

# Cannabidiol as the Substrate in Acid-Catalysed Intramolecular Cyclization

*Paola Marzullo,<sup>†</sup> Francesca Foschi,<sup>†,‡</sup> Davide Andrea Coppini, Fabiola Fanchini, Lucia*

*Magnani, Selina Rusconi,<sup>§</sup> Marcello Luzzani,<sup>§</sup> Daniele Passarella\**

Dipartimento di Chimica, Università degli Studi di Milano, 20133 Milan, Italy

<sup>‡</sup>Dipartimento di Scienza e Alta Tecnologia, Università degli Studi dell'Insubria, 22100

Como, Italy; <sup>§</sup>LINNEA SA, 6595 Riazzino (TI), Switzerland

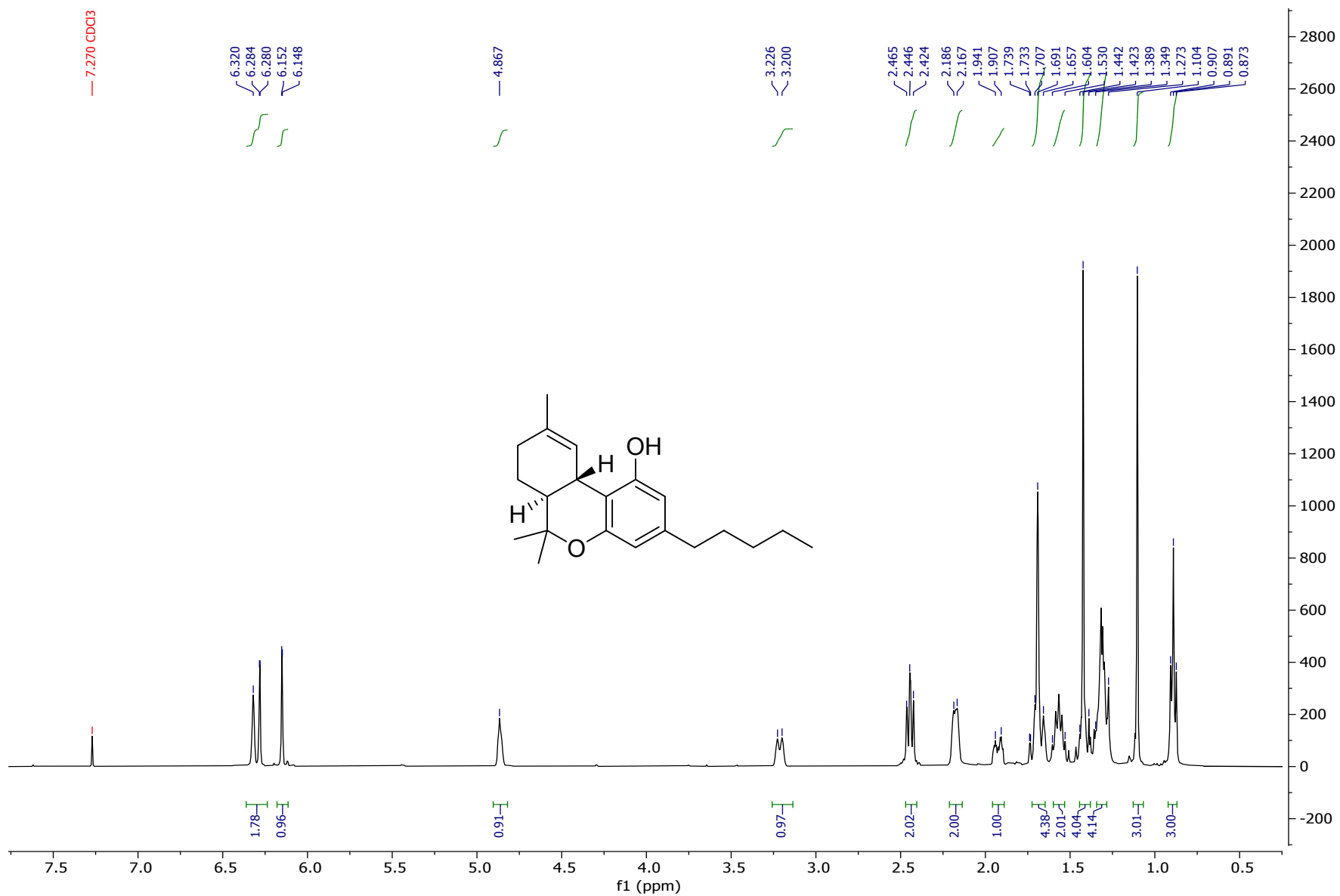


Figure S1. <sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of  $\Delta^9$ -THC

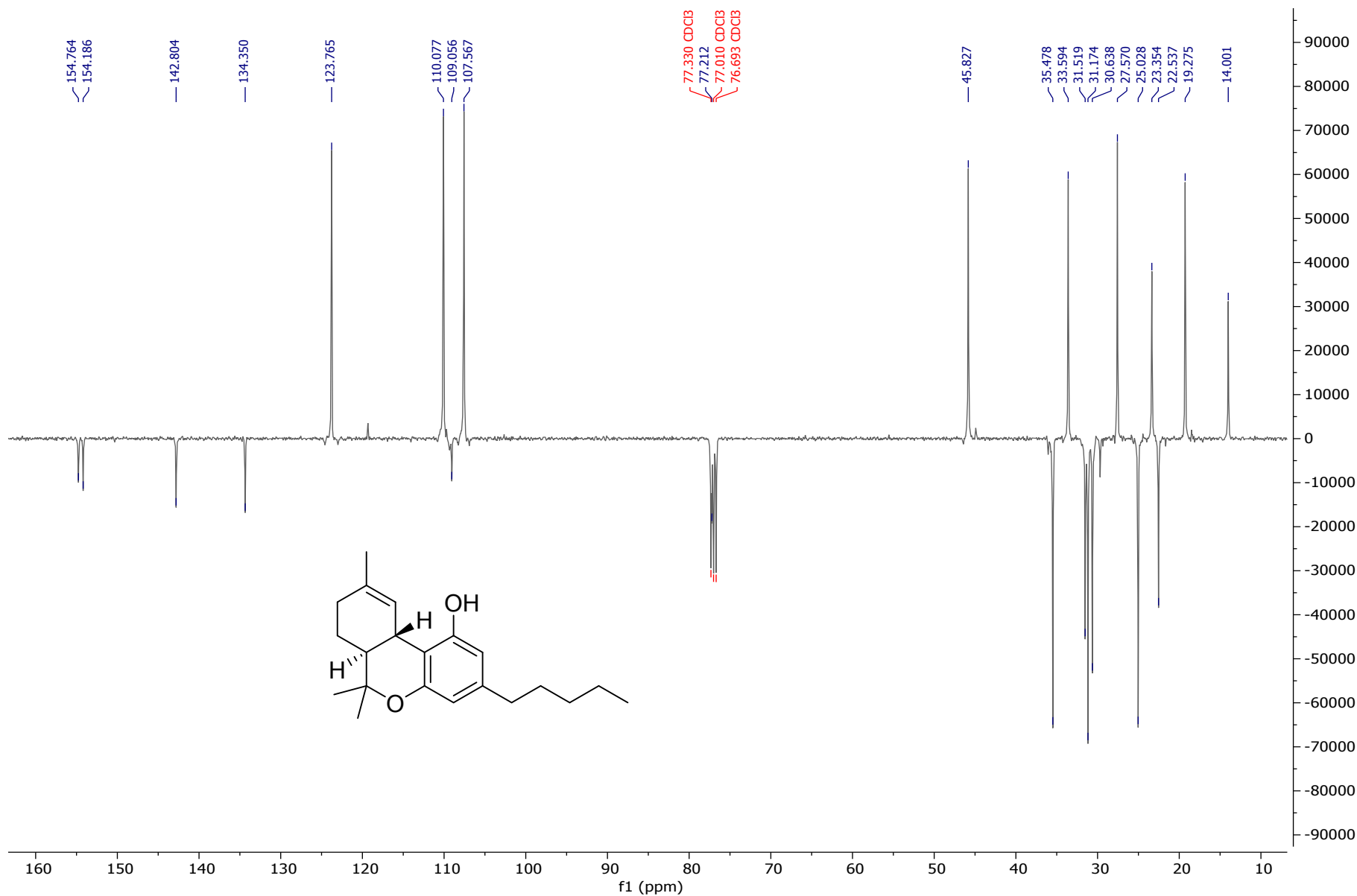
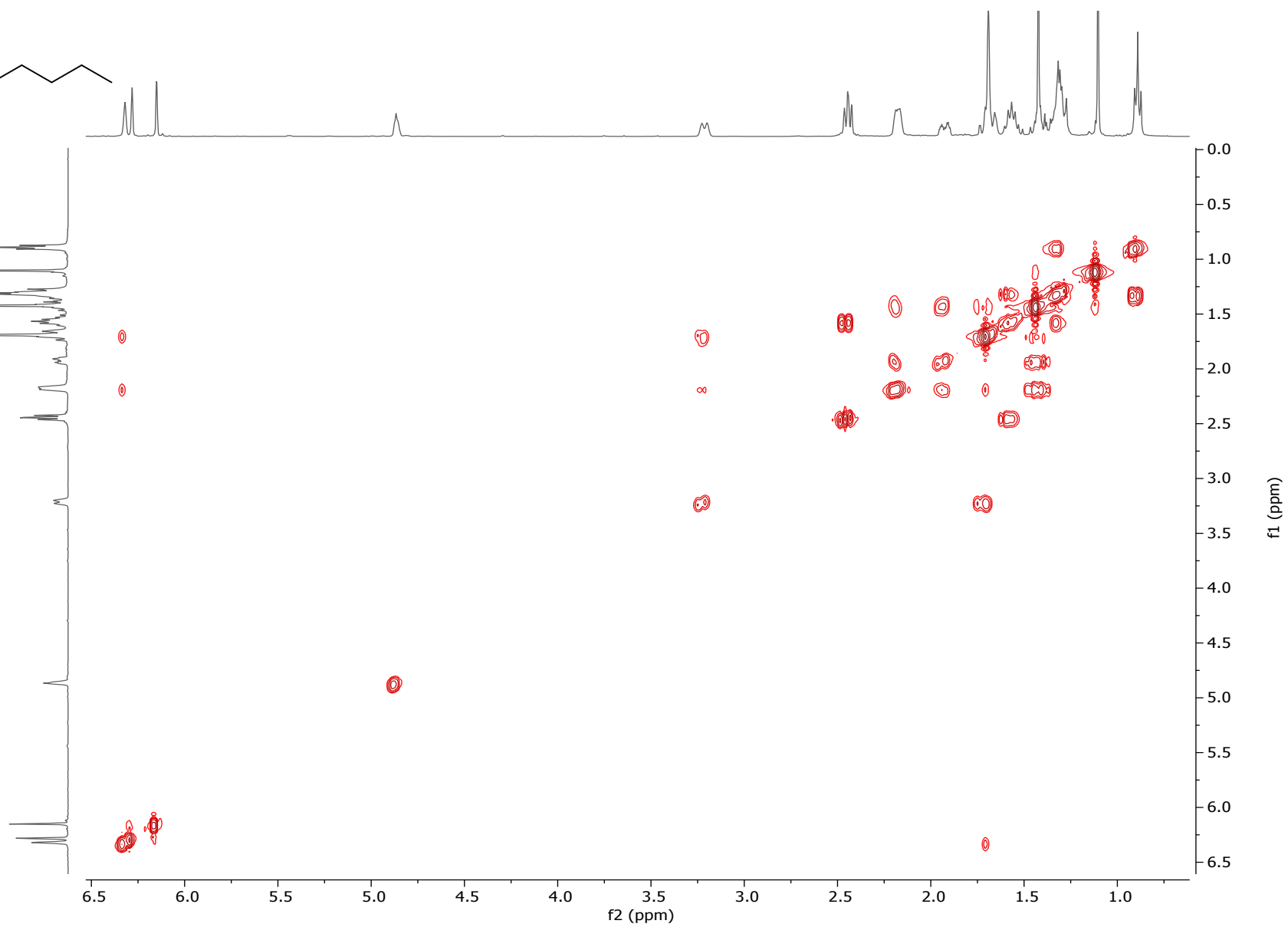
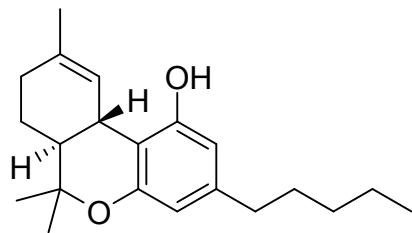


Figure S2. <sup>13</sup>C NMR APT Spectrum (101 MHz, CDCl<sub>3</sub>) of Δ<sup>9</sup>-THC



**Figure S3.**  $^1\text{H}$  COSY Spectrum in  $\text{CDCl}_3$  of  $\Delta^9$ -THC

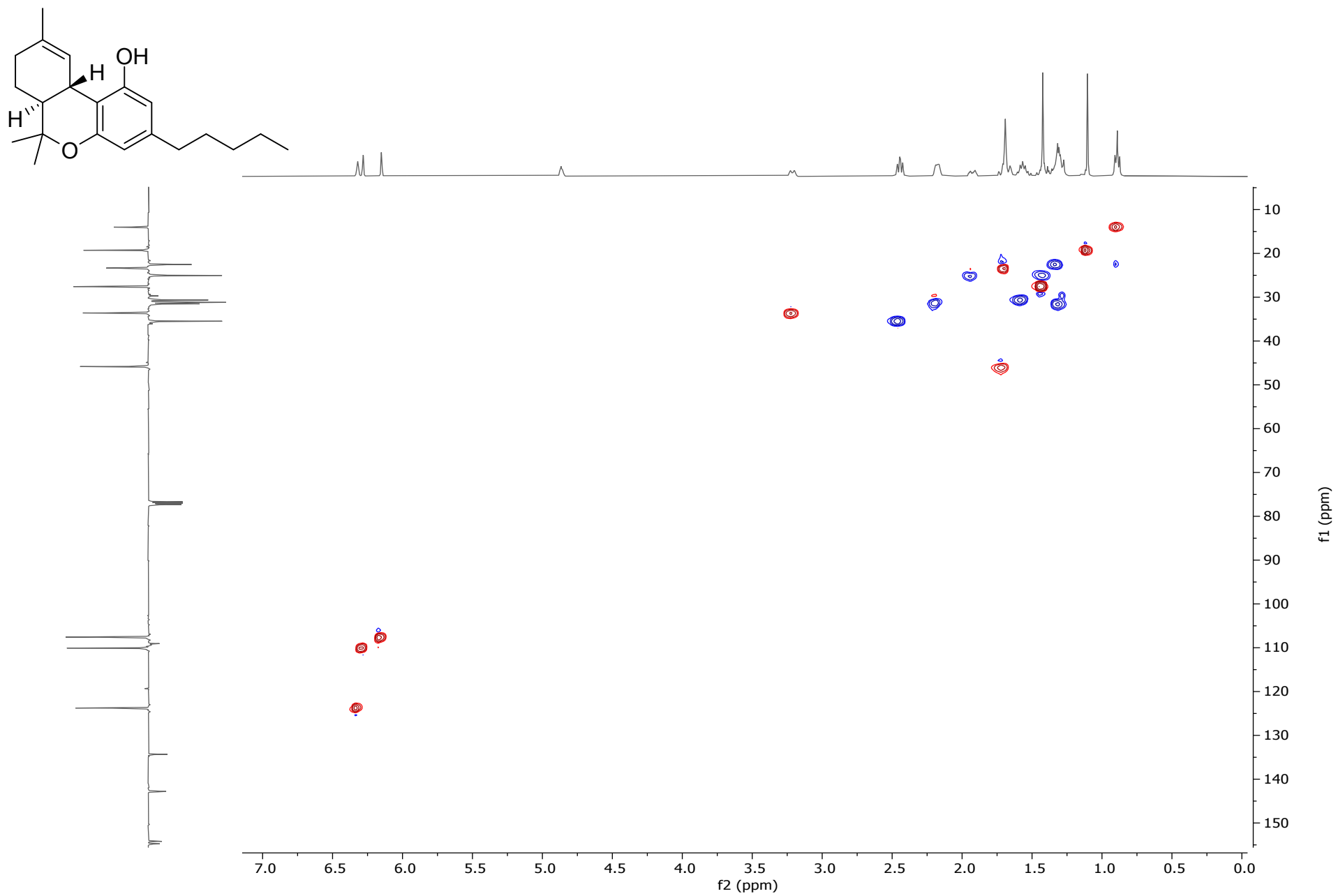


Figure S4. HSQC Spectrum in  $\text{CDCl}_3$  of  $\Delta^9$ -THC

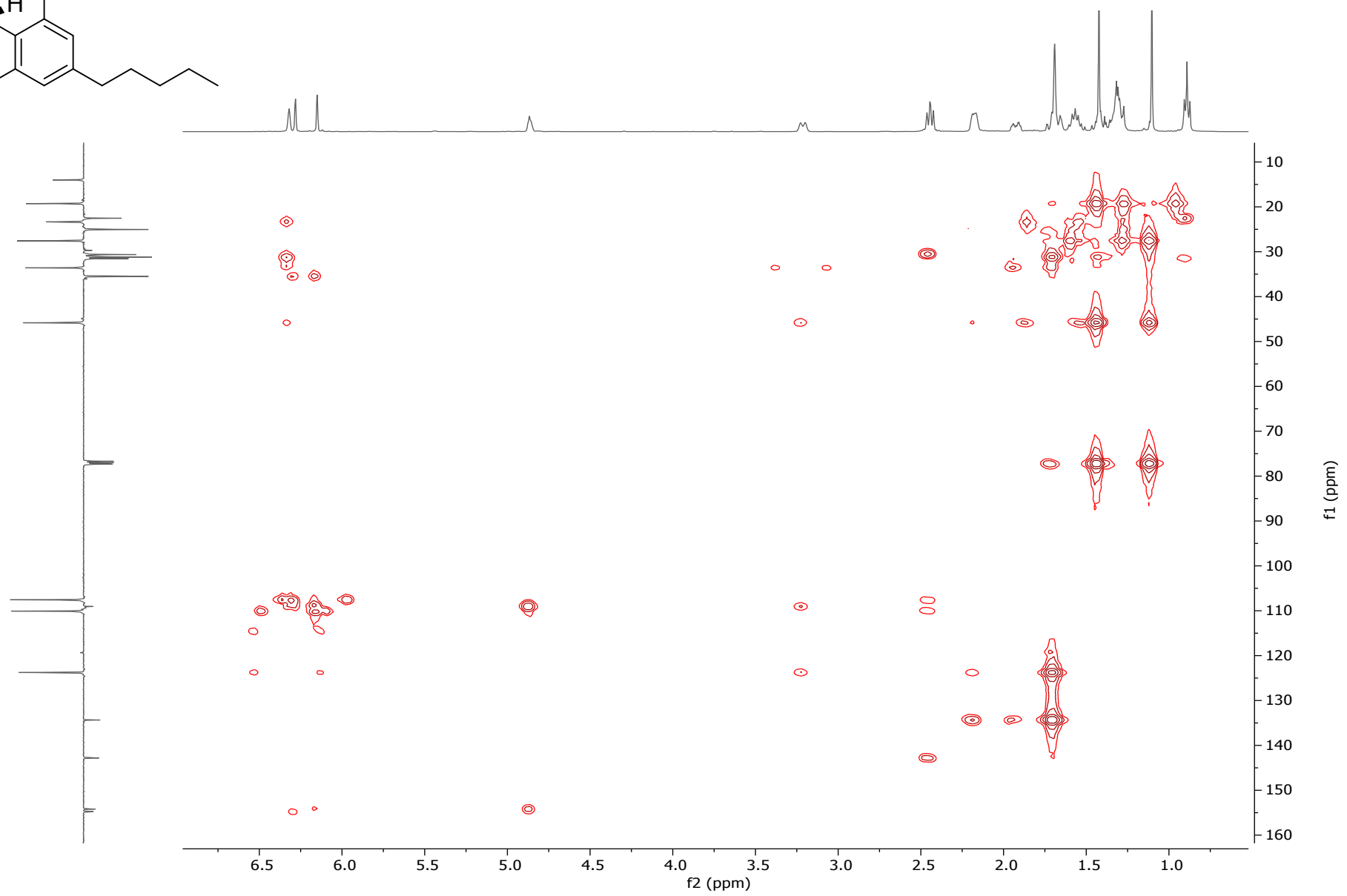
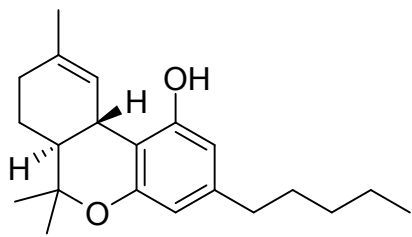


Figure S5. HMBC Spectrum in  $CDCl_3$  of  $\Delta^9$ -THC

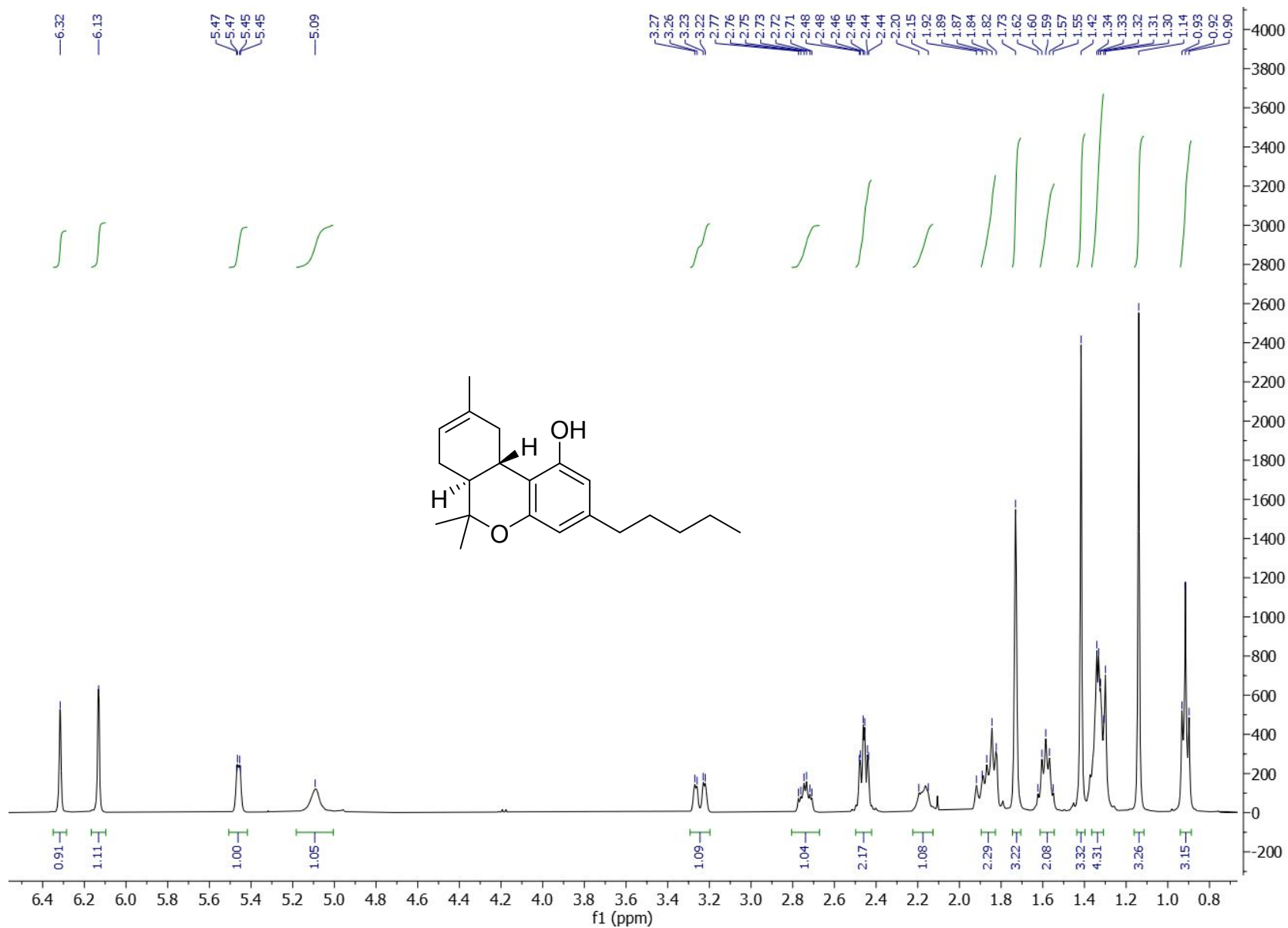


Figure S6.  $^1\text{H}$  NMR Spectrum (400 MHz,  $\text{CDCl}_3$ ) of  $\Delta^8$ -THC



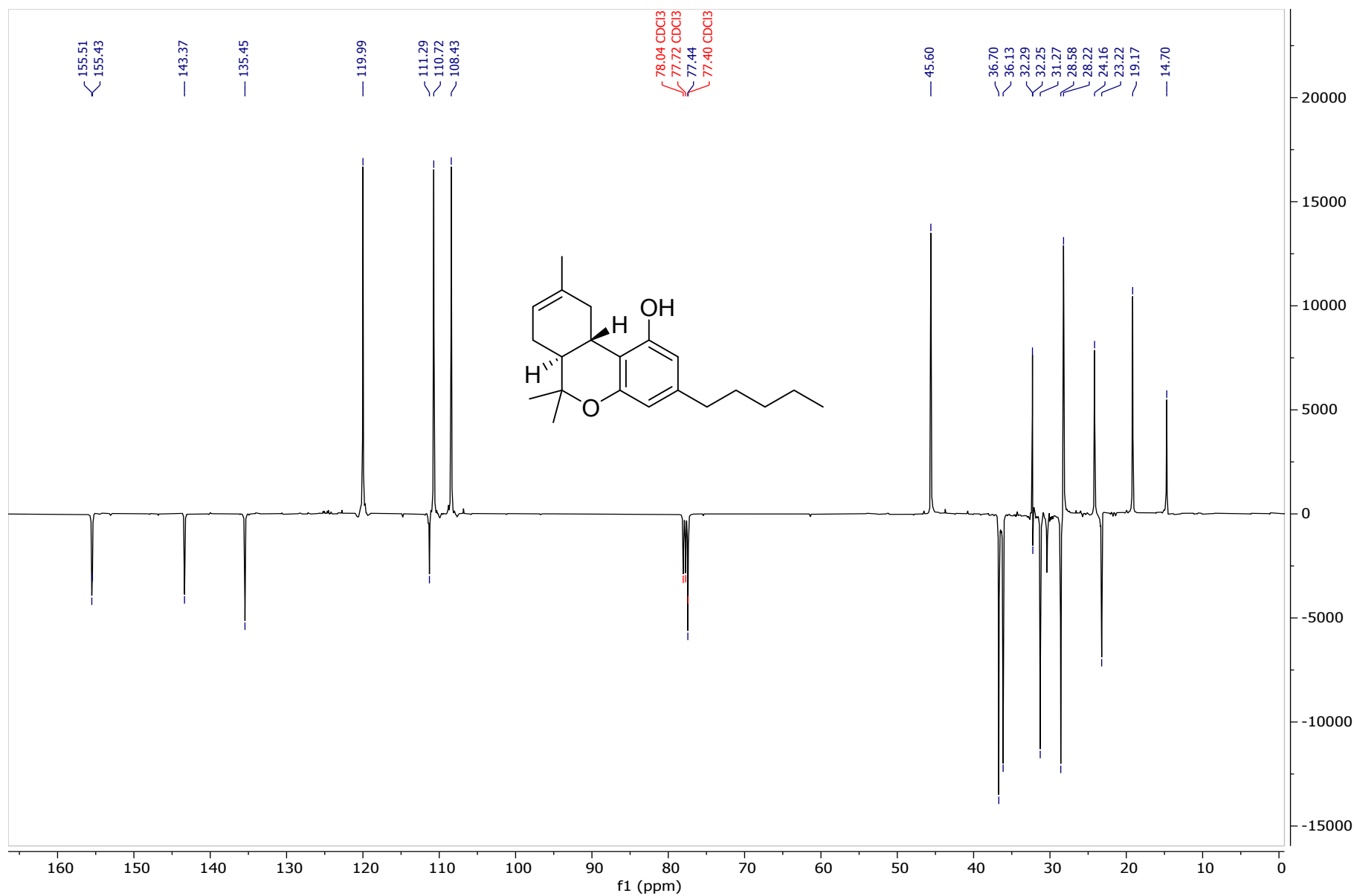


Figure S7.  $^{13}C$  NMR APT Spectrum (101 MHz,  $CDCl_3$ ) of  $\Delta^8$ -THC

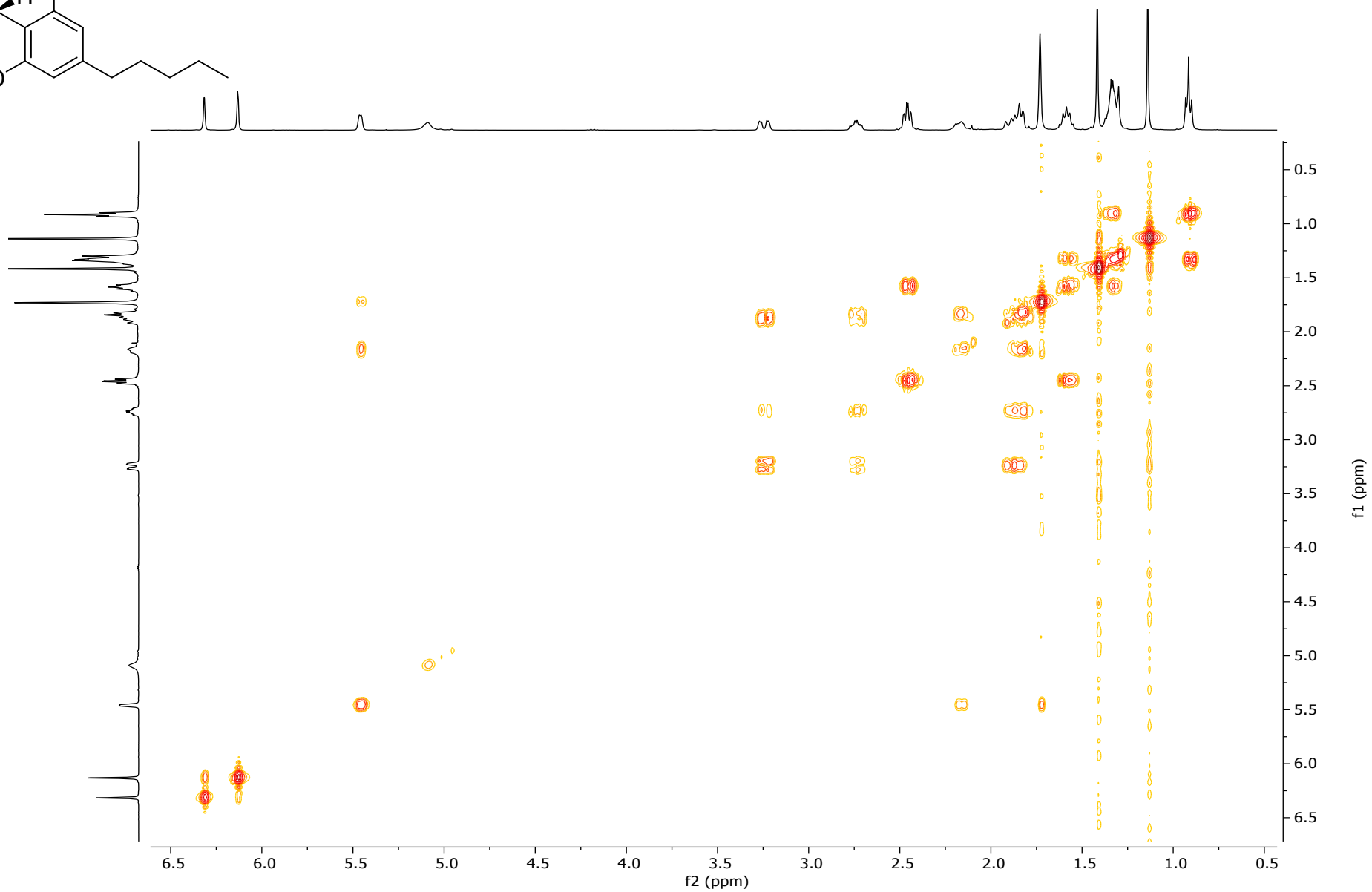
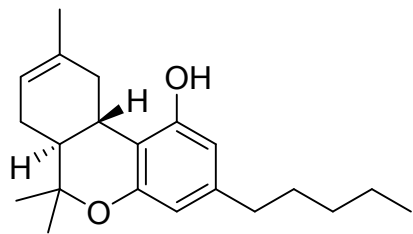


Figure S8.  $^1\text{H}$  COSY Spectrum in  $\text{CDCl}_3$  of  $\Delta^8$ -THC

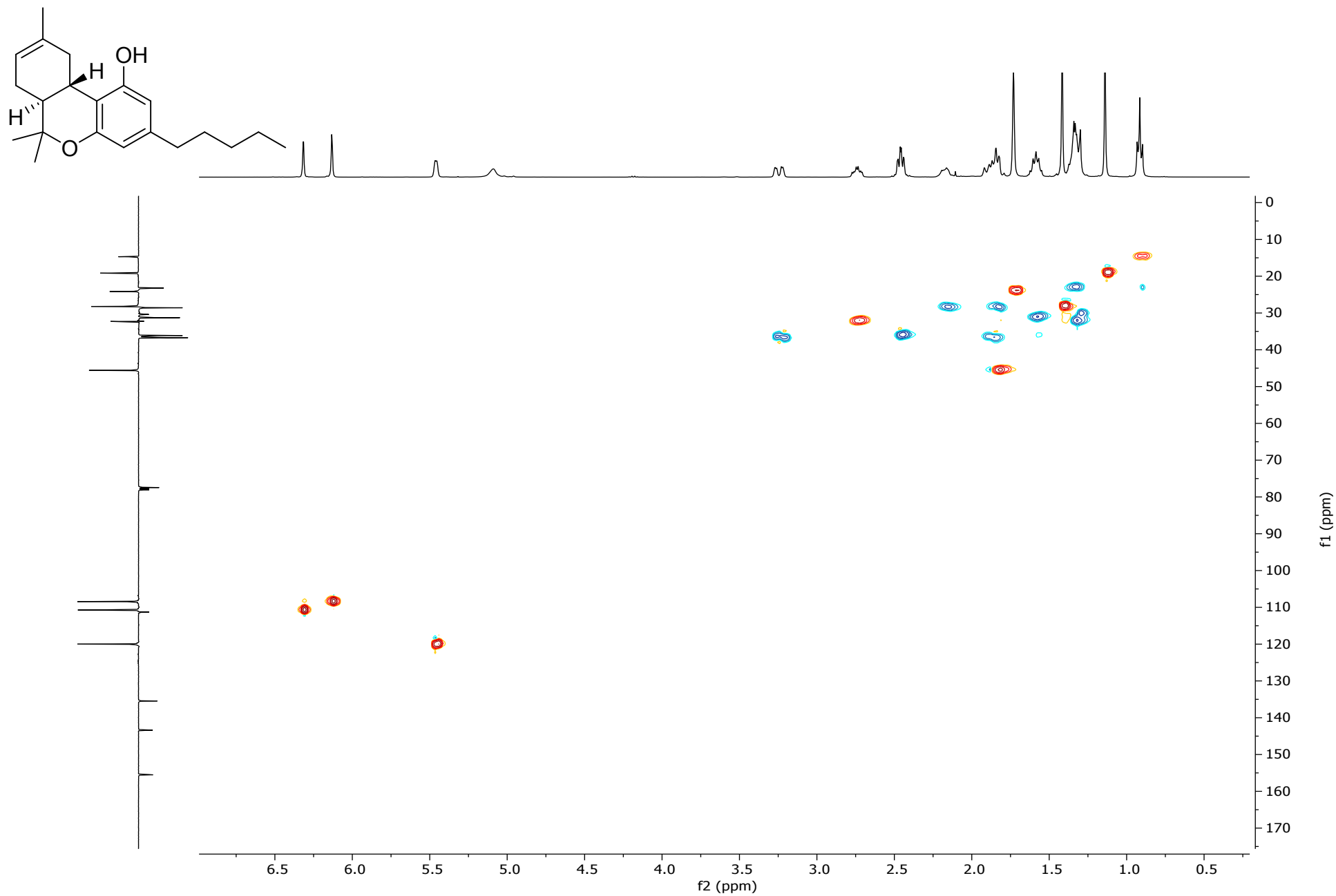


Figure S9. HSQC Spectrum in  $\text{CDCl}_3$  of  $\Delta^8$ -THC

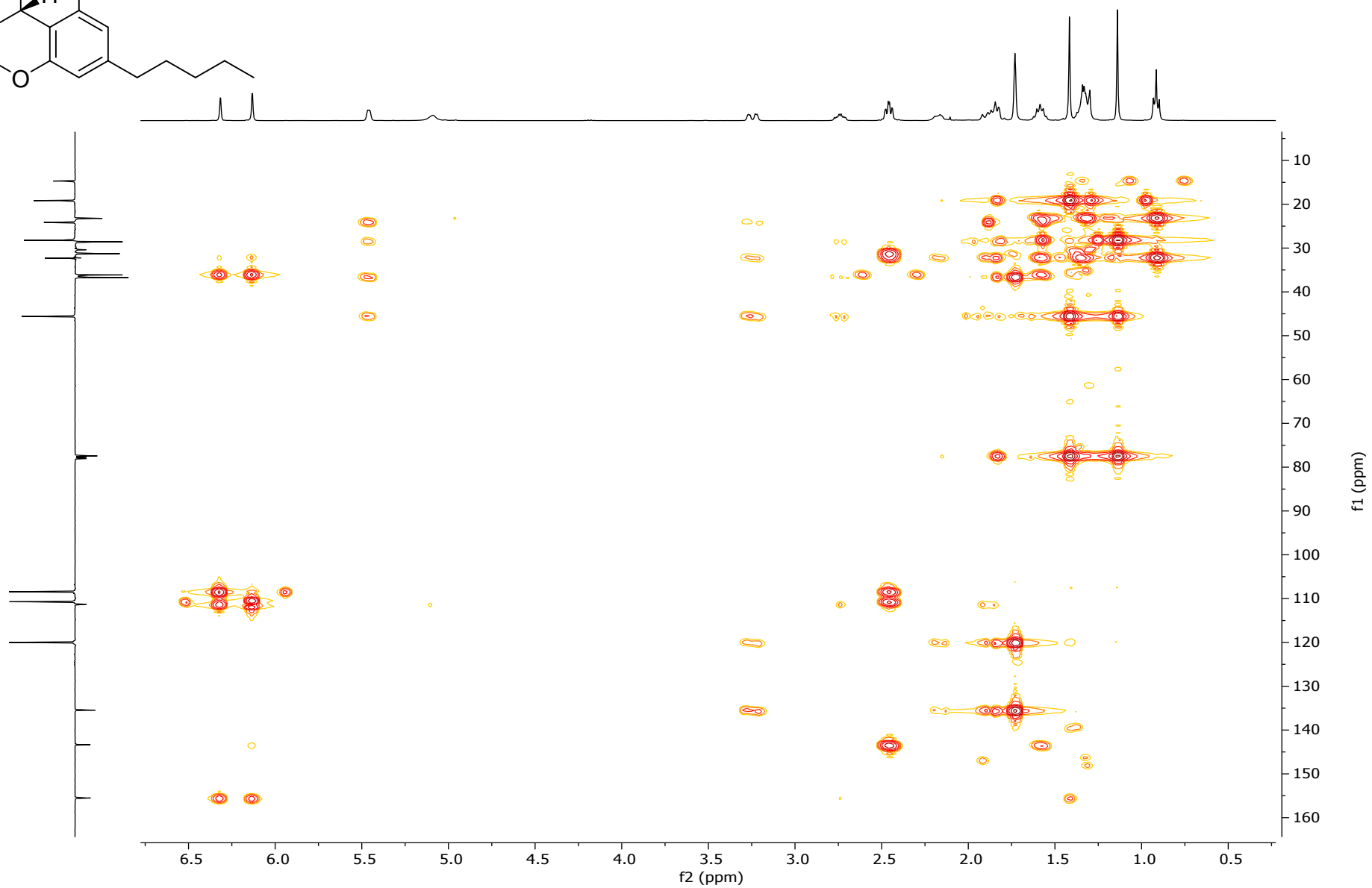
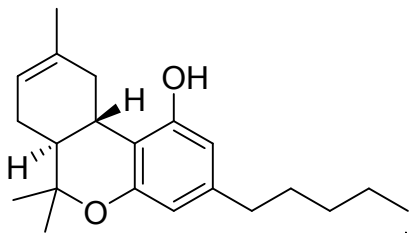


Figure S10. HMBC Spectrum in  $CDCl_3$  of  $\Delta^8$ -THC

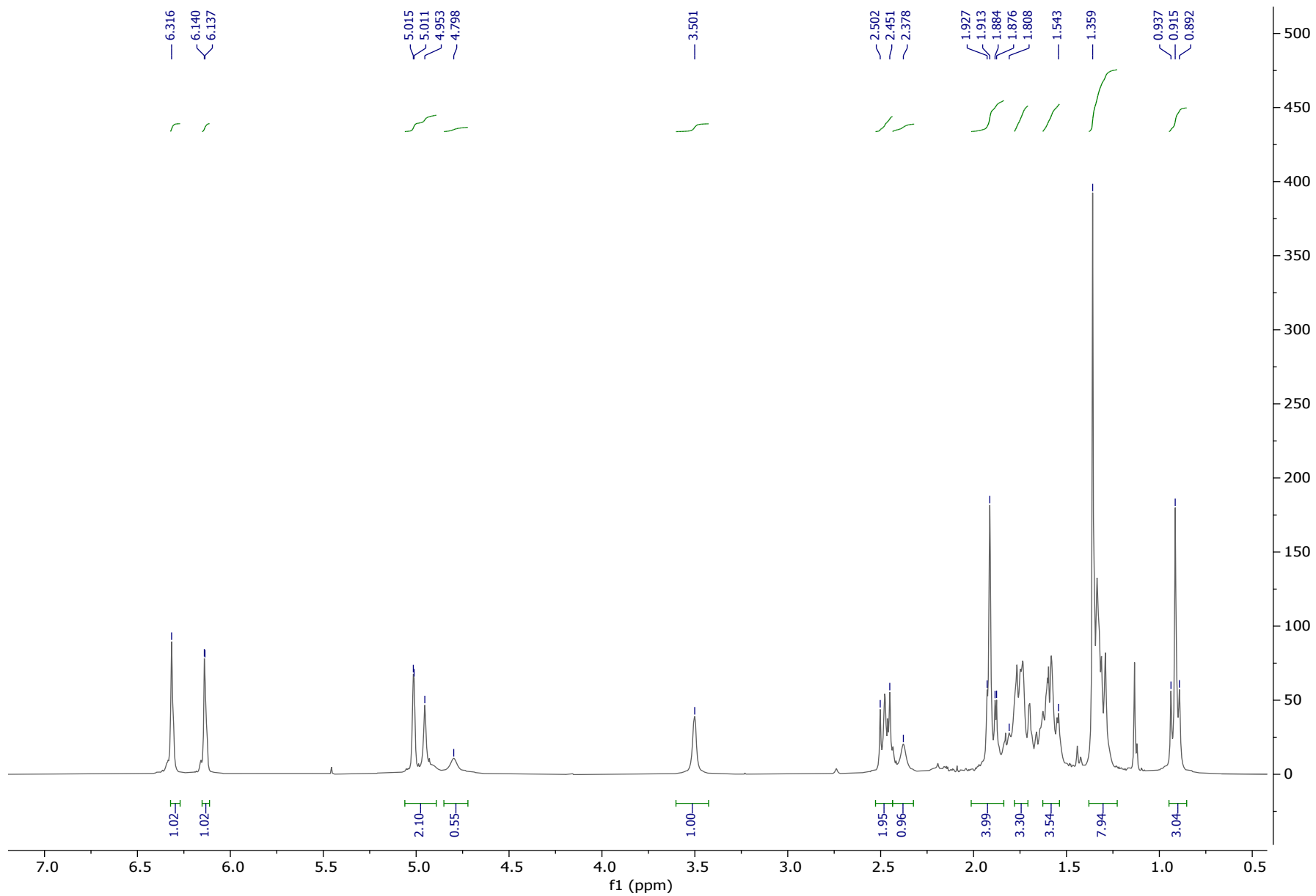
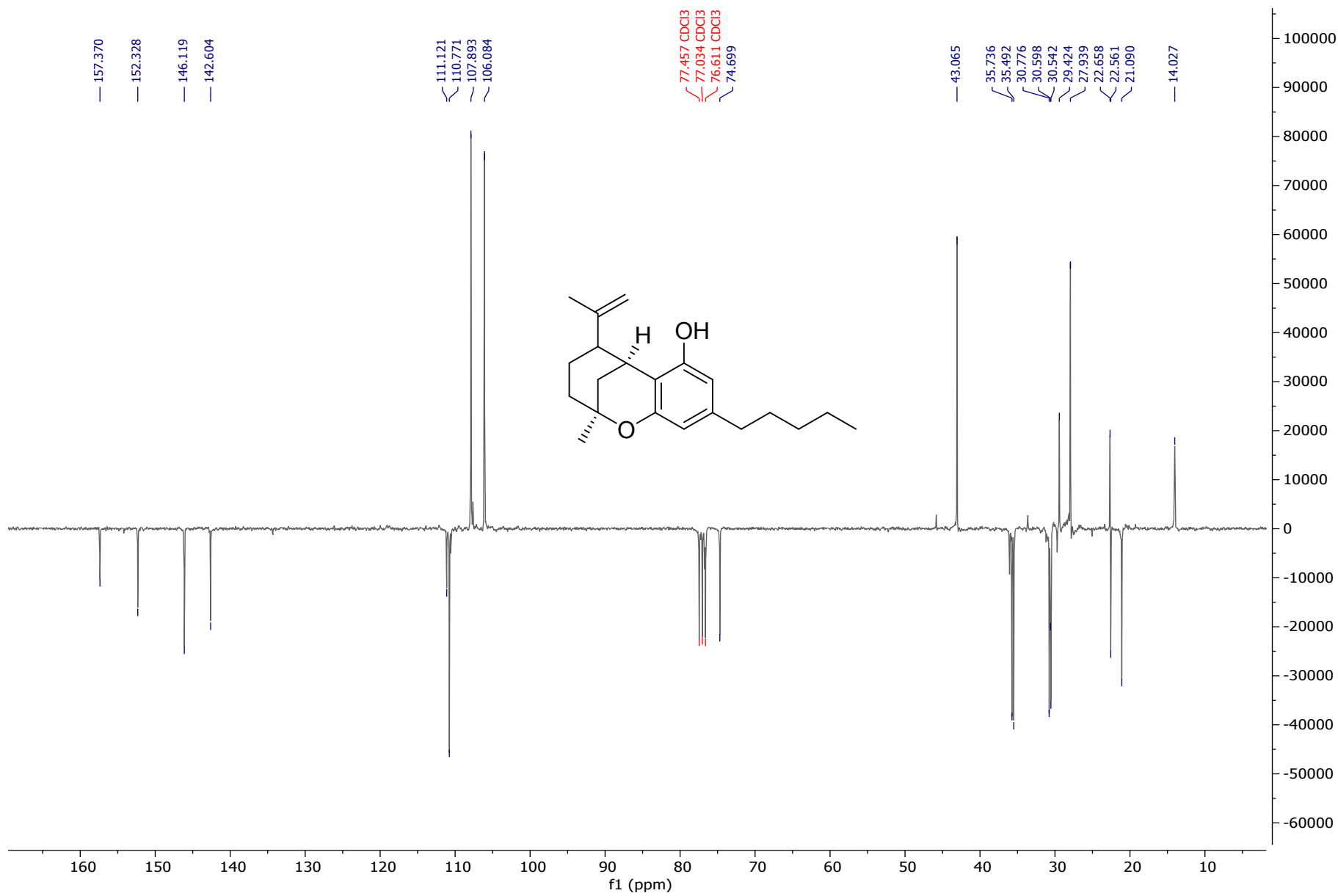
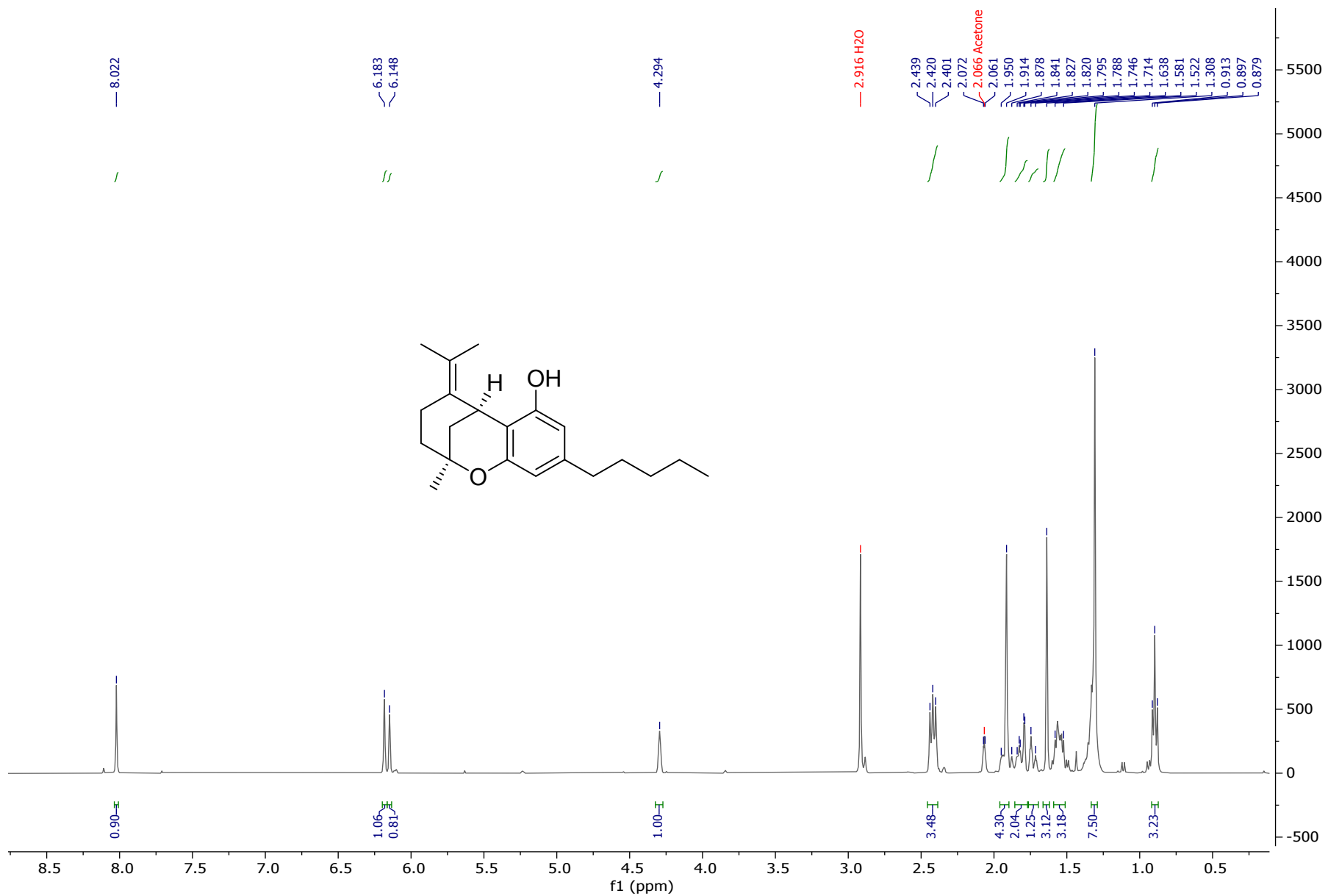


Figure S11.  $^1\text{H}$  NMR Spectrum (300 MHz,  $\text{CDCl}_3$ ) of  $\Delta^8$ -*iso*-THC

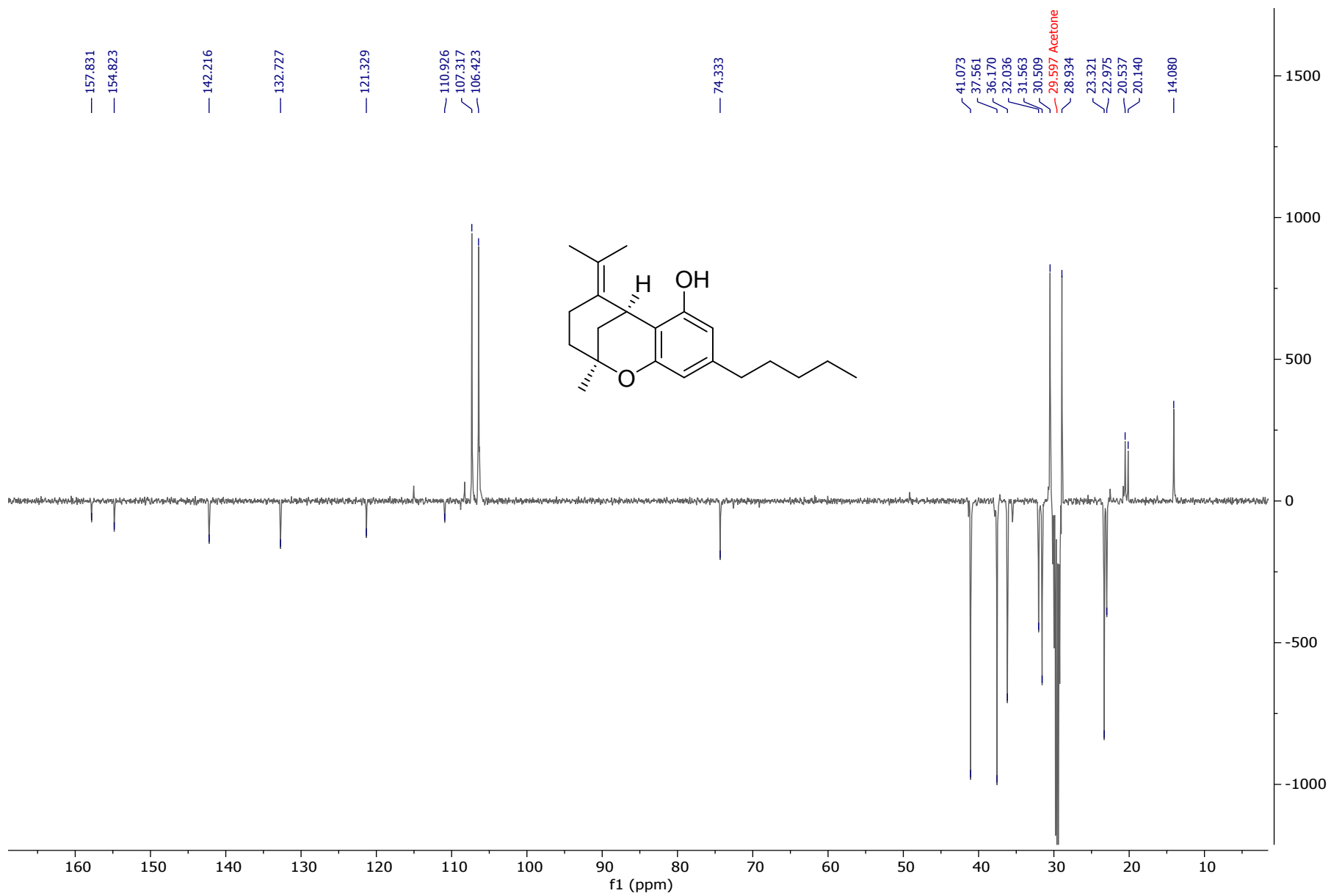


**Figure S12.**  $^{13}\text{C}$  NMR APT Spectrum (101 MHz,  $\text{CDCl}_3$ ) of  $\Delta^8$ -*iso*-THC

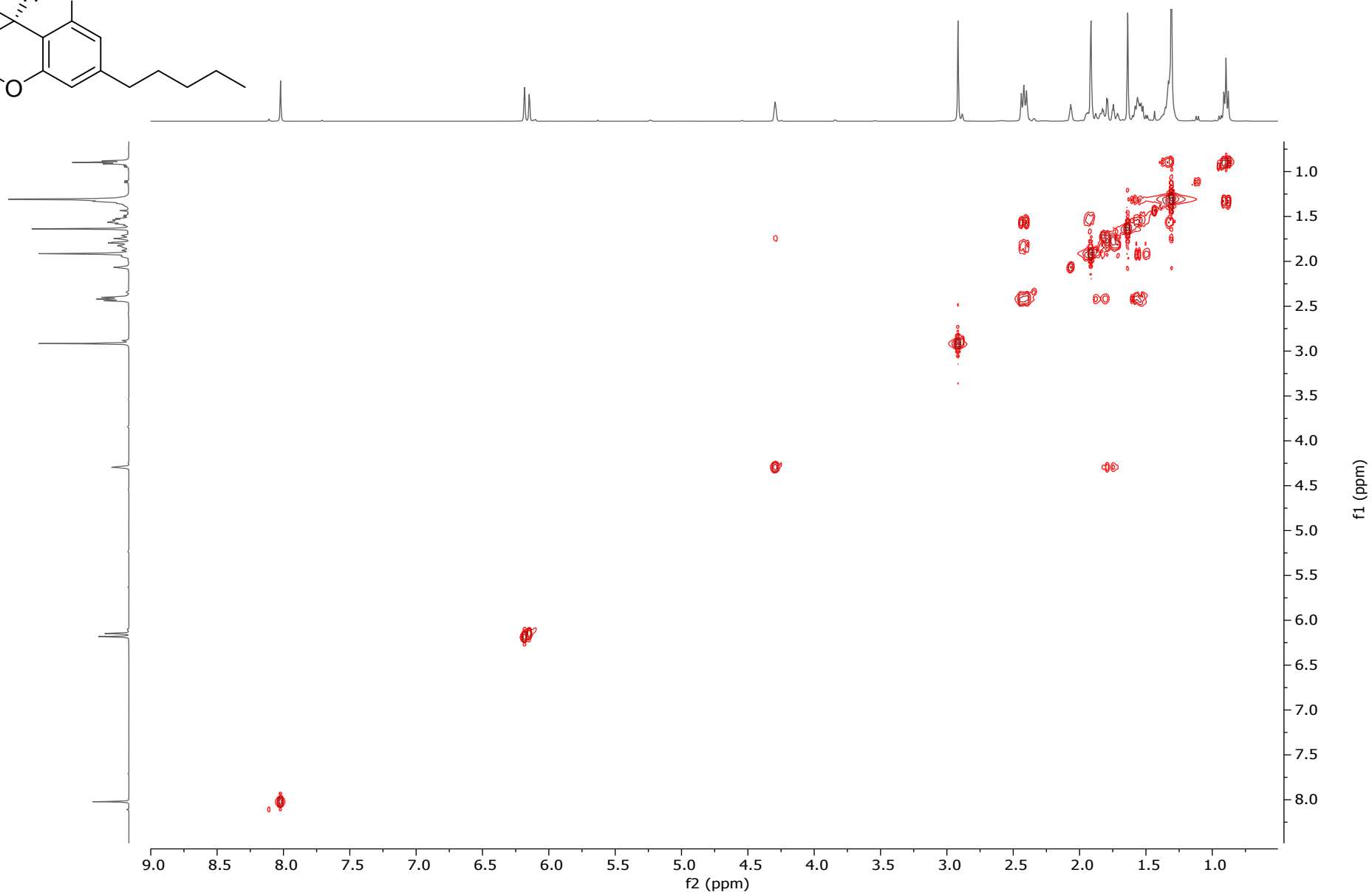
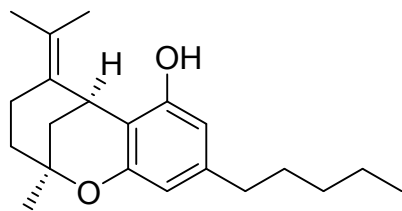




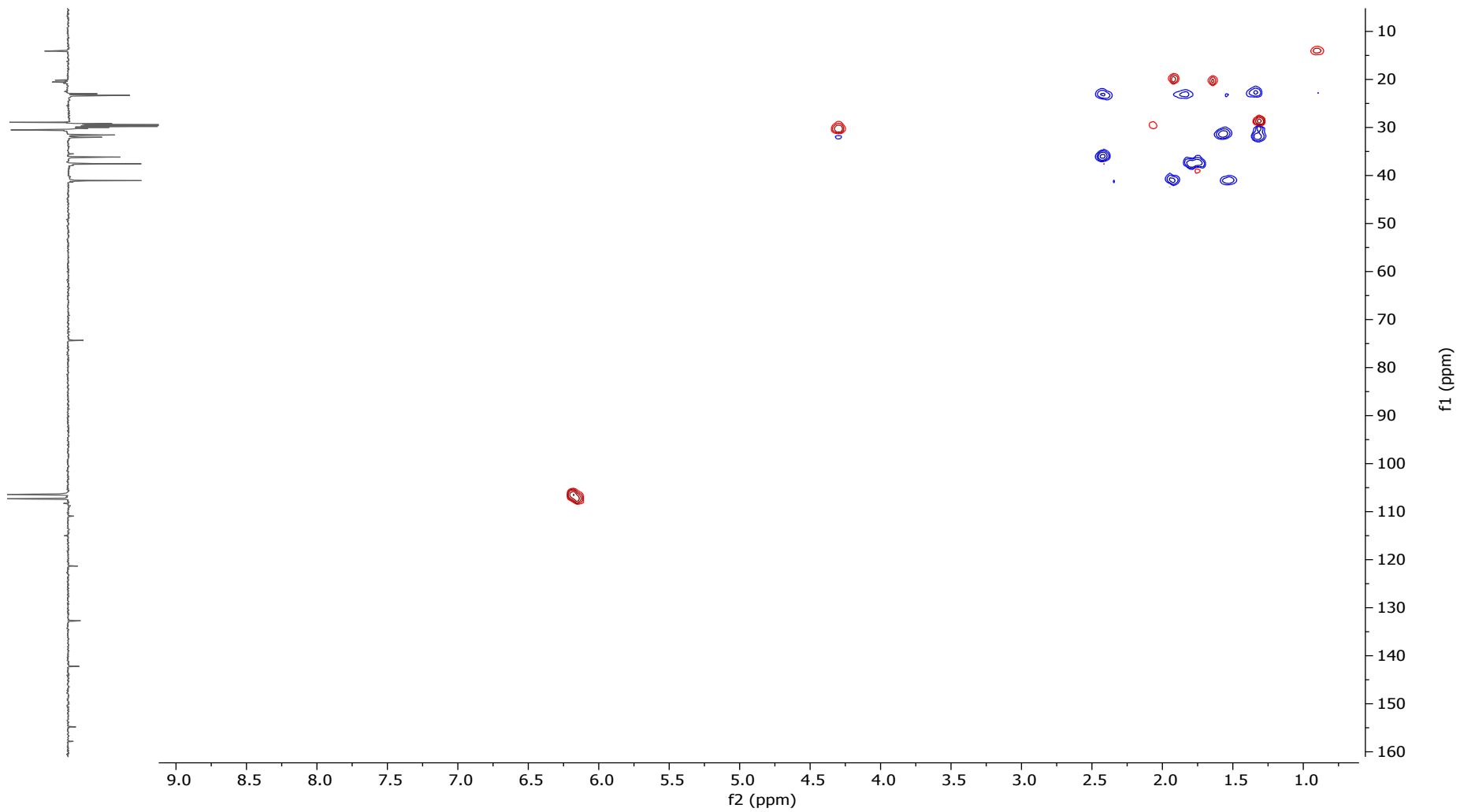
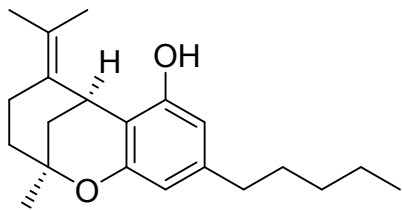
**Figure S13.**  $^1\text{H}$  NMR Spectrum (400 MHz, acetone- $d_6$ ) of  $\Delta^{4(8)}$ -*iso*-THC



**Figure S14.**  $^{13}\text{C}$  NMR APT Spectrum (101 MHz, acetone- $d_6$ ) of  $\Delta^{4(8)}$ -*iso*-THC

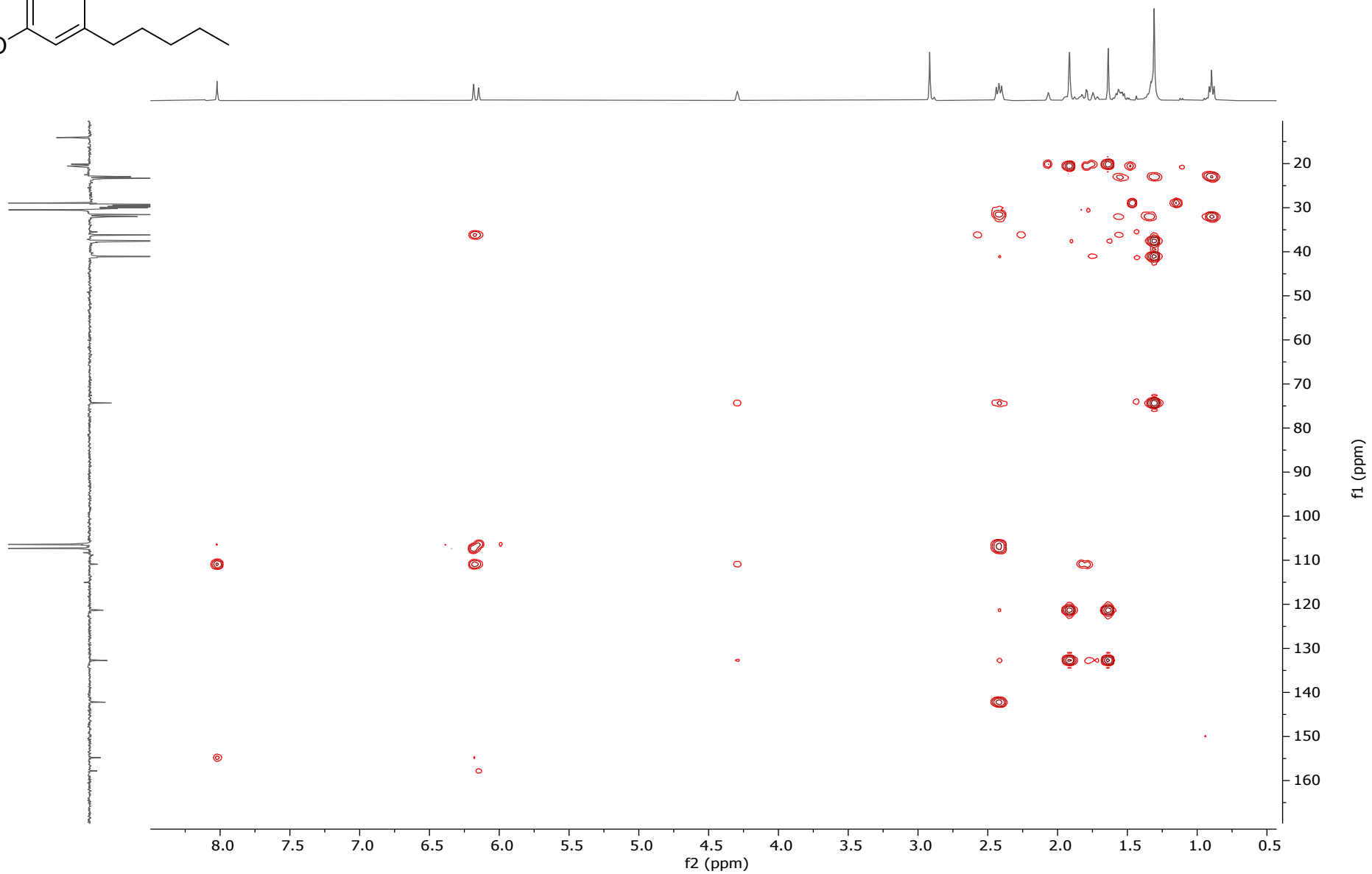
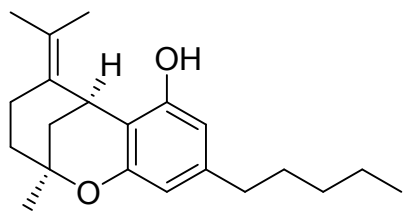


**Figure S15.**  $^1\text{H}$  COSY Spectrum in acetone- $d_6$  of  $\Delta^{4(8)}$ -*iso*-THC

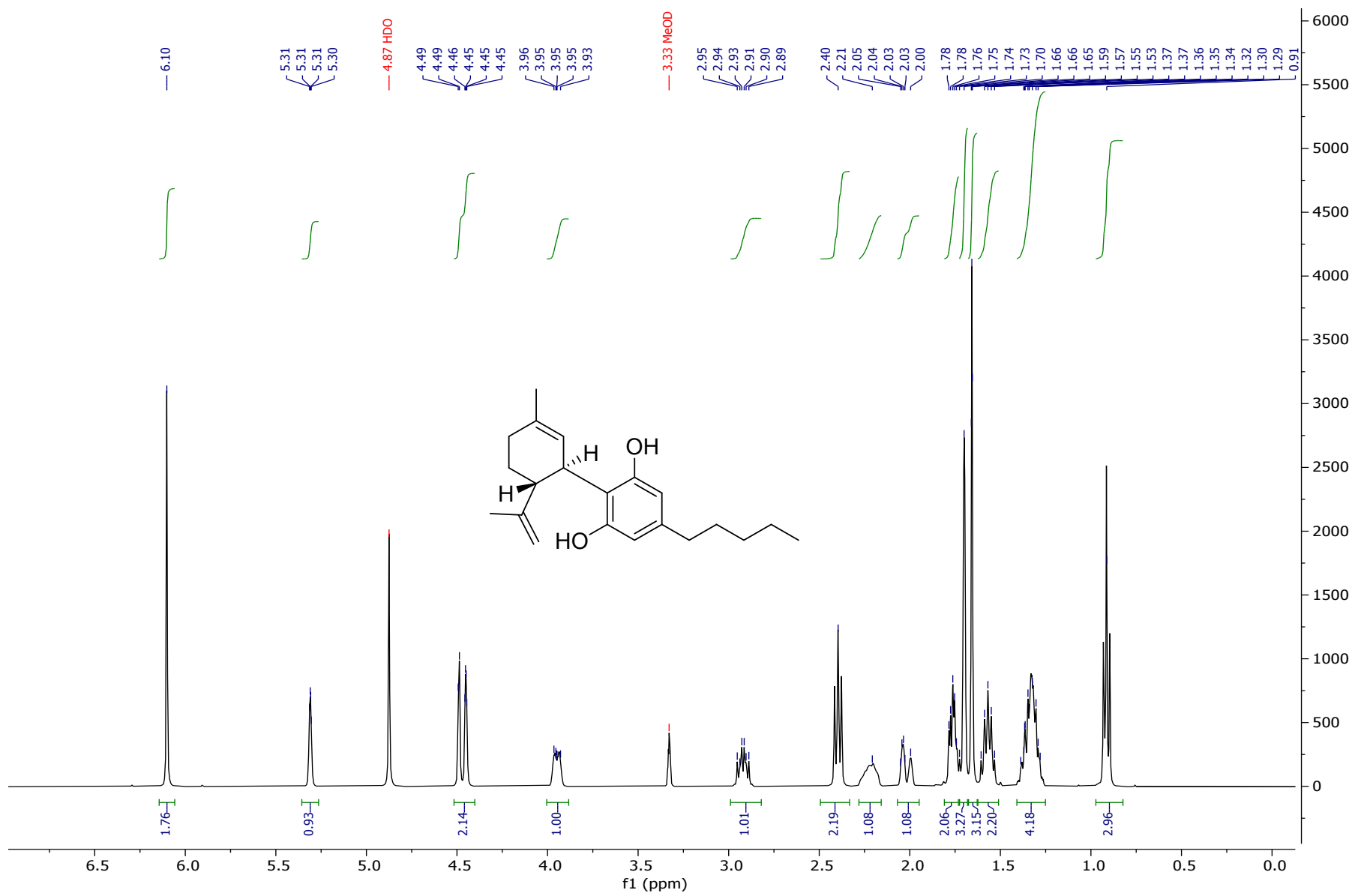


**Figure S16.** HSQC Spectrum in acetone- $d_6$  of  $\Delta^{4(8)}$ -*iso*-THC

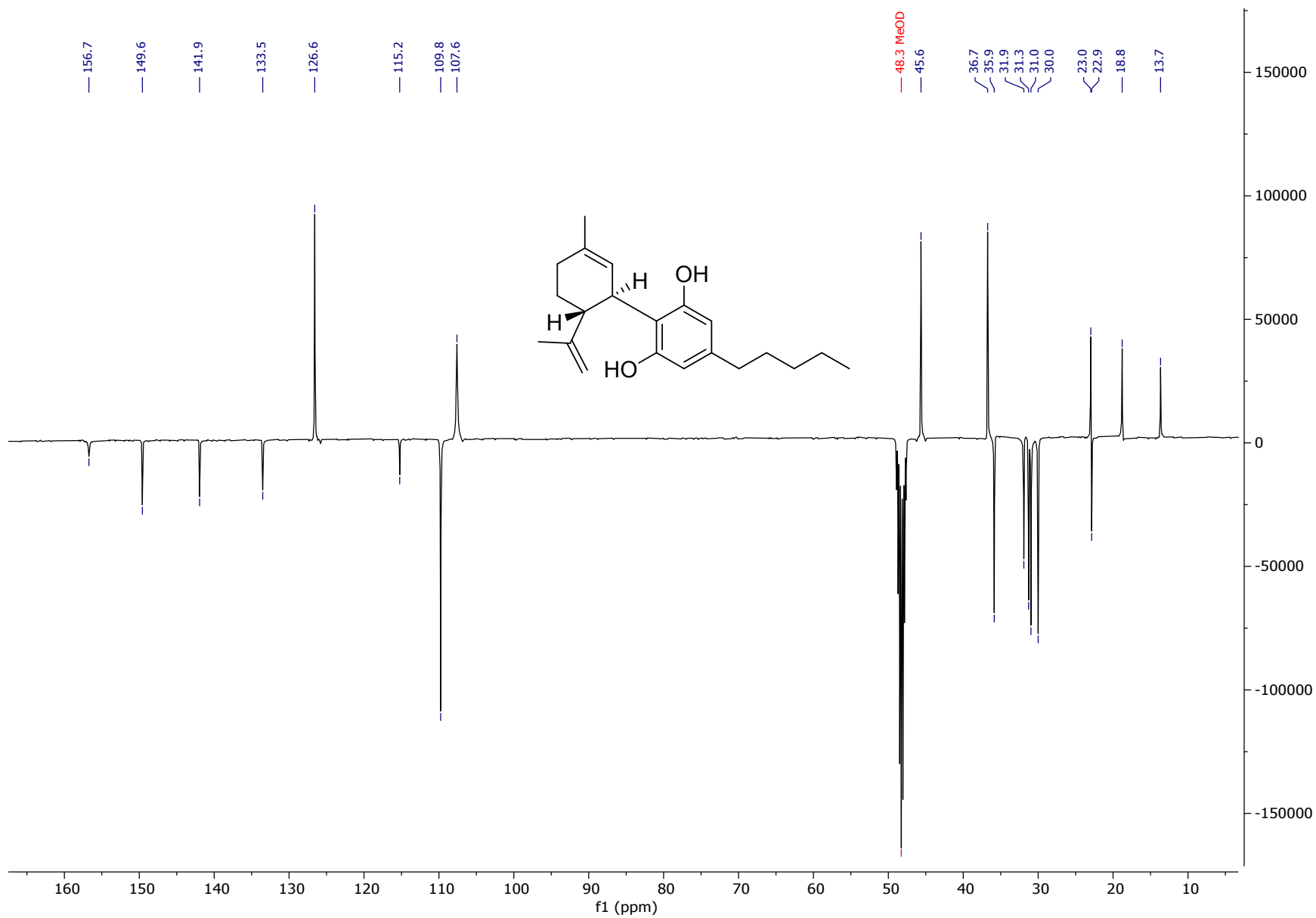




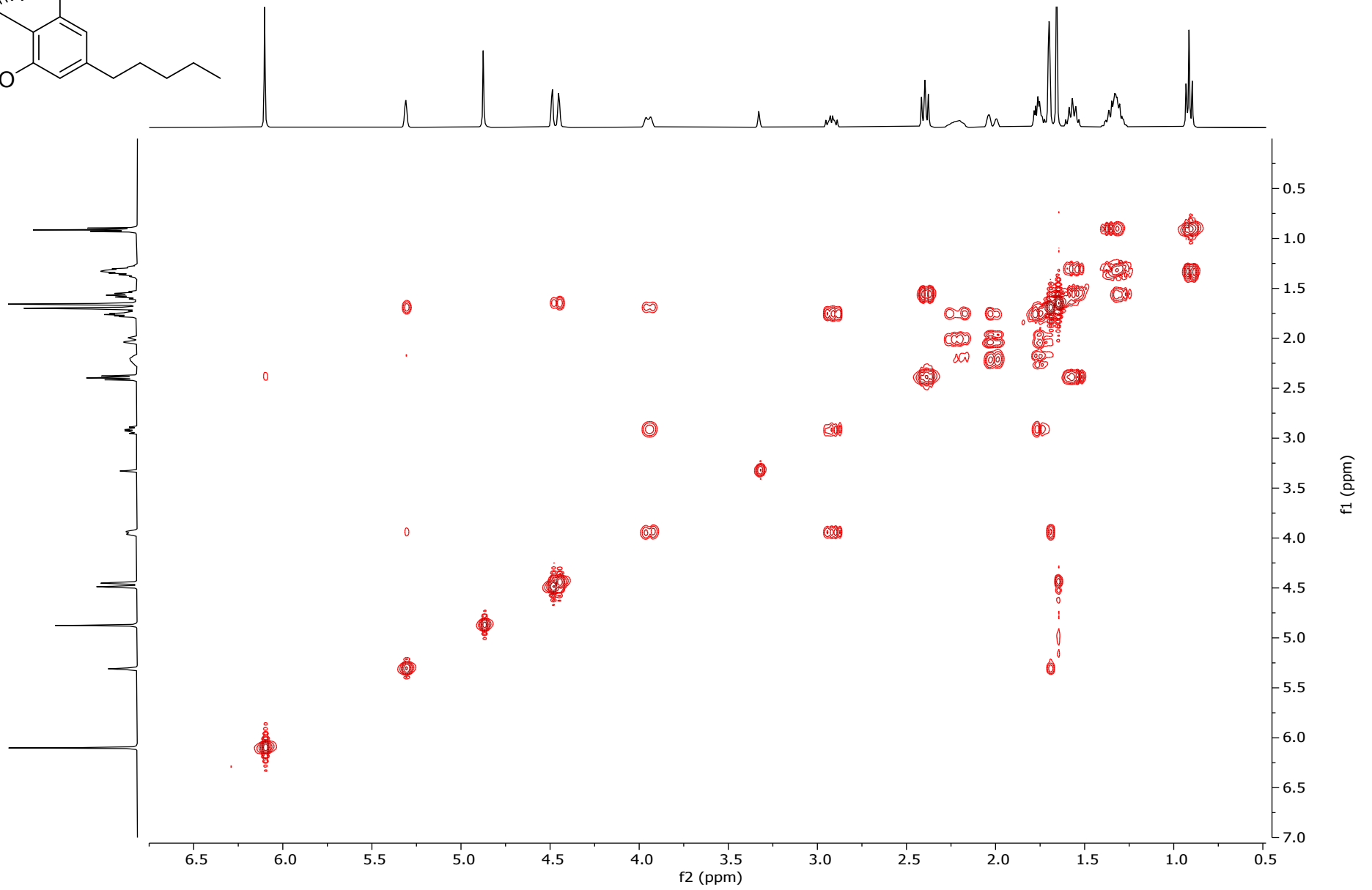
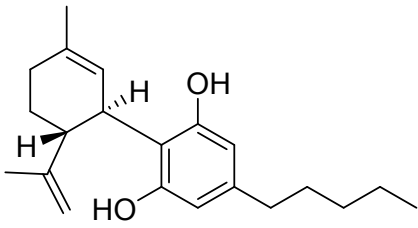
**Figure S17.** HMBC Spectrum in acetone- $d_6$  of  $\Delta^{4(8)}$ -*iso*-THC



**Figure S18.**  $^1\text{H}$  NMR Spectrum (400 MHz, methanol- $d_6$ ) of CBD

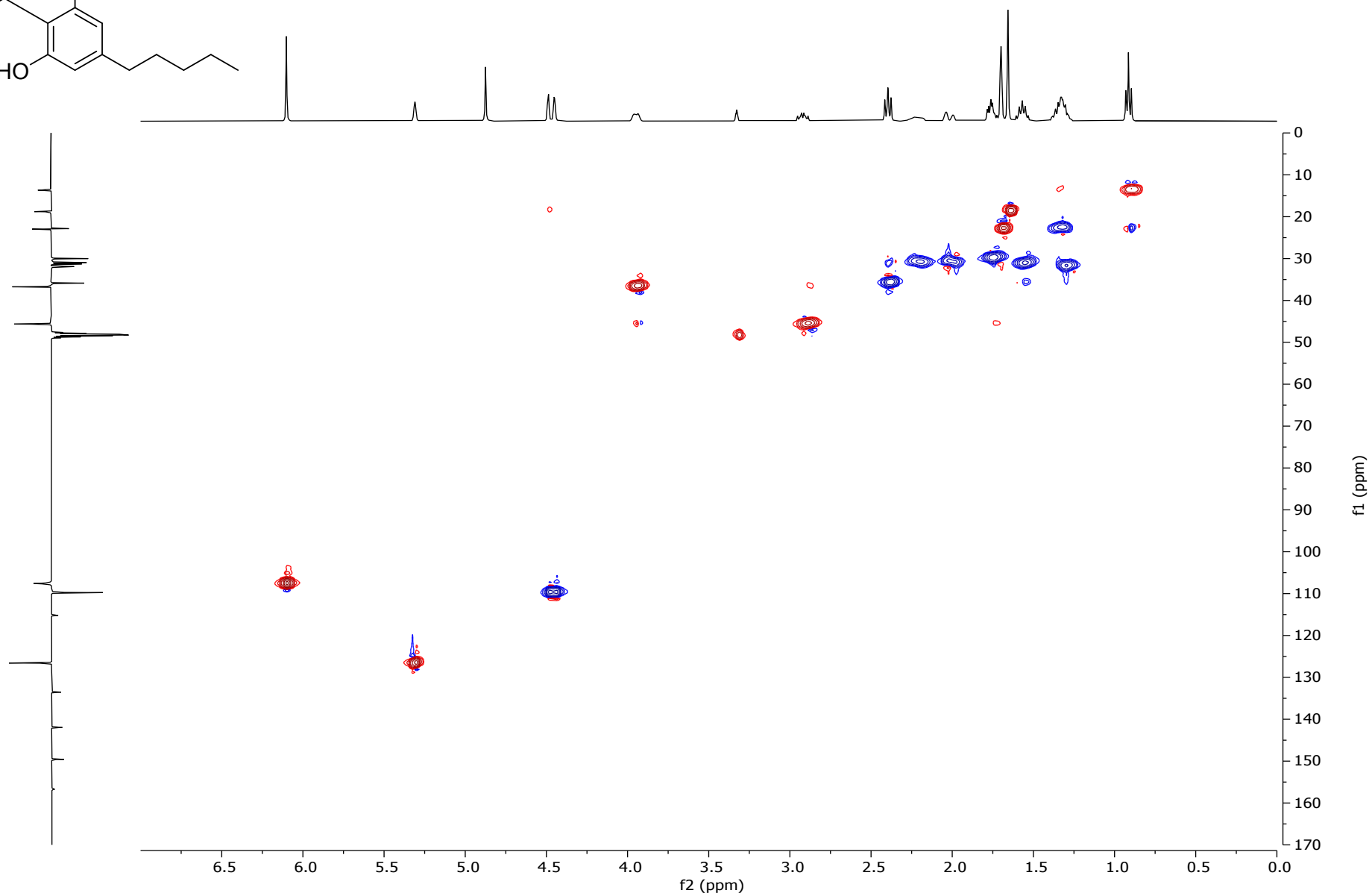
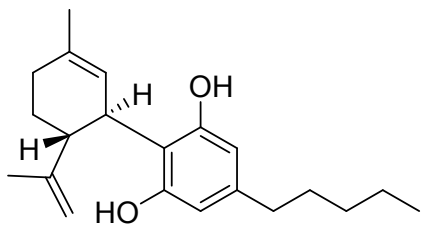


**Figure S19.**  $^{13}\text{C}$  NMR APT Spectrum (101 MHz, methanol- $d_4$ ) of CBD

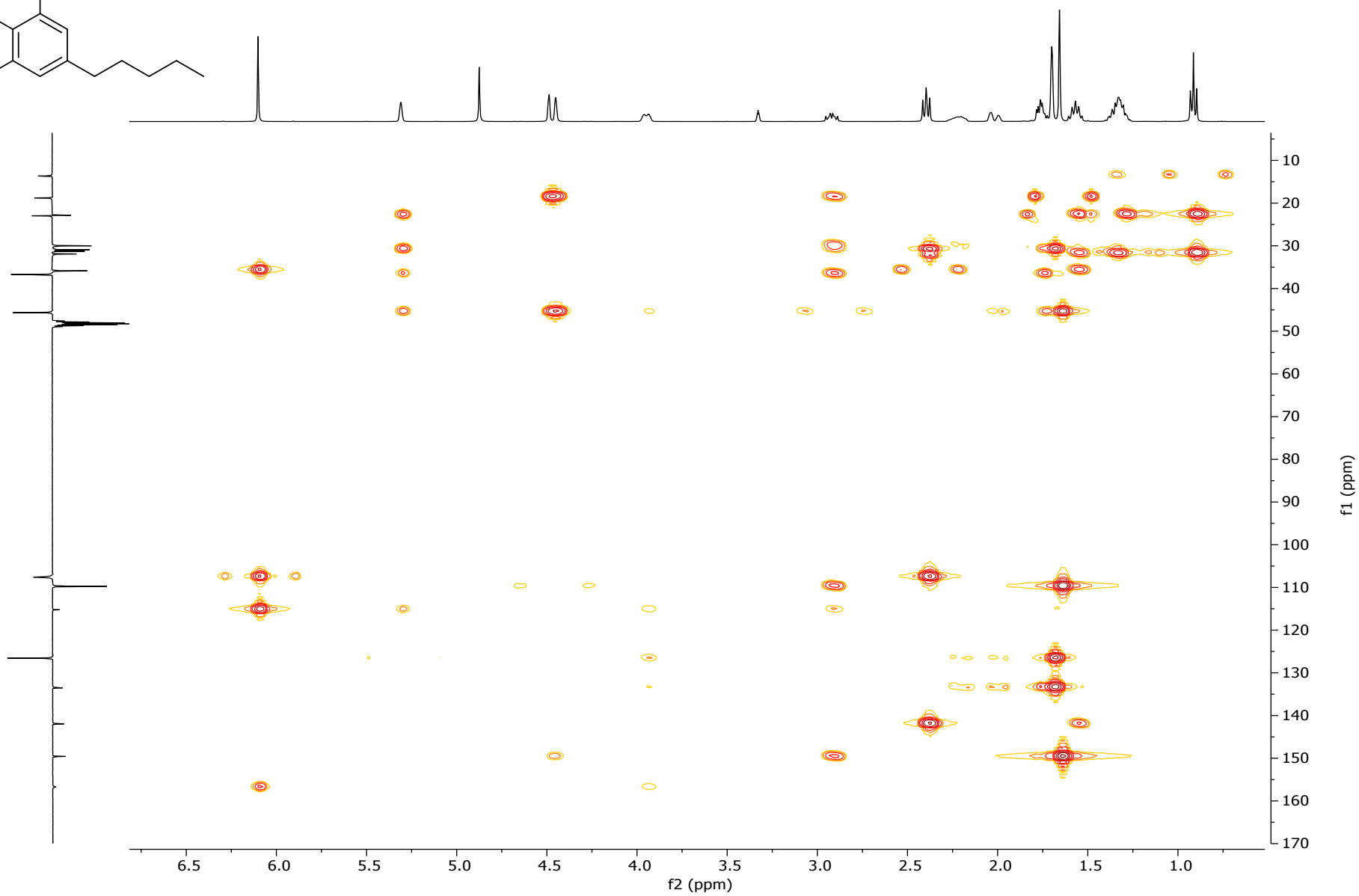
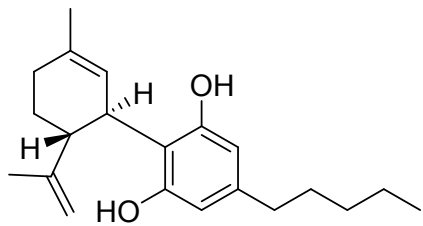


**Figure S20.**  $^1\text{H}$  COSY Spectrum in methanol- $d_4$  of CBD





**Figure S21.** HSQC Spectrum in methanol- $d_4$  of CBD



**Figure S22.** HMBC Spectrum in methanol- $d_4$  of CBD