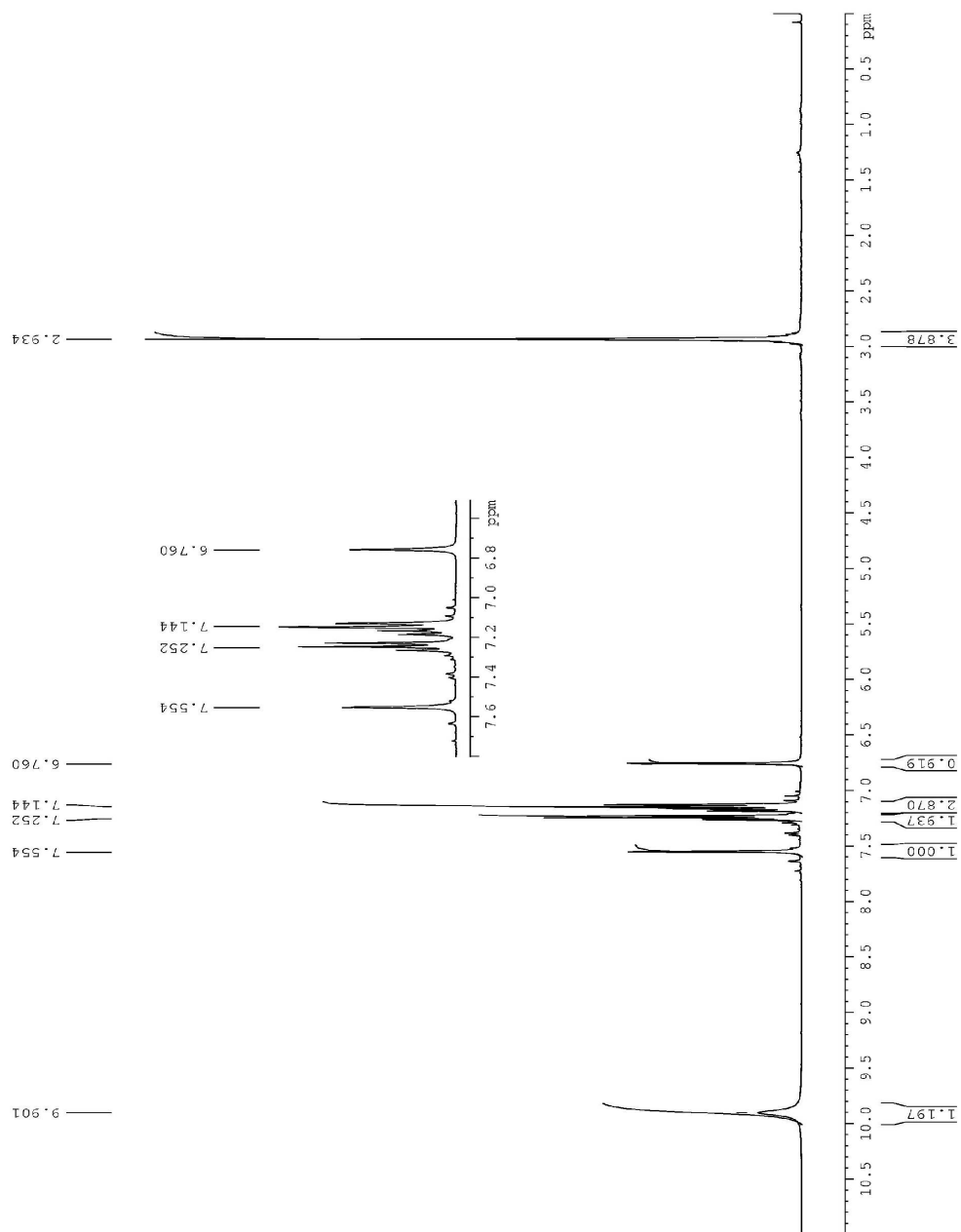
¹³C-NMR spectrum of *N*-tosyl-4-(2-phenylethyl)imidazole (15)



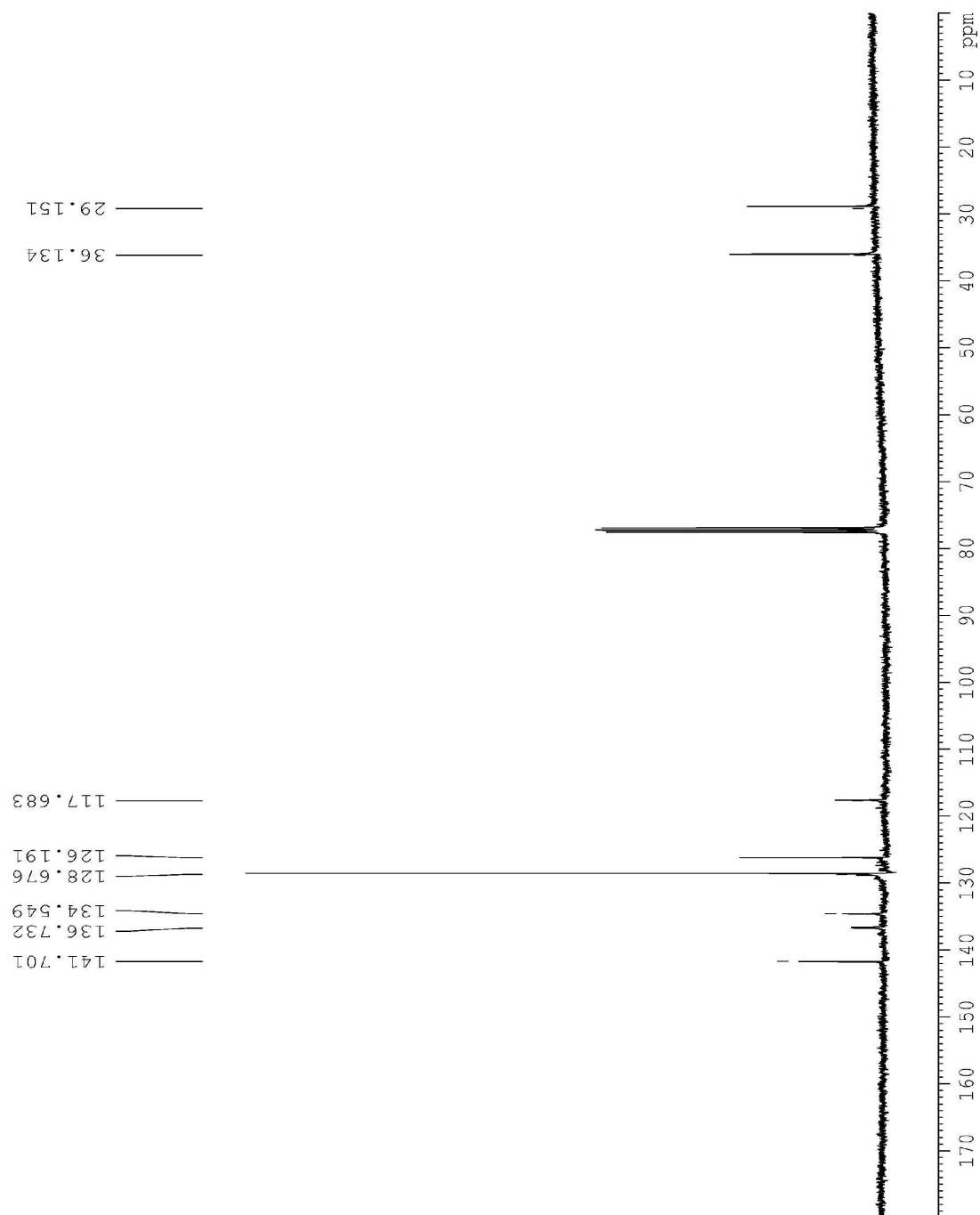
HRMS spectrum of *N*-tosyl-4-(2-phenylethyl)imidazole (15)



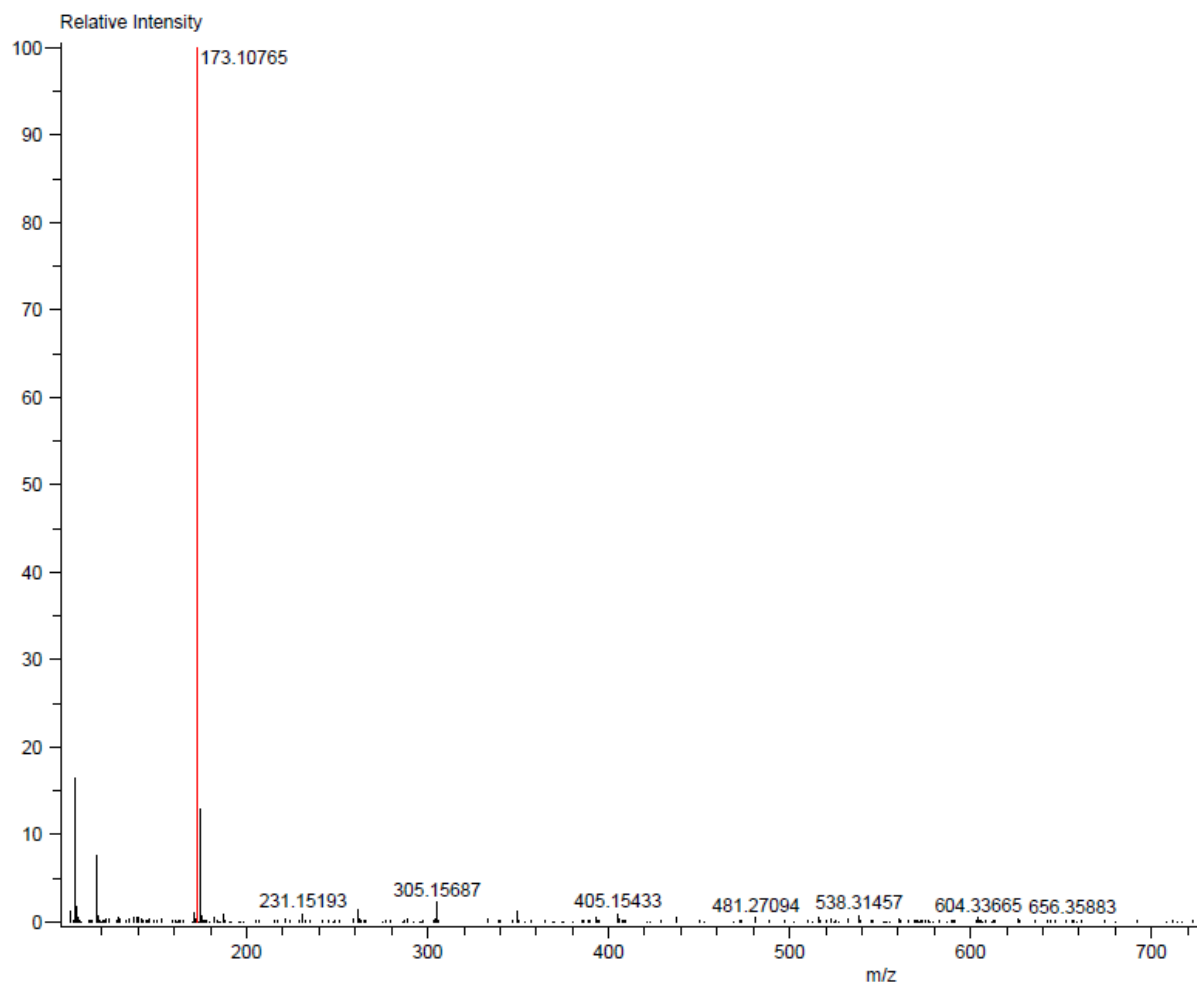
¹H-NMR spectrum of 4-(5)-(2-phenylethyl)-1H-imidazole (16)



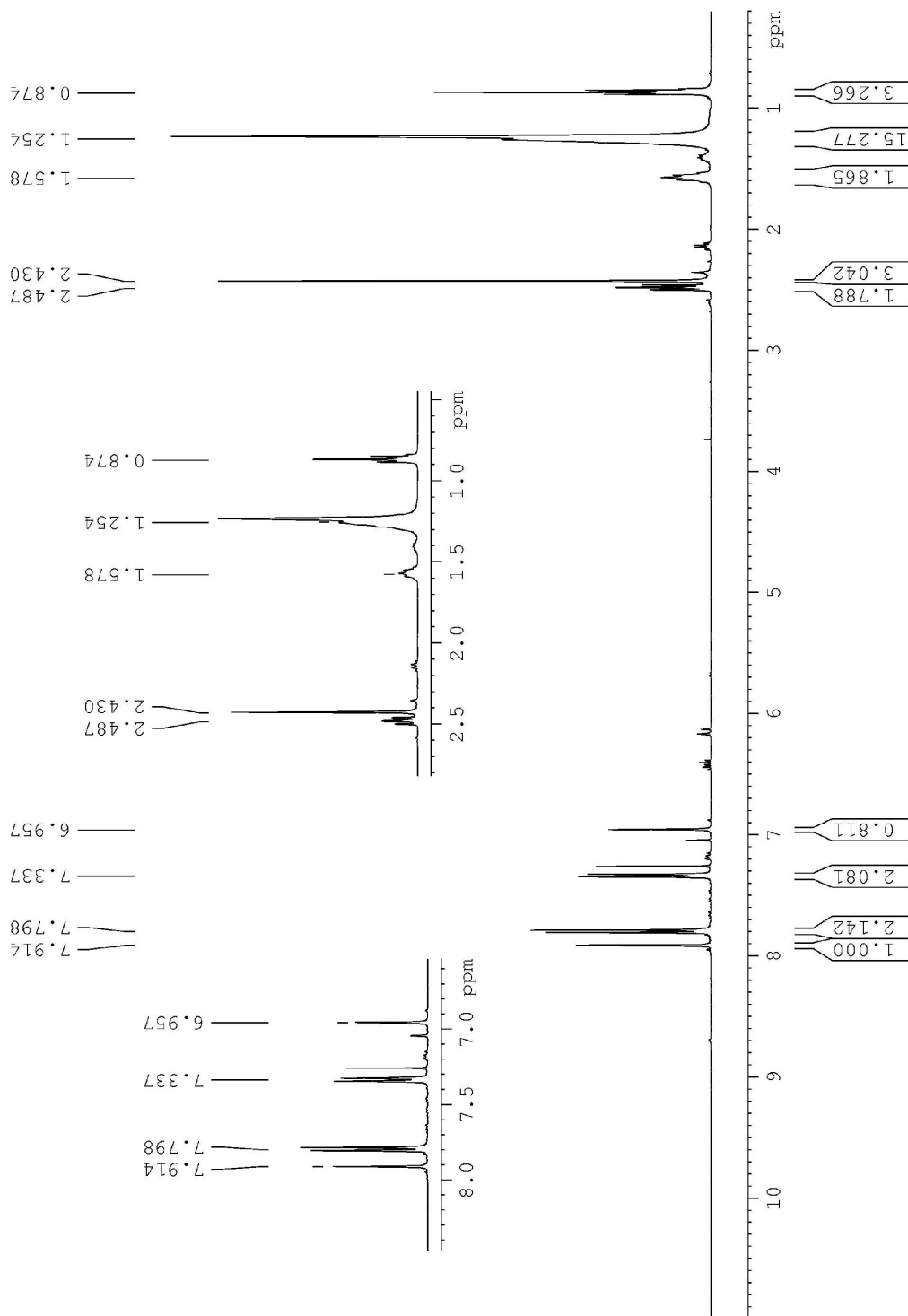
¹³C-NMR spectrum of 4-(5)-(2-phenylethyl)-1H-imidazole (16)



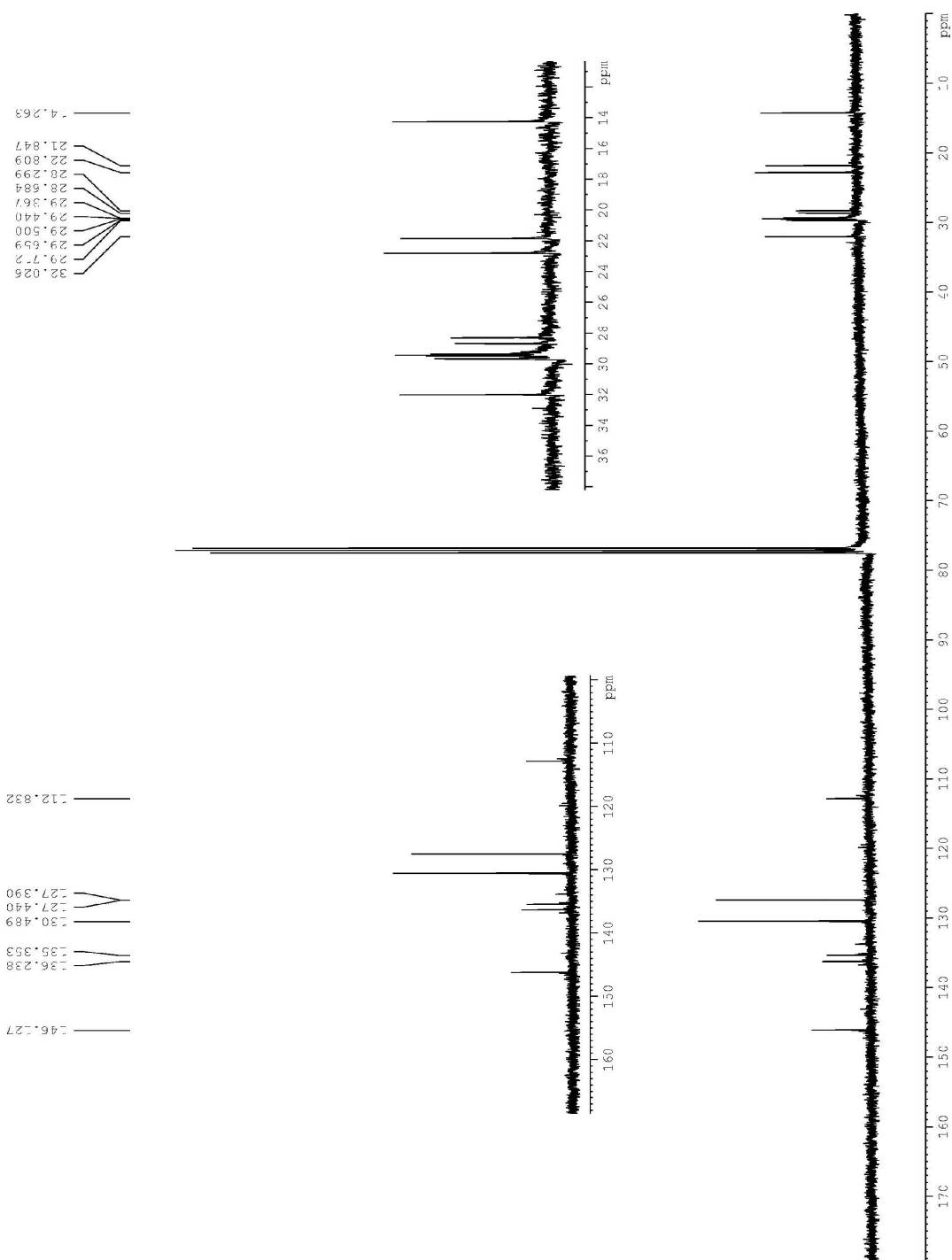
HRMS spectrum of 4-(5)-(2-phenylethyl)-1H-imidazole (16)



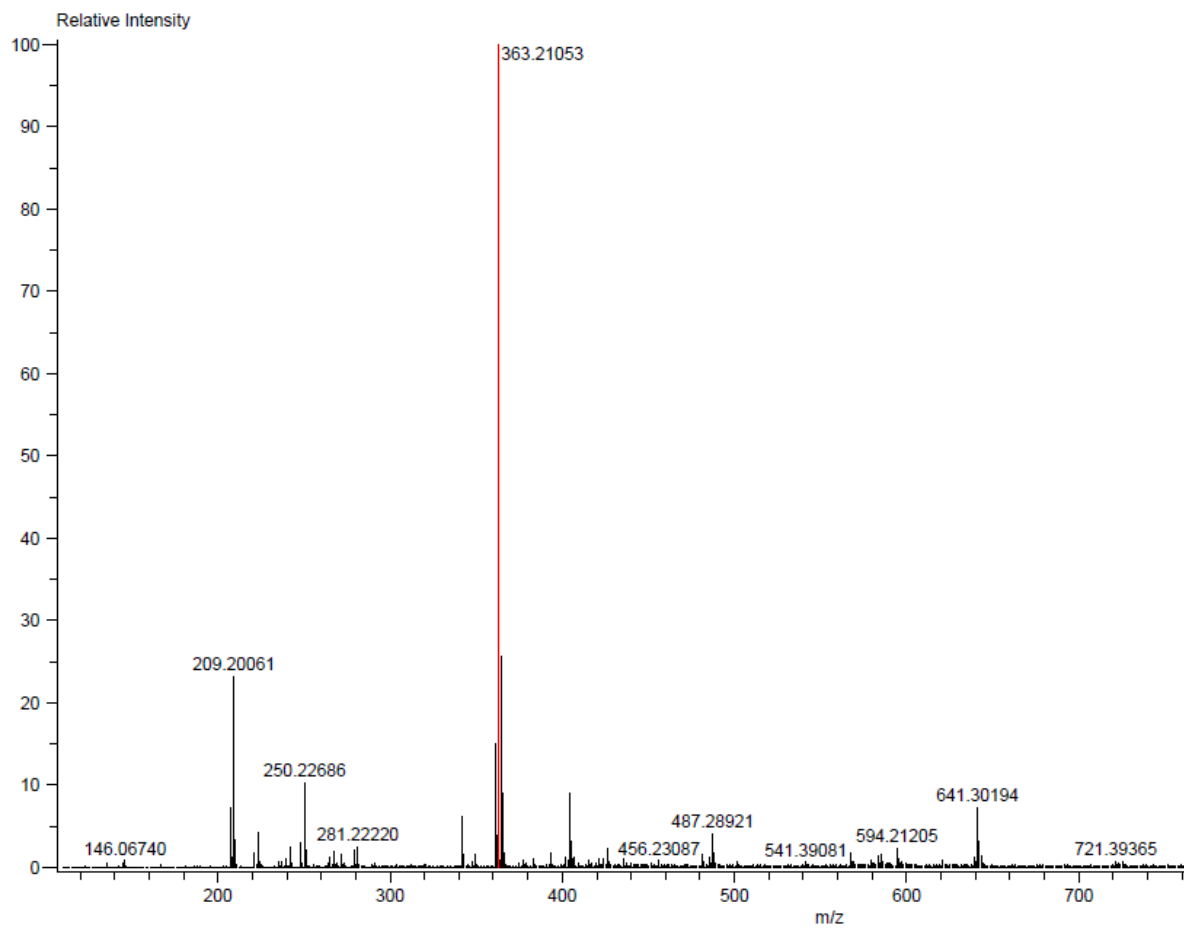
¹H-NMR spectrum of *N*-tosyl-4-decylimidazole (17)



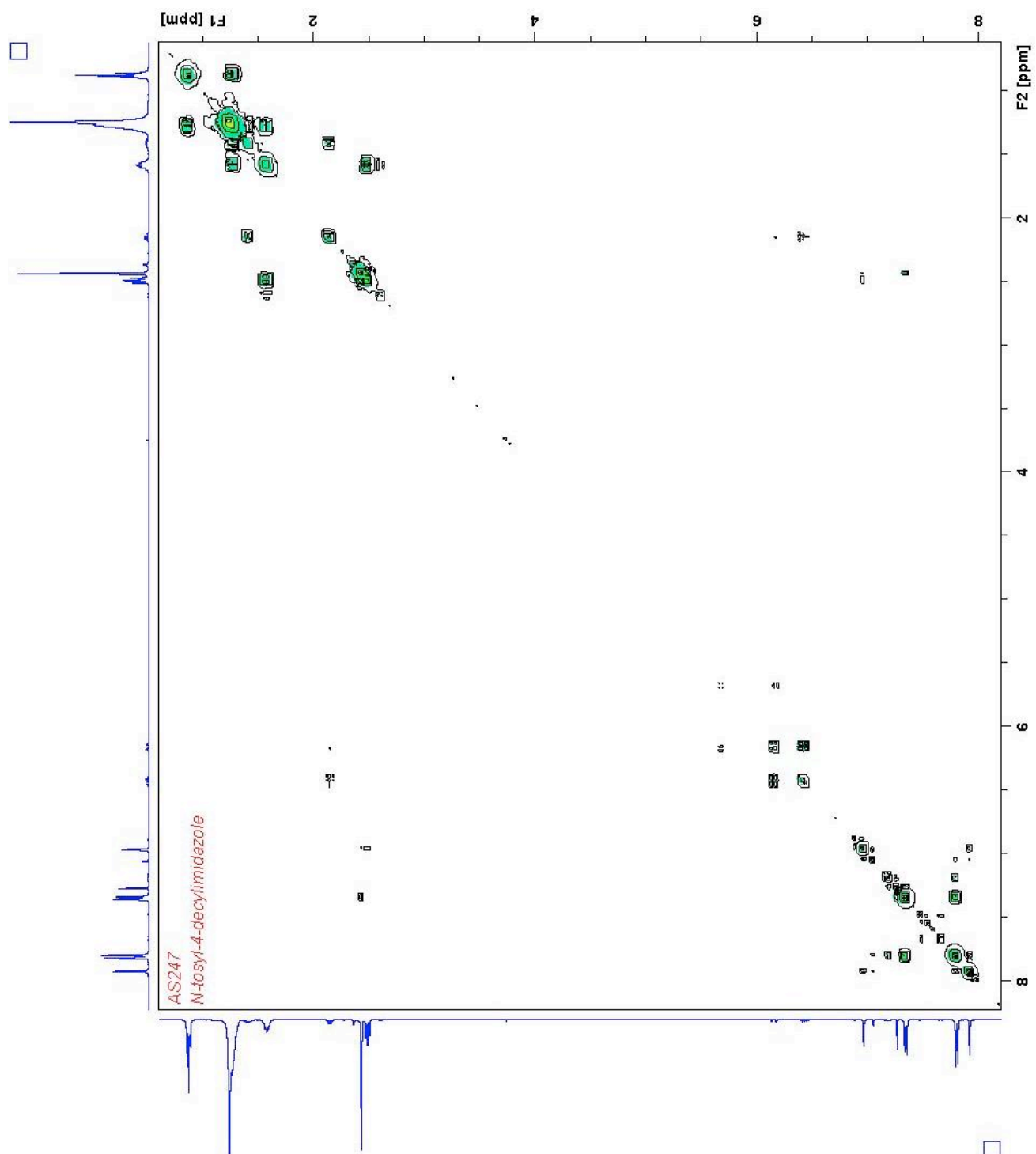
¹³C-NMR spectrum of *N*-tosyl-4-decylimidazole (17)



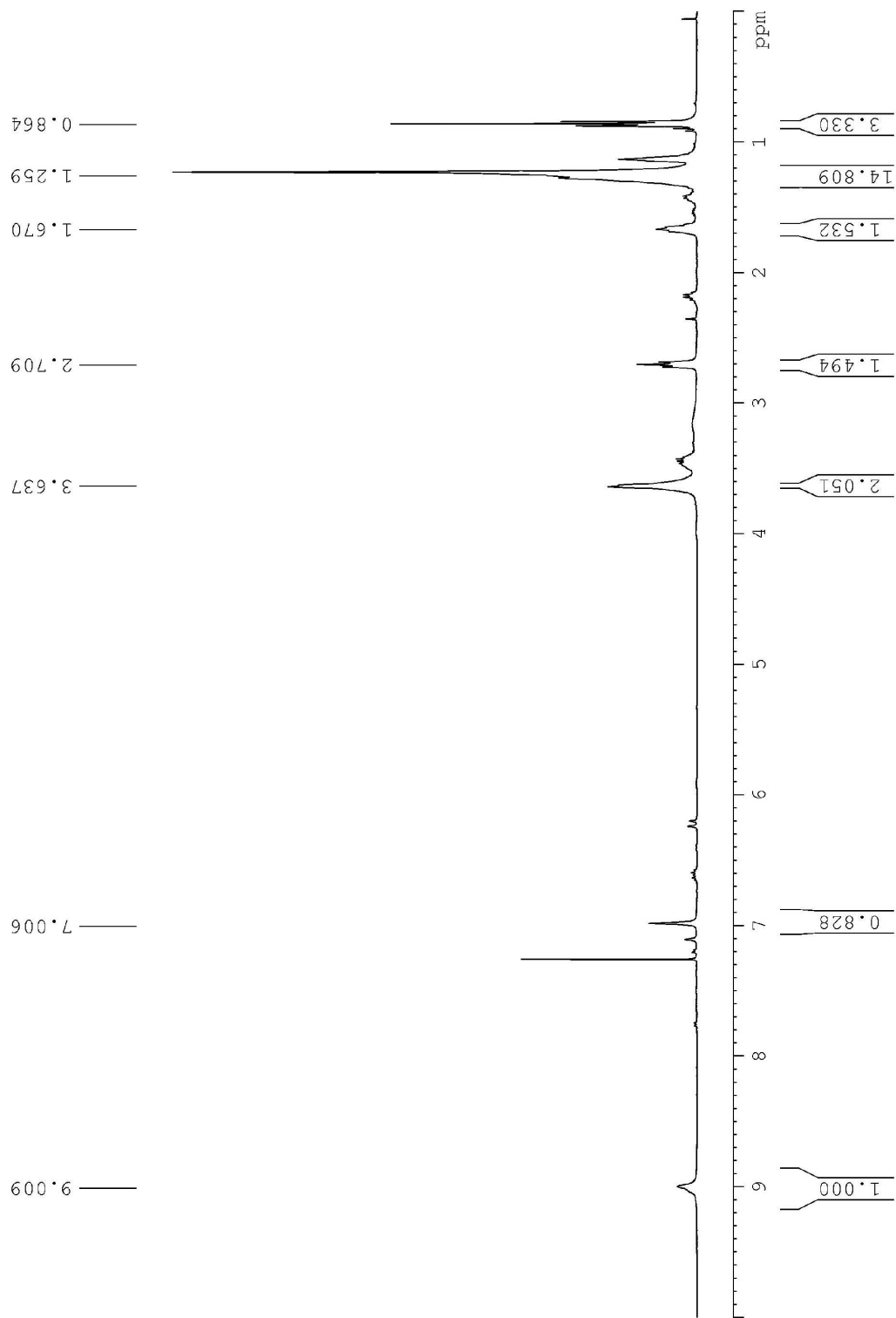
HRMS spectrum of *N*-tosyl-4-decylimidazole (17)



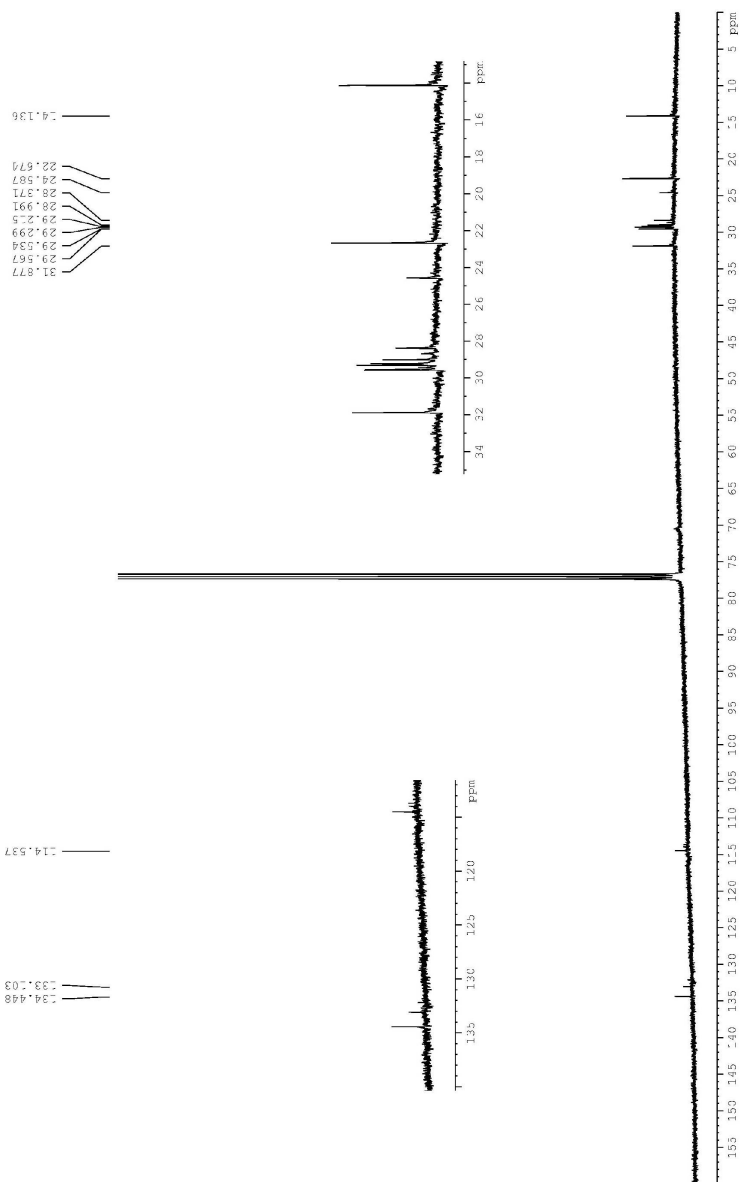
COSY-NMR spectrum of *N*-tosyl-4-decyimidazole (17)



¹H-NMR spectrum of 4-(5)-decyl-1H-imidazole (18)



¹³C-NMR spectrum of 4-(5)-decyl-1H-imidazole (18)



HRMS spectrum of 4-(5)-decyl-1H-imidazole (18)

