Supplementary Material (ESI) for Green Chemistry


# Supplementary Information

# Non-occurrence of a Zincke-like process upon treatment of 1-(2,4-dinitrophenyl)-3-methylimidazolium chloride with a chiral primary amine.

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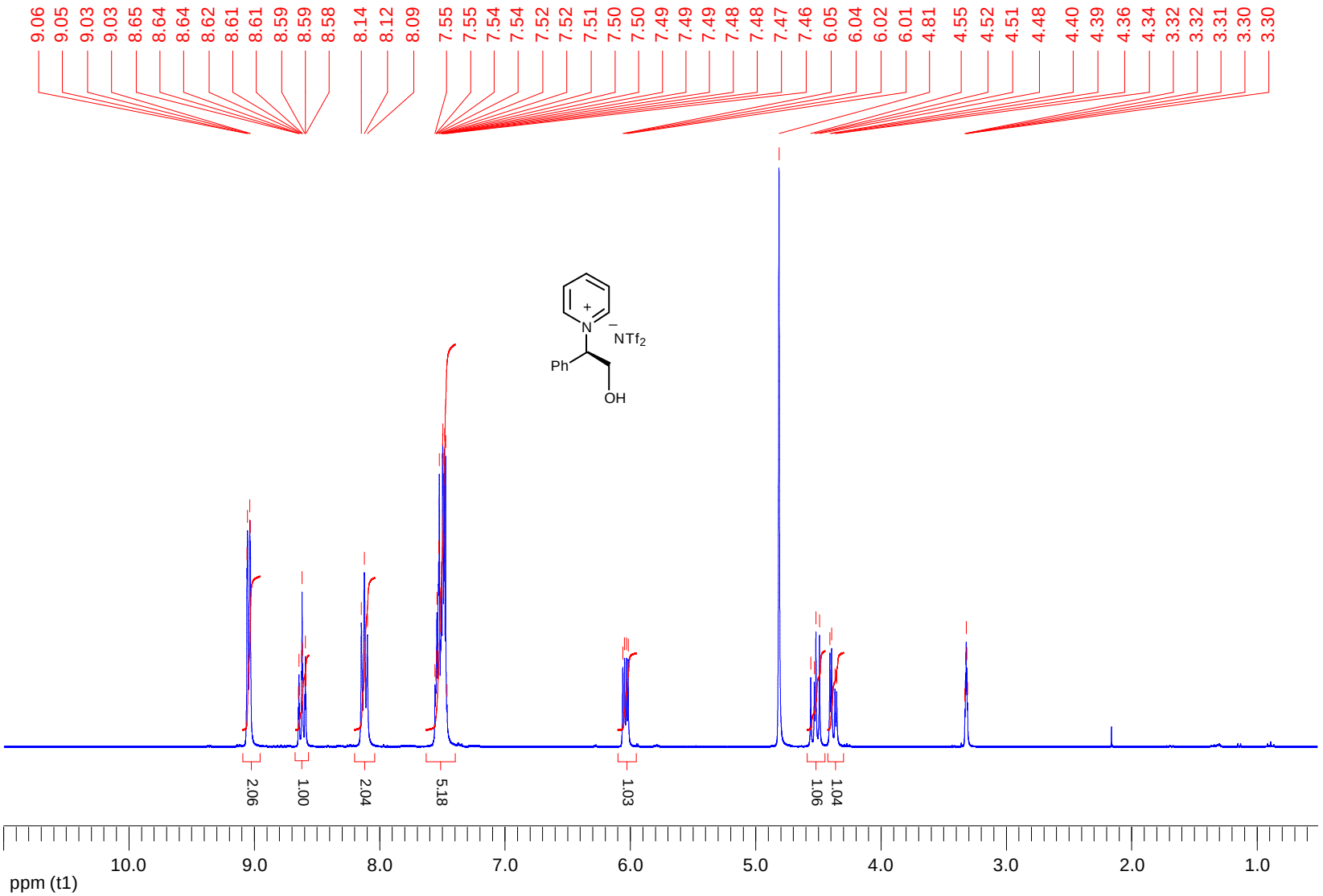
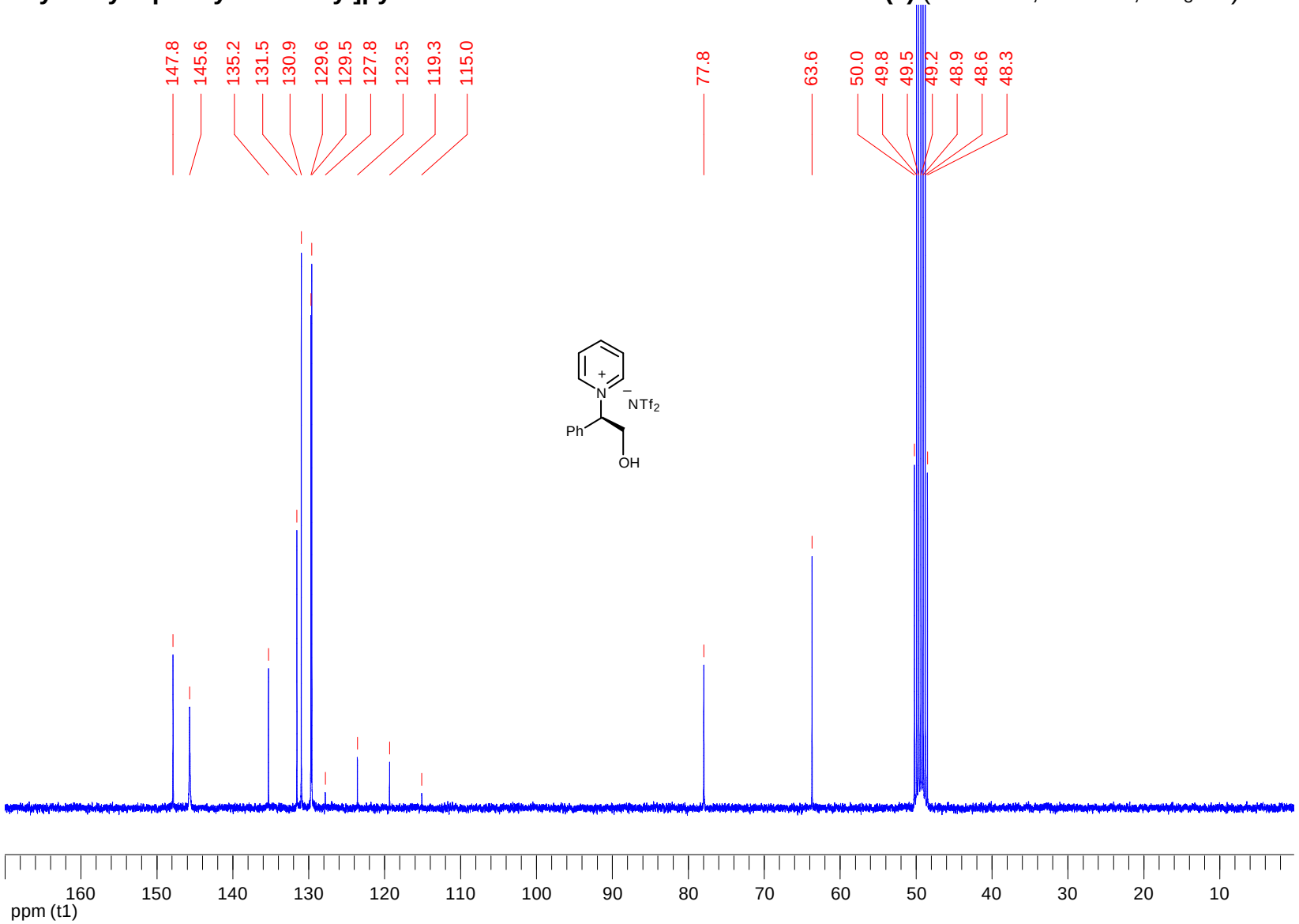
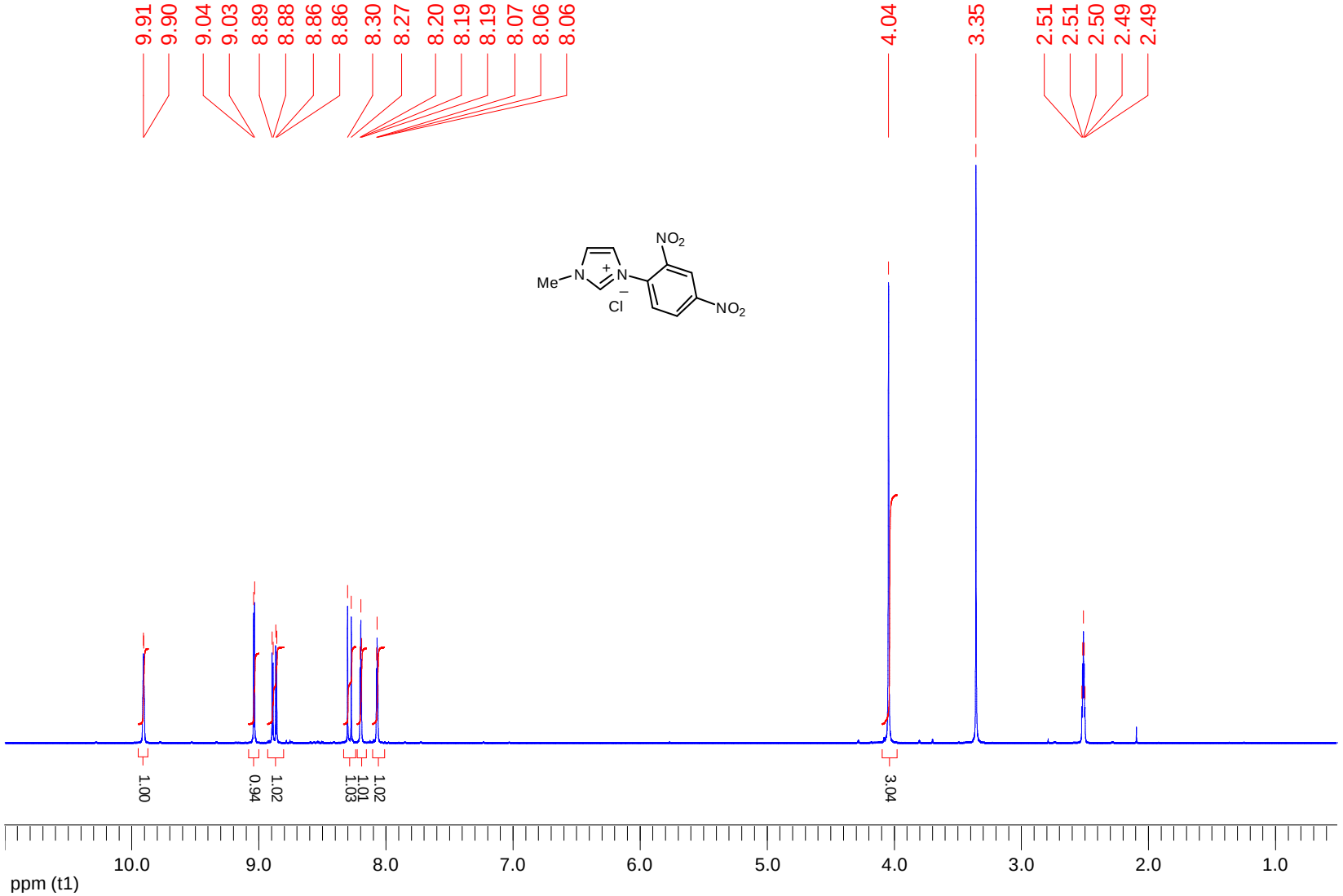
**1-[(2*R*)-1-hydroxy-2-phenyl-2-ethanyl]pyridinium bistrifluoromethanesulfonimide (3)** ($^1$H NMR, 300 MHz, $CD_3OD$).



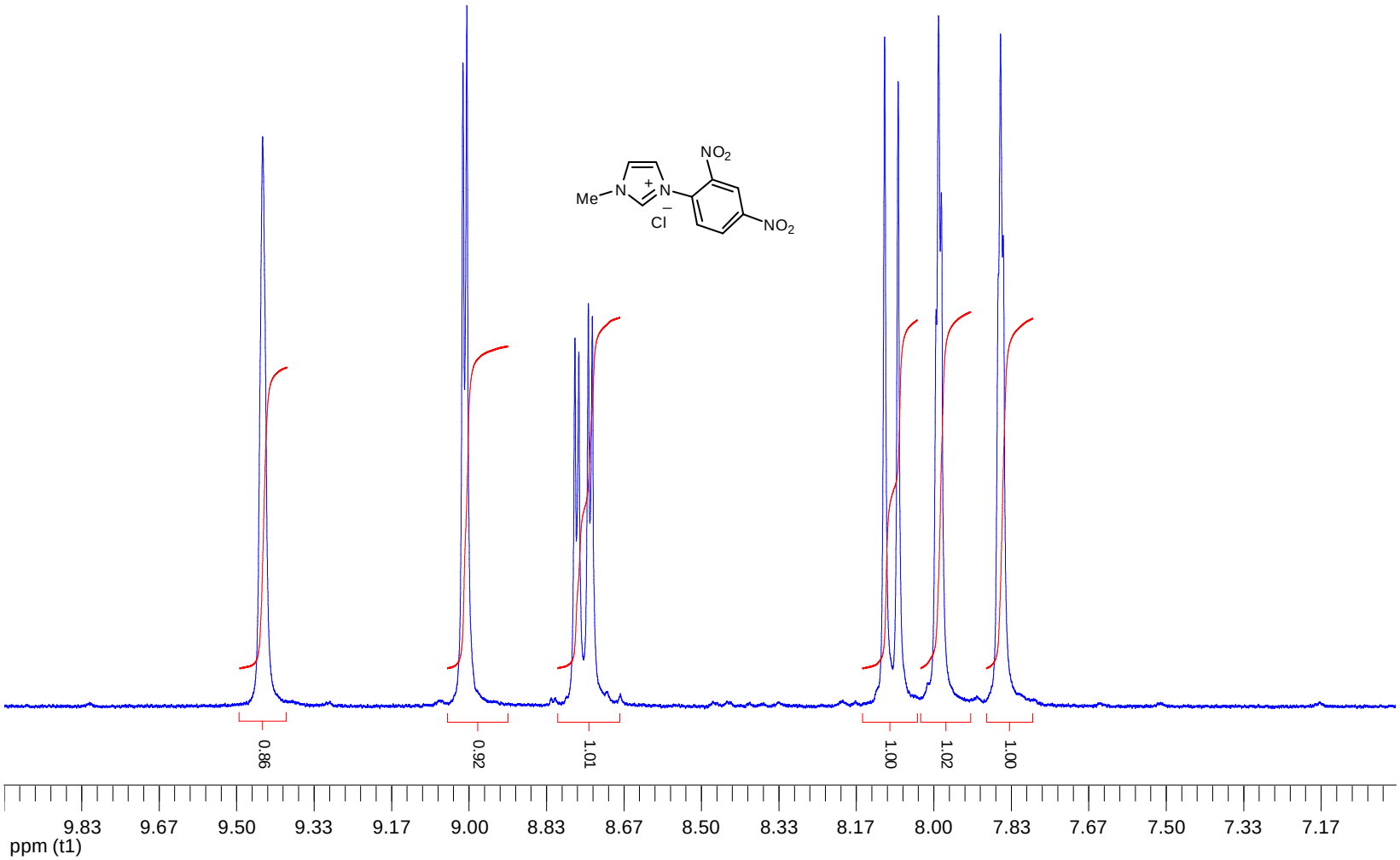
**1-[(2*R*)-1-hydroxy-2-phenyl-2-ethanyl]pyridinium bistrifluoromethanesulfonimide (3)** ($^{13}$C NMR, 75 MHz, $CD_3OD$).



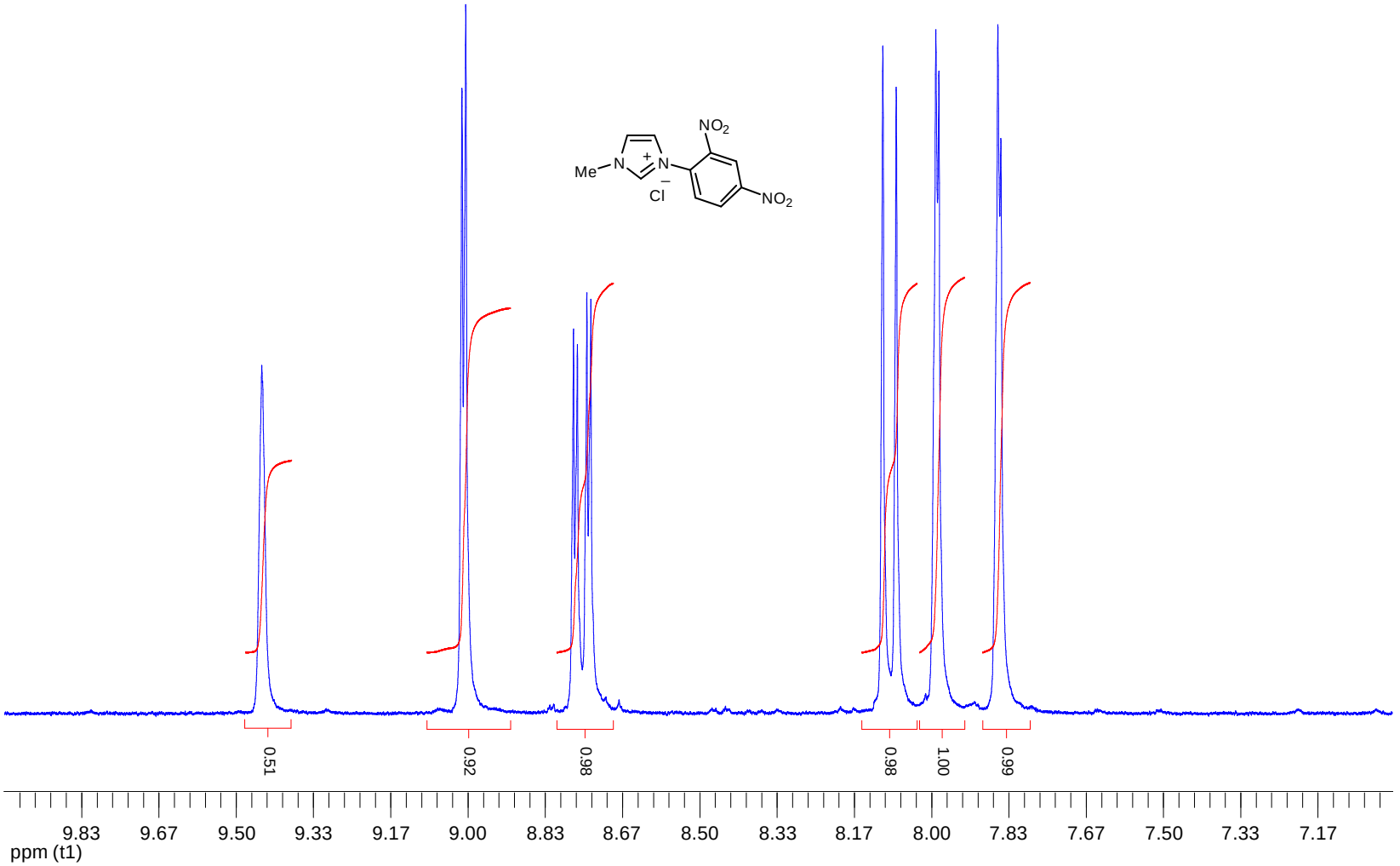
**1-(2,4-dinitrophenyl)-3-methylimidazolium chloride** (**4**) ($^1$H NMR, 300 MHz, DMSO-d6).



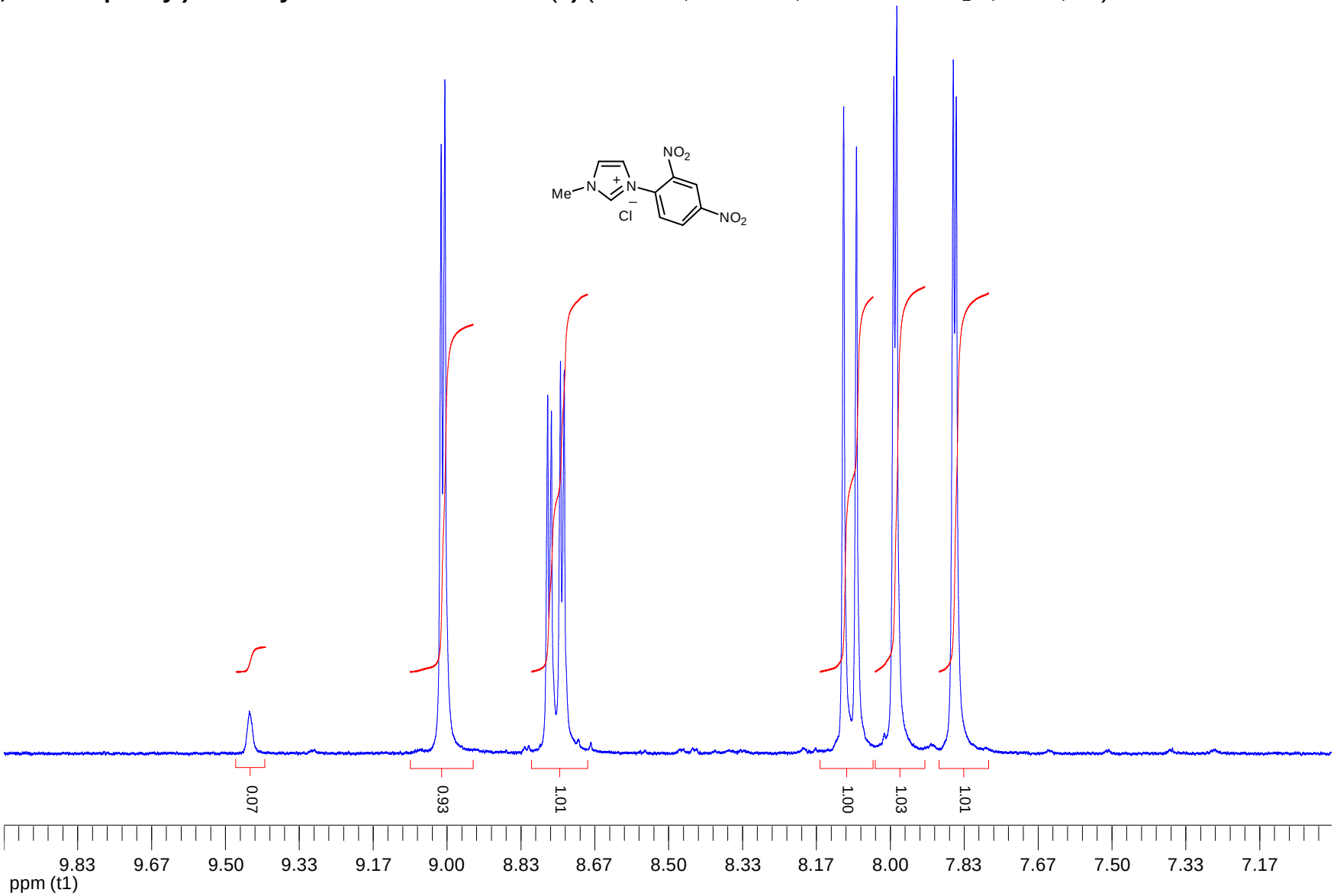
**1-(2,4-dinitrophenyl)-3-methylimidazolium chloride** (**4**) ($^1$H NMR, 300 MHz, DMSO-d6 + $D_2O$, r.t.).



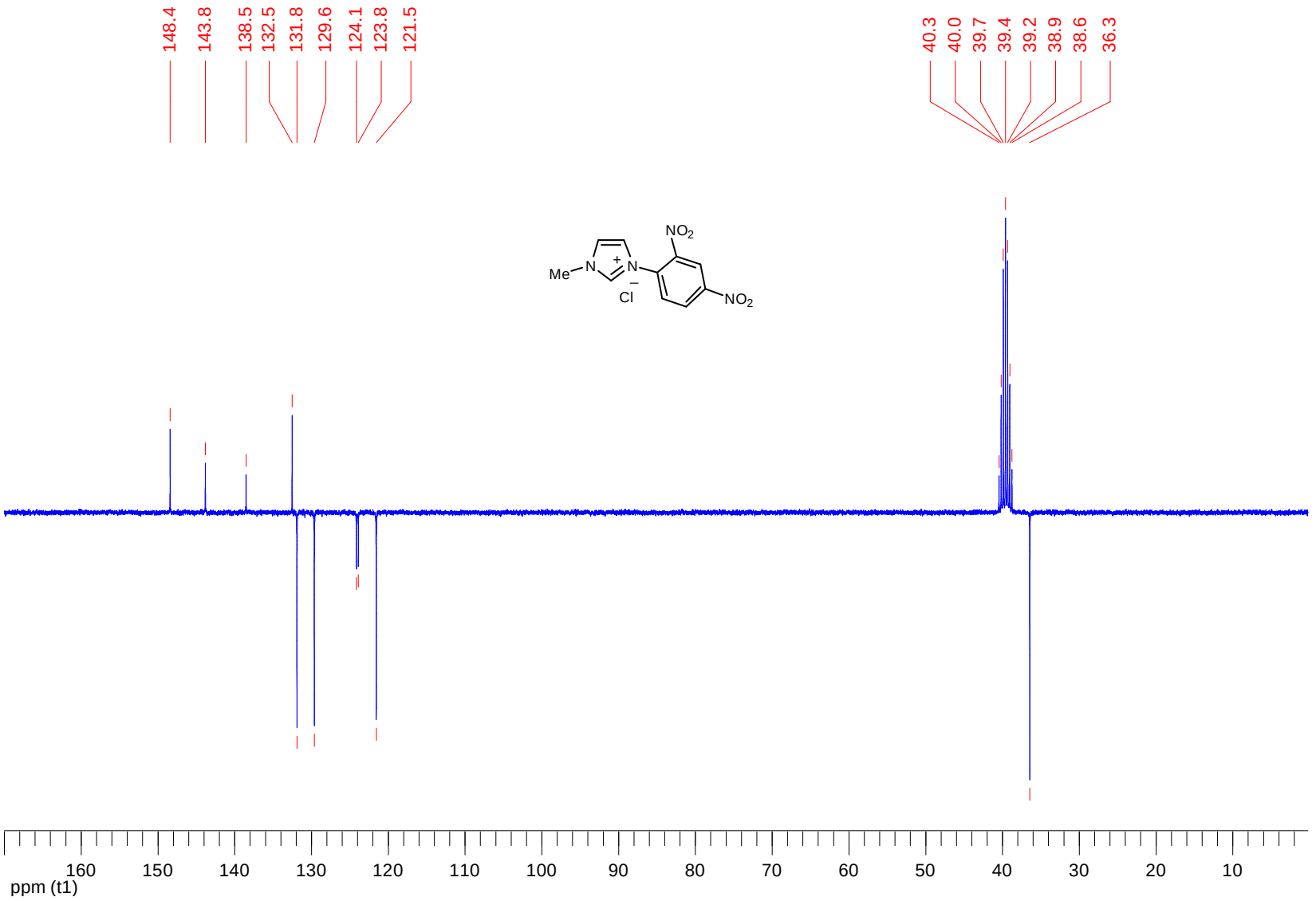
**1-(2,4-dinitrophenyl)-3-methylimidazolium chloride** (**4**) ($^1$H NMR, 300 MHz, DMSO-d6 + $D_2O$, 50 ℃, 30 min.).



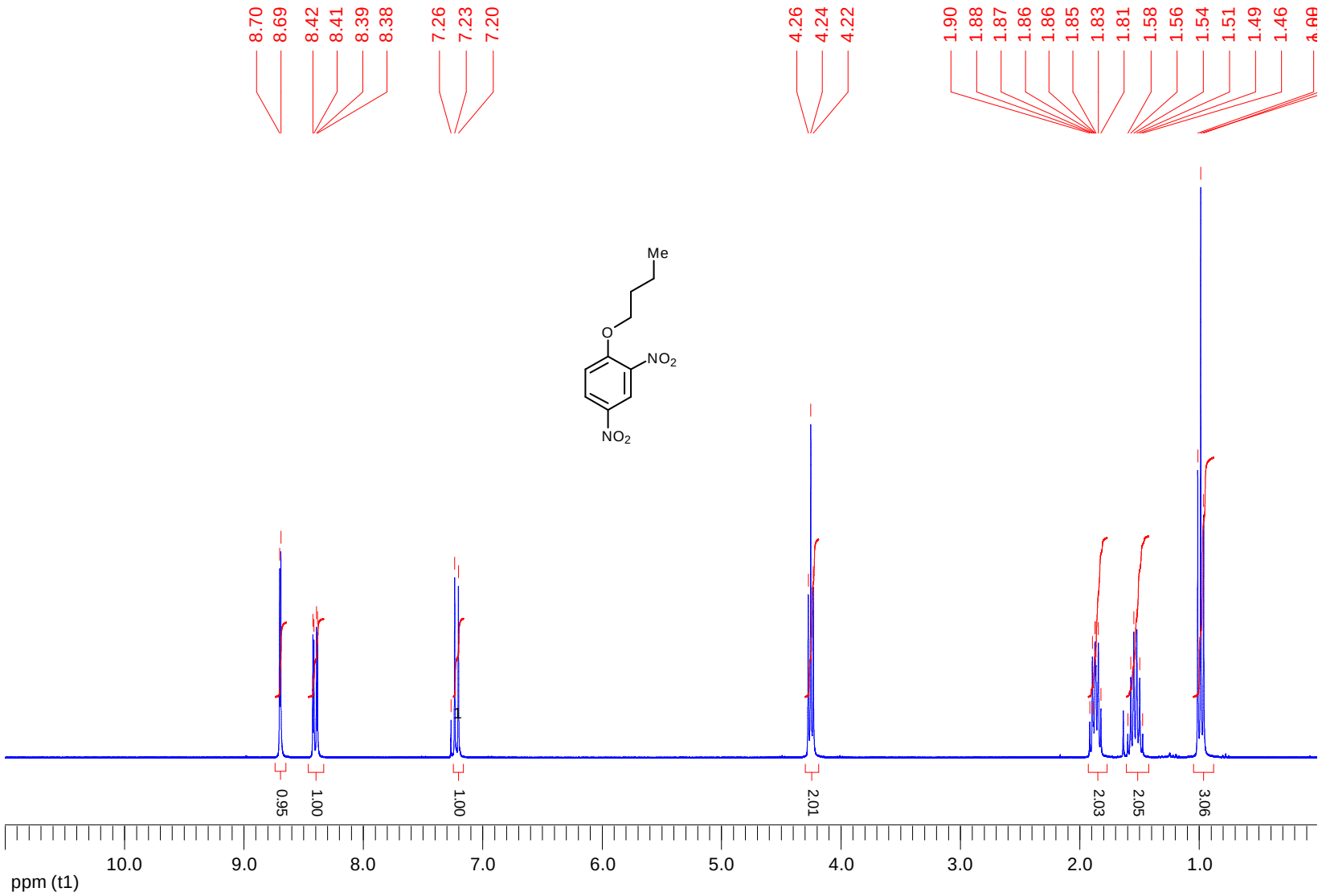
**1-(2,4-dinitrophenyl)-3-methylimidazolium chloride** (**4**) ($^1$H NMR, 300 MHz, DMSO-d6 + $D_2O$, 50 ℃, 6h).



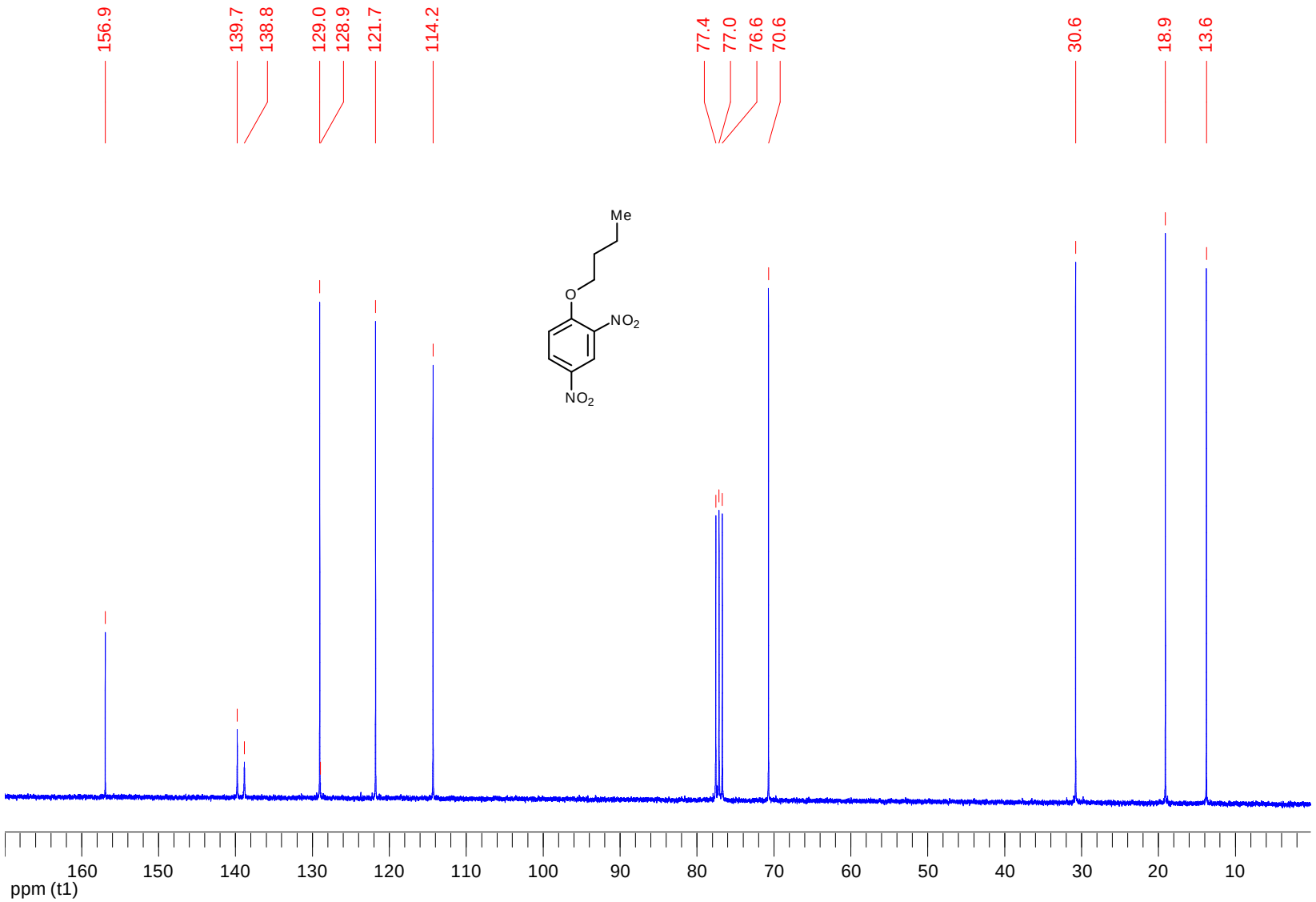
**1-(2,4-dinitrophenyl)-3-methylimidazolium chloride** (**4**) ($^{13}$C NMR, 75 MHz, DMSO-d6).



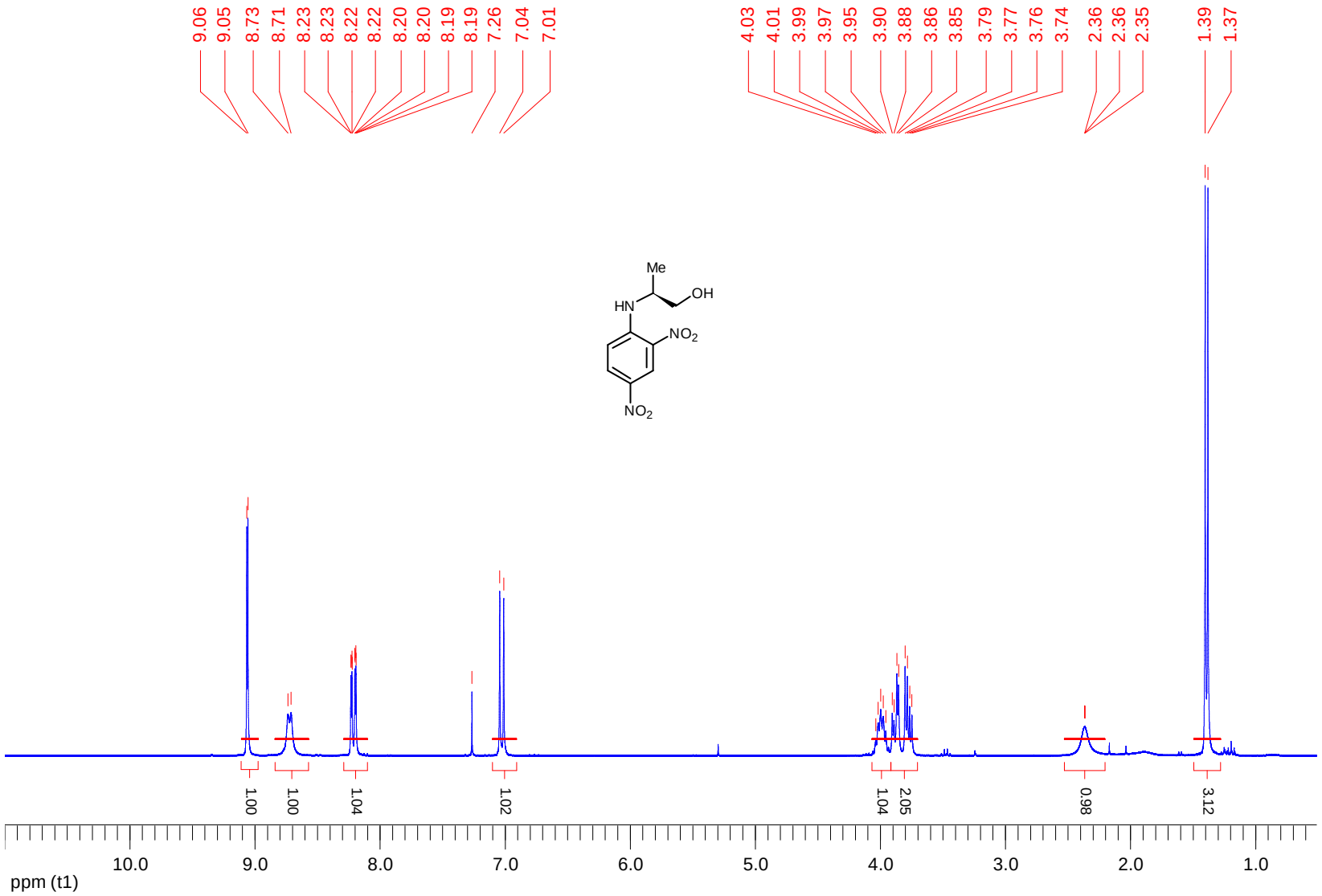
**1-butoxy-2,4-dinitrobenzene (6)** ($^1$H NMR, 300 MHz, $CDCl_3$).



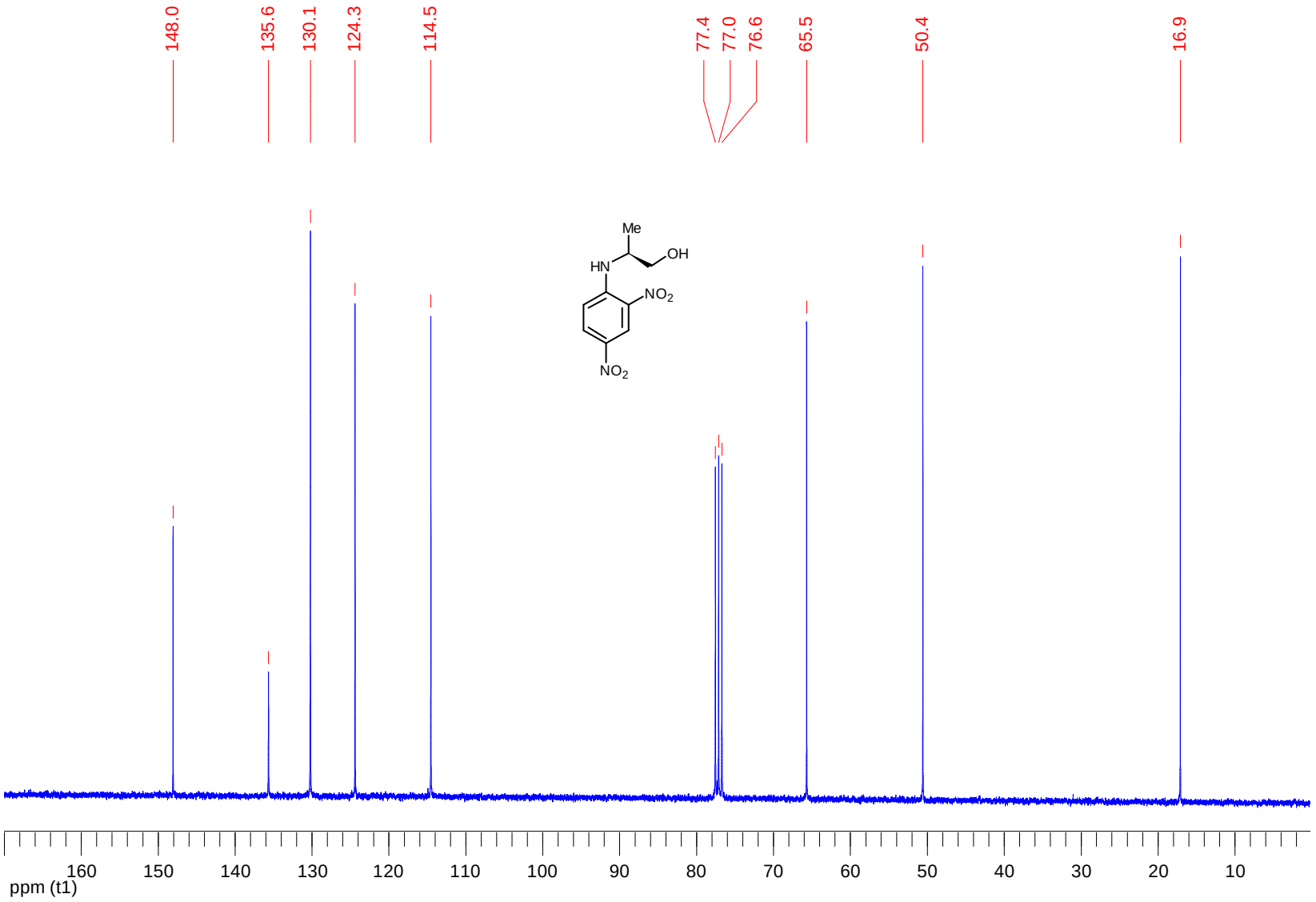
**1-butoxy-2,4-dinitrobenzene (6)** ($^{13}$C NMR, 75 MHz, $CDCl_3$).



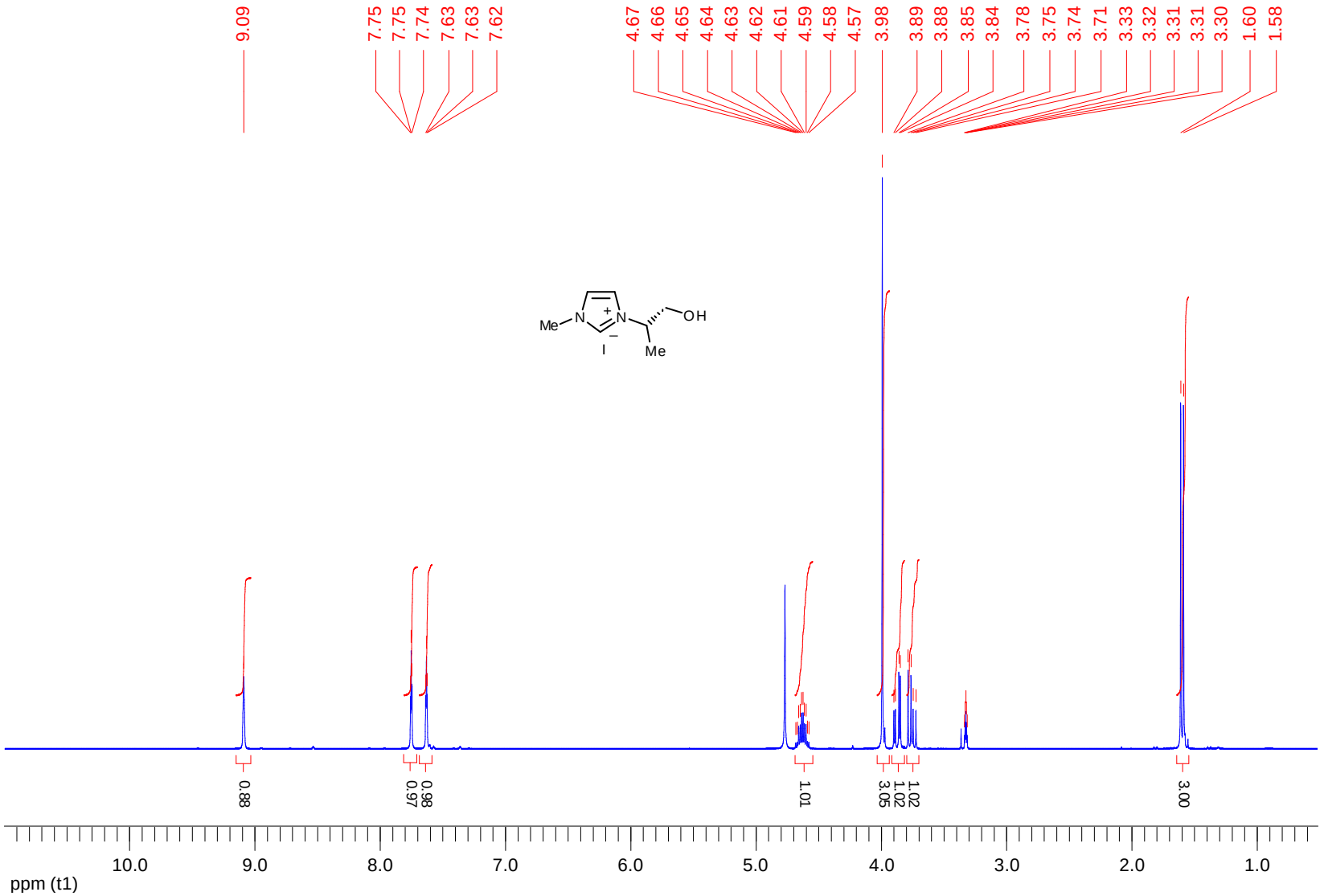
**(*S*)-2-(2,4-dinitrophenylamino)propan-1-ol (7)** ($^1$H NMR, 300 MHz, $CDCl_3$).



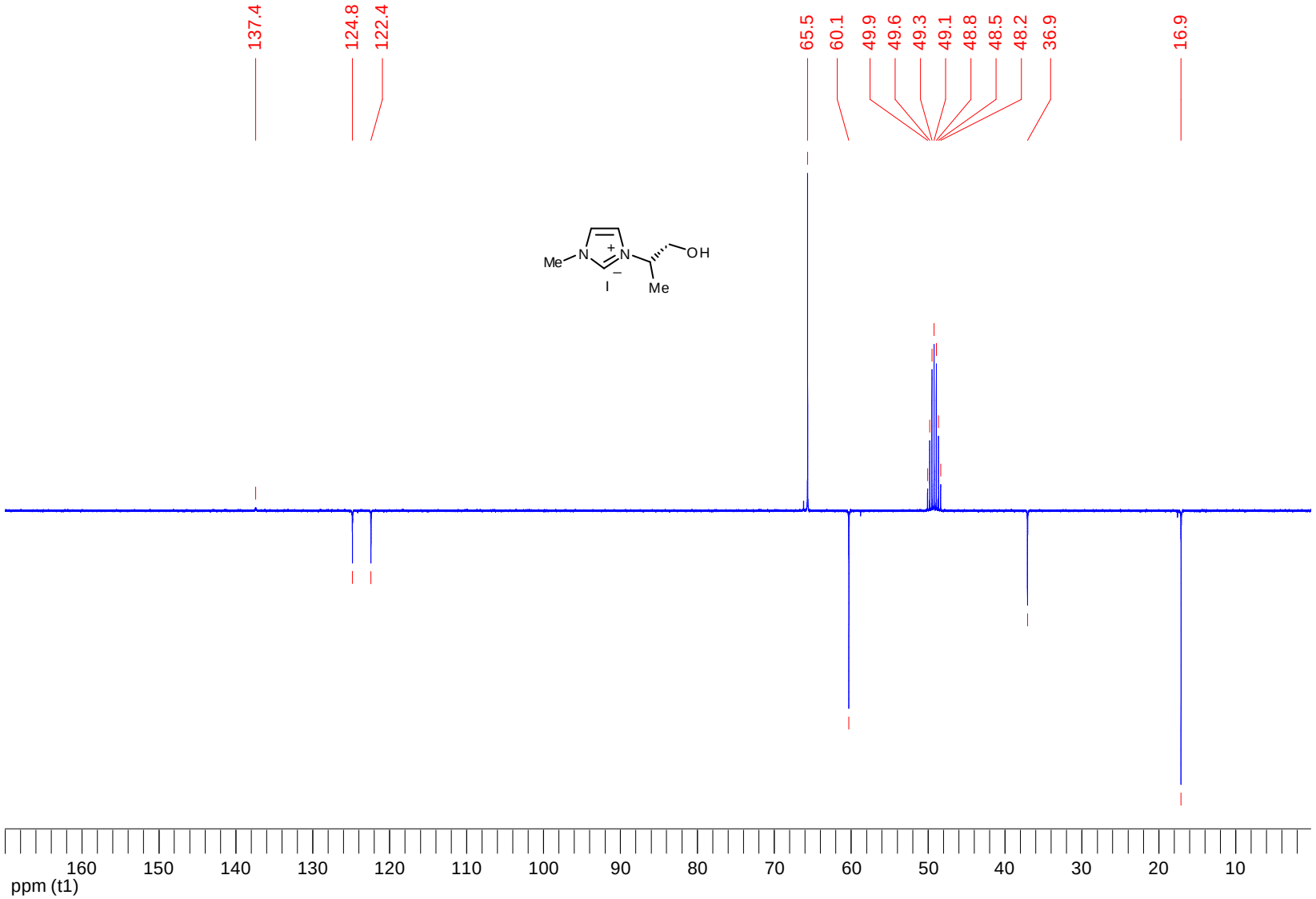
**(*S*)-2-(2,4-dinitrophenylamino)propan-1-ol (7)** ($^{13}$C NMR, 75 MHz, $CDCl_3$).



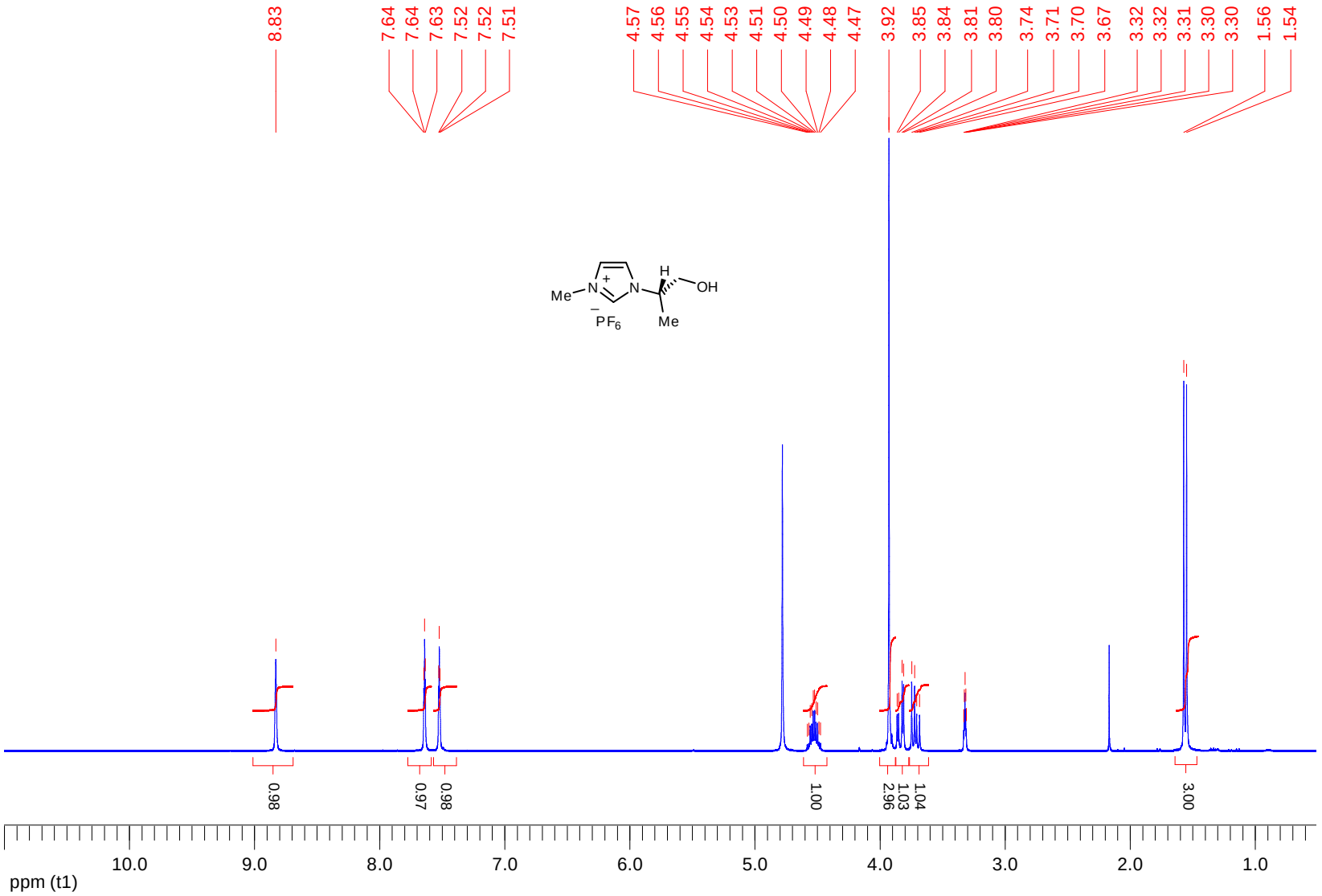
**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium iodide (9)** ($^1$H NMR, 300 MHz, $CD_3OD$).



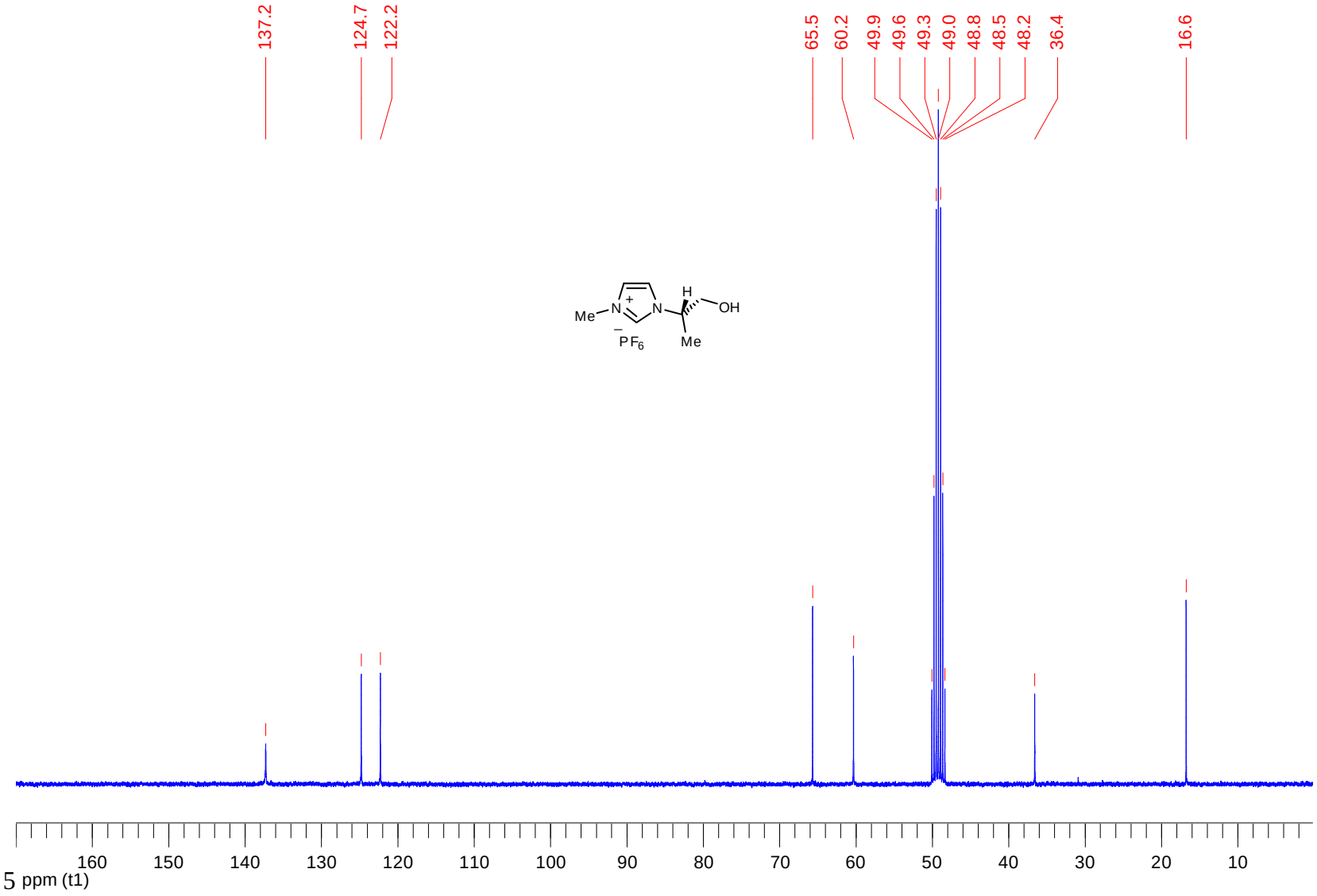
**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium iodide (9)** ($^{13}$C NMR, 75 MHz, $CD_3OD$).



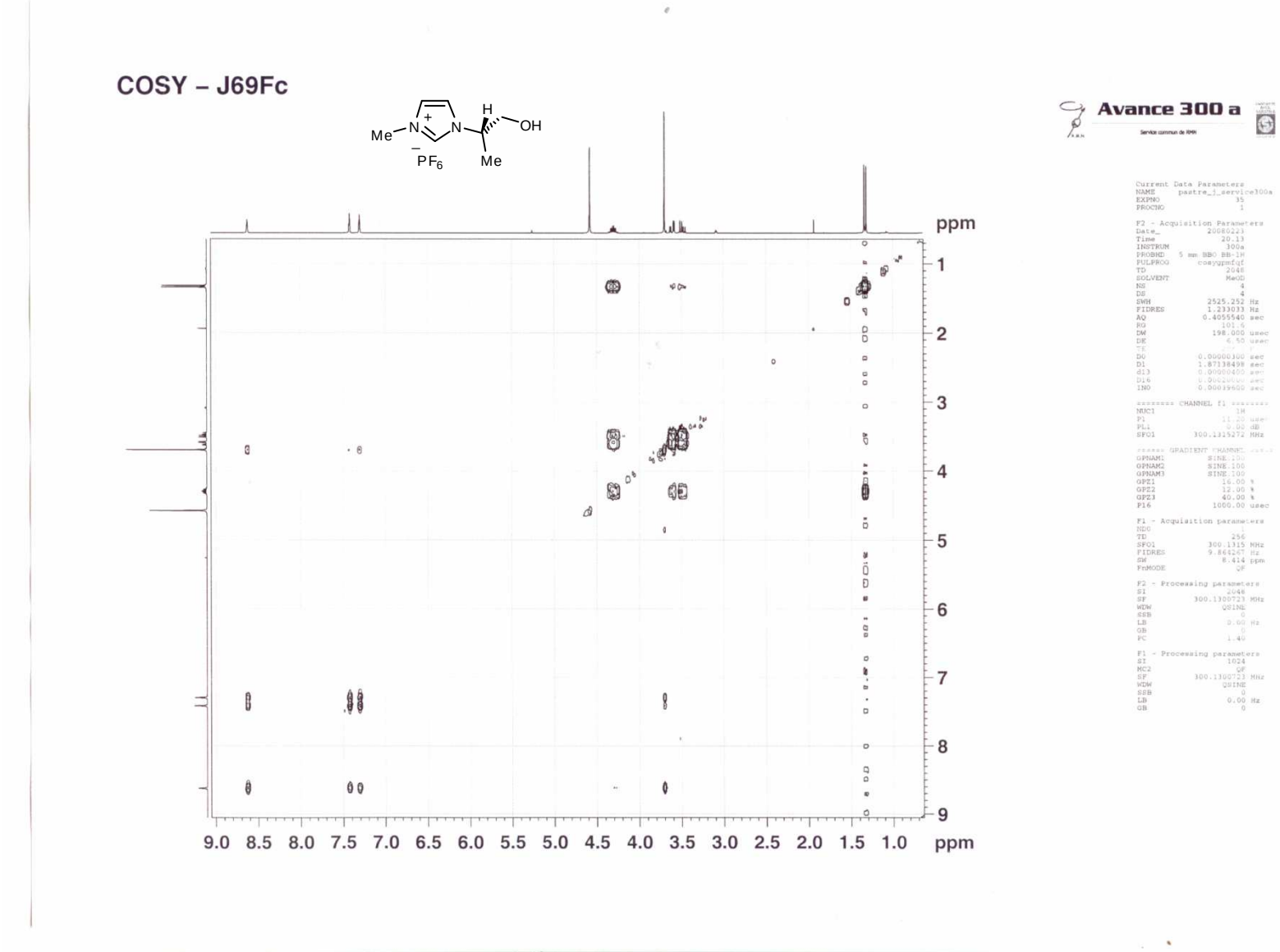
**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10)** ($^1$H NMR, 300 MHz, $CD_3OD$).



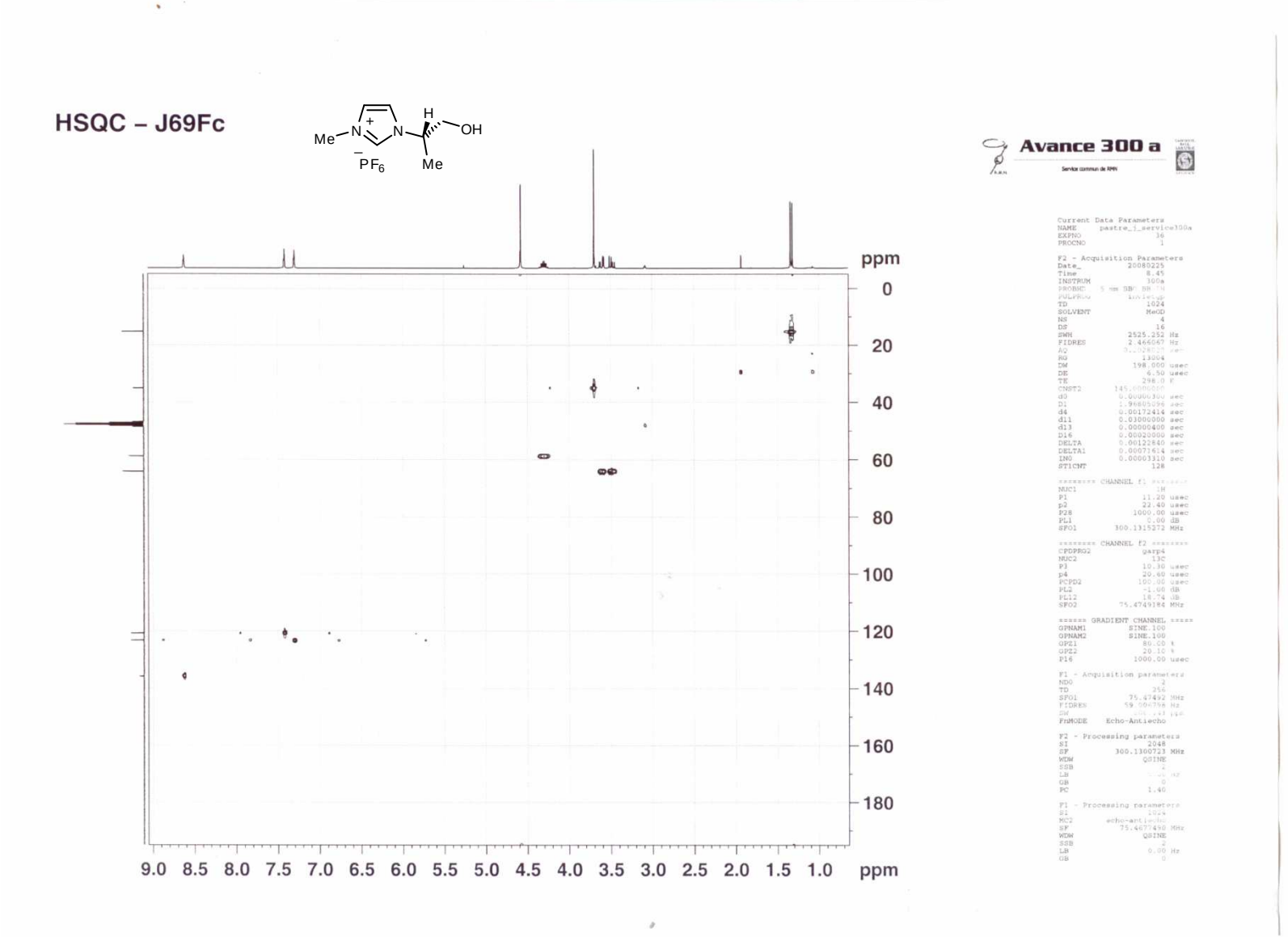
**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10)** ($^{13}$C NMR, 75 MHz, $CD_3OD$).



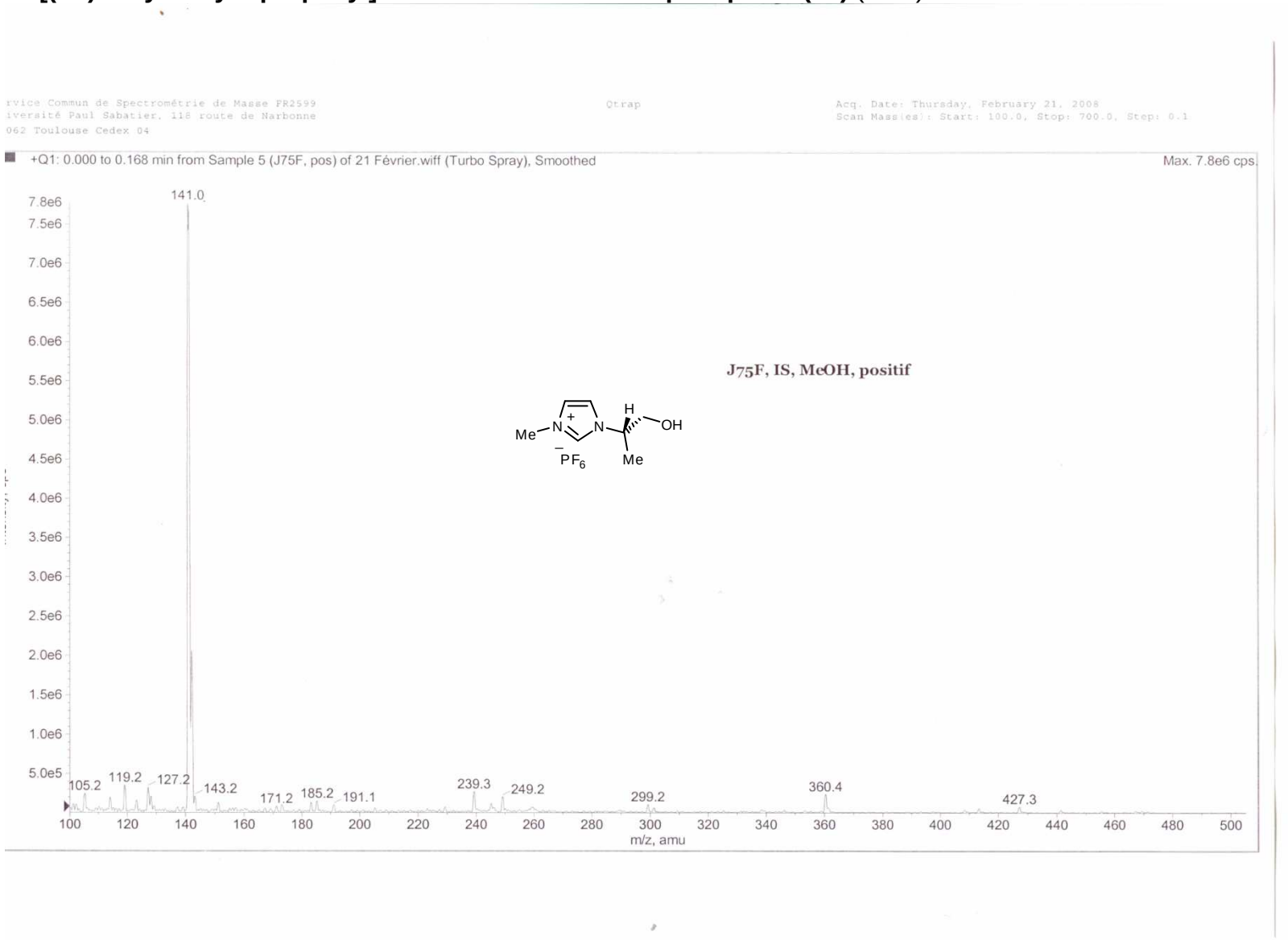
**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10)** (COSY, 300 MHz, $CD_3OD$).



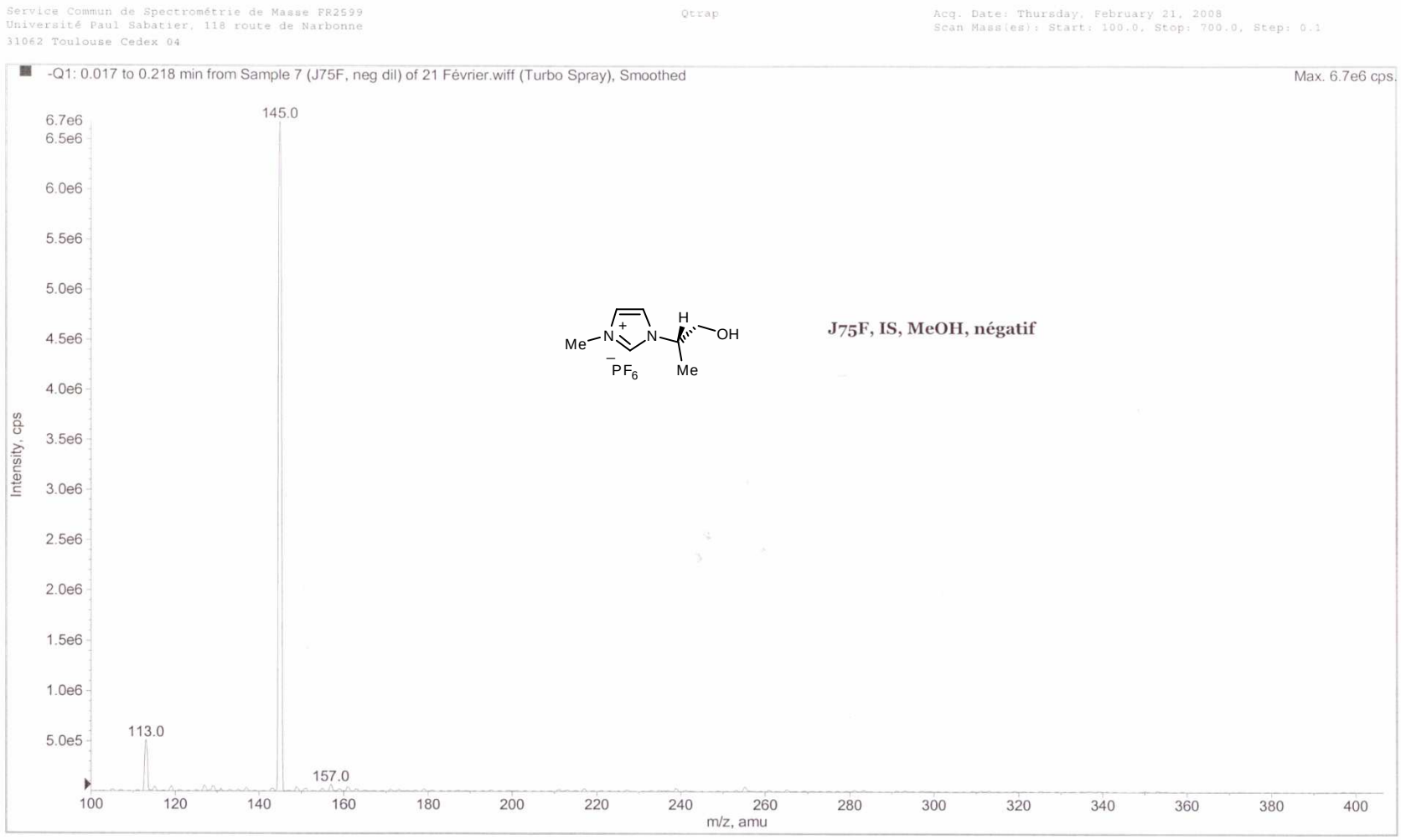
**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10)** (HSQC, 300 MHz, $CD_3OD$).



**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10)** ($ESI^+$).



**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10)** ($ESI^-$).

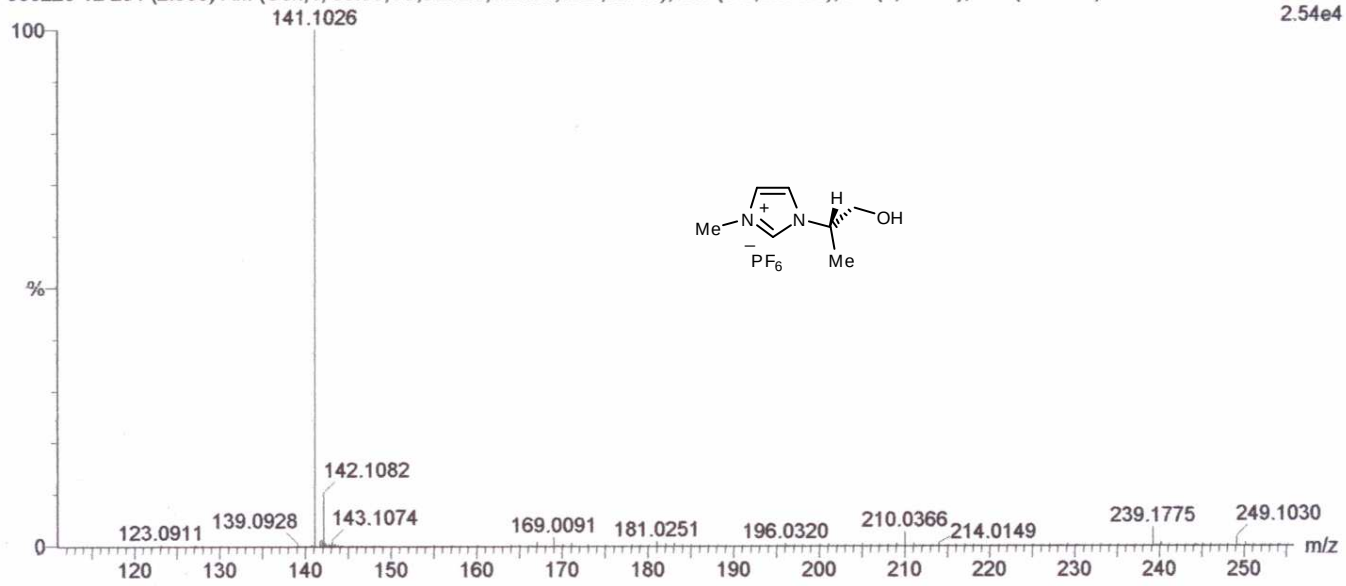


**1-Methyl-3-[(2*S*)-1-hydroxy-2-propanyl]imidazolium hexafluorophosphate (10)** (HRMS, $ESI^+$).

**Single Mass Analysis**
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
121 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

J75F
080228-12 254 (2.865) AM (Cen,4, 80.00, Ar,5000.0,196.96,0.80,LS 10); Sm (SG, 2x1.00); Sb (1,40.00 ); Cm (238:254)
1: TOF MS ES+
2.54e4







| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 5.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 141.1026 | 141.1028 | -0.2 | -1.3 | 2.5 | 1 | C7 H13 N2 O |
| | 141.1014 | 1.2 | 8.2 | 3.0 | 2 | C5 H11 N5 |
| | 141.1004 | 2.2 | 15.7 | -0.5 | 3 | C5 H14 N2 O Na |