

SUPPLEMENTARY MATERIAL

Furanocoumarins with potential antiproliferative activities from *Clausena lenis*

Yan-Ping Liu^{b,c}, Qing Wen^{b,c,d}, Shi Hu^{b,c,d}, Yan-Lei Ma^{b,c,d}, Zhi-Hua Jiang^{b,c,d}, Jin-Ying Tang^{b,c,d}, Shen-Xiang Qiu^{a,*}, Yan-Hui Fu^{a,b,c,d,*}

^a Guangdong Provincial Key Laboratory of Applied Botany, South China Botanical Garden, Chinese Academy of Sciences, Guangzhou 510650, P. R. China;

^b Key Laboratory of Tropical Medicinal Plant Chemistry of Ministry of Education, Hainan Normal University, Haikou 571158, P. R. China

^c Key Laboratory of Southern Medicinal Plants Resources of Haikou City, Hainan Normal University, Haikou 571158, P.R. China

^d College of Pharmacy, Fujian University of Traditional Chinese Medicine, Fuzhou 350122, P.R. China

*Corresponding author.

Tel./ Fax: +86-898-65889422; E-mail: fuyanhui80@126.com; sxqiu@scbg.ac.cn

ABSTRACT

A phytochemical investigation on the stems and leaves of *Clausena lenis* led to the isolation of a new furanocoumarin, clauselenisin A (**1**), together with five known analogues (**2–6**). The structure of **1** was elucidated by extensive spectroscopic methods and the known compounds were identified by comparisons with data reported in the literature. All known compounds (**2–6**) were isolated from *C. lenis* for the first time. All isolated compounds were evaluated for their antiproliferative activities against five human cancer cell lines: HL-60, SMMC-7721, A-549, MCF-7 and SW480 *in vitro*. Compounds **1–6** showed significant antiproliferative effects with IC₅₀ values ranging from 0.36 to 16.48 μM.

Keywords: *Clausena lenis*; furanocoumarin; clauselenisin A ; antiproliferative activities.

*Corresponding author. Tel.: +86-86-898-65889422; Fax: +86-898-65889422;
E-mail: fuyanhui80@163.com; sxqiu@scbg.ac.cn

List of Supplementary Material

Figure S1. Selected 2D NMR correlations for clauselenisin A (**1**).

Figure S2. ^1H -NMR spectrum of clauselenisin A (**1**) in CDCl_3 .

Figure S3. ^{13}C -NMR spectrum of clauselenisin A (**1**) in CDCl_3 .

Figure S4. DEPT spectra of clauselenisin A (**1**) in CDCl_3 .

Figure S5. HSQC spectrum of clauselenisin A (**1**) in CDCl_3 .

Figure S6. HMBC spectrum of clauselenisin A (**1**) in CDCl_3 .

Figure S7. ^1H - ^1H COSY spectrum of clauselenisin A (**1**) in CDCl_3 .

Figure S8. ROESY spectrum of clauselenisin A (**1**) in CDCl_3 .

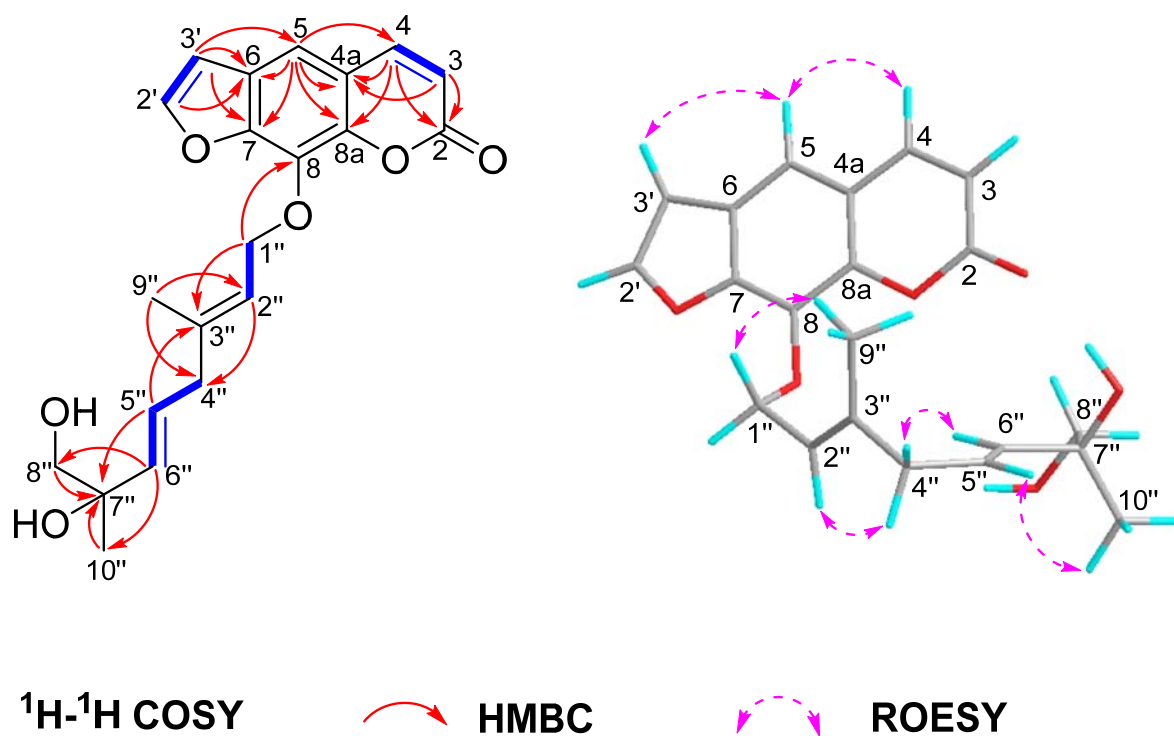


Figure S1. Selected 2D NMR correlations for clauselenisin A (**1**).

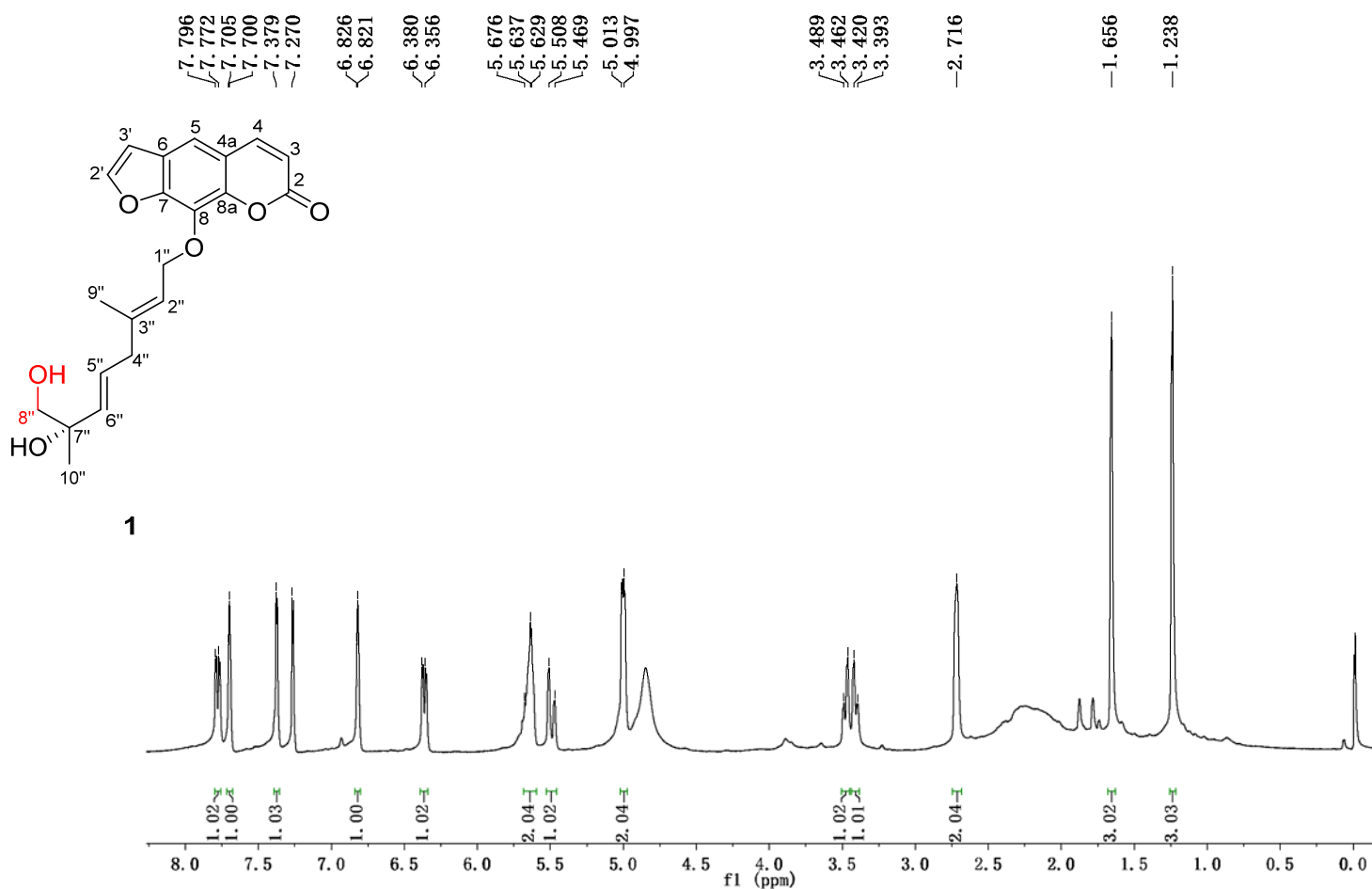


Figure S2. ^1H -NMR spectrum of clauselenisin A (**1**) in CDCl_3 .

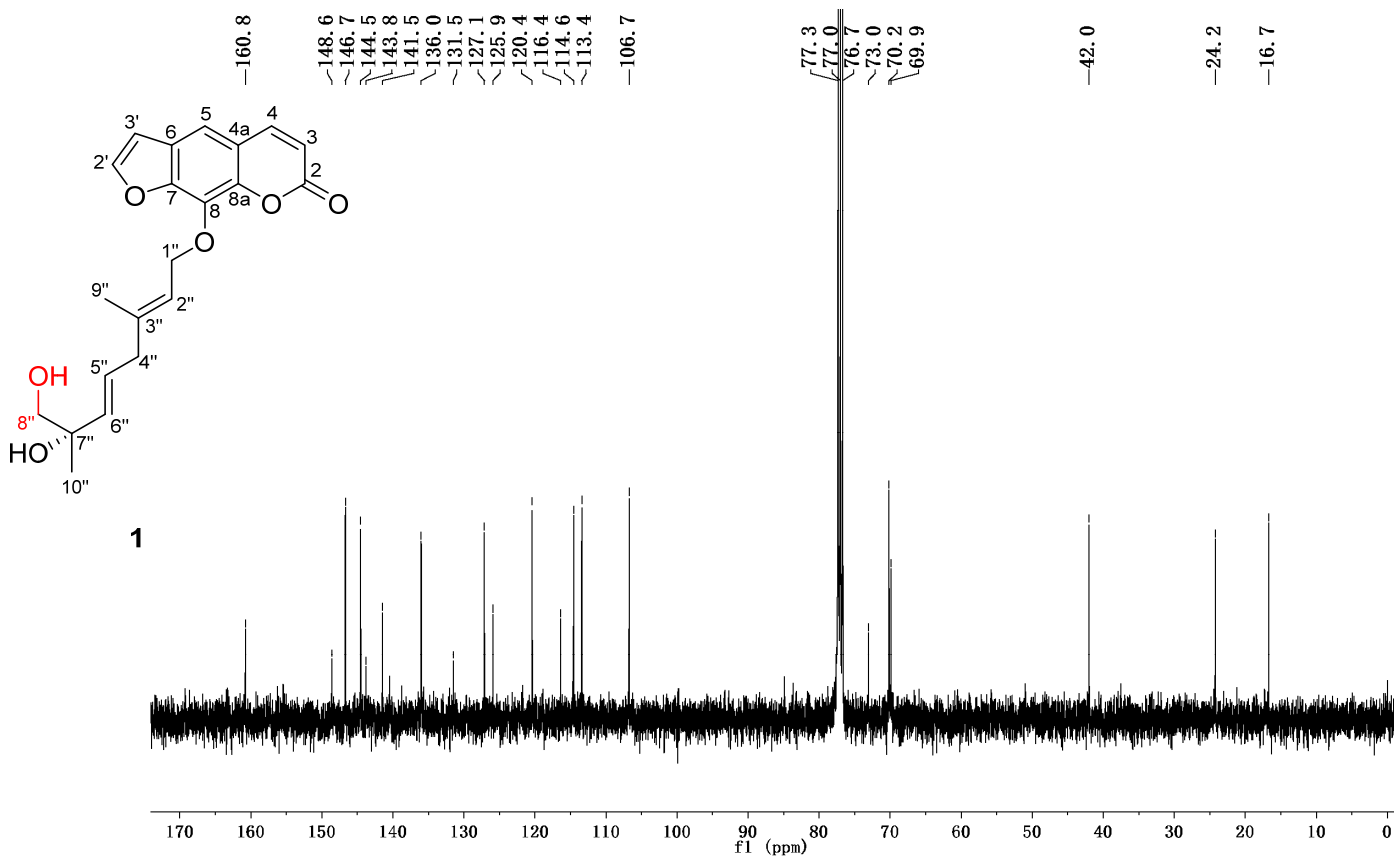


Figure S3. ^{13}C -NMR spectrum of clauselenisin A (1) in CDCl_3 .

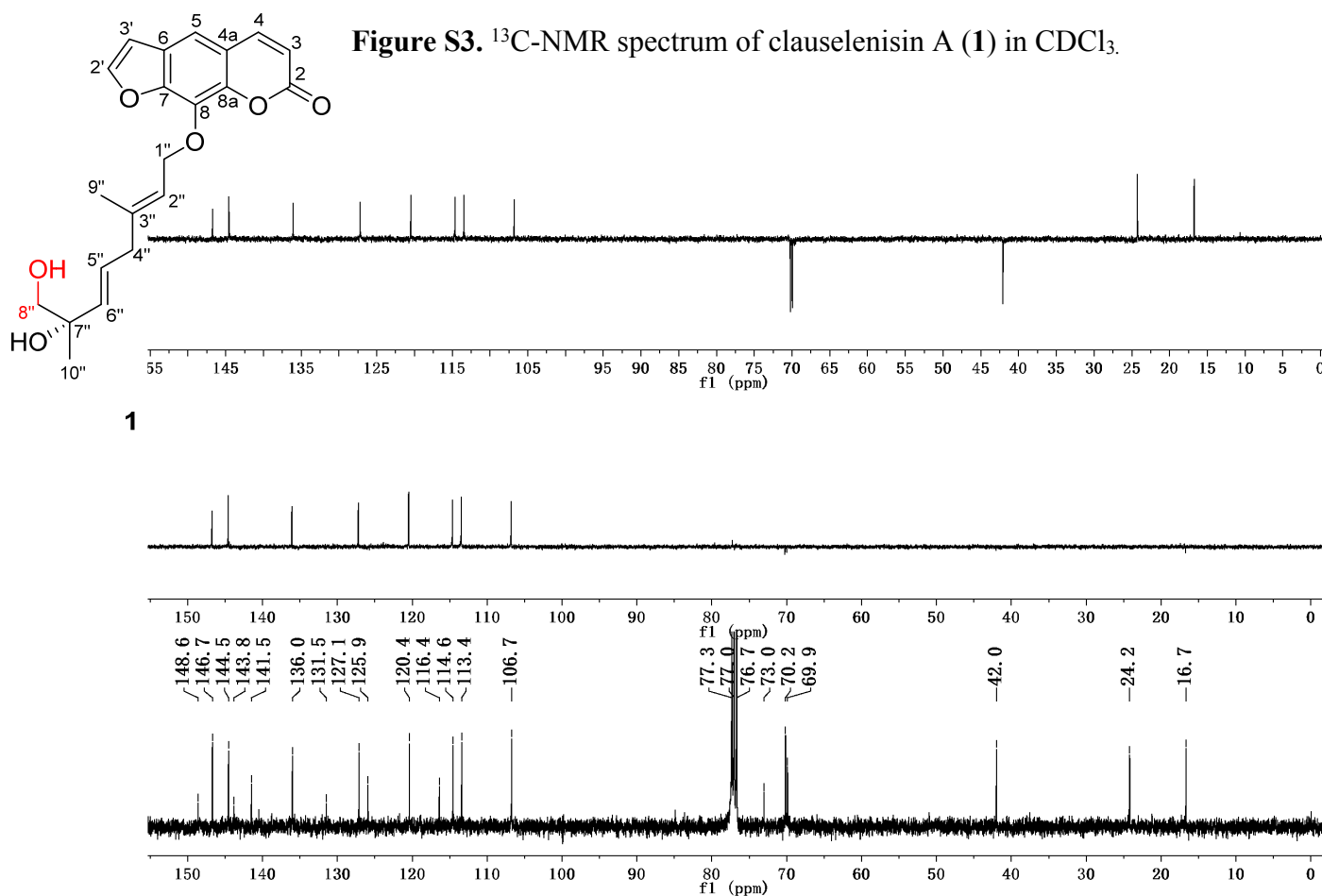


Figure S4. DEPT spectra of clauselenisin A (1) in CDCl_3 .

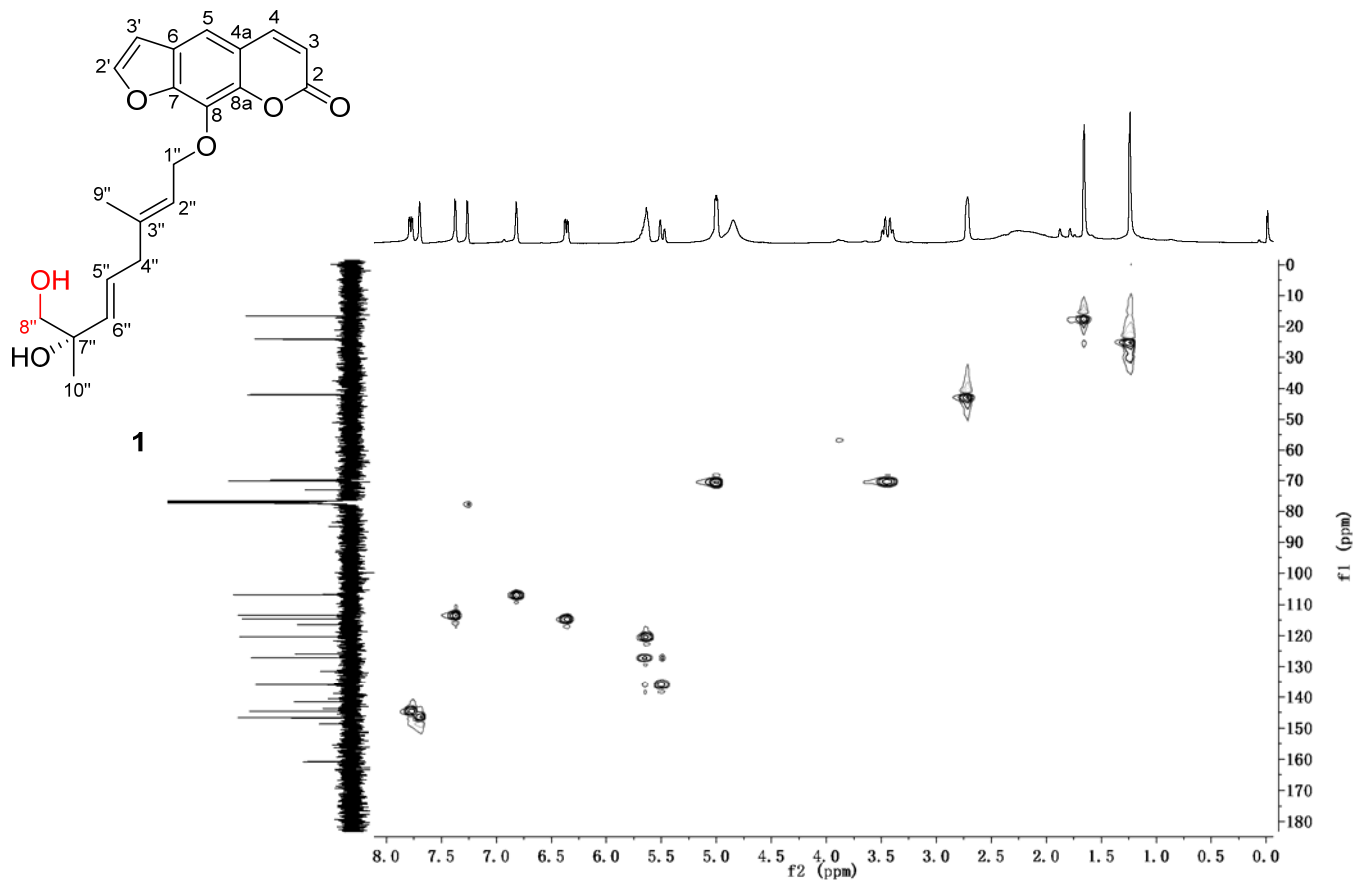


Figure S5. HSQC spectrum of clauselenisin A (**1**) in CDCl₃.

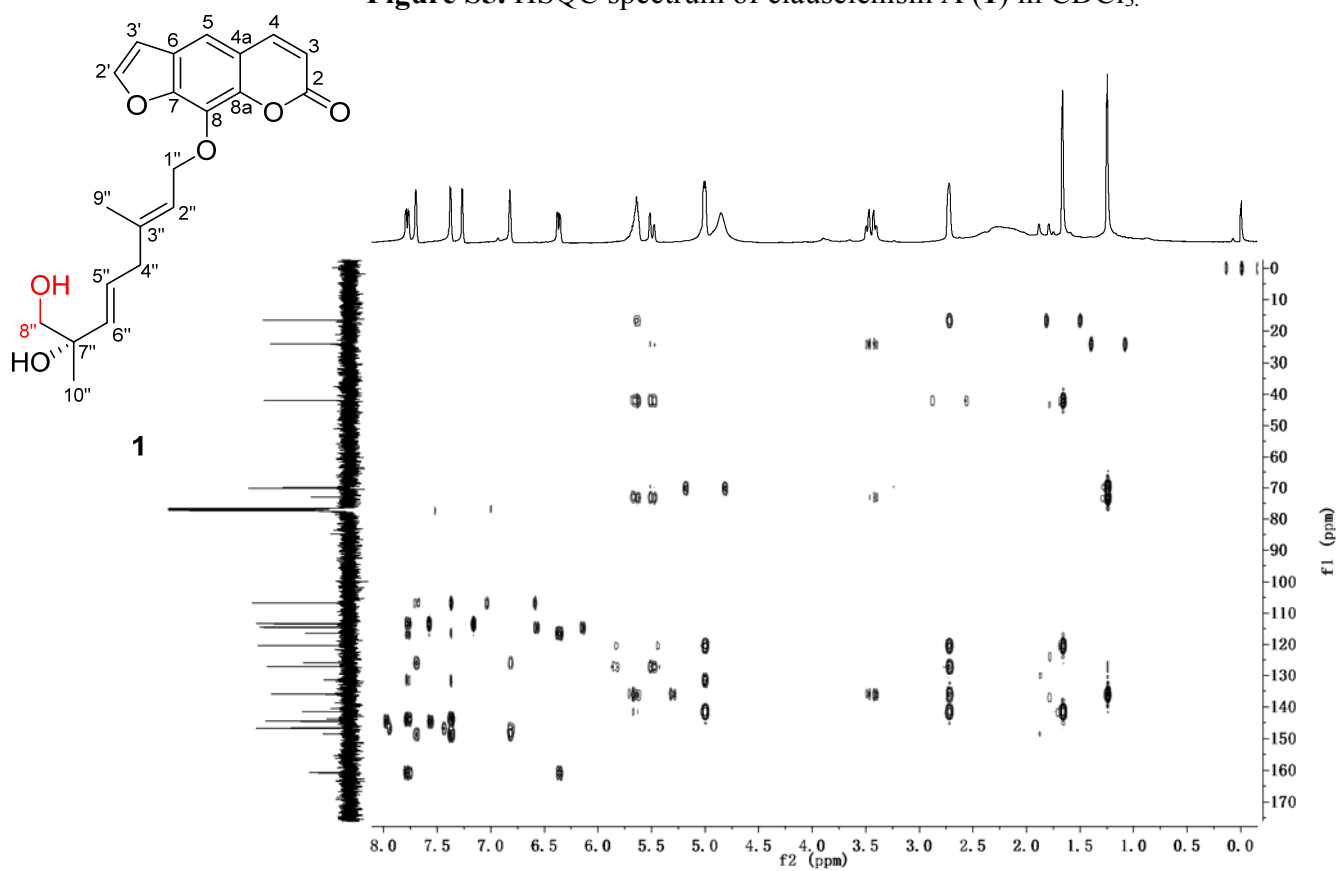


Figure S6. HMBC spectrum of clauselenisin A (**1**) in CDCl₃.

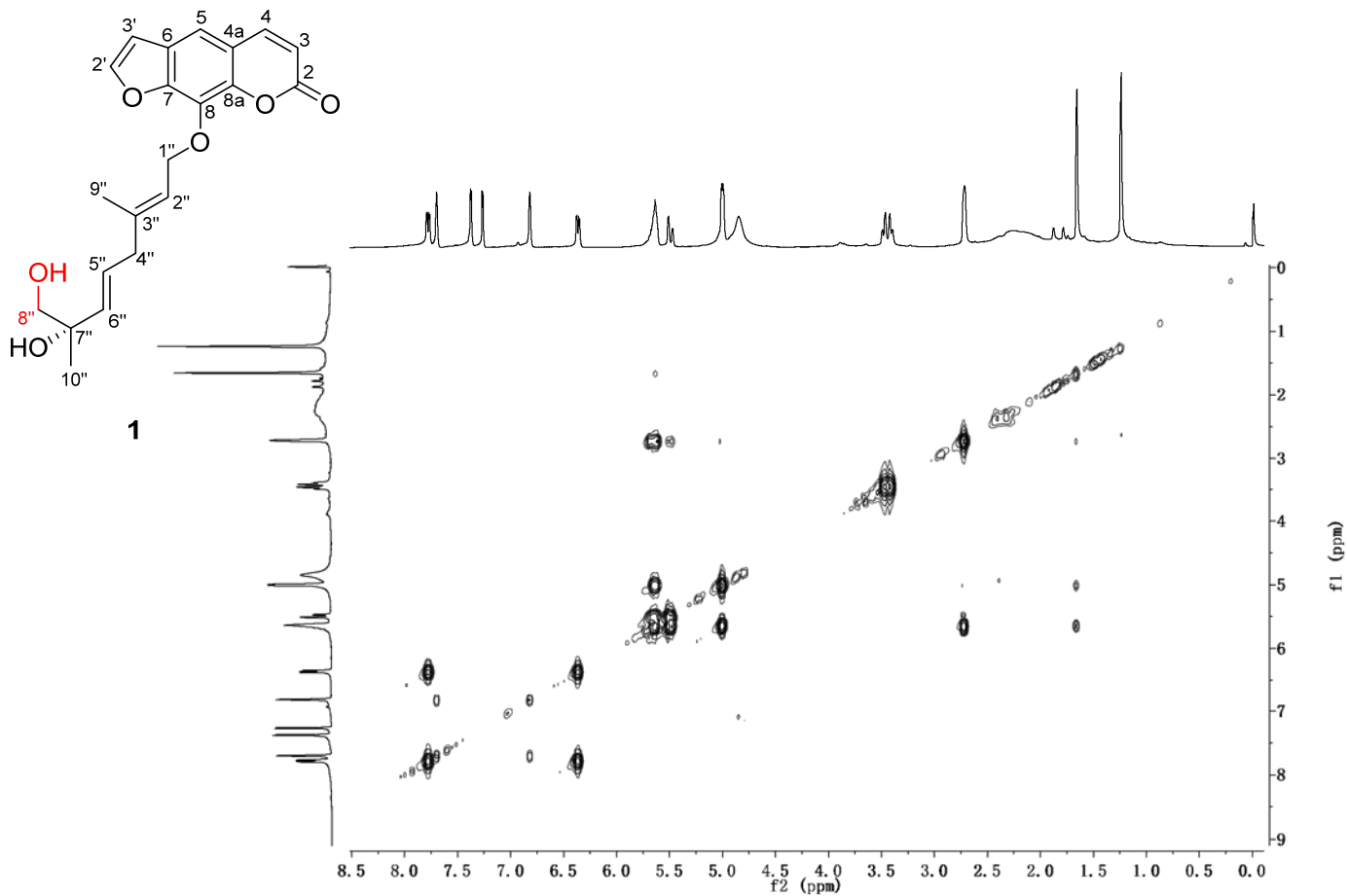


Figure S7. ^1H - ^1H COSY spectrum of clauselenisin A (**1**) in CDCl_3 .

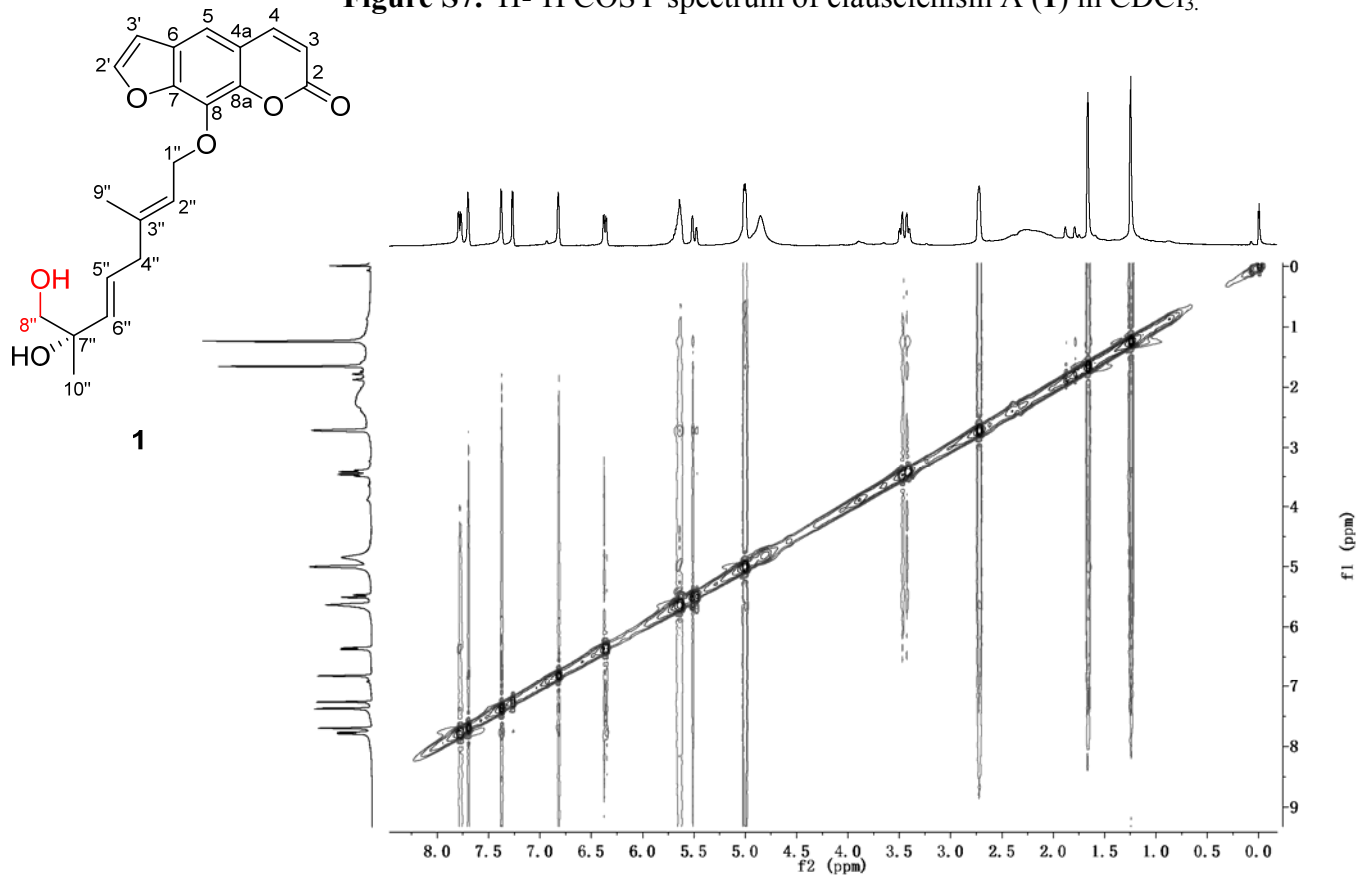


Figure S8. ROESY spectrum of clauselenisin A (**1**) in CDCl_3 .