

Supporting information

Cyclic Organic Peroxides as New Fungicides against Phytopathogenic Fungi

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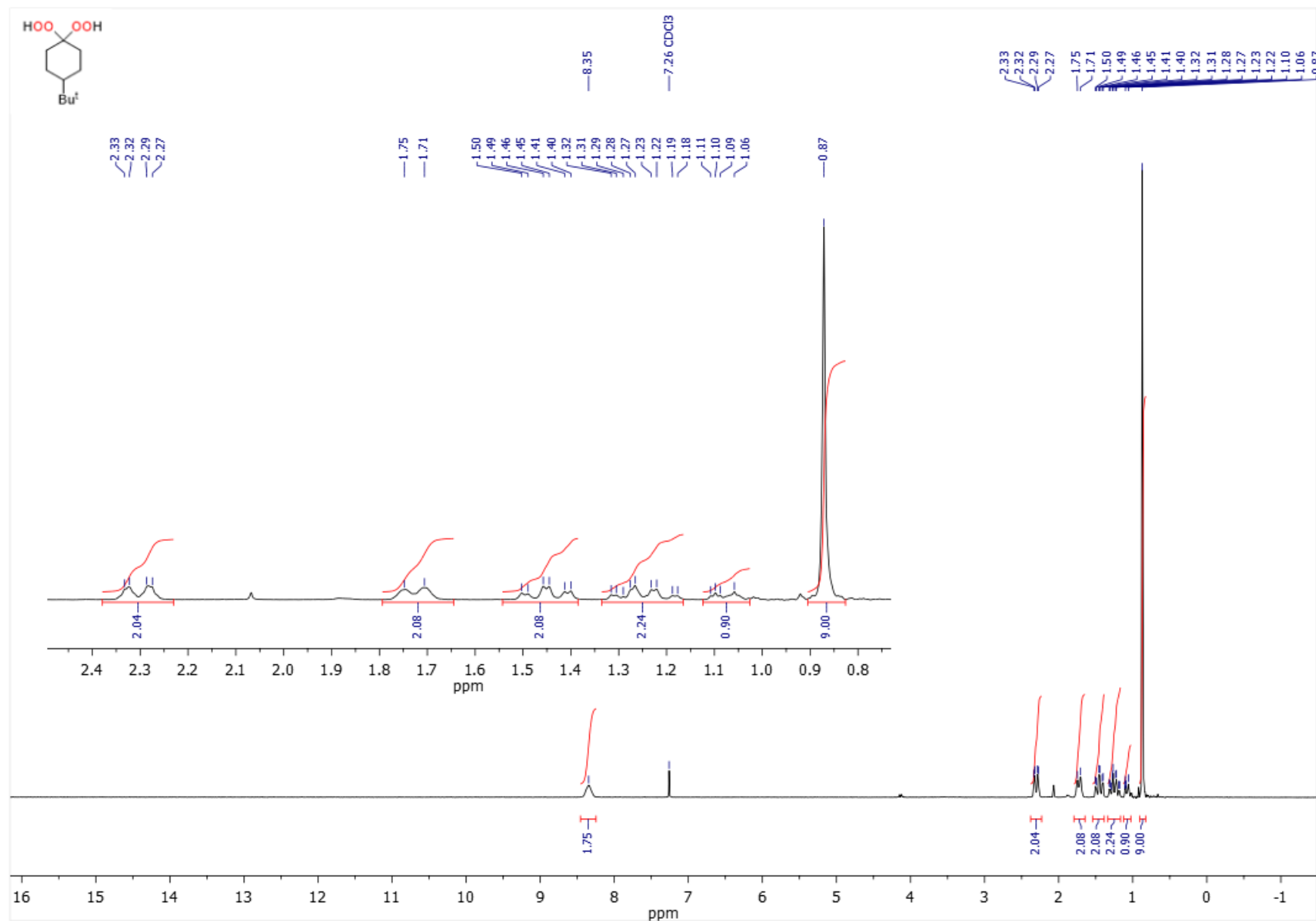
General

Caution: Although we have encountered no difficulties in working with the peroxides described below, the proper precautions, such as the use of shields, fume hoods, and the avoidance of transition metal salts, heating and shaking, should be taken whenever possible.

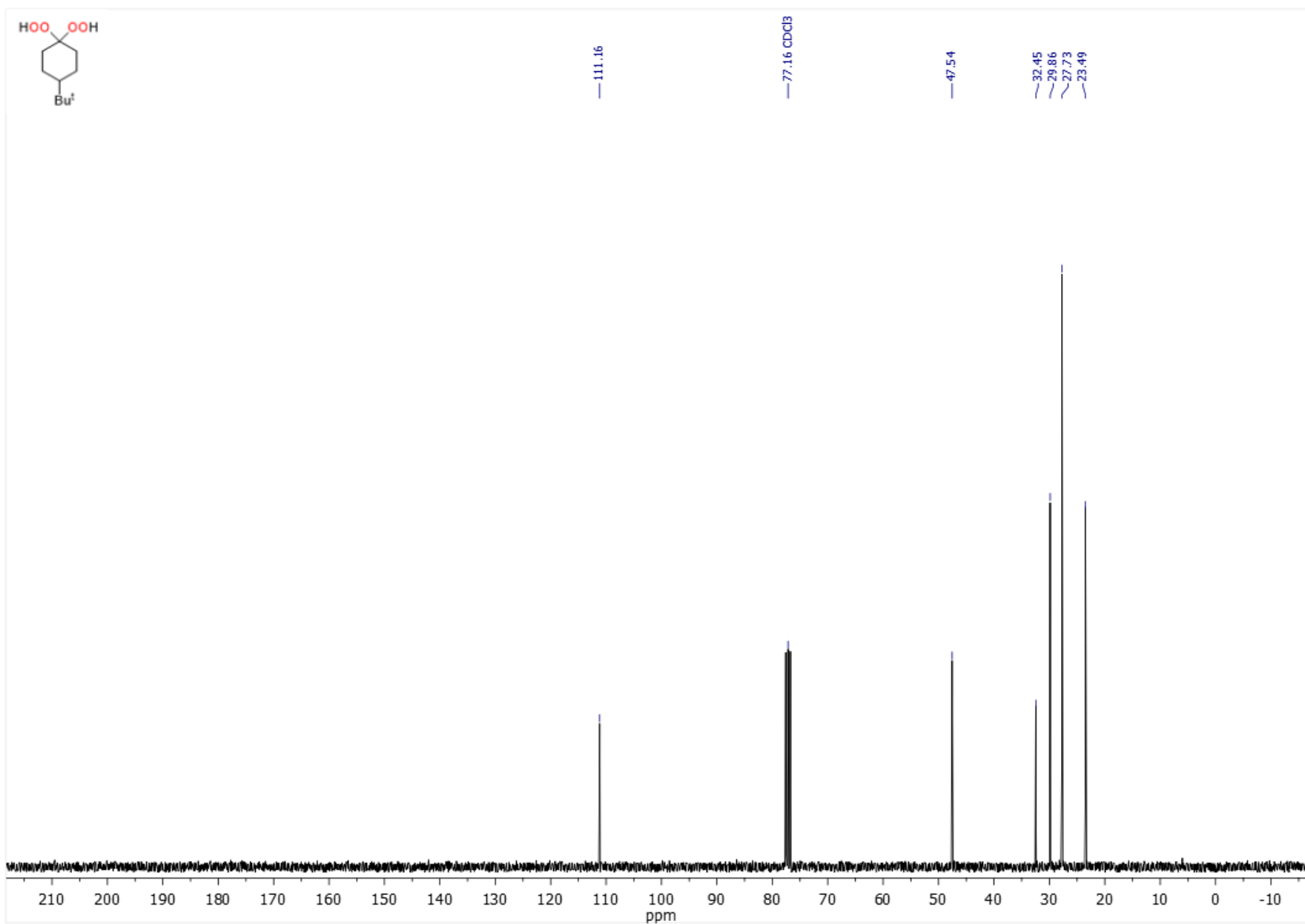
NMR spectra were recorded on a commercial instrument (300.13 MHz for ^1H , 75.48 MHz for ^{13}C) in CDCl_3 . The TLC analysis was carried out on silica gel chromatography plates Macherey-Nagel Alugram UV254; Sorbent: Silica 60, specific surface (BET) $\sim 500 \text{ m}^2/\text{g}$, mean pore size 60 \AA , specific pore volume 0.75 mL/g , particle size $5\text{--}17 \text{ }\mu\text{m}$; Binder: highly polymeric product stable in almost all organic solvents and resistant towards aggressive visualization reagents. The melting points were determined on a Kofler hot-stage apparatus. Chromatography of 1,3-diketones, β,δ' – triketones and peroxides was performed on silica gel (0.060-0.200 mm, 60 A, CAS 7631-86-9).

NMR spectra of peroxides P1-P13

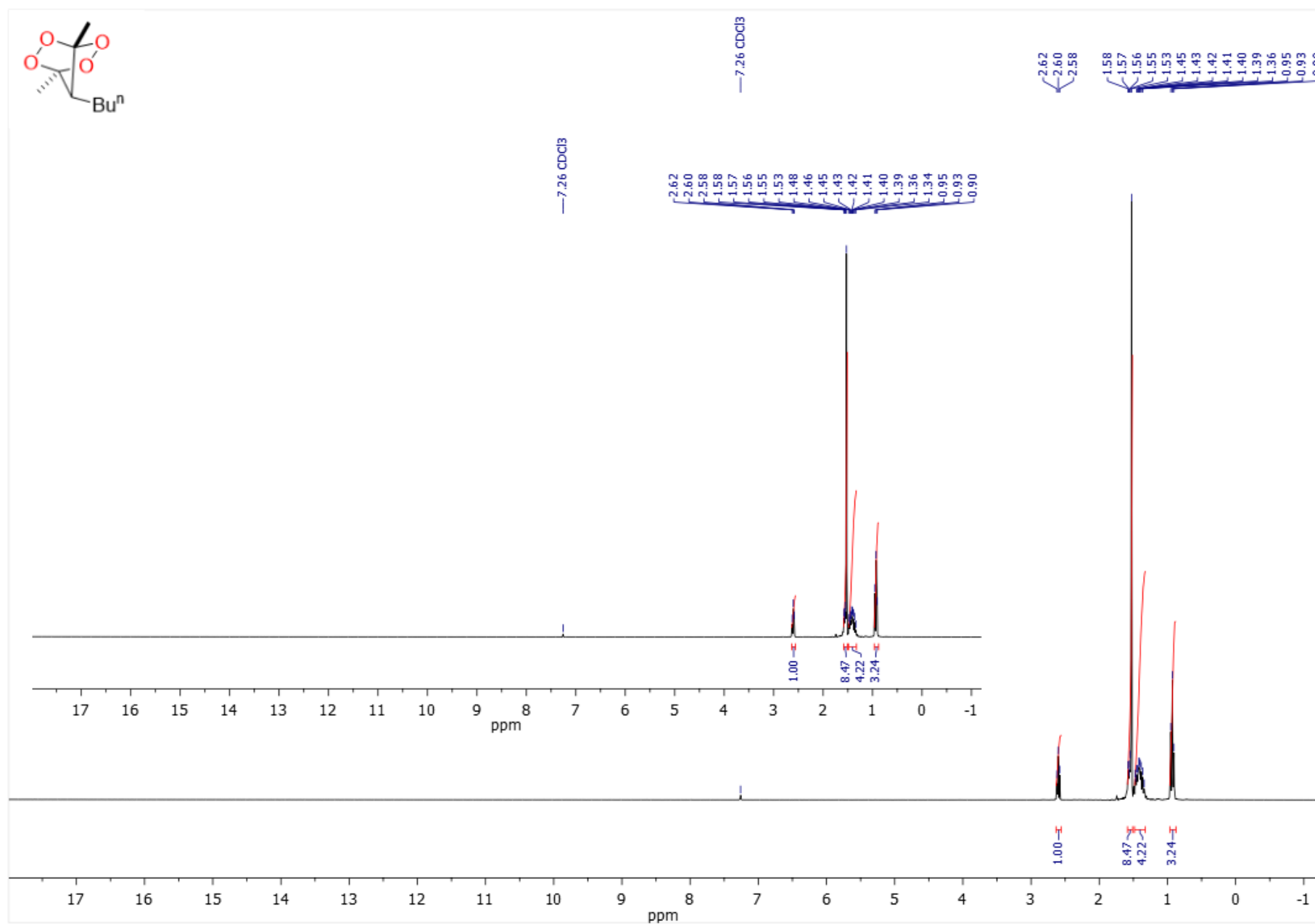
¹H NMR (300.13 MHz, CDCl₃). 4-*tert*-Butyl-1,1-dihydroperoxycyclohexane P1



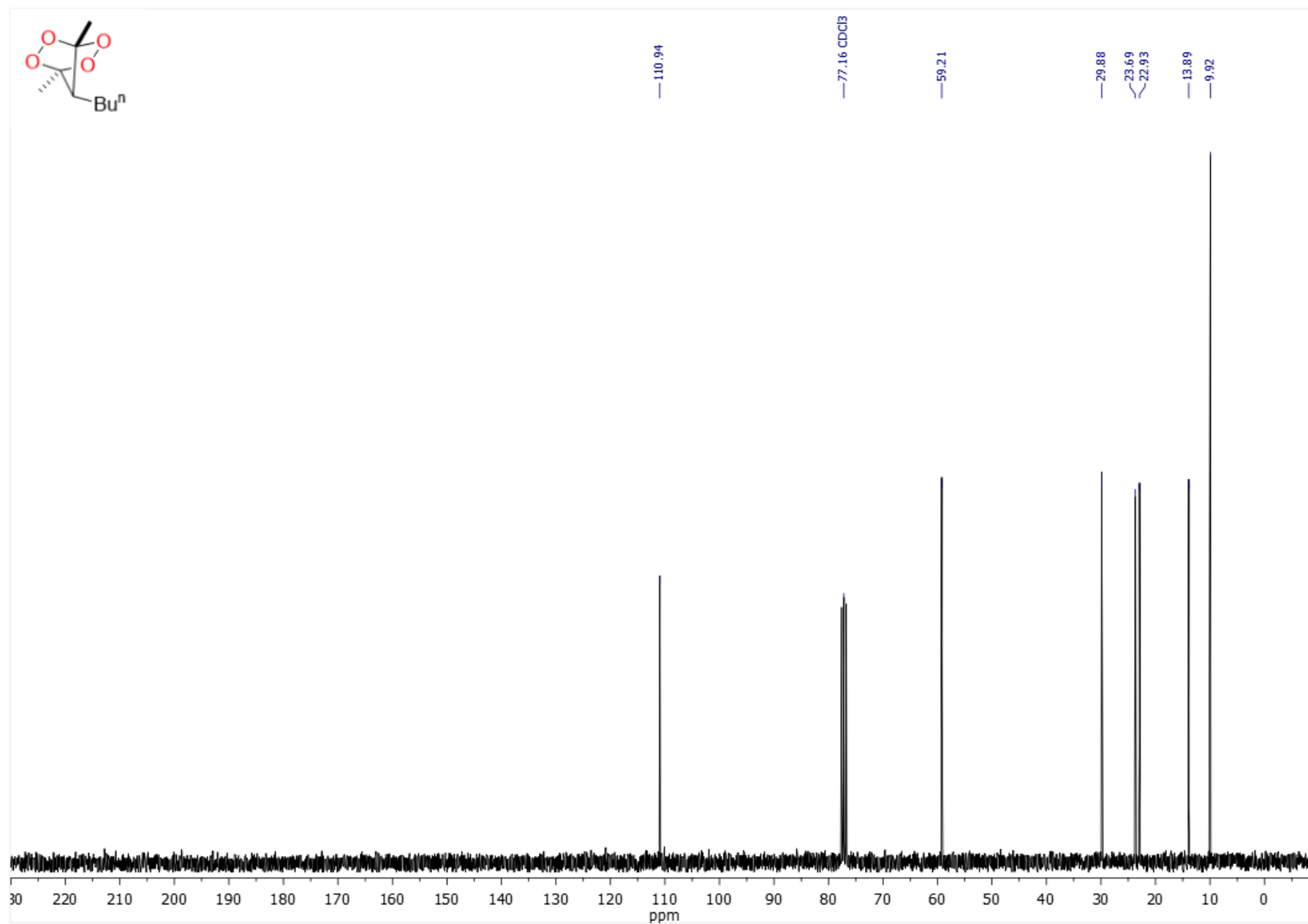
¹³C NMR (75.48 MHz, CDCl₃). 4-*tert*-Butyl-1,1-dihydroperoxycyclohexane P1



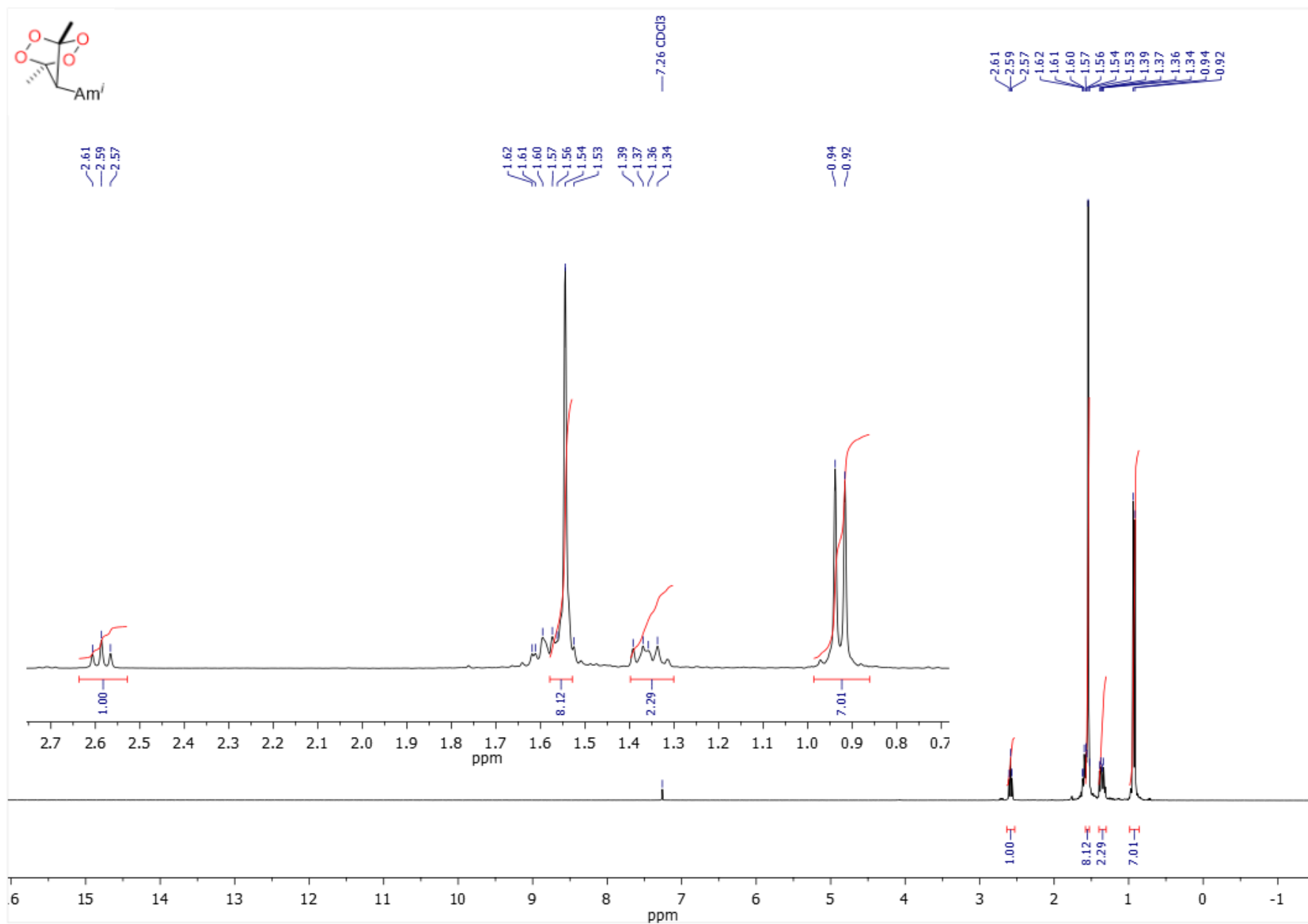
^1H NMR (300.13 MHz, CDCl_3). 7-Butyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P2



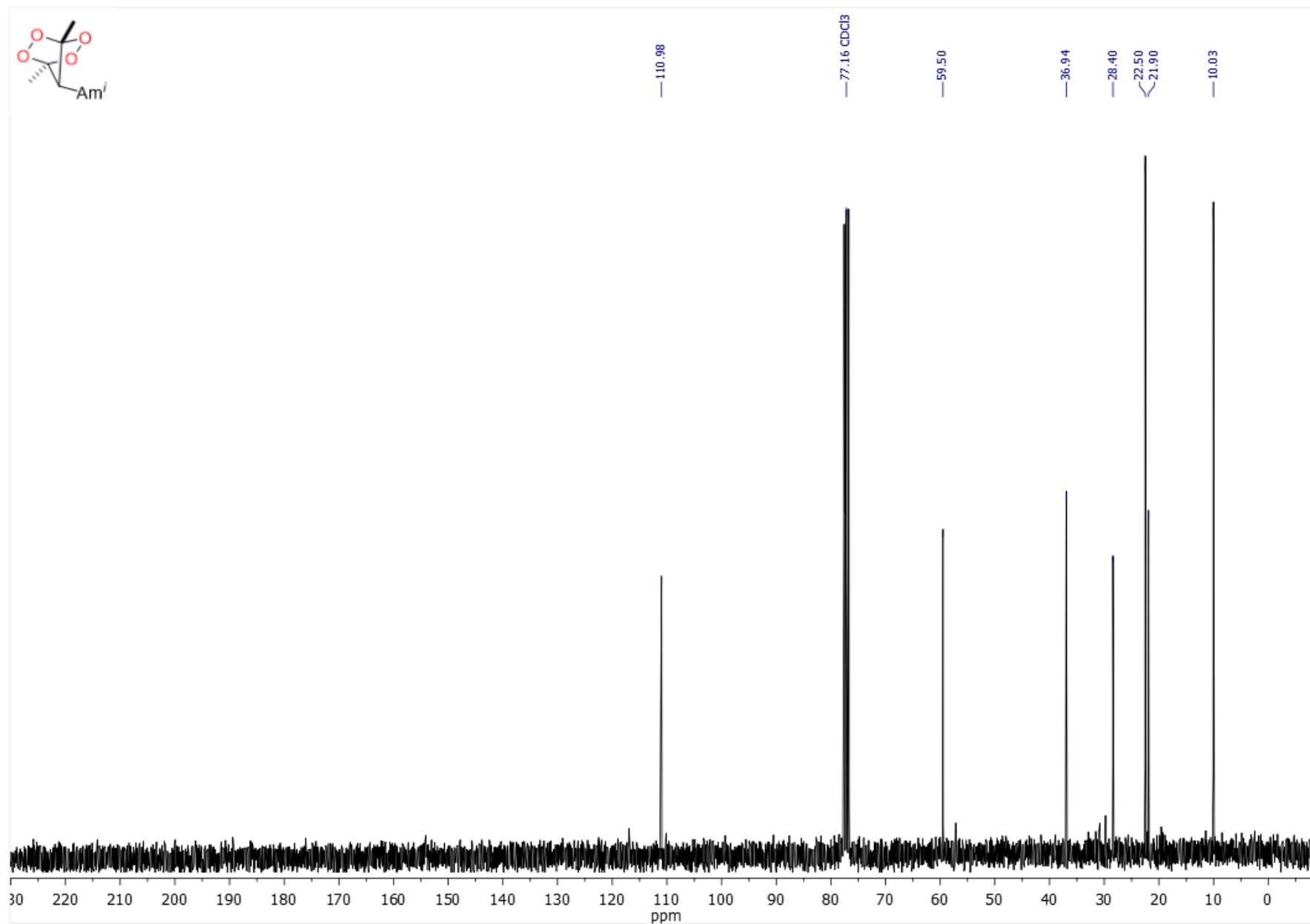
^{13}C NMR (75.48 MHz, CDCl_3). 7-Butyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P2



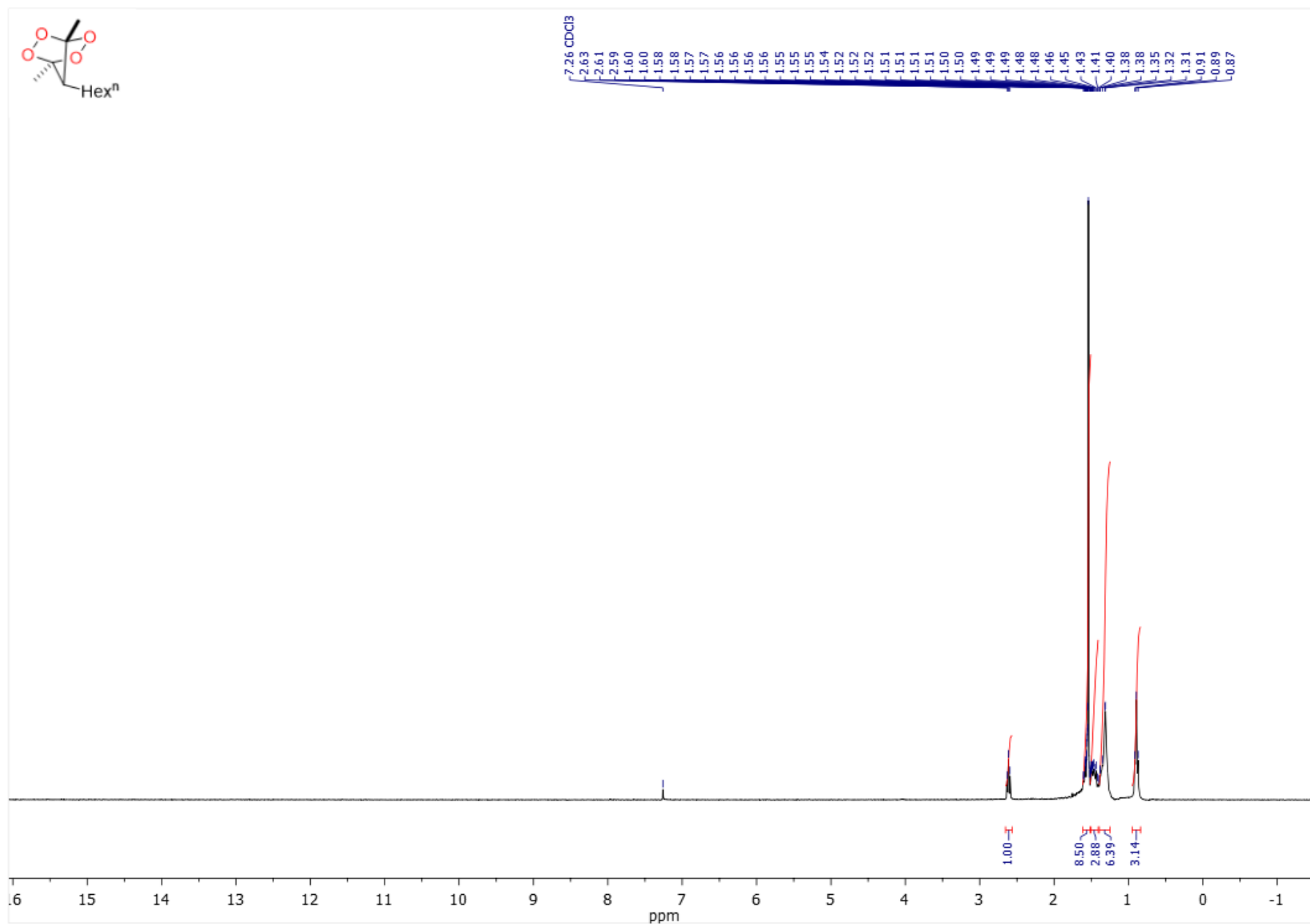
¹H NMR (300.13 MHz, CDCl₃). 7-Isopentyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P3



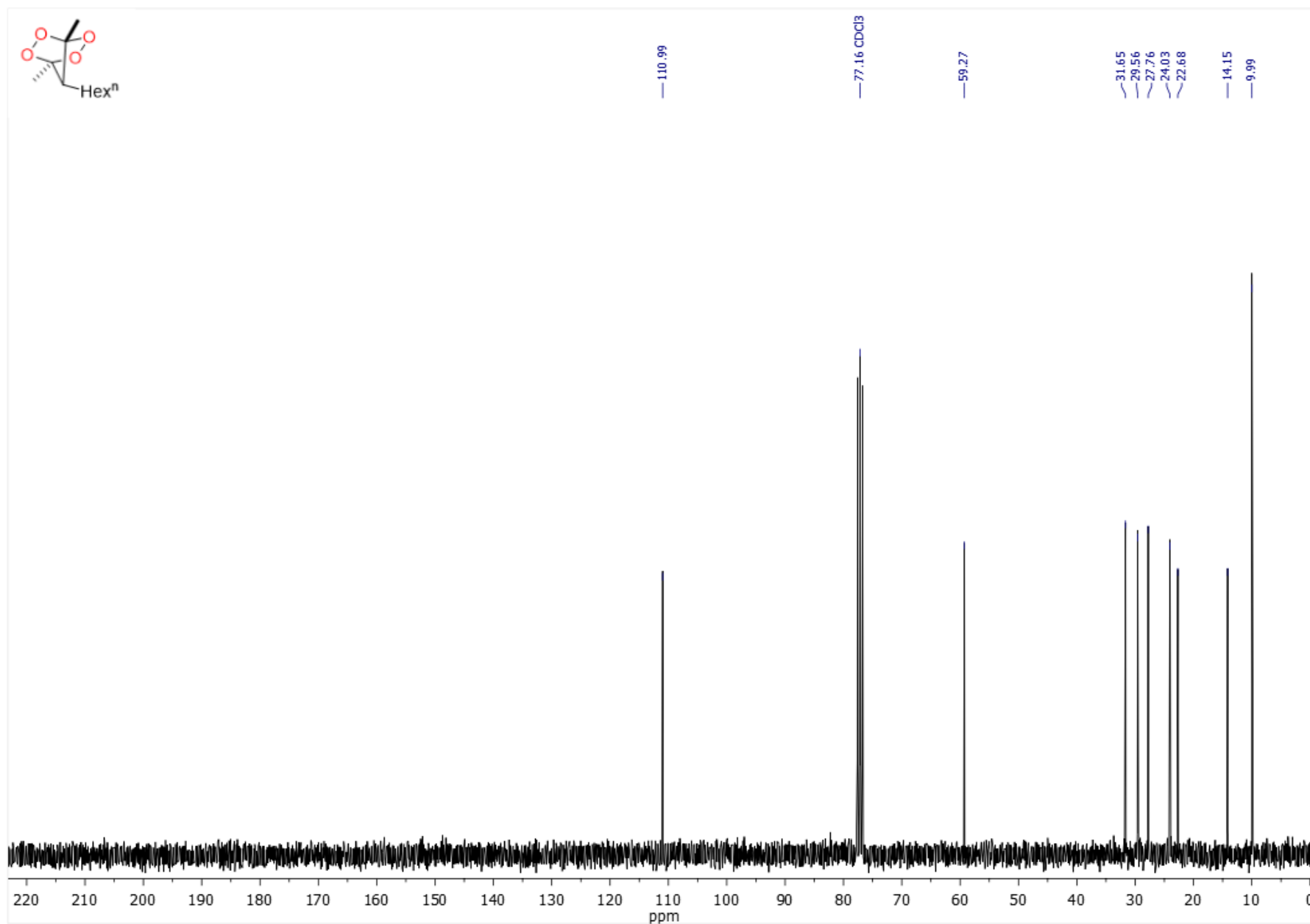
¹³C NMR (75.48 MHz, CDCl₃). 7-Isopentyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P3



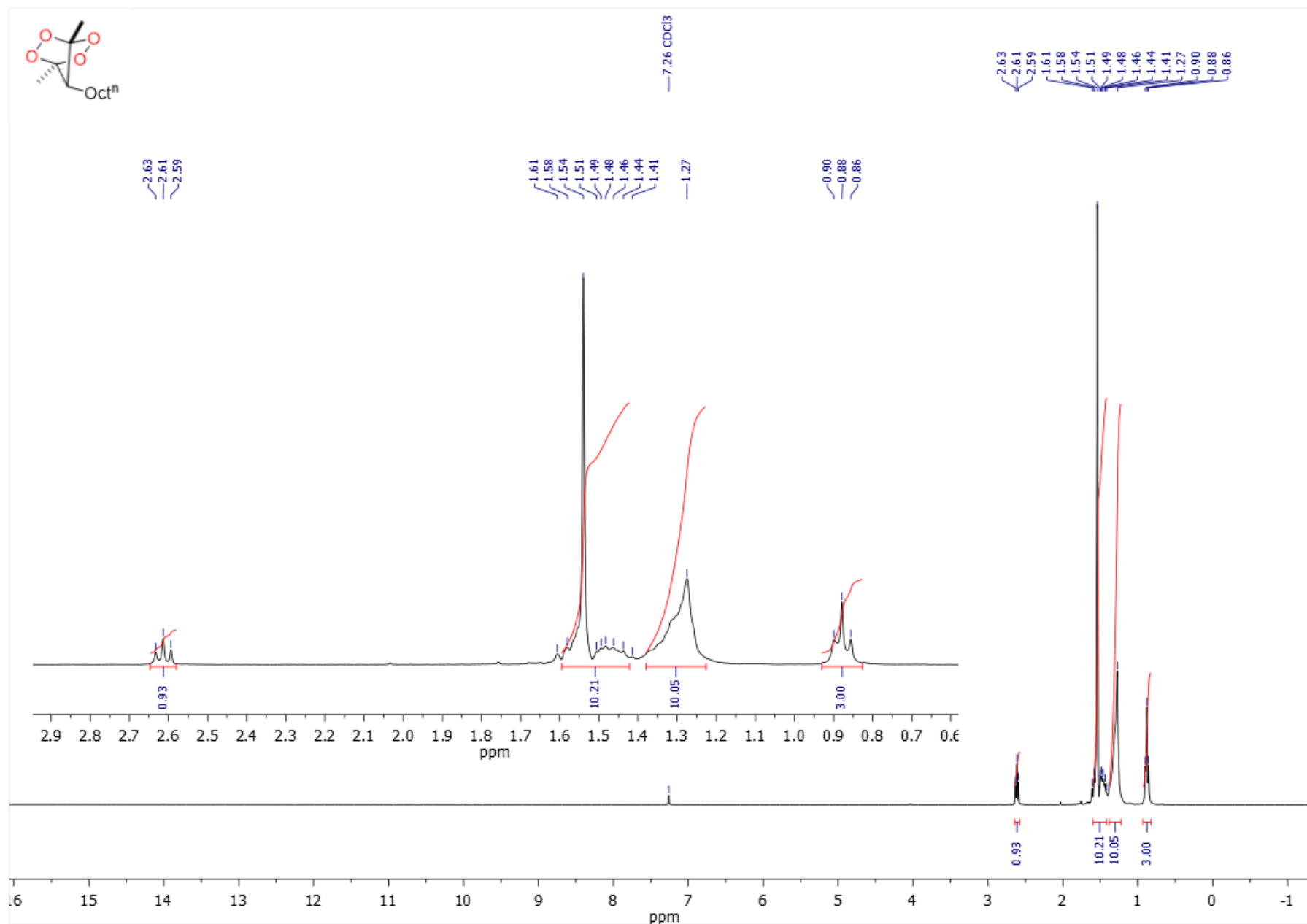
¹H NMR (300.13 MHz, CDCl₃). 7-Hexyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P4



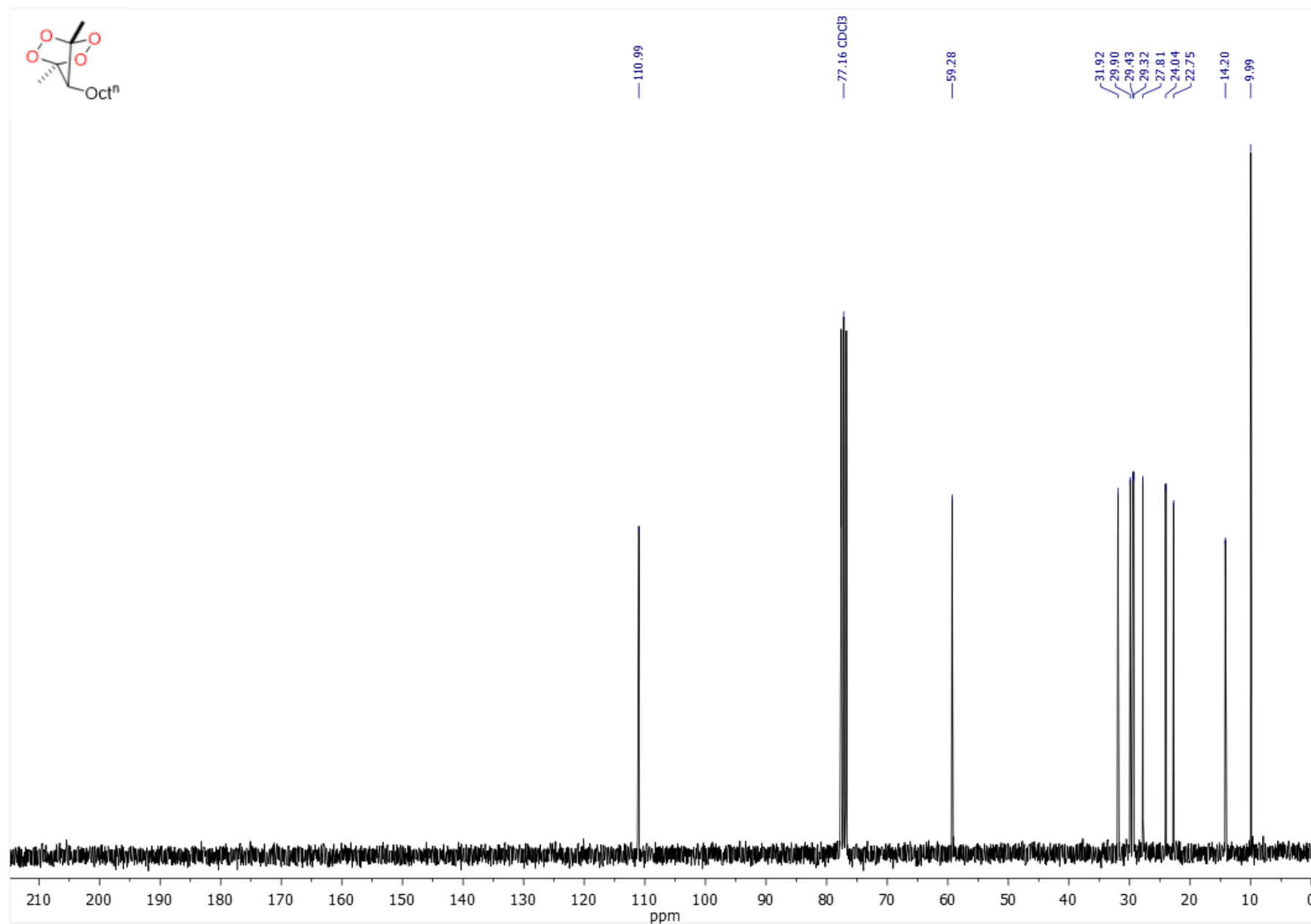
¹³C NMR (75.48 MHz, CDCl₃). 7-Hexyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P4



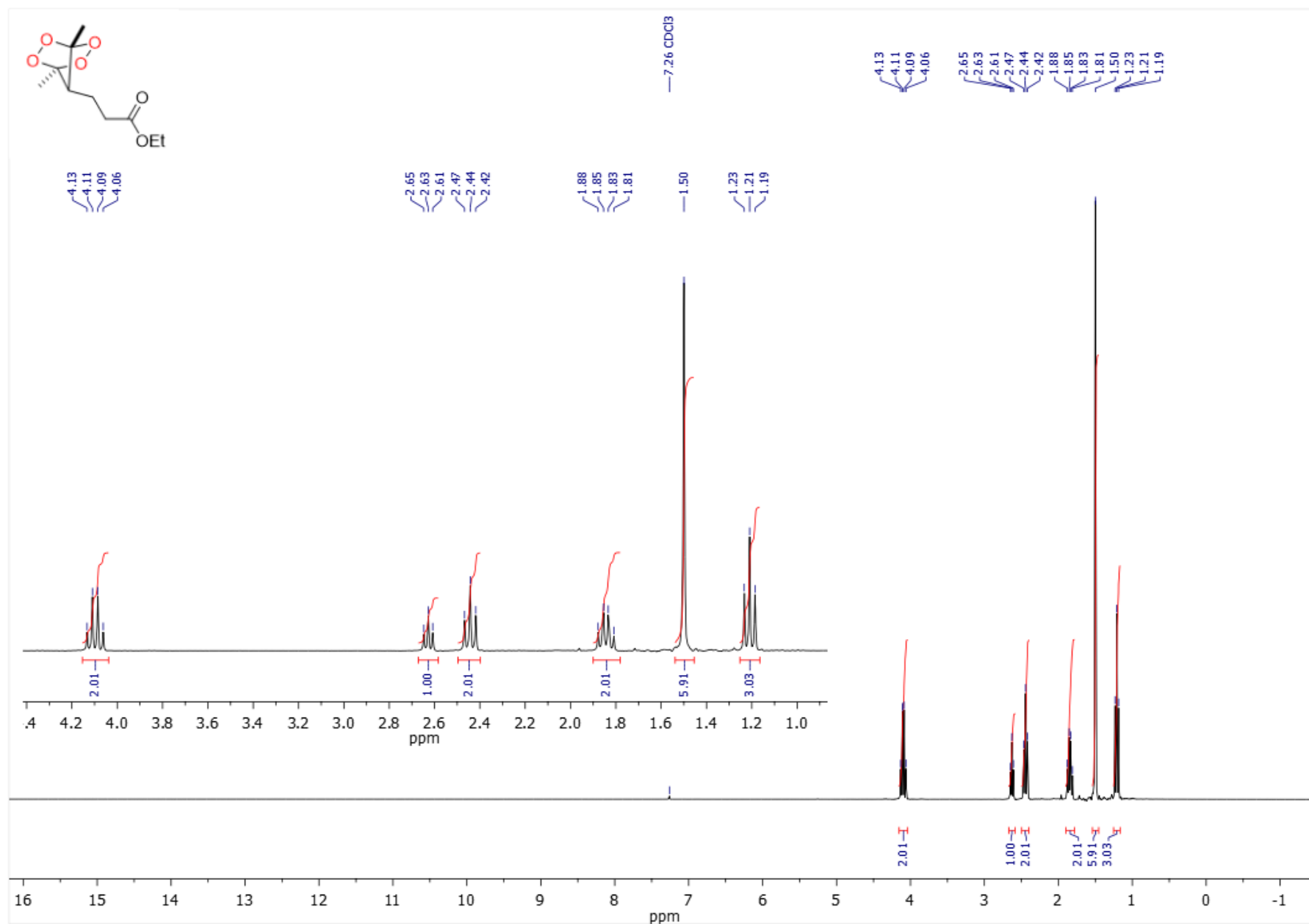
¹H NMR (300.13 MHz, CDCl₃). 1,4-Dimethyl-7-octyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P5



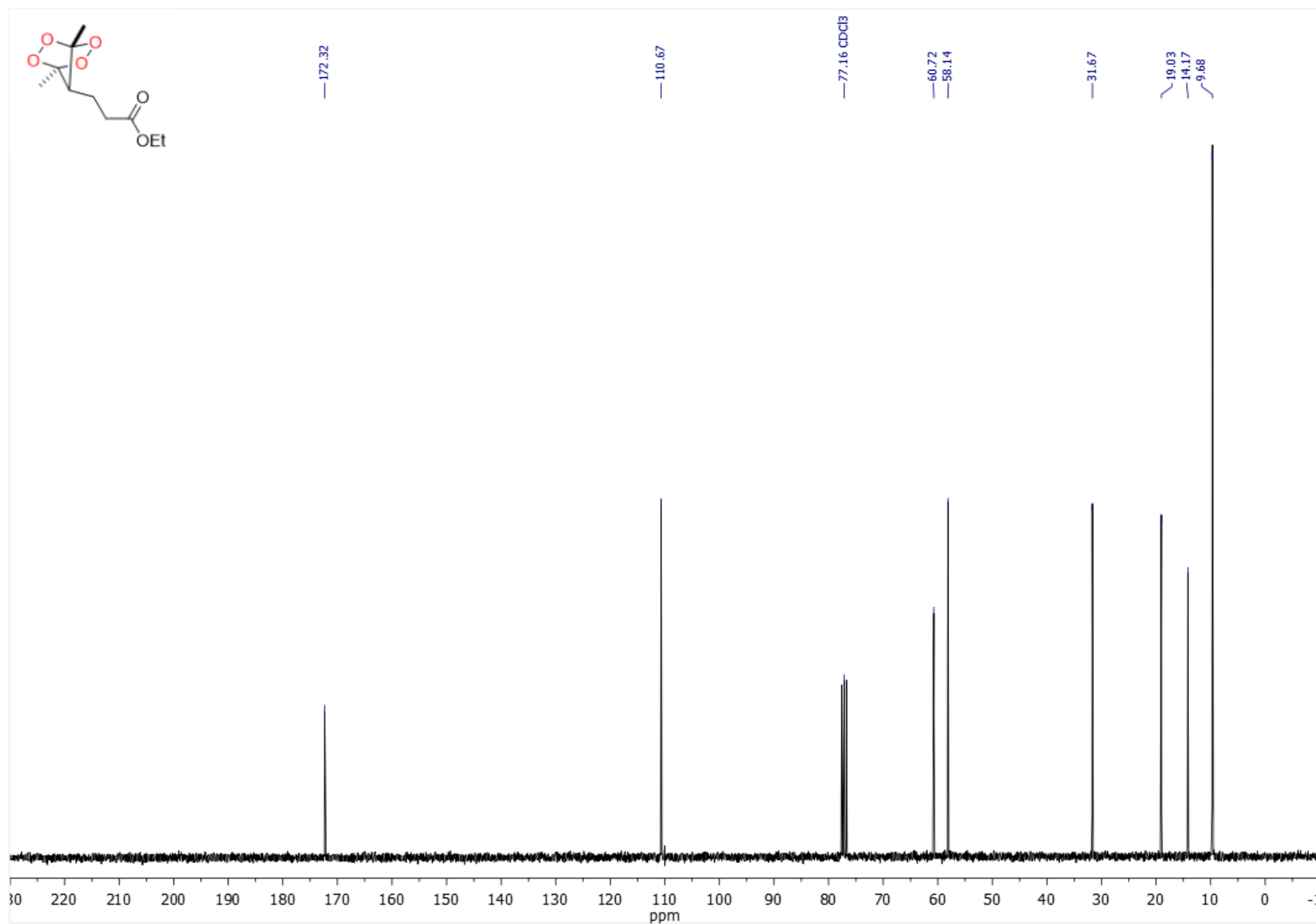
¹³C NMR (75.48 MHz, CDCl₃). 1,4-Dimethyl-7-octyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P5



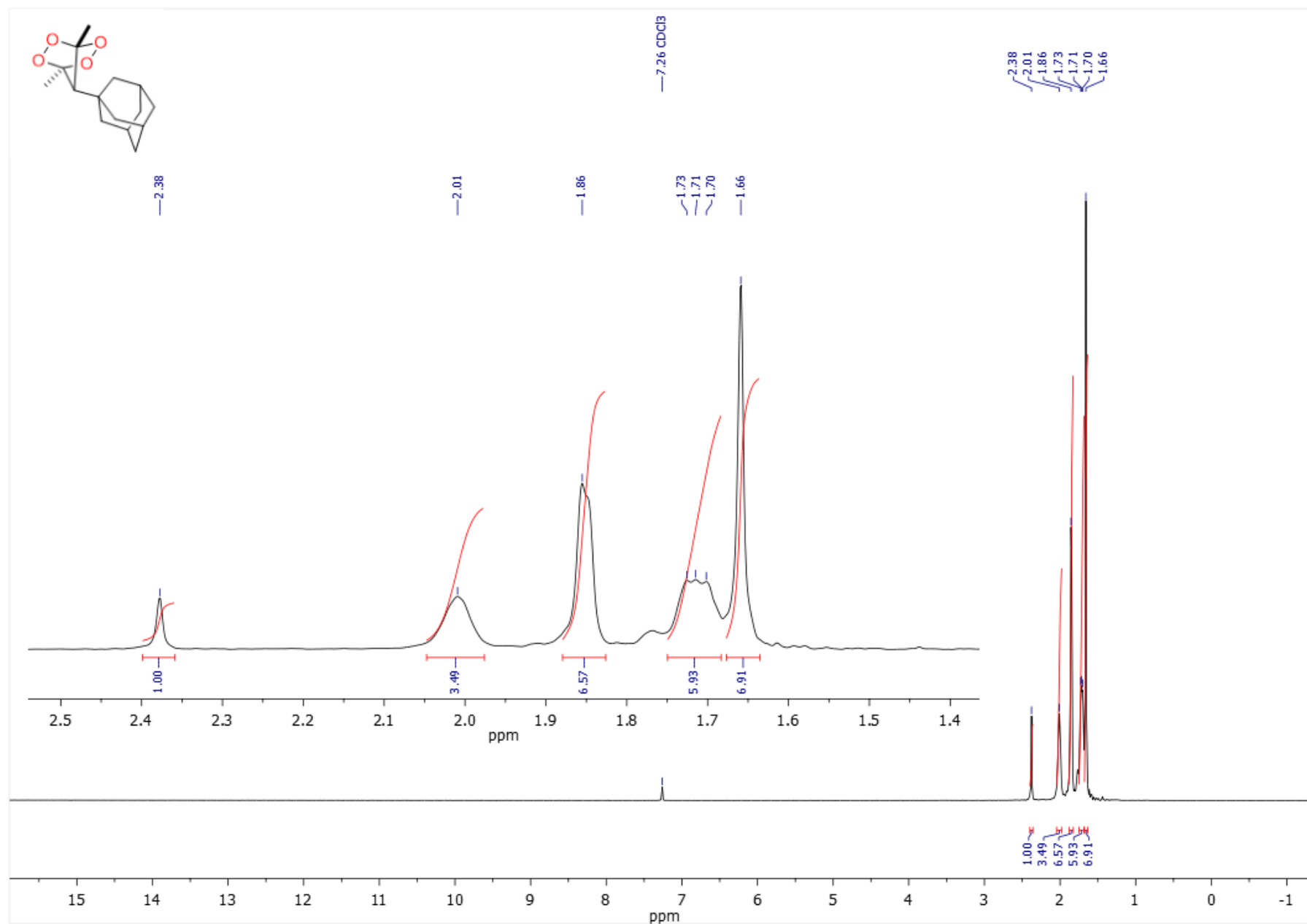
¹H NMR (300.13 MHz, CDCl₃). Ethyl 3-(1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptan-7-yl)propanoate, P6



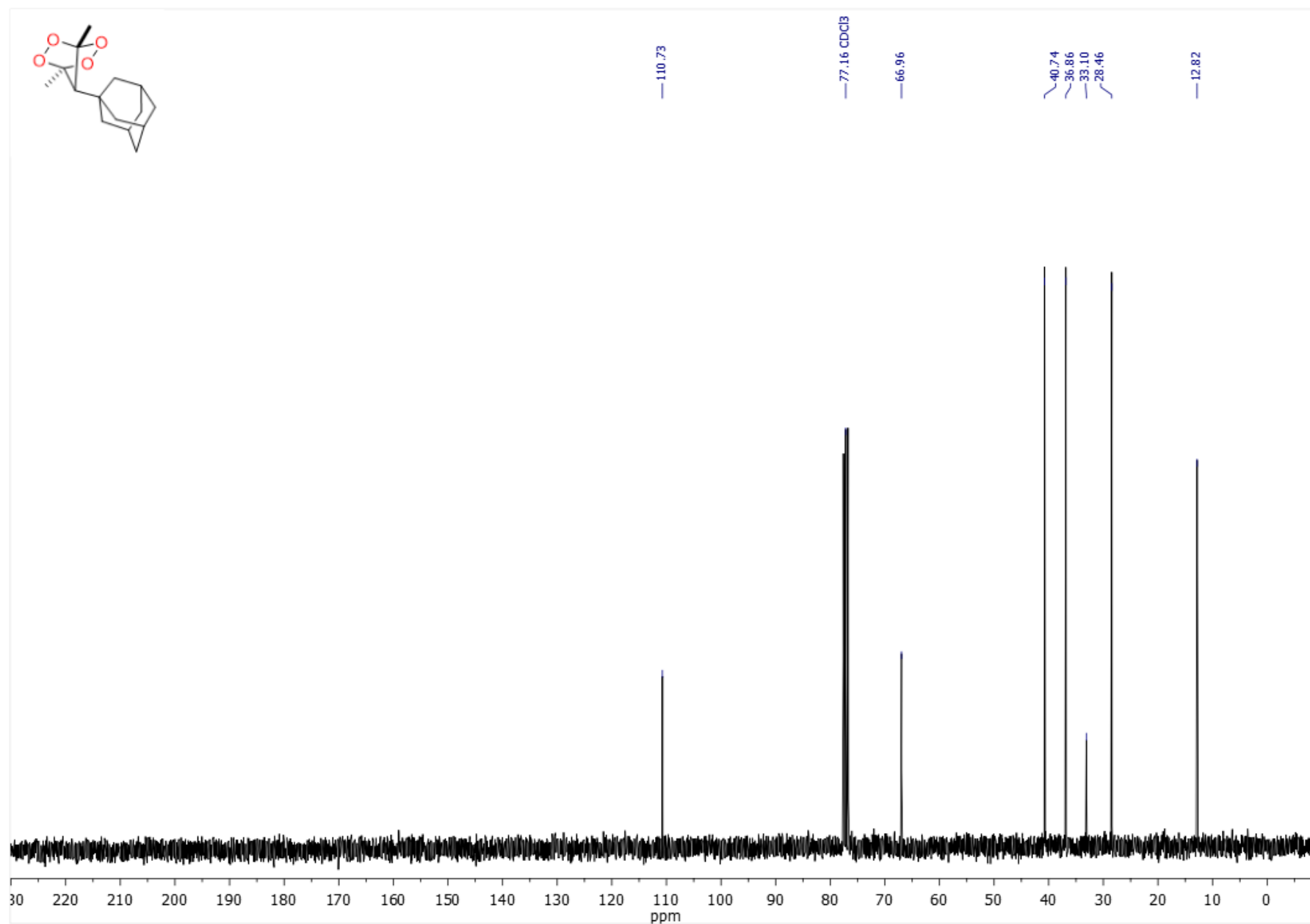
¹³C NMR (75.48 MHz, CDCl₃). Ethyl 3-(1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptan-7-yl)propanoate, P6



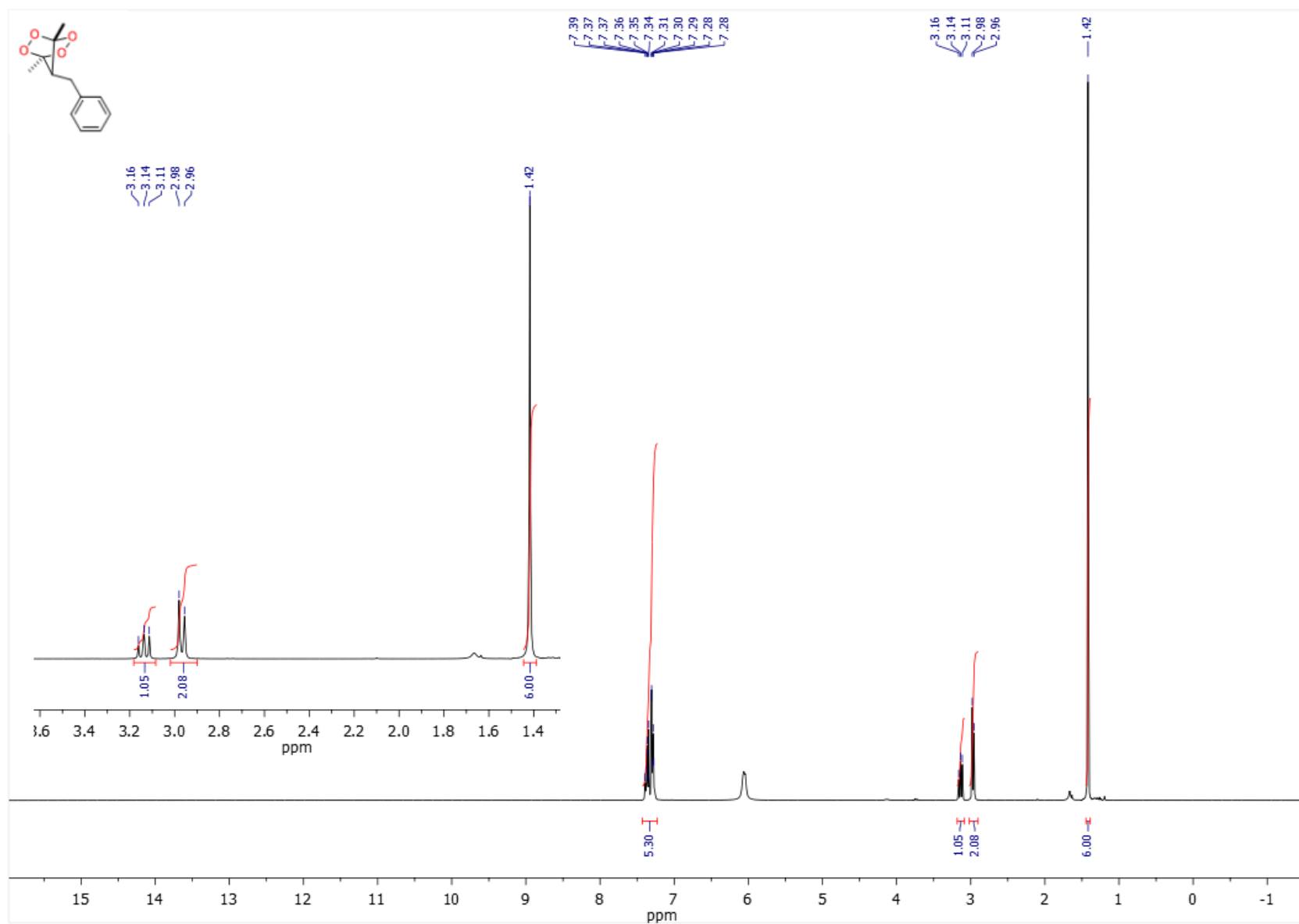
¹H NMR (300.13 MHz, CDCl₃). 7-(Adamantan-1-yl)-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P7



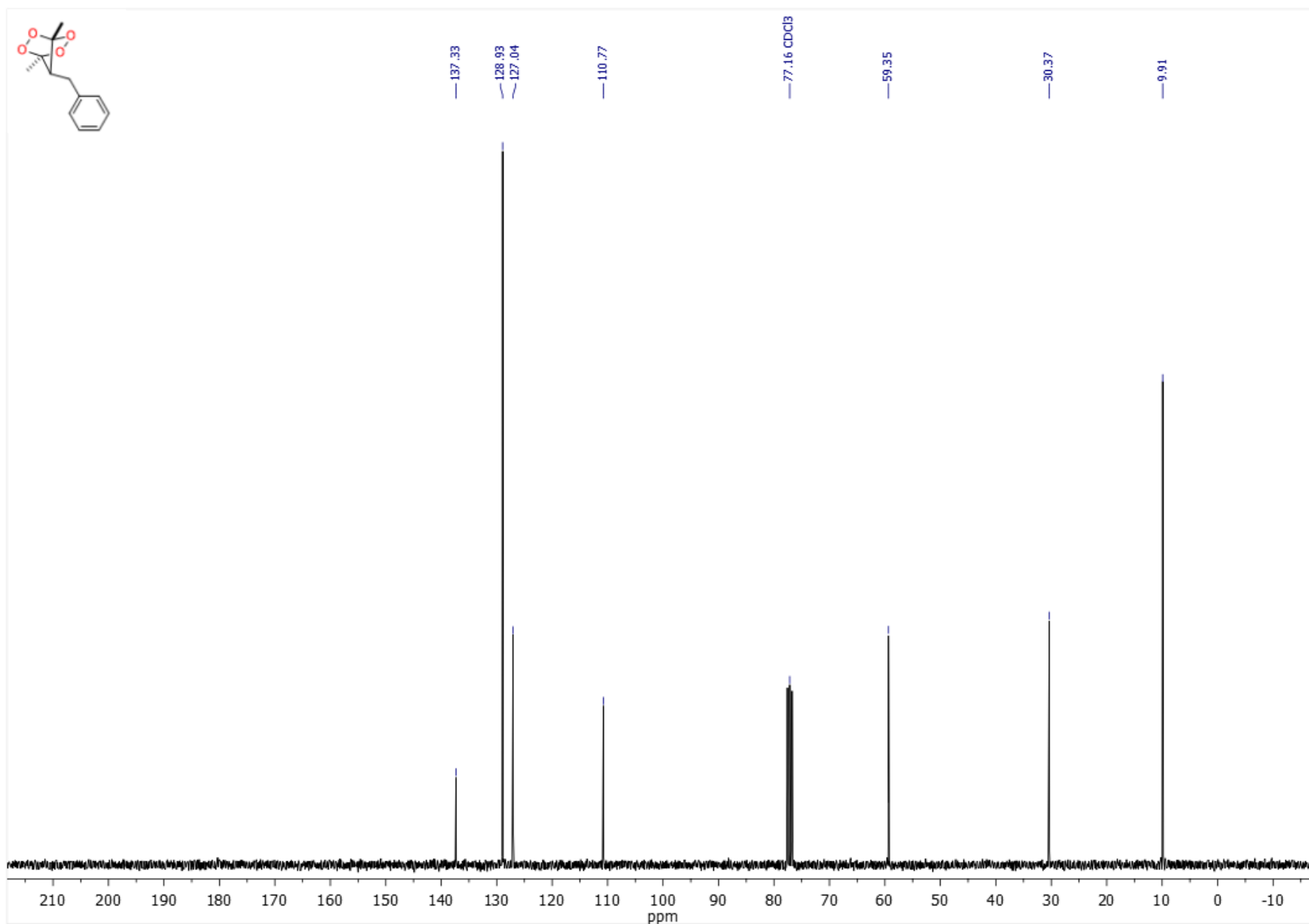
¹³C NMR (75.48 MHz, CDCl₃). 7-(Adamantan-1-yl)-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P7



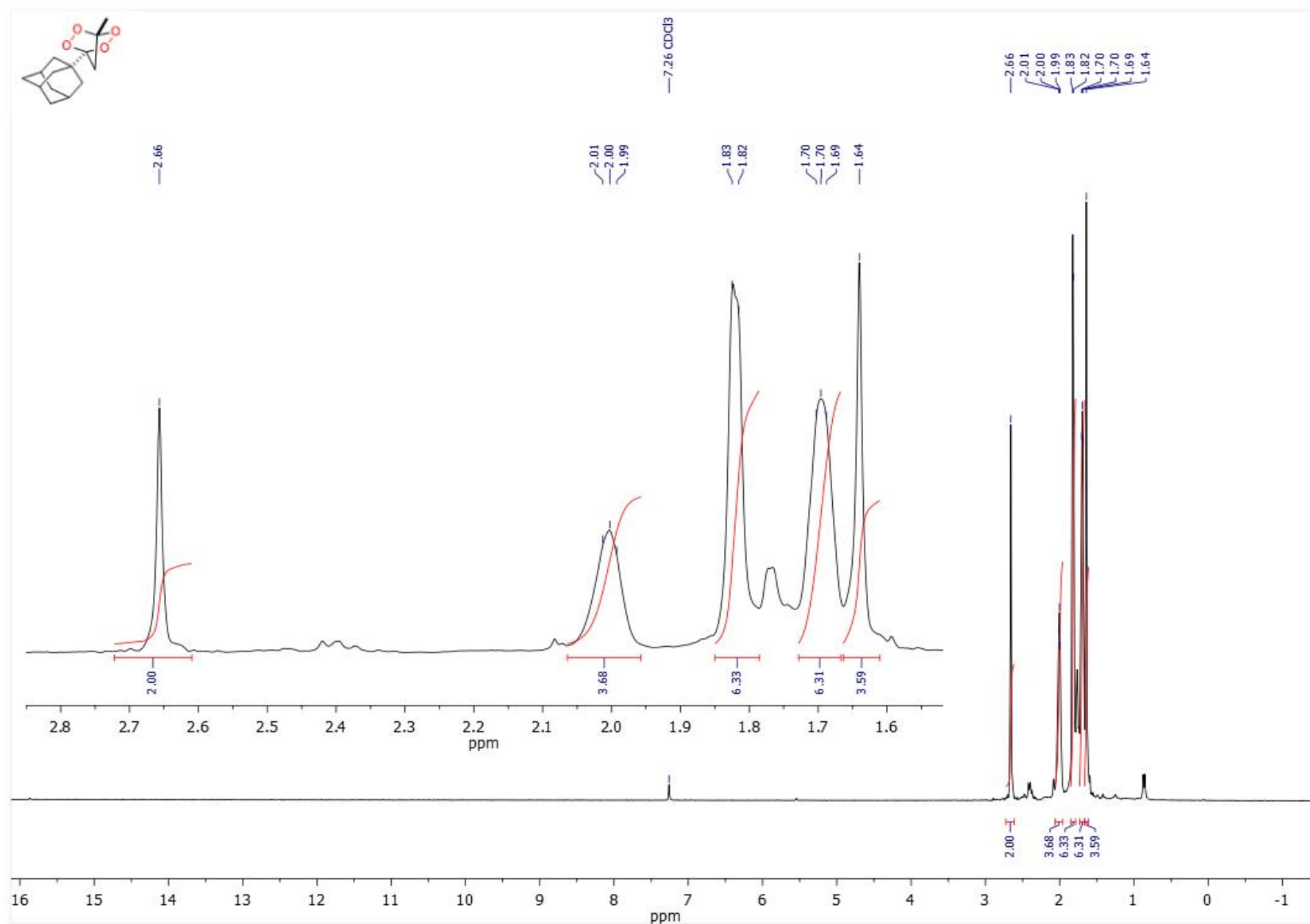
¹H NMR (300.13 MHz, CDCl₃). 7-benzyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P8



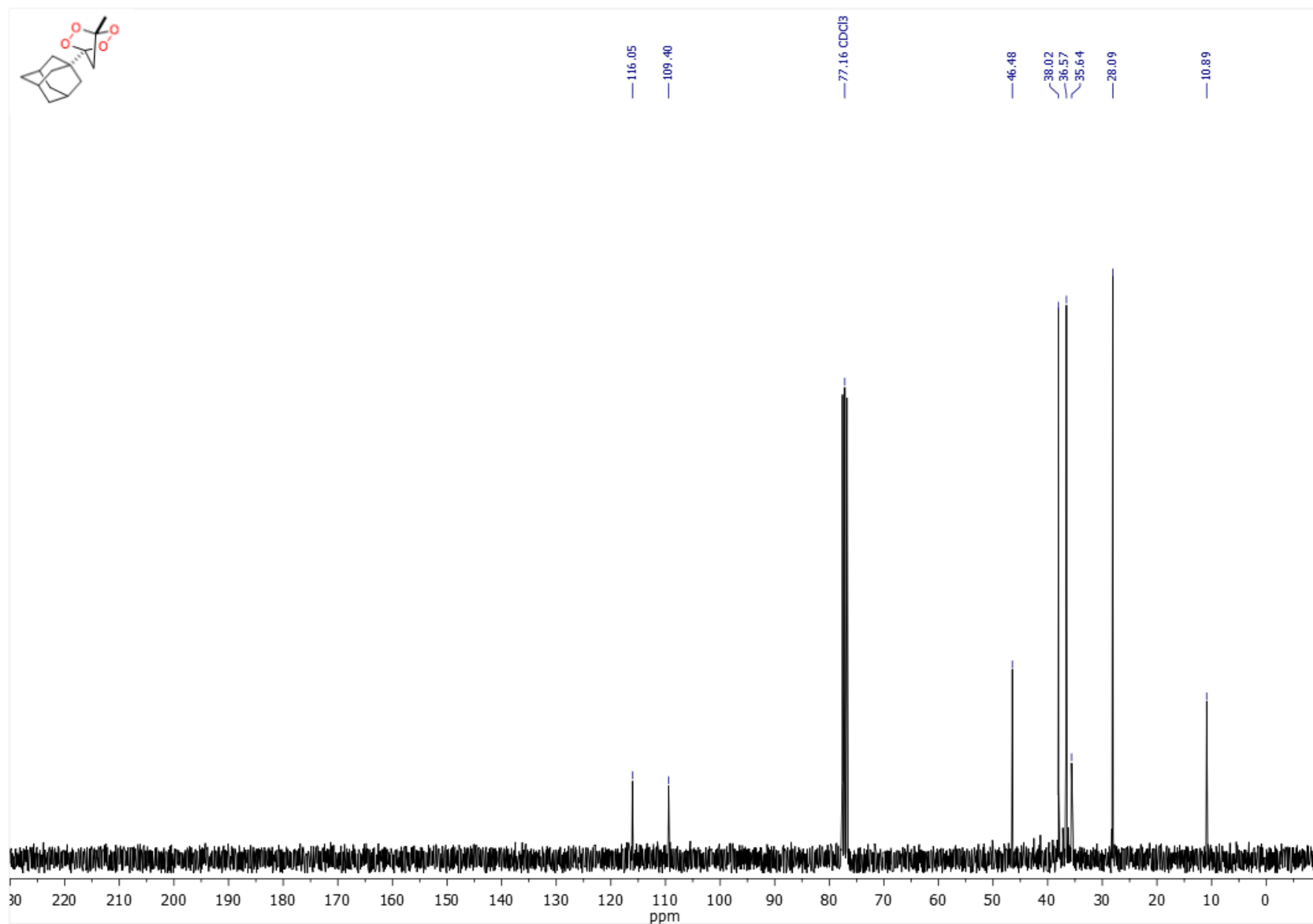
¹³C NMR (75.48 MHz, CDCl₃). 7-benzyl-1,4-dimethyl-2,3,5,6-tetraoxabicyclo[2.2.1]heptane, P8



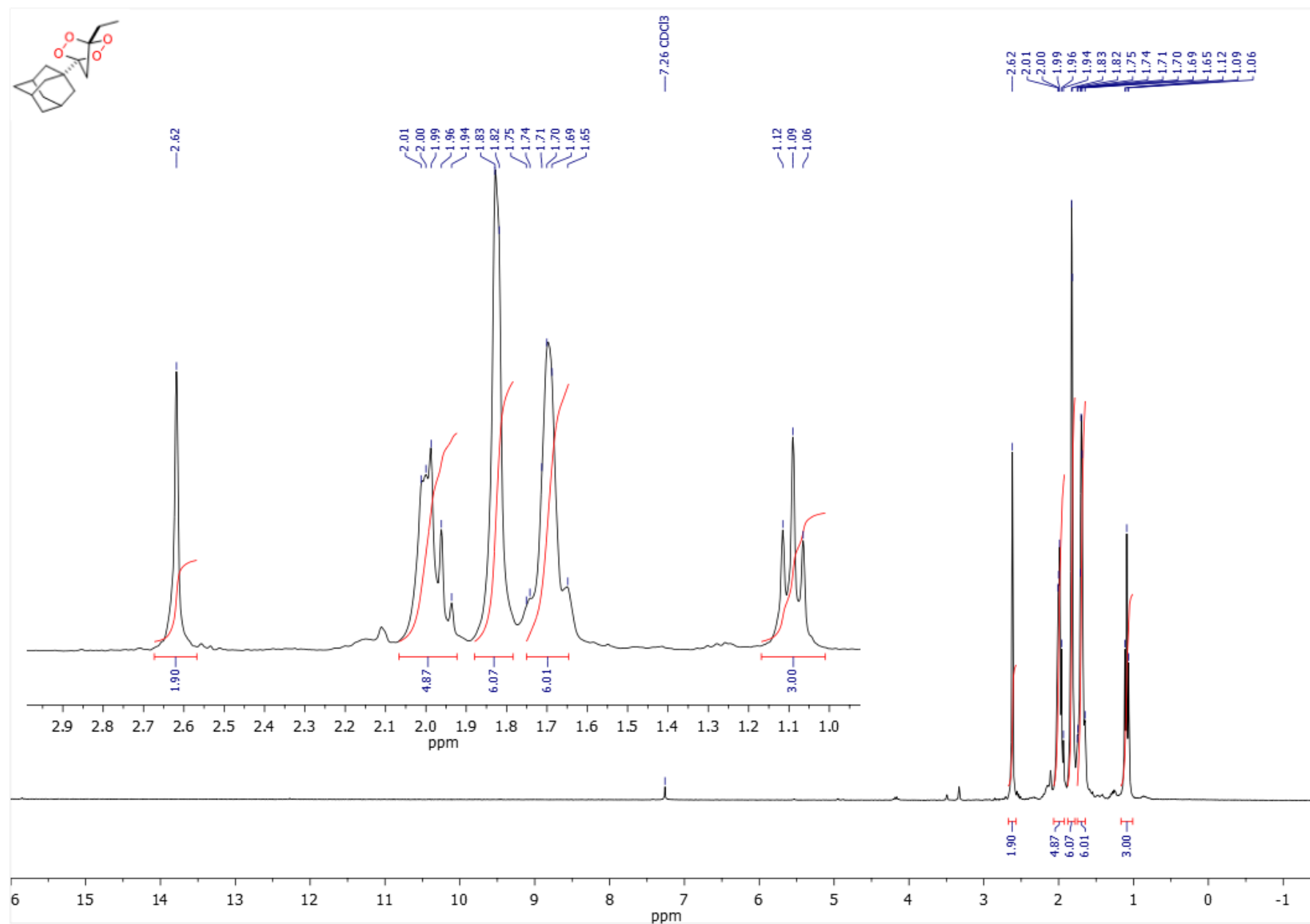
¹H NMR (300.13 MHz, CDCl₃). 4-(1-Adamantyl)-1-methyl-2,3,5,6-tetraoxabicyclo- [2.2.1]heptane, P9



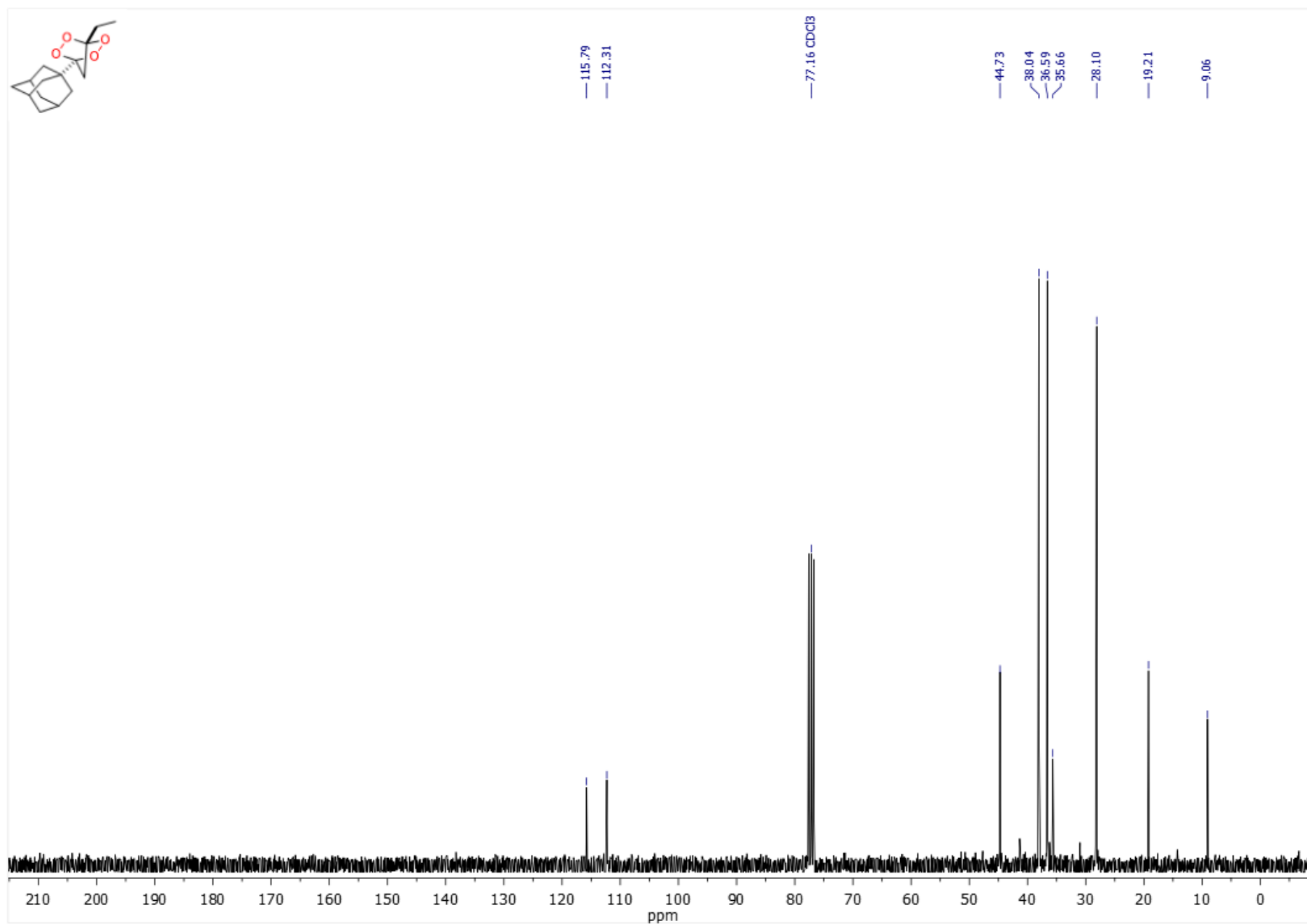
¹³C NMR (75.48 MHz, CDCl₃). 4-(1-Adamantyl)-1-methyl-2,3,5,6-tetraoxabicyclo- [2.2.1]heptane, P9



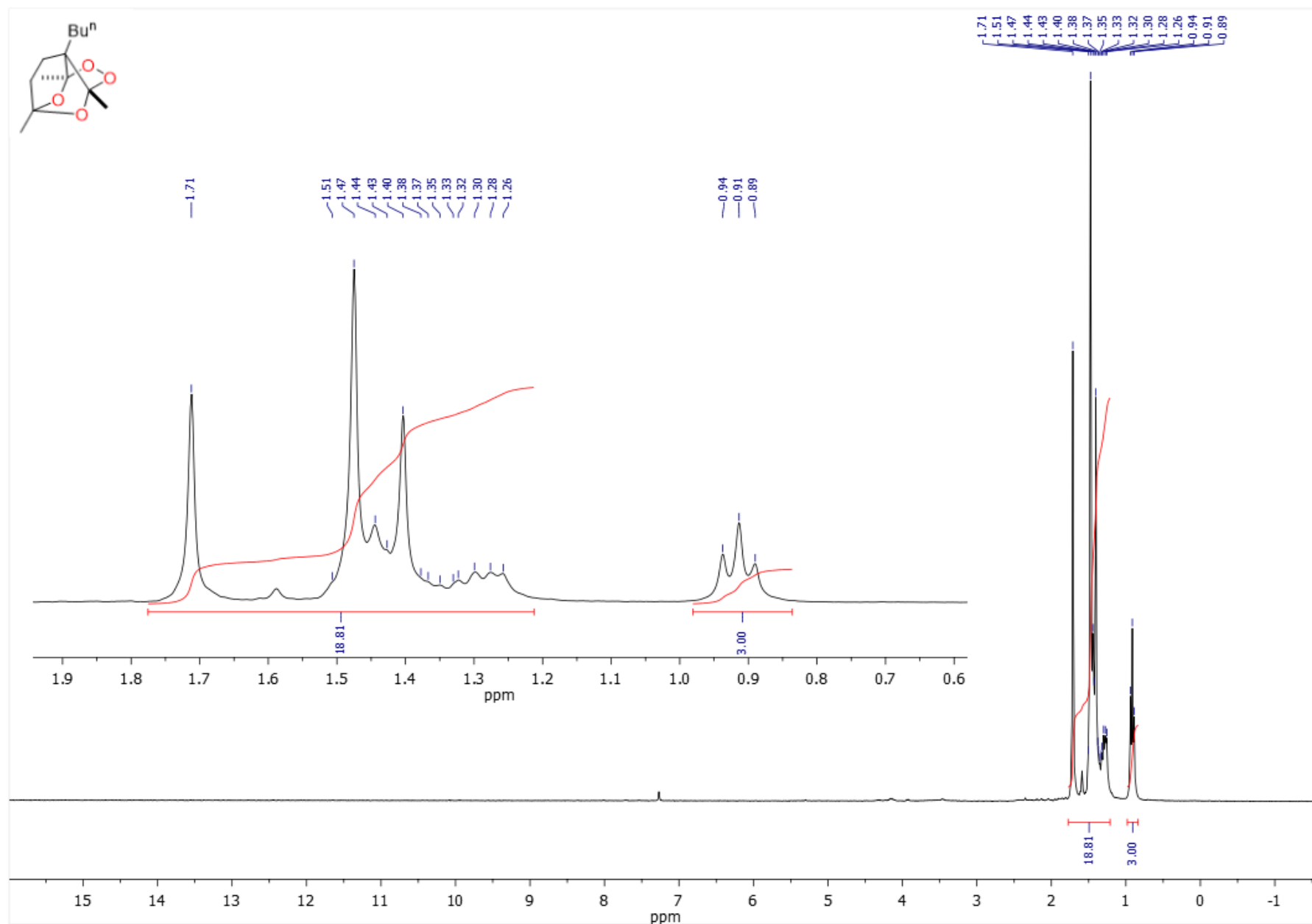
¹H NMR (300.13 MHz, CDCl₃). 4-(1-Adamantyl)-1-ethyl-2,3,5,6-tetraoxabicyclo[2.2.1]-heptane, P10



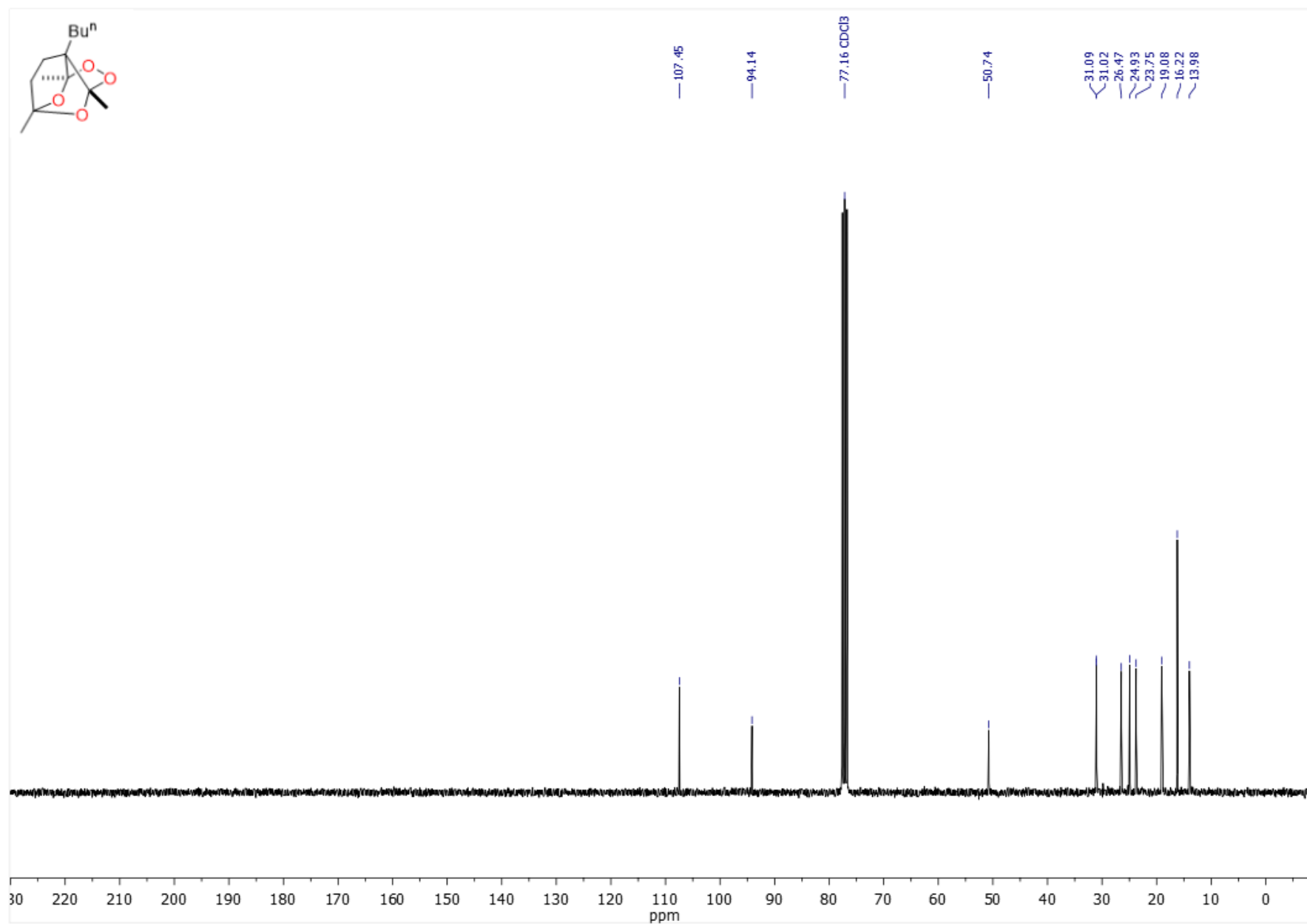
¹³C NMR (75.48 MHz, CDCl₃). 4-(1-Adamantyl)-1-ethyl-2,3,5,6-tetraoxabicyclo[2.2.1]-heptane, P10



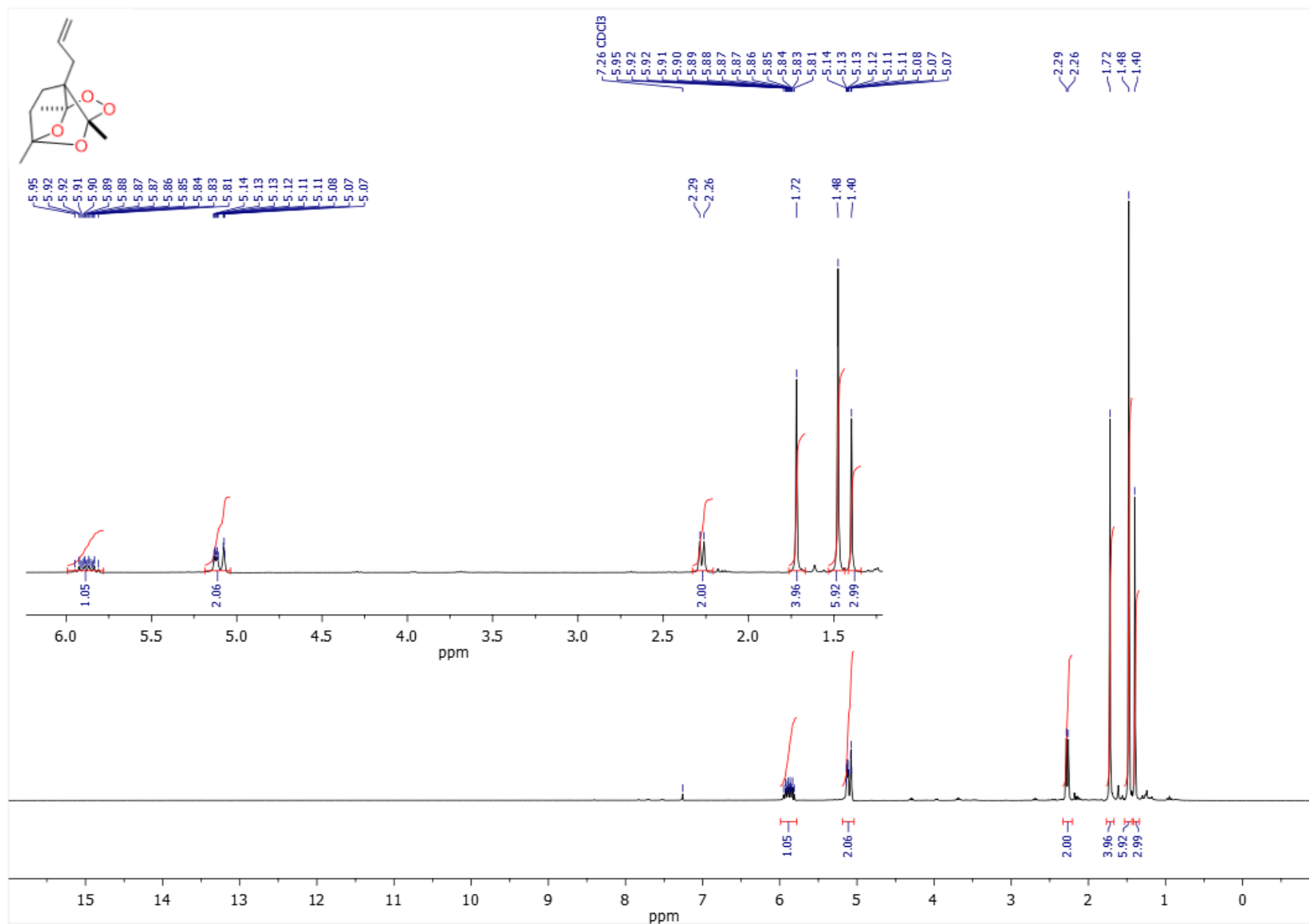
¹H NMR (300.13 MHz, CDCl₃). 3a-Butyl-3,6,7a-trimethyltetrahydro-3H,4H-3,6-epoxy[1,2]- dioxolo[3,4-b]pyran, P11



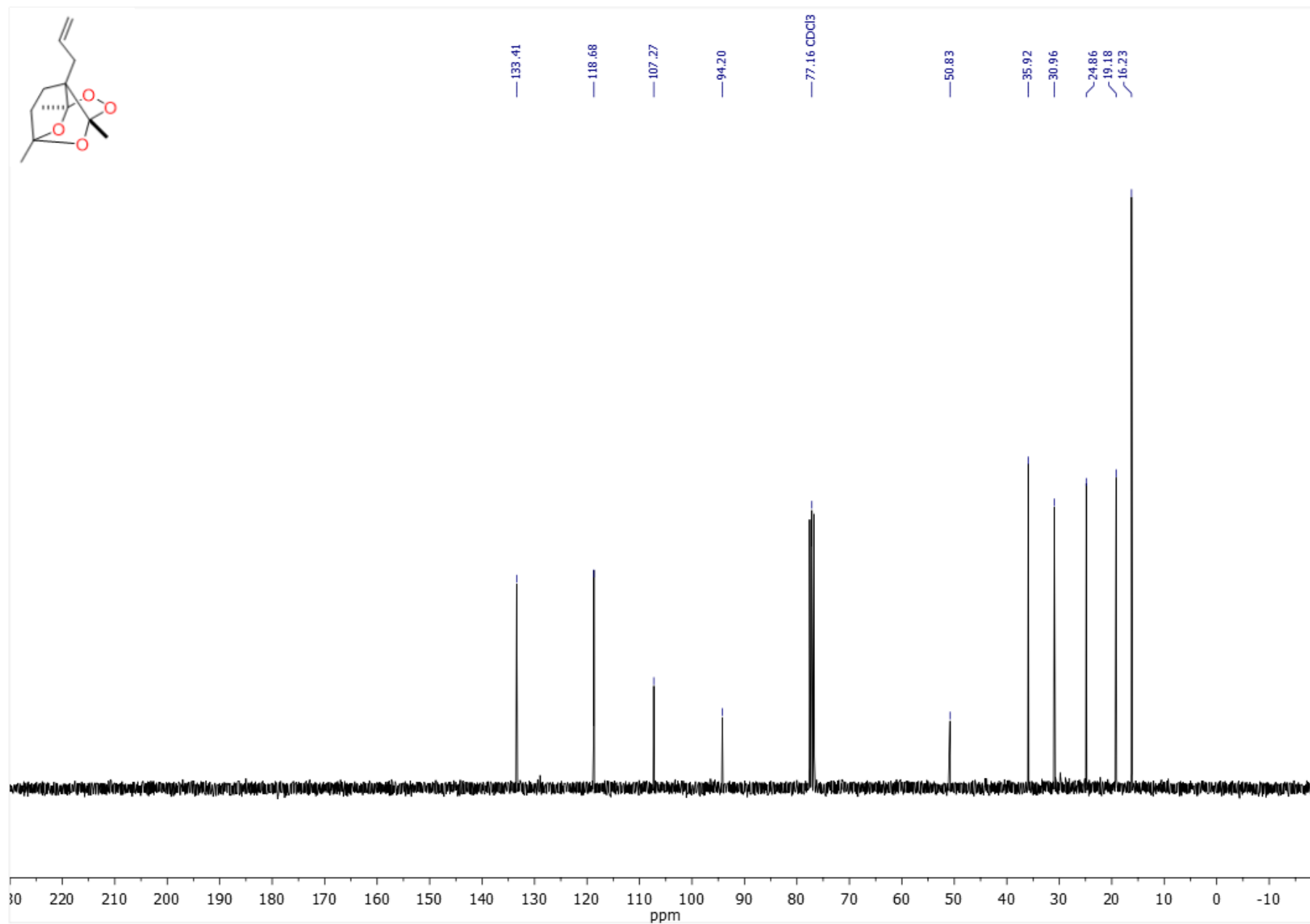
^{13}C NMR (75.48 MHz, CDCl_3). 3a-Butyl-3,6,7a-trimethyltetrahydro-3H,4H-3,6-epoxy[1,2]-dioxolo[3,4-b]pyran, P11



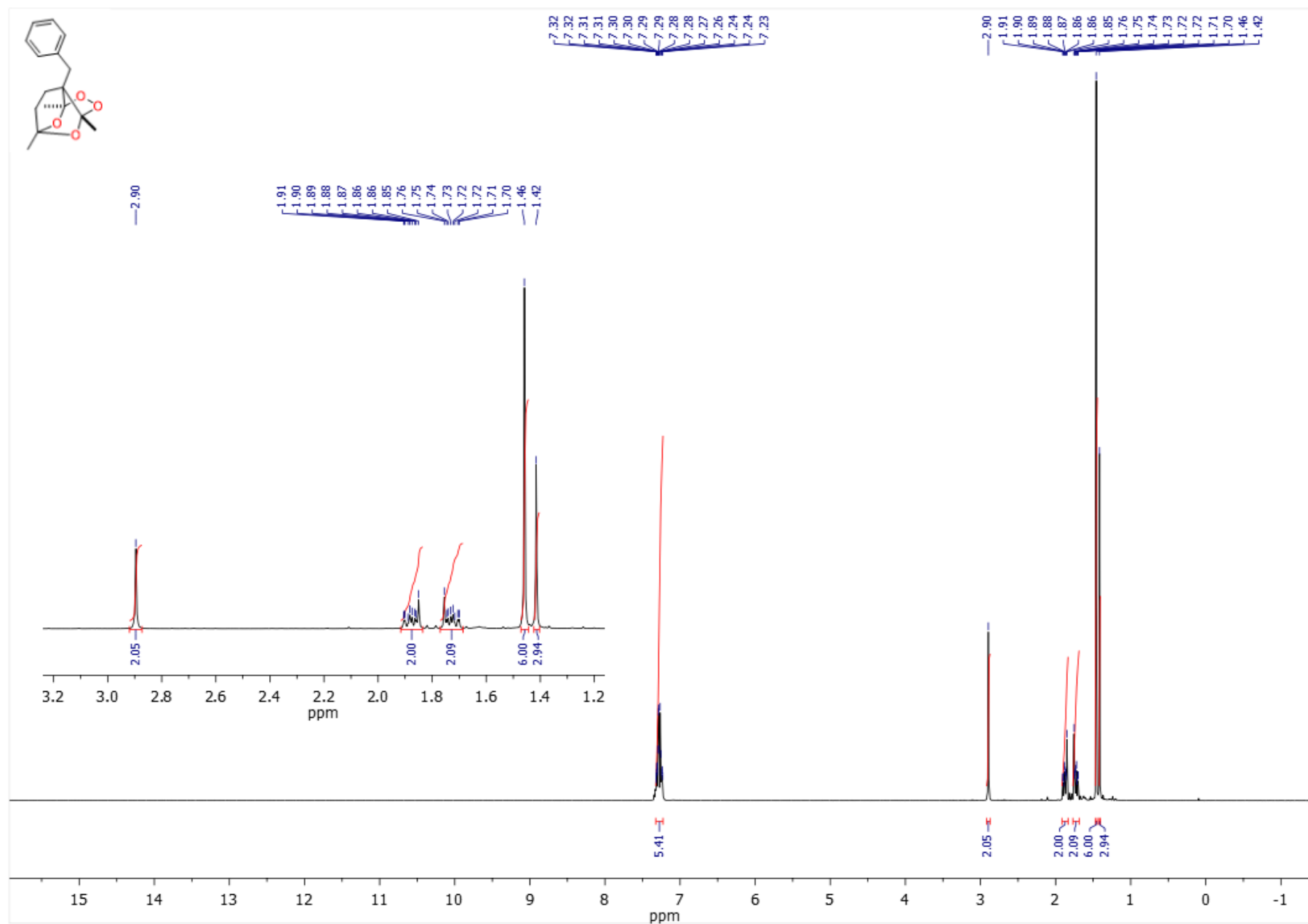
¹H NMR (300.13 MHz, CDCl₃). 3a-Allyl-3,6,7a-trimethyltetrahydro-3H,4H-3,6-epoxy[1,2]- dioxolo[3,4-b]pyran, P12



¹³C NMR (75.48 MHz, CDCl₃). 3a-Allyl-3,6,7a-trimethyltetrahydro-3H,4H-3,6-epoxy[1,2]- dioxolo[3,4-b]pyran, P12



¹H NMR (300.13 MHz, CDCl₃). 3a-benzyl-3,6,7a-trimethyltetrahydro-3H,4H-3,6-epoxy[1,2]dioxolo[3,4-b]pyran, P13



¹³C NMR (75.48 MHz, CDCl₃). 3a-benzyl-3,6,7a-trimethyltetrahydro-3H,4H-3,6-epoxy[1,2]dioxolo[3,4-b]pyran, P13

