

## Supporting Information

*Rec. Nat. Prod.* X:X (202X) XX-XX

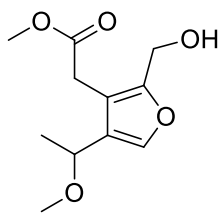
### Three Rare Furan Derivatives Transformed from Secoiridoids were Isolated from the Roots of *Gentiana macrophylla*

Wei Hu <sup>1</sup>, Yihan He <sup>1,\*</sup>, Yangyang Yin <sup>1</sup>, Ye Yang <sup>1</sup>, Huanhuan Fu <sup>1</sup>, Zhe Li <sup>1</sup>  
and Zhenggang Yue <sup>1, 2, \*</sup>

<sup>1</sup> State Key Laboratory of Research & Development of Characteristic Qin Medicine Resources  
(Cultivation), Co-construction Collaborative Innovation Center for Chinese Medicinal Resources  
Industrialization by Shaanxi & Education Ministry, Shaanxi Innovative Drug Research Center,  
School of Pharmacy, Shaanxi University of Chinese Medicine, Xianyang 712046, P.R. China

<sup>2</sup> College of Life Science, Qinghai Normal University, Xining 810016, P.R. China

| Table of Contents                                                          | Page |
|----------------------------------------------------------------------------|------|
| Figure S1: New compound (1) search report of SciFinder                     | 2    |
| Figure S2: HR-ESI-MS spectrum of 1                                         | 3    |
| Figure S3: Low-ESI-MS spectrum of 1                                        | 3    |
| Figure S4: IR spectrum of 1                                                | 4    |
| Figure S5: <sup>1</sup> H NMR (600 MHz, CD <sub>3</sub> OD) spectrum of 1  | 4    |
| Figure S6: <sup>13</sup> C NMR (150 MHz, CD <sub>3</sub> OD) spectrum of 1 | 5    |
| Figure S7: HSQC spectrum of 1                                              | 5    |
| Figure S8: HMBC spectrum of 1                                              | 6    |
| Figure S9: ROESY spectrum of 1                                             | 6    |
| Figure S10: All HMBC (H→C) correlations of 1                               | 7    |
| Table S1: HMBC data for 1                                                  | 7    |



Structure Match

As Drawn (0)

**Substructure (0)**

Similarity (80K)

Filter Content Report

Download filter data from this result set.

**Substances** (0)

Save And Alerts

We couldn't find any results. Please update your search query and try again.

[Download Task History](#) for this search or [Save your Search](#) to be informed when new content is published.

**Figure S1:** New compound (1) search report of SciFinder

## User Spectra

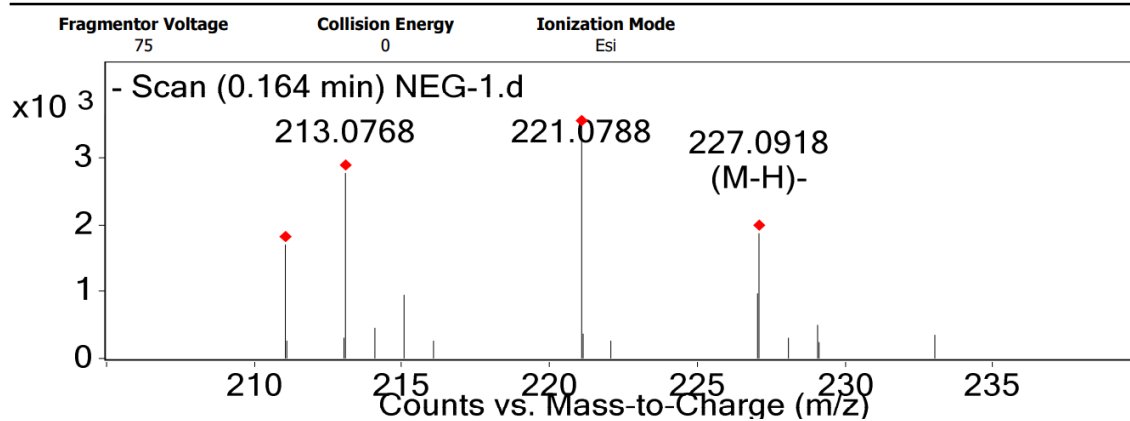


Figure S2: HR-ESI-MS spectrum of **1**

## User Spectra

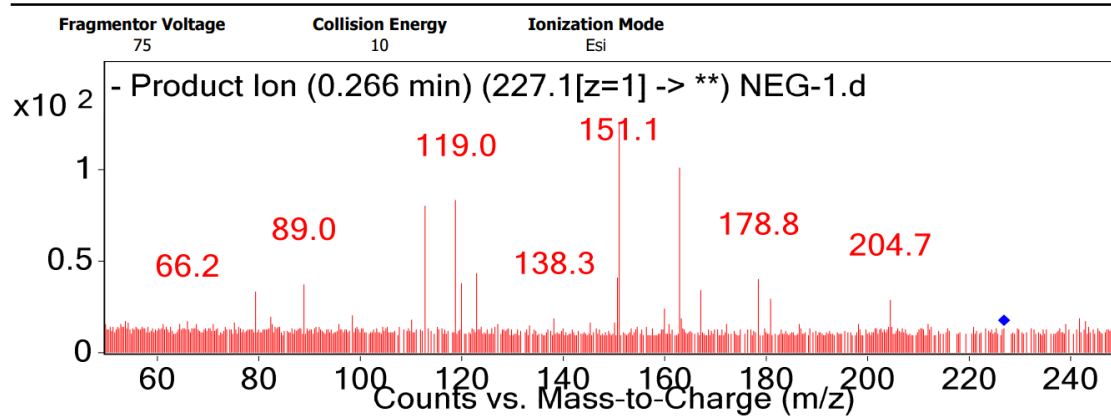


Figure S3: Low-ESI-MS spectrum of **1**

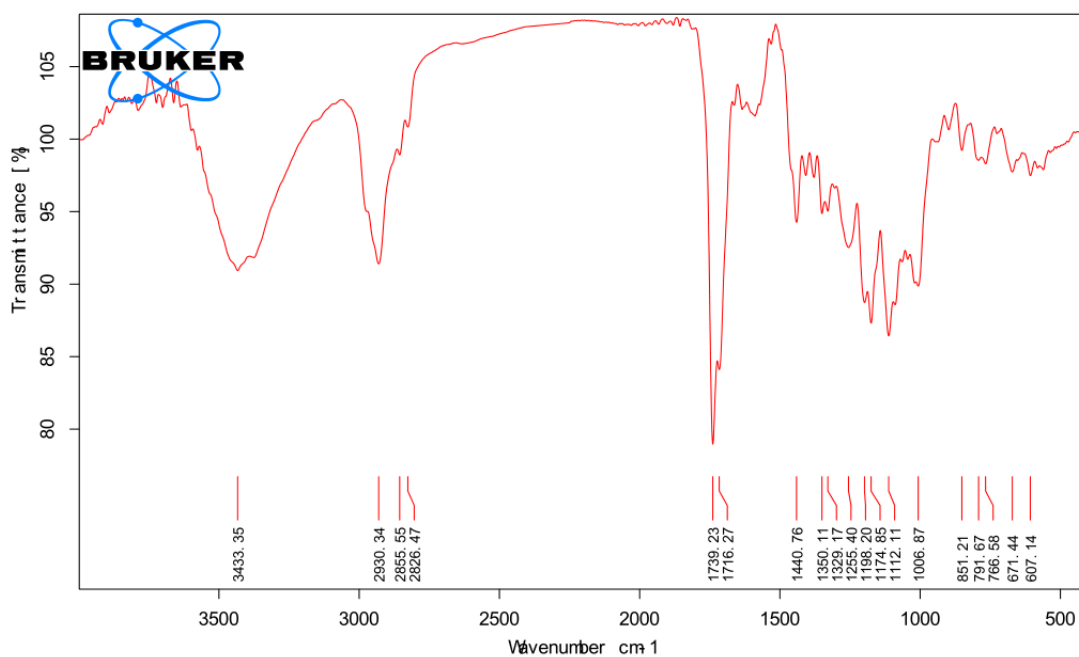


Figure S4: IR spectrum of 1

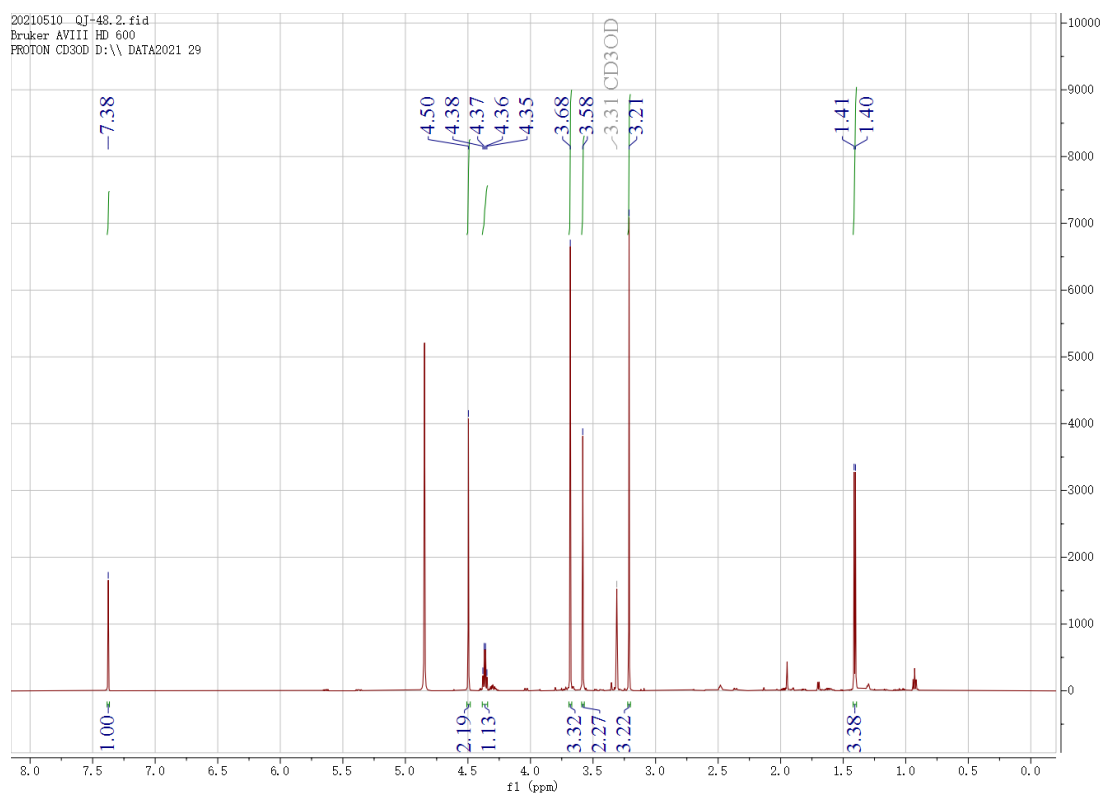
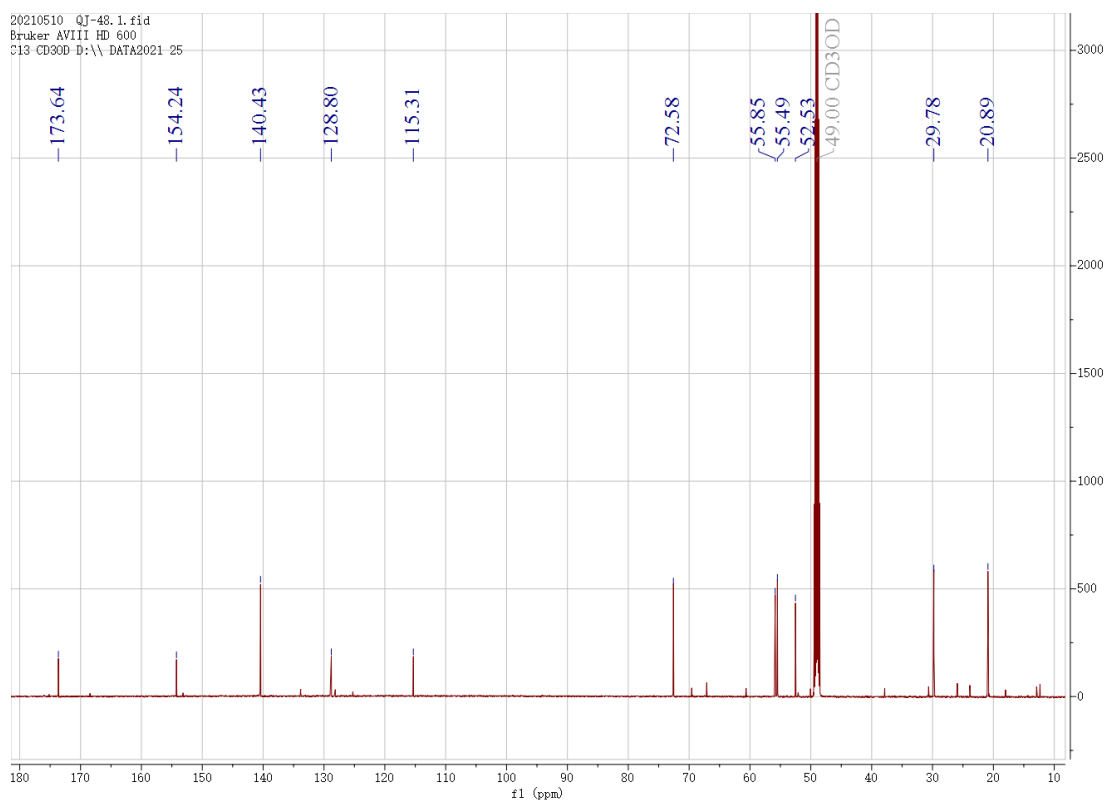
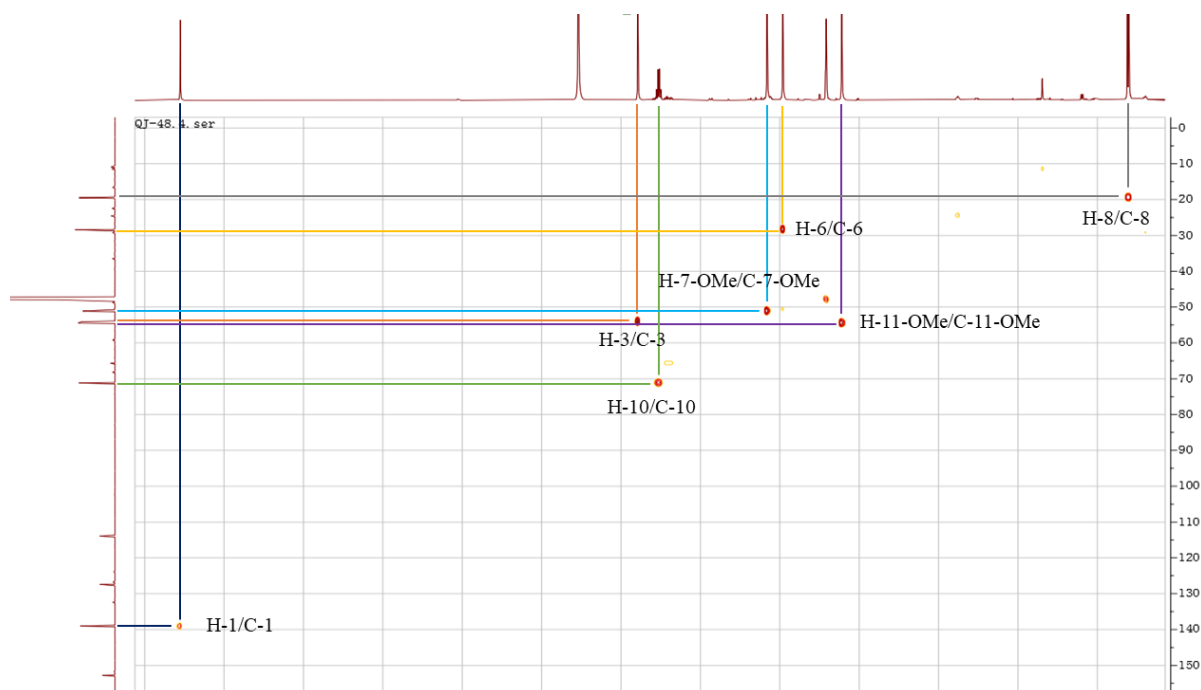


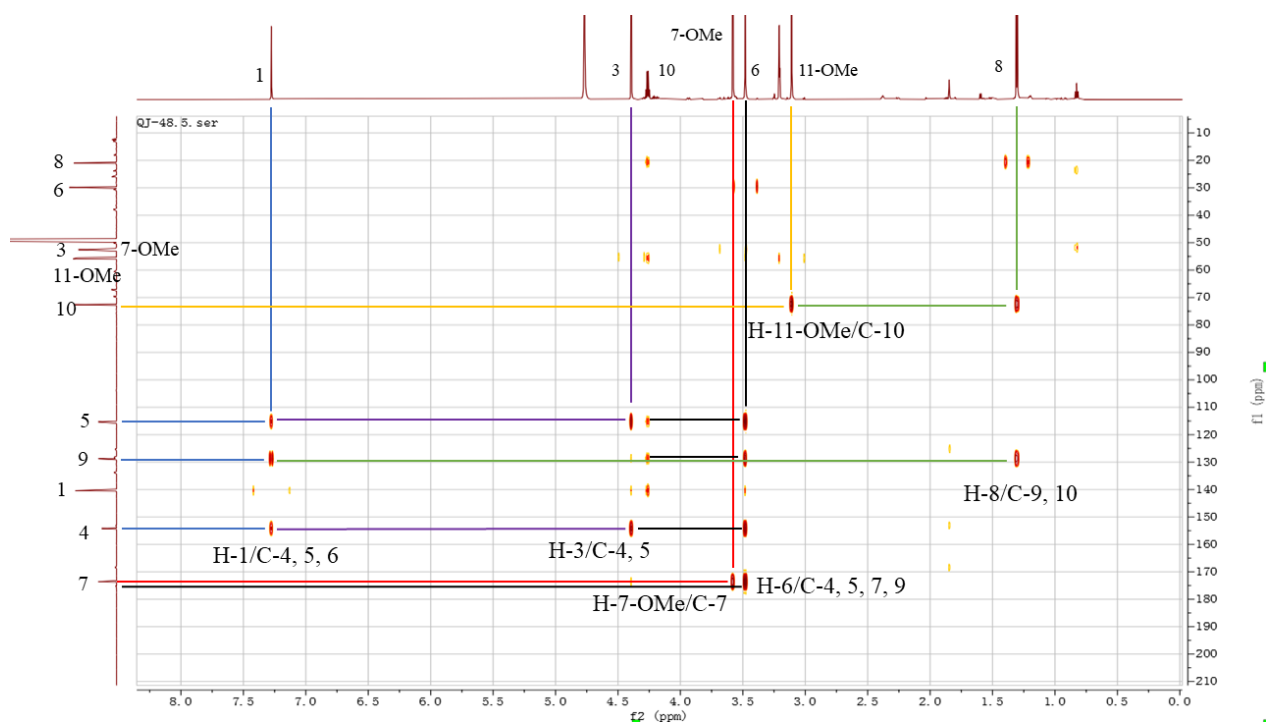
Figure S5:  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of 1



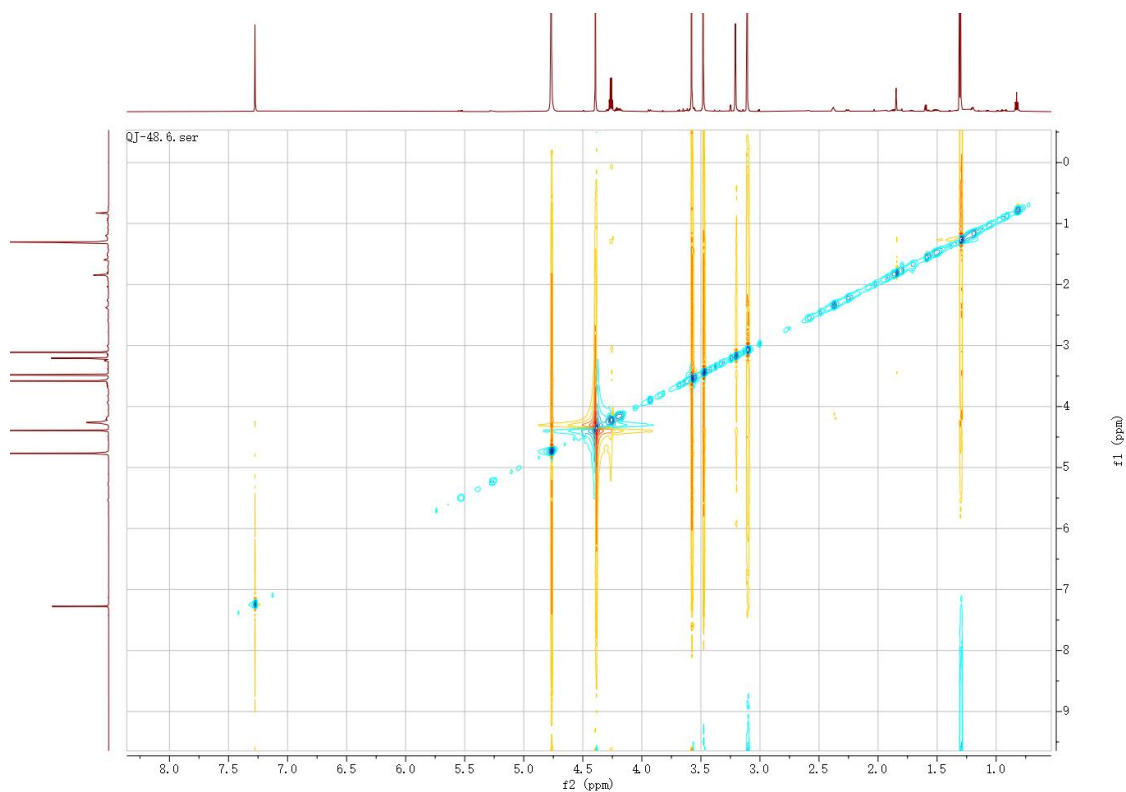
**Figure S6:**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **1**



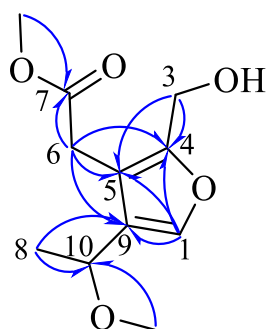
**Figure S7:** HSQC spectrum of **1**



**Figure S8: HMBC spectrum of 1**



**Figure S9: ROESY spectrum of 1**



**Figure S10** : All HMBC (H→C) correlations of **1**

**Table S1** : HMBC data for **1**

| No.    | $\delta_C$ | $\delta_H$           | HMBC               |
|--------|------------|----------------------|--------------------|
| 1      | 140.4      | 7.38 (s)             | C-9, C-5, C-4      |
| 2      |            |                      |                    |
| 3      | 55.5       | 4.50 (s)             | C-4, C-5           |
| 4      | 154.0      |                      |                    |
| 5      | 115.3      |                      |                    |
| 6      | 29.7       | 3.58 (s)             | C-4, C-5, C-7, C-9 |
| 7      | 173.6      |                      |                    |
| 8      | 20.8       | 1.41 (d, 6.6)        | C-9, C-10          |
| 9      | 128.8      |                      |                    |
| 10     | 72.5       | 4.38 (dd, 13.1, 6.6) | C-1, C-5, C-8, C-9 |
| 11     |            |                      |                    |
| 7-OMe  | 55.8       | 3.21 (s)             | C-10               |
| 11-OMe | 52.5       | 3.68 (s)             | C-7                |