Supporting Information

Oleanolic Acid Derivatives as Potential Inhibitors of HIV-1 Protease

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Figure S1. Dose / response relationships of compounds **1g**-**4g**, expressed in percentages of activity of these compounds at different concentrations (μM). Values represent means of an experiment performed in triplicate.

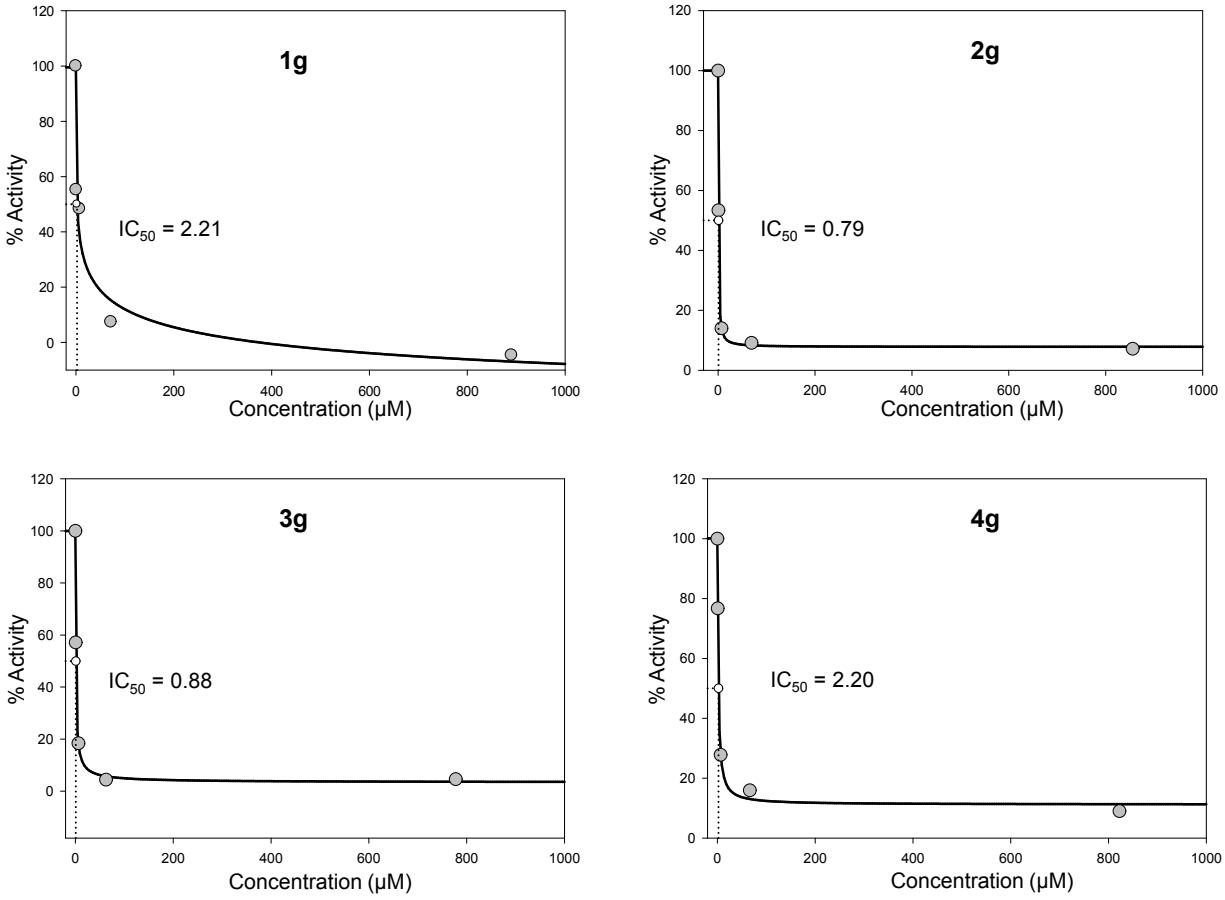


Figure S2. Dose / response relationships of compounds **5g-8g**, expressed in percentages of activity of these compounds at different concentrations (μM). Values represent means of an experiment performed in triplicate.

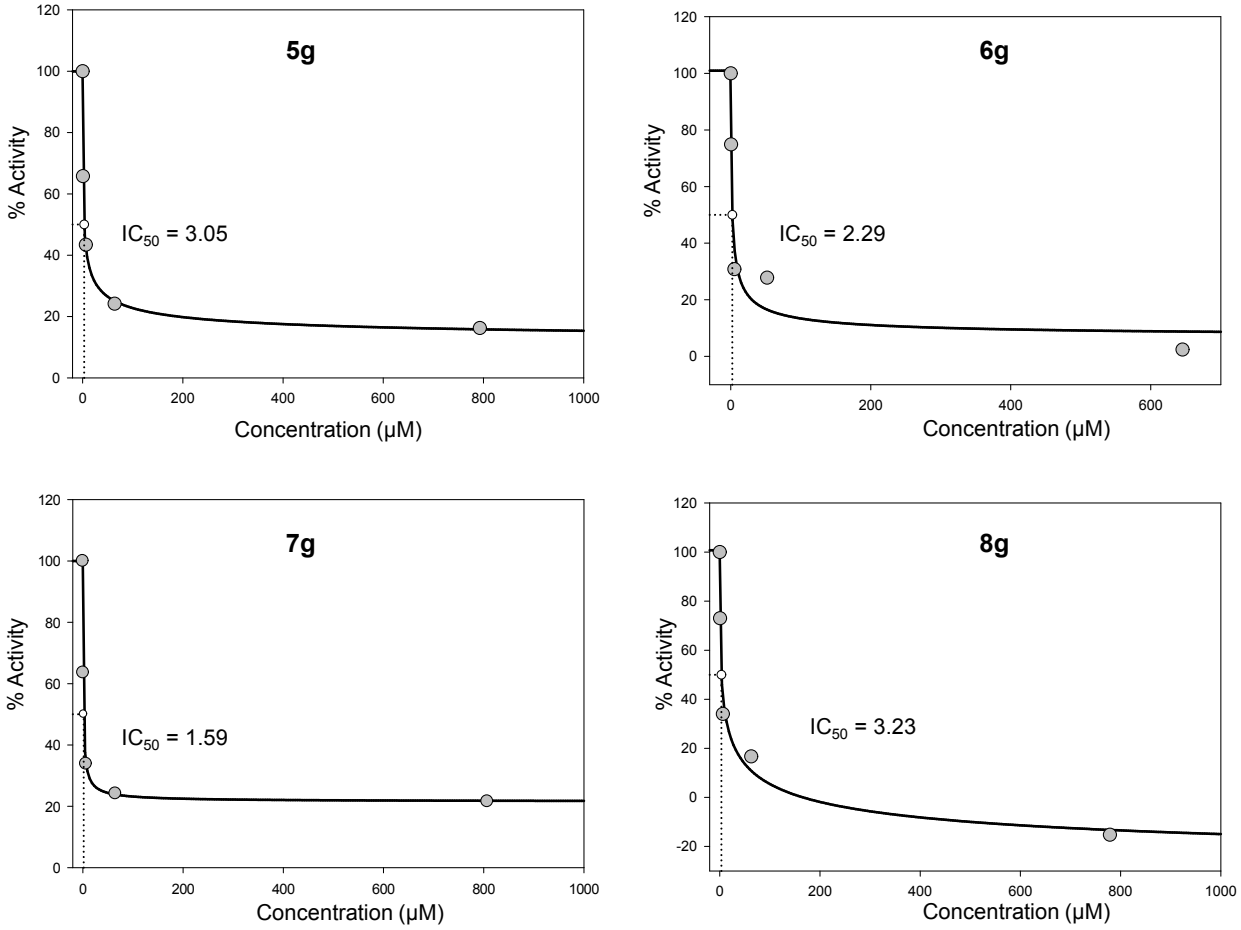


Figure S3. Dose / response relationships of compounds **9g-12g**, expressed in percentages of activity of these compounds at different concentrations (μM). Values represent means of an experiment performed in triplicate.

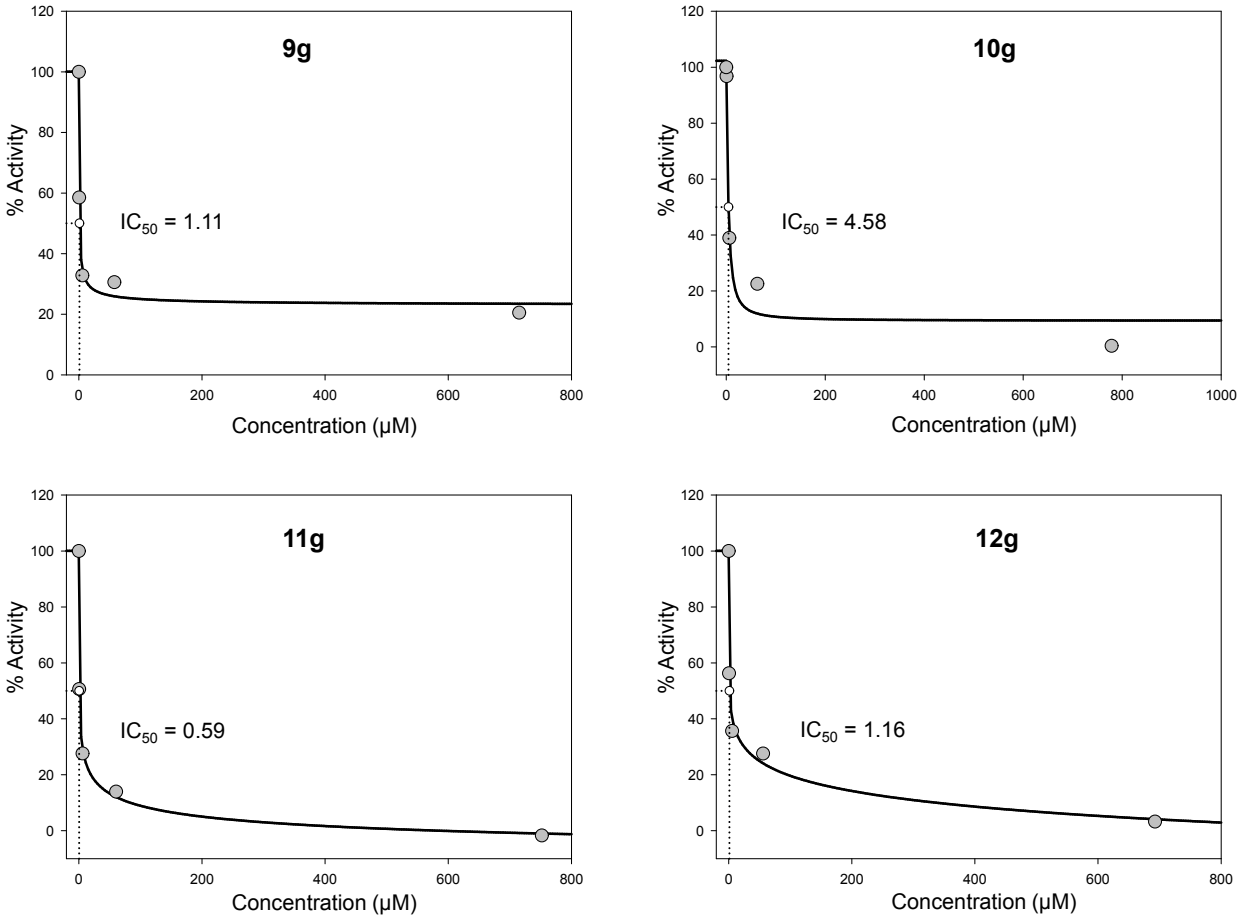


Figure S4. Dose / response relationships of compounds **2h** and **2i**, expressed in percentages of activity of these compounds at different concentrations (μM). Values represent means of an experiment performed in triplicate.

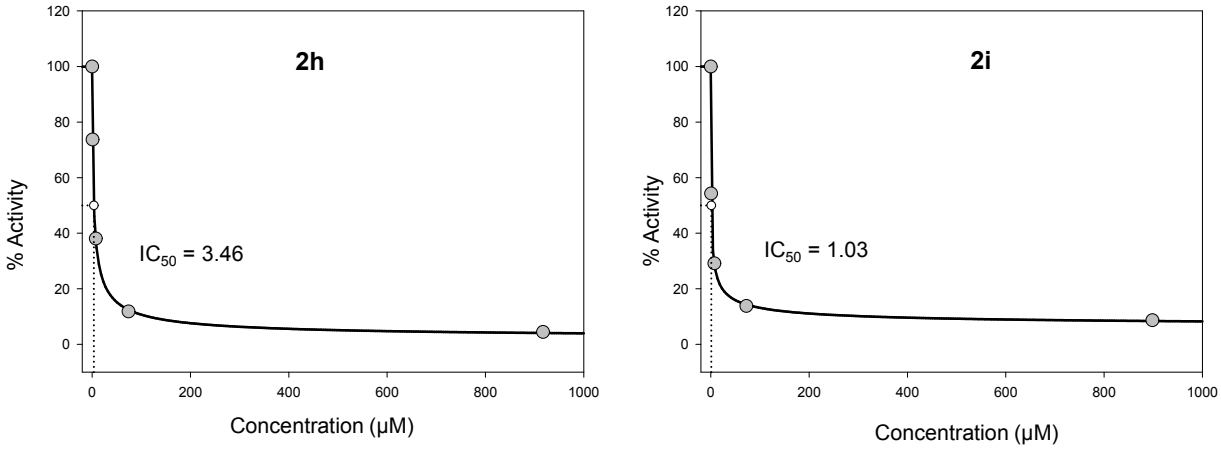
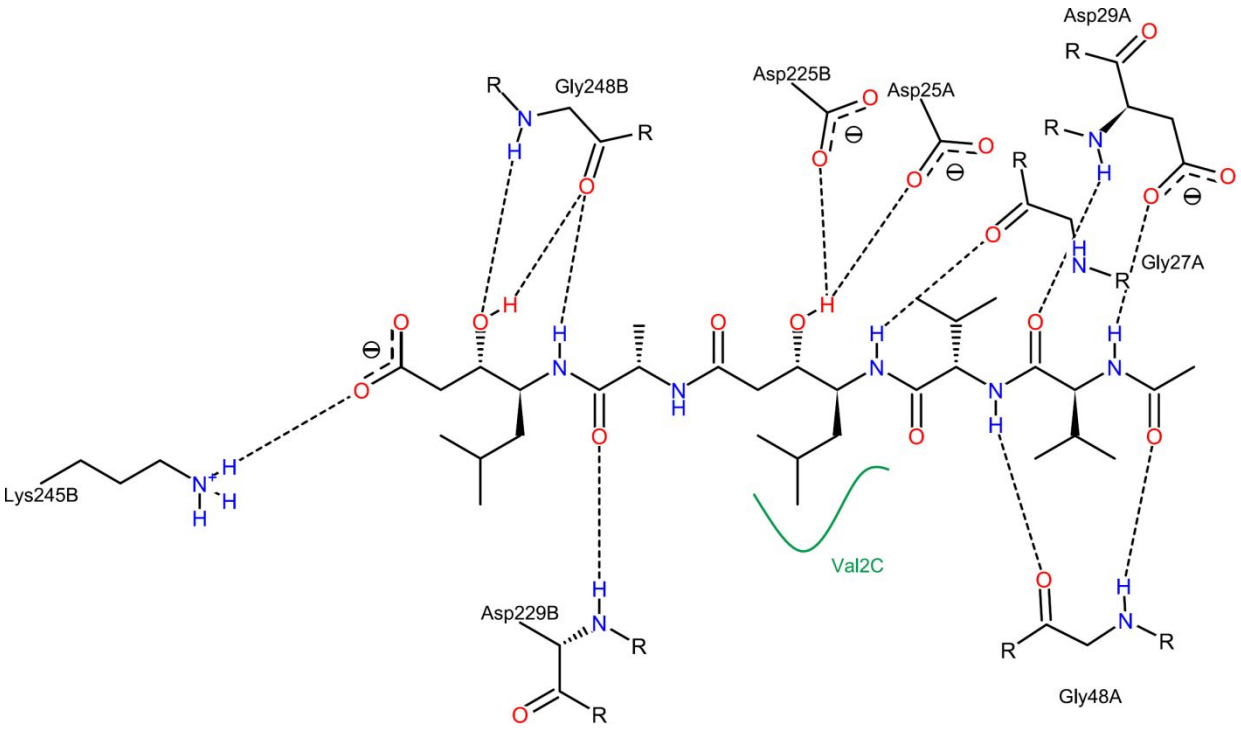


Figure S5. 2D schematic representation of the binding interactions of Acetyl-Pepstatin with the active site of the HIV-1 protease, created with PoseView.



The H-bonds are shown as black dashed lines, and residue labels and spline segments along the contacting hydrophobic ligand parts represent the hydrophobic contacts.

Figure S6. Crystallized position of acetyl-pepstatin (red sticks) and the docked position (green sticks) showing a good correlation between the two, as a positive control to validate the docking protocol.

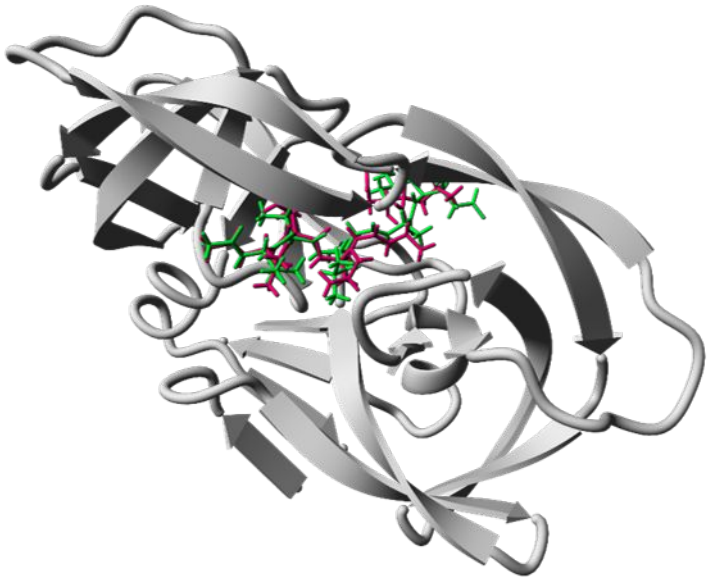


Figure S7. The docking position of acetyl-pepstatin (green sticks) and its molecular surface (translucent green), indicating the location of the active site.

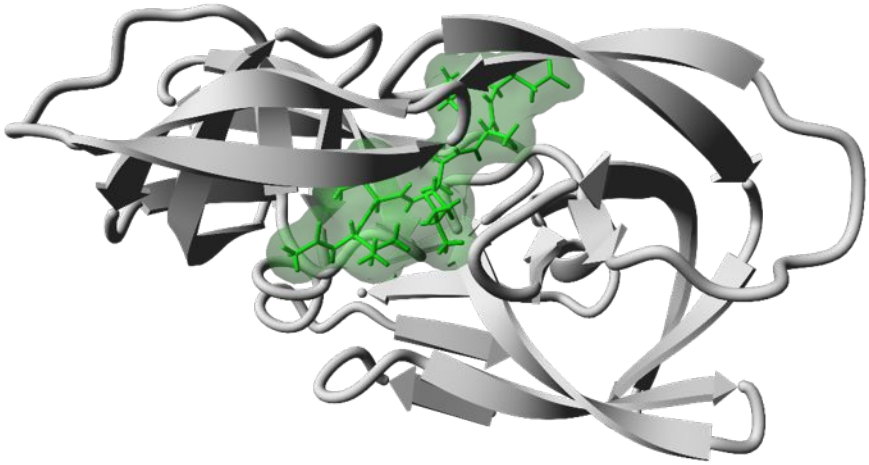


Figure S8. The 15 top-ranked OA derivatives (rainbow sticks) appear to be linked within the active site of the enzyme.

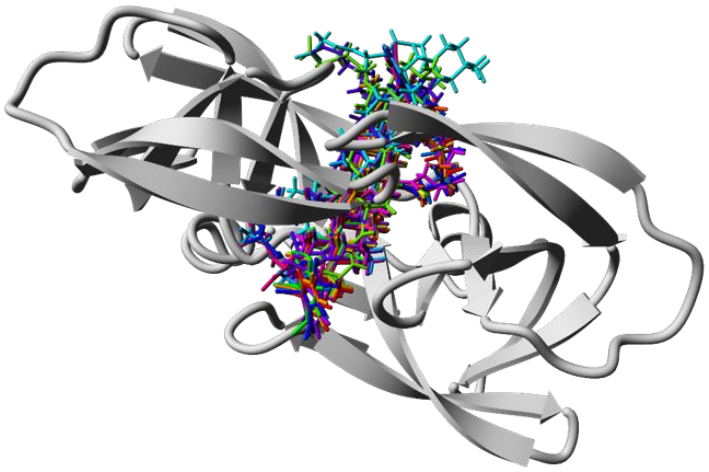


Figure S9. Frontal orientation of Figure S8, with a better visualization of the active site of the enzyme.

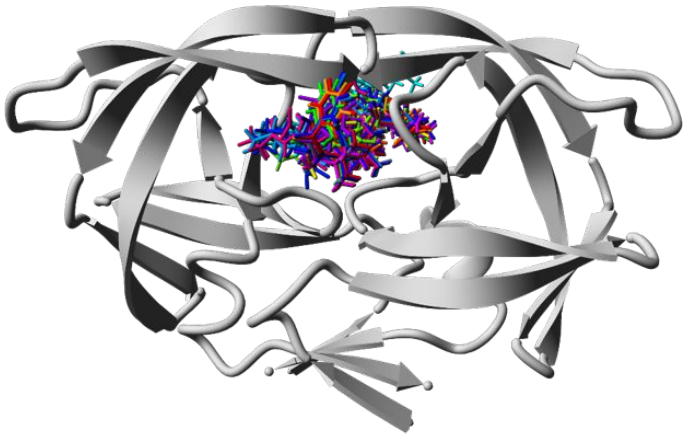


Figure S10. The best docking position for compound **11g** (blue sticks) and its molecular surface (translucent blue).

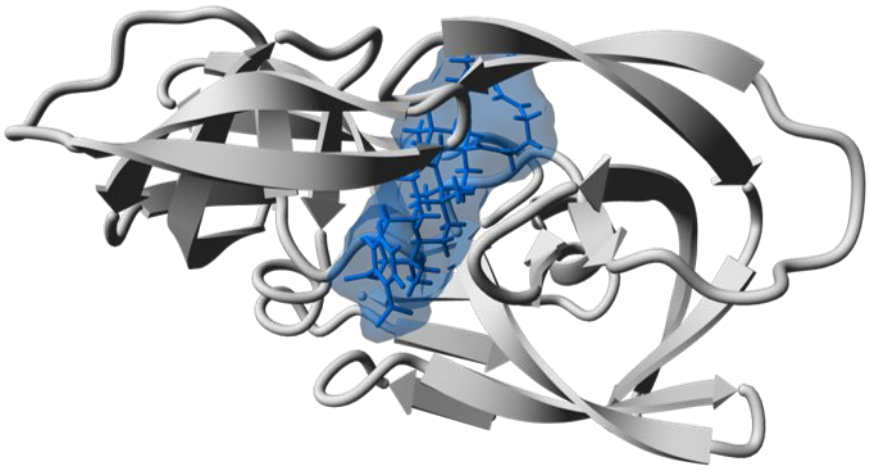


Figure S11. Superimposition of the structures of acetyl-pepstatin and compound **11g** denoting a similar binding domain, mainly within the active site of the HIV-1 protease.

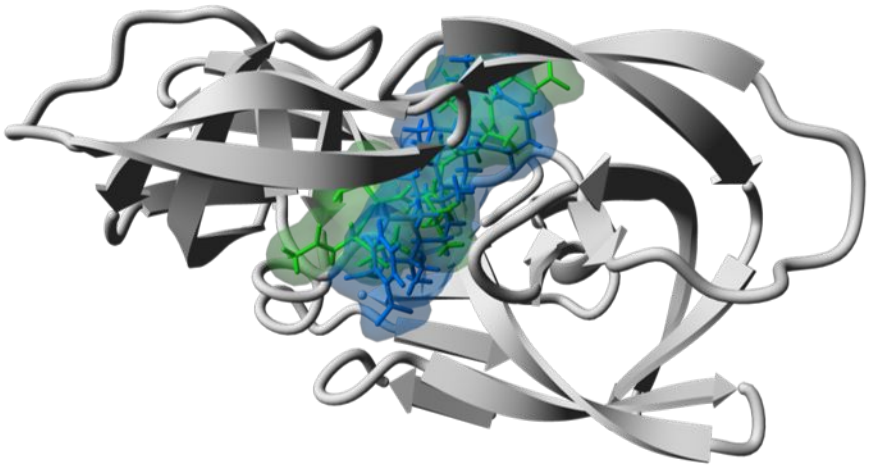


Figure S12. ^{1}H, ^{13}C NMR spectra and DEPT of compound **1g** ($CDCl_3$).

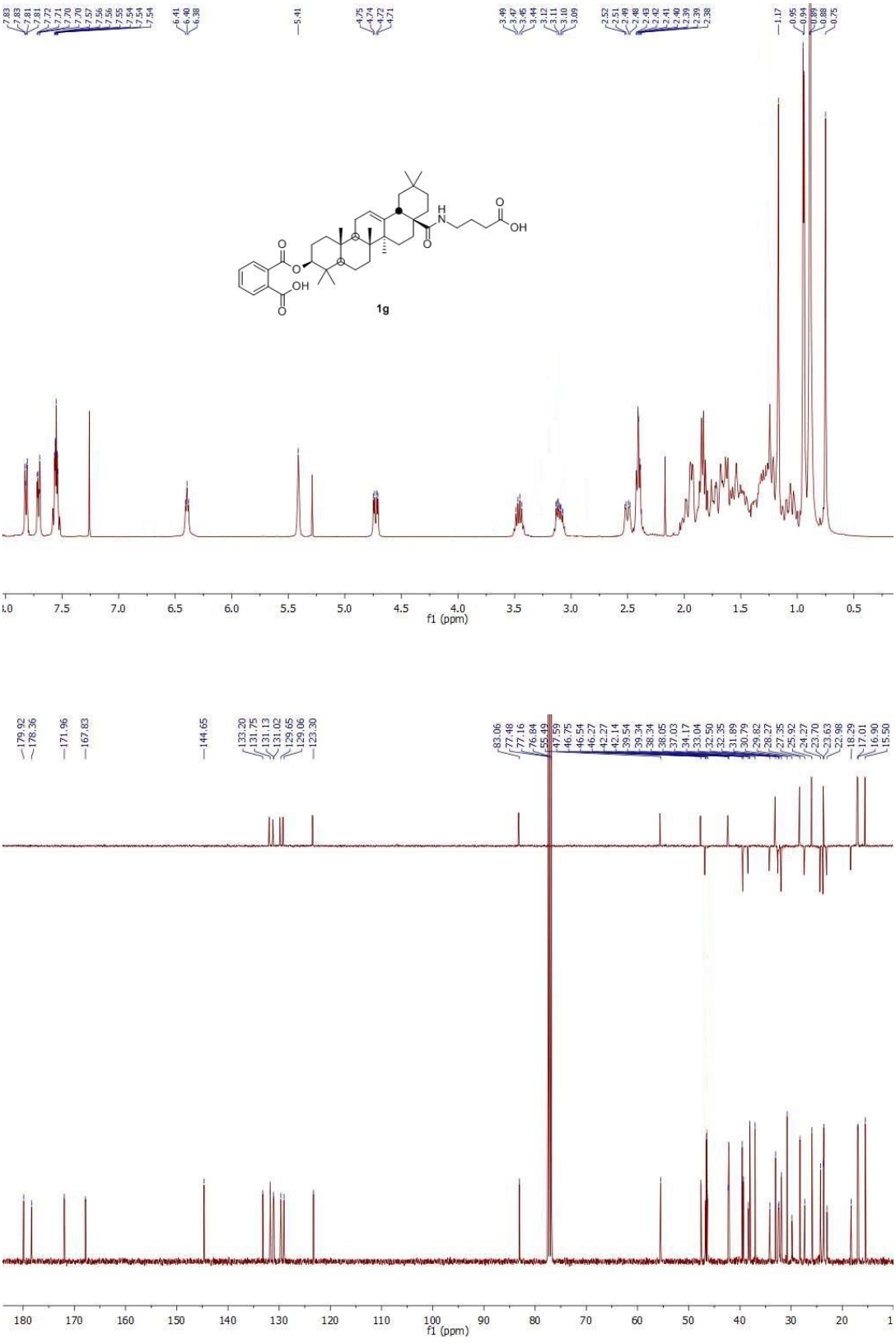


Figure S13. ^{1}H, ^{13}C NMR spectra and DEPT of compound **2g** ($CDCl_3$).

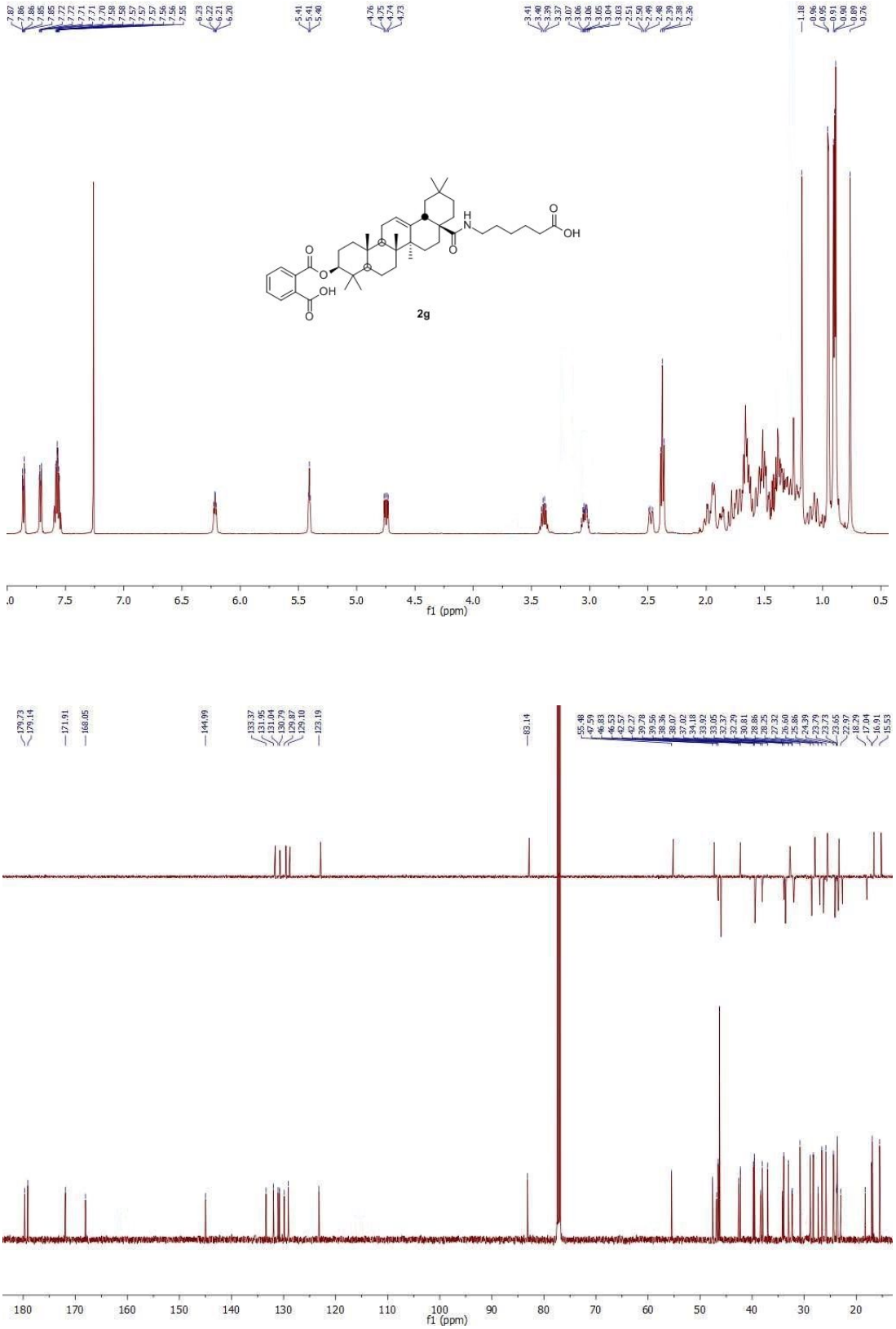


Figure S14. ^{1}H, ^{13}C NMR spectra and DEPT of compound **2h** ($CDCl_3$).

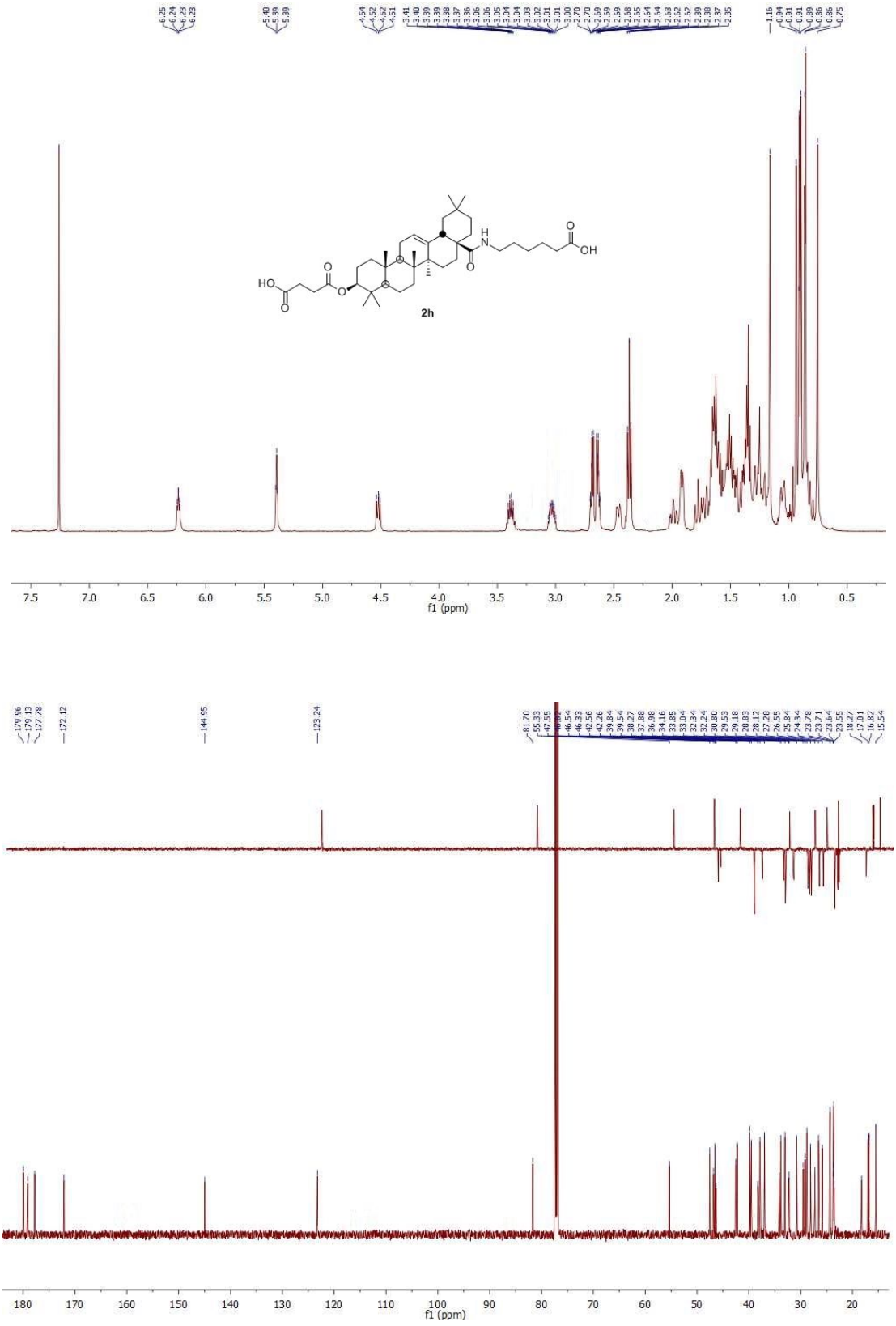


Figure S15. ^{1}H, ^{13}C NMR spectra and DEPT of compound **2i** ($CDCl_3$).

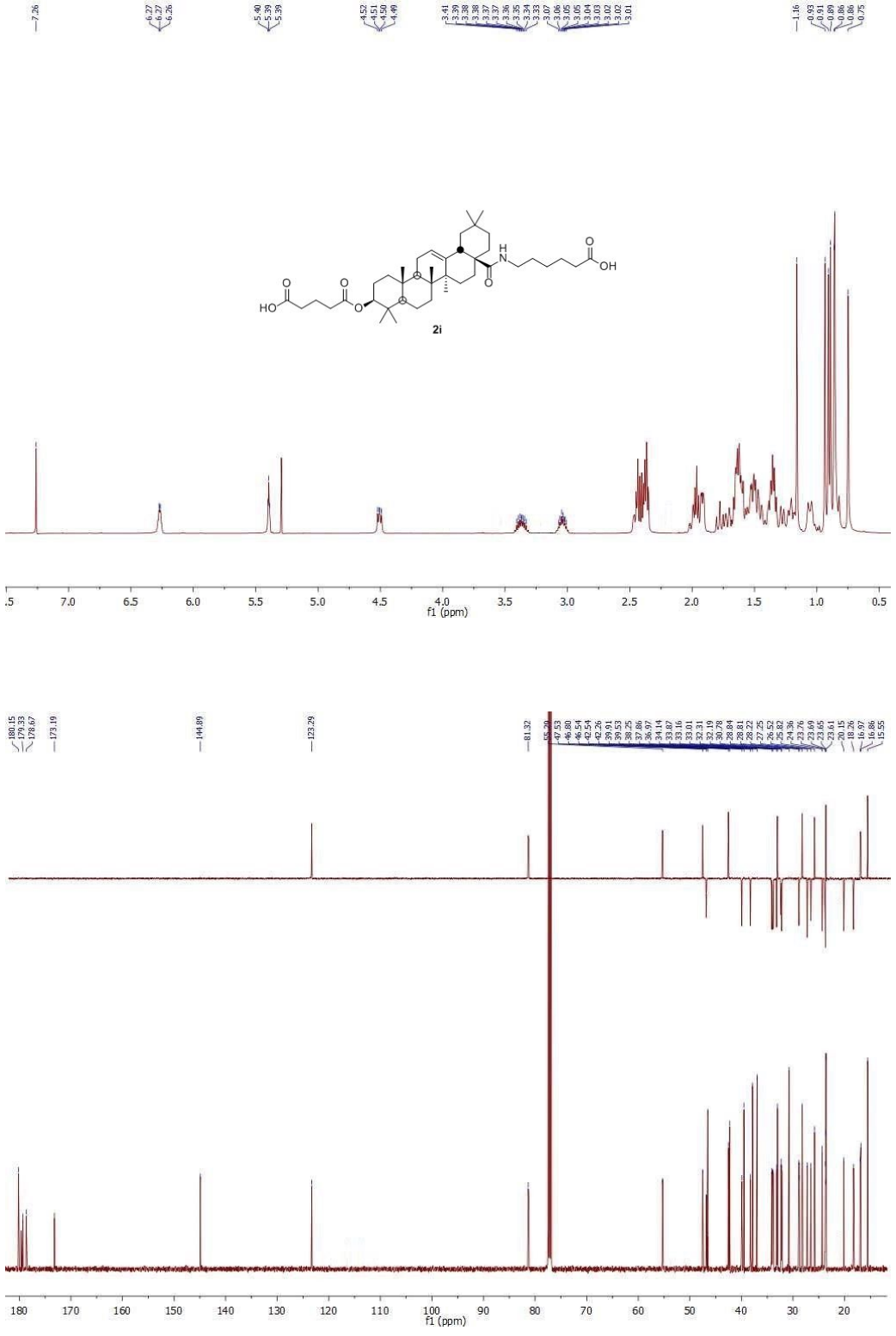


Figure S16. ^{1}H, ^{13}C NMR spectra and DEPT of compound **3g** ($CDCl_3$).

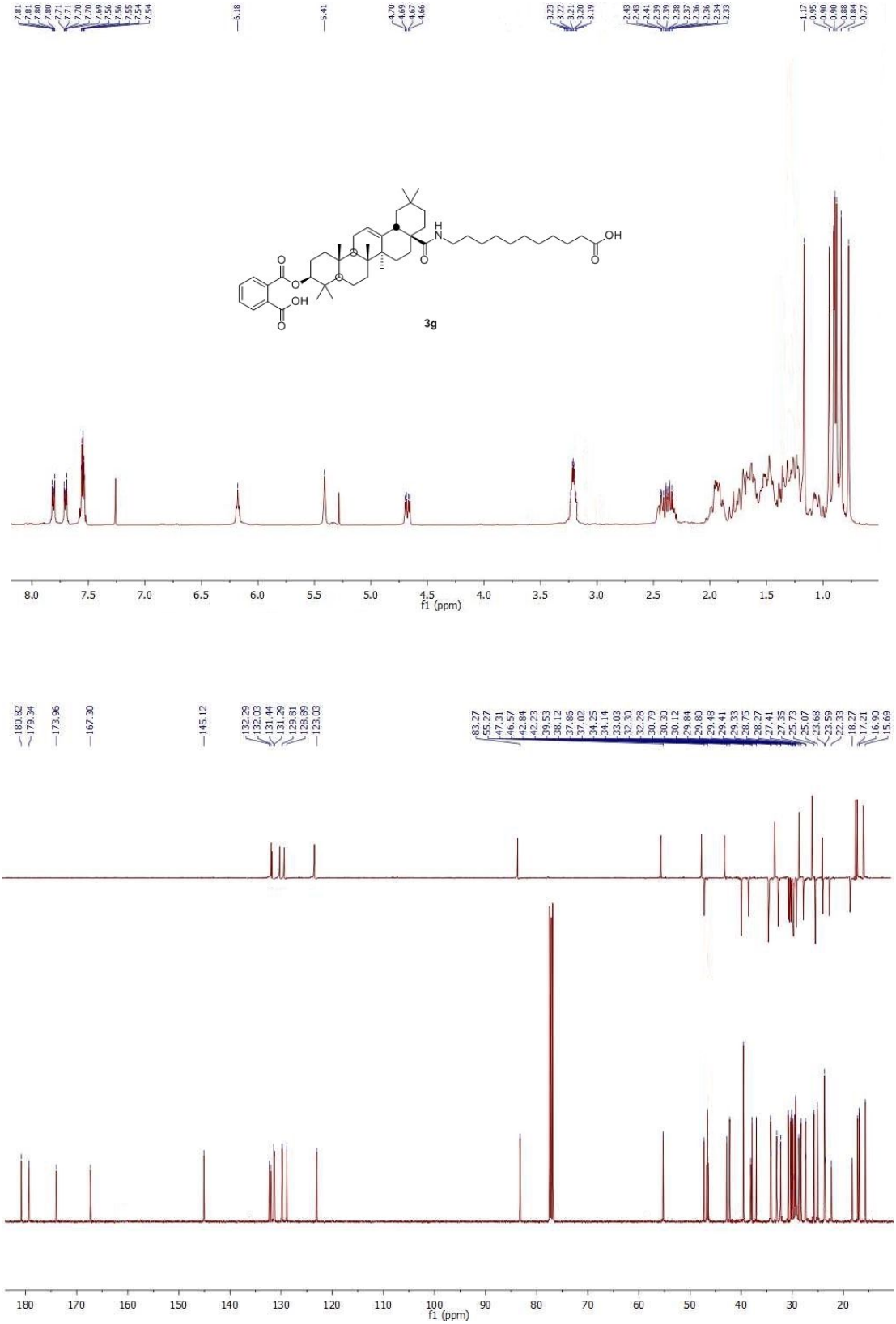


Figure S17. ^{1}H, ^{13}C NMR spectra and DEPT of compound **4g** ($CDCl_3$).

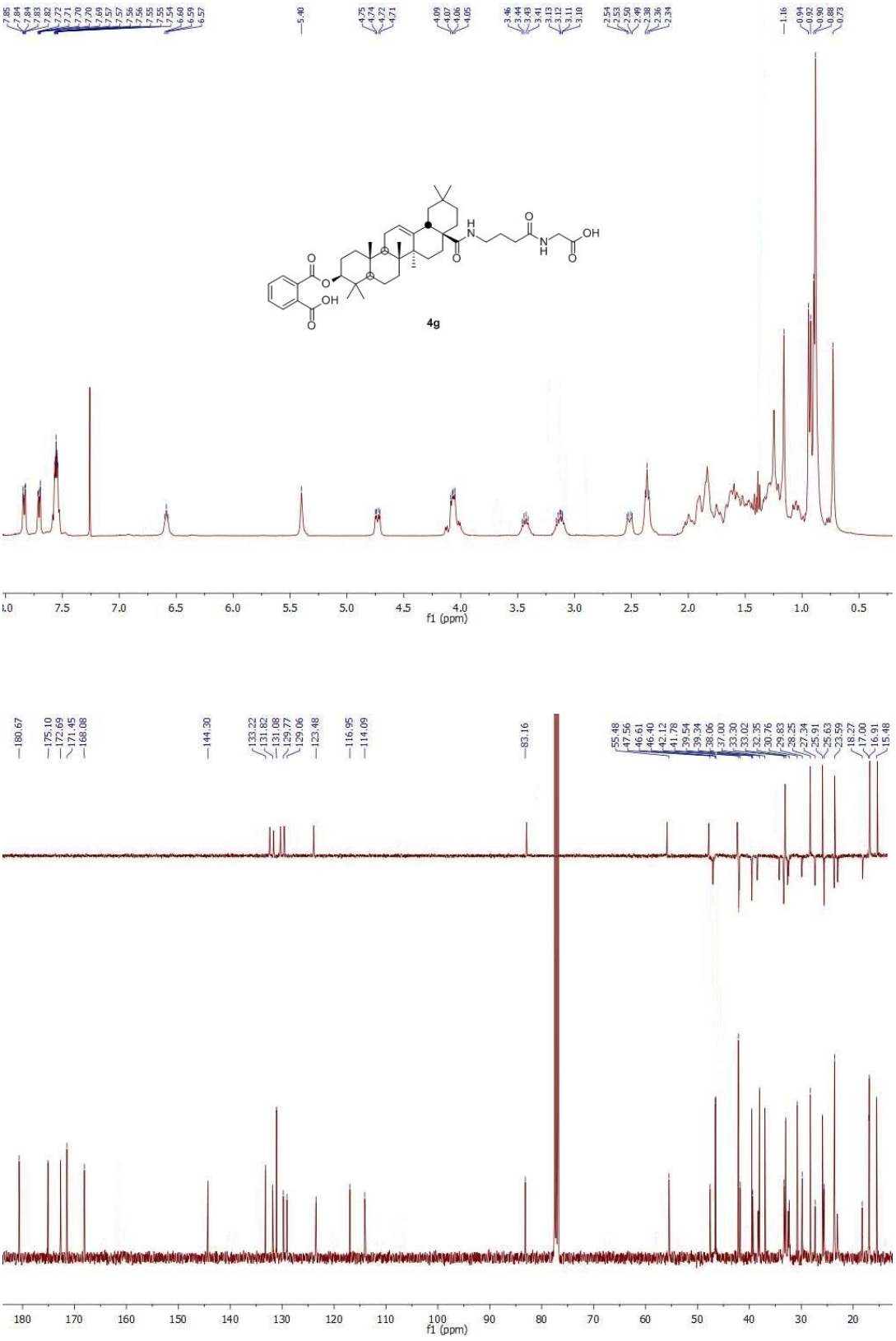


Figure S18. ^{1}H, ^{13}C NMR spectra and DEPT of compound **5g** ($CDCl_3$).

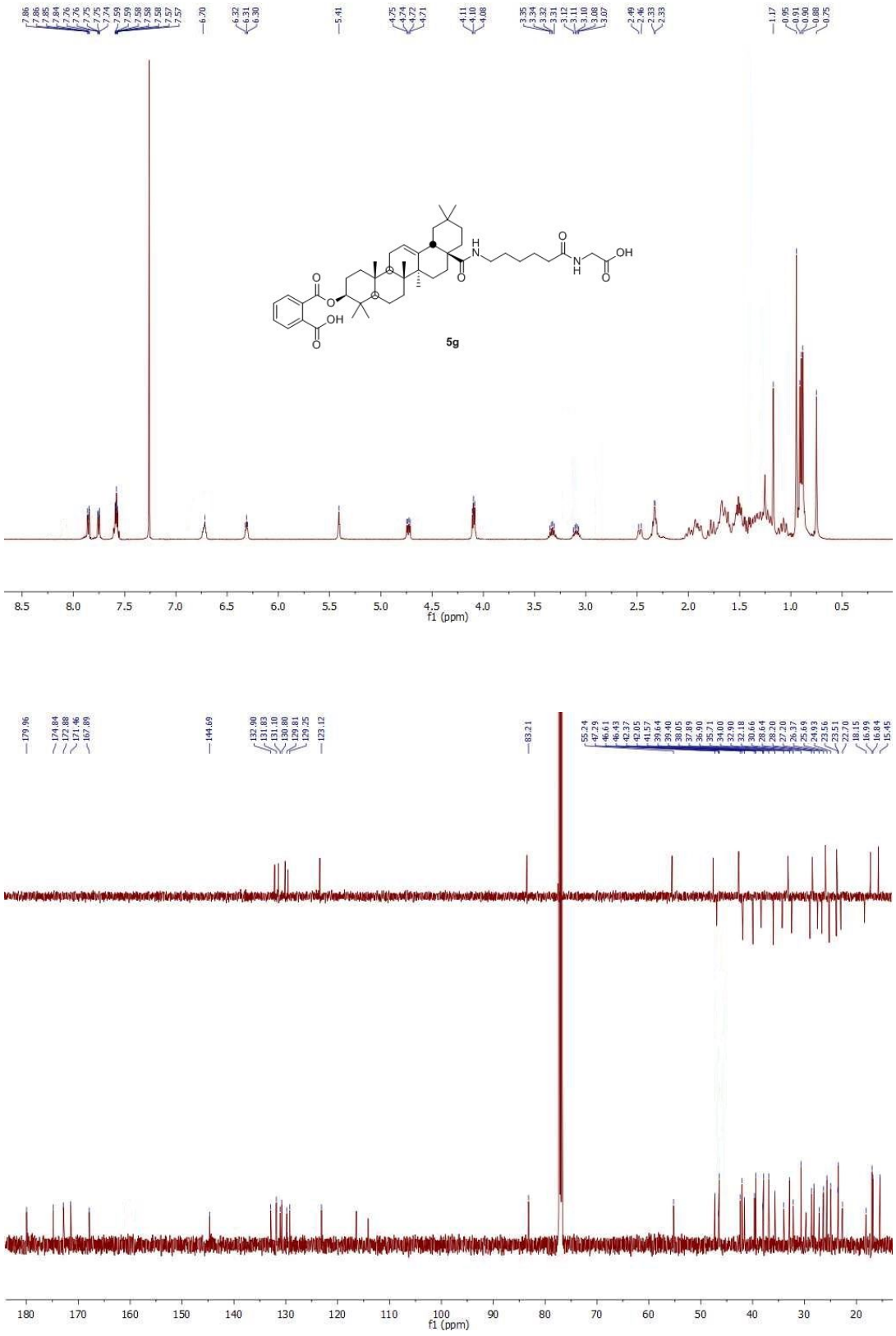


Figure S19. ^{1}H, ^{13}C NMR spectra and DEPT of compound **6g** ($CDCl_3$).

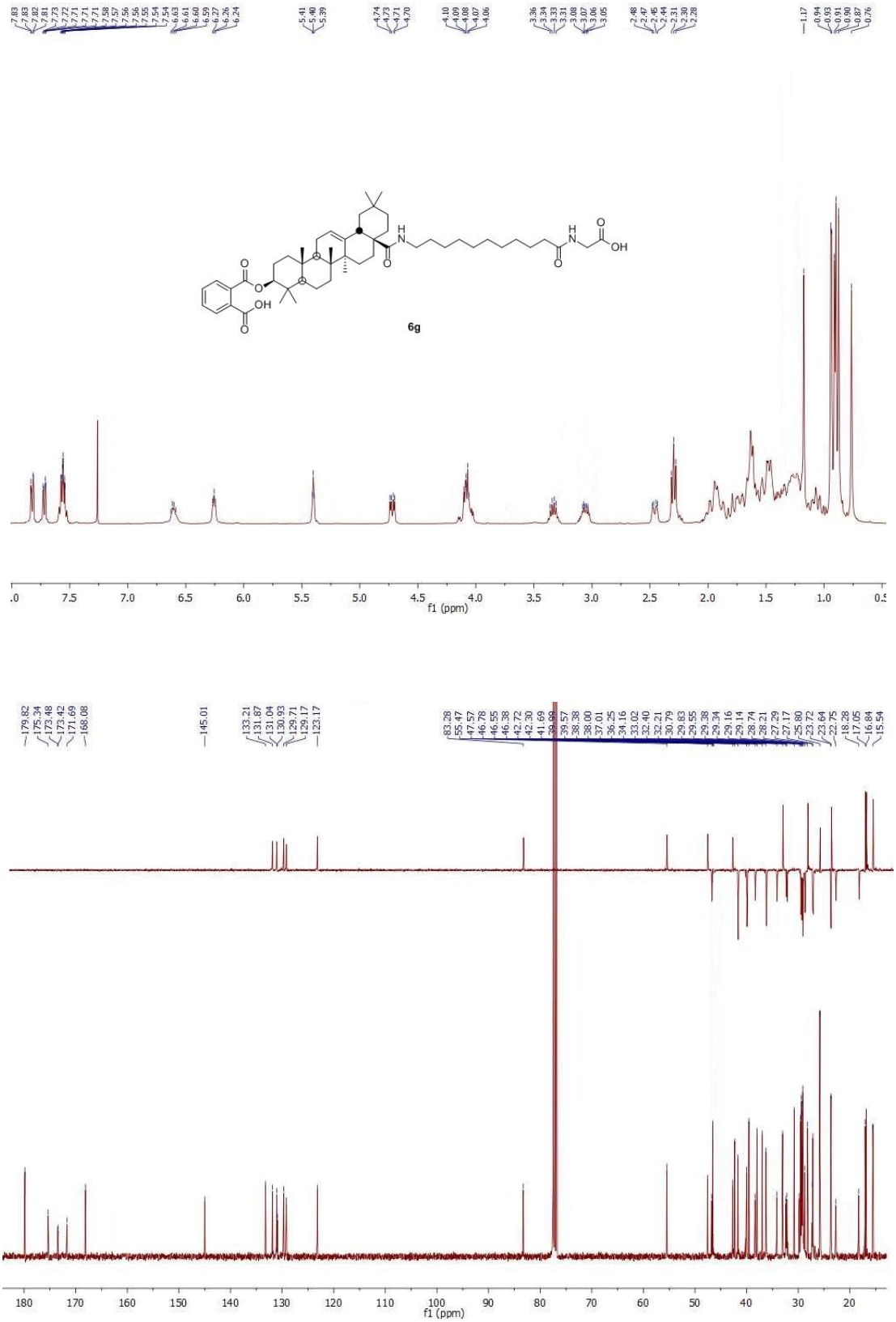


Figure S20. ^{1}H, ^{13}C NMR spectra and DEPT of compound **7g** ($CDCl_3$).

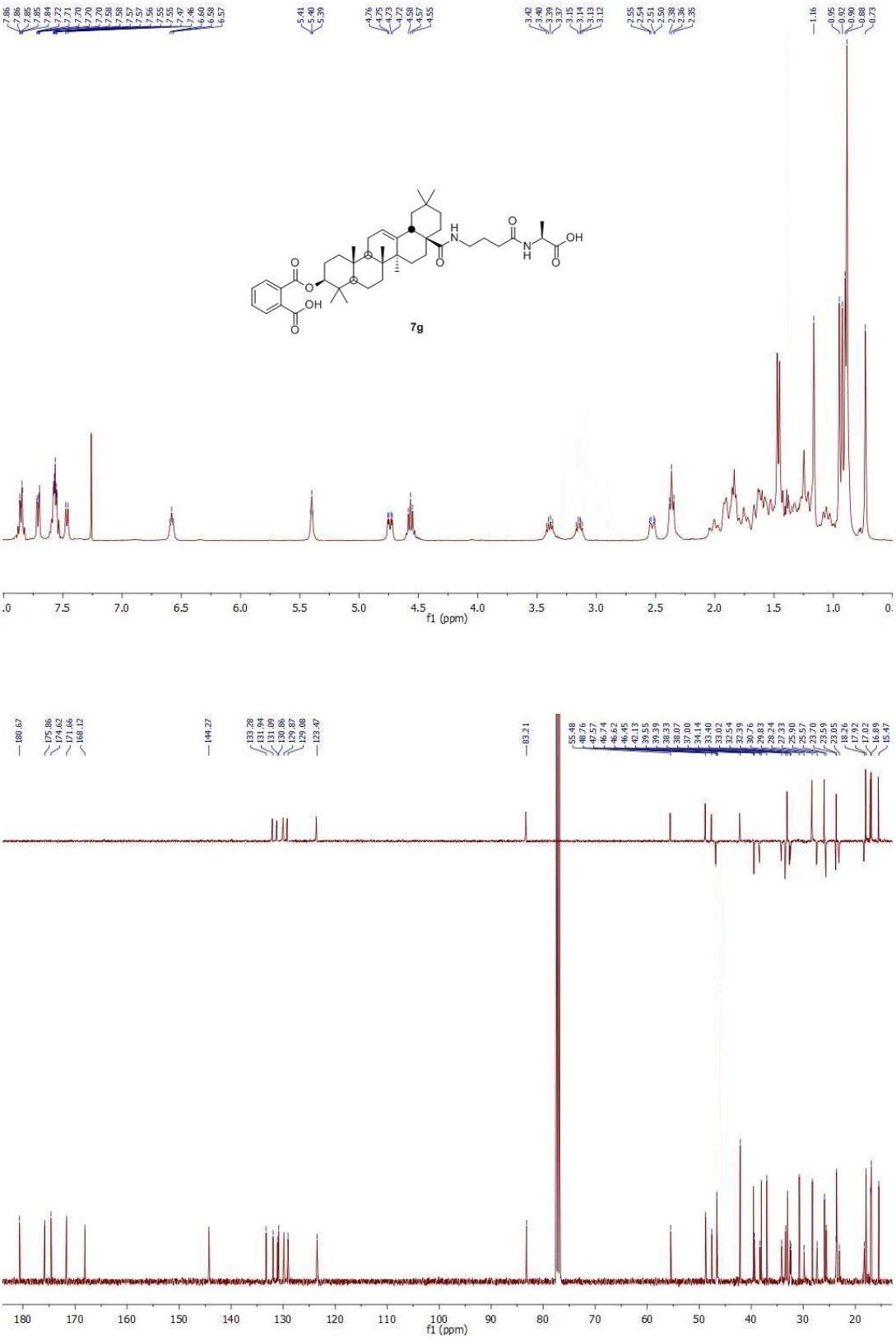


Figure S21. ^{1}H, ^{13}C NMR spectra and DEPT of compound **8g** ($CDCl_3$).

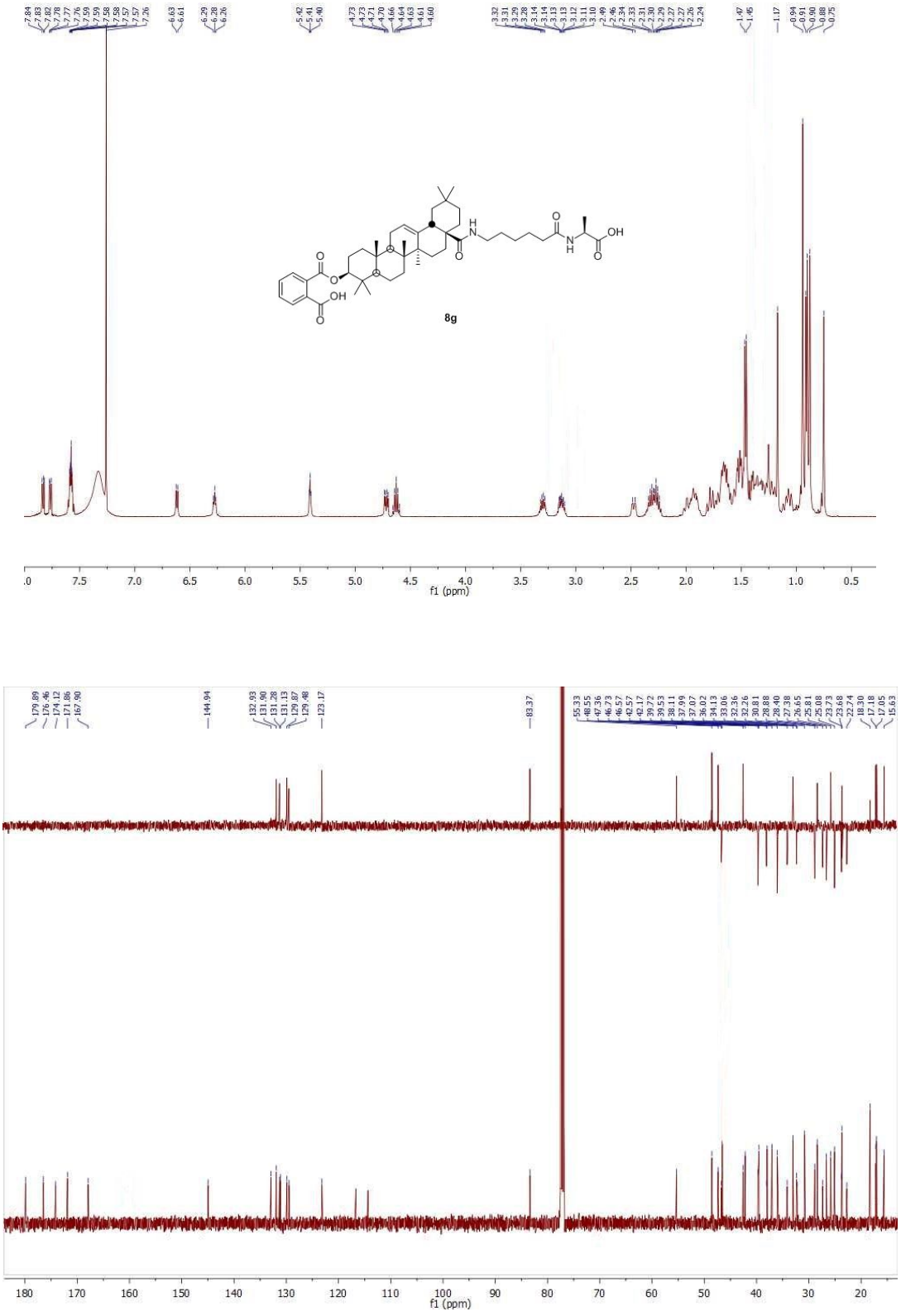


Figure S22. ^{1}H, ^{13}C NMR spectra and DEPT of compound **9g** ($CDCl_3$).

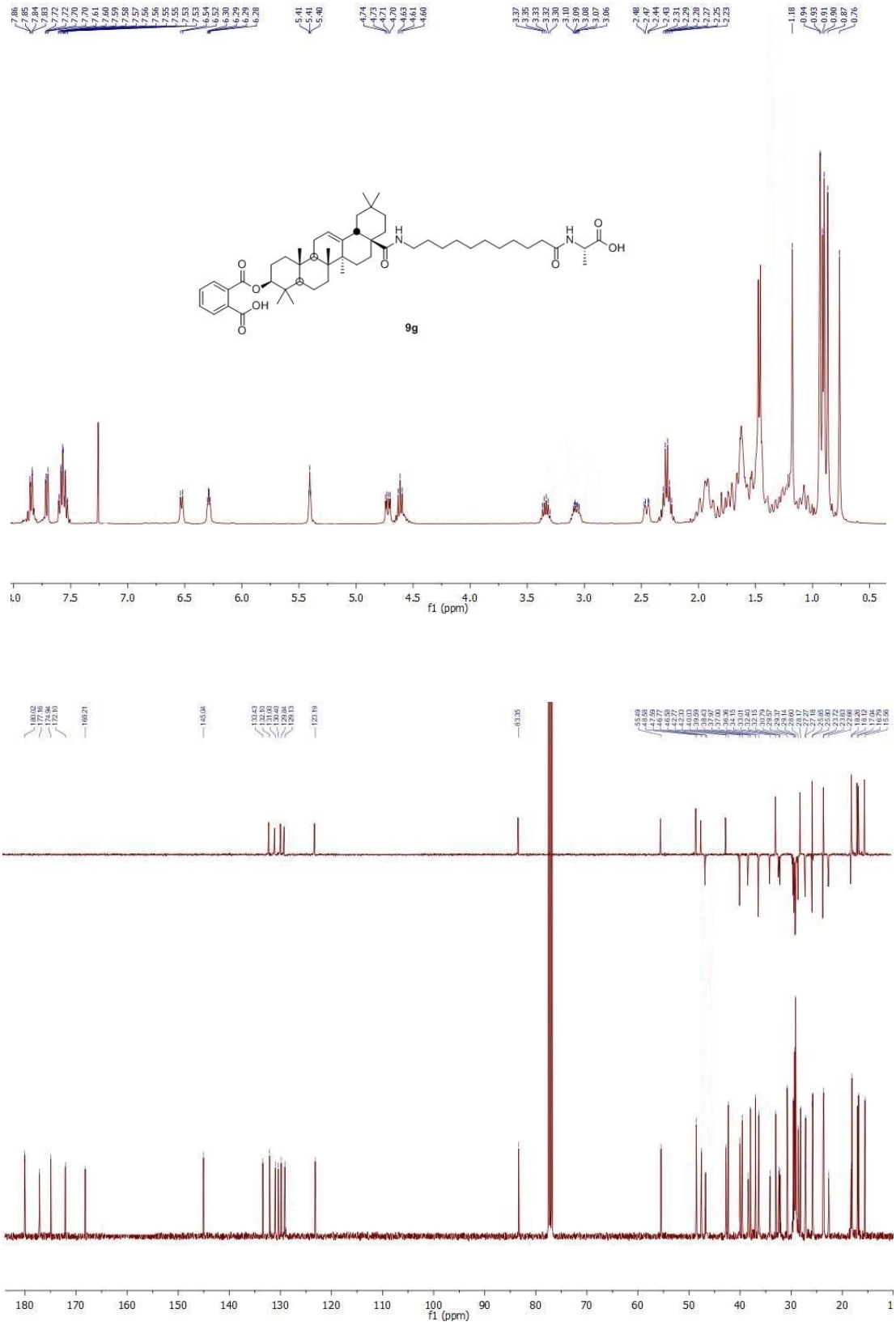


Figure S23. ^{1}H, ^{13}C NMR spectra and DEPT of compound **10g** ($CDCl_3$).

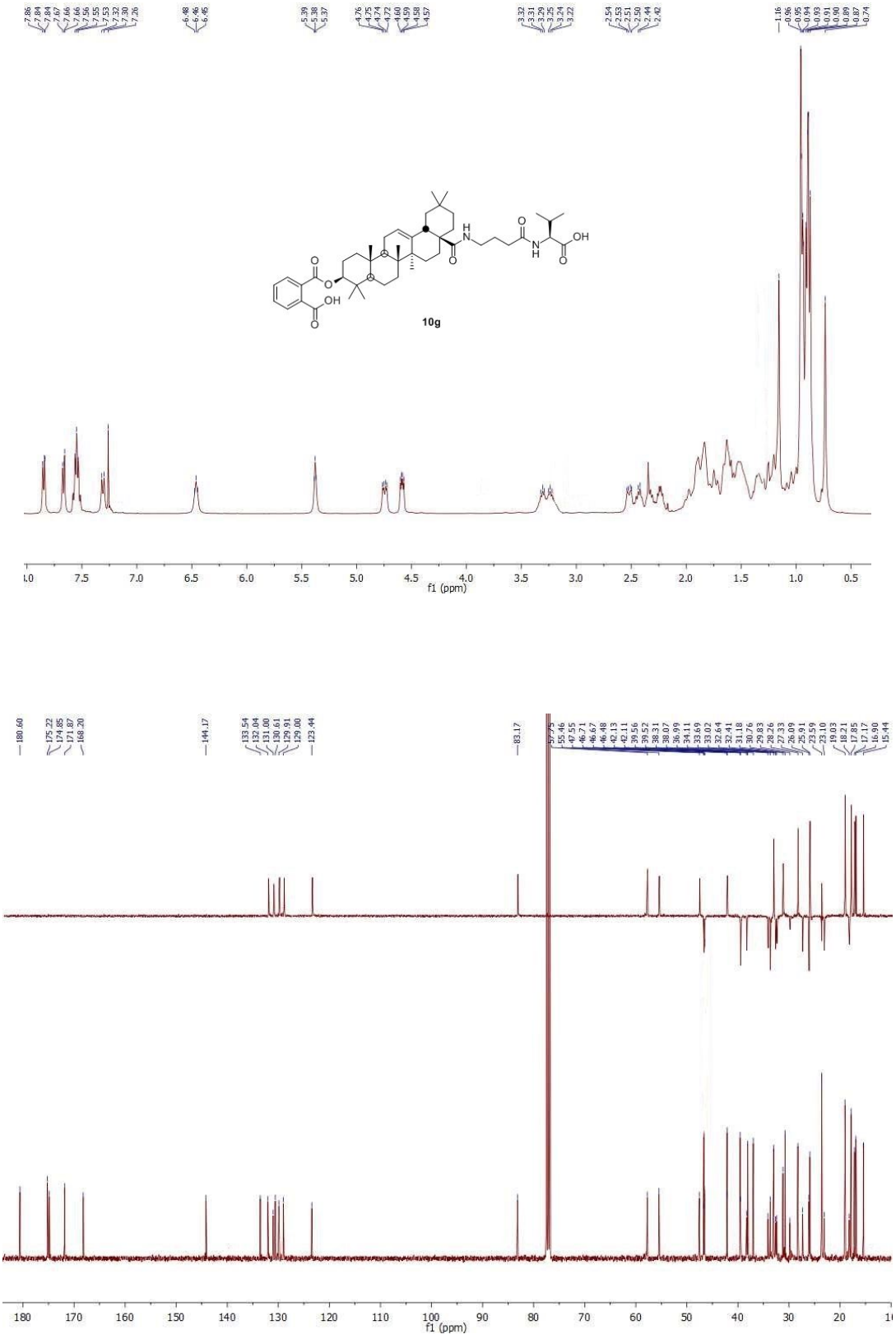


Figure S24. ^{1}H, ^{13}C NMR spectra and DEPT of compound **11g** ($CDCl_3$).

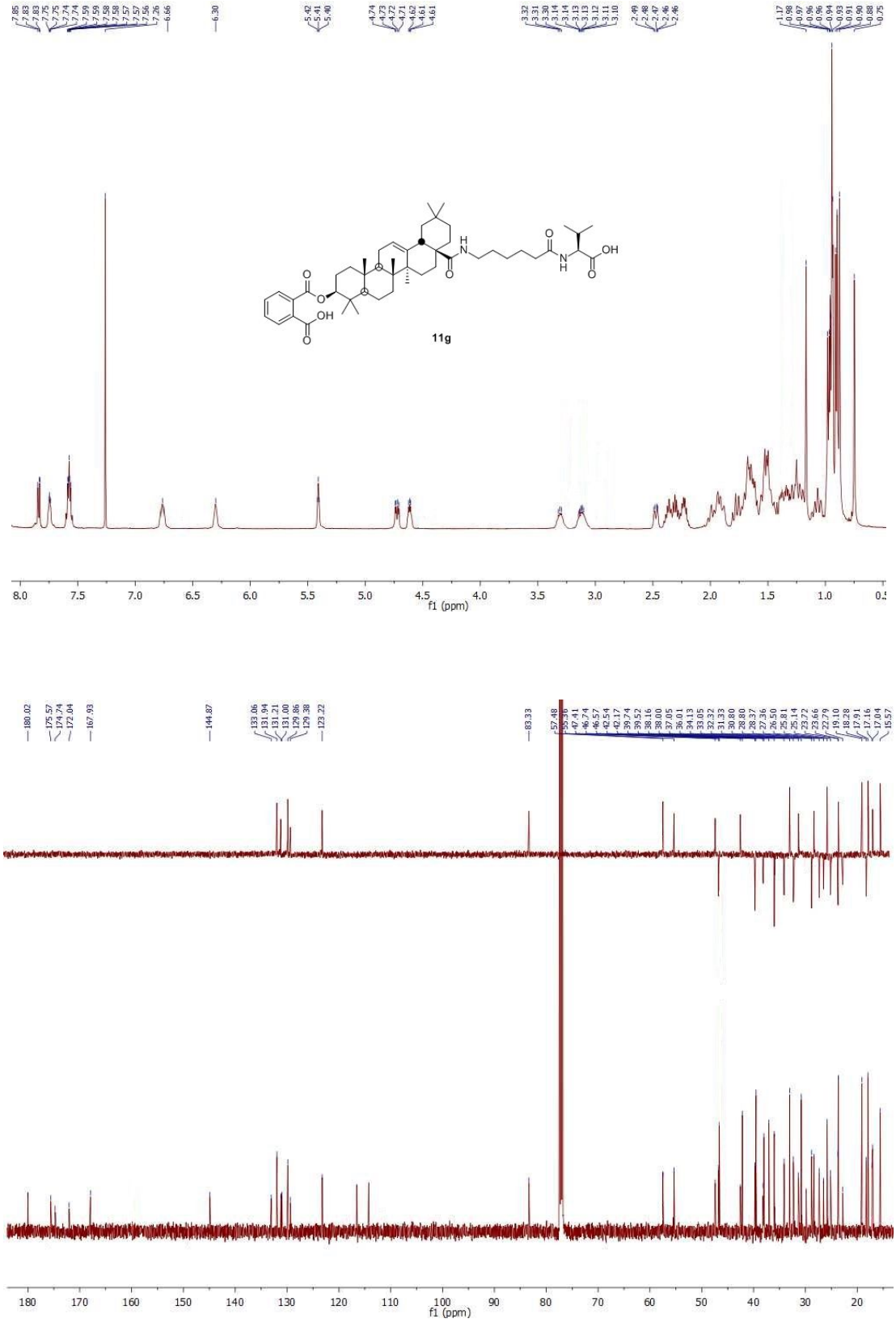


Figure S25. ^{1}H, ^{13}C NMR spectra and DEPT of compound **12g** ($CDCl_3$).