

Phytochemical analysis of methanol extracts and of essential oil from leaves of industrial hemp *Futura 75* cultivar: Isolation of a new cannabinoid derivative and biological profile using computational approaches.

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¹H NMR (CD₃OD, 400 MHz) of 2 α -hydroxy- $\Delta^{3,7}$ -cannabitol (1)

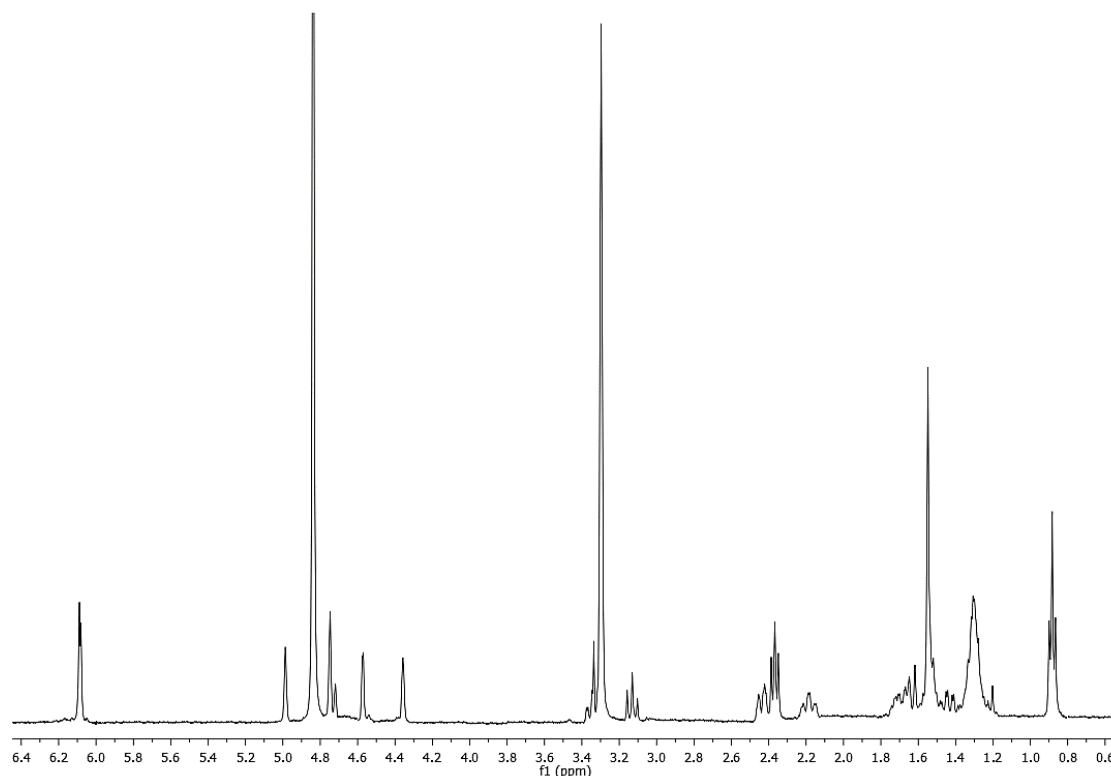


Figure S1. ¹H NMR (CD₃OD, 400 MHz) of 2 α -hydroxy- $\Delta^{3,7}$ -cannabitol (1).

^{13}C NMR (CD_3OD , 100 MHz) of 2α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1)

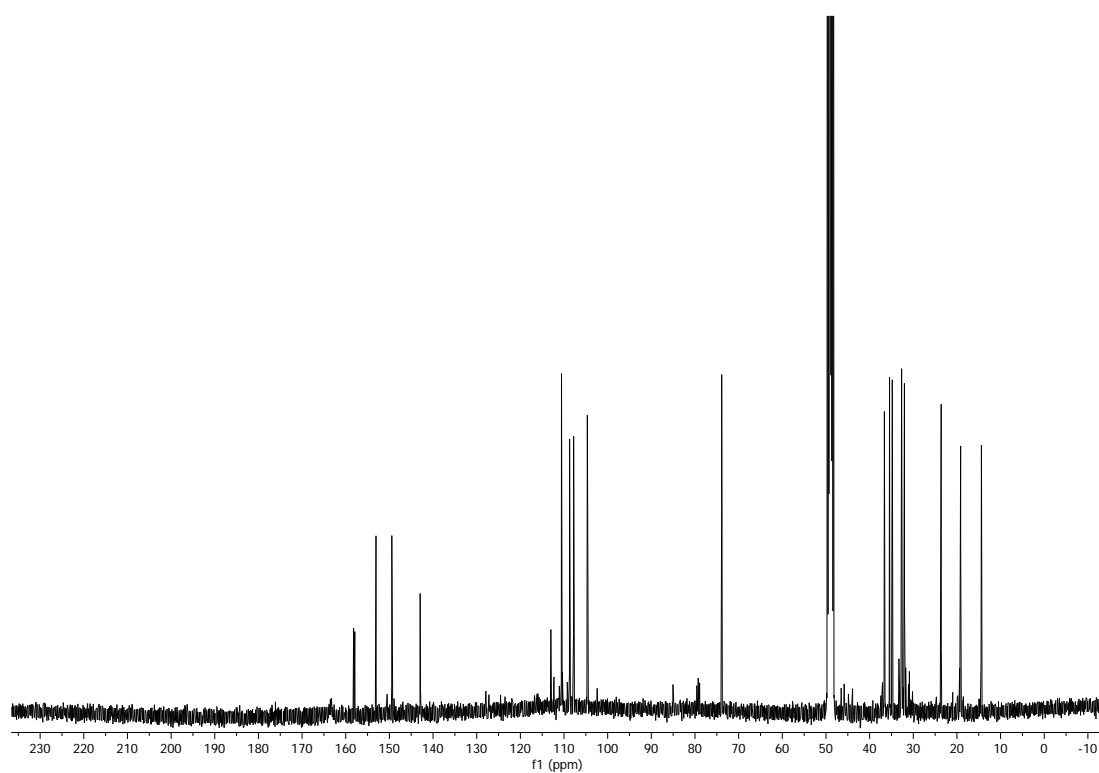


Figure S2. ^{13}C NMR (CD_3OD , 100 MHz) of 2α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1).

COSY spectrum (CD_3OD , 400 MHz) of 2α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1)

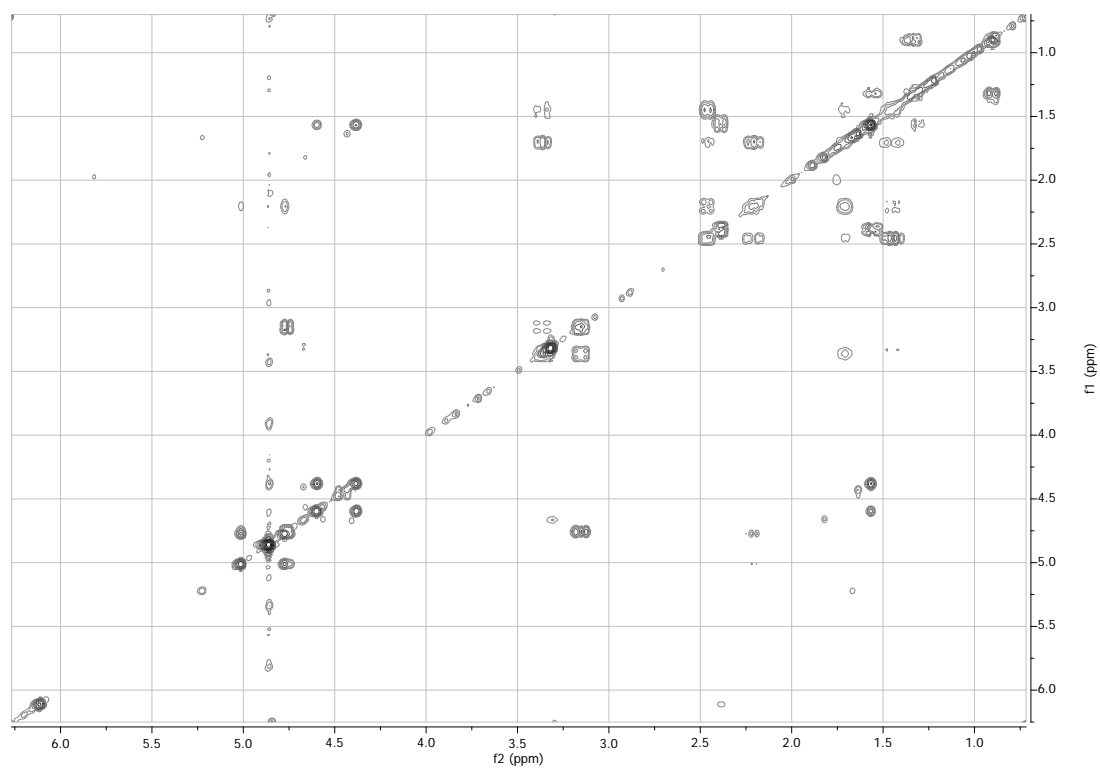


Figure S3. COSY spectrum (CD_3OD , 400 MHz) of 2α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1).

HSQC spectrum (CD₃OD, 400 MHz) of 2 α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1)

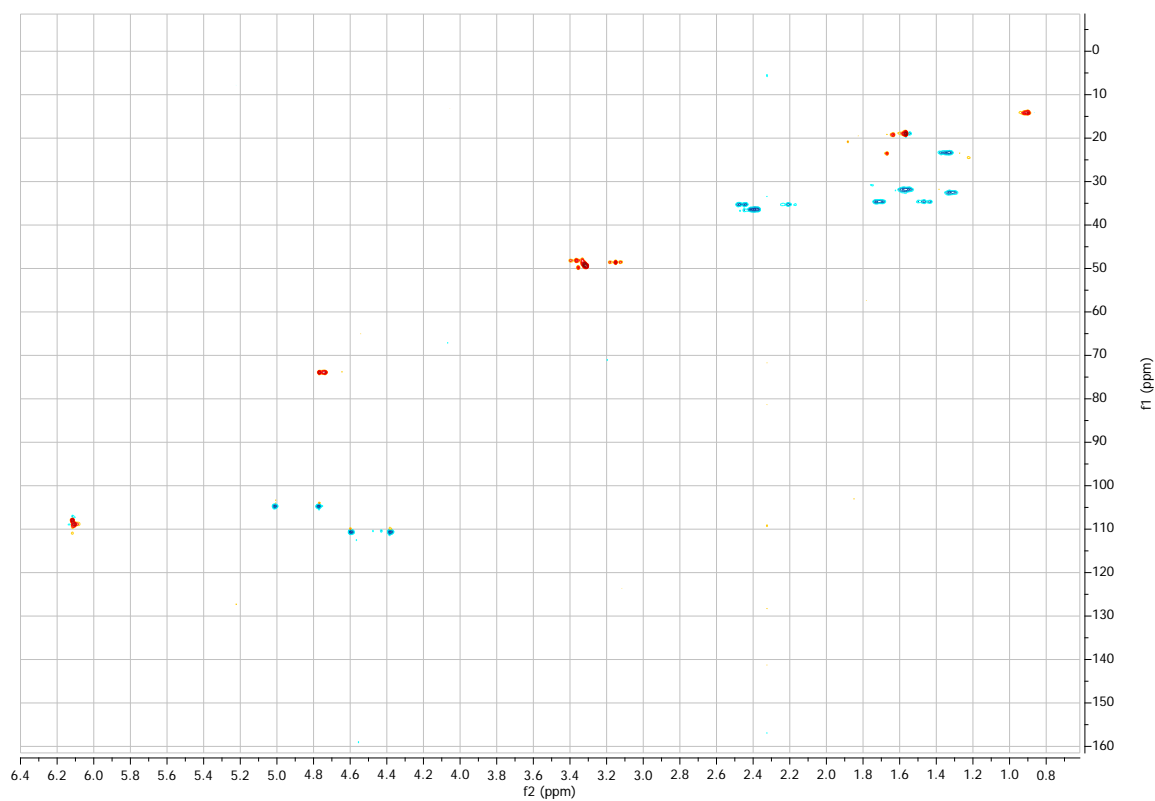


Figure S4. HSQC spectrum (CD₃OD, 400 MHz) of 2 α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1).

HMBC spectrum (CD₃OD, 400 MHz) of 2 α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1)

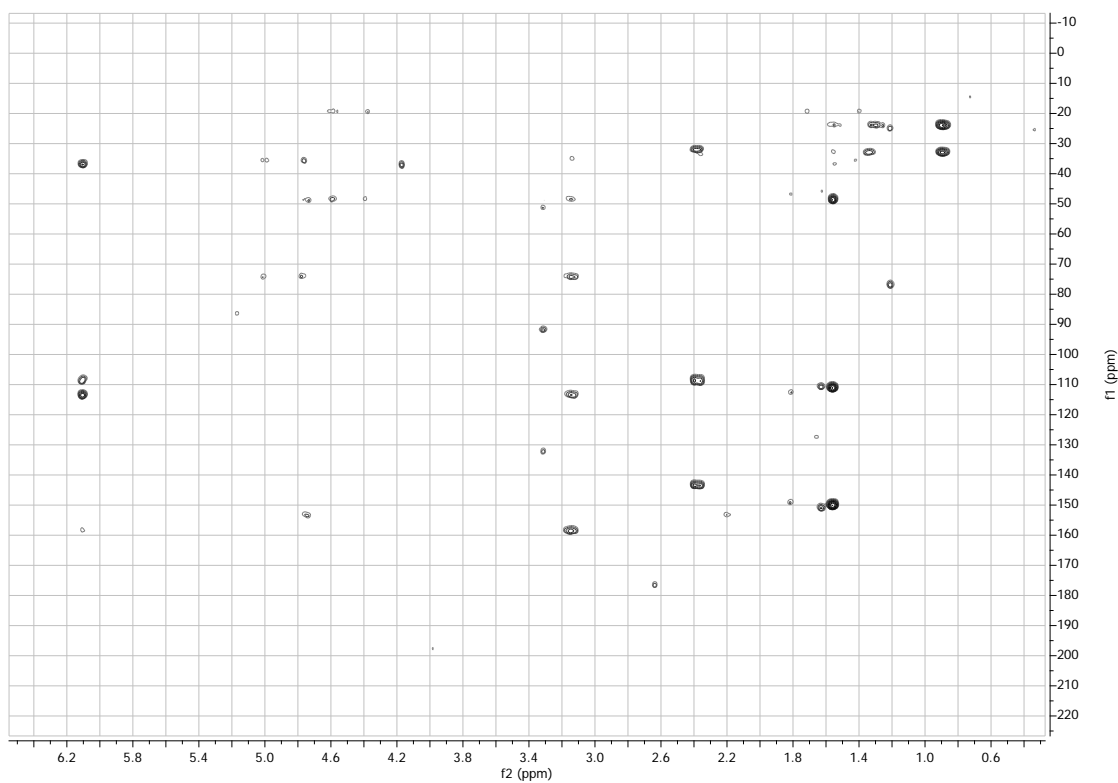


Figure S5. HMBC spectrum (CD₃OD, 400 MHz) of 2 α -hydroxy- $\Delta^{3,7}$ -cannabitrinol (1).

^1H NMR (CD_3OD , 400 MHz) of Cannabidiol (2)

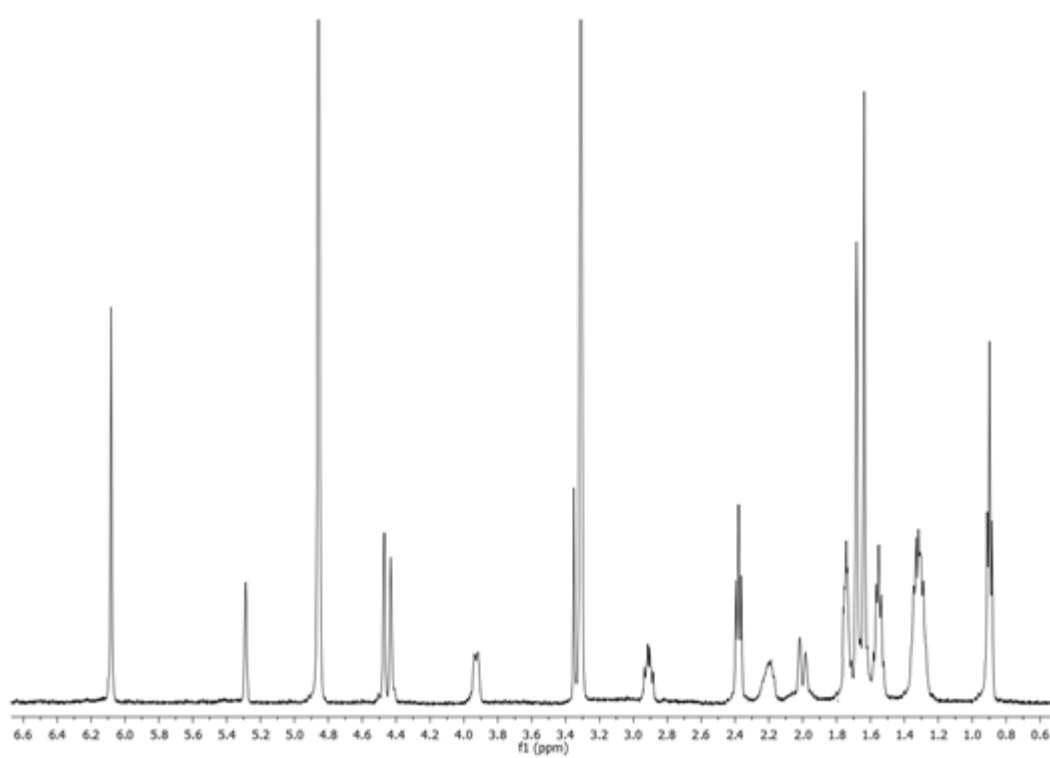


Figure S6. ^1H NMR (CD_3OD , 400 MHz) of Cannabidiol (2).

^1H NMR (CD_3OD , 400 MHz) of Cannabidiolic acid (3)

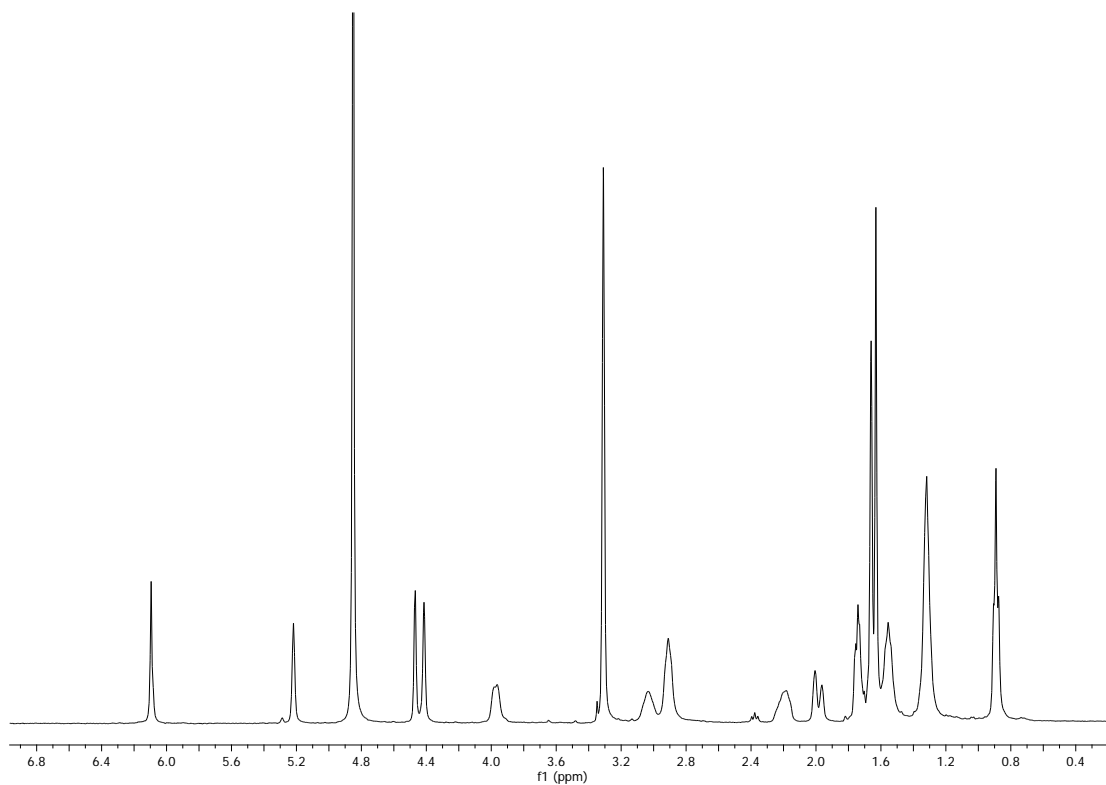


Figure S7. ^1H NMR (CD_3OD , 400 MHz) of Cannabidiolic acid (3).

^1H NMR ($\text{C}_5\text{D}_5\text{N}$, 500 MHz) of α -Cannabispiranol (4)

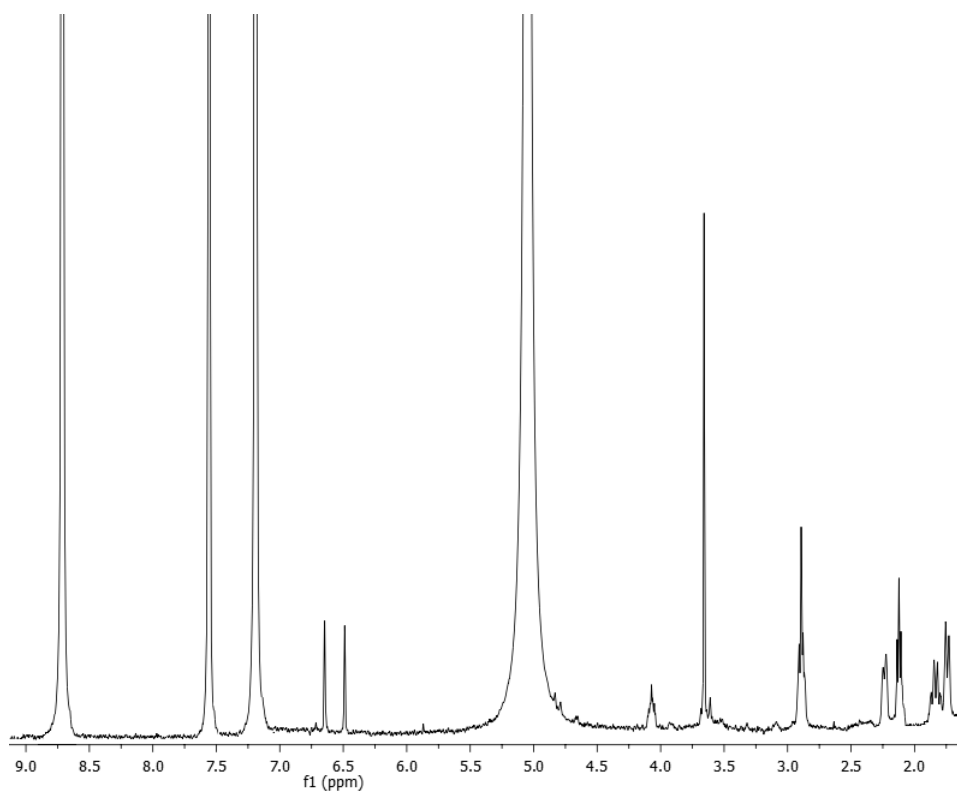


Figure S8. ^1H NMR ($\text{C}_5\text{D}_5\text{N}$, 500 MHz) of α -Cannabispiranol (4).

^1H NMR ($\text{C}_5\text{D}_5\text{N}$, 500 MHz) of β -Cannabispiranol (5)

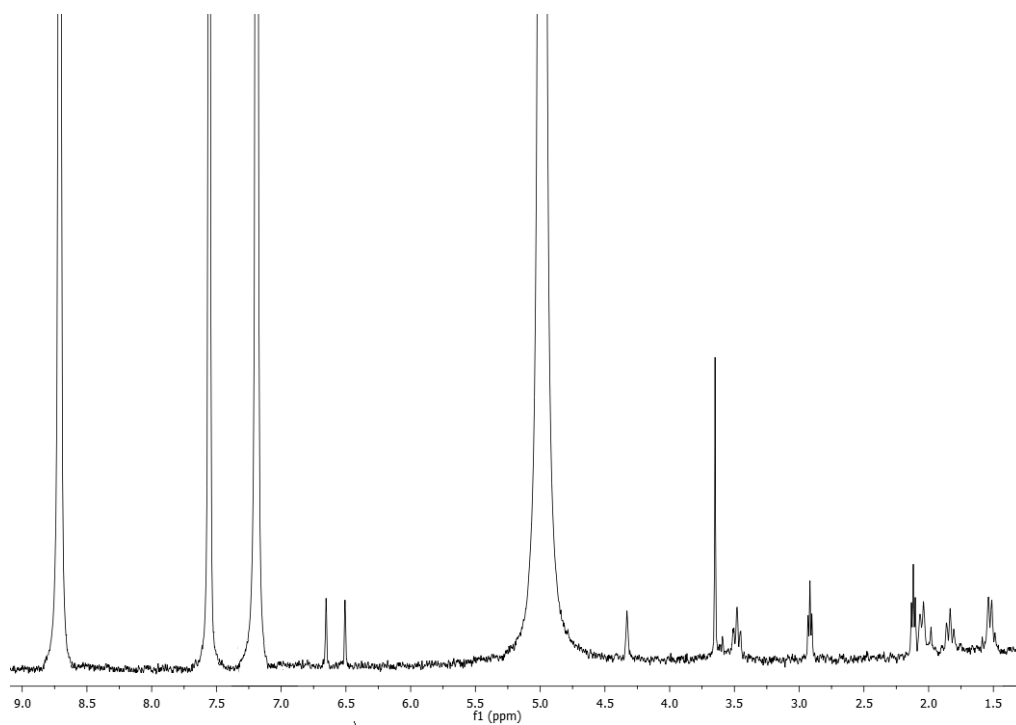


Figure S9. ^1H NMR ($\text{C}_5\text{D}_5\text{N}$, 500 MHz) of β -Cannabispiranol (5).

^1H NMR (CD_3OD , 500 MHz) of Canniprene (6)

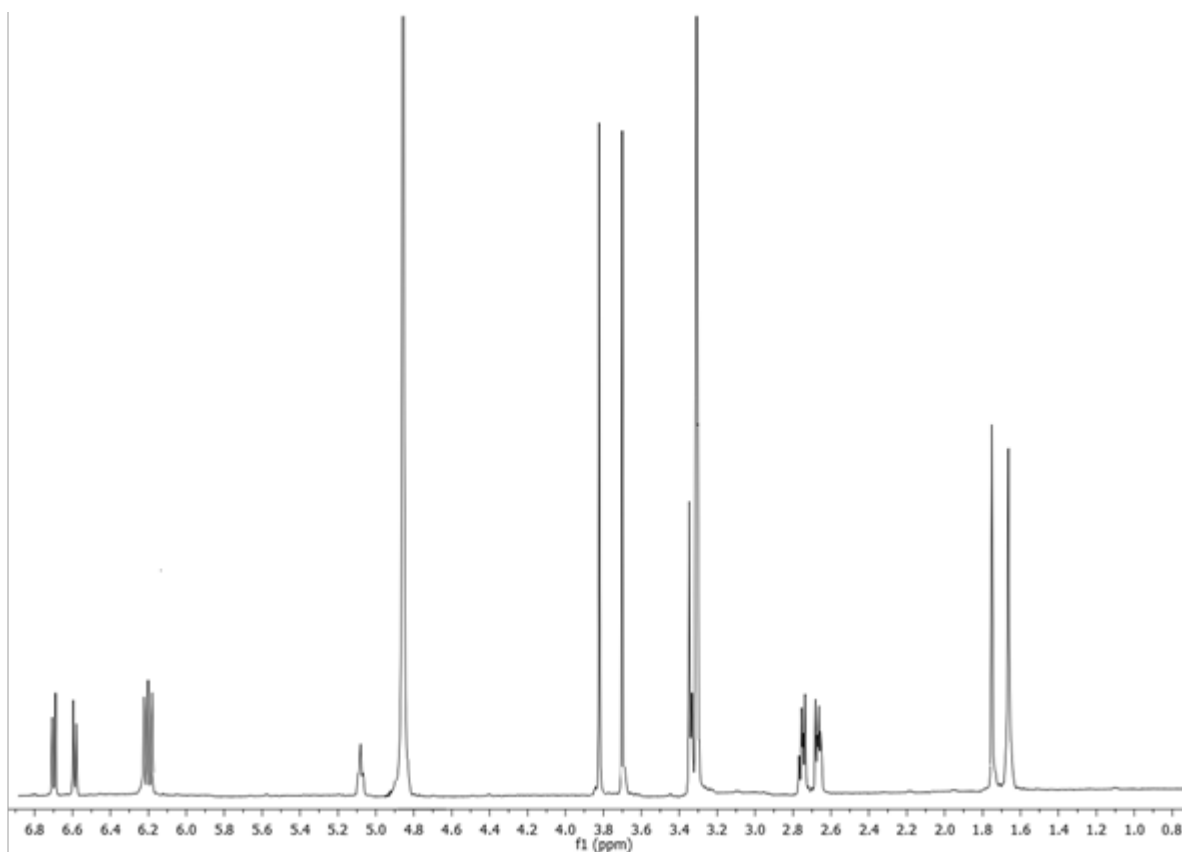


Figure S10. ^1H NMR (CD_3OD , 500 MHz) of Canniprene (6).

^1H NMR (CD_3OD , 400 MHz) of Cannabiripsol (7)

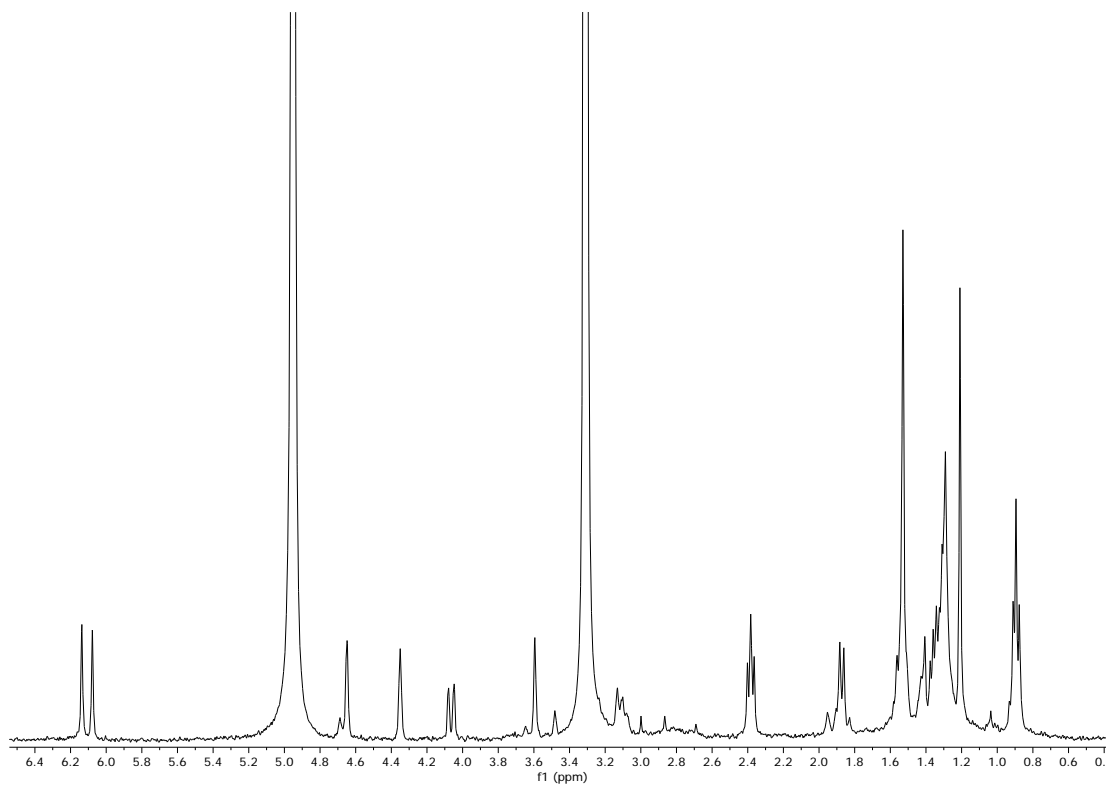


Figure S11. ^1H NMR (CD_3OD , 400 MHz) of Cannabiripsol (7).

^1H NMR (CD_3OD , 400 MHz) of Cannflavine B (8)

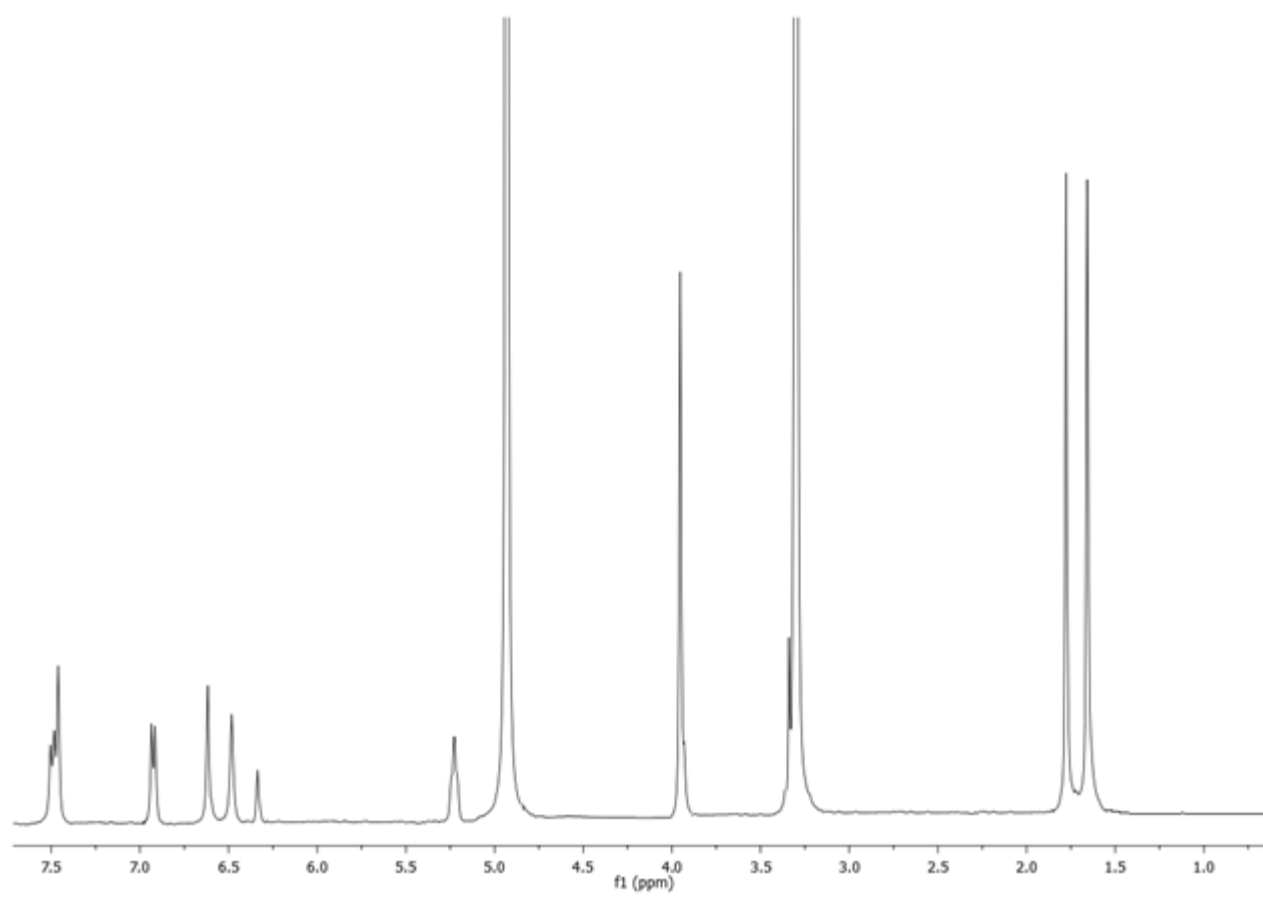


Figure S12. ^1H NMR (CD_3OD , 400 MHz) of Cannflavine B (8).

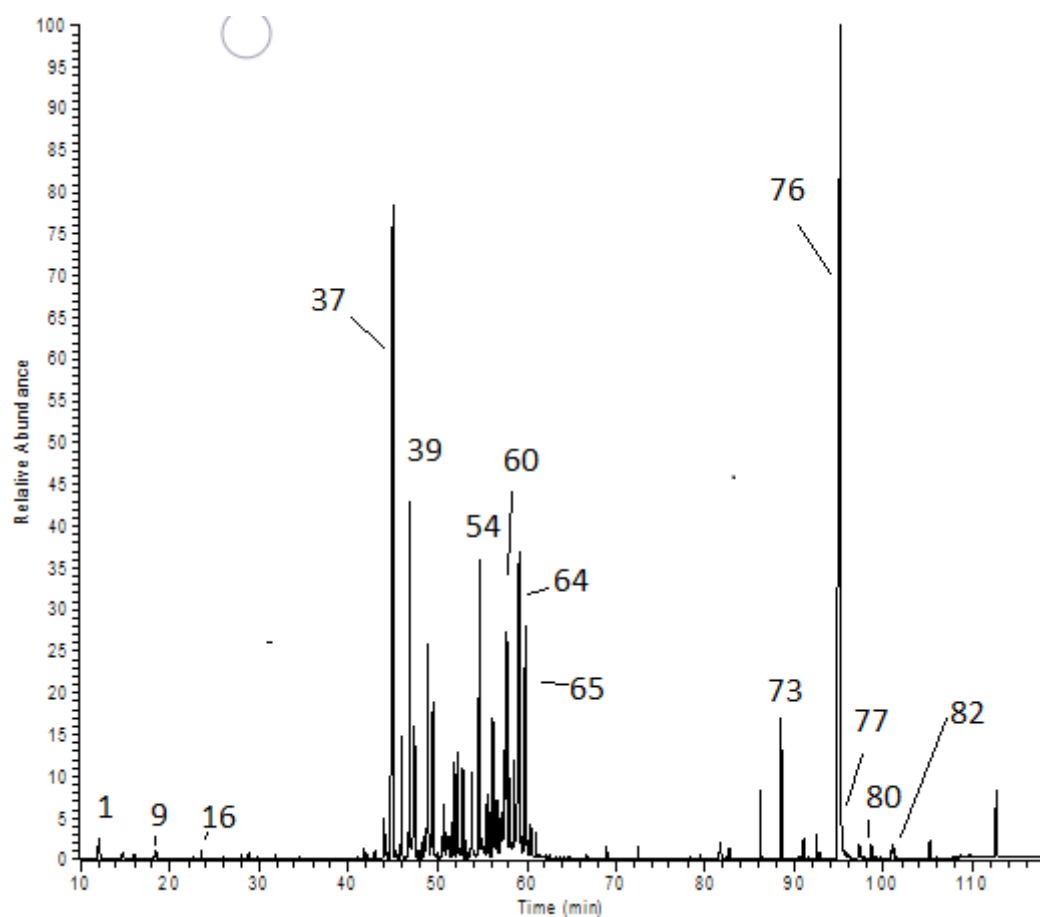


Figure S13. GC-MS TIC chromatogram of *C. sativa* L. cv. *Futura* 75. Numbers refer to those reported in Table 2.

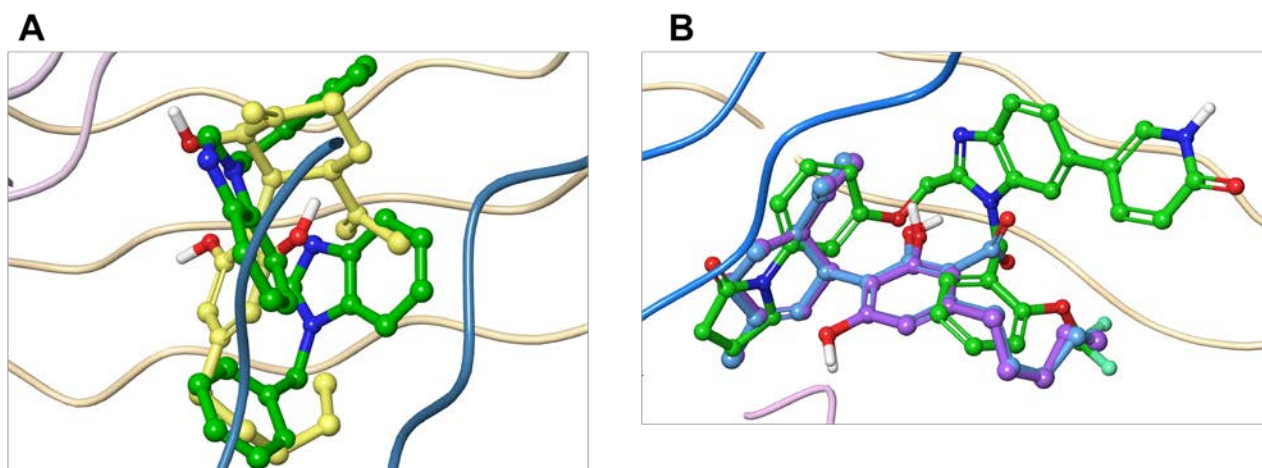


Figure S14. Superimposition of **1** (A) and **2** and **3** (B) with the co-crystallized inhibitors contained in 6X83 and 7KPA, respectively.

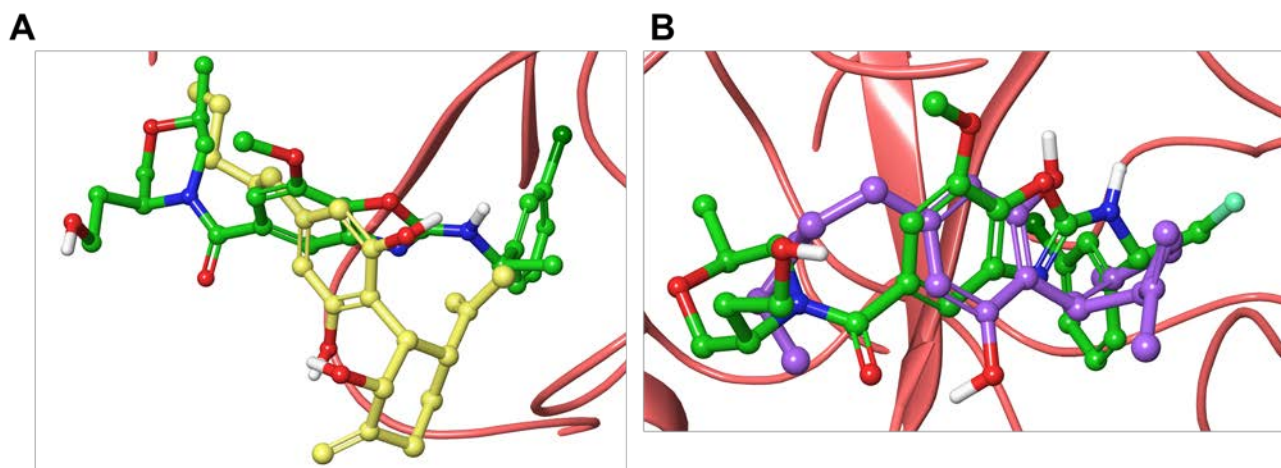


Figure S15. Superimposition of **1** (A) and **2** with the co-crystallized inhibitors contained in 6ZUX and 6ZV8, respectively.

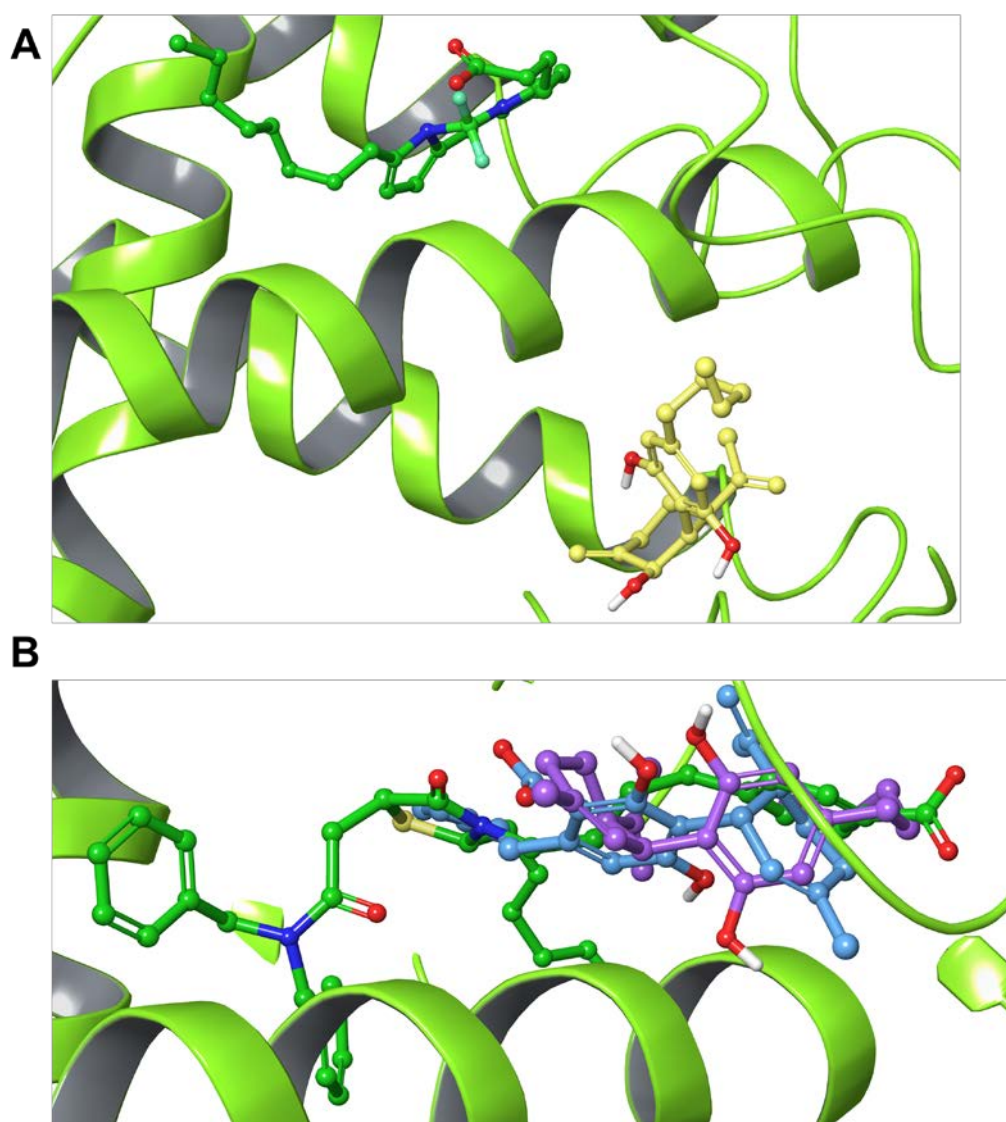


Figure S16. Superimposition of **1** (A) and **2** and **3** (B) with the co-crystallized inhibitors contained in 2ZK6 and 4PRG, respectively.