Supplementary Material

Heteroatom exchange as a scaffold-editing strategy: a matched xanthone–acridone study of aminoalkyl derivatives

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1. General experimental information

Reagents were obtained from commercial suppliers and used without further purification unless otherwise stated. Solvents were of commercial grade and distilled prior to use when required.

Thin-layer chromatography (TLC) was performed on silica gel 60 F254 plates, and compounds were visualized under UV irradiation and/or by staining with phosphomolybdic acid. Flash chromatography was performed using silica gel 60 (230–240 mesh ASTM).

Nuclear magnetic resonance (^{1}H and ^{13}C NMR) spectra were recorded at room temperature on a Bruker Avance ARX-300 spectrometer using $CDCl_3$ or DMSO-d_6 as solvents. Chemical shifts (δ) are reported in parts per million (ppm) relative to the residual solvent signals. Coupling constants (J) are reported in Hertz (Hz), and signal multiplicities are described using standard abbreviations.

Infrared spectra were obtained using a Nicolet Nexus 470 FT-IR instrument. Melting points were determined using a Büchi 510 apparatus and are uncorrected.

High-resolution mass spectra (HRMS) were recorded using Thermo Fisher LTQ Orbitrap XL and Finnigan MAT 95 spectrometers.

Characterization data for the synthesized intermediates and final aminoalkylated xanthone and acridone derivatives are provided in the following sections.

2. NMR Spectra

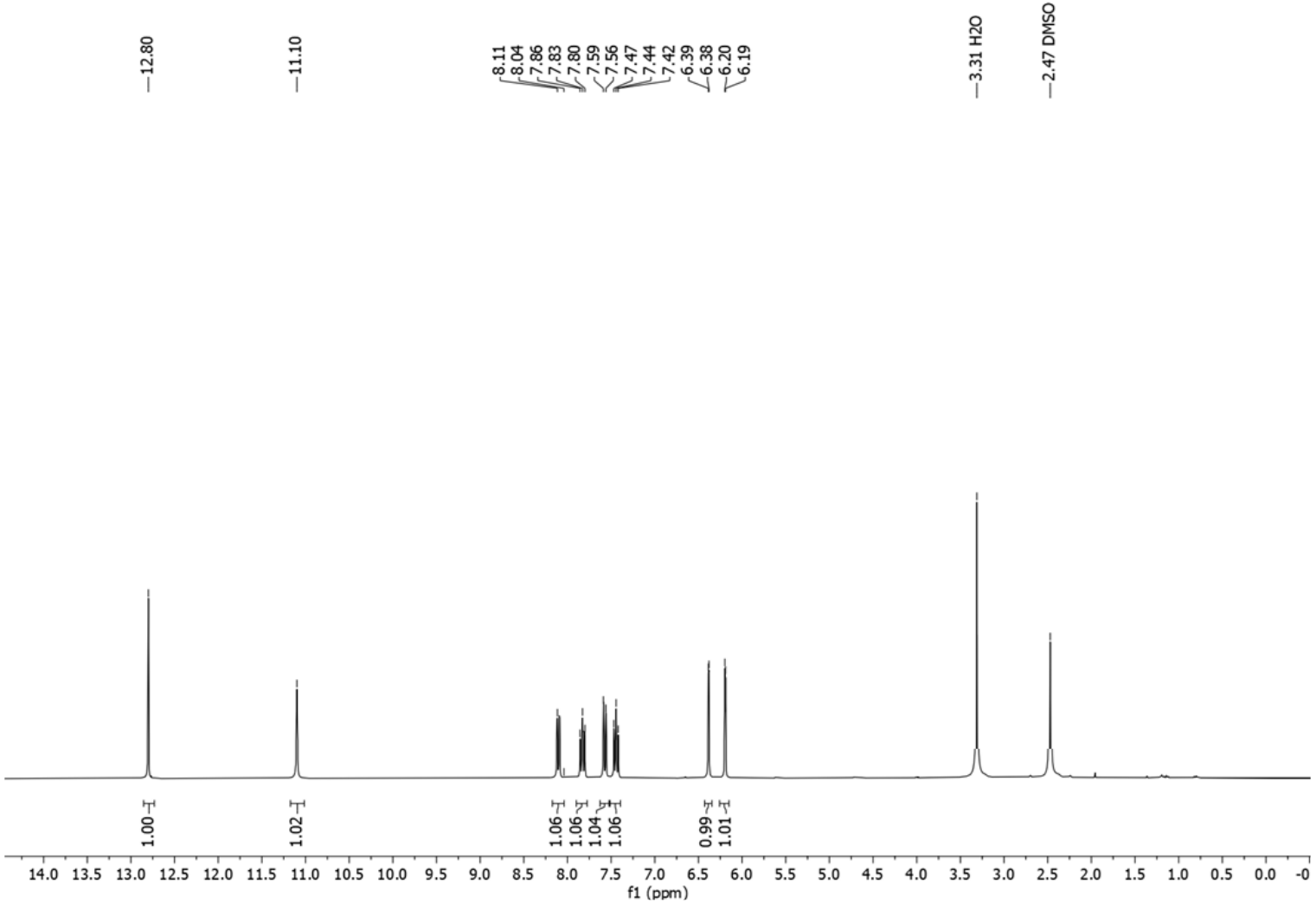

Figure 1. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of 1,3-dihydroxy-9*H*-xanthen-9-one (**1,3-DHX**).

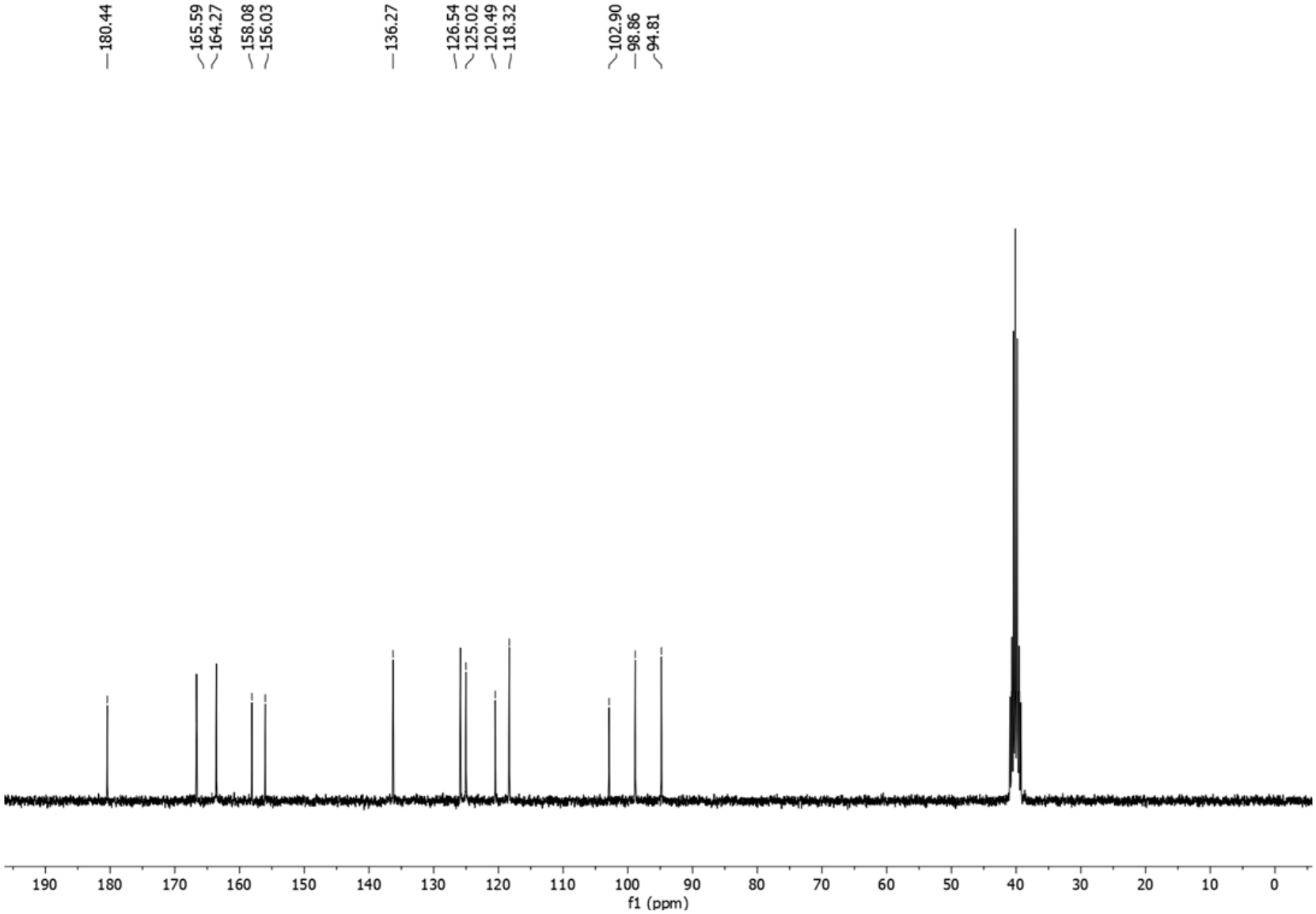

Figure 2. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of 1,3-dihydroxy-9*H*-xanthen-9-one (**1,3-DHX**).

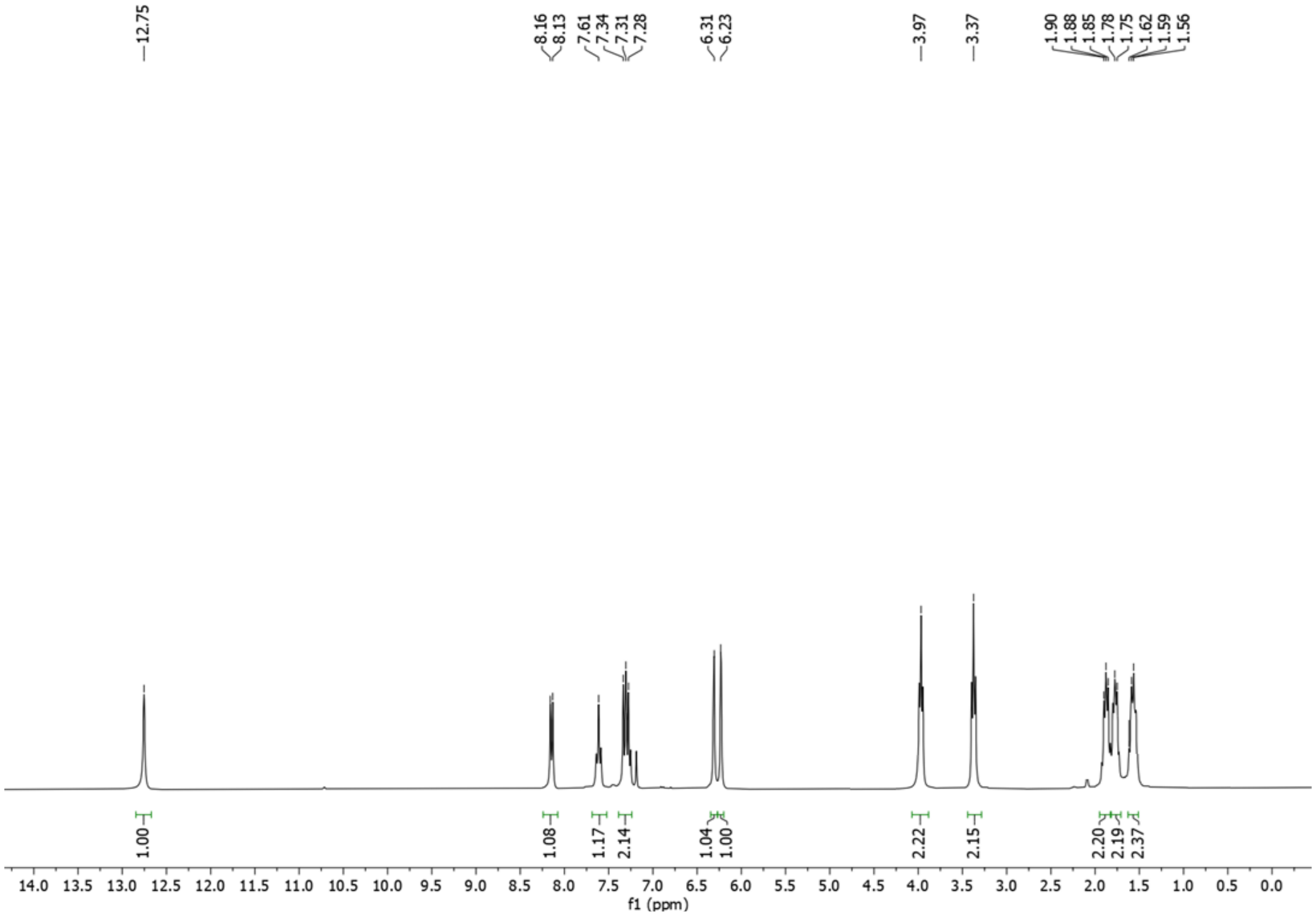

Figure 3. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of 3-((5-bromopentyl)oxy)-1-hydroxy-9*H*-xanthen-9-one (**X5Br**).

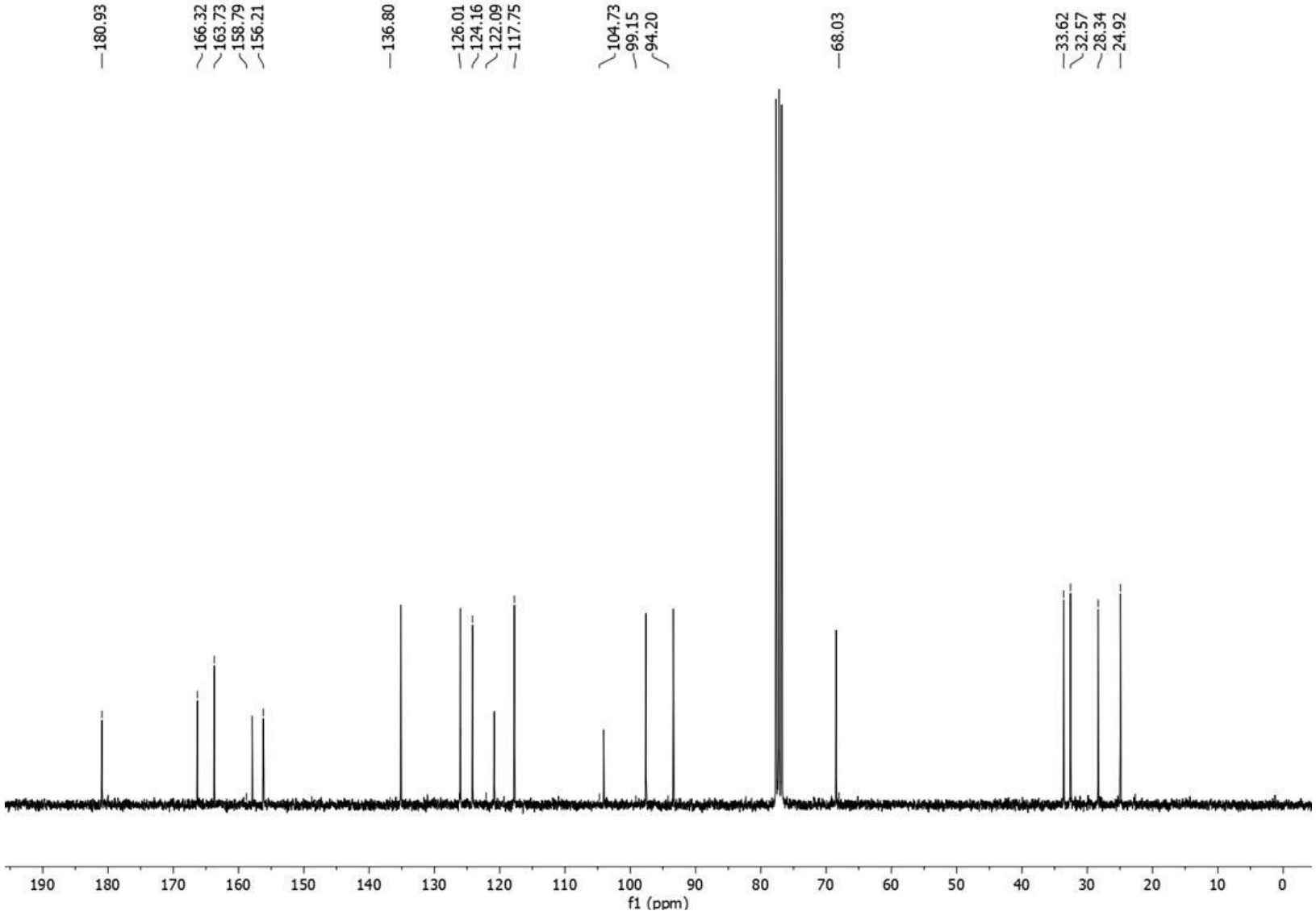

Figure 4. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of 3-((5-bromopentyl)oxy)-1-hydroxy-9*H*-xanthen-9-one (**X5Br**).

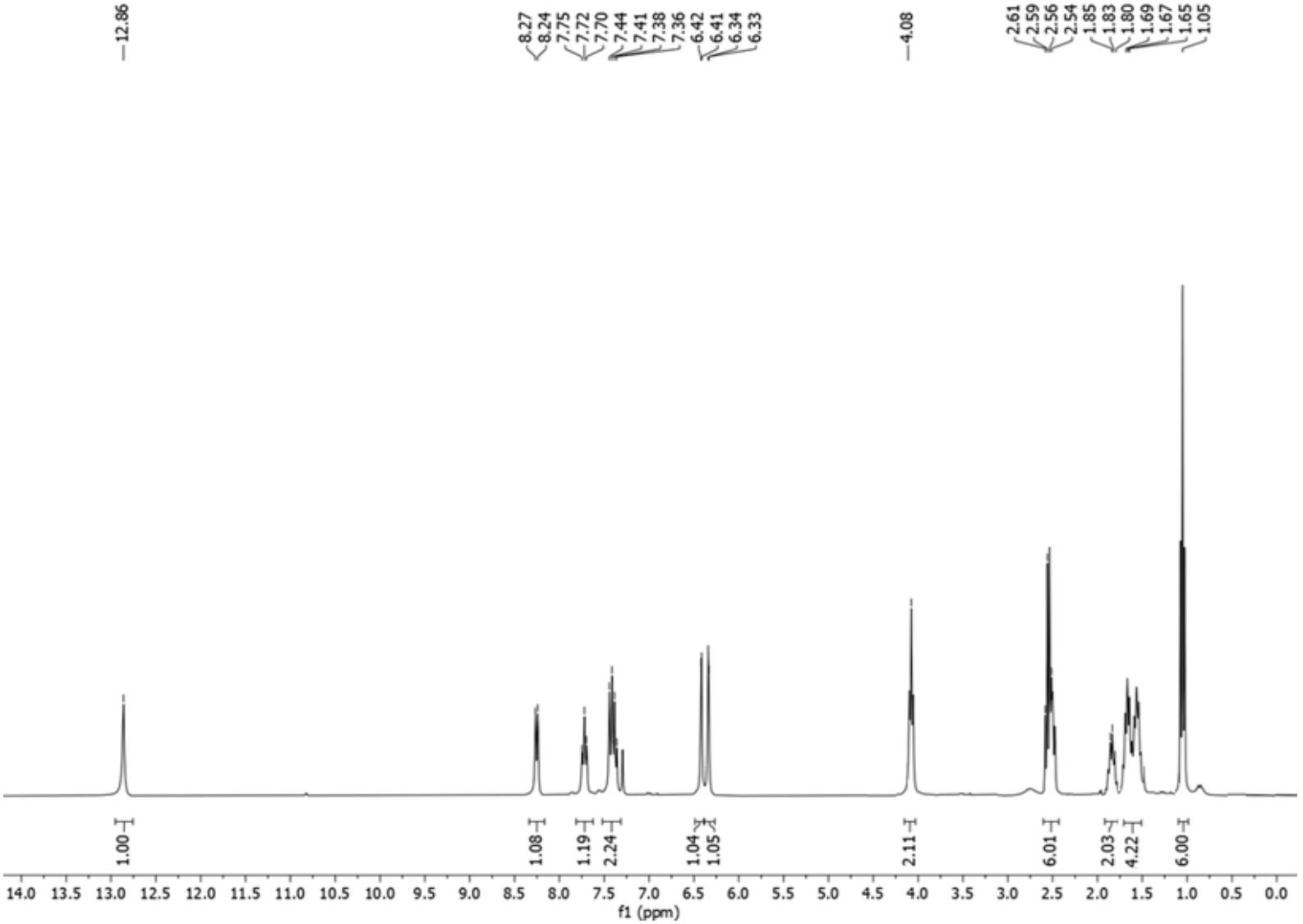

Figure 5. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of 3-((5-(diethylamino)pentyl)oxy)-1-hydroxy-9*H*-xanthen-9-one (**X5DE**).

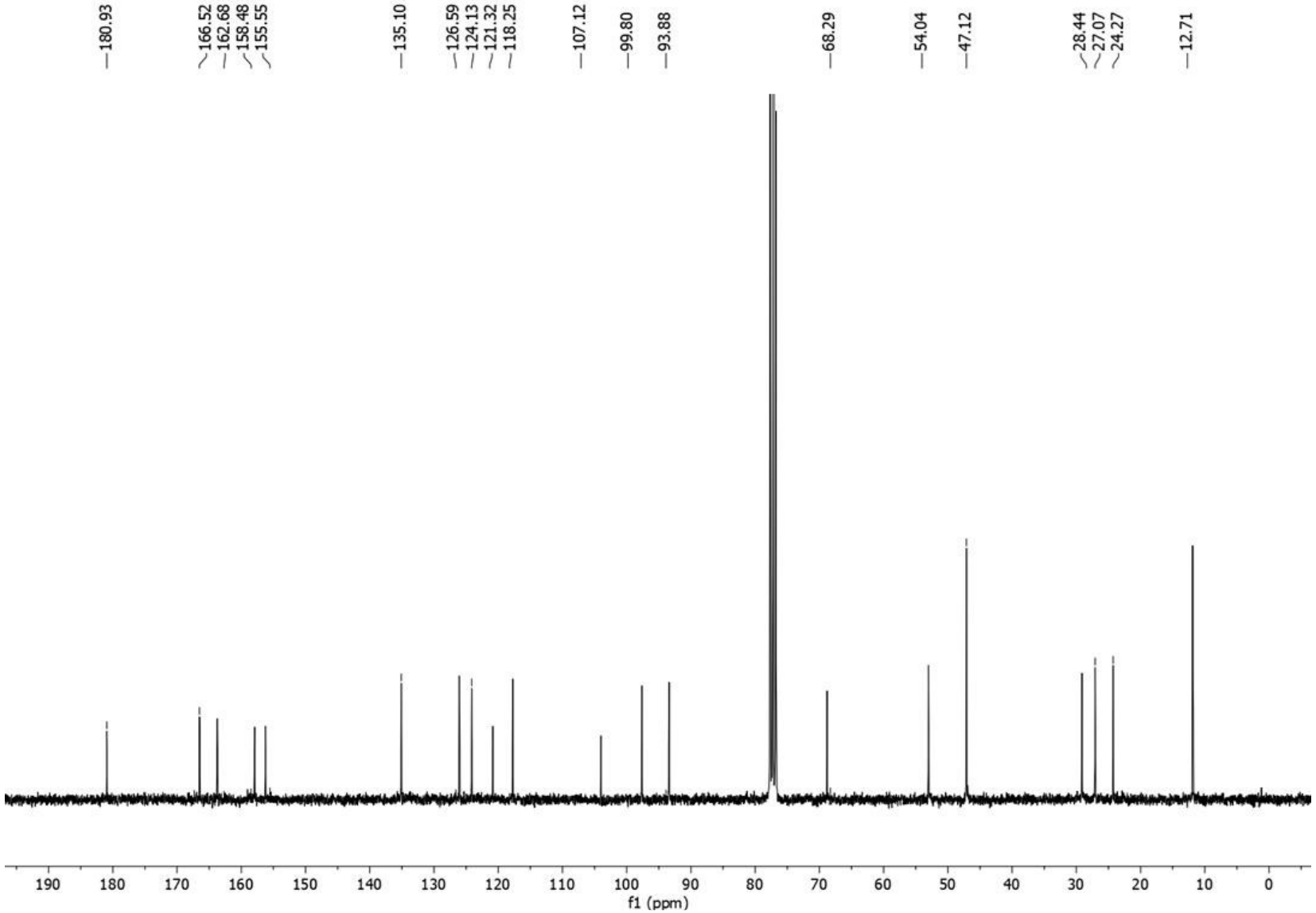

Figure 6. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of 3-((5-(diethylamino)pentyl)oxy)-1-hydroxy-9*H*-xanthen-9-one (**X5DE**).

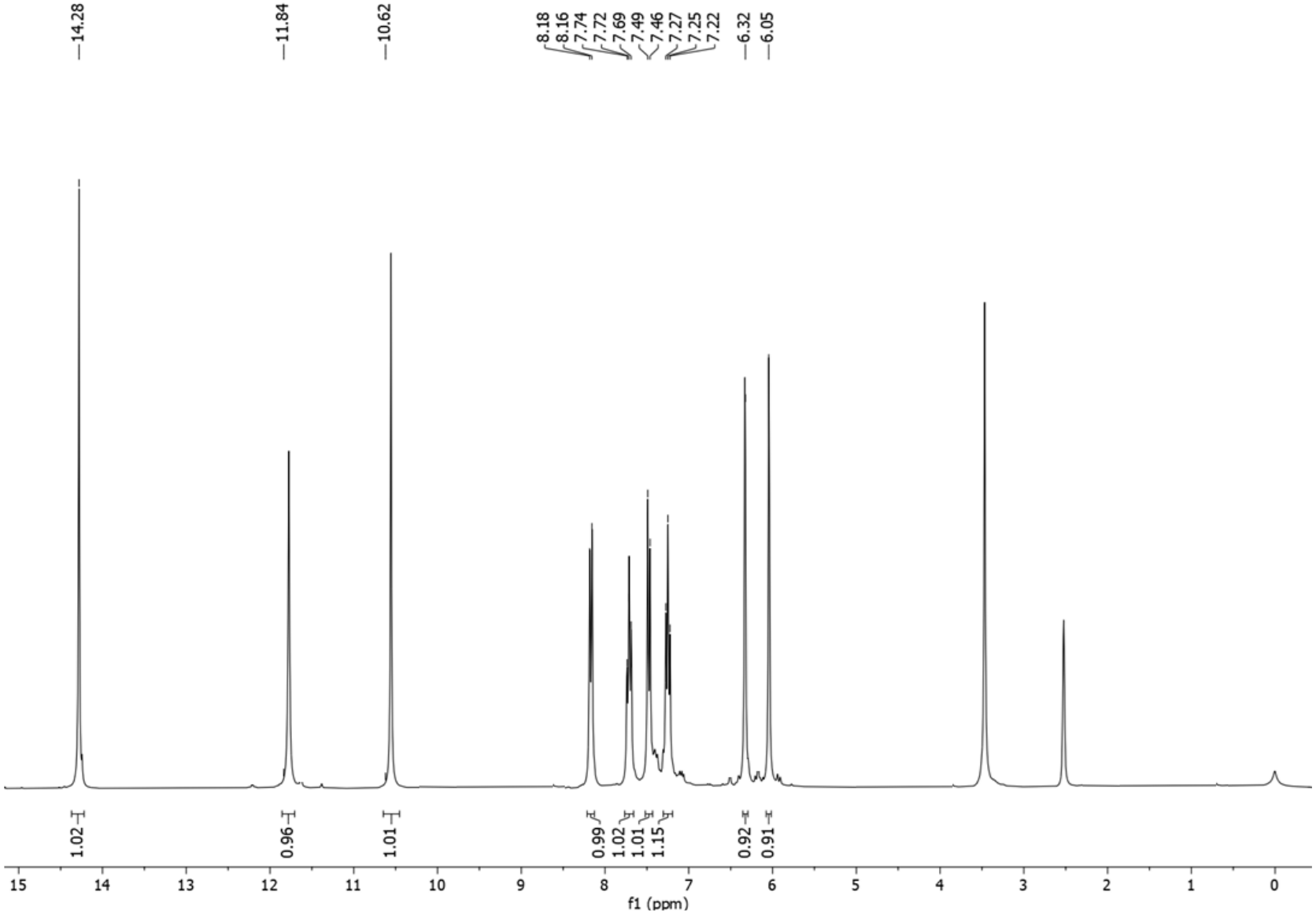

Figure 7. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of 1,3-dihydroxyacridin-9(10*H*)-one (**1,3-DHA**).

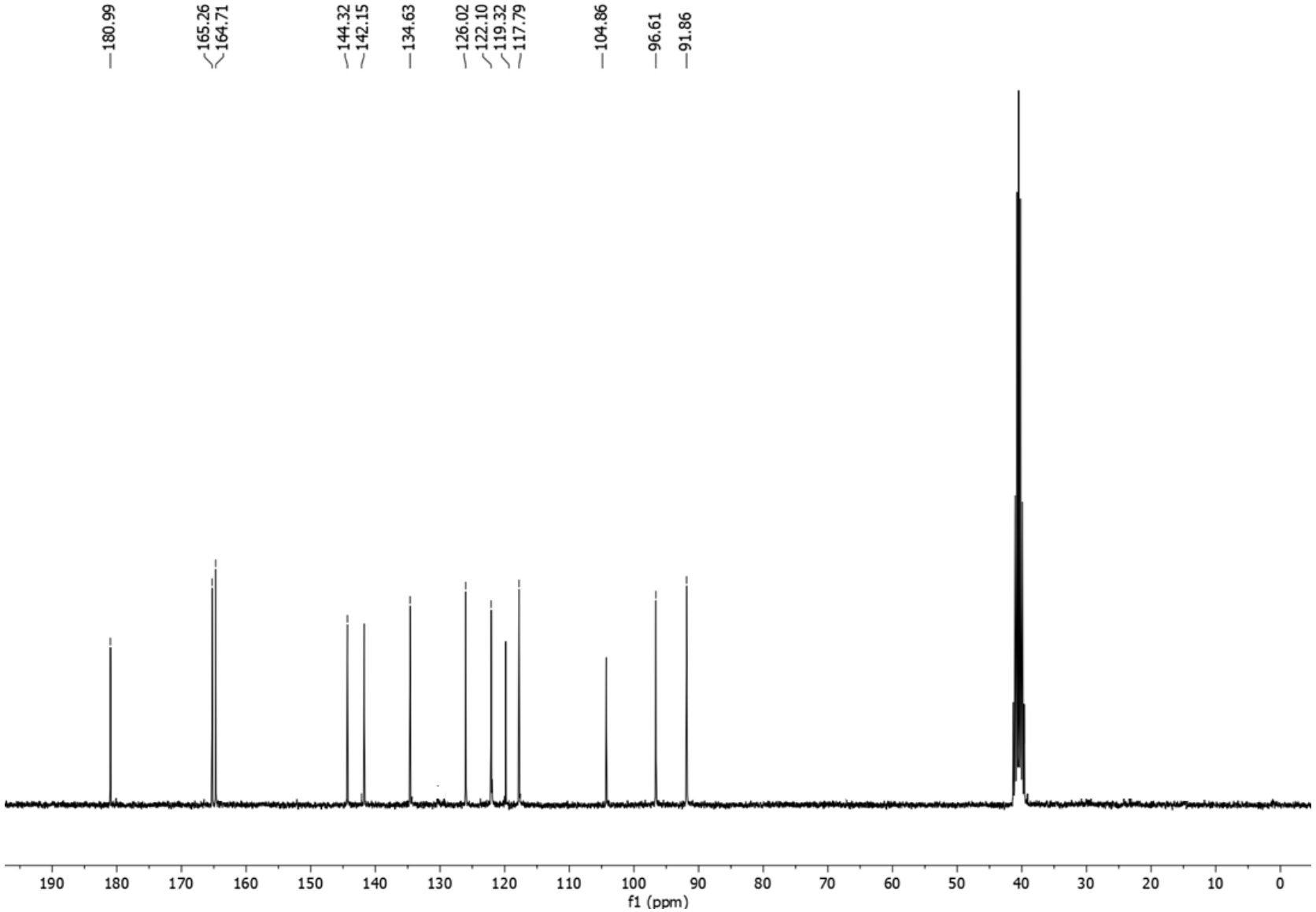

Figure 8. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of 1,3-dihydroxyacridin-9(10*H*)-one (**1,3-DHA**).

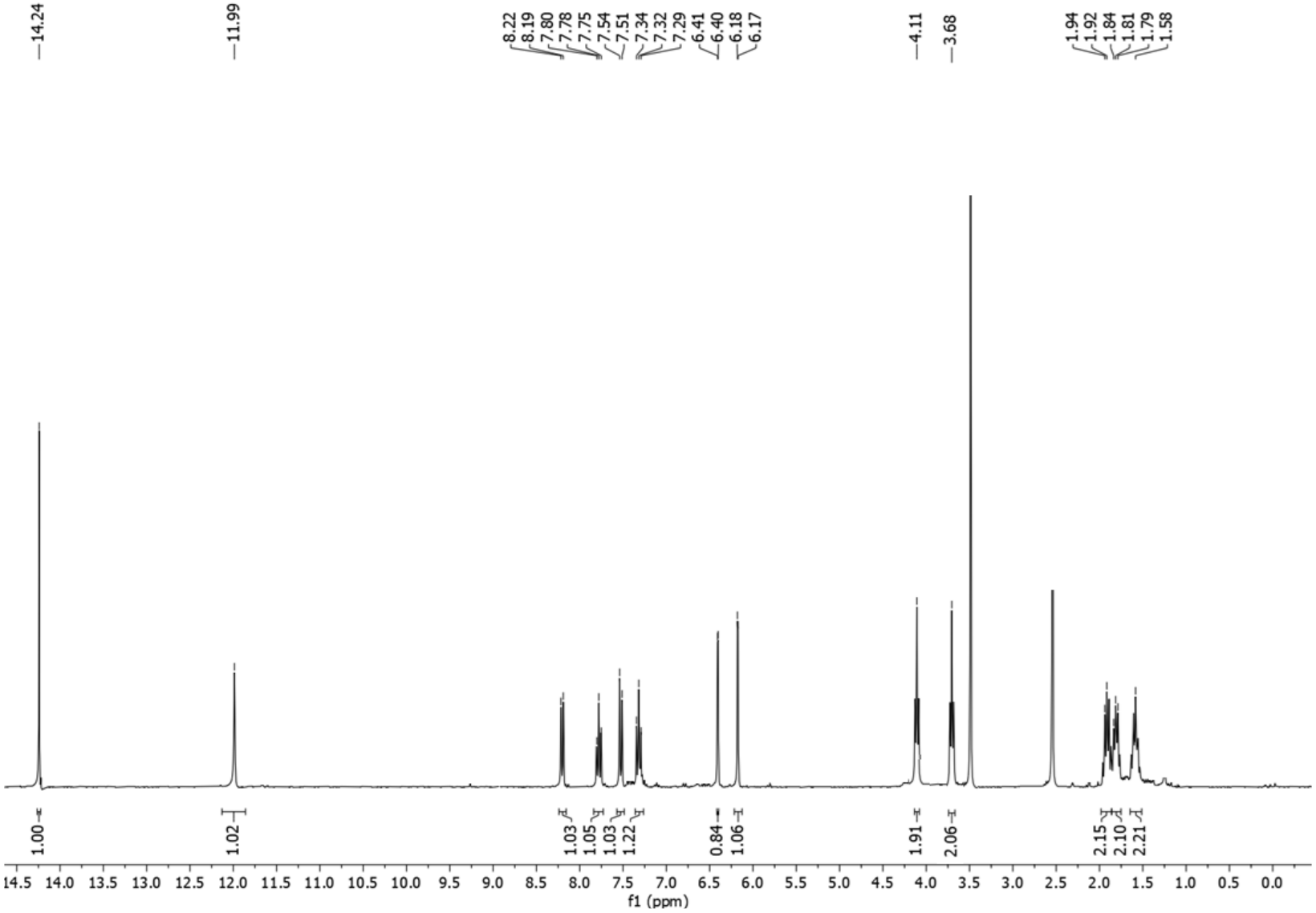

Figure 9. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of 3-((5-bromopentyl)oxy)-1-hydroxy-acridin-9(10*H*)-one (**A5Br**).

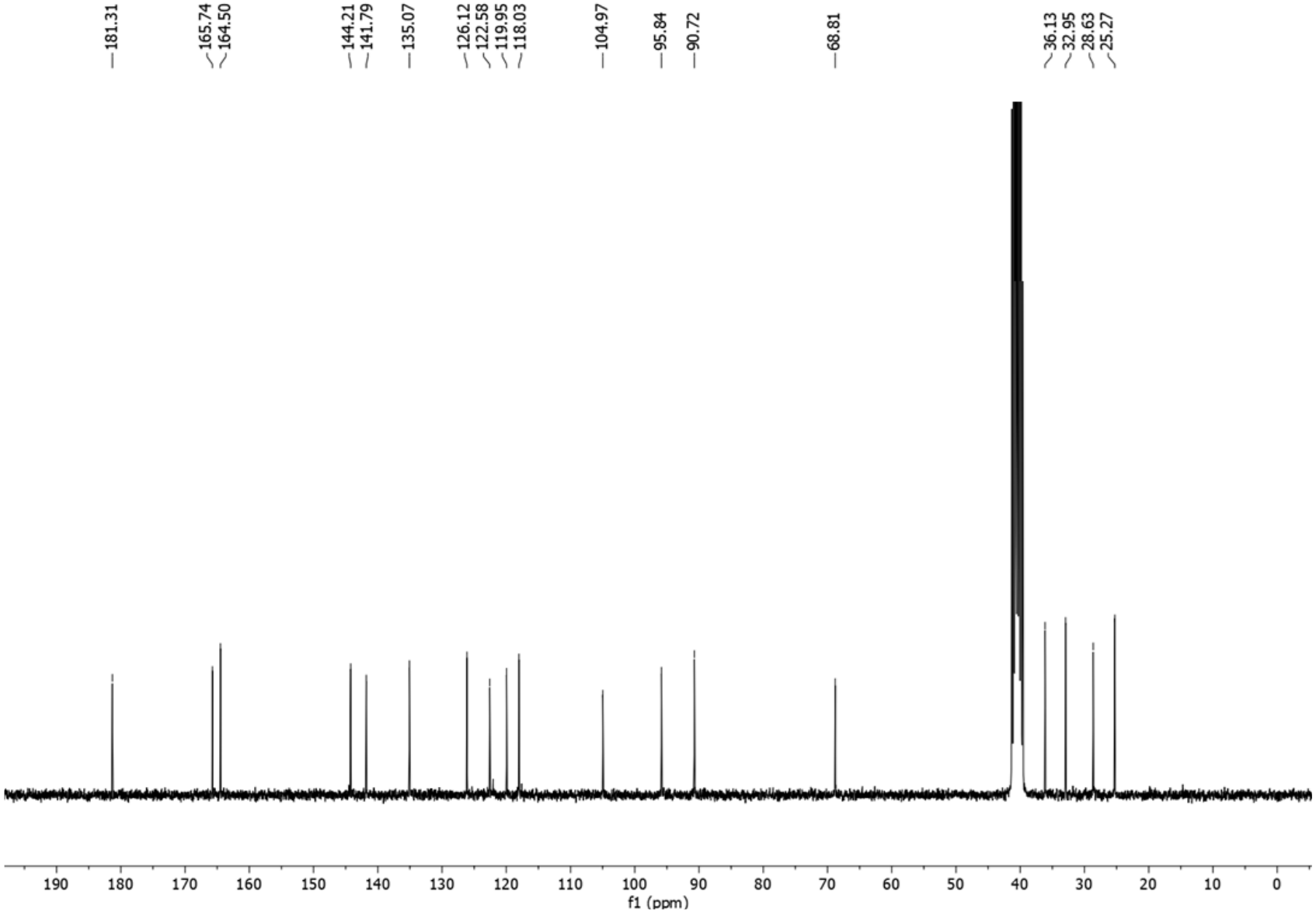

Figure 10. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of 3-((5-bromopentyl)oxy)-1-hydroxy-acridin-9(10*H*)-one (**A5Br**).

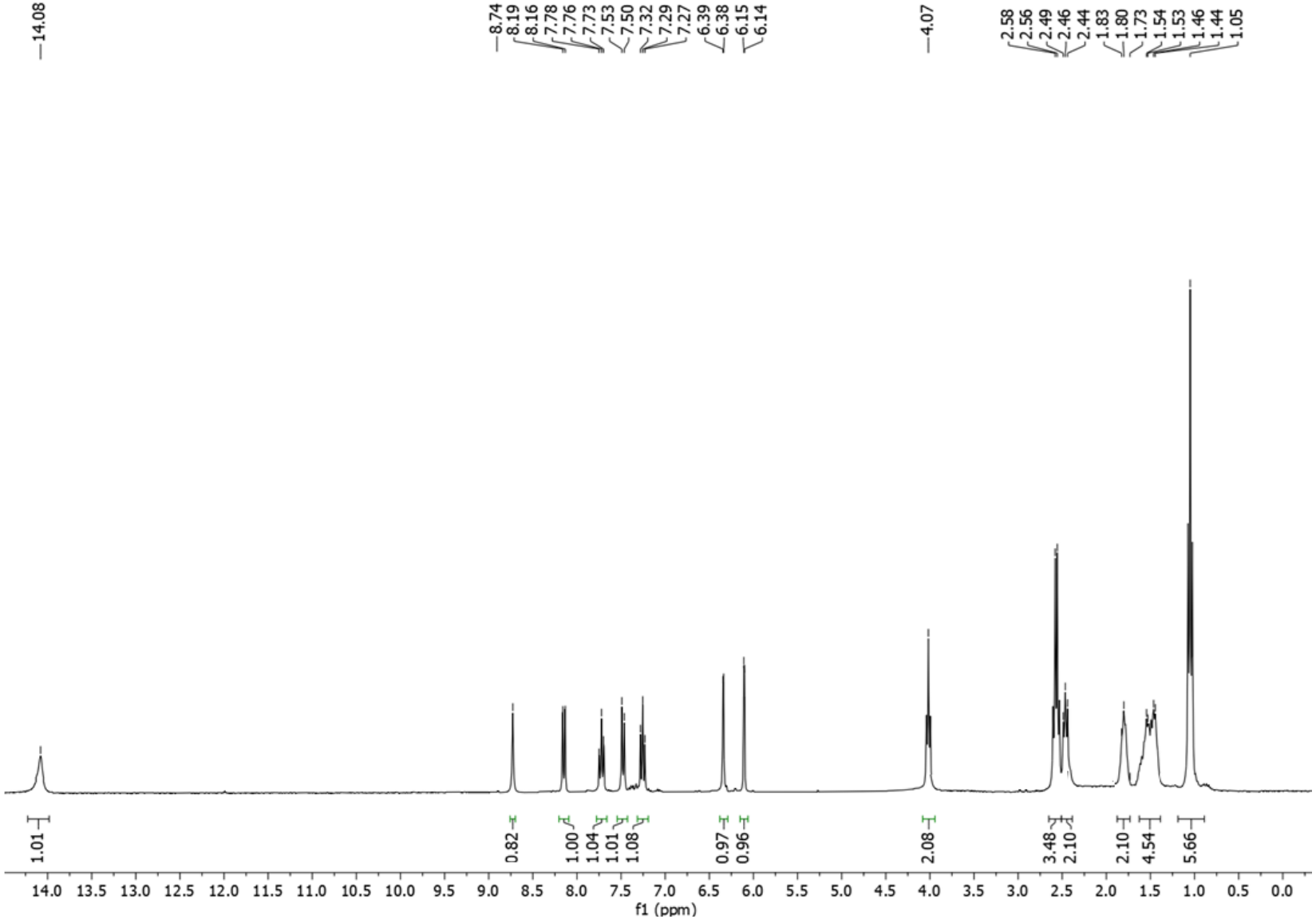

Figure 11. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of 3-((5-(diethylamino)pentyl)oxy)-1-hydroxyacridin-9(10*H*)-one (**A5DE**).

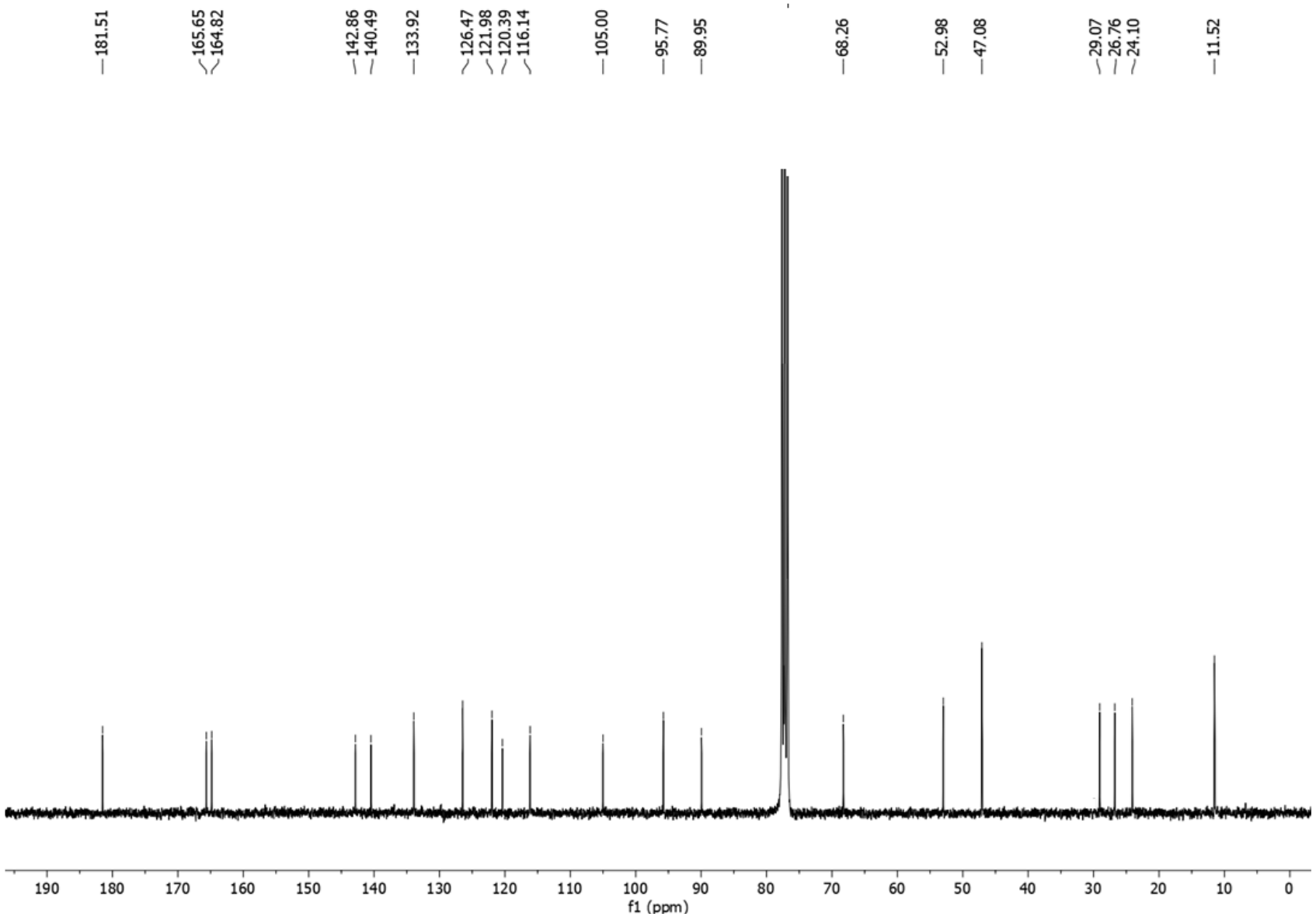

Figure 12. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of 3-((5-(diethylamino)pentyl)oxy)-1-hydroxyacridin-9(10*H*)-one (**A5DE**).