# Supplementary Materials

# Structurally Diverse Metabolites from the *Ophiorrhiza japonica* Bl. and Their Antioxidant Activities In Vitro and PPARα Agonistic Activities In Silico

**Qing Bu [1,†], Yang Jin [2,†], Meng-Juan Xu [1], Lei Wu [3] and Lin-Fu Liang [1,*]**

[1] College of Materials Science and Engineering, Central South University of Forestry and Technology, Changsha 410004, China
[2] School of Chinese Materia Medica, Nanjing University of Chinese Medicine, Nanjing 210023, China
[3] College of Forestry, Central South University of Forestry and Technology, Changsha 410004, China
* Correspondence: lianglinfu@csuft.edu.cn
† These authors contributed equally to this work

# Table of contents

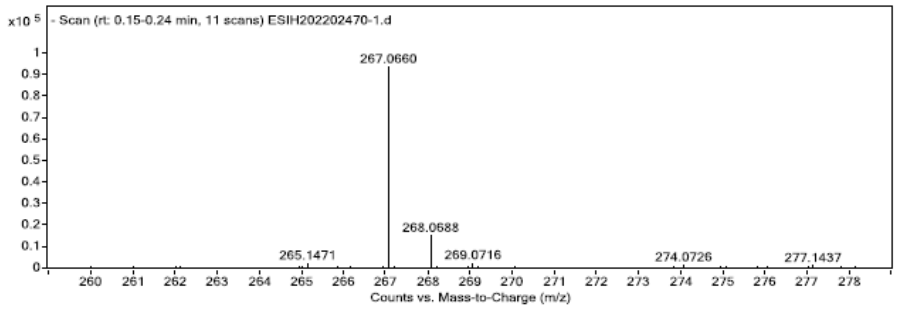
**Figure S1.** HRESIMS spectrum of compound **1**
**Figure S2.** $^{1}H$ NMR spectrum (600 MHz) of compound **1** in $CDCl_3$
**Figure S3.** $^{13}C$ NMR (BB+DEPT) spectrum (125 MHz) of compound **1** in $CDCl_3$
**Figure S4.** HSQC spectrum (600 MHz) of compound **1** in $CDCl_3$
**Figure S5.** $^{1}H$–$^{1}H$ COSY spectrum (600 MHz) of compound **1** in $CDCl_3$
**Figure S6.** HMBC spectrum (600 MHz) of compound **1** in $CDCl_3$
**Figure S7.** NOESY spectrum (600 MHz) of compound **1** in $CDCl_3$
**Figure S8.** IR spectrum of compound **1**
**Figure S9.** UV spectrum of compound **1**

## Qualitative Analysis Report

| | | | |
|---|---|---|---|
| **Data Filename** | ESIH202202470-1.d | **Sample Name** | A8-A8-RE1 |
| **Sample ID** | | **Position** | P1-A4 |
| **Instrument Name** | Agilent G6520 Q-TOF | **Acq Method** | 20160324_MS_ESIH_NEG_1min.m |
| **Acquired Time** | 7/25/2022 15:01:10 | **IRM Calibration Status** | Success |
| **DA Method** | small molecular data analysis method.m | **Comment** | ESIH by fangsu |

**User Spectra**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |




**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 267.066 | 267.0663 | 0.33 | 1.22 | C16 H11 O4 | (M-H)- |

--- End Of Report ---



**Figure S1.** HRESIMS spectrum of compound **1**

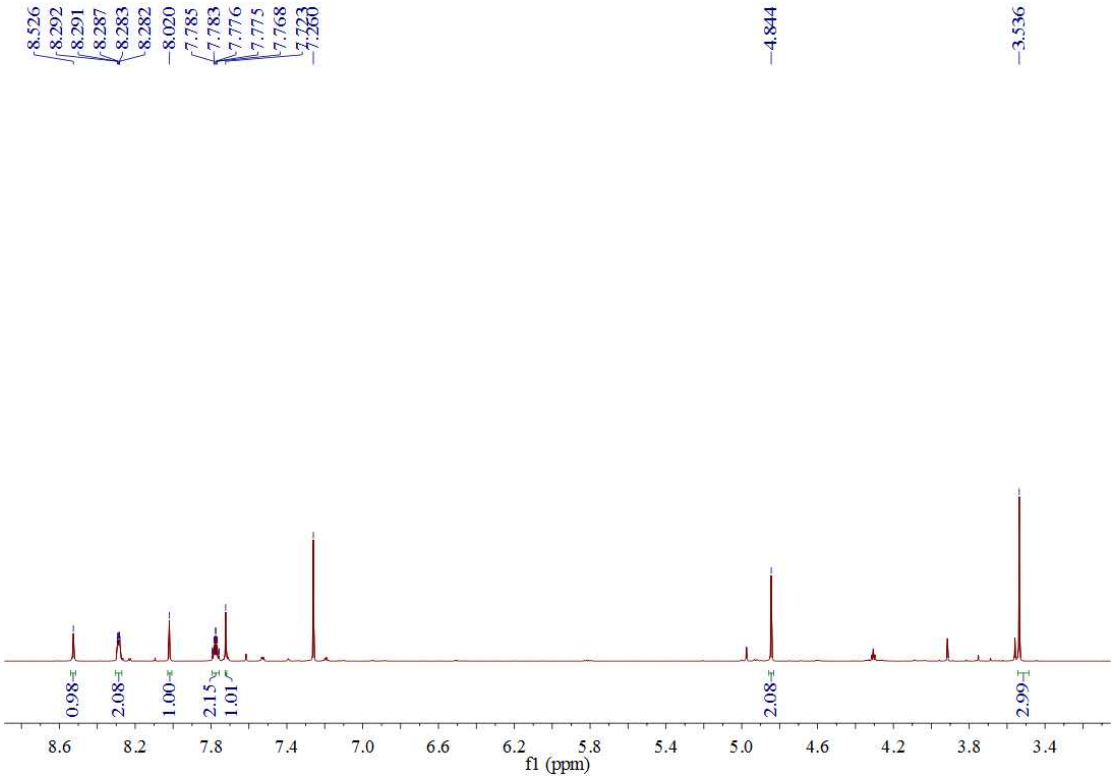



**Figure S2.** $^{1}$H NMR spectrum (600 MHz) of compound **1** in $CDCl_3$

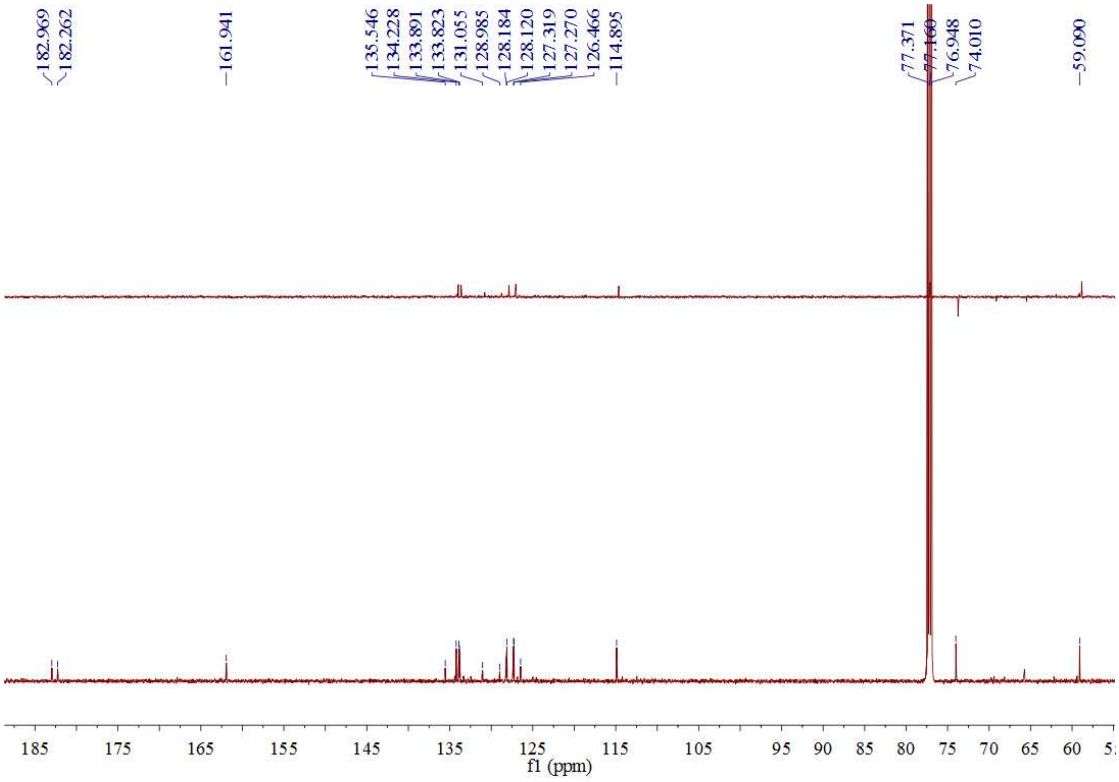



**Figure S3.** $^{13}C$ NMR (BB+DEPT) spectrum (125 MHz) of compound **1** in $CDCl_3$

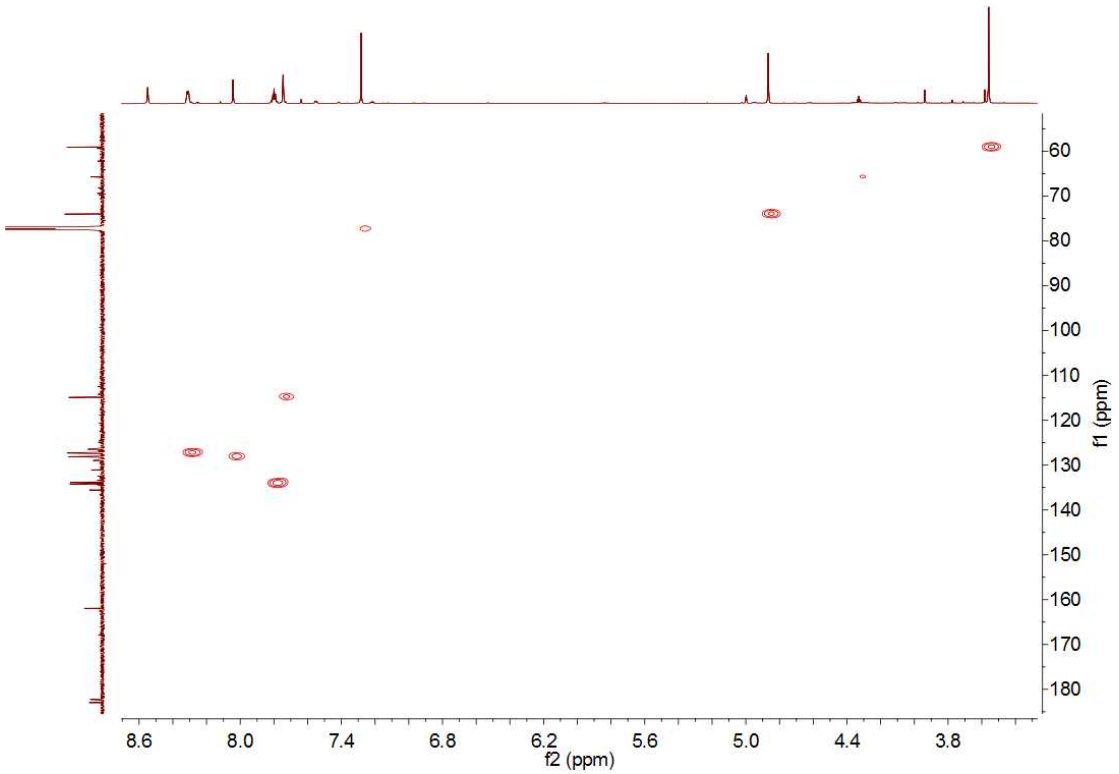



**Figure S4.** HSQC spectrum (600 MHz) of compound **1** in $CDCl_3$

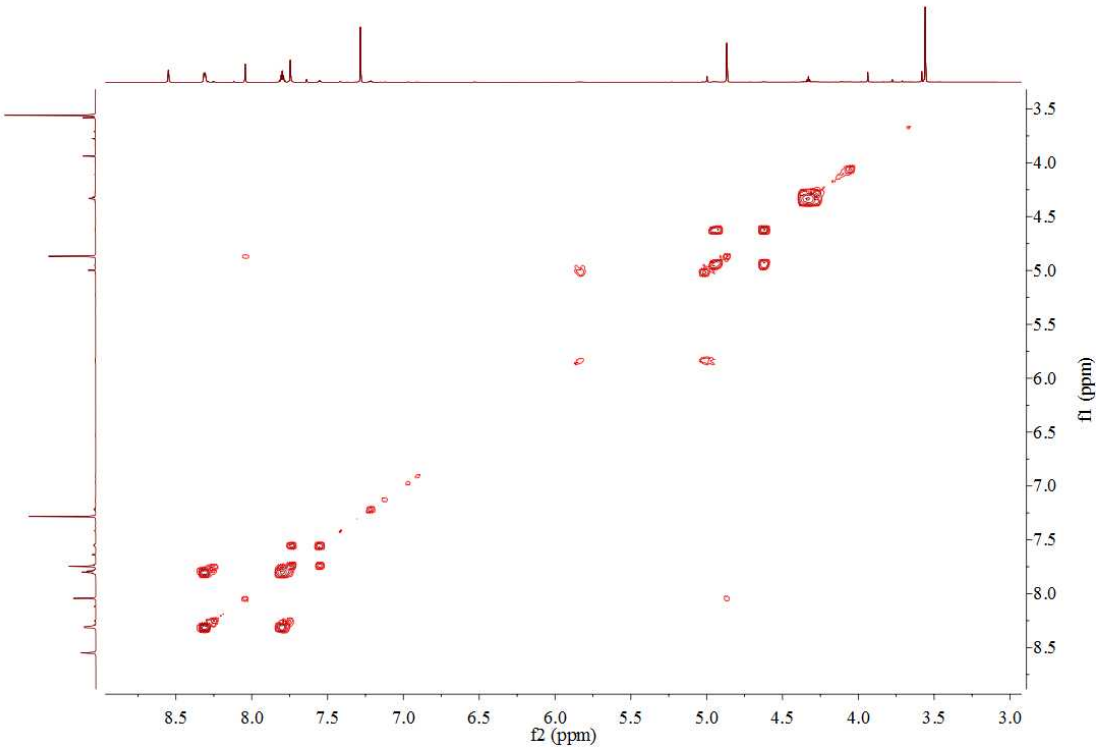



**Figure S5.** $^{1}H$–$^{1}H$ COSY spectrum (600 MHz) of compound **1** in $CDCl_3$

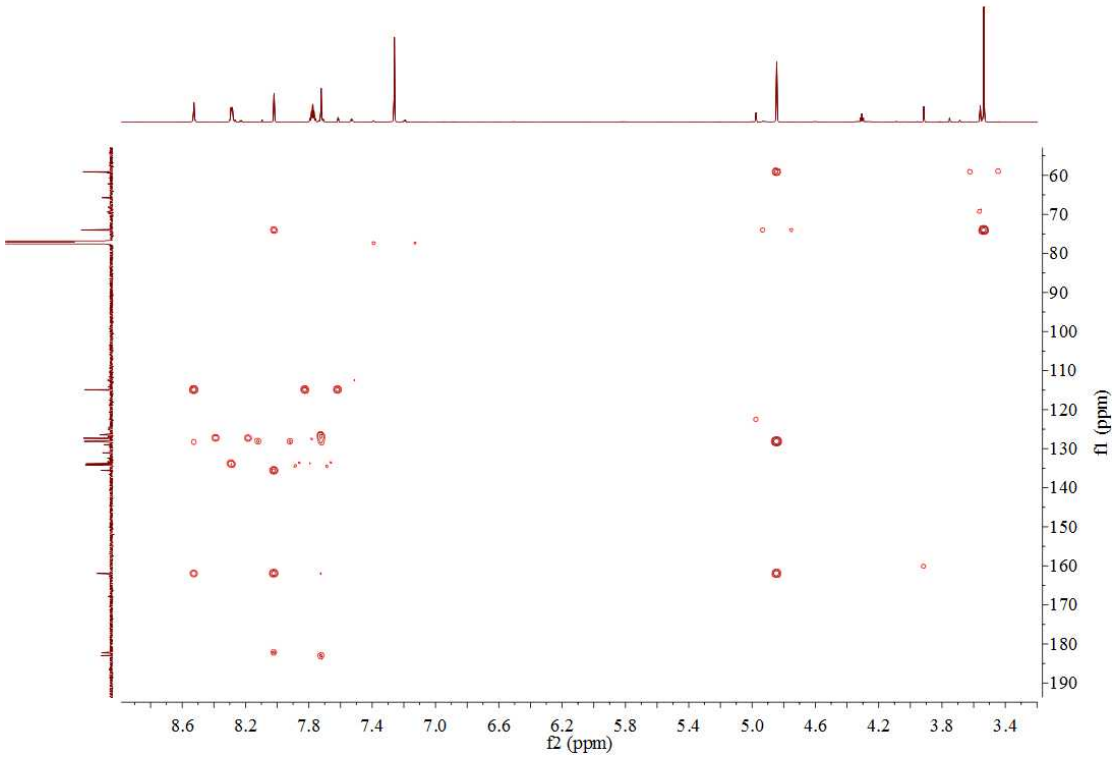



**Figure S6.** HMBC spectrum (600 MHz) of compound **1** in $CDCl_3$

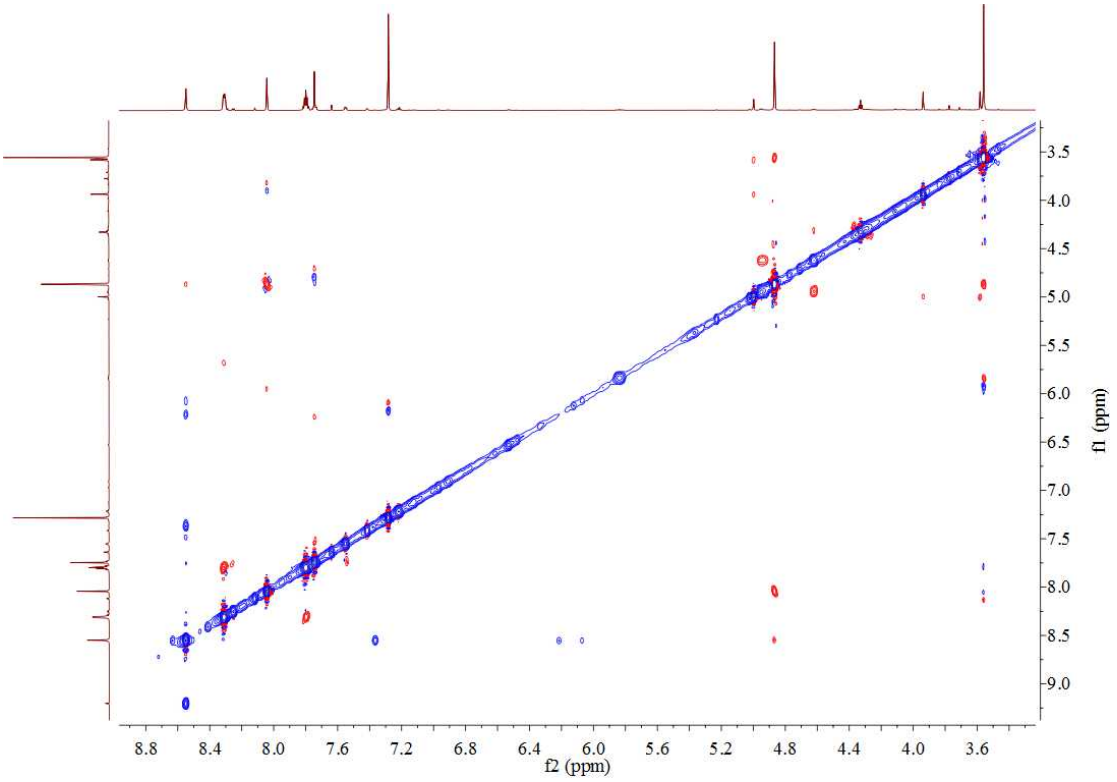



**Figure S7.** NOESY spectrum (600 MHz) of compound **1** in $CDCl_3$

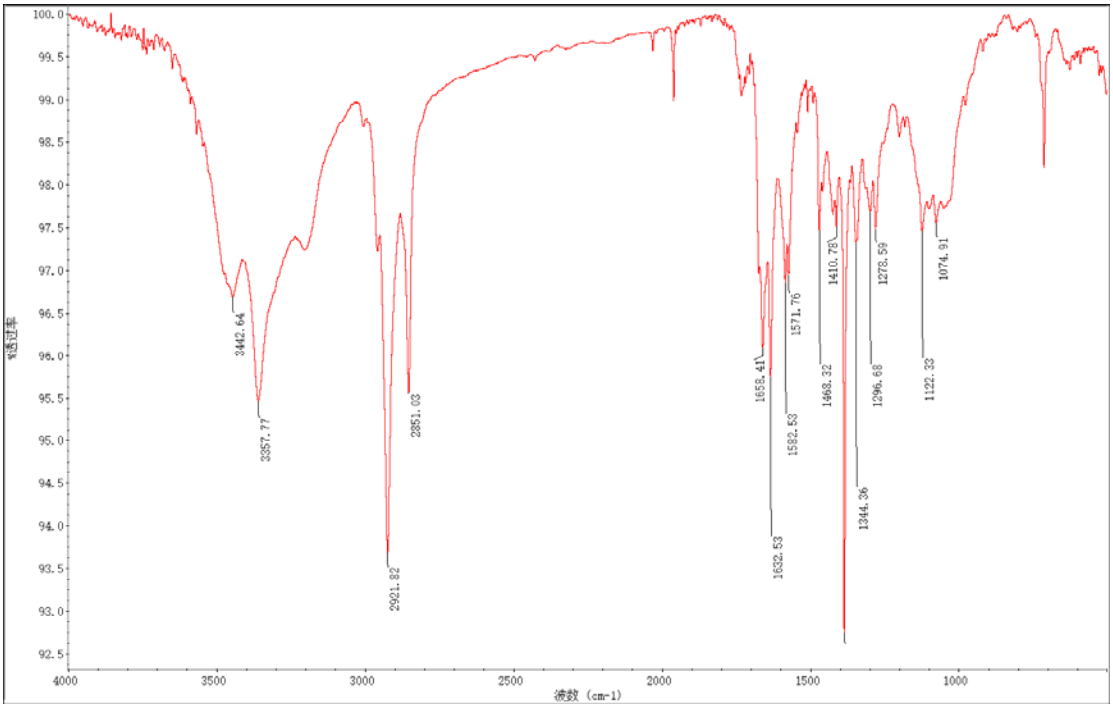



**Figure S8.** IR spectrum of compound **1**

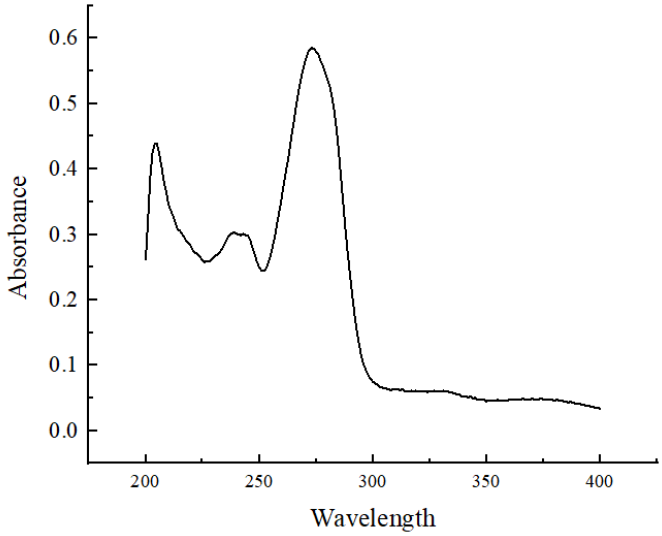



**Figure S9.** UV spectrum of compound **1**