Electronic supplementary materials *Mendeleev Commun.*, 2019, **29**, 150–152

Synthesis and structure of stereoisomers of 3,4-benzo-5,10-diphenyl-1,3-diaza-7-oxa-6-phosphabicyclo[4.3.1]decane-2,6-dione

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General remarks. NMR spectra were recorded on a Bruker Avance-400 instrument (400 MHz, ^{1}H; 161.0 MHz, ^{31}P; and 100.6 MHz, ^{13}C) in $CDCl_3$ relative to the residual signals of the solvent. Mass spectra (EI) were taken on a DFS Thermo Electron Corporation instrument (Germany). The energy of ionizing electrons was 70 eV, the temperature of the ion source was 290°C, a system of direct input of the sample into the ion source was used, temperature of the evaporator was 250°C. Elemental analysis was performed on a EuroVector-3000 instrument (C, H, N) or manually by pyrolysis in an oxygen stream (P).

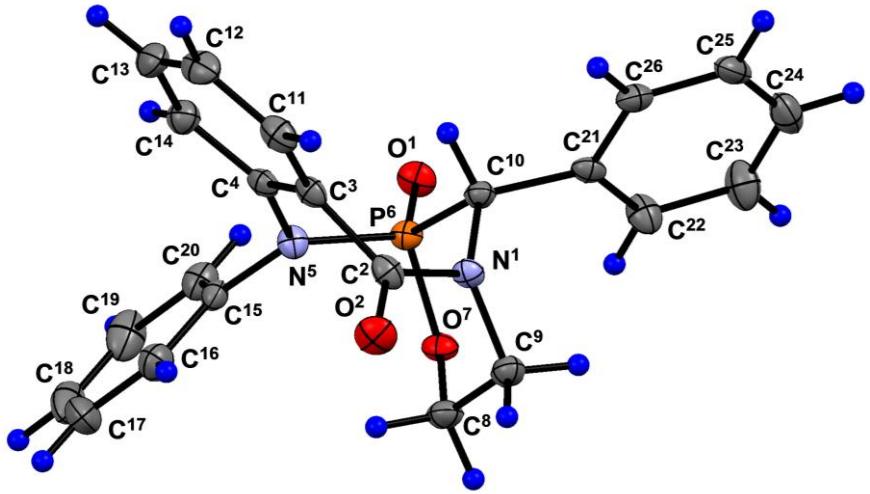

Figure S1. Geometry of diastereoisomer **4** (d_1, P_RC_R/P_SC_S) in the crystal, P_RC_R-enantiomer is shown (hereafter non-hydrogen atoms are presented as thermal ellipsoids with 50% probability). Selected bond lengths (Å), bond and torsion angles (deg): P^6–O^1 1.461(2), P^6–O^7 1.586(2), P^6–N^5 1.674(2), P^6–C^{10} 1.805(3), O^2–C^2 1.225(3), N^1–C^2 1.372(3), N^1–C^{10} 1.477(3), N^5–C^4 1.441(3), O^1–P^6–O^7 110.5(1), O^1–P^6–N^5 117.9(1), O^1–P^6–C^{10} 117.5(1), O^7–P^6–N^5 105.01(9), O^7–P^6–C^{10} 103.8(1), N^5–P^6–C^{10} 100.5(1), P^6–O^7–C^8 119.7(1), P^6–C^{10}–N^1 105.5(2), O^1–P^6–O^7–C^8 174.4(2), O^1–P^6–N^5–C^4 –102.0(2), O^2–C^2–C^3–C^{11} 52.2(4), C^{10}–P^6–N^5–C^4 27.0(2), C^9–N^1–C^2–O^2 32.9(3), C^2–N^1–C^{10}–P^6 –85.3(2).

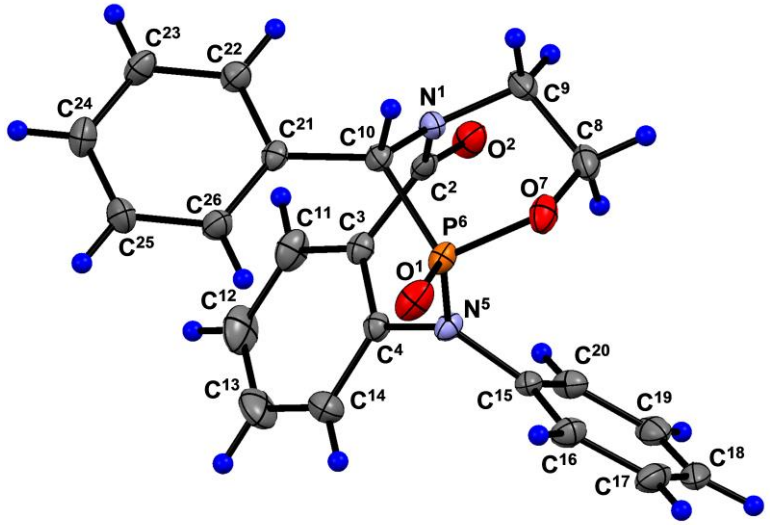

Figure S2. Geometry of diastereoisomer **4** (d_2, P_SC_R/P_RC_S) in the crystal, P_SC_R-enantiomer is shown. Selected bond lengths (Å) and bond and torsion angles (deg): P^6–O^1 1.462(1), P^6–O^7 1.596(1), P^6–N^5 1.667(1), P^6–C^{10} 1.814(2), O^2–C^2 1.226(2), N^1–C^2 1.365(2), N^1–C^{10} 1.474(2), N^5–C^4 1.439(2), O^1–P^6–O^7 109.66(7), O^1–P^6–N^5 117.86(7), O^1–P^6–C^{10} 118.49(7), O^7–P^6–N^5 105.20(6), O^7–P^6–C^{10} 99.95(7), N^5–P^6–C^{10} 103.53(6), P^6–O^7–C^8 121.3(1), P^6–C^{10}–N^1 104.52(9), O^1–P^6–O^7–C^8 –176.2(1), O^1–P^6–N^5–C^4 102.3(1), O^2–C^2–C^3–C^{11} –54.7(2), C^{10}–P^6–N^5–C^4 –30.8(1), C^9–N^1–C^2–O^2 –30.6(2), C^2–N^1–C^{10}–P^6 80.2(1).

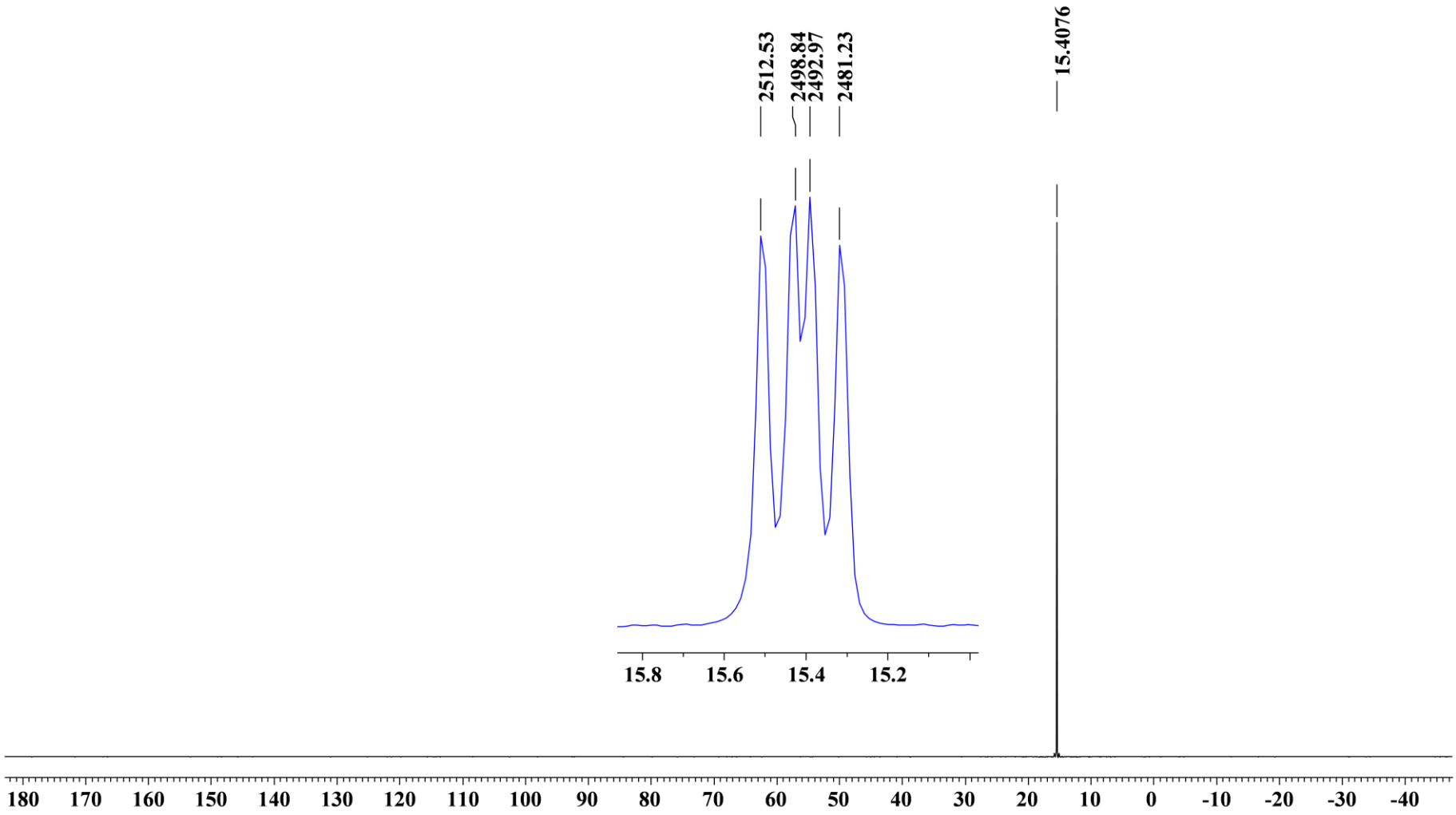

Figure S3. ^{31}P-{^{1}H} and ^{31}P NMR spectra (162.0 MHz, $CDCl_3$) of compound **4**(d_1).

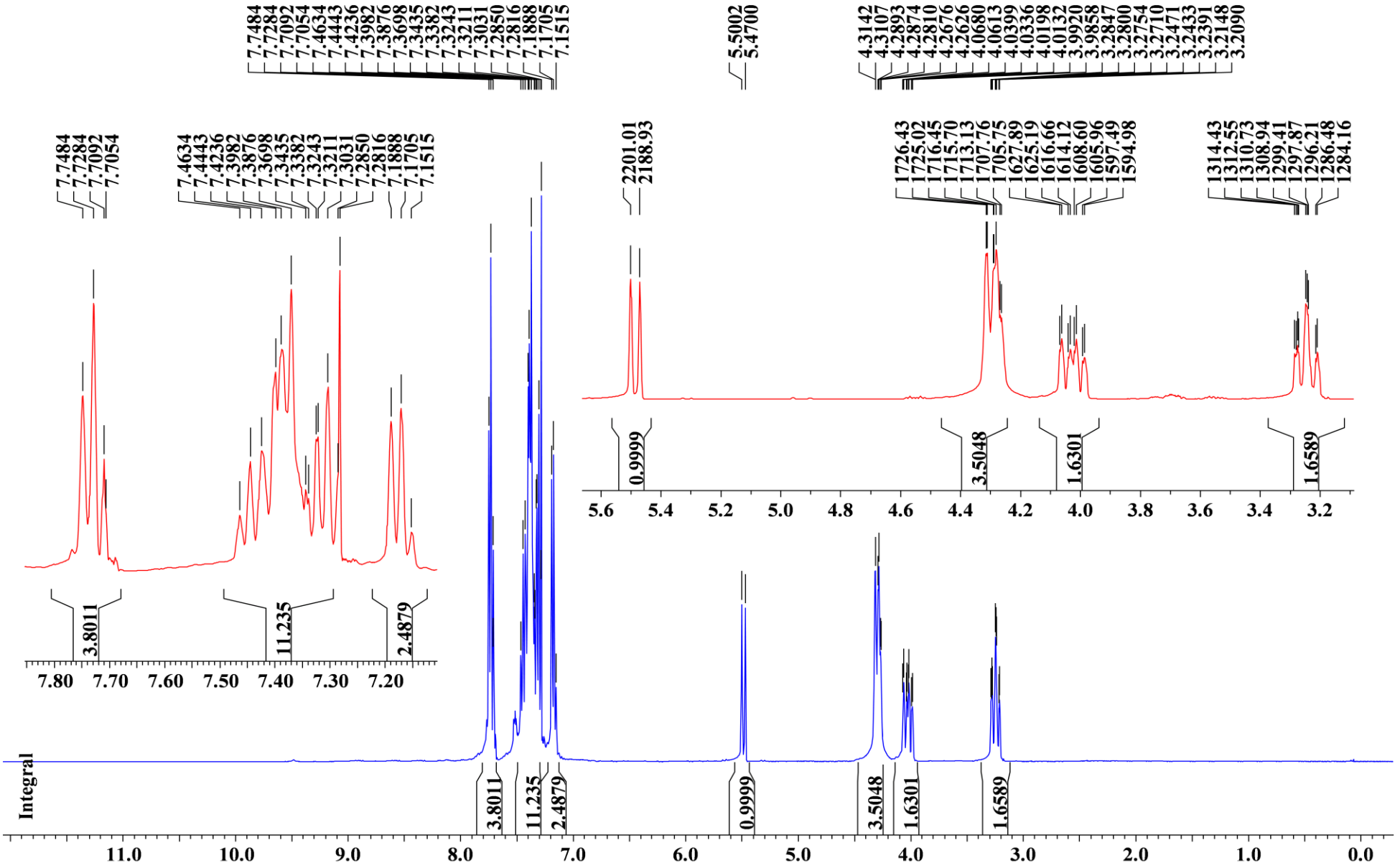

Figure S4. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **4**(d_1).

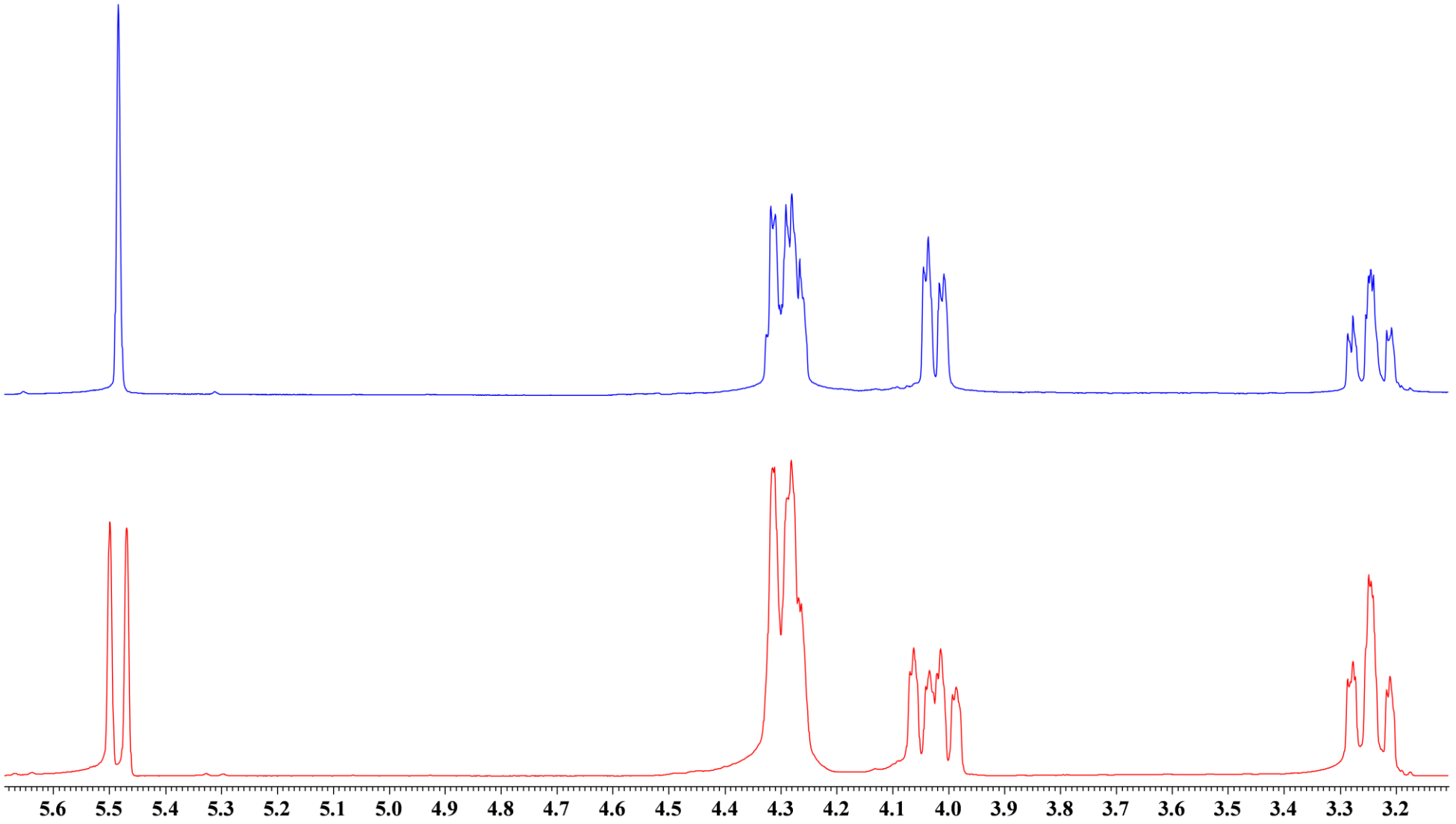

Figure S5. ^{1}H NMR (red) and ^{1}H-{^{31}P}spectra (400 MHz, $CDCl_3$) of compound **4**(d_1).

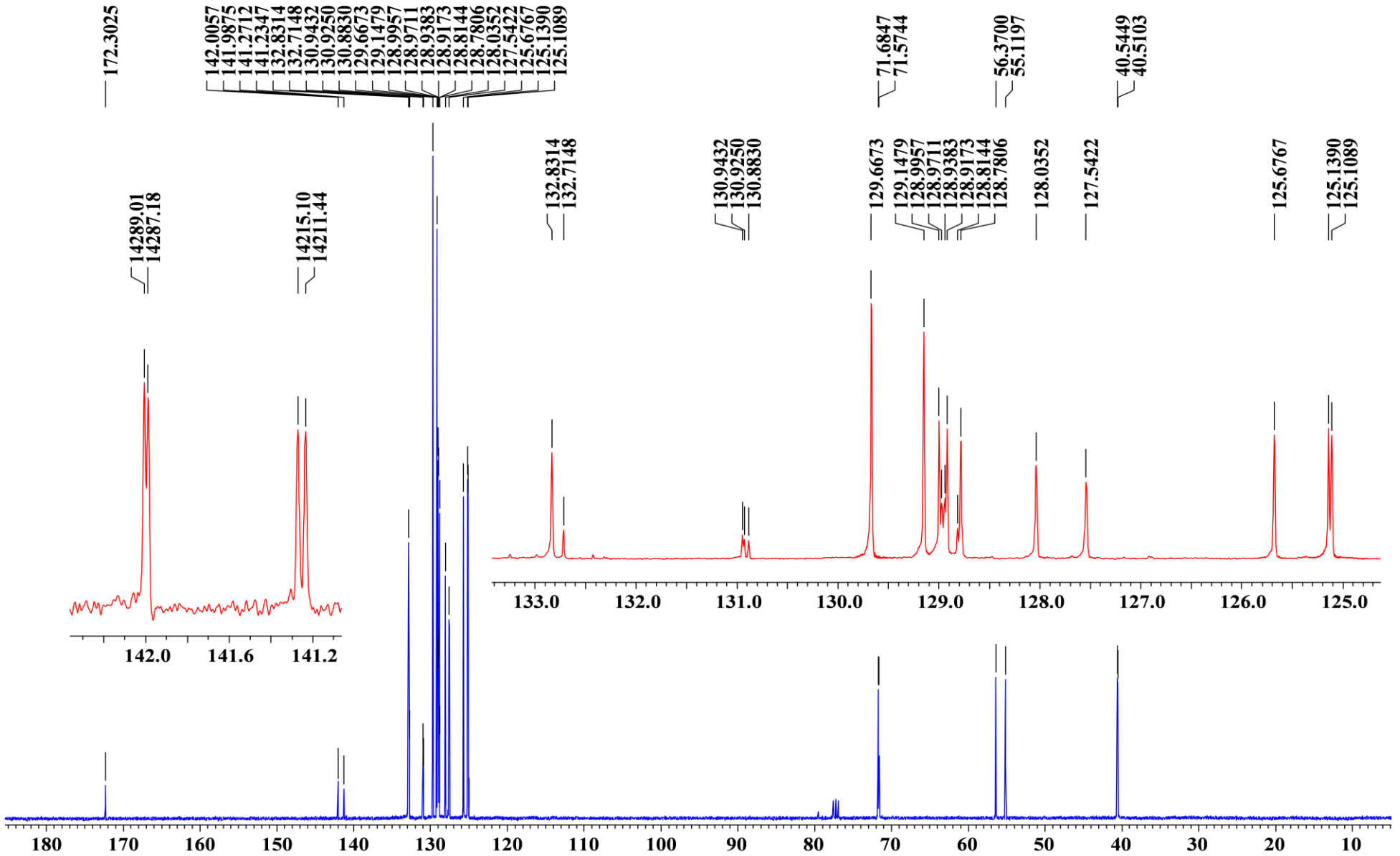

Figure S6. ^{13}C-{^{1}H} NMR spectrum (100.6 MHz, $CDCl_3$) of compound **4**(d_1).

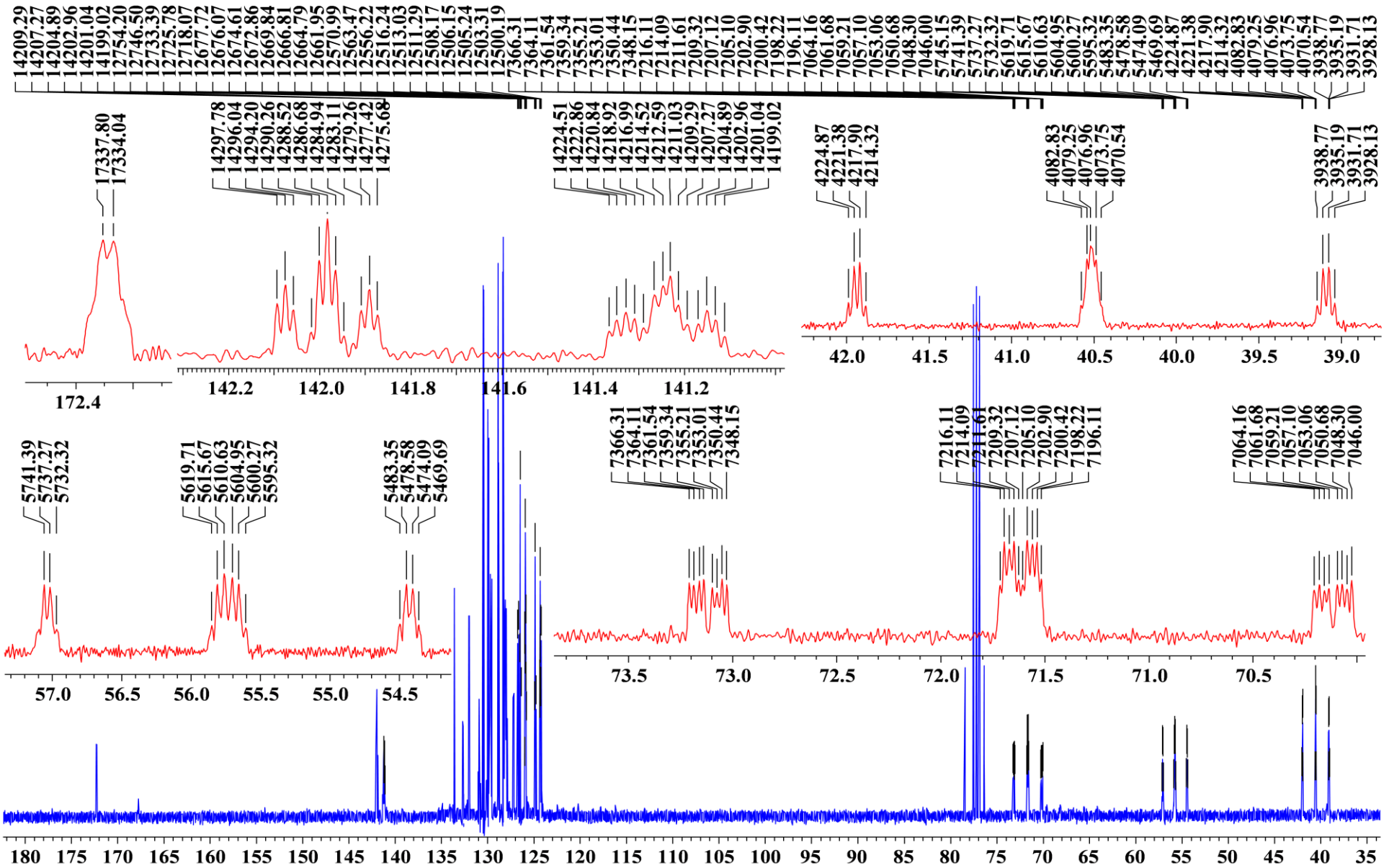

Figure S7. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of compound **4**(d_1).

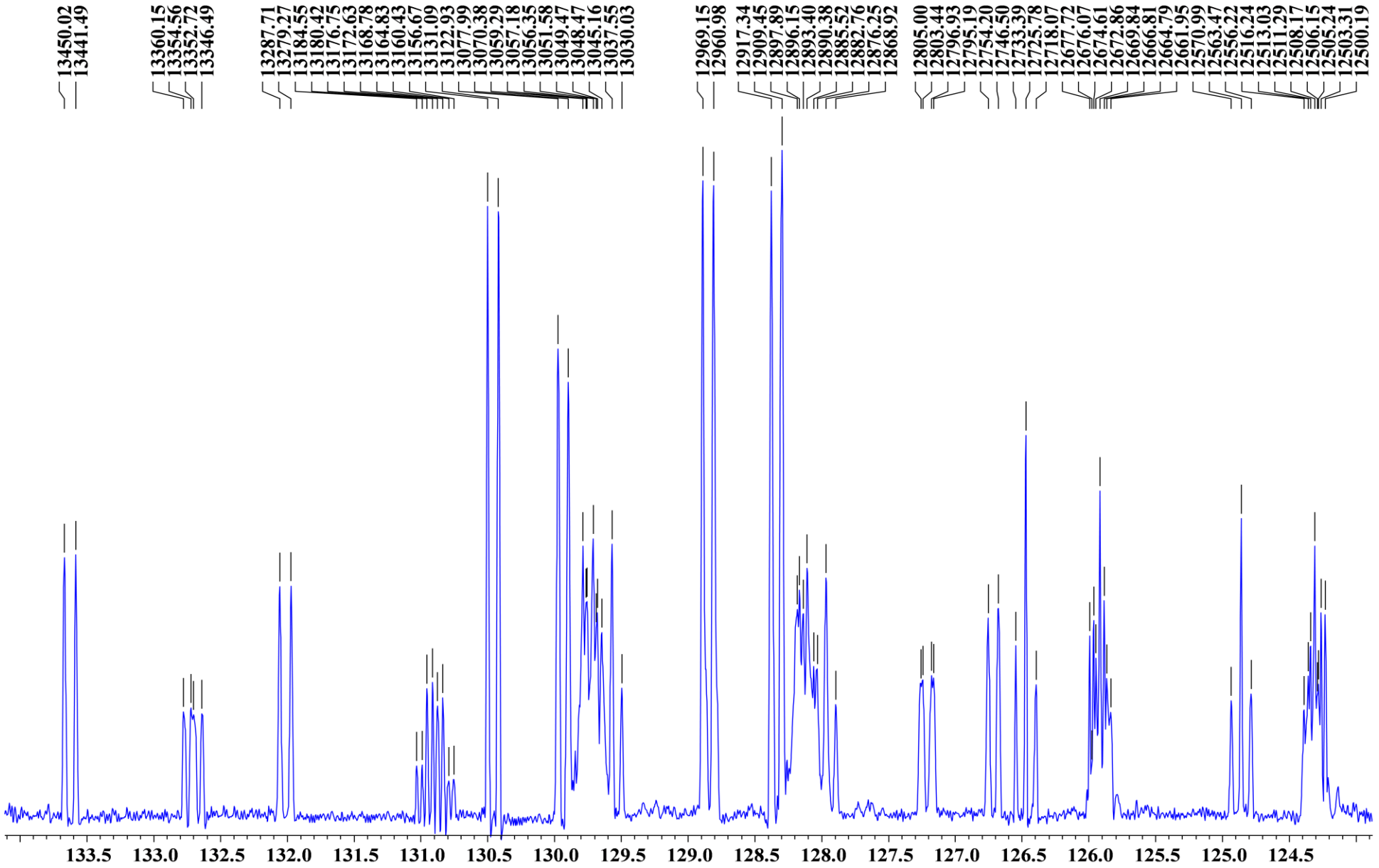

Figure S8. 123-134 ppm region of ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of compound **4**(d_1).

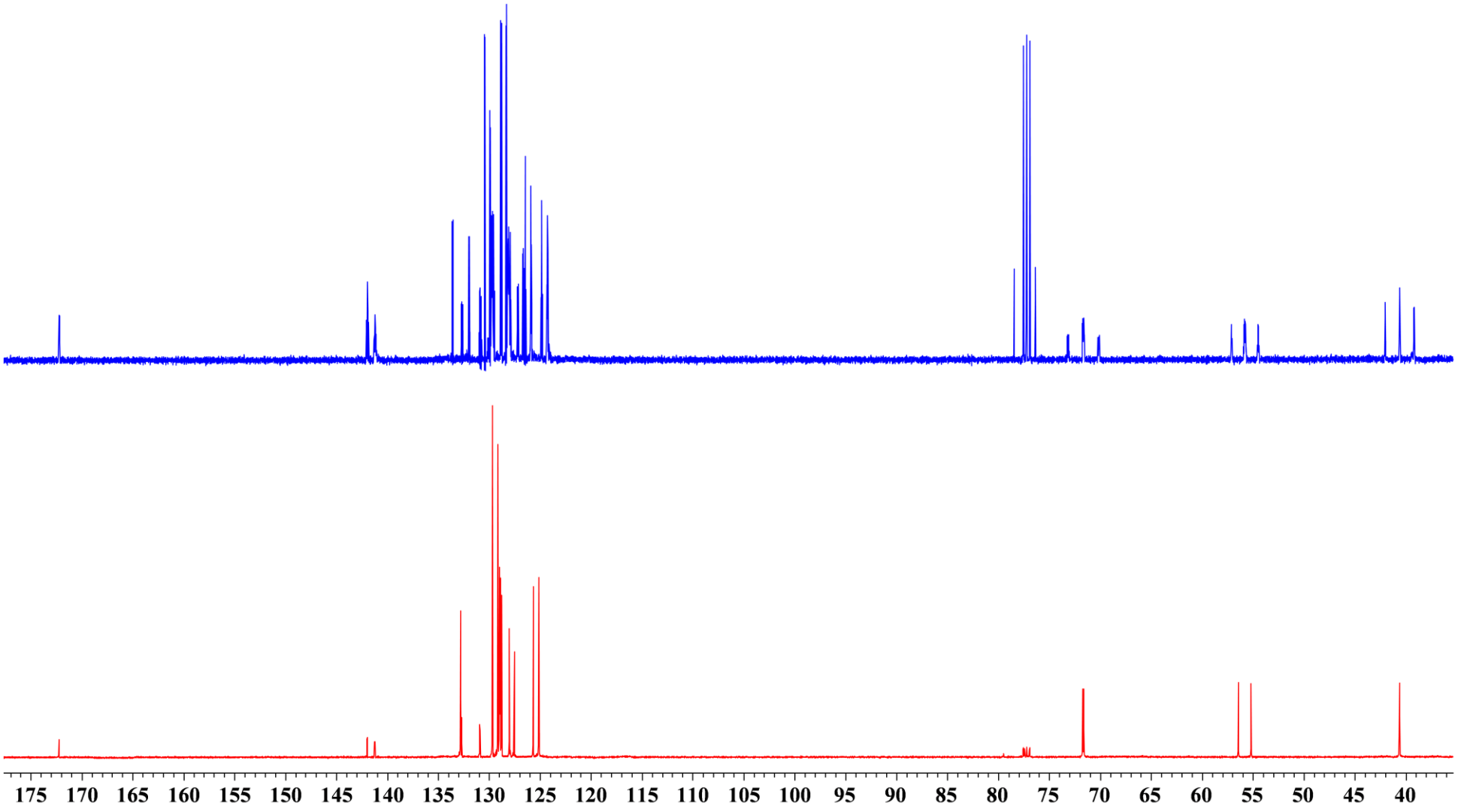

Figure S9. ^{13}C and ^{13}C-{^{1}H} NMR spectra (100.6 MHz, $CDCl_3$) of compound **4**(d_1).

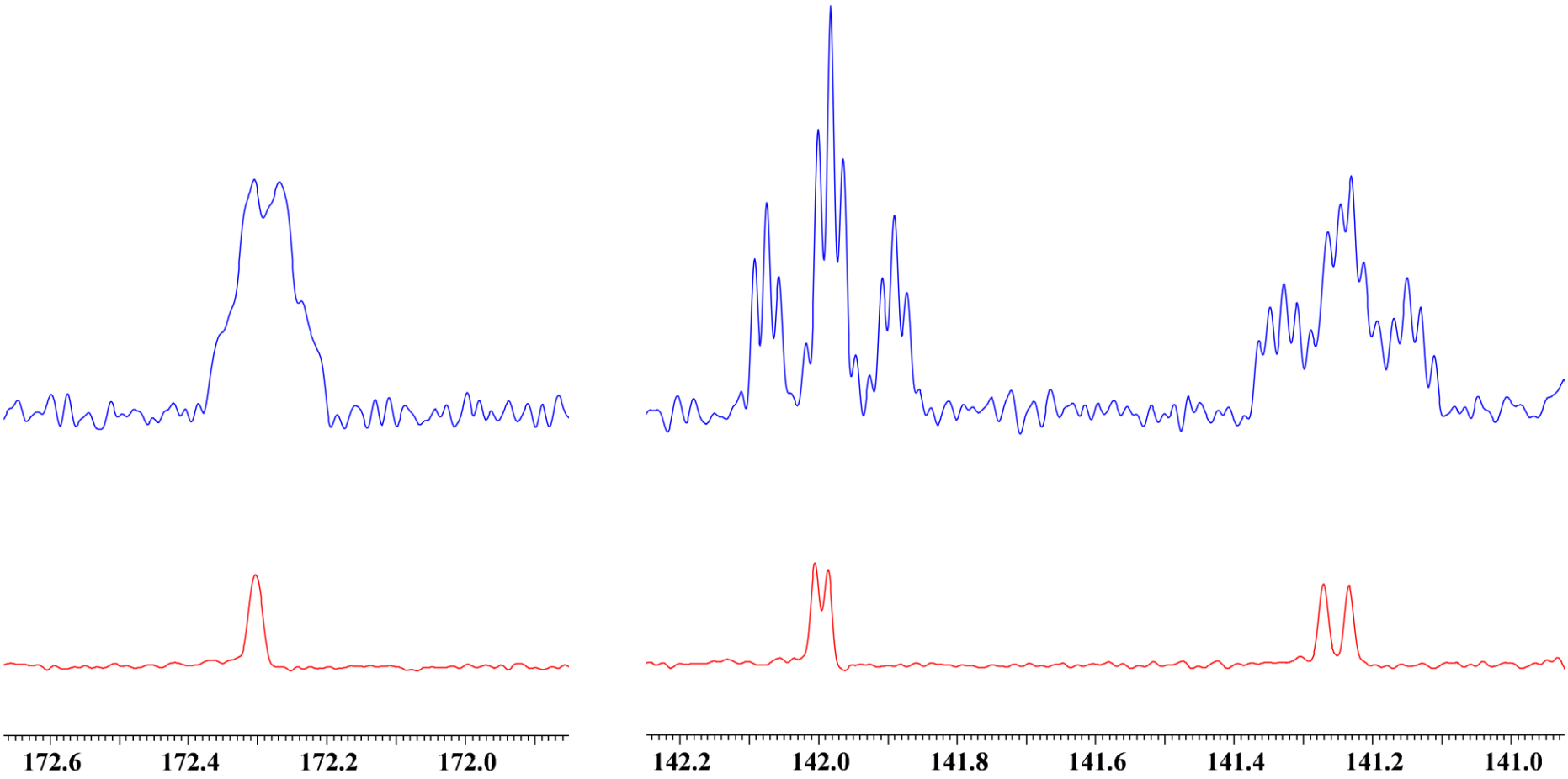

Figure S10. Fragments of ^{13}C and ^{13}C-{^{1}H} NMR spectra (100.6 MHz, $CDCl_3$) of compound **4**(d_1).

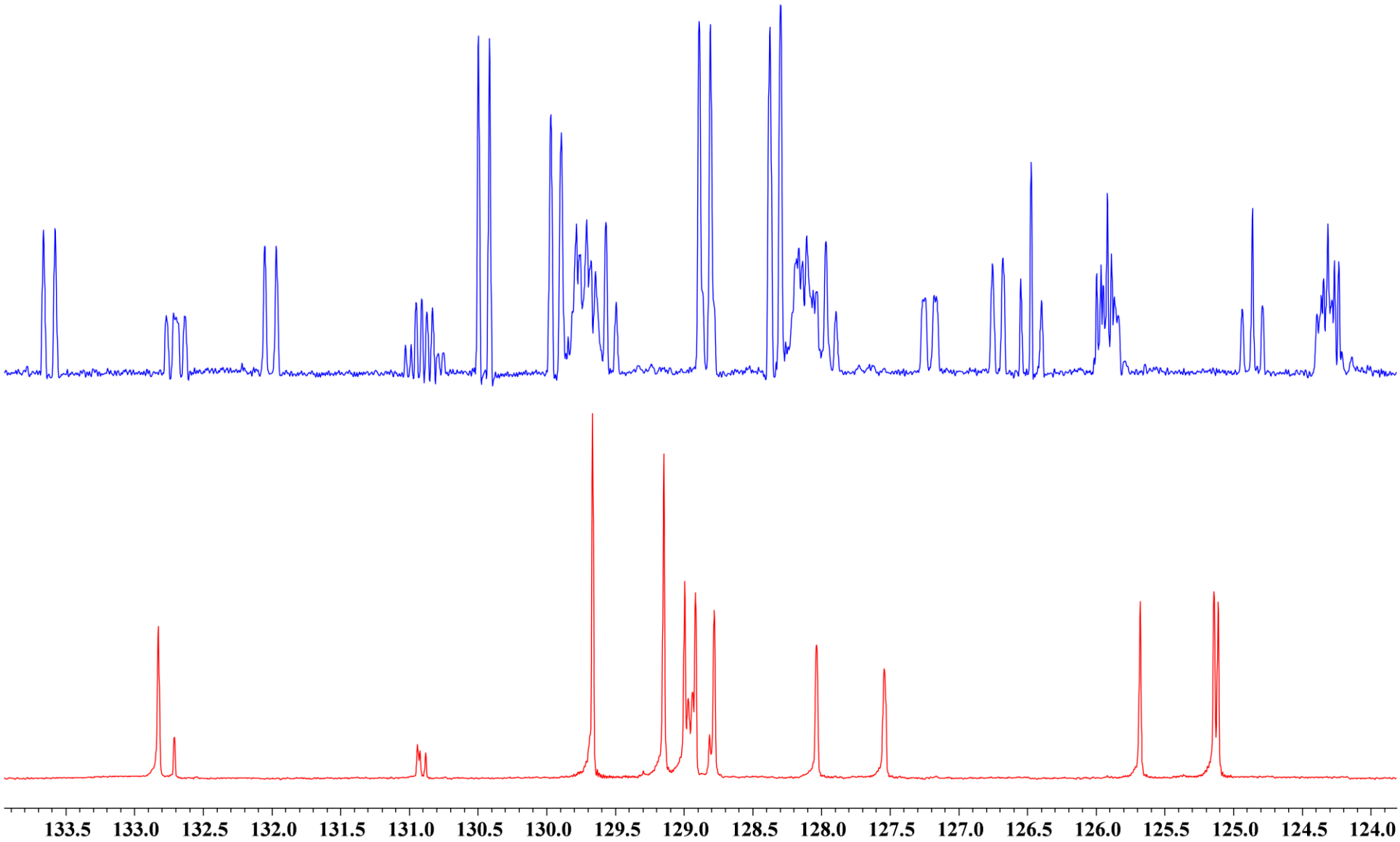

Figure S11. 123-134 ppm region of ^{13}C and ^{13}C-{^{1}H} NMR spectra (100.6 MHz, $CDCl_3$) of compound **4**(d_1).

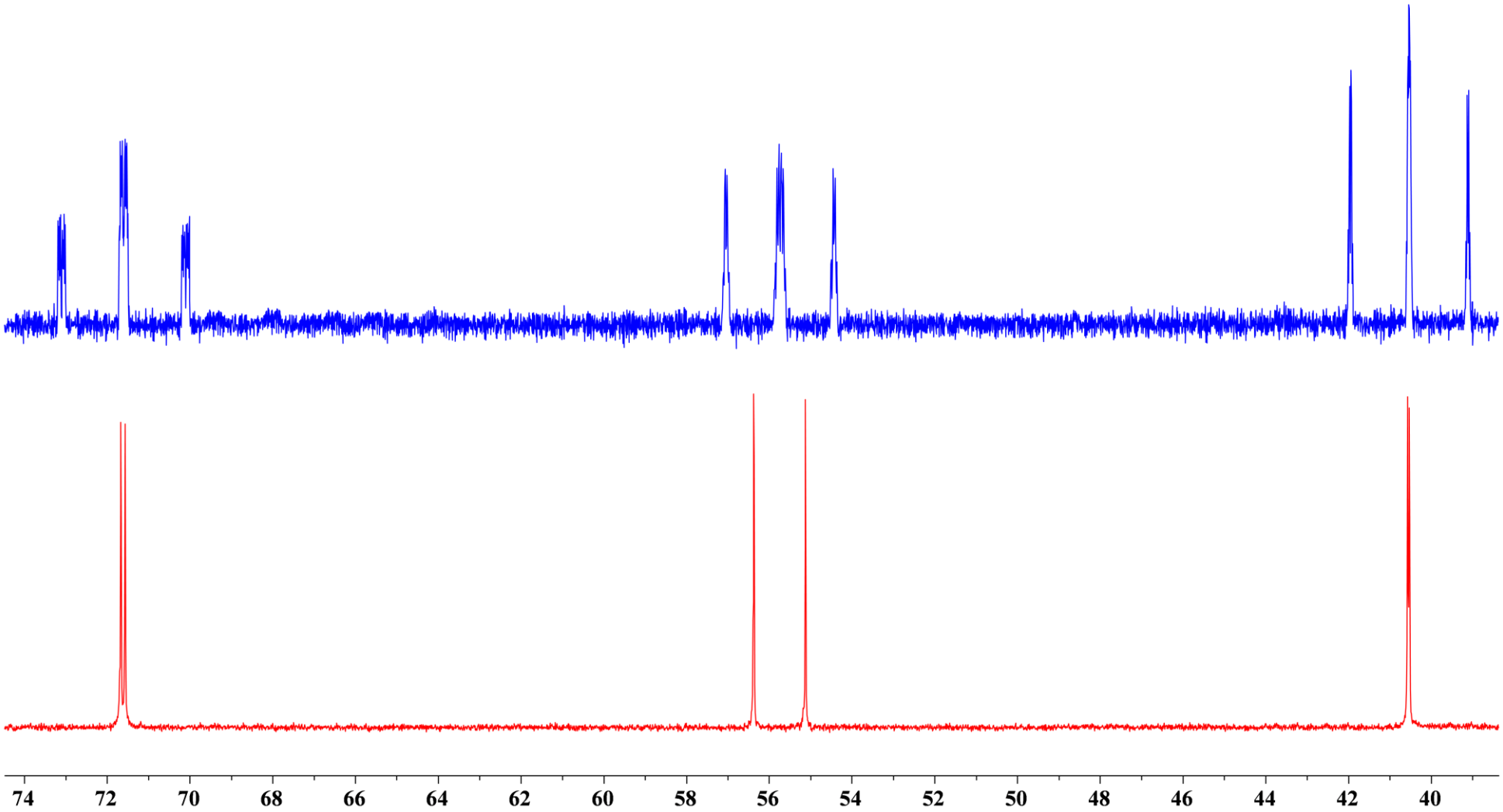

Figure S12. High-field regions of ^{13}C and ^{13}C-{^{1}H} NMR spectra (100.6 MHz, $CDCl_3$) of compound **4**(d_1).

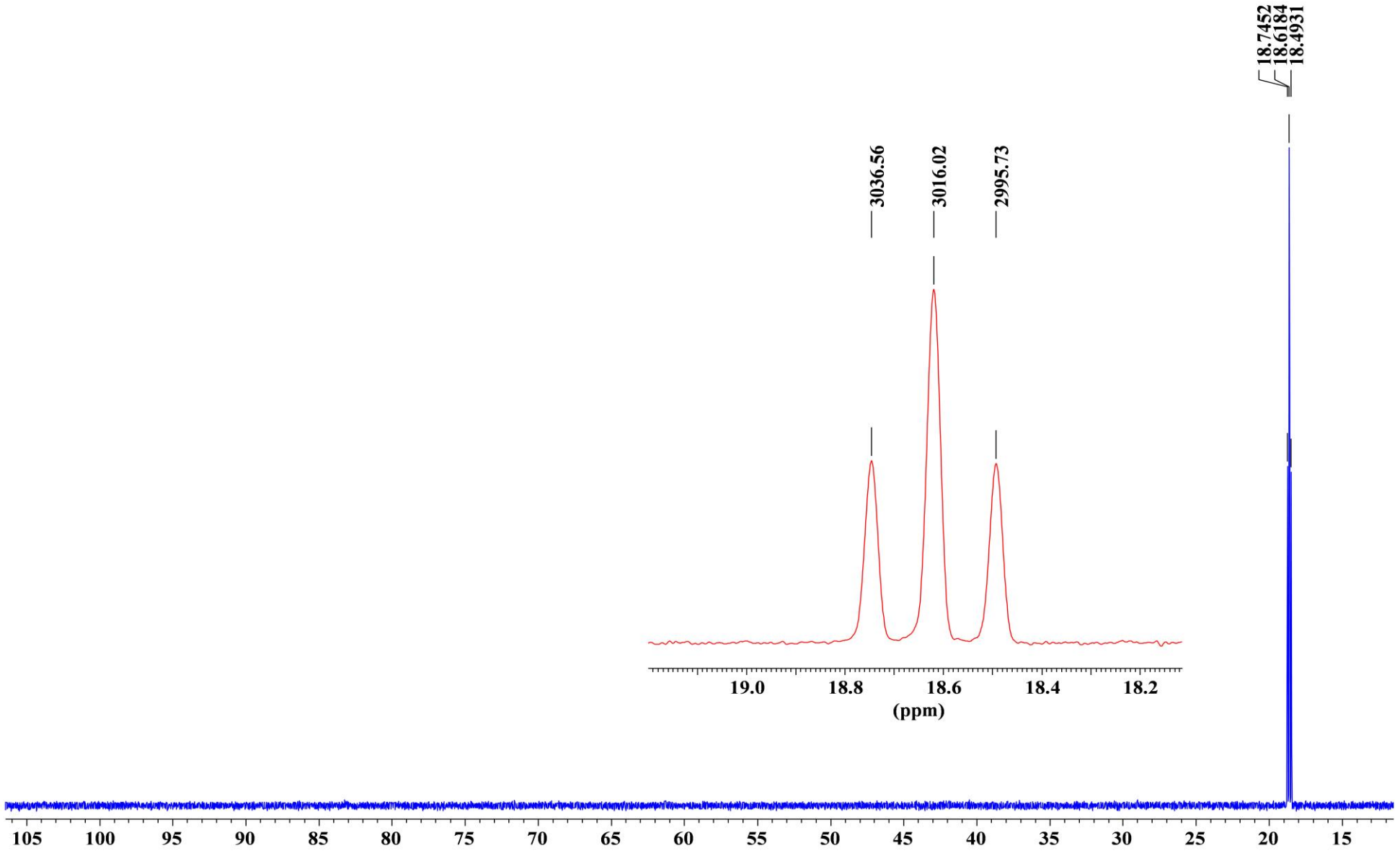

Figure S13. ^{31}P NMR spectrum (162.0 MHz, $CDCl_3$) of compound **4**(d_2).

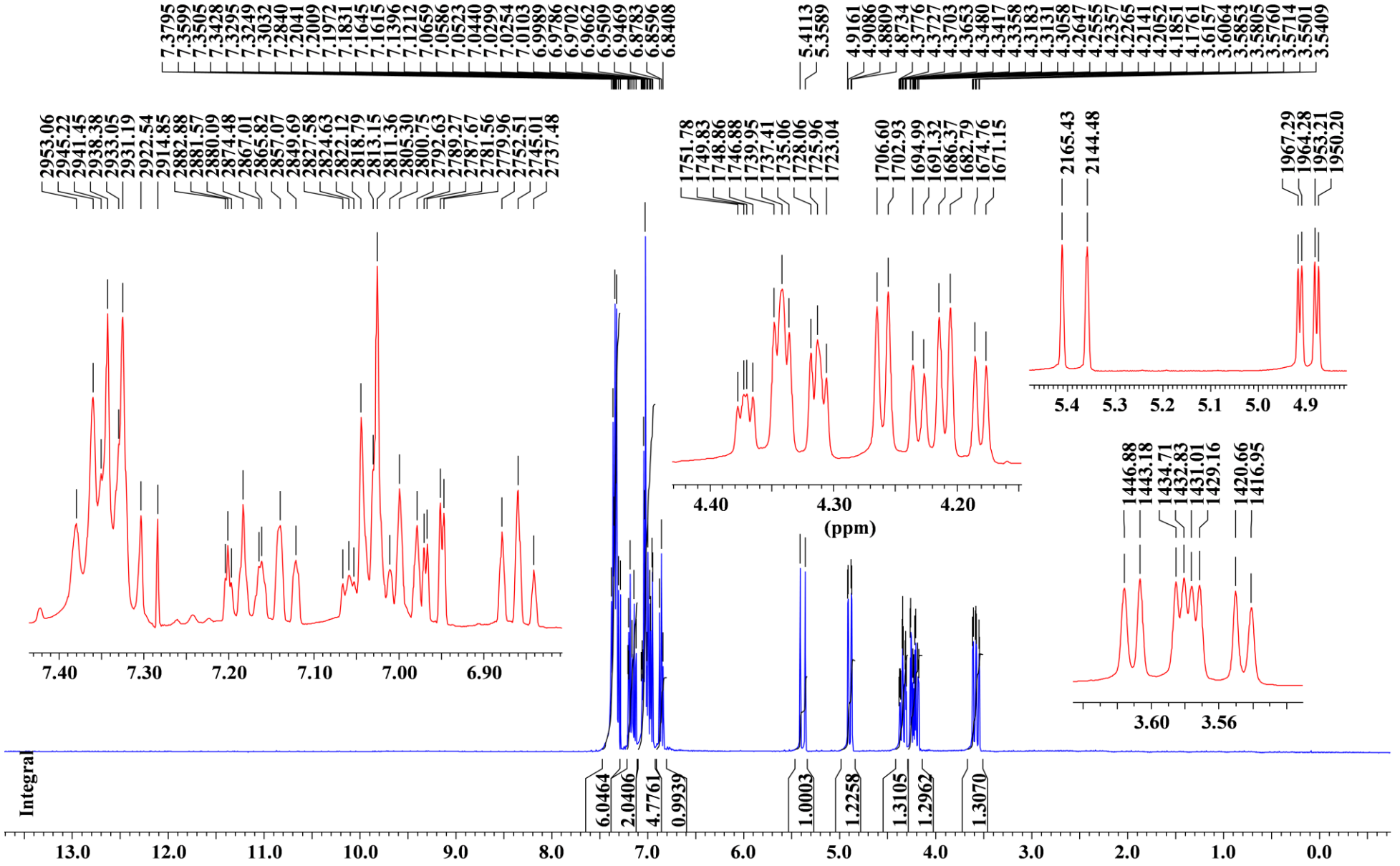

Figure S14. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **4**(d_2).

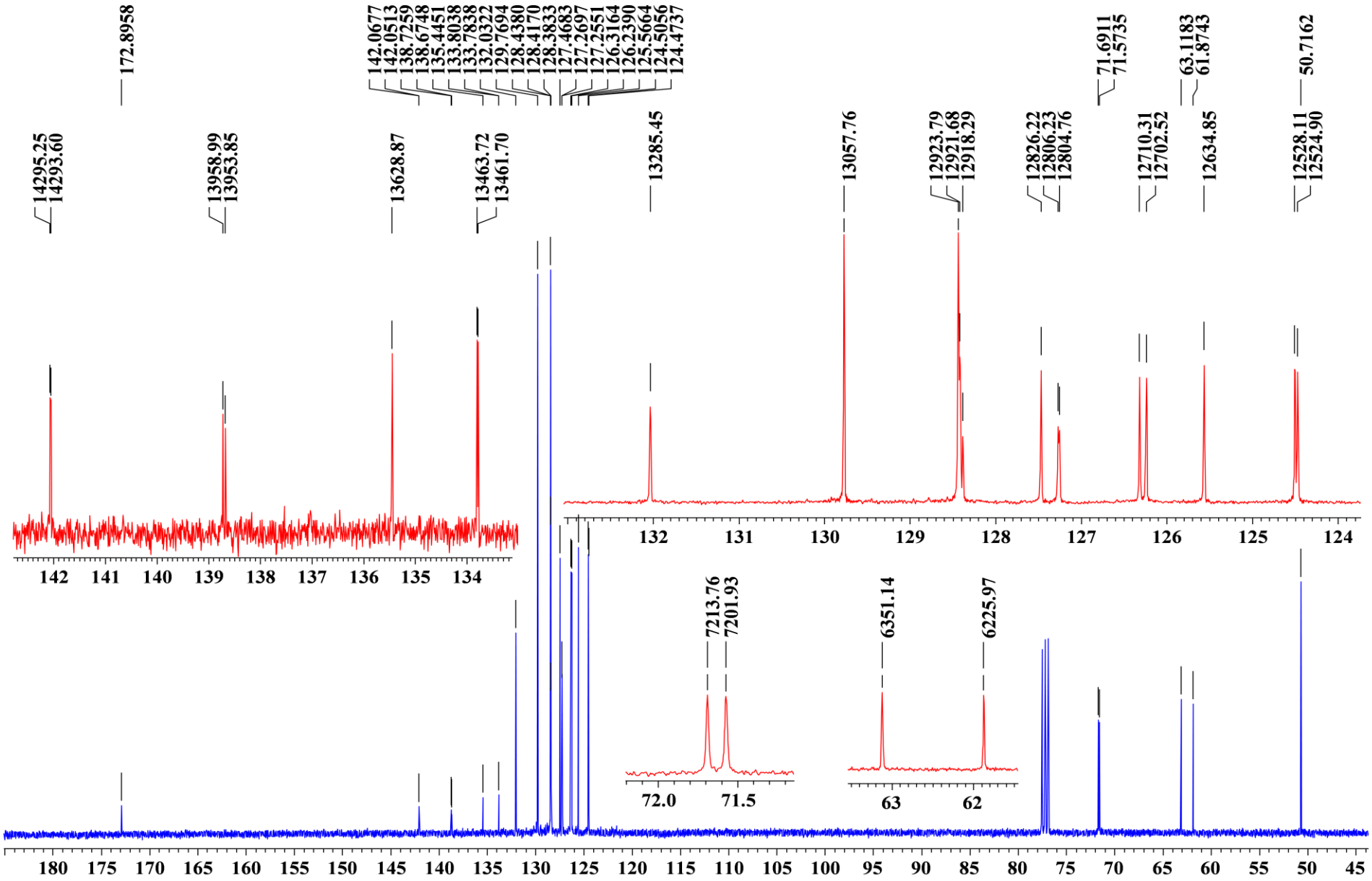

Figure S15. ^{13}C-{^{1}H} NMR spectrum (100.6 MHz, $CDCl_3$) of compound **4**(d_2).

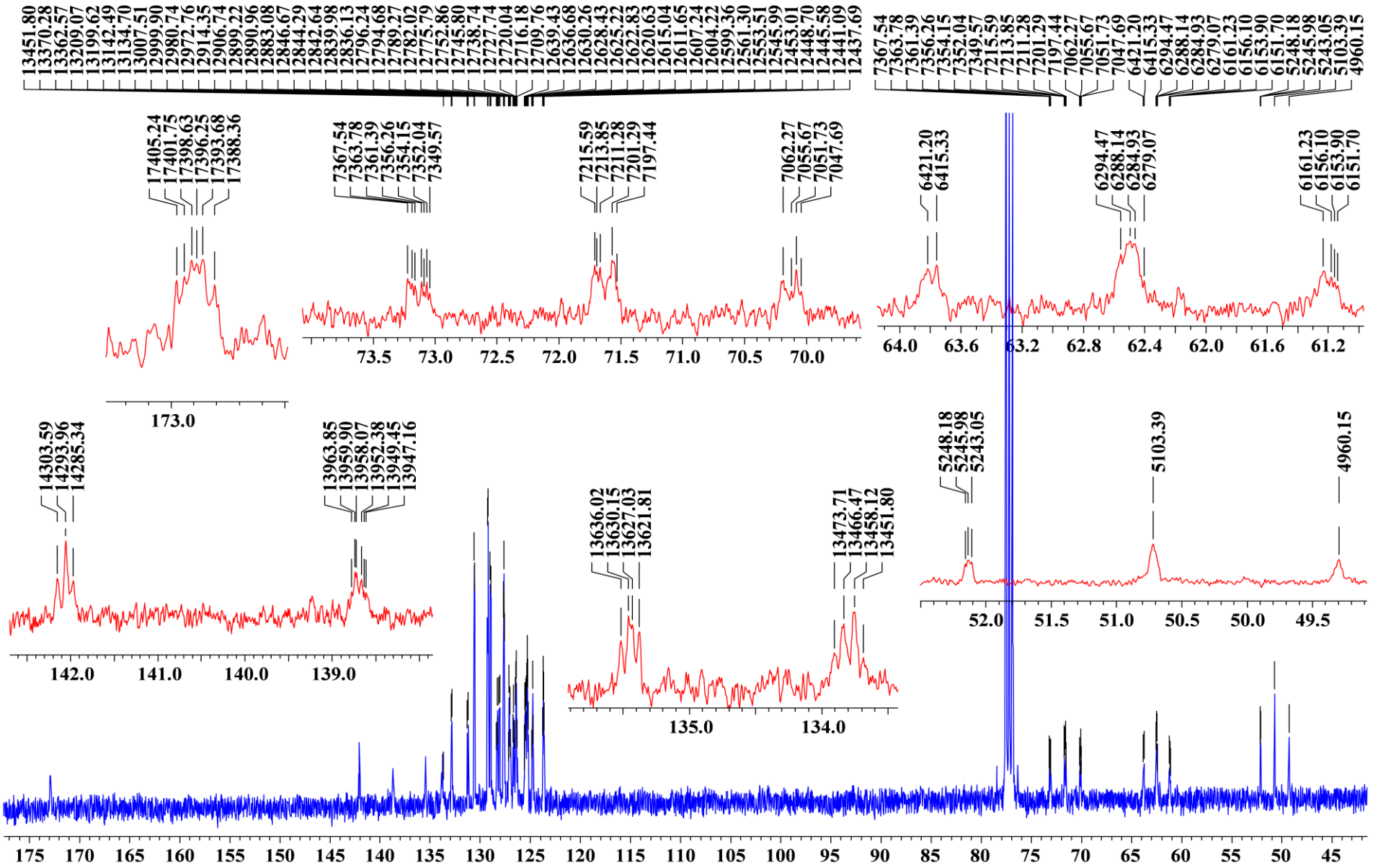

Figure S16. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of compound **4**(d_2).

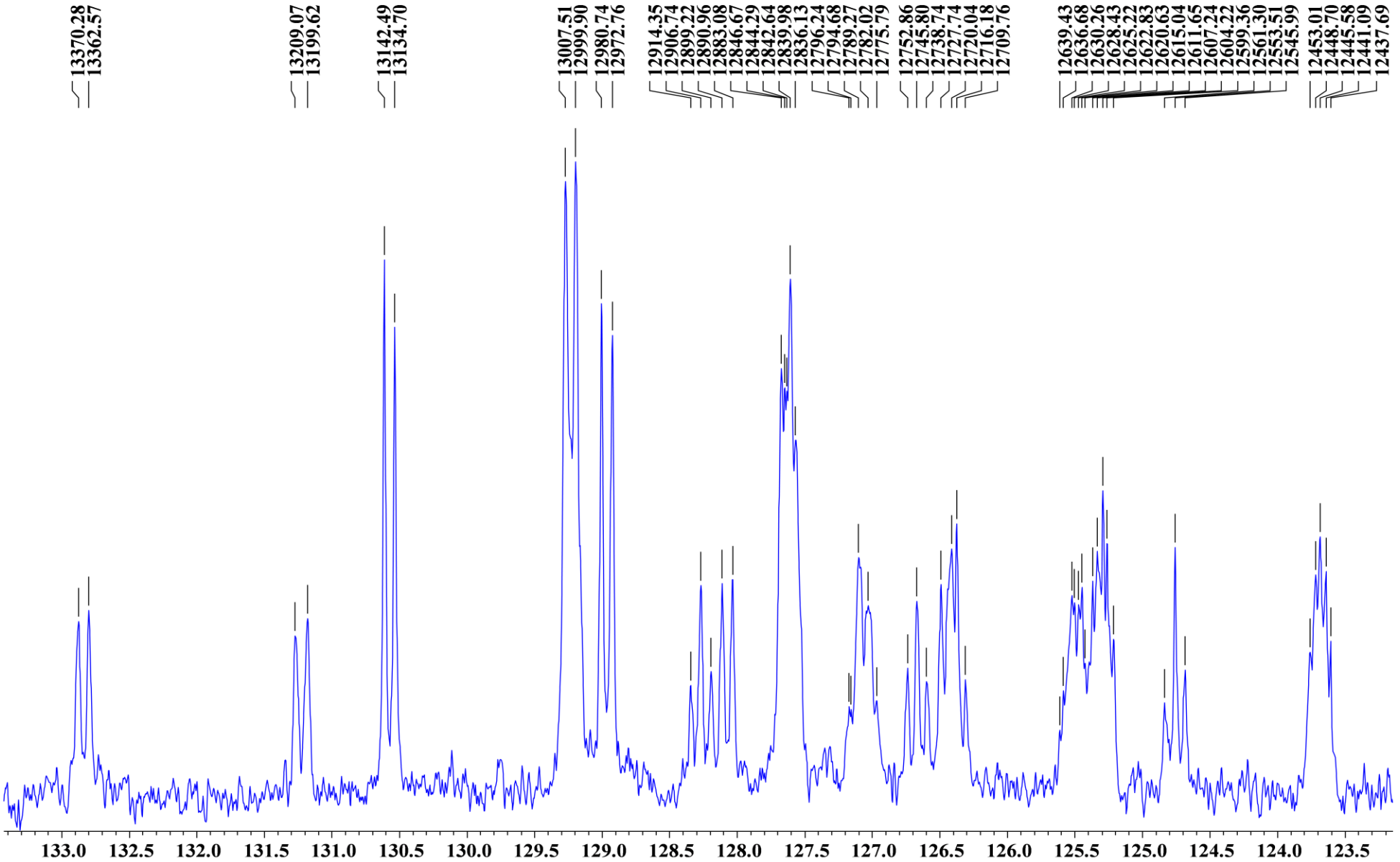

Figure S17. 123-134 ppm region of ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of compound **4**(d_2).

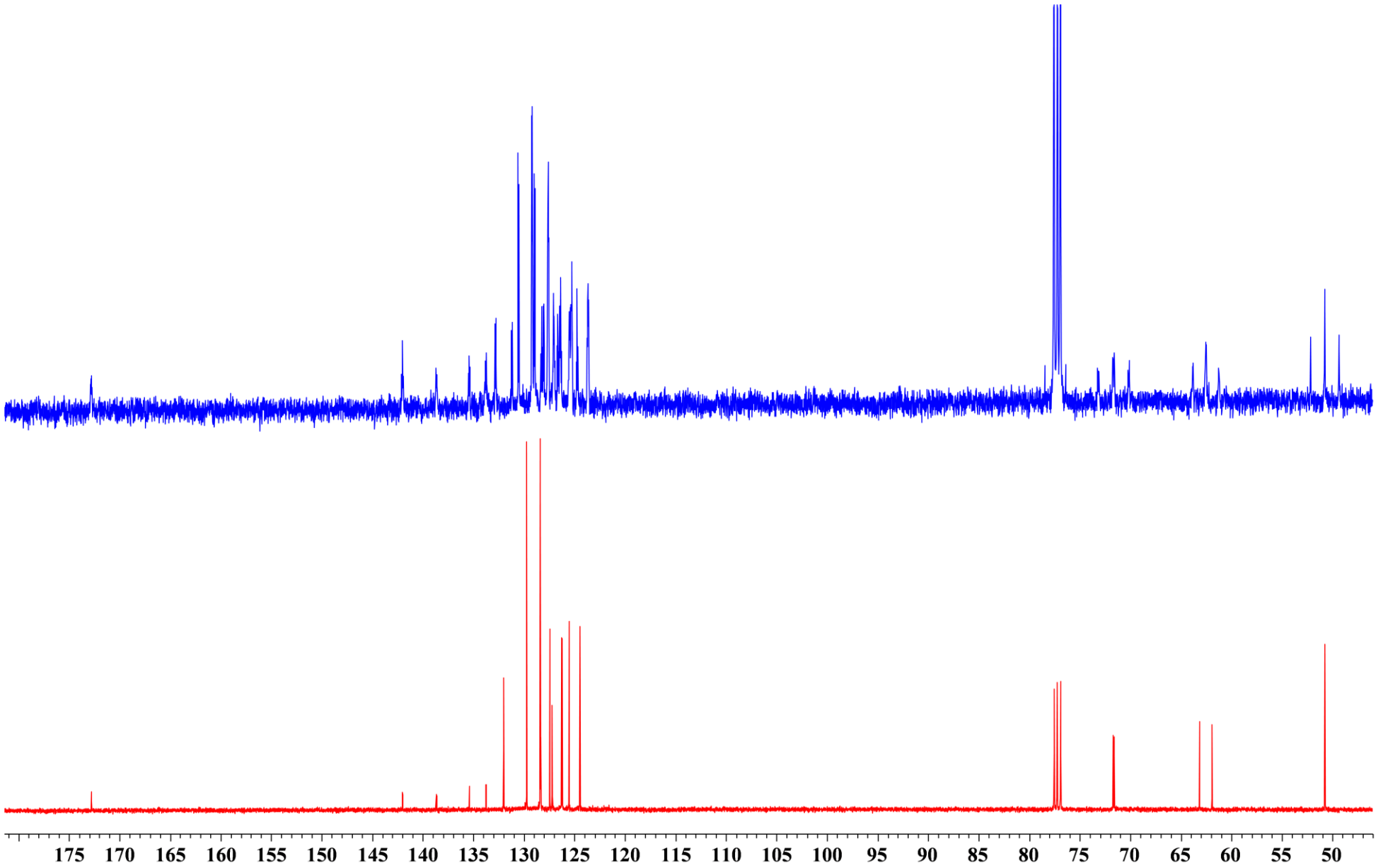

Figure S18. ^{13}C and ^{13}C-{^{1}H} NMR spectra (100.6 MHz, $CDCl_3$) of compound **4**(d_2).

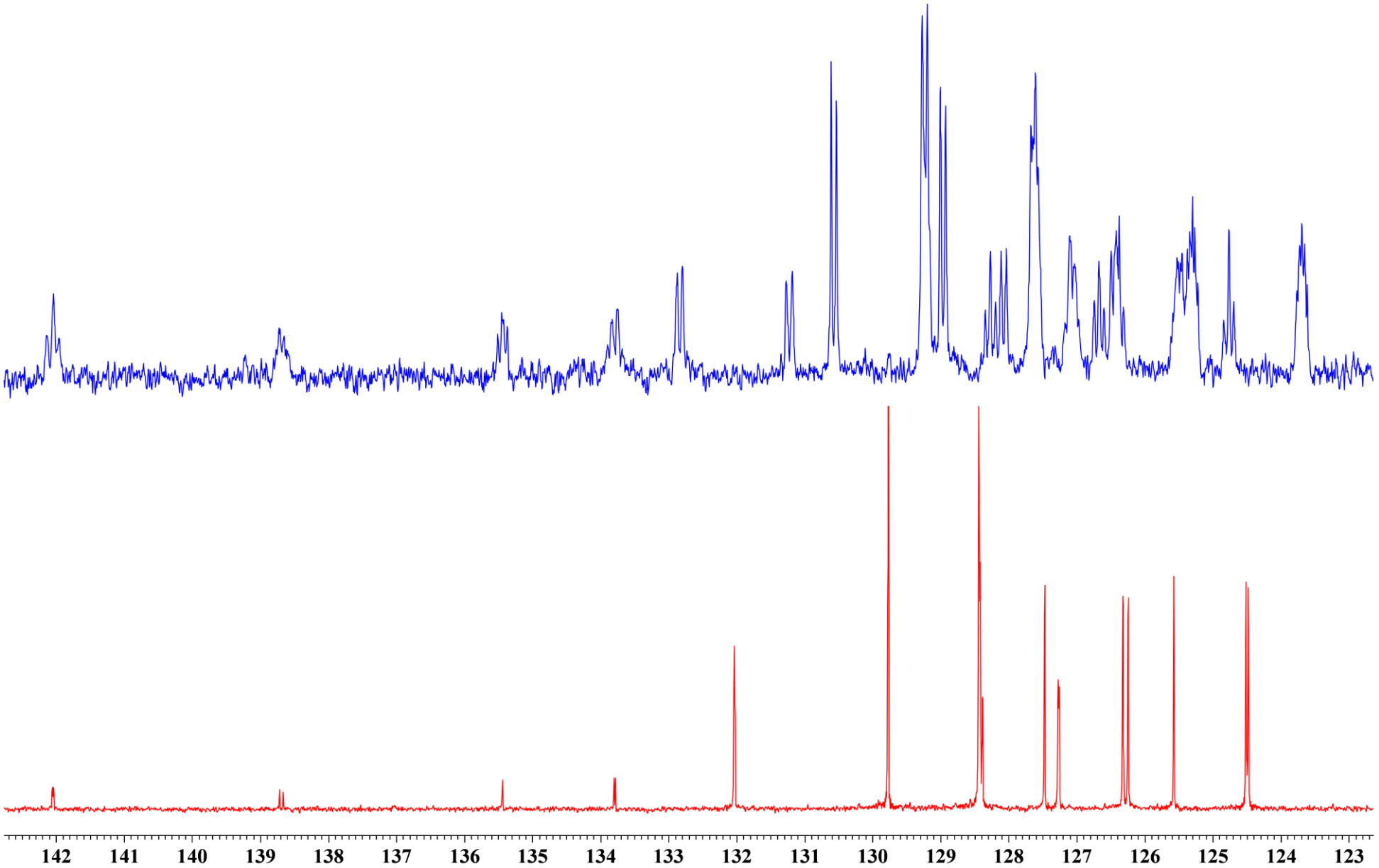

Figure S19. 123-143 ppm region of ^{13}C and ^{13}C-{^{1}H} NMR spectra (100.6 MHz, $CDCl_3$) of compound **4**(d_2).

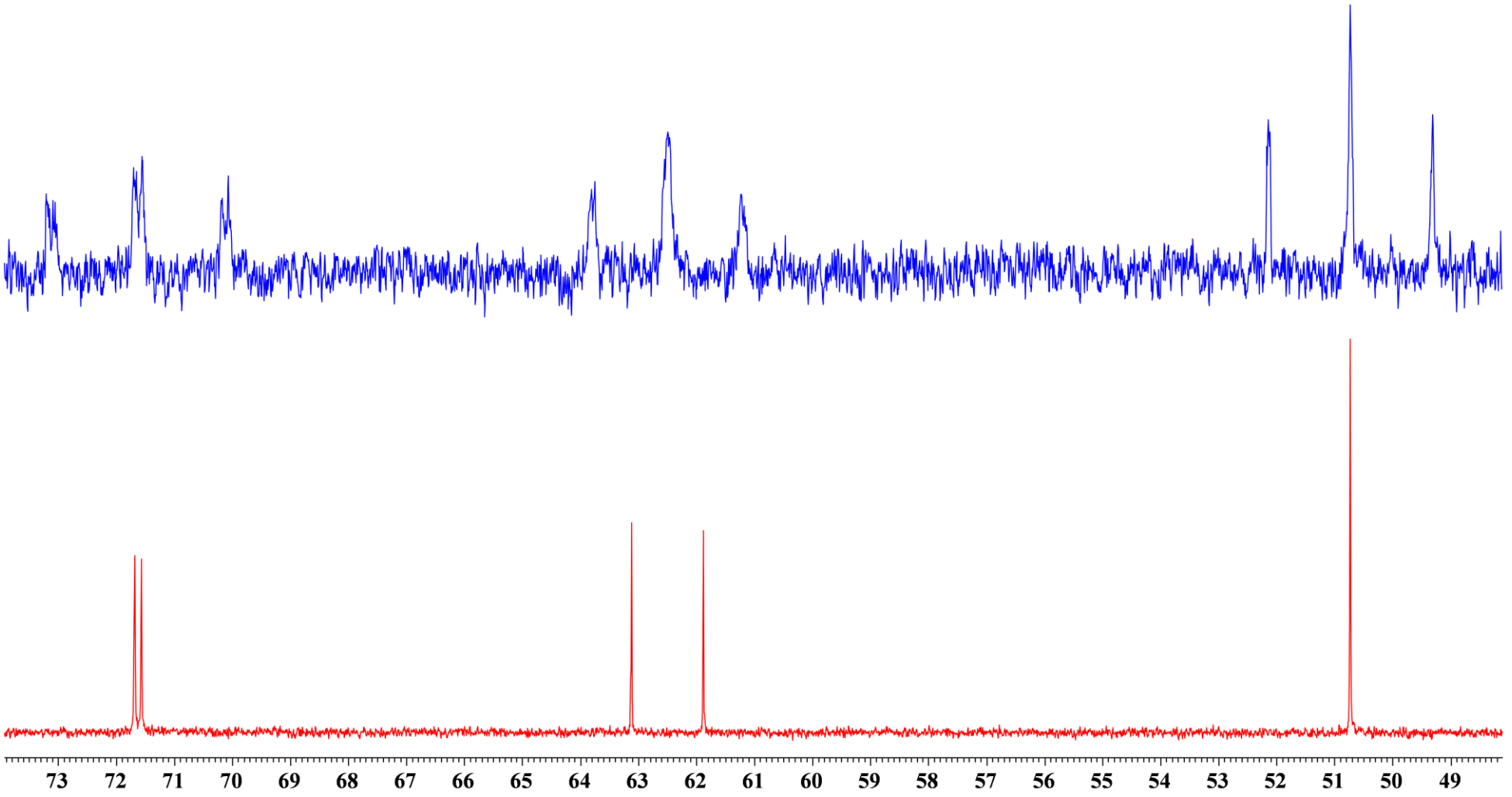

Figure S20. High-field regions of ^{13}C and ^{13}C-{^{1}H} NMR spectra (100.6 MHz, $CDCl_3$) of compound **4**(d_2).