Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

A novel spirocyclic triterpenoid and a new taraxerane triterpenoid from *Teucrium viscidum*

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Supporting Information Contents

Experimental section

General Experimental Procedures: Melting points were determined on an X-4 digital display micro-melting point apparatus which 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 Bruker AVANCE III-400 NMR spectrometer. HR-ESI-MS data were recorded on a Thermo LTQ Orbitrap Elite mass spectrometer. The X-ray crystallographic data were collected on an Agilent Technologies SuperNova, Dual source, EOS CCD with mirror optics using graphite monochromated Cu-Kα radiation. Silica gel (200-300 mesh) used for column chromatography, and silica gel GF_{254} used for TLC were both supplied by the Qingdao Marine Chemical Factory, Qingdao, China.

Plant Material: The whole plants of *Teucrium viscidum* were purchased from Hebei Anguo Medicine Market in Anguo County, Hebei Province, China, in August, 2014 and identified by Dr. Jian-Yin Li, a doctor at school of Pharmacy, Lanzhou University. A voucher specimen (No. 20140821TV) is deposited in the school of Pharmacy, Lanzhou University.

Extraction and Isolation: The dried whole plants of *Teucrium viscidum* (20 kg) were percolated four times (each one week) with 95% EtOH at room temperature to give 2520 g crude extract. After removal of organic solvents, the extract was suspended in H_2O (1.5L) and extracted with EtOAc (3×1.5L) and *n*-BuOH (3×1.5L).The EtOAc fraction (852 g) was chromatographed on a silica gel column with a stepwise gradient of petroleum ether-acetone (40:1-1:1) to give six major fractions (A-F). The fraction A (70g) was subjected to silica gel column chromatograph (CC) and eluted with petroleum ether-acetone successively to give Fr.A1-Fr.A3. The Fr.A1 (13.6 g) was separated by silica gel CC (petroleum ether/acetone, 20:1-10:1) to afford three fractions. The Fr.A1.1 (3.0 g) was subjected to silica gel CC (petroleum ether/EtOAc, 30:1-2:1) to yield **1** (8 mg). Fraction C was subjected to silica gel CC and eluted with

$CHCl_3$/EtOAc (80:1-10:1) to give three fractions. The subfraction Fr.C2 was further applied to a silica gel CC ($CHCl_3$/acetone, 100:1-10:1) to yield **2** (20 mg).

Bioactivity Assay for Delaying Paralysis in Transgenic Alzheimer Disease *Caenorhabditis elegans* Procedure: The transgenic *Caenorhabditis elegans* strains CL2006 (unc-54/Aβ1-42), CL4176 (smg-1ts [myo-3/Aβ1-42 long 3′-untranslated region (UTR)]) is obtained from Caenorhabditis Genetics Center (CGC) (University of Minnesota, Minneapolis, MN). Worms were propagated at 16 ^oC on nematode growth medium (NGM) seeded with *E. coli* (OP50) as standard food resource. 100 eggs of CL4176 were added onto NGM containing tested compound at concentration of 100 μM in 0.1% DMSO, and 0.1% DMSO was used as control group. The animals were kept at 16 ^oC till they are at their L3 larval stage, then transferred into a 25 ^oC incubator for 34 h. Paralysis worms were counted under a dissecting stereo microscope at 2 h intervals until all animals got into paralysis. A paralysis worm did not respond to any mechanical stimulus or only moved its head. The anti-AD bioactivity was described as the capacity of tested compound delaying worm paralysis. More worms are not paralysis, higher anti-AD bioactivity of the tested compounds have.

Fig. 1S ^{1}H NMR (400MHz, $CDCl_3$) of compound **1**

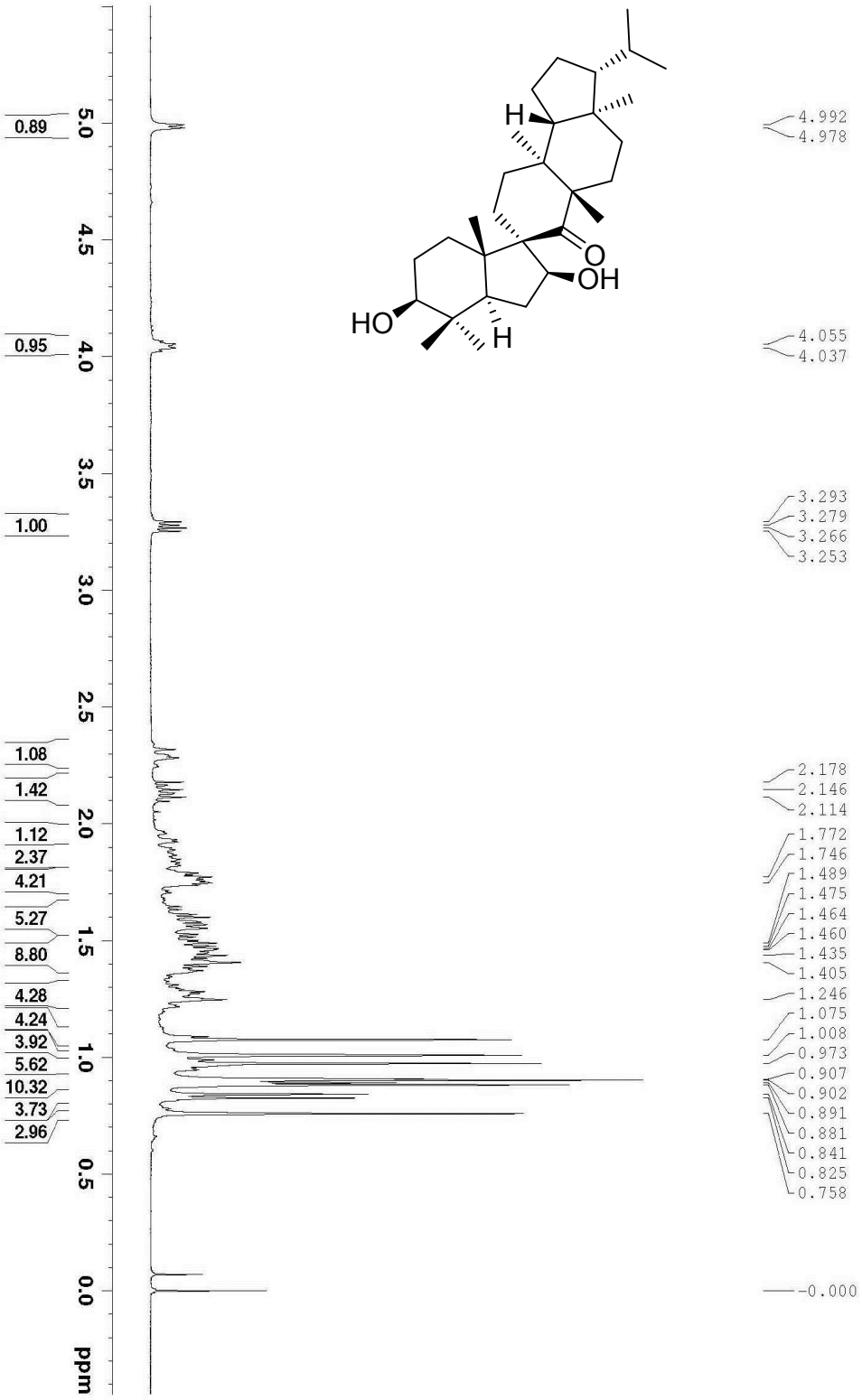

Fig. 2S ^{13}C NMR and DEPT135 (100MHz, $CDCl_3$) of compound **1**

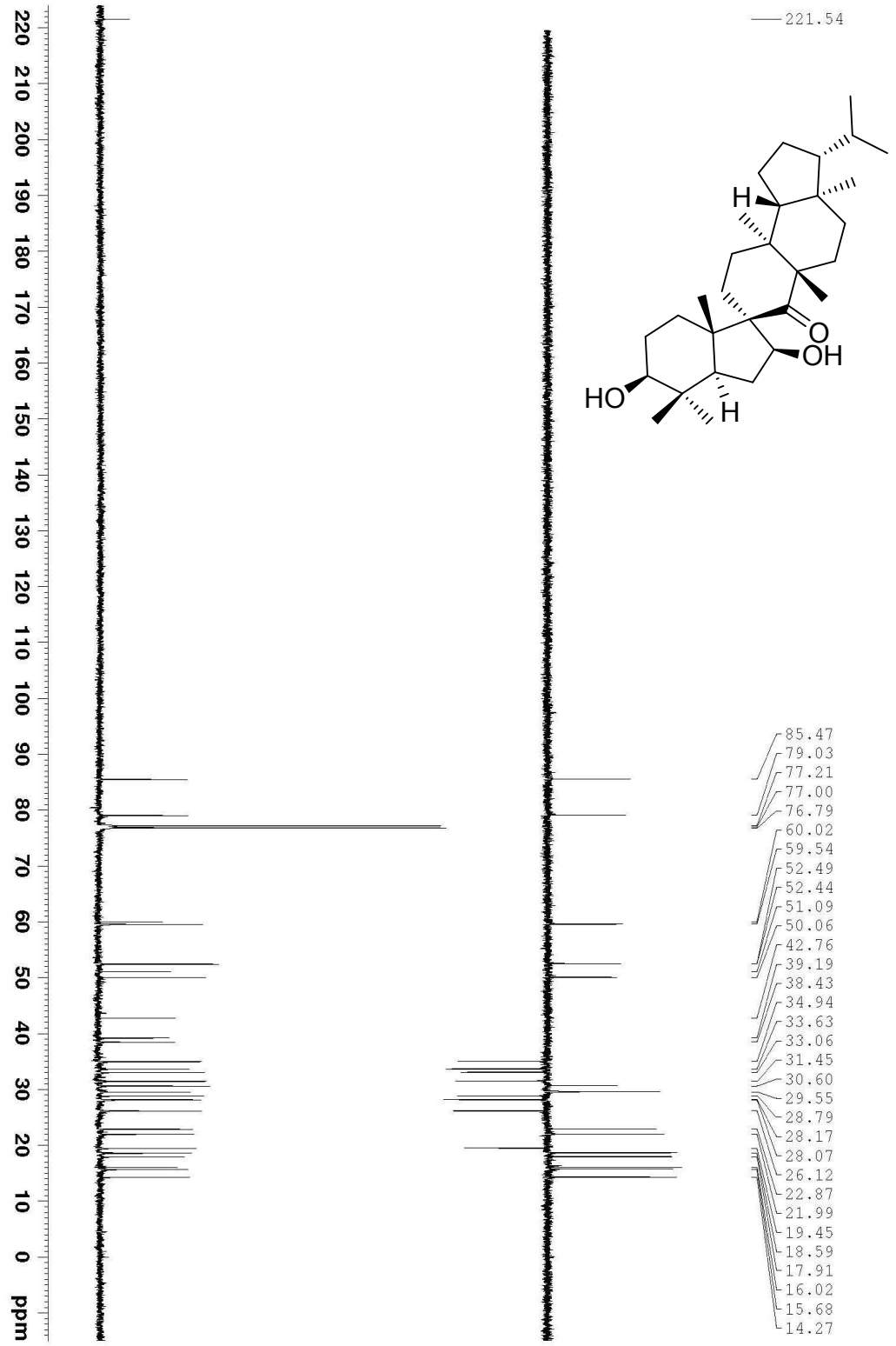

Fig. 3S ^{1}H-^{1}H COSY spectrum of compound **1**

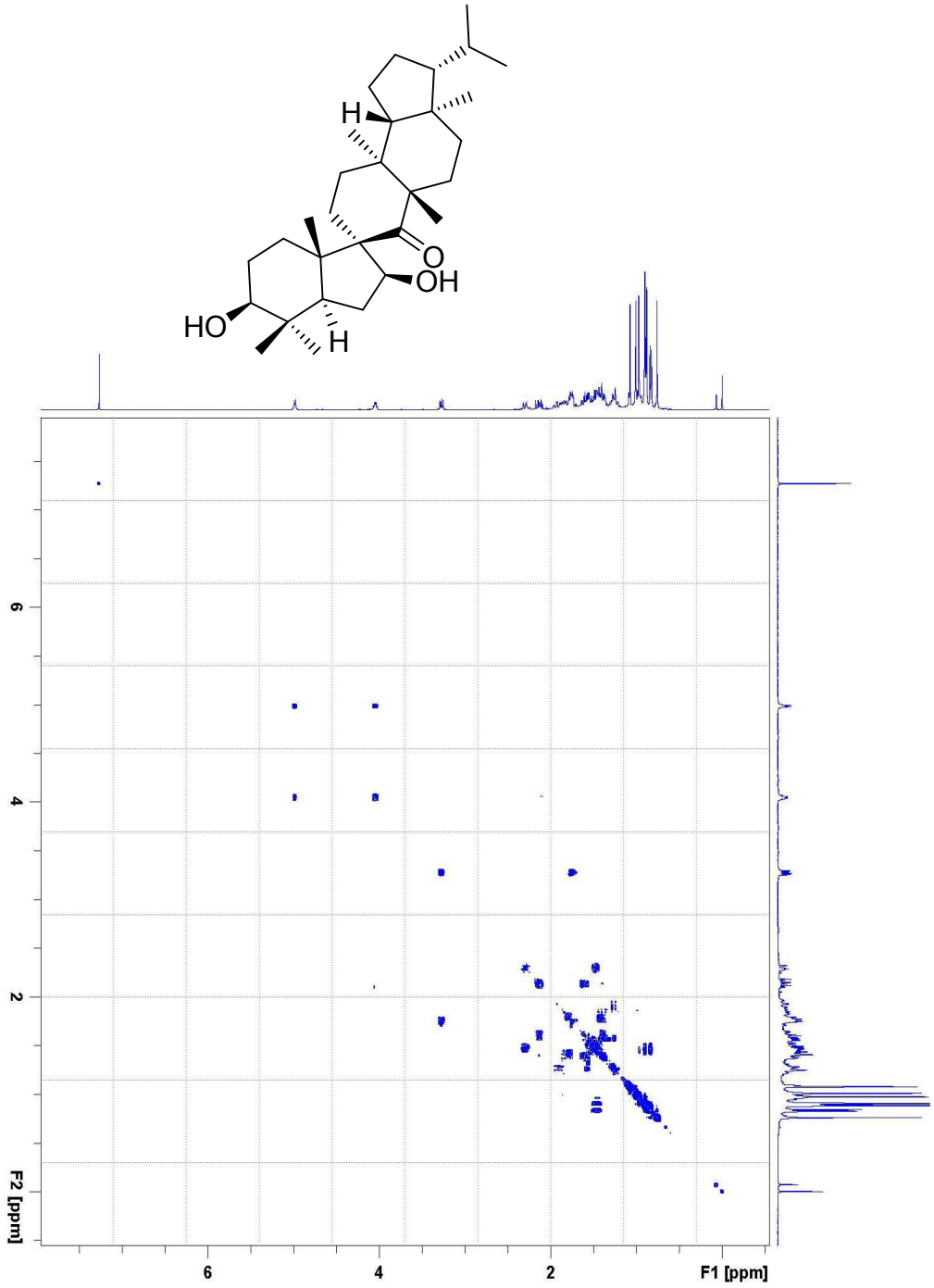

Fig. 4S HSQC spectrum of compound **1**

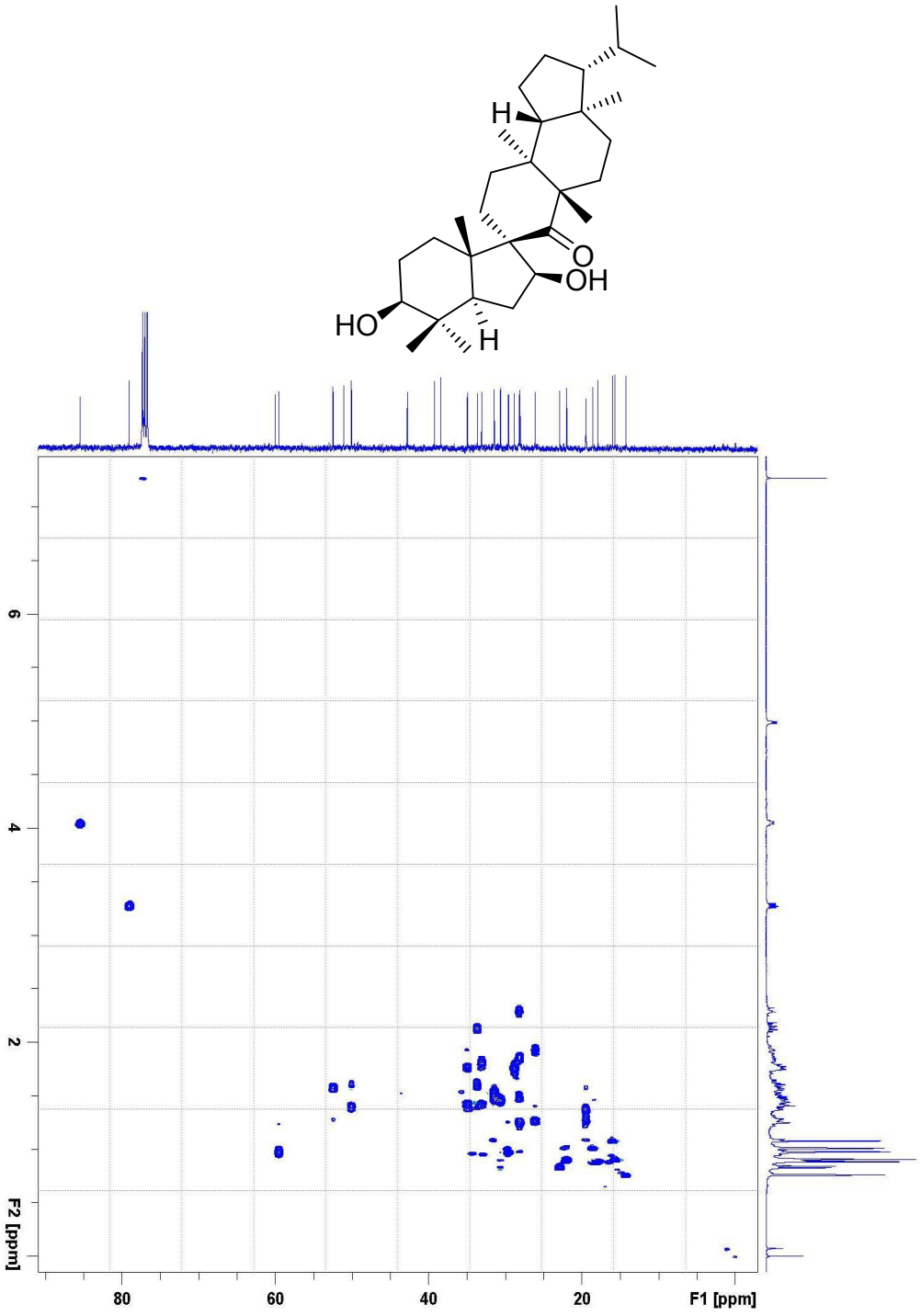

Fig. 5S HMBC spectrum of compound **1**

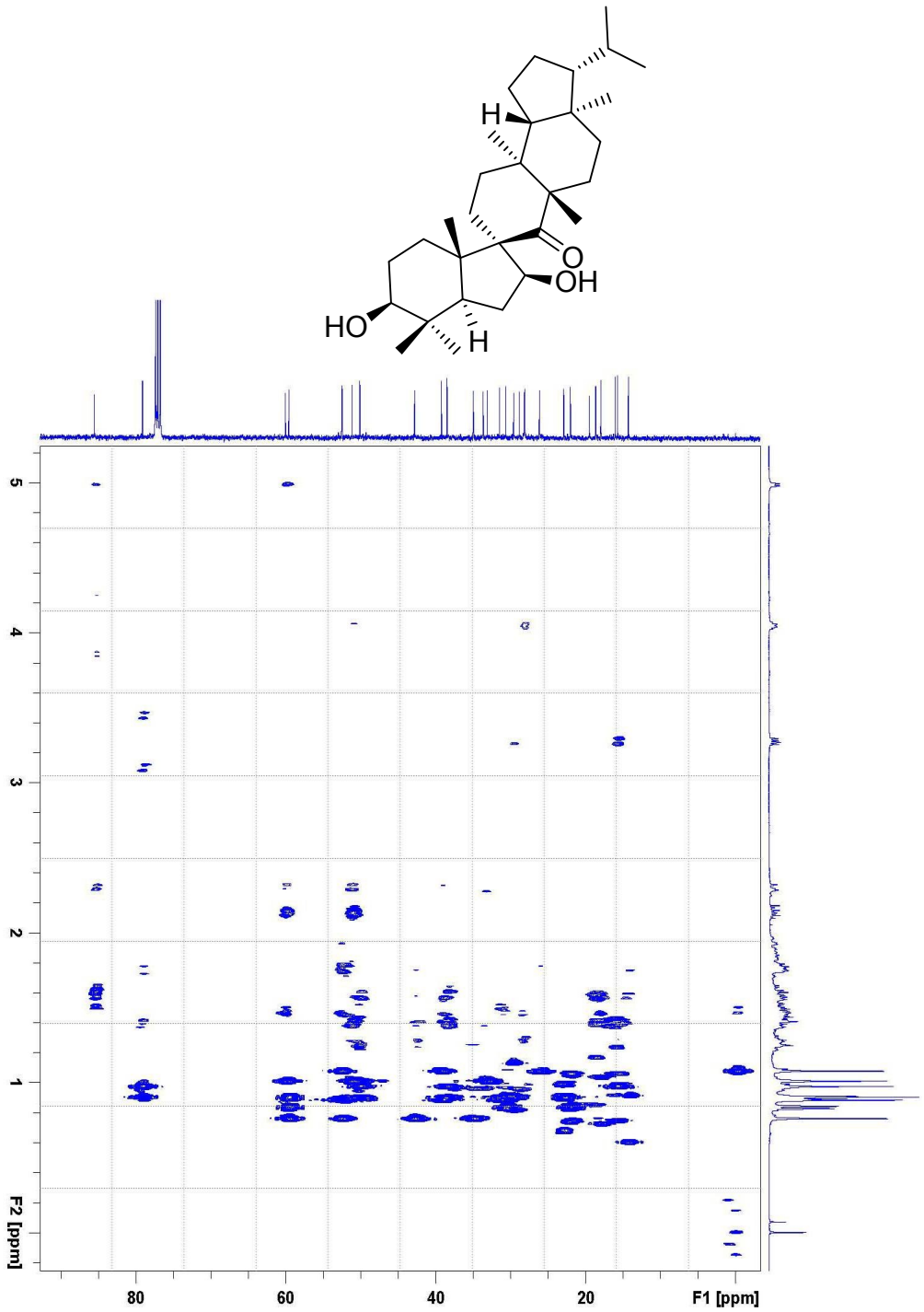

Fig. 6S NOESY spectrum of compound **1**

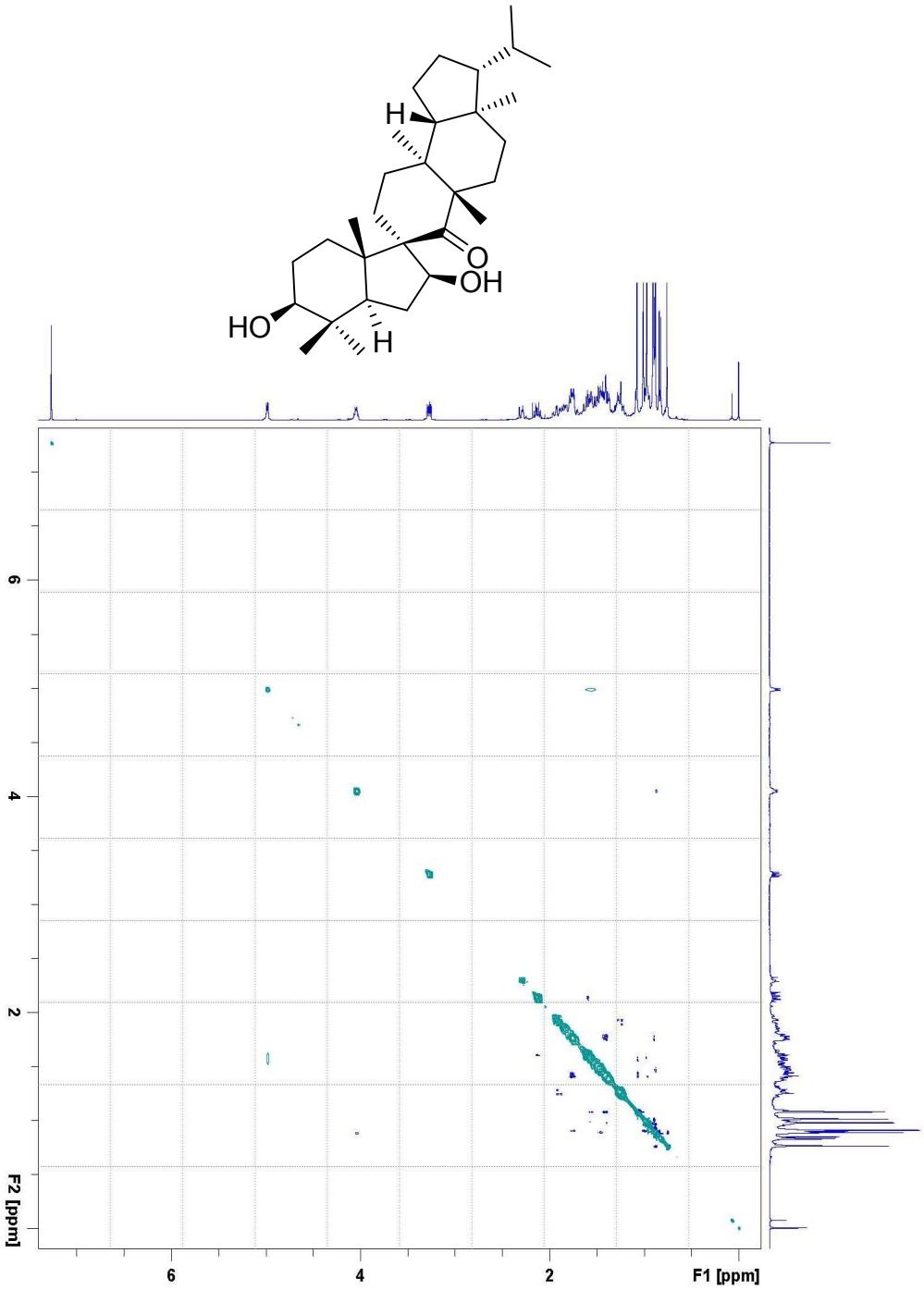

Fig. 7S HR-ESI-MS spectrum of compound **1**

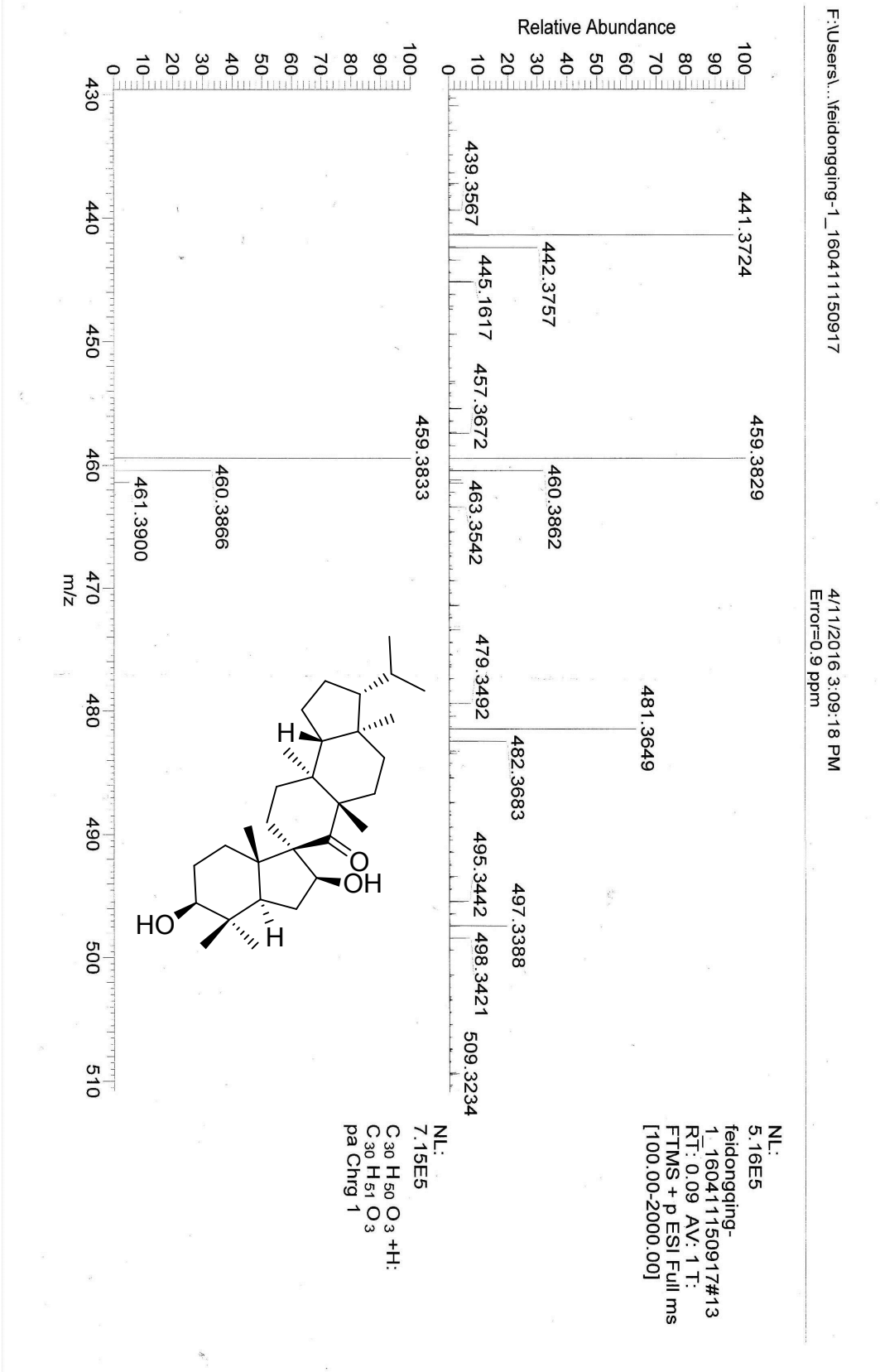

Fig. 8S IR spectrum of compound **1**

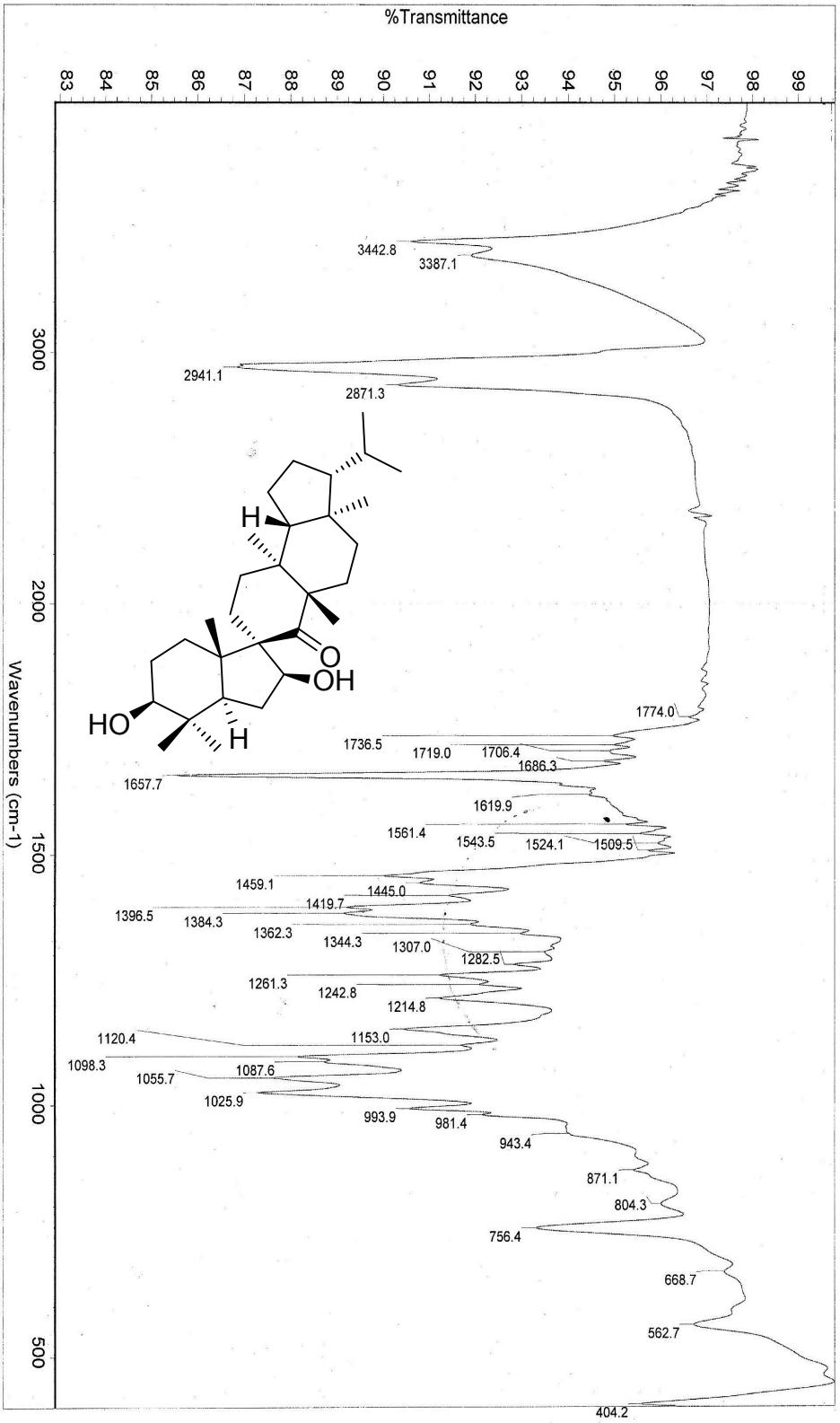

Fig. 9S ^{1}H NMR (400MHz, C_5D_5N) of compound **2**

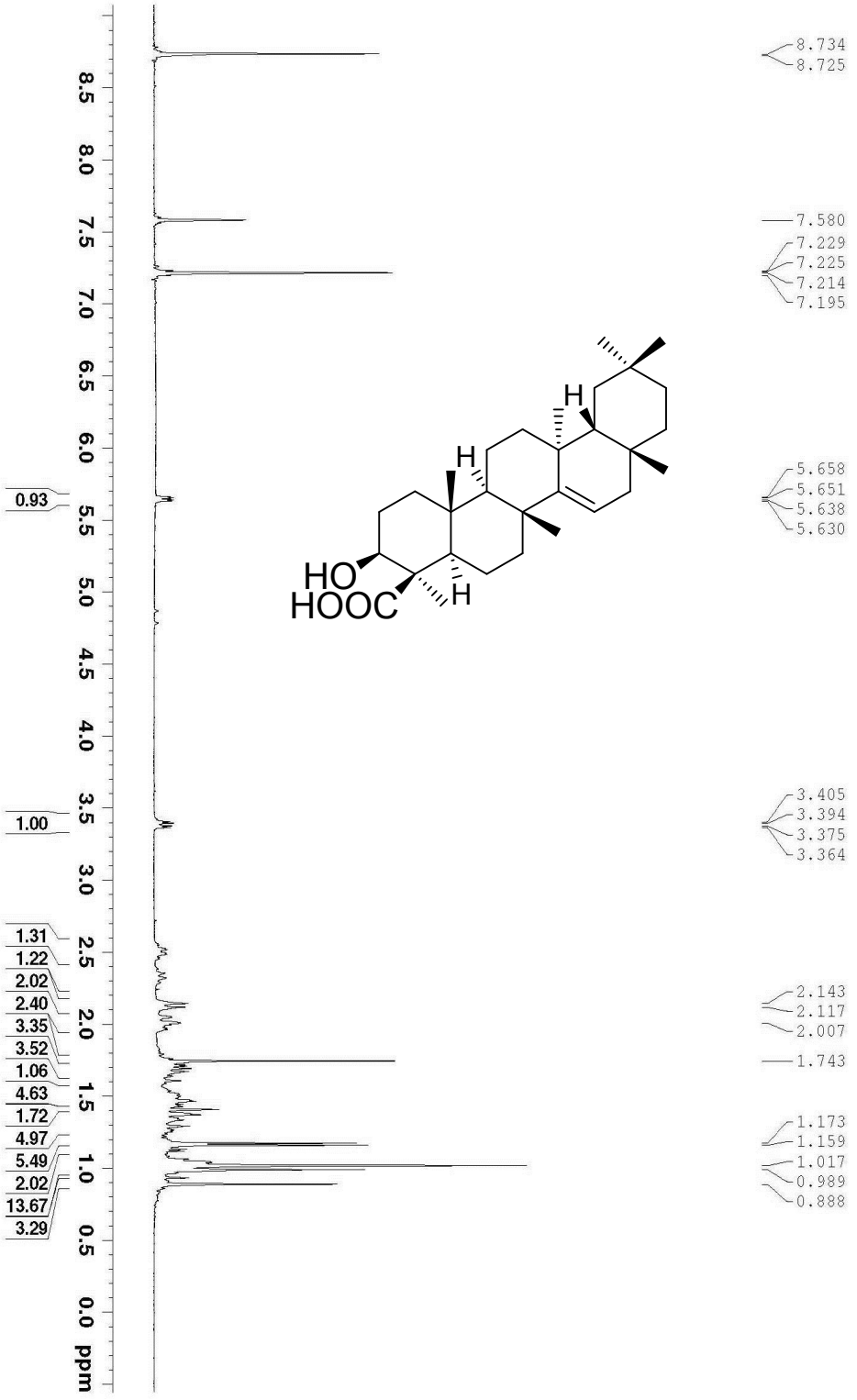

Fig. 10S ^{13}C NMR and DEPT135 (100MHz, C_5D_5N) of compound **2**

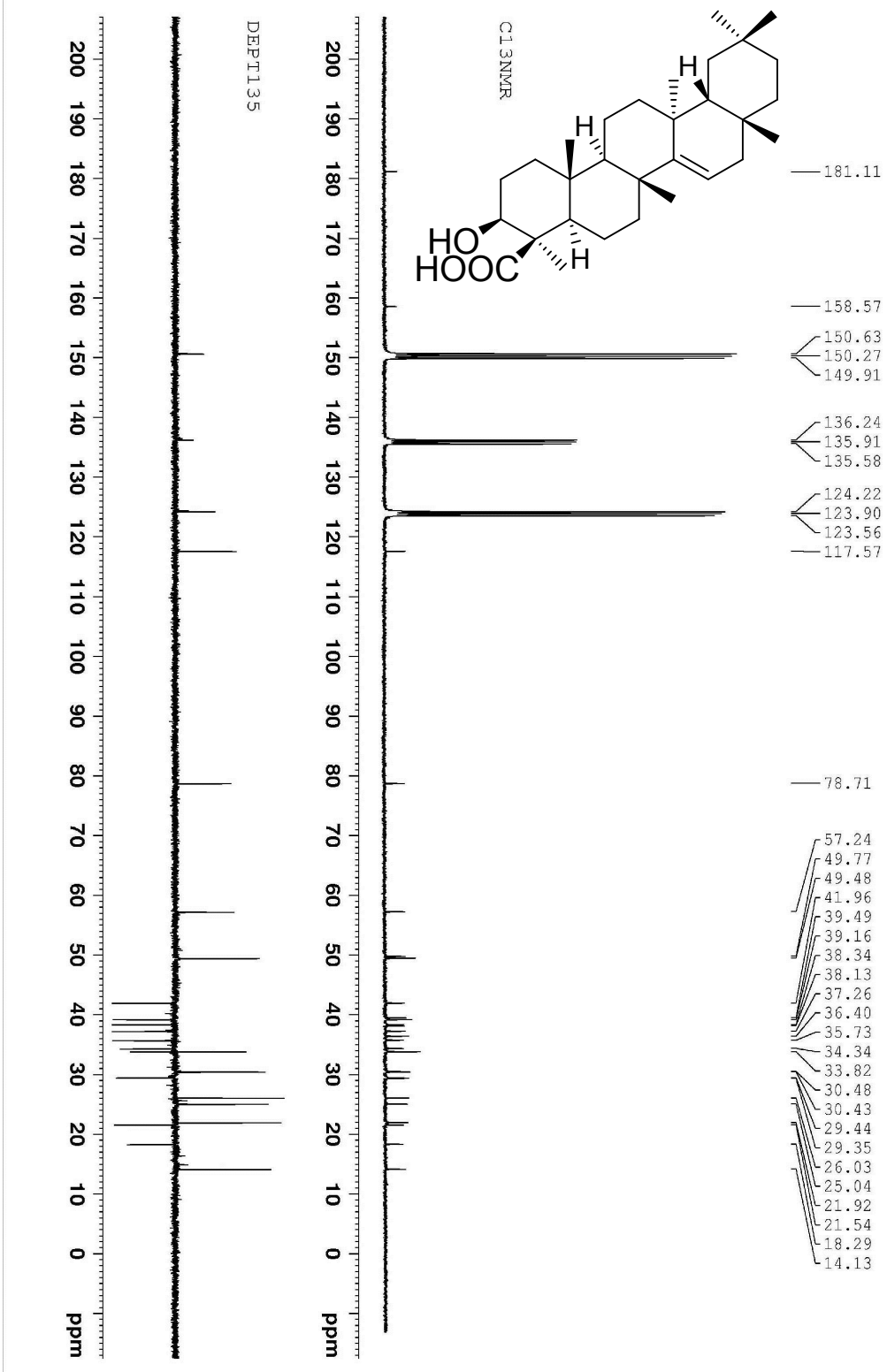

Fig. 11S ^{1}H-^{1}H COSY spectrum of compound **2**

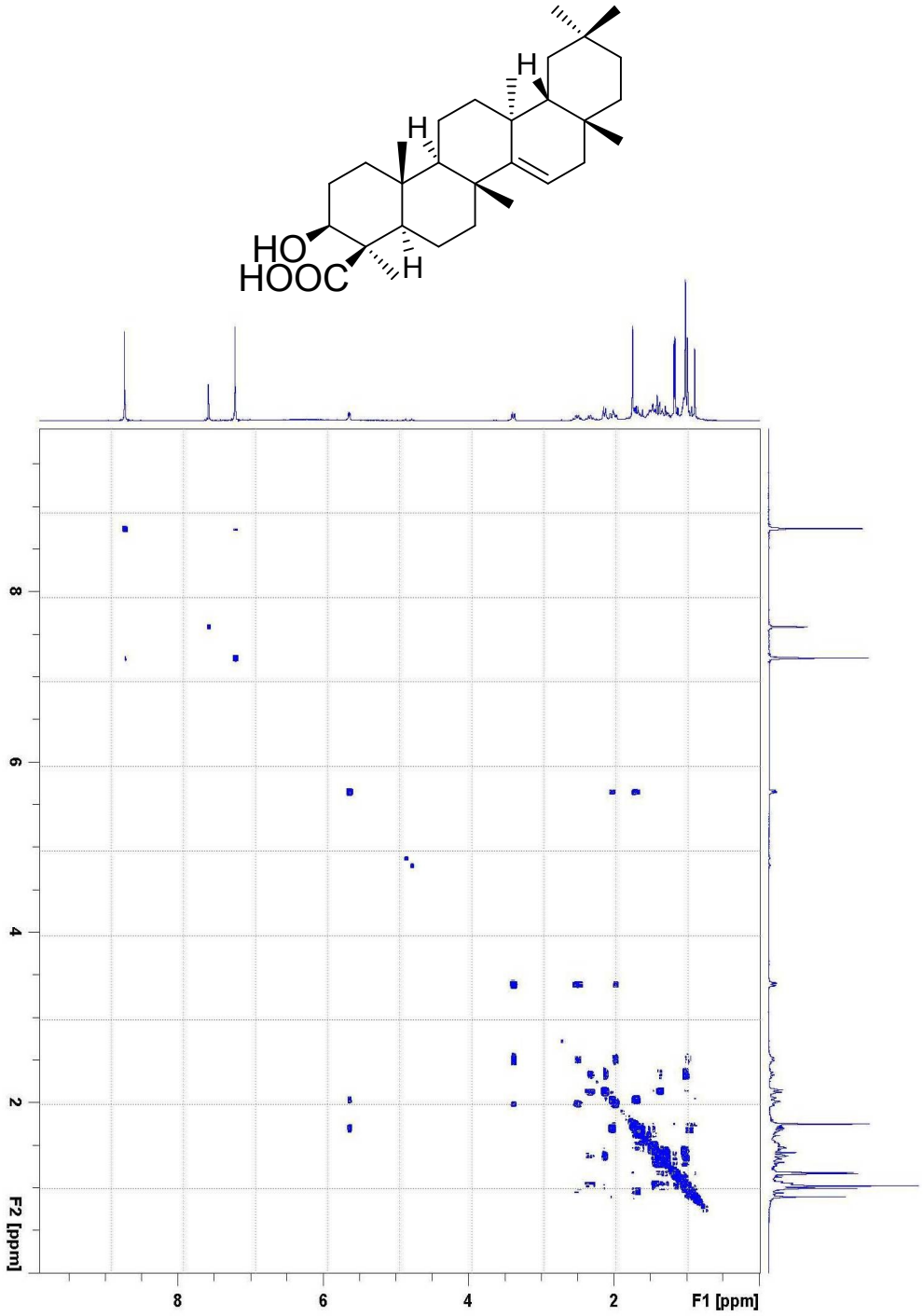

Fig. 12S HSQC spectrum of compound **2**

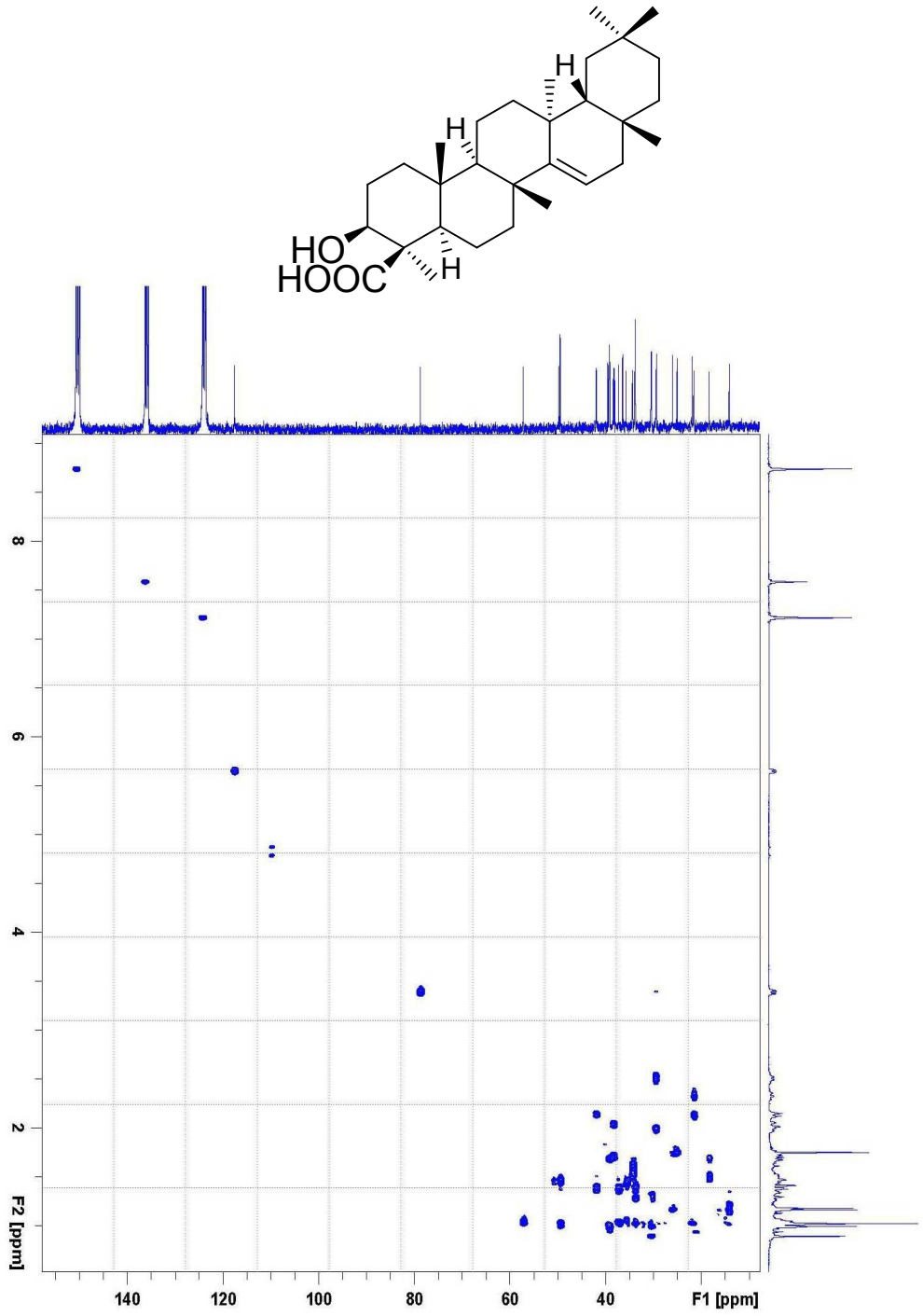

Fig. 13S HMBC spectrum of compound **2**

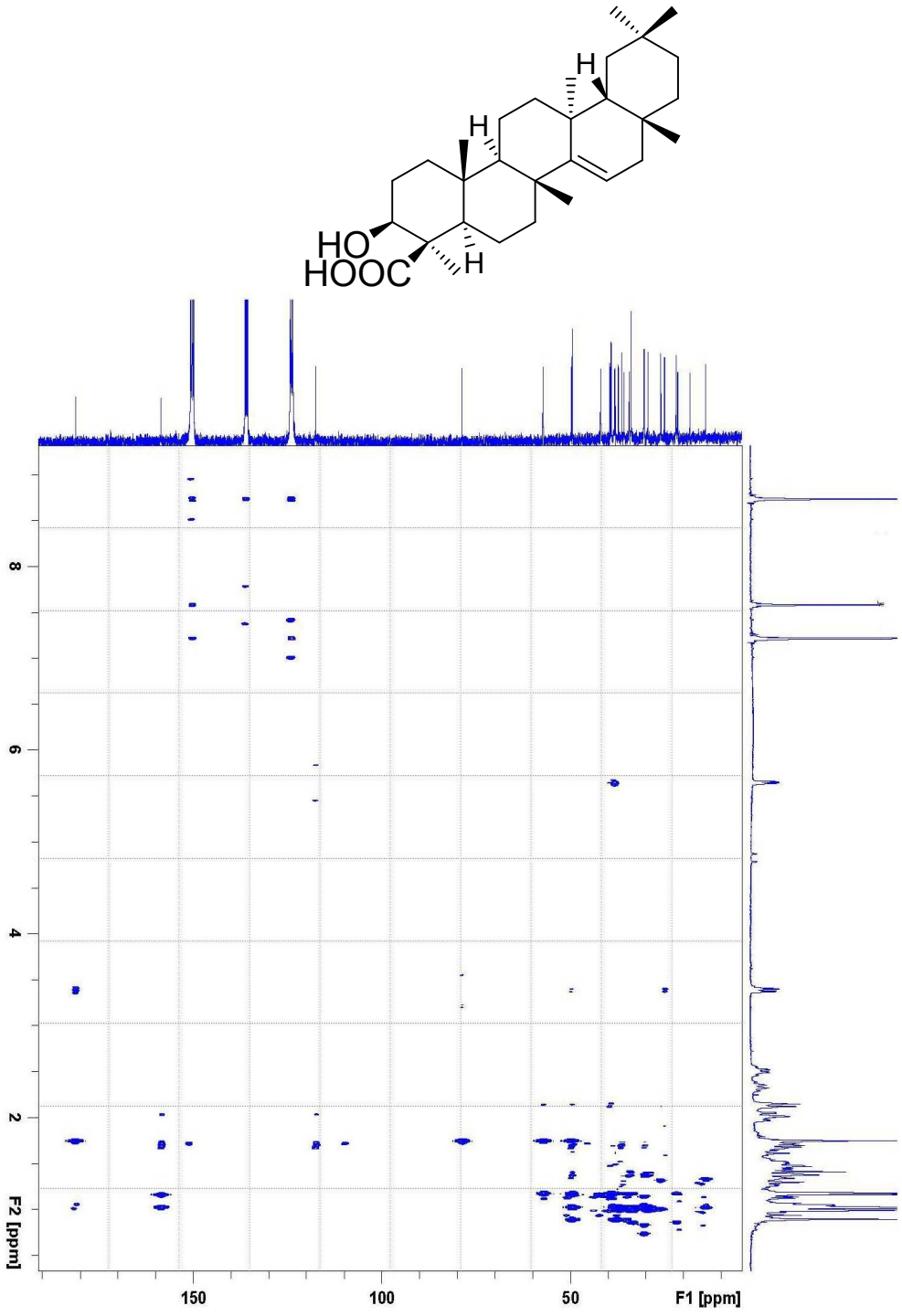

Fig. 14S NOESY spectrum of compound **2**

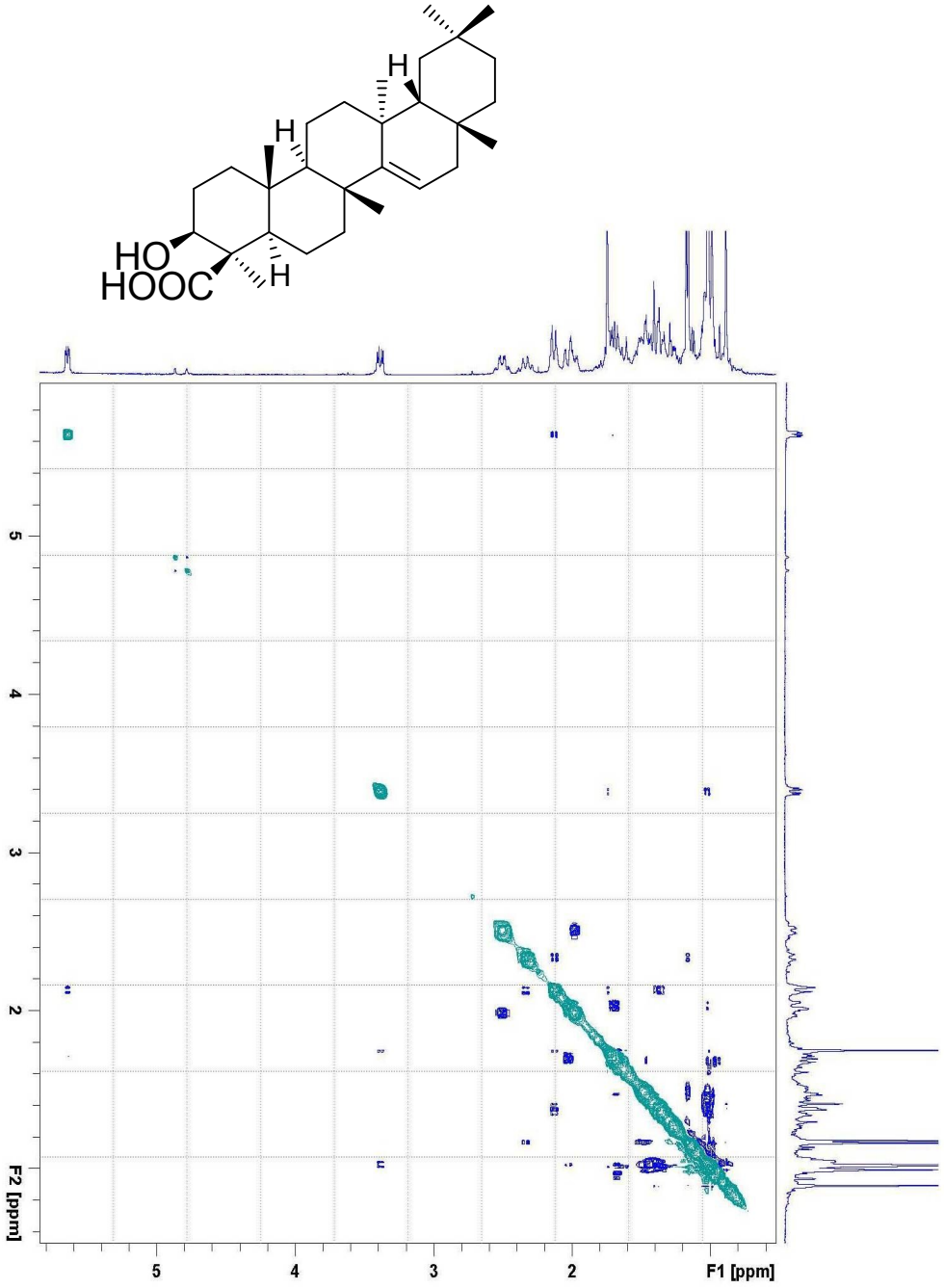

Fig. 15S HR-ESI-MS spectrum of compound **2**

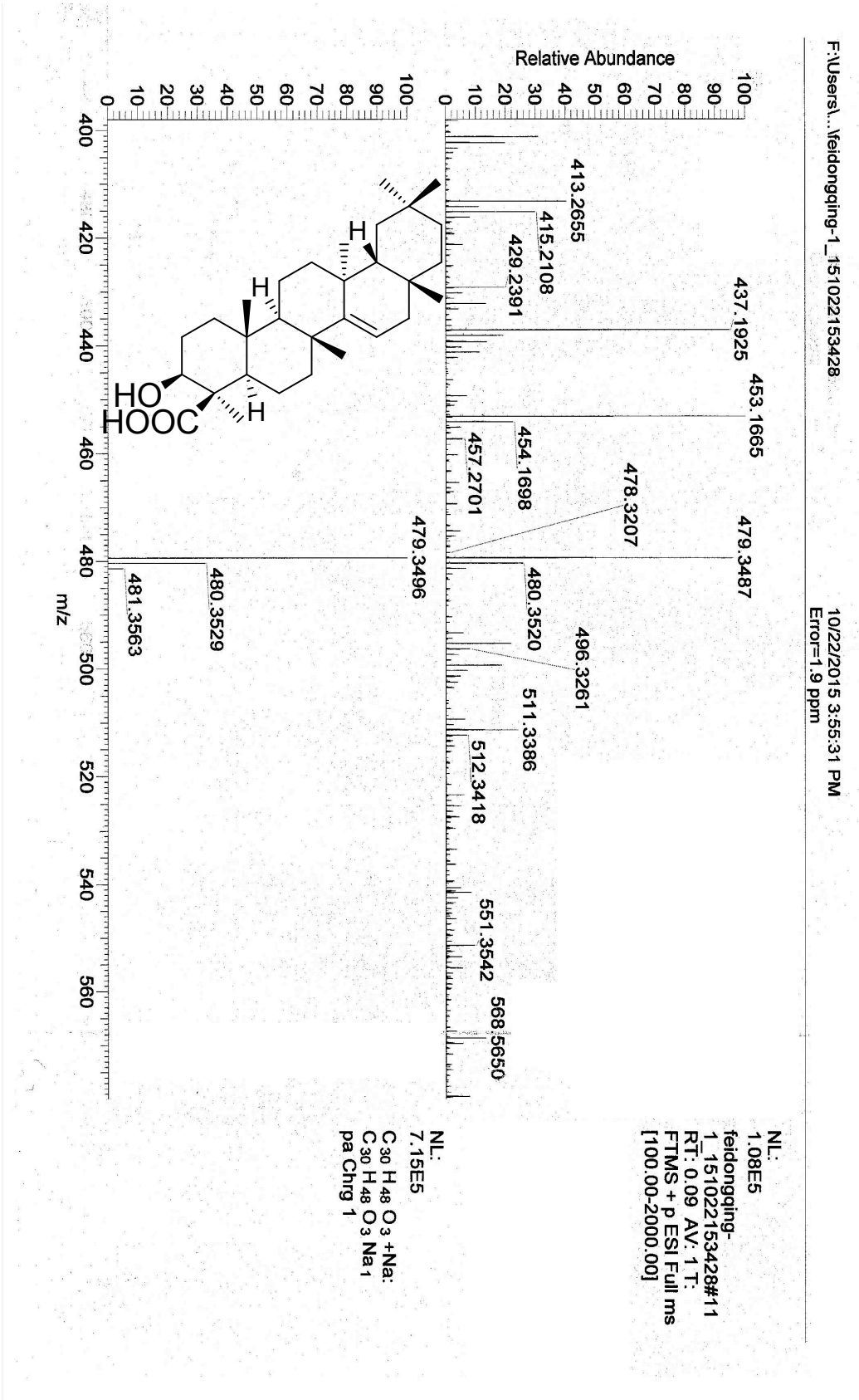

Fig. 16S IR spectrum of compound **2**