

**Unexpected formation of bicyclo[3.2.0]heptane topology products in the reaction of
2,3,5-trichloro-4,4-ethylenedioxcyclopent-4-en-1-one with alkyl acrylates under
Heck reaction conditions**

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SUPPLEMENTARY MATERIAL

NMR-data

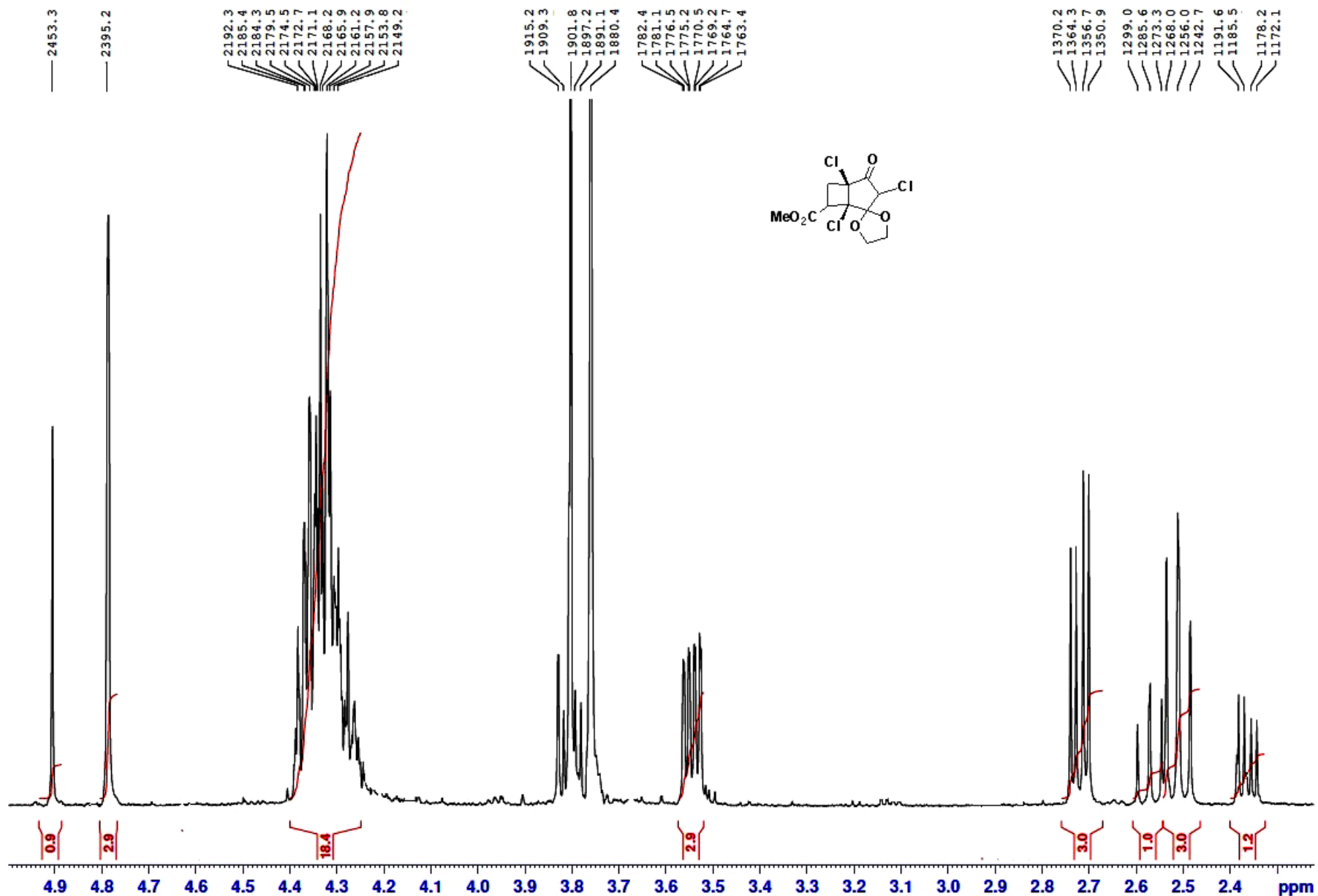


Figure S1. Complete ¹H NMR spectrum of compound 4a in CDCl₃, 500MHz

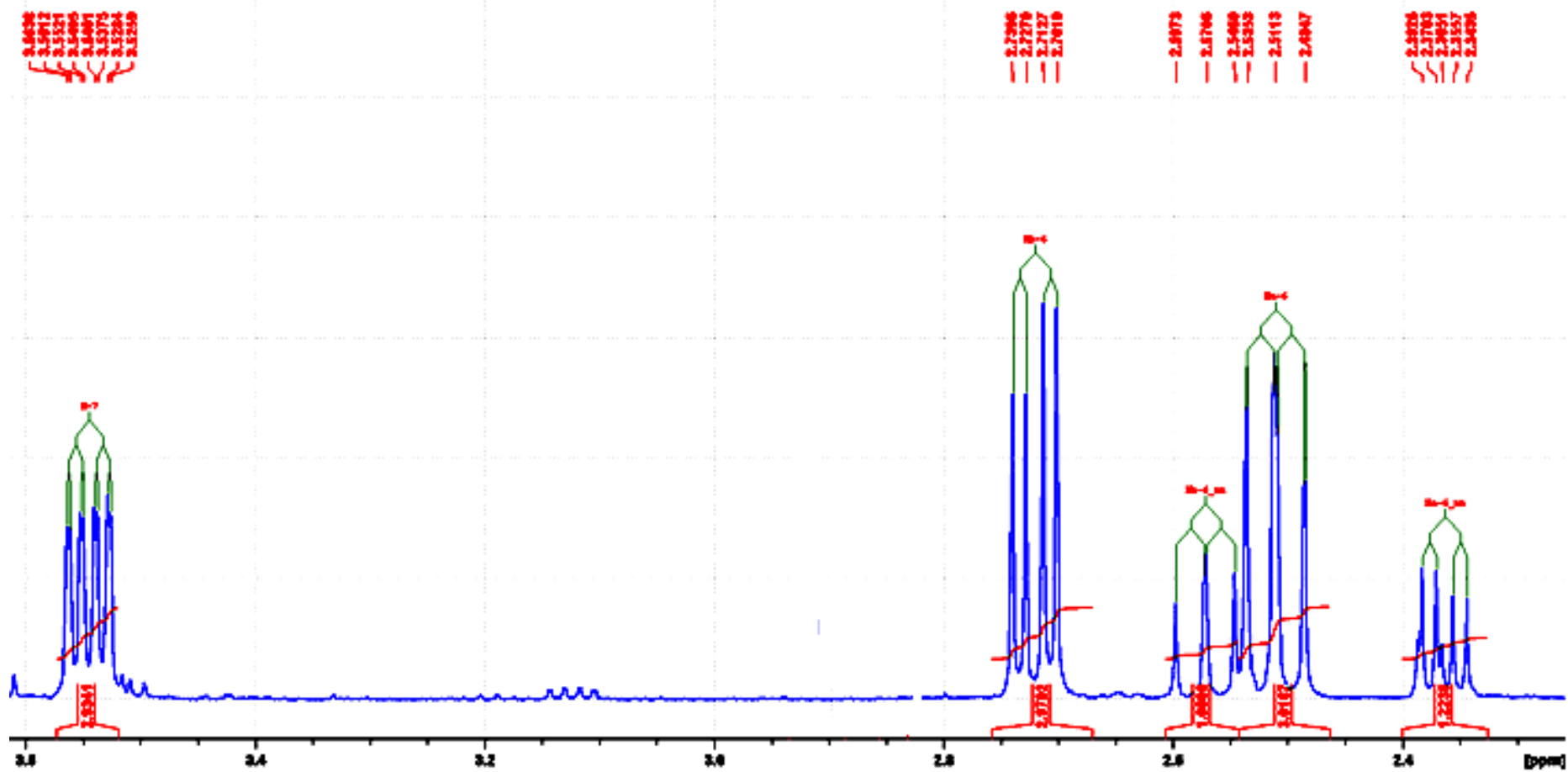
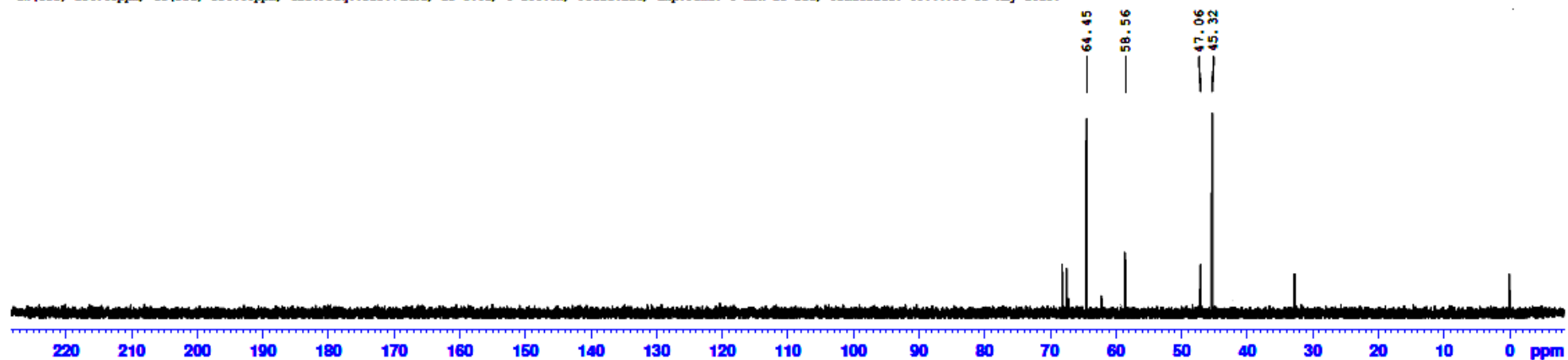


Figure S2. Expanded ¹H NMR spectrum of compound 4a in CDCl₃, 500 MHz

Sp-404 Egorov V-1126(31) 12mg in CDCl₃, TMS 13C{1H} dept90 AV500 13.05.2025 LAN

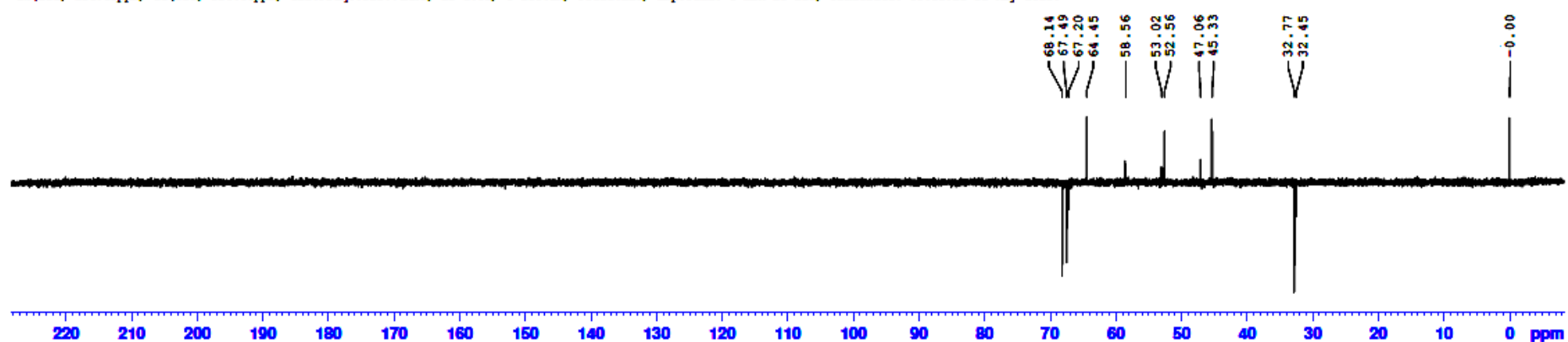
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SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=3.0s; T=298.9K; Probe:BBQ; Exp.Time: 9 min 25 sec; Time4Date: 09:44:50 13 May 2025.



Sp-404 Egorov V-1126(31) 12mg in CDCl₃, TMS 13C{1H} dept135 AV500 13.05.2025 LAN

SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=299.2K; Probe:BBQ; Exp.Time: 9 min 28 sec; Time4Date: 09:35:23 13 May 2025.



Sp-404 Egorov V-1126(31) 12mg in CDCl₃, TMS 13C{1H} com AV500 13.05.2025 LAN

SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=0.9s; T=299.7K; Probe:BBQ; Exp.Time:35 min 14 sec; Time4Date: 09:25:52 13 May 2025.

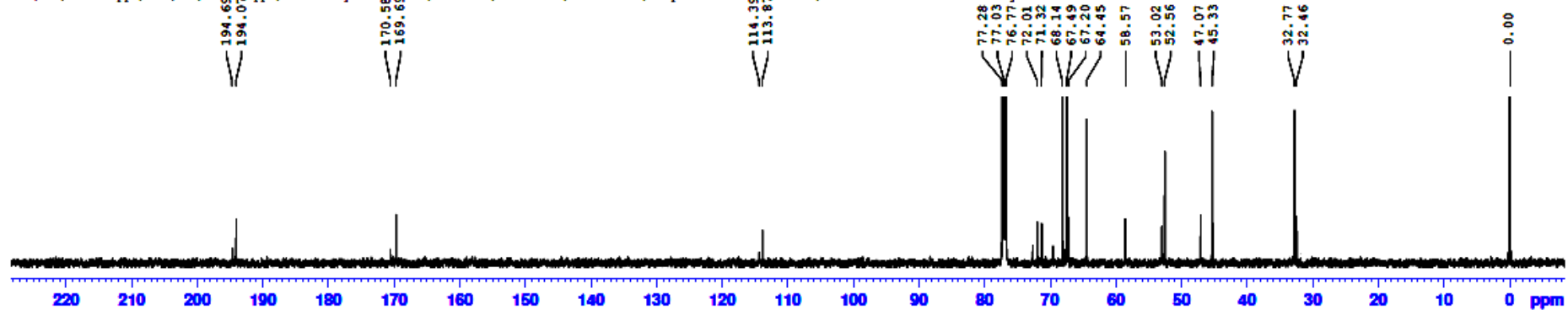
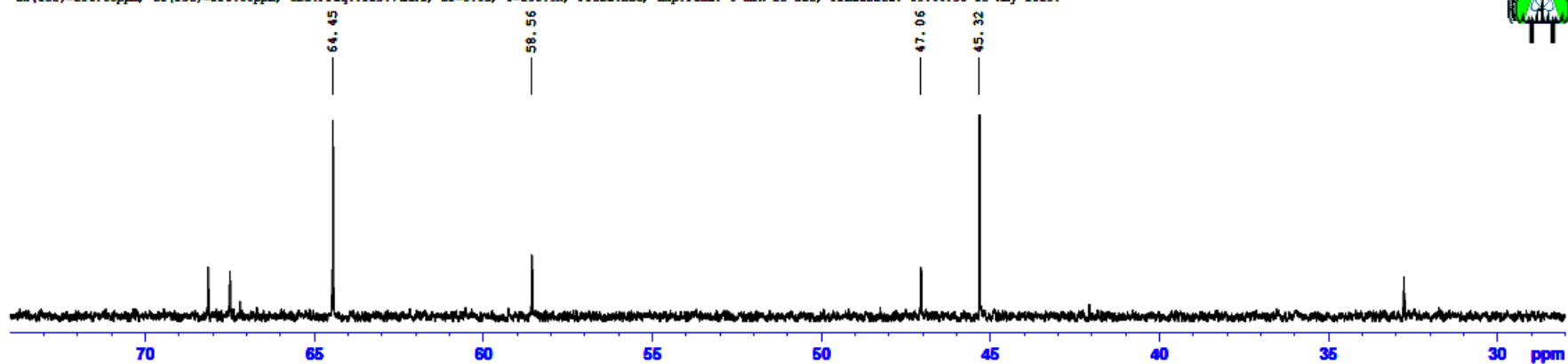


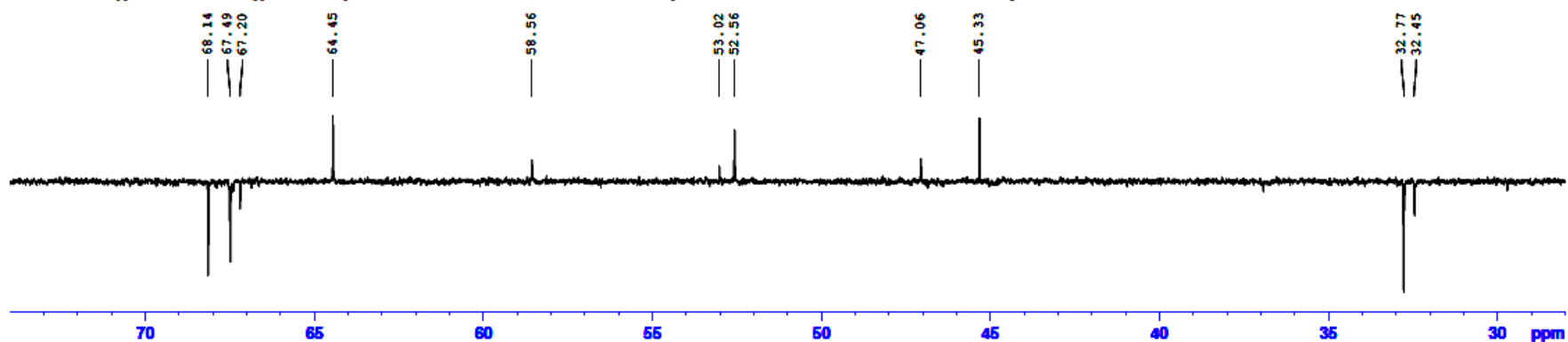
Figure S3. ¹³C{¹H}, DEPT-135 and DEPT-90 spectra of compound 4a in CDCl₃, 125 MHz

Sp-404 Egorov V-1126(31) 12mg in CDCl₃, TMS 13C{1H} dept90 AV500 13.05.2025 LAN
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=3.0s; T=298.9K; Probe:BBQ; Exp.Time: 9 min 25 sec; Time&Date: 09:44:50 13 May 2025.

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Sp-404 Egorov V-1126(31) 12mg in CDCl₃, TMS 13C{1H} dept135 AV500 13.05.2025 LAN
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=1.0s; T=299.2K; Probe:BBQ; Exp.Time: 9 min 28 sec; Time&Date: 09:35:23 13 May 2025.



Sp-404 Egorov V-1126(31) 12mg in CDCl₃, TMS 13C{1H} com AV500 13.05.2025 LAN
SW(13C)=236.63ppm; O1(13C)=110.00ppm; Obs.Freq.:125.76MHz; D1=0.9s; T=299.7K; Probe:BBQ; Exp.Time:35 min 14 sec; Time&Date: 09:25:52 13 May 2025.

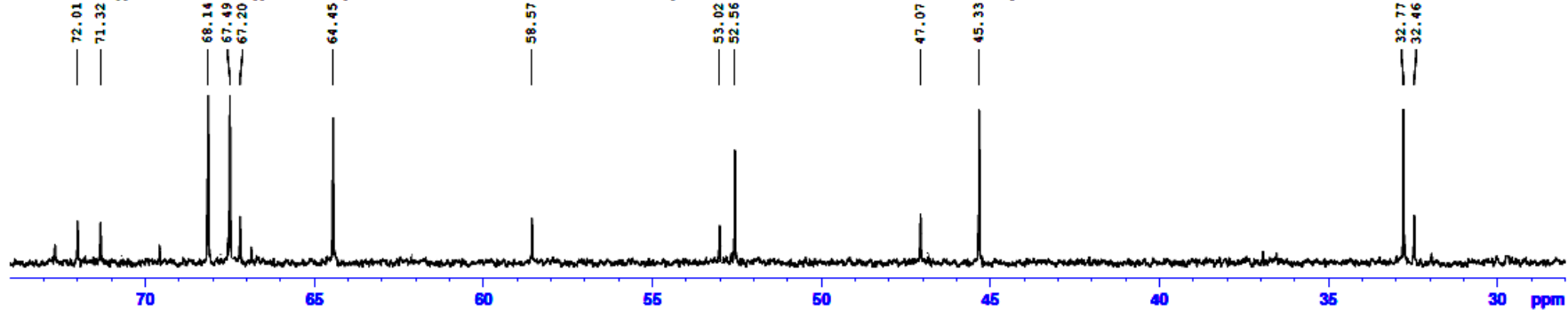


Figure S4. Expanded ¹³C{¹H}, DEPT-135 and DEPT-90 spectra of compound 4a in CDCl₃, 125 MHz

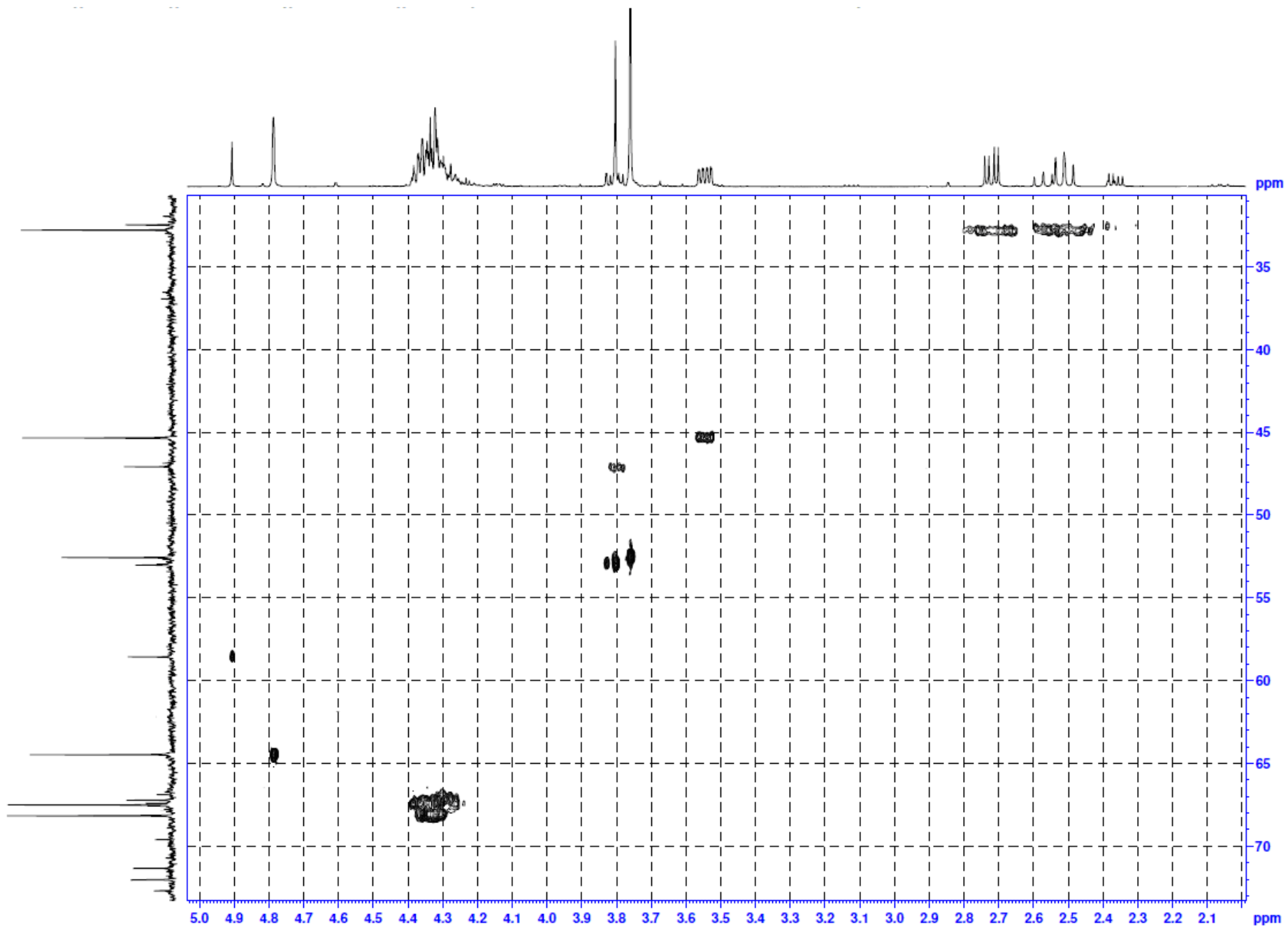


Figure S5. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC spectrum of compound **4a** in CDCl_3 , 500 MHz

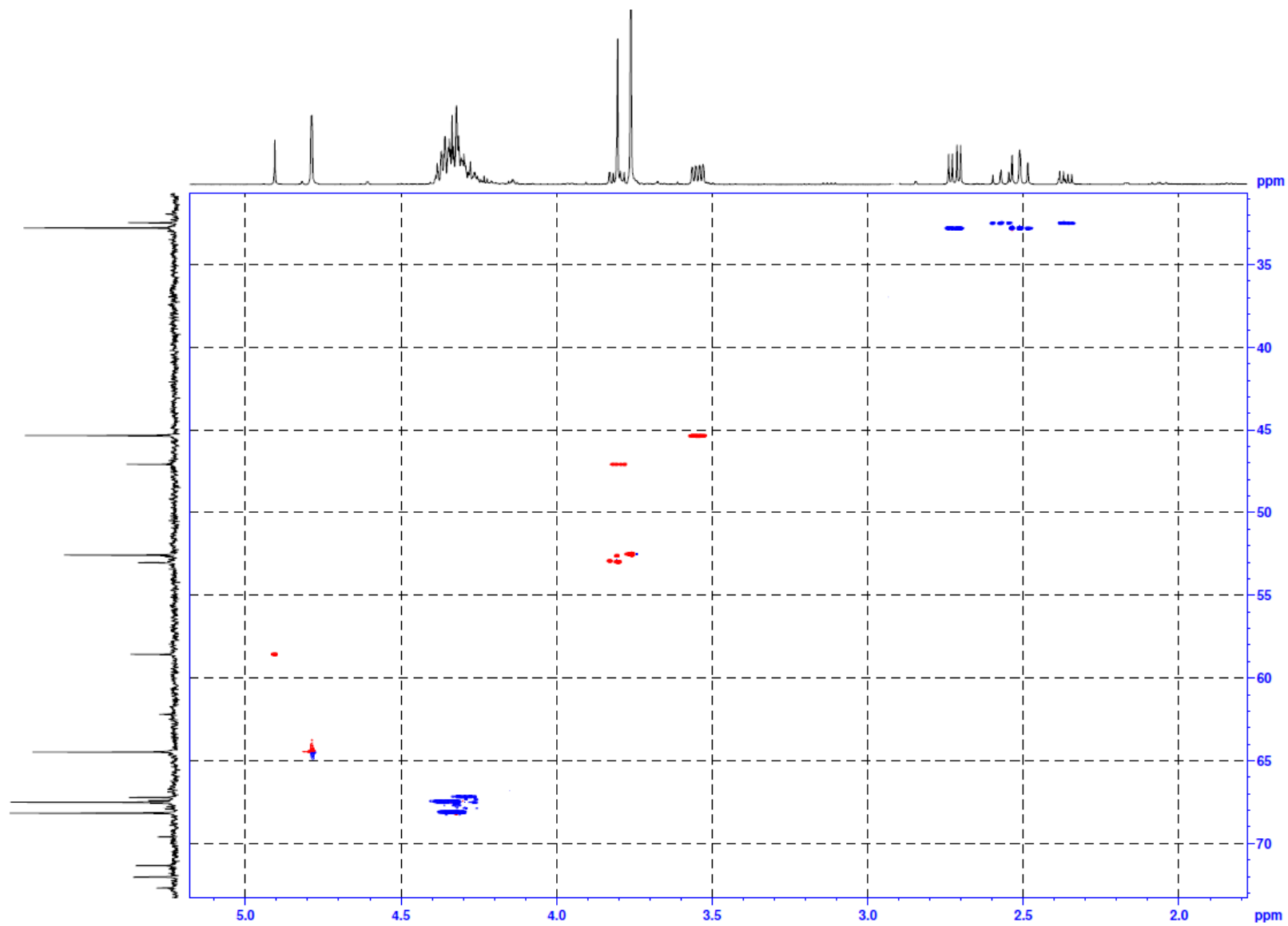


Figure S6. $\{^1\text{H}, ^{13}\text{C}\}$ HSQCED spectrum of compound **4a** in CDCl_3 , 500 MHz

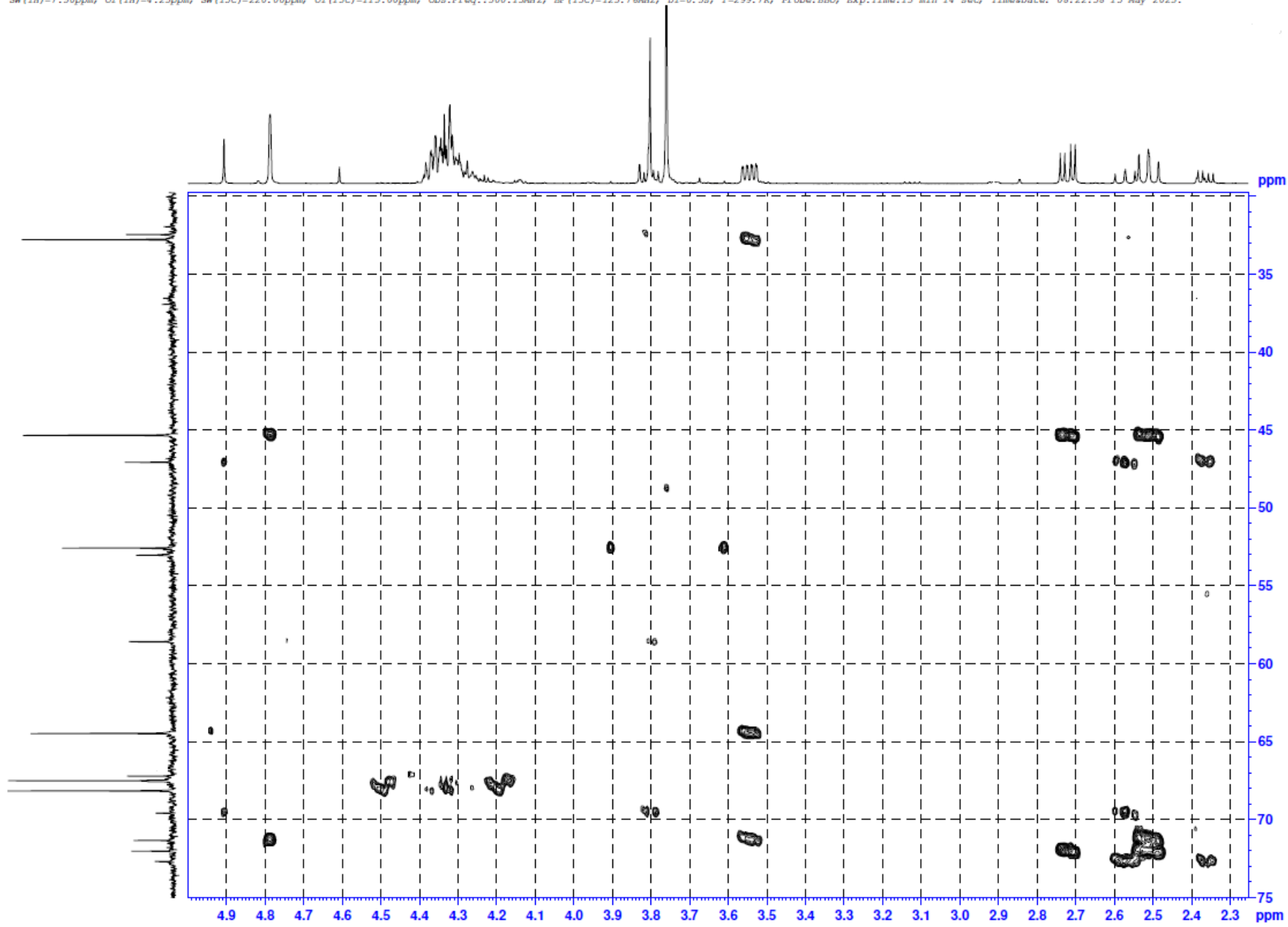


Figure S7. {¹H, ¹³C} HMBS spectrum of compound 4a in CDCl₃, 500 MHz

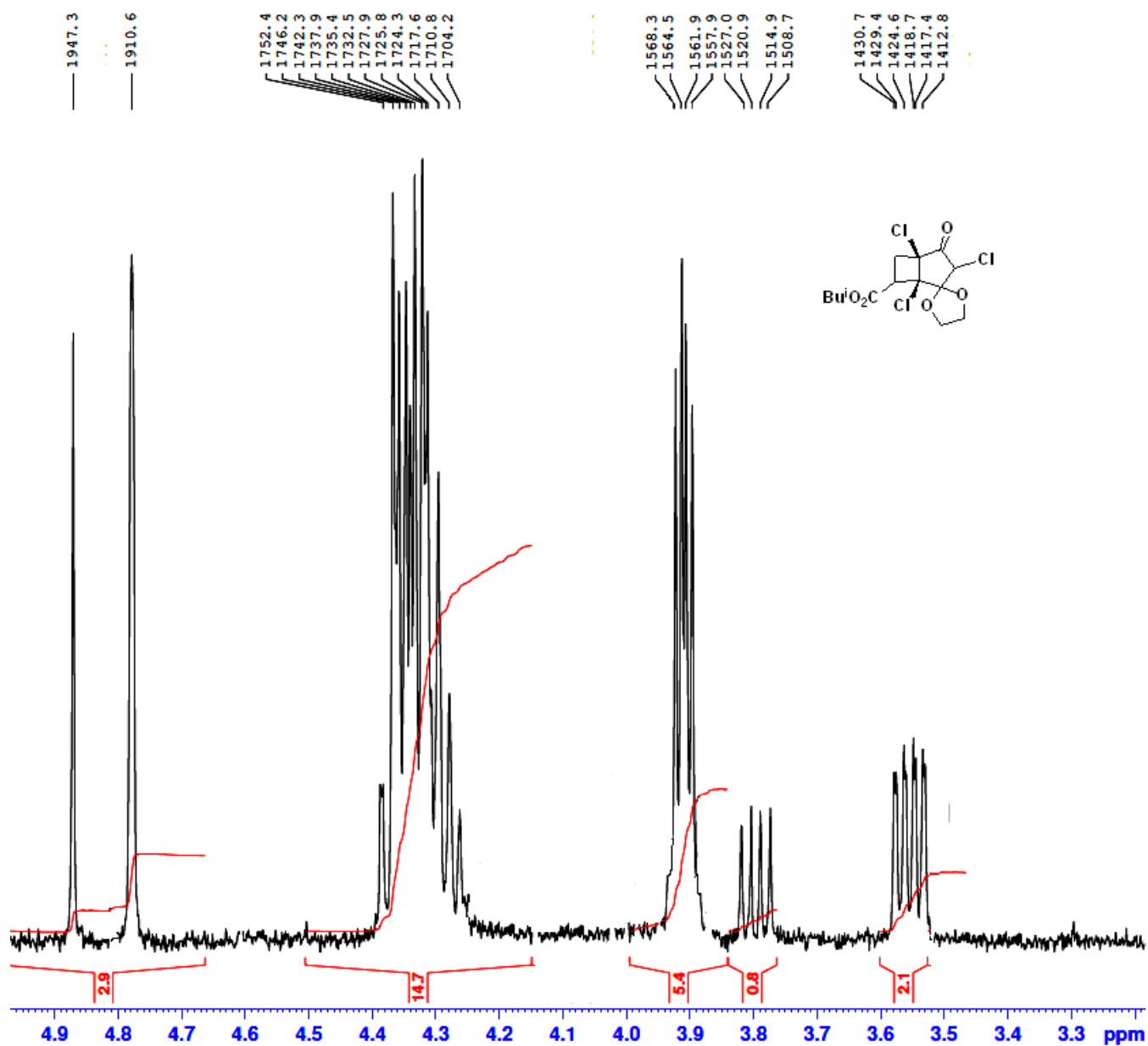


Figure S8. Expanded ¹H NMR spectrum of compound **4b** in CDCl₃, 400 MHz

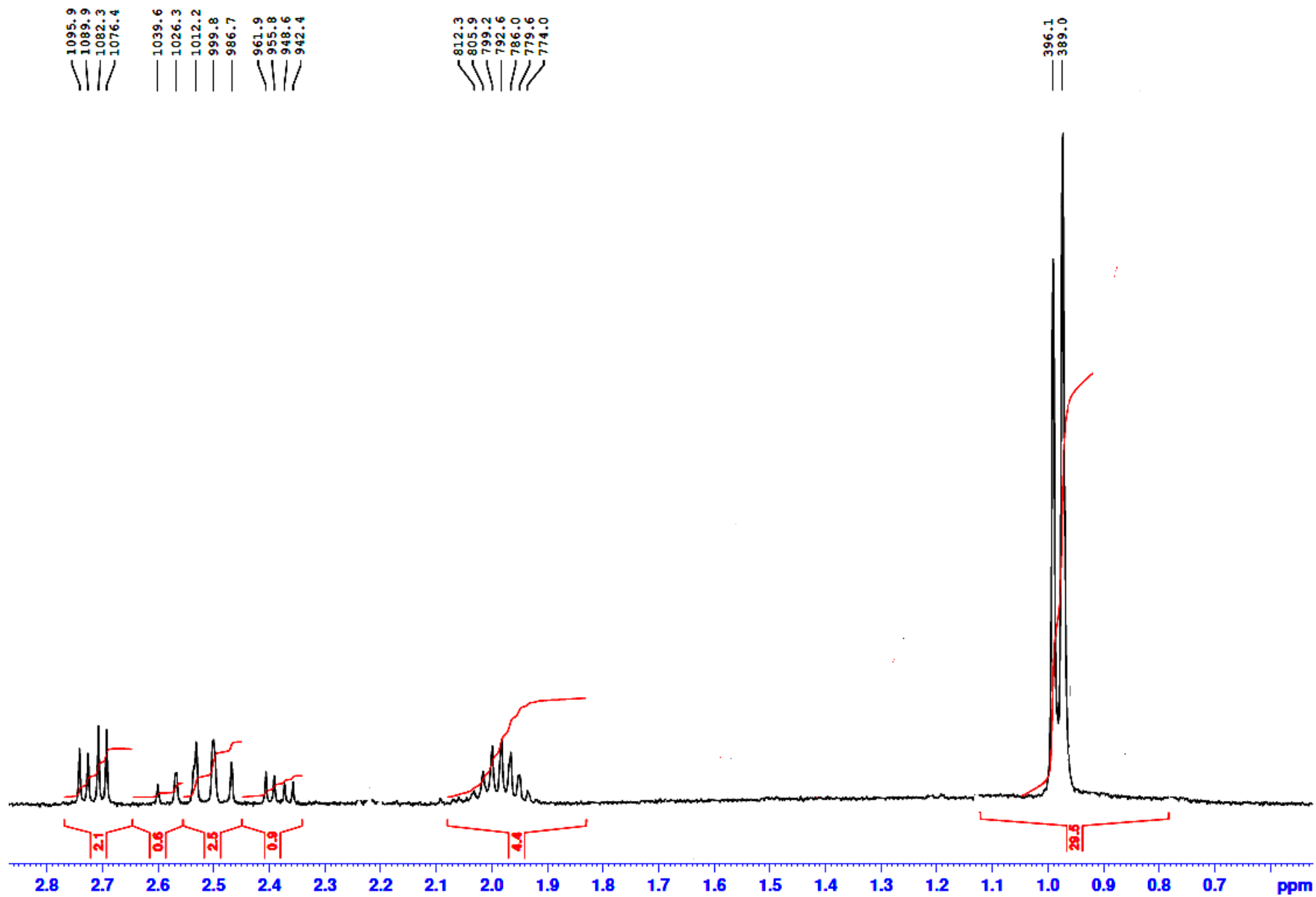


Figure S9. Expanded ¹H NMR spectrum of compound **4b** in CDCl₃, 400 MHz

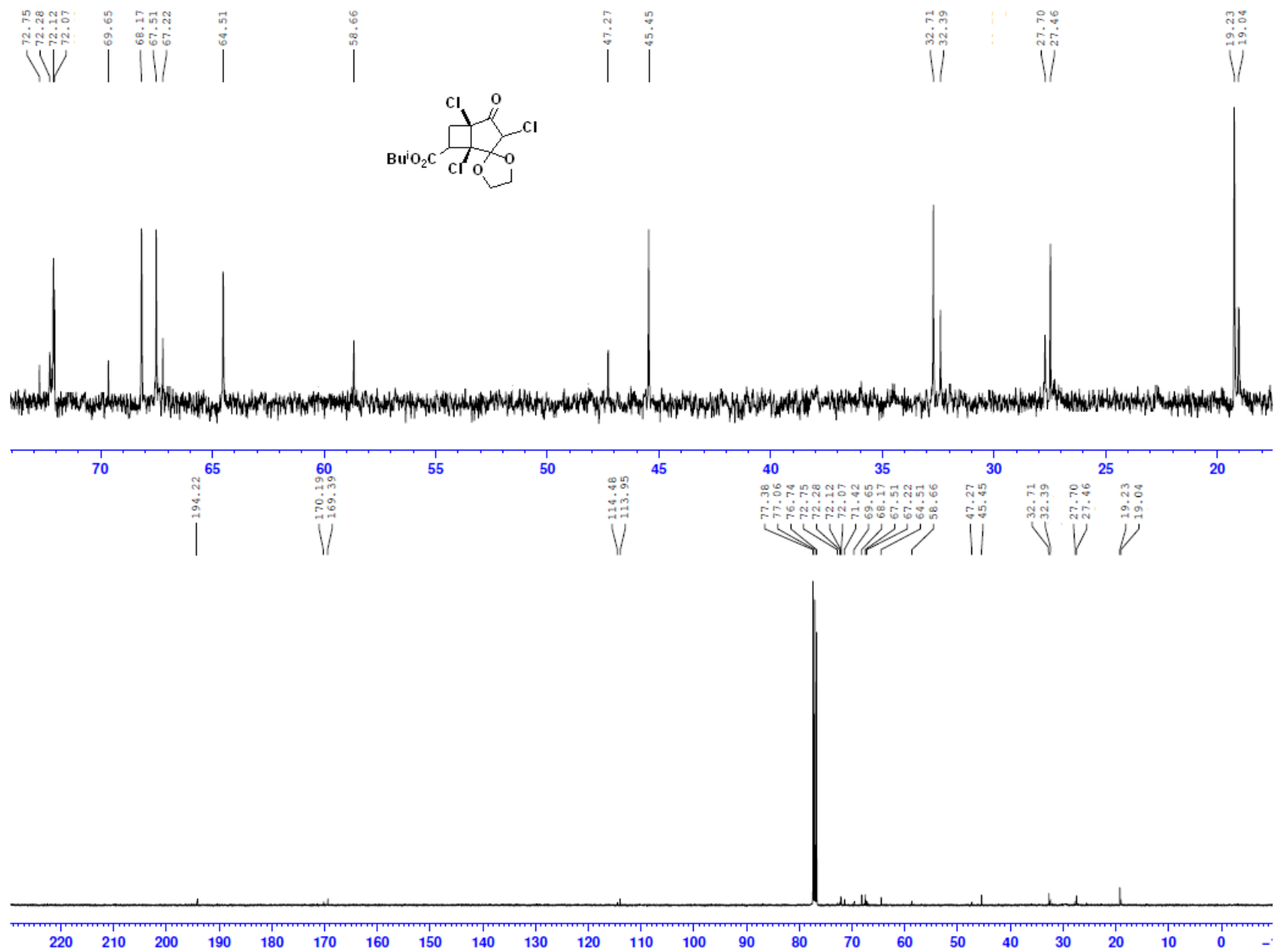


Figure S10. ¹³C{¹H} spectrum of compound **4b** in CDCl₃, 100 MHz

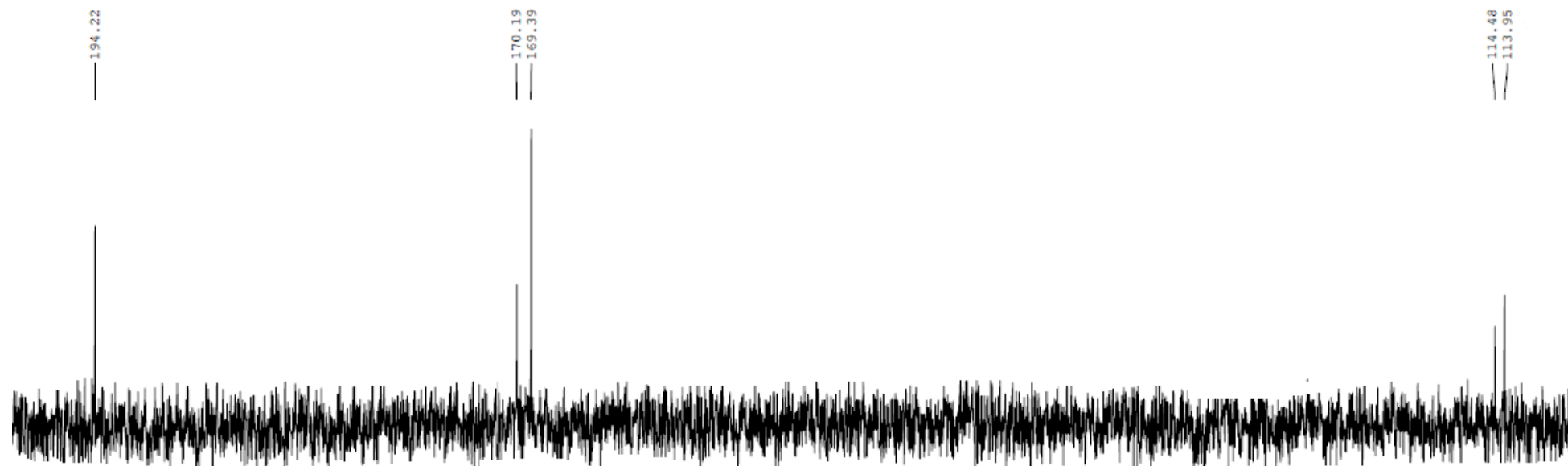


Figure S11. Expanded ¹³C{¹H} spectrum of compound **4b** in CDCl₃, 100 MHz

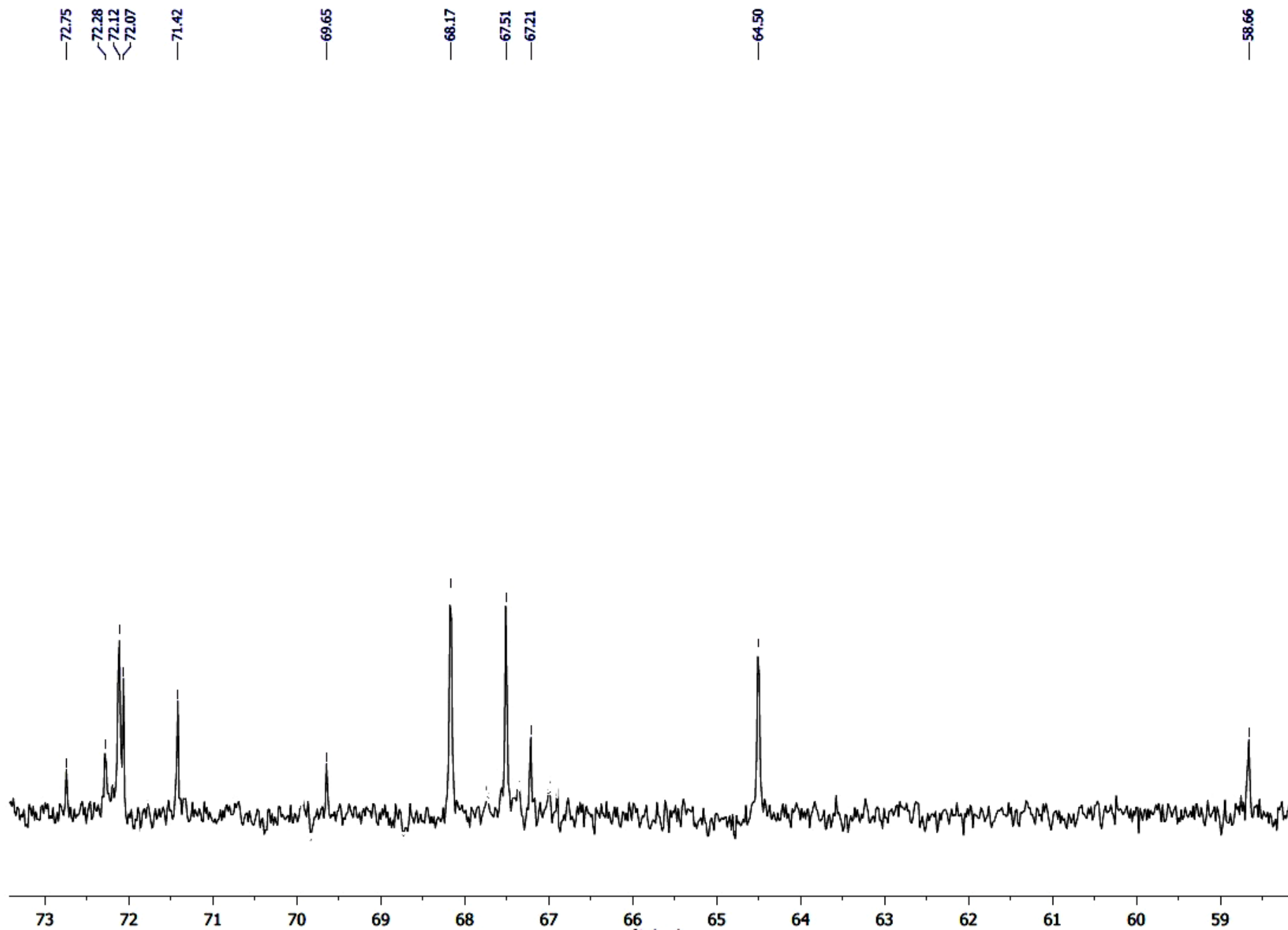


Figure S12. Expanded $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound **4b** in CDCl_3 , 100 MHz

Mass spectra

Egorov V-1126.15
25.04.2025 22:15:24

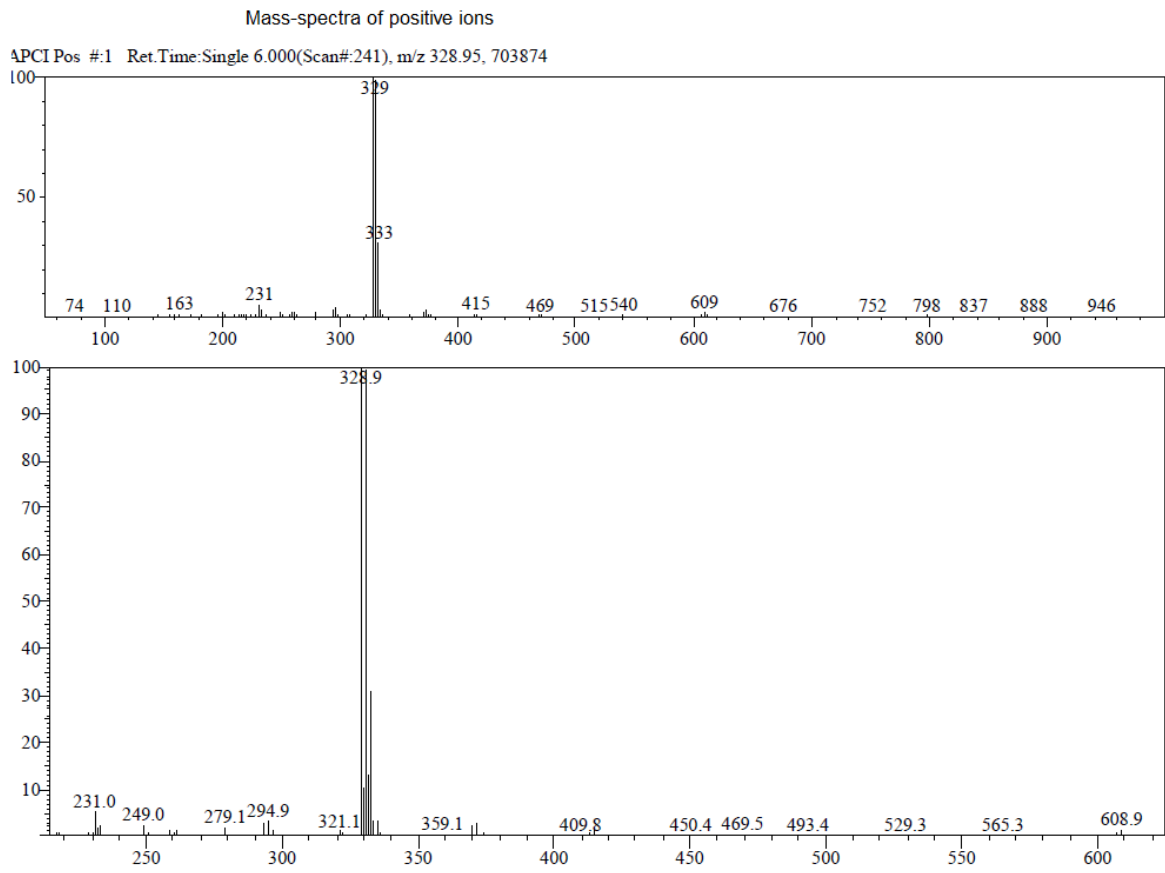


Figure S12. Mass spectra (APCI) of compound 4a