Supporting Information (SI)

Euphorikanin A, a Diterpenoid Lactone with a Fused 5/6/7/3 Ring System from *Euphorbia kansui*

Dong-Qing Fei*,†, Le-Le Dong,† Feng-Ming Qi,‡ Gai-Xia Fan,† Hui-Hong Li,† Zheng-Yu Li,† and Zhan-Xin Zhang,*,†

†School of Pharmacy, Lanzhou University, Lanzhou 730000, People's Republic of China

‡State Key Laborratory of Applied Organic Chemistry, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, People's Republic of China

* To whom correspondence should be addressed. Tel:+86-931-8915686. Fax: Tel:+86-931-8915686. E-mail: feidq@lzu.edu.cn (D.-Q. F.); zhangzhx@lzu.edu.cn (Z.-X. Z.)

TABLE OF CONTENTS

1. Detailed experimental procedures

1.1 General Experimental Procedures

Melting points were determined on an X-4 digital display micromelting point apparatus, and are uncorrected. Optical rotations were measured on a Perkin Elmer 341 polarimeter. IR spectra were taken on a Nicolet NEXUS 670 FT-IR spectrometer. NMR spectra were recorded on a Varian INOVA-600 NMR spectrometer with TMS as internal standard. HRESIMS data were recorded on a Thermo LTQ Orbitrap Elite mass spectrometer. Sephadex LH-20 was supplied by Amersham Pharmacia Biotech. Silica gel (200-300 mesh) used for column chromatography and silica gel GF_{254} (10-40 μM) used for TLC were supplied by the Qingdao Marine Chemical Factory, Qingdao, China. Spots were detected on TLC under UV light or by heating after spraying with 5% H_2SO_4 in C_2H_5OH (v/v).

1.2 Plant Material

The dry roots of *Euphorbia kansui* were purchased in September 2012 from Hebei Anguo Medicine Market, Anguo, China. The plant material was identified by Dr. Jian-Yin Li, School of Pharmacy, Lanzhou University, Lanzhou, China. A voucher specimen (No. 201209EK) was deposited at the School of Pharmacy, Lanzhou University.

1.3 Extraction and isolation

The dried and pulverized roots of *E. kansui* (25 kg) were extracted with 95% aqueous EtOH at room temperature four times (each time for 7 days). The solvent was evaporated under reduced pressure to yield a crude extract (470 g), which was suspended in water and then extracted with EtOAc and n-BuOH, sequentially. The EtOAc-soluble extract (324 g) was obtained after evaporation of the EtOAc solution under reduced pressure. The EtOAc extract was subjected to column chromatography over silica gel eluting with a petroleum ether-acetone step gradient system (40:1 to 1:1) to give six main fractions A-F. Fraction B (21 g) was chromatographed over silica gel column, eluted with a gradient solvent system of increasing polarity (petroleum ether-acetone, 30:1 to 4:1), yielding two subfractions B1 and B2. Subfraction B1 was subjected to repeated chromatography over silica gel (petroleum ether-EtOAc, 20:1 to 2:1) to give subfractions B1A-B1C. Subfraction B1A was purified by silica gel CC (petroleum ether-acetone, 20:1 to 2:1) followed by gel permeation chromatography (GPC) on Sephadex LH-20 in $CHCl_3$-MeOH (1:1) to yield an inseparable mixture. This mixture was subjected to silica gel preparative TLC using petroleum ether-acetone (5:1) to afford compound **1** (2 mg).

2. NMR, HRESIMS, and IR spectra of compound 1

Figure S1. ^{1}H NMR spectrum of euphorikanin A (**1**) in $CDCl_3$

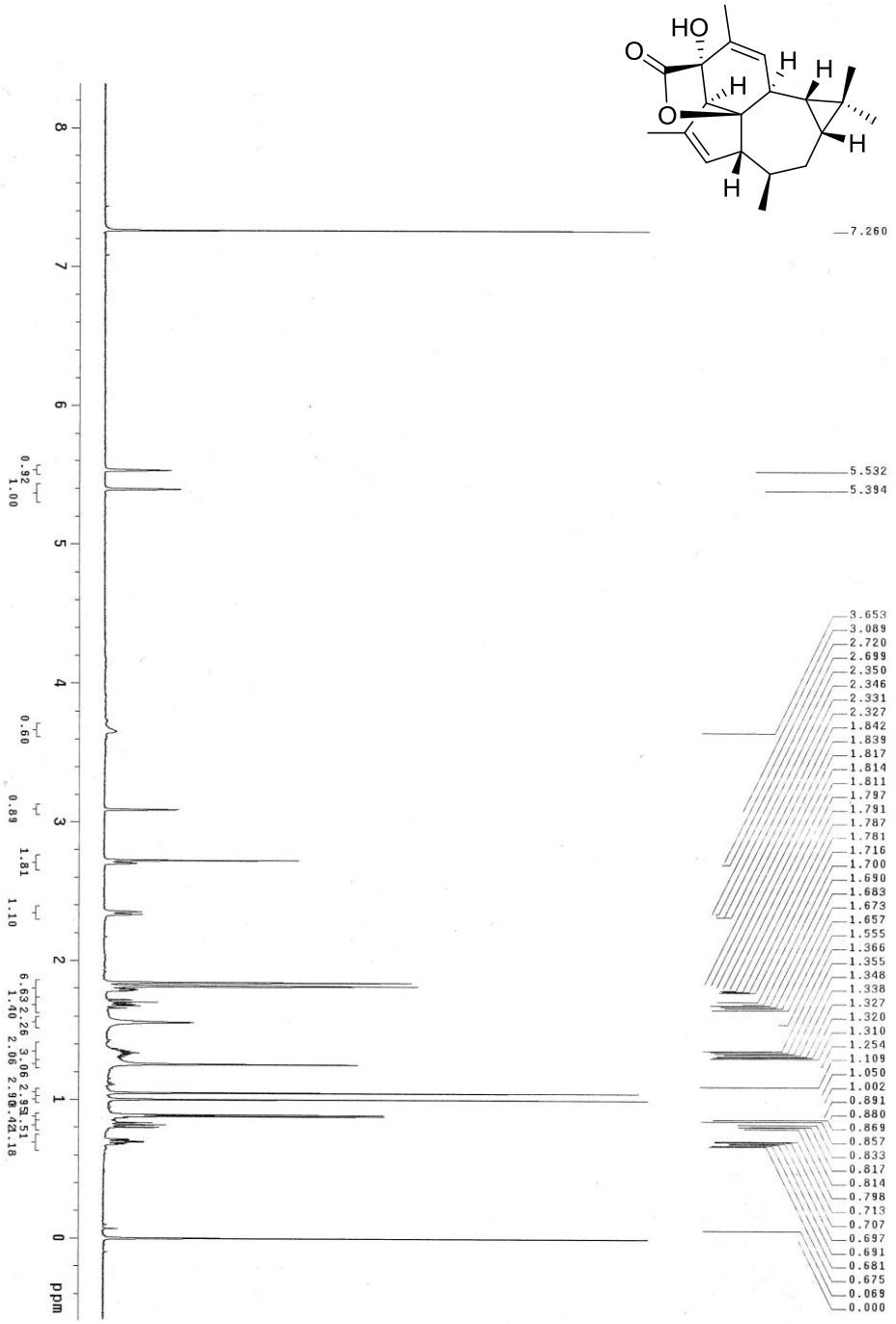

Figure S2. ^{13}C NMR spectrum of euphorikanin A (**1**) in $CDCl_3$

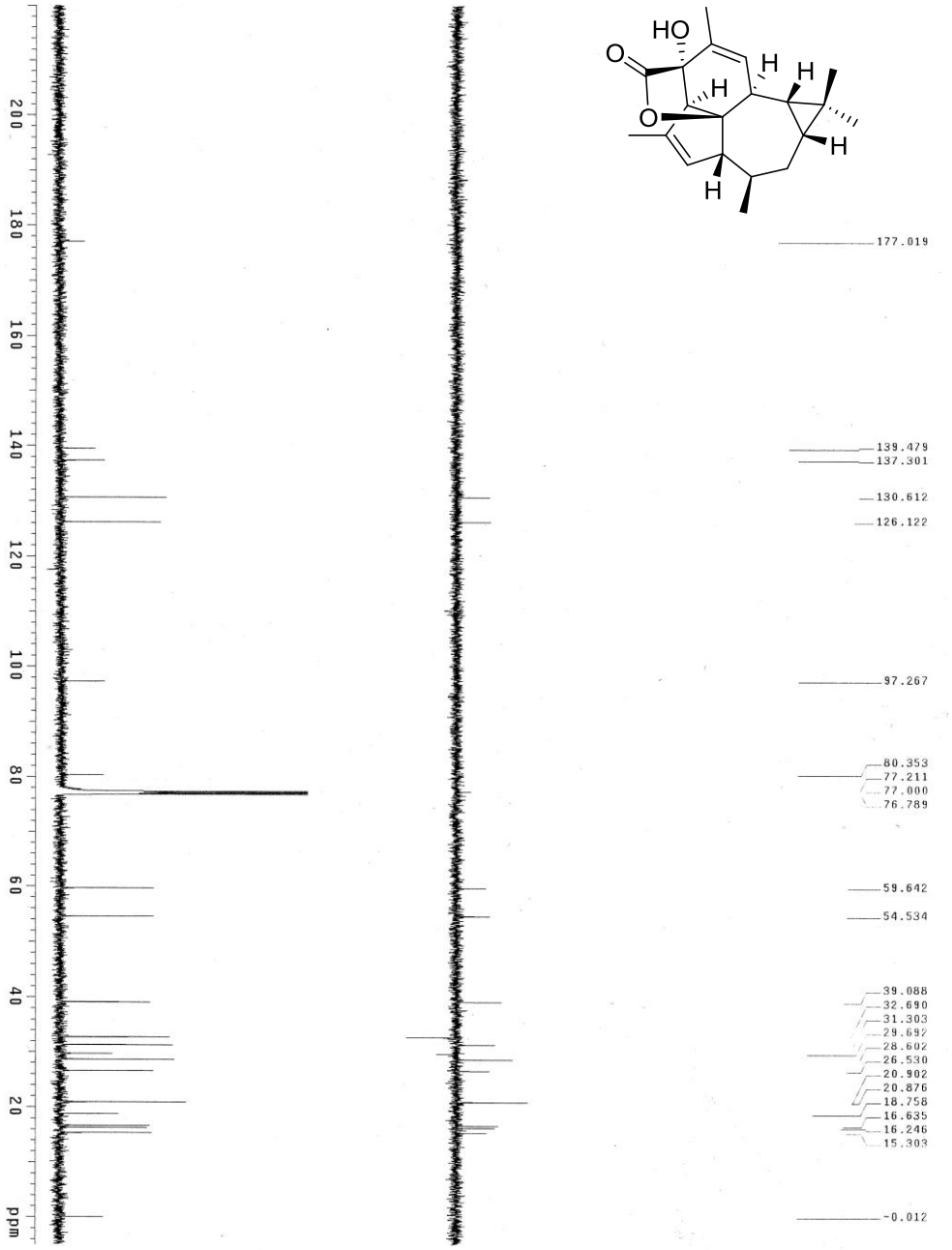

Figure S3. HSQC spectrum of euphorikanin A (**1**) in $CDCl_3$

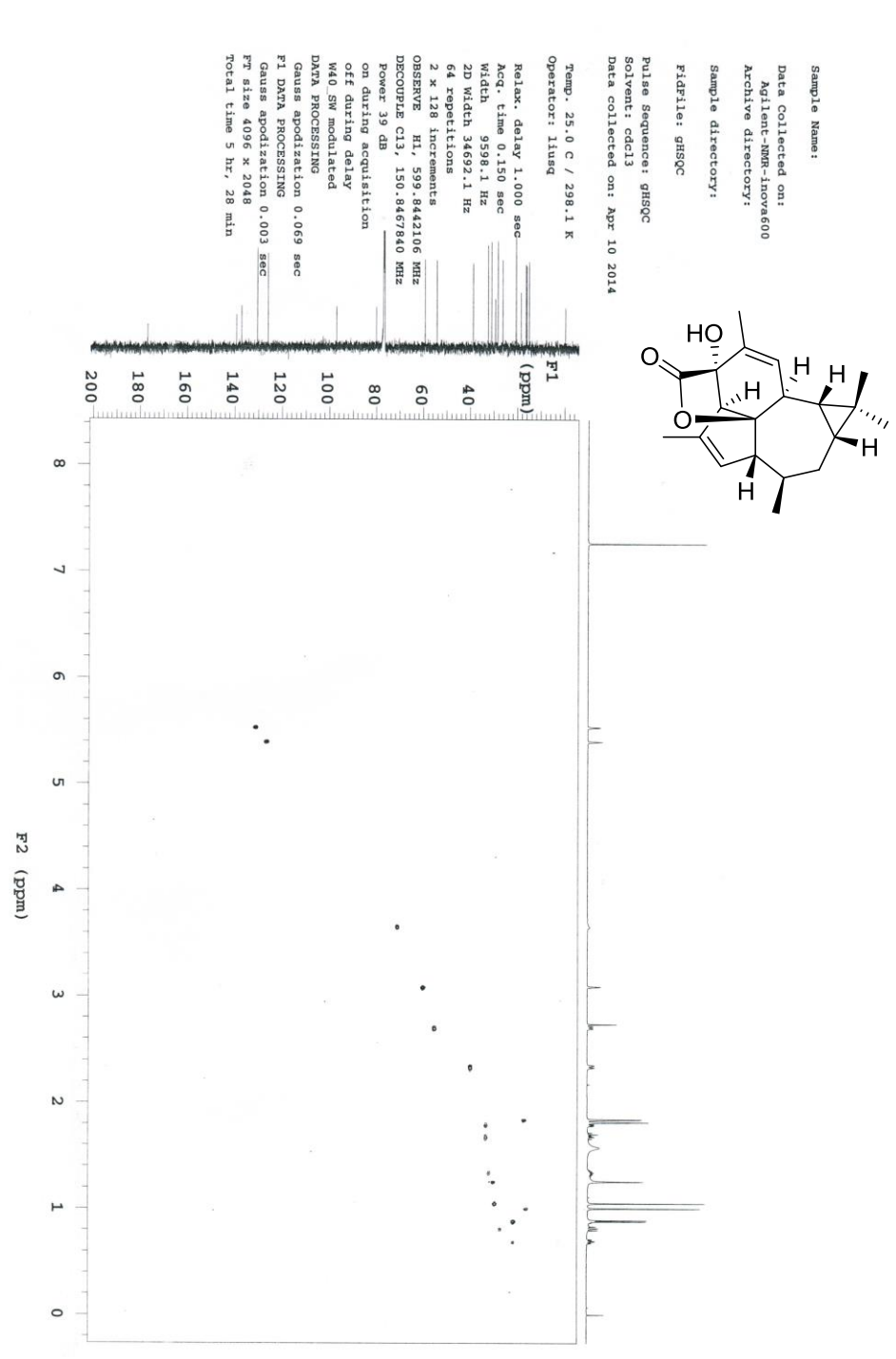

Figure S4. HMBC spectrum of euphorikanin A (**1**) in $CDCl_3$

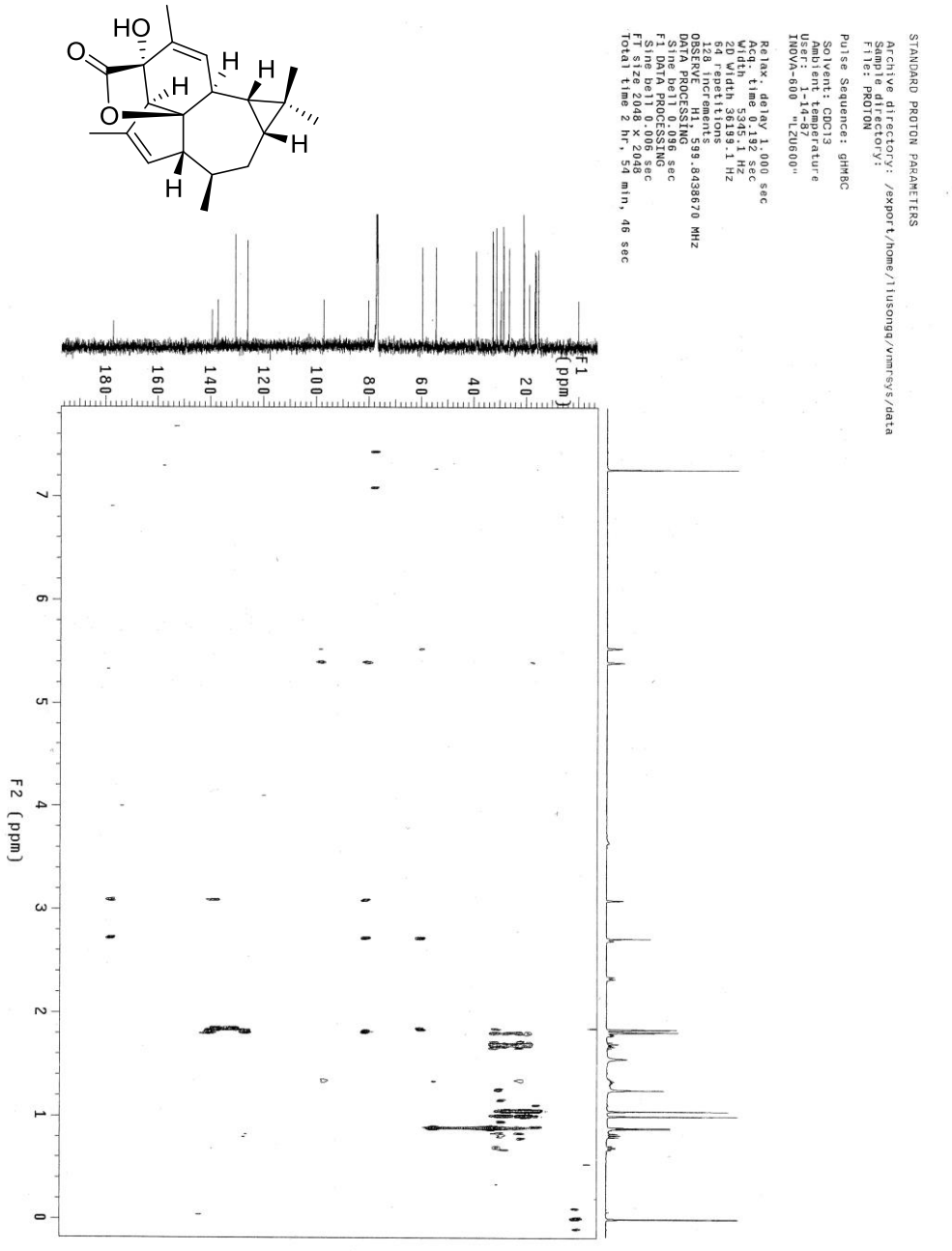

Figure S5. ^{1}H-^{1}H COSY spectrum of euphorikanin A (**1**) in $CDCl_3$

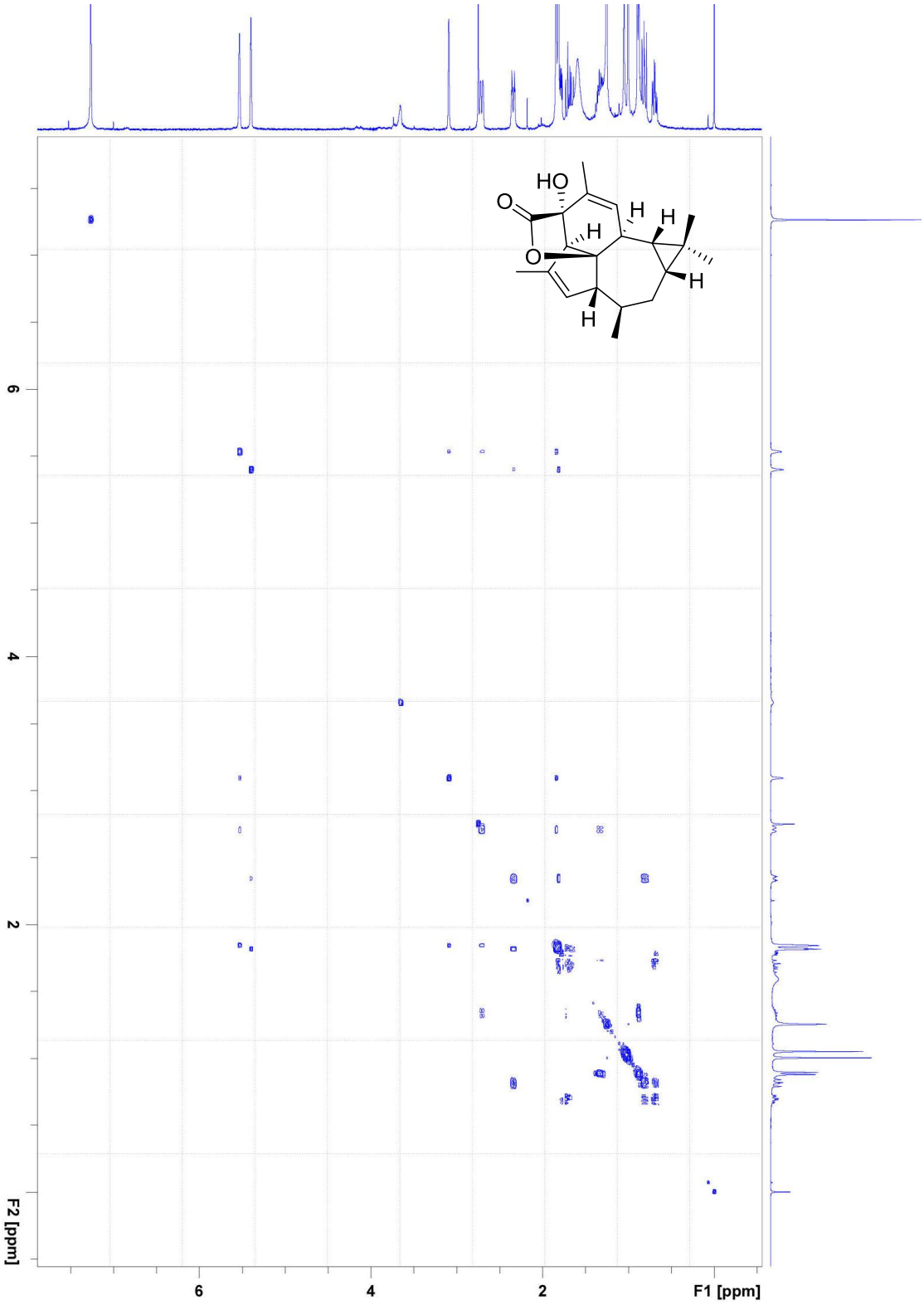

Figure S6. NOESY spectrum of euphorikanin A (**1**) in $CDCl_3$

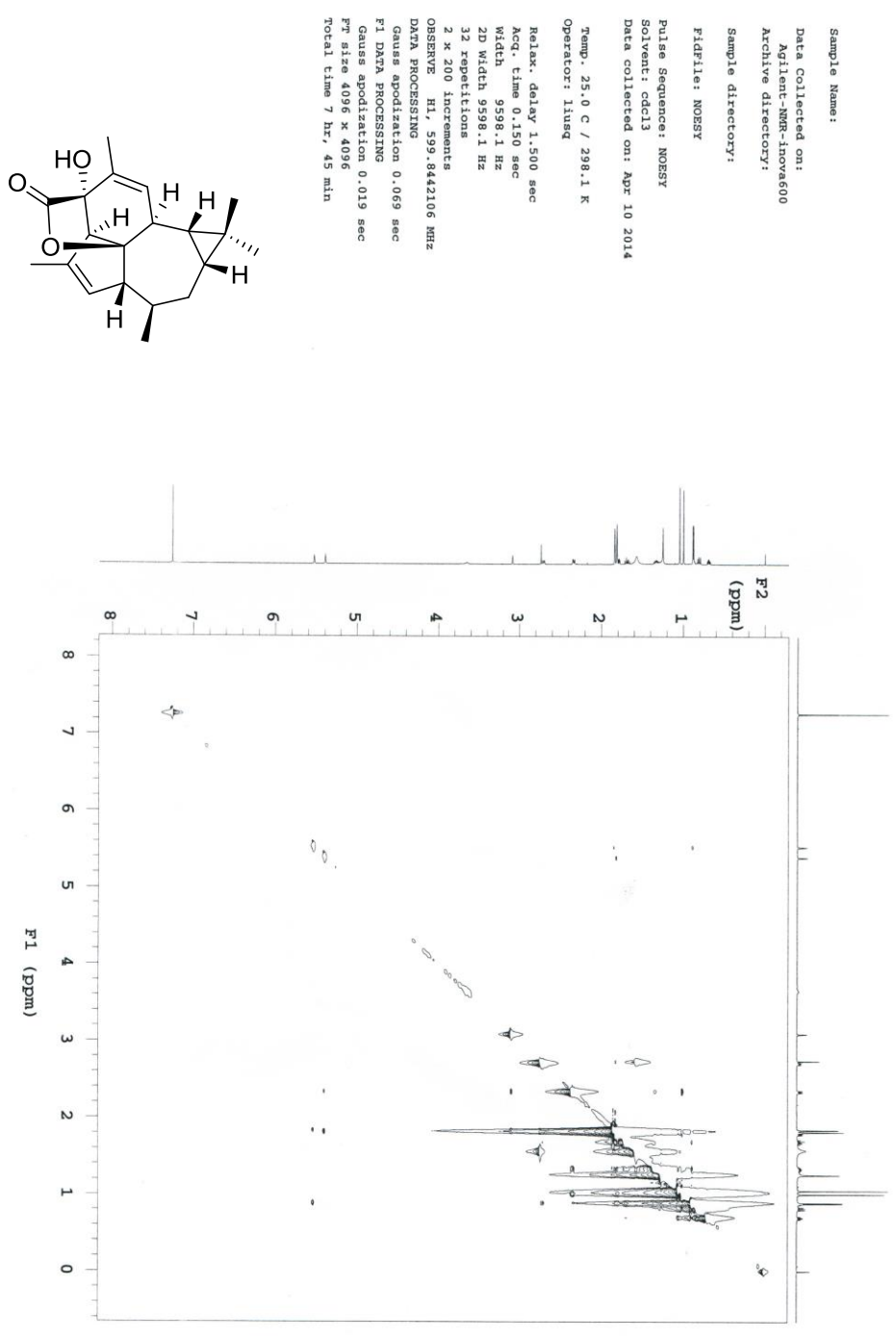

Figure S7. HRESIMS spectrum of euphorikanin A (**1**)

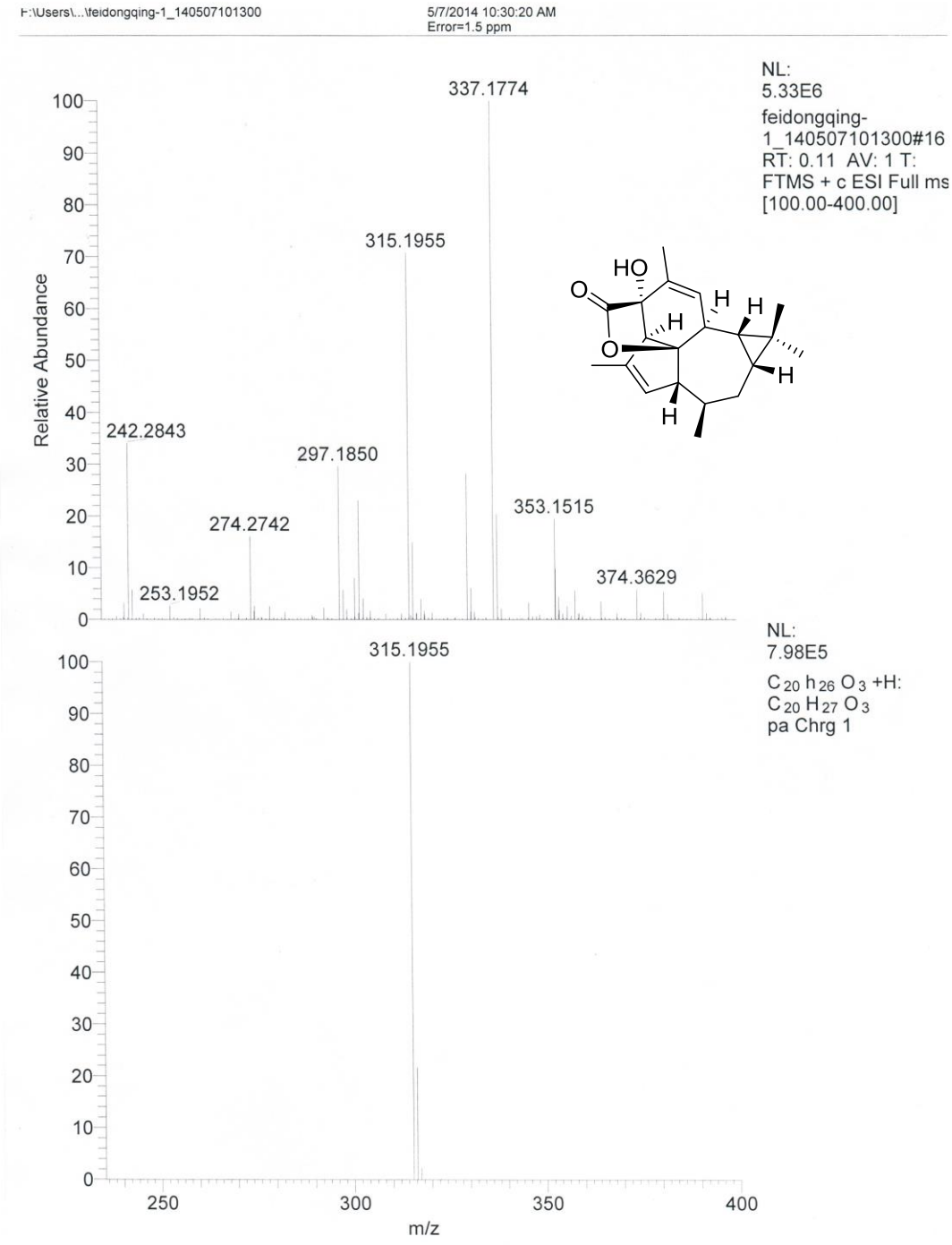

Figure S8. IR spectrum of euphorikanin A (**1**)