

## Supporting Information

*Rec. Nat. Prod.* 9:4 (2015) 609-613

### Two new flavone glycosides from *Chenopodium ambrosioides* growing wildly in Egypt

Hala M. Hammoda<sup>\*1</sup>, Fathalla M. Harraz<sup>1</sup>, Maged G. Al Ghazouly<sup>1,2</sup>,  
Mohamed M. Radwan<sup>1,4</sup>, Mahmoud A. ElSohly<sup>3,4</sup>, Amira S. Wanas<sup>4,5</sup>,  
Samar M. Bassam<sup>2</sup>

<sup>1</sup> Department of Pharmacognosy, Faculty of Pharmacy, Alexandria University 21521, Alexandria, Egypt

<sup>2</sup> Department of Pharmacognosy, Faculty of Pharmacy, Pharos University, Alexandria, Egypt

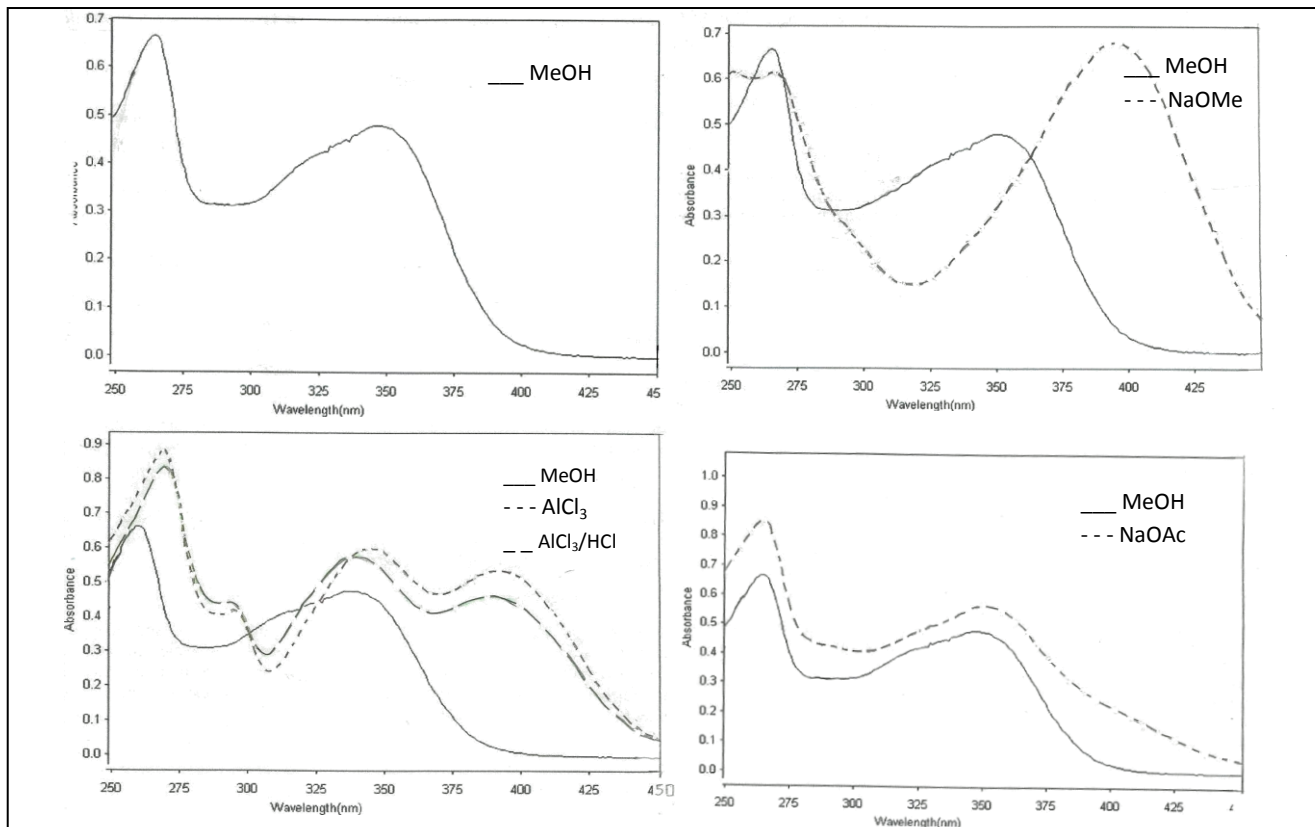
<sup>3</sup> Department of Pharmaceutics, School of Pharmacy, University of Mississippi, MS 38677, USA

<sup>4</sup> National Center for Natural Products Research, School of pharmacy, University of Mississippi, University MS 38655, USA

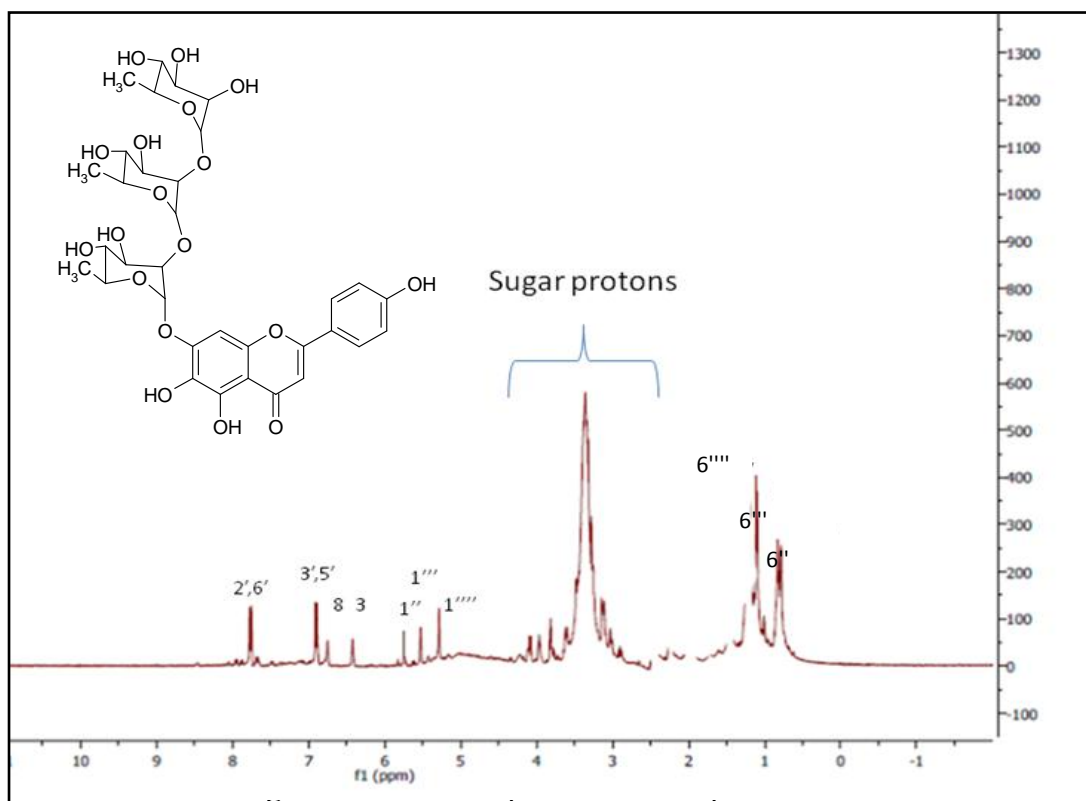
<sup>5</sup> Department of Pharmacognosy, Faculty of Pharmacy, University of Minia, Egypt

Table of Contents	Page
<b>S1:</b> UV spectra of compound <b>1</b>	3
<b>S2:</b> <sup>1</sup> H-NMR spectrum (400 MHz, DMSO-d <sub>6</sub> ) of compound <b>1</b>	4
<b>S3:</b> COSY spectrum (400 MHz) of compound <b>1</b>	5
<b>S4:</b> Broad band decoupled <sup>13</sup> C- NMR (100 MHz) of compound <b>1</b>	6
<b>S5:</b> DEPT spectrum of compound <b>1</b> (from 15 to 210)	7
<b>S6:</b> HMQC spectra of compound <b>1</b>	8
<b>S7:</b> NOESY spectrum of compound <b>1</b>	9
<b>S8:</b> HRESI-MS spectrum of <b>1</b> (positive mode)	10
<b>S9:</b> HRESI-MS spectrum of <b>1</b> (negative mode)	11
<b>S10:</b> UV spectra of compound <b>2</b>	12
<b>S11:</b> <sup>1</sup> H-NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of compound <b>2</b>	13
<b>S12:</b> COSY spectrum (400 MHz) of compound <b>2</b>	14

<b>S13:</b> Broad band decoupled $^{13}\text{C}$ -NMR spectra (100 MHz) of compound <b>2</b>	15
<b>S14:</b> DEPT spectrum of compound <b>2</b> (from 0 to 135)	16
<b>S15:</b> HRESI-MS spectrum of <b>1</b> (positive mode)	17
<b>S16:</b> S7: HRESI-MS spectrum of <b>1</b> (negative mode)	18

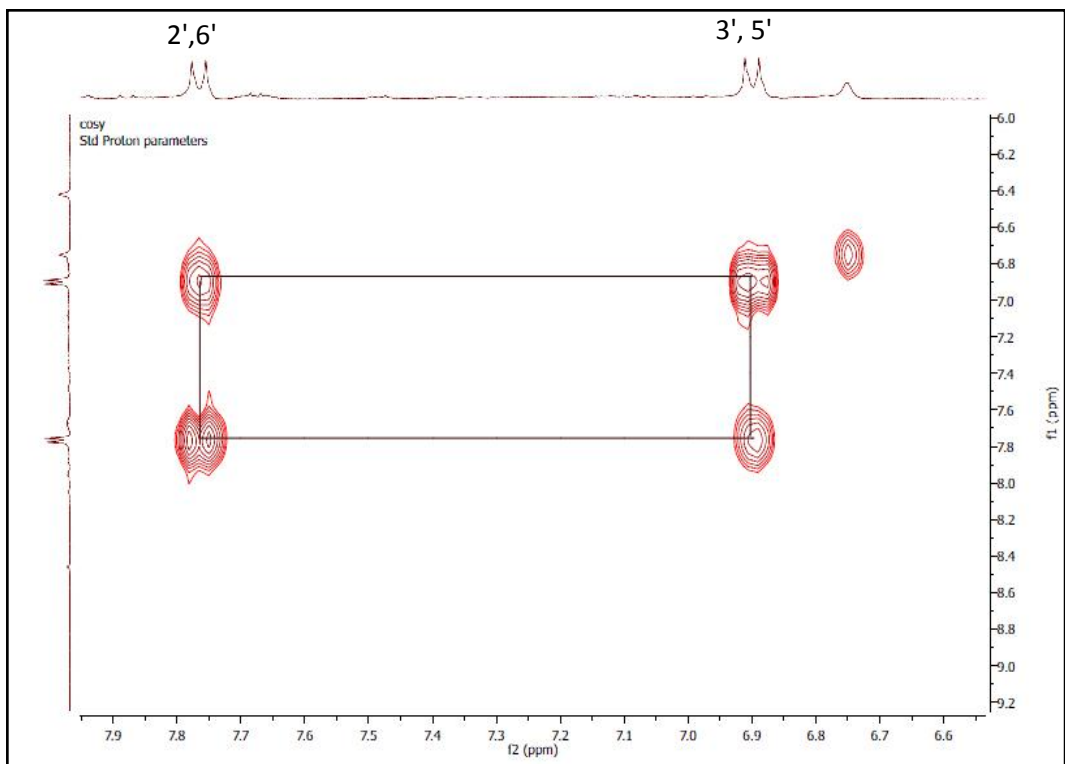


S1: UV spectra of compound 1

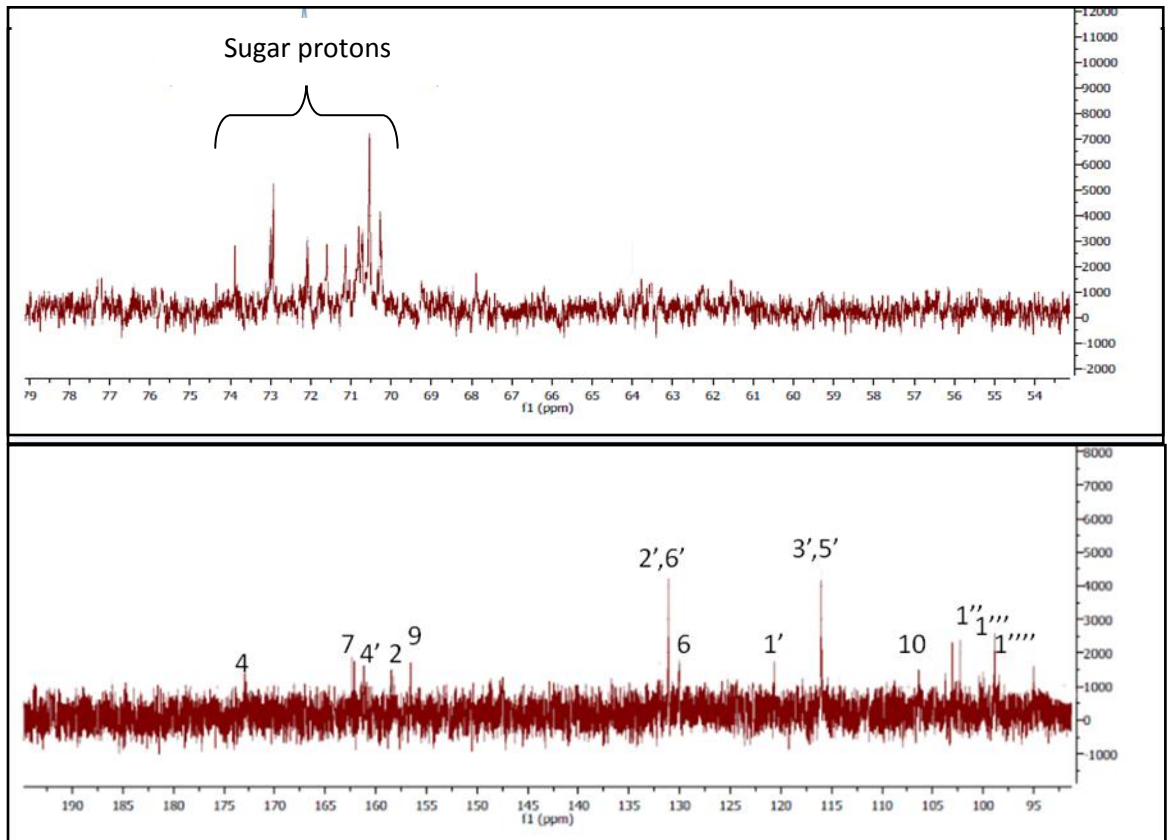
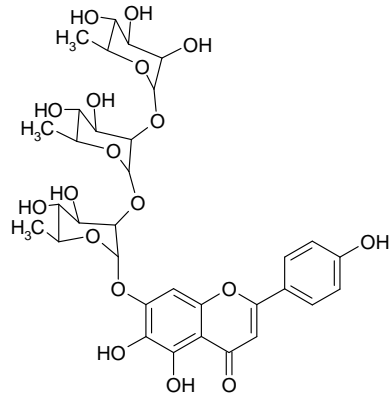


S2:  $^1\text{H-NMR}$  spectrum (400MHz, DMSO- $d_6$ ) of compound **1**

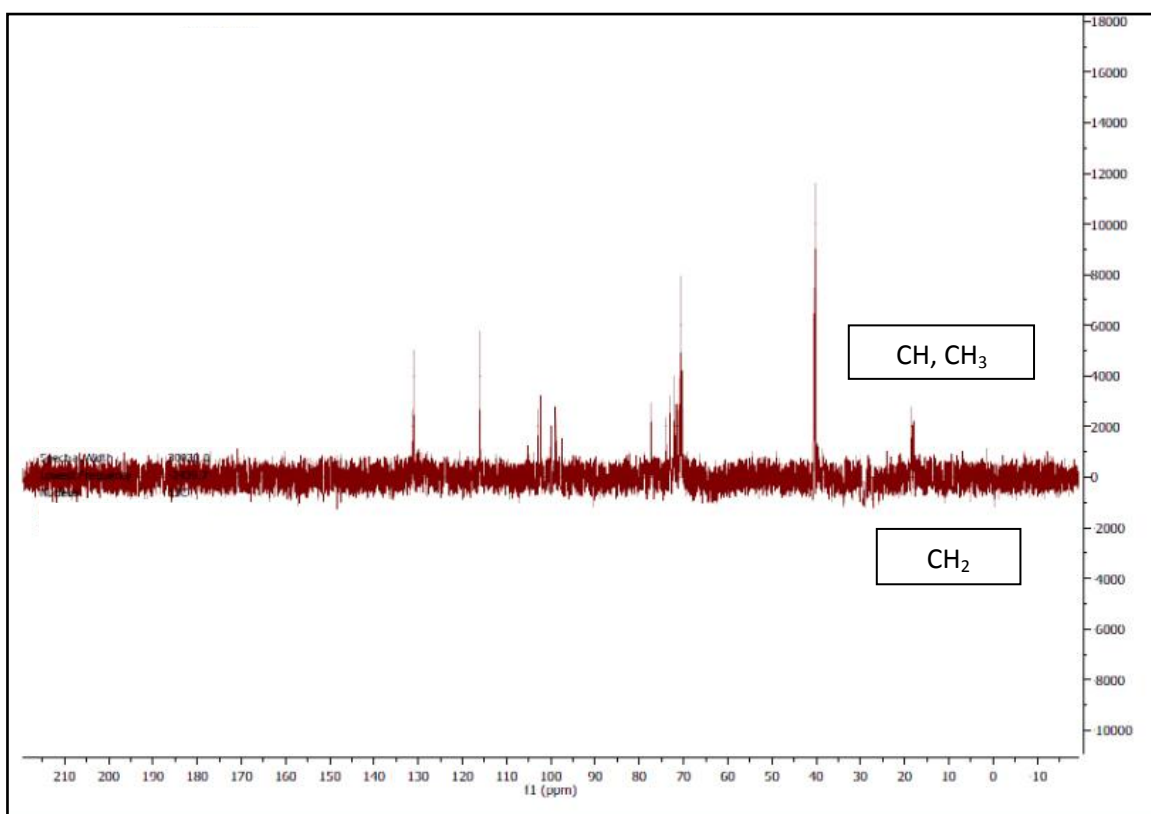
*Scutellarein-7-O-rhamnosyl (1→2) rhamnosyl (1→2) rhamnoside (1)*: yellowish white amorphous powder. UV (MeOH):  $\lambda_{\text{max}}$  (A) 349 (0.158), 265 (0.371). UV (MeOH/MeONa): 397 (0.232), 270 (0.399). UV (MeOH/ $\text{AlCl}_3$ ): 389 (0.163), 339 (0.214), 272 (0.403). UV (MeOH/ $\text{AlCl}_3/\text{HCl}$ ): 388 (0.219), 330 (0.228), 274 (0.410). UV (MeOH/ $\text{AcONa}$ ): 352 (0.191), 265 (0.467).  $^1\text{H NMR}$  (400 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) = 6.42 (1H, s, H-3); 6.74 (1H, s, H-8); 7.75 (2H, d,  $J=8.4$  Hz, H-2', H-6'); 6.90 (2H, d,  $J=8.4$  Hz, H-3', H-5'); 5.75 (1H, br.s, H-1''), 3.81 (1H, s, H-2''), 0.79 (3H, d,  $J=5.4$ , H-6''), 5.52 (1H, br.s, H-1'''), 3.96 (1H, s, H-2'''), 0.84 (3H, d,  $J=5.2$ , H-6'''), 5.28 (1H, br.s, H-1''''), 1.10 (3H, d,  $J=5.2$ , H-6'''), 3.15-4.35 (overlapped remaining protons of sugars).  $^{13}\text{C NMR}$  (100 MHz, DMSO- $d_6$ ):  $\delta$  (ppm) = 158.2 (C, C-2); 103.1 (CH, C-3); 172.9 (C, C-4); 158.2 (C, C-5); 130.1 (C, C-6); 162.1 (C, C-7); 94.9 (CH, C-8); 156.6 (C, C-9); 109.5 (C, C-10); 120.6 (C, C-1'); 131.1 (CH, C-2',C-6'); 115.9 (CH, C-3', C-5'), 162.1 (C, C-4'), 102.3 (CH, C-1''), 77.3 (CH, C-2''), 71.1 (CH, C-3''), 72.9 (CH, C-4''), 70.3 (CH, C-5''), 18.0 (CH<sub>3</sub>, C-6''), 99.9 (CH, C-1'''), 77.2 (CH, C-2'''), 71.6 (CH, C-3'''), 73.0 (CH, C-4'''), 70.5 (CH, C-5'''), 18.4 (CH<sub>3</sub>, C-6'''), 98.9 (CH, C-1''''), 70.8 (CH, C-2'''), 72.1 (CH, C-3'''), 73.8 (CH, C-4'''), 70.7 (CH, C-5'''), 18.7 (CH<sub>3</sub>, C-6'''). HRMS: positive ion mode:  $m/z$  747. 224 [ $\text{M} + \text{Na}$ ] $c^+$ , negative ion mode:  $m/z$  577.1666 [ $\text{M-Rha}$ ].



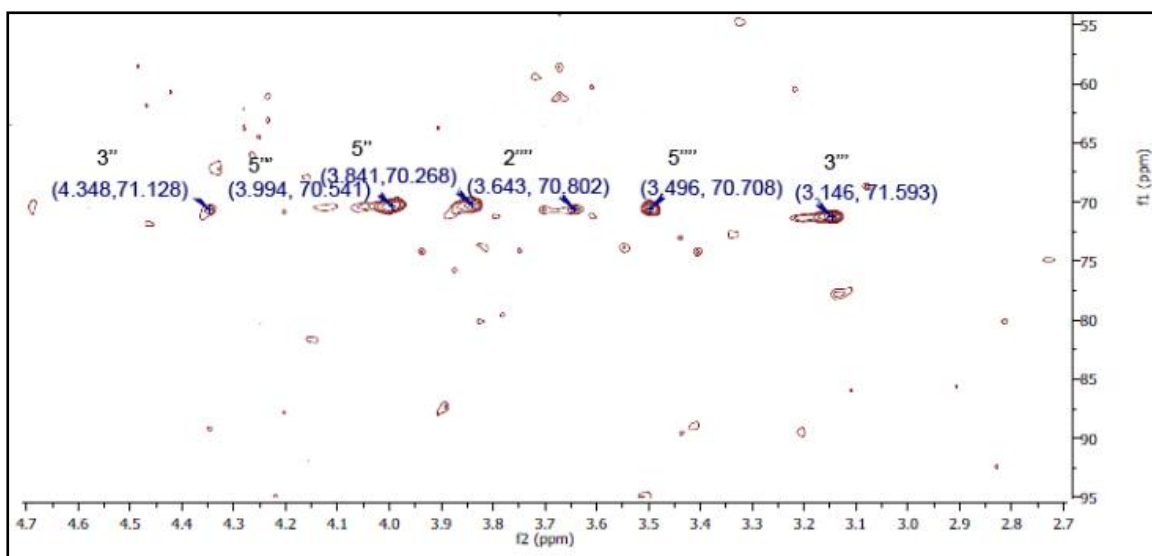
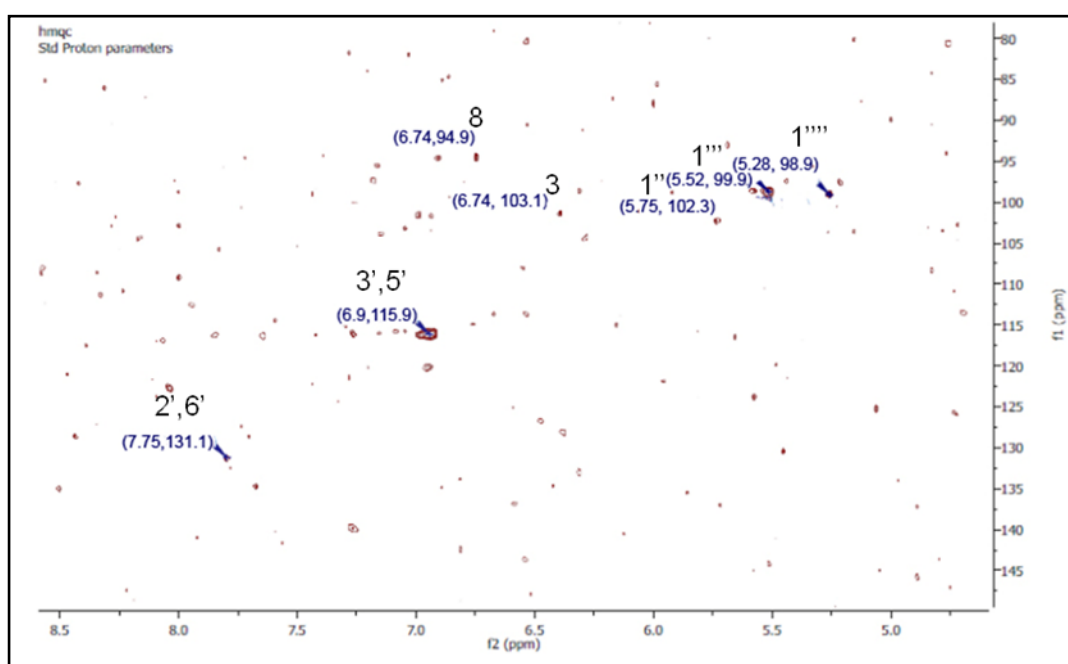
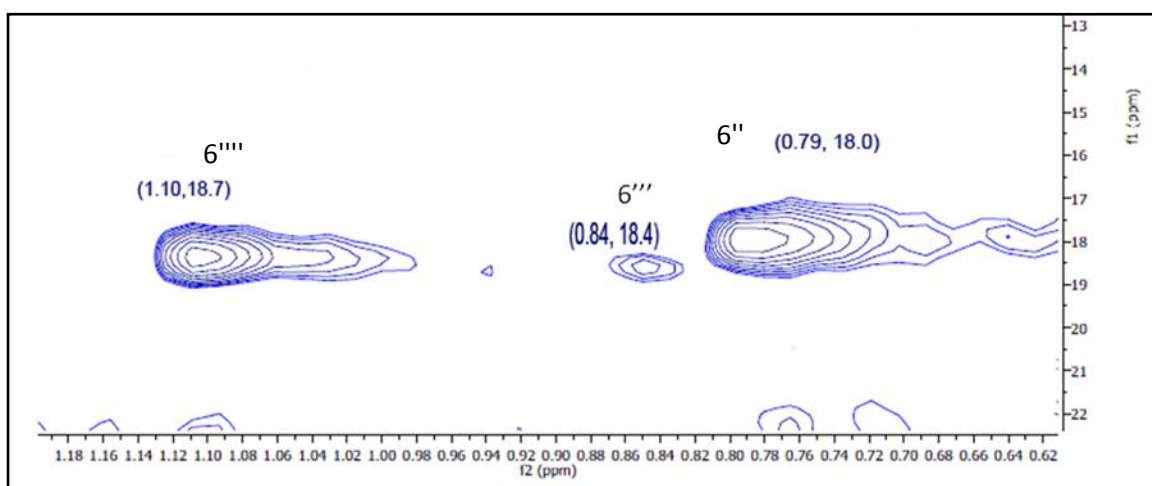
S3: COSY spectrum (400 MHz) of compound "A2"



S4: Broad band decoupled  $^{13}\text{C}$ -NMR spectra (100 MHz) of compound **1**

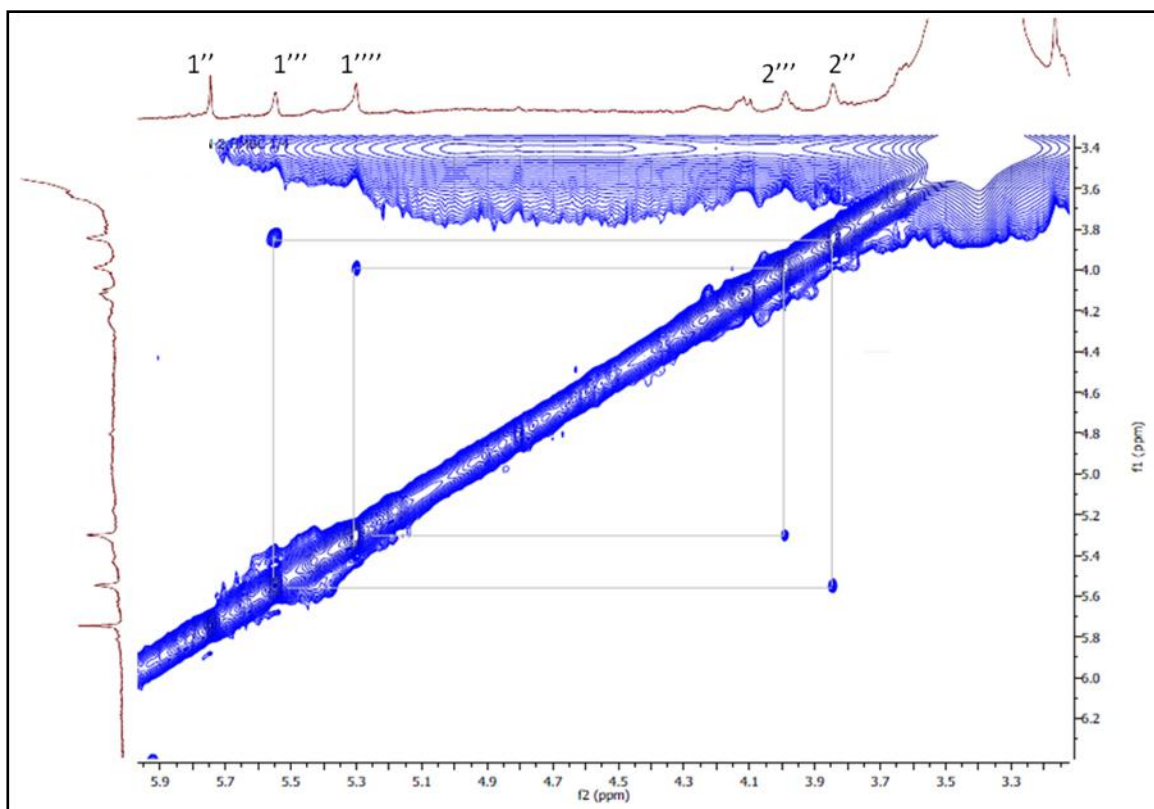
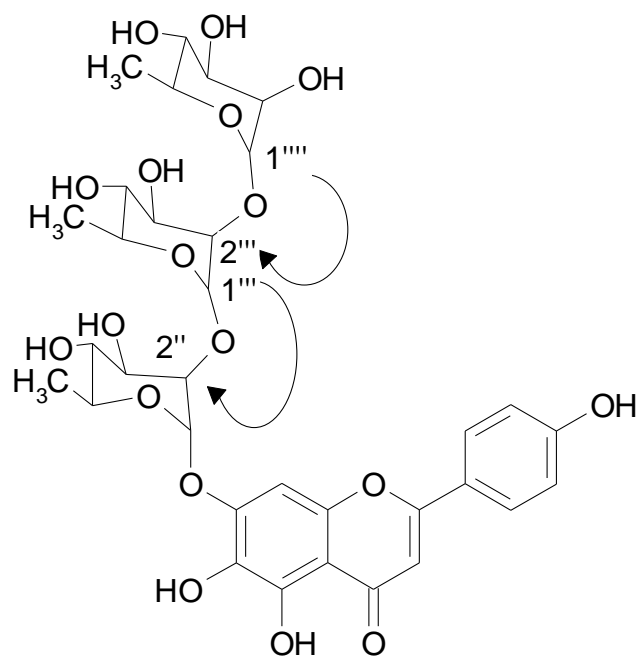


S5: DEPT spectrum of compound **1** (from 0 to 210)

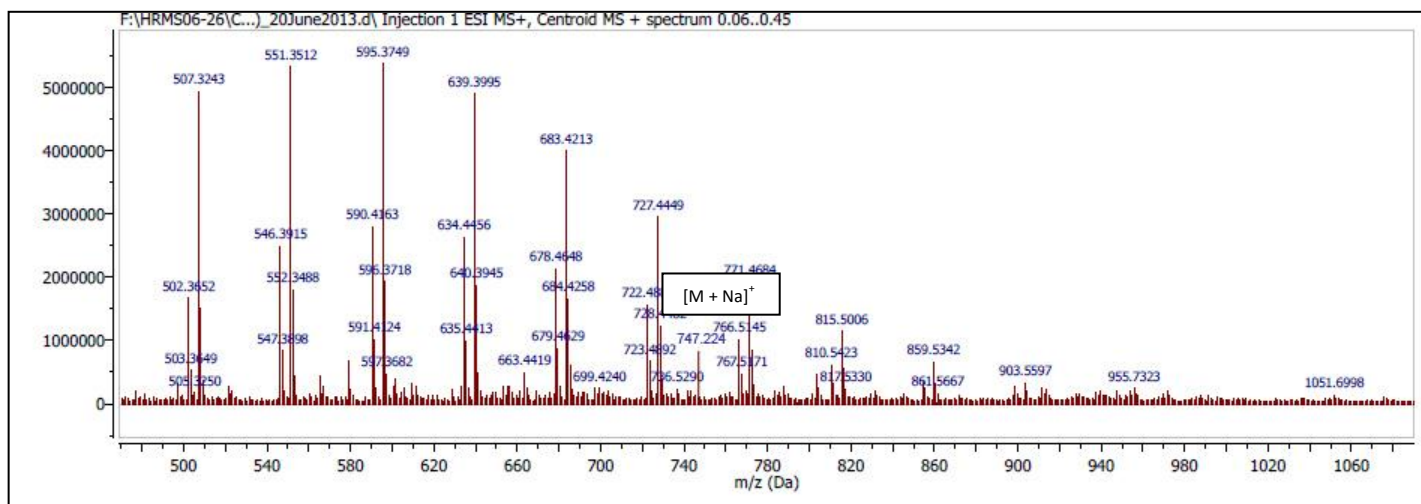


S6: HMQC spectra of compound **1**

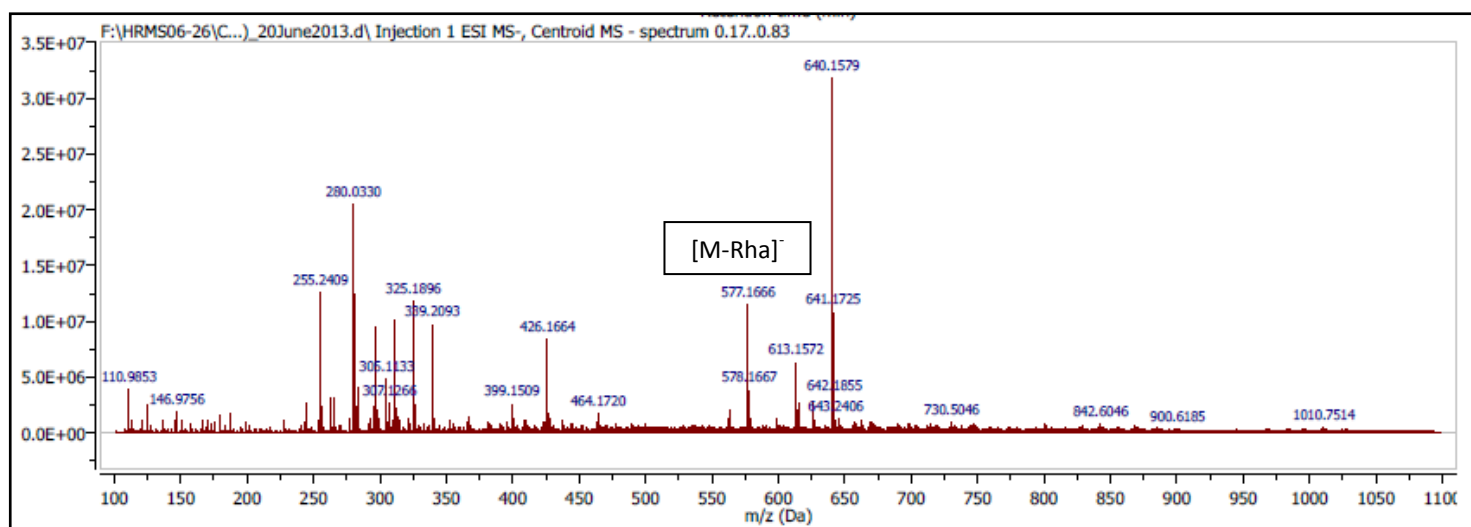




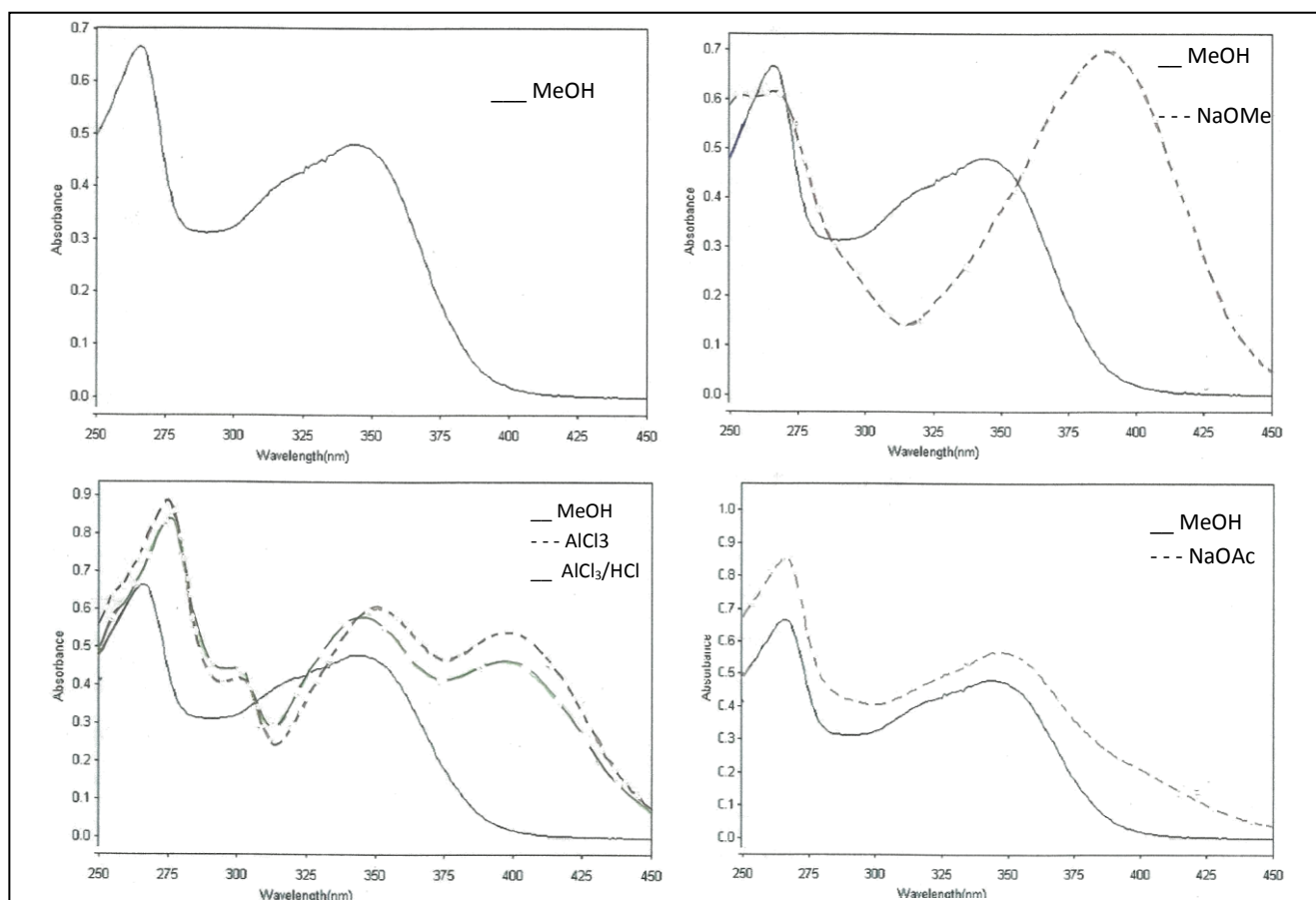
S7: NOESY spectrum of compound 1



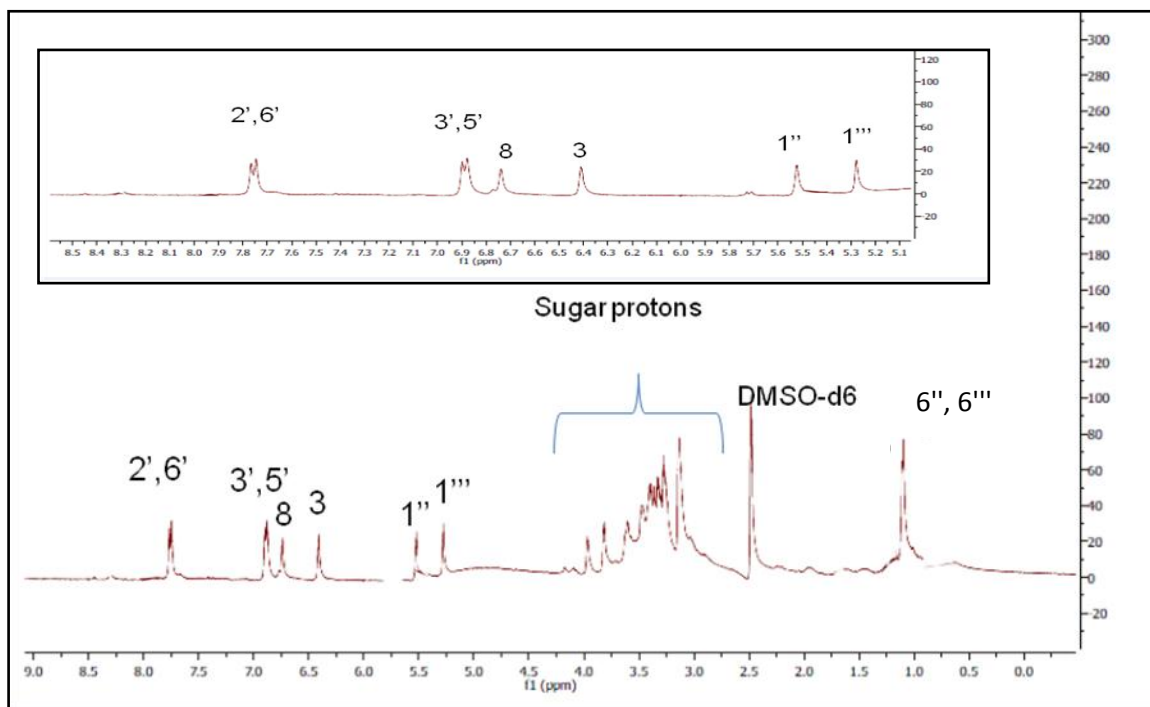
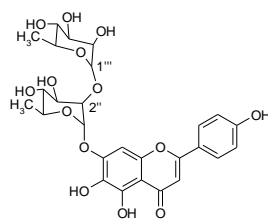
S8: HRESI-MS spectrum of **1** (positive mode)



S9: HRESI-MS spectrum of **1** (negative mode)

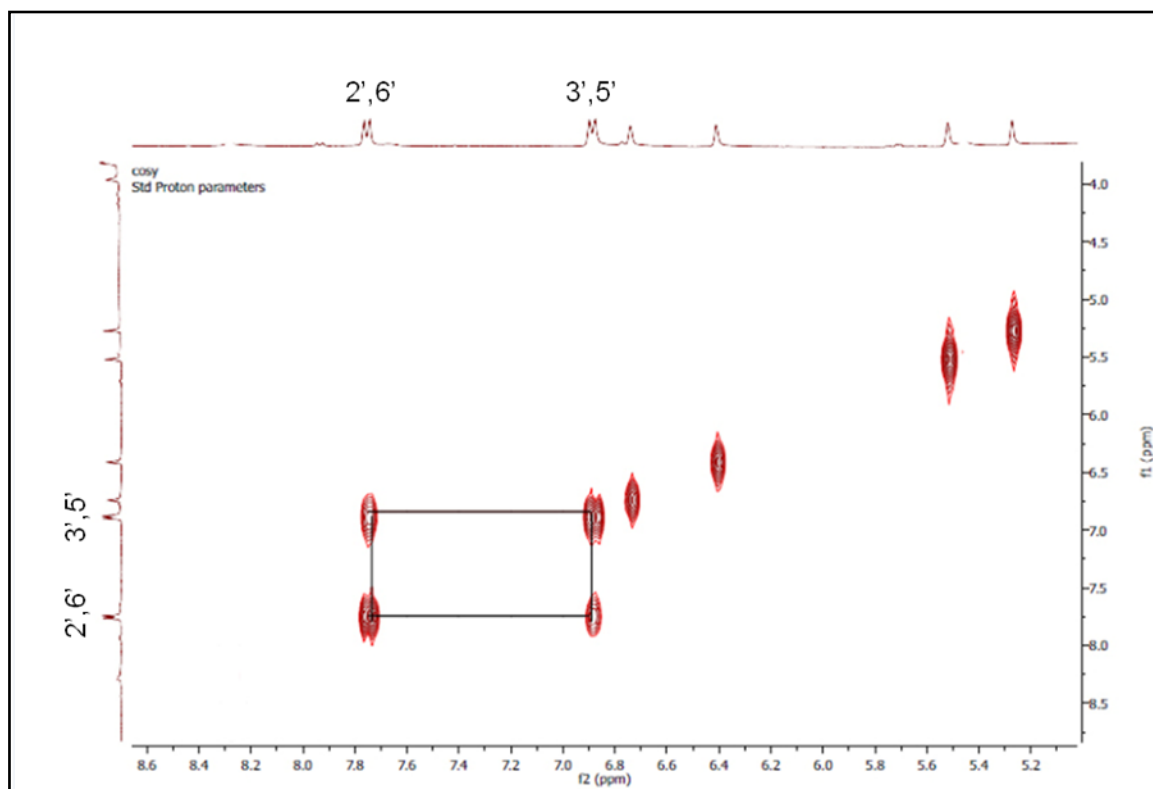


**S10:** UV spectra of compound 2

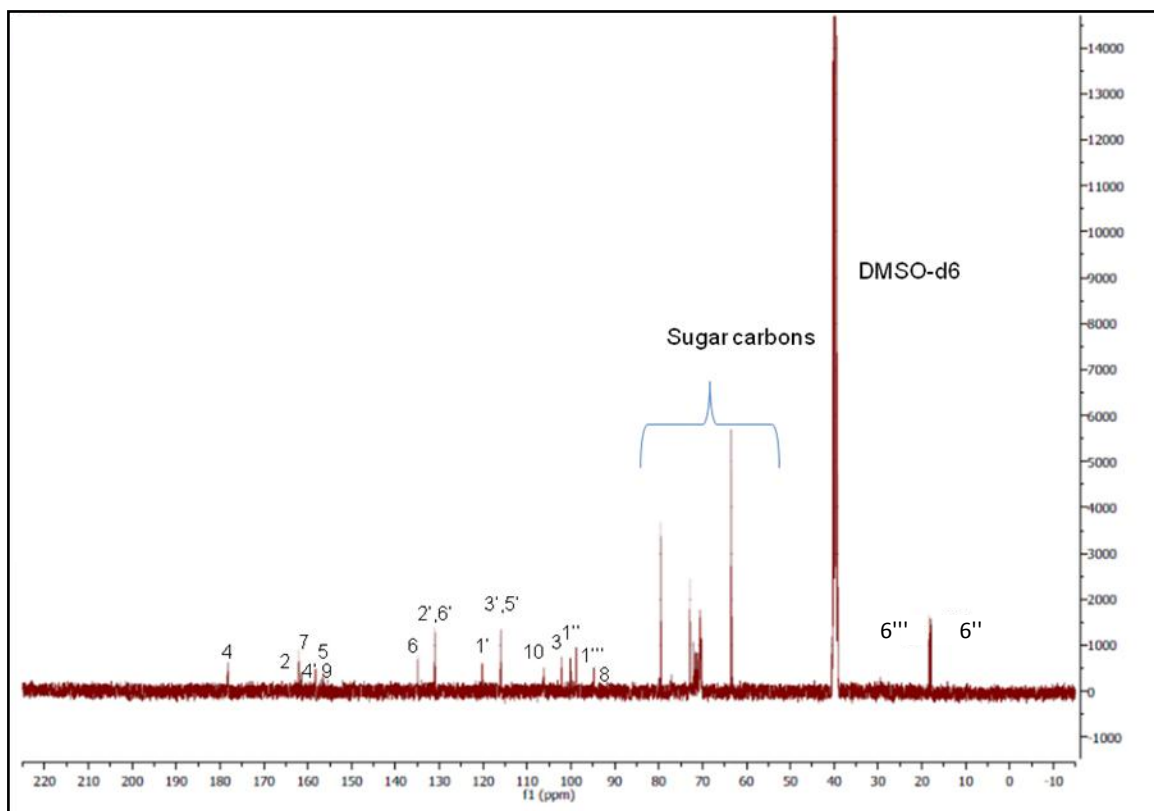
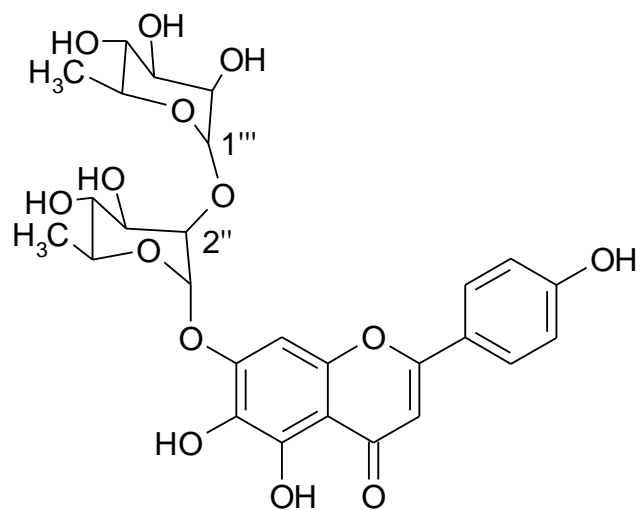


**S11:**  $^1\text{H-NMR}$  spectrum (400 MHz,  $\text{DMSO-d}_6$ ) of compound 2

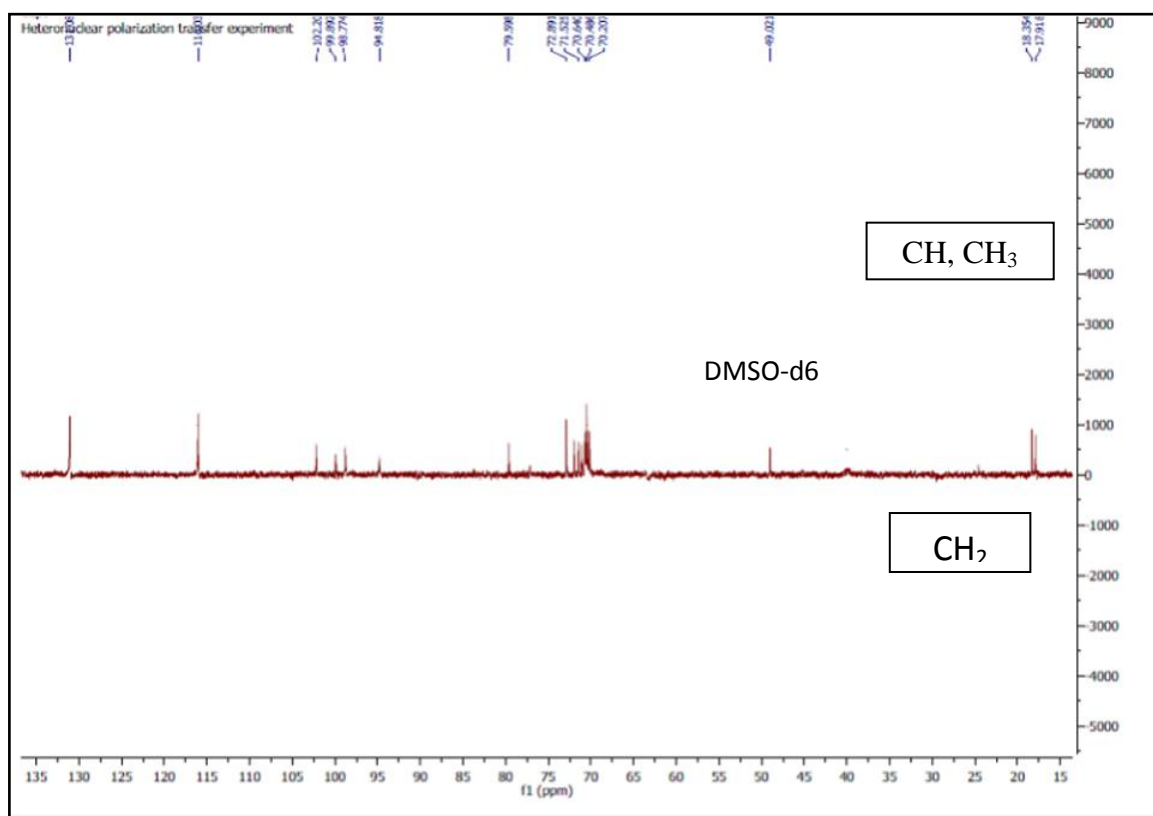
*Scutellarein-7-O-rhamnosyl (1→2) rhamnoside (2)*: yellowish white amorphous powder. UV (MeOH):  $\lambda_{\text{max}}$  (A) 344 (0.055), 267 (0.181). UV (MeOH/ MeONa): 389 (0.060), 268 (0.280). UV (MeOH/  $\text{AlCl}_3$ ): 399 (0.060), 352 (0.109), 276 (0.246). UV (MeOH/  $\text{AlCl}_3/\text{HCl}$ ): 395 (0.079), 347 (0.142), 276 (0.285). UV (MeOH/ AcONa): 347 (0.068), 266 (0.263).  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  (ppm) = 6.41 (1H, s, H-3); 6.74 (1H, s, H-8); 7.75 (2H, d,  $J=8.4$ , H-2', H-6'); 6.68 (2H, d,  $J=8.4$ , H-3', H-5'); 5.52 (1H, br.s, H-1''), 1.15 (6H, d,  $J=5.2$ , H-6'', H-6'''), 5.28 (1H, br.s, H-1'''), 3.00-4.00 (overlapped remaining protons of sugars).  $^{13}\text{C NMR}$  (125 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  (ppm) = 162.1 (C, C-2); 102.2 (CH, C-3); 178.2 (C, C-4); 158.2 (C, C-5); 134.8 (C, C-6); 161.4 (C, C-7); 94.8 (CH, C-8); 156.5 (C, C-9); 106.3 (C, C-10); 120.2 (C, C-1'); 131.1 (CH, C-2', C-6''); 116.0 (CH, C-3', C-5'), 161.5 (C, C-4'), 99.9 (CH, C-1''), 79.5 (CH, C-2''), 70.7 (CH, C-3''), 72.0 (CH, C-4''), 70.5 (CH, C-5''), 17.9 ( $\text{CH}_3$ , C-6''), 98.8 (CH, C-1'''), 71.1 (CH, C-2'''), 71.6 (CH, C-3'''), 72.8 (CH, C-4'''), 70.6 (CH, C-5'''), 18.4 ( $\text{CH}_3$ , C-6'''). HRMS: positive ion mode:  $m/z$  579.1692  $[\text{M}+\text{H}]^+$ , negative ion mode:  $m/z$  577.1608  $[\text{M}-\text{H}]^-$ .



S12: COSY spectrum (400 MHz) of compound **2**

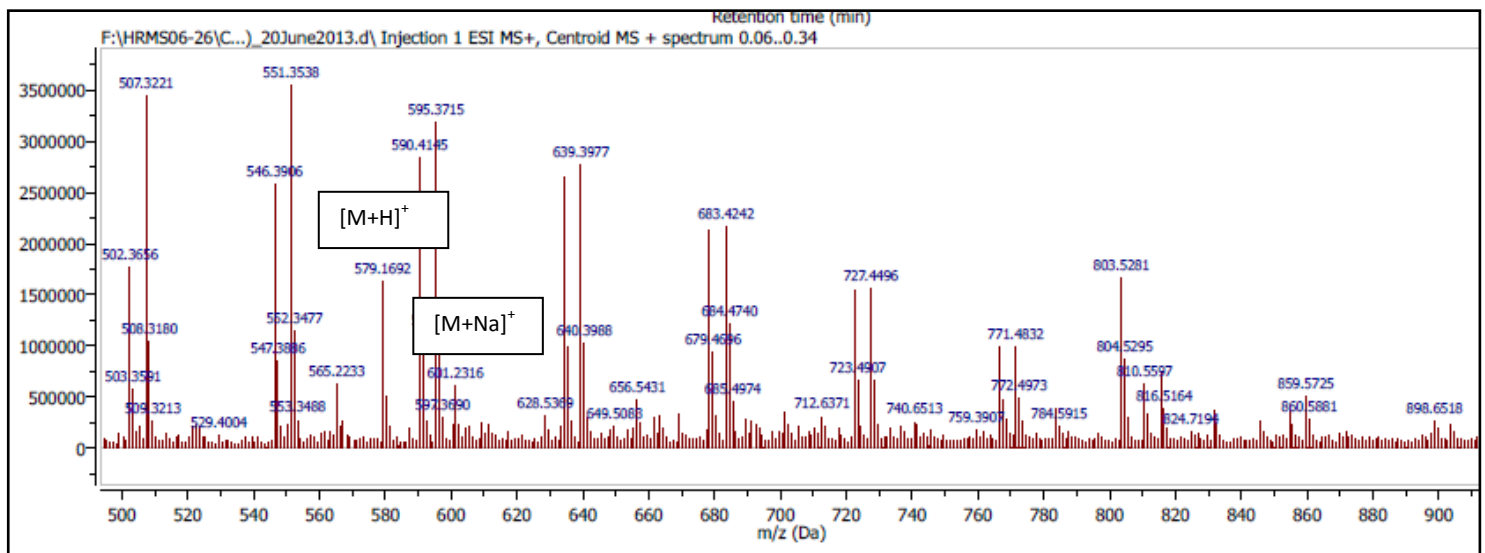
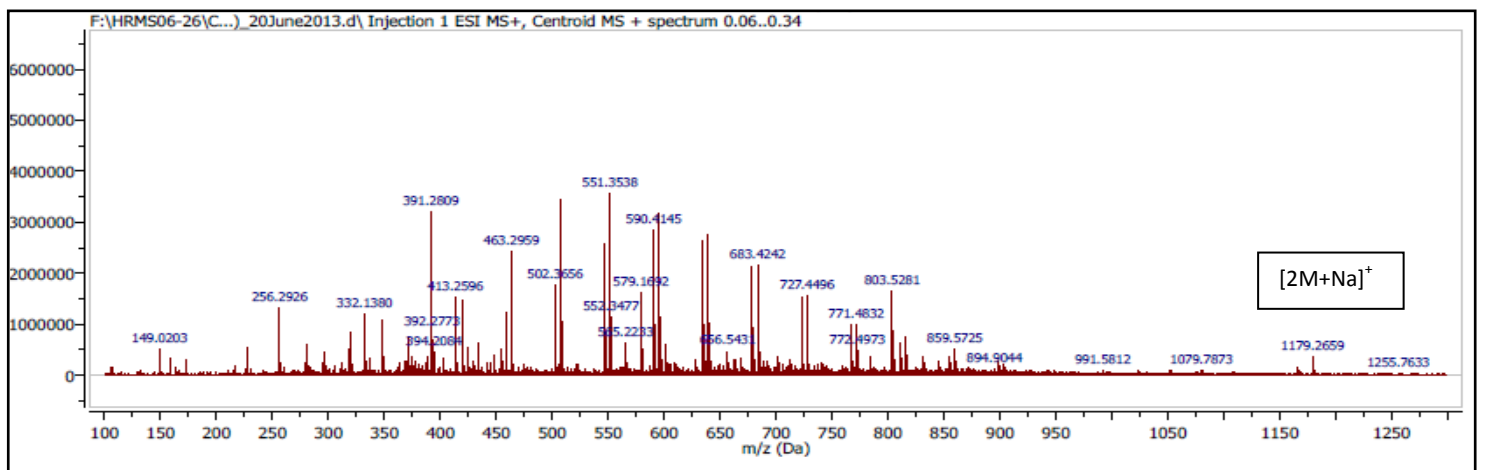


S13: Broad band decoupled  $^{13}\text{C}$ - NMR (100 MHz) of compound **2**

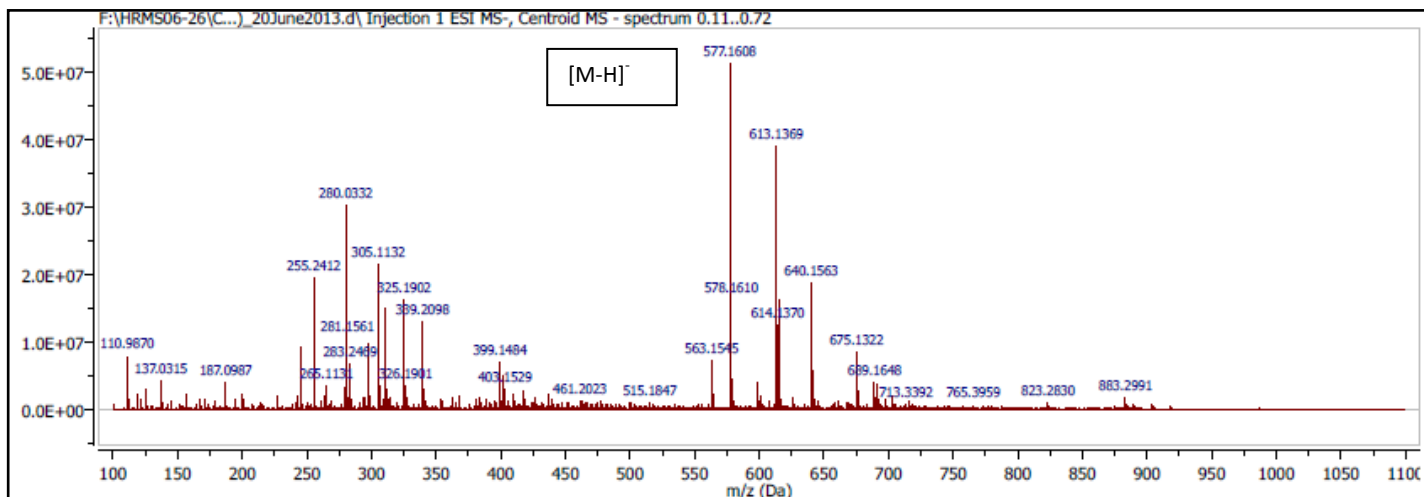


S14: DEPT spectrum of compound **2** (from 15 to 135)





S15: HRESI-MS spectrum of **2** (positive mode)



S16: HRESI-MS spectrum of **2** (negative mode)

