

SUPPLEMENTARY DATA

Triterpenoids from *Aglaia shawiana* with their Cytotoxicity against MDA-MB-468 and MCF-7 Cancer Cell Lines

Ricson Pemimpin Hutagaol^{1*}, Tjandrawati Moze², Gian Primahana², Sofa Fajriah², Muhammad Eka Prastya², Fitri Nur Aini¹, Desy Satyaningsih¹

¹Department of Chemistry, Faculty of Mathematics and Natural sciences, Nusa Bangsa University, Bogor 16166, Indonesia

²Research Center for Pharmaceutical Ingredients and Traditional Medicine, National Research and Innovation Agency (BRIN), Serpong Tangerang Selatan 15314, Indonesia

*Corresponding author email: ricsonpemimpin70@gmail.com

Triterpenoids from *Aglaia shawiana* with their Cytotoxicity against MDA-MB468 and MCF-7 Cancer Cell Lines

Table of contents	Page
Figure S1. HR-TOF MS of compound 1 .	2.
Figure S2. IR Spectrum of compound 1 .	3
Figure S3A. ¹ H-NMR Spectrum of 1 (700 MHz in CDCl ₃).	4
Figure S3B. ¹ H-NMR Spectrum of 1 (b) (700 MHz in CDCl ₃).	5
Figure S4. ¹³ C-NMR Spectrum of 1 (175 MHz in CDCl ₃).	6
Figure S5. DEPT-135° Spectrum of 1 (in CDCl ₃).	7
Figure S6. HMQC Spectrum of 1 .	8
Figure S7. HMBC Spectrum of 1 .	9
Figure S8. ¹ H- ¹ H COSY Spectrum of 1	10
Figure S9. NOESY Spectrum of 1	11
Figure S10A. ¹ H-NMR Spectrum of 2 (700 MHz in CDCl ₃).	12
Figure S10B. ¹ H-NMR Spectrum of 2 (700 MHz in CDCl ₃).	13
Figure S11. ¹³ C-NMR Spectrum of 2 (175 MHz in CDCl ₃).	14
Figure S12. DEPT-135° Spectrum of 2 (in CDCl ₃).	15

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

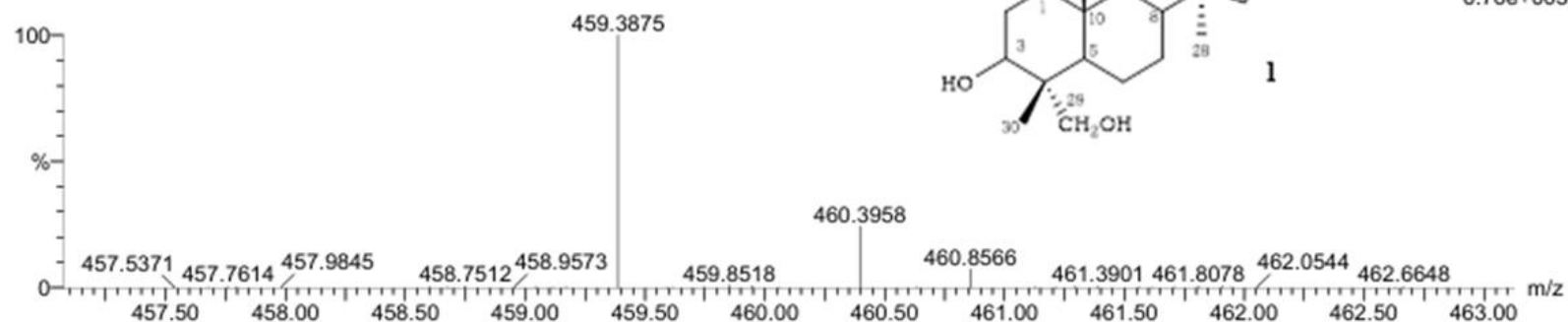
114 formula(e) evaluated with 1 results within limits (up to 100 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

RC 7 13 (0.238) Cm (13:14)

TOF MS ES+



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
459.3875	459.3838	3.7	8.1	5.5	107.9	0.0	C30 H51 O3

Figure S1. HR-TOF MS of compound 1.

Pak Ricson sampel 4 (RC-7) 4 September 2024

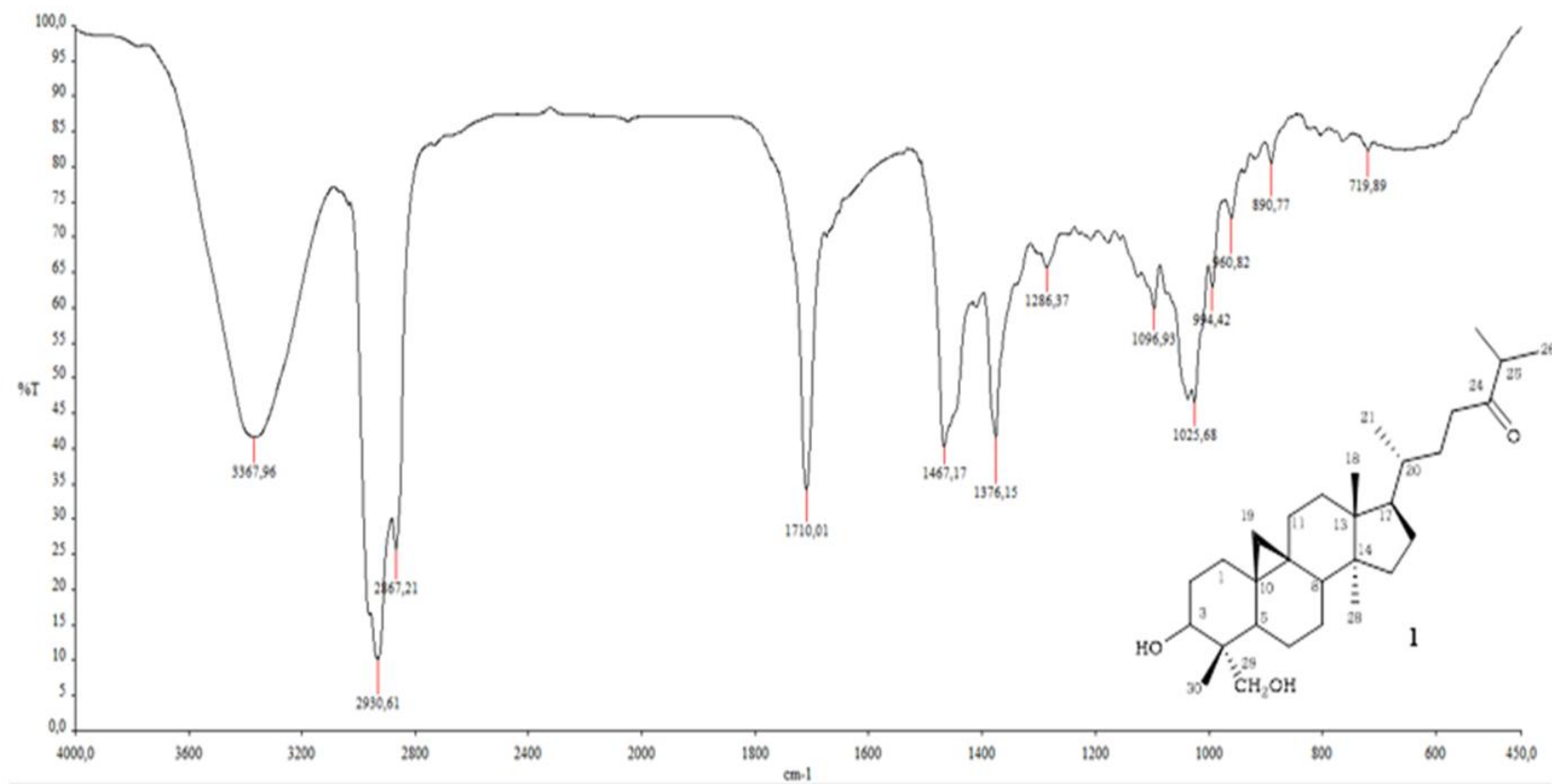


Figure S2. IR spectrum of compound 1.

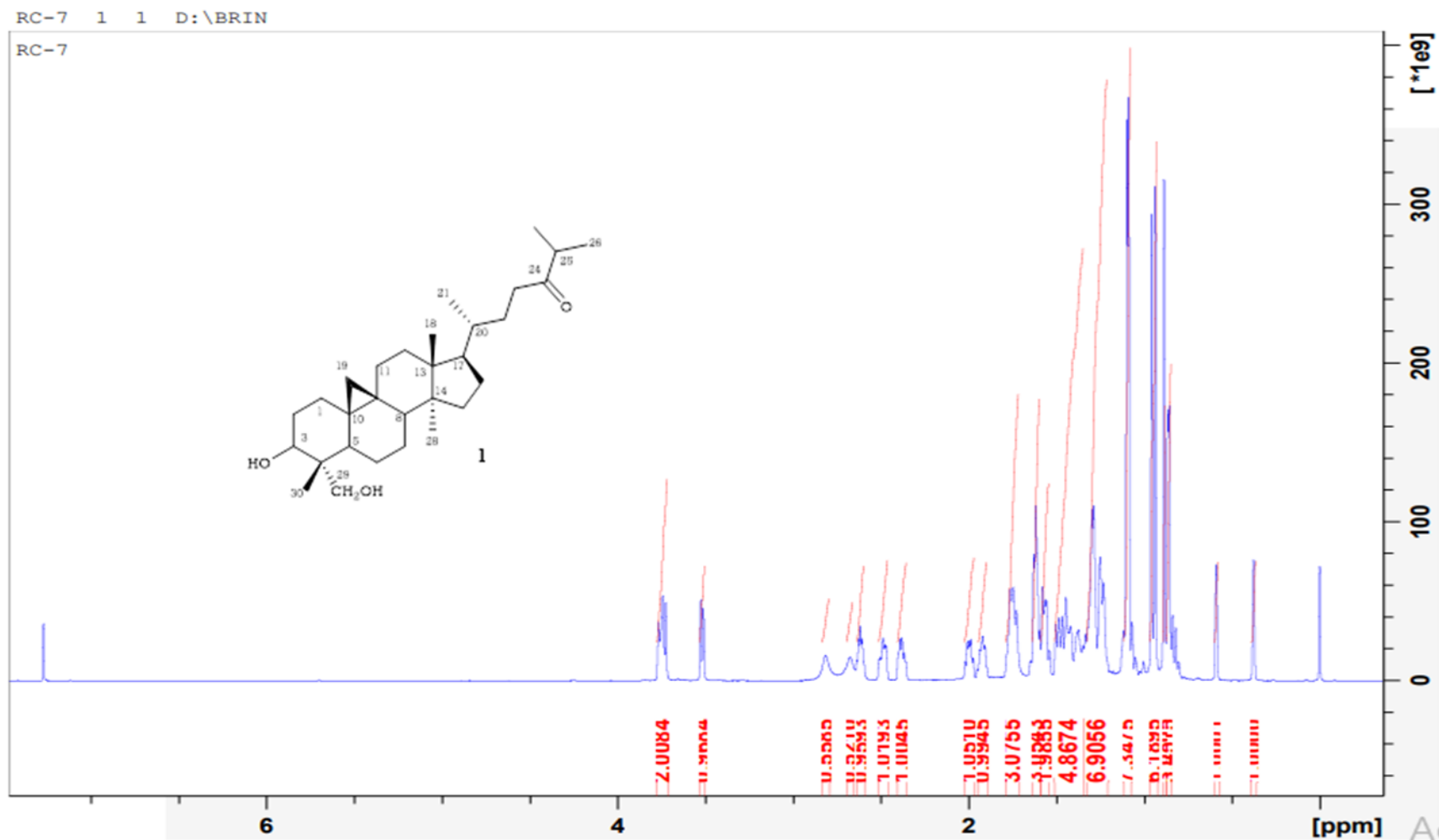


Figure 3a. ^1H -NMR Spectrum of **1** (δ_{H} 0-8 ppm, 700 MHz in CDCl_3).

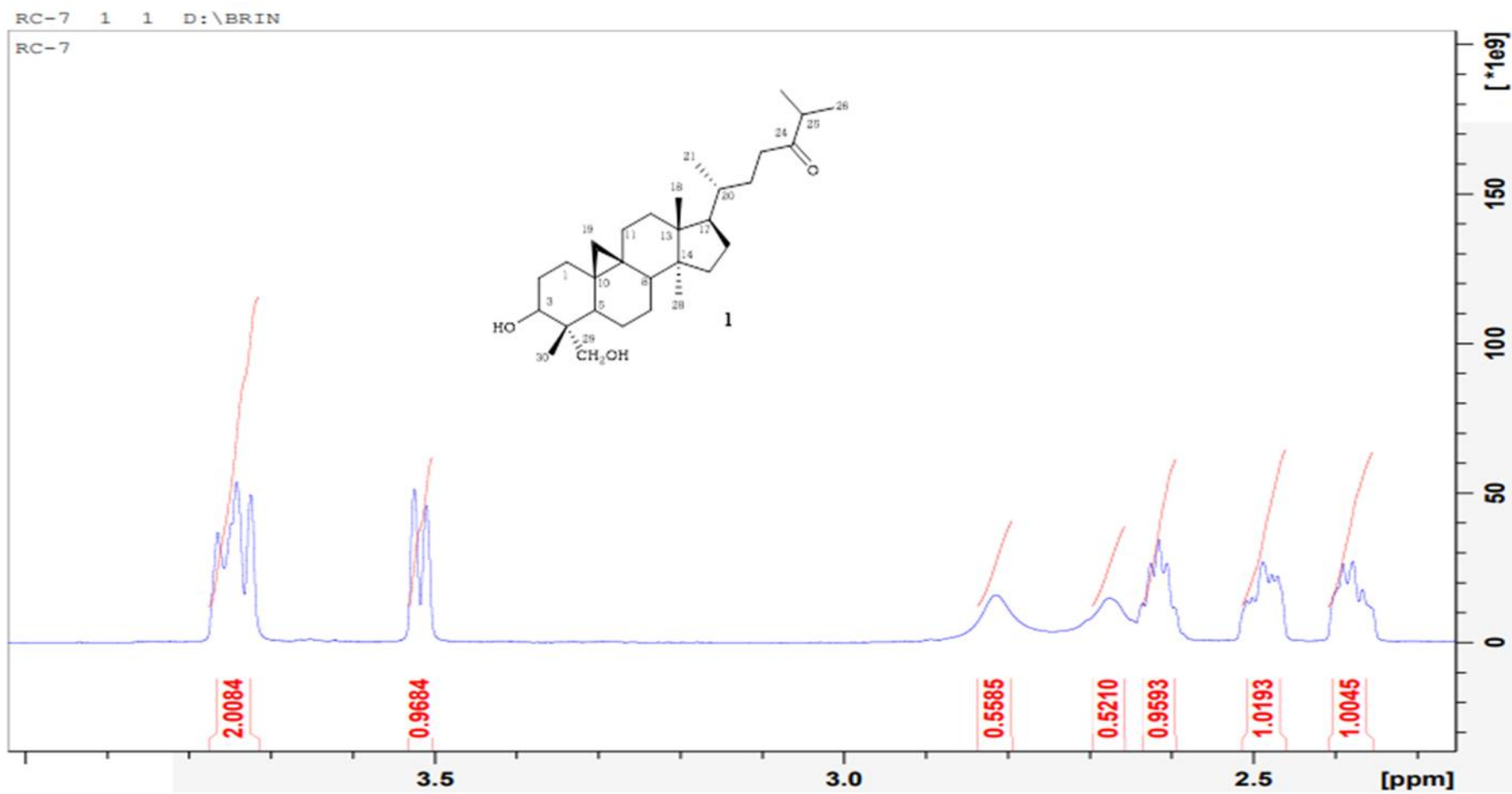


Figure 3b. ¹H-NMR Spectrum of **1** (δ_{H} 2-4 ppm, 700 MHz in CDCl₃).

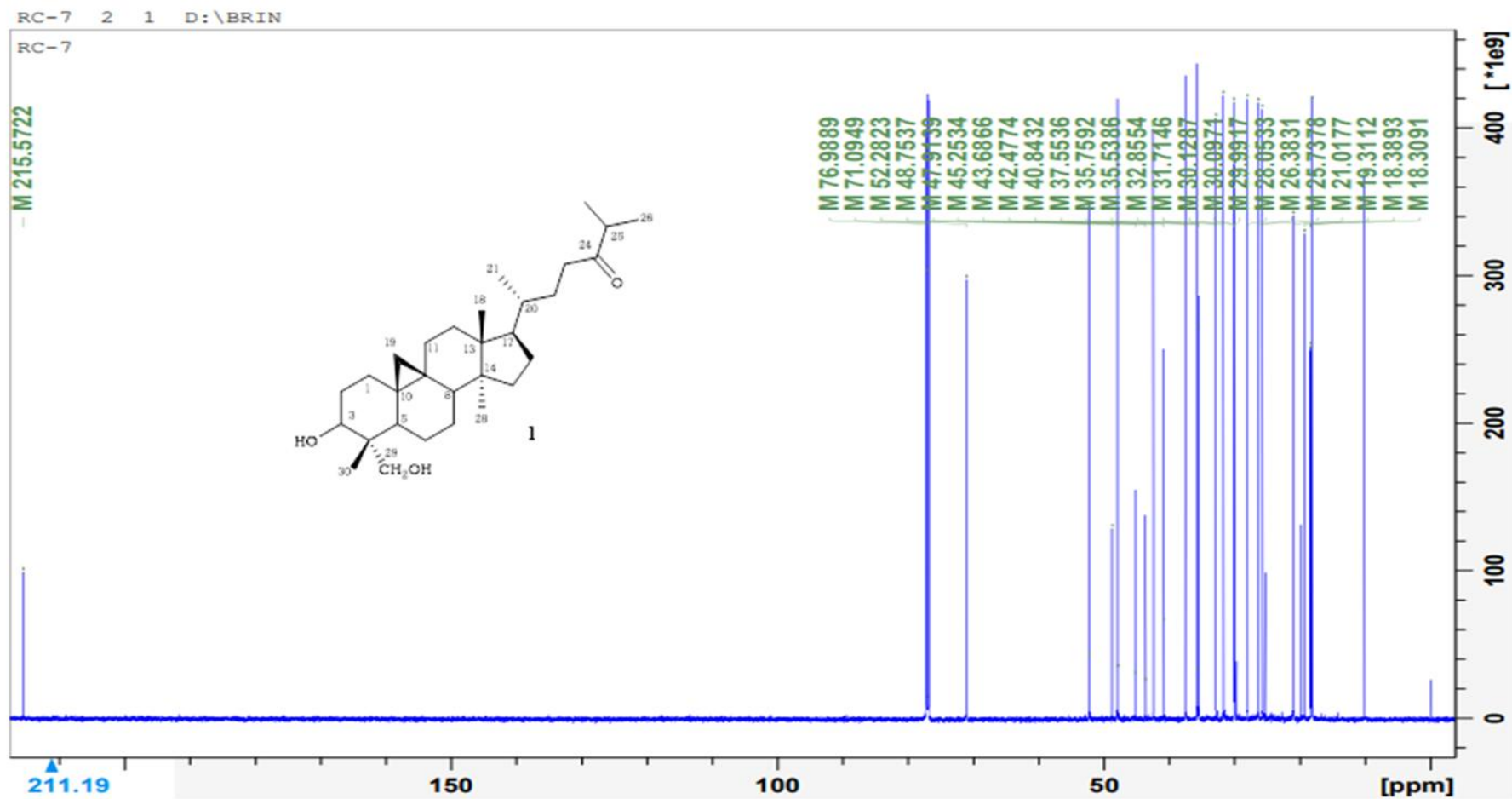


Figure S4. ^{13}C -NMR Spectrum of **1** (175 MHz in CDCl_3).

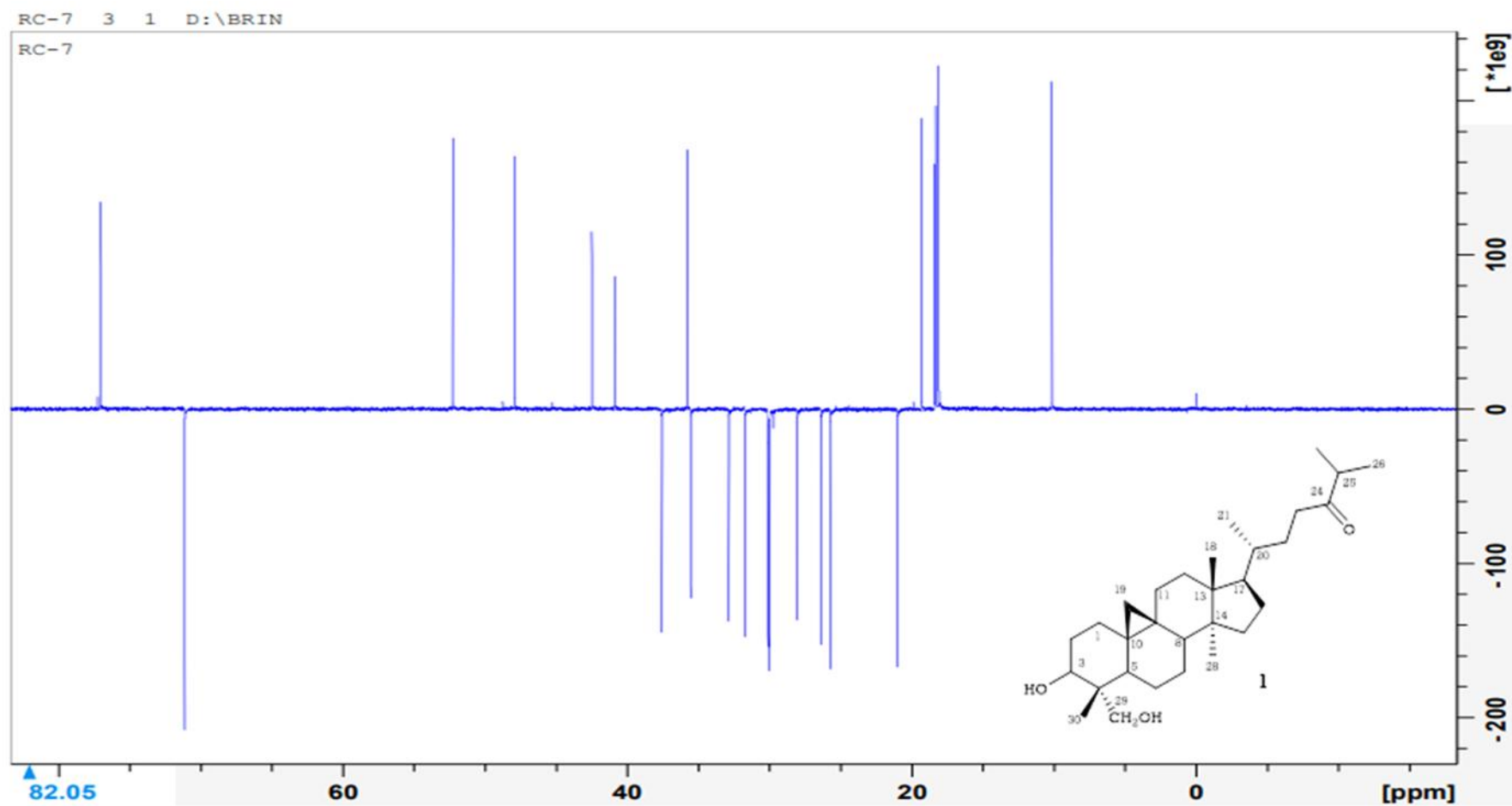


Figure S5. DEPT-135° Spectrum of **1** (in CDCl₃).

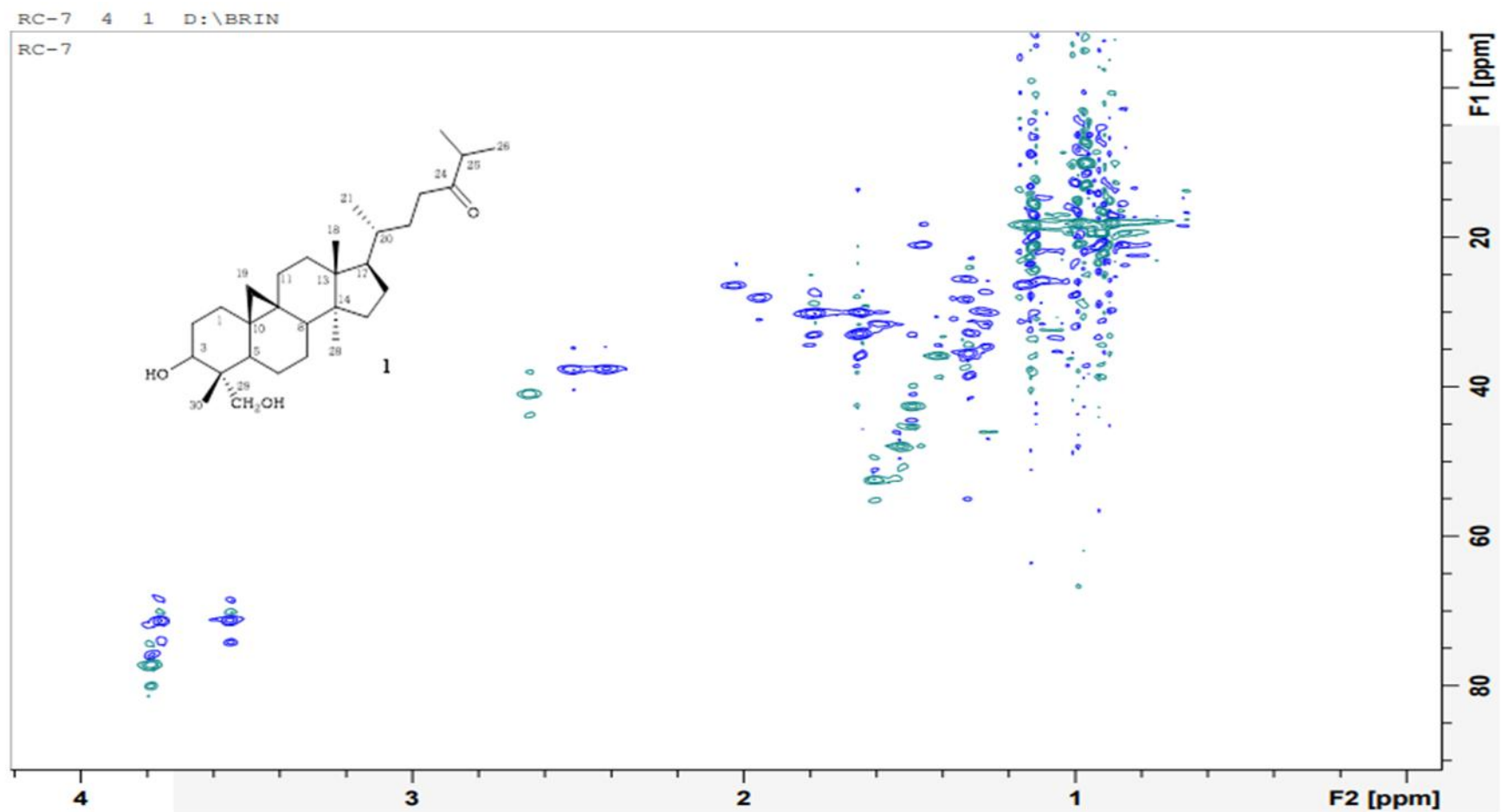


Figure S6. HMQC Spectrum of 1.

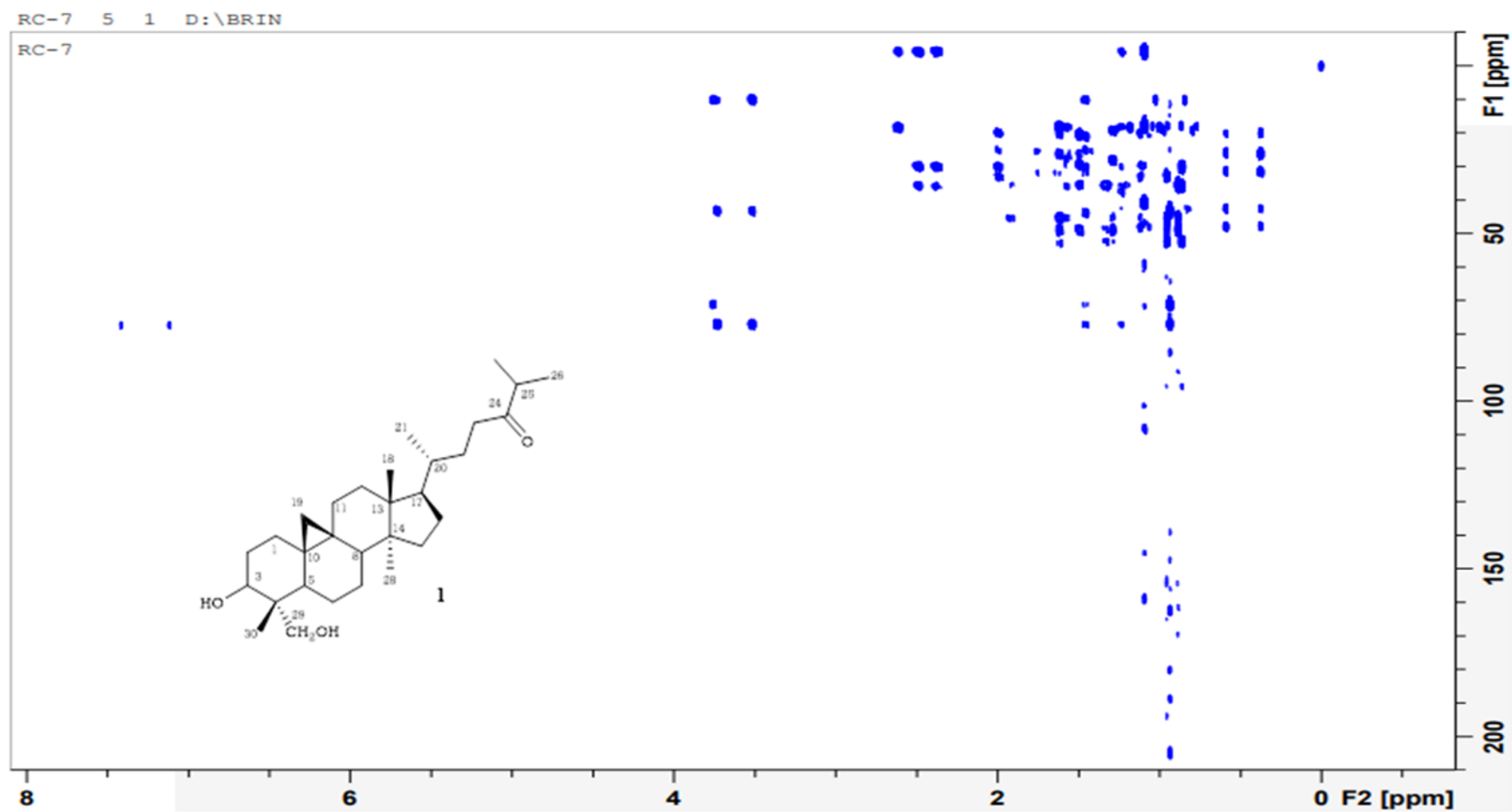
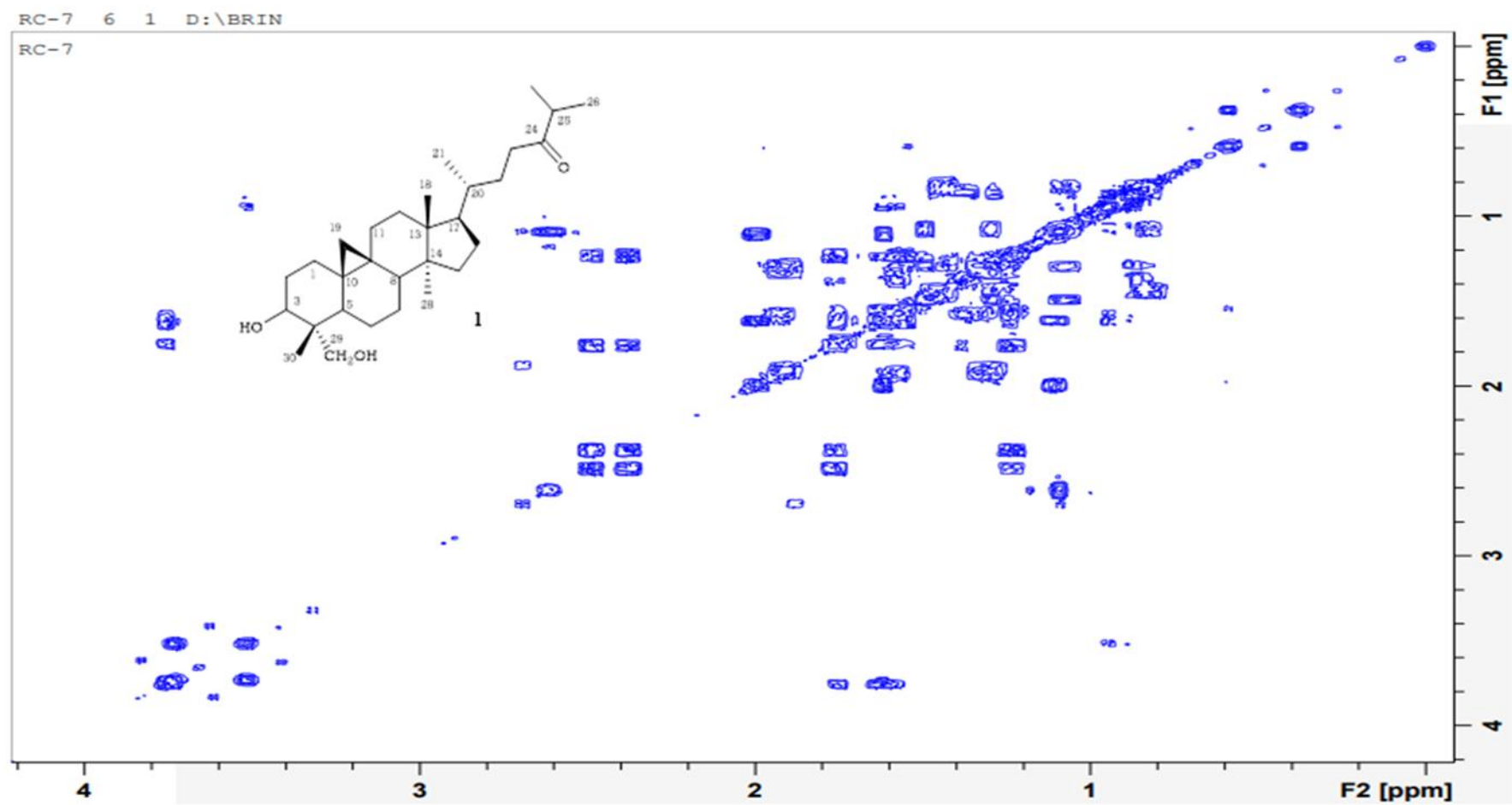


Figure S7. HMBC Spectrum of 1.



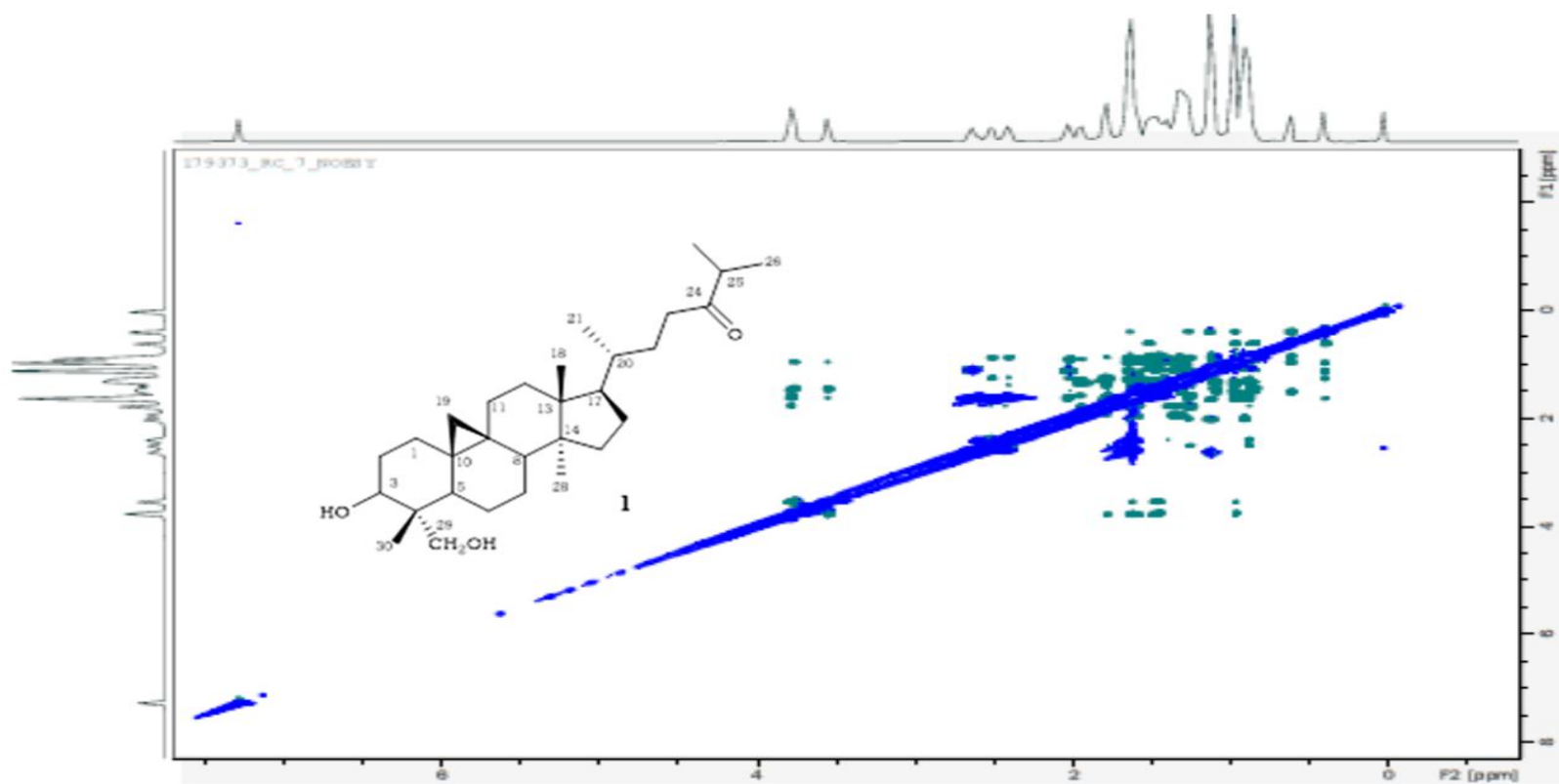


Figure S9. NOESY Spectrum of **1** (700 MHz in CDCl₃).

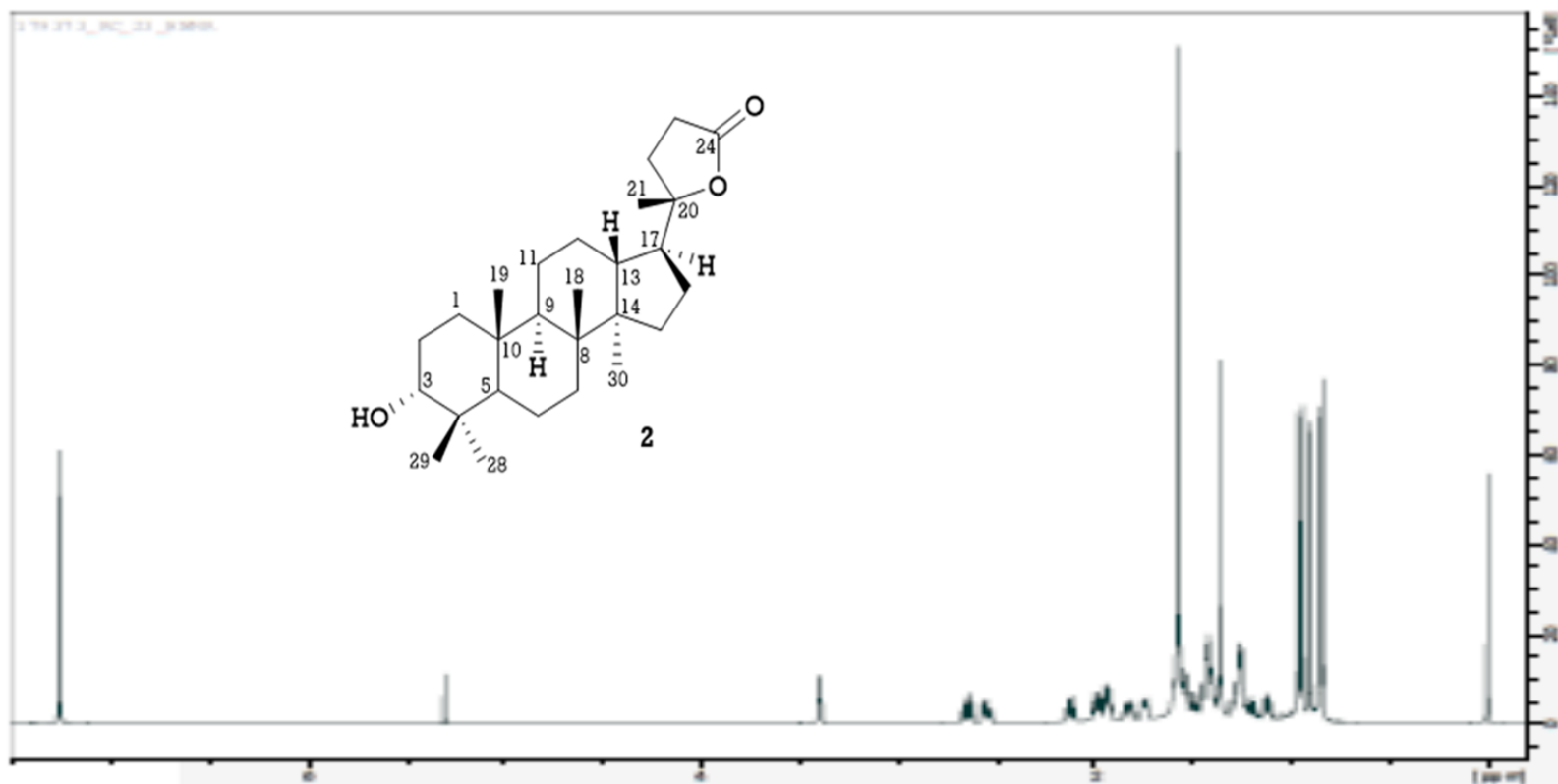


Figure S10a. ¹H-NMR Spectrum of **2** (δ_H 0-8 ppm, 700 MHz in CDCl₃).

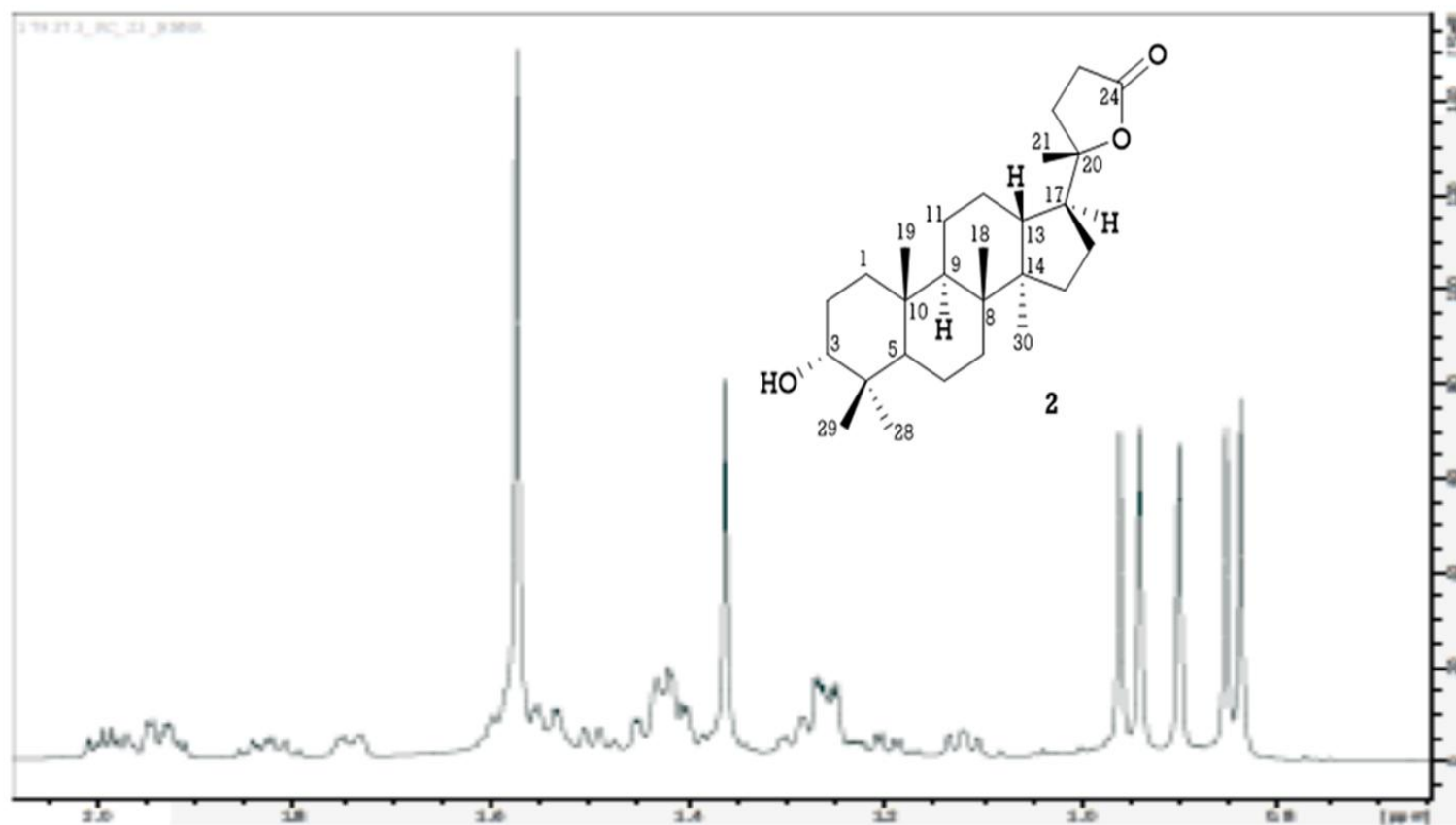


Figure S10b. ^1H -NMR Spectrum of **2** (δ_{H} 0.6-2.0 ppm 700 MHz in CDCl_3).

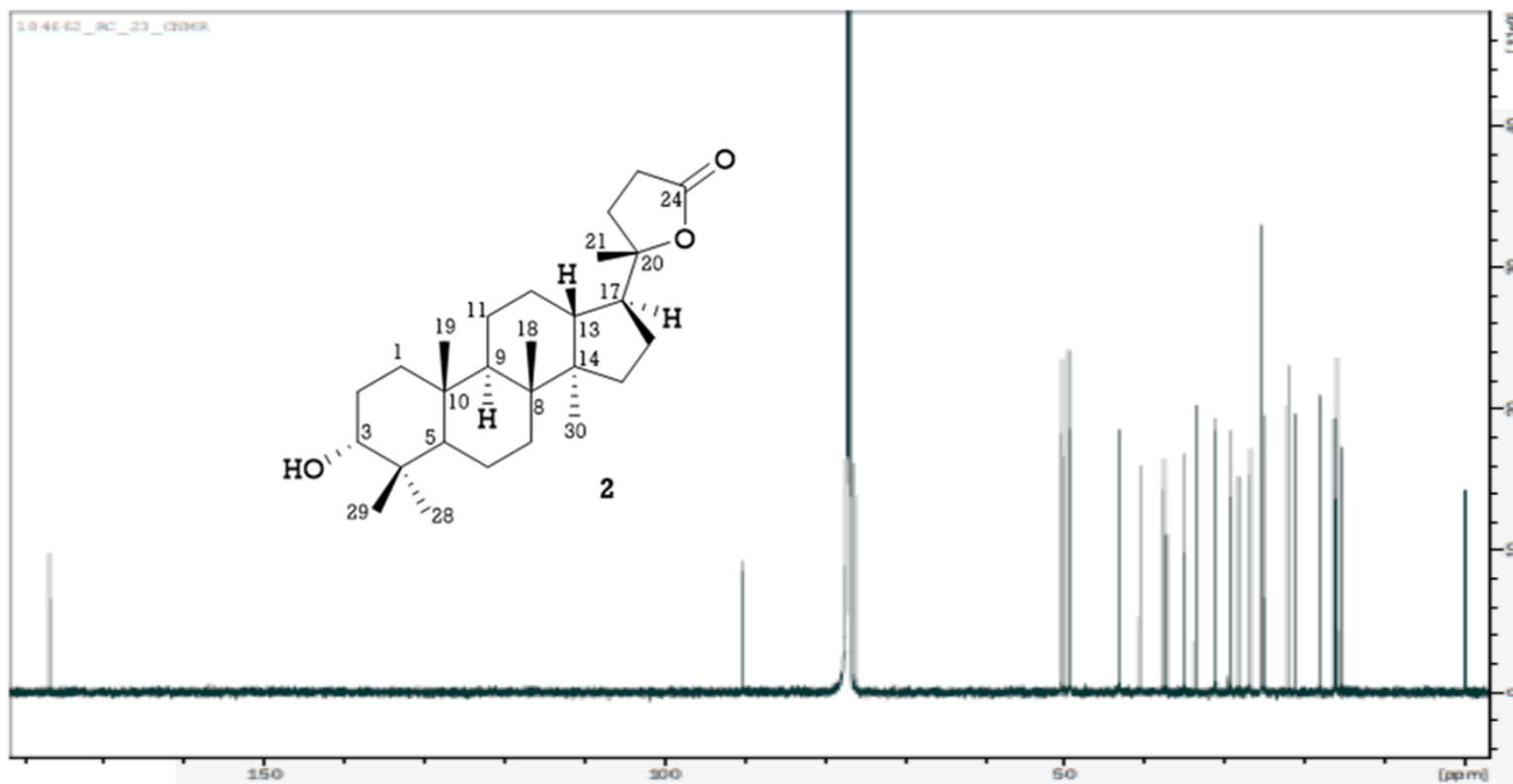


Figure S11. ^{13}C -NMR Spectrum of **2** (175 MHz in CDCl_3).

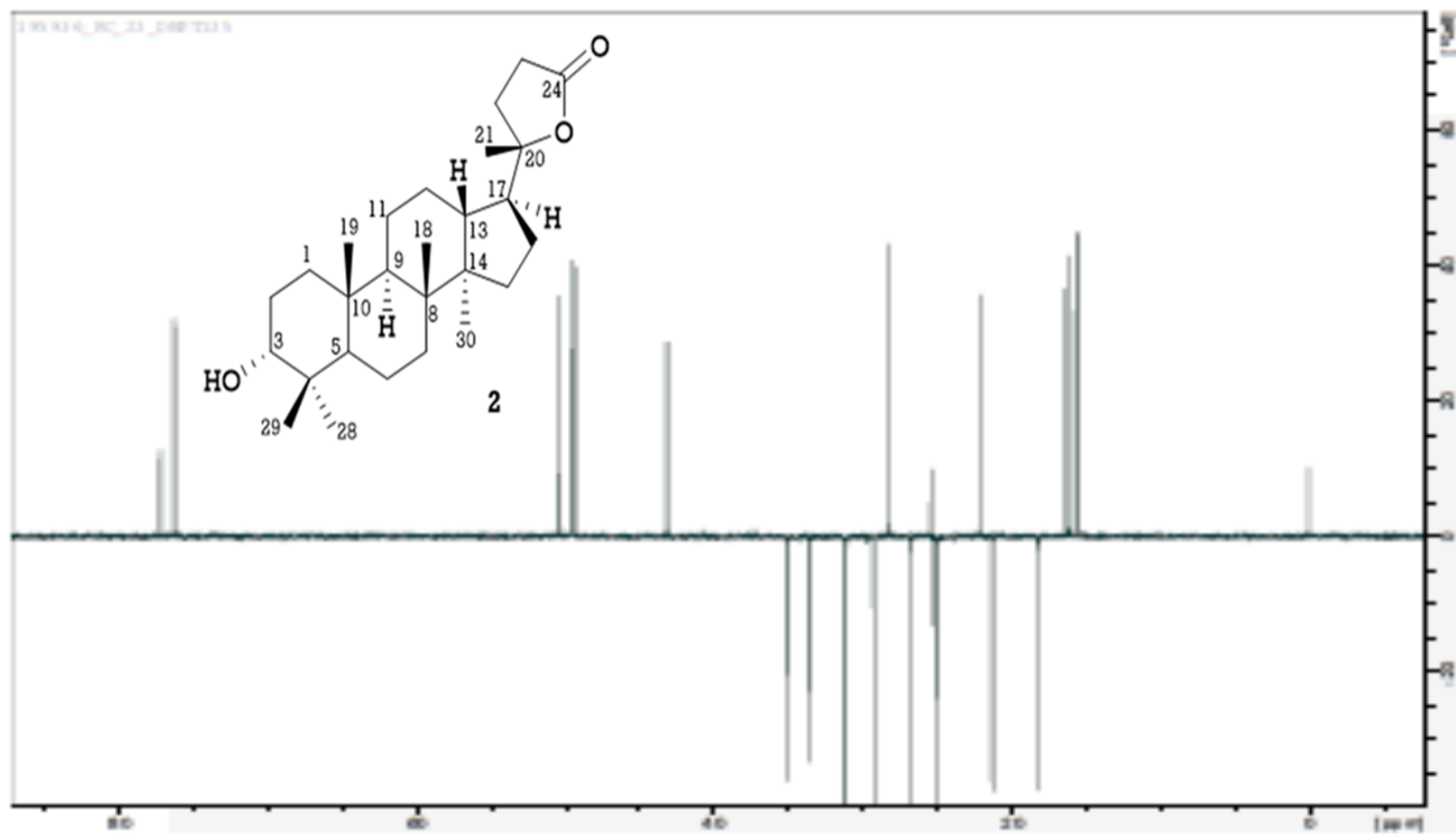


Figure S12. DEPT Spectrum of **2** (175 MHz in CDCl₃).