Supporting Information

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

Lyratin D, A New 4-Hydroxyisoflavan from the Whole Plant of *Solanum lyratum* Thunb.

Nguyen Minh Trang [1, 2], Le Ba Vinh [1], Nguyen Viet Phong [1,3 *]

and Seo Young Yang [3 *]

[1] *Institute of Marine Biochemistry, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Hanoi 10072, Vietnam*

[2] *College of Pharmacy, Chungnam National University, Daejeon 34134, Republic of Korea*

[3] *Deparment of Biology Education, Teachers College and Institute for Phylogenomics and Evolution, Kyungpook National University, Daegu 41566, Republic of Korea*

Table of Contents	Page

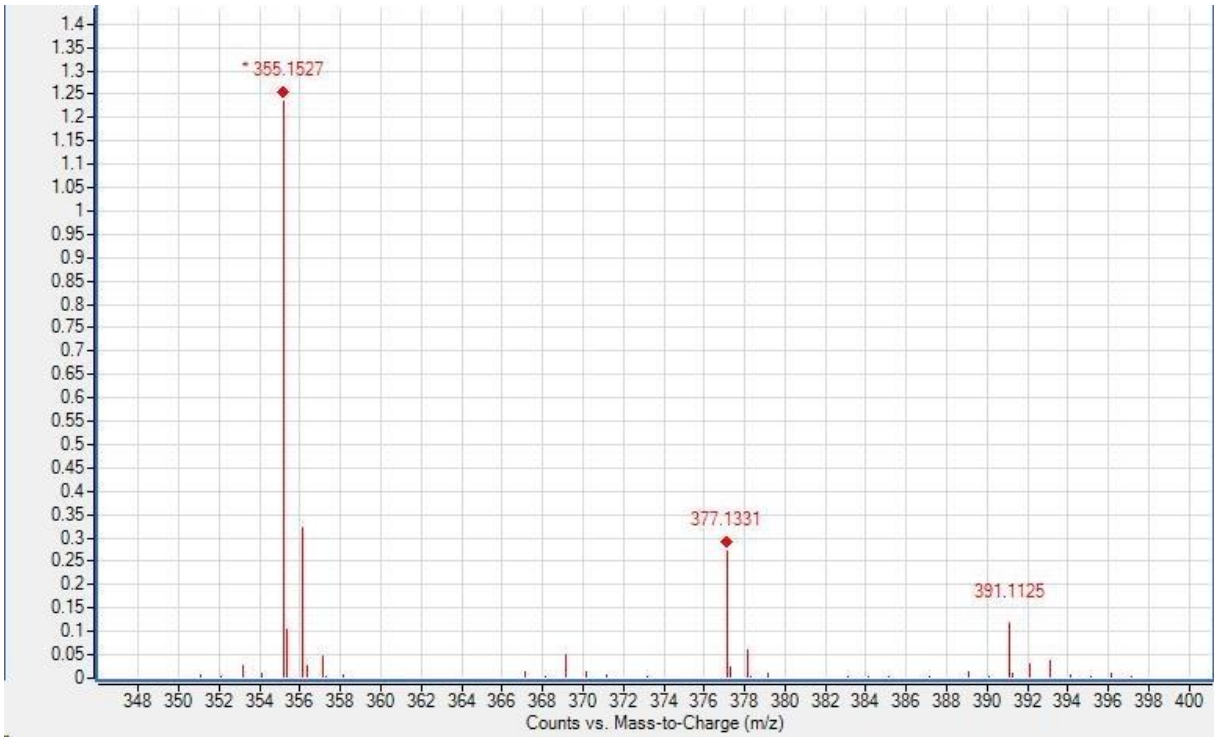


Figure S1: HR-ESI-MS spectrum of **1** (lyratin D)

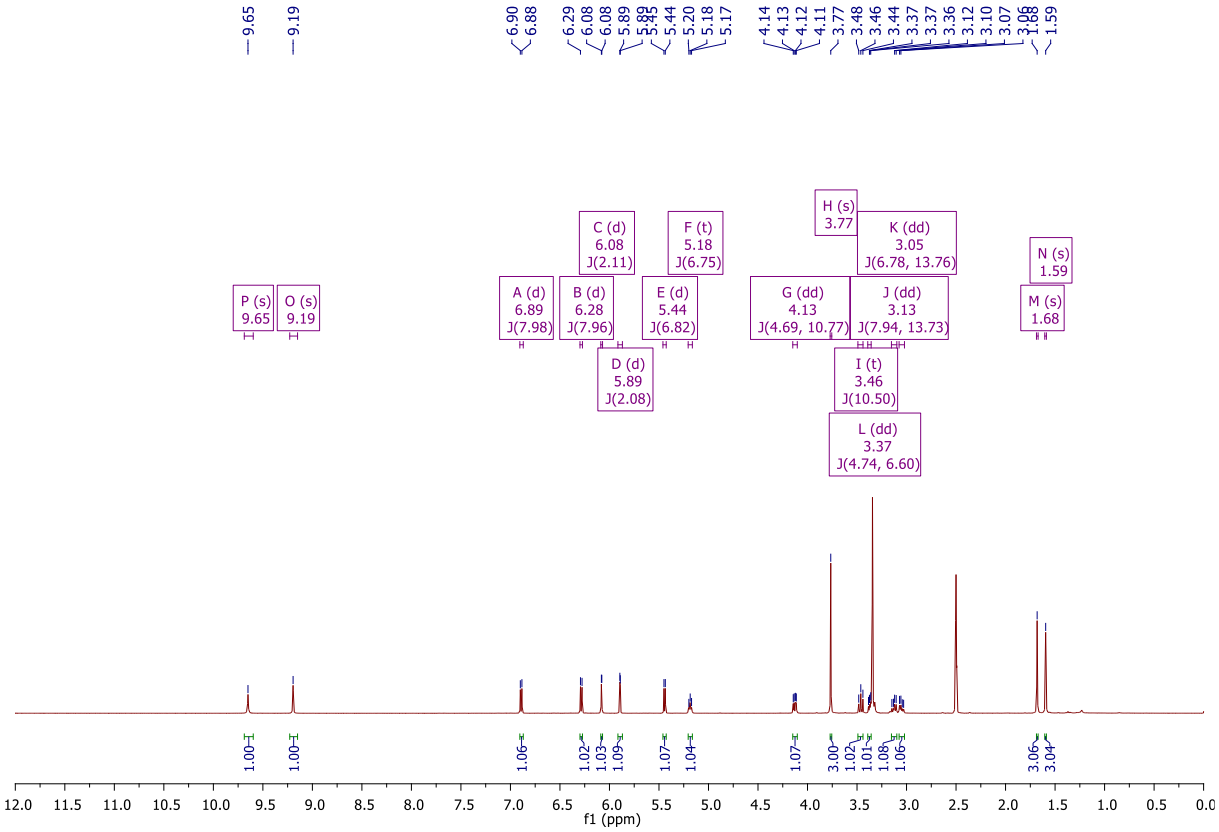


Figure S2: ^{1}H-NMR (500 MHz, DMSO-d_6) spectrum of **1** (lyratin D)

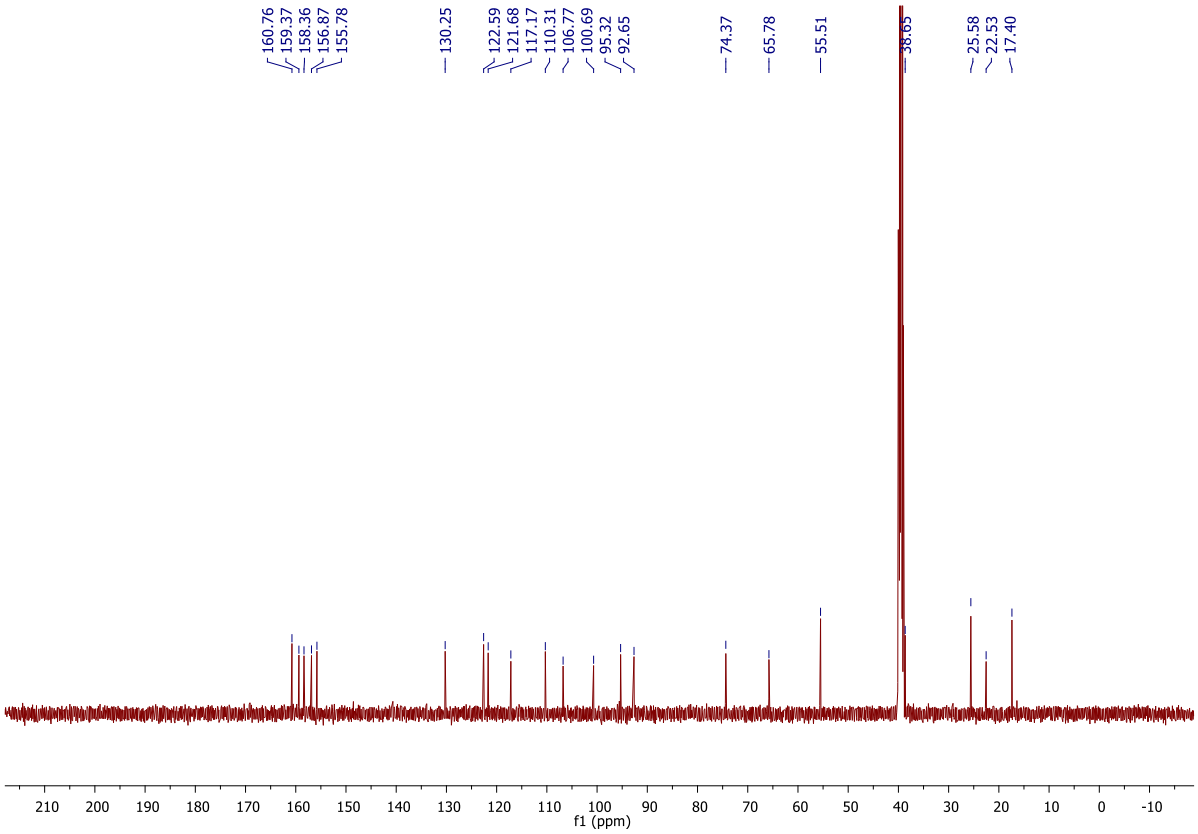


Figure S3: ^{13}C-NMR (125 MHz, DMSO-d_6) spectrum of **1** (lyratin D)

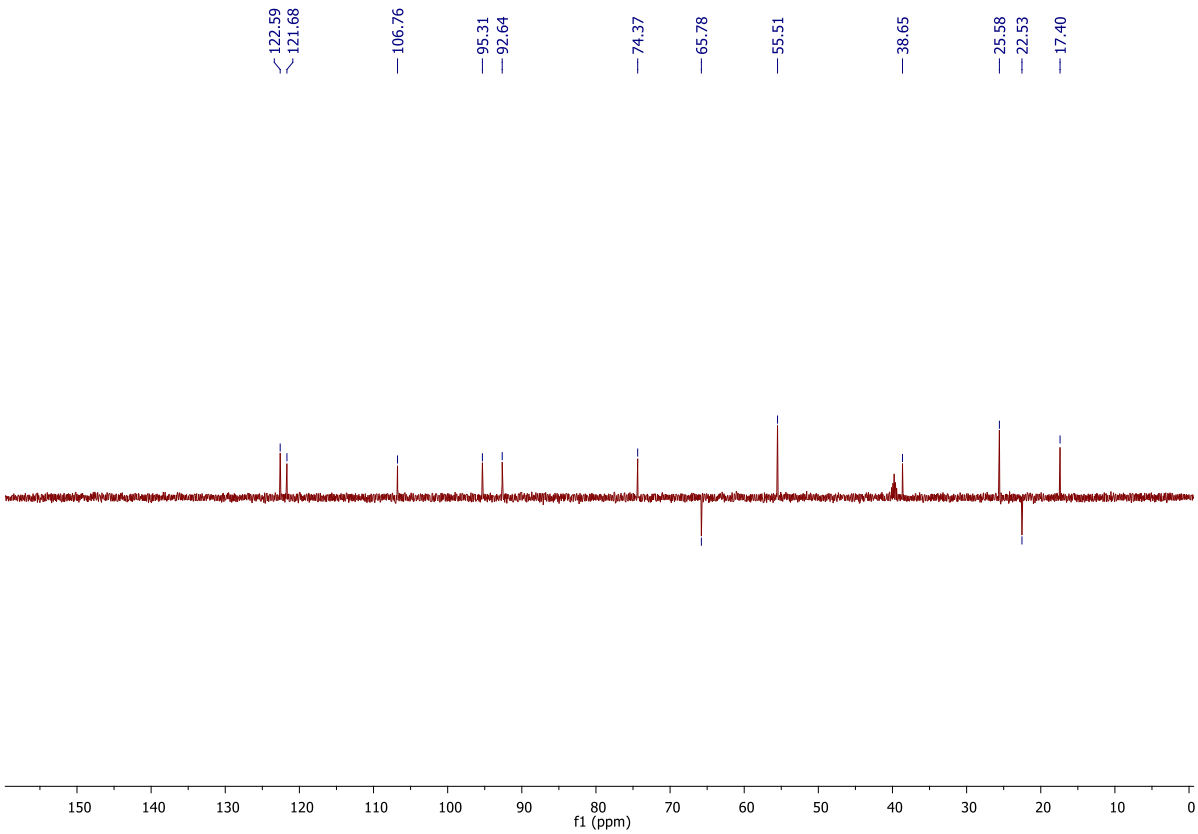


Figure S4: DEPT-135 (125 MHz, DMSO-d_6) spectrum of **1** (lyratin D)

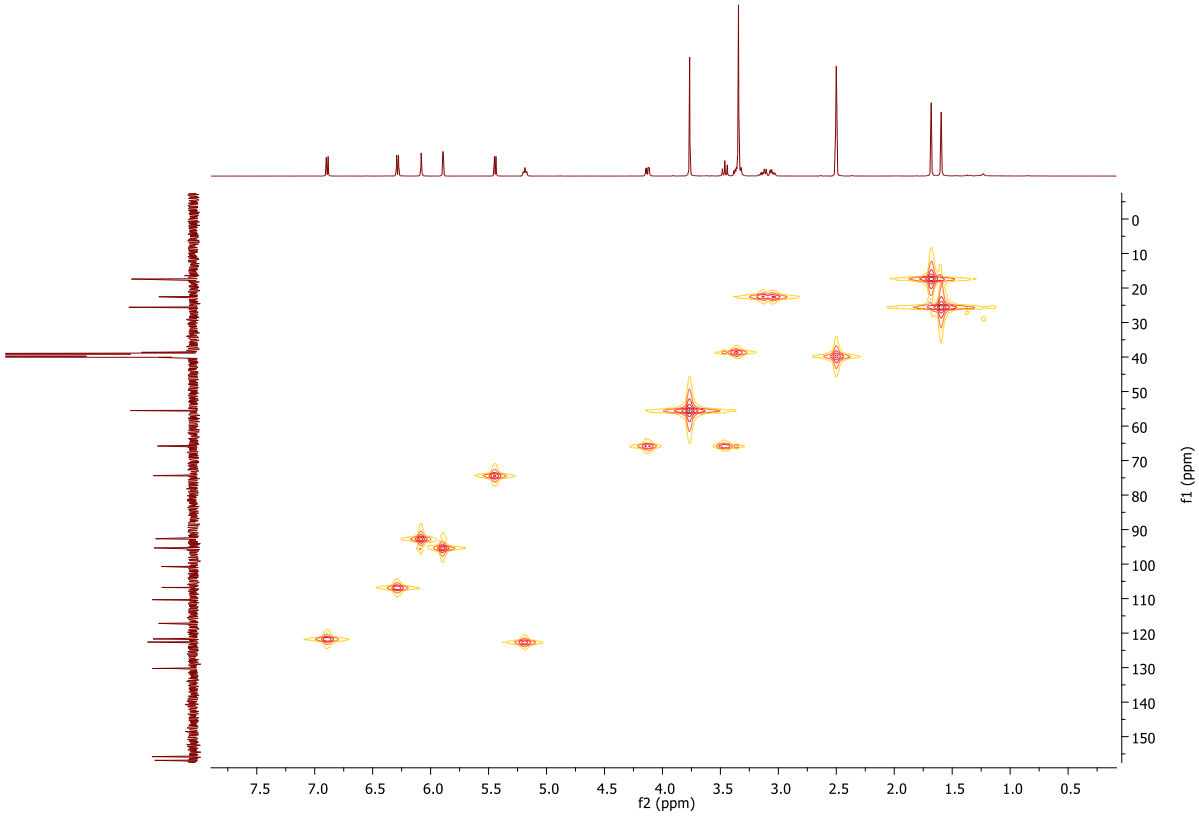


Figure S5: HMQC spectrum of **1** (lyratin D)

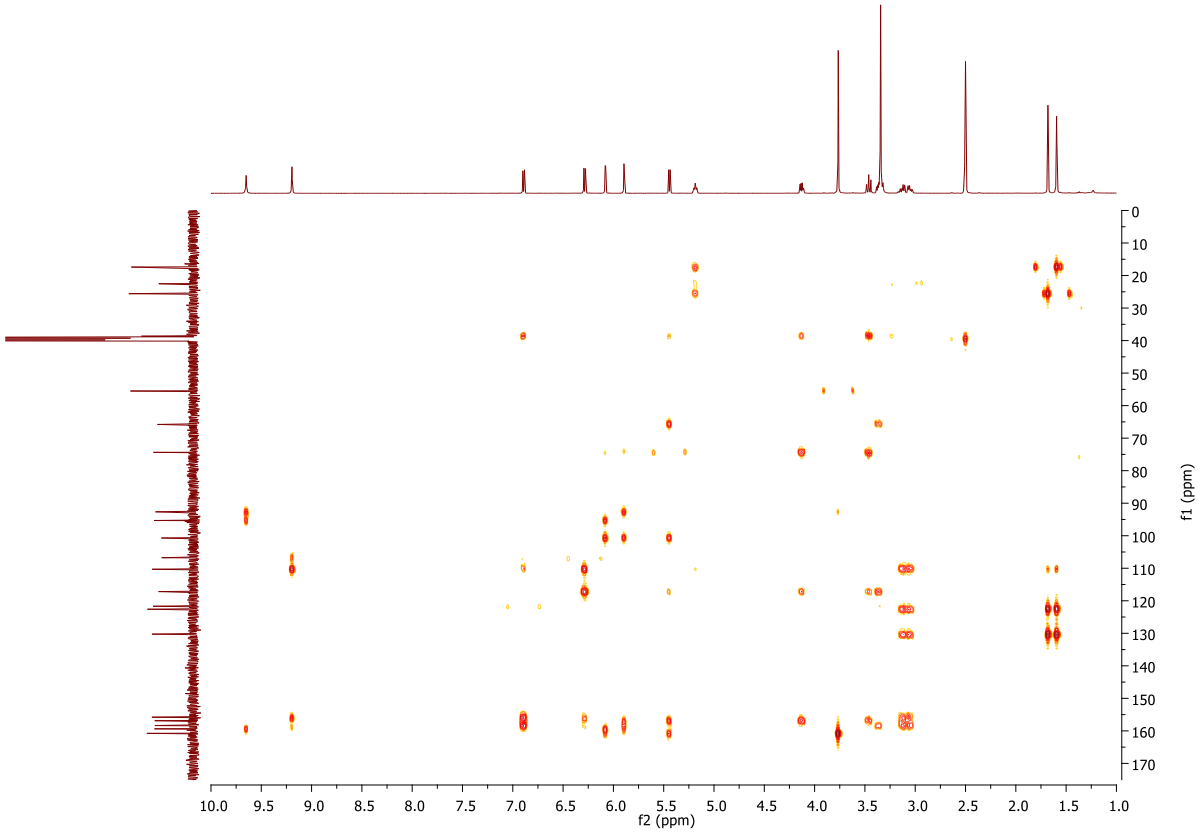


Figure S6: HMBC spectrum of **1** (lyratin D)

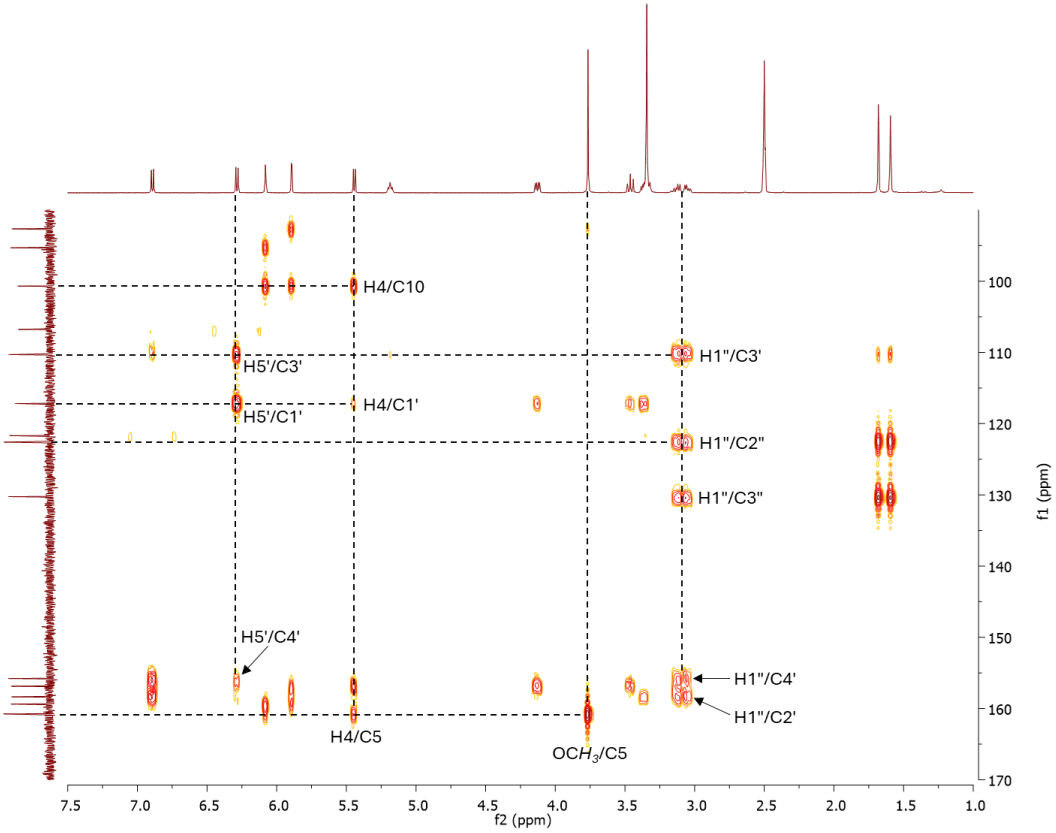


Figure S7: HMBC spectrum of **1** (lyratin D) (From δ_C 90 ppm to δ_C 170 ppm)

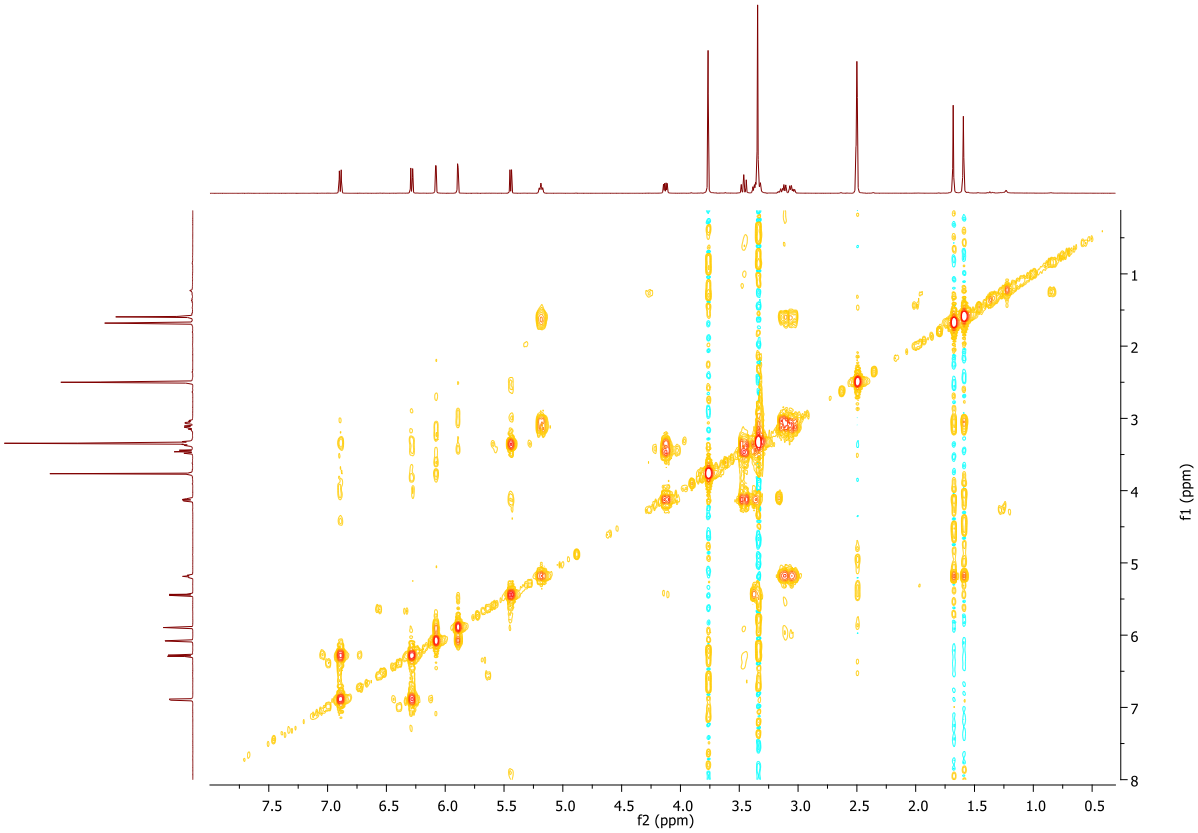


Figure S8: ^{1}H-^{1}H COSY spectrum of **1** (lyratin D)

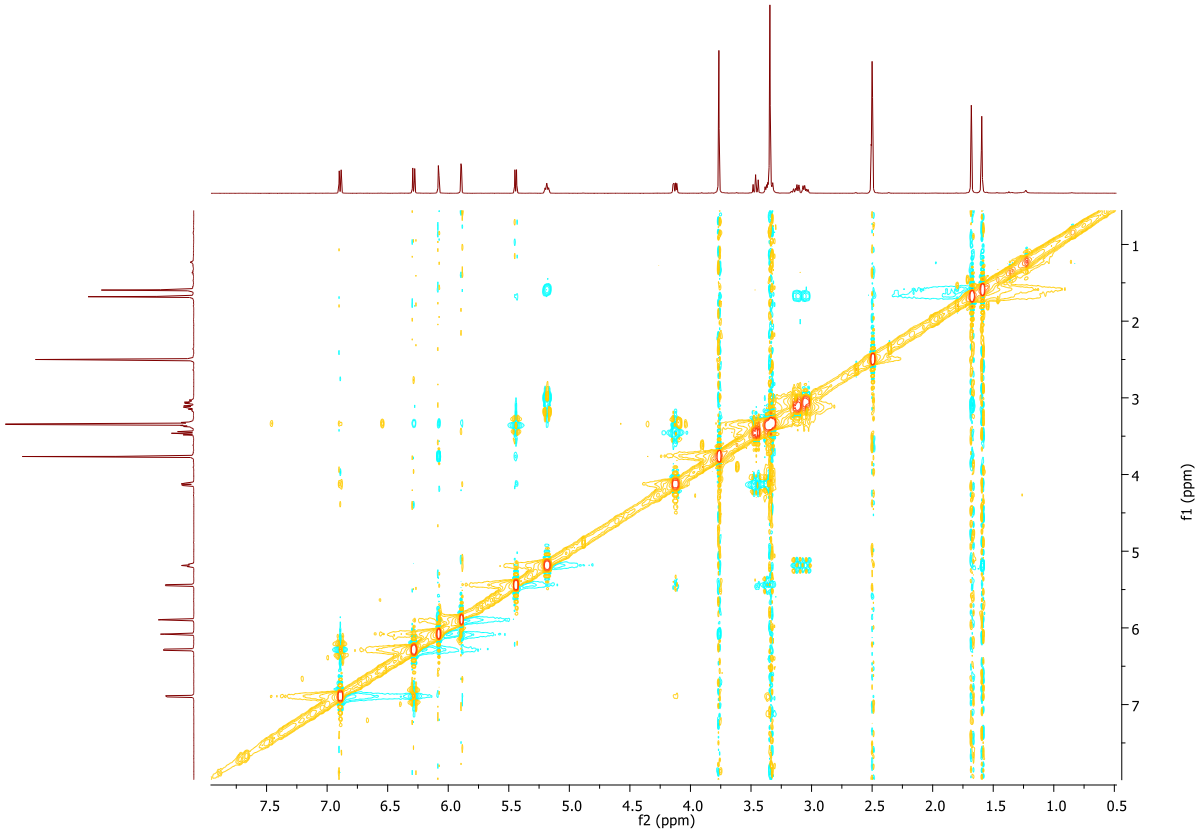


Figure S9: NOESY spectrum of **1** (lyratin D)

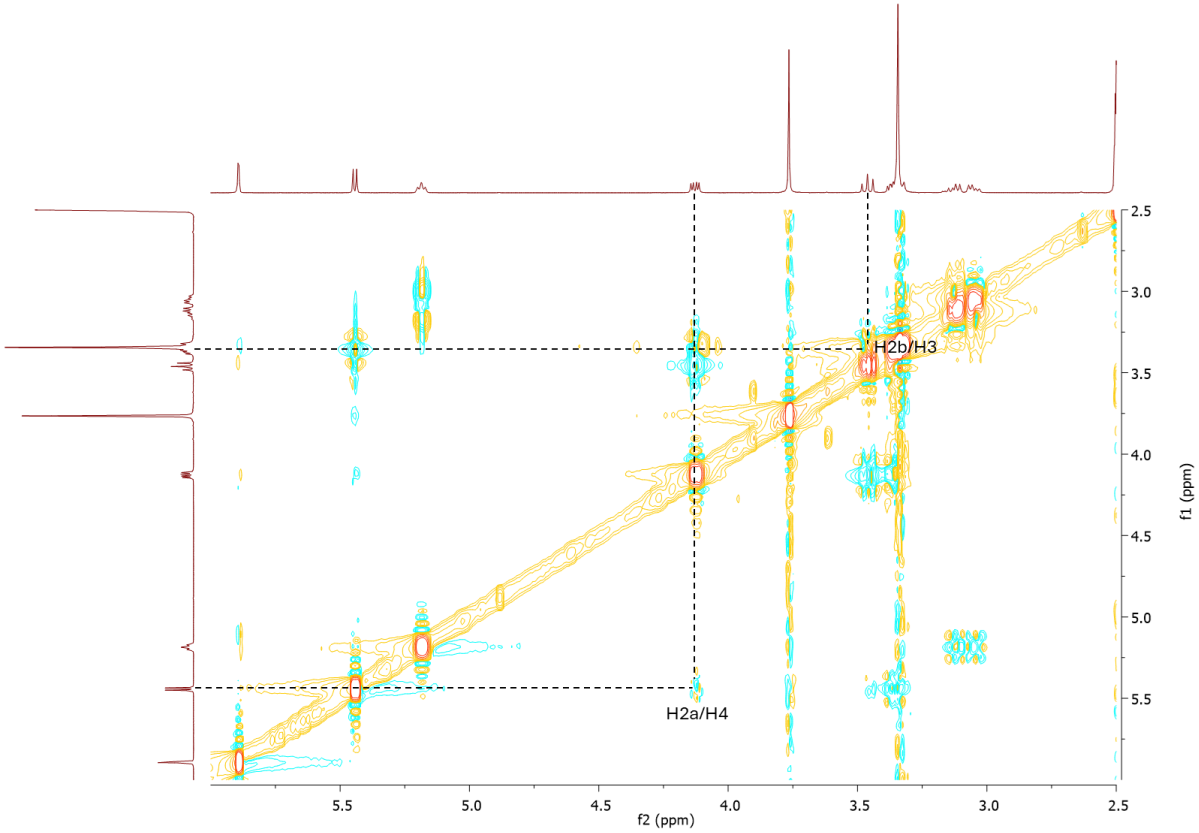


Figure S10: NOESY spectrum of **1** (lyratin D) (From δ_H 2.5 ppm to δ_H 6.0 ppm)

CAS SciFinder

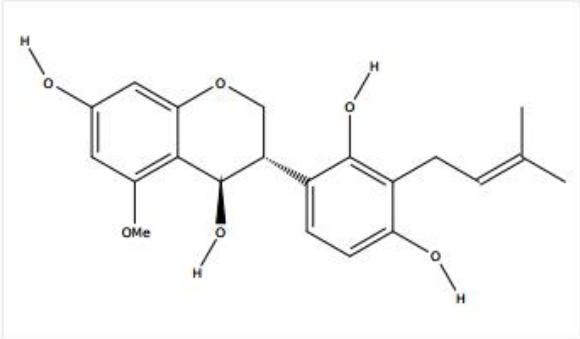
Task History

Initiating Search

July 11, 2024, 5:24 PM

Substances:

Filtered By:



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	Substances	View Results

CAS SciFinder

Substances (0)

View in CAS SciFinder

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

Substances with (0) results

Figure S11: Search report from SciFinder for **1** (lyratin D) (accessed on July 11, 2024)

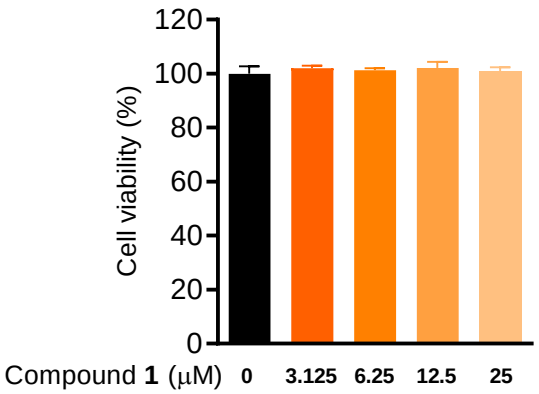


Figure S12: Cytotoxic effect of lyratin D (**1**) on RAW264.7 cells

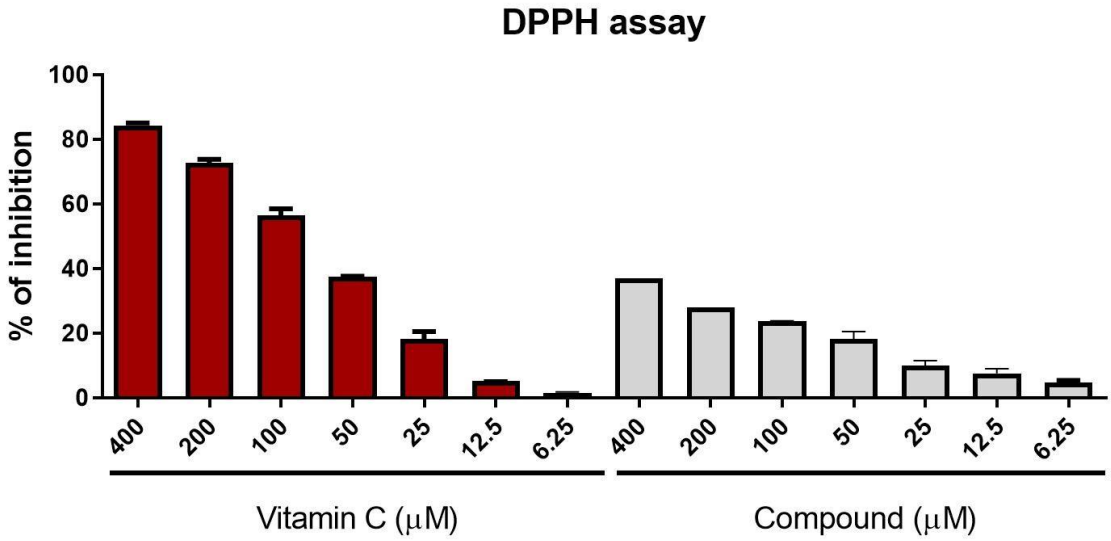
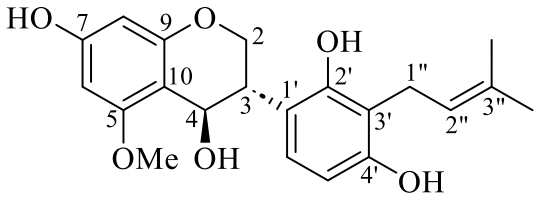
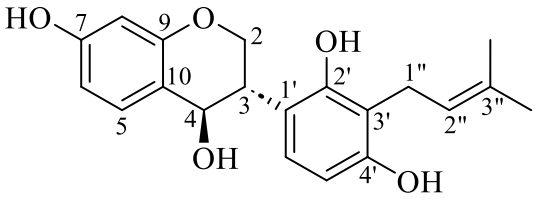


Figure S13: DPPH radical scavenging activity of lyratin D (**1**) and the positive control (vitamin C)

Table S1: NMR spectroscopic data (recorded in DMSO-d_6) for lyratin D (**1**) and lyratin A (δ in ppm).



Lyratin D (**1**)



Lyratin A

Position	Lyratin D (**1**)		Lyratin A [1]	
	δ_C, type[a]	δ_H (J in Hz)[b]	δ_C, type[c]	δ_H (J in Hz)[d]
2	65.8, CH_2	4.13, dd (10.5, 4.7)	65.8, CH_2	4.19, dd (11.0, 5.0)
		3.46, d (10.5)		3.57, dd (11.1, 11.0)
3	38.7, CH	3.37, dd (6.8, 4.7)	39.3, CH	3.52, m
4	74.4, CH	5.44, d (6.8)	77.4, CH	5.45, d (6.6)
5	160.8, C	–	132.0, CH	7.25, d (8.4)
6	92.6, CH	6.08, d (2.1)	109.6, CH	6.48, dd (8.4, 2.0)
7	159.4, C	–	158.6, C	–
8	95.3, CH	5.89, d (2.1)	102.3, CH	6.25, d (2.0)
9	156.9, C	–	156.2, C	–
10	100.7, C	–	111.6, C	–
1′	117.2, C	–	117.2, C	–
2′	158.4, C	–	158.2, C	–
3′	110.3, C	–	110.4, C	–
4′	155.8, C	–	155.8, C	–
5′	106.8, CH	6.28, d (8.0)	107.0, CH	6.32, d (8.0)
6′	121.7, CH	6.89, d (8.0)	121.7, CH	6.92, d (8.0)
1″	22.5, CH_2	3.13, dd (13.7, 8.0)	22.4, CH_2	3.12, d (6.9, 2H)
		3.05, dd (13.7, 6.8)		
2″	122.6, CH	5.18, t (6.8)	122.6, CH	5.15, t (6.9)
3″	130.3, C	–	130.0, C	–
4″	17.4, CH_3	1.68, s	17.6, CH_3	1.67, s
5″	25.6, CH_3	1.59, s	25.4, CH_3	1.59, s
5-OMe	55.5, CH_3	3.77, s		
7-OH		9.65, br s		9.59, br s
4′-OH		9.19, br s		9.21, br s

The assignments were based on DEPT, HMQC and HMBC experiments.

[a] 125 MHz.

[b] 500 MHz.

[c] 100 MHz.

[d] 400 MHz.

[1] D.-W. Zhang, G.-H. Li, Q.-Y. Yu and S.-J. Dai (2010). New anti-inflammatory 4-hydroxyisoflavans from *Solanum lyratum*, *Chem. Pharm. Bull.* **58**, 840-842.