

Supplementary Materials

3-Hydroxy-8,14-secogammacera-7,14-dien-21-one: A New Onoceranoid Triterpenes from *Lansium domesticum* Corr. cv *Kokossan*

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Abstract: A new onoceranoid triterpenes, namely 3-hydroxy-8,14-secogammacera-7,14-dien-21-one (**1**), has been isolated from the fruit peels of *Lansium domesticum* Corr. cv *kokossan*. The structure of **1** was determined on the basis of spectroscopic data including infrared, 1D and 2D-NMR as well as high resolution mass spectroscopy analysis. Compound **1** showed a weak activity against the MCF-7 breast cancer cell lines.

Keywords: *Lansium domesticum*; Meliaceae; MCF-7; triterpene onoceranoid

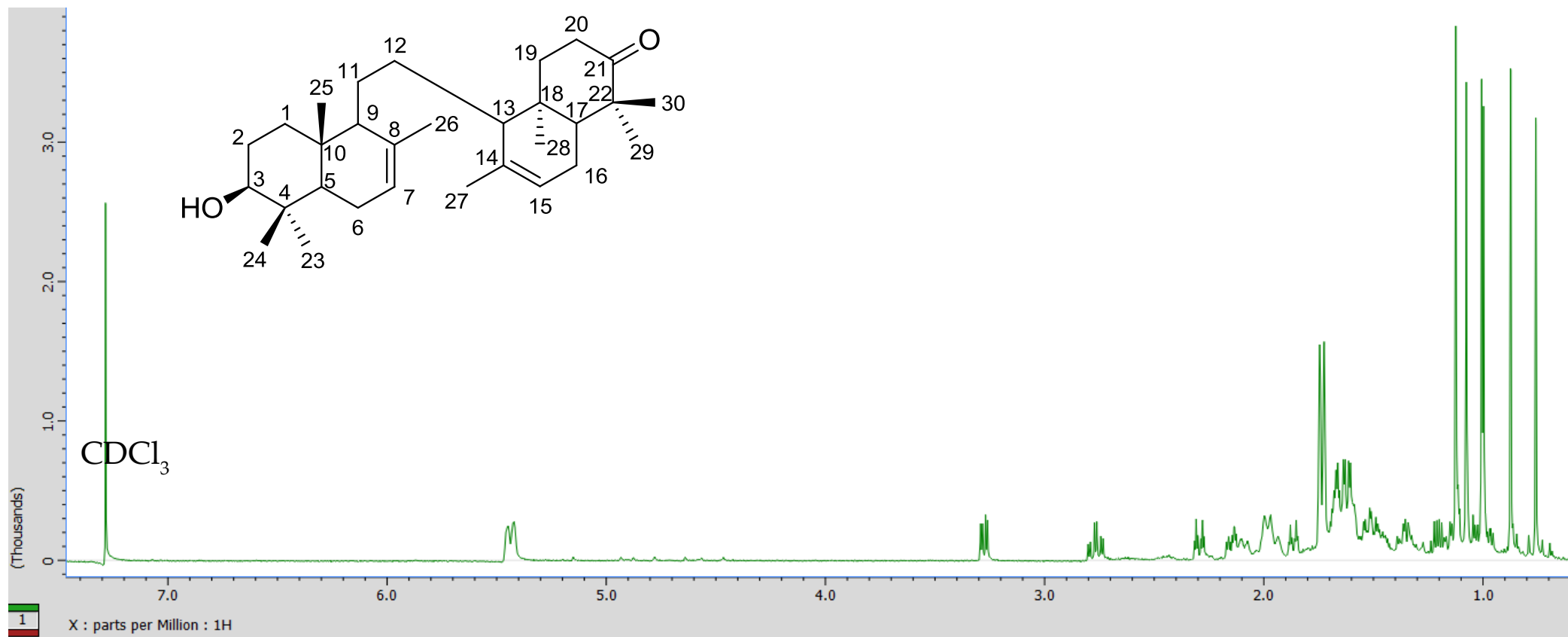


Figure S1. ¹H-NMR spectra of compound **1** in CDCl₃ (500 MHz)

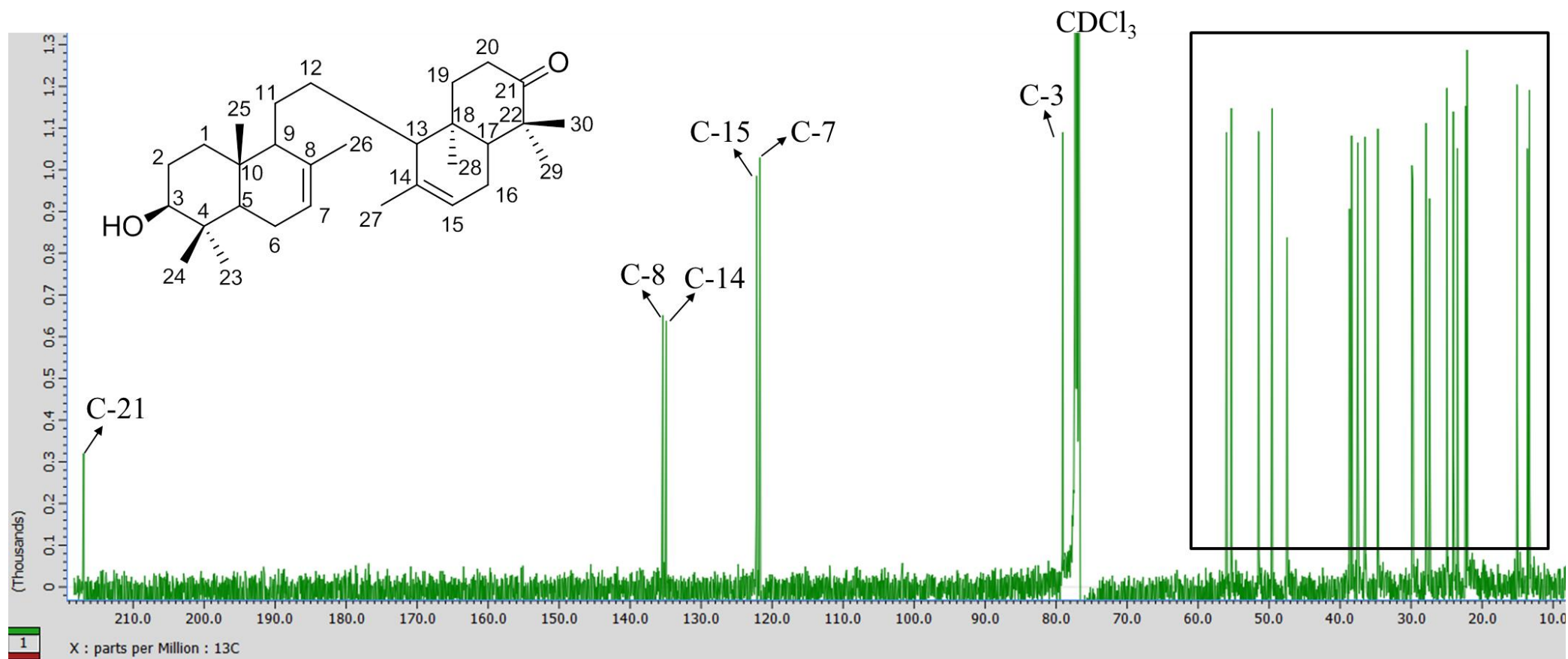


Figure S2. ^{13}C -NMR spectra of compound **1** in CDCl_3 (125 MHz)

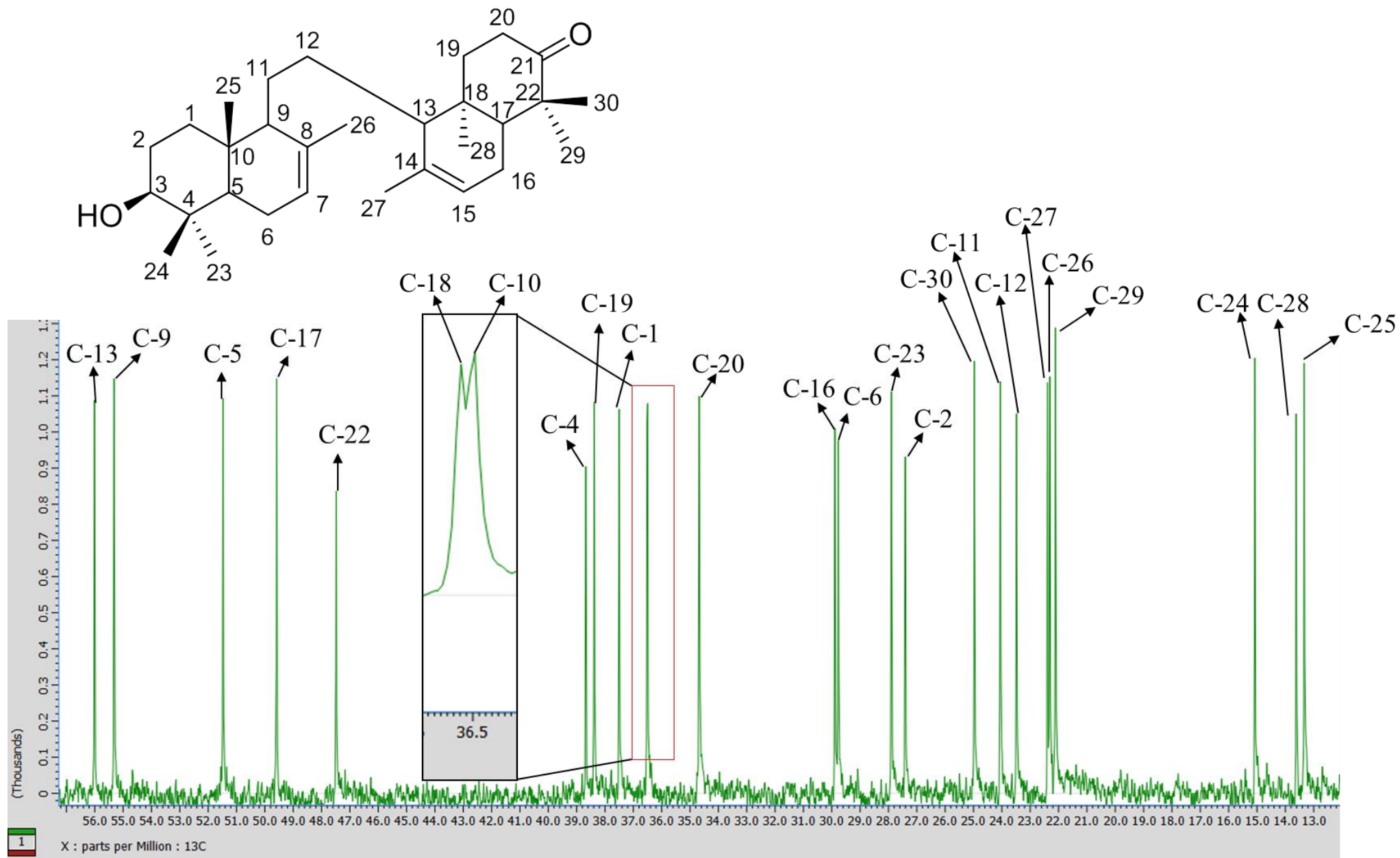


Figure S2. Cont.

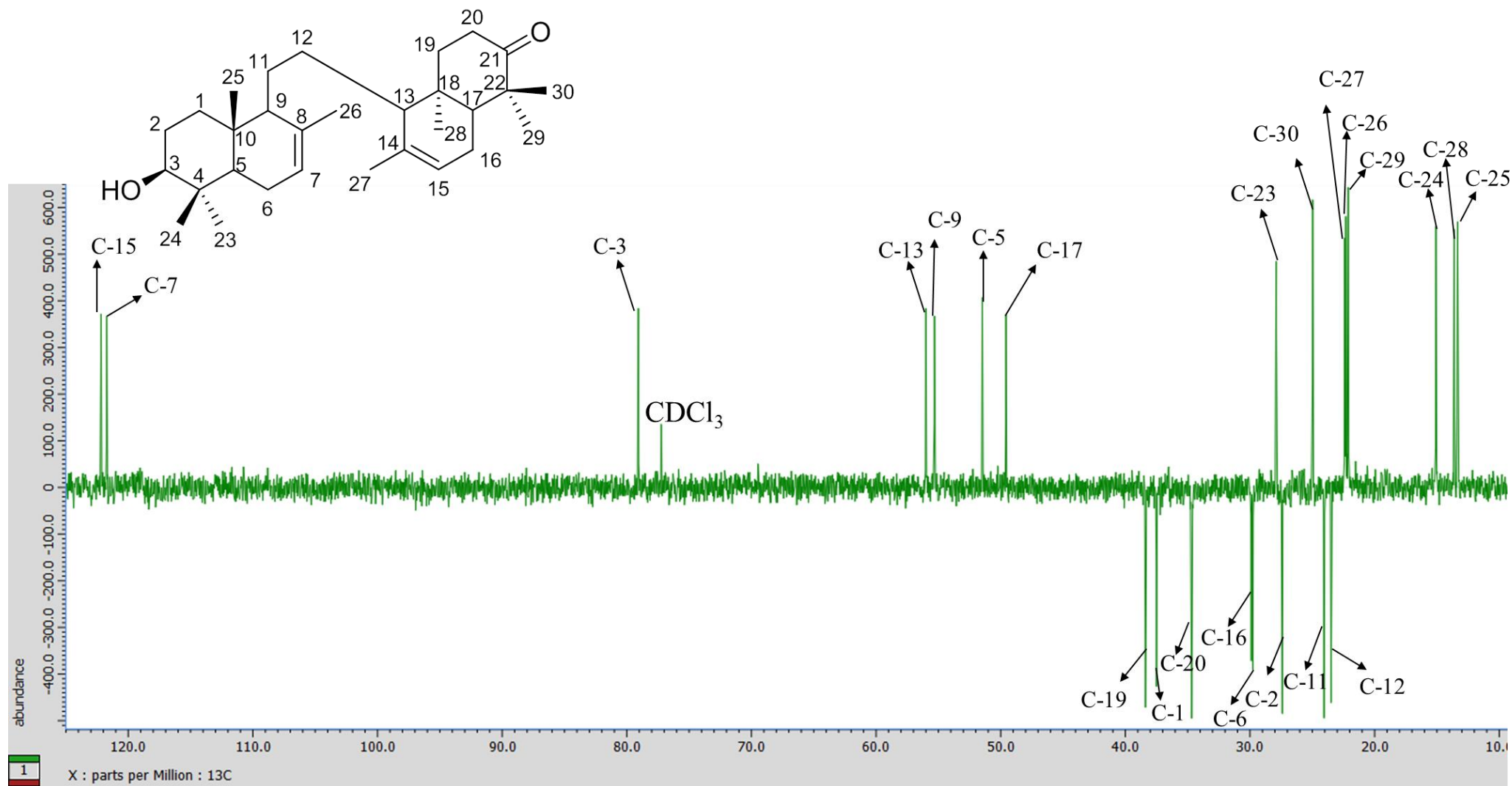


Figure S3. DEPT-135° spectra of compound 1 in CDCl₃

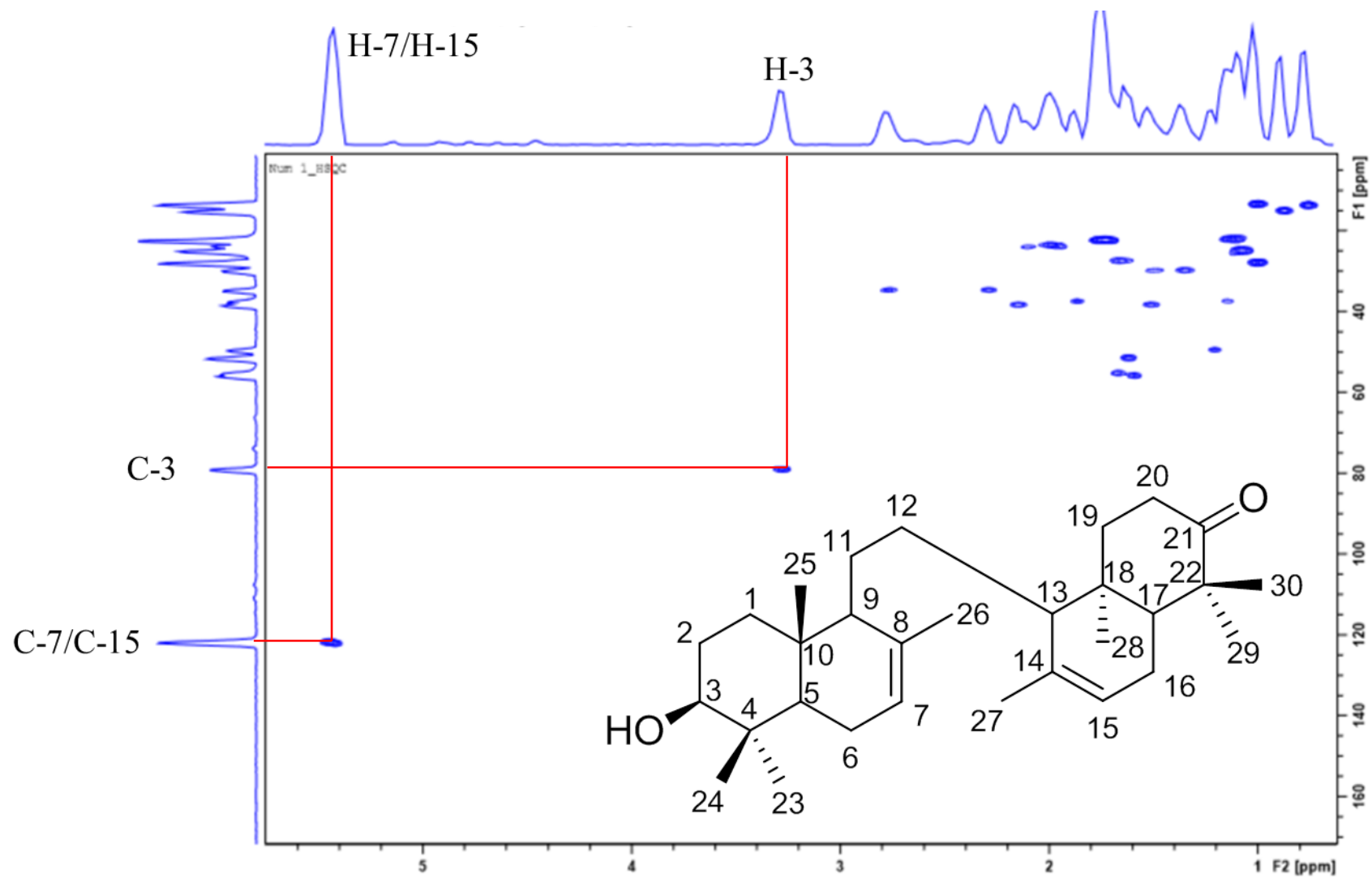


Figure S4. HSQC spectra of compound 1 in CDCl₃

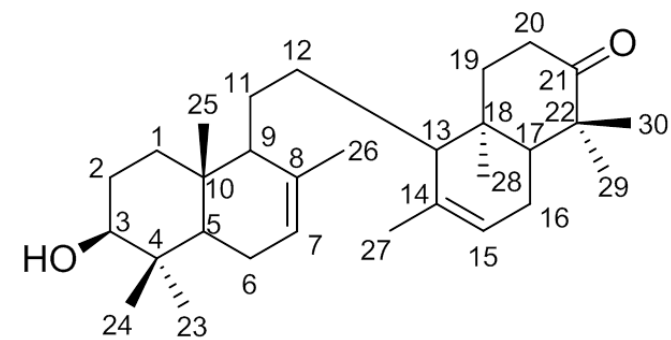
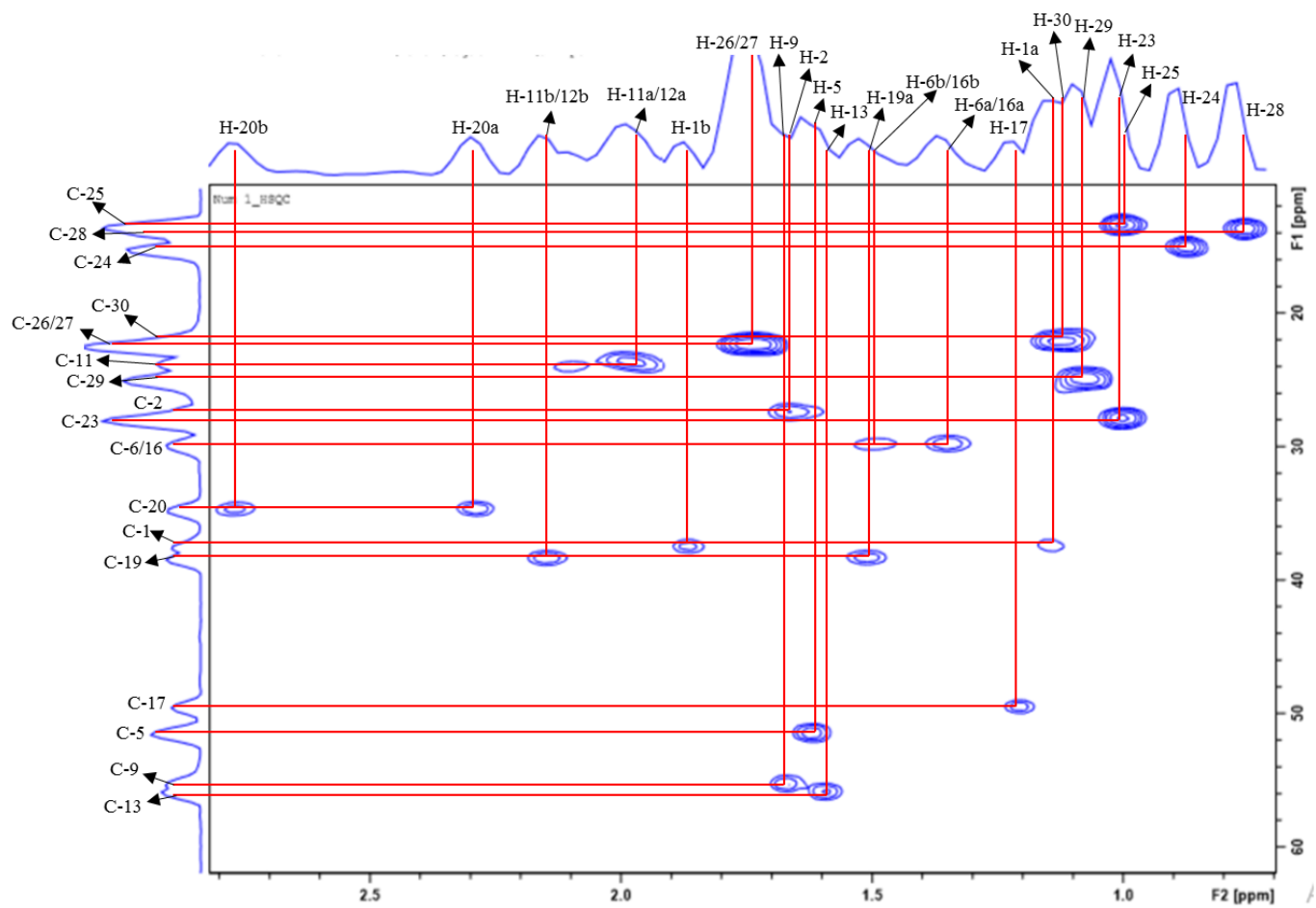


Figure S4. Cont.

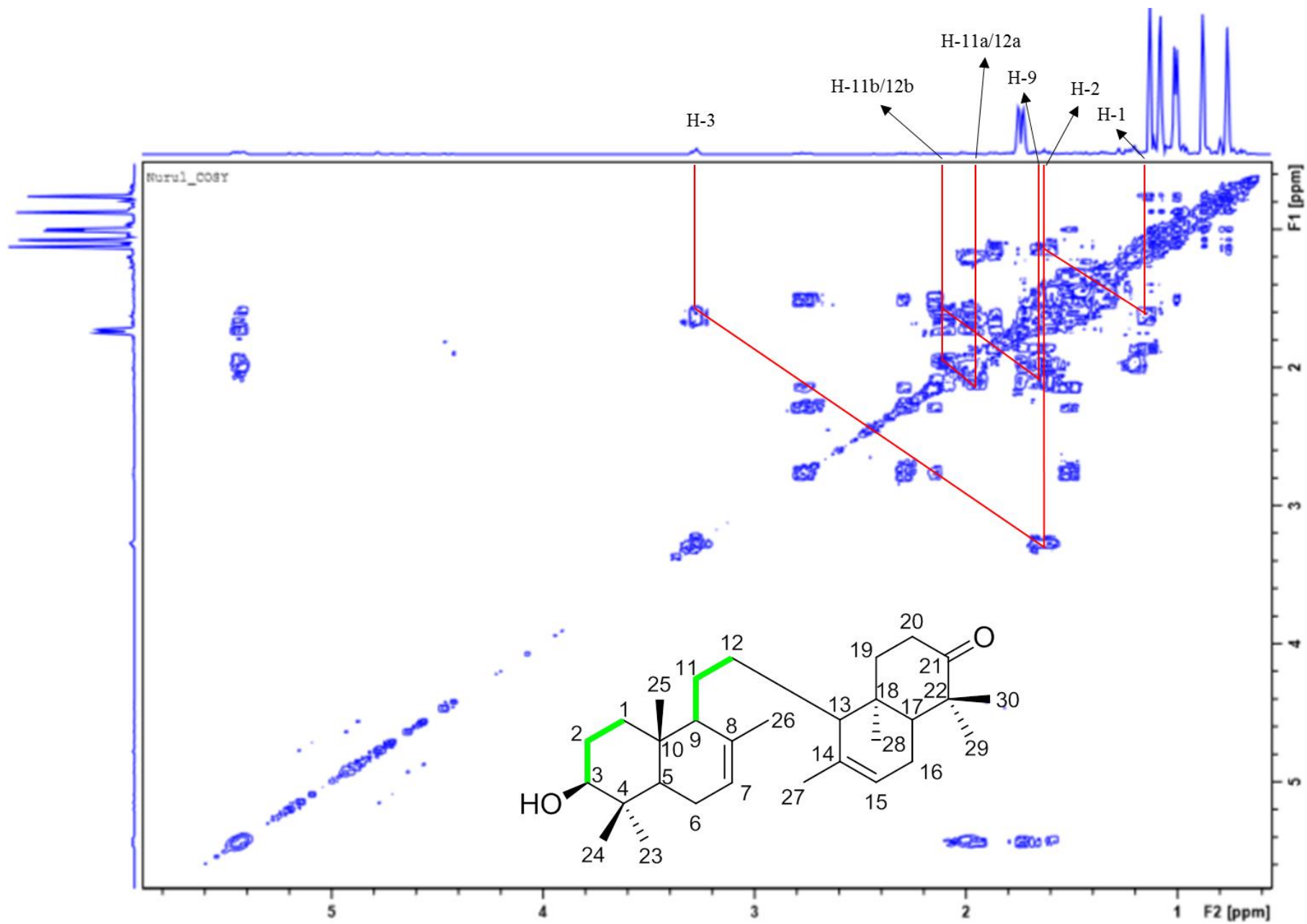


Figure S5. ^1H - ^1H COSY spectra of compound 1 in CDCl_3

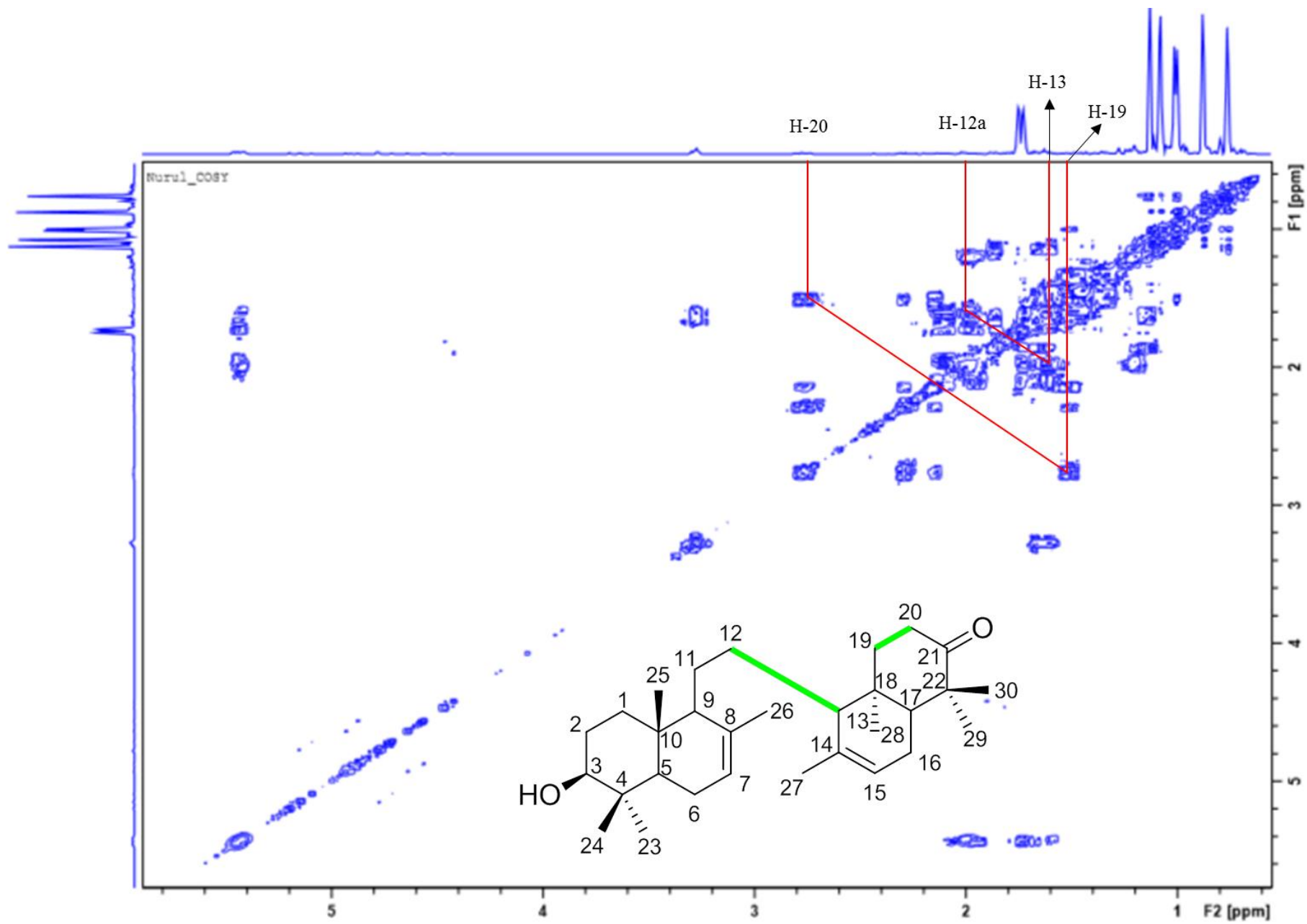


Figure S5. *Cont.*

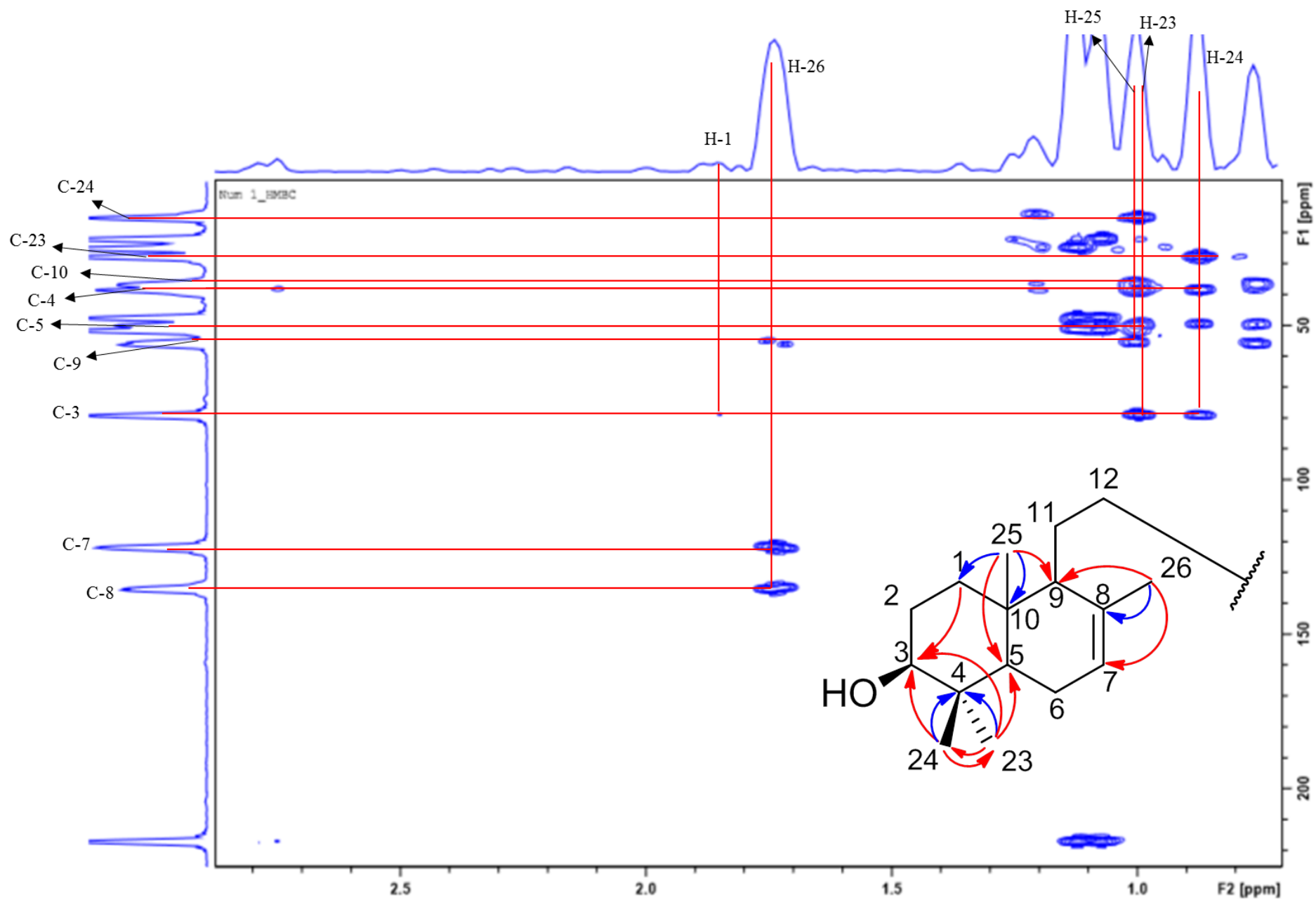


Figure S6. HMBC spectra of compound 1 in CDCl₃

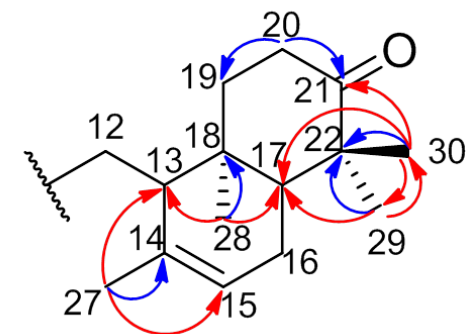
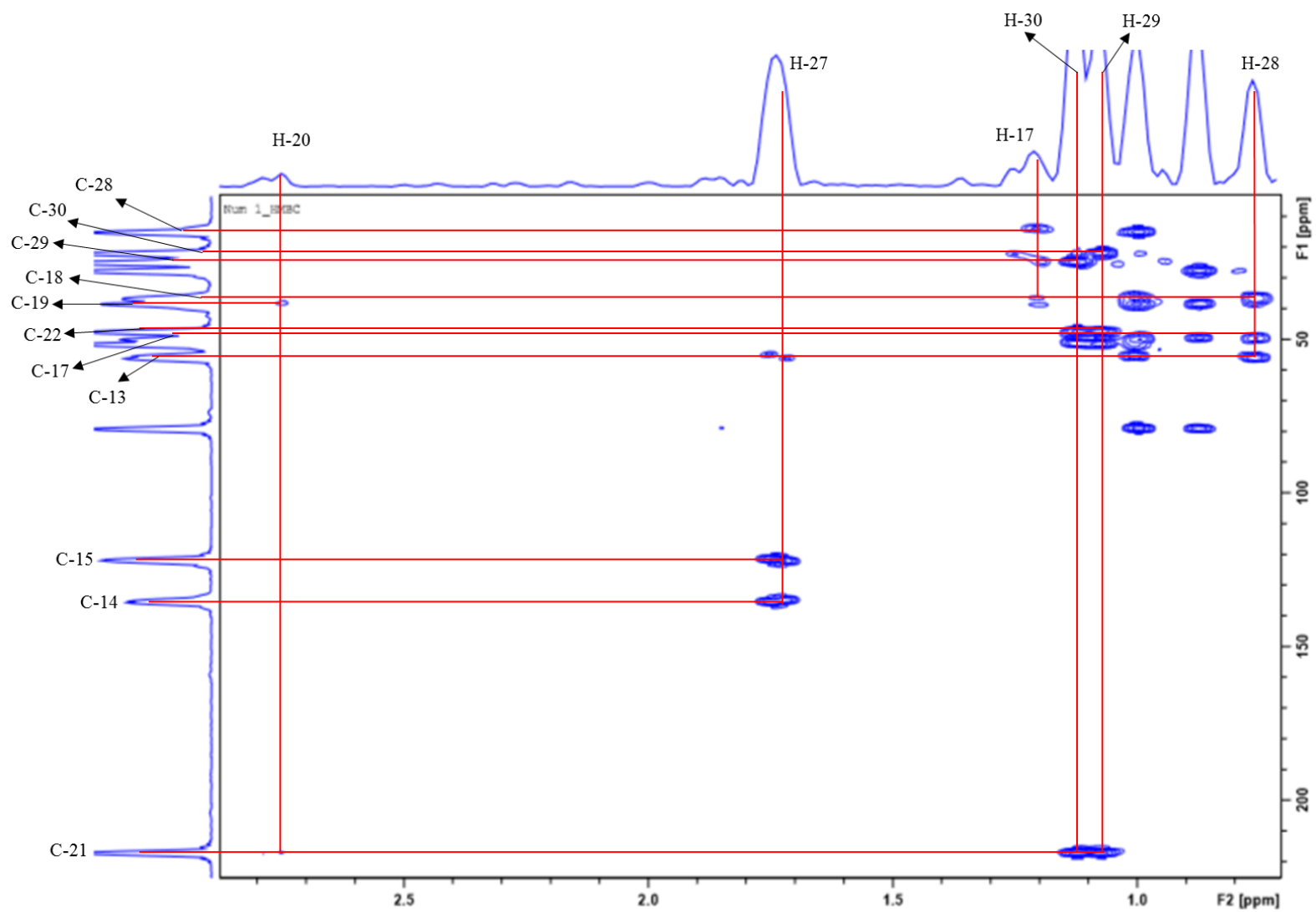


Figure S6. Cont.

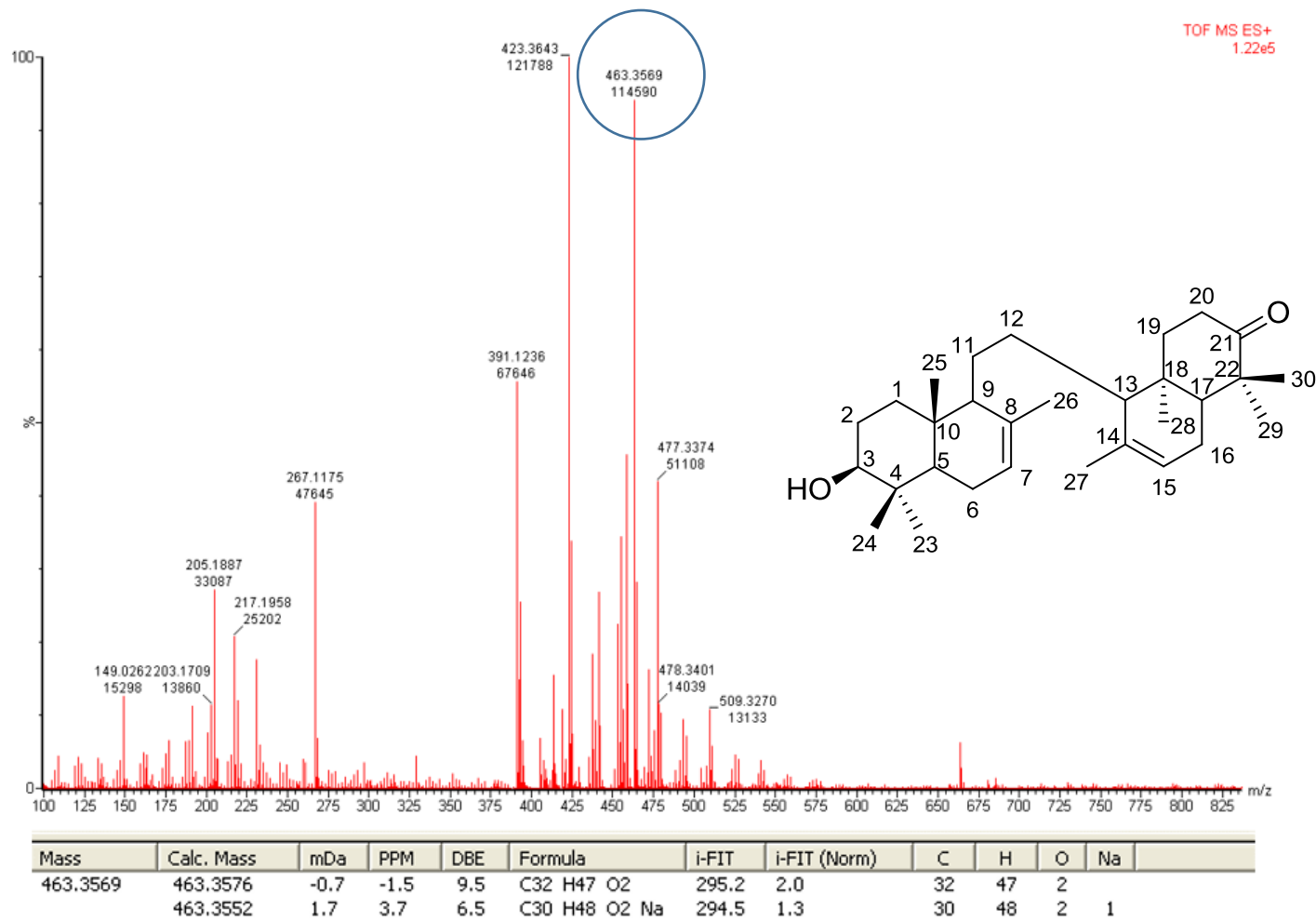


Figure S7. HRTOFMS spectra of compound 1

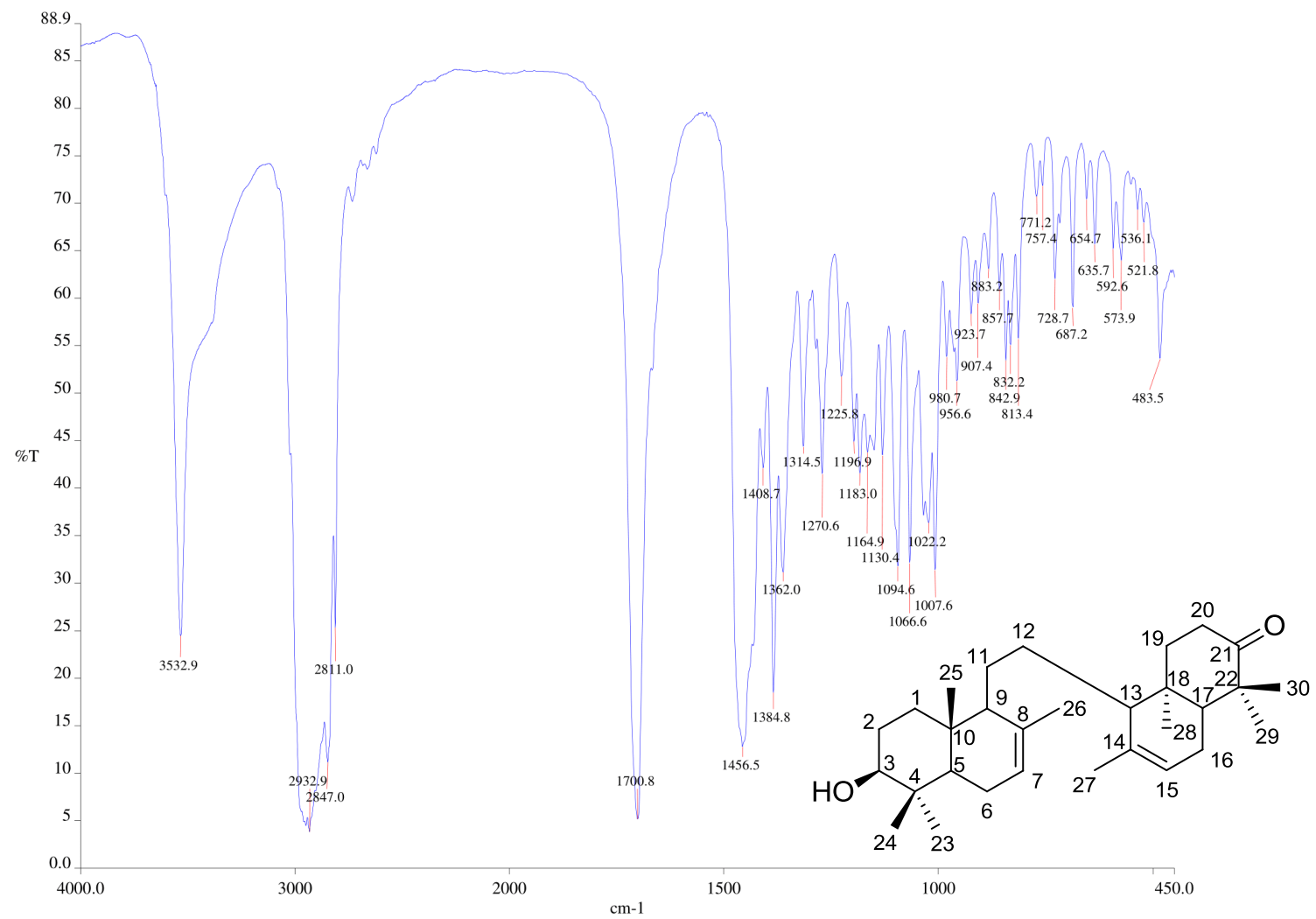
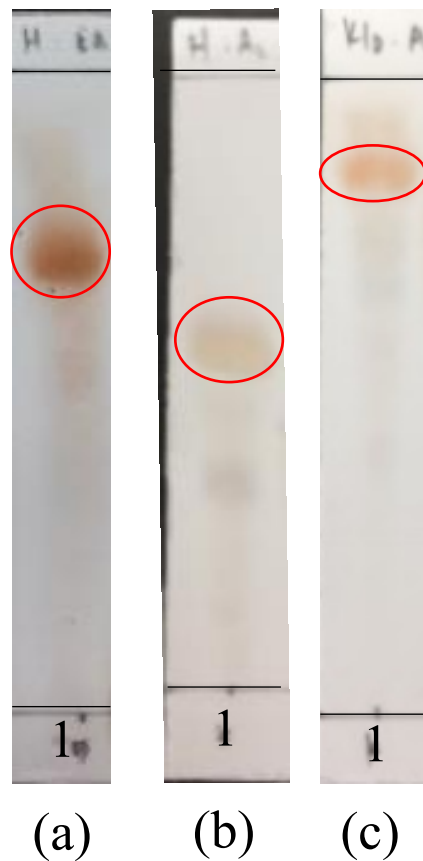


Figure S8. IR (KBr disc) spectra of compound 1



No.	Mobile Phase	Rf
a	n-Hexane : ethyl acetate (7:3 v/v)	0,71
b	n-Hexane : acetone (7:3 v/v)	0,54
c	Chloroform : acetone (8:2 v/v)	0,83

Figure S9. TLC Profile of **1** after spraying with H₂SO₄ 10% in EtOH and heating.