

## Supporting Information

*Rec. Nat. Prod.* 7:3 (2013) 242-244

### Secondary metabolites of *Centaurea cadmea* Boiss.

**Kaveh Alizadeh Astari<sup>1</sup>, Sura Baykan Erel<sup>1</sup>, Erdal Bedir<sup>2</sup> and  
Canan Karaalp<sup>1\*</sup>**

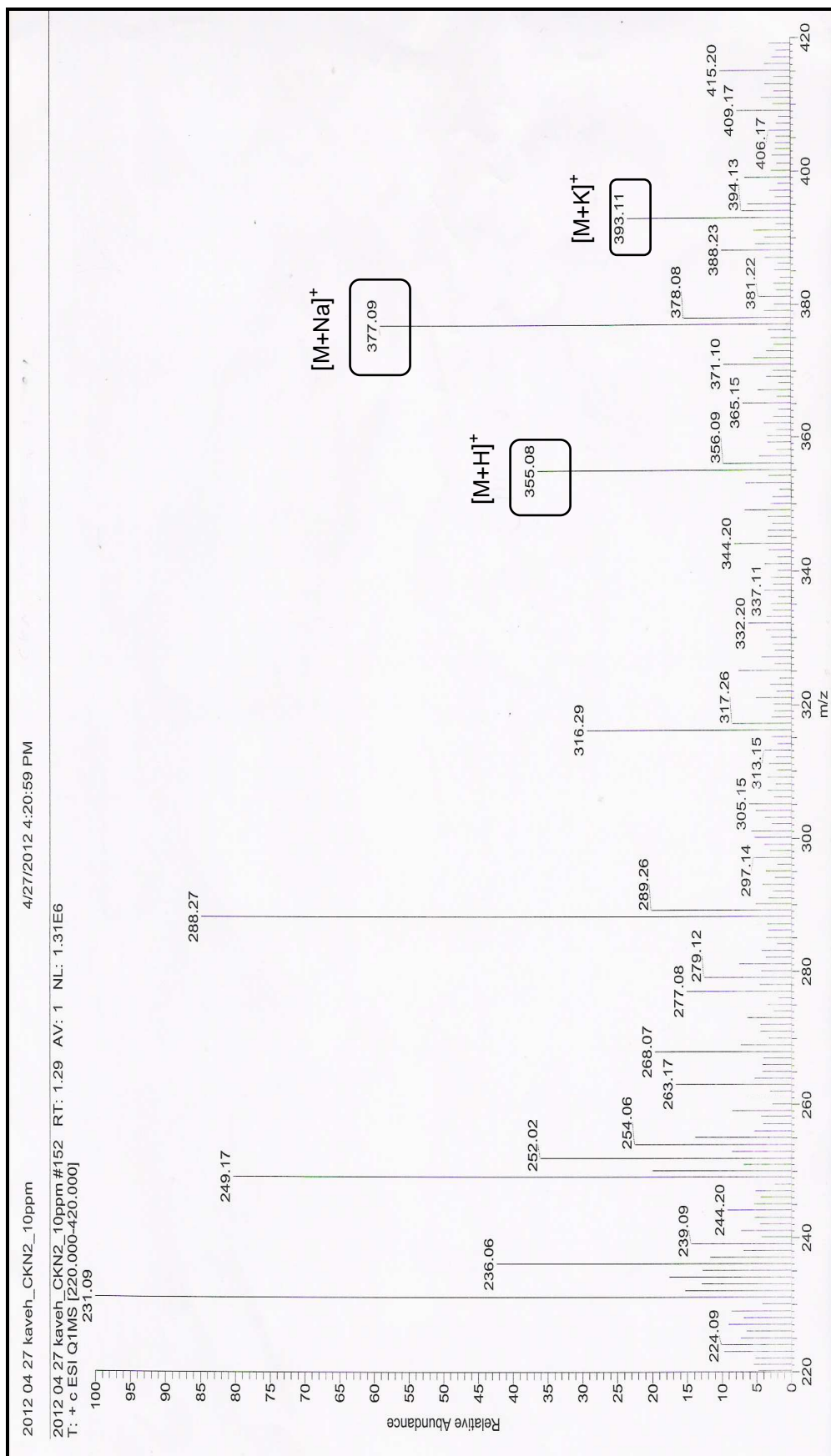
<sup>1</sup>*Department of Pharmaceutical Botany, Faculty of Pharmacy, Ege University,  
35100 Bornova-Izmir, Türkiye*

<sup>2</sup>*Department of Bioengineering, Faculty of Engineering, Ege University, 35100  
Bornova-Izmir, Türkiye*

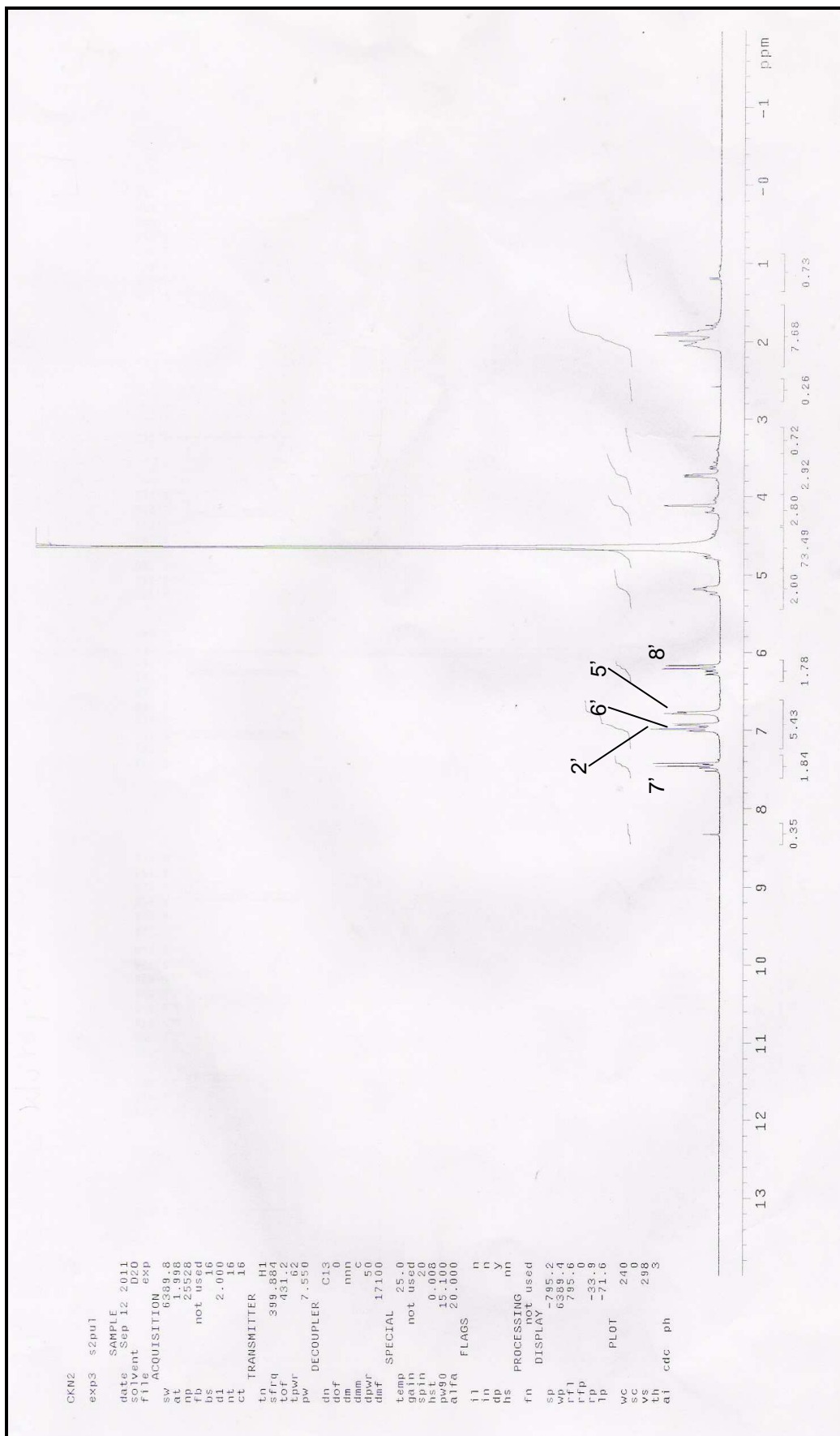
#### Table of contents

<b>S 1:</b> ESI mass spectrum of compound <b>1</b> (chlorogenic acid) .....	3
<b>S 2:</b> <sup>1</sup> H NMR spectrum (D <sub>2</sub> O, 400 MHz) of compound <b>1</b> (chlorogenic acid).....	4
<b>S 3:</b> <sup>13</sup> C NMR spectrum (D <sub>2</sub> O, 100 MHz) of compound <b>1</b> (chlorogenic acid).....	5
<b>S 4:</b> ESI mass spectrum (CD <sub>3</sub> OD, 400 MHz) of compound <b>2</b> (scutellarin). .....	6
<b>S 5:</b> <sup>1</sup> H NMR spectrum (CD <sub>3</sub> OD, 400 MHz) of compound <b>2</b> (scutellarin) .....	7
<b>S 6:</b> <sup>13</sup> C NMR spectrum (DMSO, 100 MHz) of compound <b>2</b> (scutellarin).....	8
<b>S 7:</b> ESI mass spectrum of compound <b>3</b> (syringin) .....	9
<b>S 8:</b> <sup>1</sup> H-NMR spectrum (CD <sub>3</sub> OD, 400 MHz) of compound <b>3</b> (syringin) .....	10
<b>S 9:</b> Expansion of the <sup>1</sup> H-NMR spectrum (CD <sub>3</sub> OD, 400 MHz) of compound <b>3</b> (syringin).....	11
<b>S 10:</b> ESI mass spectrum of compound <b>4</b> (roseoside) .....	12
<b>S 11:</b> <sup>1</sup> H NMR spectrum (CD <sub>3</sub> OD, 400 MHz) of compound <b>4</b> (roseoside).....	13
<b>S 12:</b> <sup>13</sup> C NMR spectrum (CD <sub>3</sub> OD, 100 MHz) of compound <b>4</b> (roseoside) .....	14
<b>S 13:</b> Expansion of the <sup>13</sup> C NMR spectrum of (CD <sub>3</sub> OD, 100 MHz) compound <b>4</b> (roseoside).....	15
<b>S 14:</b> COSY spectrum of compound <b>4</b> (roseoside).....	16

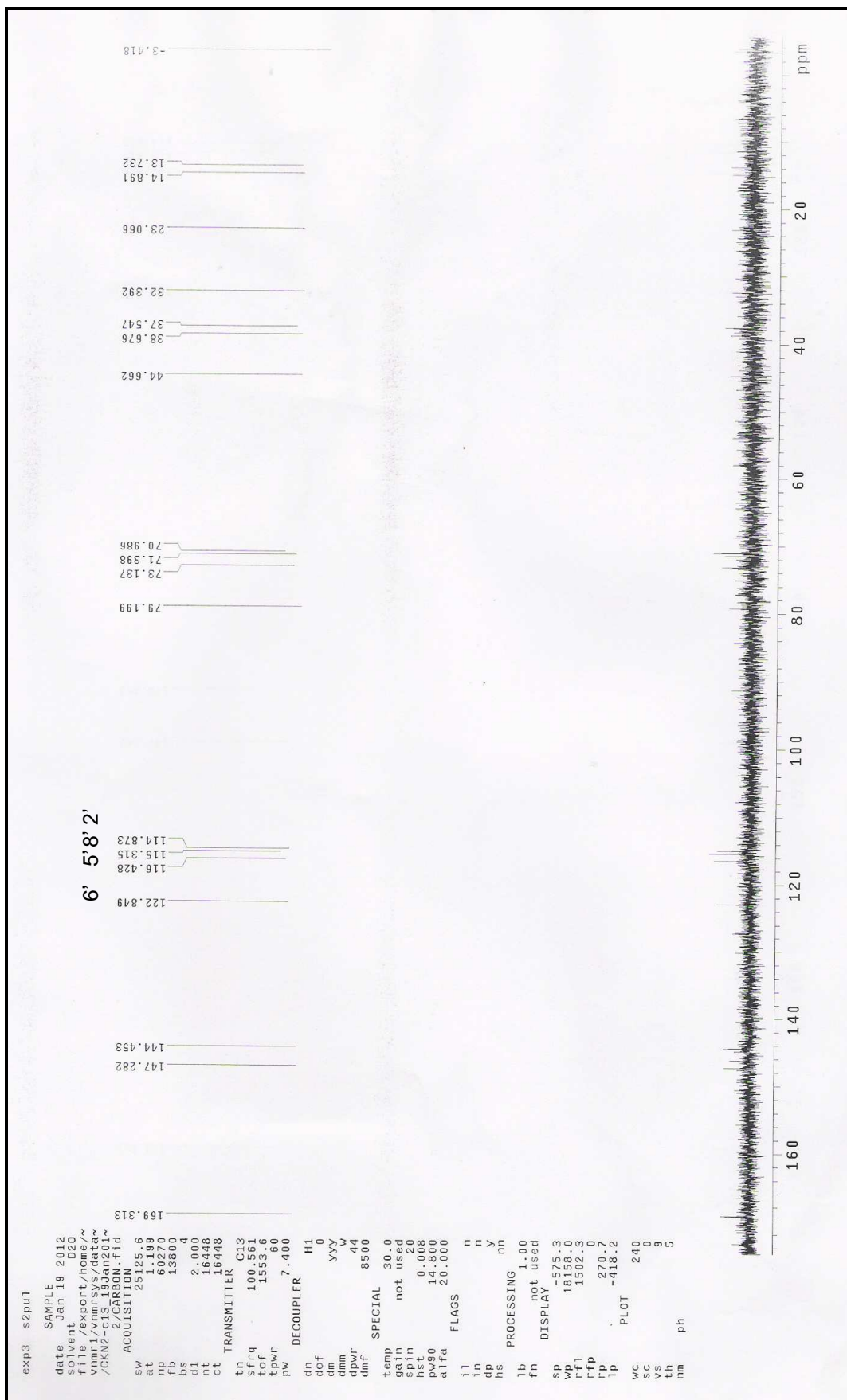
<b>S 15:</b> HMBC spectrum of compound <b>4</b> (roseoside).....	17
<b>S 16:</b> HMQC spectrum of compound <b>4</b> (roseoside) .....	18
<b>Picture 1:</b> TLC profile of compound <b>3</b> (syringin) (silica gel plate, CHCl <sub>3</sub> /MeOH/H <sub>2</sub> O, 61:32:7).....	18
<b>Picture 2:</b> TLC profile of compound <b>5</b> ( $\beta$ -sitosterol-3- <i>O</i> - $\beta$ -D-glucopyranoside) (silica gel plate, CH <sub>2</sub> Cl <sub>2</sub> /MeOH, 9:1) .....	18



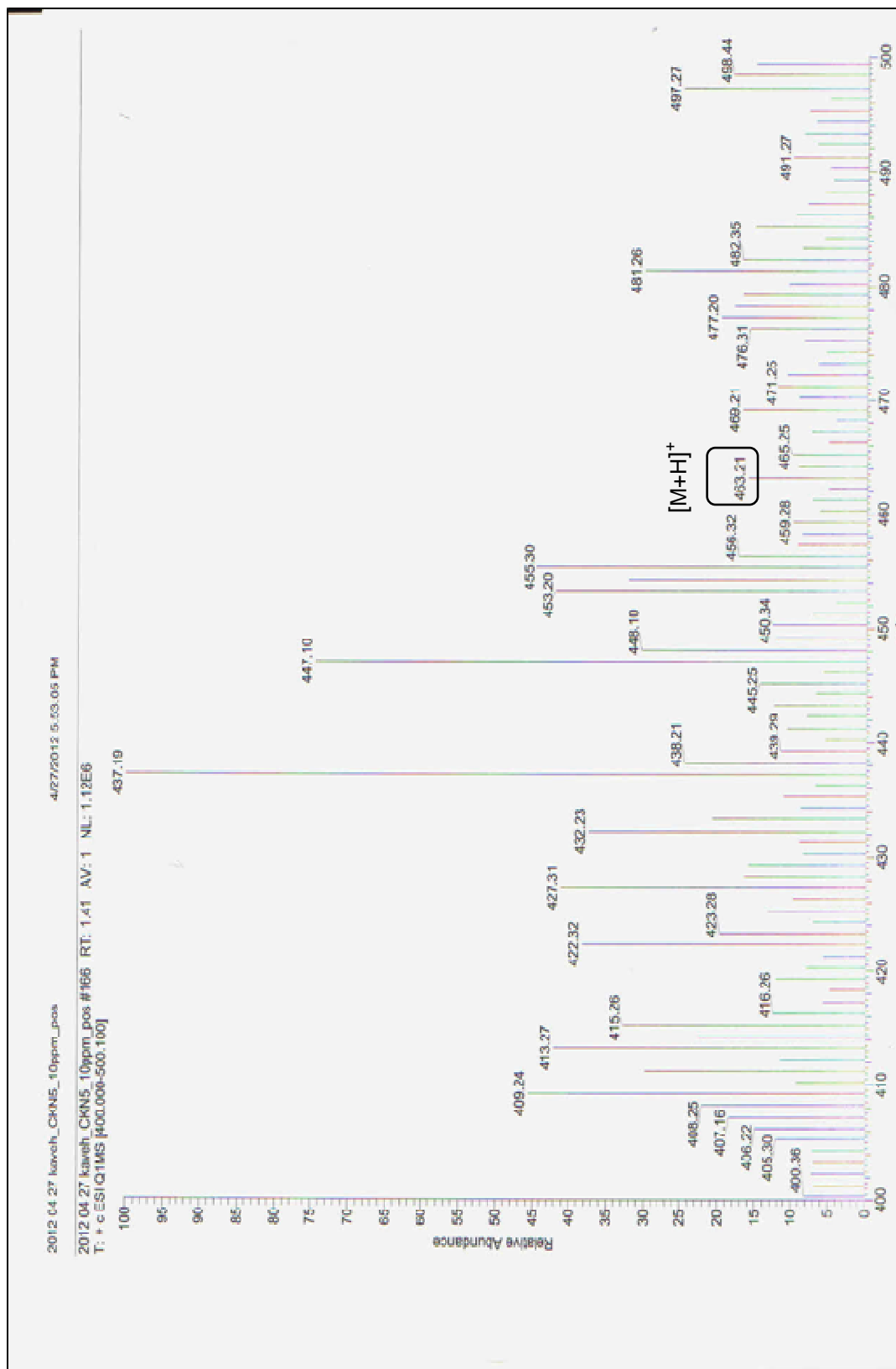
**S 1:** ESI mass spectrum of compound 1 (chlorogenic acid)



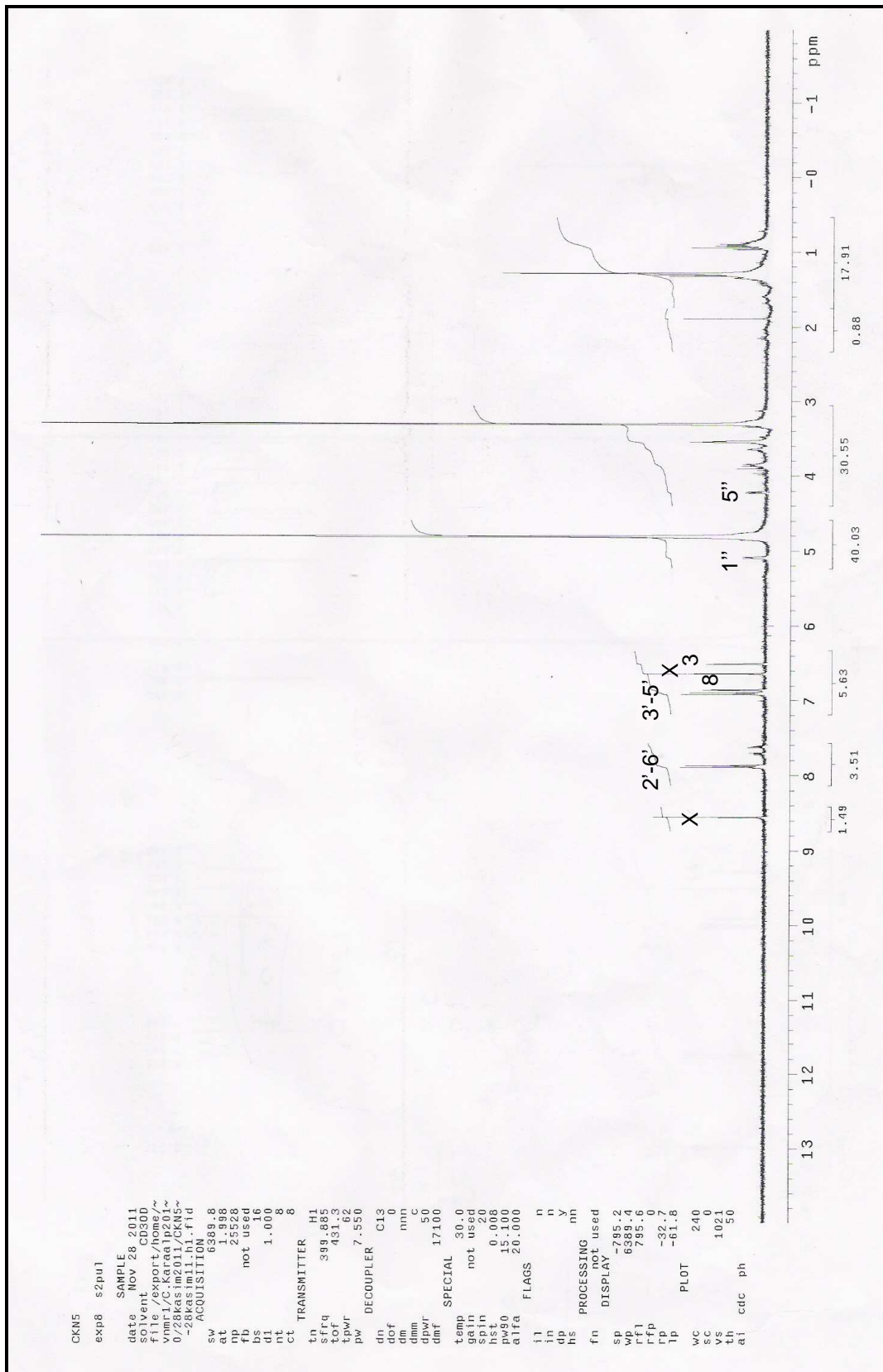
S 2:  $^1\text{H}$  NMR spectrum ( $\text{D}_2\text{O}$ , 400 MHz) of compound 1 (chlorogenic acid)



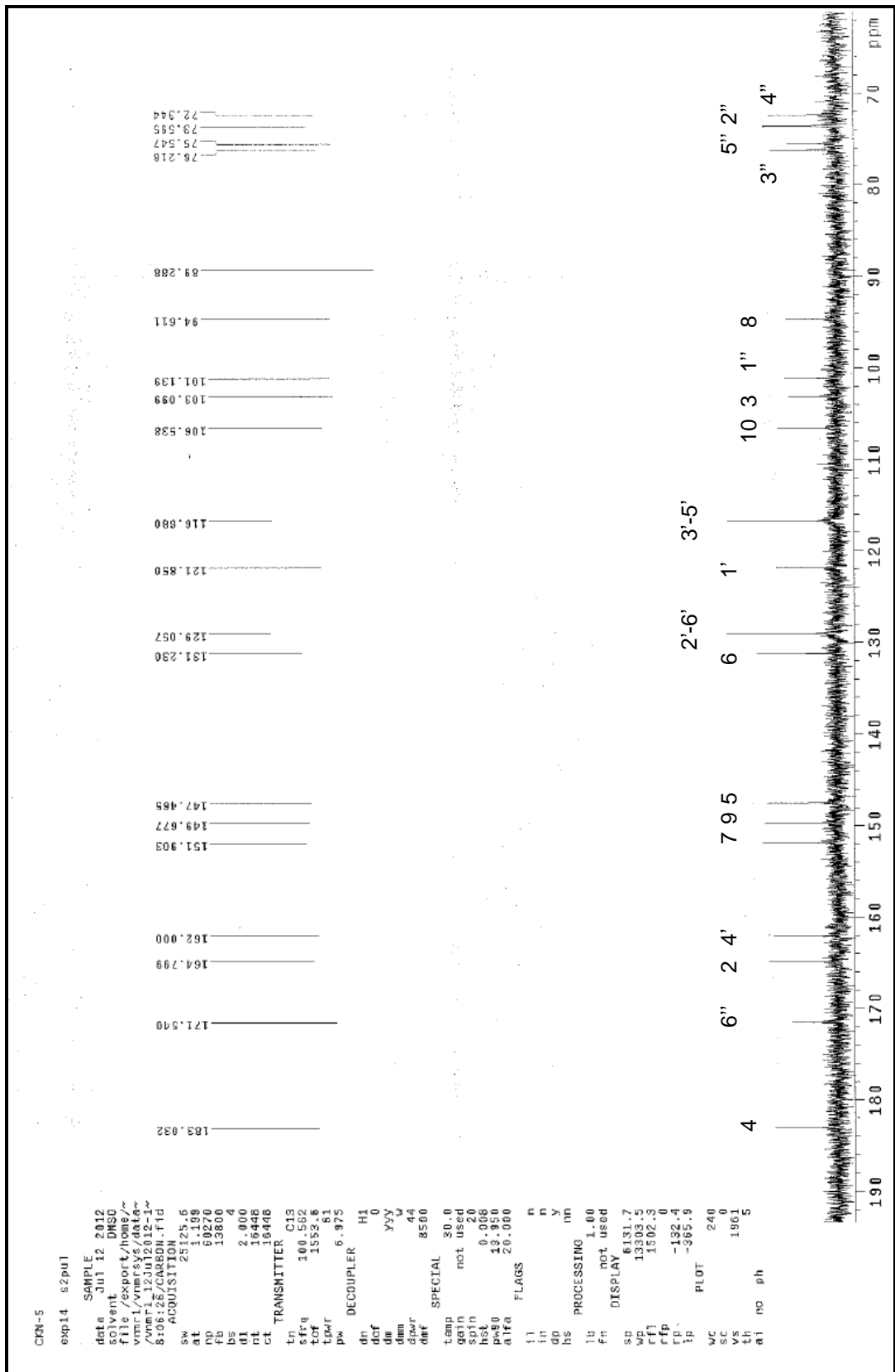
S 3:  $^{13}\text{C}$  NMR spectrum ( $\text{D}_2\text{O}$ , 100 MHz) of compound 1 (chlorogenic acid)



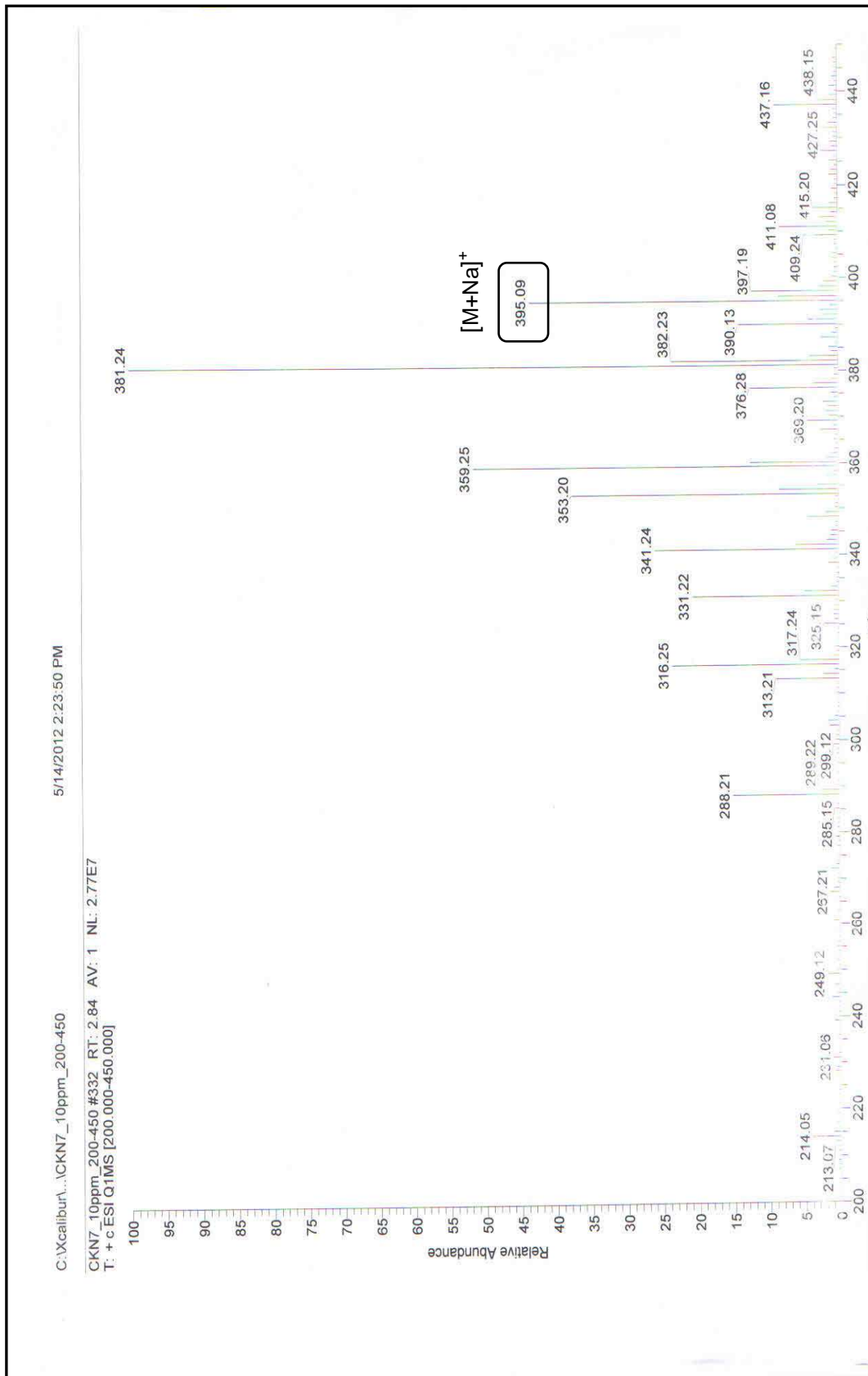
**S 4:** ESI mass spectrum (CD<sub>3</sub>OD, 400 MHz) of compound 2 (scutellarin).



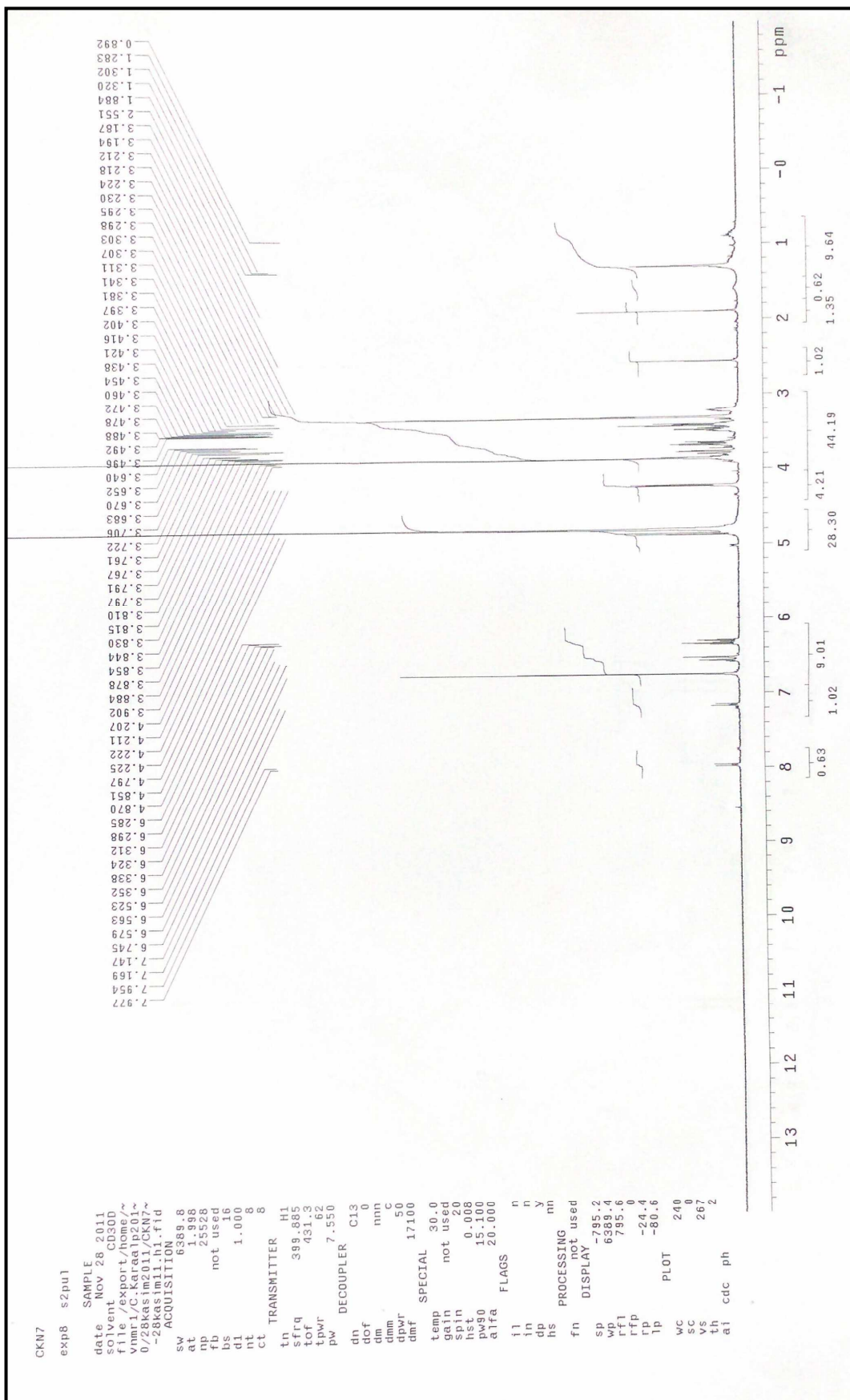
S 5:  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 400 MHz) of compound 2 (scutellarin)



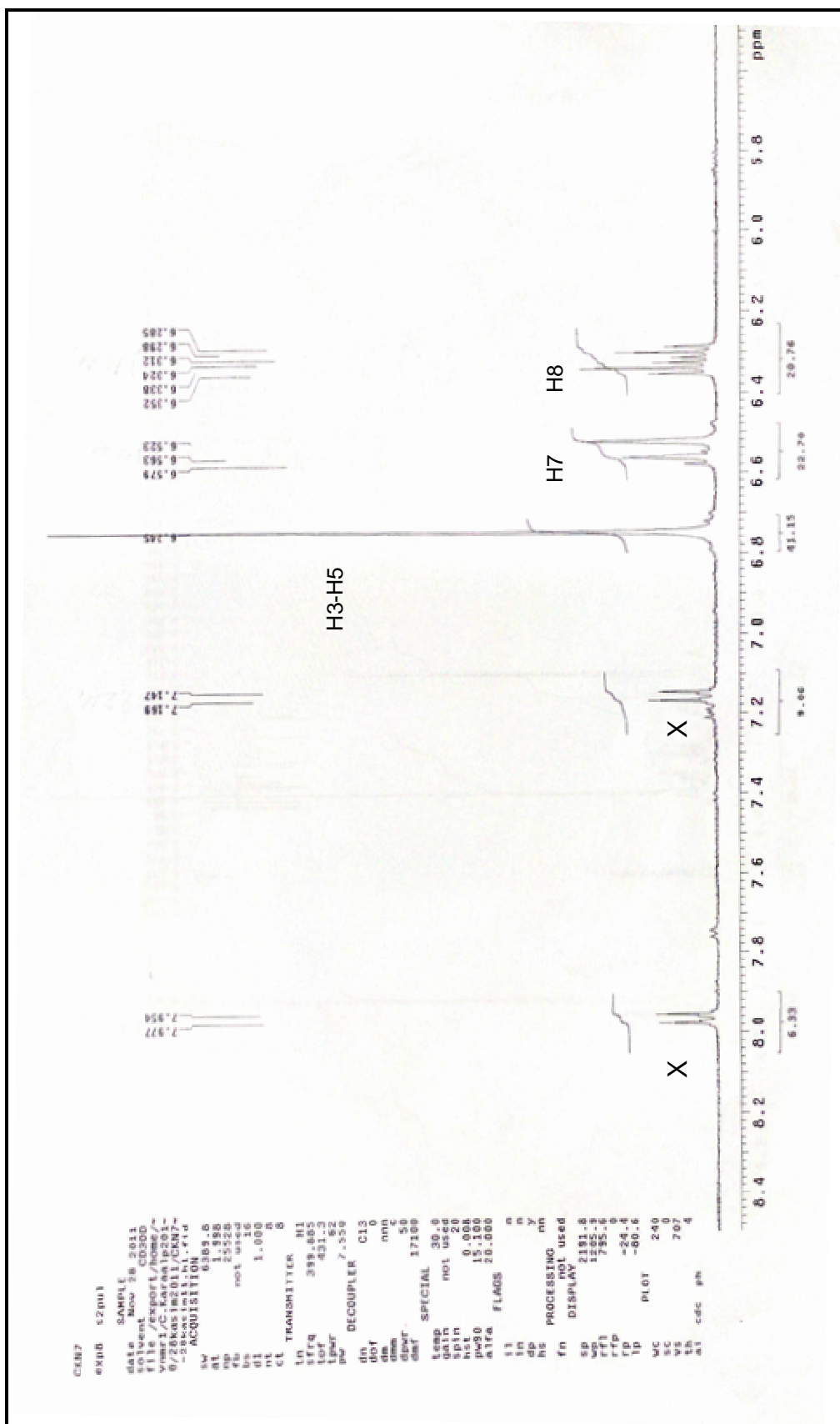




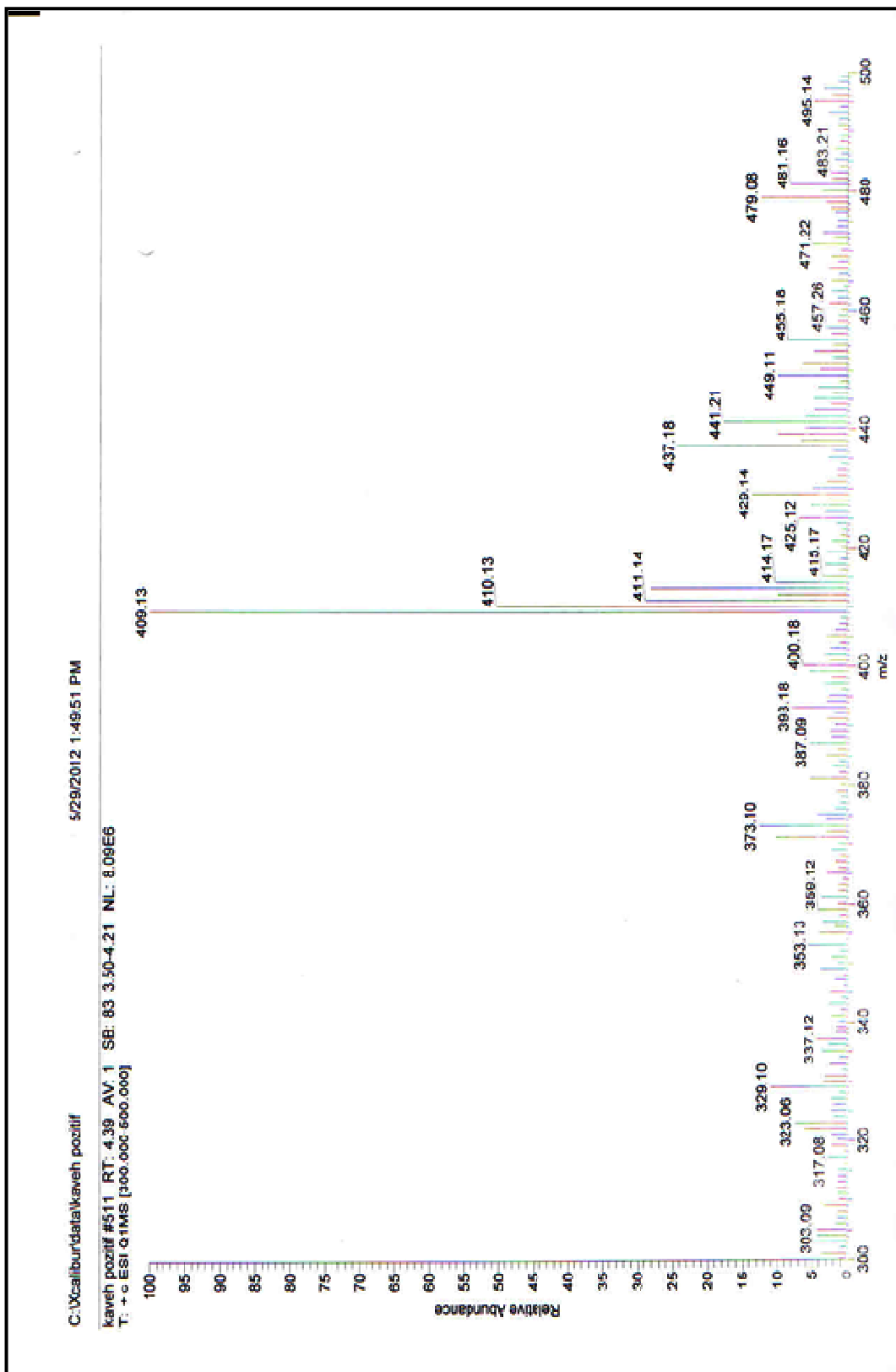
S 7: ESI mass spectrum of compound 3 (syringin)



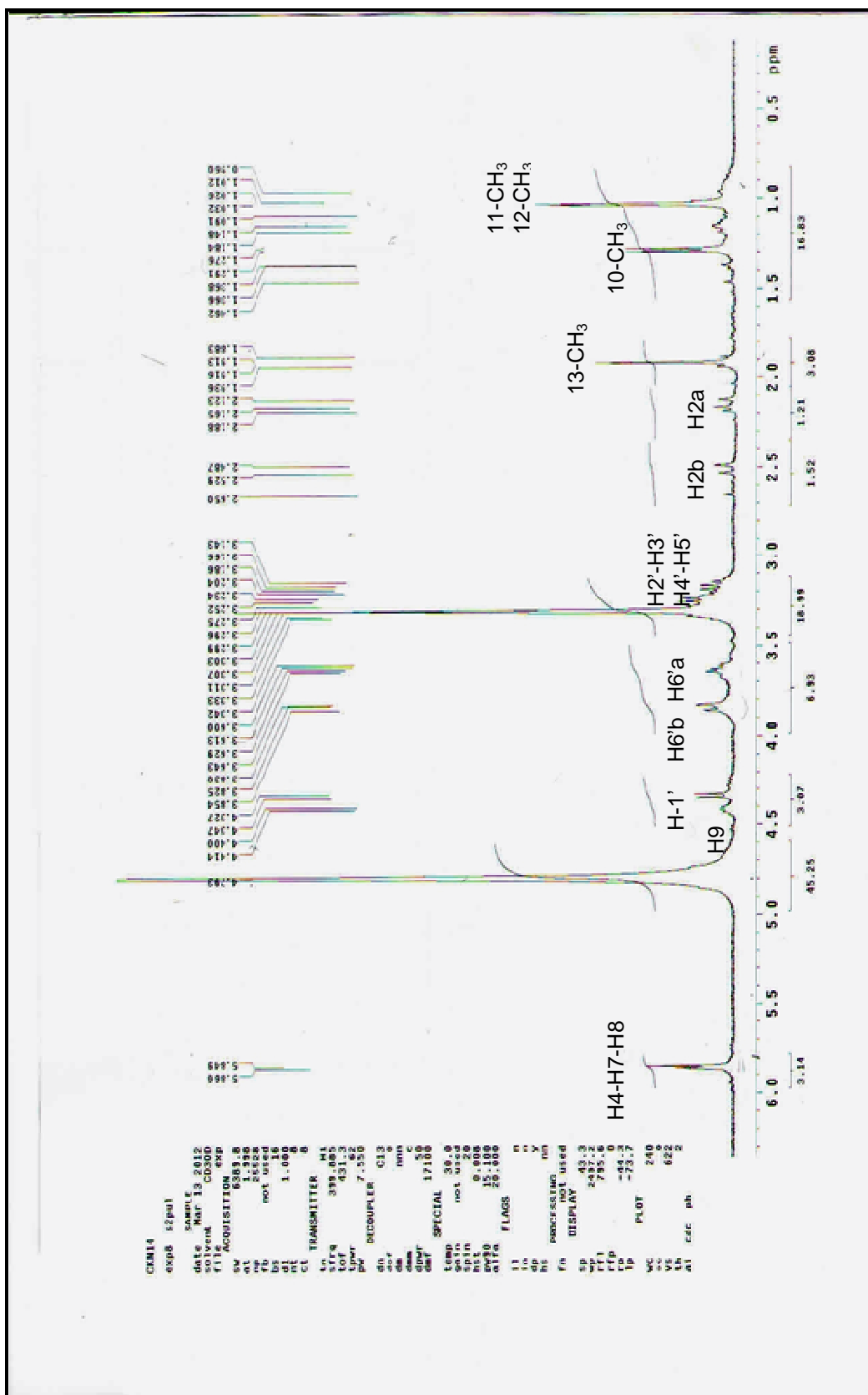
S 8:  $^1\text{H-NMR}$  spectrum ( $\text{CD}_3\text{OD}$ , 400 MHz) of compound 3 (syringin)

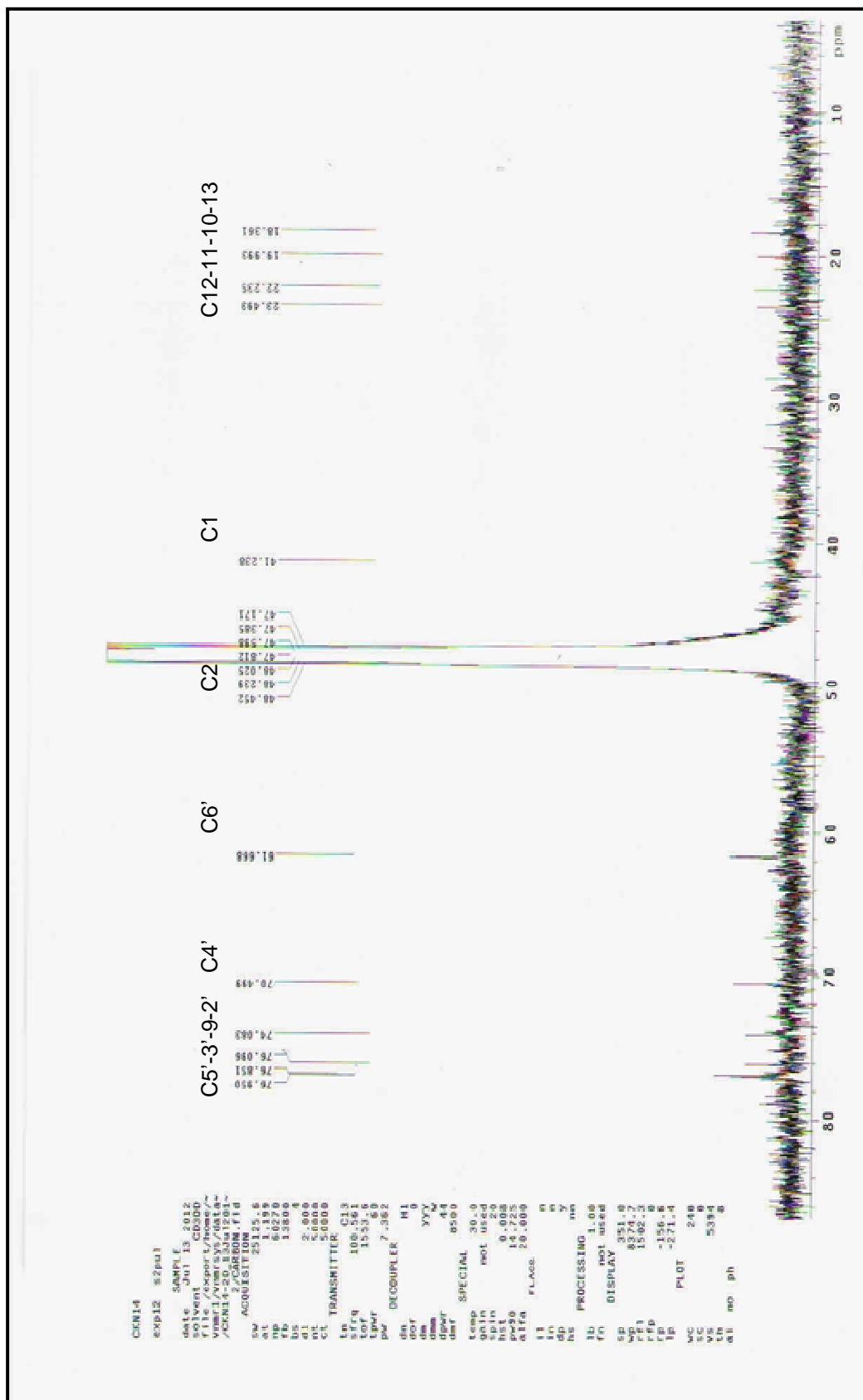


**S 9:** Expansion of the  $^1\text{H-NMR}$  spectrum ( $\text{CD}_3\text{OD}$ , 400 MHz) of compound 3 (syringin)



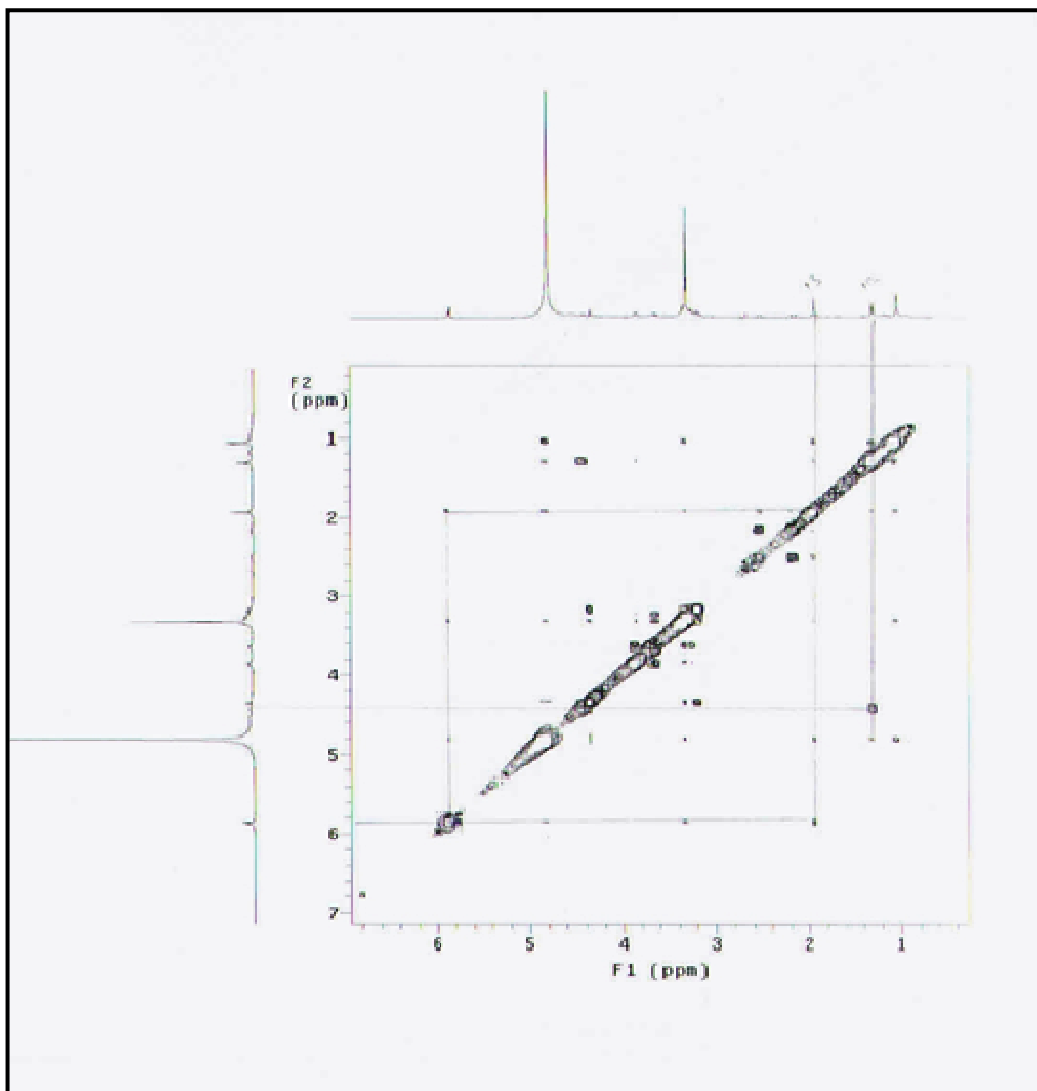
**S 10:** ESI mass spectrum of compound 4 (roseoside)





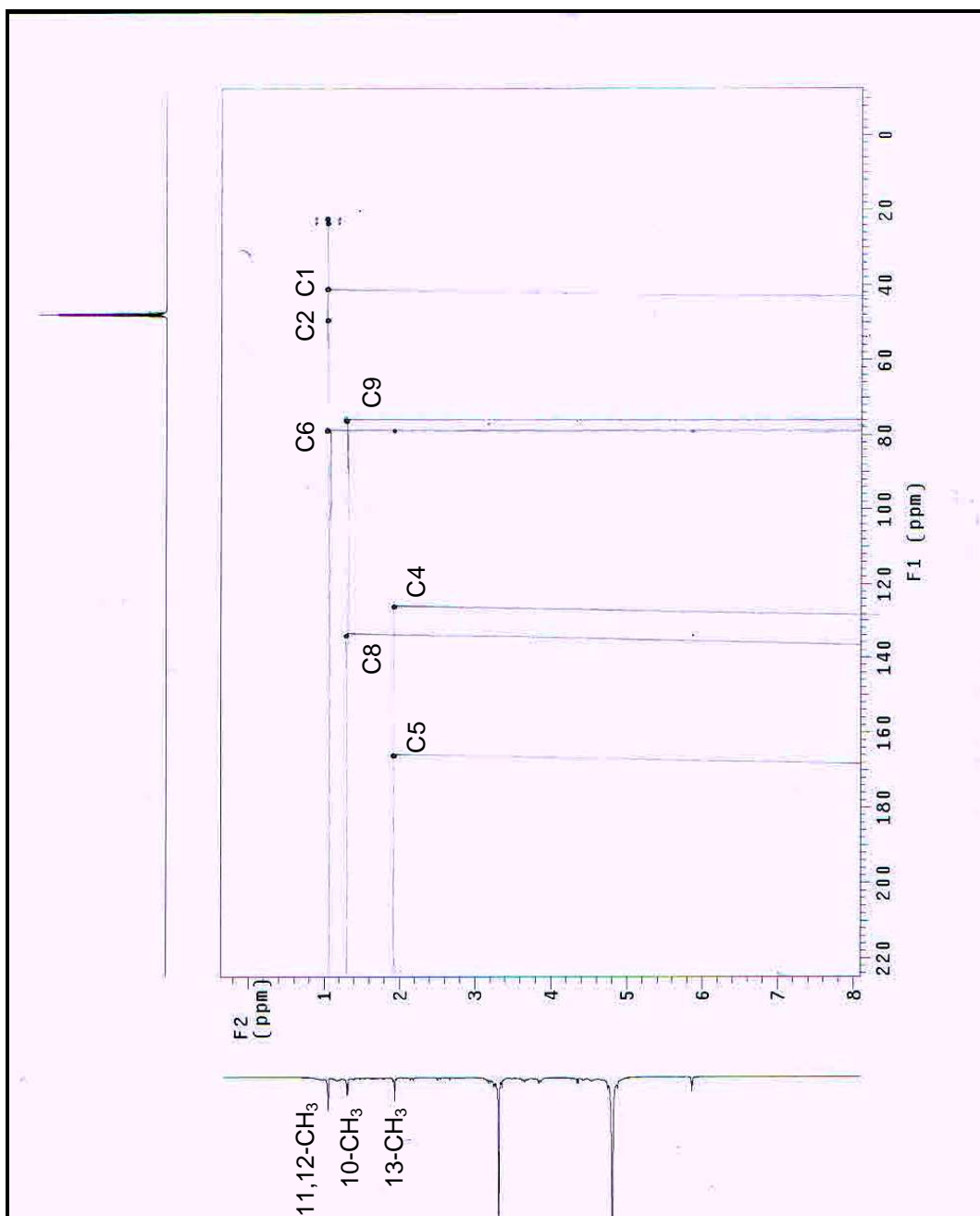
S 12:  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 100 MHz) of compound 4 (roseoside)



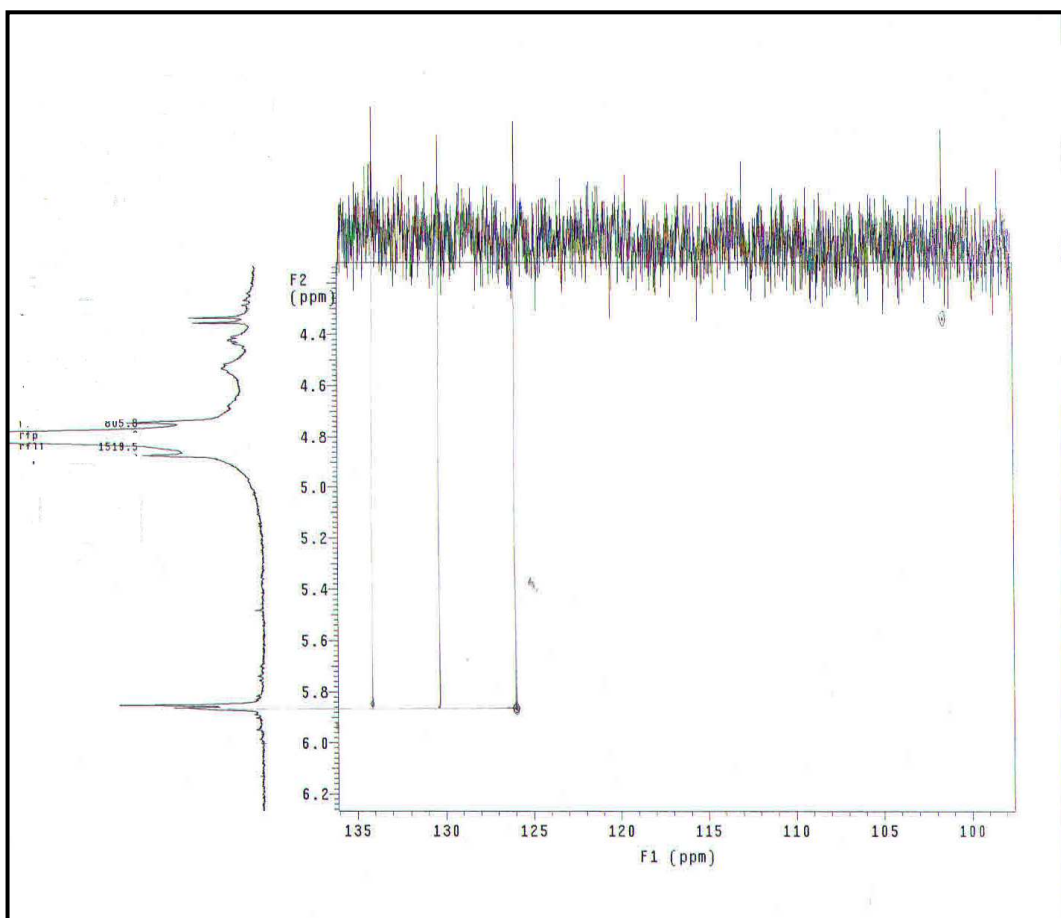


**S 14:** COSY spectrum of compound 4 (roseoside)





S 15: HMBC spectrum of compound 4 (roseoside)



**S 16:** HMQC spectrum of compound 4 (roseoside)



**Picture 1.** TLC profile of compound 3 (syringin)  
 (silica gel plate,  $\text{CHCl}_3/\text{MeOH}/\text{H}_2\text{O}$ , 61:32:7)



**Picture 2.** TIC profile of compound 5 ( $\beta$ -sitosterol-3-*O*- $\beta$ -D-glucopyranoside)  
 (silica gel plate,  $\text{CH}_2\text{Cl}_2/\text{MeOH}$ , 9:1).