

Supplementary Materials

($3\beta,16\alpha$)-3,16-Dihydroxypregn-5-en-20-one from the Twigs of *Euonymus alatus* (Thunb.) Sieb.

Exerts Anti-inflammatory Effects in LPS-stimulated RAW-264.7 Macrophages

Seulah Lee^{1,†}, Dahae Lee^{1,†}, Su Cheol Baek¹, Mun Seok Jo¹, Ki Sung Kang^{2,*}, and Ki Hyun Kim^{1,*}

¹School of Pharmacy, Sungkyunkwan University, Suwon 16419, Republic of Korea

² College of Korean Medicine, Gachon University, Seongnam 13120, Republic of Korea

* Corresponding author:

Ki Sung Kang, Tel.: +82-31-750-5402; E-mail: : kkang@gachon.ac.kr

Ki Hyun Kim, Tel: +82-31-290-7700; Fax: +82-31-290-7730; E-mail: khkim83@skku.edu

† These authors contributed equality to this work.

Supporting Information Contents:

Figure S1. HR-ESIMS data of 1	S3
Figure S2. ^1H NMR spectrum of 1 (CD_3OD , 700 MHz).....	S4
Figure S3. DEPT spectrum of 1 (CD_3OD , 175 MHz).....	S5
Figure S4. ^1H - ^1H COSY spectrum of 1 (CD_3OD).....	S6
Figure S5. NOESY spectrum of 1 (CD_3OD).....	S7
Figure S6. HSQC spectrum of 1 (CD_3OD).....	S8
Figure S7. HMBC spectrum of 1 (CD_3OD).....	S9

Figure S1. HR-ESIMS data of **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

63 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O
333.2430	333.2430	0.0	0.0	5.5	C21 H33 O3	250.1	n/a	n/a	21	33	3

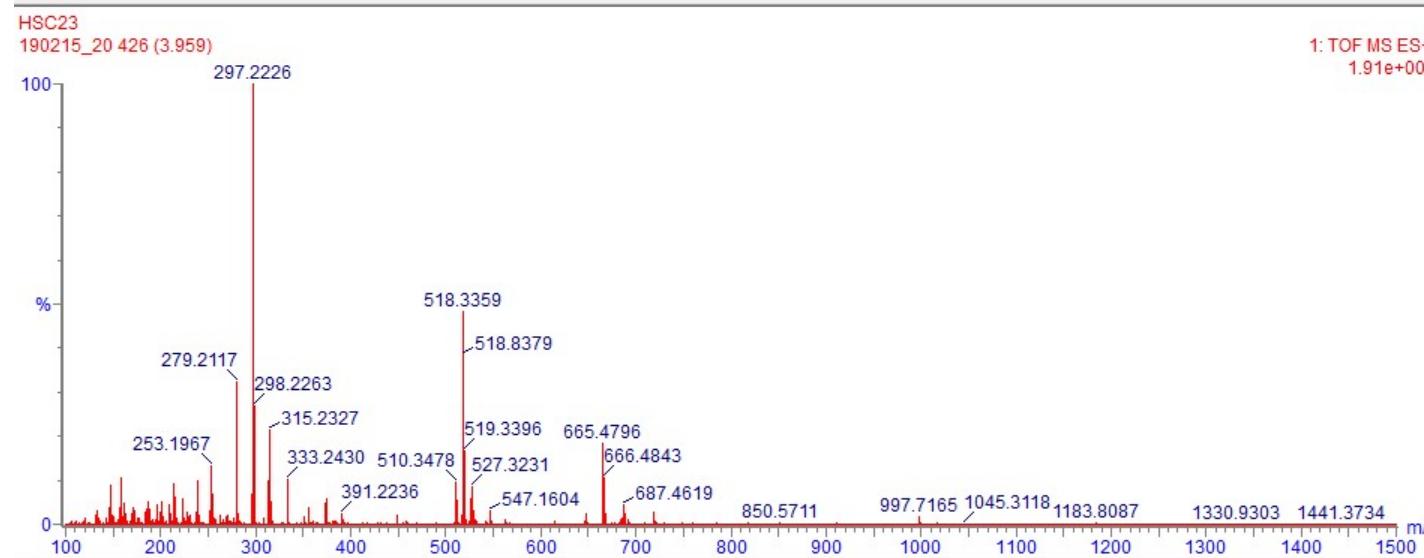


Figure S2. ^1H NMR spectrum of **1** (CD_3OD , 700 MHz).

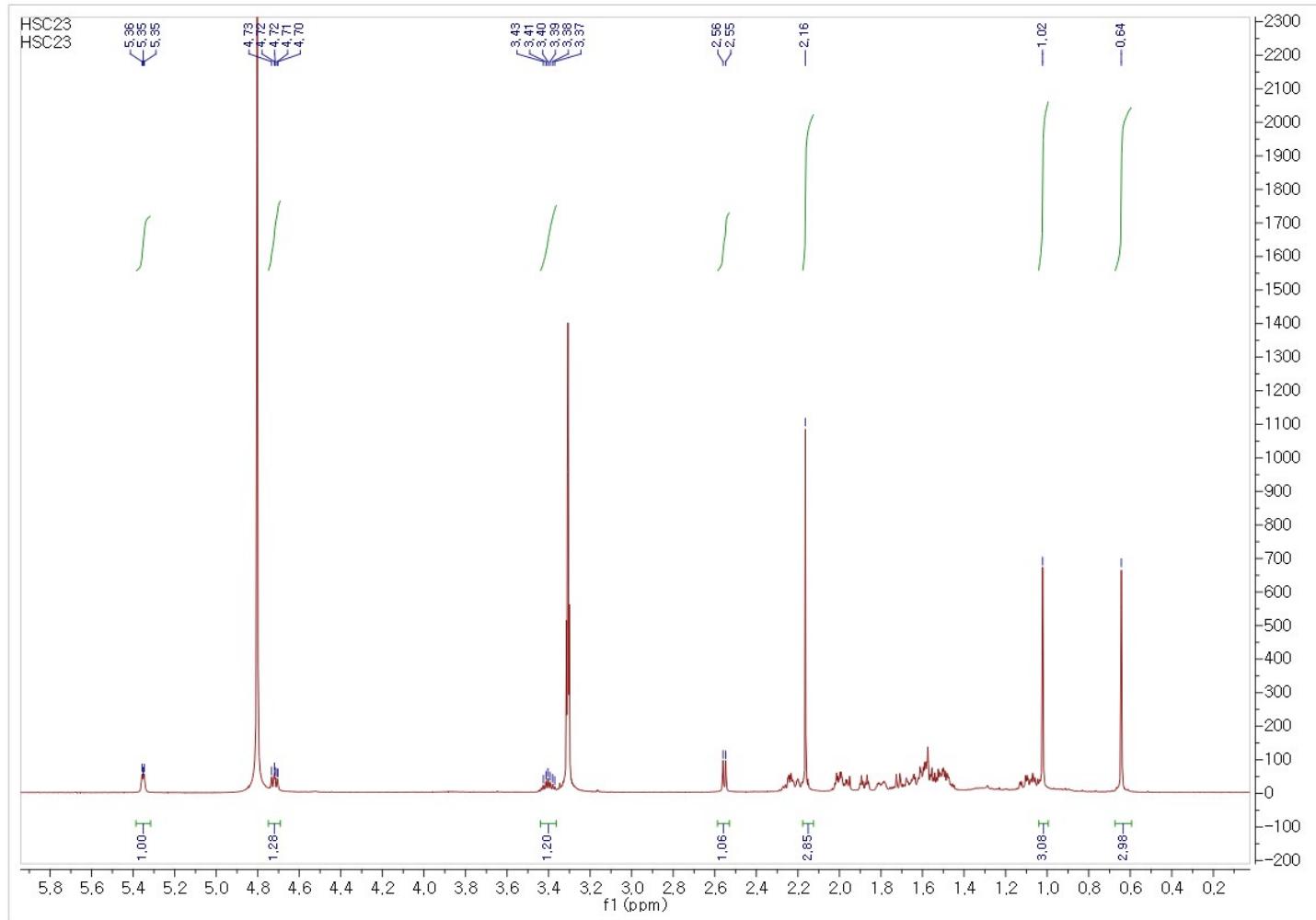


Figure S3. DEPT spectrum of **1** (CD_3OD , 175 Hz).

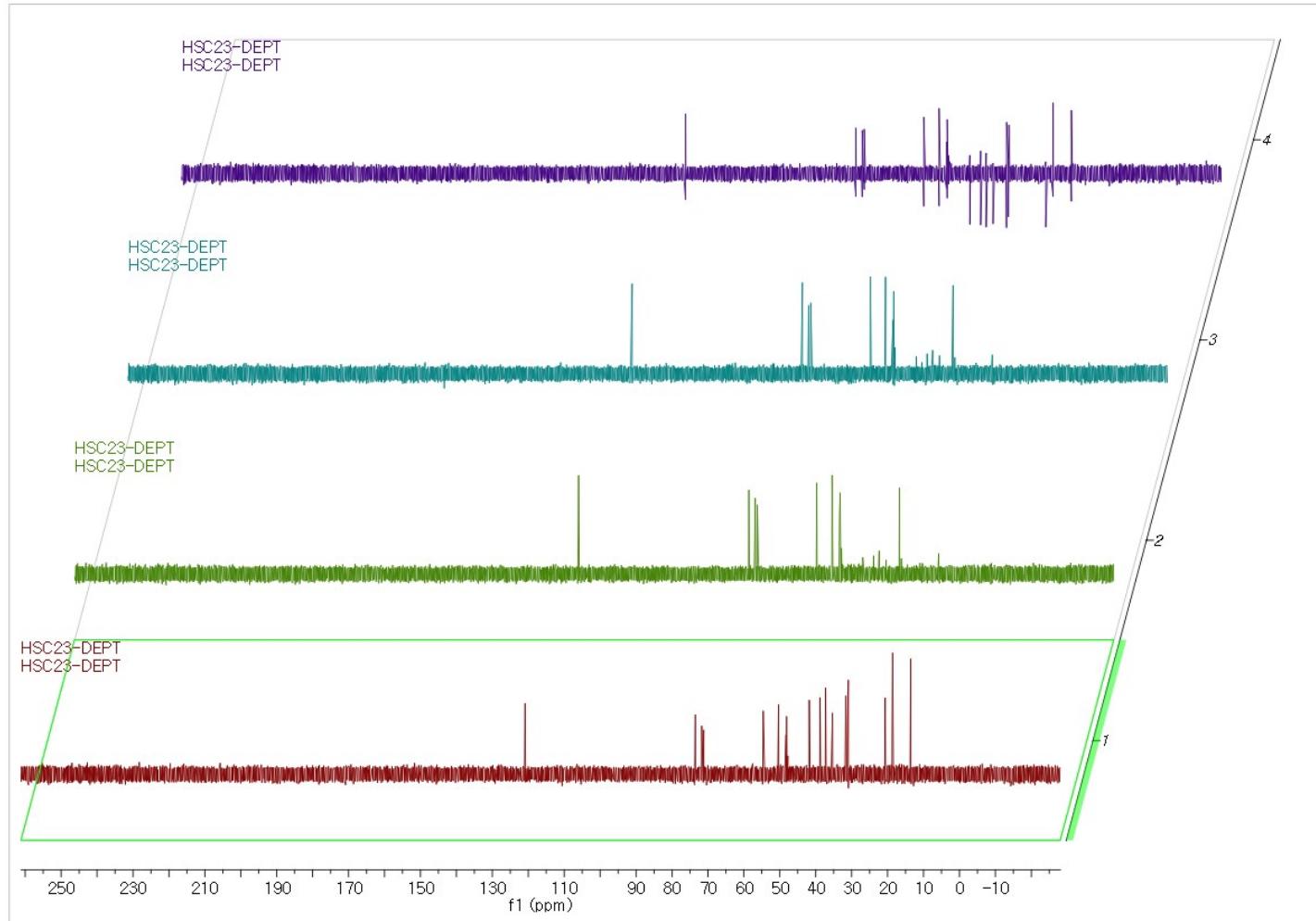


Figure S4. ^1H - ^1H COSY spectrum of **1** (CD_3OD).

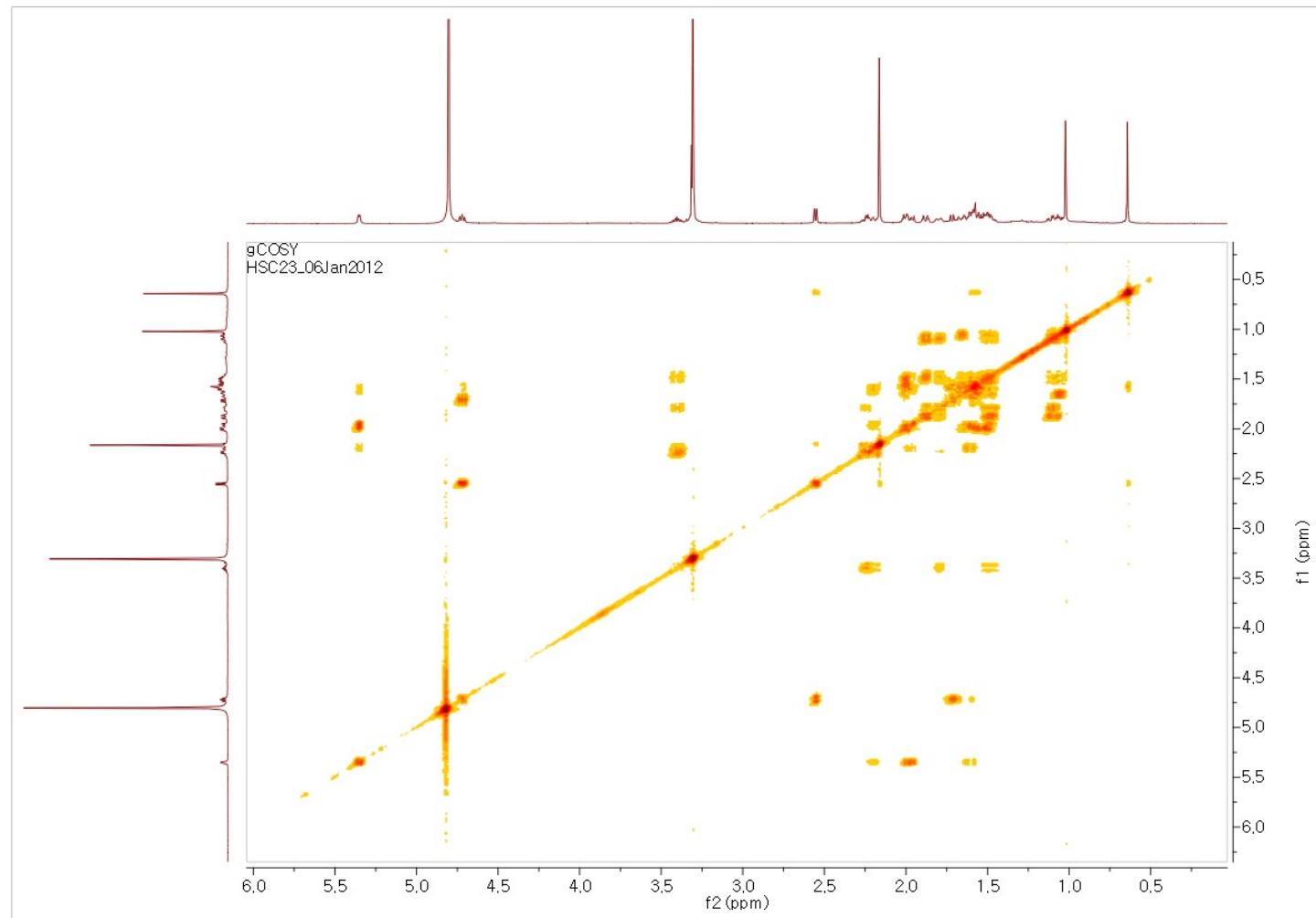


Figure S5. NOESY spectrum of **1** (CD_3OD).

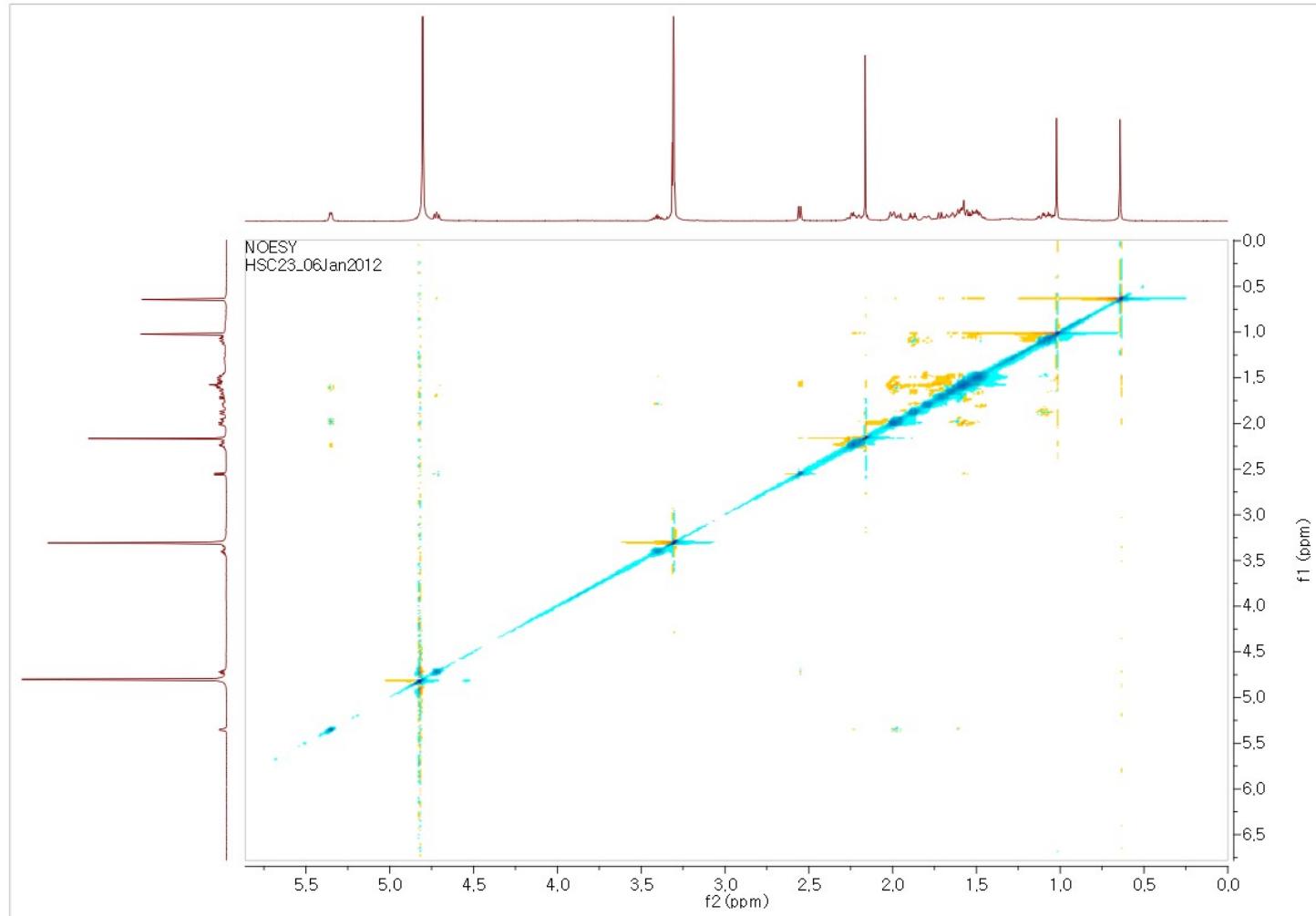


Figure S6. HSQC spectrum of **1** (CD_3OD).

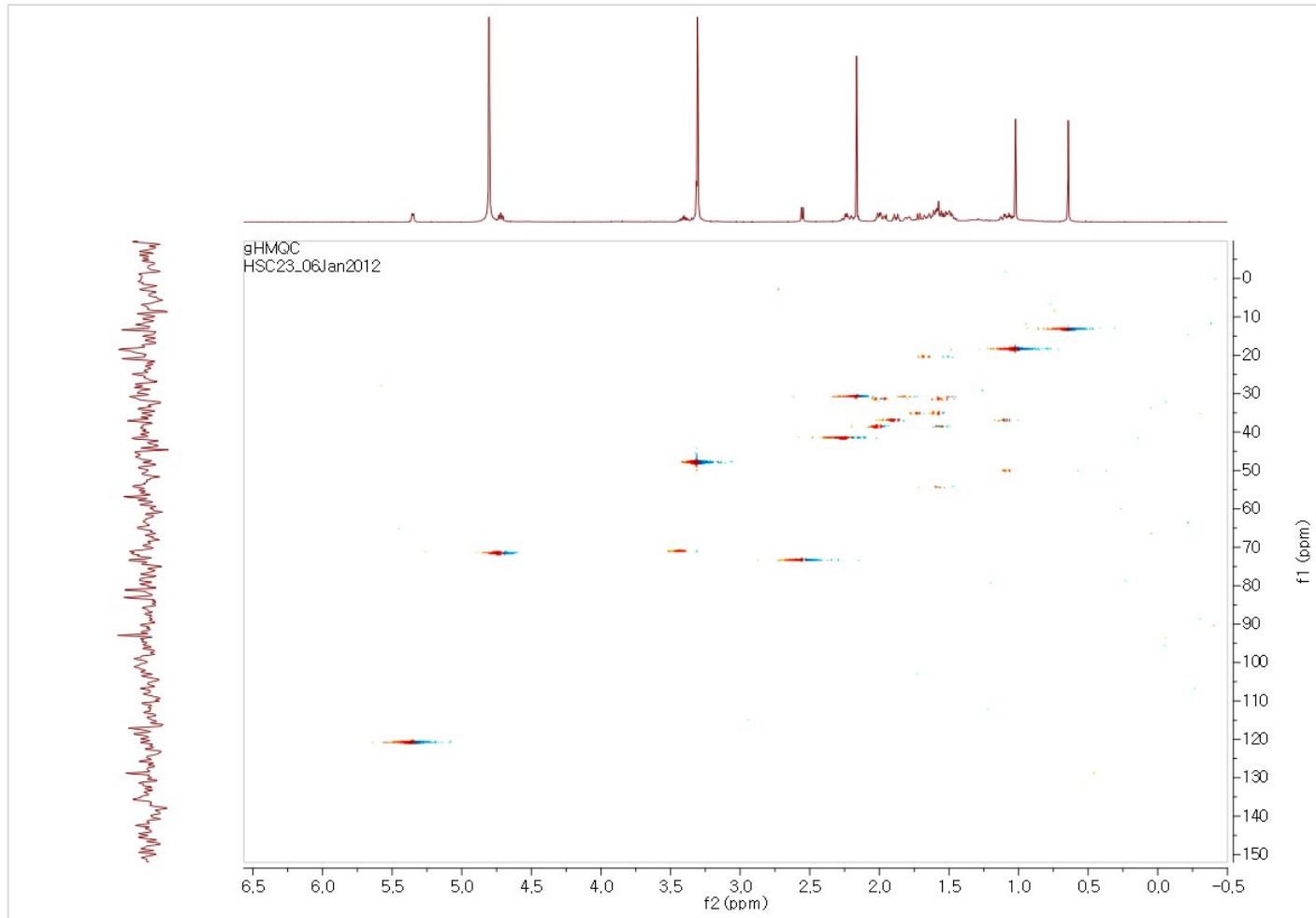


Figure S7. HMBC spectrum of **1** (CD_3OD).

