

## Supplementary Data

*Rec. Nat. Prod.* 16:4 (2022) 393-397

### A New Iridoid Glycoside Isolated from *Valeriana officinalis* L.

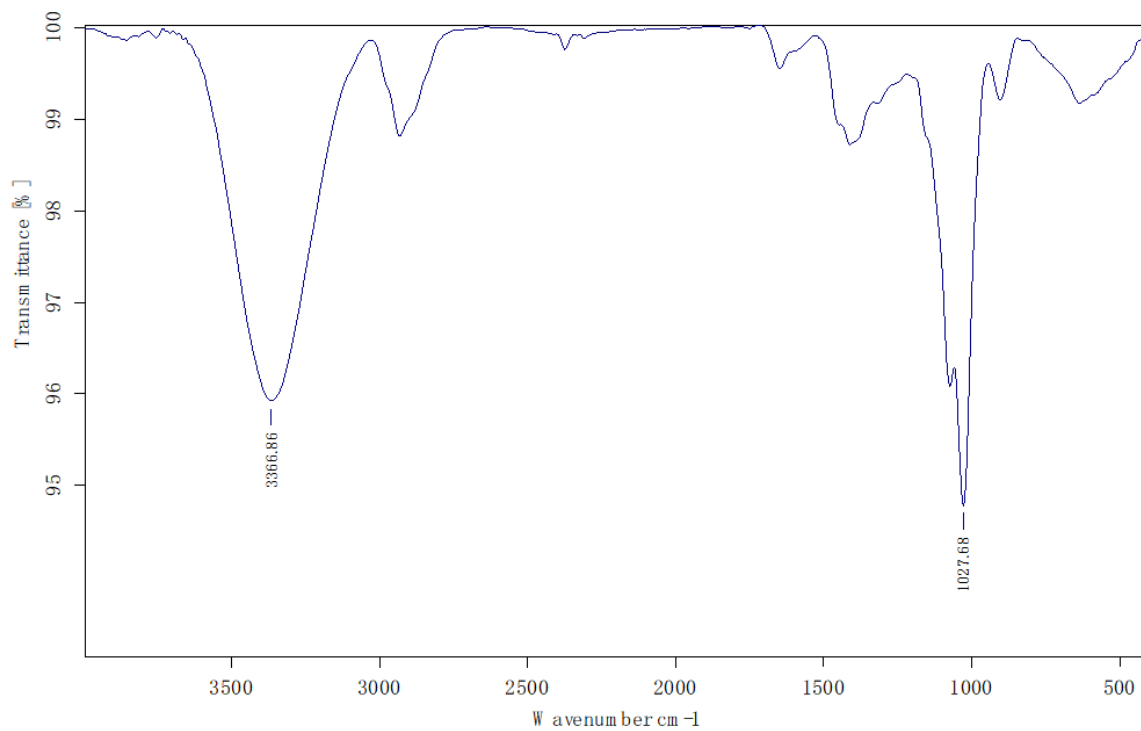
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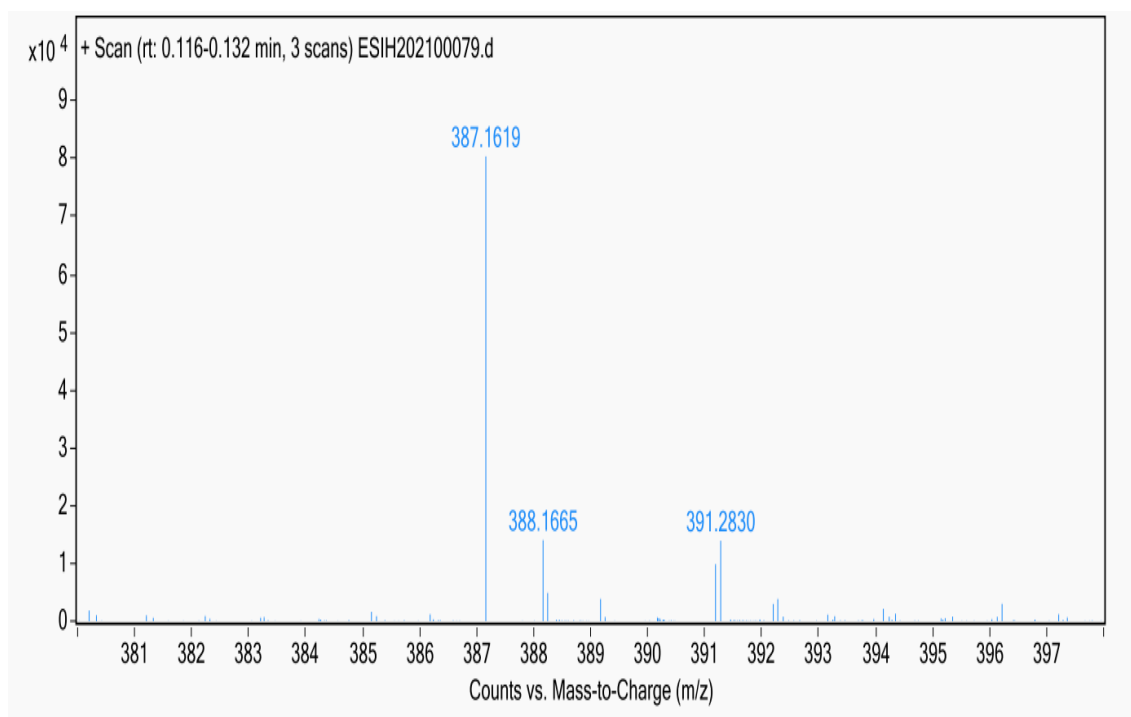
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<sup>#</sup>These authors contributed equally to this work

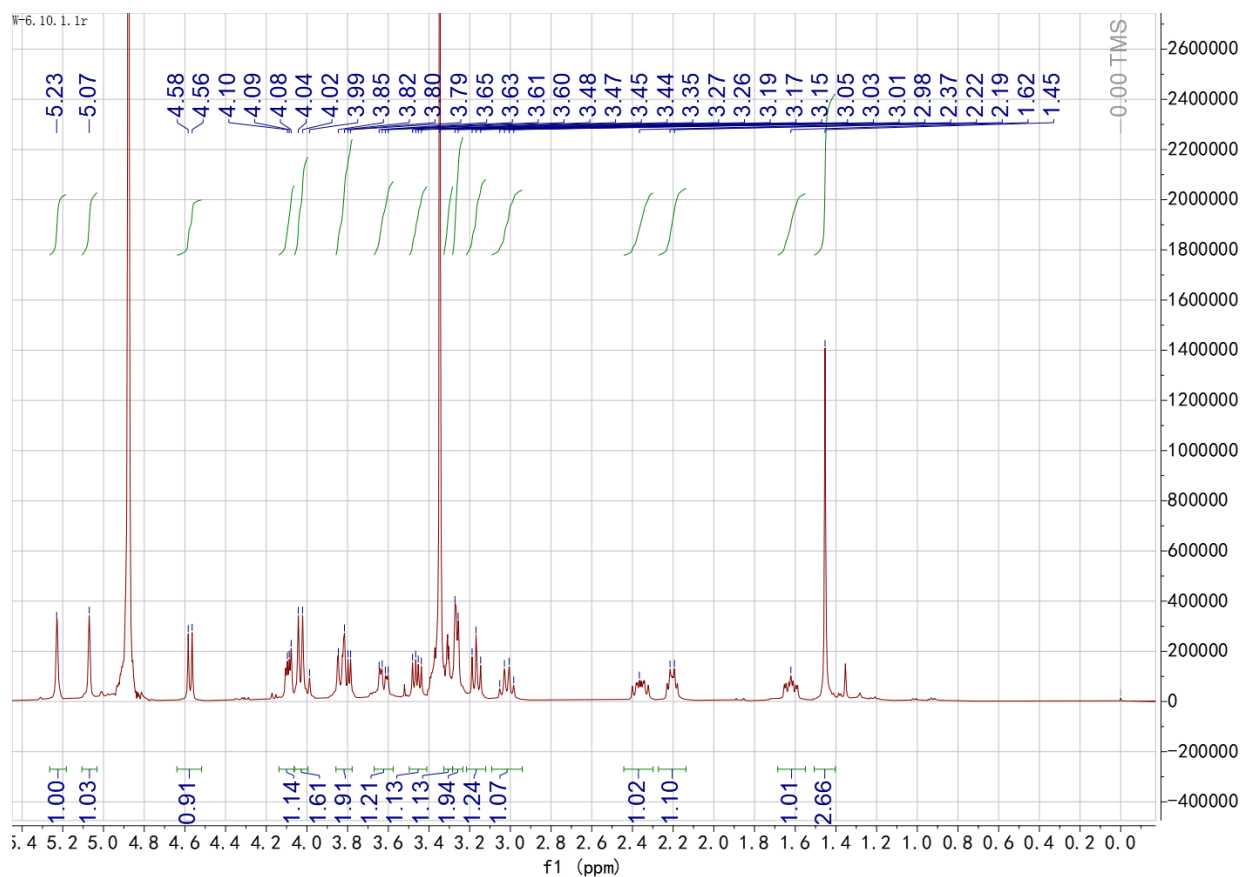
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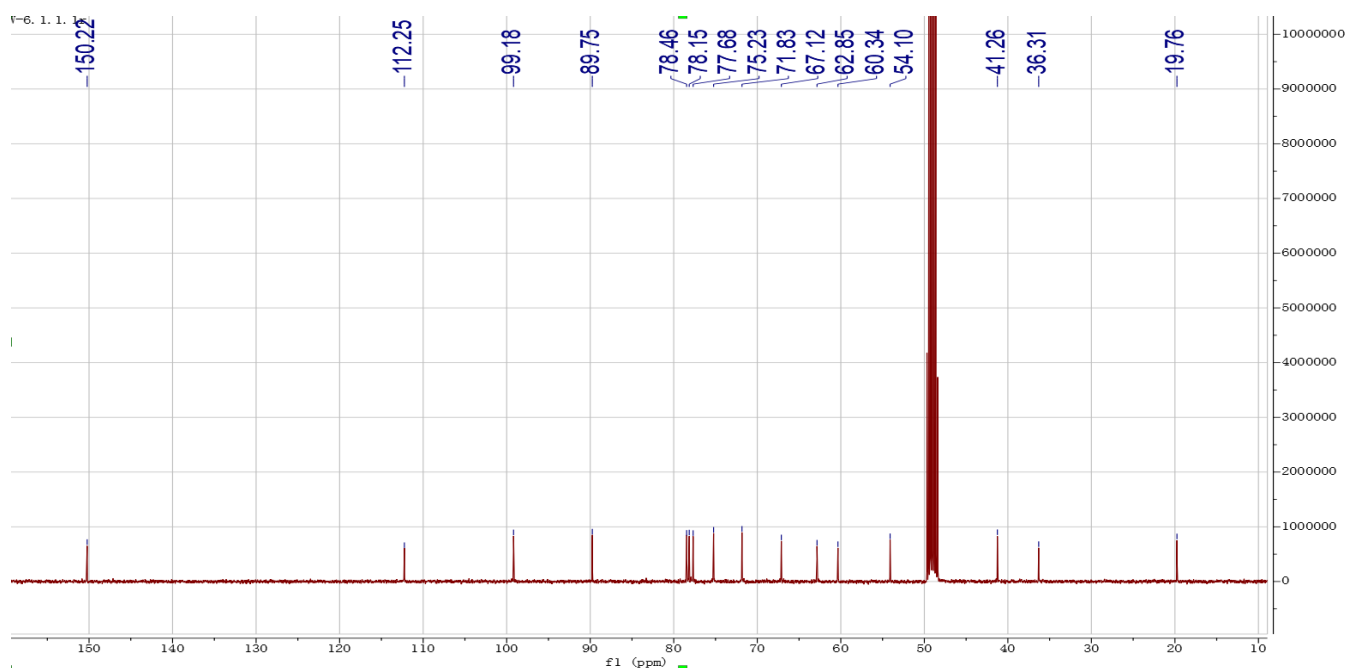
**Figure S1:** The IR spectrum of **1** (in KBr)



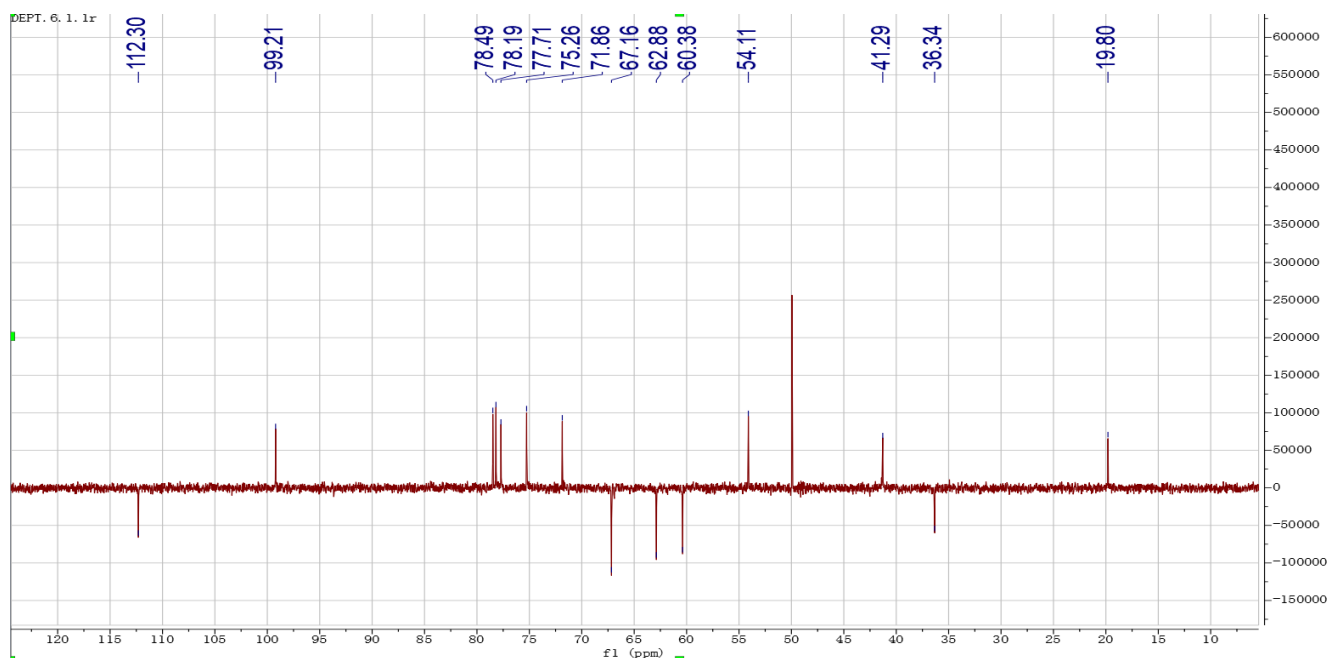
**Figure S2:** The HR-ESI-MS spectrum of **1** (in MeOH)



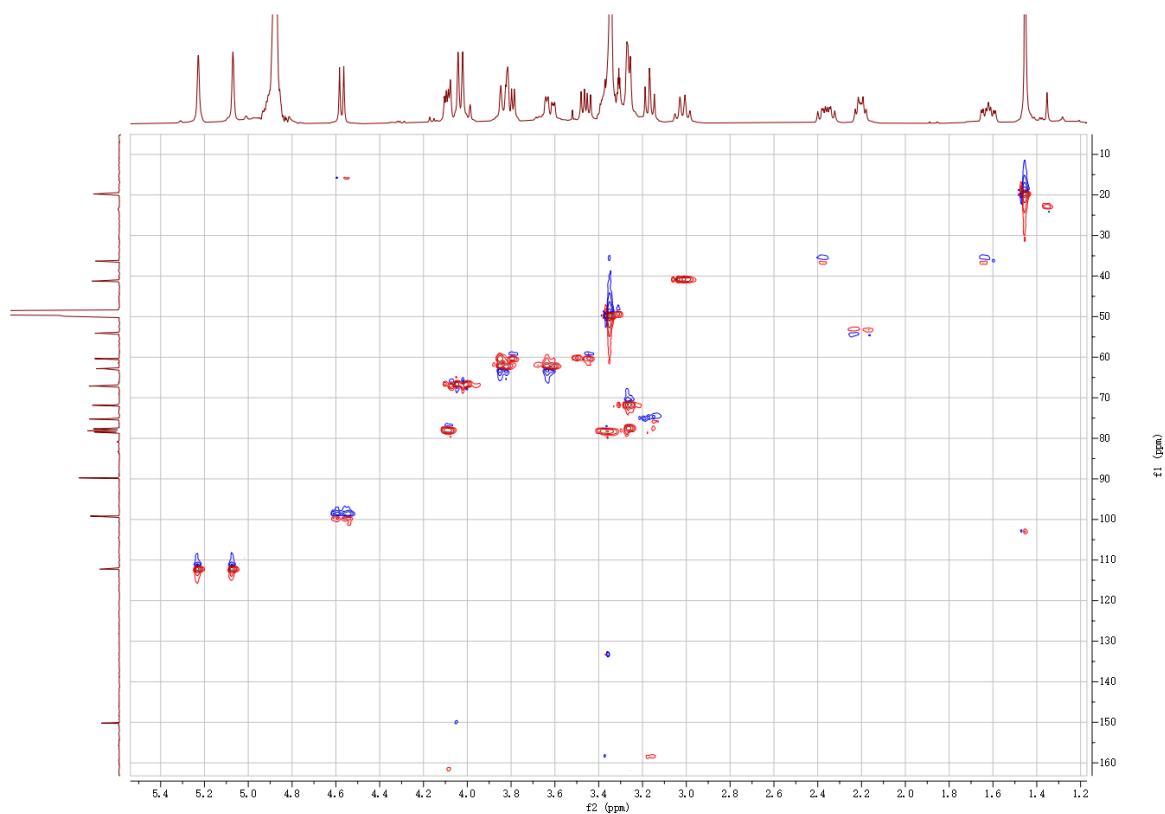
**Figure S3:** The  $^1\text{H}$  NMR spectrum of **1** (in MeOD)



**Figure S4:** The  $^{13}\text{C}$  NMR spectrum of **1** (in MeOD)



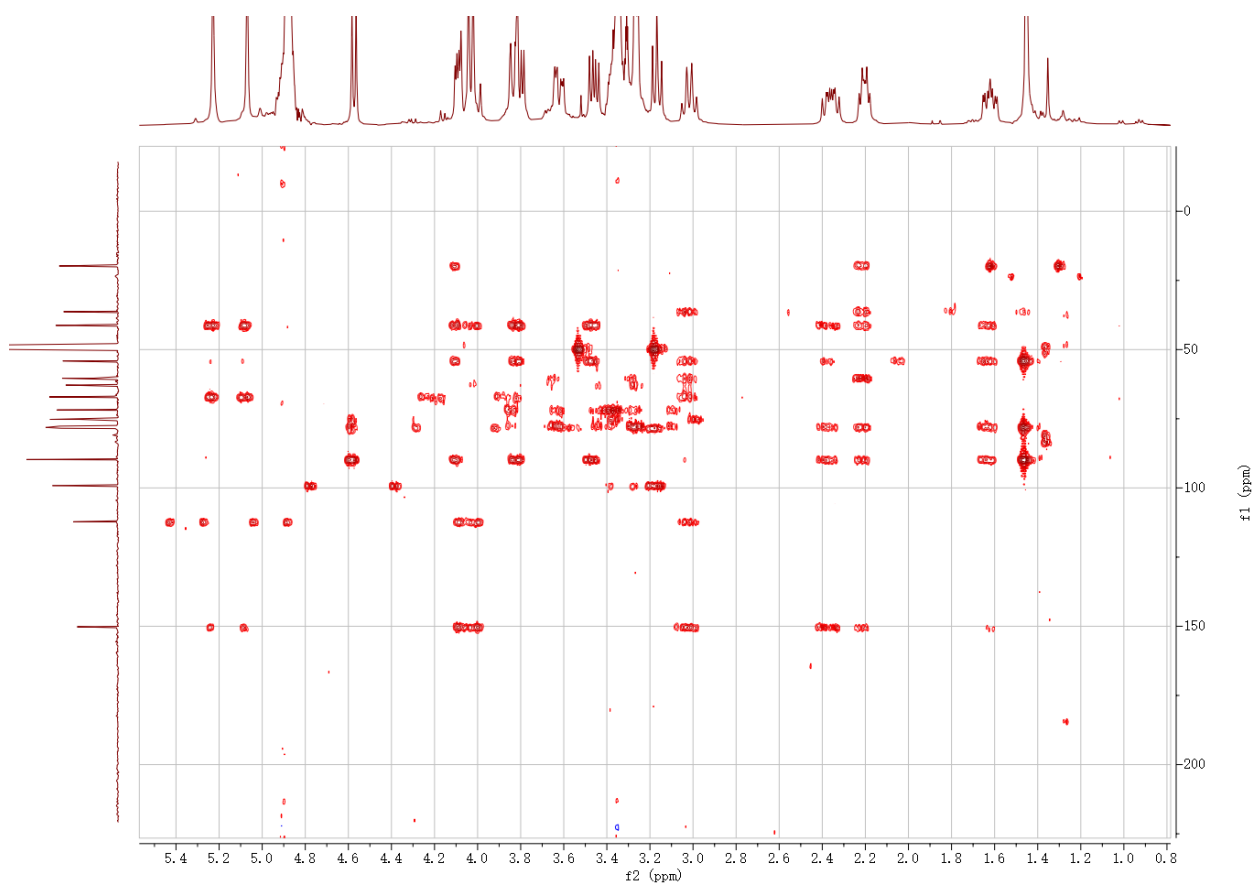
**Figure S5:** The DEPT spectrum of **1** (in MeOD)



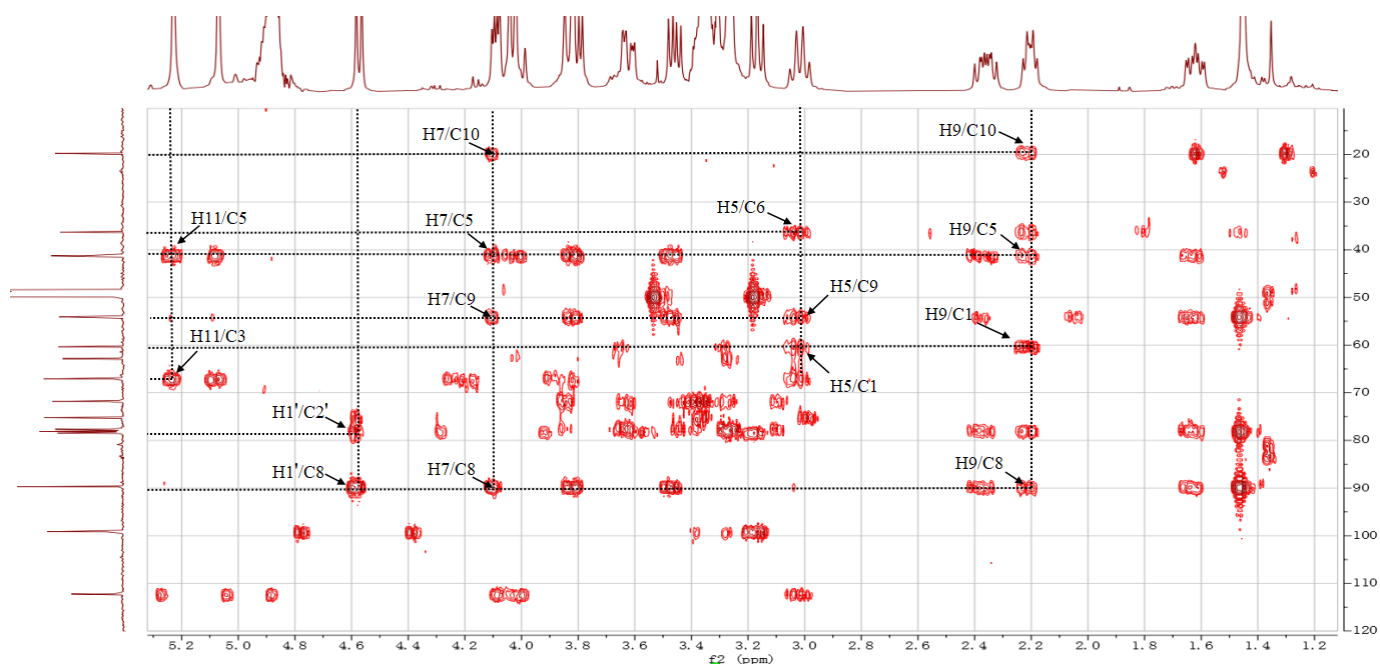
**Figure S6:** The HSQC spectrum of **1** (in MeOD)



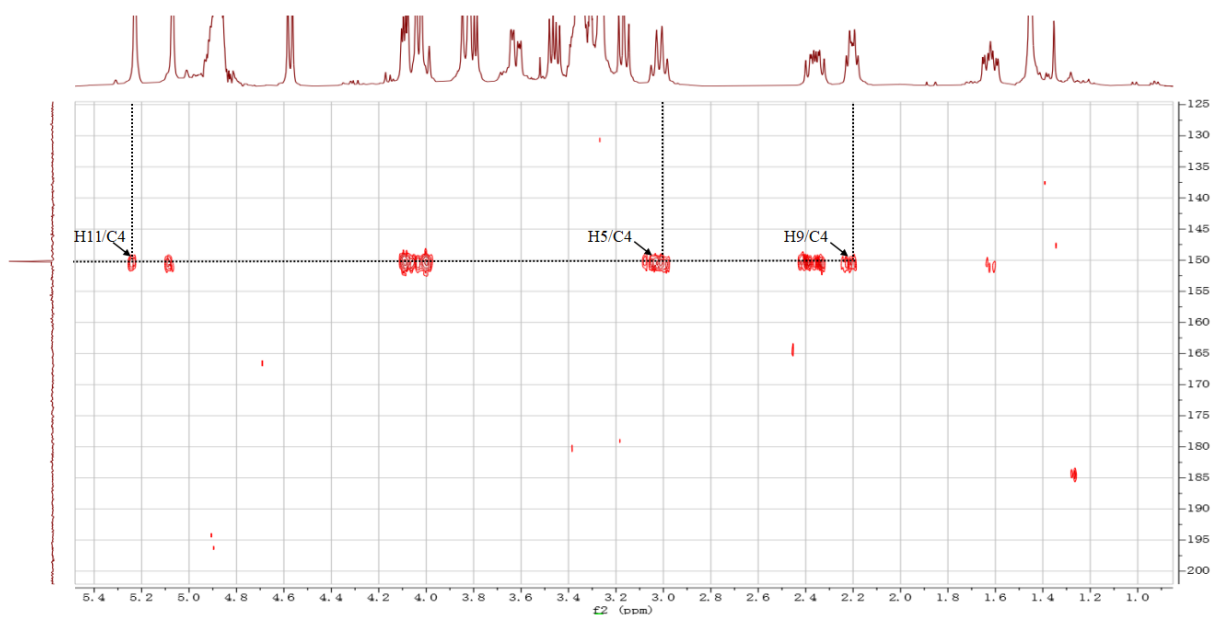
**Figure S7:** The HSQC spectrum of **1** (in MeOD) (From  $\delta_C$  90 ppm to  $\delta_C$  160 ppm)



**Figure S8:** The HMBC spectrum of **1** (in MeOD)

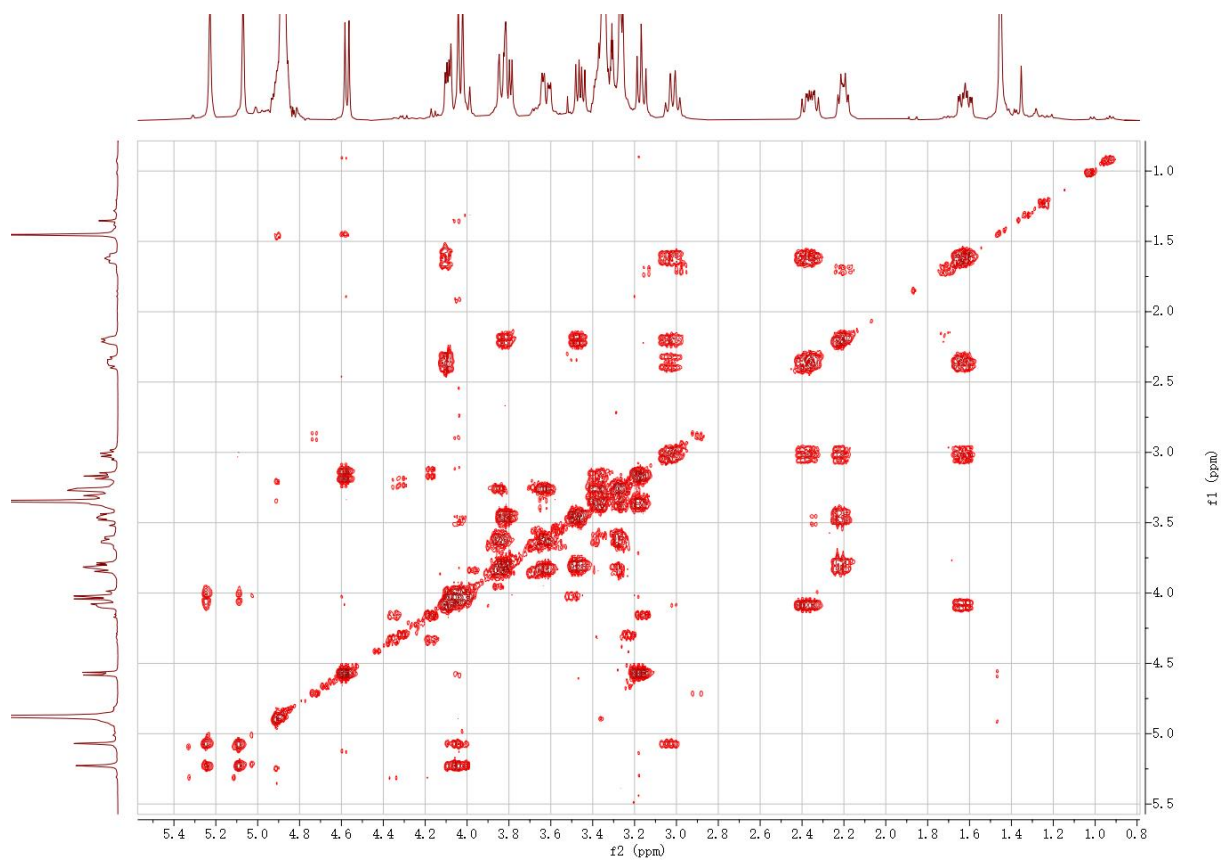


**Figure S9:** The HMBC spectrum of **1** (in MeOD) (From  $\delta_c$ 20ppm to  $\delta_c$  120 ppm)

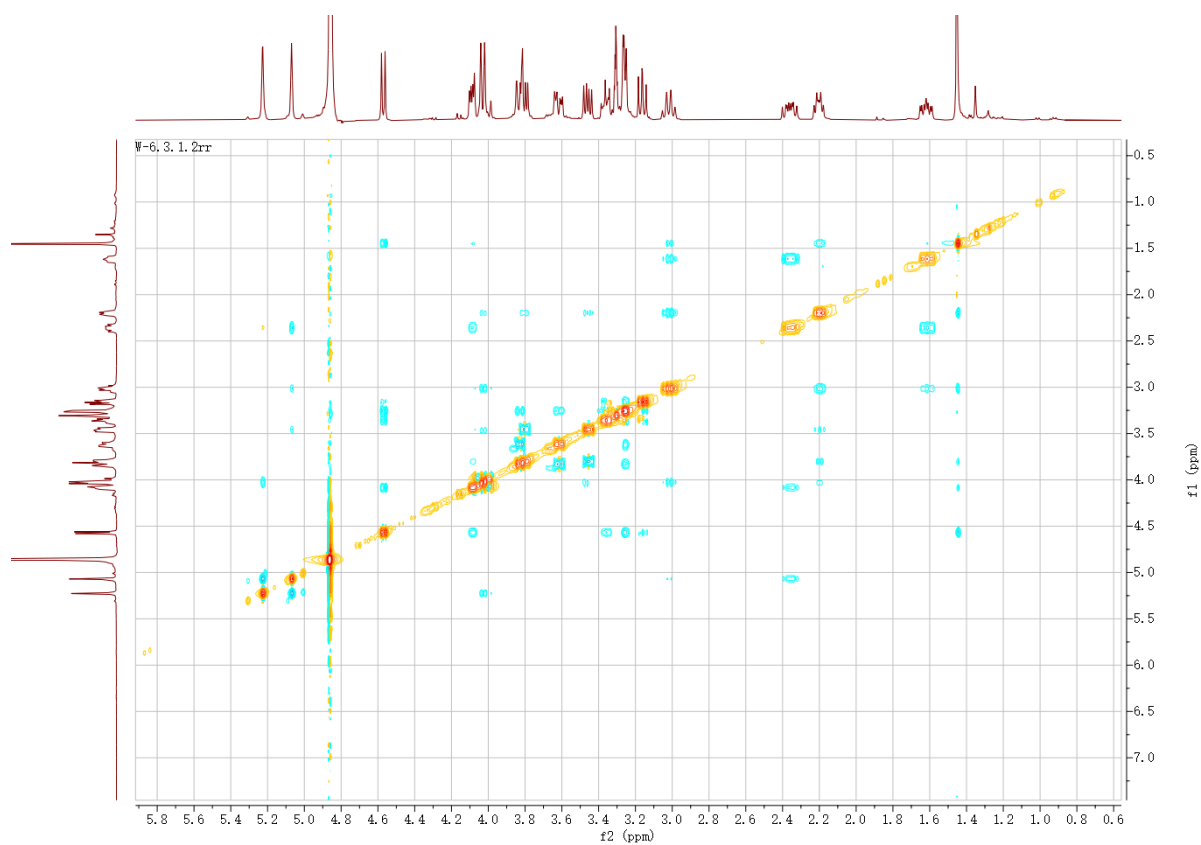


**Figure S10:** The HMBC spectrum of **1** (in MeOD) (From  $\delta_c$ 125ppm to  $\delta_c$  200 ppm)





**Figure S11:** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (in MeOD)



**Figure S12:** The NOESY spectrum of **1** (in MeOD)

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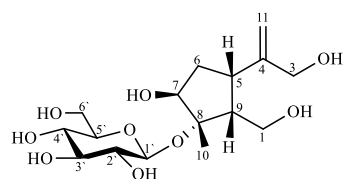
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Key Physical Properties  
 Search

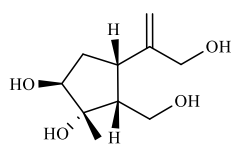
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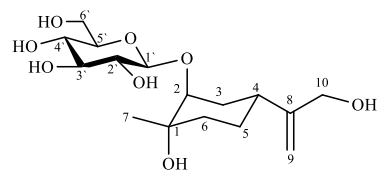
S1: Search report of SciFinder of 1



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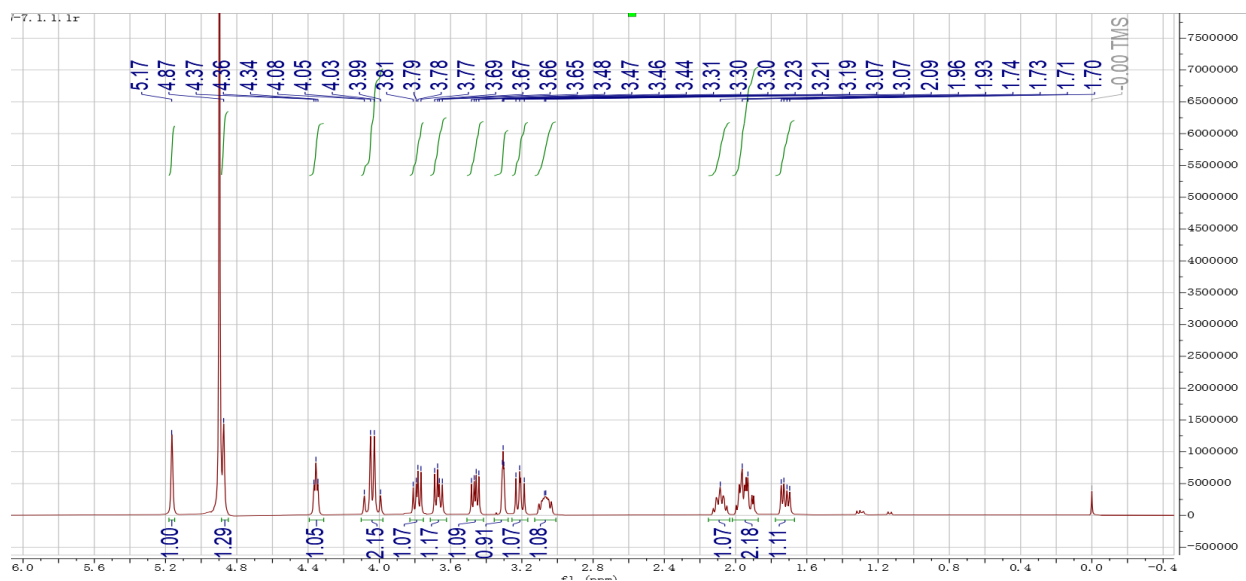
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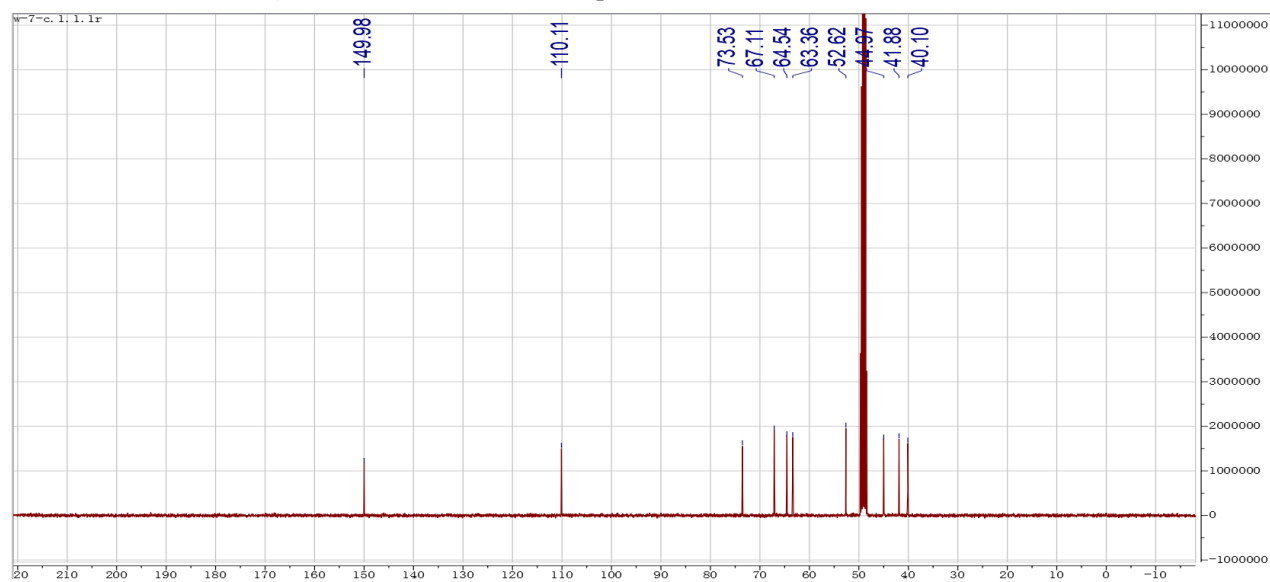
similar compound

**Table 1:**  $^{13}\text{C}$  NMR data for compound 1 and similar compound

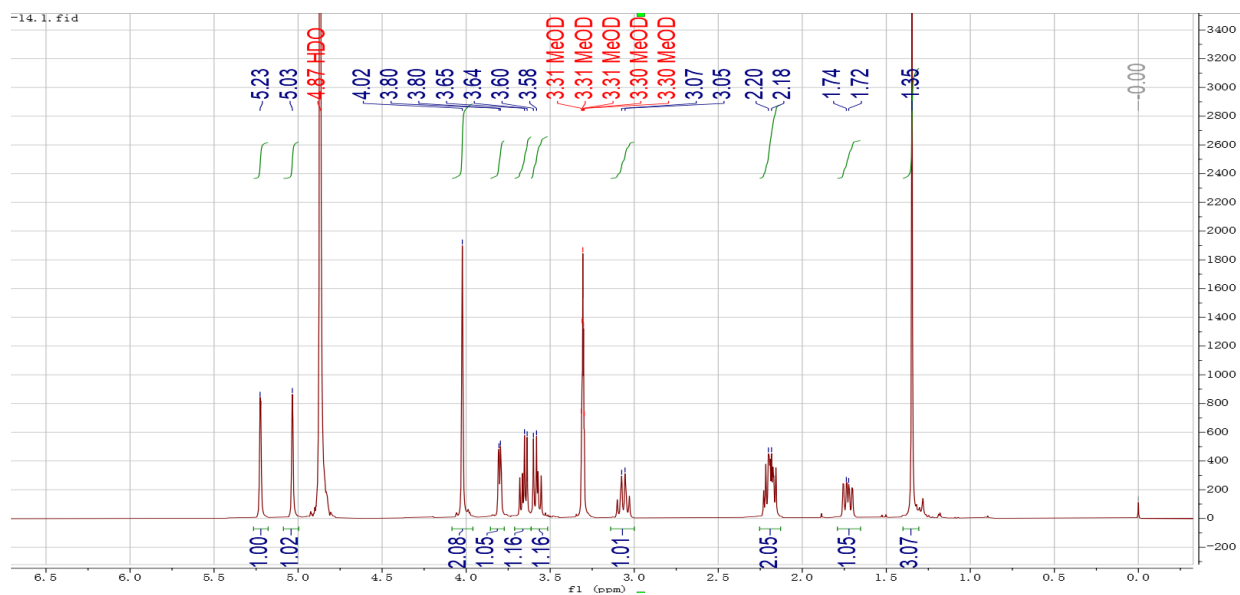
	<b>1</b>	<b>3</b>	<b>similar compound</b>
<b>Position</b>	$\delta_{\text{C}}$	$\delta_{\text{C}}$	$\delta_{\text{C}}$
1	60.4	61.0	70.4
2	-	-	84.1
3	67.1	67.5	33.9
4	150.2	150.6	34.4
5	41.3	41.5	27.6
6	36.3	38.9	35.3
7	78.2	81.0	28.3
8	89.8	83.5	156.1
9	54.1	51.3	107.0
10	19.8	23.5	64.8
11	112.3	112.4	-
1'	99.2		106.3
2'	75.2		75.7
3'	77.7		78.7
4'	71.8		71.7
5'	78.5		78.3
6'	62.9		62.9



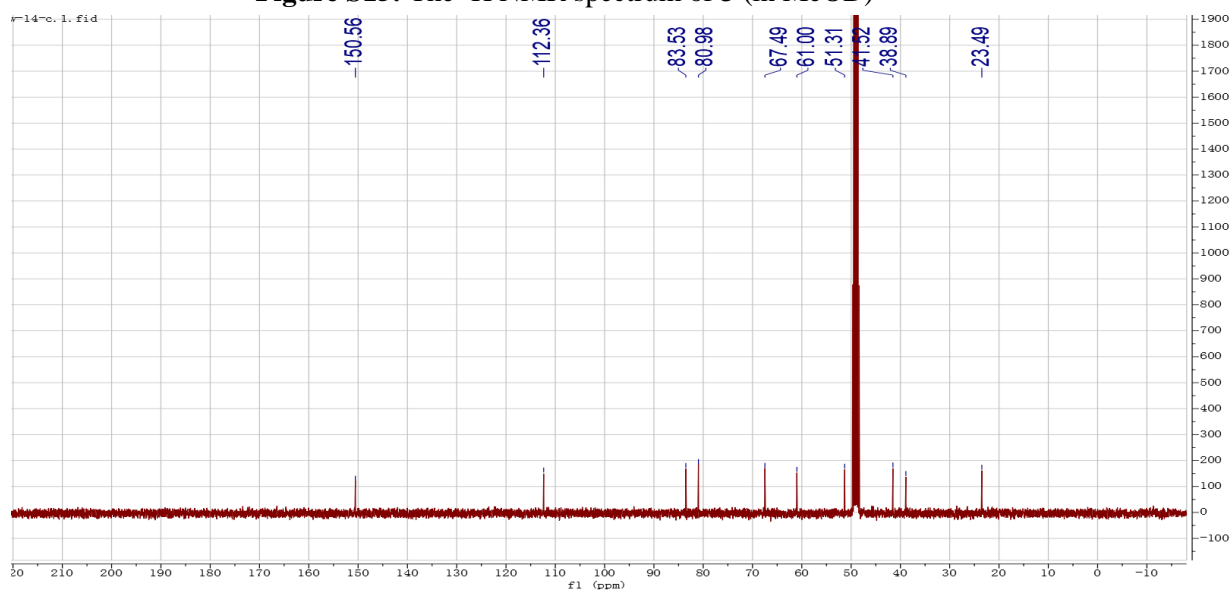
**Figure S13:** The  $^1\text{H}$  NMR spectrum of **2** (in MeOD)



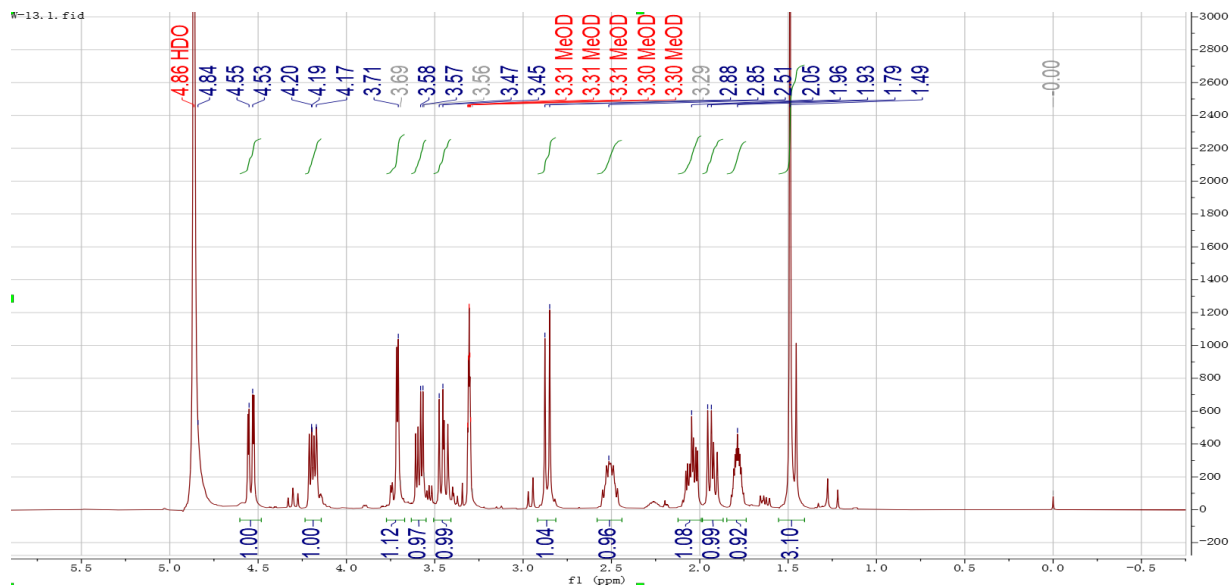
**Figure S14:** The  $^{13}\text{C}$  NMR spectrum of **2** (in MeOD)



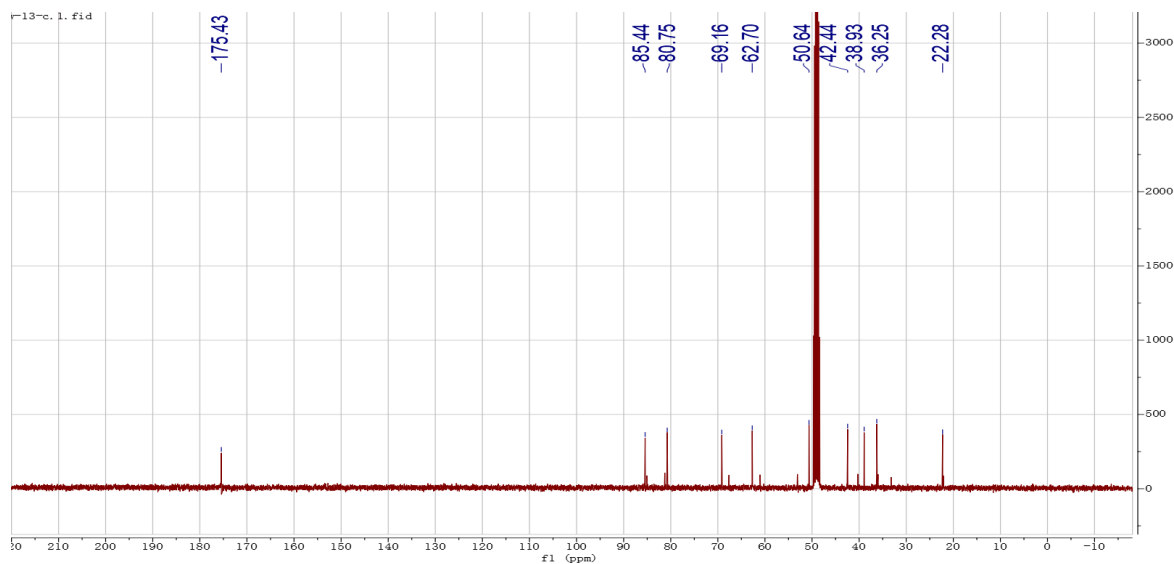
**Figure S15:** The  $^1\text{H}$  NMR spectrum of **3** (in MeOD)



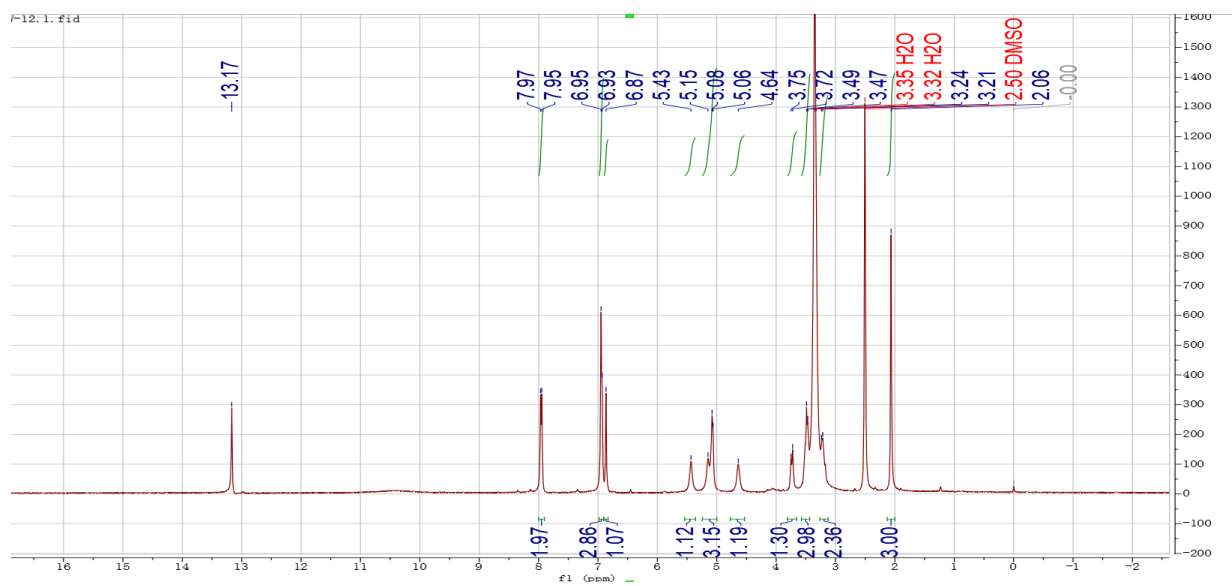
**Figure S16:** The  $^{13}\text{C}$  NMR spectrum of **3** (in MeOD)



**Figure S17:** The  $^1\text{H}$  NMR spectrum of **4** (in MeOD)

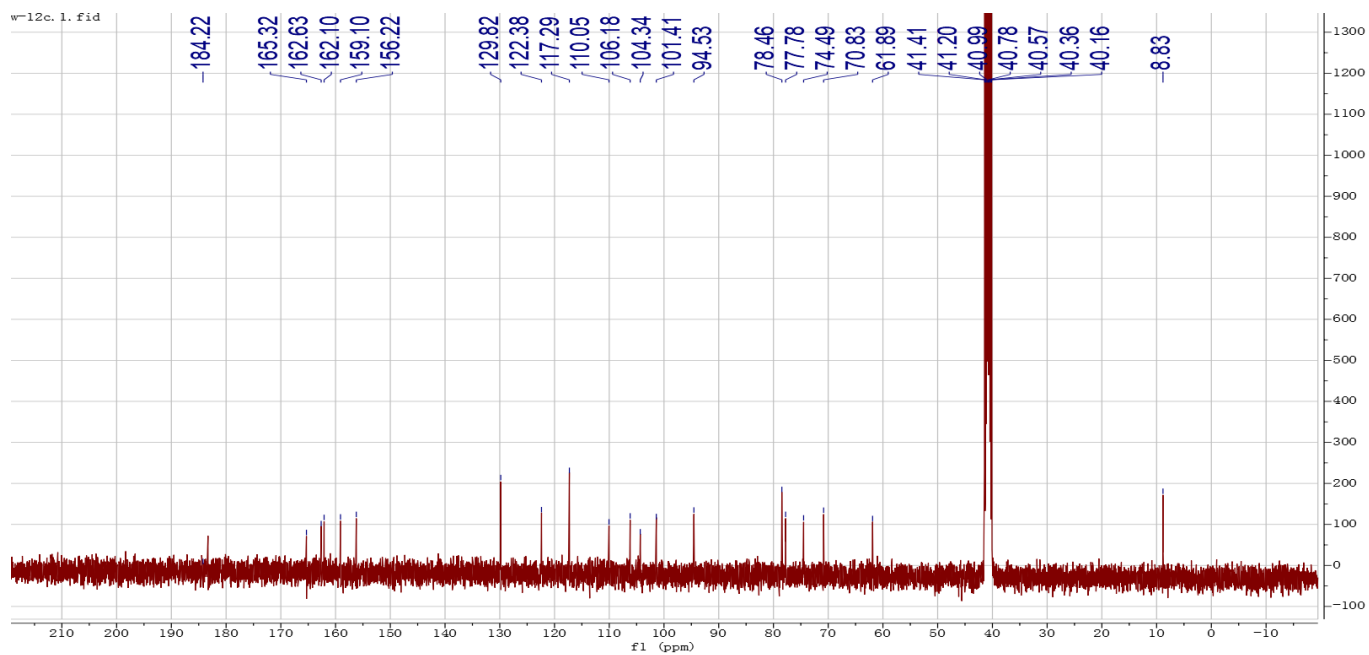


**Figure S18:** The  $^{13}\text{C}$  NMR spectrum of **4** (in MeOD)

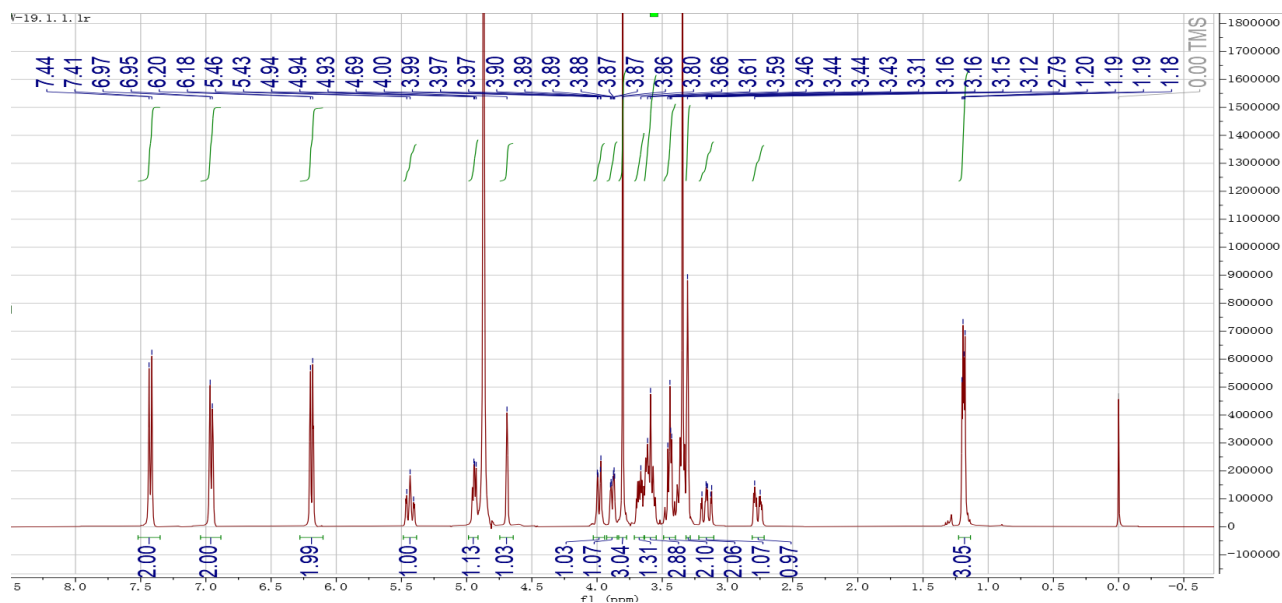


**Figure S19:** The  $^1\text{H}$  NMR spectrum of **5** (in  $\text{DMSO-}d_6$ )

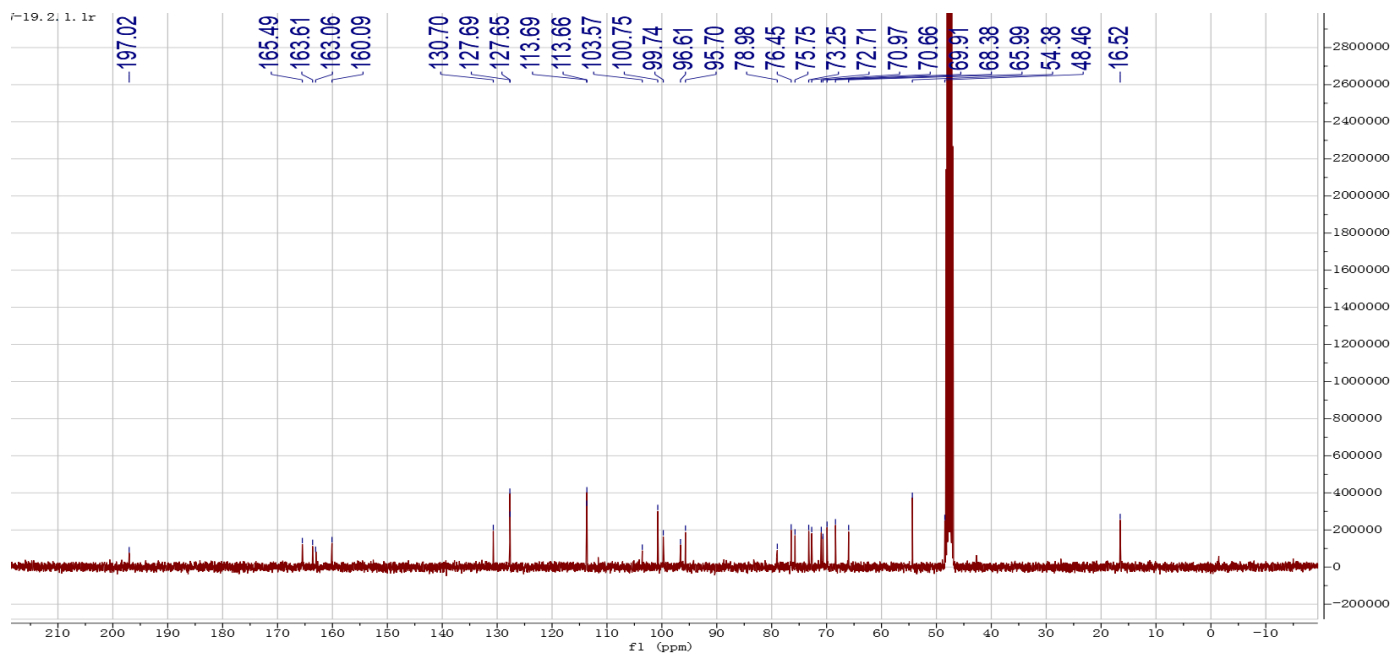




**Figure S20:** The  $^{13}\text{C}$  NMR spectrum of **5** (in  $\text{DMSO-}d_6$ )



**Figure S21:** The  $^1\text{H}$  NMR spectrum of **6** (in MeOD)



**Figure S22:** The <sup>1</sup>H NMR spectrum of **6** (in MeOD)

## S2: Spectroscopic Data of 2-6

*Dioscoridin A (2)*:  $C_{10}H_{18}O_4$ , colorless oil,  $[\alpha]_D^{27} = +8.0$  (c 0.1, MeOH), HR-ESI-MS  $m/z$  225.1095 ( $[M+Na]^+$ ).  $^1H$ -NMR (400 MHz, MeOD)  $\delta_H$ : 5.17 (1H, s, H-11a), 4.87 (1H, s, H-11b), 3.46 (1H, dd,  $J = 10.6, 6.1$  Hz, H-1a), 3.21 (1H, dd,  $J = 10.6, 8.2$  Hz, H-1b), 4.06 (2H, dd,  $J = 14.0, 8.6$  Hz, H-3), 3.07 (1H, m, H-5), 1.92 (1H, dd,  $J = 13.0, 4.0$  Hz, H-6a), 1.72 (1H, dd,  $J = 13.0, 6.1$  Hz, H-6b), 4.36 (1H, t,  $J = 4.6$  Hz, H-7), 1.97 (1H, m, H-8), 2.09 (1H, m, H-9), 3.79 (1H, dd,  $J = 10.6, 6.9$  Hz, H-10a), 3.67 (1H, dd,  $J = 10.6, 6.7$  Hz, H-10b).  $^{13}C$ -NMR (100 MHz, MeOD)  $\delta_C$ : 64.5 (C-1), 67.1 (C-3), 149.9 (C-4), 41.9 (C-5), 40.1 (C-6), 73.5 (C-7), 52.6 (C-8), 45.0 (C-9), 63.4 (C-10), 110.1 (C-11).

*Jatamanin J (3)*:  $C_{10}H_{18}O_4$ , yellow oil,  $[\alpha]_D^{20} +87.0$  (c 0.36, MeOH), HR-ESI-MS  $m/z$  225.1102 ( $[M+Na]^+$ ).  $^1H$ -NMR (400 MHz, MeOD)  $\delta_H$ : 3.66 (1H, dd,  $J = 11.1, 6.3$  Hz, H-1a), 3.58 (1H, dd,  $J = 11.1, 7.4$  Hz, H-1b), 4.02 (2H, s, H-3), 3.06 (1H, dd,  $J = 10.4, 7.9$  Hz, H-5), 2.19 (1H, ddd,  $J = 13.2, 9.6, 4.8$  Hz, H-6a), 1.72 (1H, ddd,  $J = 13.2, 7.9, 1.8$  Hz, H-6b), 3.80 (1H, dd,  $J = 5.2, 1.8$  Hz, H-7), 2.19 (1H, ddd,  $J = 10.2, 7.2, 6.0$  Hz, H-9), 1.34 (3H, s, H-10), 5.23 (1H, s, H-11a), 5.03 (1H, s, H-11b).  $^{13}C$ -NMR (100 MHz, MeOD)  $\delta_C$ : 61.0 (C-1), 67.5 (C-3), 150.6 (C-4), 41.5 (C-5), 38.9 (C-6), 81.0 (C-7), 83.5 (C-8), 51.3 (C-9), 23.5 (C-10), 112.4 (C-11).

*Longiflorone (4)*:  $C_{10}H_{16}O_5$ , yellow oil,  $[\alpha]_D^{20} +61.9$  (c 1.1, MeOH), DCI-MS  $m/z$  234.1 ( $[M+NH_3+H]^+$ ).  $^1H$ -NMR (400 MHz, MeOD)  $\delta_H$ : 4.54 (1H, dd,  $J = 10.9, 2.9$  Hz, H-3a), 4.19 (1H, dd,  $J = 10.9, 5.7$  Hz, H-3b), 1.76 (1H, m, H-4), 2.52 (1H, m, H-5), 2.05 (1H, ddd,  $J = 13.4, 9.4, 4.0$  Hz, H-6a), 1.93 (1H, dd,  $J = 13.4, 8.3$  Hz, H-6b), 3.71 (1H, d,  $J = 3.9$  Hz, H-7), 2.86 (1H, d,  $J = 10.9$  Hz, H-9), 1.49 (3H, s, H-10), 3.59 (1H, dd,  $J = 11.2, 5.4$  Hz, H-11a), 3.45 (1H, dd,  $J = 11.2, 8.4$  Hz, H-11b).  $^{13}C$ -NMR (100 MHz, MeOD)  $\delta_C$ : 175.4 (C-1), 69.2 (C-3), 42.4 (C-4), 36.2 (C-5), 38.9 (C-6), 80.8 (C-7), 85.4 (C-8), 50.6 (C-9), 22.3 (C-10), 62.7 (C-11).

*Apigenin-8-O- $\beta$ -D-glucopyranoside (5)*:  $C_{22}H_{23}O_{10}$ , colorless oil,  $[\alpha]_D^{20} -115.8$  (c 0.41, MeOH), HR-FAB-MS  $m/z$  447.1285 ( $[M+H]^+$ ).  $^1H$ -NMR (400 MHz, MeOD)  $\delta_H$ : 6.87 (1H, s, H-3), 7.96 (1H, d,  $J = 8.4$  Hz, H-6), 7.96 (1H, d,  $J = 8.4$  Hz, H-8), 6.93 (1H, d,  $J = 2.1$  Hz, H-2'), 6.94 (1H, d,  $J = 7.3$  Hz, H-5'), 6.94 (1H, dd,  $J = 7.3, 2.1$  Hz, H-6'), 5.08 (1H, d,  $J = 7.5$  Hz, H-1''), 4.64 (1H, m, H-2''), 3.75 (1H, m, H-3''), 3.49 (1H, m, H-4''), 3.49 (1H, m, H-5''), 3.24 (2H, m, H-6''), 2.06 (3H, s, Me-3').  $^{13}C$ -NMR (100 MHz, MeOD)  $\delta_C$ : 162.6 (C-2), 106.2 (C-3), 184.2 (C-4), 159.1 (C-5), 104.3 (C-6), 94.5 (C-7), 165.3 (C-8), 162.1 (C-9), 110.1 (C-10), 129.8 (C-1'), 117.3 (C-2'), 129.8 (C-3'), 156.2 (C-4'), 117.3 (C-5'), 122.4 (C-6'), 101.4 (C-1''), 77.8 (C-2''), 74.5 (C-3''), 70.8 (C-4''), 78.5 (C-5''), 61.9 (C-6''), 8.8 (3'-CH<sub>3</sub>).

*Isosakuranetin-5-O-rutinoside (6)*: C<sub>28</sub>H<sub>34</sub>O<sub>14</sub>, white needles,  $[\alpha]_D^{20}$  -105.3 (c 0.16, MeOH), FAB-MS  $m/z$  594.2 ([M]<sup>+</sup>). <sup>1</sup>H-NMR (400 MHz, MeOD)  $\delta_H$ : 7.43 (2H, d,  $J$  = 8.7 Hz, H-2', 6'), 6.96 (2H, d,  $J$  = 8.8 Hz, H-3', 5'), 6.20 (1H, d,  $J$  = 2.2 Hz, H-6), 6.18 (1H, d,  $J$  = 2.2 Hz, H-8), 5.57 (1H, dd,  $J$  = 11.9, 2.9 Hz, H-2), 4.96 (1H, d,  $J$  = 7.5 Hz, H-1''), 4.51 (1H, brs, H-1'''), 3.80 (3H, s, 4'-OCH<sub>3</sub>), 1.19 (3H, m, H-6'''). <sup>13</sup>C-NMR (100 MHz, MeOD)  $\delta_C$ : 78.9 (C-2), 48.5 (C-3), 197.0 (C-4), 163.6 (C-5), 96.6 (C-6), 165.5 (C-7), 95.7 (C-8), 163.1 (C-9), 103.6 (C-10), 130.7 (C-1'), 127.6 (C-2'), 113.6 (C-3'), 160.1 (C-4'), 113.7 (C-5'), 127.7 (C-6'), 100.7 (C-1''), 73.2 (C-2''), 75.8 (C-3''), 69.9 (C-4''), 76.4 (C-5''), 66.0 (C-6''), 99.7 (C-1'''), 70.9 (C-2'''), 70.7 (C-3'''), 72.7 (C-4'''), 68.4 (C-5'''), 16.5 (C-6'''), 54.4 (4'-OCH<sub>3</sub>).