

Supplementary data

Antioxidant Phenylpropanoid Glycosides from *Ginkgo biloba* Fruit and Identification of a New Phenylpropanoid Glycoside, Ginkgopanoside

Akida Alishir, and Ki Hyun Kim*

School of Pharmacy, Sungkyunkwan University, Suwon 16419, Korea; akida.alishir@gmail.com (A.A.)

* Corresponding author: khkim83@skku.edu; Tel.: +82-31-290-7700

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Figure S1. The HRESIMS data of **1**

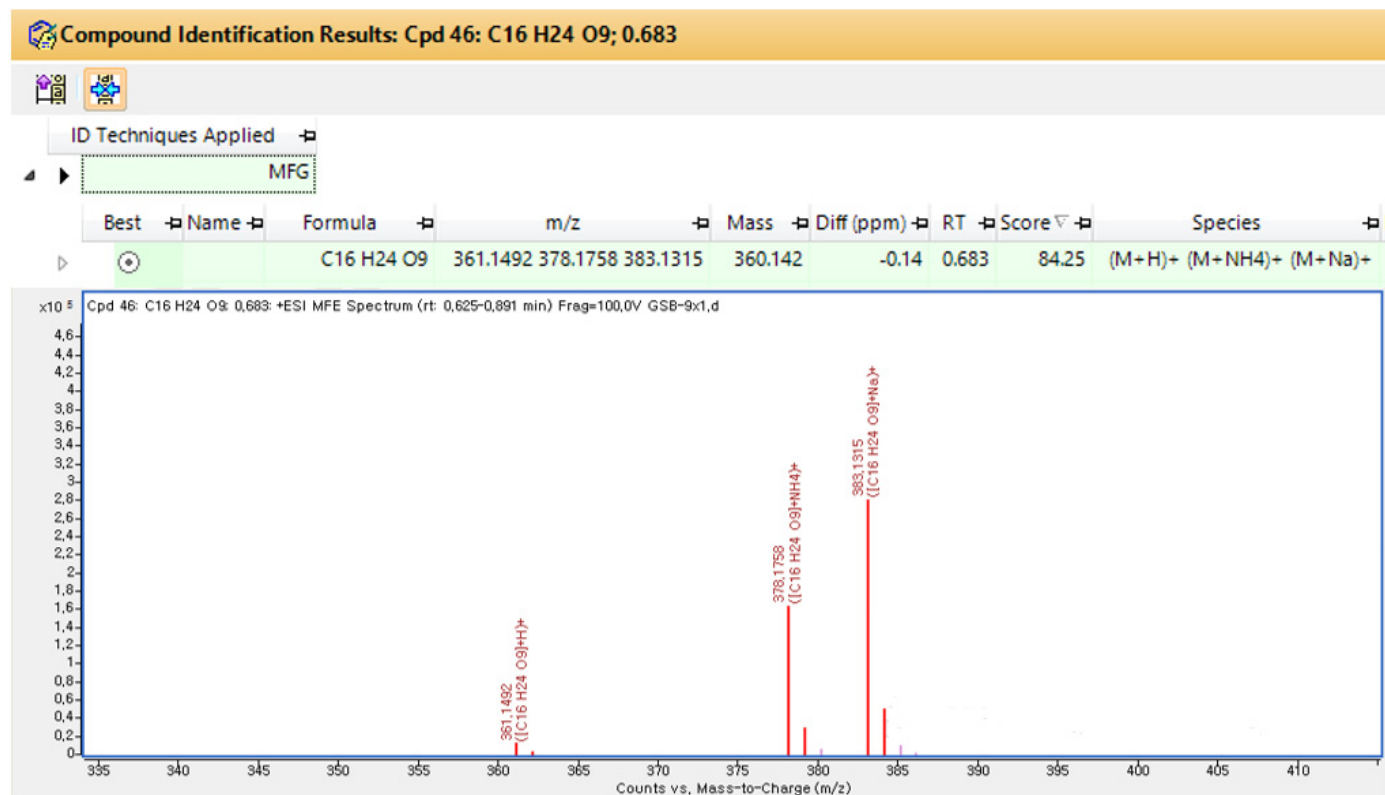


Figure S2. The ^1H NMR spectrum of **1** (D_2O , 850 MHz)

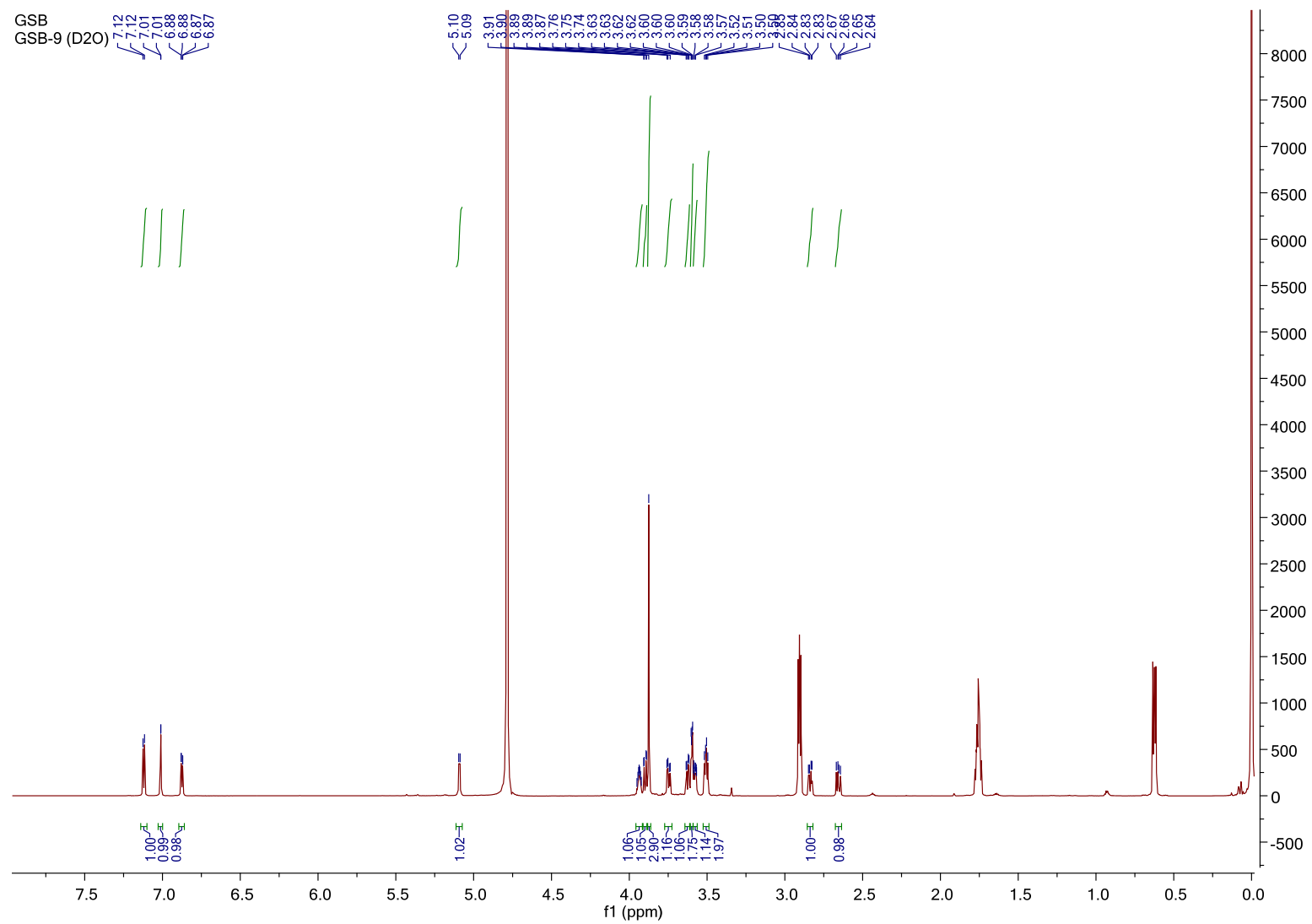


Figure S3. The HSQC spectrum of **1** (D₂O)

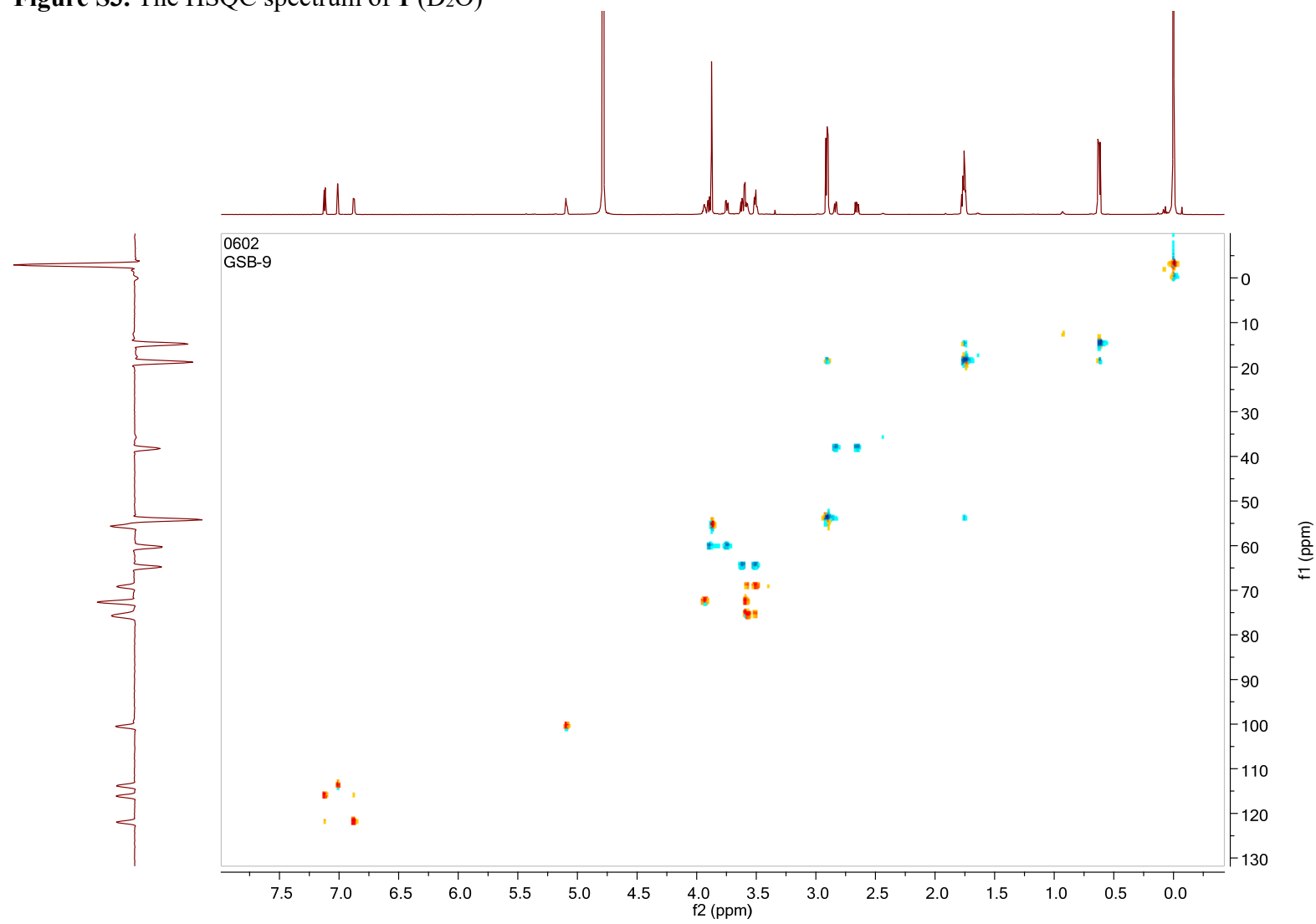


Figure S4. The HMBC spectrum of **1** (D₂O)

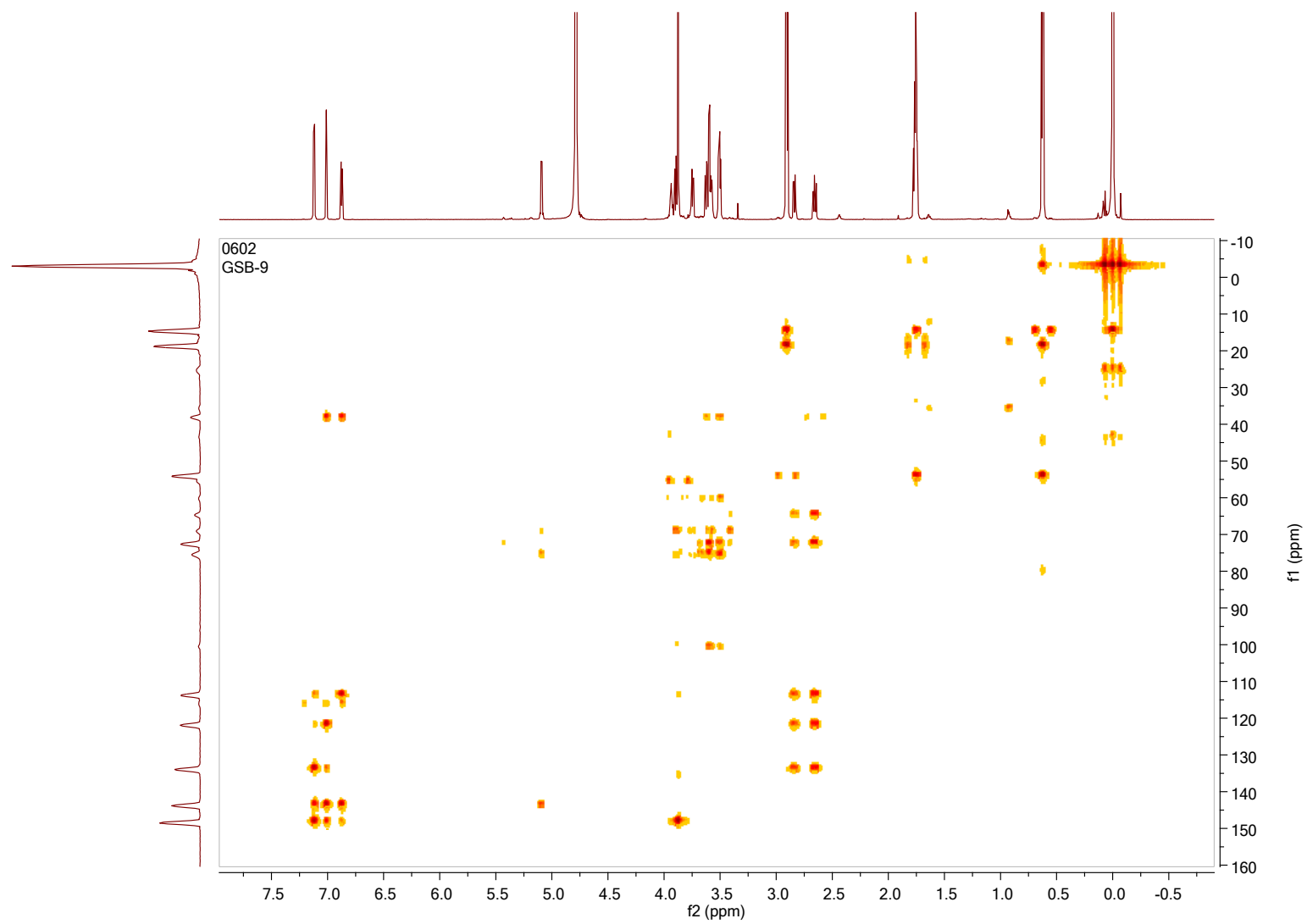


Figure S5. The ^1H - ^1H COSY spectrum of **1** (D_2O)

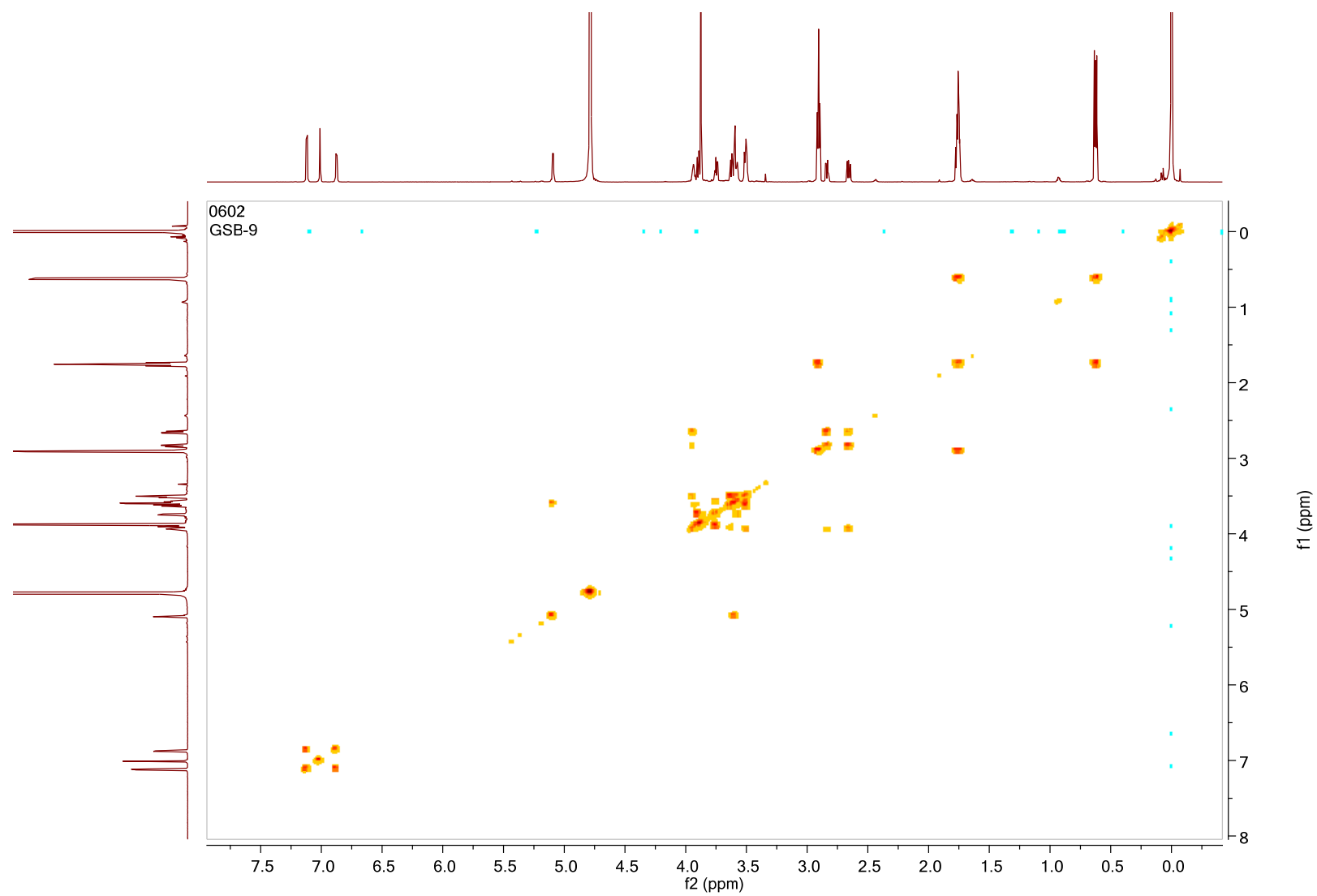
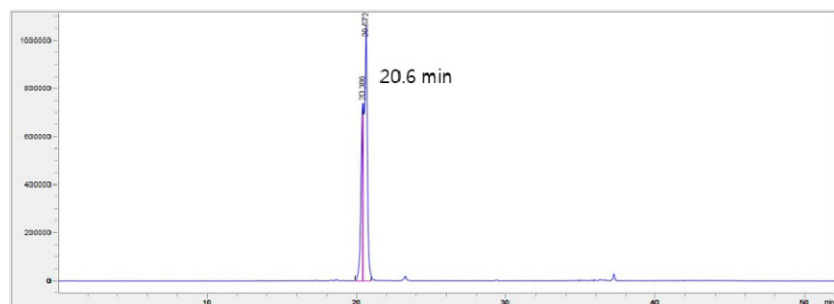
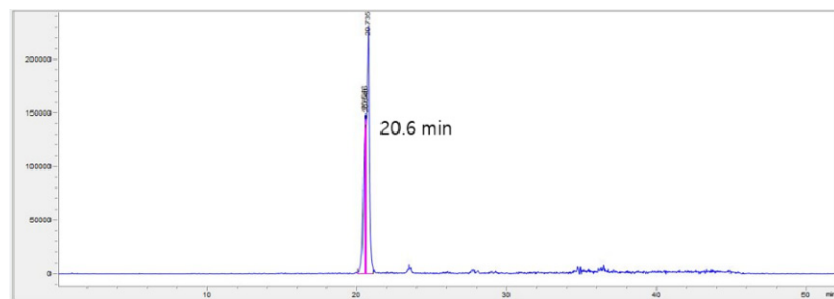


Figure S6. Retention time of reaction products of thiocarbamoyl-thiazolidine derivatives of D-glucopyranose standard and glucopyranose from compound **1**

Positive

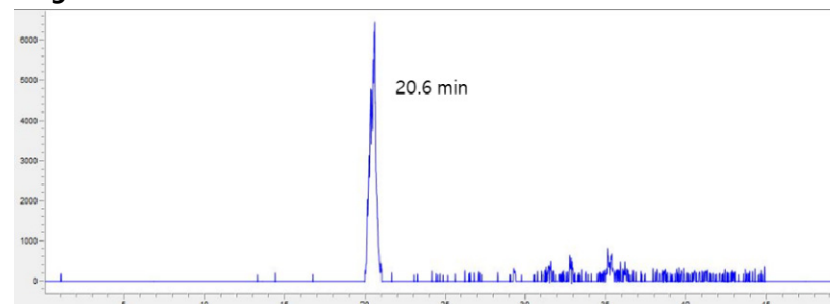


Reaction product of D-glucopyranose standard

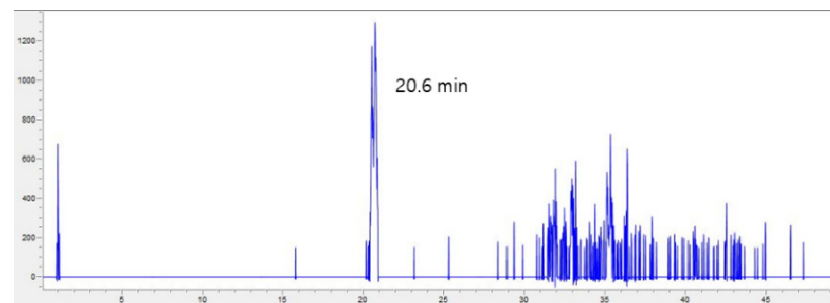


Reaction product of glucopyranose from compound **1**

Negative



Reaction product of D-glucopyranose standard



Reaction product of glucopyranose from compound **1**

Figure S7. The circular dichroism spectrum of compound **1**

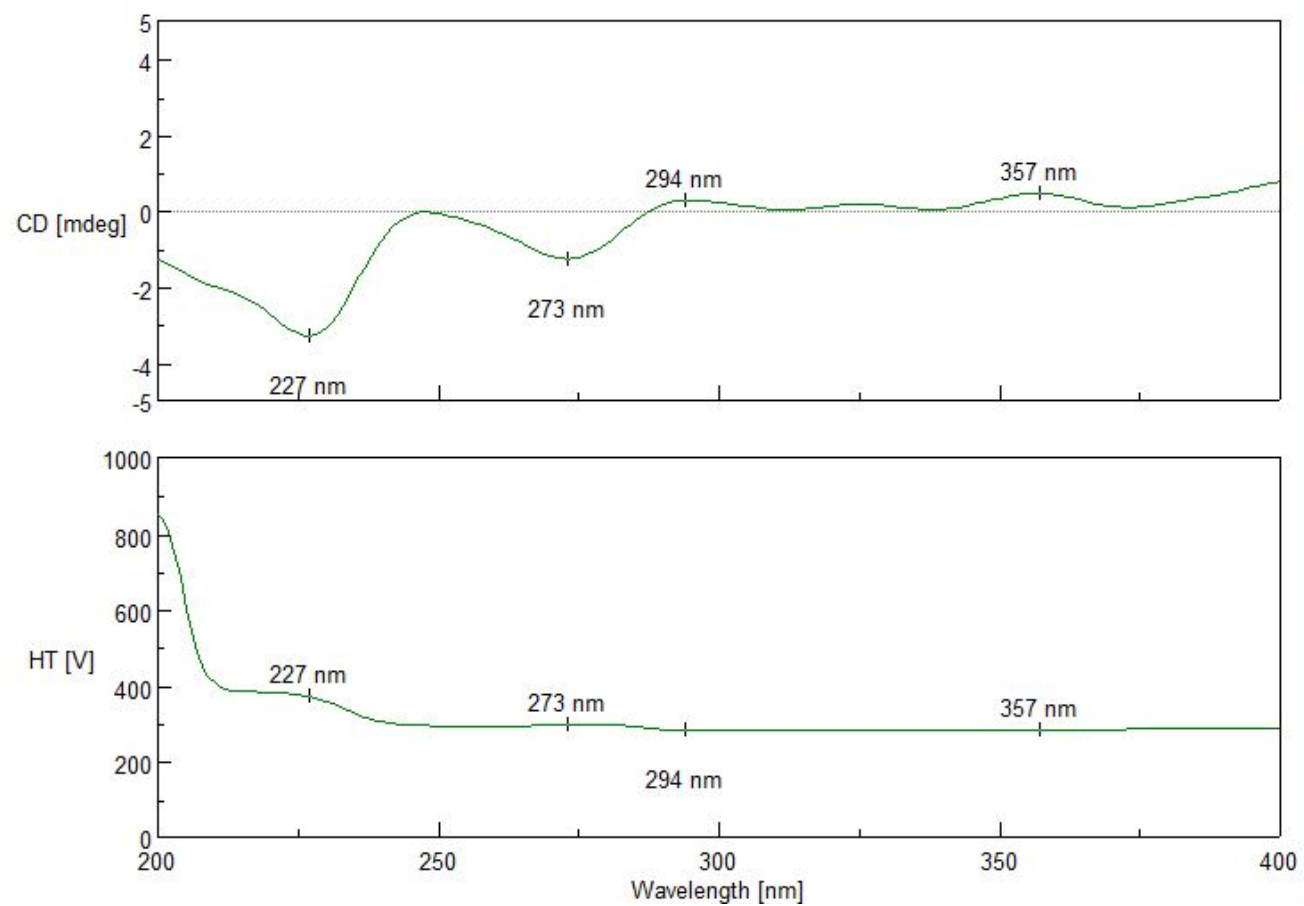


Figure S8. The ESIMS data of **2** (negative-ion mode)

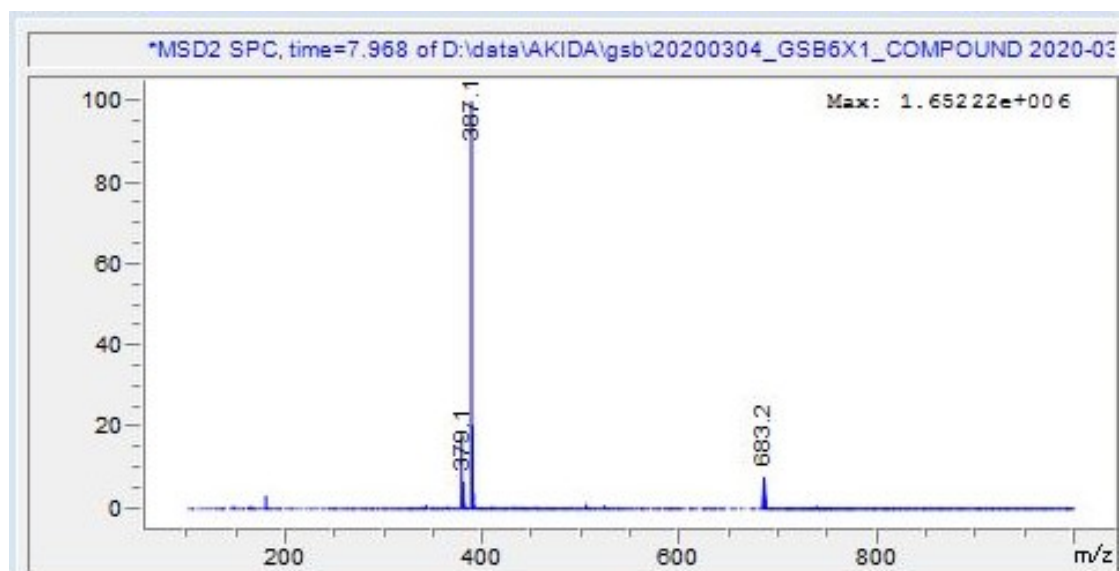


Figure S9. The ^1H NMR spectrum of **2** (CD_3OD , 850 MHz)

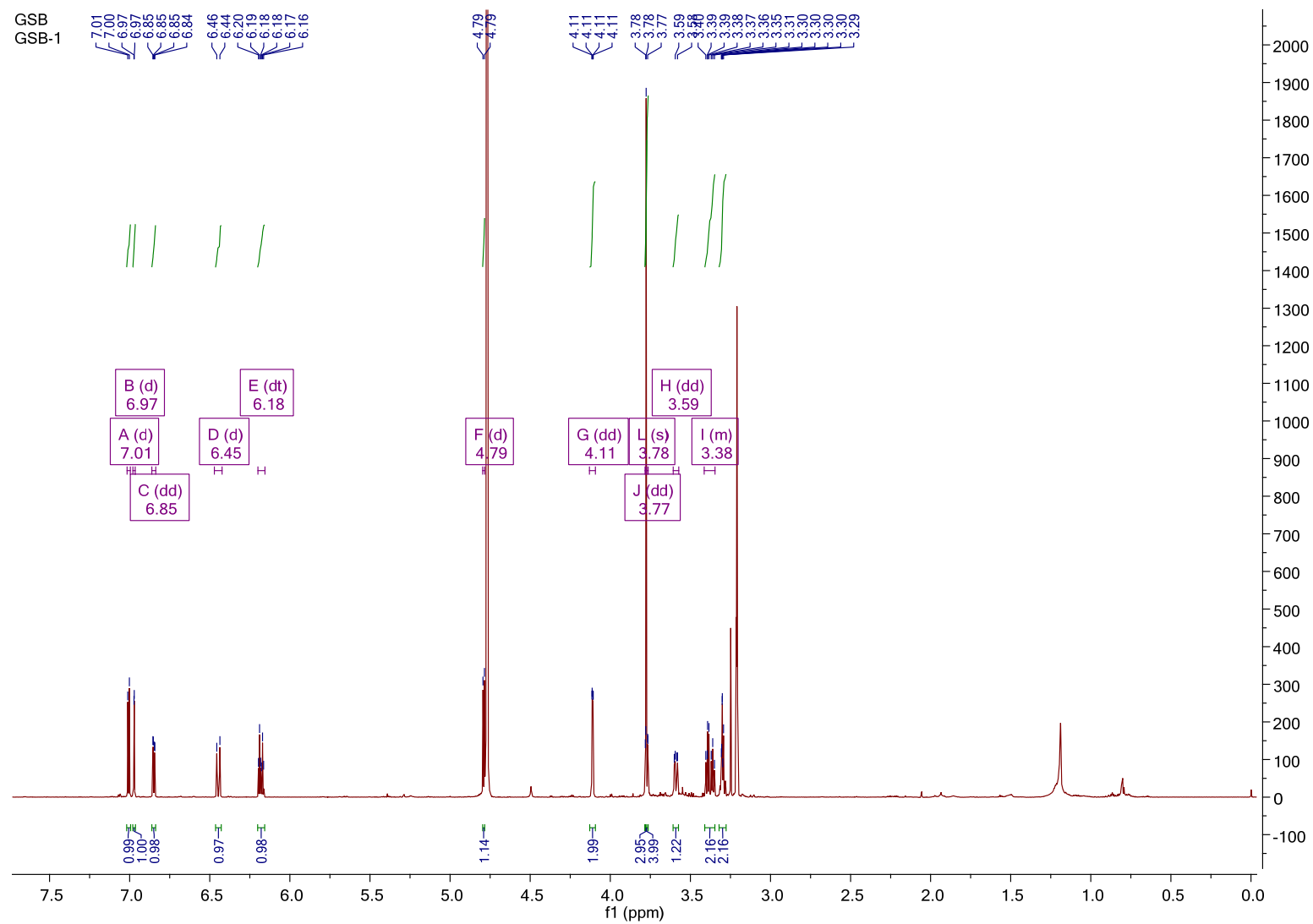
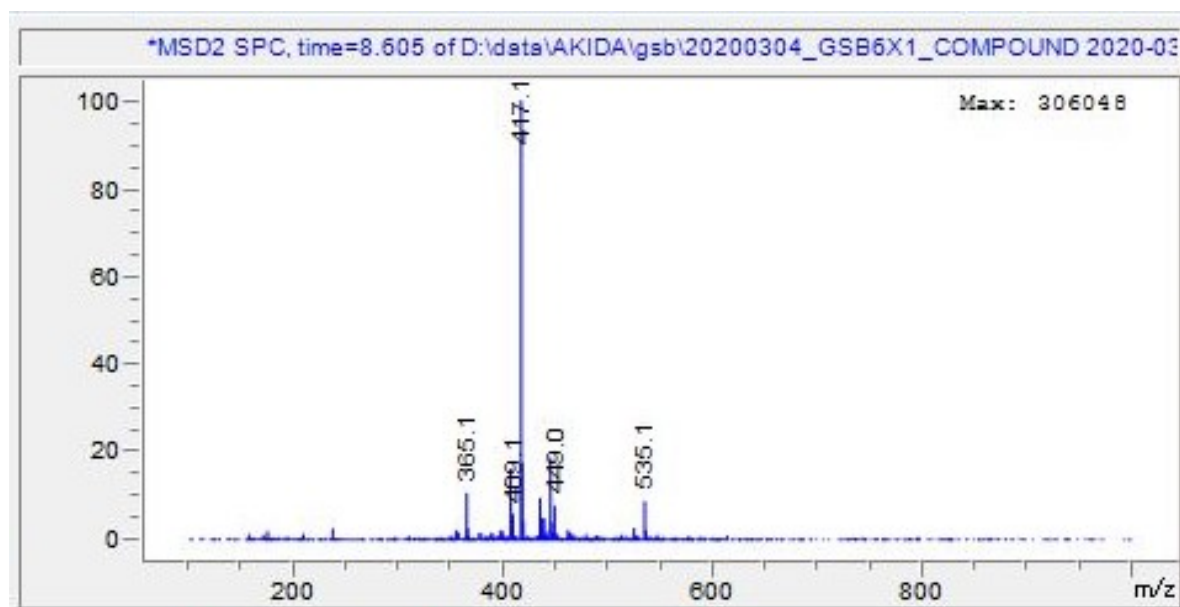


Figure S10. The ESIMS data of **3** (negative-ion mode)



1H NMR spectrum of compound 10a in CDCl₃. The spectrum shows peaks from 0 to 7 ppm. Key peaks are labeled: C (s) at 6.66 ppm, A (d) at 6.45 ppm, B (dt) at 6.23 ppm, F (s) at 4.78 ppm, D (dd) at 4.12 ppm, E (m) at 3.75 ppm, and G (m) at 3.51 ppm. Integration values are shown below the baseline: 1.95, 0.99, 1.00, 1.20, 2.10, and 6.01. A list of chemical shifts (delta) is provided at the top: 6.66, 6.46, 6.44, 6.25, 6.24, 6.23, 6.23, 6.22, 4.13, 4.12, 4.12, 3.76, 3.69, 3.57, 3.57, 3.56, 3.55, 3.53, 3.31, 3.31.

Figure S12. The ESIMS data of **4** (negative-ion mode)

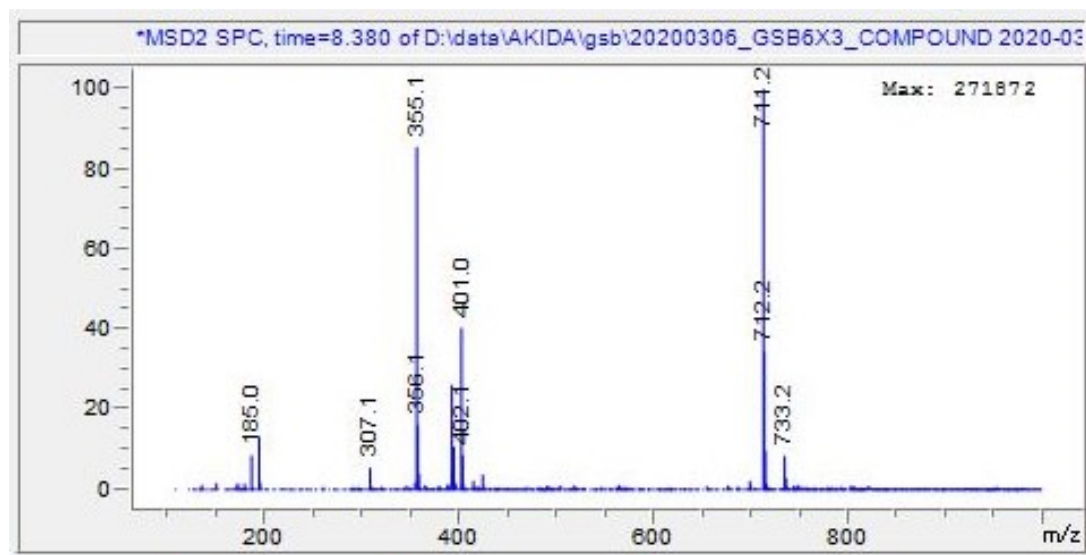


Figure S13. The ^1H NMR spectrum of **4** (CD_3OD , 850 MHz)

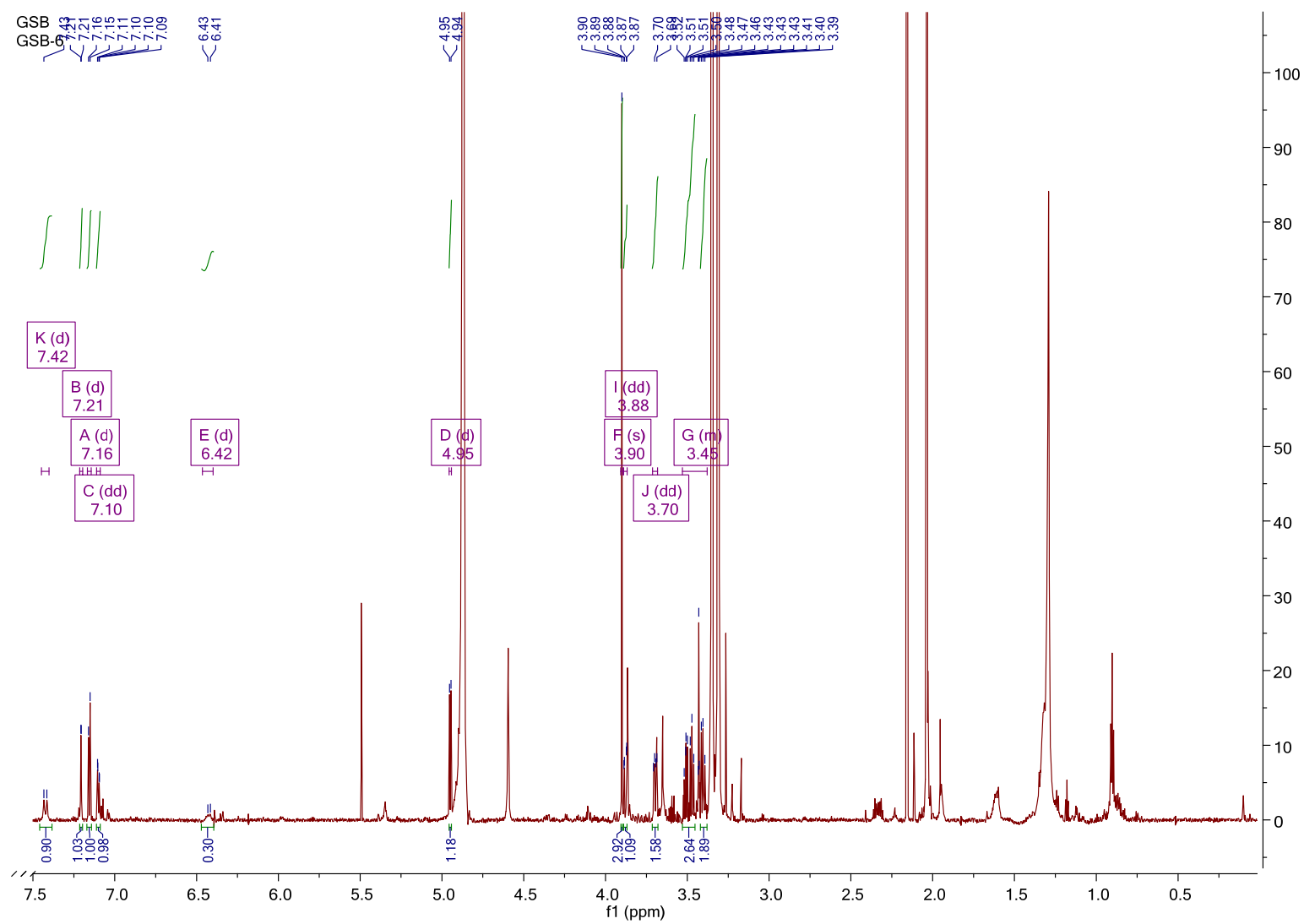


Figure S14. The ESIMS data of **5** (negative-ion mode)

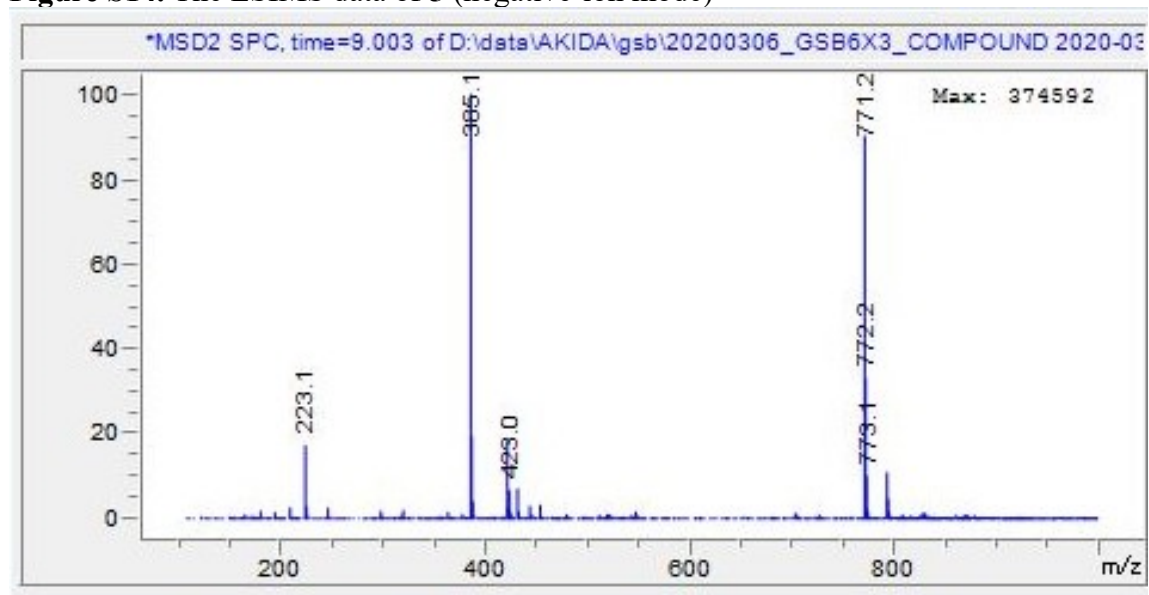


Figure S15. The ^1H NMR spectrum of **5** (CD_3OD , 850 MHz)

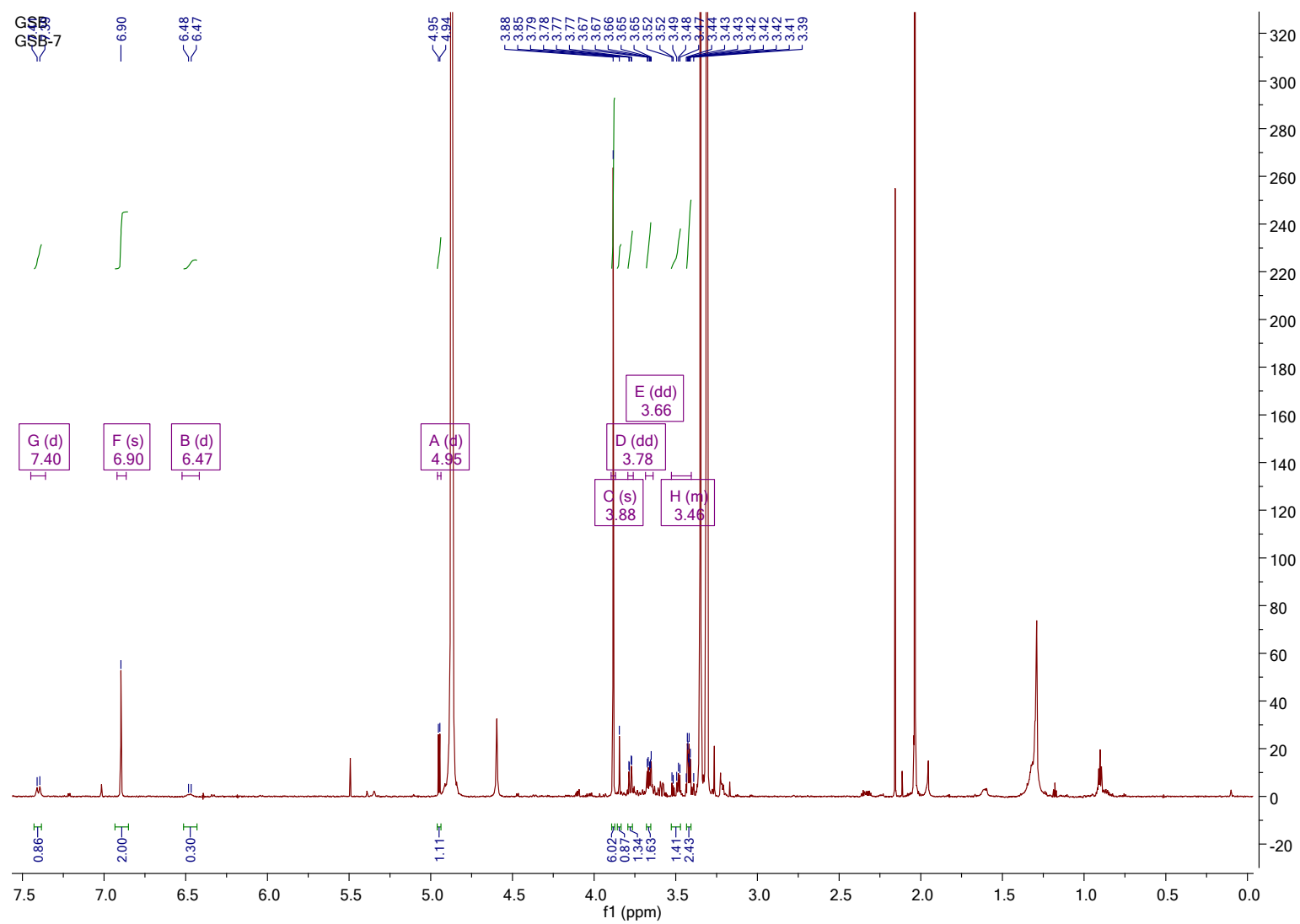


Figure S16. The ESIMS data of **6** (positive-ion mode)

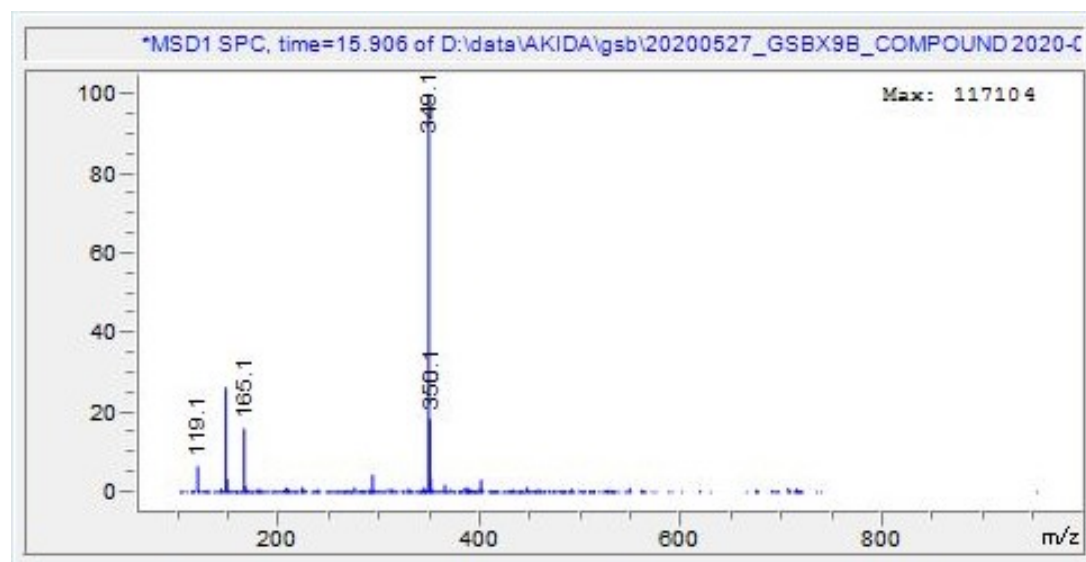
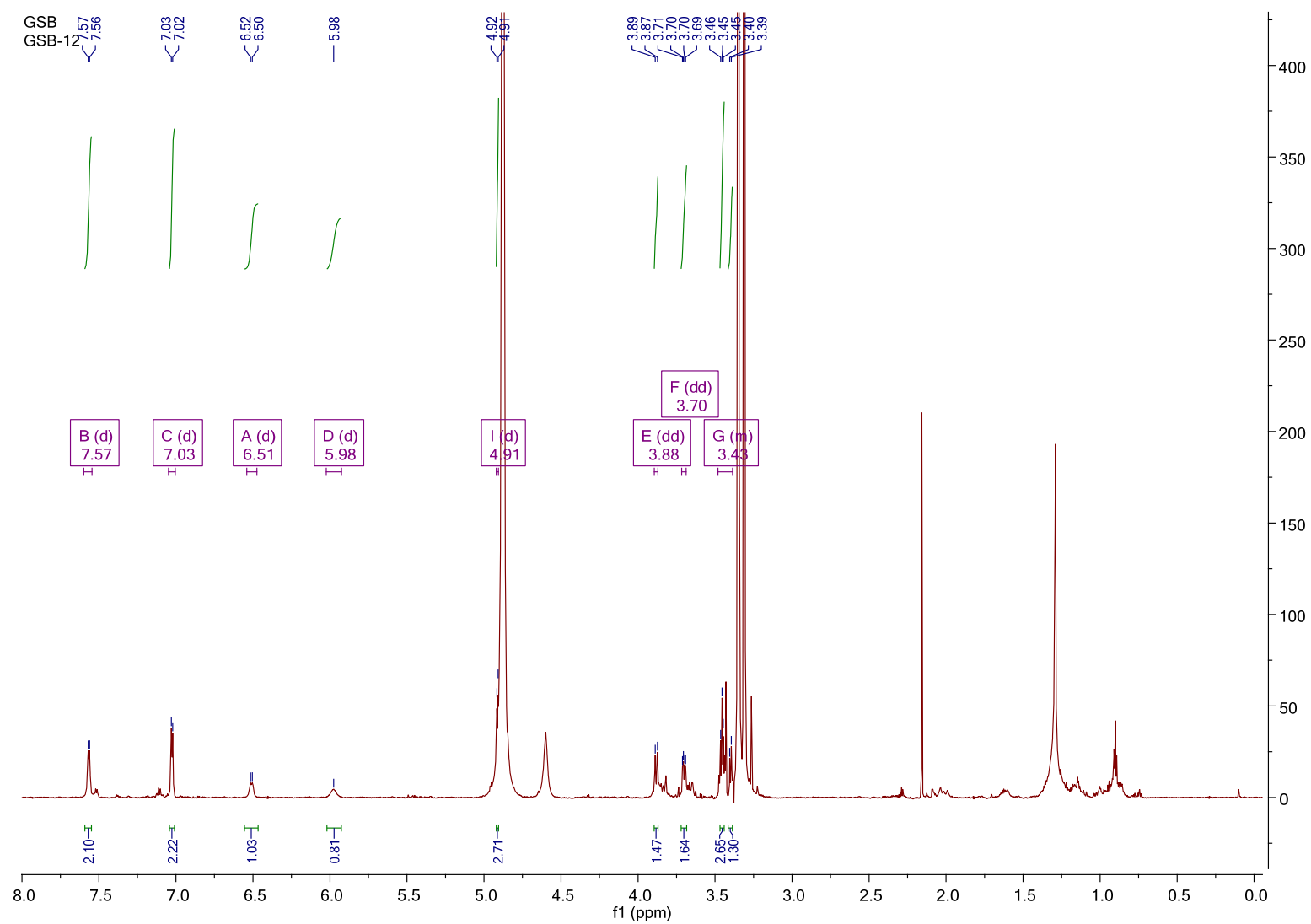


Figure S17. The ^1H NMR spectrum of **6** (CD_3OD , 850 MHz)



General experimental procedure

Optical rotations were measured using a Jasco P-2000 polarimeter (Jasco, Easton, MD, USA). Infrared (IR) spectra were recorded with a Bruker IFS-66/S FT-IR spectrometer (Bruker, Karlsruhe, Germany). Ultraviolet (UV) spectra were acquired on an Agilent 8453 UV-visible spectrophotometer (Agilent Technologies, Santa Clara, CA, USA). Circular dichroism spectra were measured on a Jasco J-1500 spectropolarimeter (Jasco). NMR spectra were recorded using a Bruker AVANCE III HD 850 NMR spectrometer with a 5 mm TCI CryoProbe, operated at 850 MHz (^1H) and 212.5 MHz (^{13}C). The chemical shifts were represented in ppm (δ) for ^1H and ^{13}C NMR analyses. Preparative and semi-preparative HPLC was performed using a Waters 1525 Binary HPLC pump with a Waters 996 photodiode array detector (Waters Corporation, Milford, MA, USA) using an Agilent Eclipse C18 column (250 \times 21.2 mm, 5 μm ; flow rate: 5 mL/min; Agilent Technologies) and a Phenomenex Luna Phenyl-hexyl 100 Å column (250 \times 10 mm, 5 μm ; flow rate: 2 mL/min; Phenomenex, Torrance, CA, USA). LC/MS analysis was performed on an Agilent 1200 Series HPLC system, equipped with a diode array detector and 6130 Series ESI mass spectrometer, and an analytical Kinetex C18 100 Å column (100 \times 2.1 mm, 5 μm ; flow rate: 0.3 mL/min; Phenomenex). All HRESIMS data were obtained using an Agilent G6545B quadrupole time-of-flight (Q-TOF) mass spectrometer (Agilent Technologies). Silica gel 60 (230-400 mesh; Merck, Darmstadt, Germany) was used for column chromatography. Diaion HP-20 (Mitsubishi Chemical, Tokyo, Japan) was used for open-column chromatography. Thin-layer chromatography was performed with precoated silica gel F₂₅₄ plates and RP-C₁₈ F_{254s} plates (Merck) and spots were detected under UV light or by heating, after spraying with anisaldehyde-sulfuric acid.

Plant material

The whole fruits of *G. biloba* were collected in the campus of Sungkyunkwan University, Suwon, Korea, in October 2019, and the plant was identified by one of the authors (K.H.K.). A voucher specimen of the material (GBF-2019-10) was deposited in the herbarium of the School of Pharmacy, Sungkyunkwan University, Suwon, Korea