Electronic Supplementary Information

Lithocholic acid derivatives as potent modulators of the nuclear receptor RORγt

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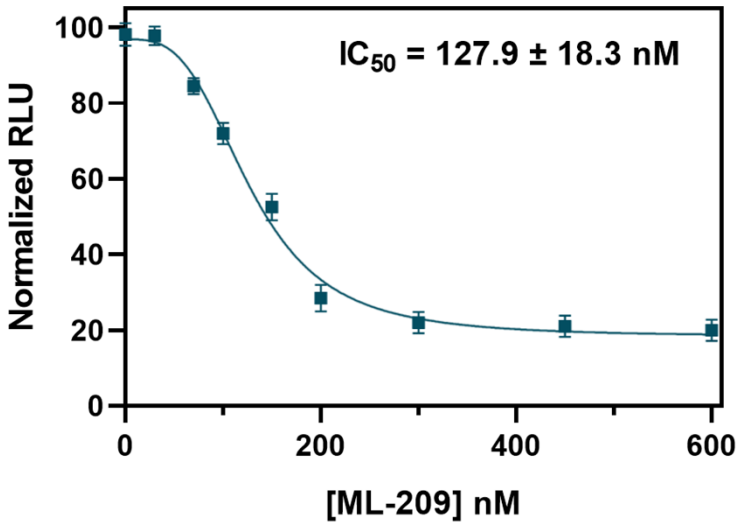


Figure S1. Dose-response curve of ML-209 in the RORγt reporter luciferase assay. Error bars represent standard deviation (n=3).

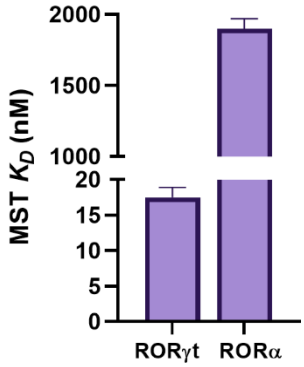


Figure S2. MST binding analysis of the binding of **A2** to RORγt and RORα. The binding affinity (K_D) is represented in nM. Error bars represent standard deviation (n = 3).

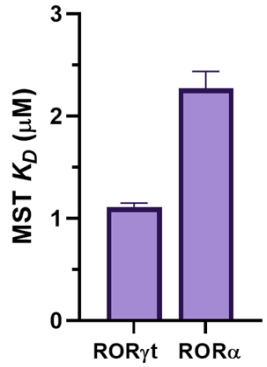
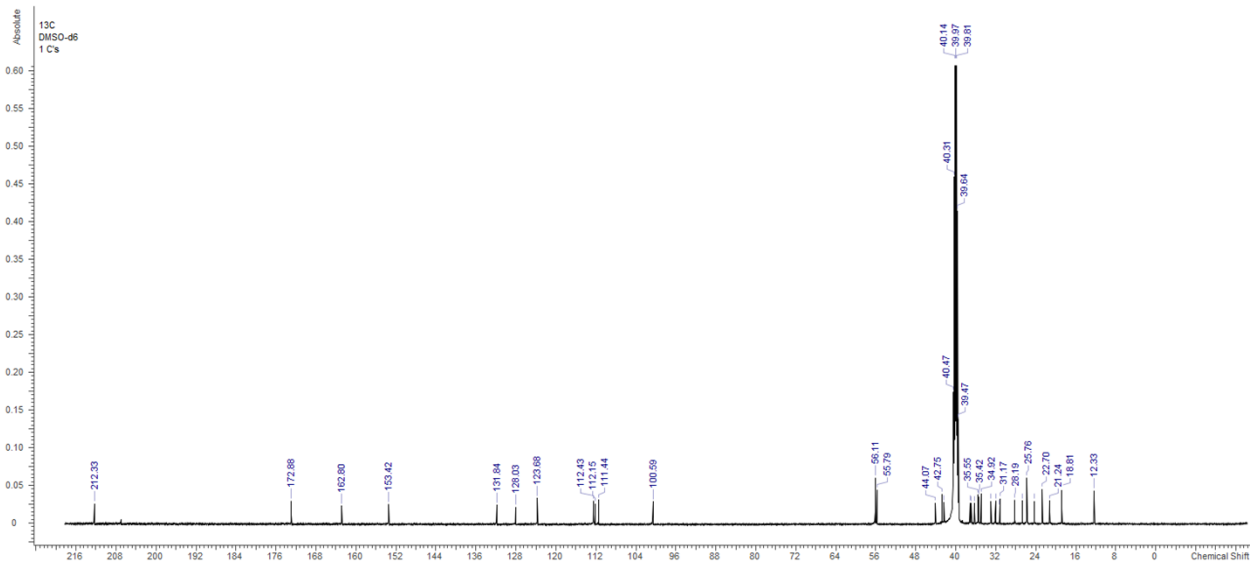
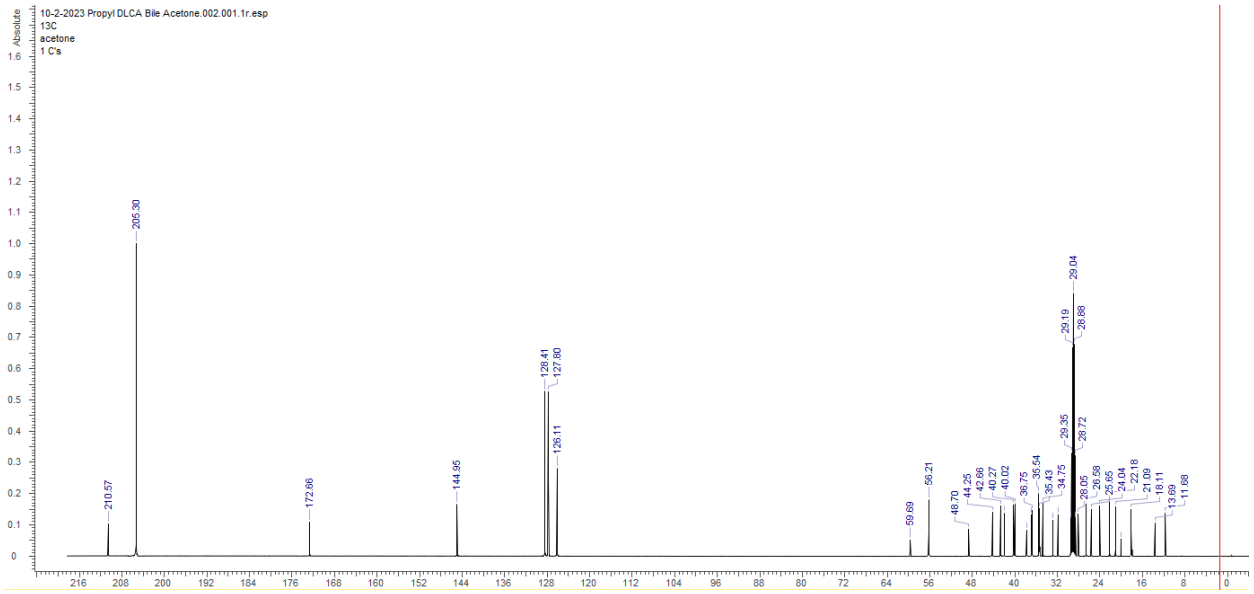


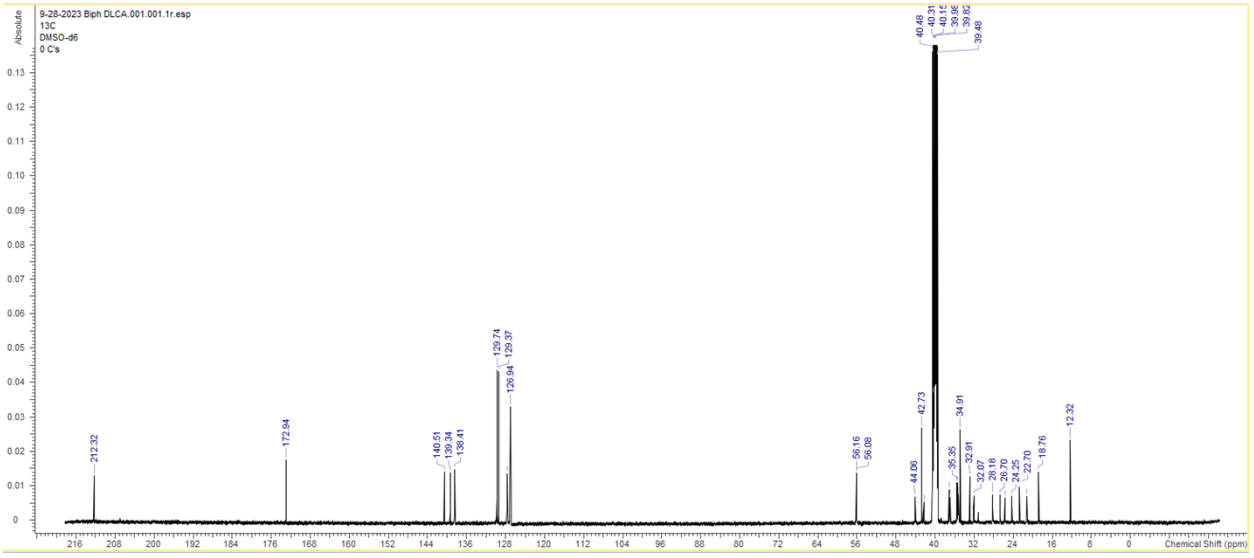
Figure S3. MST binding analysis of the binding of 3-oxoLCA to RORγt and RORα. The binding affinity (K_D) is represented in μM. Error bars represent standard deviation (n = 3).



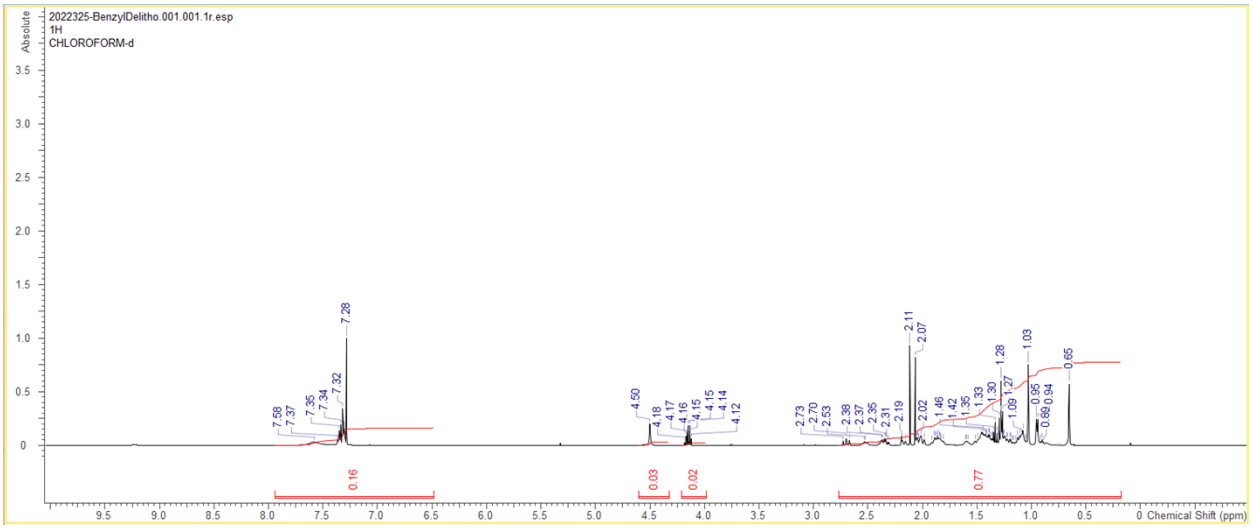
^{13}C NMR spectrum of compound **A2**.



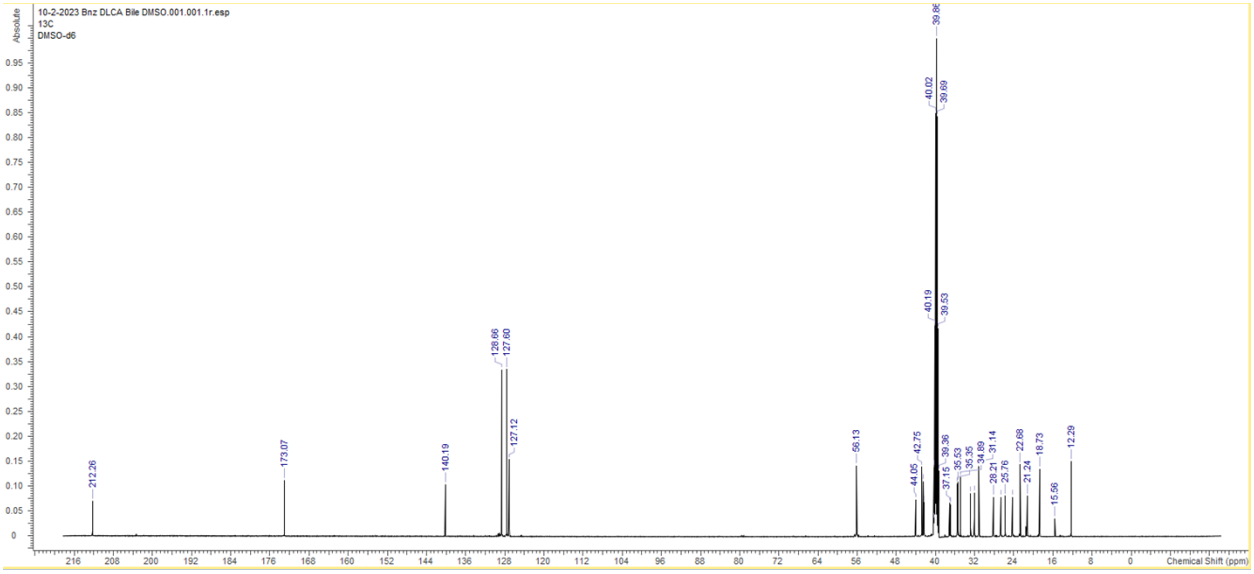
^{13}C NMR spectrum of compound **A3**.



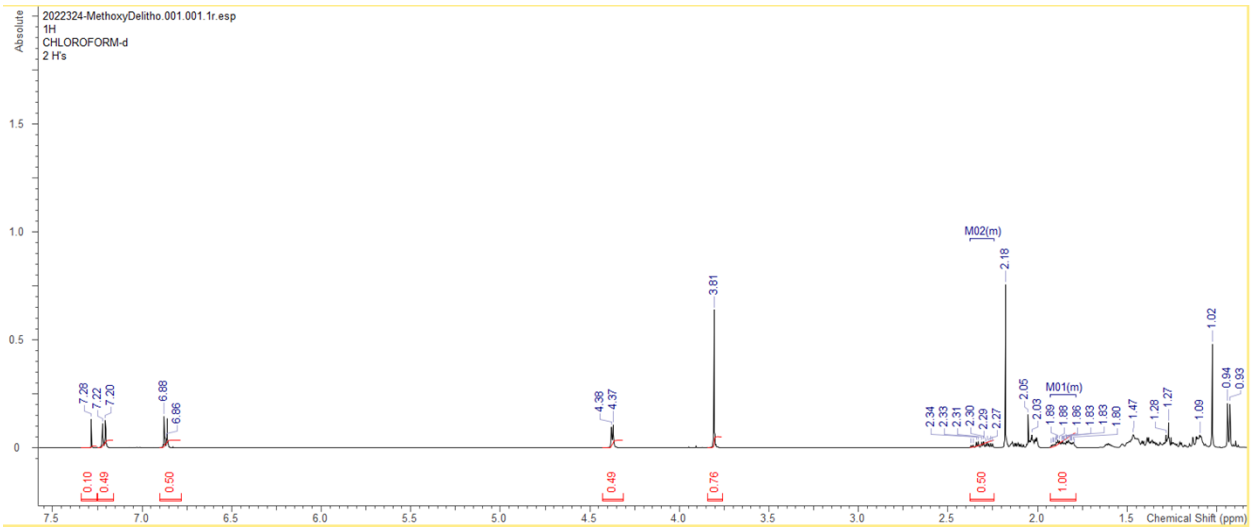
^{13}C NMR spectrum of compound **A4**.



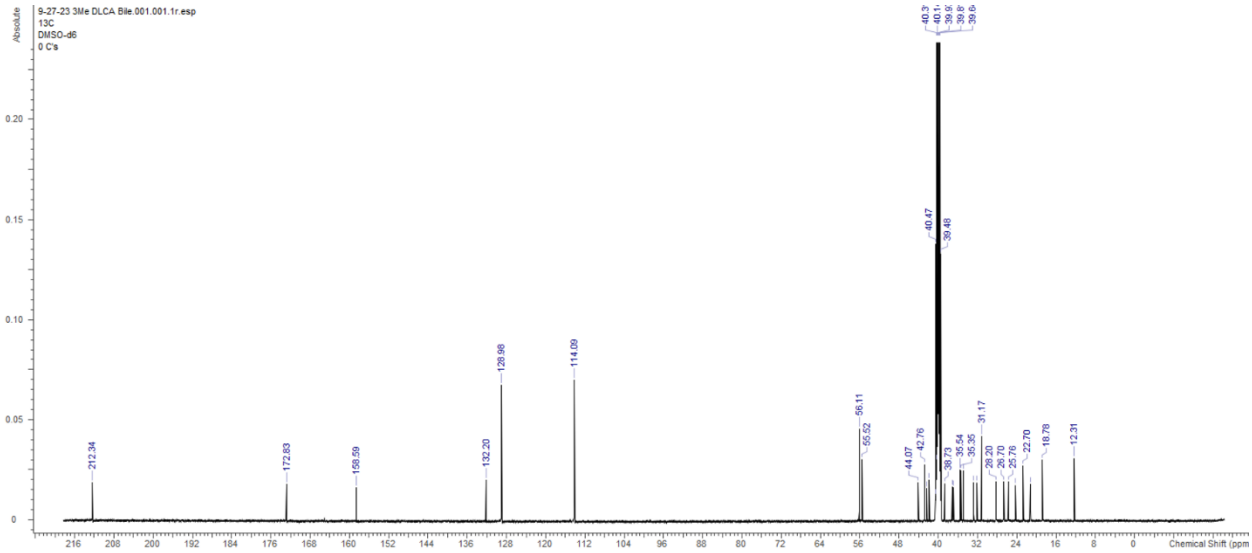
^{1}H NMR spectrum of compound **A5**.



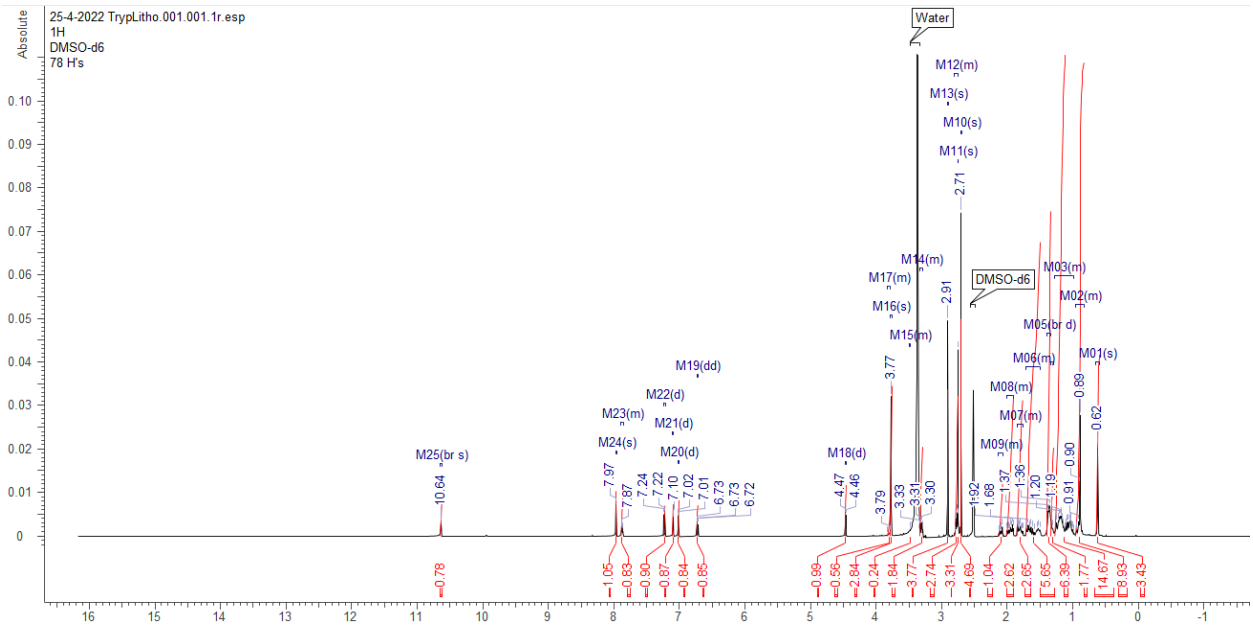
^{13}C NMR spectrum of compound **A5**.



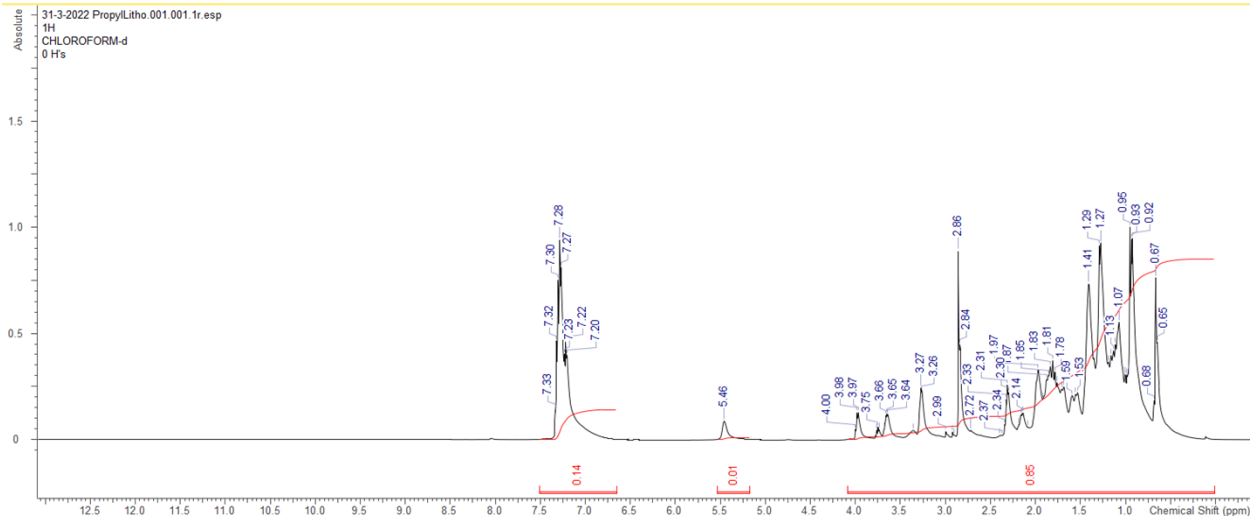
^{1}H NMR spectrum of compound **A6**.



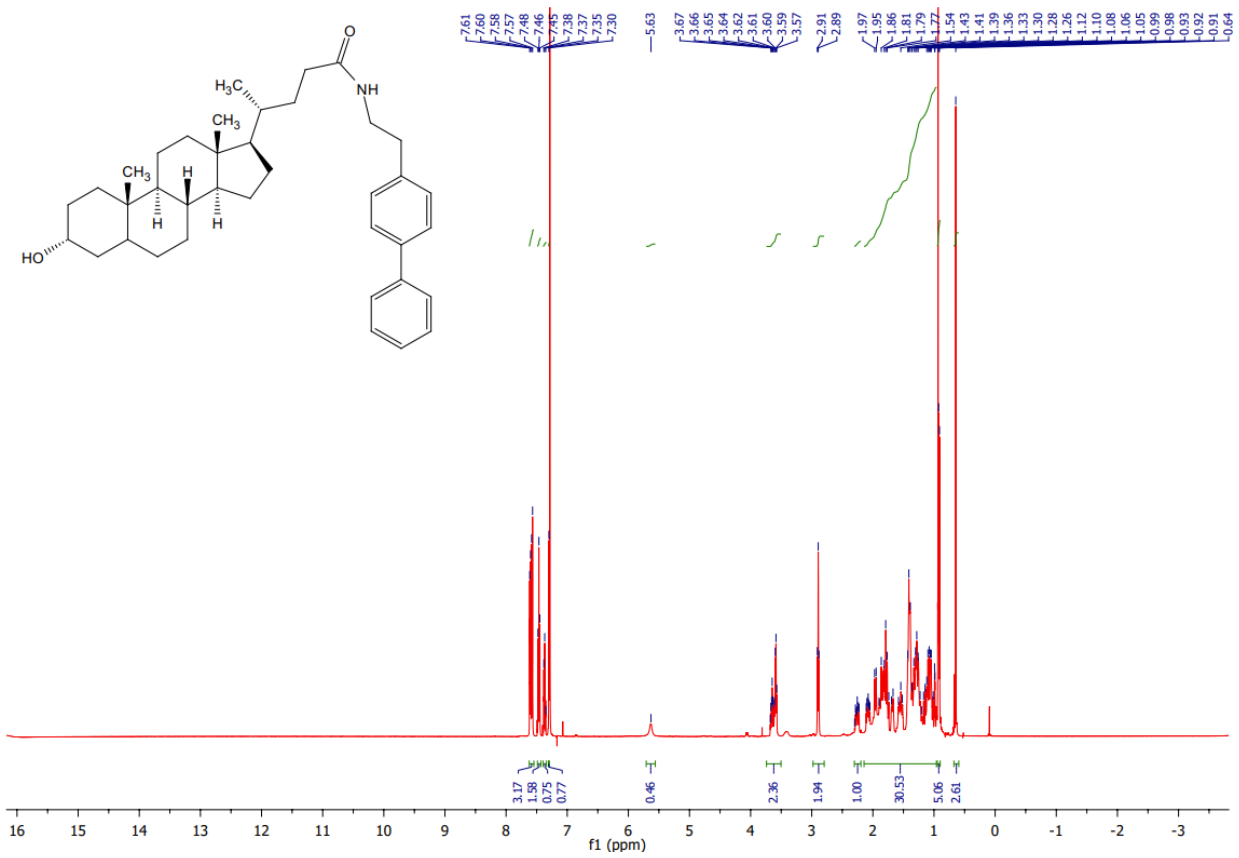
^{13}C NMR spectrum of compound **A6**.



^{1}H NMR spectrum of compound **B2**.



^{1}H NMR spectrum of compound **B3**.



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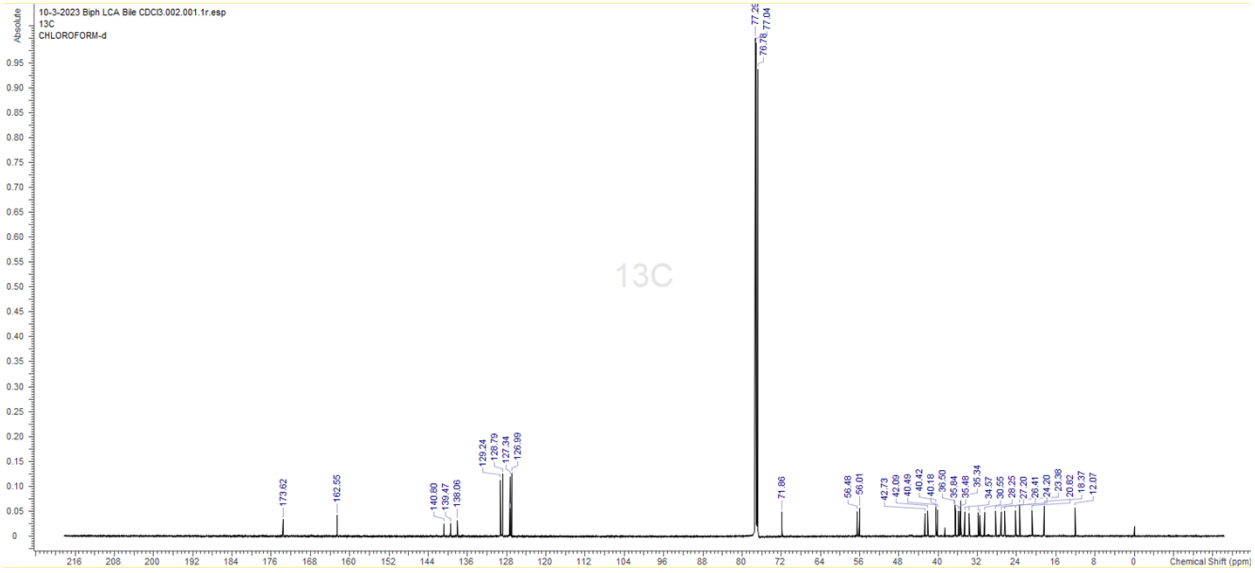
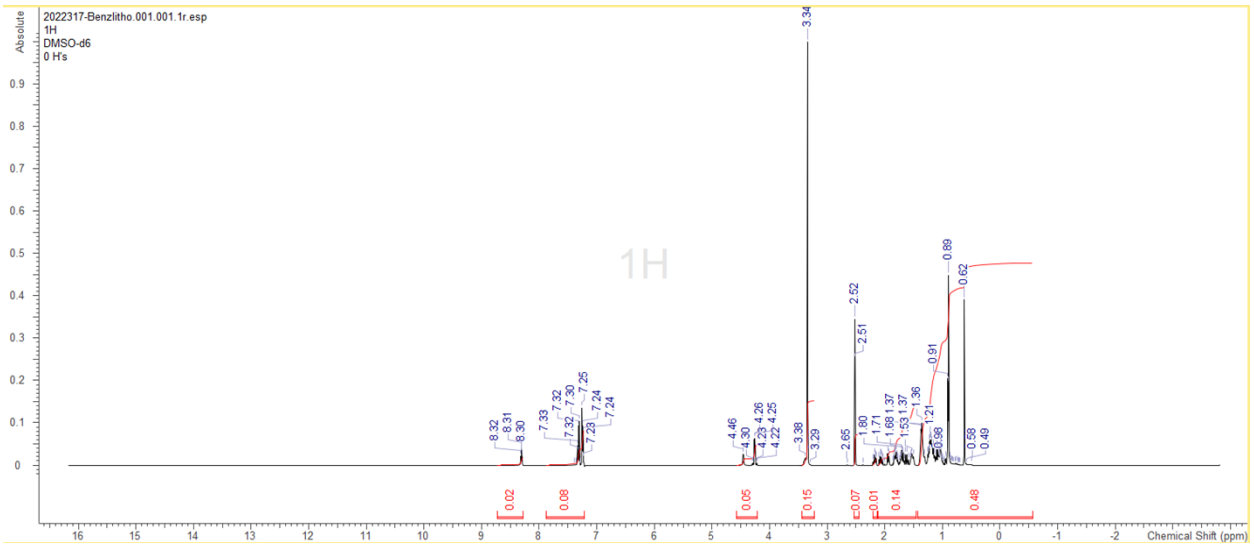
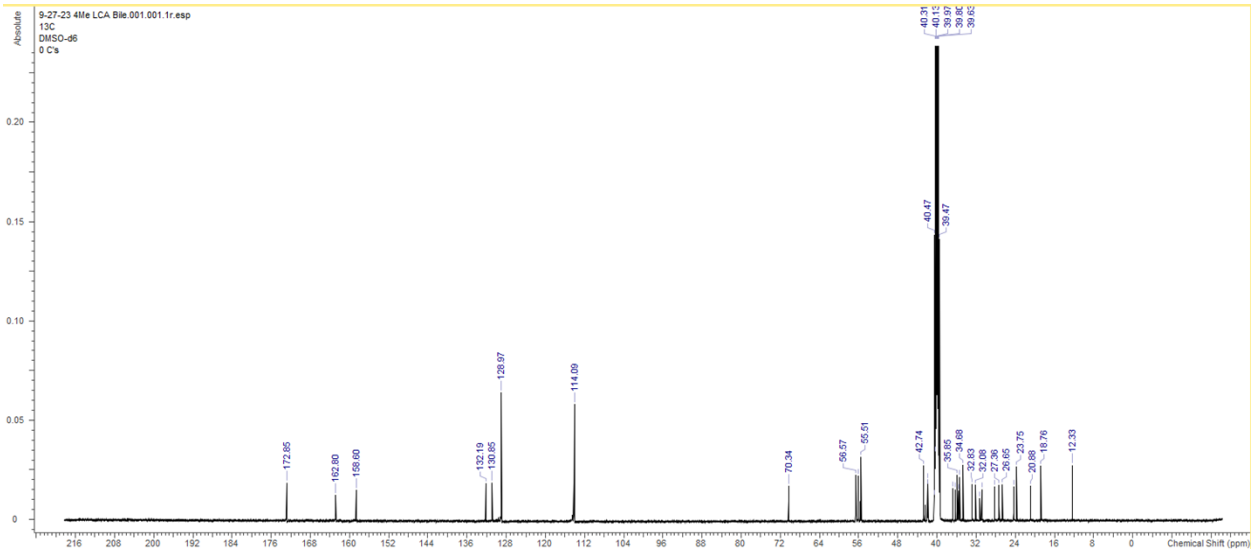


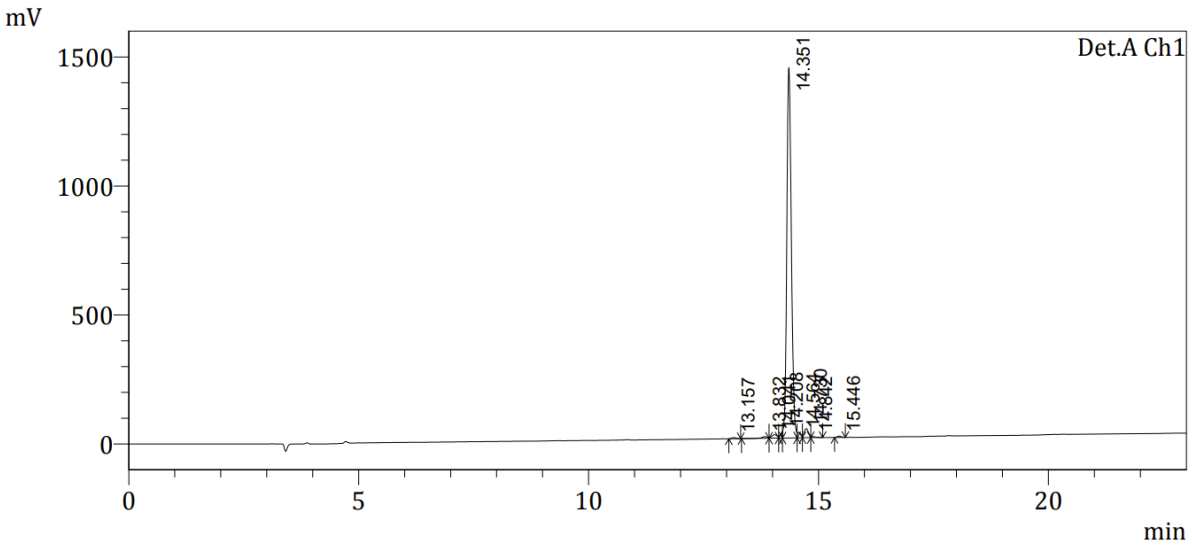
^{13}C NMR spectrum of compound **B4**.



^{1}H NMR spectrum of compound **B5**.

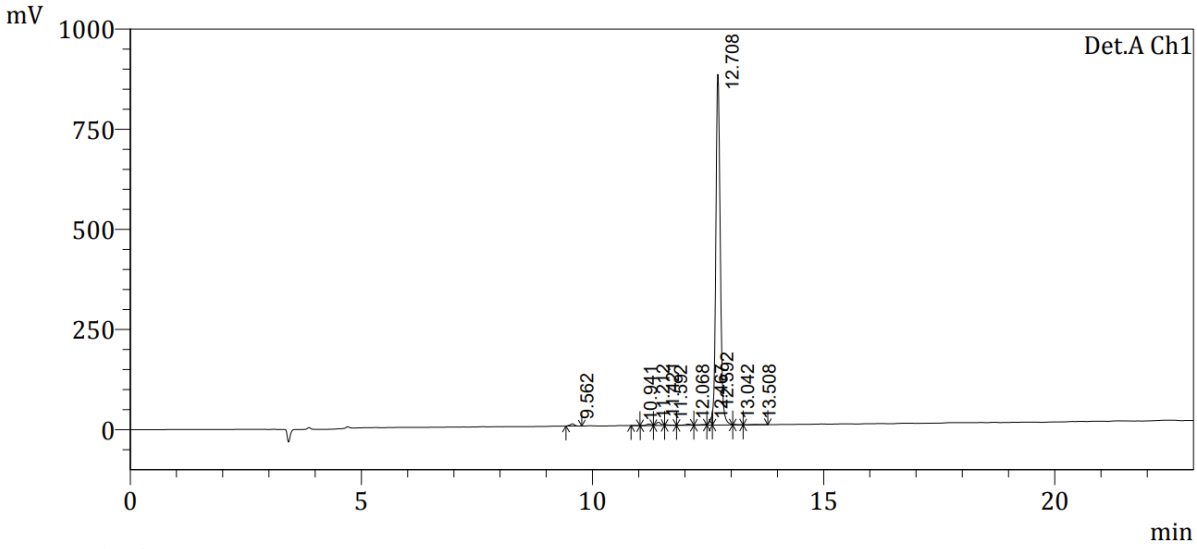


^{13}C NMR spectrum of compound **B6**.



1 Det.A Ch1/220nm

HPLC trace for compound **A2**.



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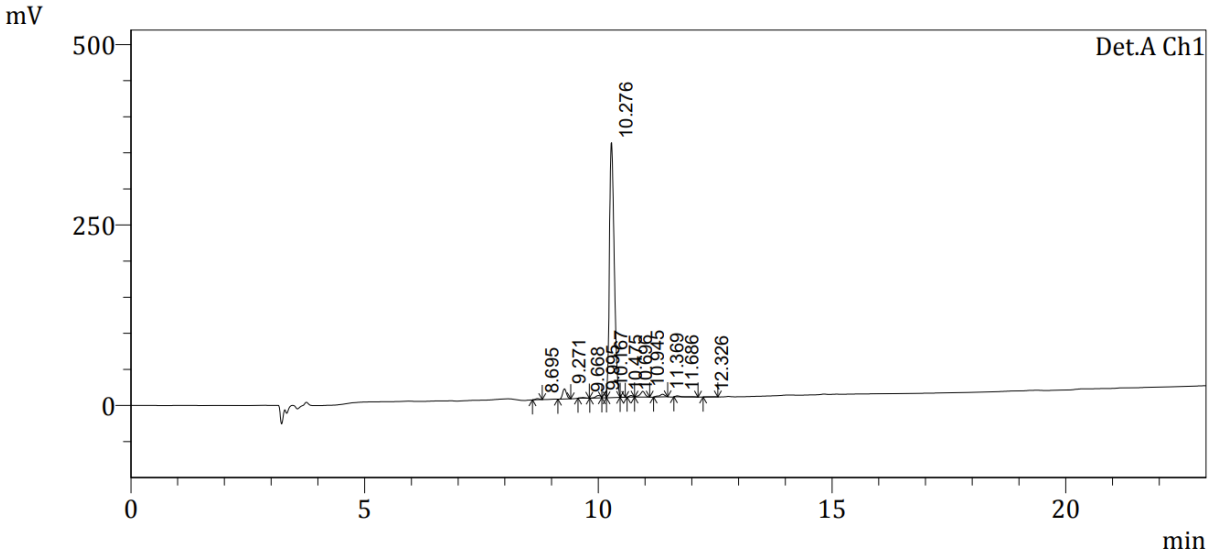

1 Det.A Ch1/220nm

HPLC trace for compound **A4**.