

## Supporting Information

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

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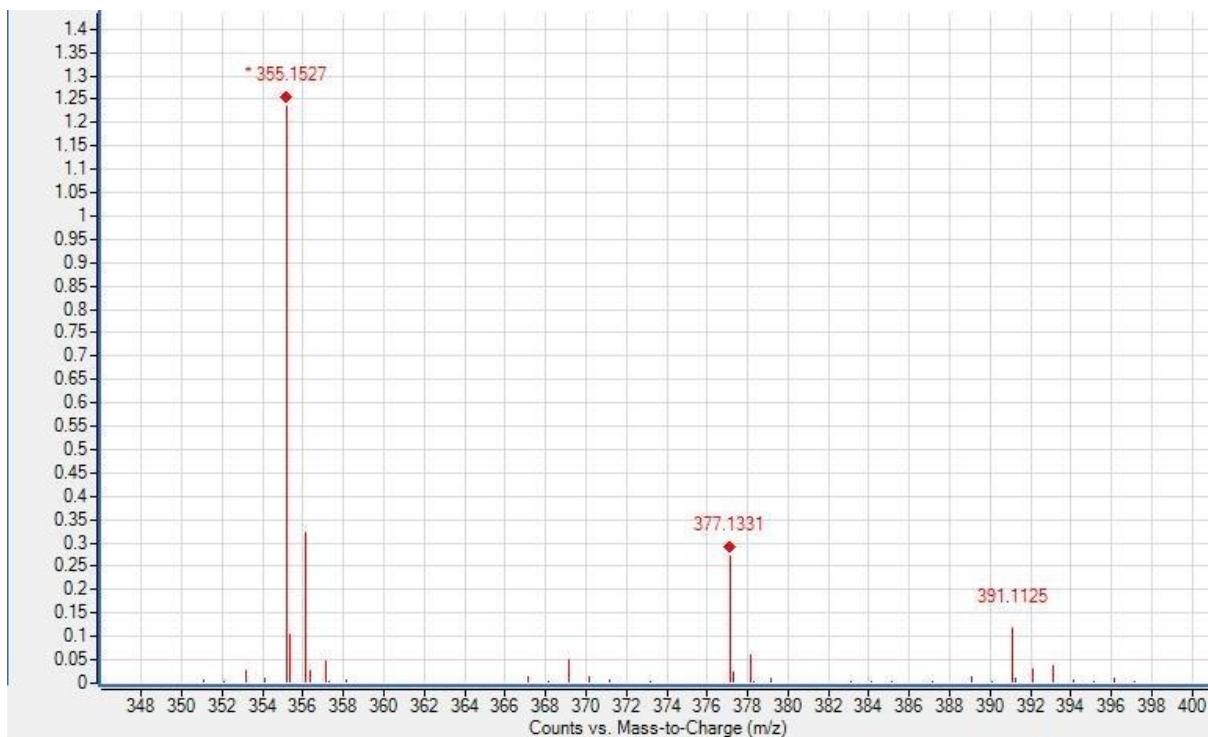
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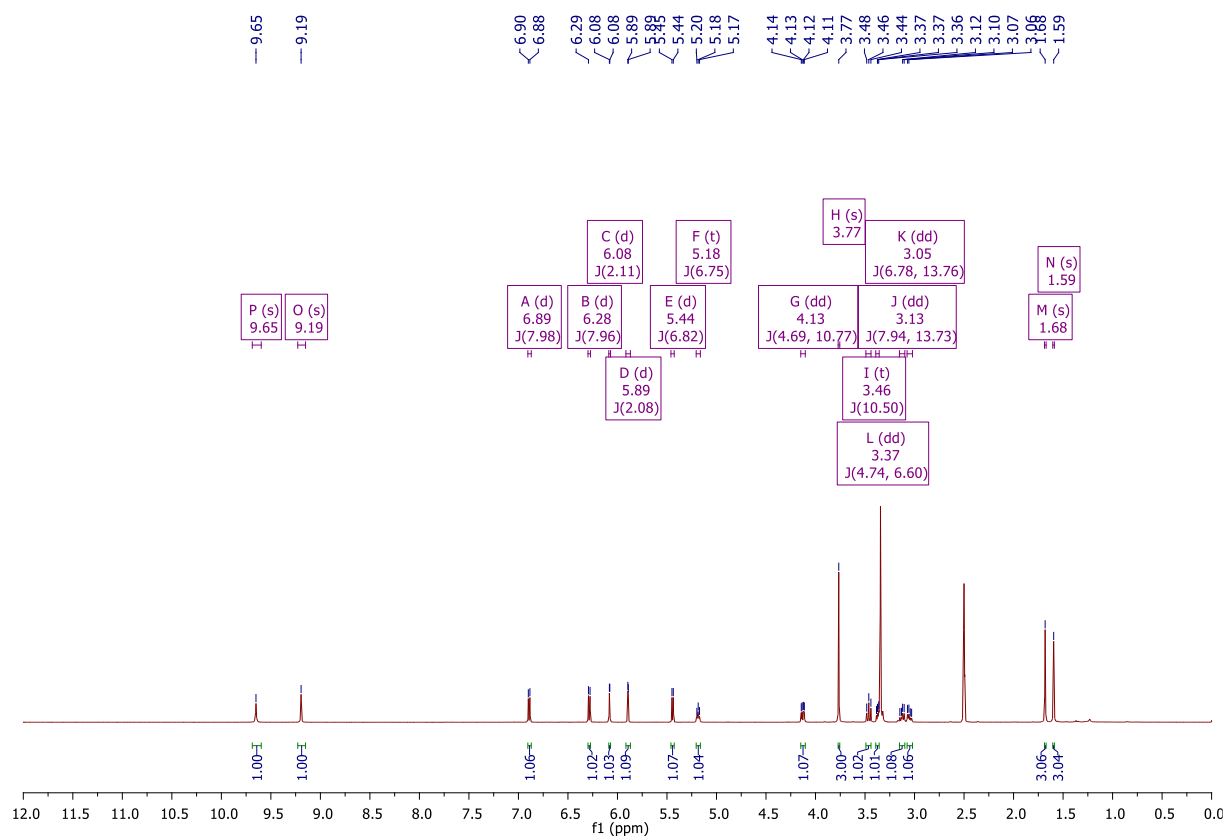
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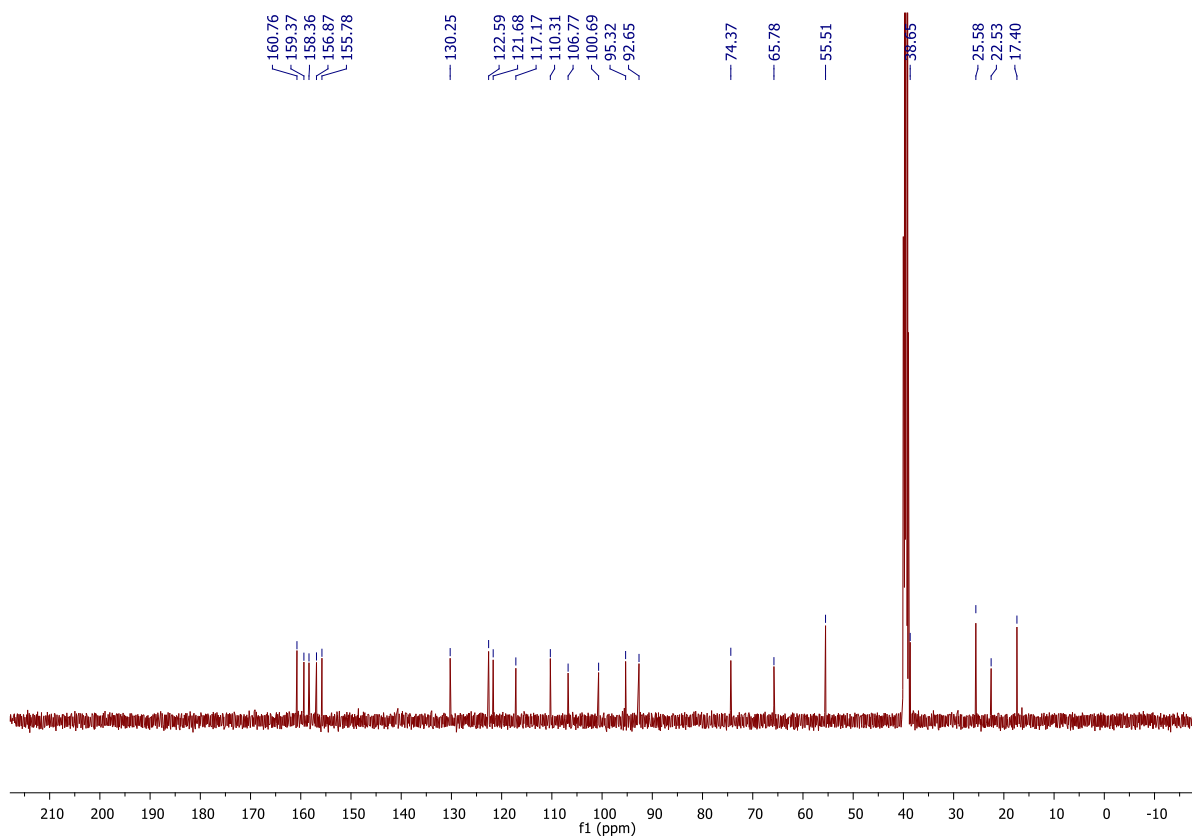
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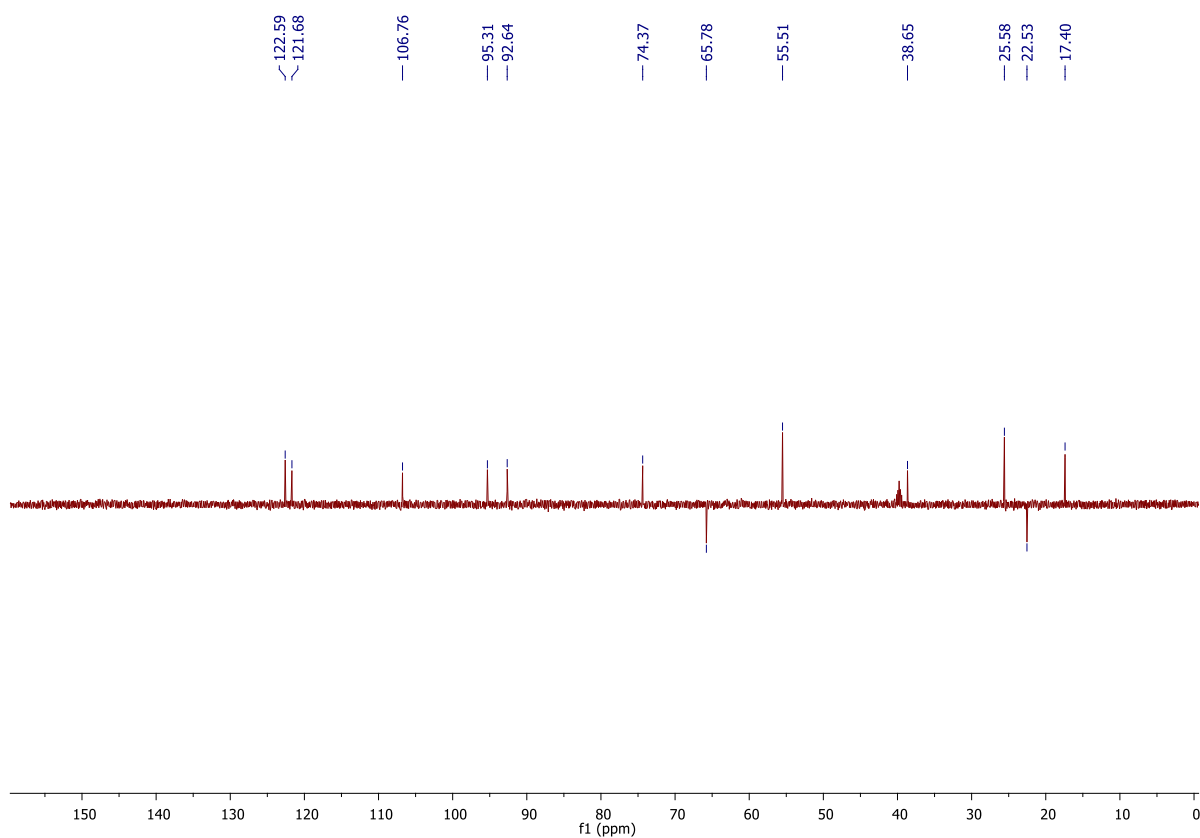
**Figure S1:** HR-ESI-MS spectrum of **1** (lyratin D)



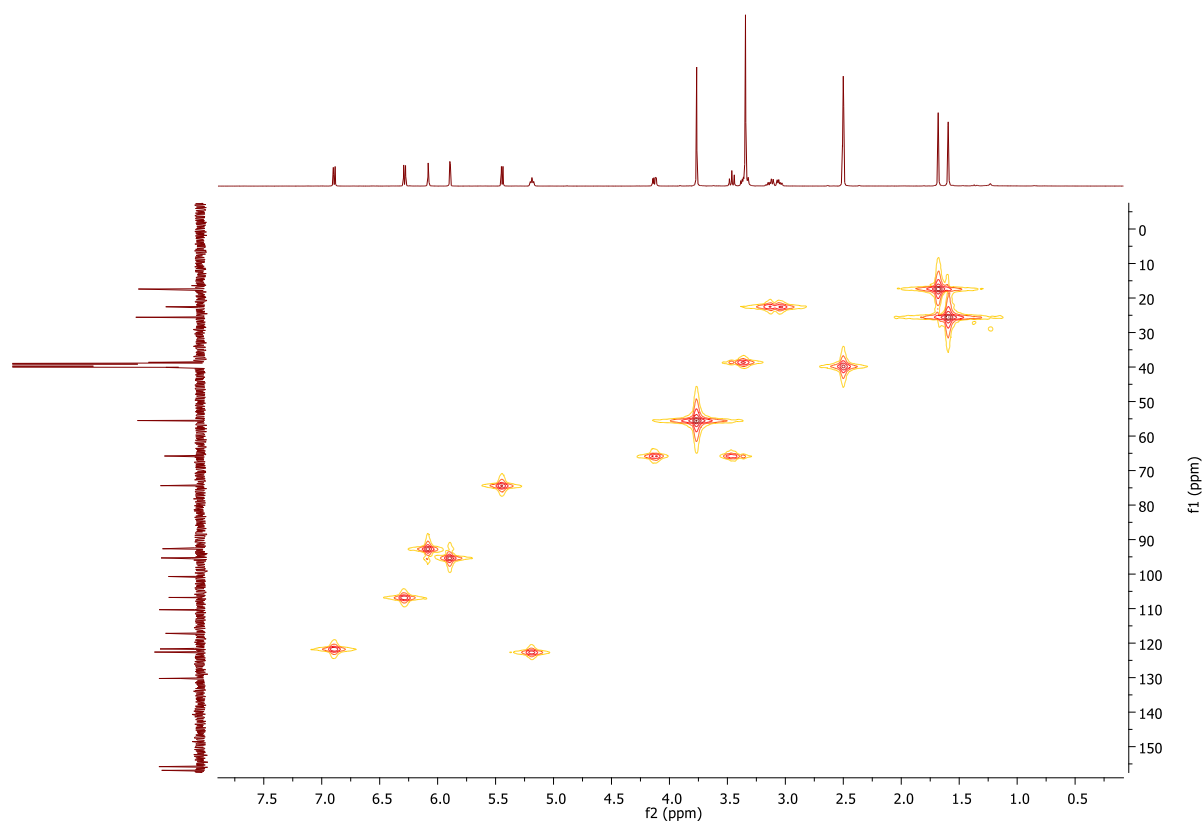
**Figure S2:**  $^1\text{H-NMR}$  (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of **1** (lyratin D)



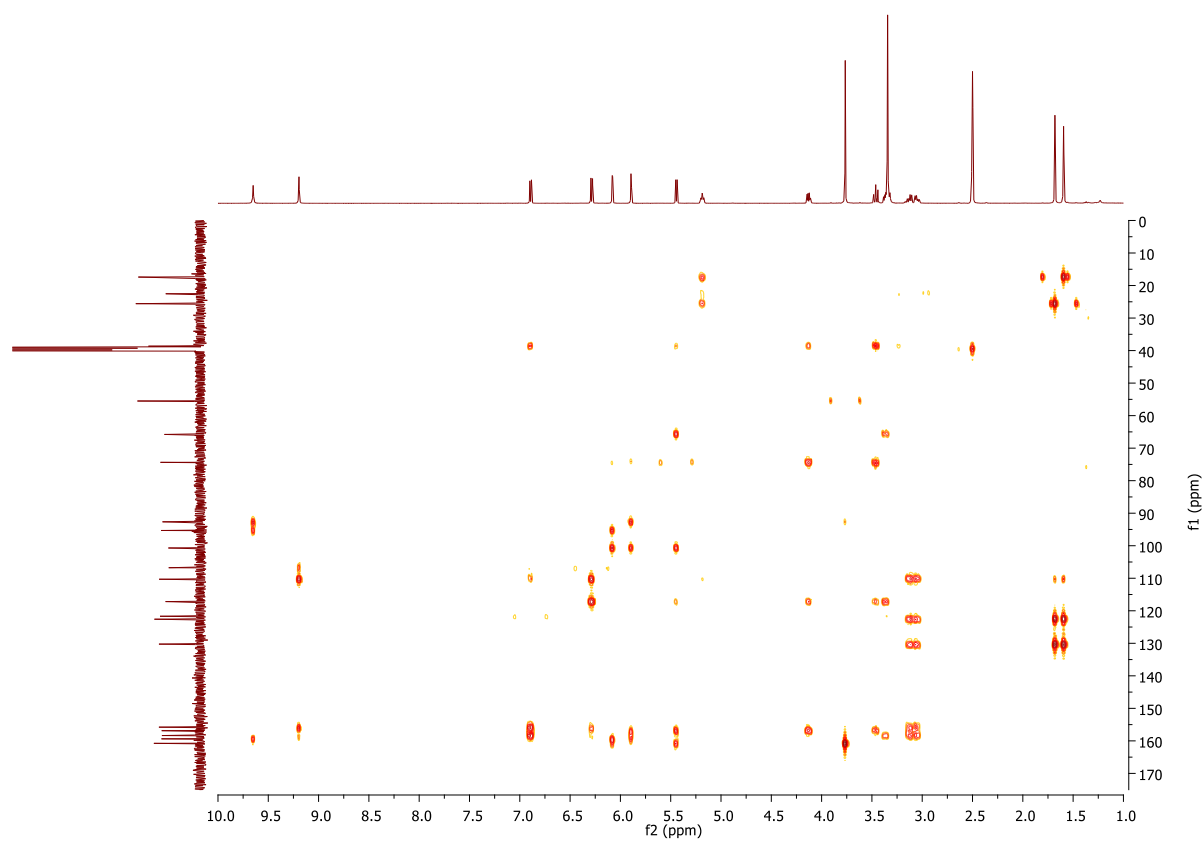
**Figure S3:**  $^{13}\text{C}$ -NMR (125 MHz,  $\text{DMSO-}d_6$ ) spectrum of **1** (lyratin D)



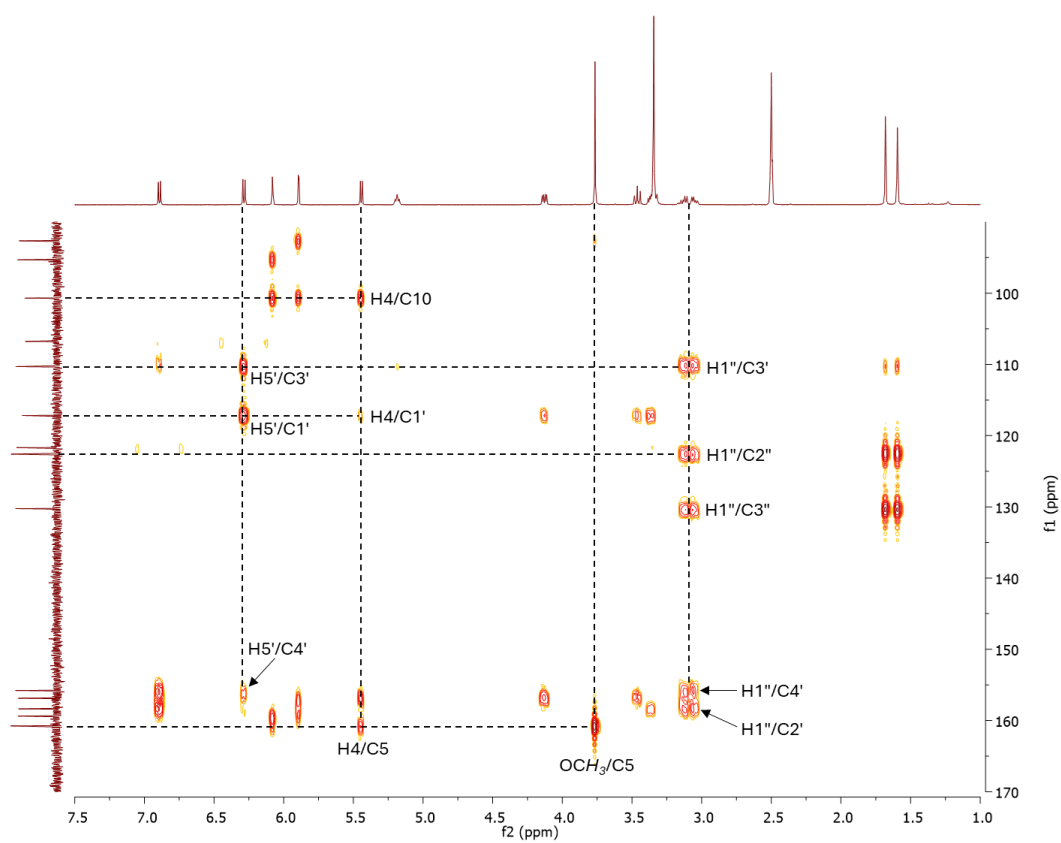
**Figure S4:** DEPT-135 (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of **1** (lyratin D)



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

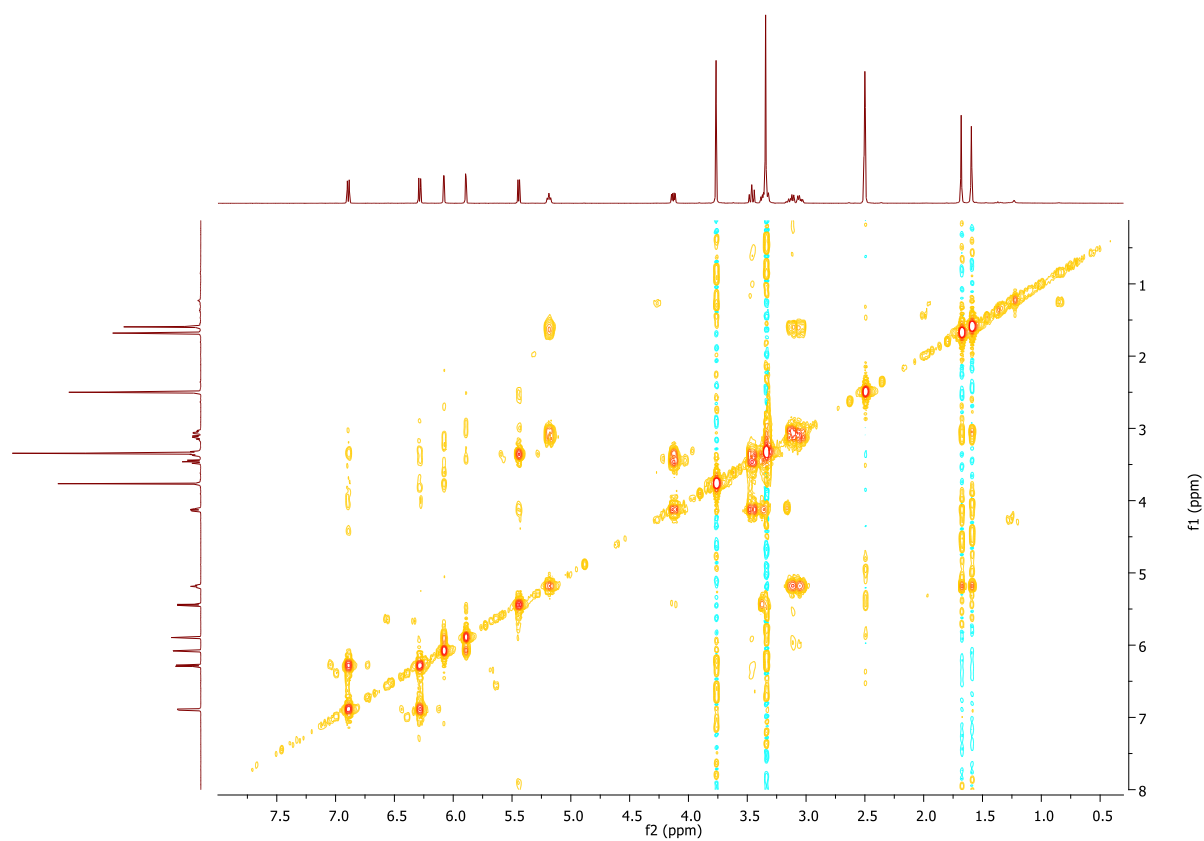


**Figure S6:** HMBC spectrum of **1** (lyratin D)

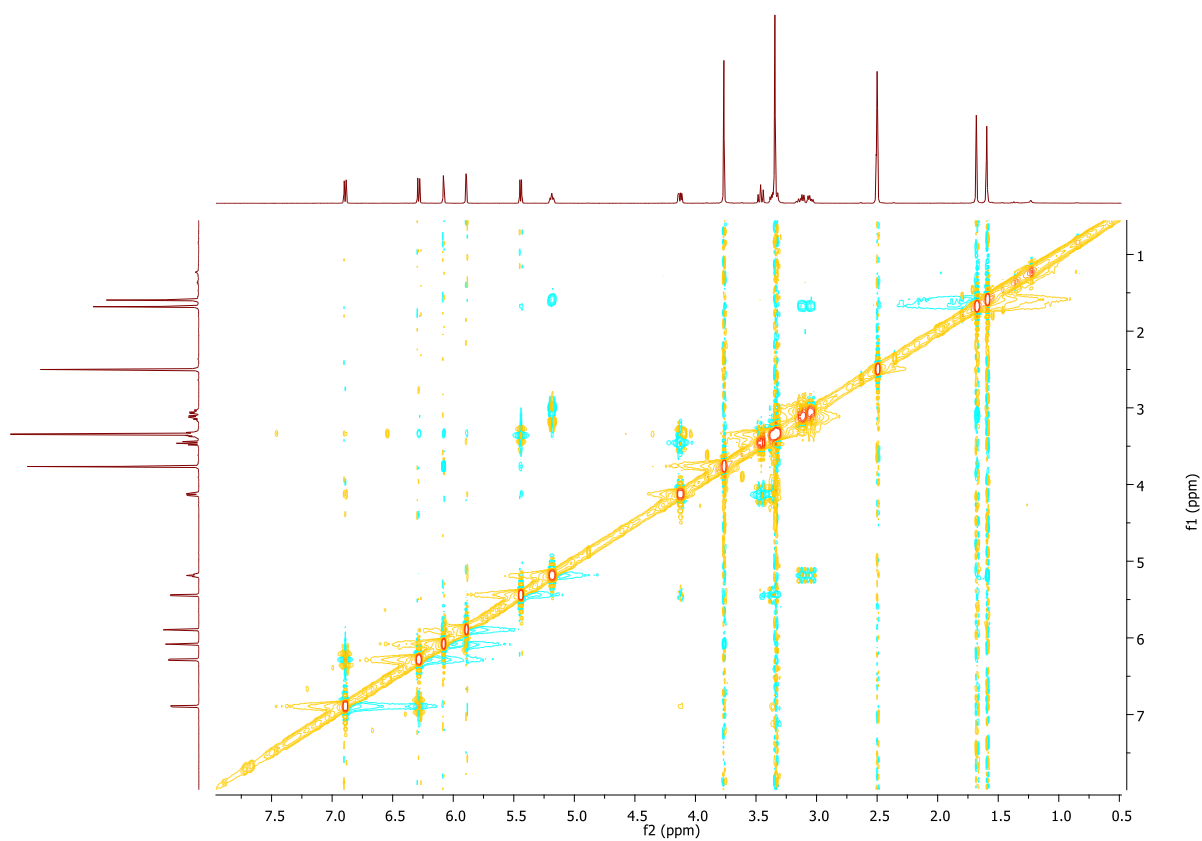


**Figure S7:** HMBC spectrum of **1** (lyratin D) (From  $\delta_C$  90 ppm to  $\delta_C$  170 ppm)

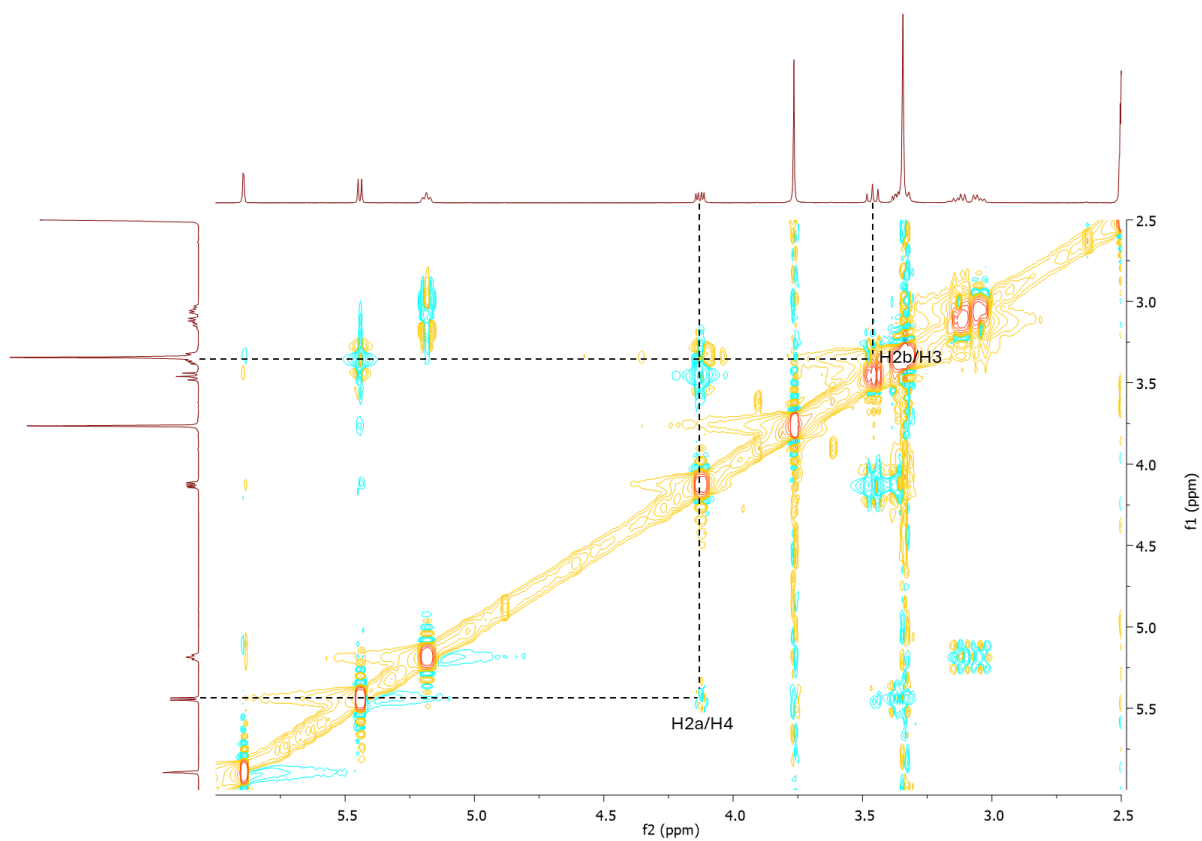




**Figure S8:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (lyratin D)



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



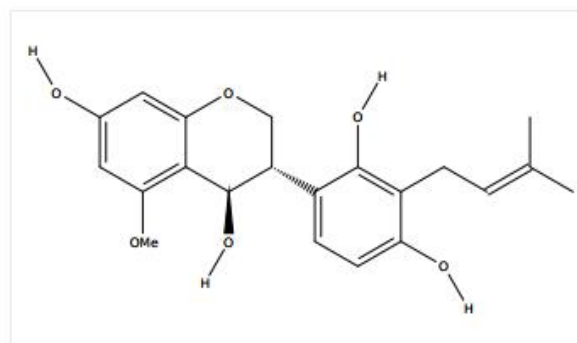
**Figure S10:** NOESY spectrum of **1** (lyratin D) (From  $\delta_{\text{H}}$  2.5 ppm to  $\delta_{\text{H}}$  6.0 ppm)

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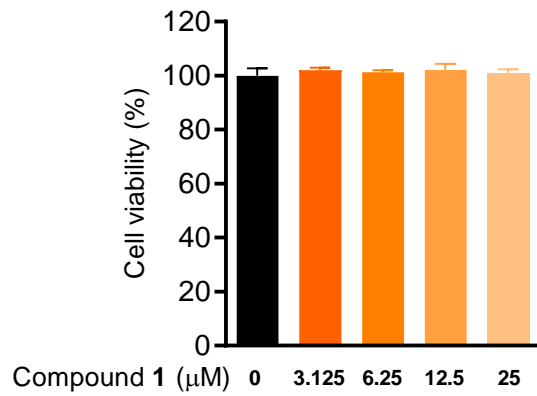
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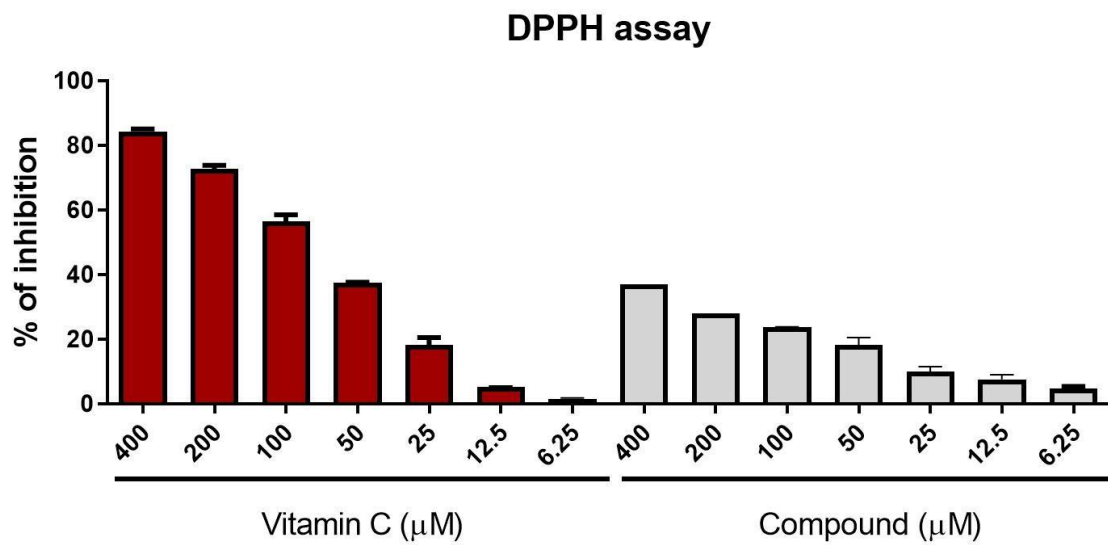
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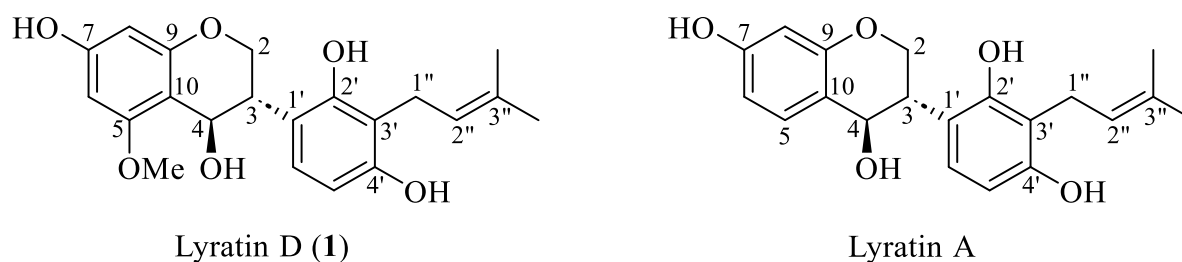
**Figure S11:** Search report from SciFinder for **1** (lyratin D) (accessed on July 11, 2024)



**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*<sub>6</sub>) for lyratin D (**1**) and lyratin A ( $\delta$  in ppm).

Position	Lyratin D ( <b>1</b> )		Lyratin A [1]	
	$\delta_C$ , type <sup>a</sup>	$\delta_H$ ( <i>J</i> in Hz) <sup>b</sup>	$\delta_C$ , type <sup>c</sup>	$\delta_H$ ( <i>J</i> in Hz) <sup>d</sup>
2	65.8, CH <sub>2</sub>	4.13, dd (10.5, 4.7) 3.46, d (10.5)	65.8, CH <sub>2</sub>	4.19, dd (11.0, 5.0) 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 <sub>2</sub>	3.13, dd (13.7, 8.0) 3.05, dd (13.7, 6.8)	22.4, CH <sub>2</sub>	3.12, d (6.9, 2H)
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 <sub>3</sub>	1.68, s	17.6, CH <sub>3</sub>	1.67, s
5''	25.6, CH <sub>3</sub>	1.59, s	25.4, CH <sub>3</sub>	1.59, s
5-OMe	55.5, CH <sub>3</sub>	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.

<sup>a</sup> 125 MHz.

<sup>b</sup> 500 MHz.

<sup>c</sup> 100 MHz.

<sup>d</sup> 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.