

Synthesis of cannabinoid metabolites: ajulemic acid and HU-210

Wenbin Shao^{1,2}, Pingyong Liao^{1,2}, Xiaoyan Zhang³, Binbin Fan³, Ruijia Chen^{1,2}, Xilong Chen^{1,2},
Xuejun Zhao^{1,2,*}, Wenbin Liu^{1,2,*}

¹ Shanghai Key Laboratory of Crime Scene Evidence, Shanghai Research Institute of Criminal Science and Technology,
Shanghai 200072, China

² Shanghai Yuansi Standard Science and Technology Co., Ltd, Shanghai, 200072, China

³ State Key Laboratory of Bio-Fibers and Eco-Textiles & Institute of Marine Biobased Materials & Collage of Materials
Science and Engineering, Qingdao University, Qingdao 266071, China

* Correspondence: wblu1981@163.com (W.L.); xjzhao1201@163.com (X.Z.)

Table of contents

Figure S1-S2. NMR spectra of intermediate 5.

Figure S3-S4. NMR spectra of intermediate 6.

Figure S5-S6. NMR spectra of intermediate 7.

Figure S7-S8. NMR spectra of intermediate 8.

Figure S9-S10. NMR spectra of intermediate 10.

Figure S11-S12. NMR spectra of intermediate 11.

Figure S13-S14. NMR spectra of intermediate 12.

Figure S15-S16. NMR spectra of intermediate 14.

Figure S17. ¹HNMR spectra of intermediate 15.

Figure S18-S19. NMR spectra of intermediate 3.

Figure S20-S21. NMR spectra of intermediate 9.

Figure S22-S23. NMR spectra of intermediate 4.

Figure S24-S25. NMR spectra of intermediate Δ^8 -THC.

Figure S26-S27. NMR spectra of intermediate 11-Nor- Δ^8 -THC-carboxylic acid.

Figure S28-S29. NMR spectra of intermediate Δ^9 -THC.

Figure S30-S31. NMR spectra of intermediate Δ^9 -THC- carboxylic acid.

NMR spectra for the synthesized compounds

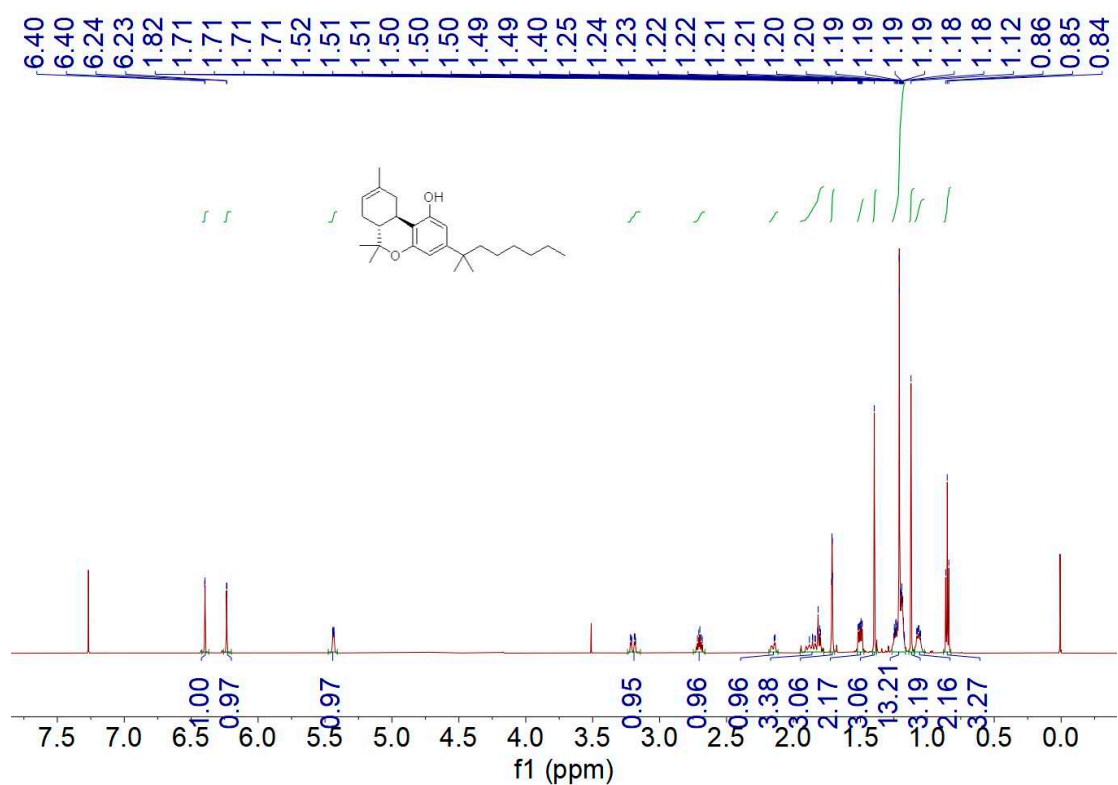


Figure S1 ¹H-NMR of compound **5** (CDCl₃)

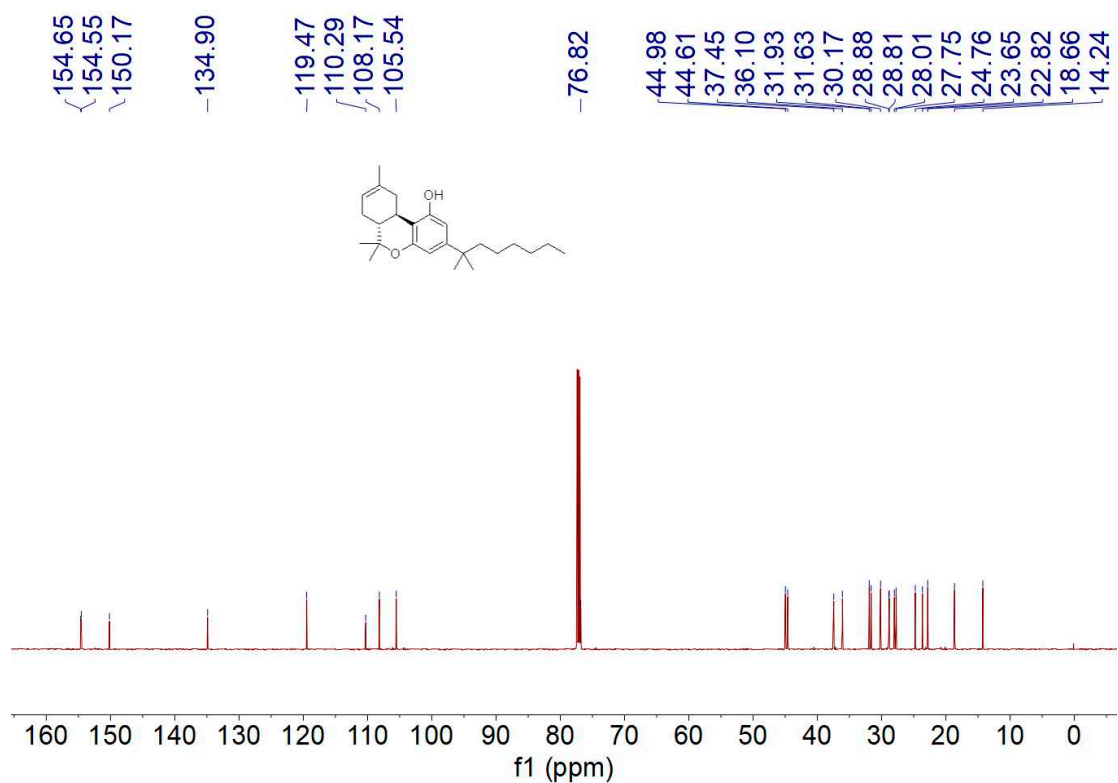


Figure S2 ¹³C-NMR of compound **5** (CDCl₃)

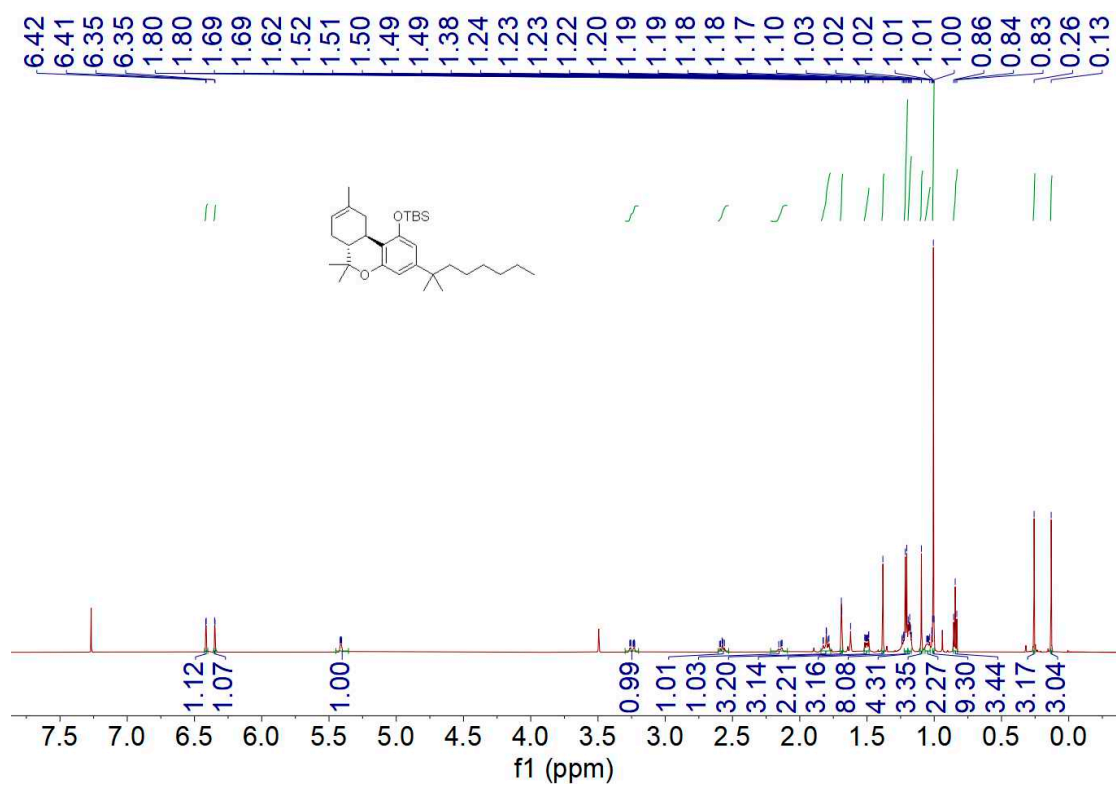


Figure S3 ¹H-NMR of compound **6** (CDCl₃)

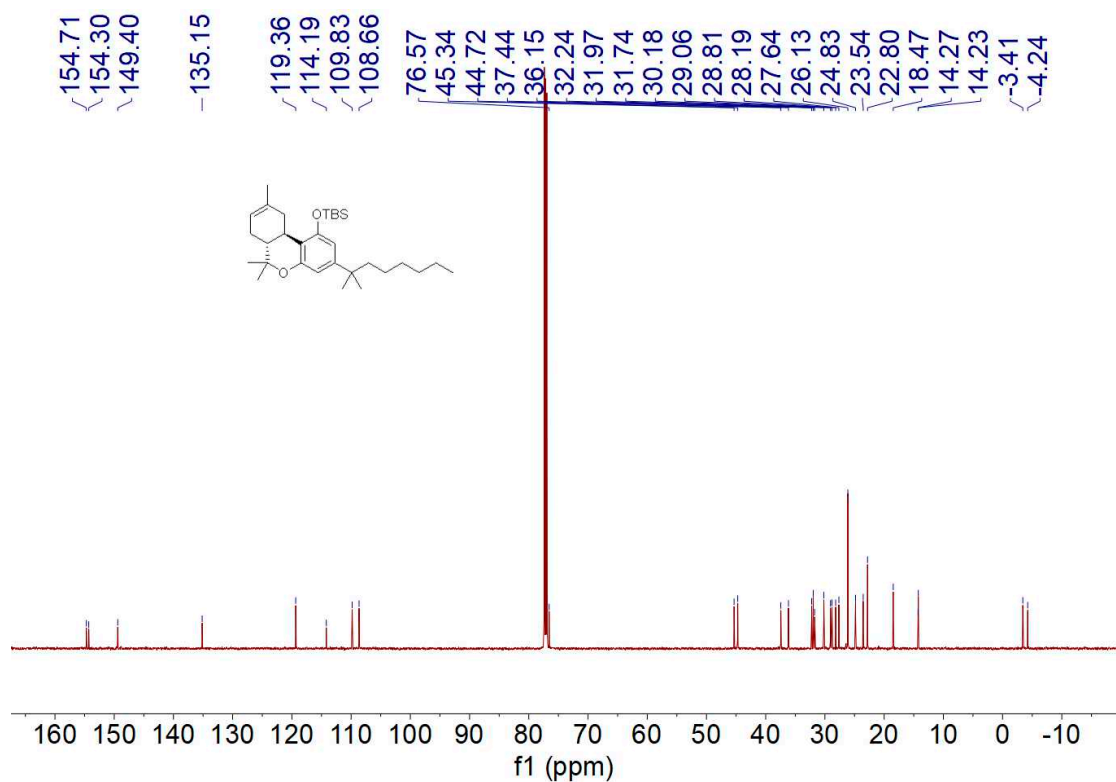


Figure S4 ¹³C-NMR of compound **6** (CDCl₃)

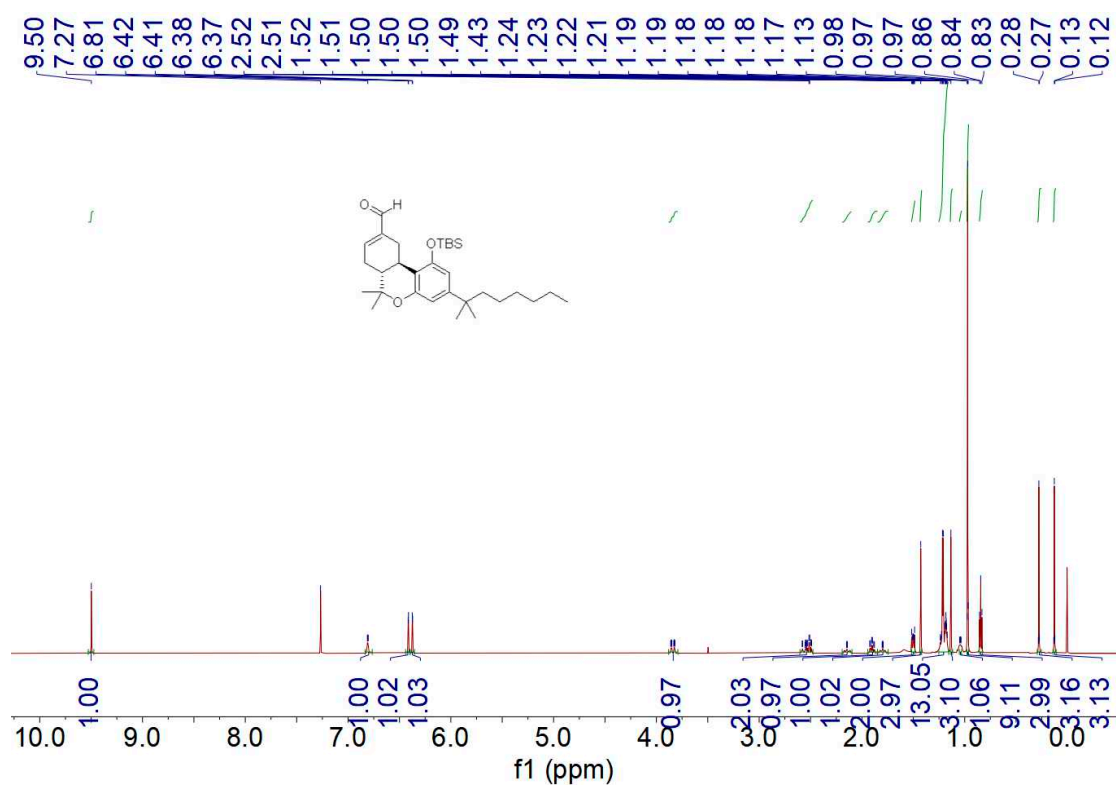


Figure S5 ¹H-NMR of compound 7 (CDCl₃)

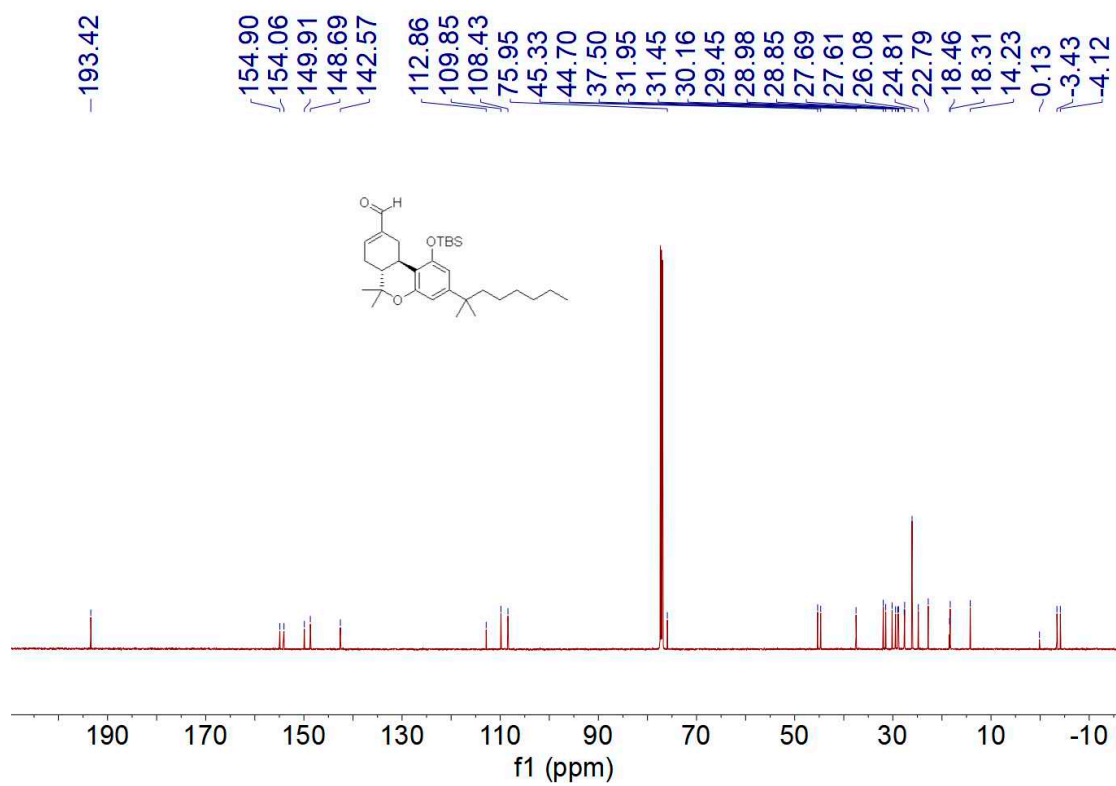


Figure S6 ¹³C-NMR of compound 7 (CDCl₃)

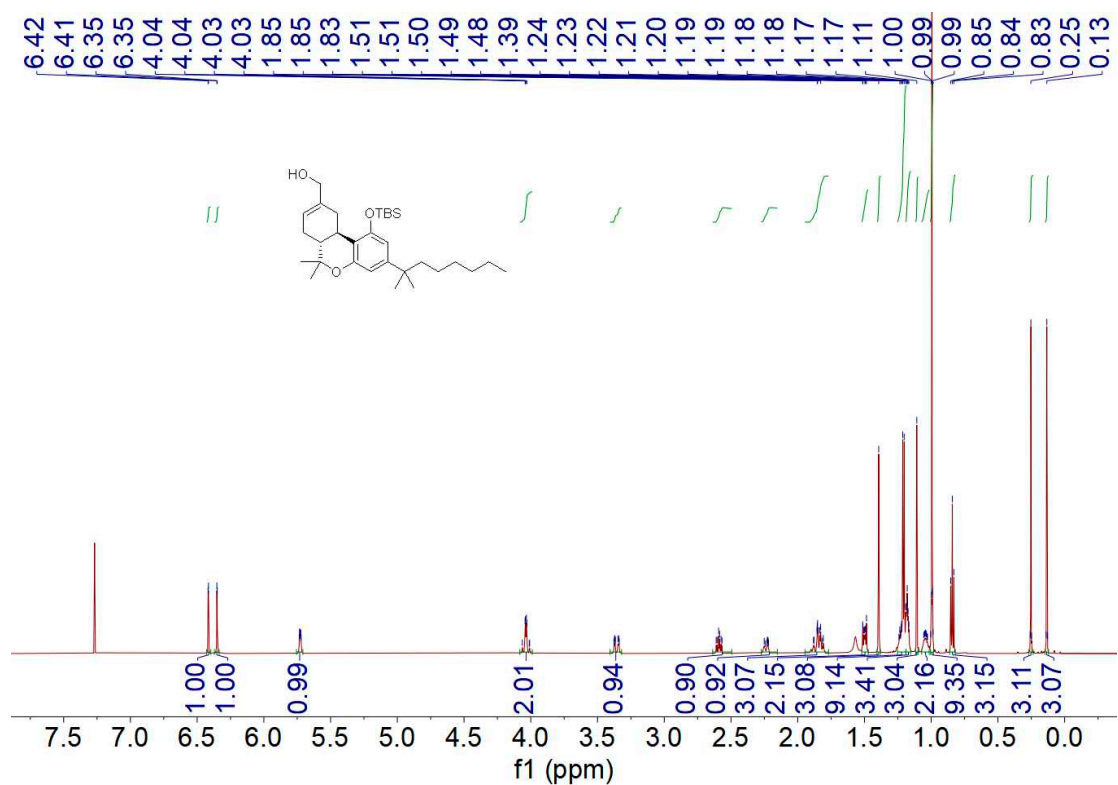


Figure S7 ¹H-NMR of compound 8 (CDCl₃)

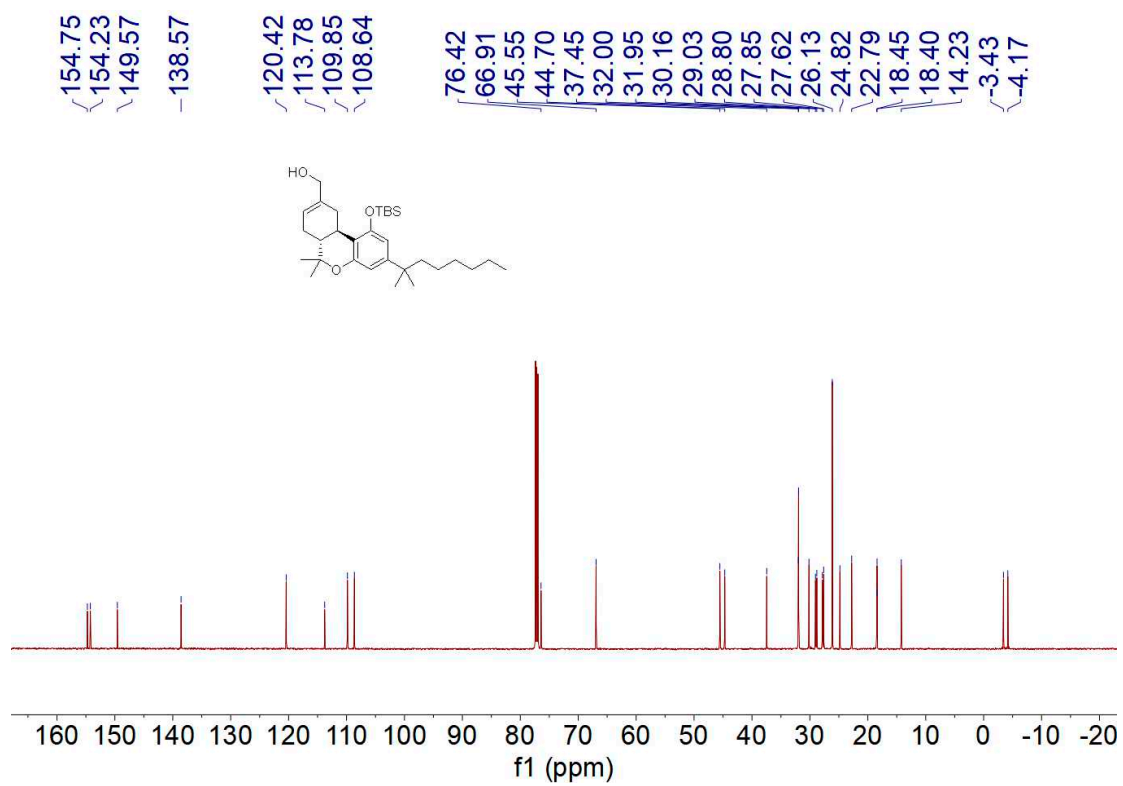


Figure S8 ¹³C-NMR of compound 8 (CDCl₃)

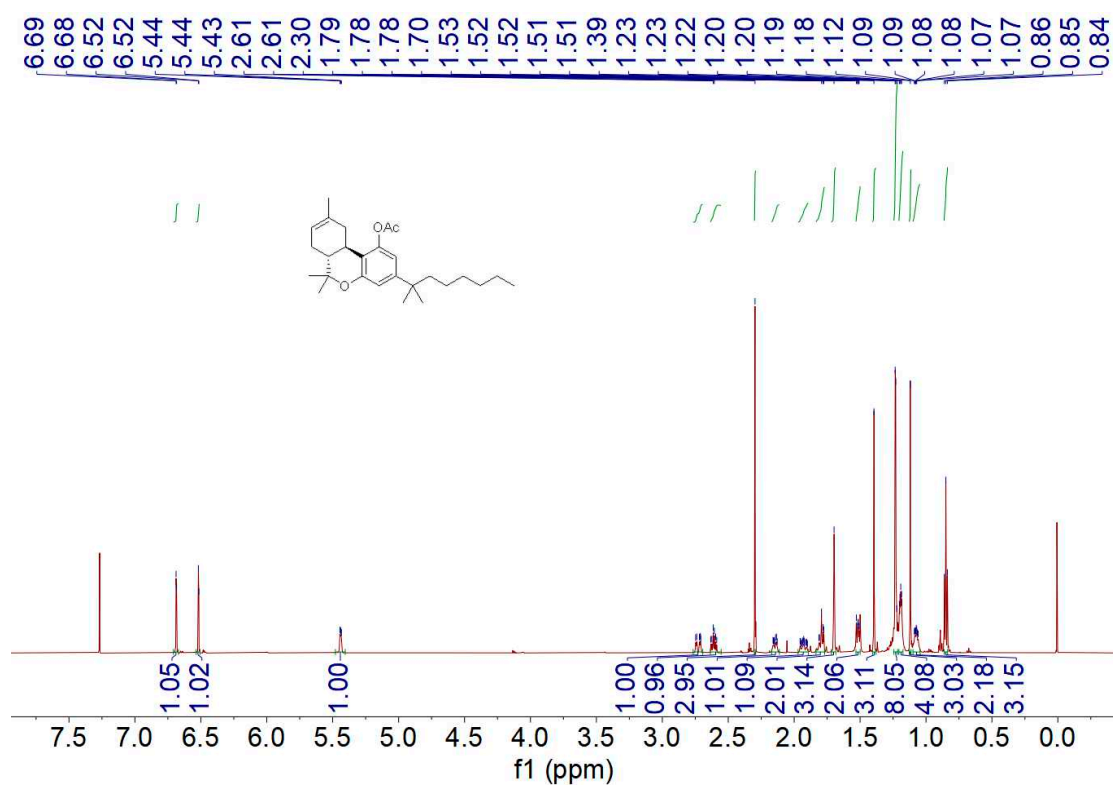


Figure S9 ¹H-NMR of compound **10** (CDCl₃)

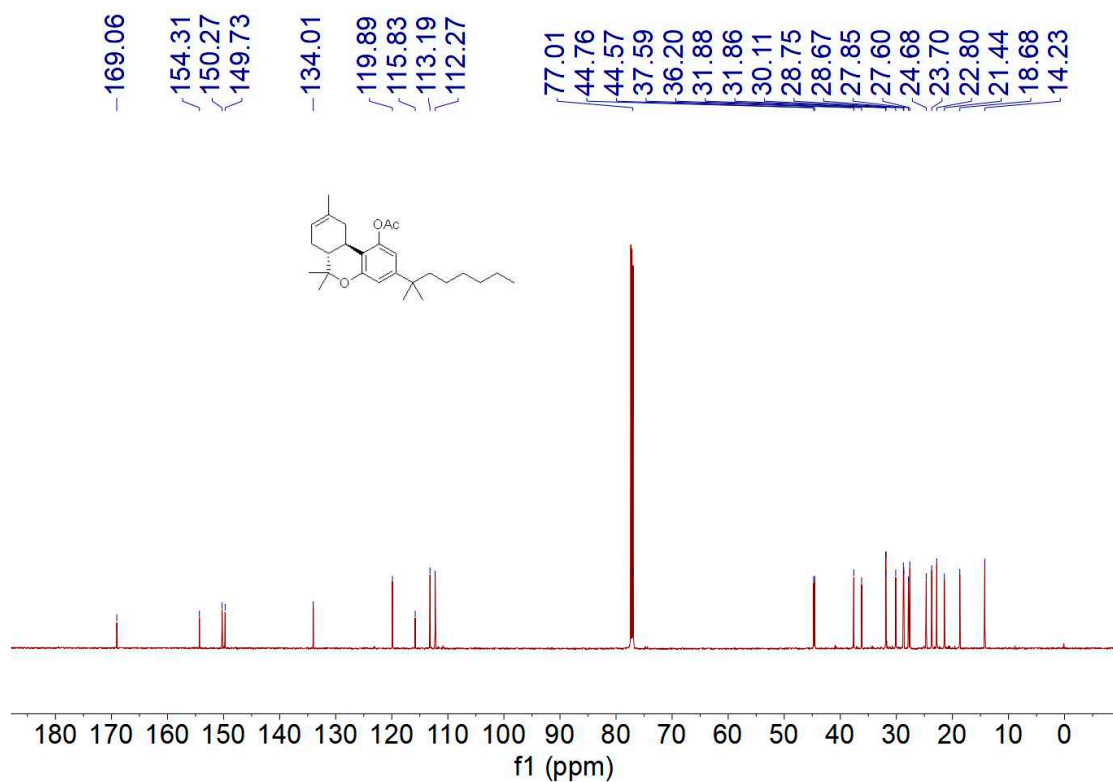


Figure S10 ¹³C-NMR of compound **10** (CDCl₃)

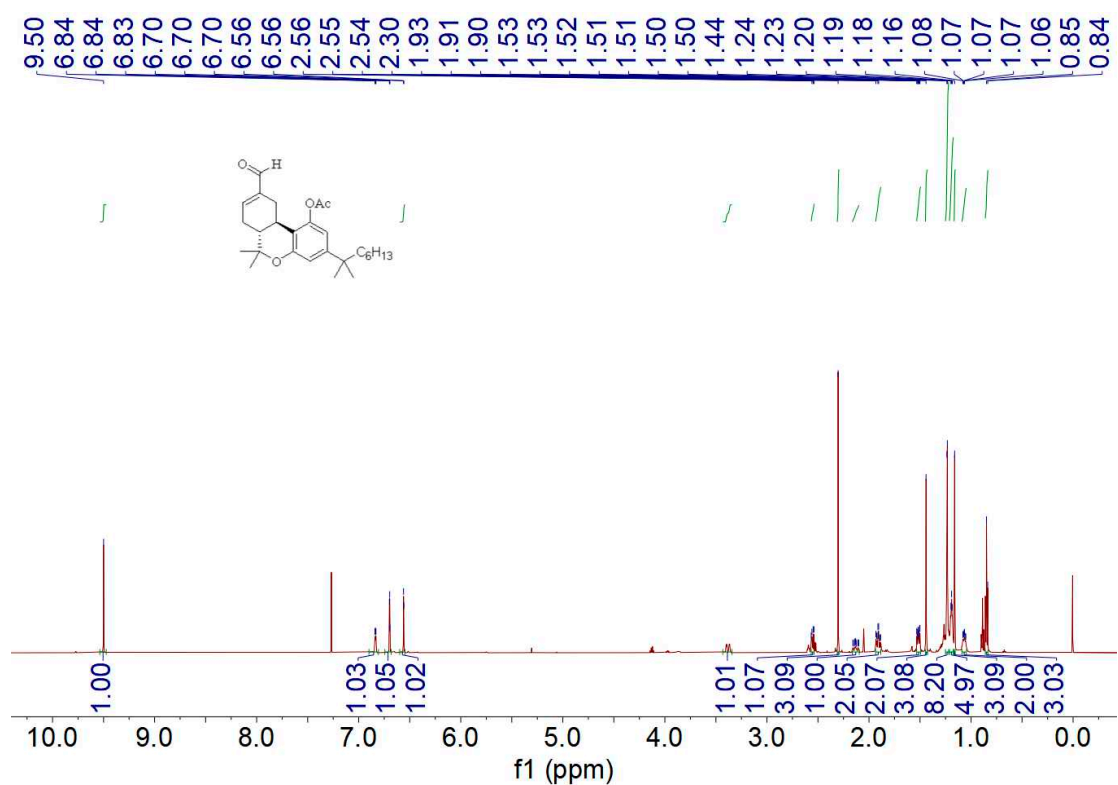


Figure S11 ¹H-NMR of compound 11 (CDCl₃)

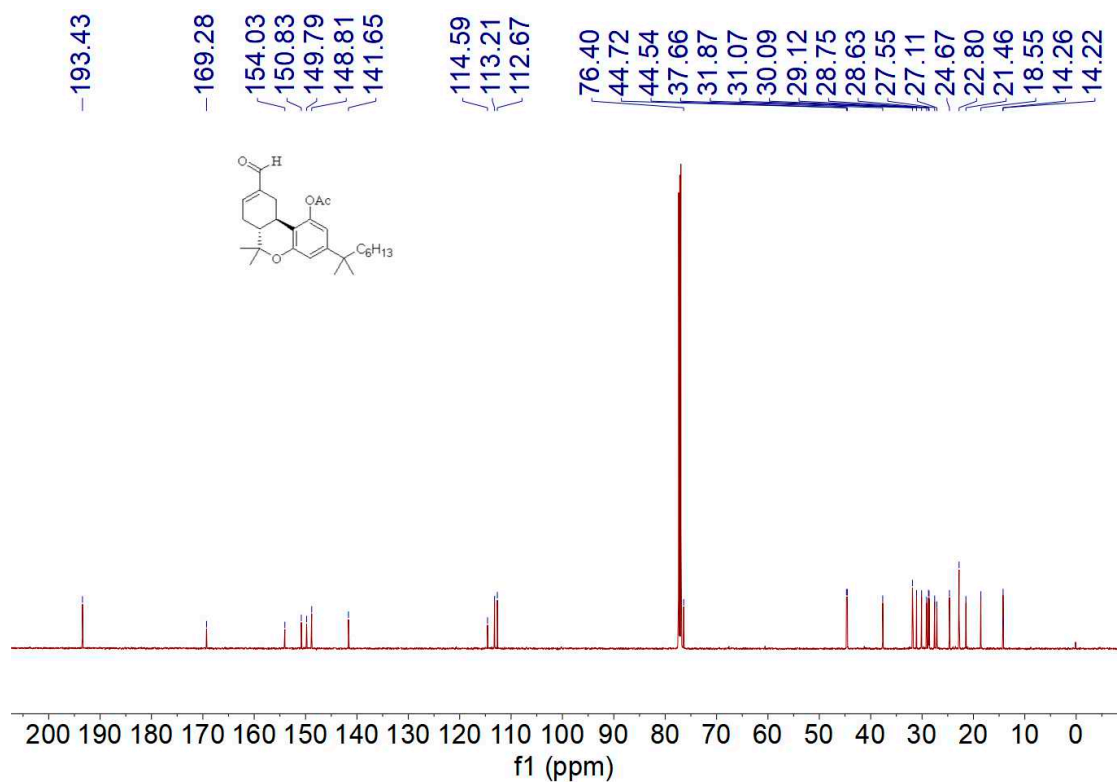


Figure S12 ¹³C-NMR of compound 11 (CDCl₃)

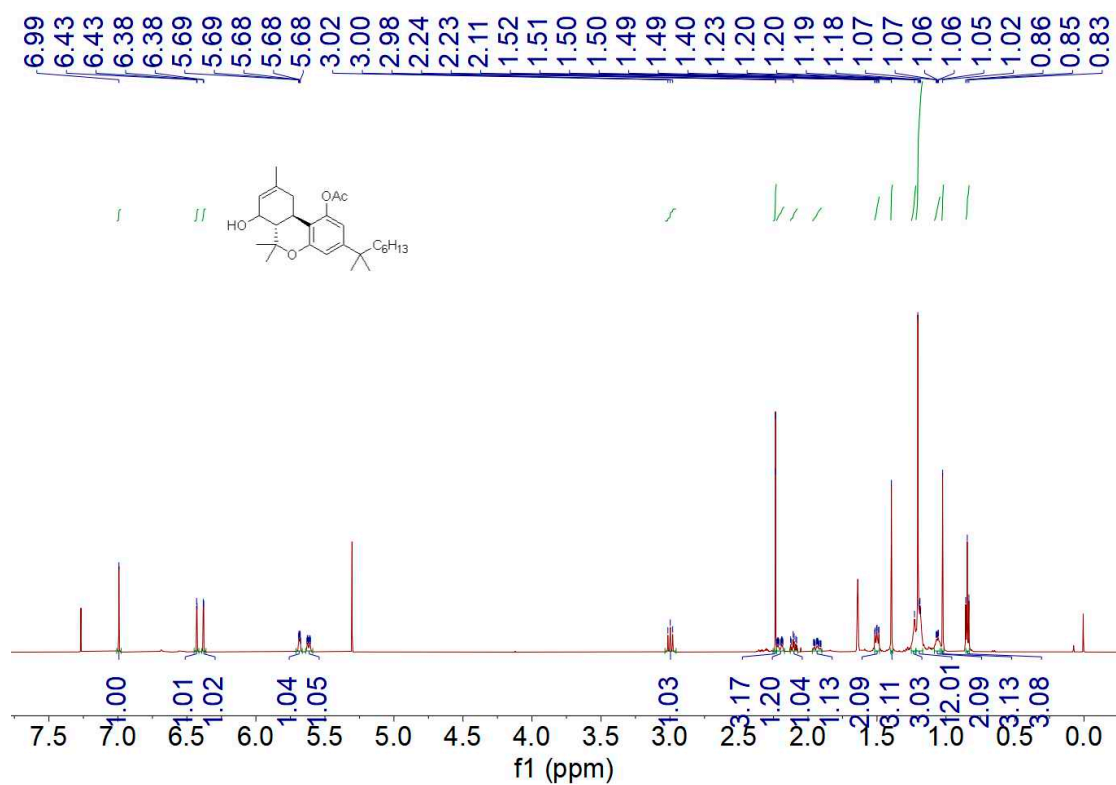


Figure S13 ¹H-NMR of compound **12** (CDCl₃)

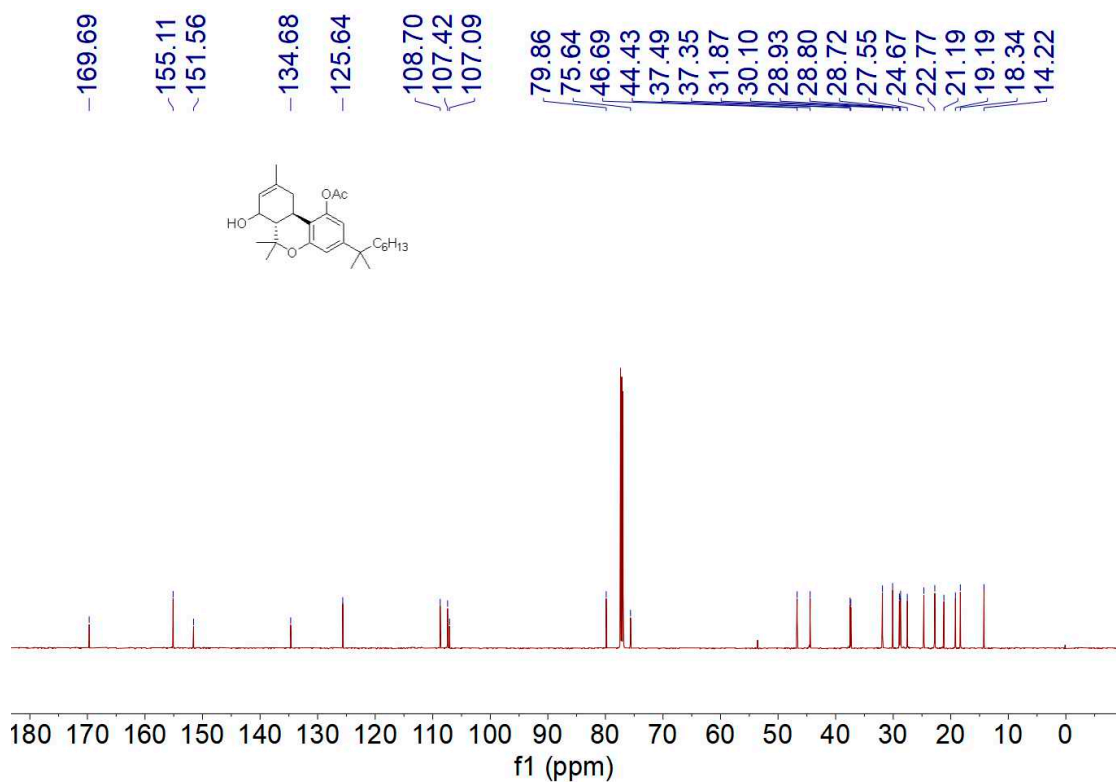


Figure S14 ¹³C-NMR of compound **12** (CDCl₃)

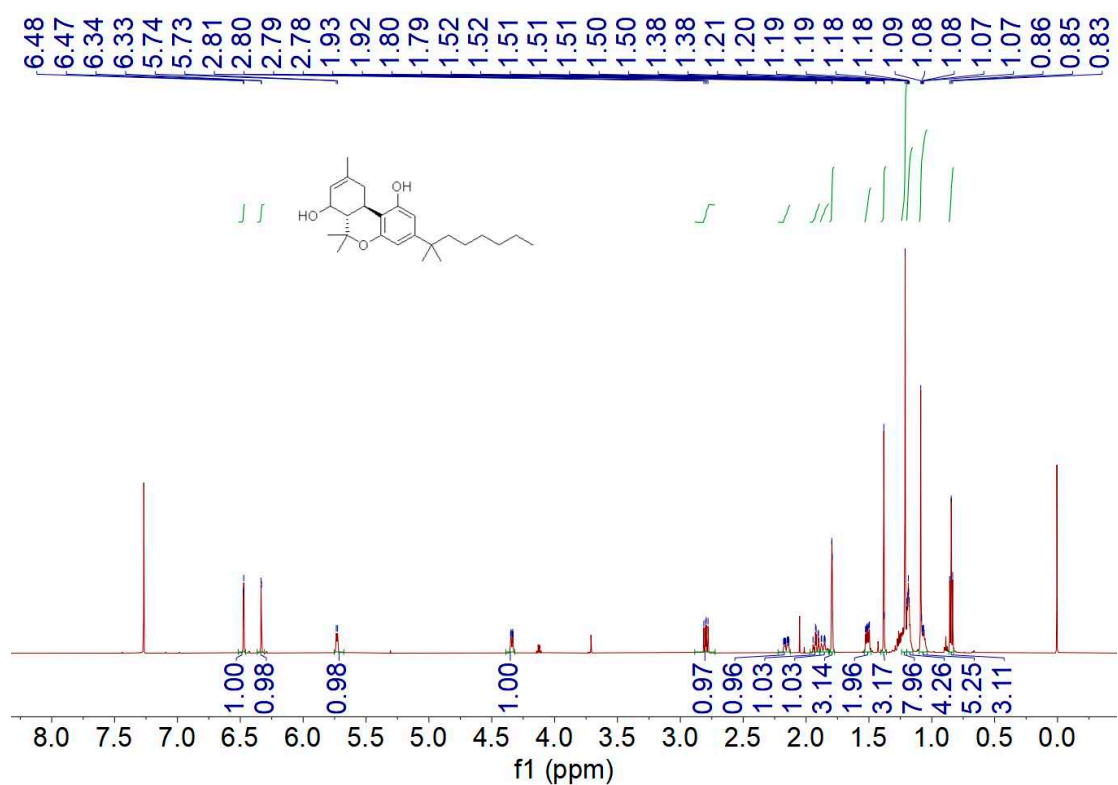


Figure S15 ^1H -NMR of compound **14** (CDCl_3)

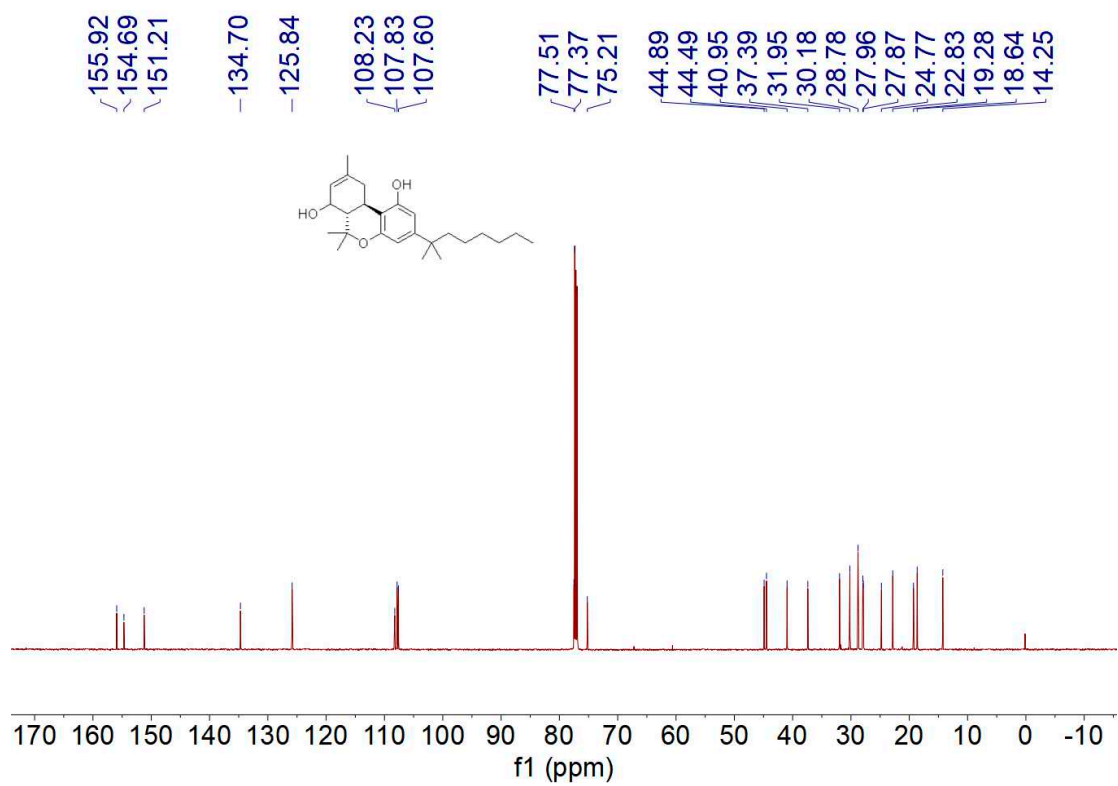


Figure S16 ^{13}C -NMR of compound **14** (CDCl_3)

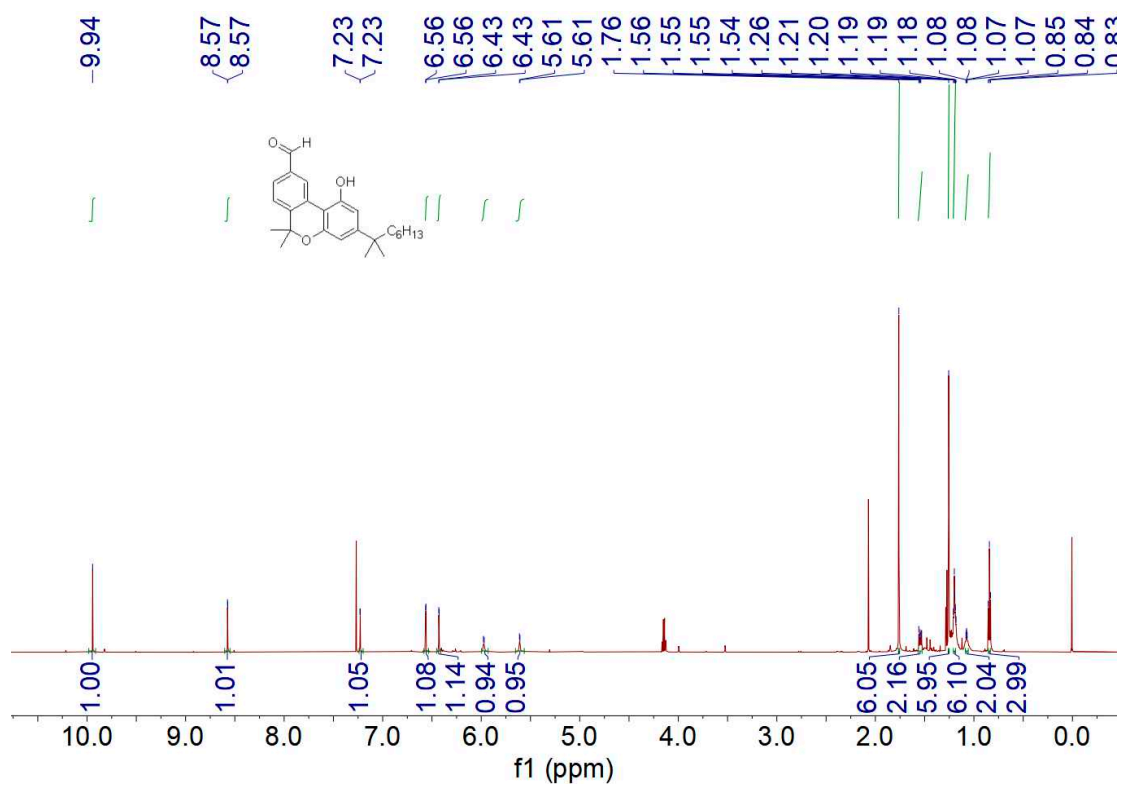


Figure S17 ¹H-NMR of compound **15** (CDCl₃)

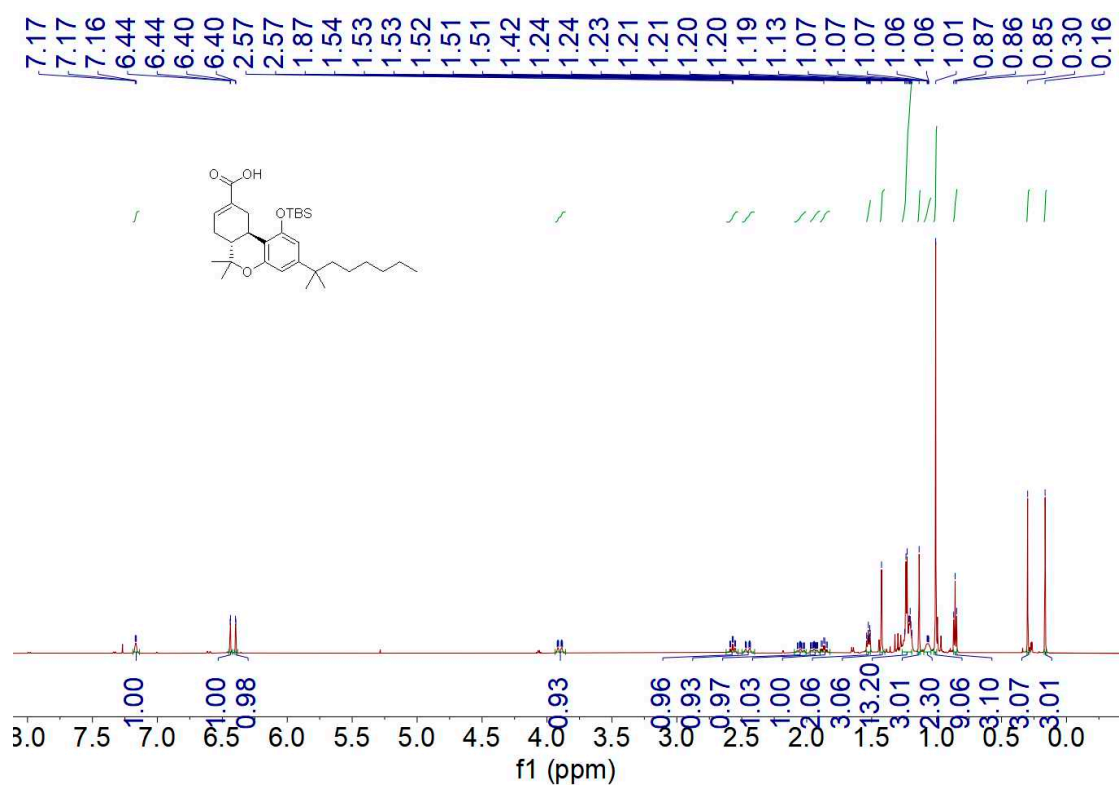


Figure S20 ¹H-NMR of compound **9** (CDCl₃)

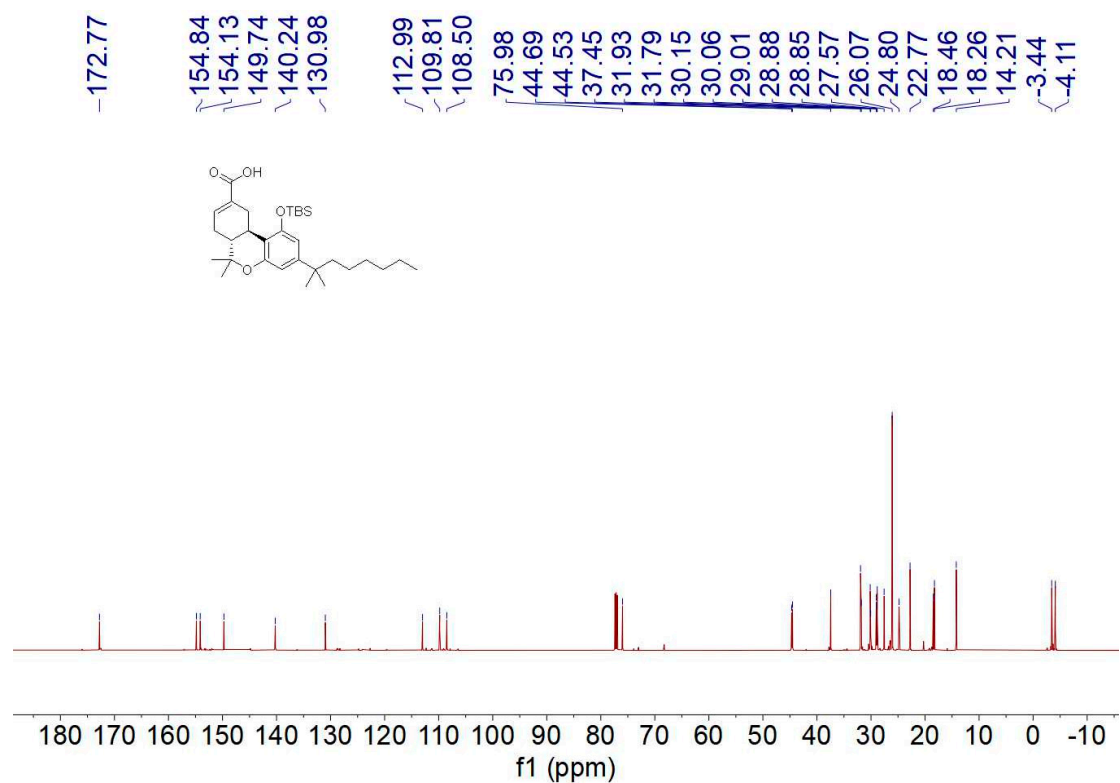


Figure S21 ¹³C-NMR of compound **9** (CDCl₃)

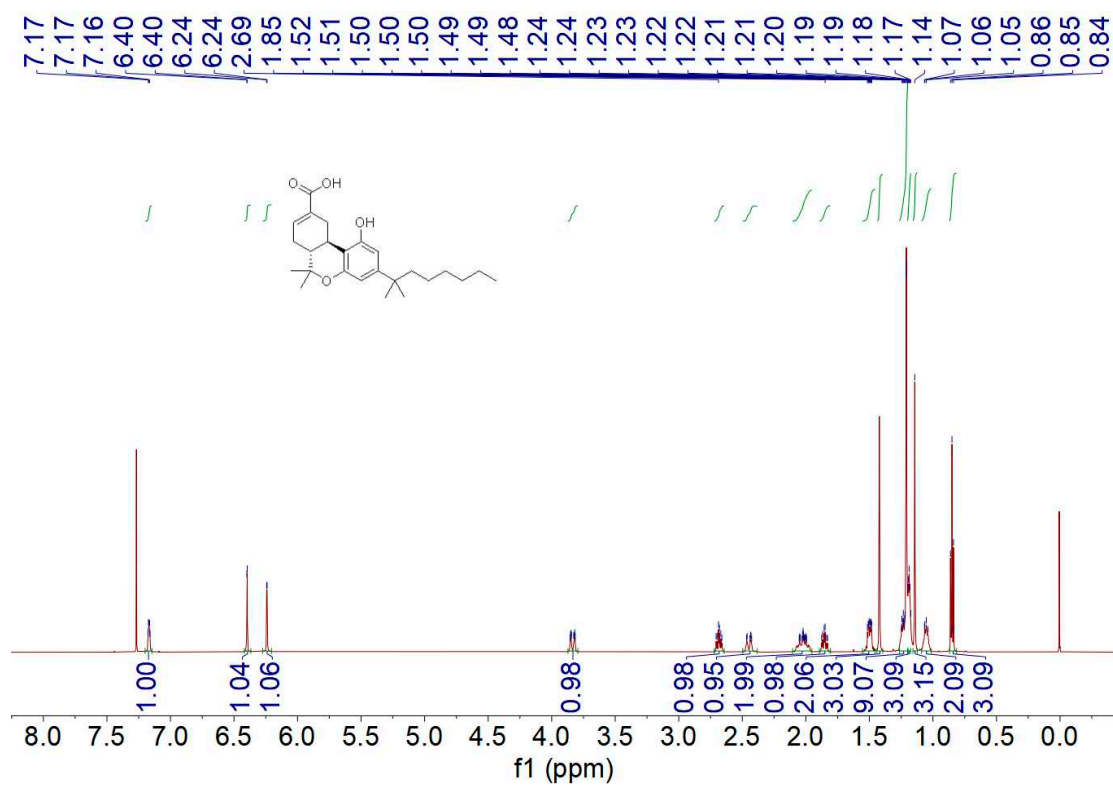


Figure S22 ^1H -NMR of compound 4 (CDCl_3)

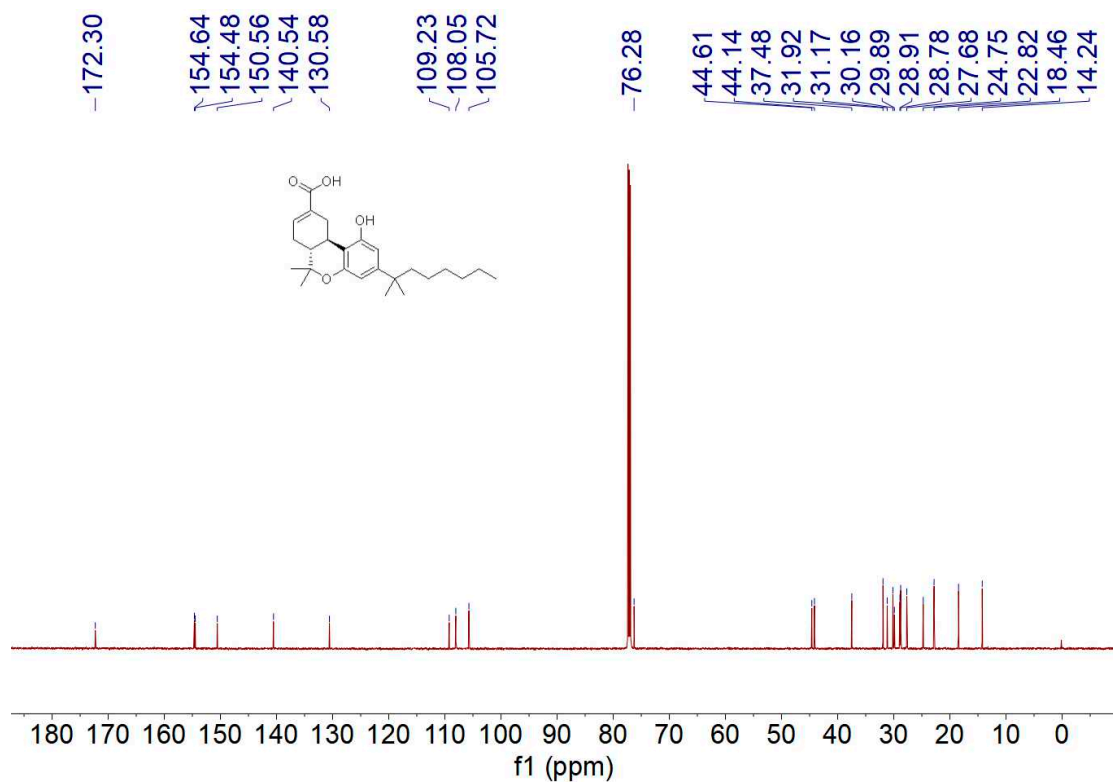


Figure S23 ^{13}C -NMR of compound 4 (CDCl_3)

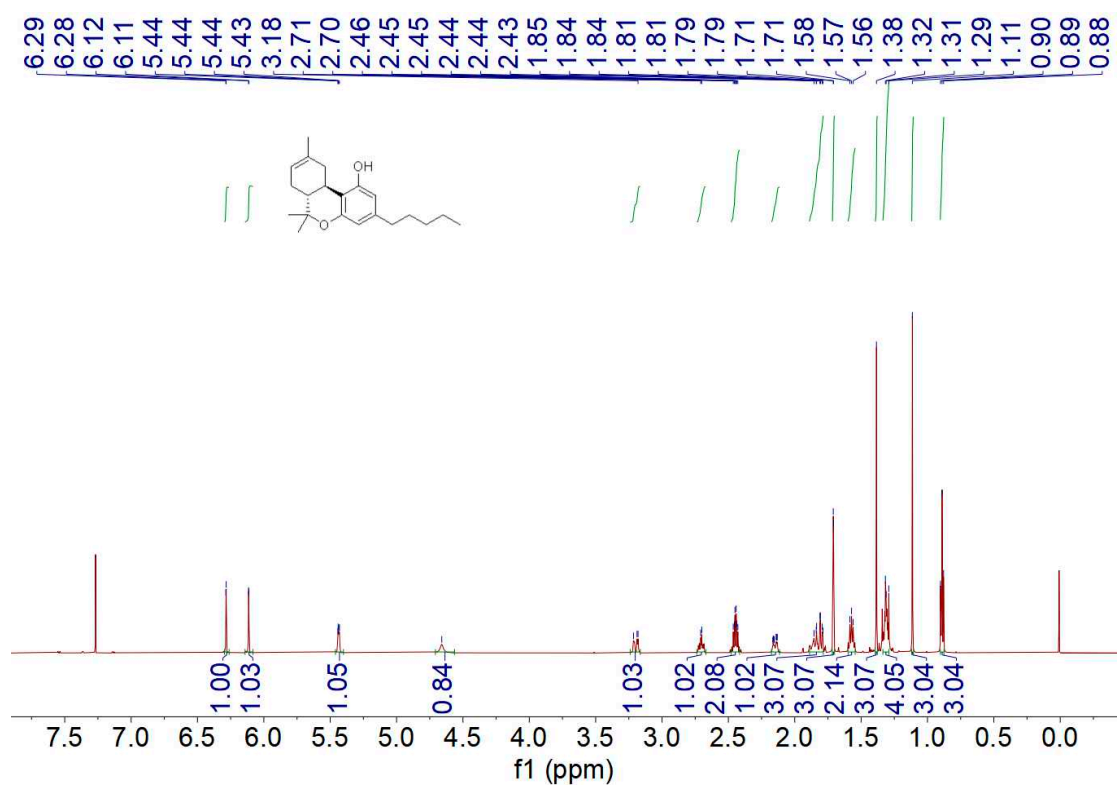


Figure S24 ^1H -NMR of compound Δ^8 -THC (CDCl_3)

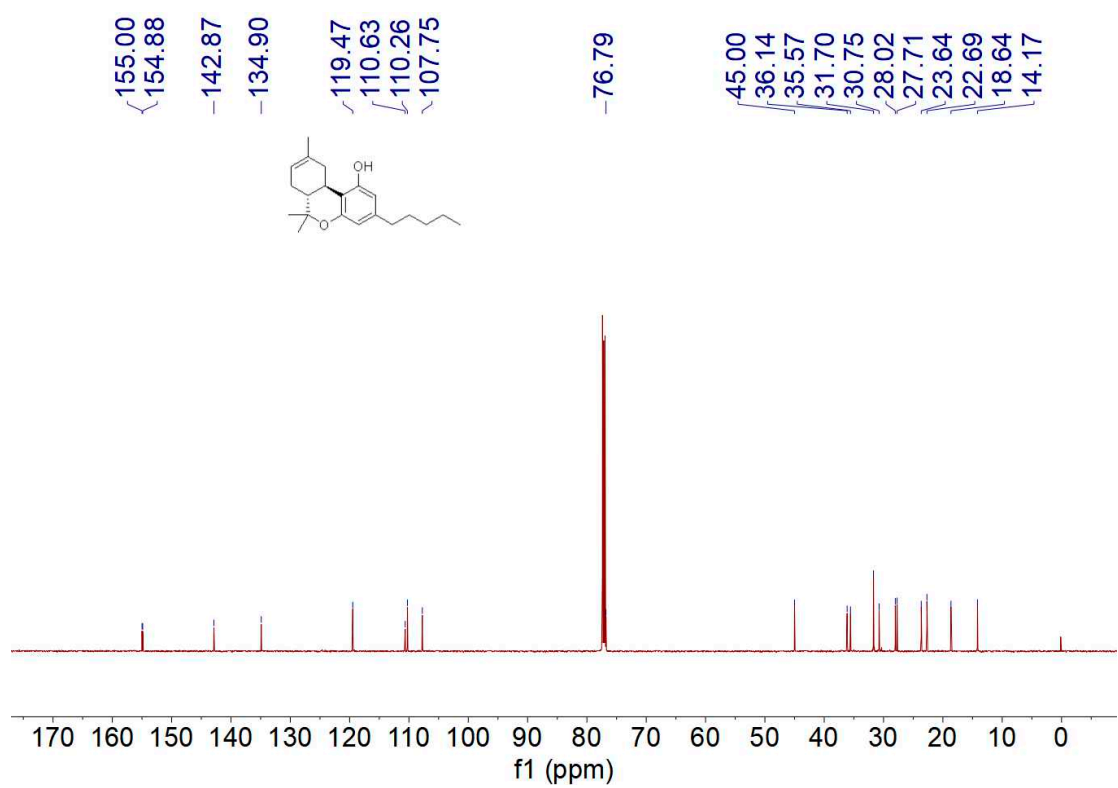


Figure S25 ^{13}C -NMR of compound Δ^8 -THC (CDCl_3)

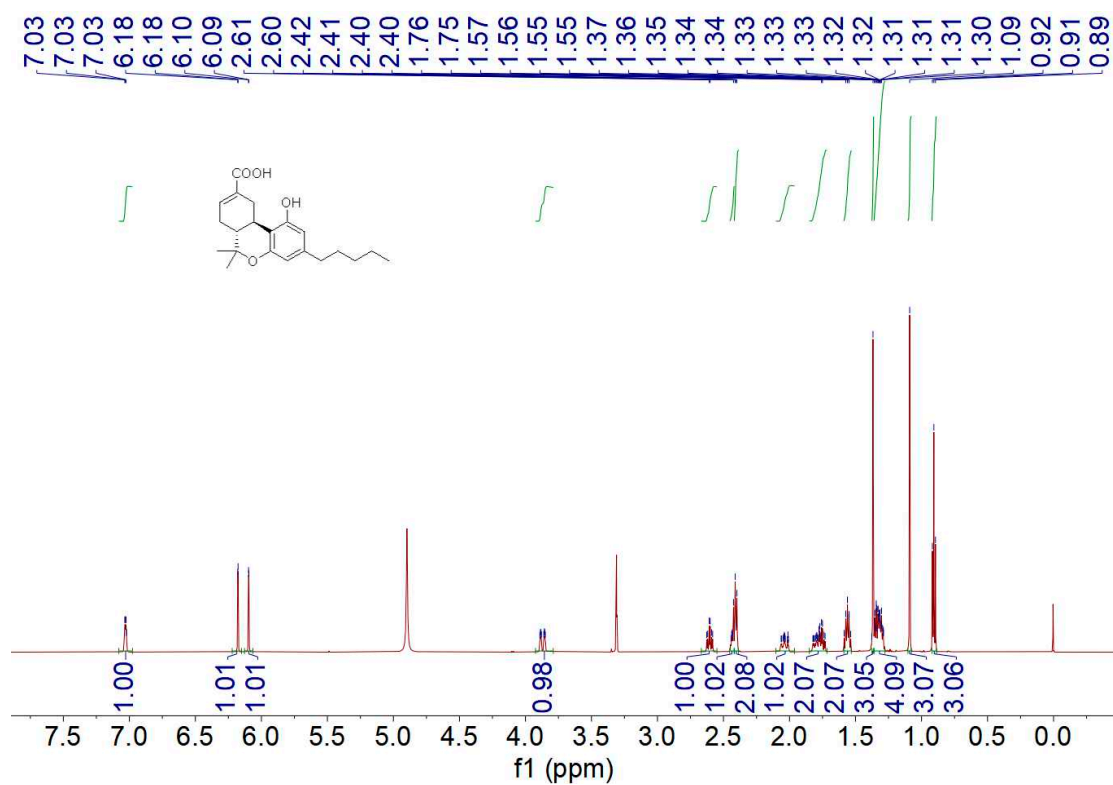


Figure S26 ¹H-NMR of compound 11- nor- Δ^8 -THC-carboxylic acid (CD₃OD)

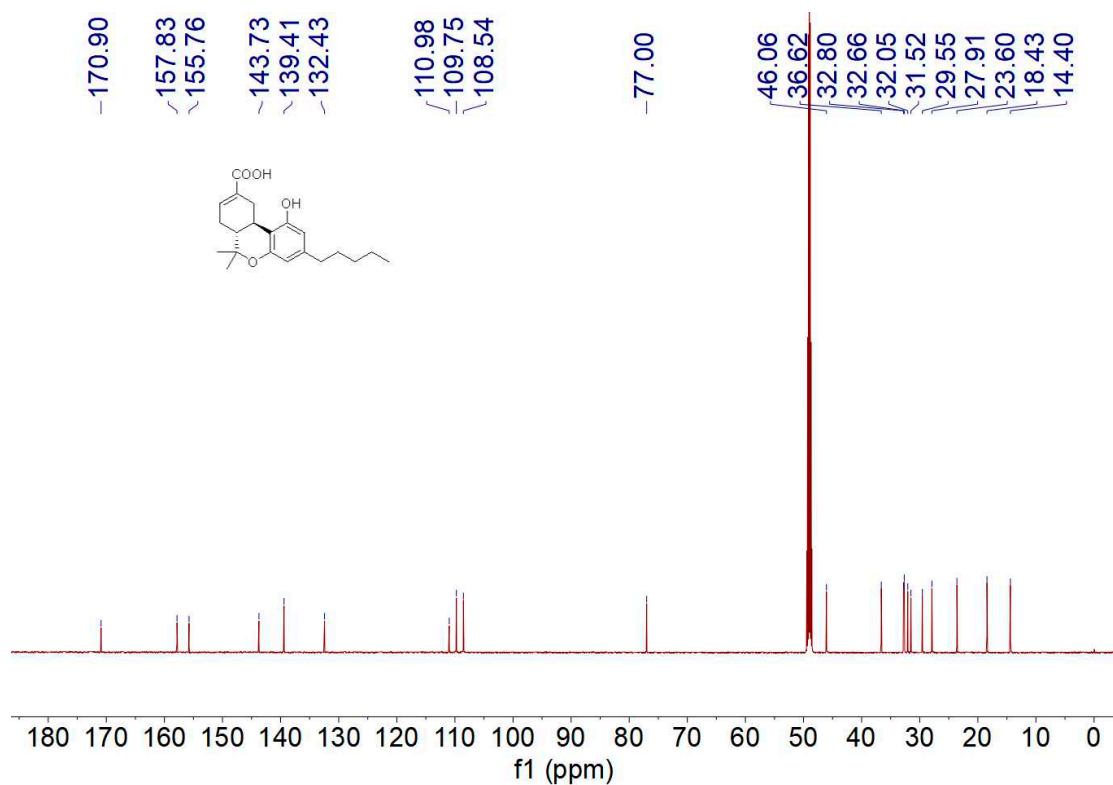


Figure S27 ¹³C-NMR of compound 11-nor- Δ^8 -THC-carboxylic acid (CD₃OD)

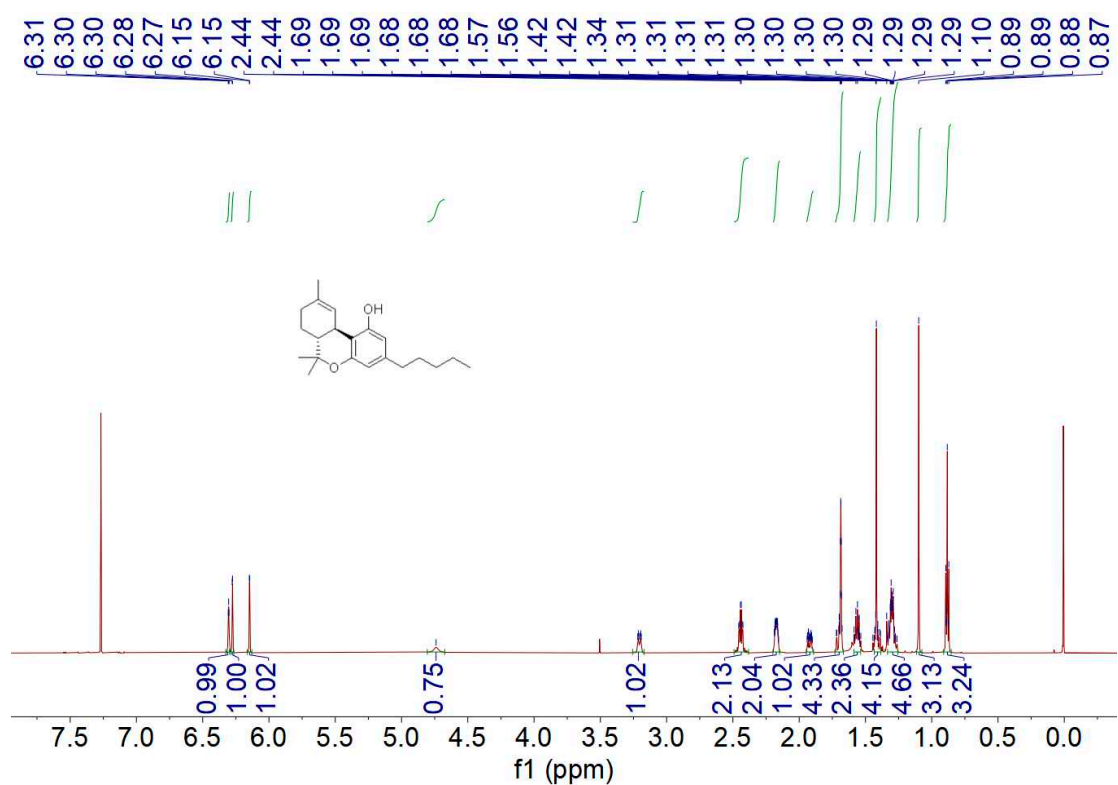


Figure S28 ^1H -NMR of compound Δ^9 -THC (CDCl_3)

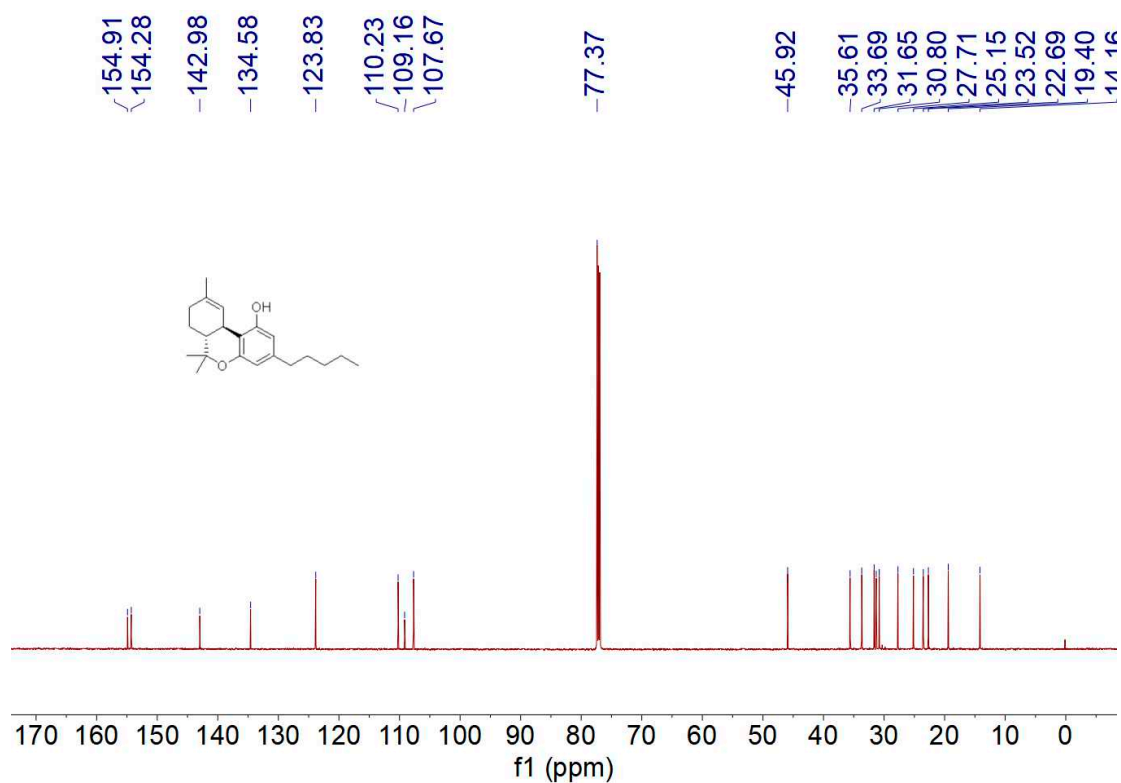


Figure S29 ^{13}C -NMR of compound Δ^9 -THC (CDCl_3)

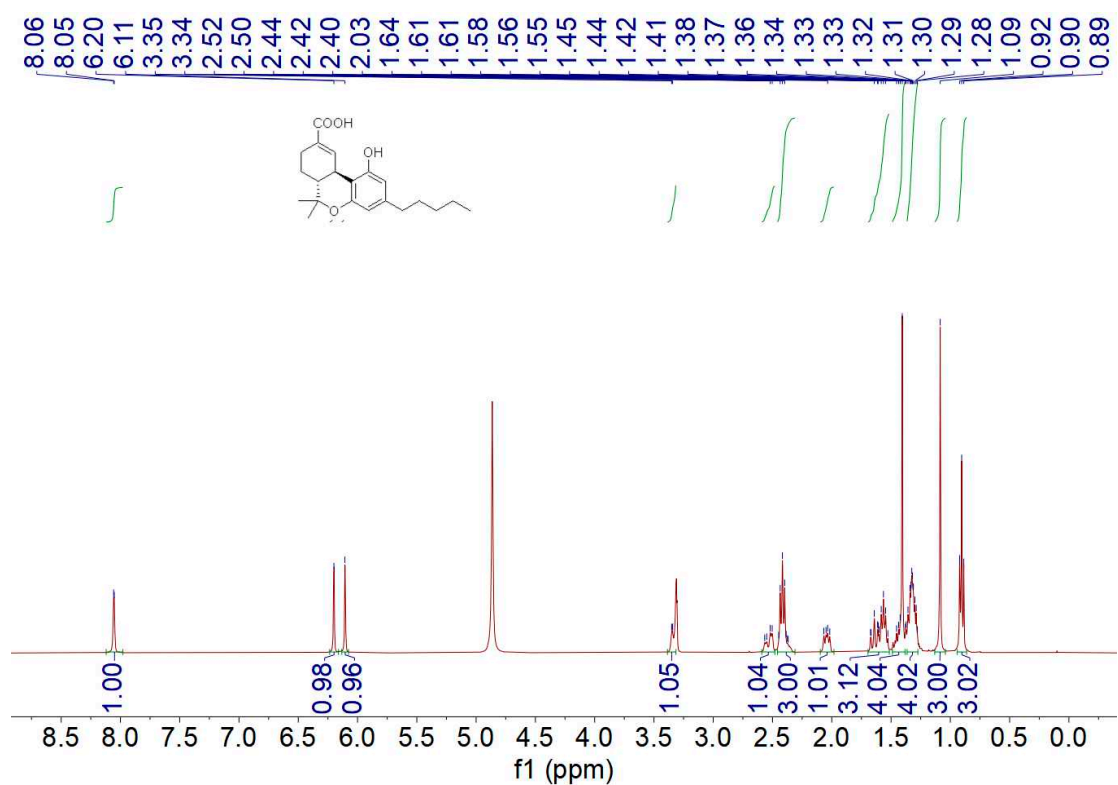


Figure S30 ¹H-NMR of compound Δ^9 -THC- carboxylic acid (CDCl₃)

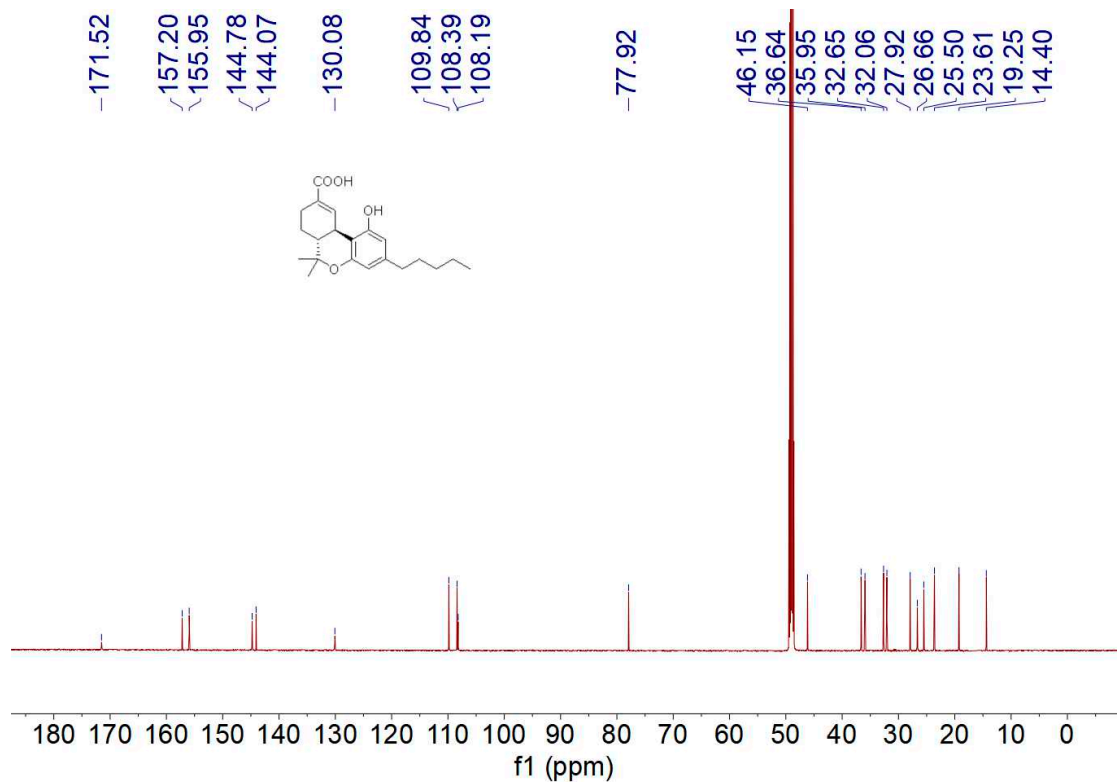


Figure S31 ¹³C-NMR of compound Δ^9 -THC- carboxylic acid (CDCl₃)