

Supporting Information for

A Versatile and Scalable Method for Producing N-functionalized Imidazoles

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Contents

- Spectroscopic data for compounds 1 – 21
- ¹H NMR Spectra images for compounds 1 – 21

Sodium imidazolate (Nalm) (**1**): ^1H NMR (360 MHz, DMSO) δ 6.99 (s, 1H), 6.60 (d, $J = 0.7$ Hz, 2H). ^{13}C NMR (126 MHz, DMSO) δ 143.70 (d, $J = 6.8$ Hz), 125.35 (d, $J = 8.0$ Hz). ESI(-) MS: Calculated as 67.1 for $[\text{C}_3\text{H}_3\text{N}_2]^-$; Found for $[\text{C}_3\text{H}_3\text{N}_2(\text{C}_3\text{H}_3\text{N}_2\text{Na})_n]^-$ ($n=0, 1, 2, 3, 4$): 67.2, 157.1, 247.1, 337.1, 427.1, 517.1.

1-ethylimidazole (**2**): ^1H NMR (500 MHz, CDCl_3) δ 7.35 (s, 1H), 6.87 (dd, $J = 58.1, 0.8$ Hz, 2H), 3.86 (qd, $J = 7.3, 1.5$ Hz, 2H), 1.32 (td, $J = 7.4, 1.7$ Hz, 3H).

1-propylimidazole (**3**): ^1H NMR (500 MHz, CDCl_3) δ 7.37 (s, 1H), 6.96 (s, 1H), 6.82 (d, $J = 1.0$ Hz, 1H), 3.84 – 3.77 (m, 2H), 1.76 – 1.67 (m, 2H), 0.87 – 0.80 (m, 3H).

1-butylimidazole (**4**): ^1H NMR (500 MHz, CDCl_3) δ 7.43 (s, 1H), 6.95 (dd, $J = 73.0, 0.9$ Hz, 2H), 3.90 (t, $J = 7.1$ Hz, 2H), 1.73 (dt, $J = 14.9, 7.3$ Hz, 2H), 1.49 – 1.11 (m, 2H), 0.91 (t, $J = 7.4$ Hz, 3H).

1-pentylimidazole (**5**): ^1H NMR (500 MHz, CDCl_3) δ 7.45 (s, 1H), 7.05 (s, 1H), 6.90 (s, 1H), 3.91 (t, $J = 7.2$ Hz, 2H), 1.85 – 1.69 (m, 2H), 1.49 – 1.16 (m, 4H), 0.89 (t, $J = 7.2$ Hz, 3H).

1-hexylimidazole (**6**): ^1H NMR (500 MHz, CDCl_3) δ 7.43 (s, 1H), 7.12 – 6.79 (m, 2H), 4.07 – 3.70 (m, 2H), 1.83 – 1.63 (m, 2H), 1.27 (d, $J = 2.9$ Hz, 6H), 0.85 (dd, $J = 6.8, 5.4$ Hz, 3H).

1-octylimidazole (**7**): ^1H NMR (500 MHz, CDCl_3) δ 7.44 (s, 1H), 7.04 (d, $J = 0.8$ Hz, 1H), 6.89 (d, $J = 0.9$ Hz, 1H), 3.90 (t, $J = 7.2$ Hz, 2H), 1.75 (p, $J = 7.0$ Hz, 2H), 1.26 (dd, $J = 12.2, 5.6$ Hz, 10H), 0.86 (t, $J = 6.7$ Hz, 3H).

1-decylimidazole (**8**): ^1H NMR (500 MHz, CDCl_3) δ 7.43 (s, 1H), 6.92 (dd, $J = 39.0, 37.9$ Hz, 2H), 4.09 – 3.71 (m, 2H), 1.83 – 1.64 (m, 2H), 1.46 – 1.04 (m, 14H), 0.86 (td, $J = 6.9, 1.3$ Hz, 3H).

1-dodecylimidazole (**9**): ^1H NMR (500 MHz, CDCl_3) δ 7.43 (s, 1H), 6.95 (dd, $J = 75.8, 0.7$ Hz, 2H), 3.89 (t, $J = 7.2$ Hz, 2H), 1.74 (p, $J = 7.0$ Hz, 2H), 1.45 – 1.04 (m, 20H), 0.86 (t, $J = 6.8$ Hz, 3H).

1-tetradecylimidazole (**10**): ^1H NMR (500 MHz, CDCl_3) δ 7.46 (s, 1H), 7.06 (s, 1H), 6.90 (s, 1H), 3.92 (t, $J = 7.2$ Hz, 2H), 1.85 – 1.69 (m, 2H), 1.44 – 1.07 (m, 24H), 0.88 (t, $J = 6.9$ Hz, 3H).

1-(2-methoxyethyl)imidazole (**11**): ^1H NMR (500 MHz, CDCl_3) δ 7.44 (s, 1H), 7.09 – 6.74 (m, 2H), 4.02 (t, $J = 5.2$ Hz, 2H), 3.56 (t, $J = 5.2$ Hz, 2H), 3.27 (d, $J = 0.9$ Hz, 3H).

1-[2-(2-methoxyethoxy)ethyl]imidazole (**12**): ^1H NMR (500 MHz, CDCl_3) δ 7.51 (s, 1H), 6.99 (d, $J = 26.3$ Hz, 2H), 4.09 (t, $J = 5.3$ Hz, 2H), 3.71 (t, $J = 5.3$ Hz, 2H), 3.55 (dd, $J = 5.5, 3.1$ Hz, 2H), 3.51 – 3.46 (m, 2H), 3.34 (s, 3H).

1-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]imidazole (**13**): ^1H NMR (500 MHz, CDCl_3) δ 7.49 (s, 1H), 6.97 (d, $J = 18.7$ Hz, 2H), 4.06 (t, $J = 5.2$ Hz, 2H), 3.70 (t, $J = 5.2$ Hz, 2H), 3.63 – 3.53 (m, 6H), 3.50 (dd, $J = 5.8, 3.4$ Hz, 2H), 3.33 (d, $J = 5.2$ Hz, 3H).

1-benzylimidazole (**14**): ^1H NMR (500 MHz, CDCl_3) δ 7.55 (s, 1H), 7.42 – 7.29 (m, 3H), 7.16 (dd, $J = 7.6, 1.0$ Hz, 2H), 7.10 (s, 1H), 6.91 (s, 1H), 5.12 (s, 2H).

1,1'-(1,4-butanediyl)bis(imidazole) (**15**): ^1H NMR (500 MHz, CDCl_3) δ 7.46 (s, 2H), 7.09 (s, 2H), 6.88 (d, $J = 1.0$ Hz, 2H), 3.96 (d, $J = 6.1$ Hz, 4H), 1.86 – 1.71 (m, 4H).

1,1'-(1,6-hexanediyil)bis(imidazole) (**16**): ^1H NMR (500 MHz, CDCl_3) δ 7.39 (s, 2H), 6.93 (d, $J = 83.8$ Hz, 4H), 3.87 (t, $J = 7.0$ Hz, 4H), 1.93 – 1.50 (m, 4H), 1.44 – 1.07 (m, 4H).

1,1'-(1,8-octanediyil)bis(imidazole) (**17**): ^1H NMR (500 MHz, CDCl_3) δ 7.44 (s, 2H), 7.05 (s, 2H), 6.89 (s, 2H), 3.91 (t, $J = 7.1$ Hz, 4H), 1.83 – 1.65 (m, 4H), 1.37 – 1.15 (m, 8H).

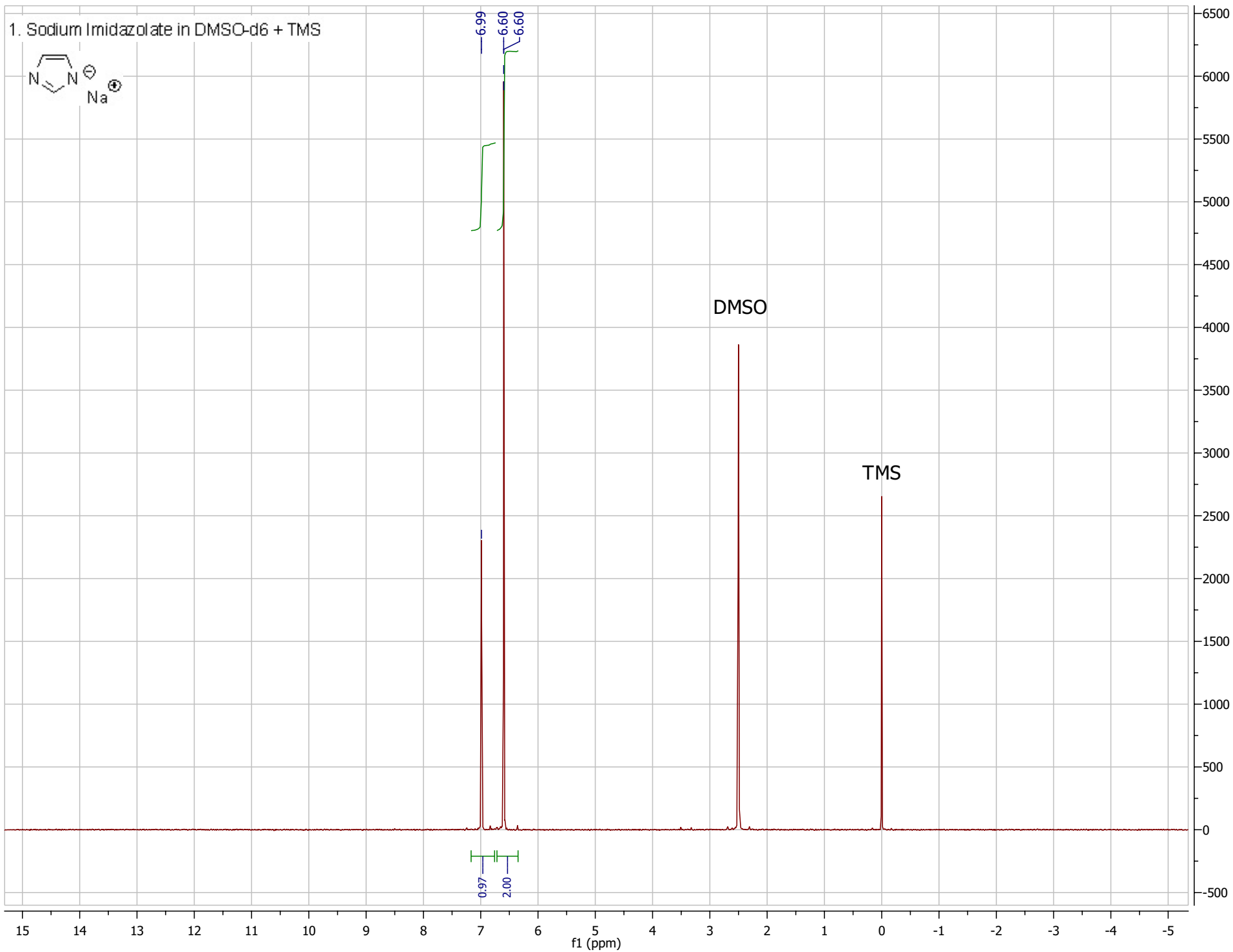
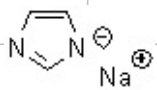
1,1'-(1,10-decanediyil)bis(imidazole) (**18**): ^1H NMR (500 MHz, CDCl_3) δ 7.43 (s, 2H), 6.92 (dd, $J = 39.3, 38.1$ Hz, 4H), 4.09 – 3.71 (m, 4H), 1.84 – 1.65 (m, 4H), 1.25 (dd, $J = 9.8, 5.1$ Hz, 12H).

1,1'-(oxydi-2,1-ethanediyil)bis(imidazole) (**19**): ^1H NMR (500 MHz, CDCl_3) δ 7.44 (s, 2H), 7.03 (s, 2H), 6.86 (s, 2H), 4.05 (t, $J = 5.1$ Hz, 4H), 3.62 (t, $J = 5.1$ Hz, 4H).

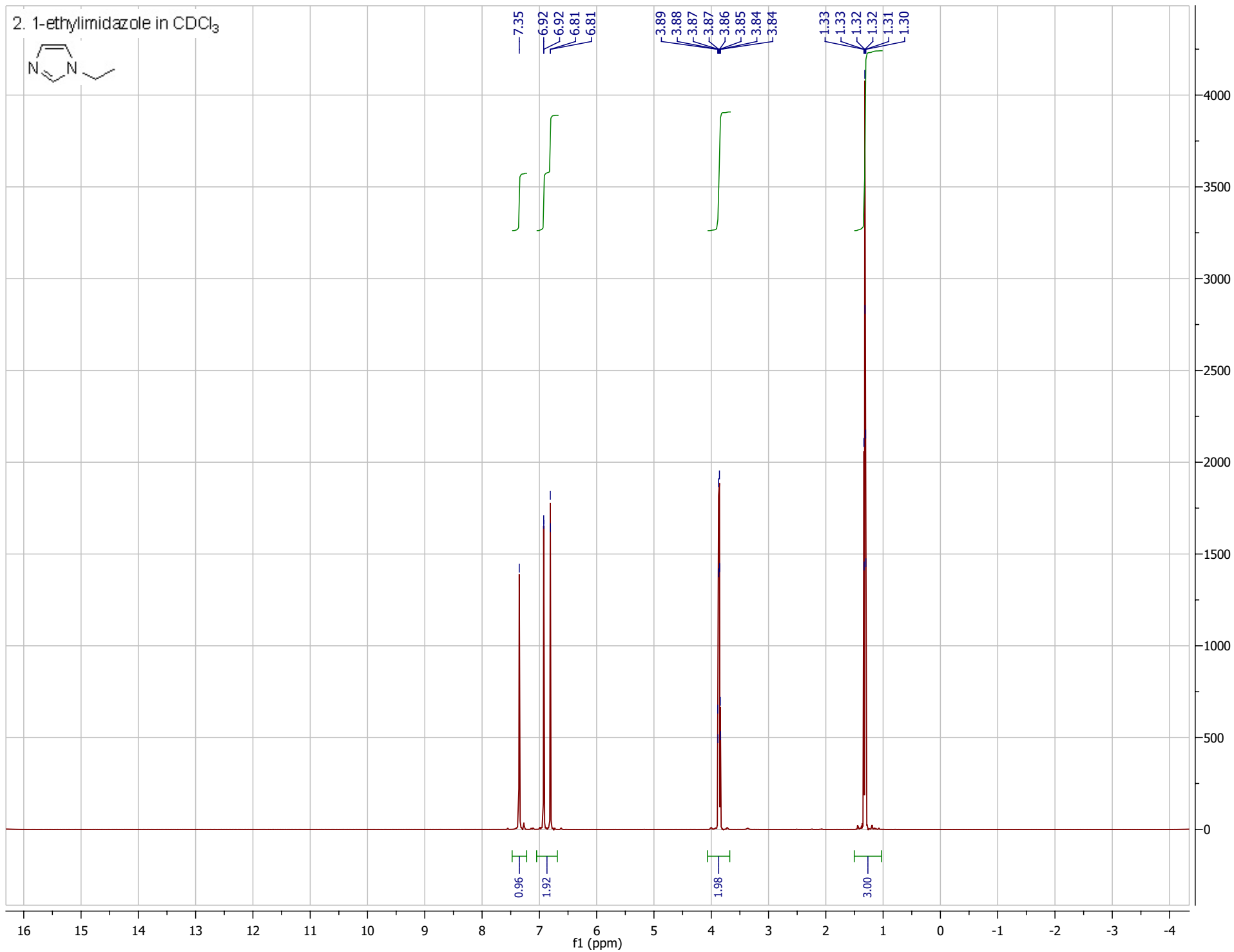
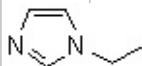
1,1'-[1,2-ethanediyilbis(oxy-2,1-ethanediyil)]bis(imidazole) (**20**): ^1H NMR (500 MHz, CDCl_3) δ 7.51 (s, 2H), 6.99 (d, $J = 41.8$ Hz, 4H), 4.07 (t, $J = 5.1$ Hz, 4H), 3.67 (t, $J = 5.1$ Hz, 4H), 3.52 (s, 4H).

1,1'-[oxybis(2,1-ethanediyloxy-2,1-ethanediyil)]bis(imidazole) (**21**): ^1H NMR (500 MHz, CDCl_3) δ 7.49 (s, 2H), 7.09 – 6.78 (m, 4H), 4.06 (t, $J = 5.2$ Hz, 4H), 3.69 (dd, $J = 7.2, 3.1$ Hz, 4H), 3.53 (d, $J = 1.3$ Hz, 8H).

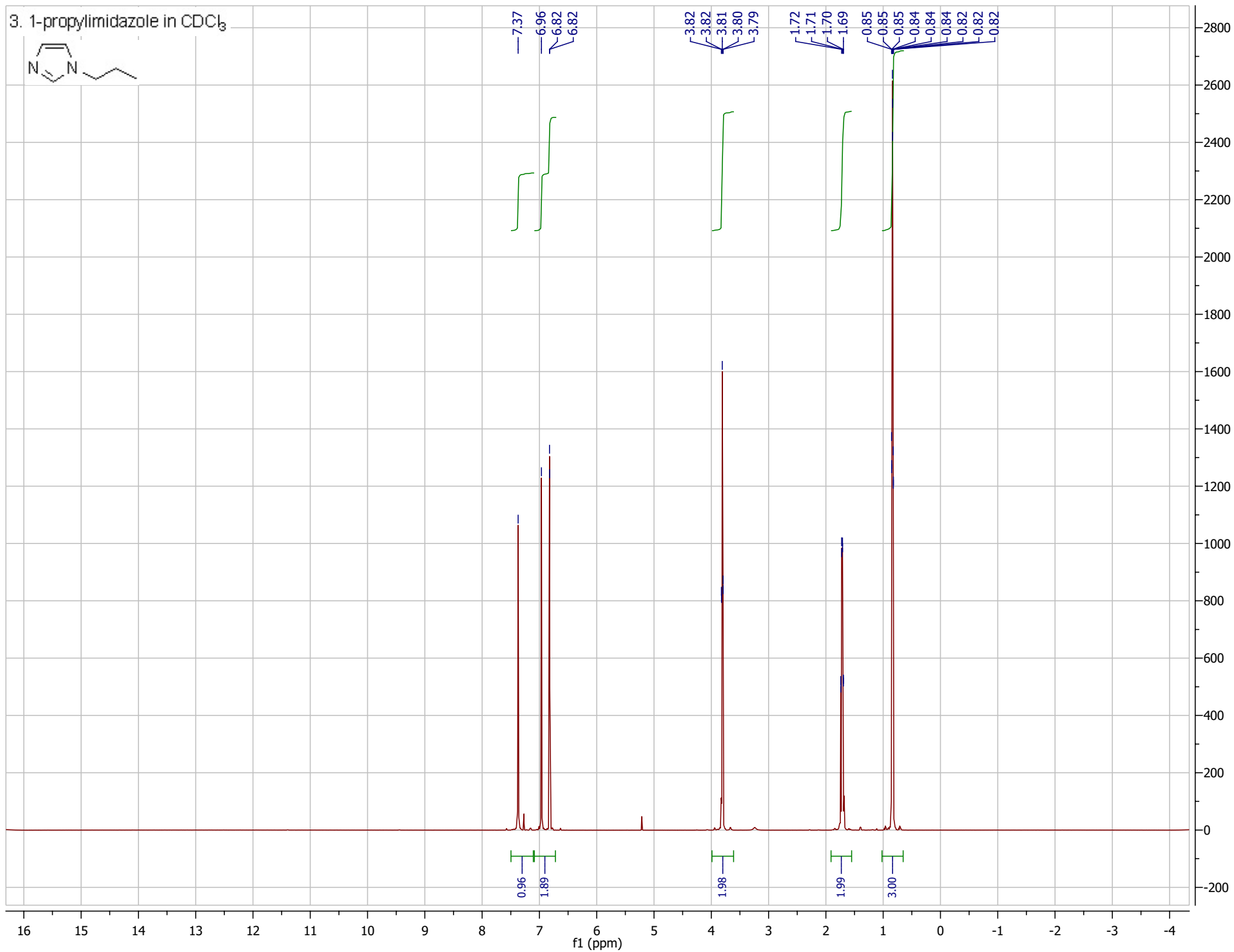
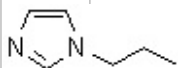
1. Sodium Imidazolate in DMSO-d6 + TMS



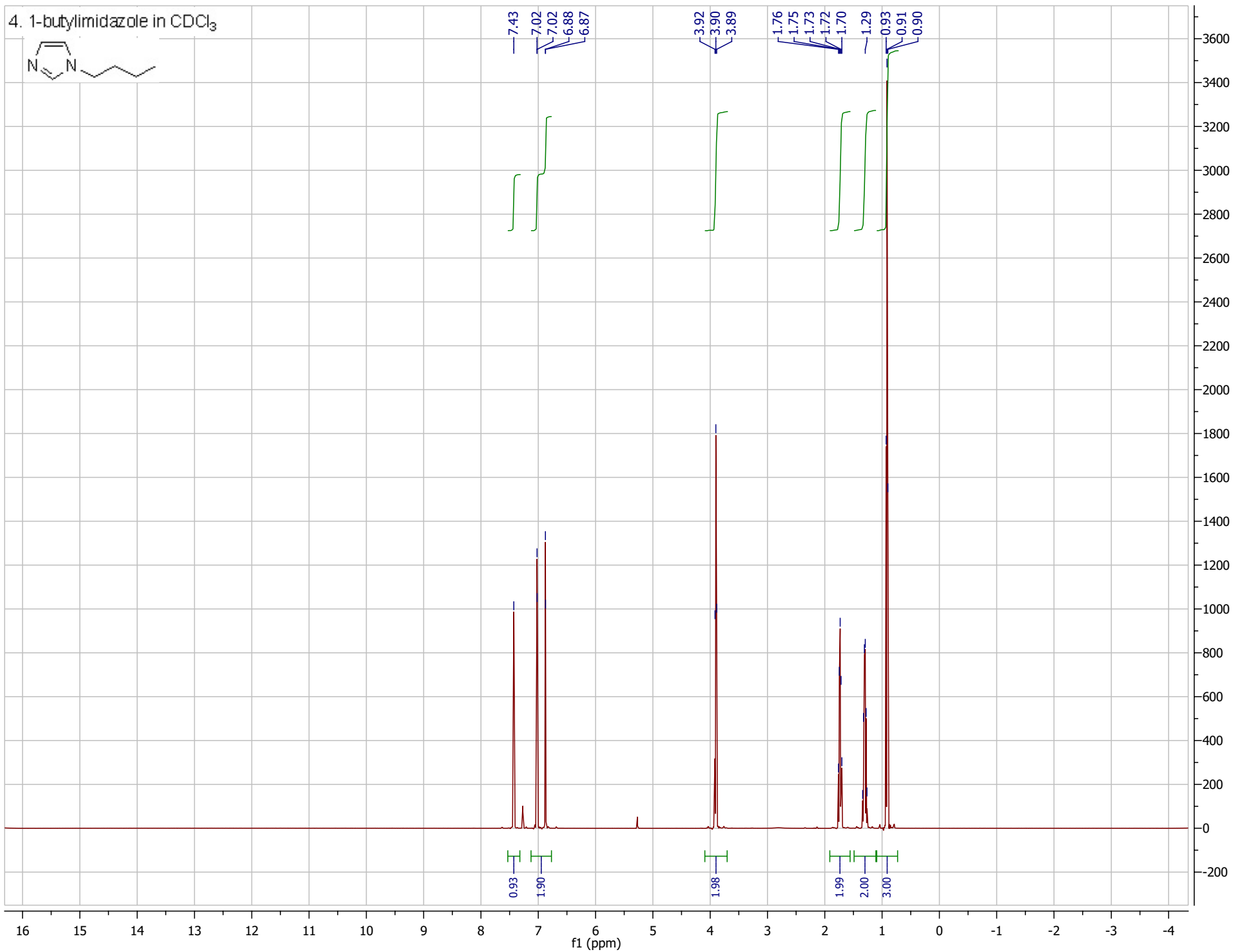
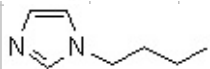
2. 1-ethylimidazole in CDCl₃



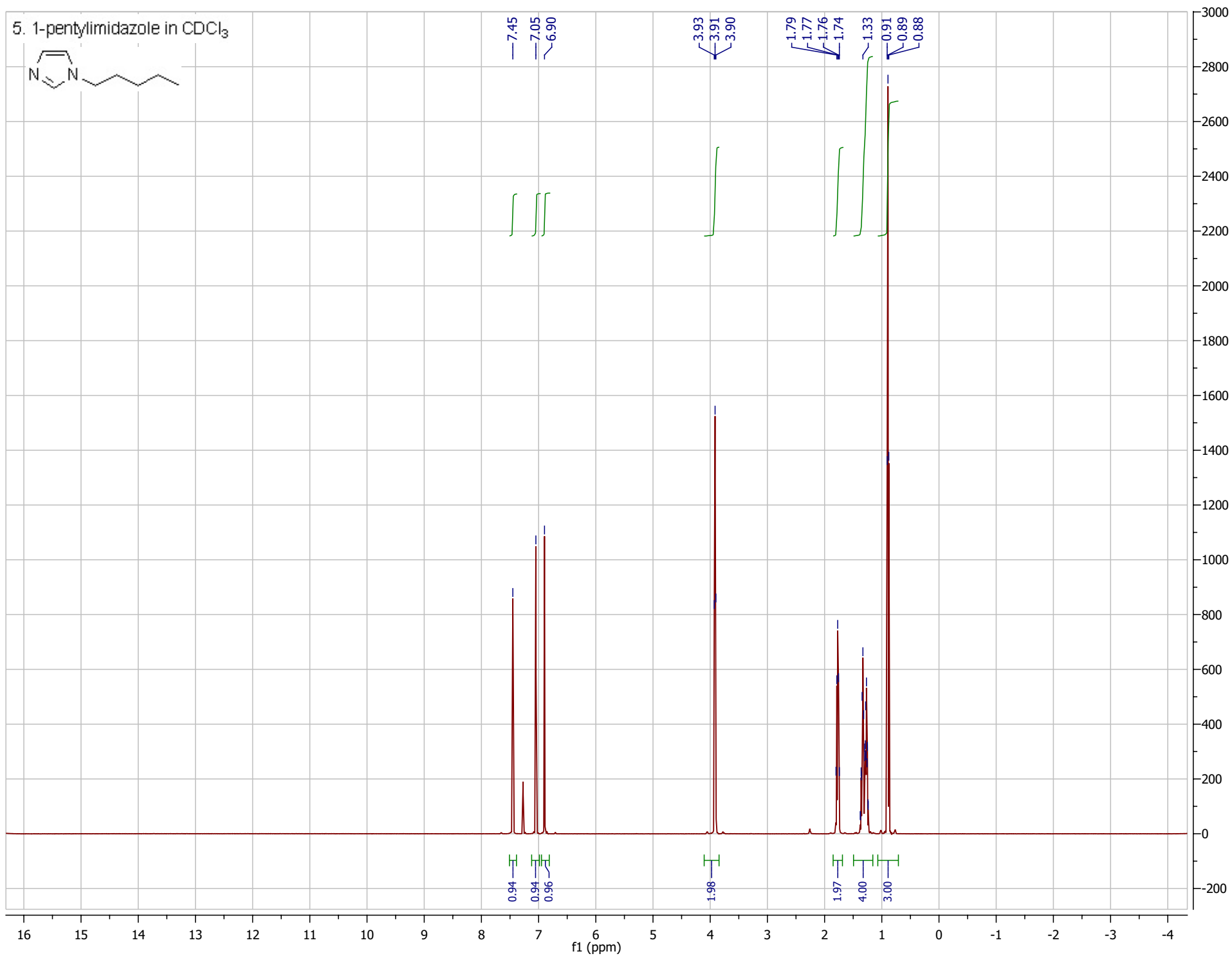
3. 1-propylimidazole in CDCl₃



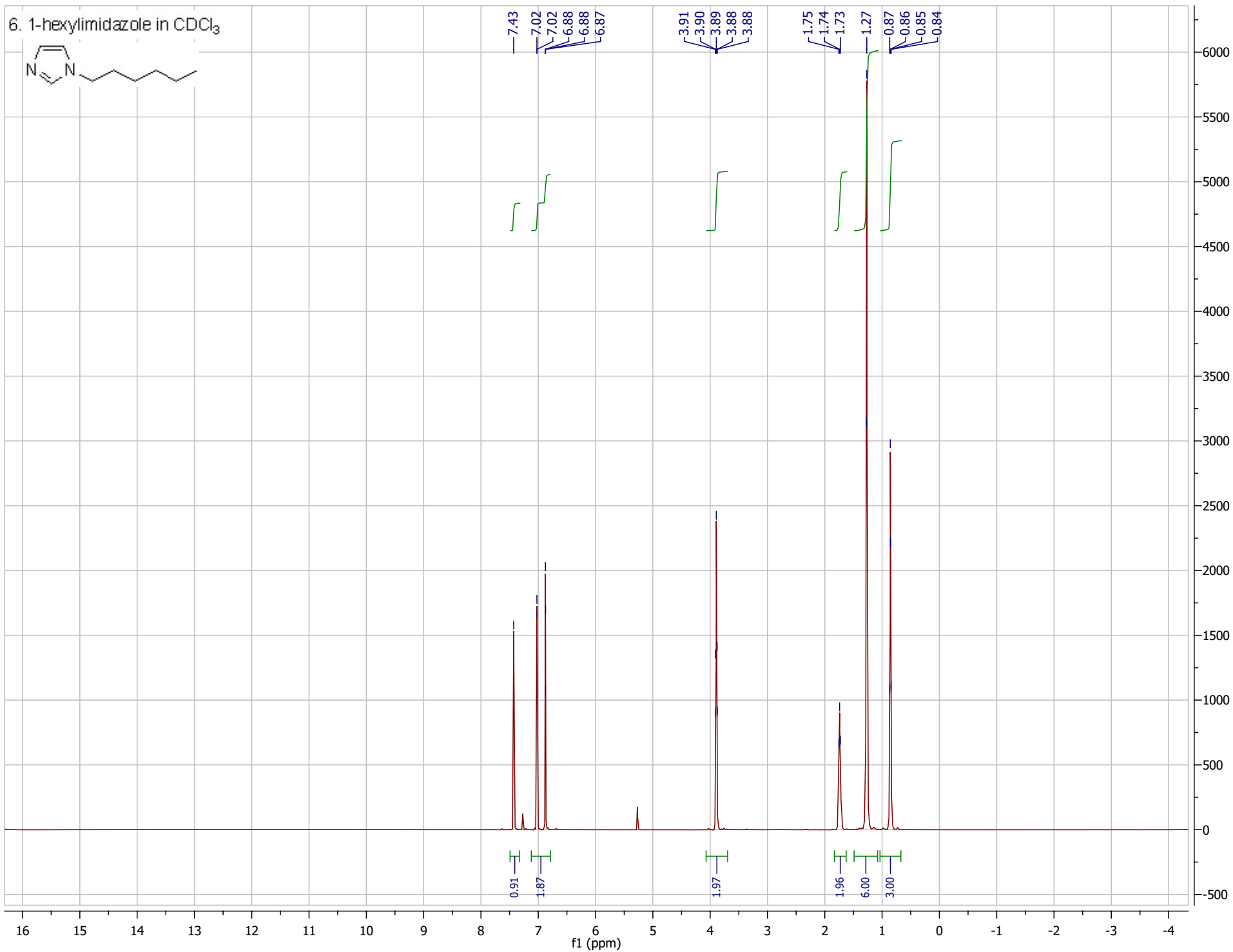
4. 1-butylimidazole in CDCl₃



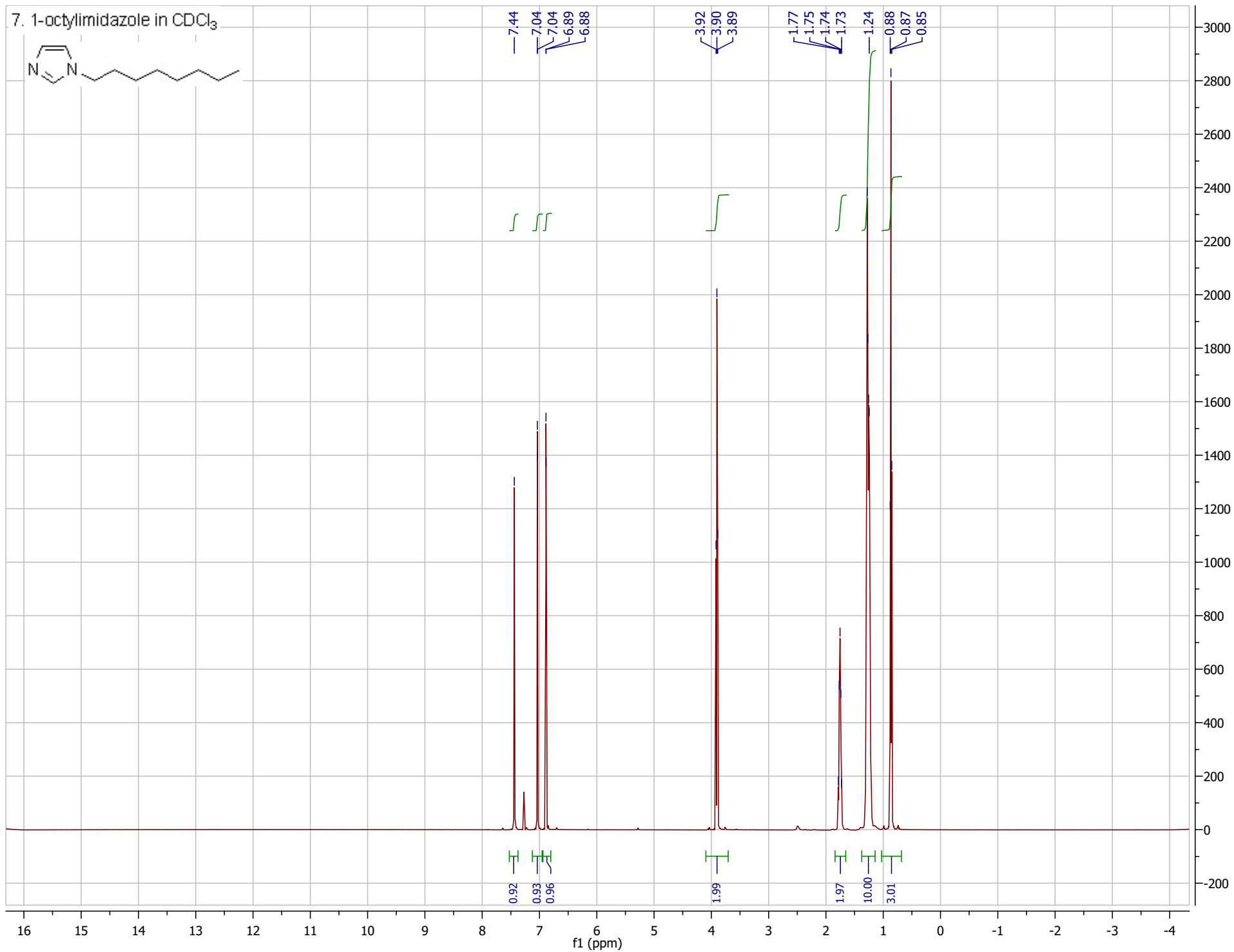
5. 1-pentylimidazole in CDCl_3



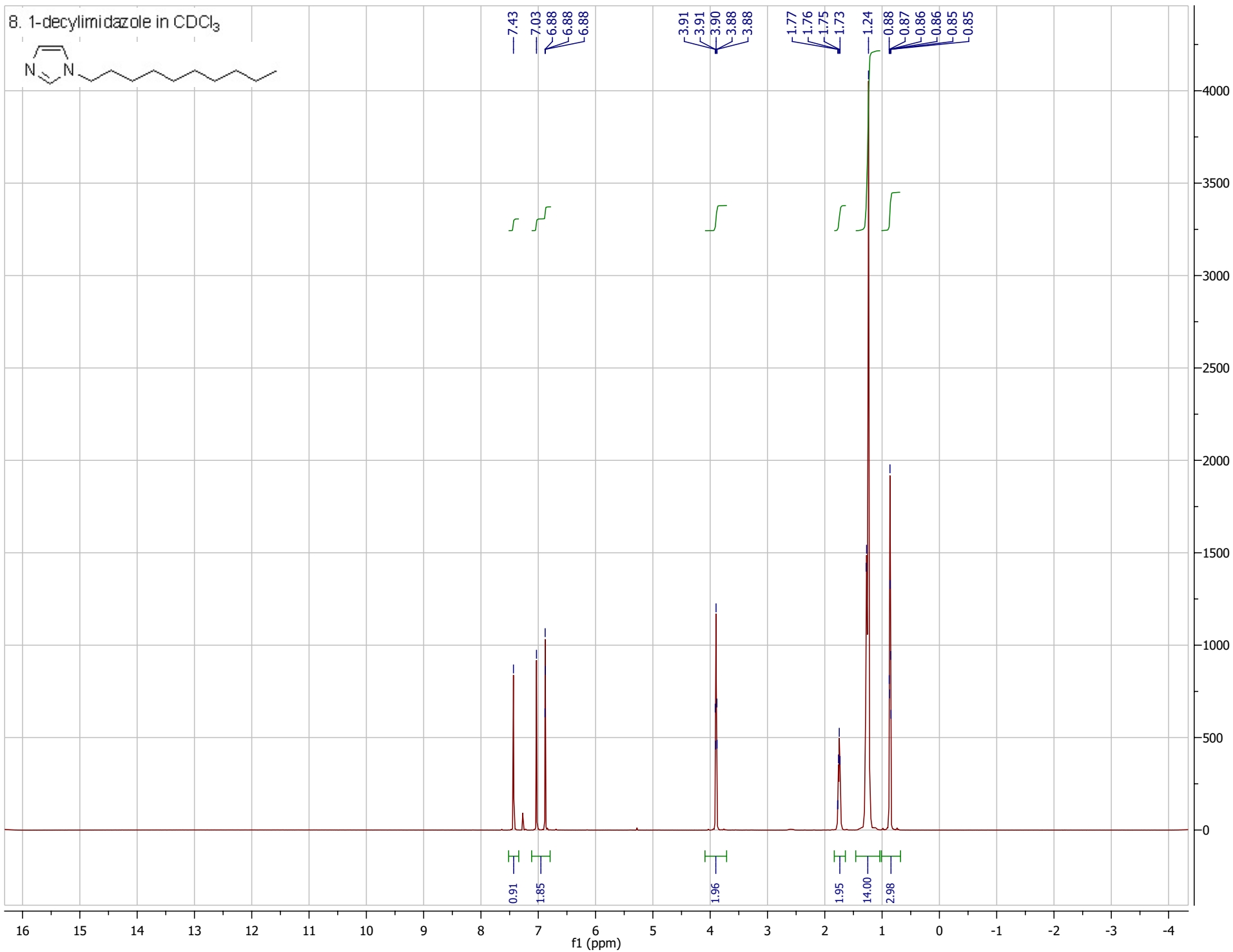
6. 1-hexylimidazole in CDCl₃



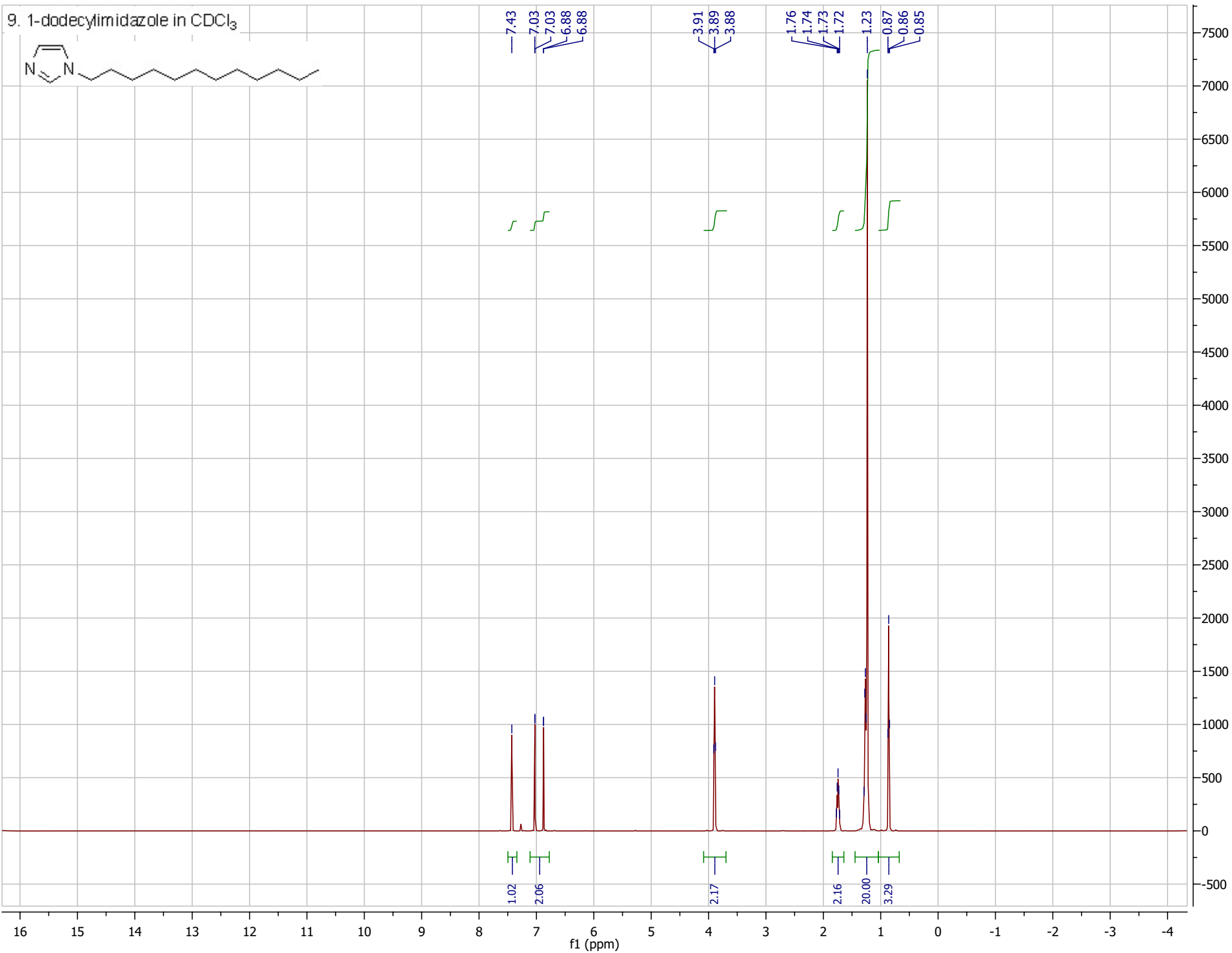
7. 1-octylimidazole in CDCl₃



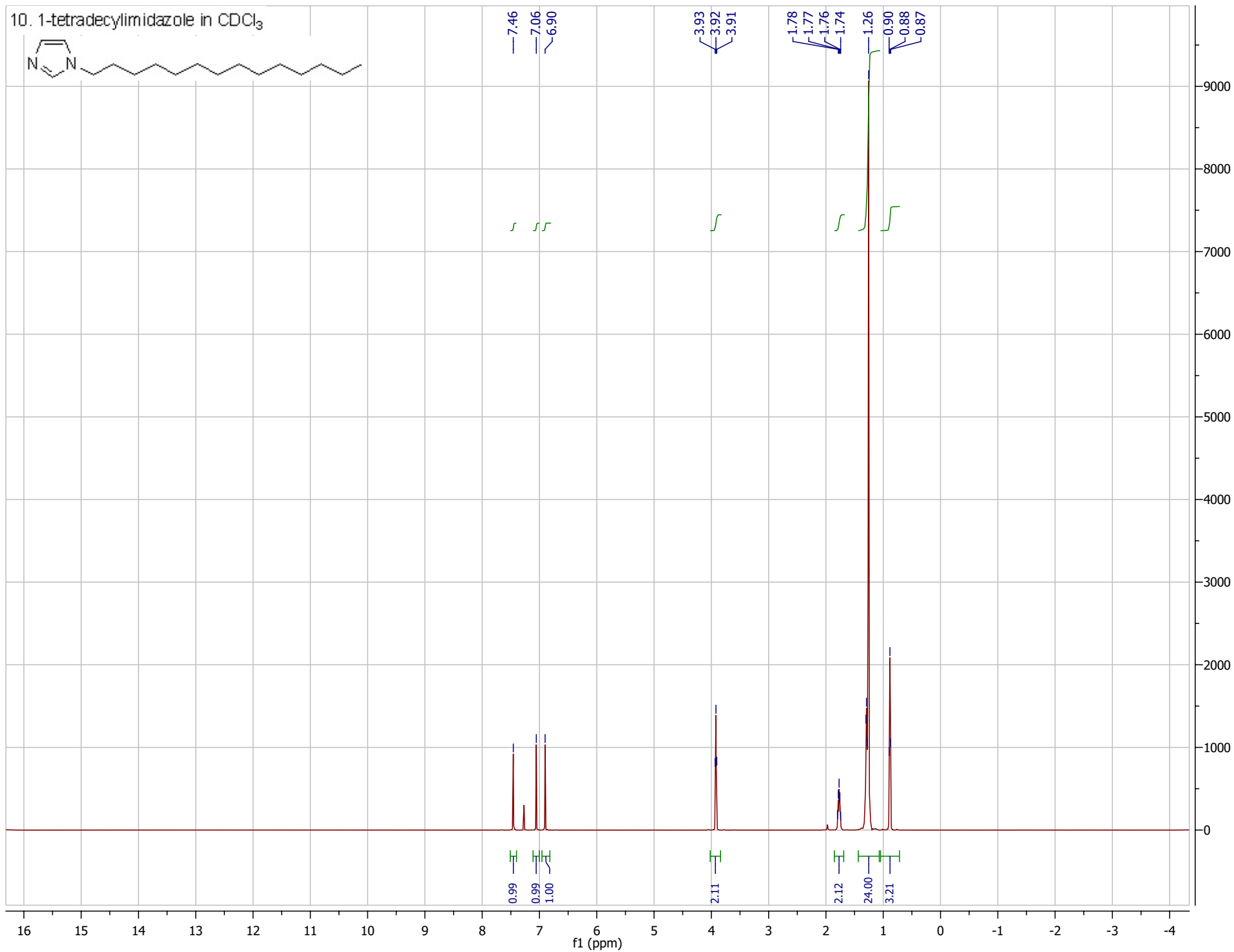
8. 1-decylimidazole in CDCl₃



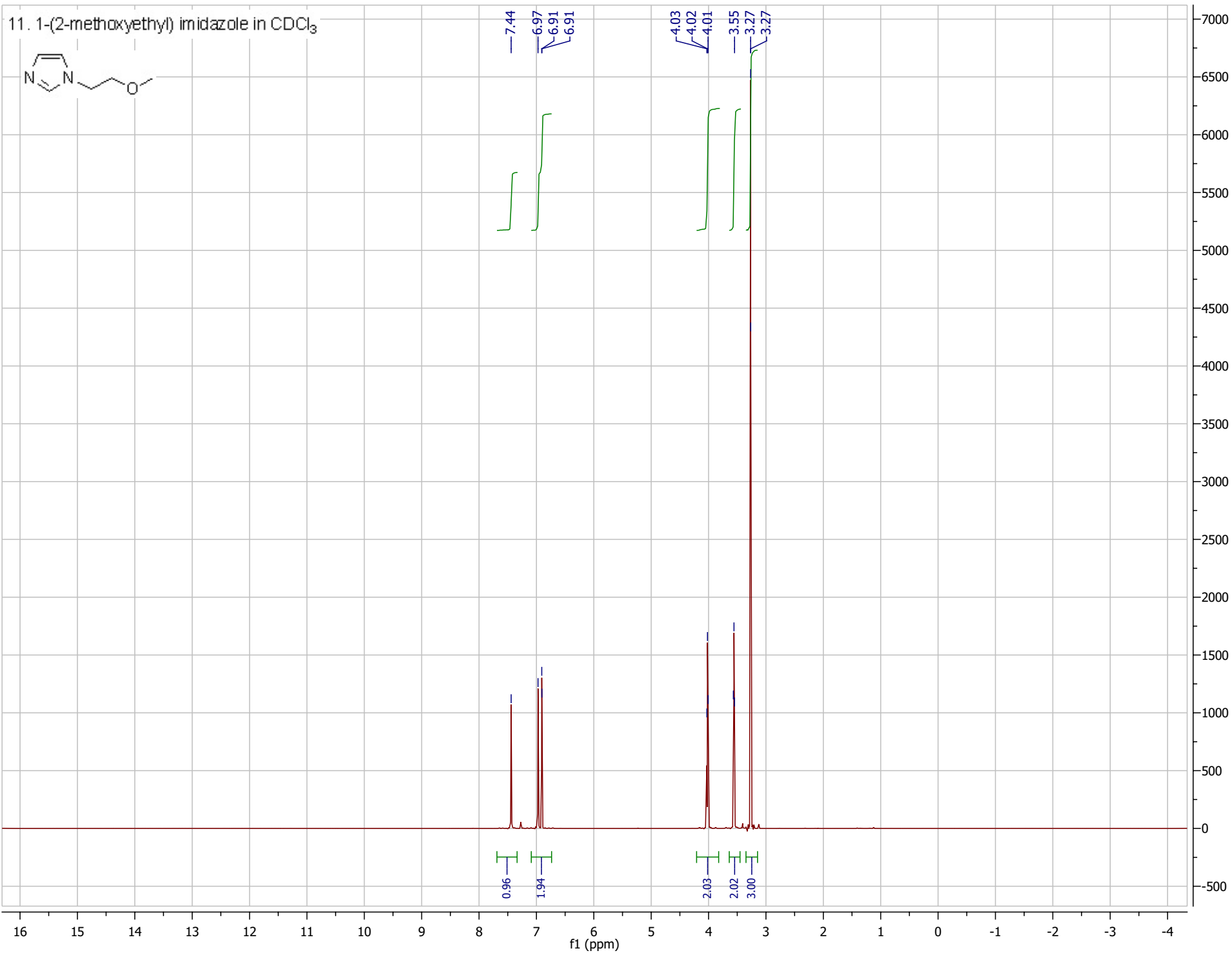
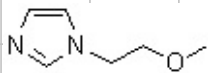
9. 1-dodecylimidazole in CDCl₃



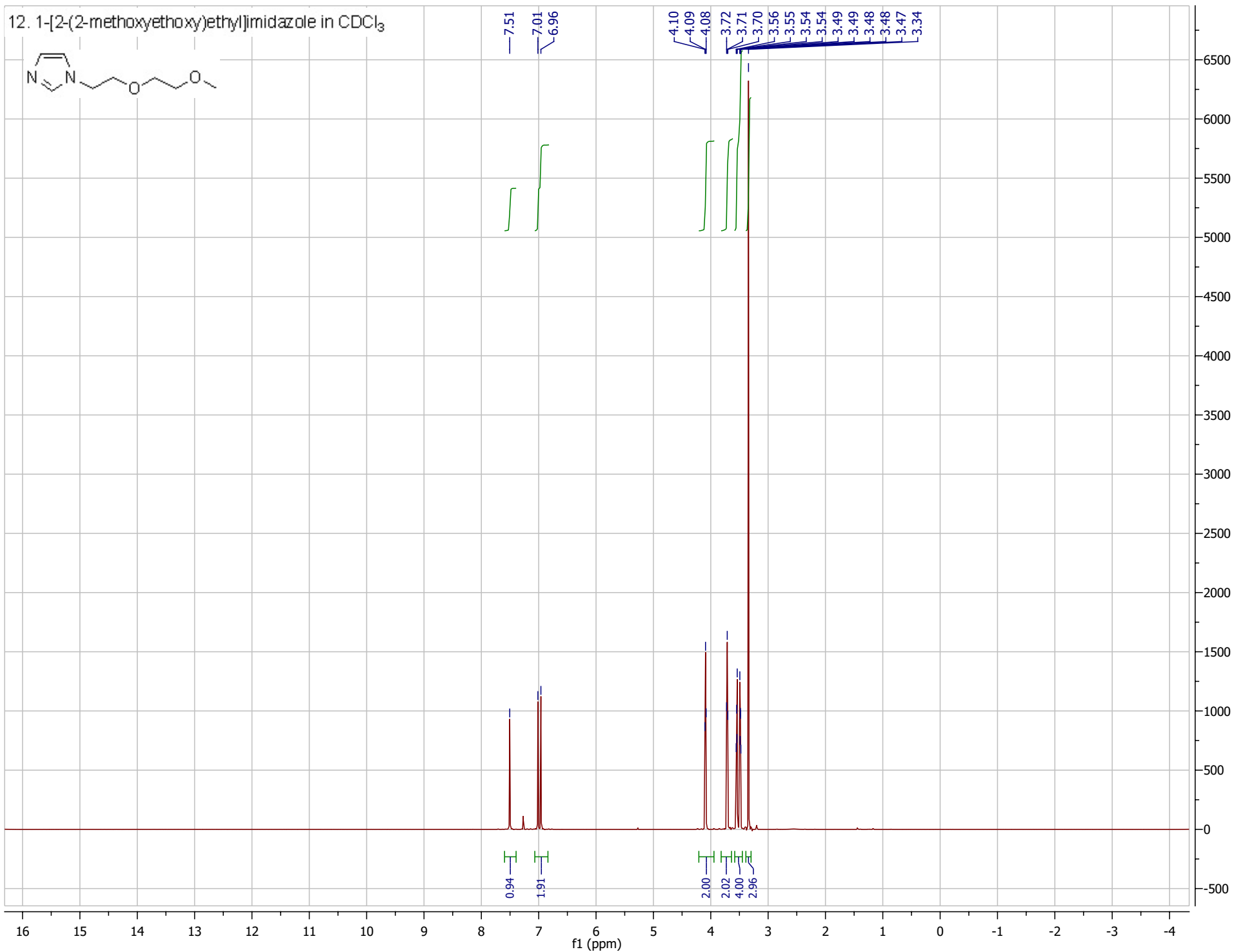
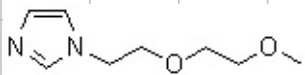
10. 1-tetradecylimidazole in CDCl₃



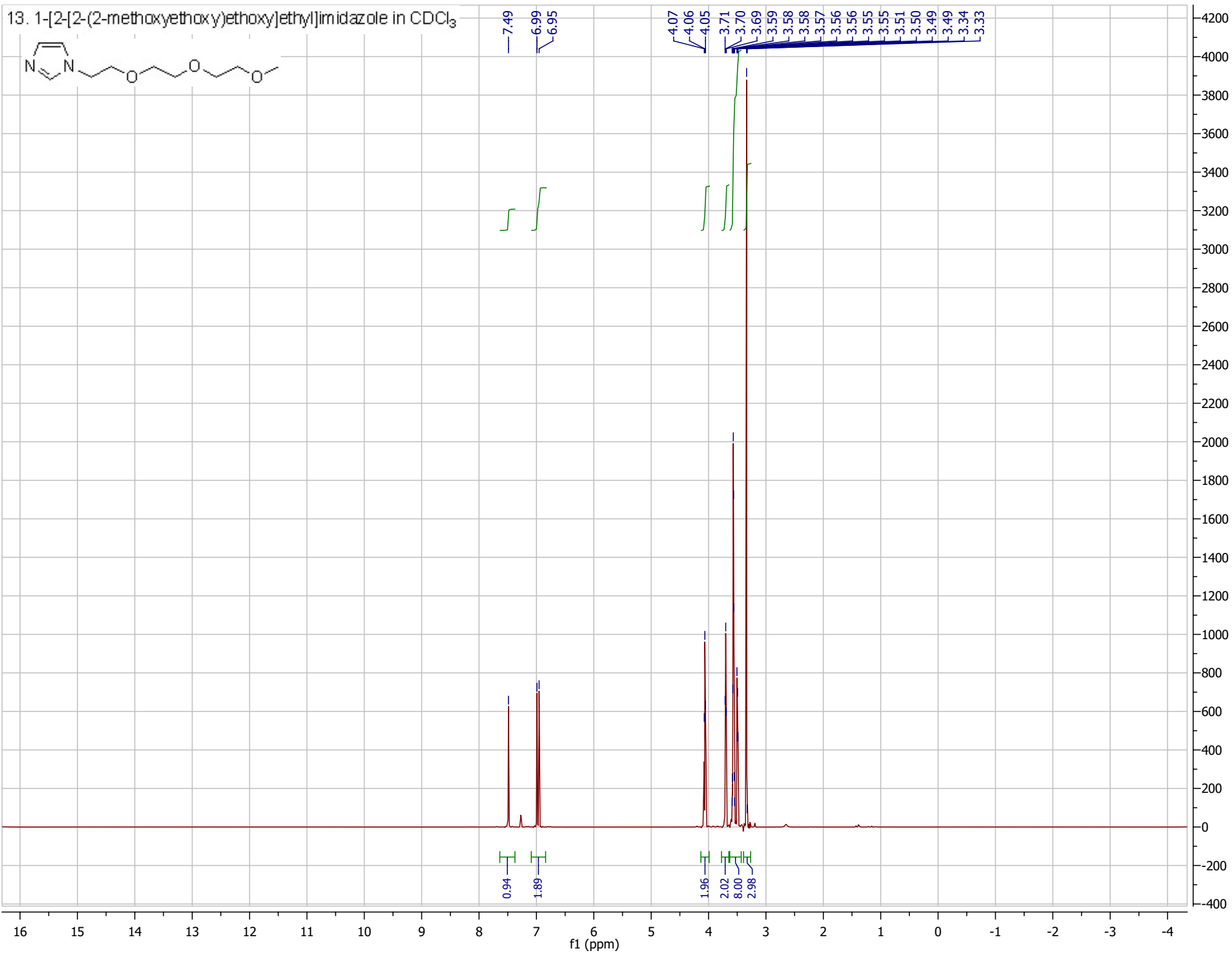
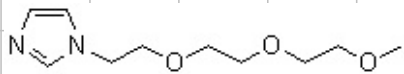
11. 1-(2-methoxyethyl) imidazole in CDCl₃



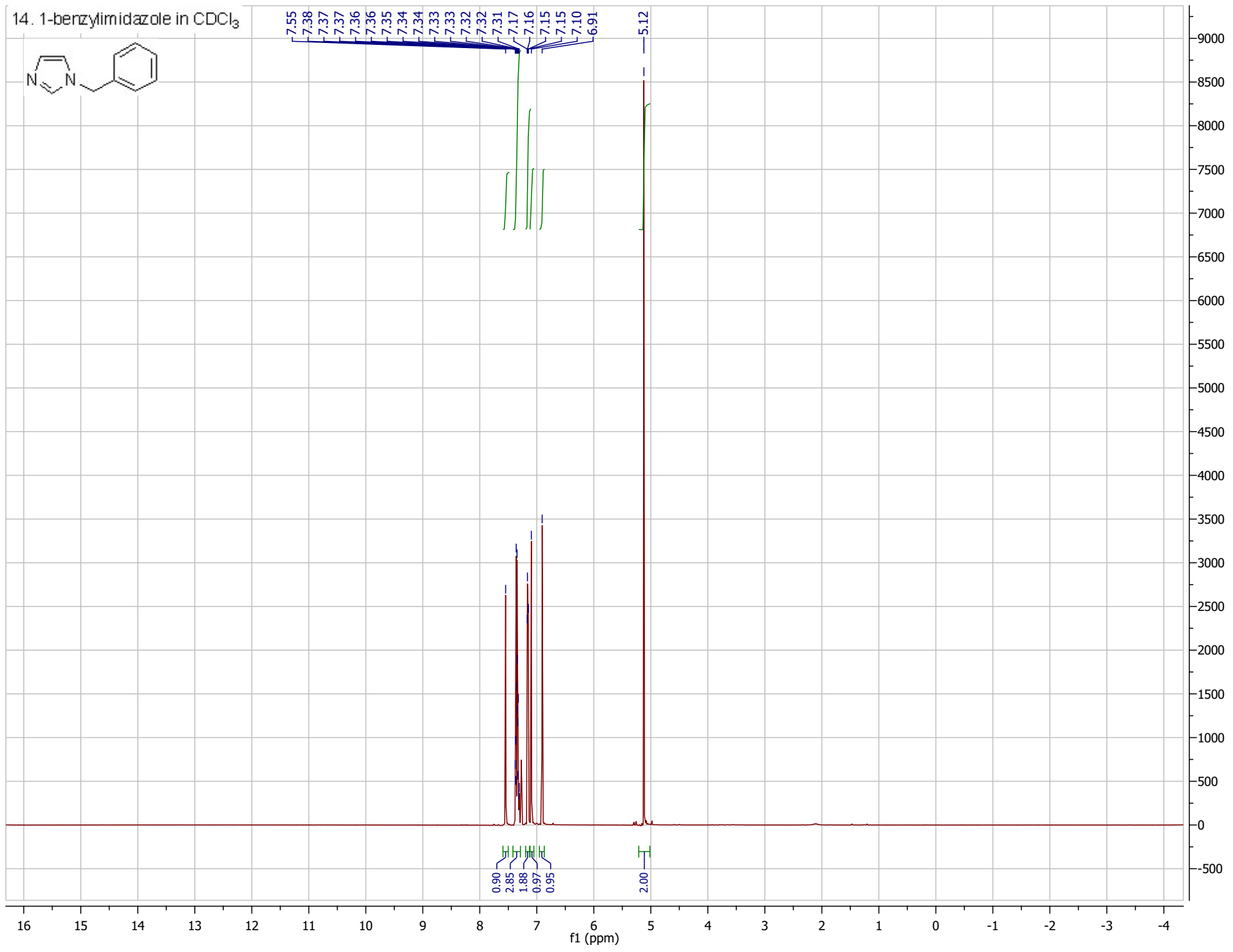
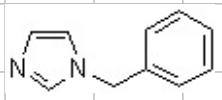
12. 1-[2-(2-methoxyethoxy)ethyl]imidazole in CDCl₃



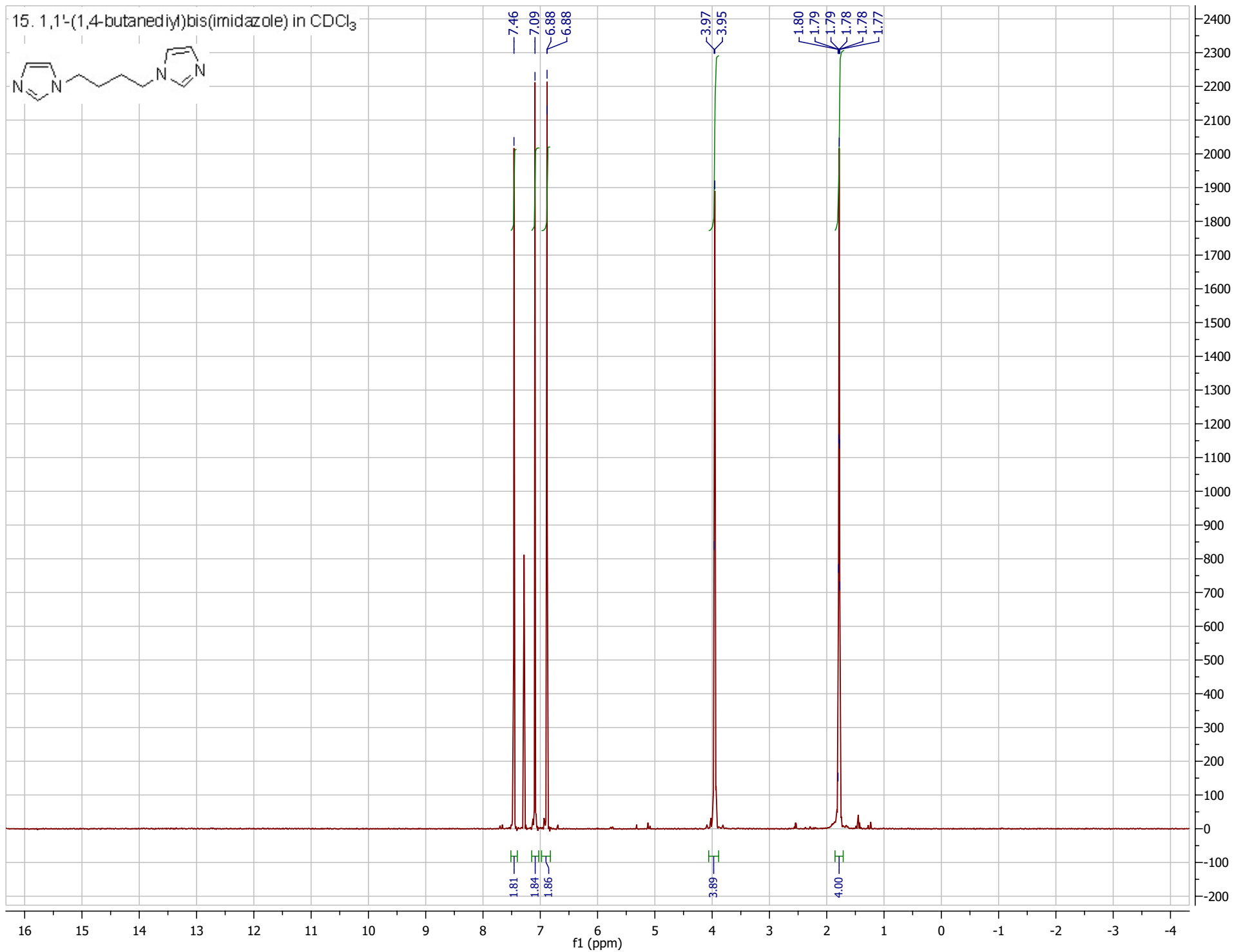
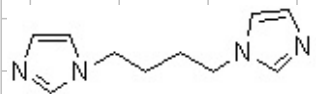
13. 1-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]imidazole in CDCl₃



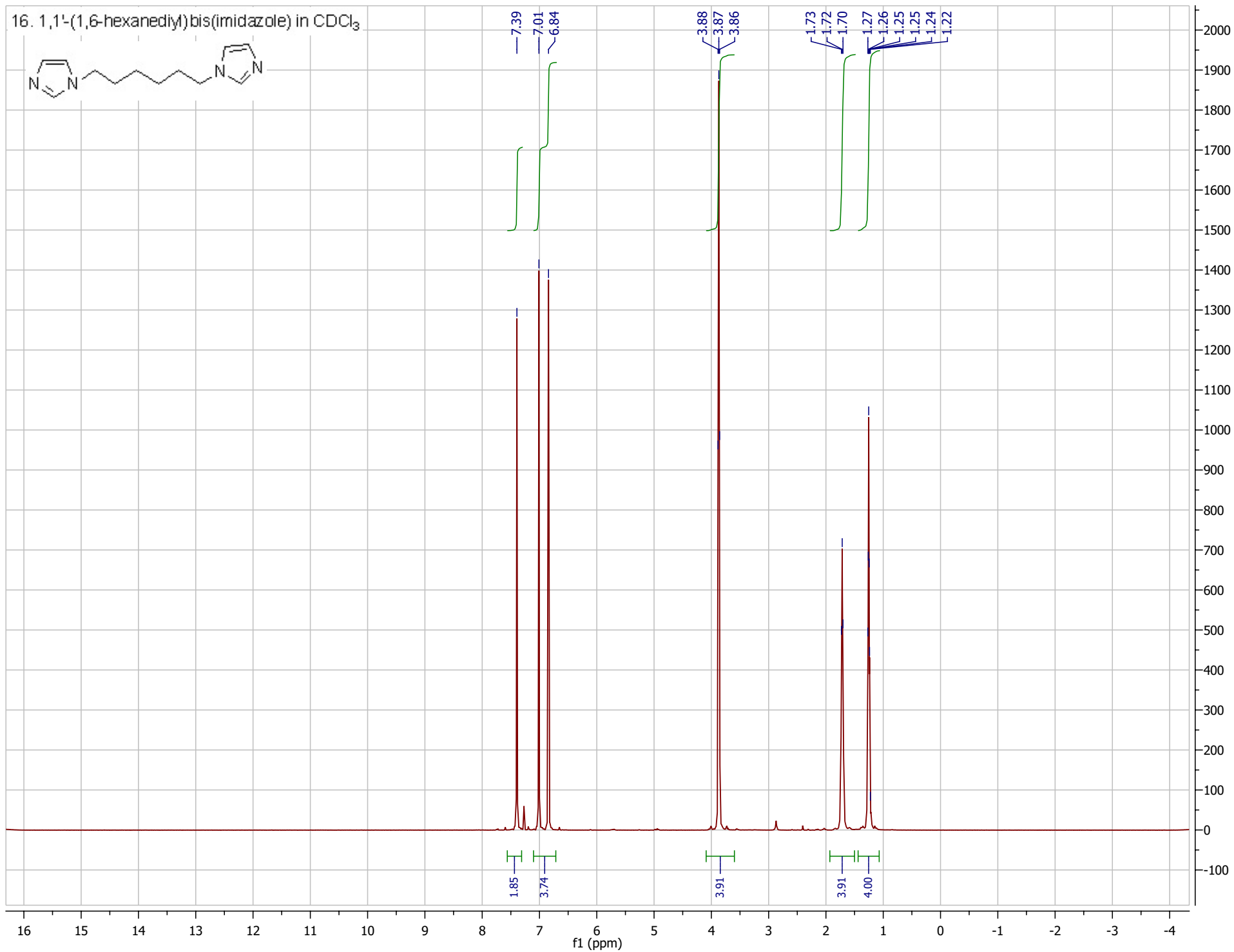
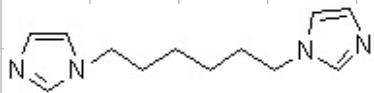
14. 1-benzylimidazole in CDCl₃



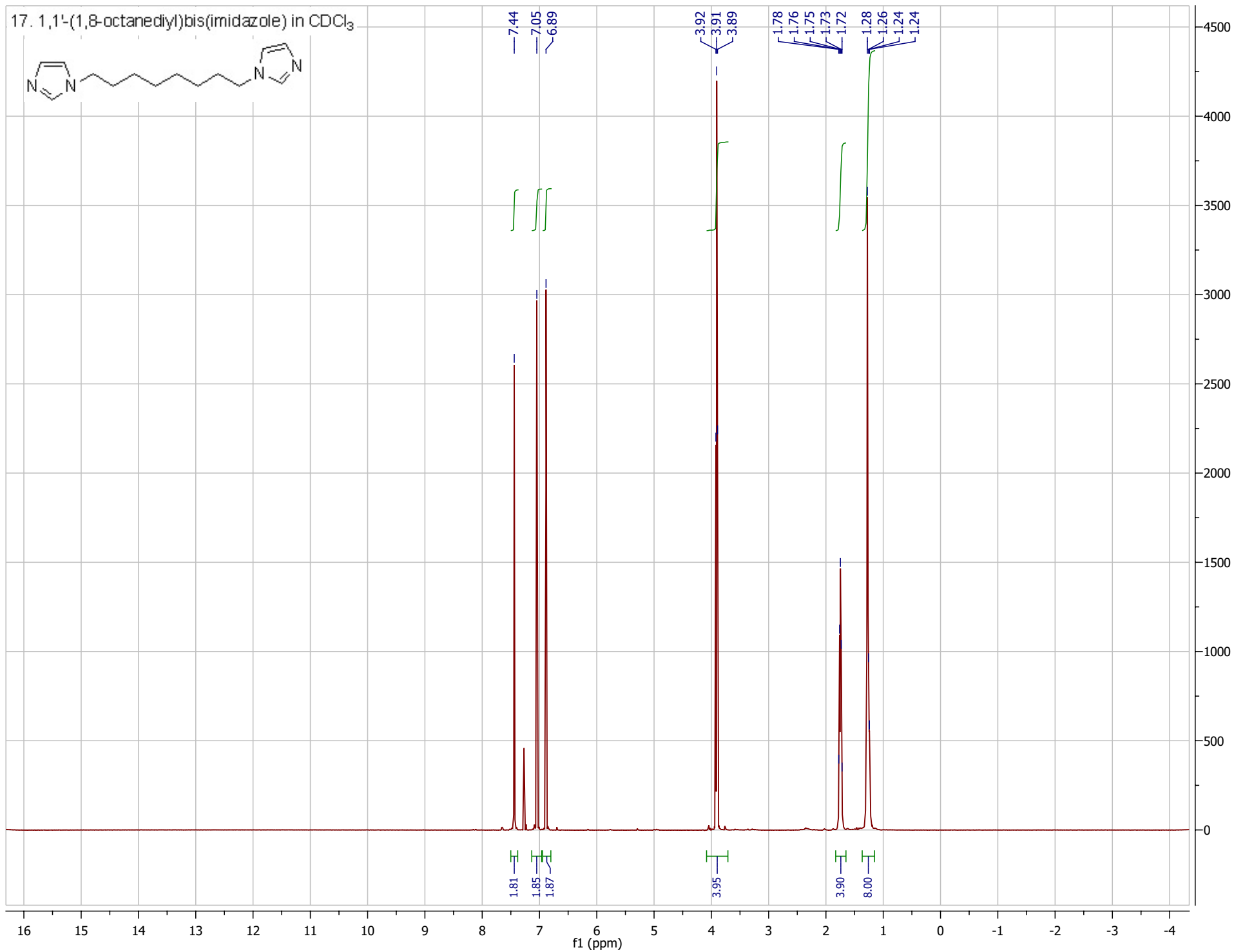
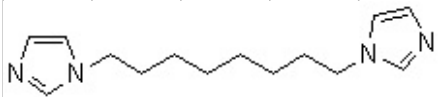
15. 1,1'-(1,4-butanediyl)bis(imidazole) in CDCl₃



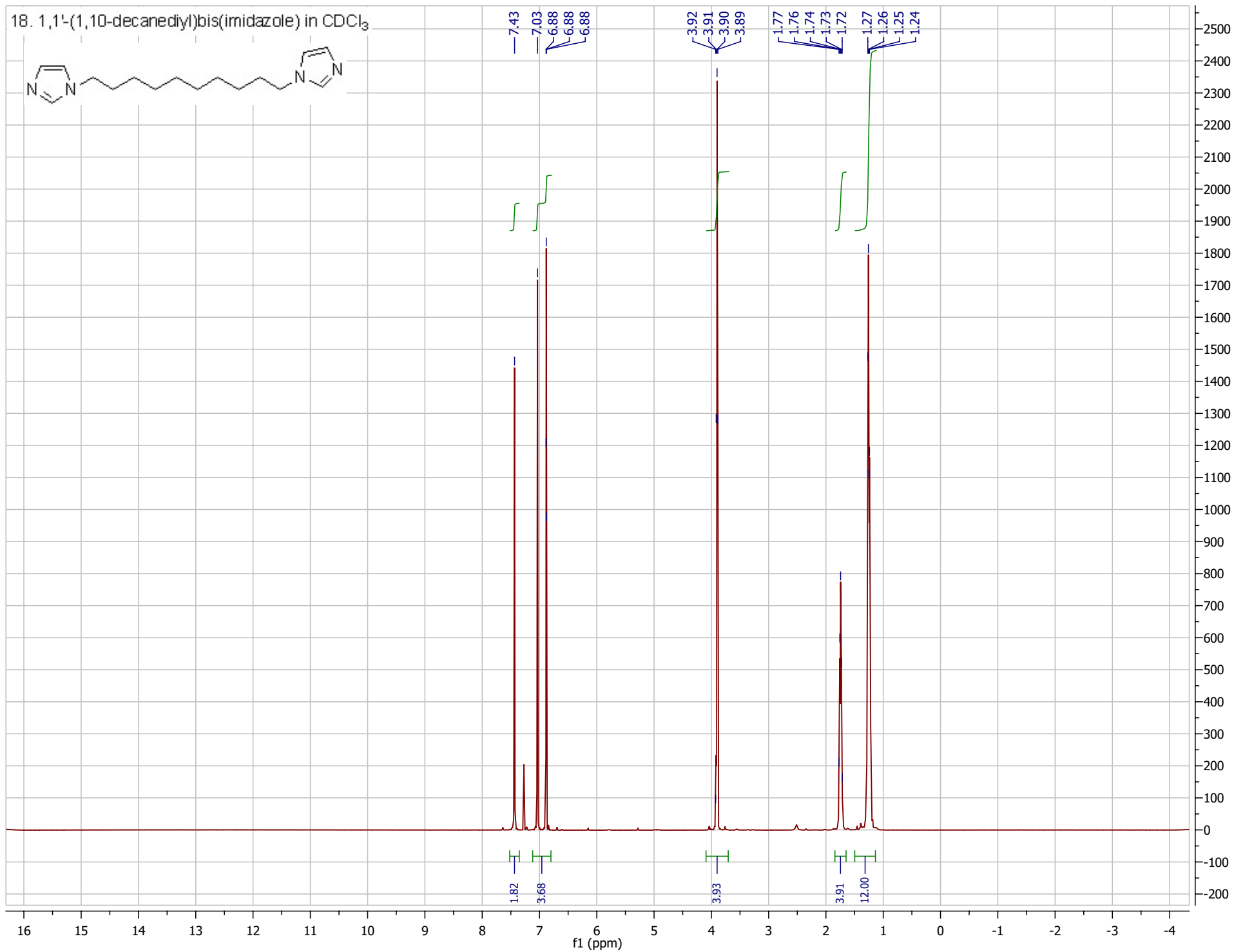
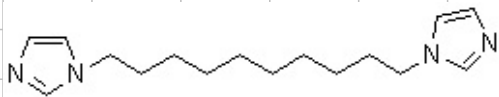
16. 1,1'-(1,6-hexanediyl)bis(imidazole) in CDCl₃



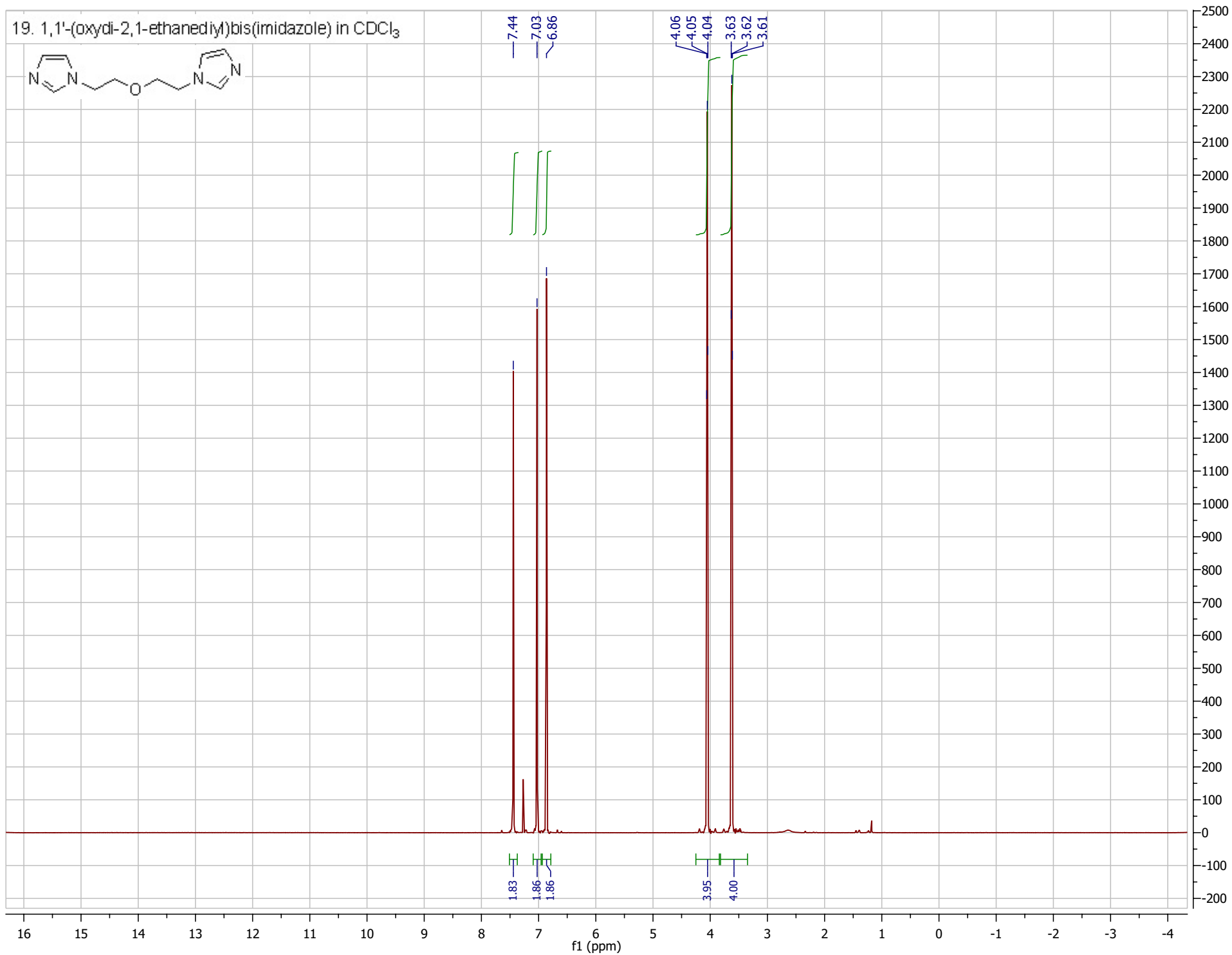
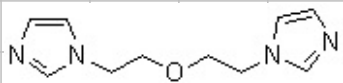
17. 1,1'-(1,8-octanediyl)bis(imidazole) in CDCl₃



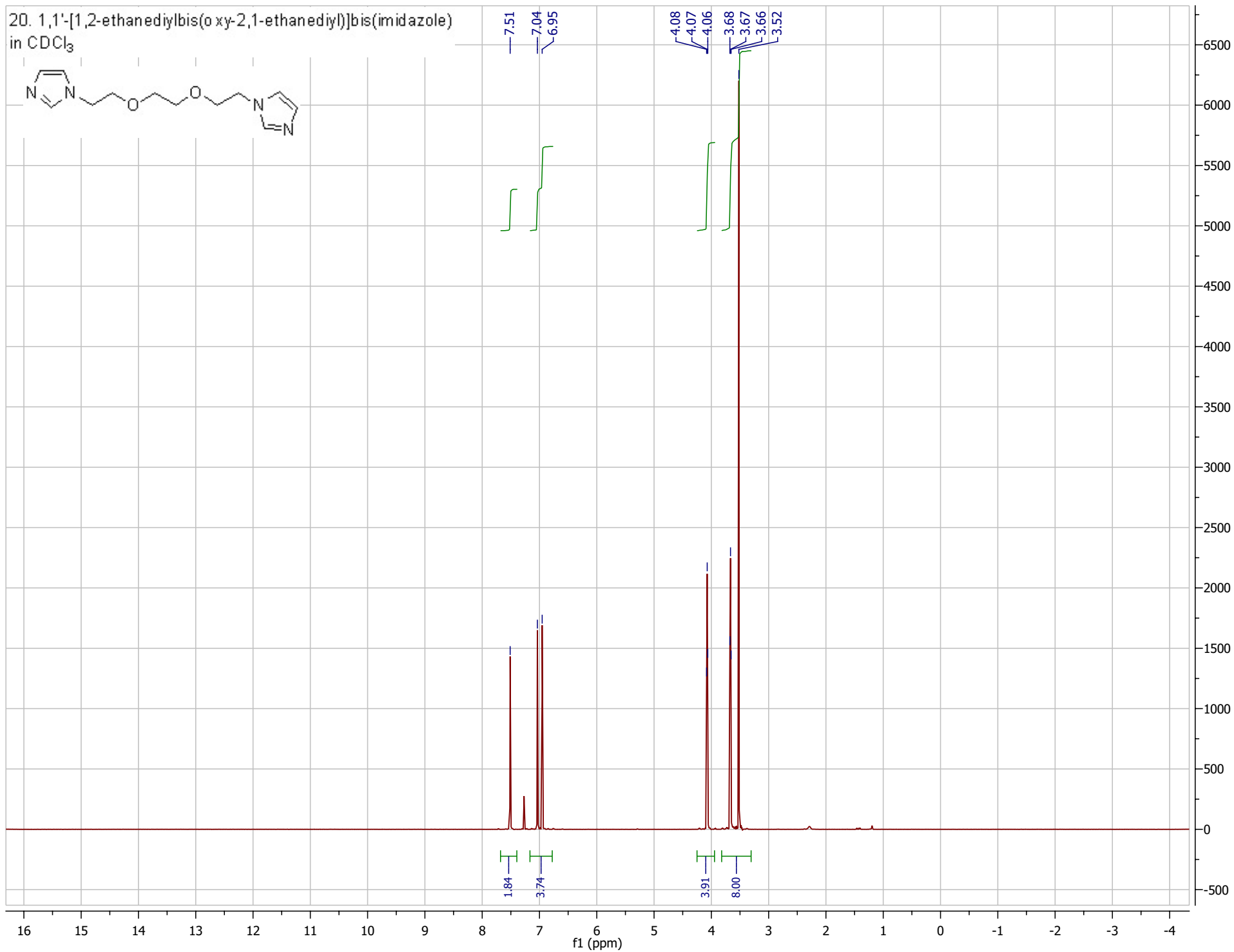
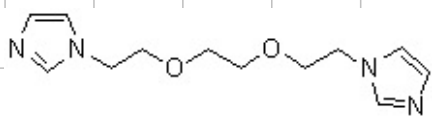
18. 1,1'-(1,10-decanediyl)bis(imidazole) in CDCl₃



19. 1,1'-(oxydi-2,1-ethanediy)bis(imidazole) in CDCl₃



20. 1,1'-[1,2-ethanediylbis(o xy-2,1-ethanediyl)]bis(imidazole)
in CDCl₃



21. 1,1'-[oxybis(2,1-ethanedioxy-2,1-ethanedioyl)]bis(imidazole)
in CDCl₃

