

Synthesis of Cucurbitacin B Derivatives as Potential Anti-hepatocellular Carcinoma Agents

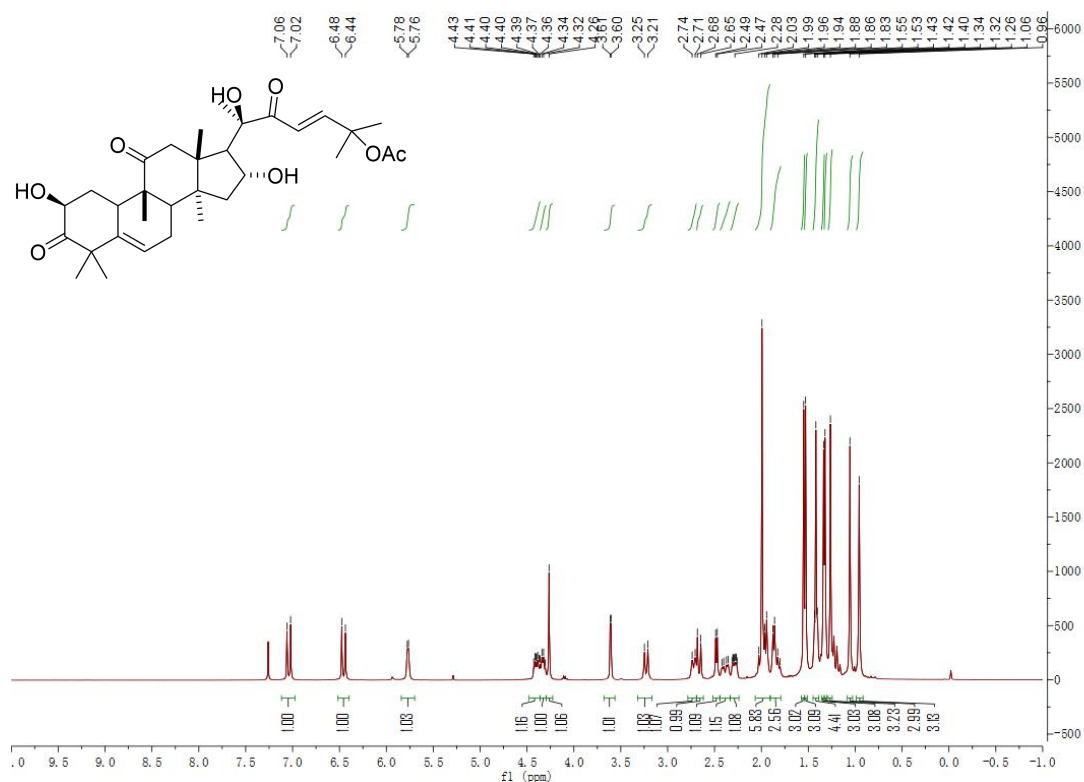
*Weizhi Ge,^a Xinyi Chen,^a Fangzhi Han,^a Zhongquan Liu,^a Tianpeng Wang,^a
Mengmeng Wang,^b Yue Chen,^{a,*} Yahui Ding^{a,*} and Quan Zhang^{a,*}*

*^aState Key Laboratory of Medicinal Chemical Biology, College of Pharmacy and
Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Haihe
Education Park, 38 Tongyan Road, Tianjin 300353, People's Republic of China*

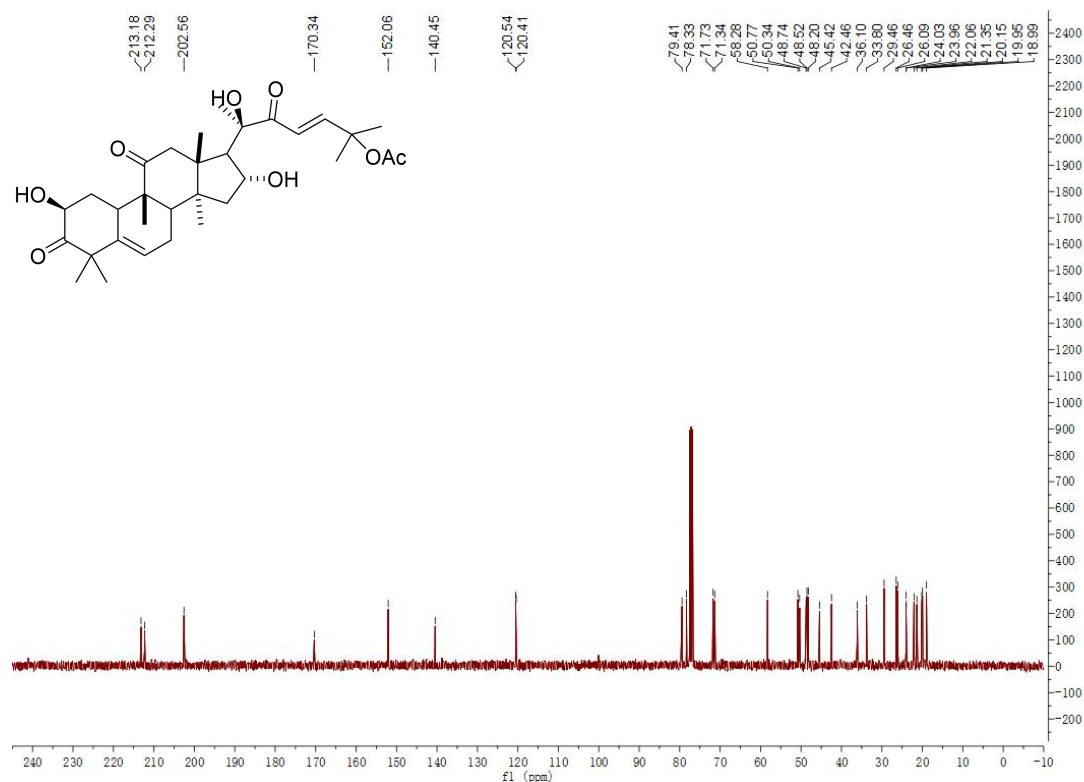
^bAccendatech Company, Ltd., Tianjin 300384, People's Republic of China

SUPPORTING INFORMATION

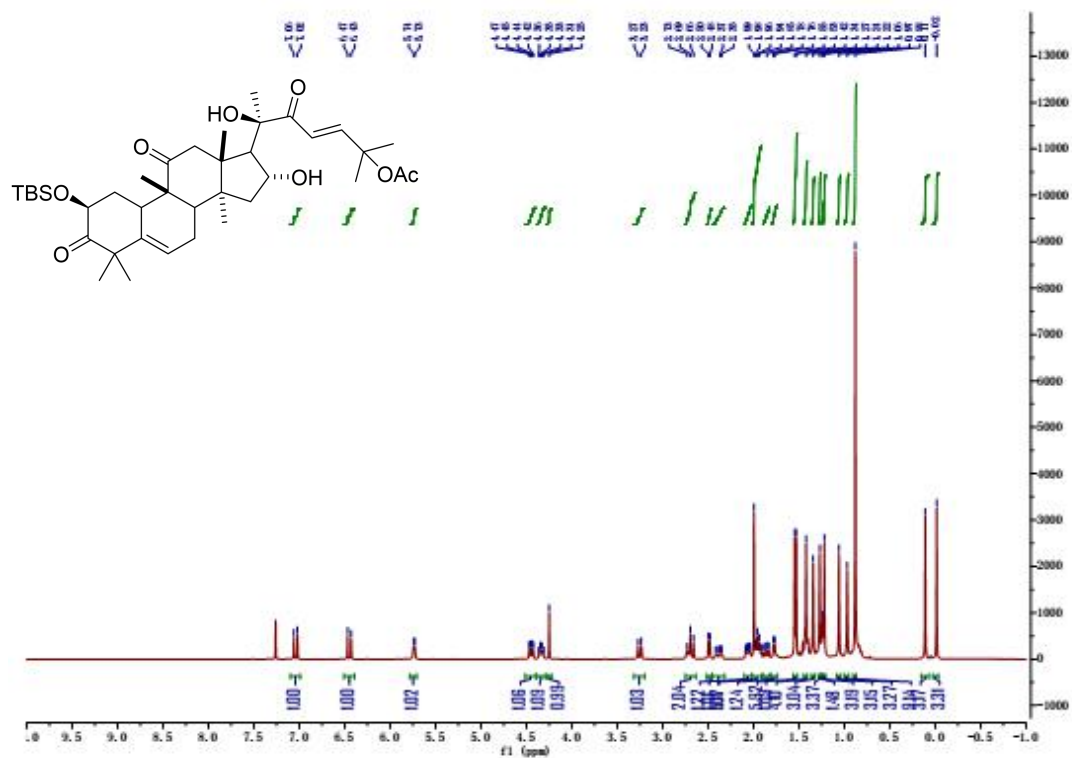
1. Copies of ¹HNMR and ¹³C NMR	S2
2. The purity of the compounds tested by HPLC	S44
3. The dose-response curves of compounds	S54



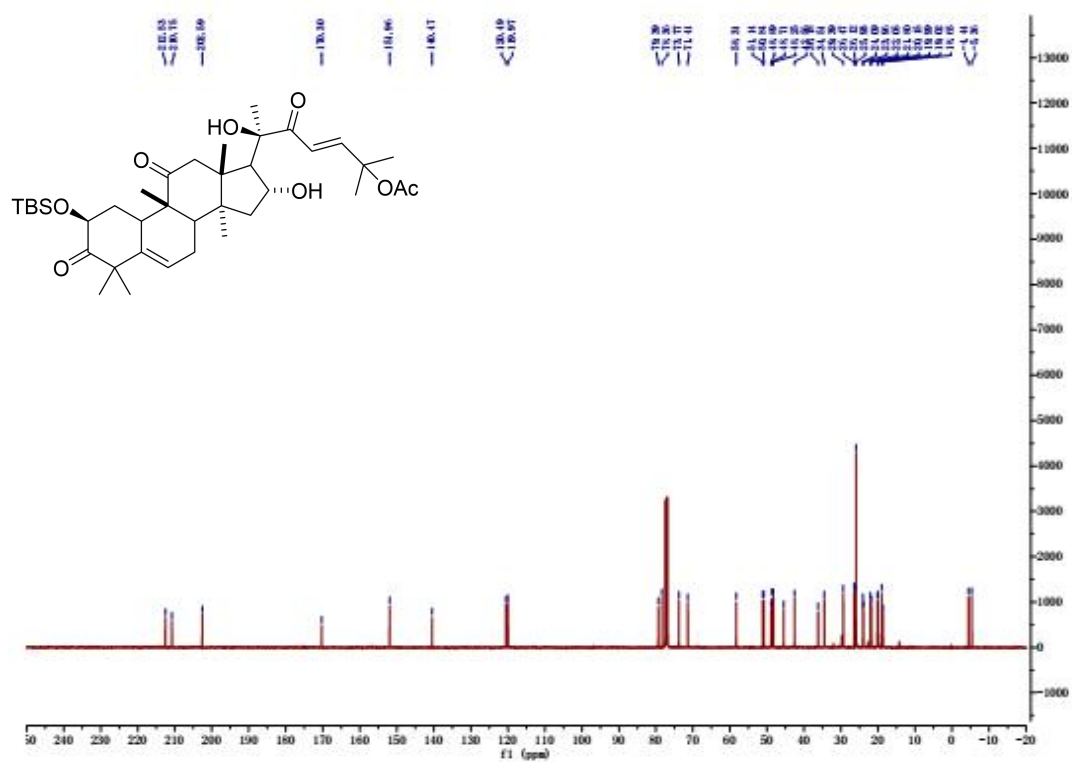
¹H NMR of cucurbitacin B (1)



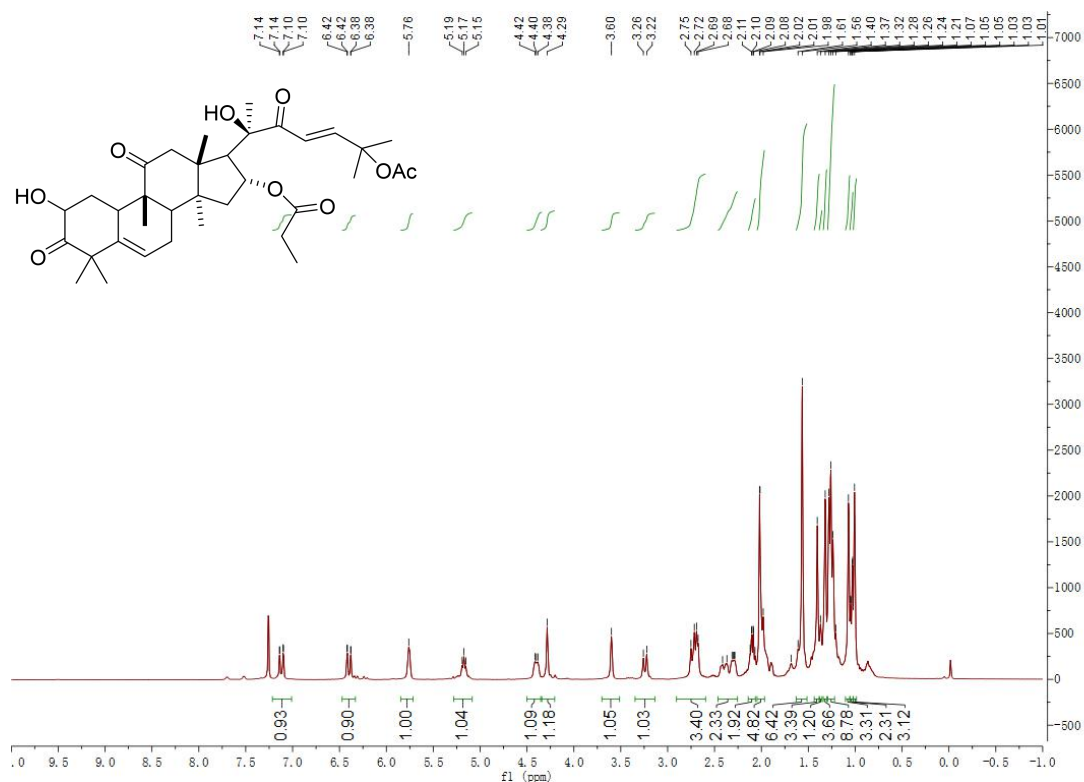
¹³C NMR of cucurbitacin B (1)



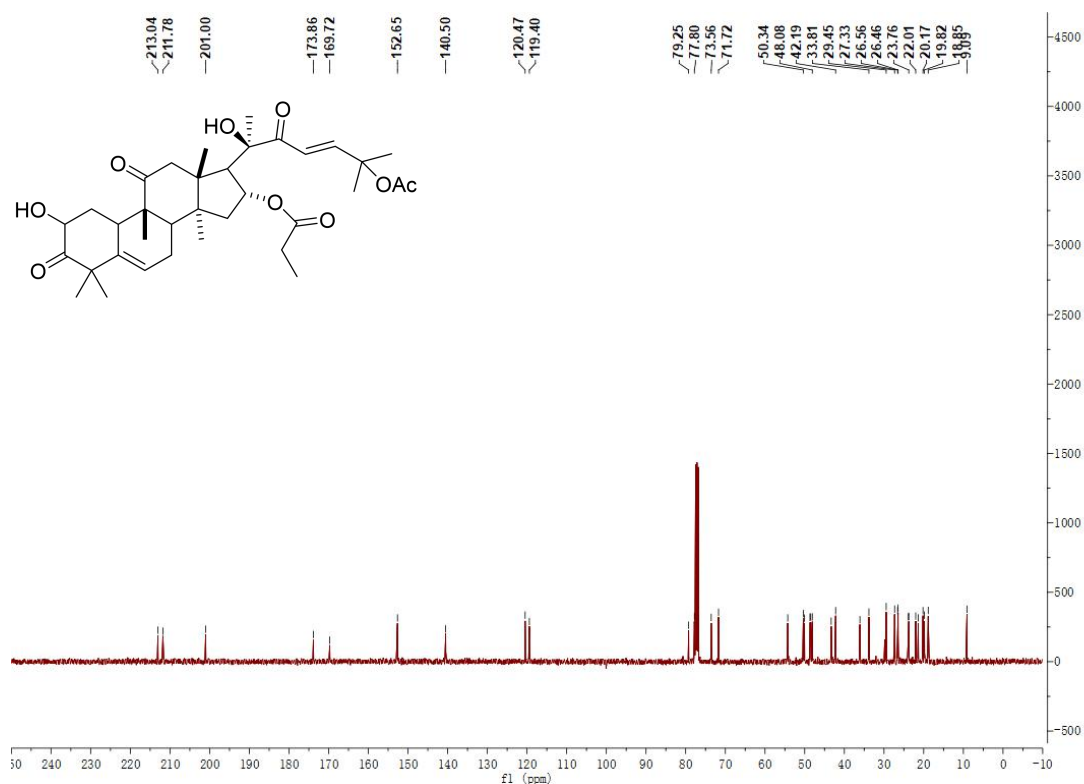
¹H NMR of compound 2



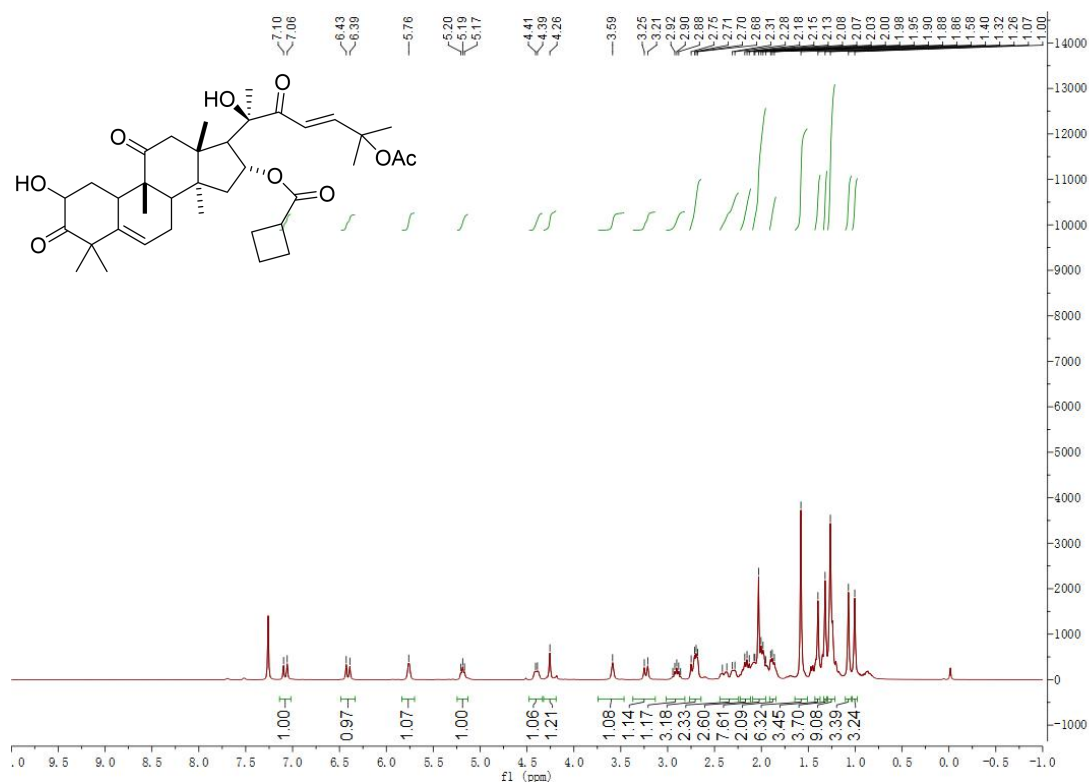
¹³C NMR of compound 2



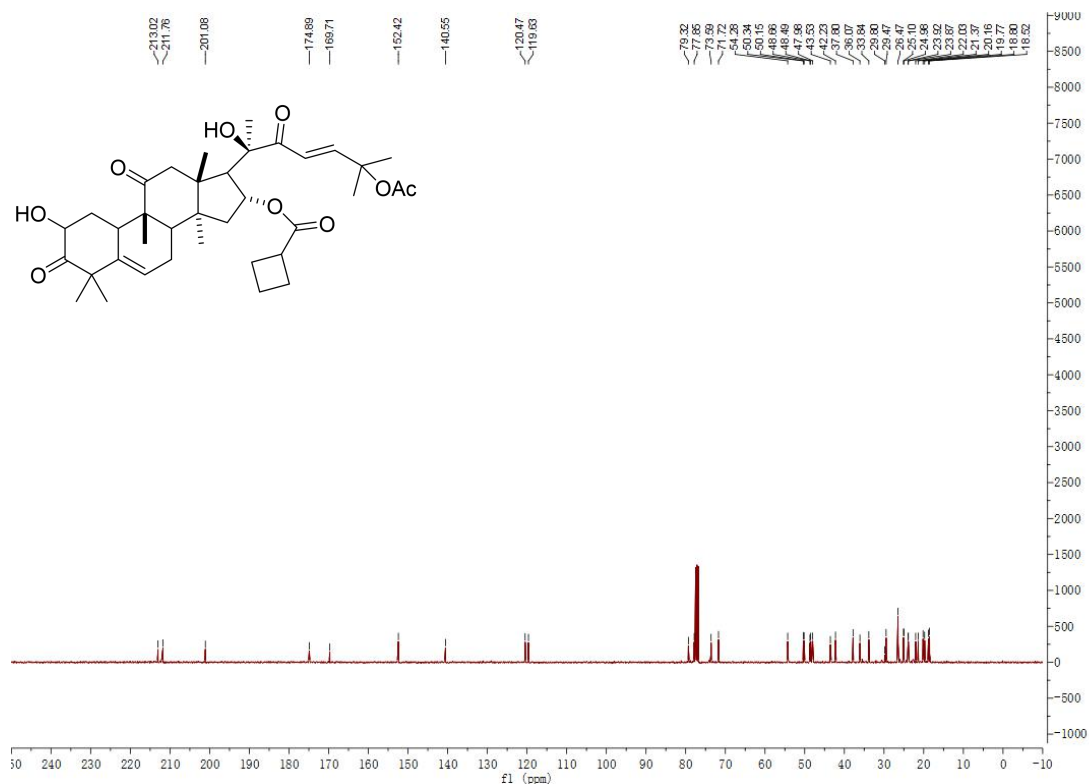
¹H NMR of compound 3a



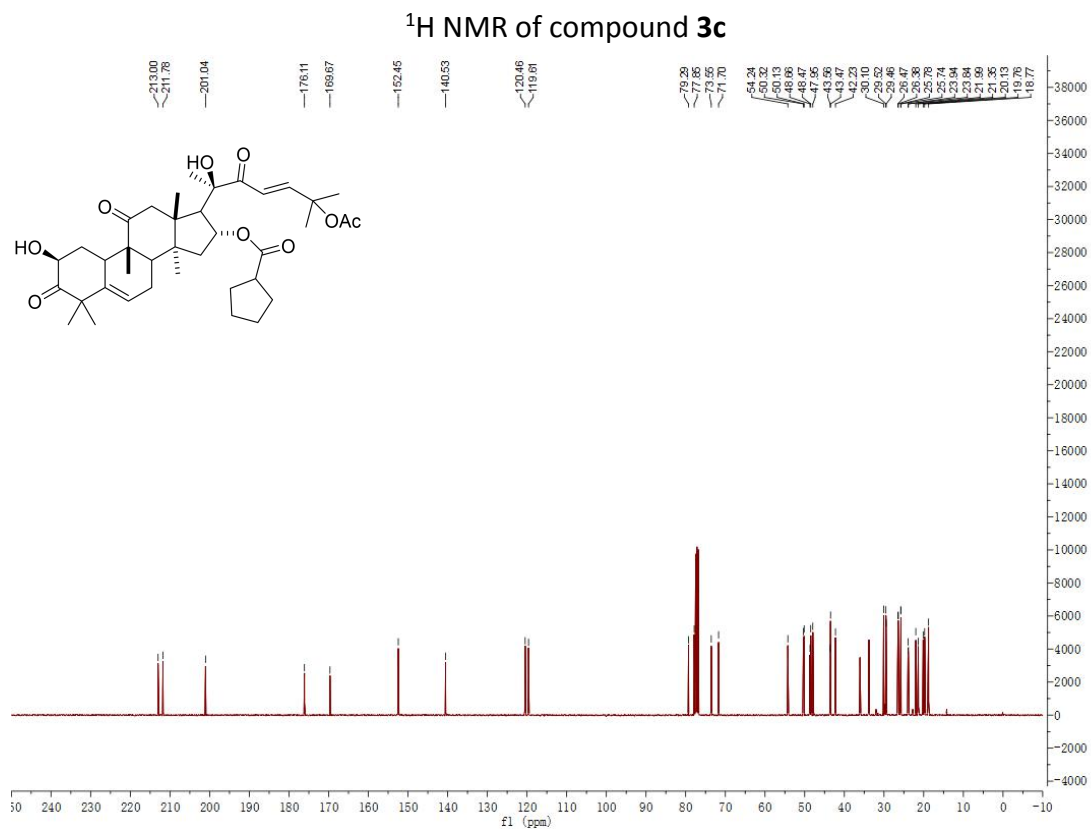
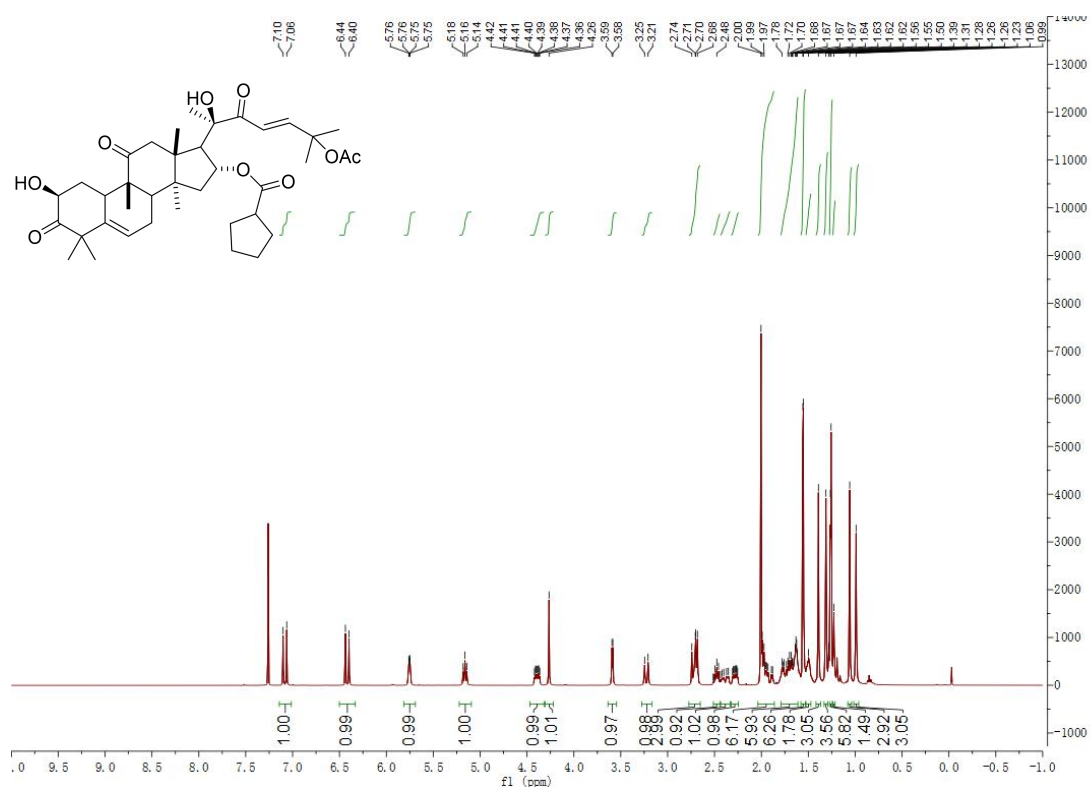
¹³C NMR of compound 3a



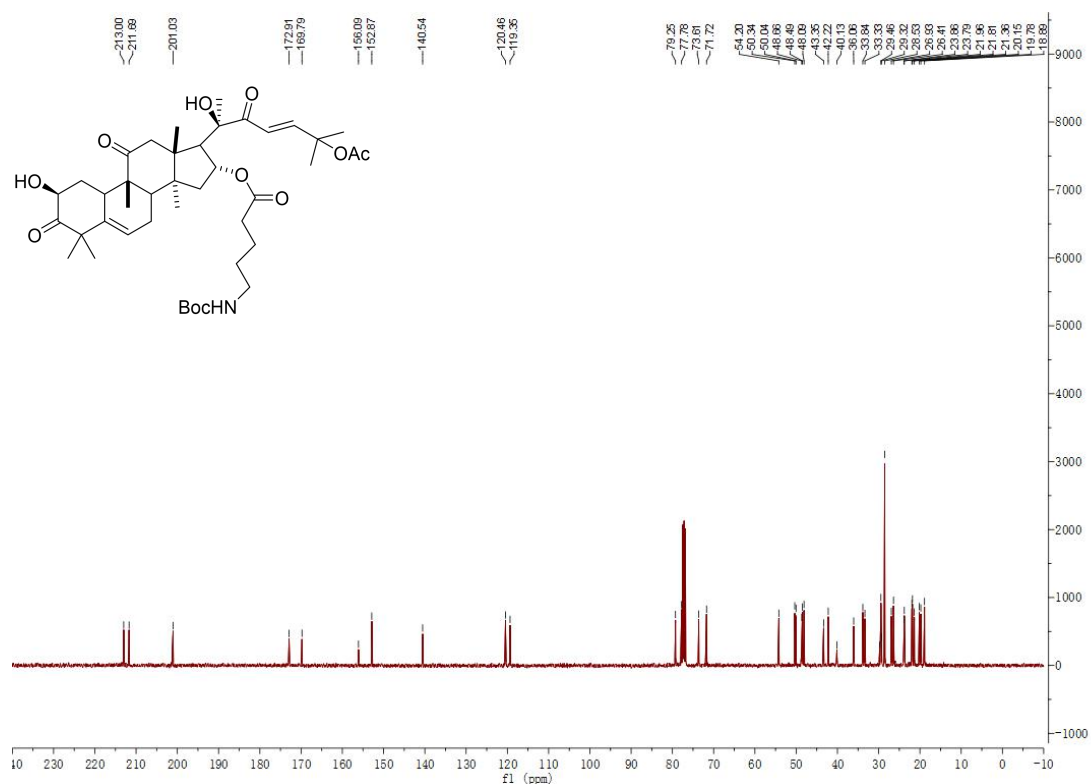
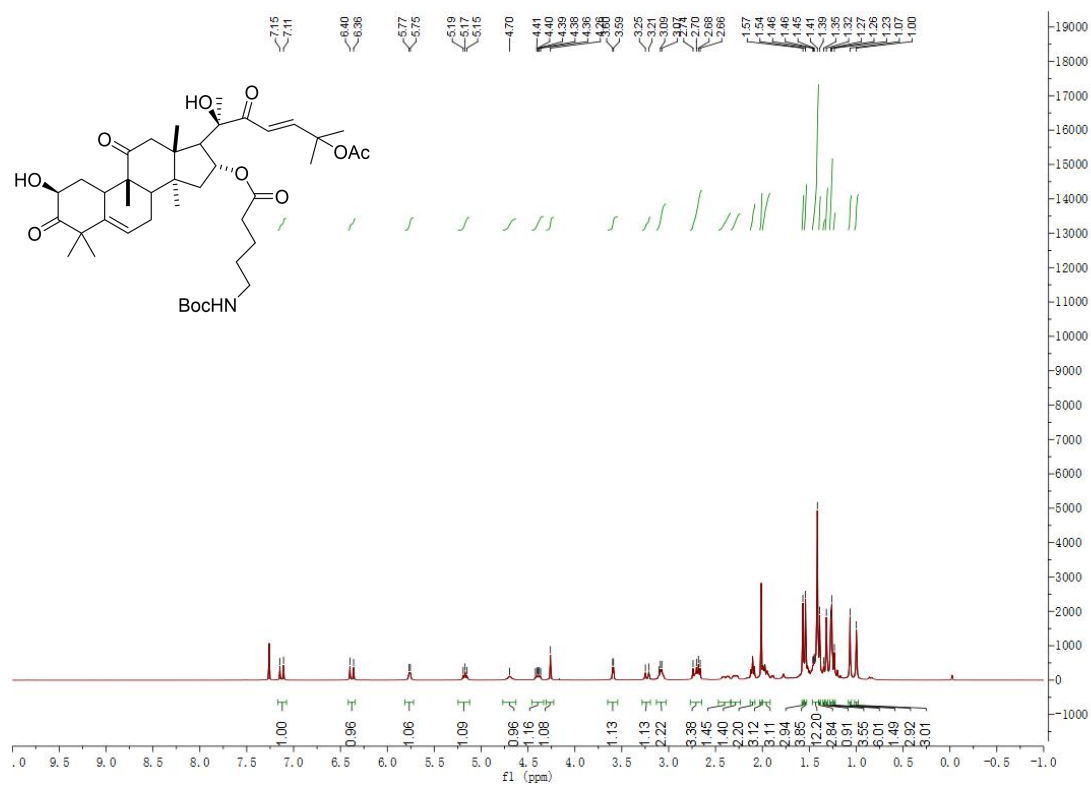
¹H NMR of compound 3b

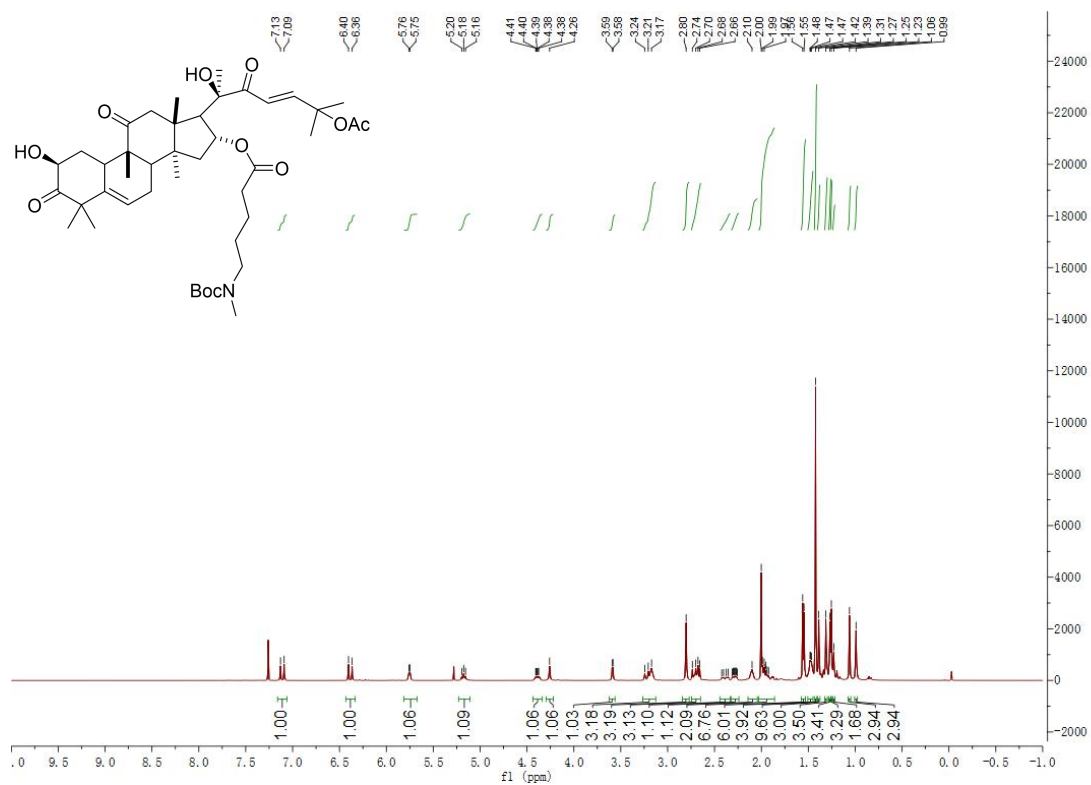


¹³C NMR of compound 3b

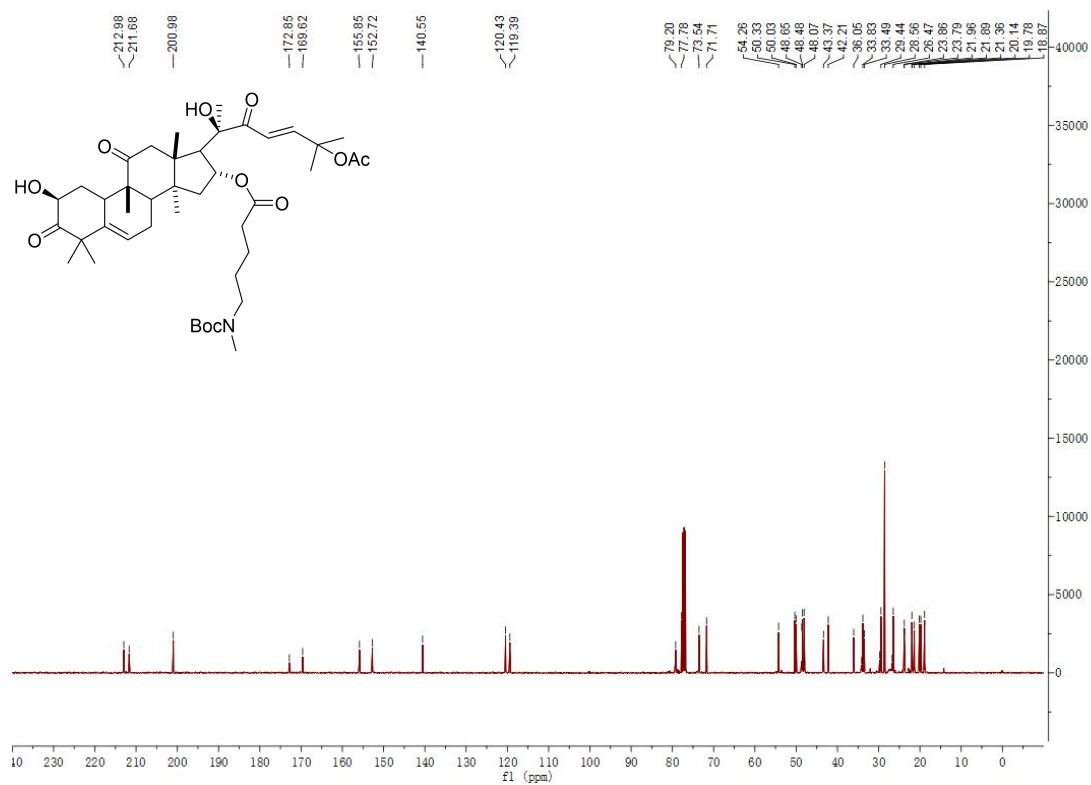


¹³C NMR of compound 3c

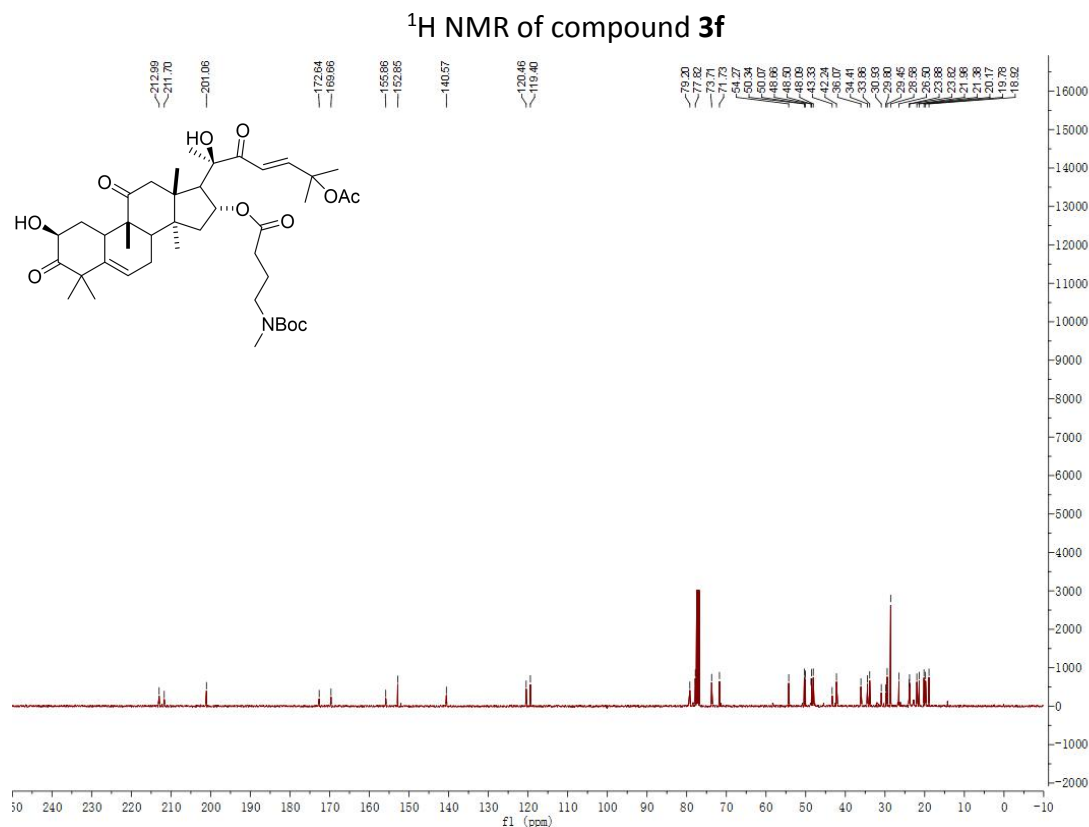
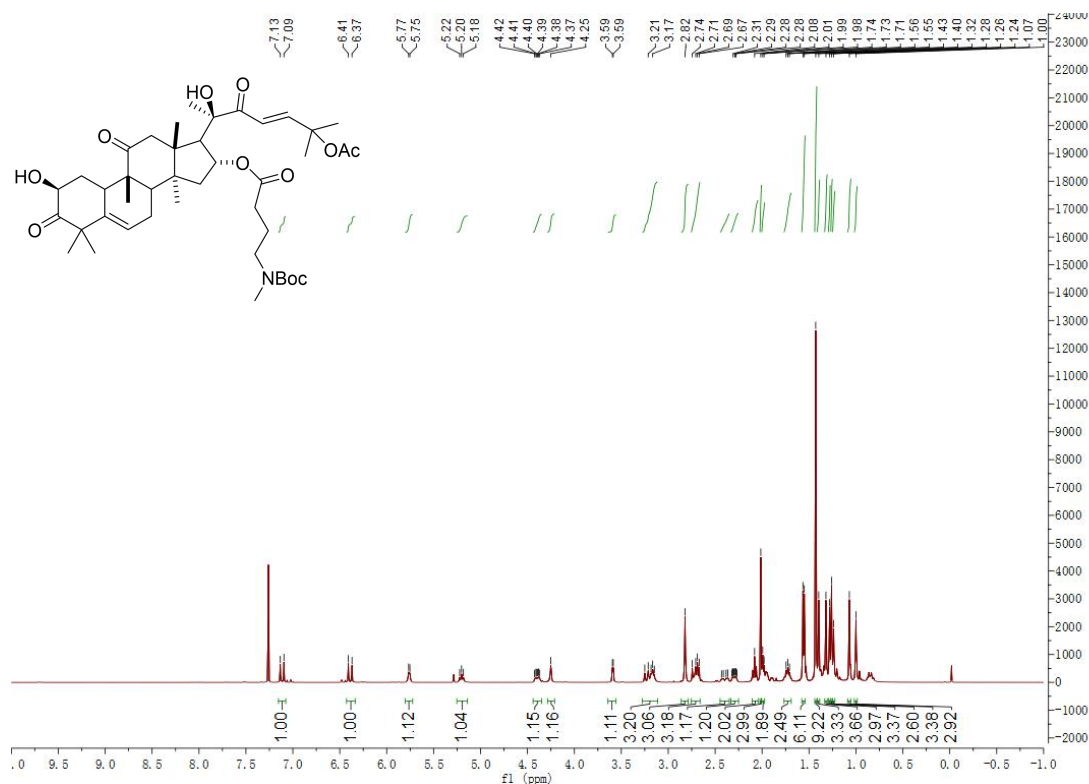


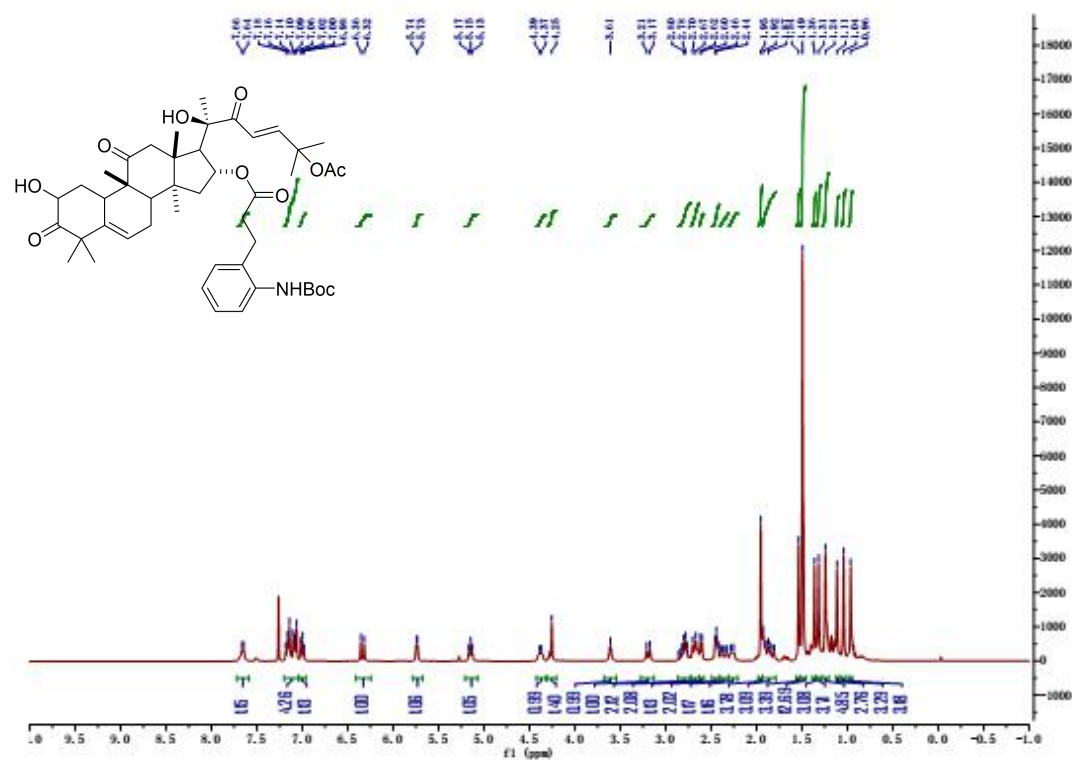


¹H NMR of compound 3e

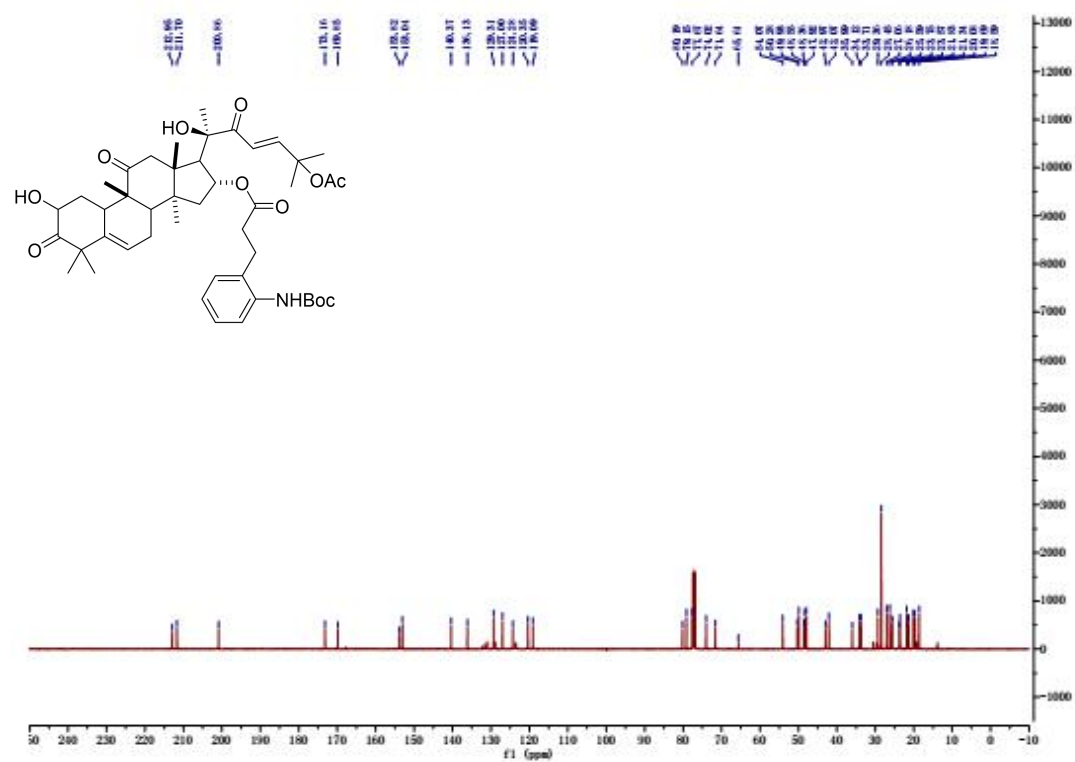


¹³C NMR of compound 3e

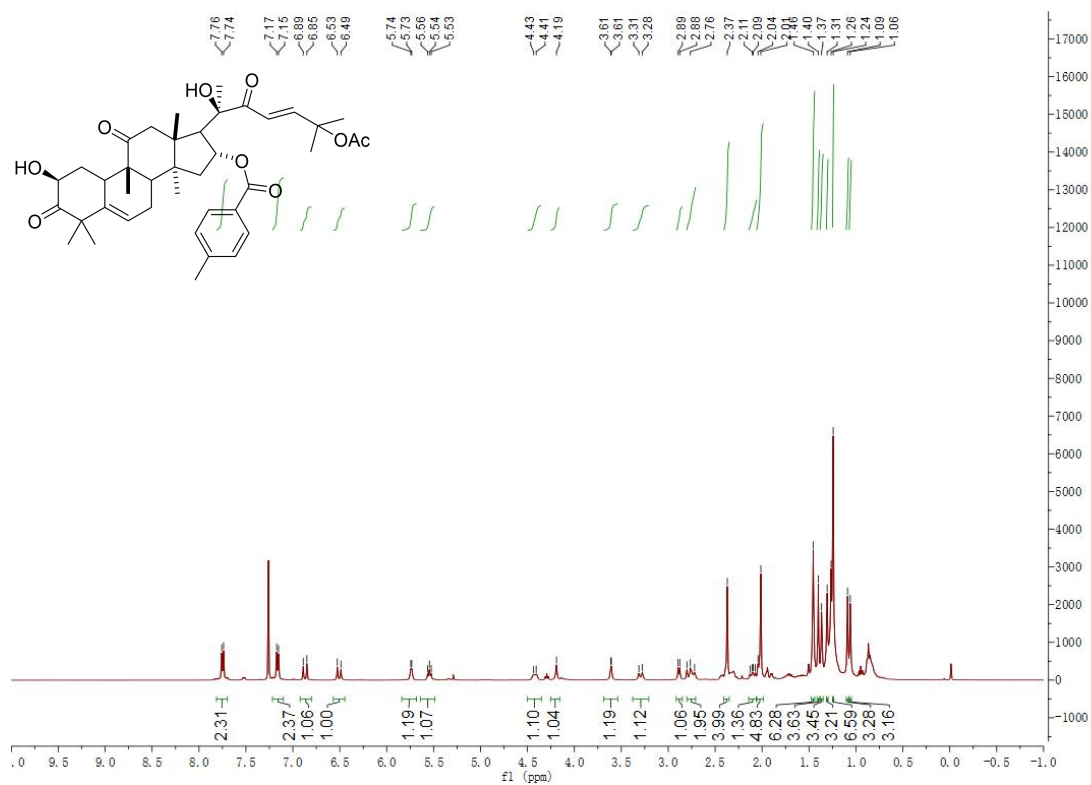




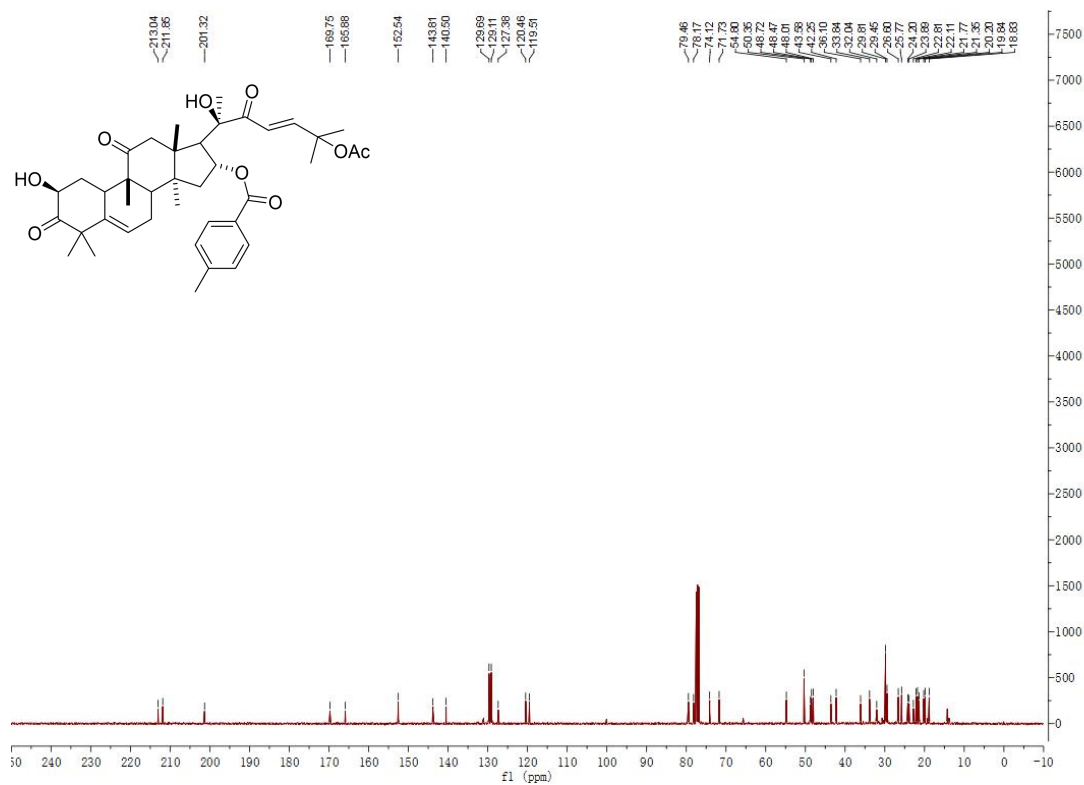
¹H NMR of compound **3g**



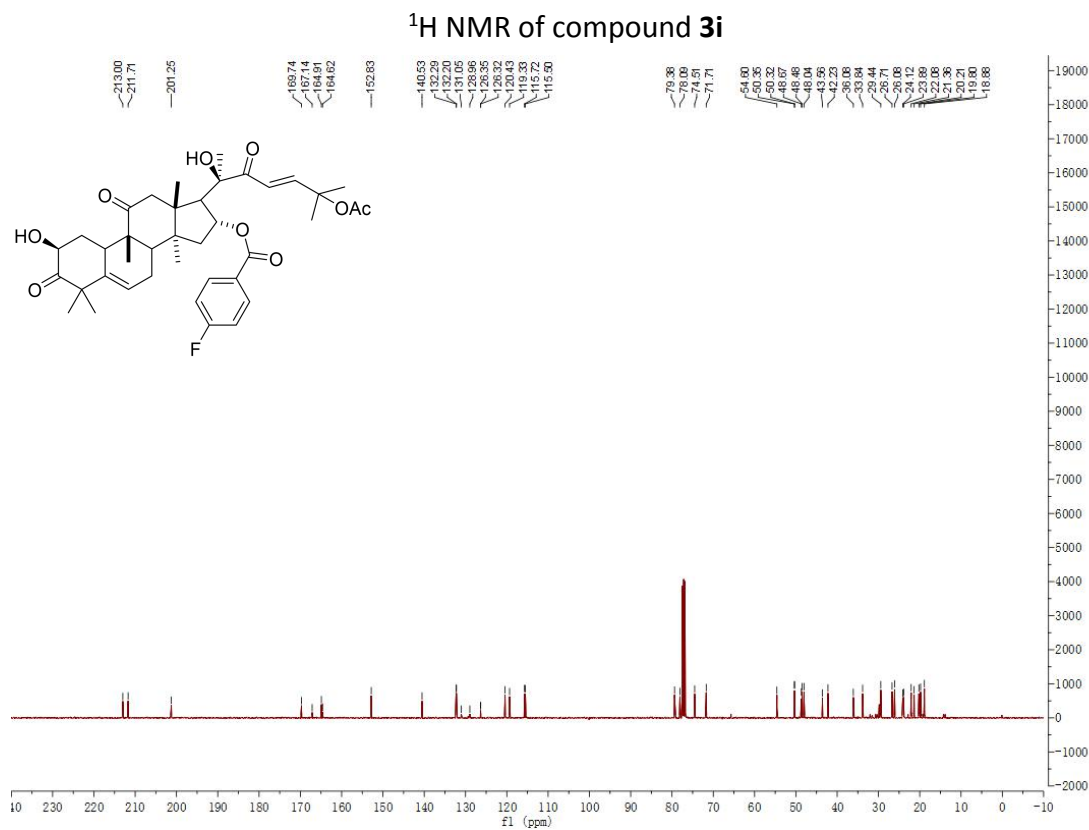
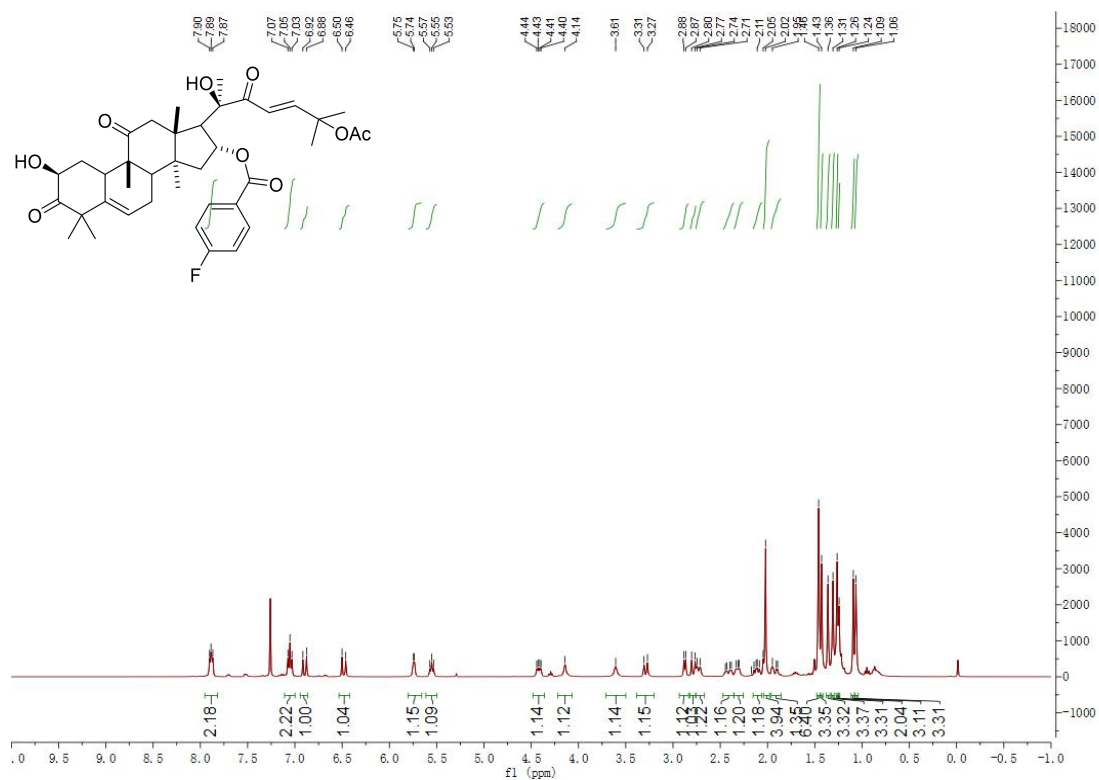
¹³C NMR of compound **3g**

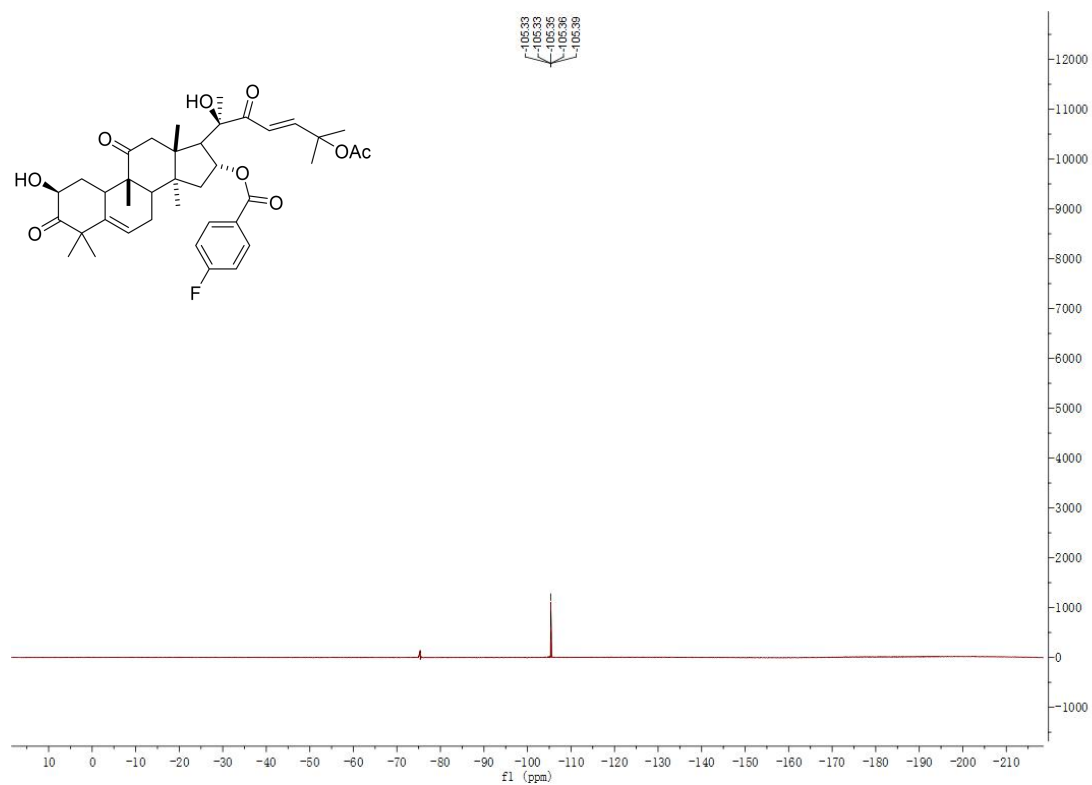


¹H NMR of compound 3h

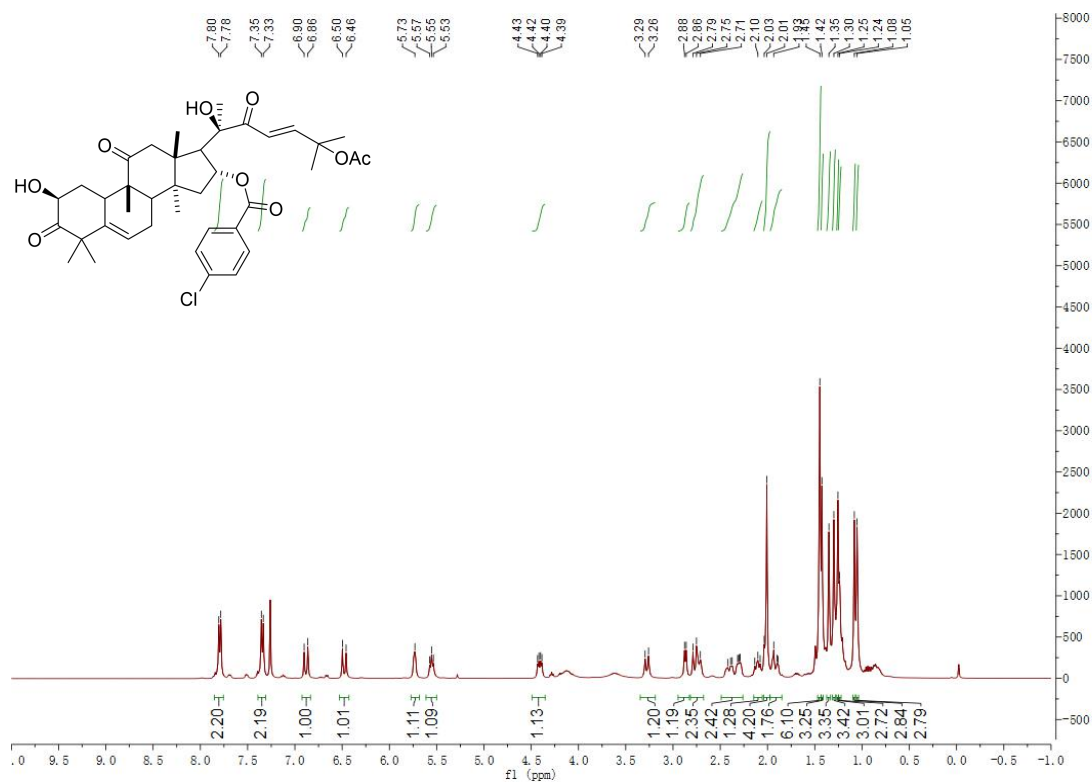


¹³C NMR of compound 3g

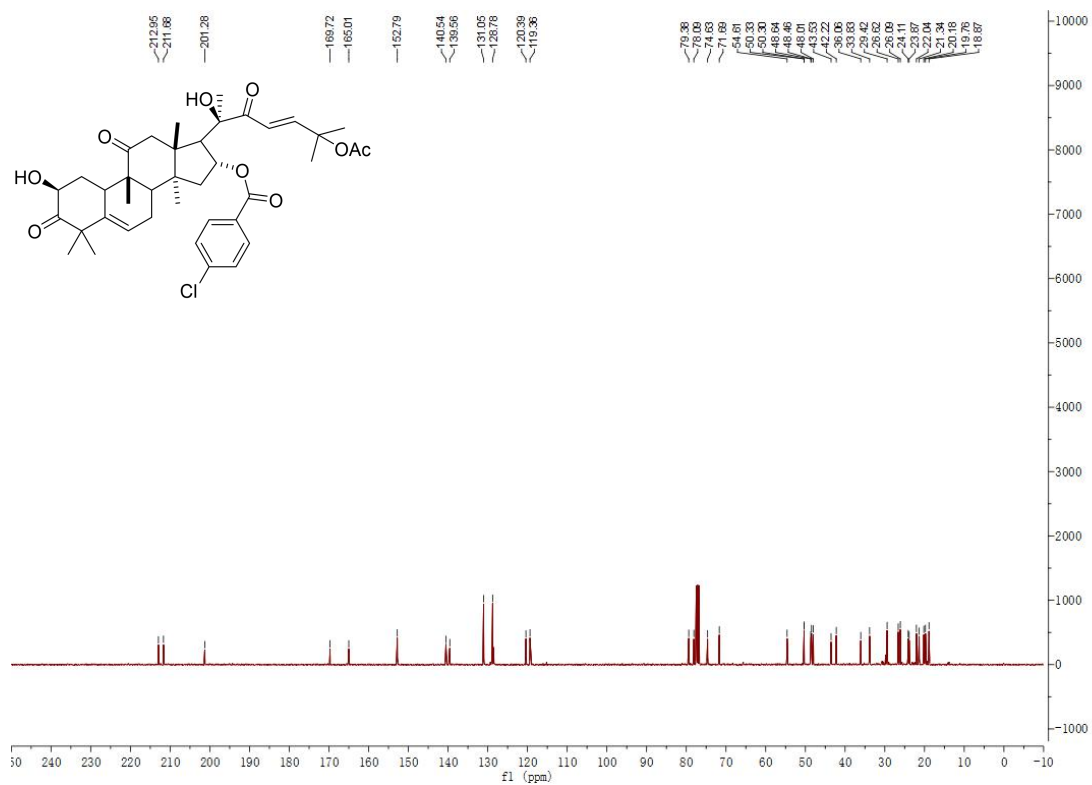




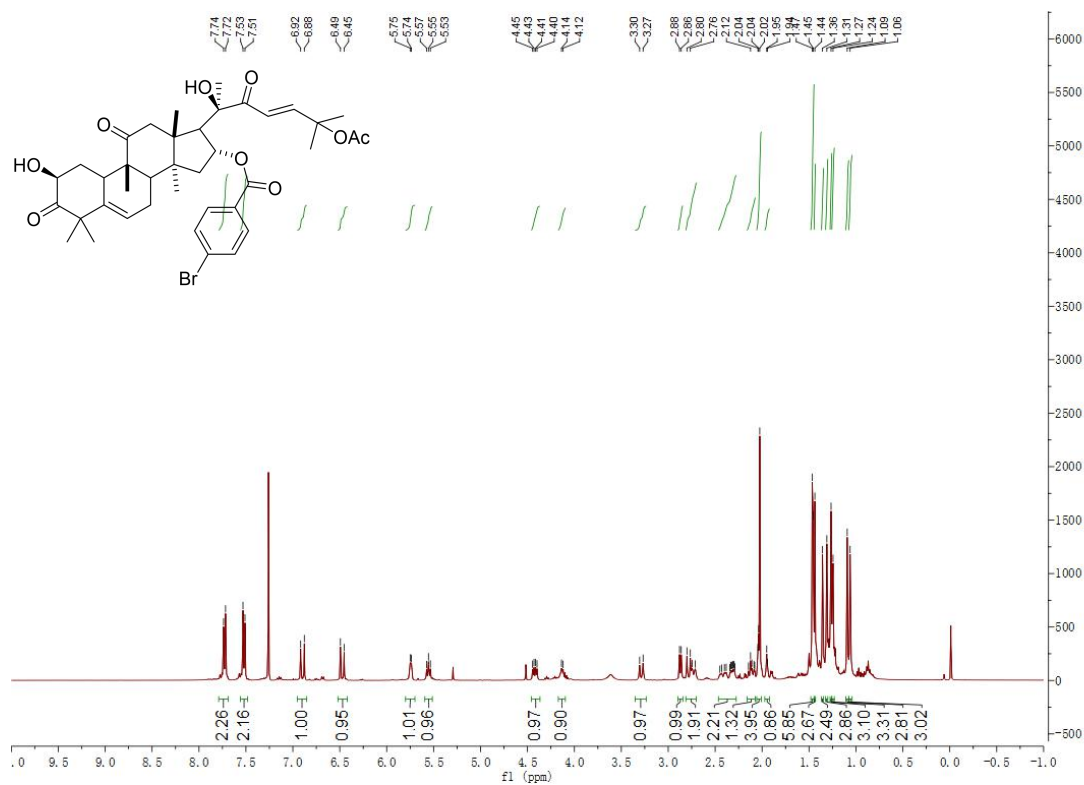
^{19}F NMR of compound **3i**



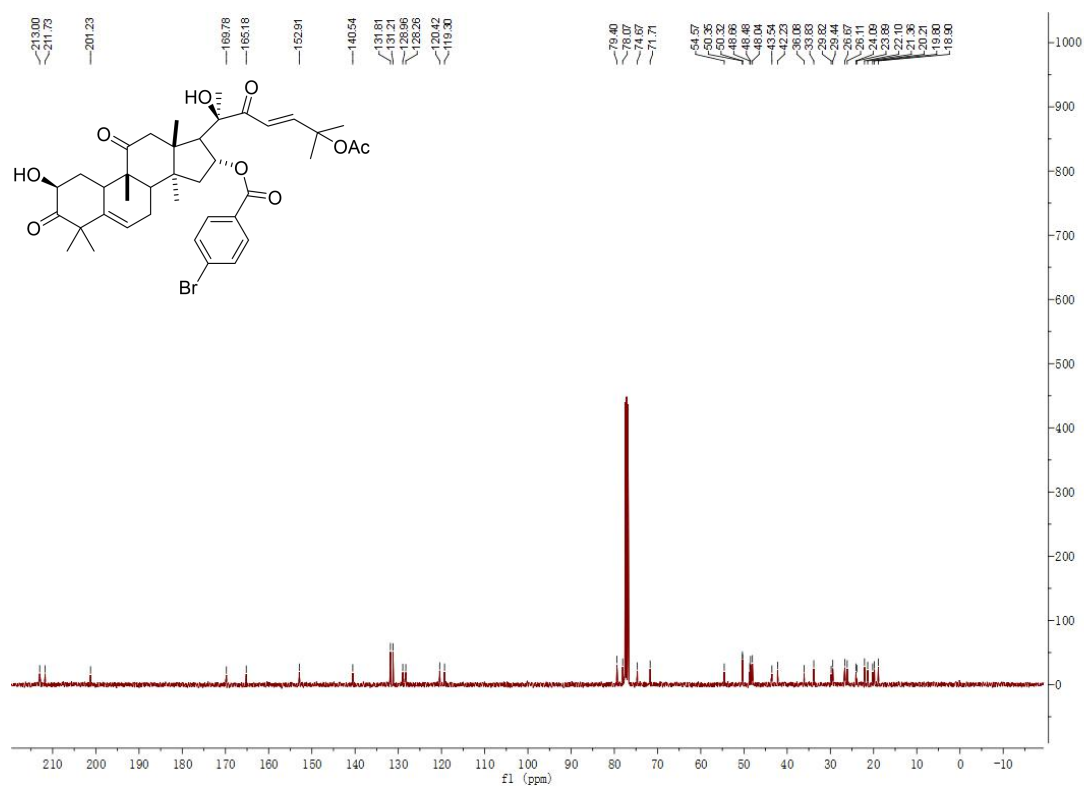
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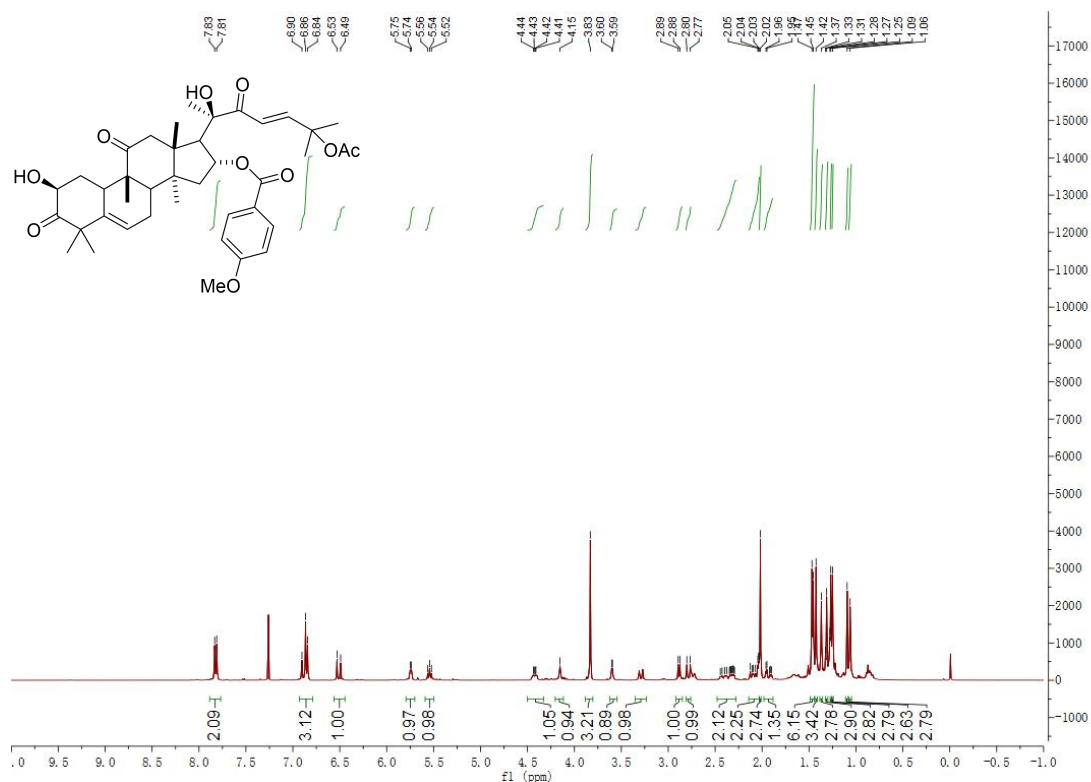
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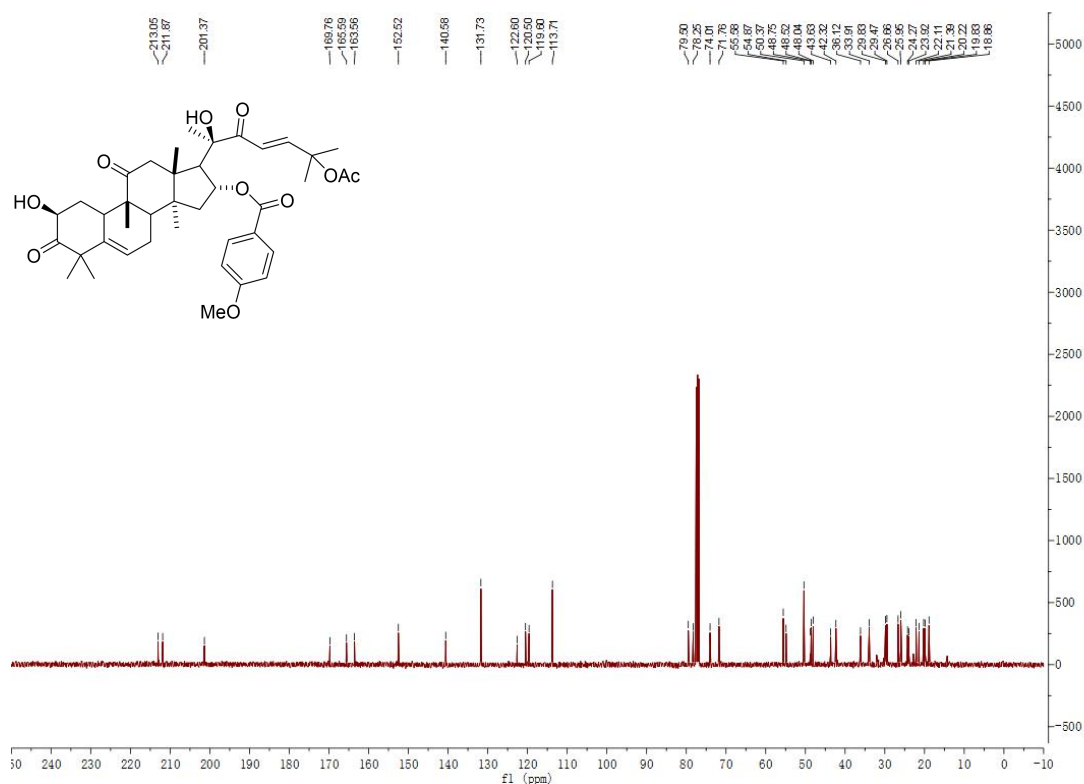
¹H NMR of compound 3k



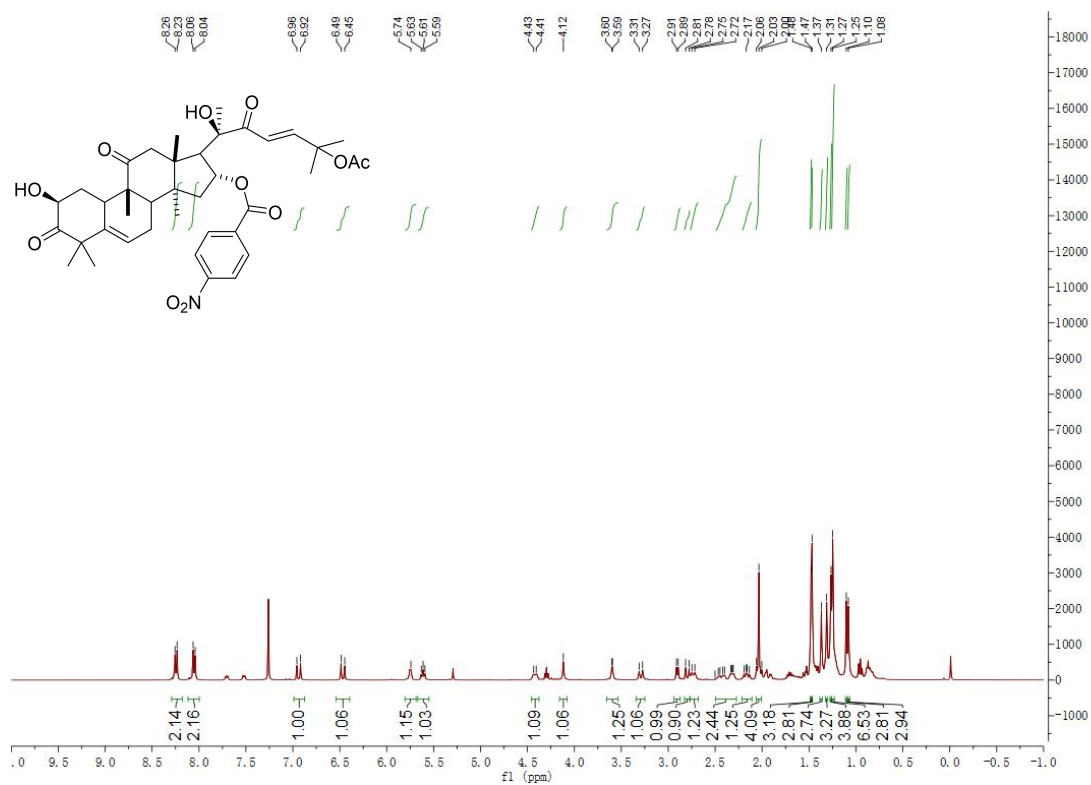
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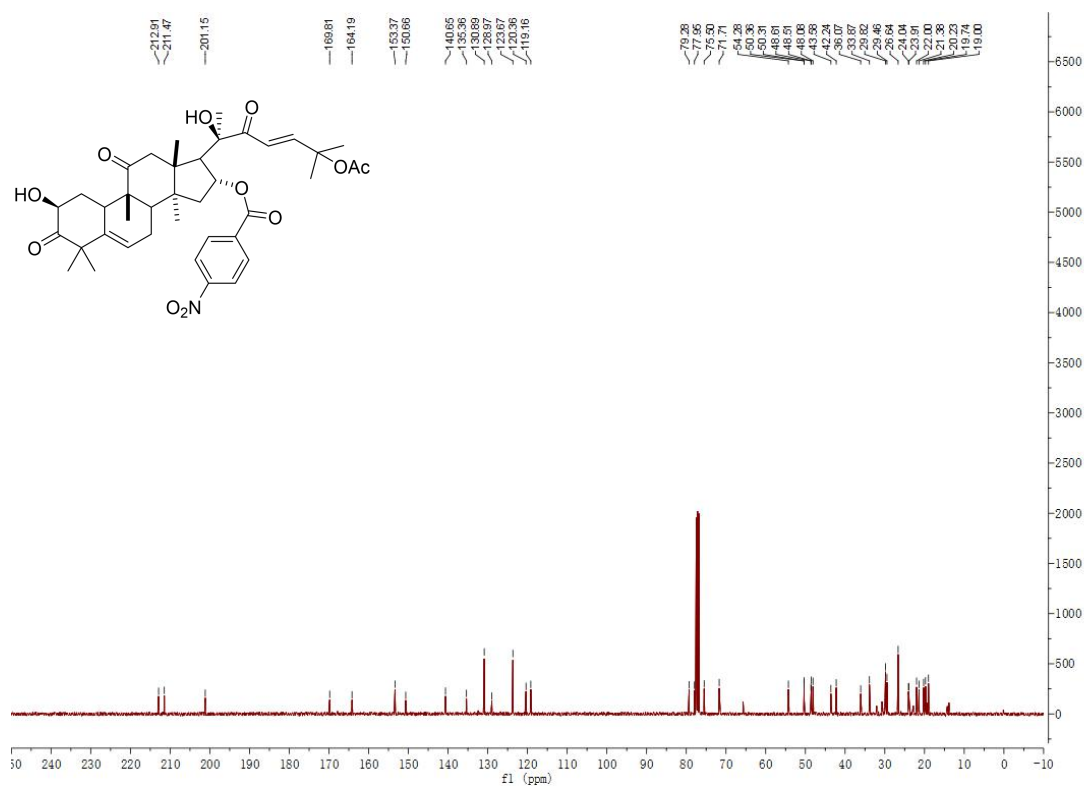
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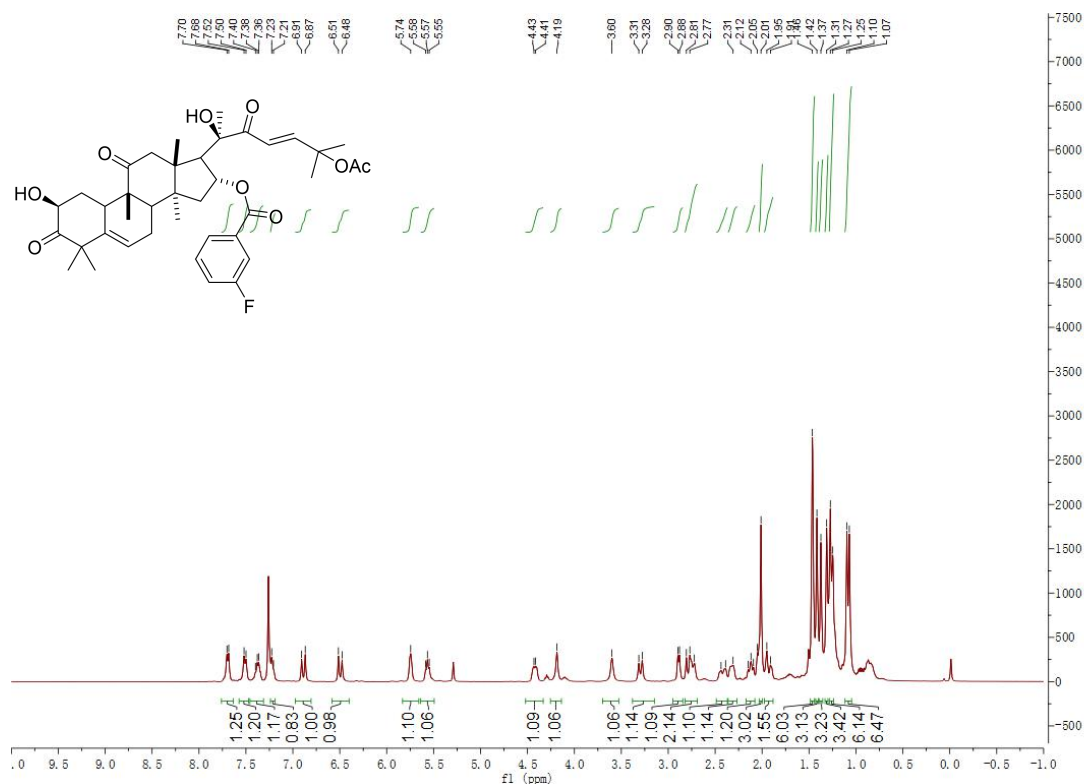
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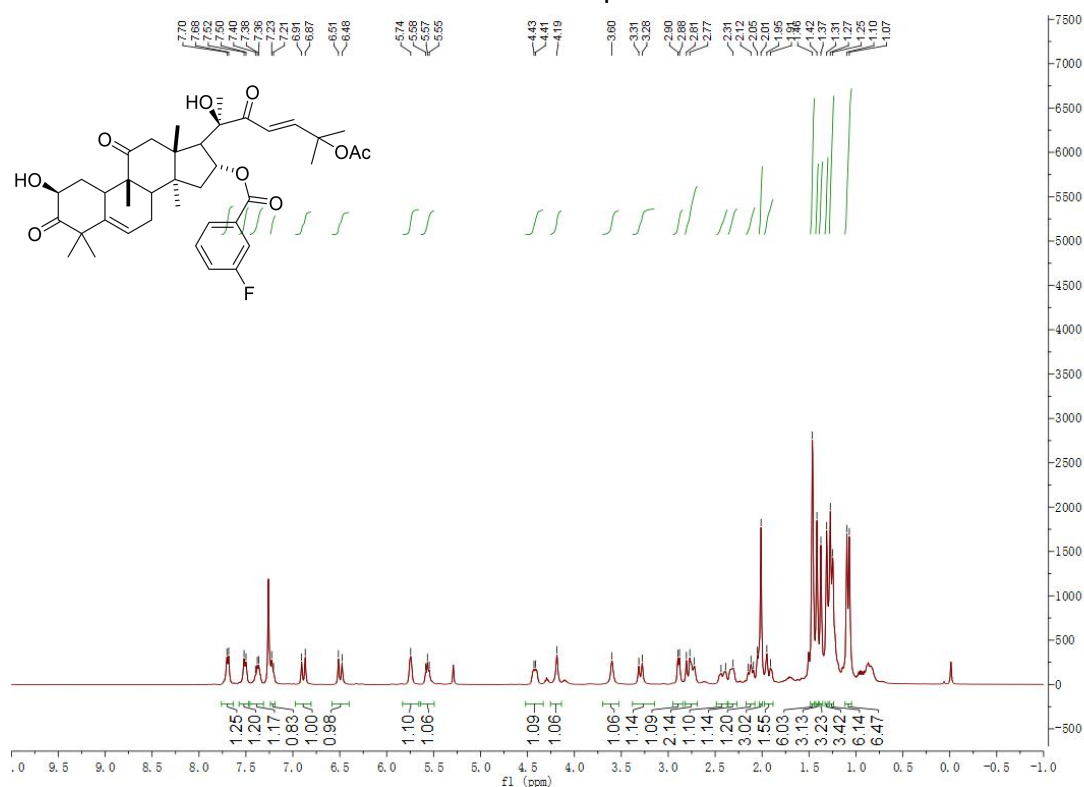
¹H NMR of compound 3m



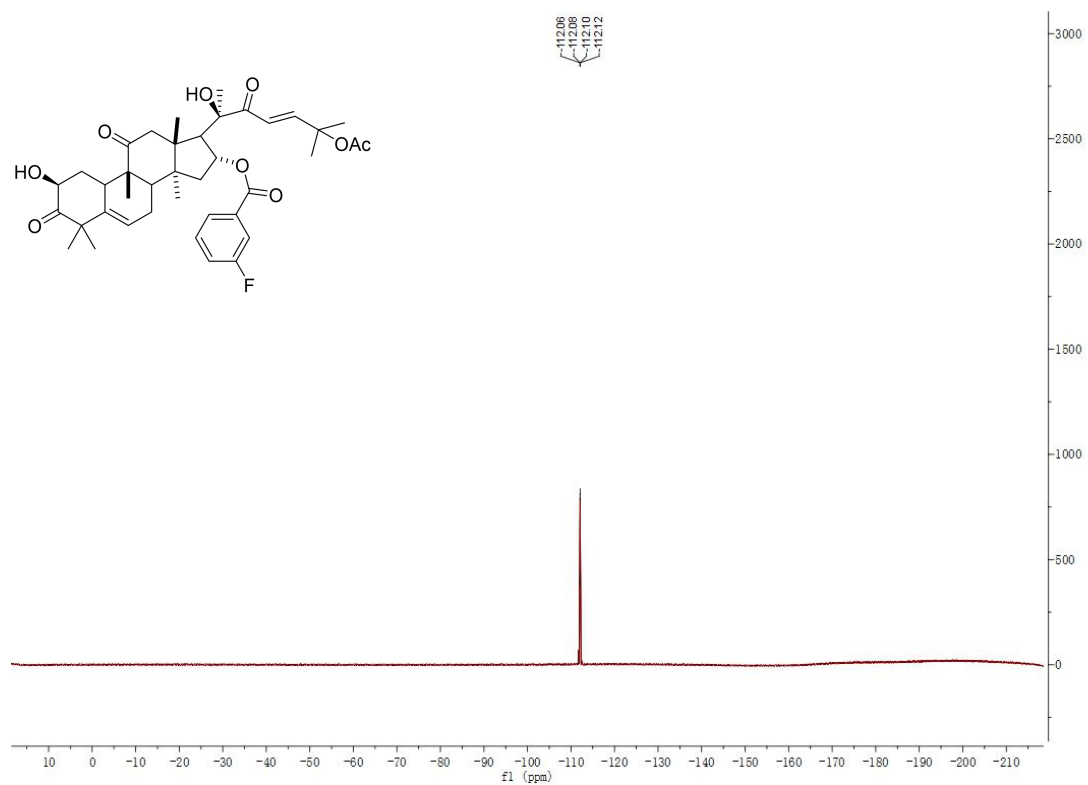
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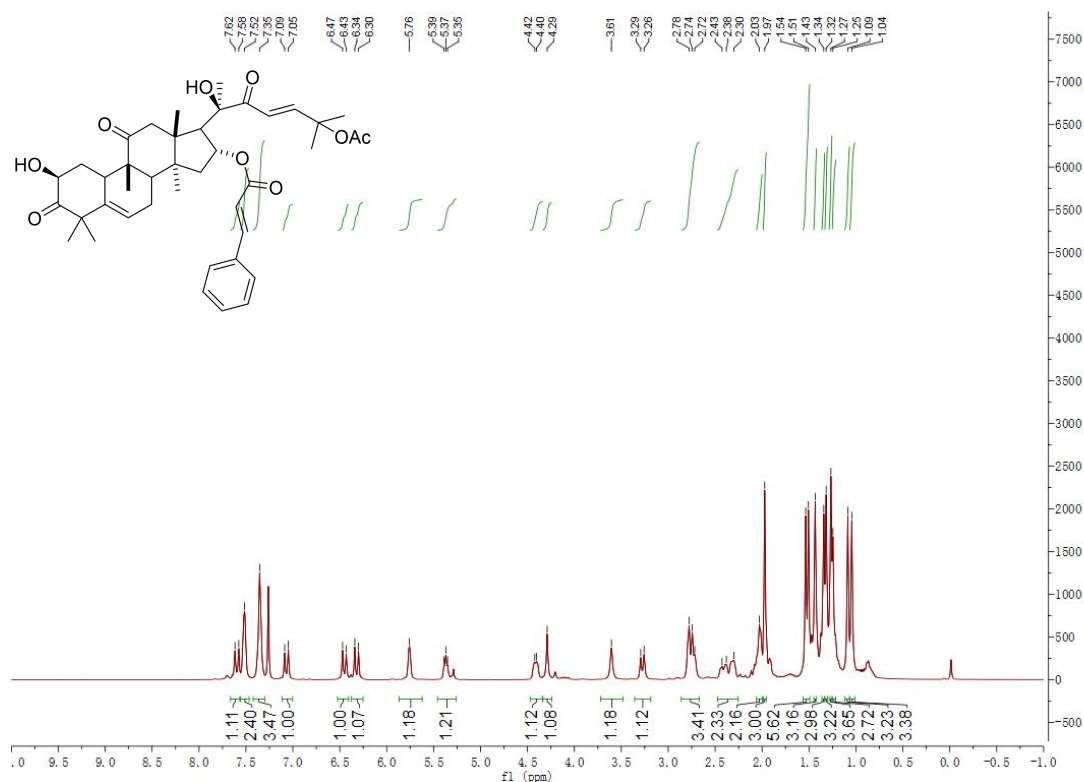
¹H NMR of compound 3n



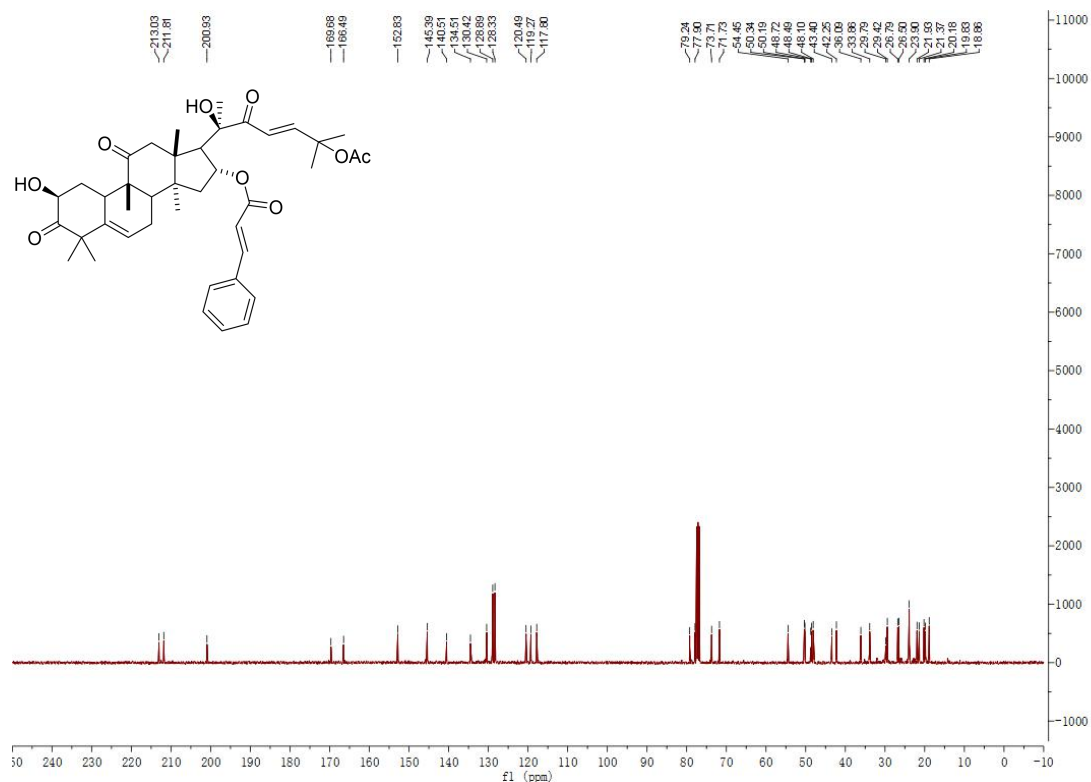
¹³C NMR of compound 3n



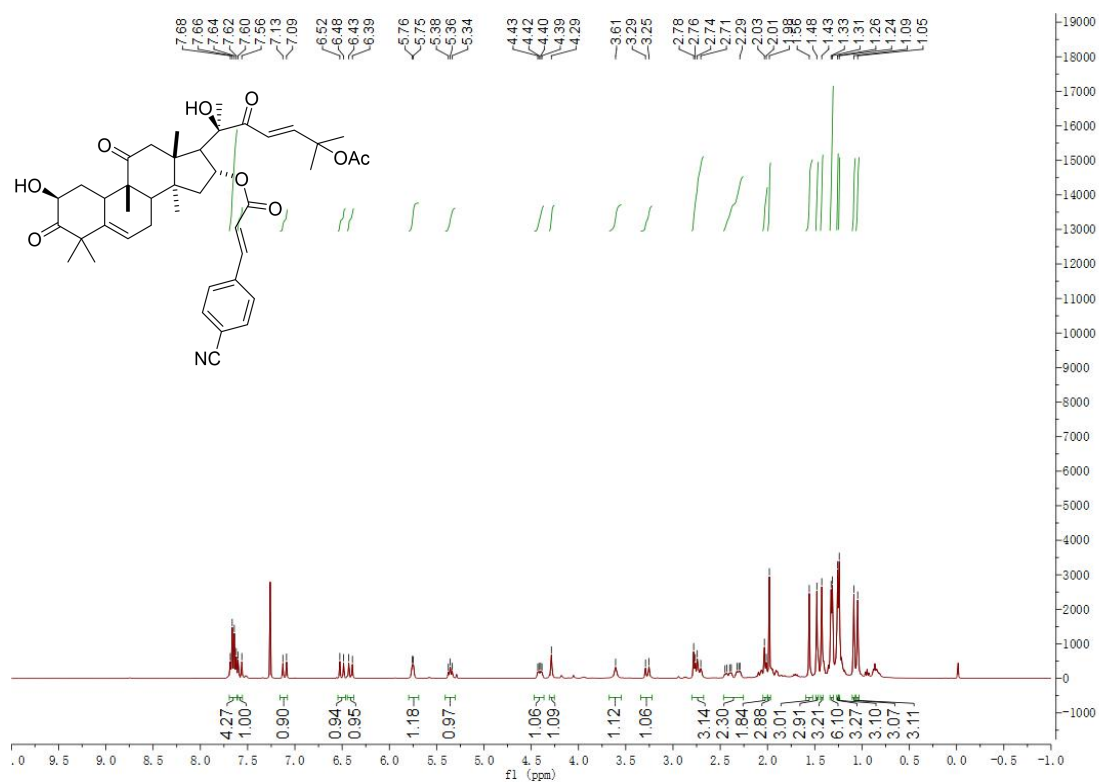
^{19}F NMR of compound **3n**



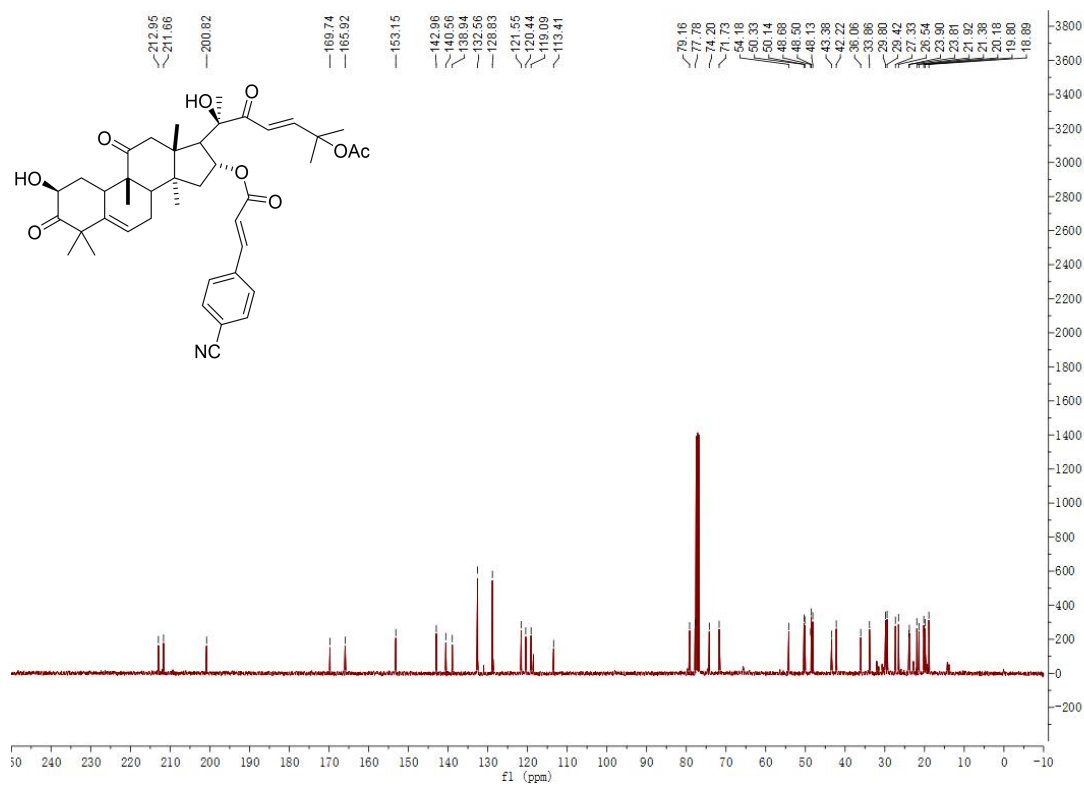
¹H NMR of compound 3o



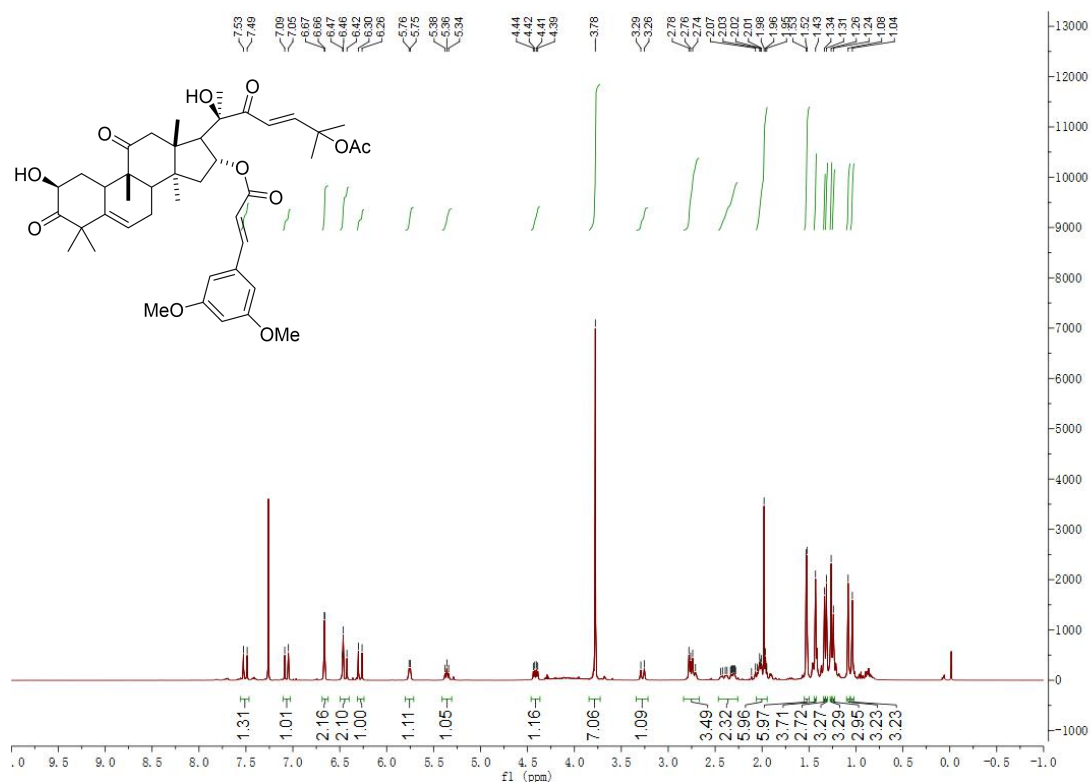
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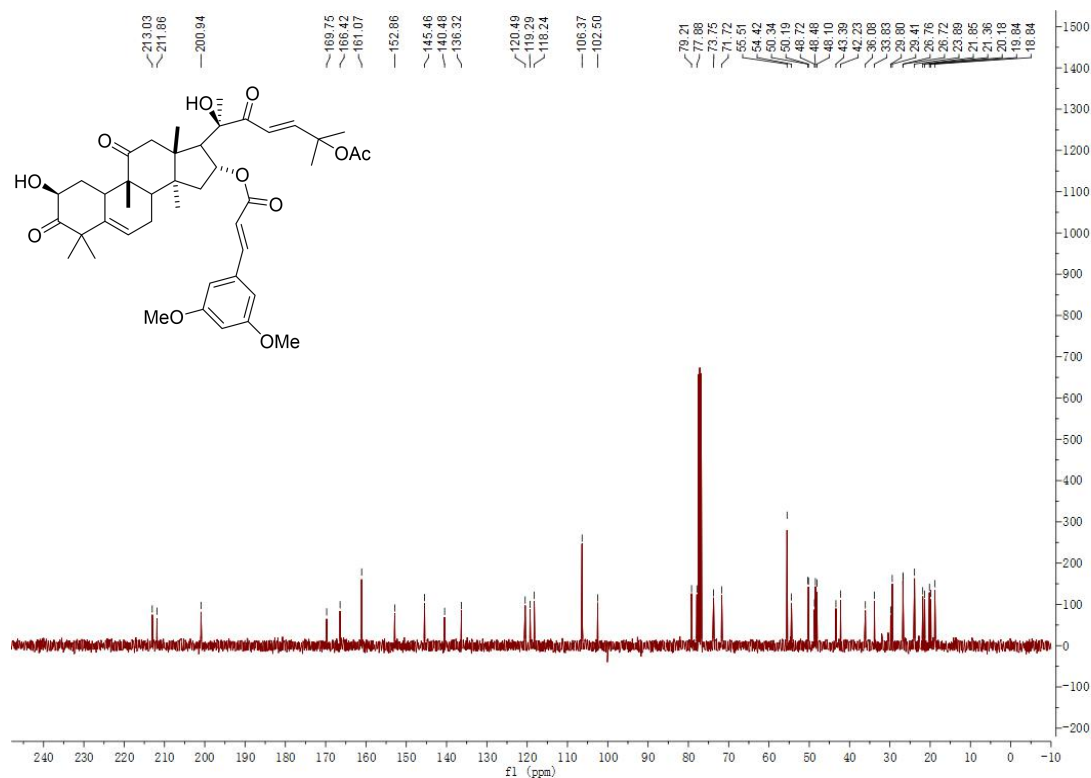
¹H NMR of compound 3p



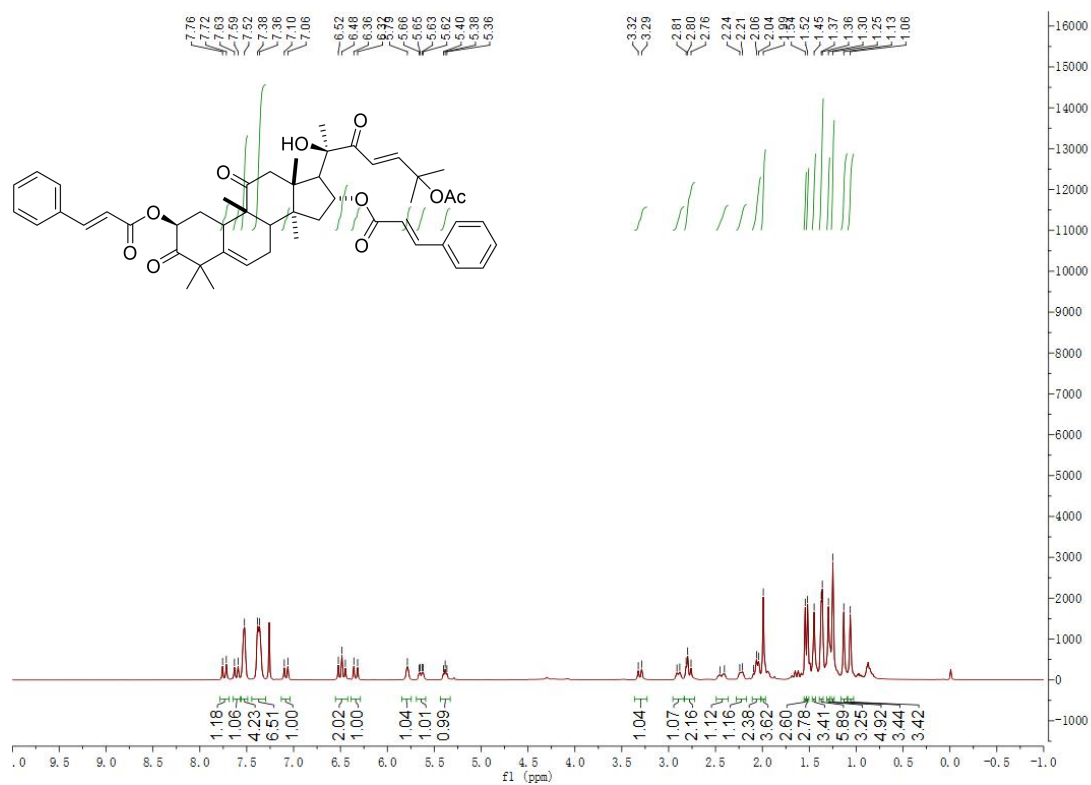
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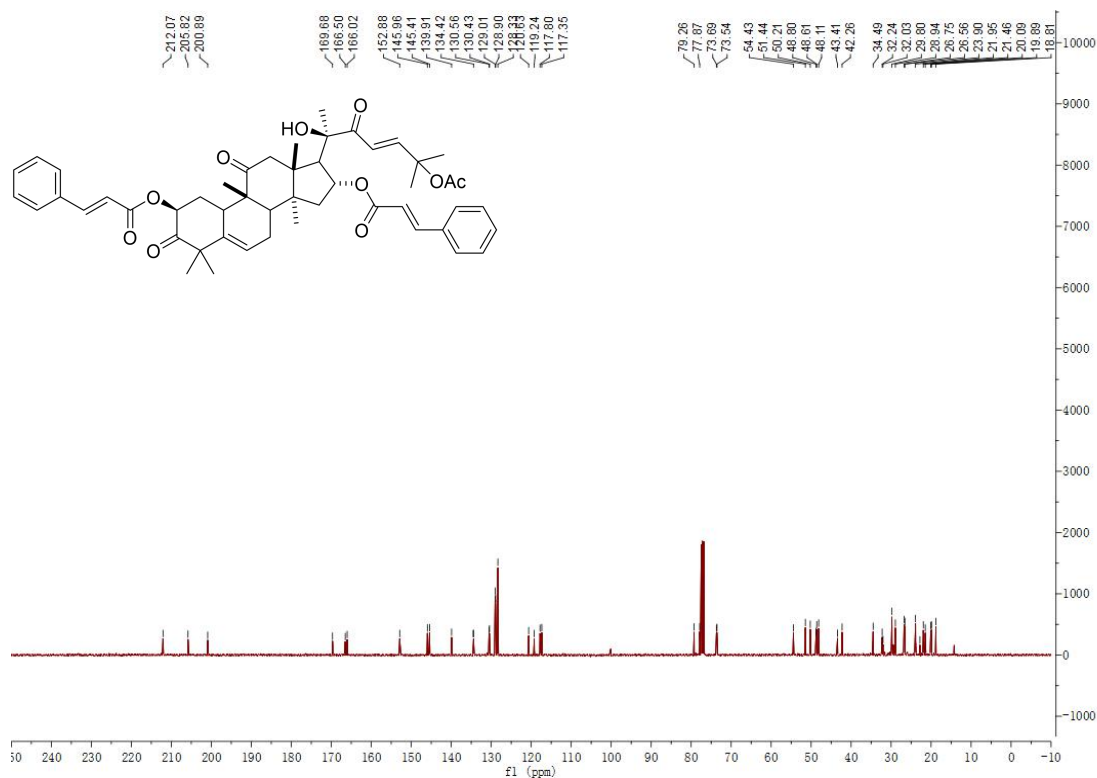
¹H NMR of compound 3q



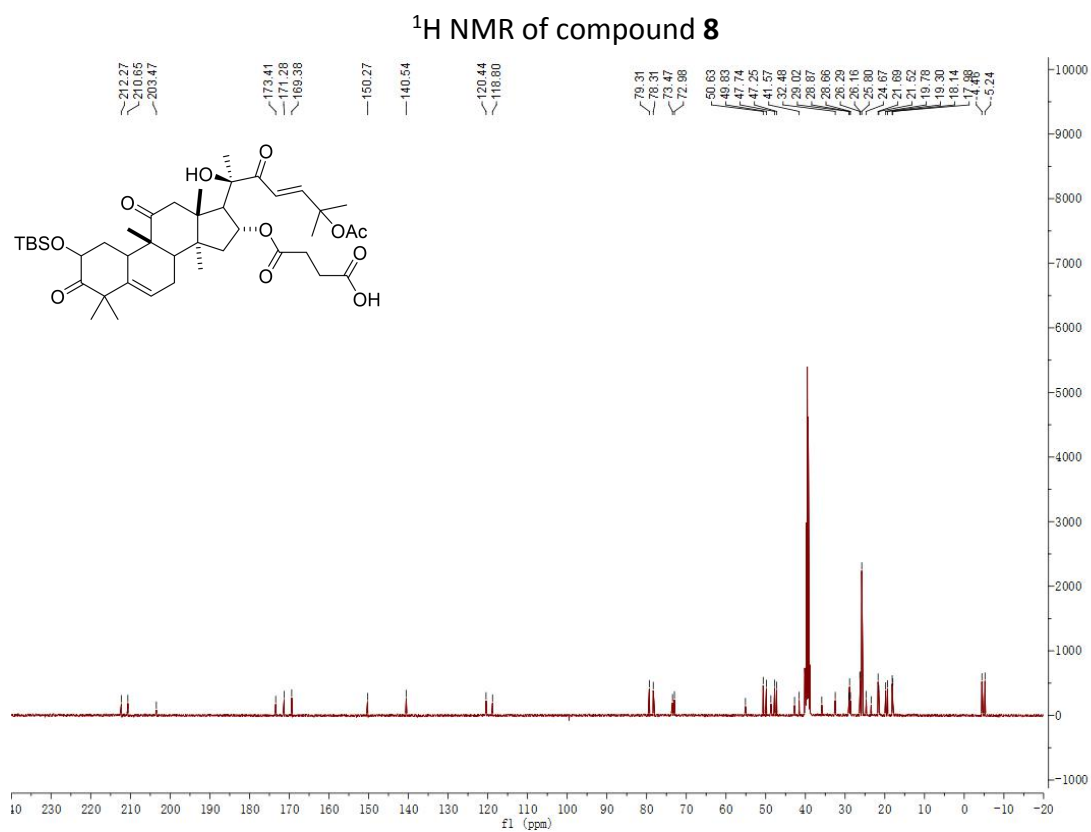
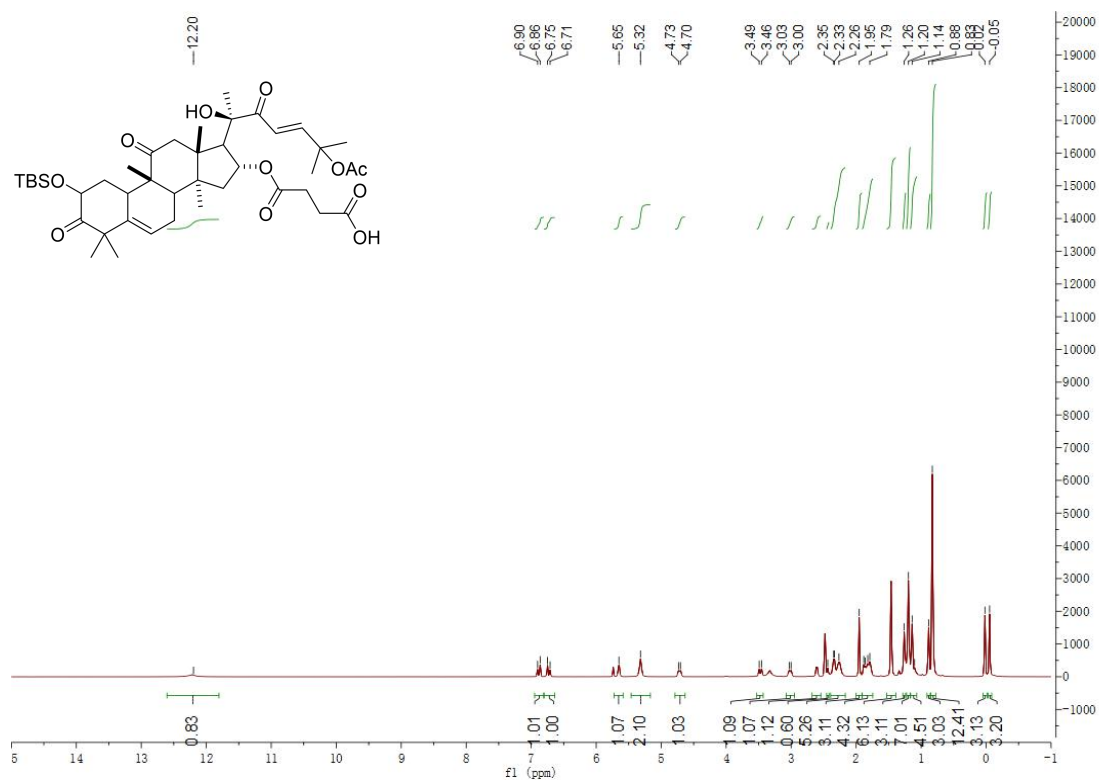
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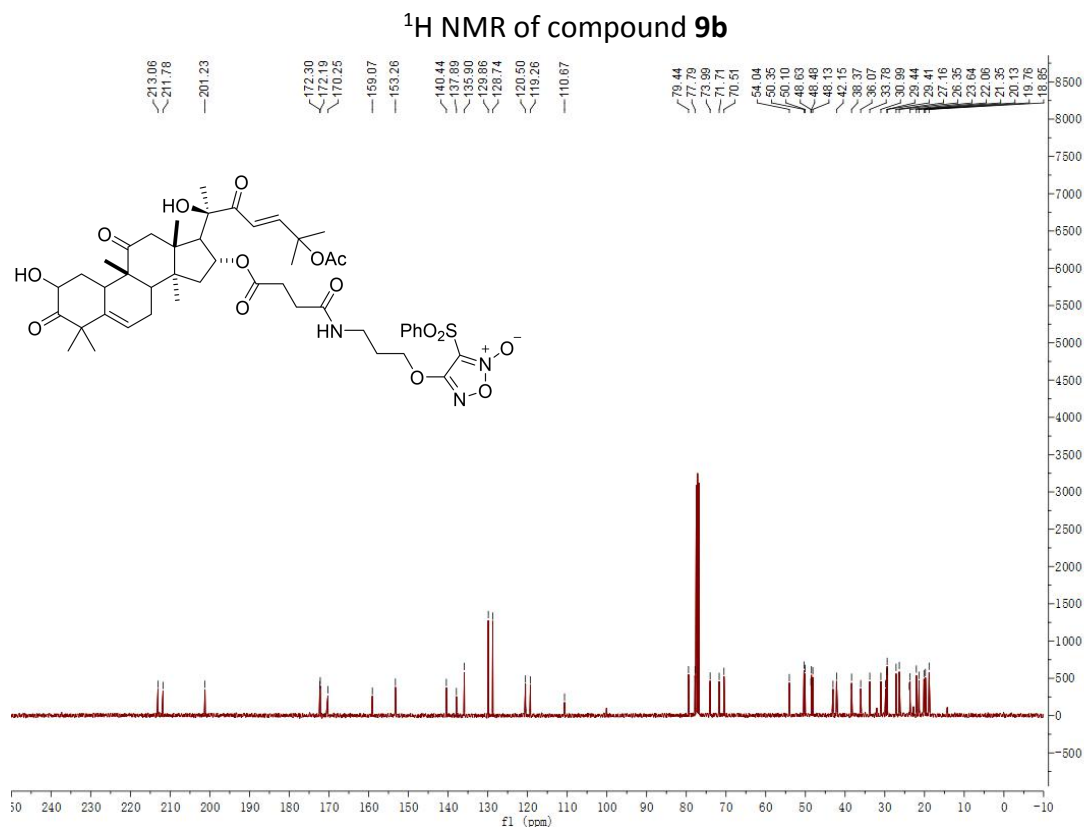
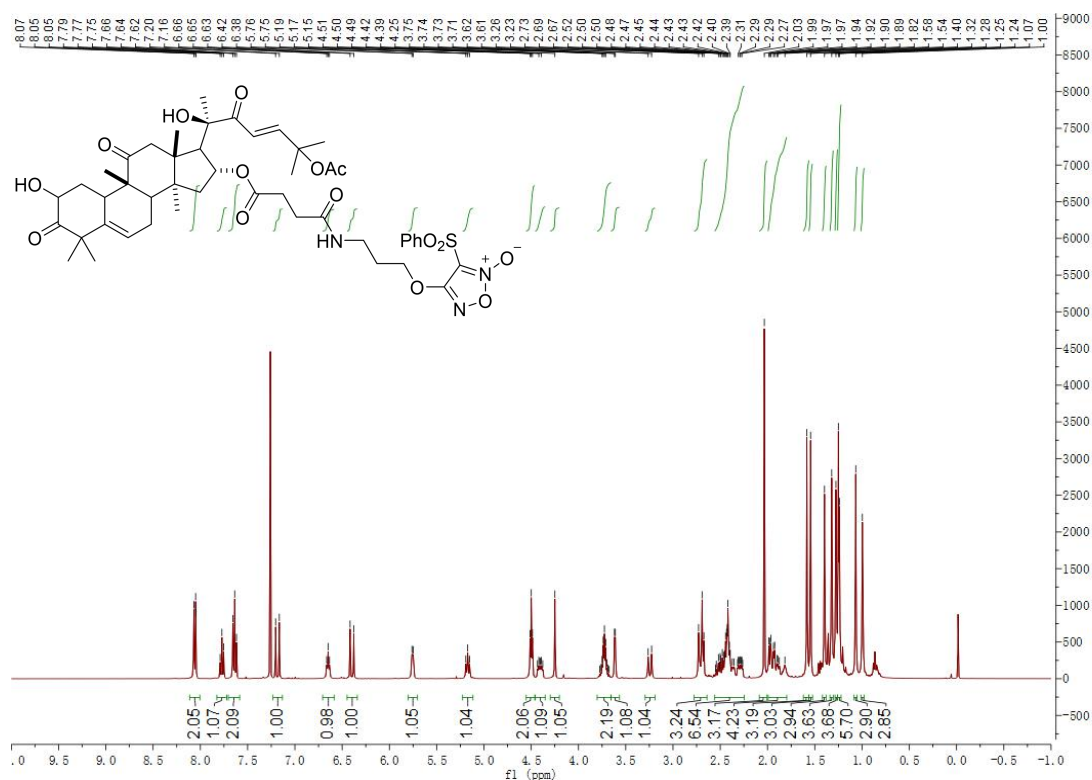


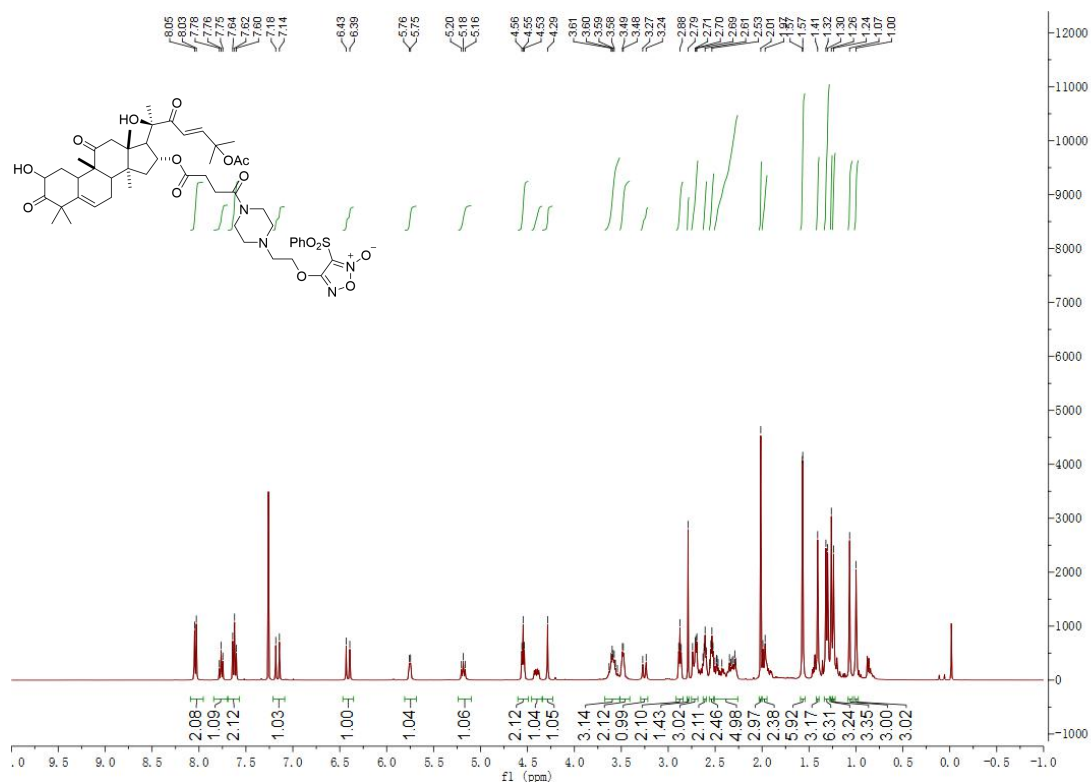
¹H NMR of compound 4



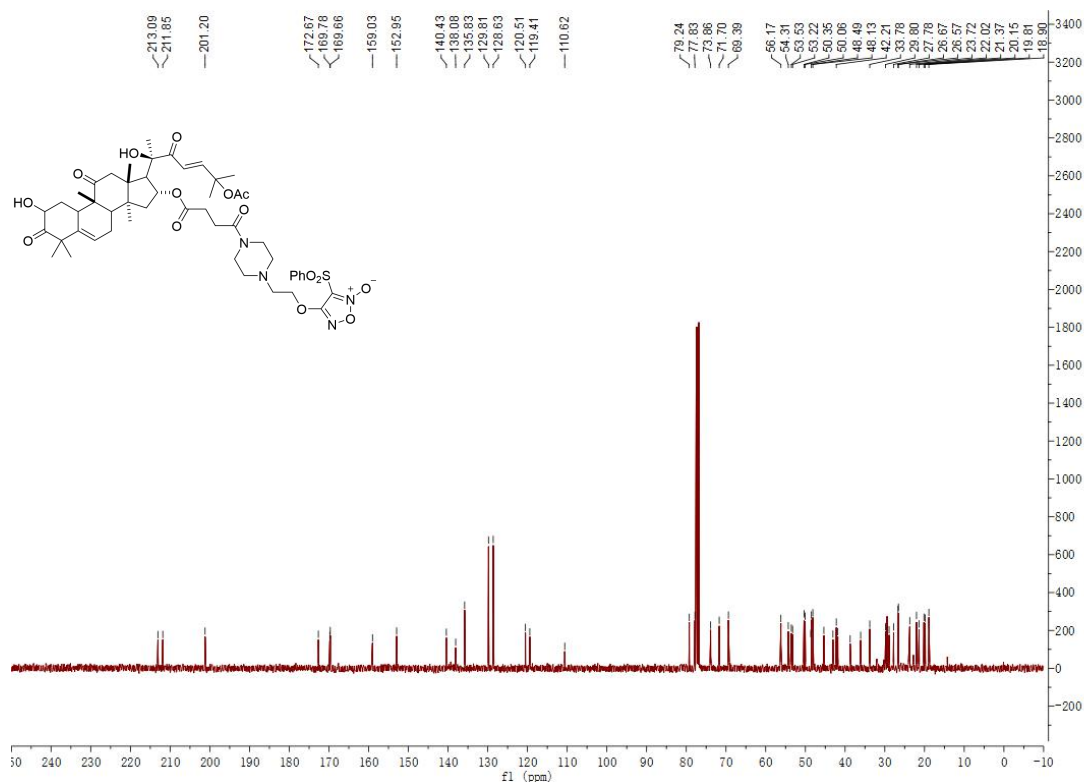
¹³C NMR of compound 3q



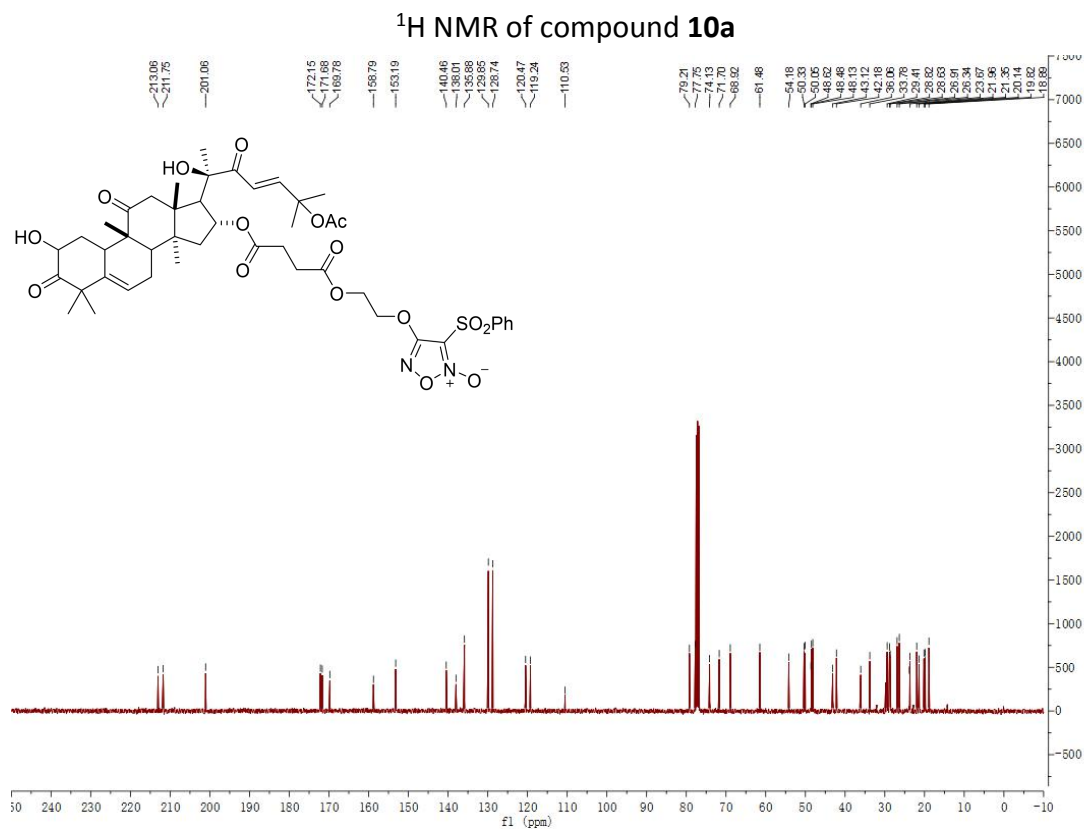
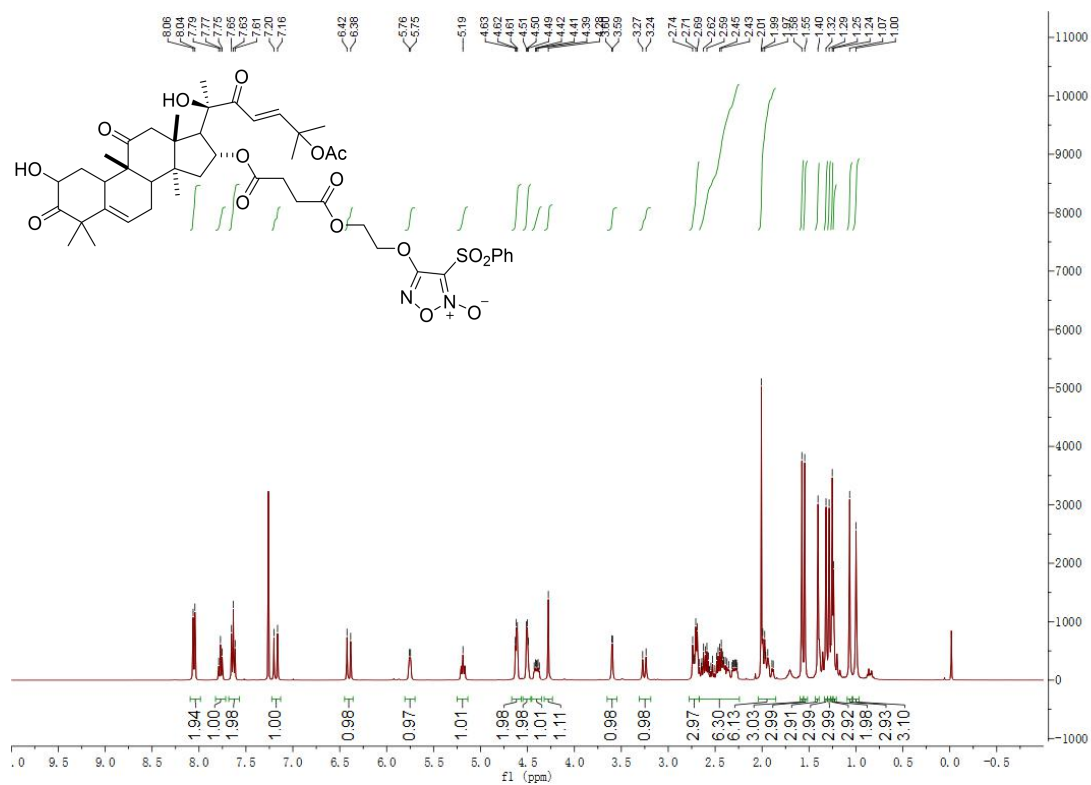


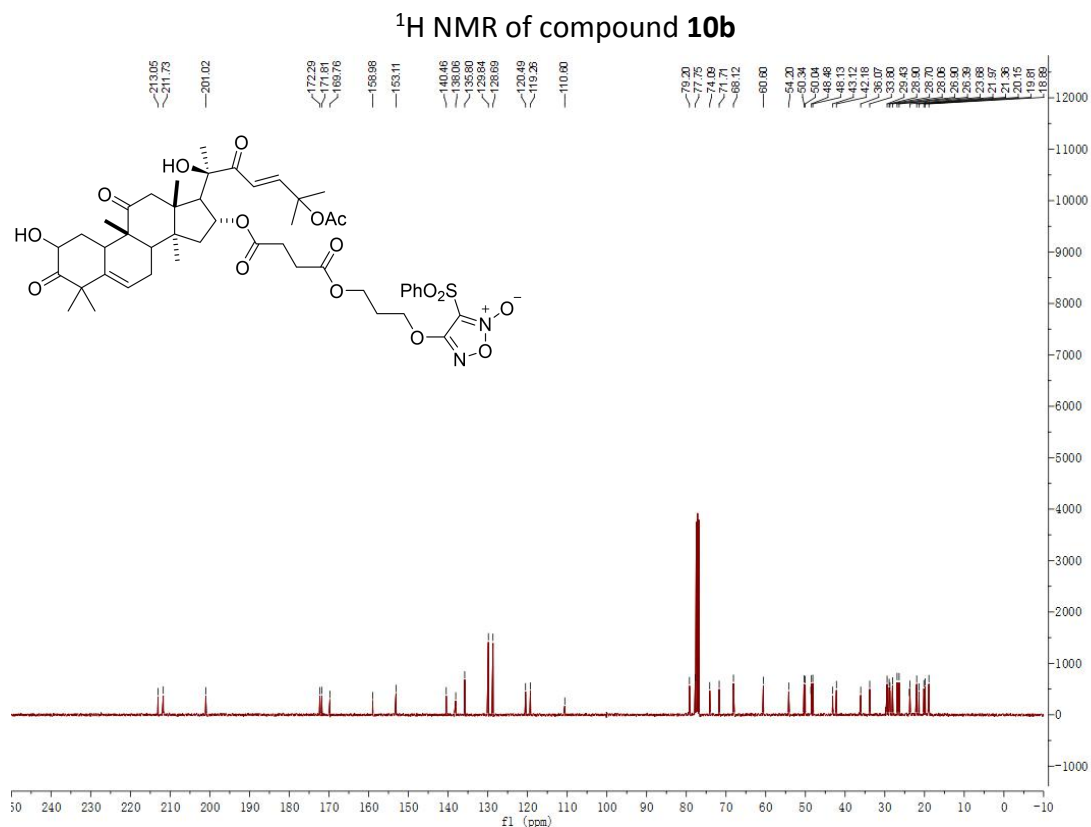
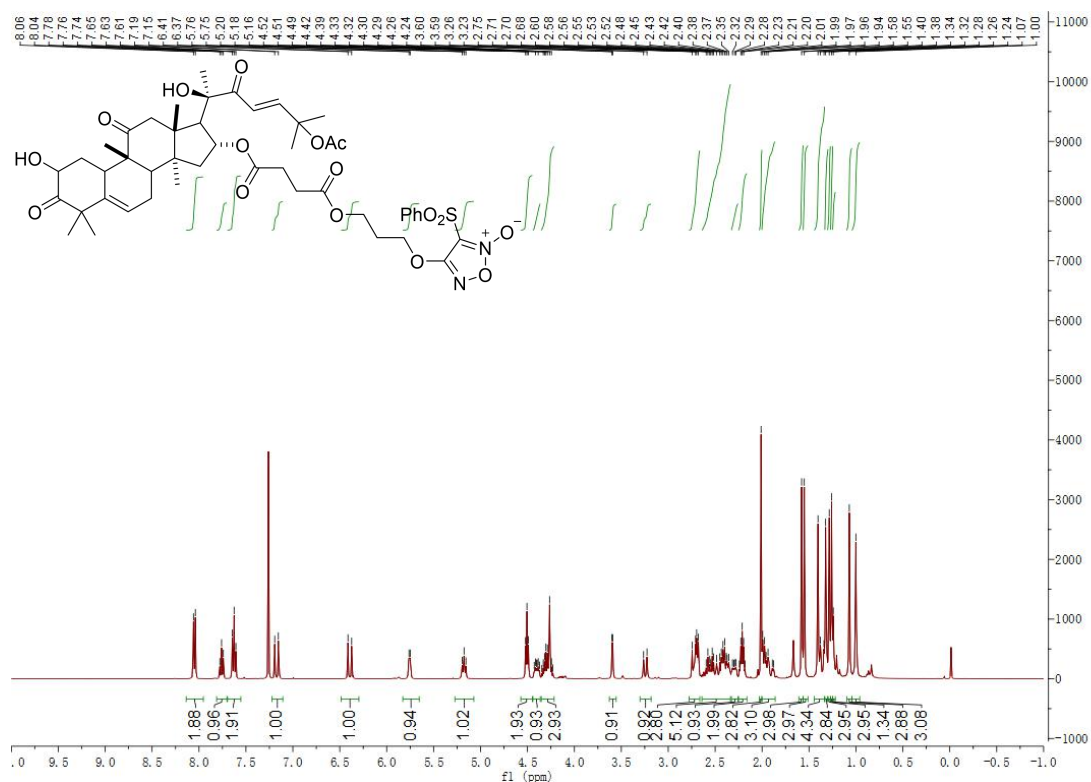


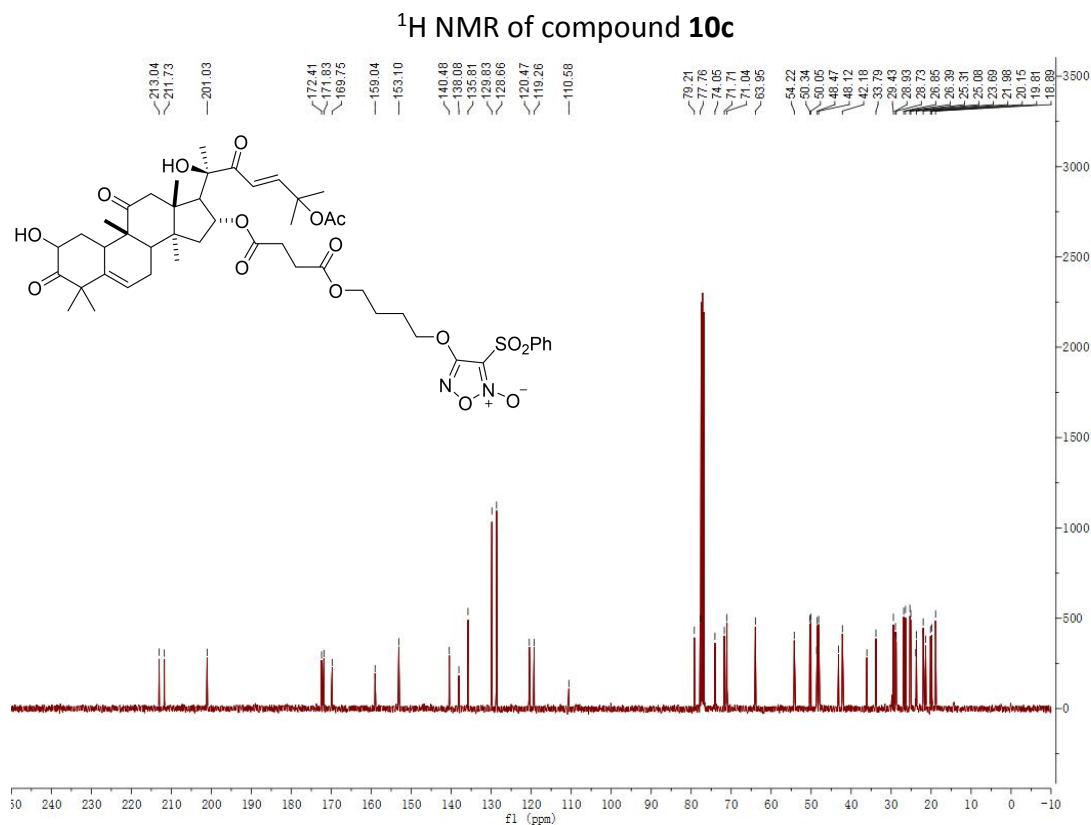
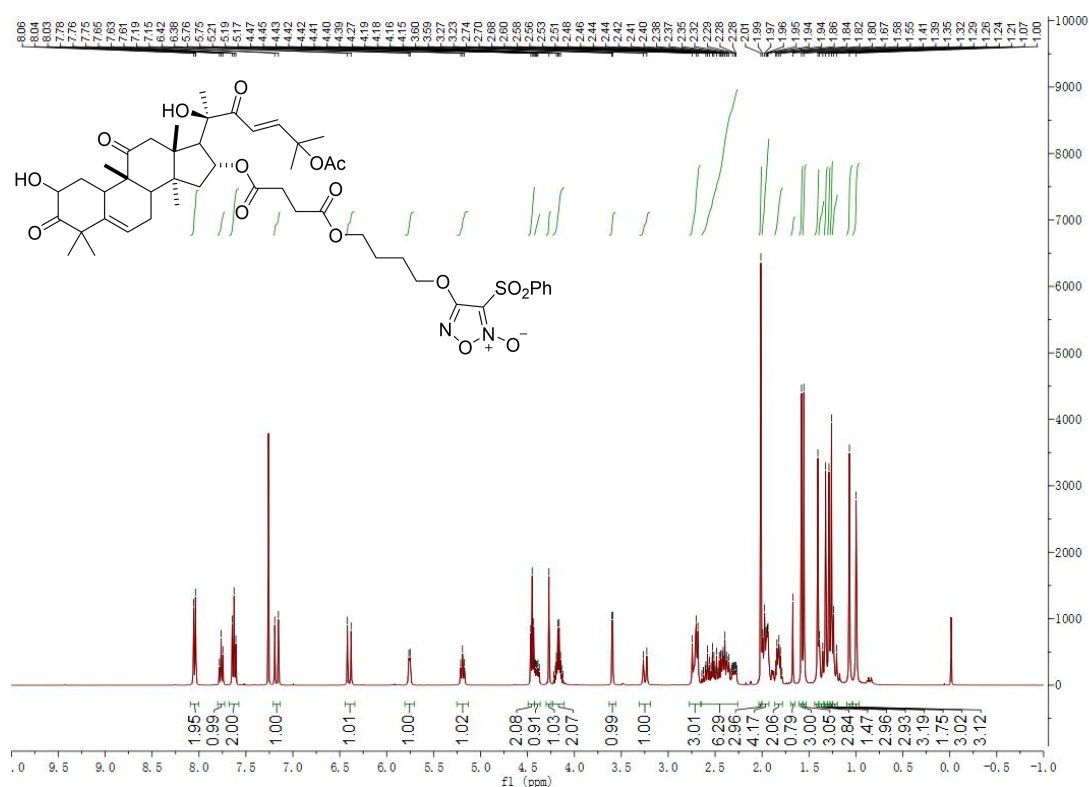
¹H NMR of compound 9c

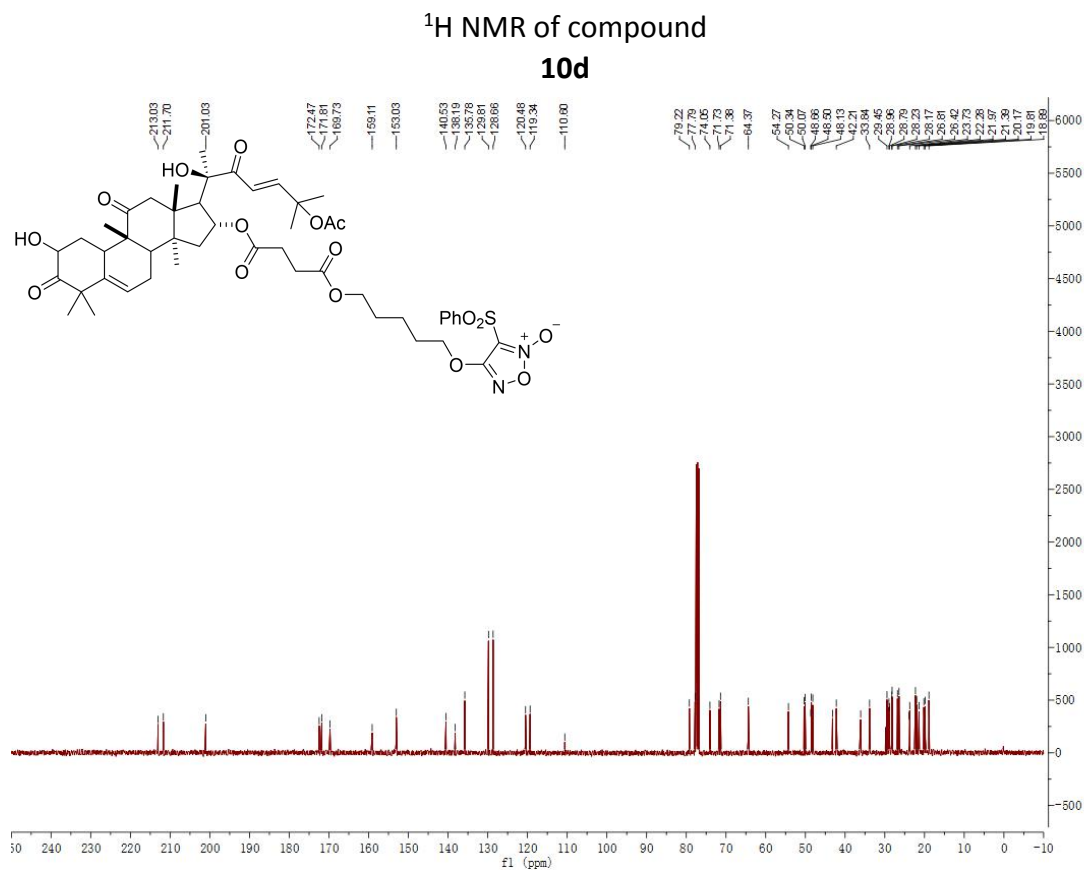
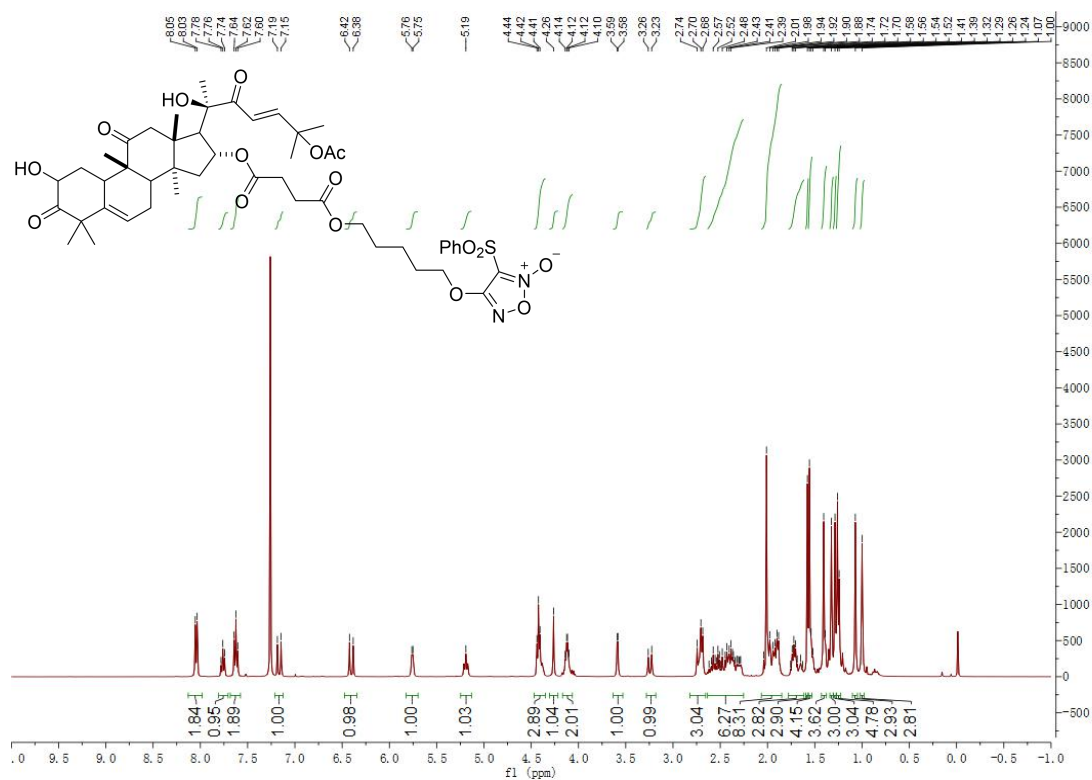


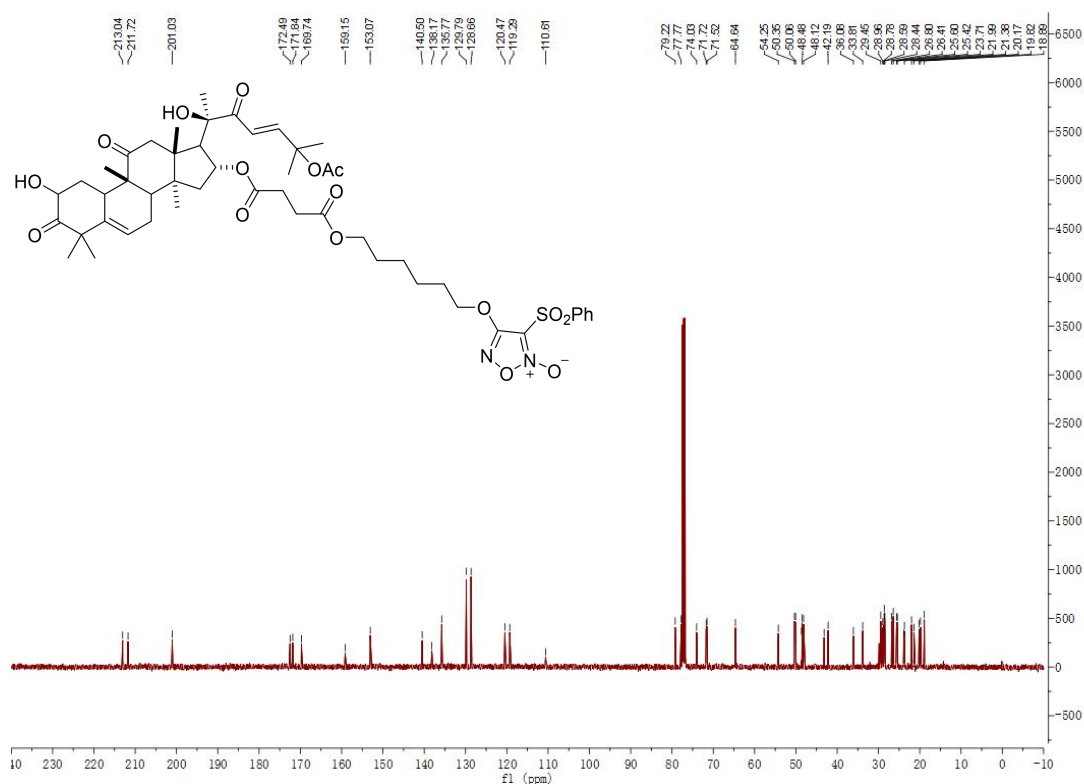
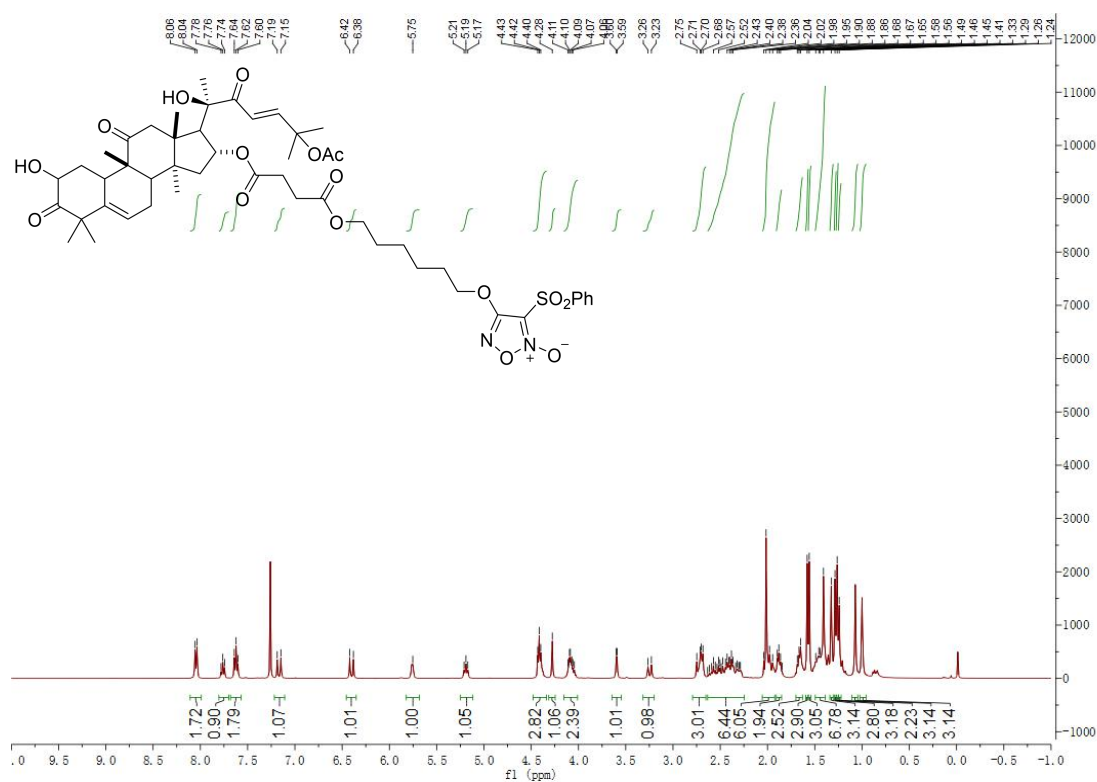
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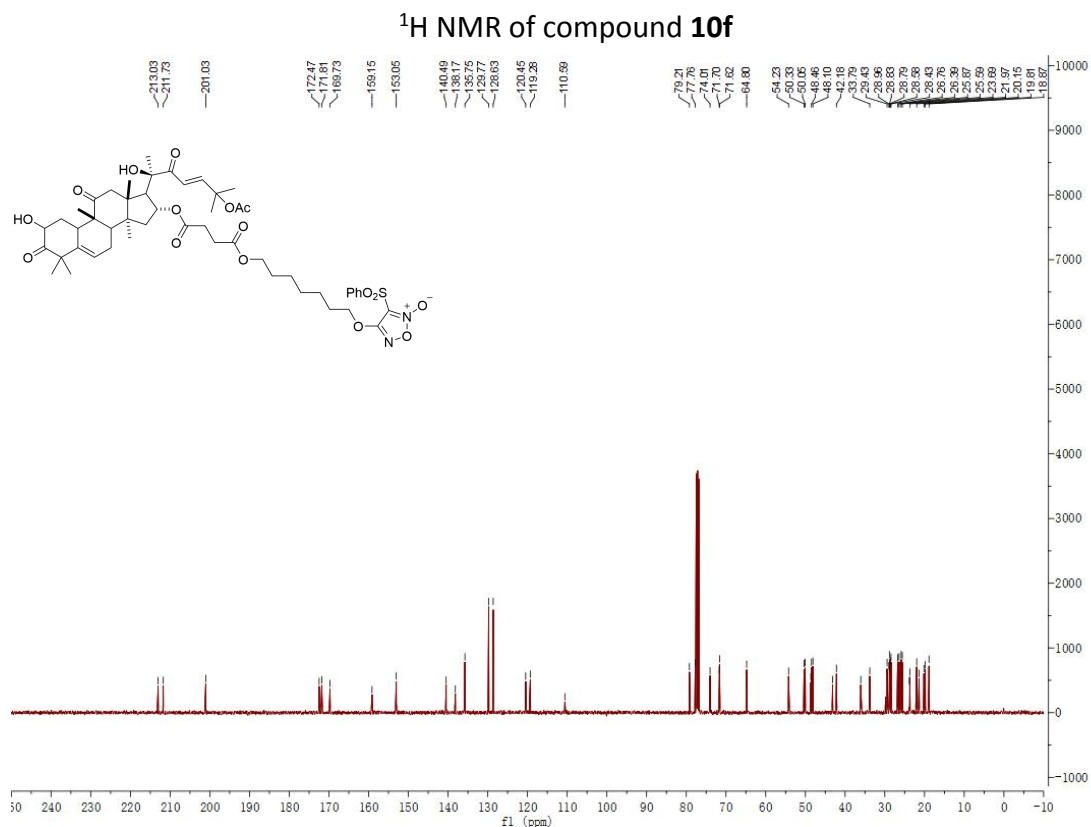
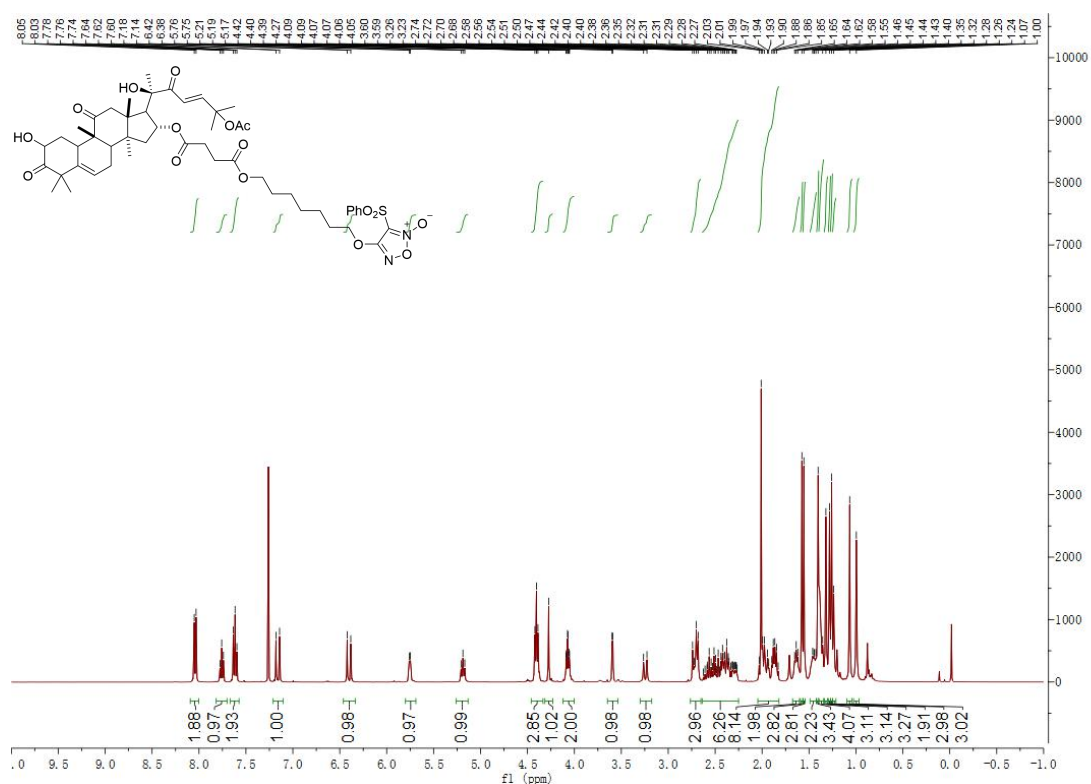


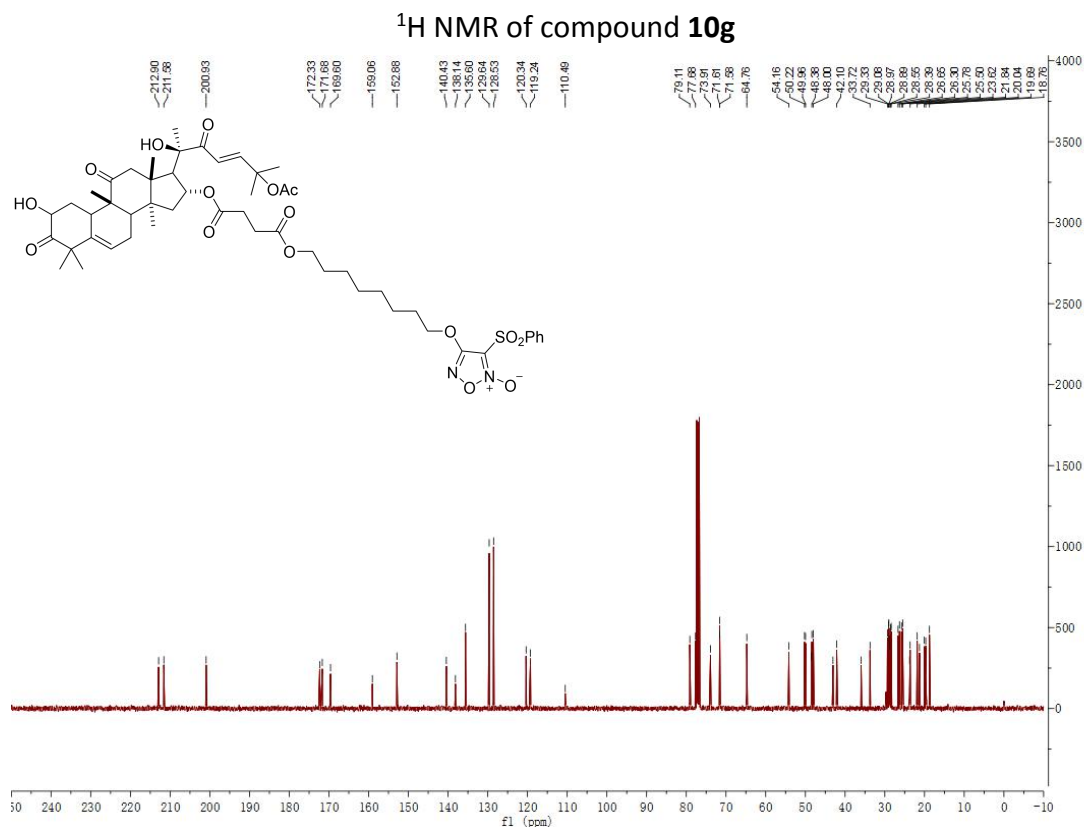
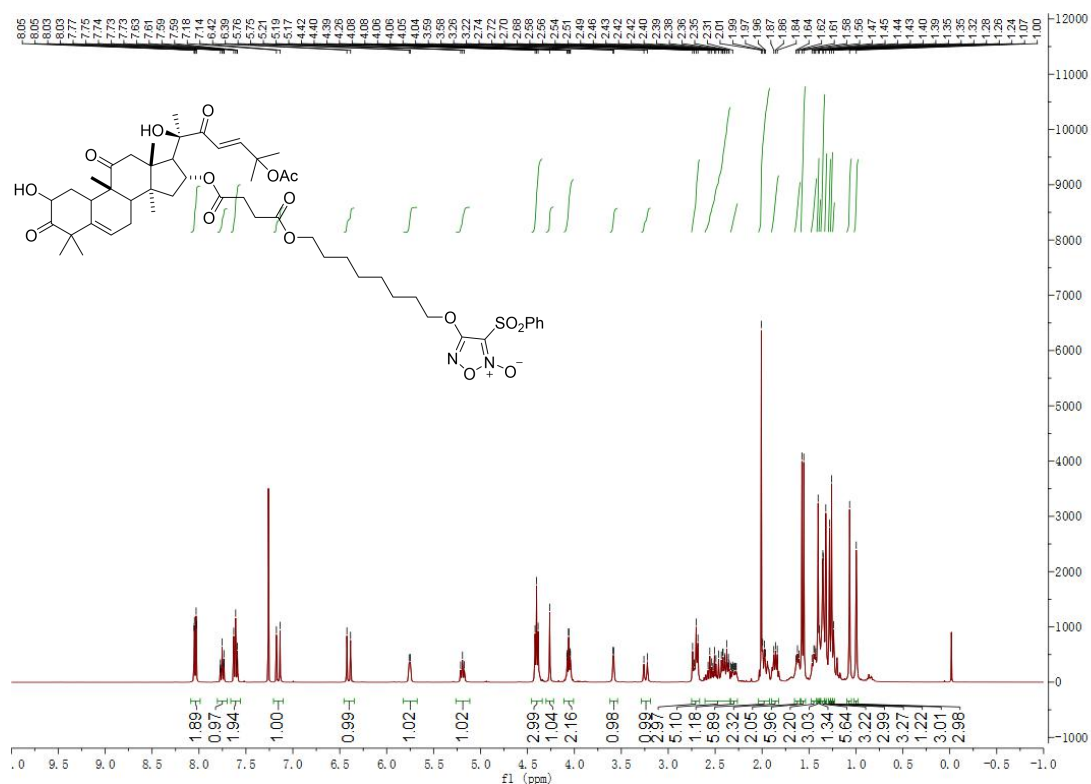


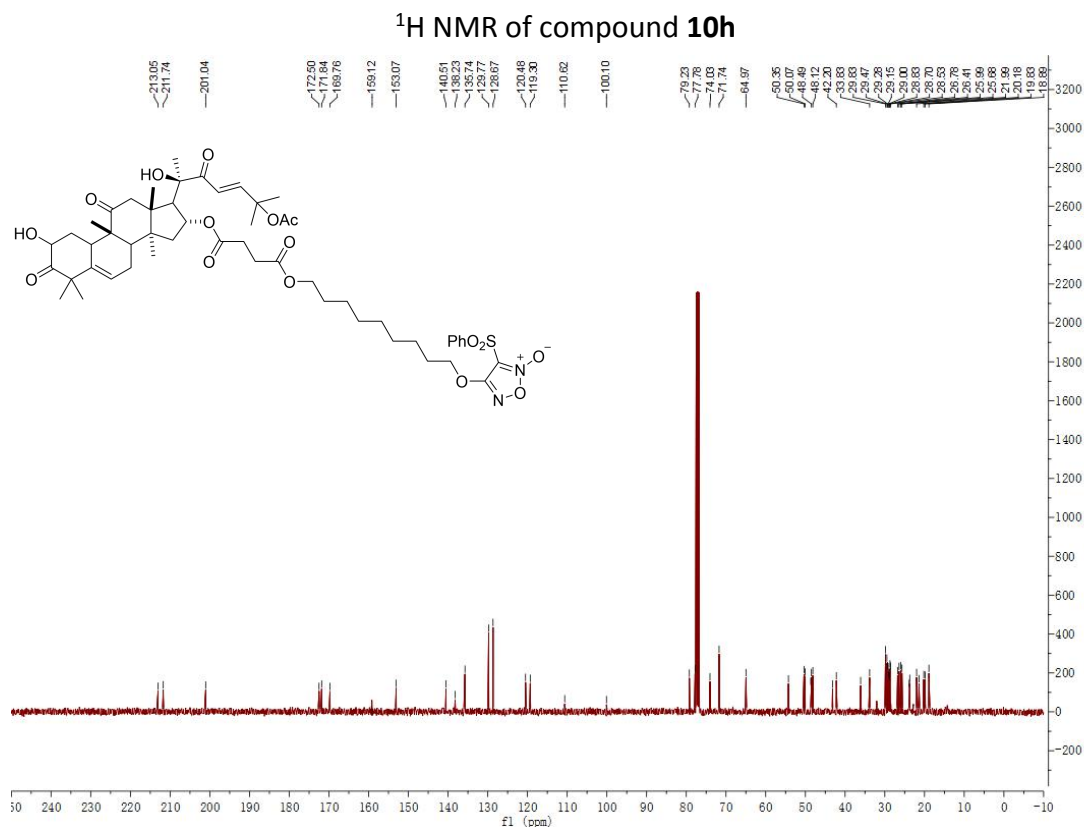
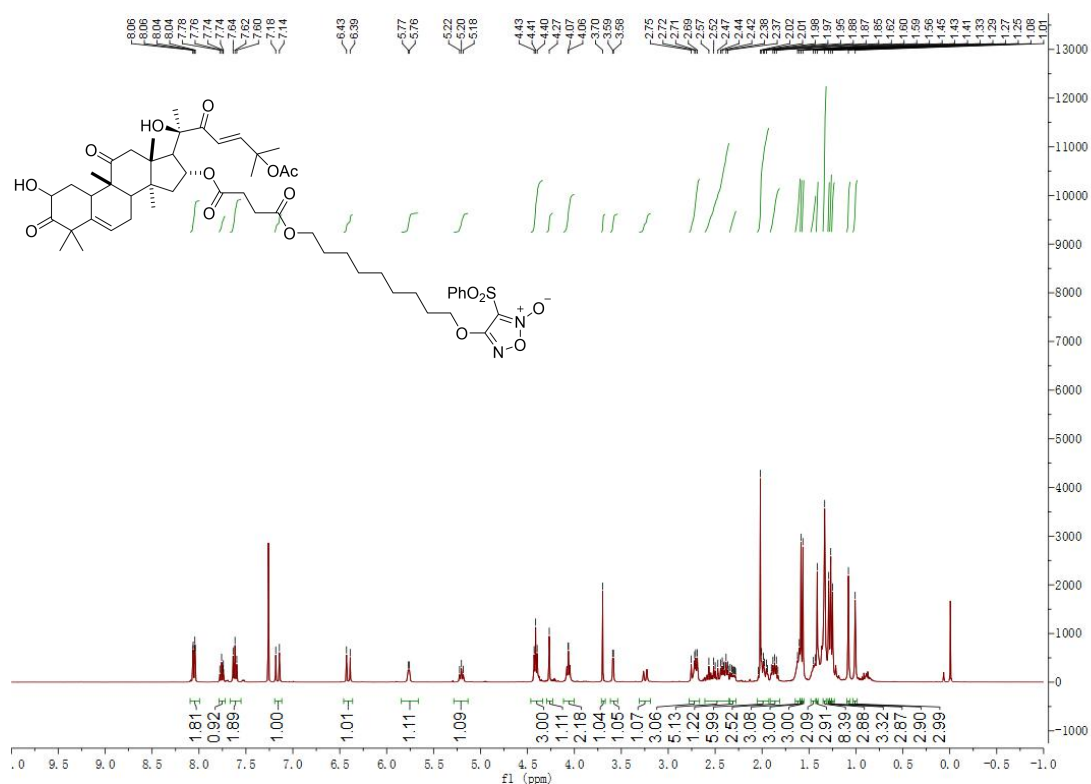


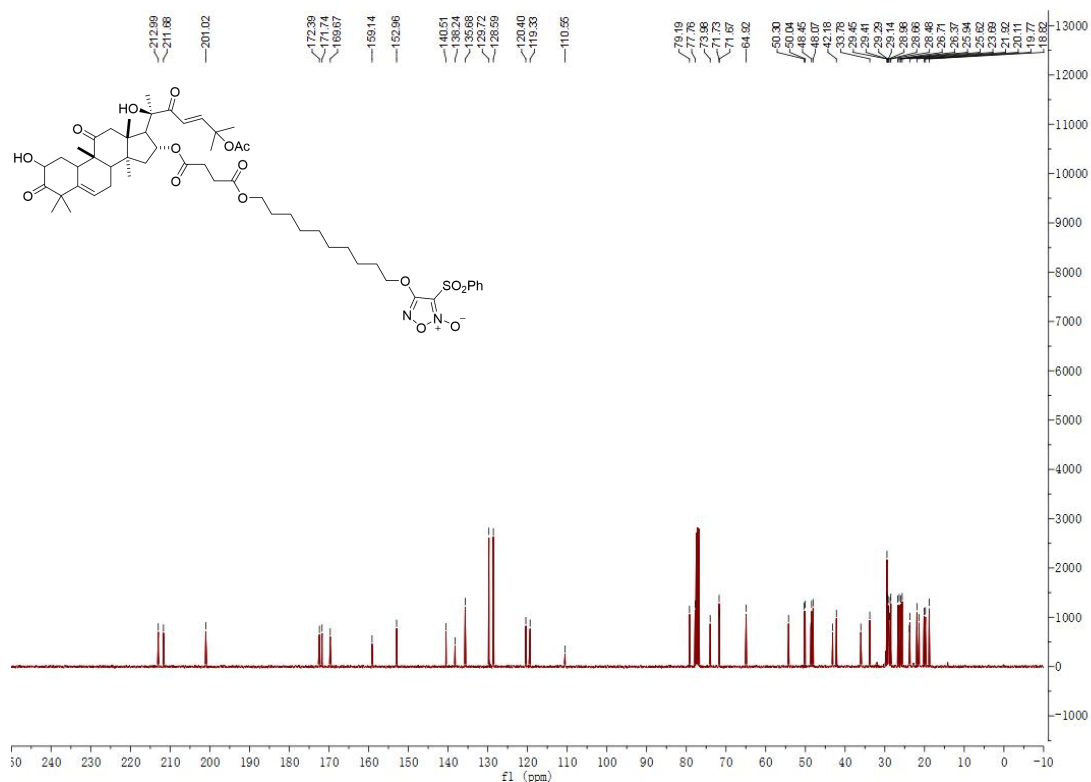
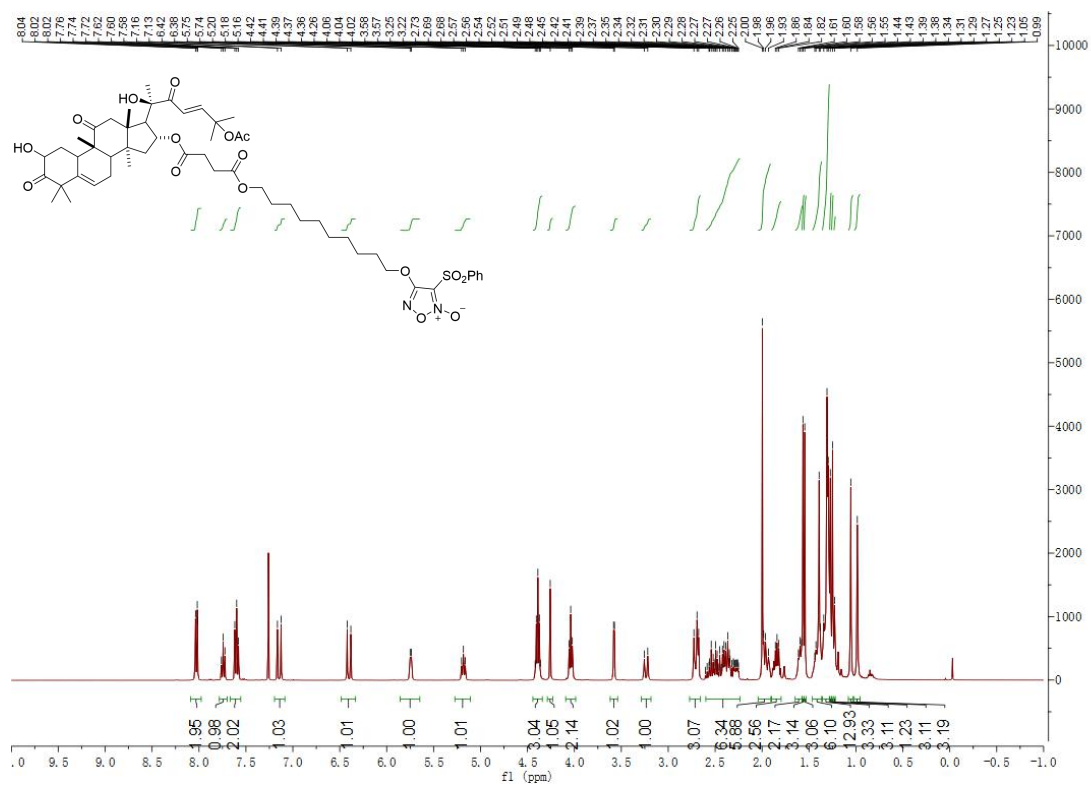


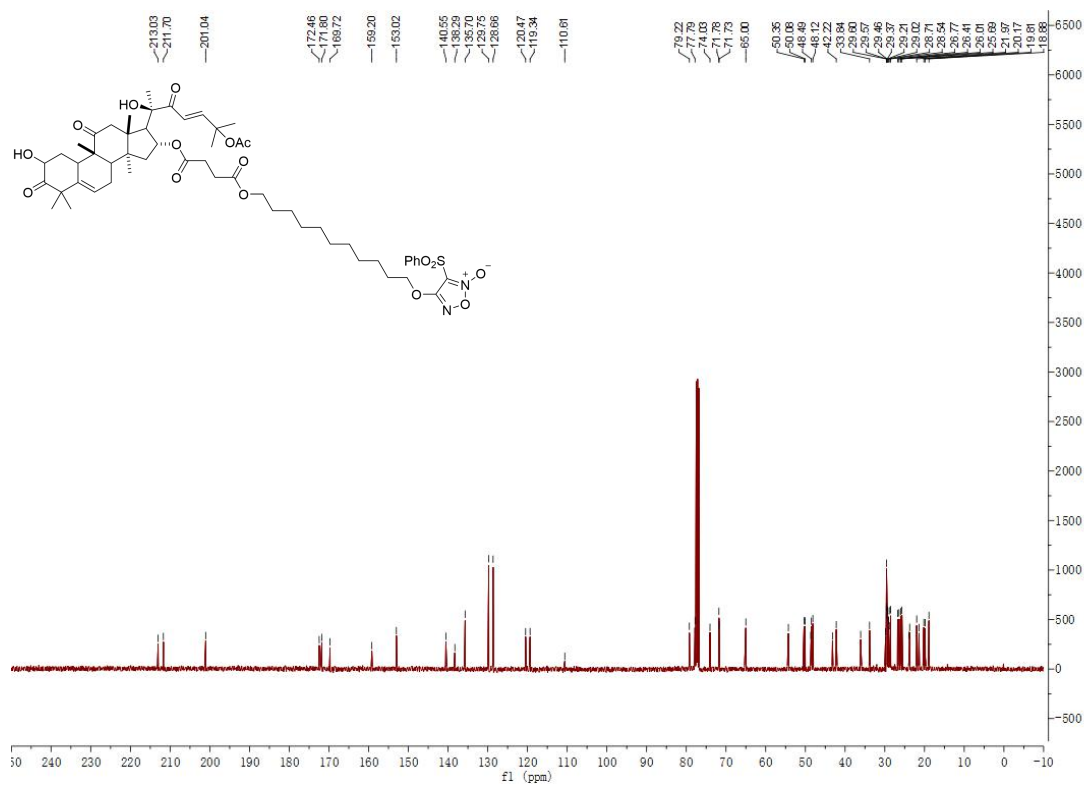
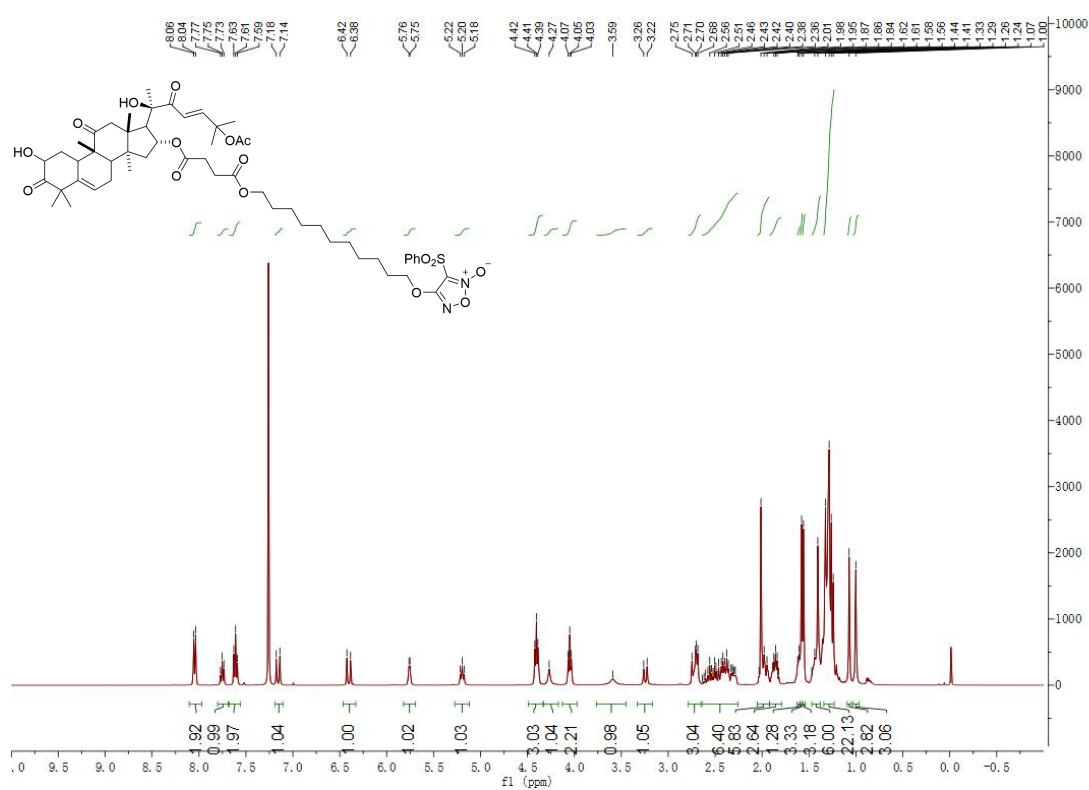


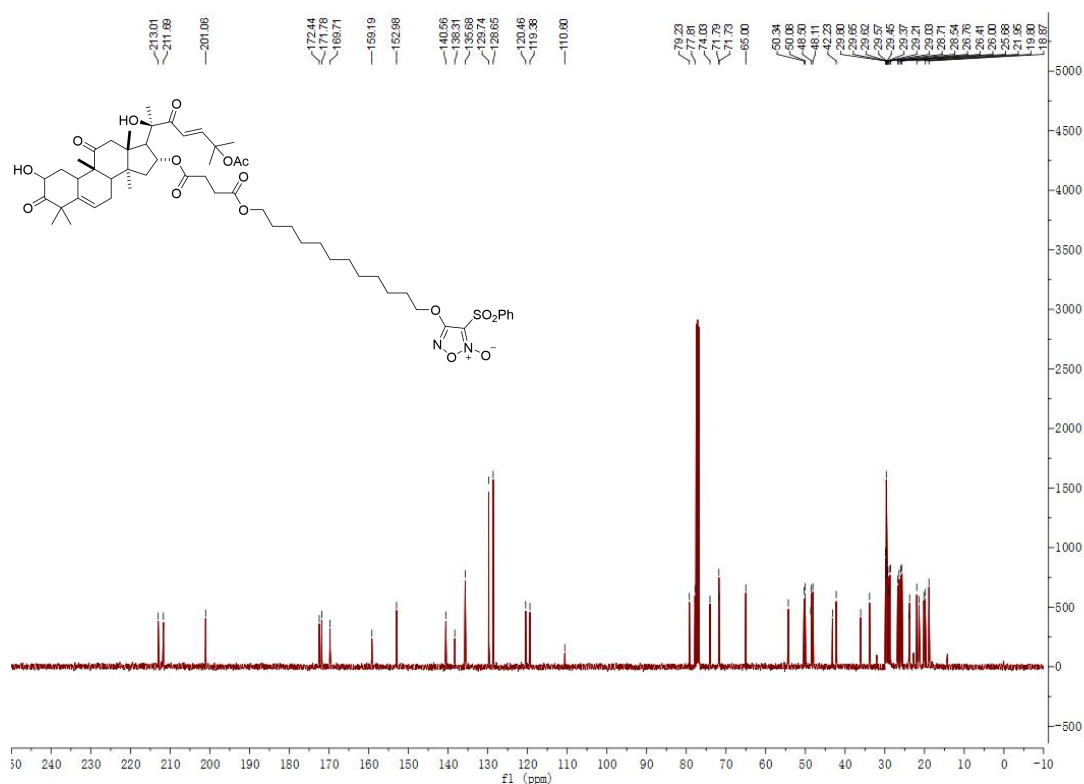
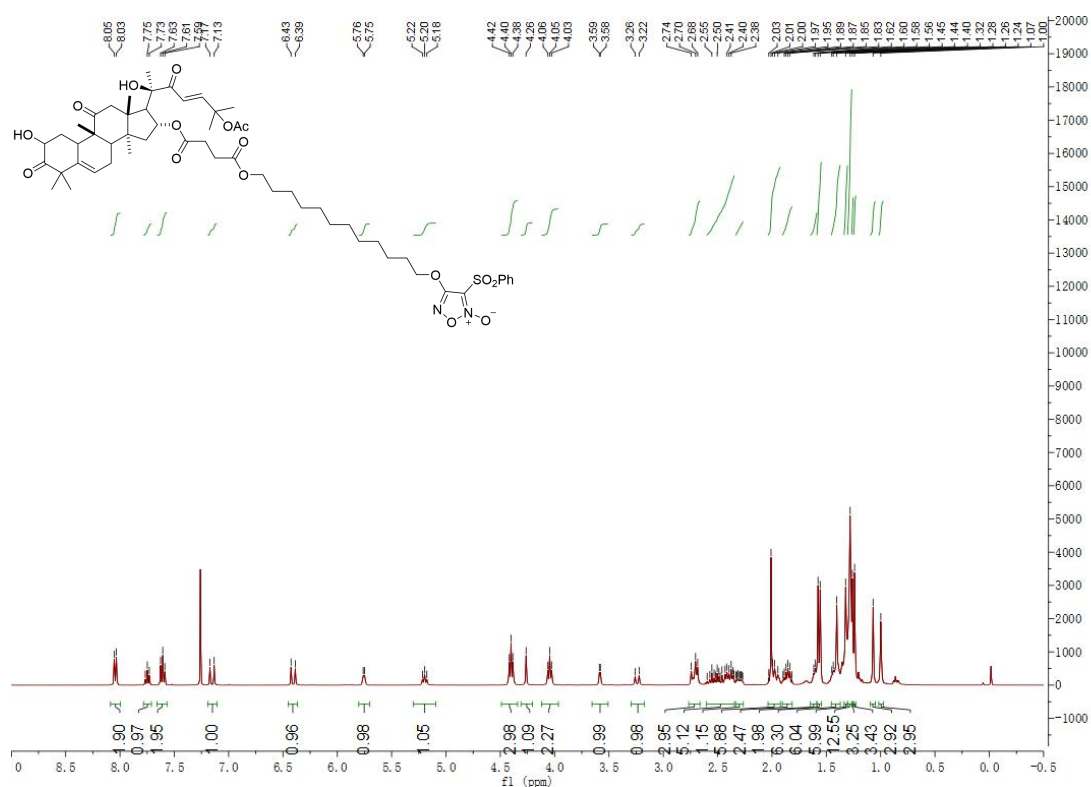


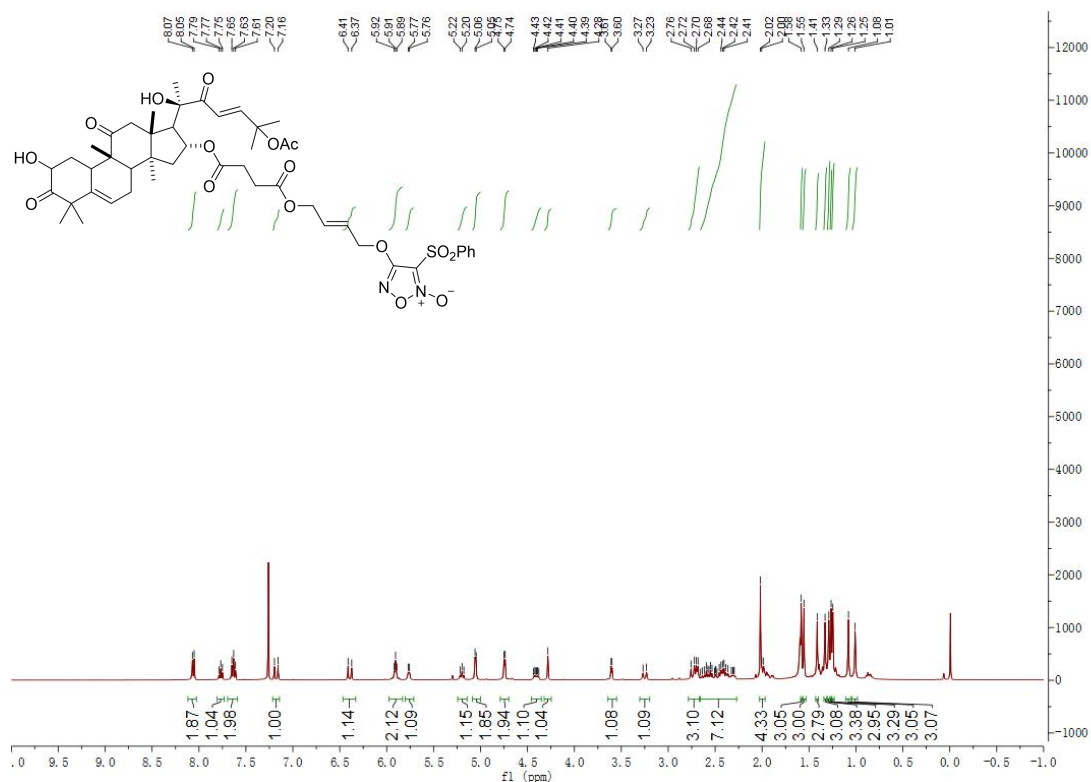




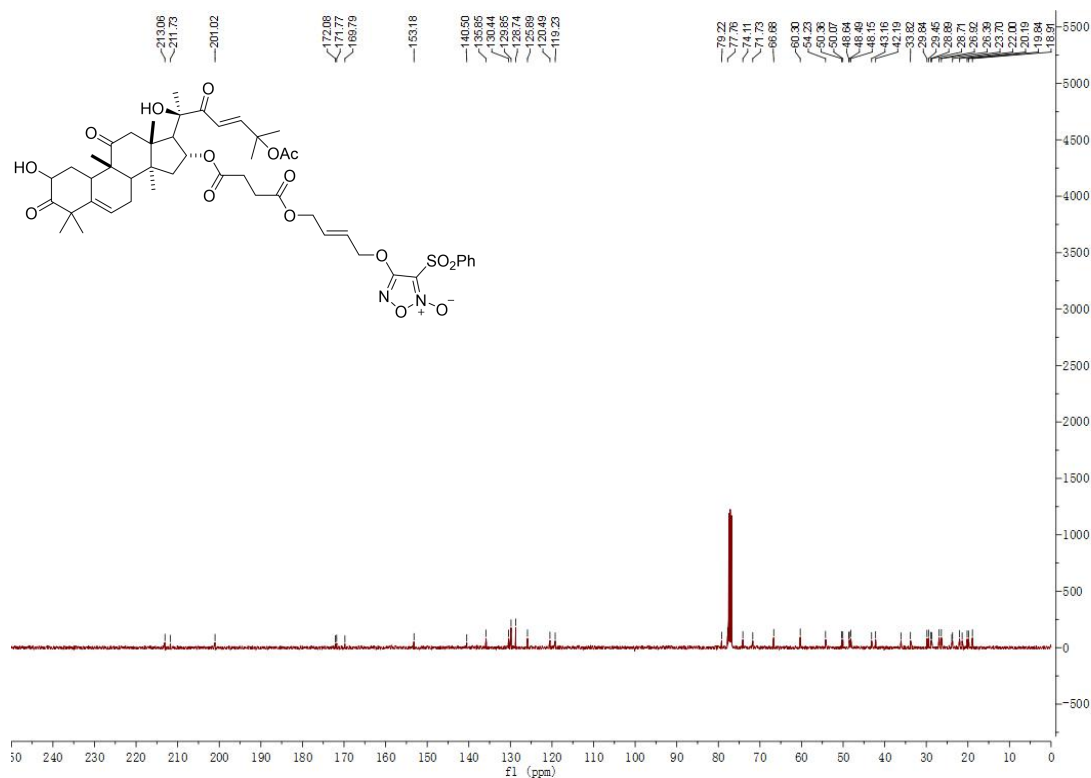




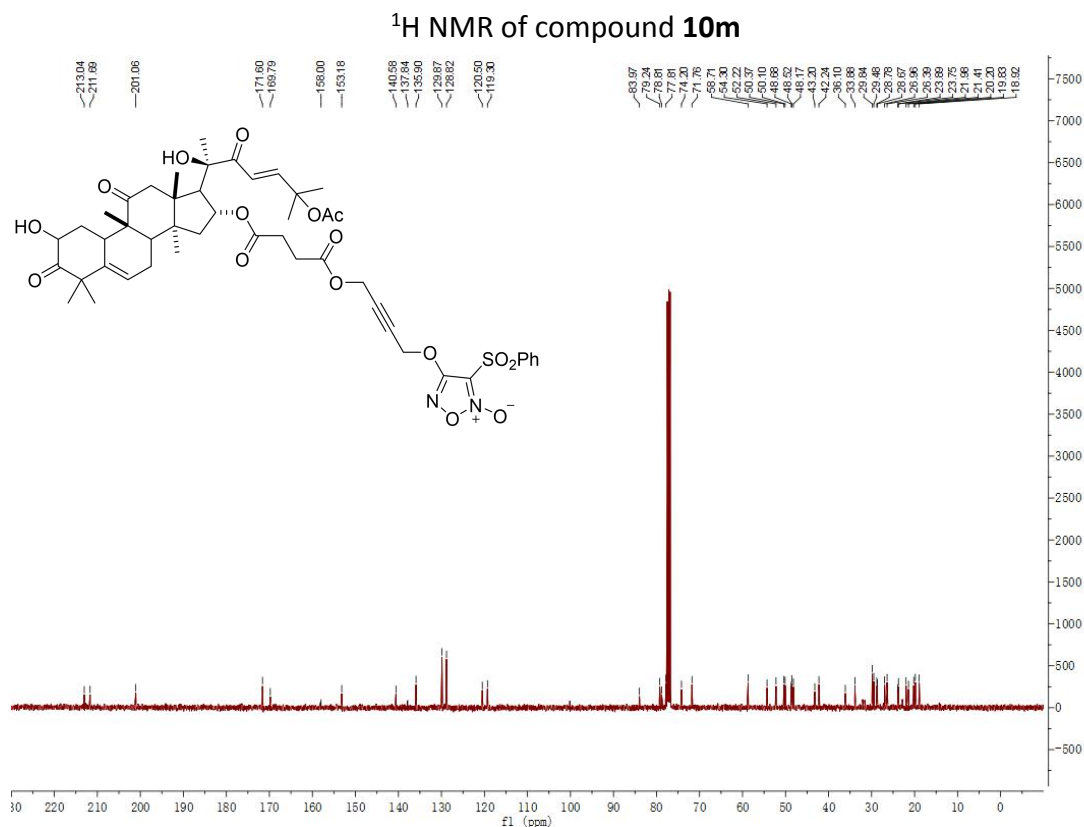
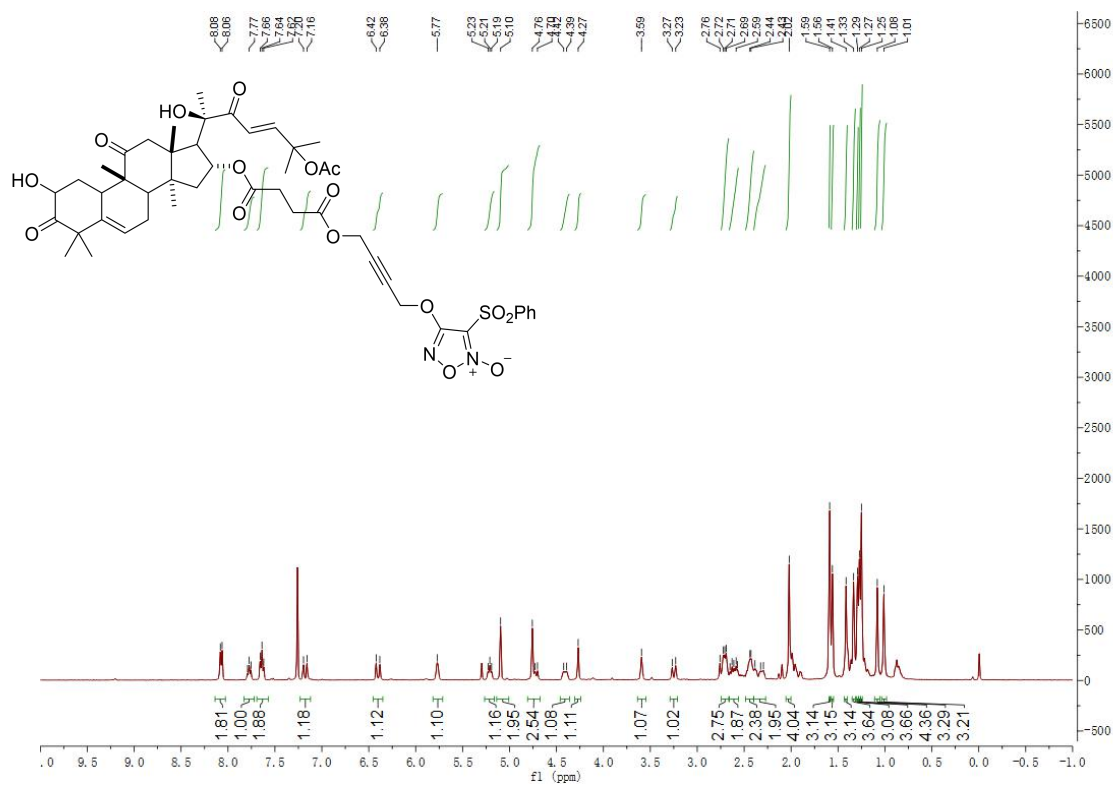


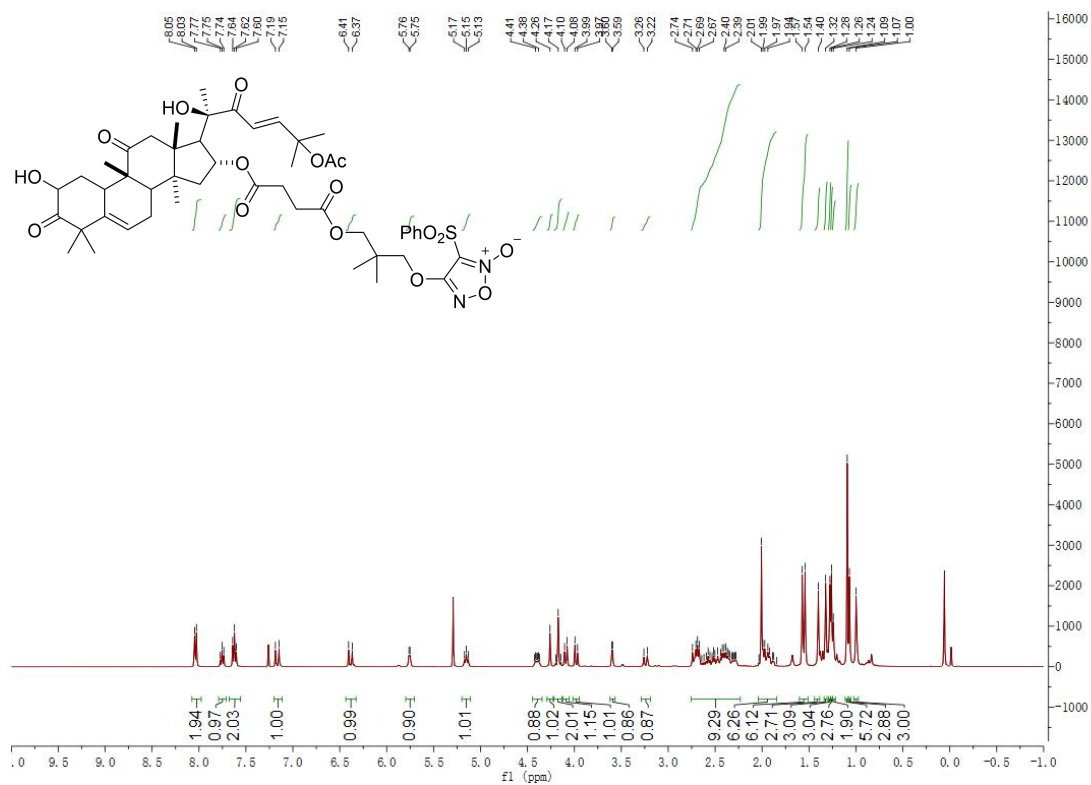


¹H NMR of compound 10I

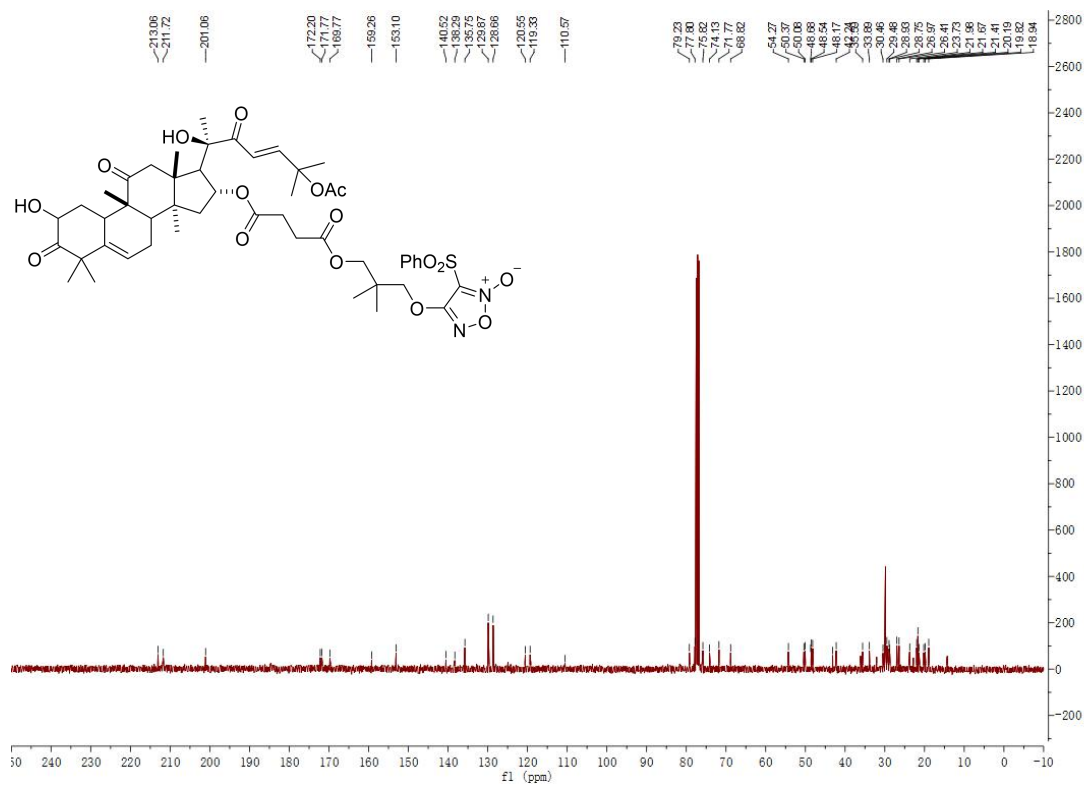


¹³C NMR of compound 10I

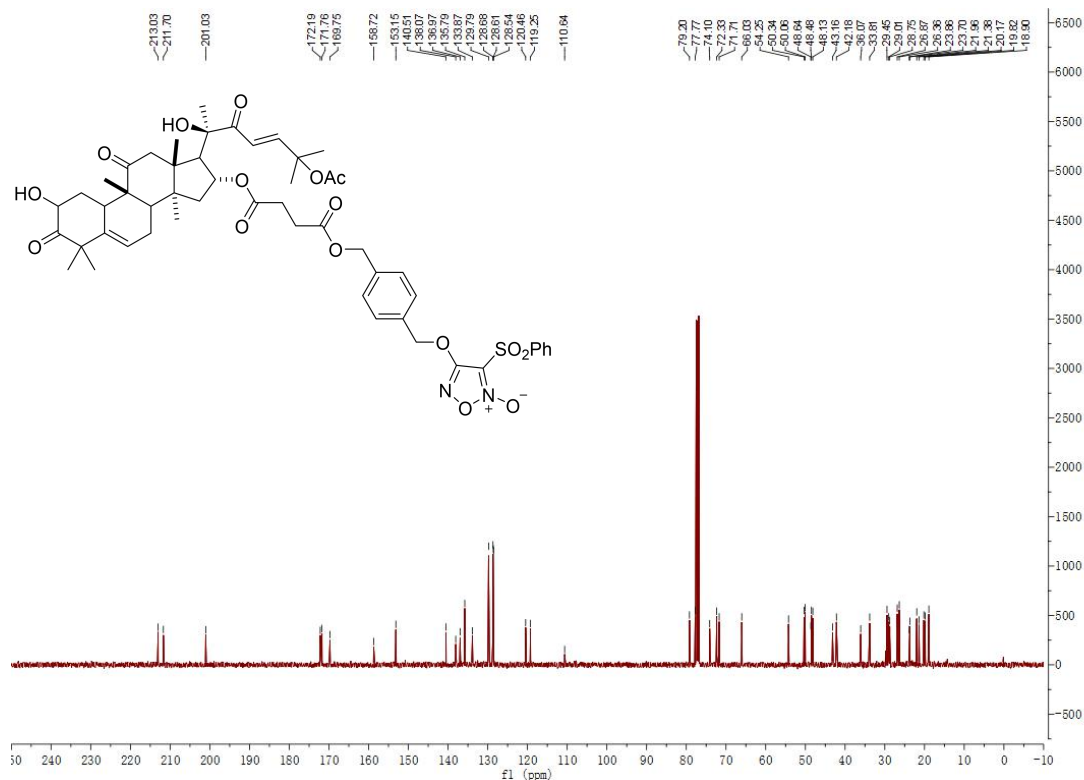
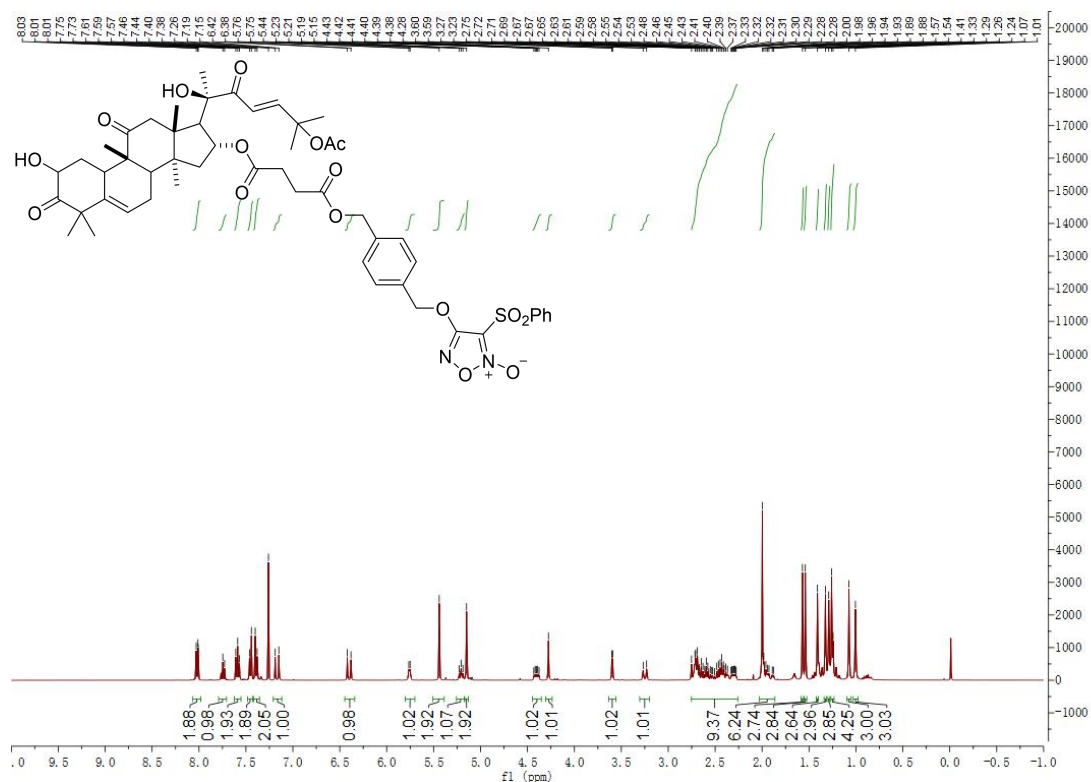


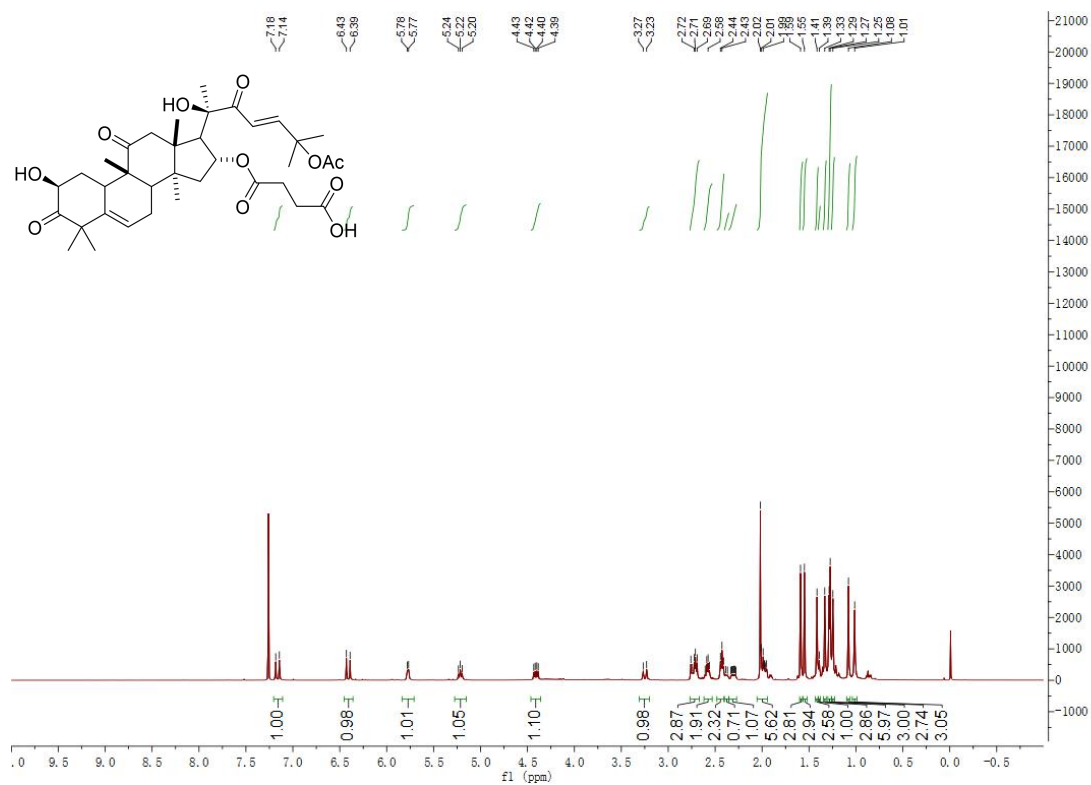


¹H NMR of compound 10n

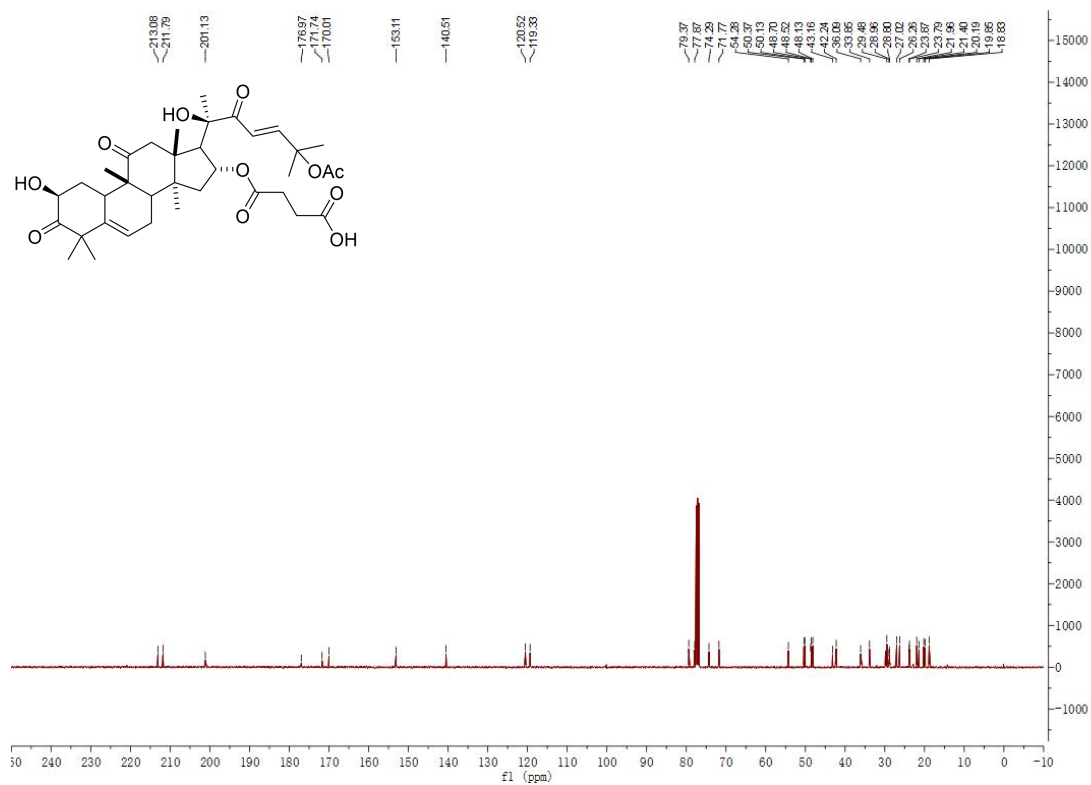


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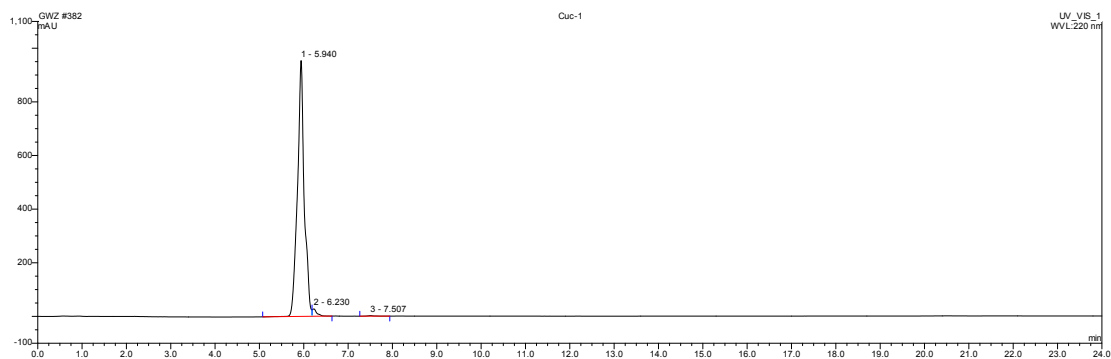




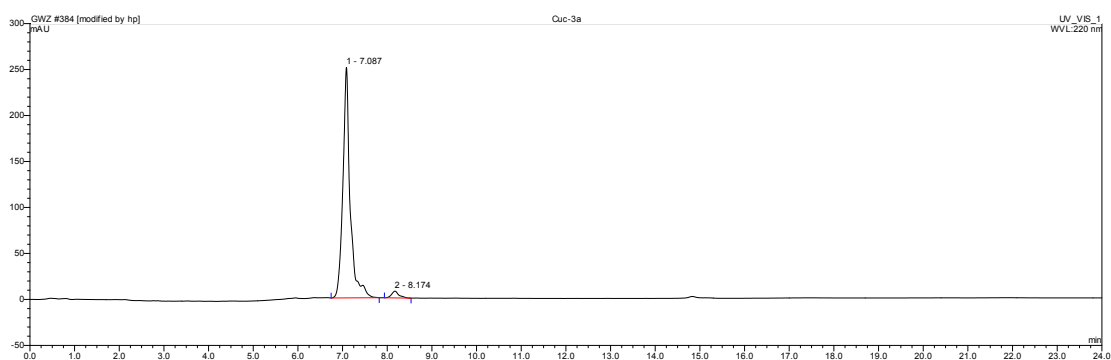
¹H NMR of compound 11



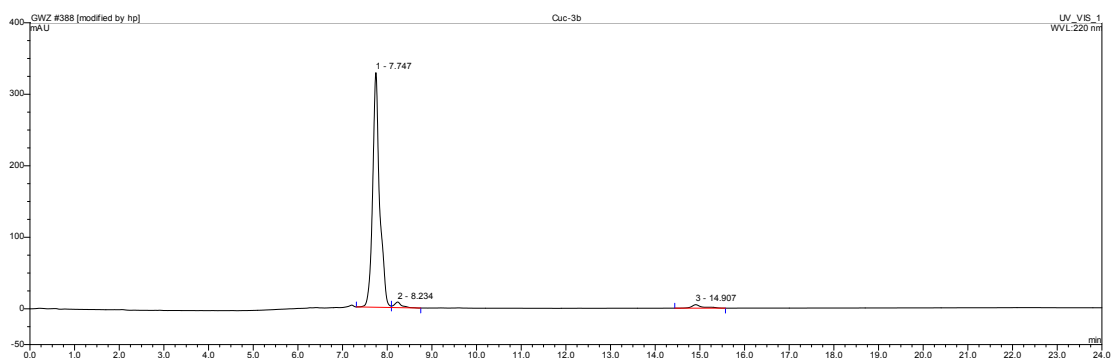
¹³C NMR of compound 11



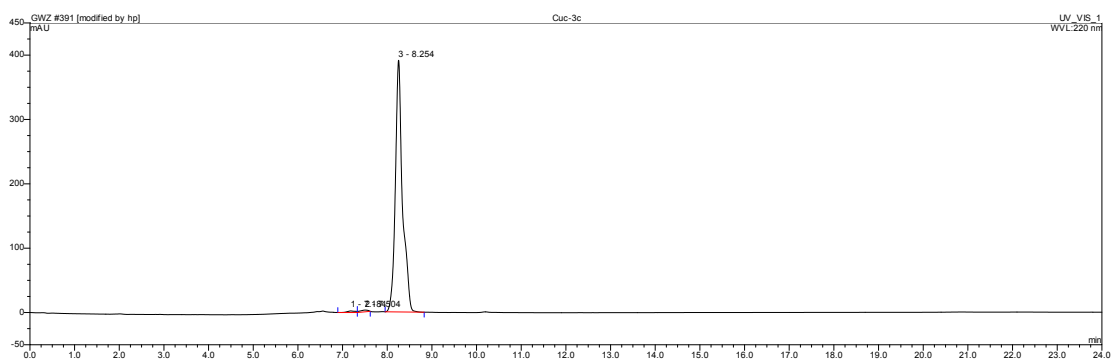
Compound 1



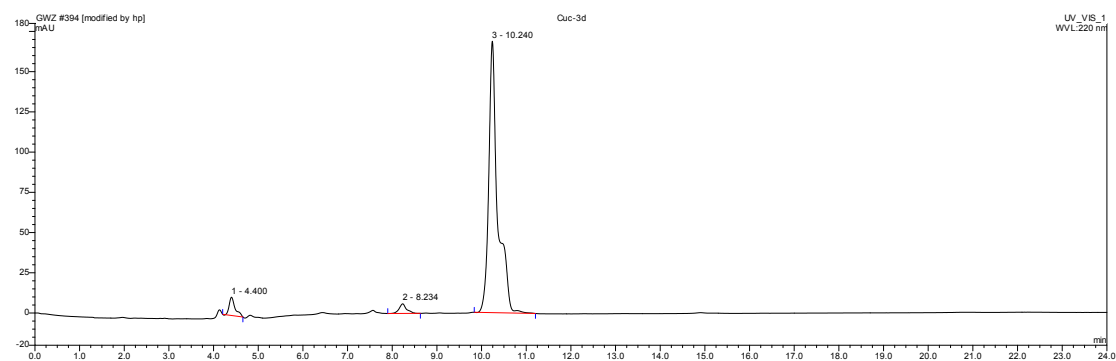
Compound 3a



Compound 3b

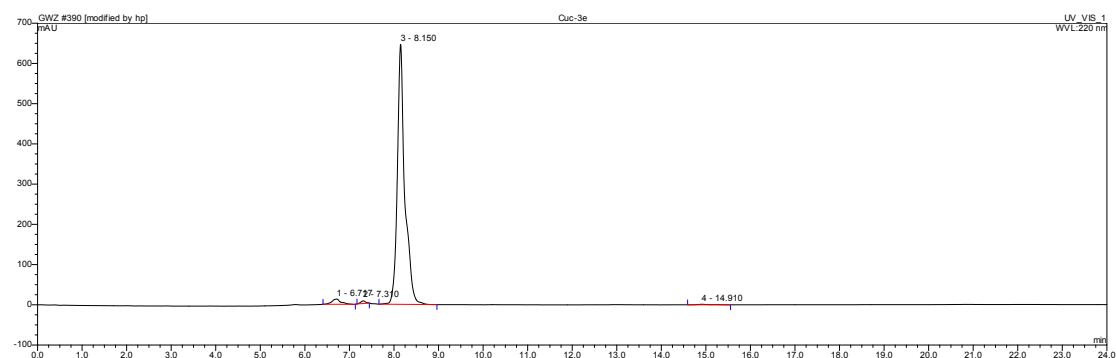


Compound 3c

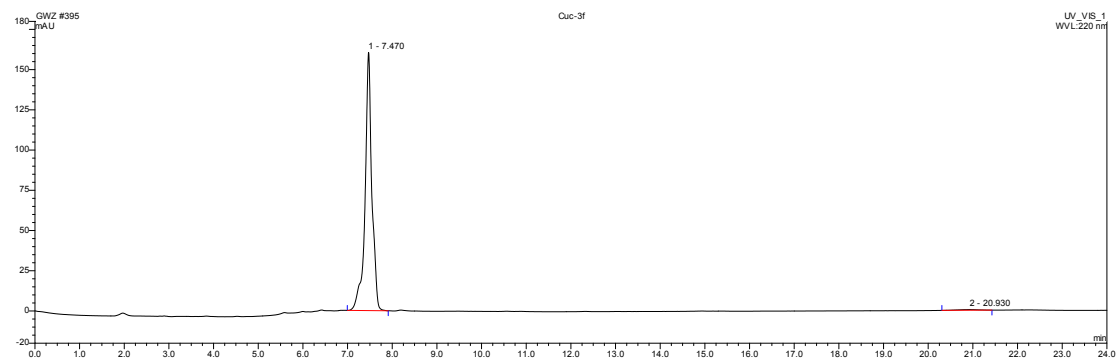


Compound

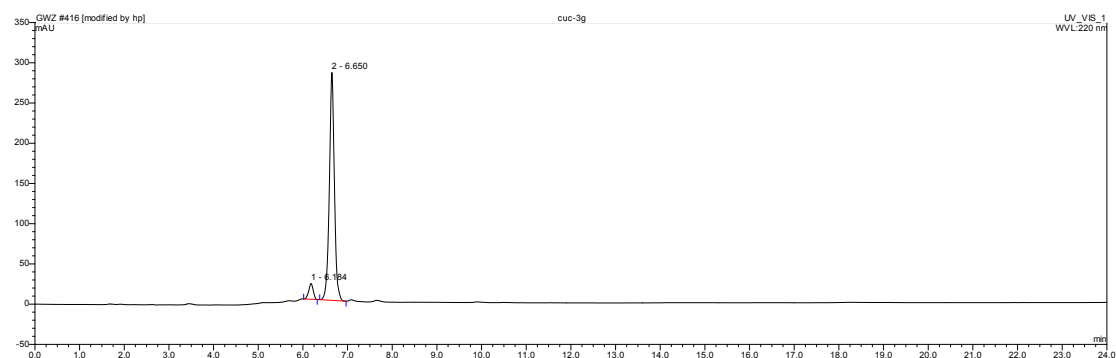
3d



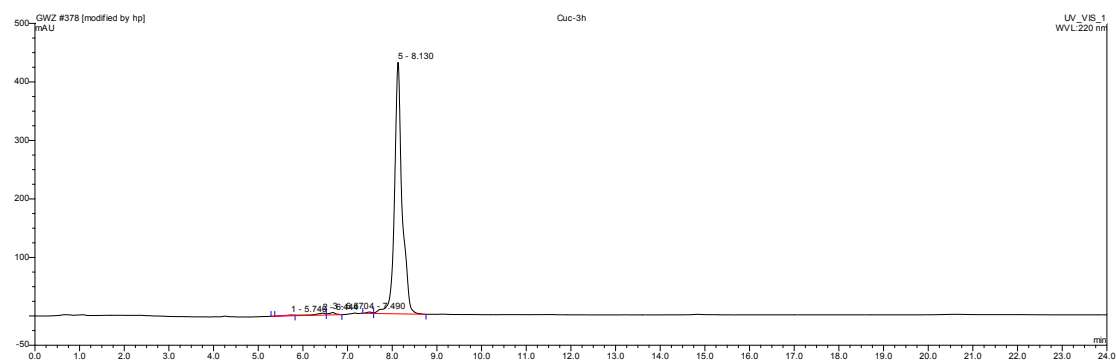
Compound **3e**



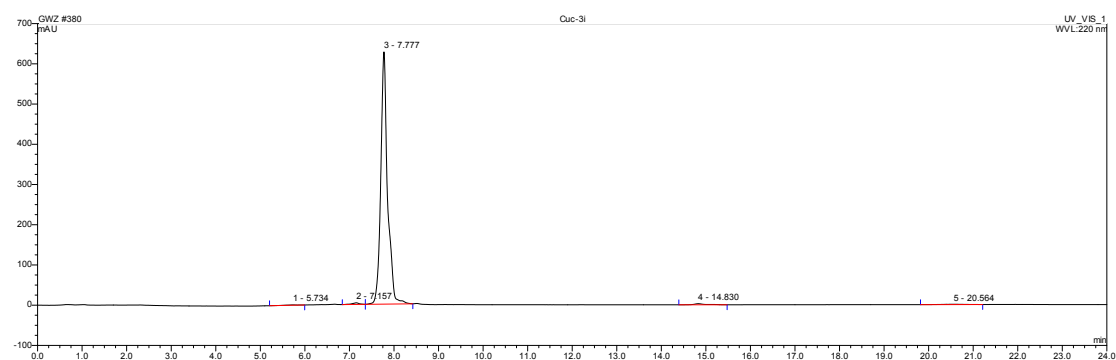
Compound **3f**



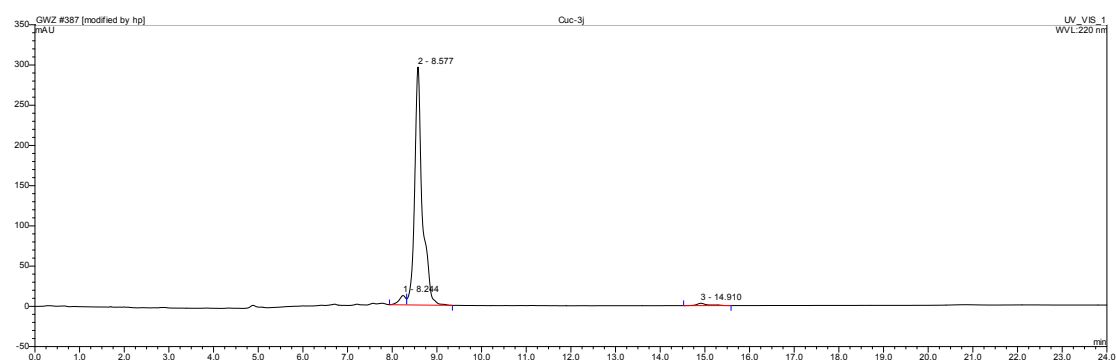
Compound **3g**



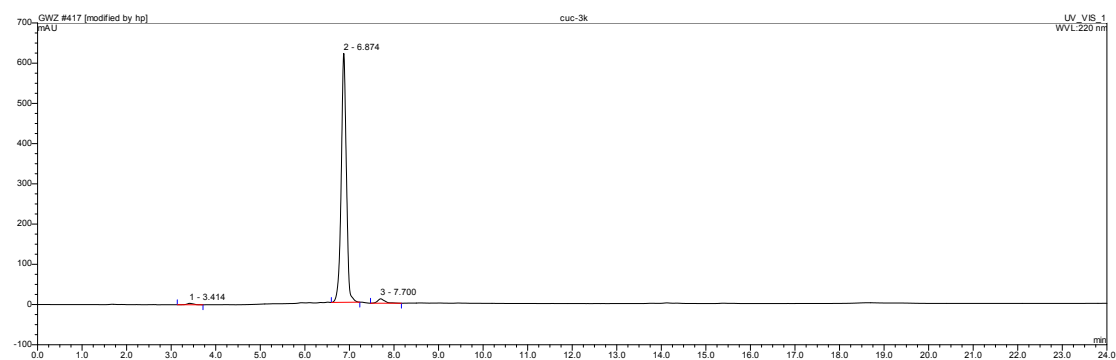
Compound 3h



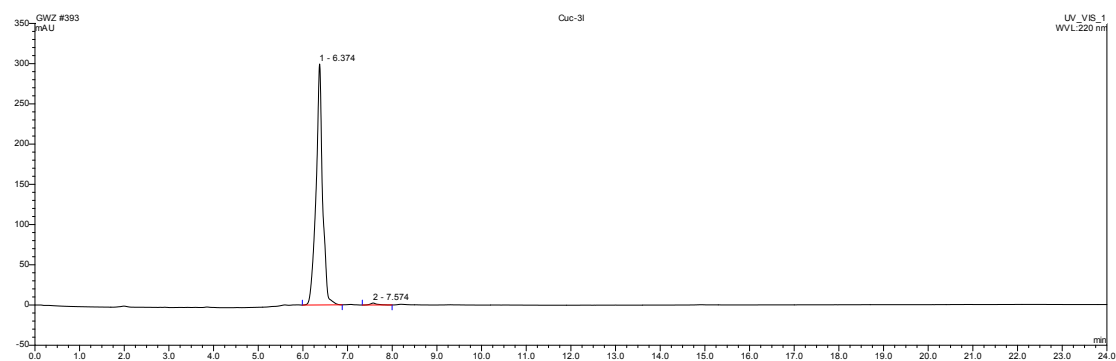
Compound 3i



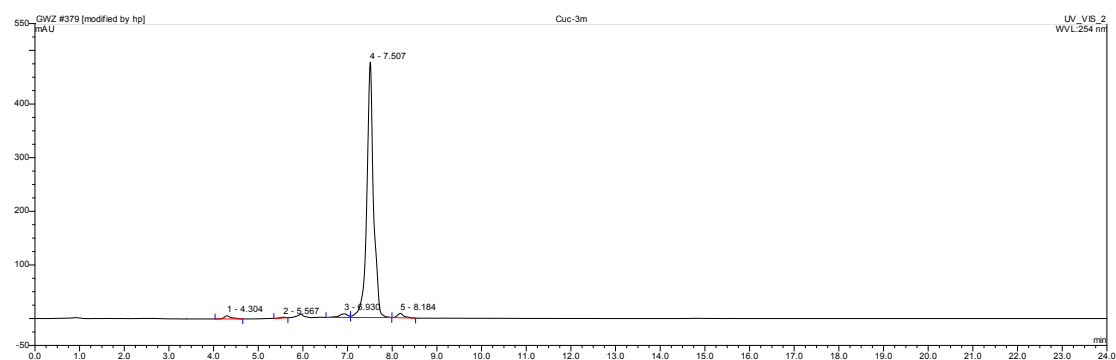
Compound 3j



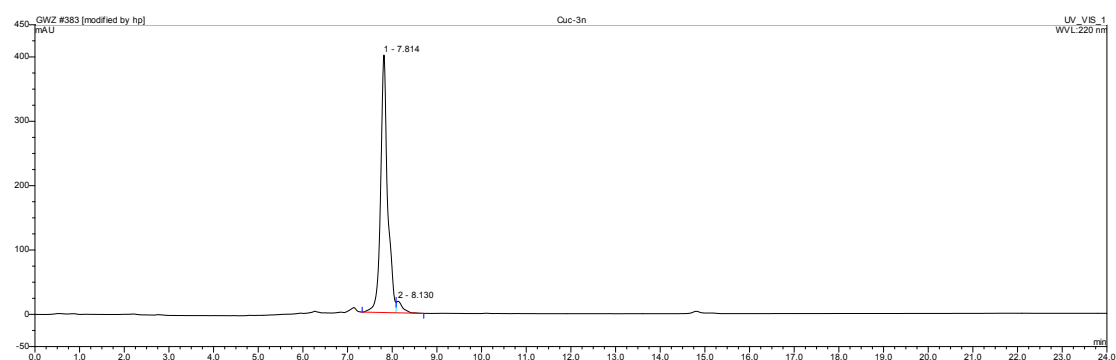
Compound 3k



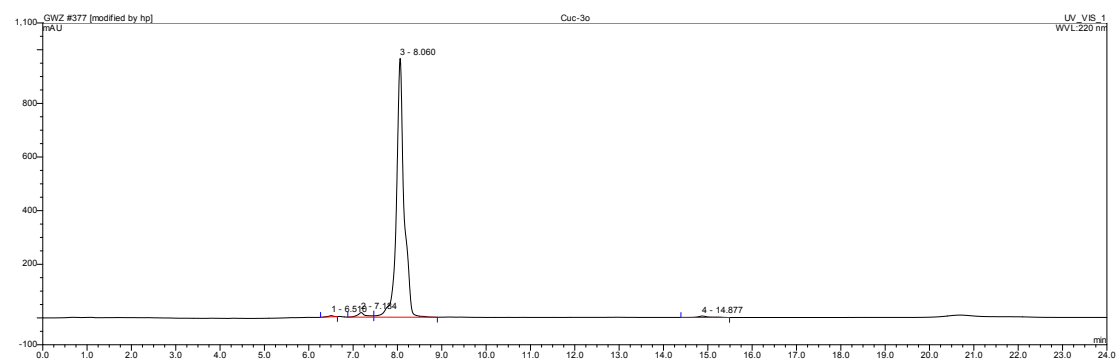
Compound 3I



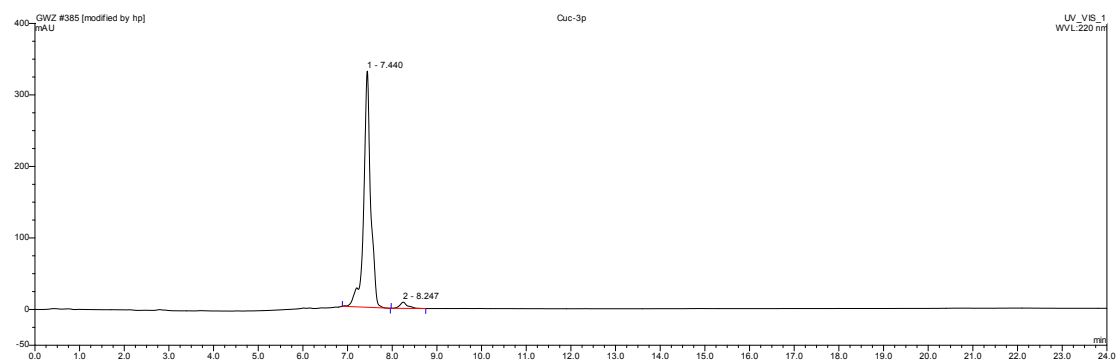
Compound 3m



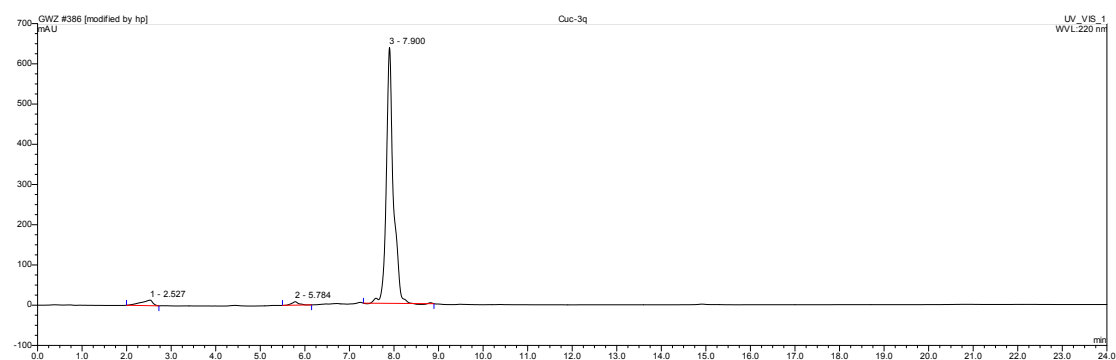
Compound 3n



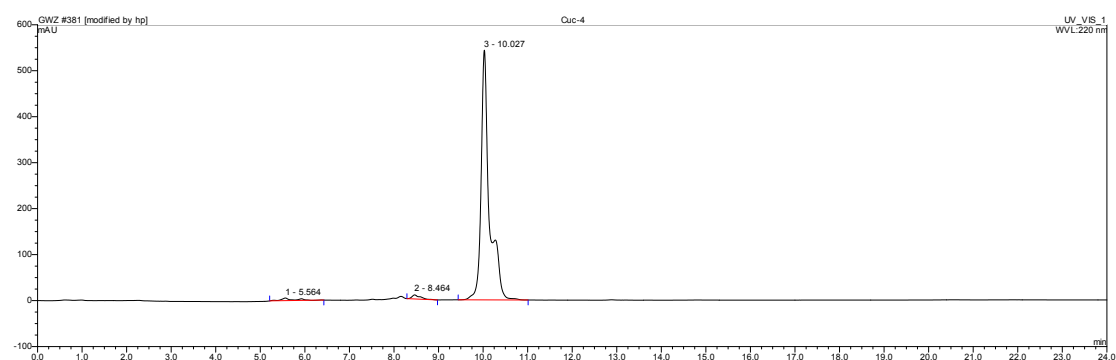
Compound 3o



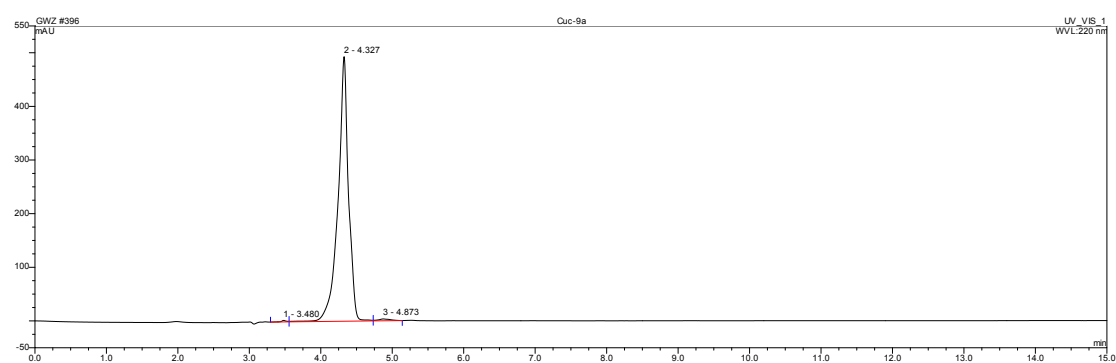
Compound 3p



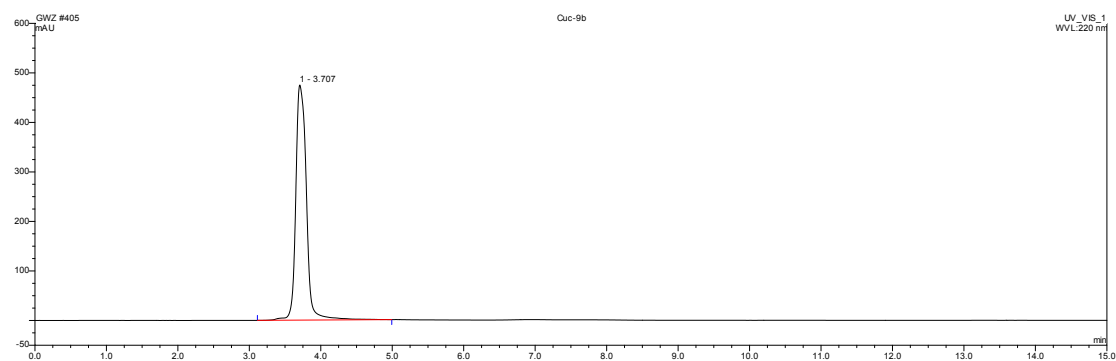
Compound 3q



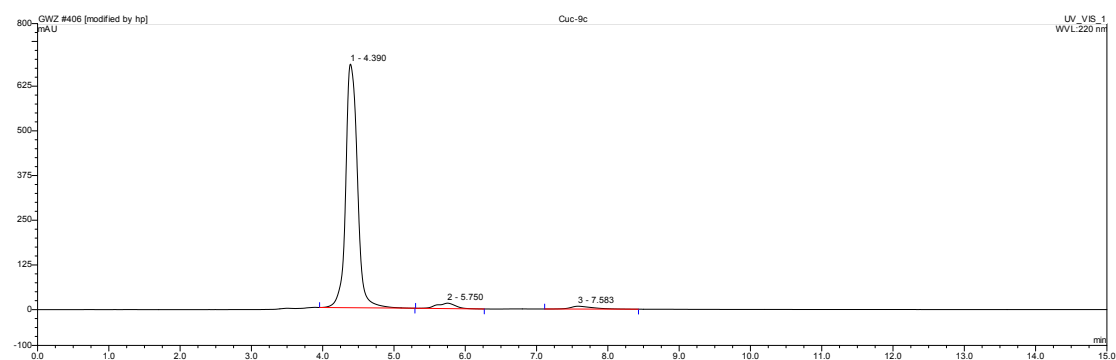
Compound 4



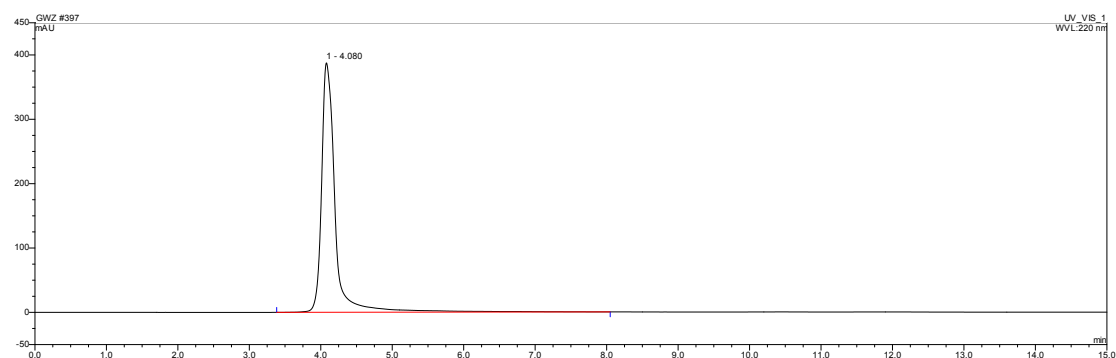
Compound 9a



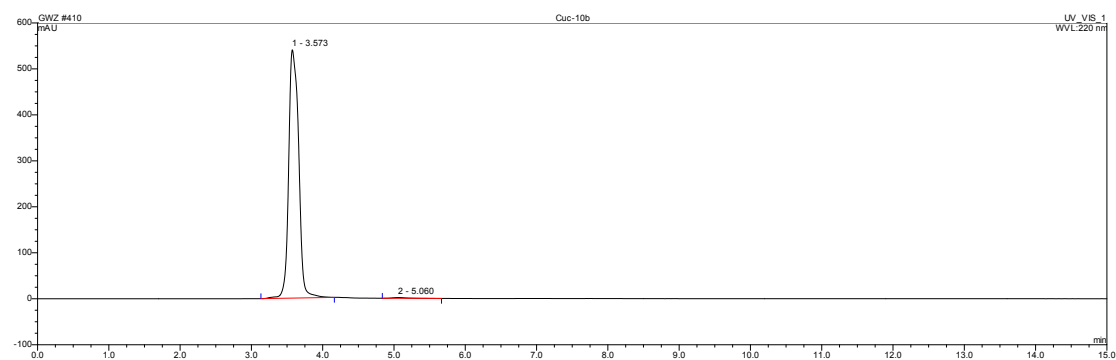
Compound 9b



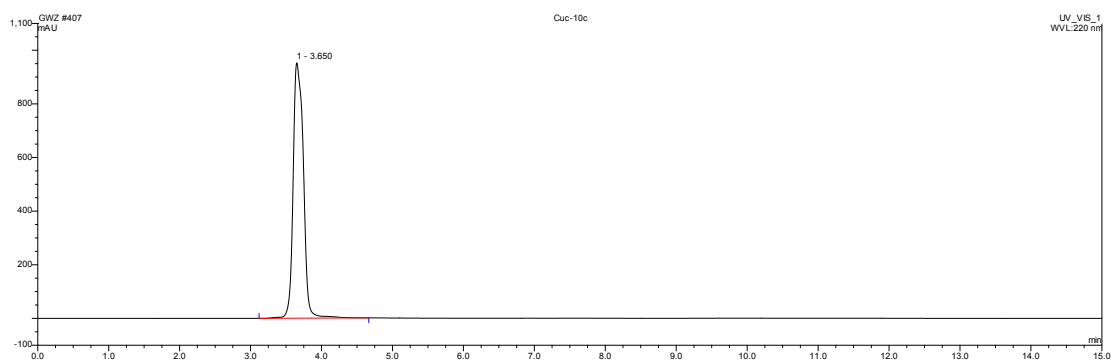
Compound 9c



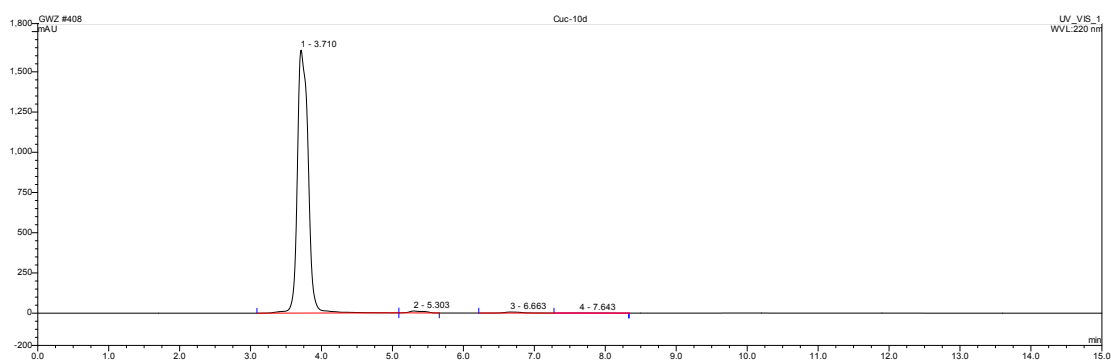
Compound 10a



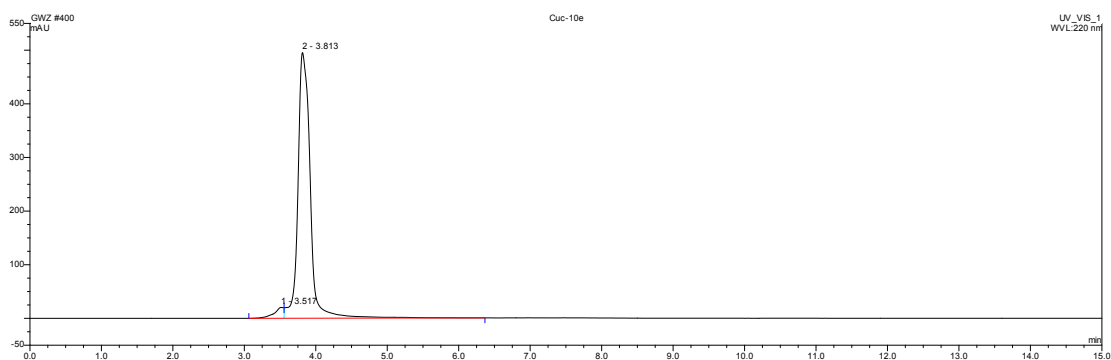
Compound 10b



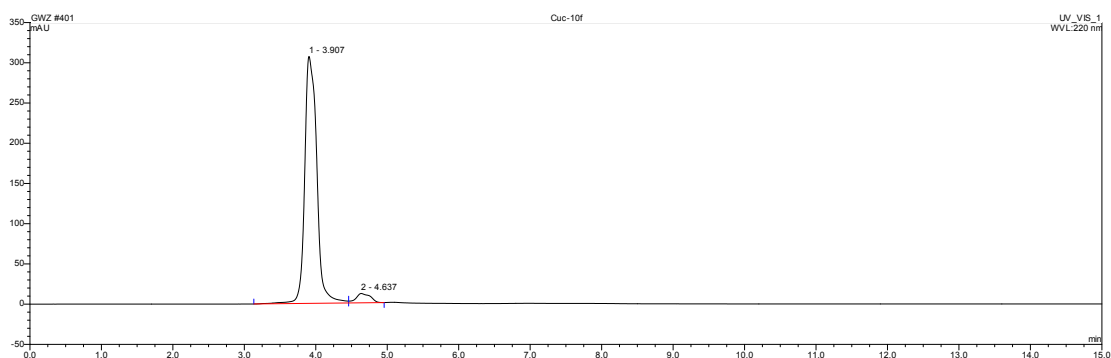
Compound 10c



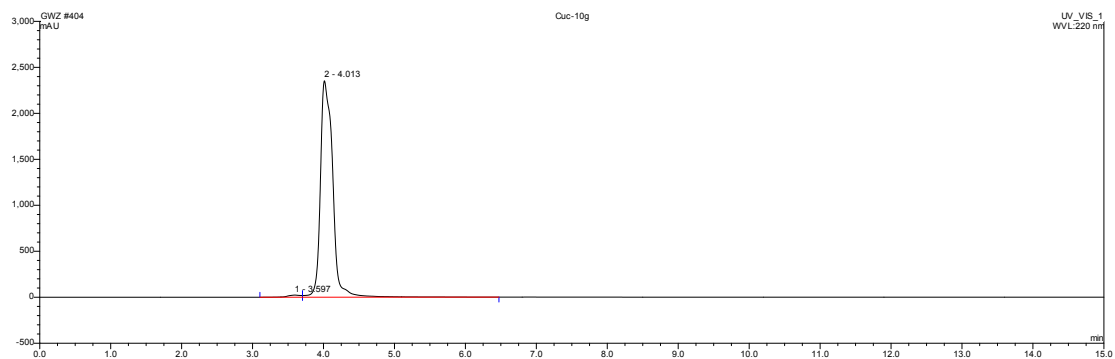
Compound 10d



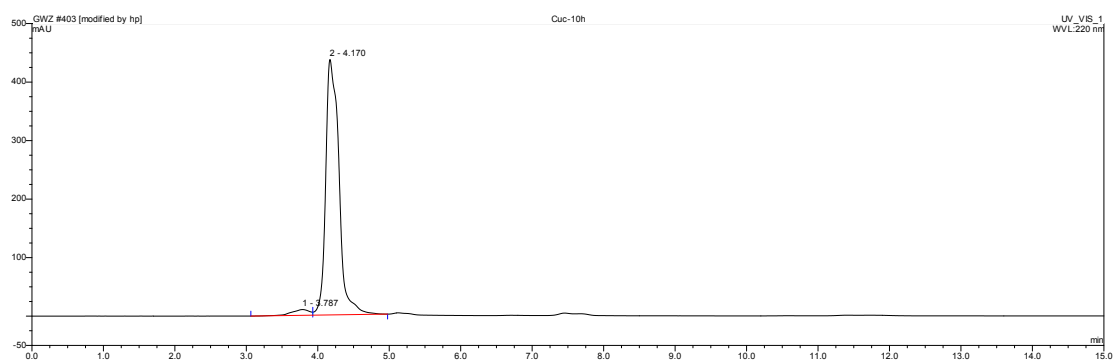
Compound 10e



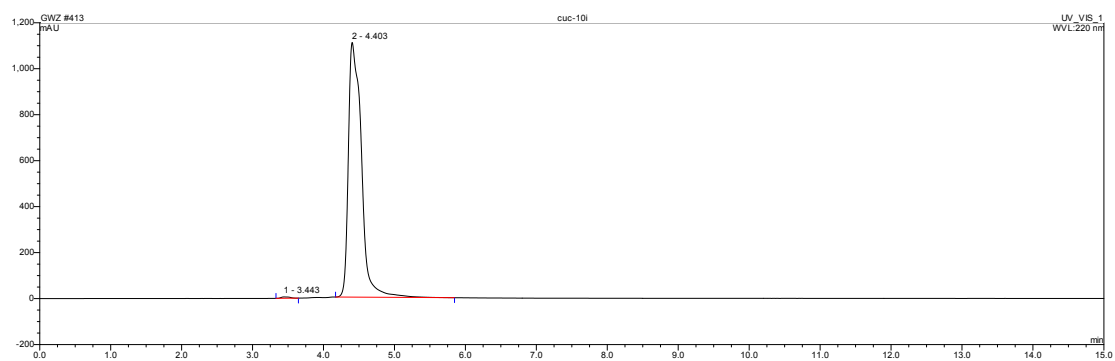
Compound 10f



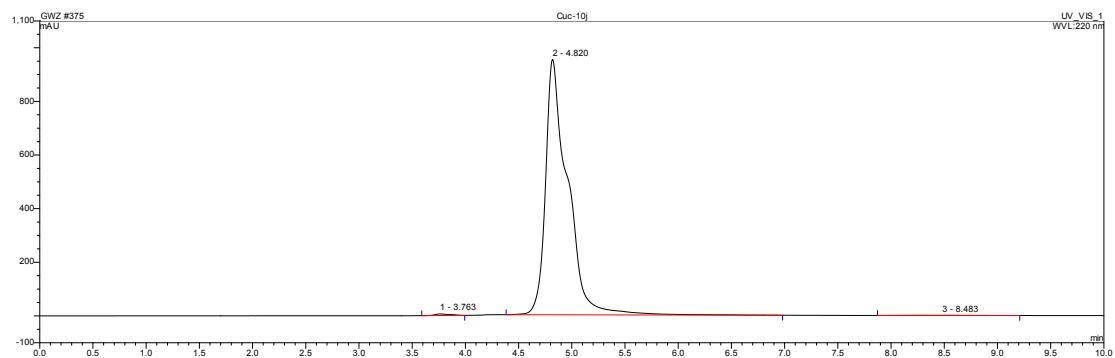
Compound 10g



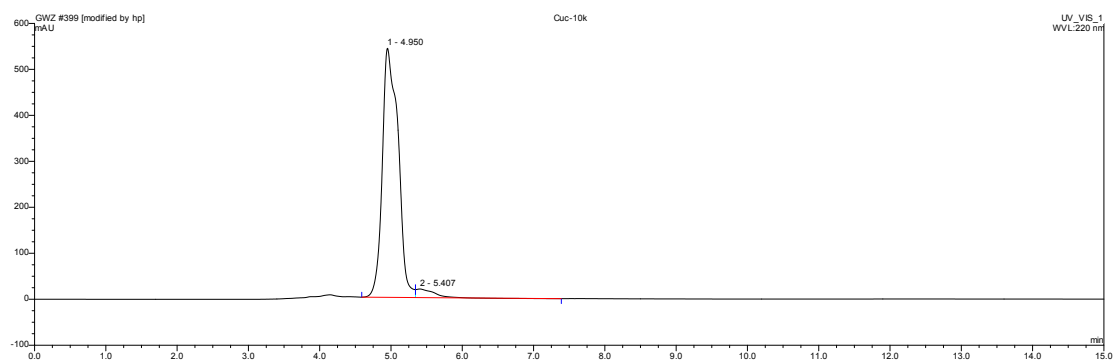
Compound 10h



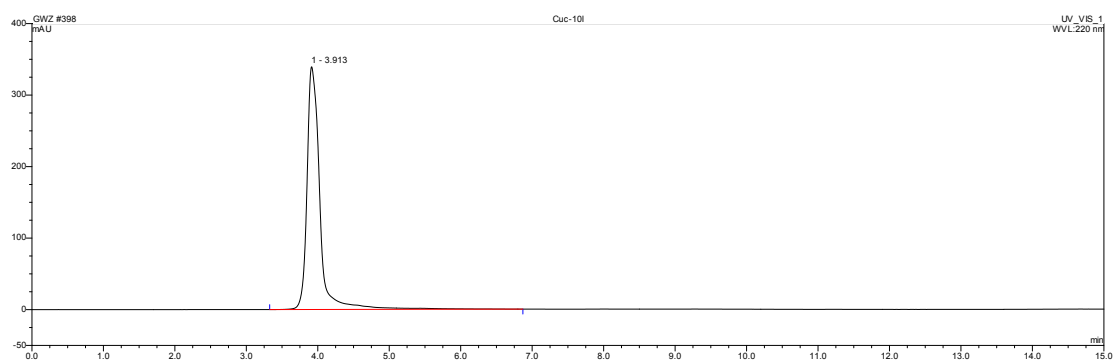
Compound 10i



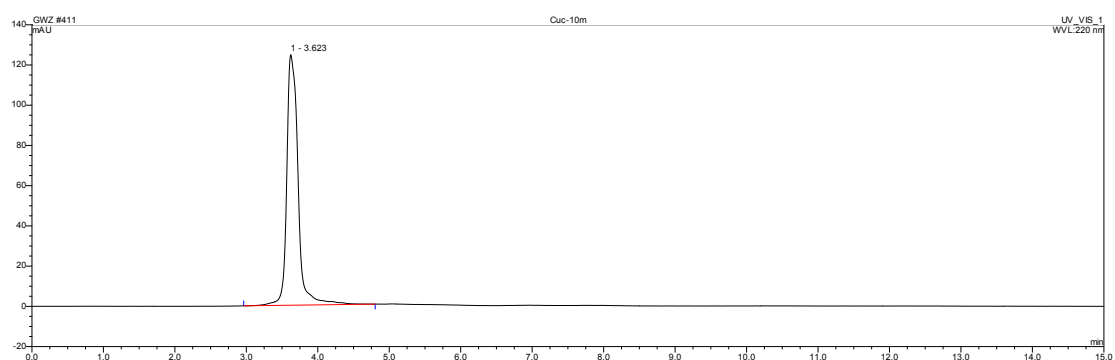
Compound 10j



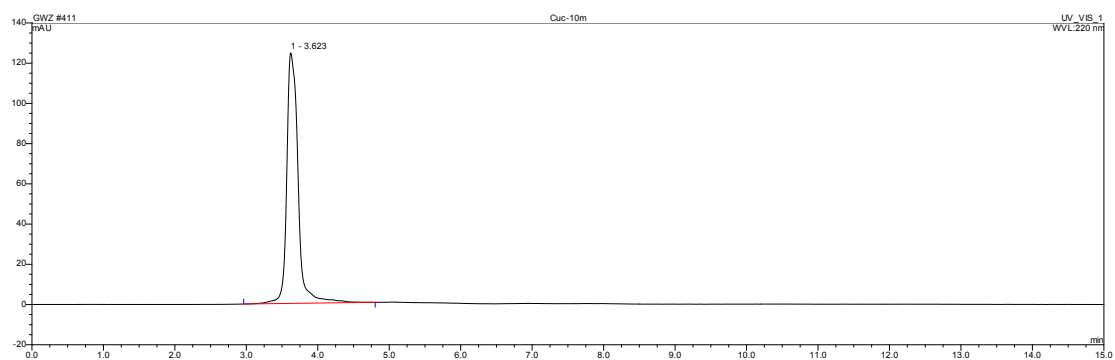
Compound 10k



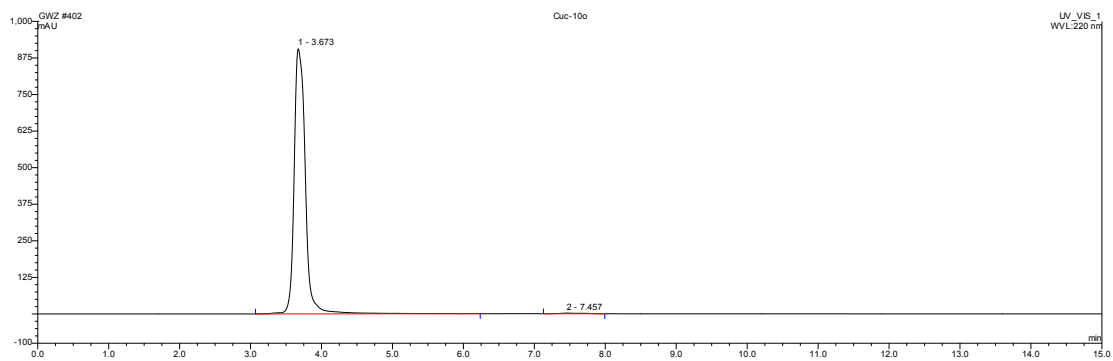
Compound 10l



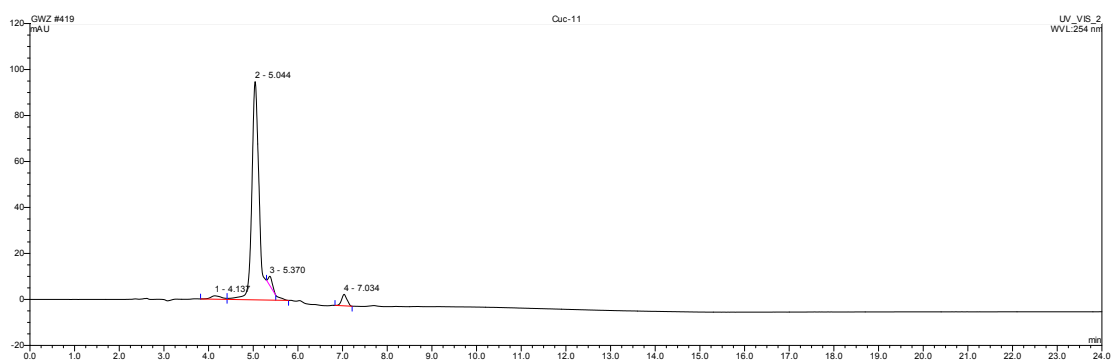
Compound 10m



Compound 10n



Compound 10o



Compound 11

3. The dose-response curves of compounds

