

Supporting Information

Rec. Nat. Prod. 16:6 (2022) 651-656

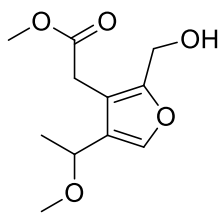
Three Rare Furan Derivatives Transformed from Secoiridoids were Isolated from the Roots of *Gentiana macrophylla*

Wei Hu ¹, Yihan He ^{1,*}, Yangyang Yin ¹, Ye Yang ¹, Huanhuan Fu ¹, Zhe Li ¹
and Zhenggang Yue ^{1,2,*}

¹ 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

² 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: ¹ H NMR (600 MHz, CD ₃ OD) spectrum of 1	4
Figure S6: ¹³ C NMR (150 MHz, CD ₃ 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)

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

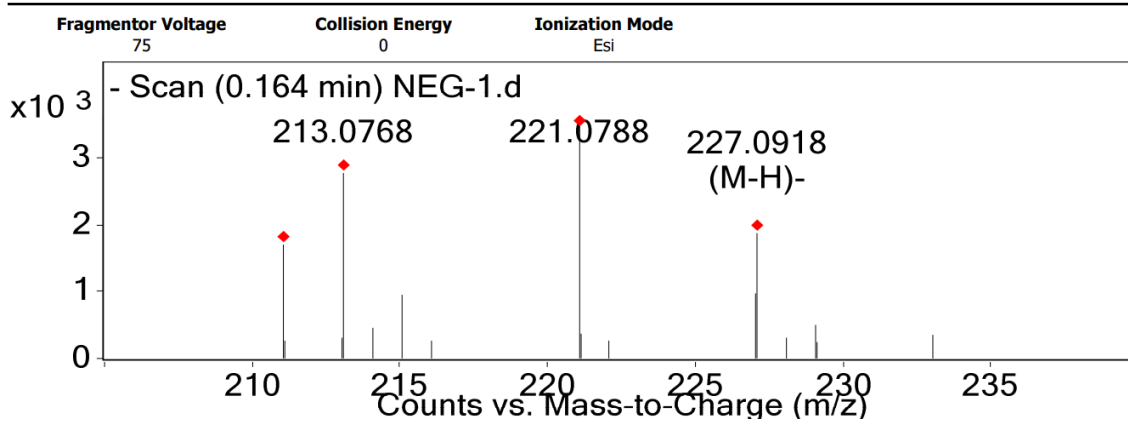


Figure S2: HR-ESI-MS spectrum of 1

User Spectra

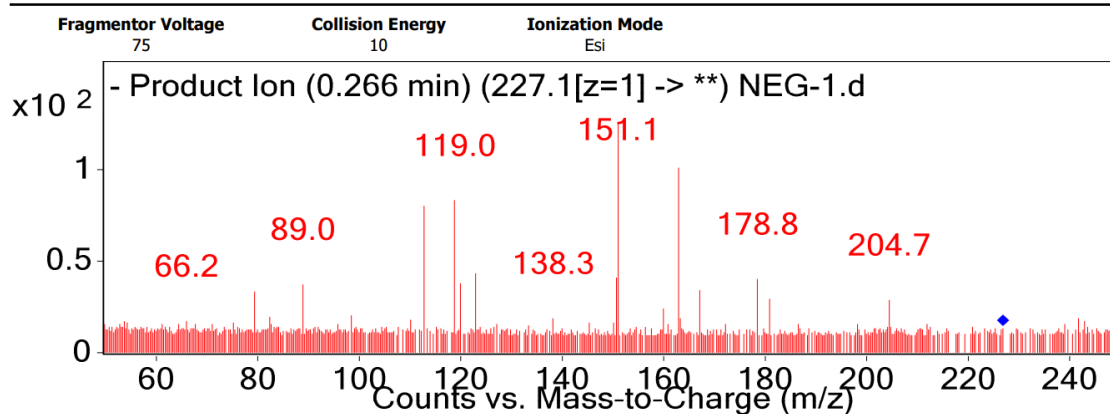


Figure S3: Low-ESI-MS spectrum of 1

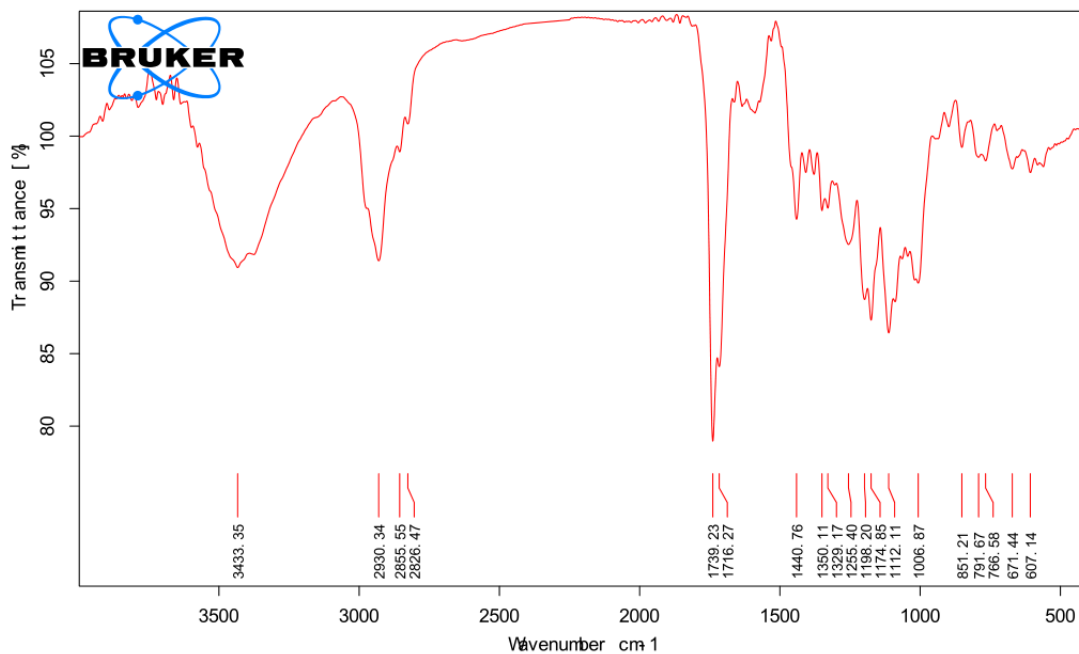


Figure S4: IR spectrum of **1**

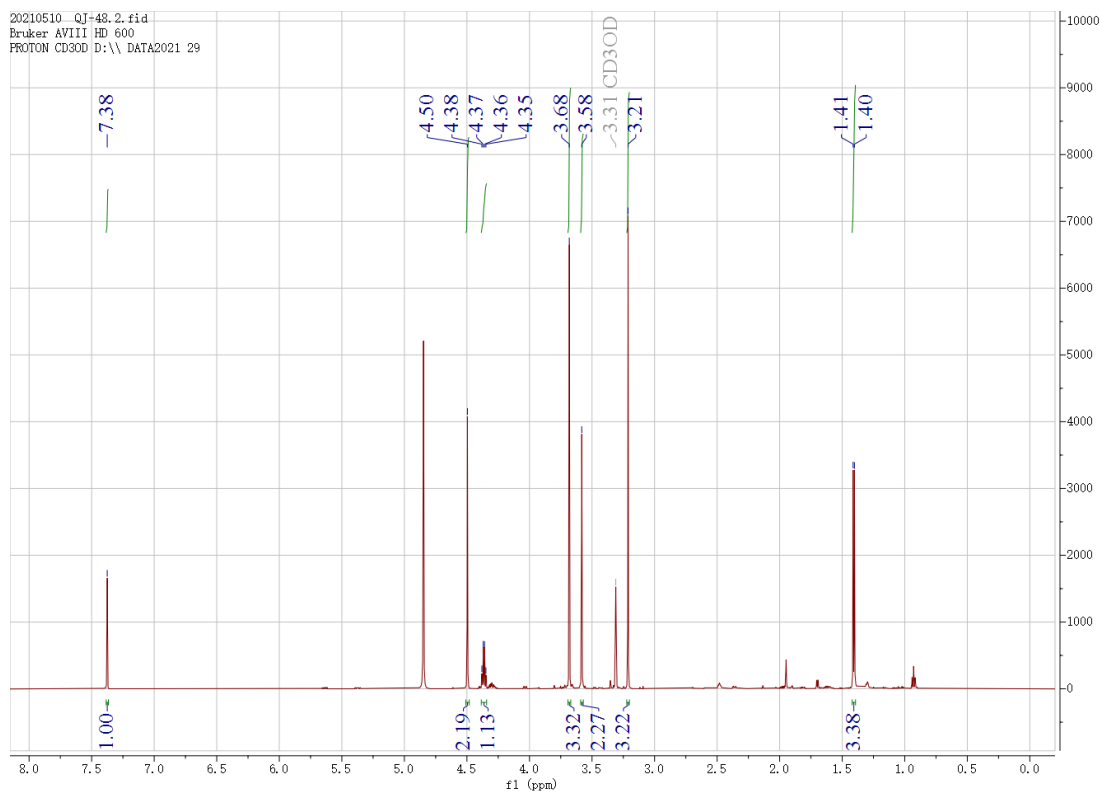


Figure S5: ^1H NMR (600 MHz, CD_3OD) spectrum of **1**

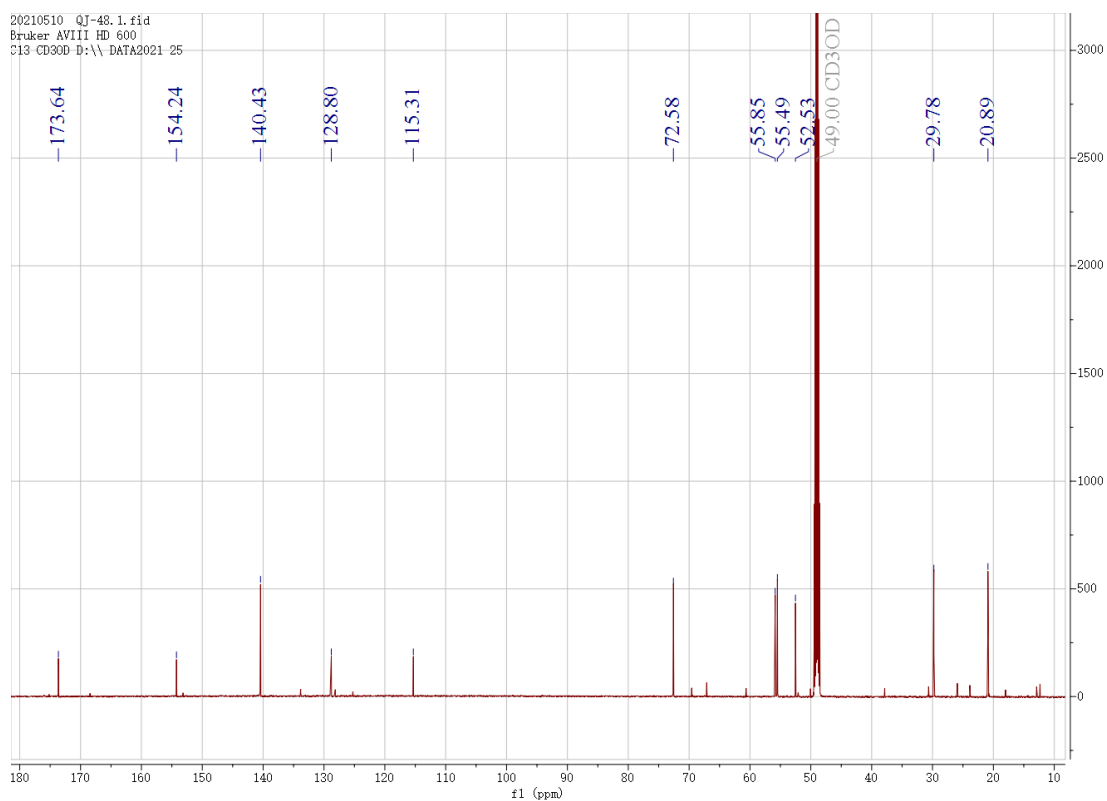


Figure S6: ^{13}C NMR (150 MHz, CD_3OD) spectrum of **1**

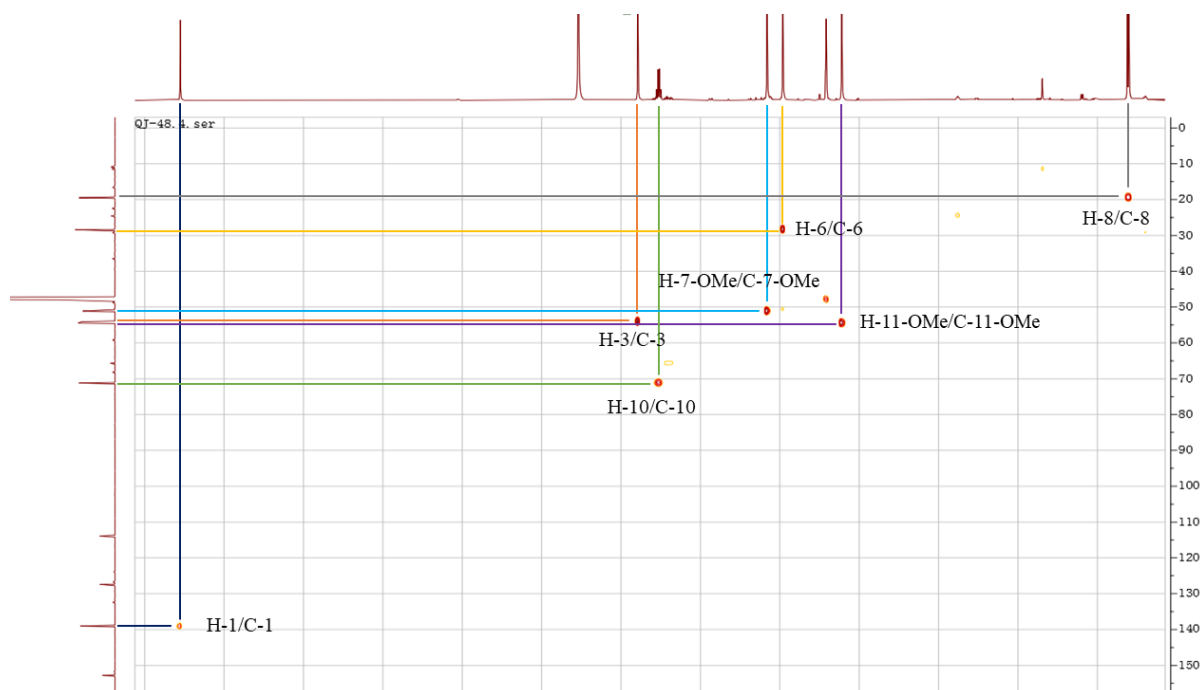


Figure S7: HSQC spectrum of **1**

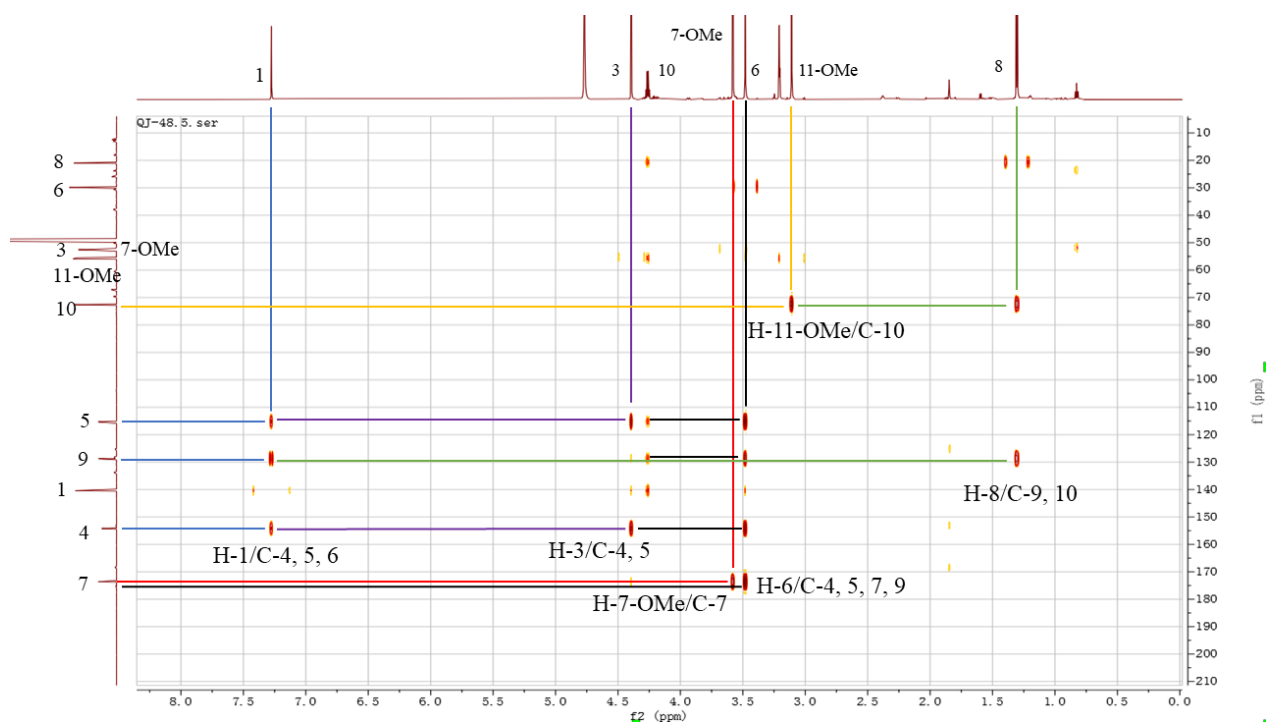


Figure S8: HMBC spectrum of **1**

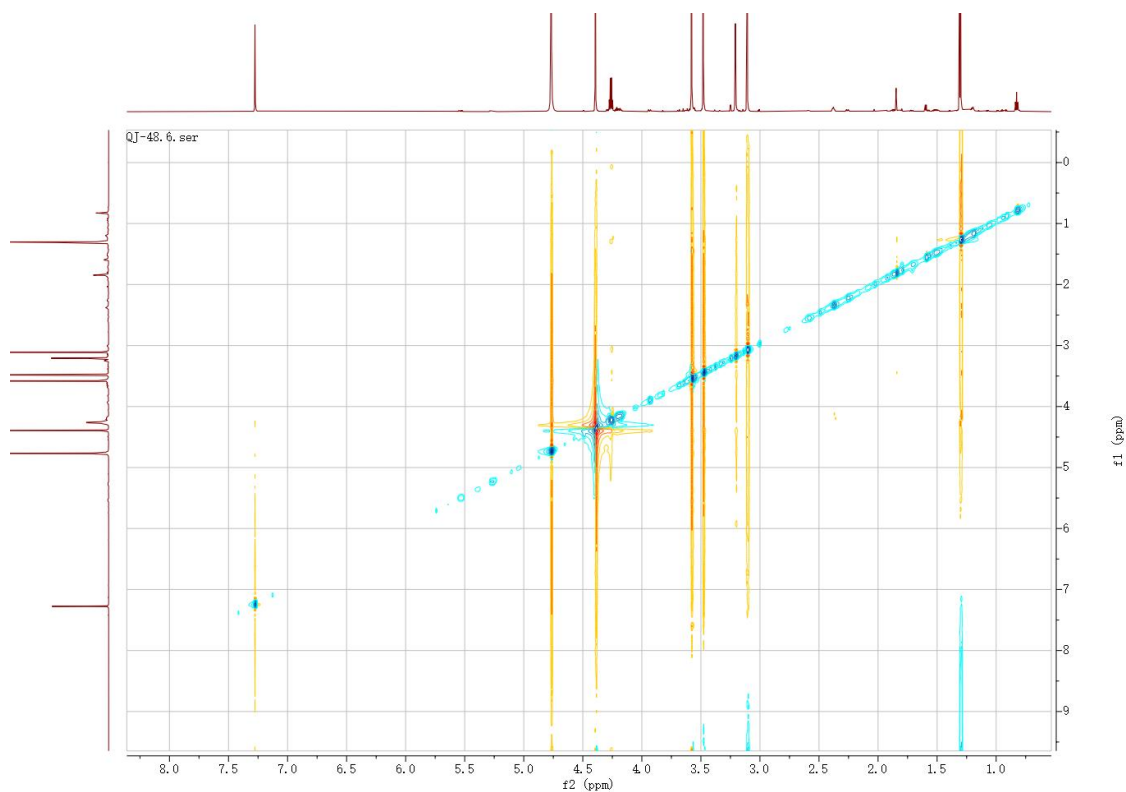


Figure S9: ROESY spectrum of **1**

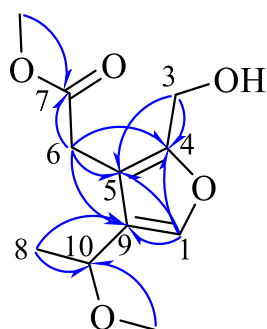


Figure S10 : All HMBC (H→C) correlations of **1**

Table S1 : HMBC data for **1**

No.	δ_C	δ_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