

## SUPPLEMENTARY MATERIAL

# Phytotoxic Compounds Isolated from Leaves of the Invasive Weed *Xanthium Spinosum*

Zhuogeng Yuan<sup>1</sup>, Xiangwei Zheng<sup>2</sup>, Yu Zhao<sup>1</sup>, Ying Liu<sup>1</sup>, Shixing Zhou<sup>3</sup>, Caixia Wei<sup>3</sup>, Yunxia Hu<sup>1,\*</sup> and Hua Shao<sup>3,\*</sup>

<sup>1</sup> Yili Normal University, Yining, 835000, China; Emails: yzg821871139@outlook.com (Z.Y.); 2001 zhaoyu@sohu.com(Y.Z.); zylyzhllily@126.com(Y.L.).

<sup>2</sup> Engineering Research Center of Modern Preparation Technology of TCM, Ministry of Education, Shanghai University of Traditional Chinese Medicine, Shanghai,201203, China; Email: zhengxwsh@hotmail.com (X.Z.);

<sup>3</sup> Key Laboratory of Biogeography and Bioresource in Arid Land, Xinjiang Institute of Ecology and Geography, Chinese Academy of Sciences, Urumqi 830011, China; E-Mails:zhoushixing16@mails.ucas.ac.cn (S.Z.); weicaixia16@mails.ucas.ac.cn (C.W.)

\* Correspondence: yunxiahu1214@163.com (Y.H.);shaohua@ms.xjb.ac.cn (H.S.); Tel.: +86-991-7823155

## List of content

- Figure S1.** <sup>1</sup>H NMR spectrum of xanthatin (**1**) (CDCl<sub>3</sub>, 400 MHz).  
**Figure S2.** <sup>13</sup>C NMR spectrum of xanthatin (**1**) (CDCl<sub>3</sub>, 100 MHz).  
**Figure S3.** Mass spectrum of xanthatin (**1**).  
**Figure S4.** <sup>1</sup>H NMR spectrum of 1 $\alpha$ , 5 $\alpha$ -epoxyxanthatin (**2**) (CDCl<sub>3</sub>, 400 MHz).  
**Figure S5.** <sup>13</sup>C NMR spectrum of 1 $\alpha$ , 5 $\alpha$ -epoxyxanthatin (**2**) (CDCl<sub>3</sub>, 100 MHz).  
**Figure S6.** Mass spectrum of 1 $\alpha$ , 5 $\alpha$ -epoxyxanthatin (**2**).  
**Figure S7.** <sup>1</sup>H NMR spectrum of 4-epiisoxanthanol (**3**) (CD<sub>3</sub>OD, 400 MHz).  
**Figure S8.** <sup>13</sup>C NMR spectrum of 4-epiisoxanthanol (**3**) (CD<sub>3</sub>OD, 100 MHz).  
**Figure S9.** Mass spectrum of 4-epiisoxanthanol (**3**).  
**Figure S10.** <sup>1</sup>H NMR spectrum of 4-epixanthanol (**4**) (CD<sub>3</sub>OD, 400 MHz).  
**Figure S11.** <sup>13</sup>C NMR spectrum of 4-epixanthanol (**4**) (CD<sub>3</sub>OD, 100 MHz).  
**Figure S12.** Mass spectrum of 4-epixanthanol (**4**).  
**Figure S13.** <sup>1</sup>H NMR spectrum of loliolide (**5**) (CD<sub>3</sub>OD, 400 MHz).  
**Figure S14.** <sup>13</sup>C NMR spectrum of loliolide (**5**) (CD<sub>3</sub>OD, 100 MHz).  
**Figure S15.** Mass spectrum of loliolide (**5**).  
**Figure S16.** <sup>1</sup>H NMR spectrum of dehydrovomifoliol (**6**) (CD<sub>3</sub>OD, 400 MHz).  
**Figure S17.** <sup>13</sup>C NMR spectrum of dehydrovomifoliol (**6**) (CD<sub>3</sub>OD, 100 MHz).  
**Figure S18.** Mass spectrum of dehydrovomifoliol (**6**) .

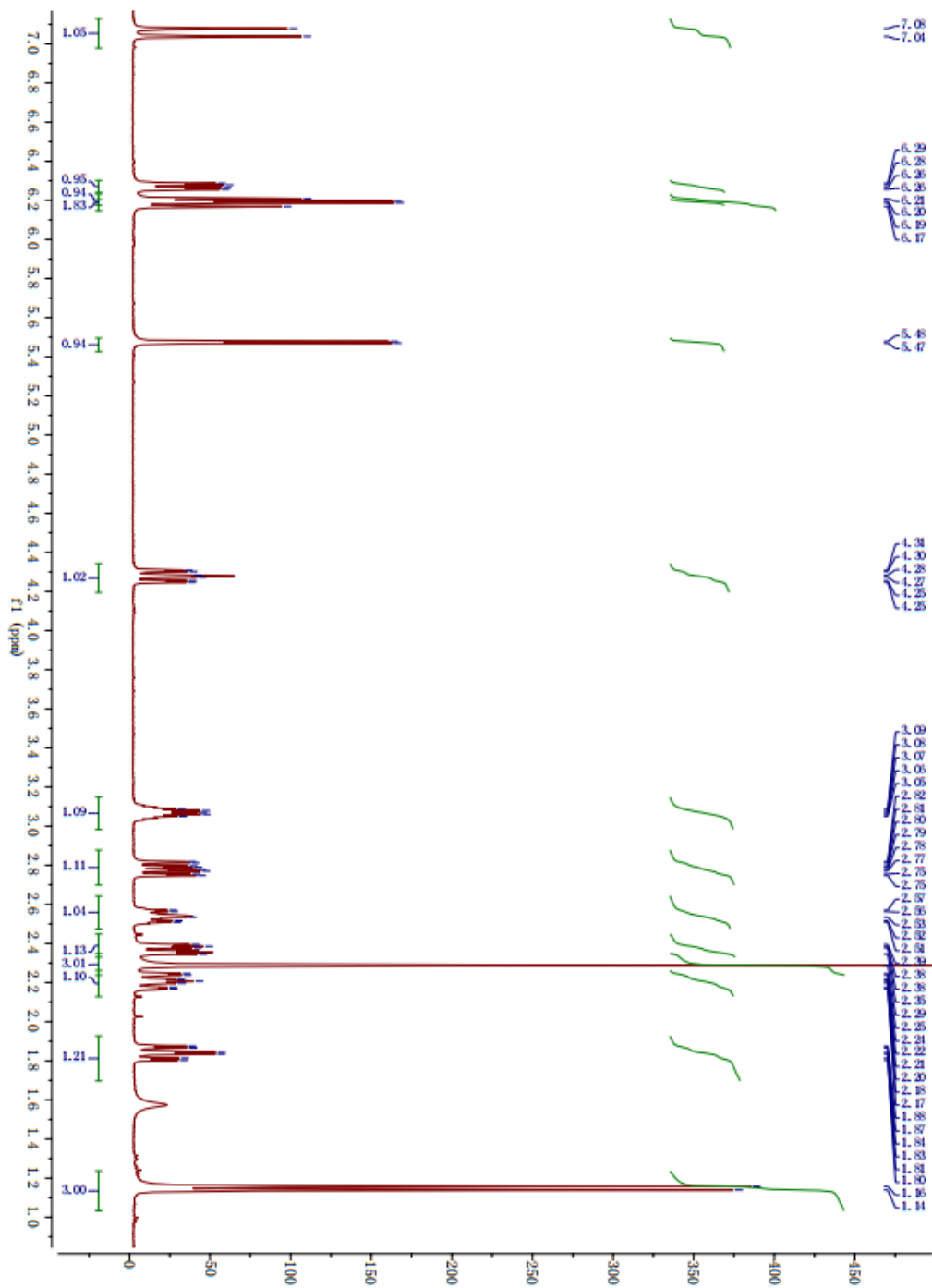
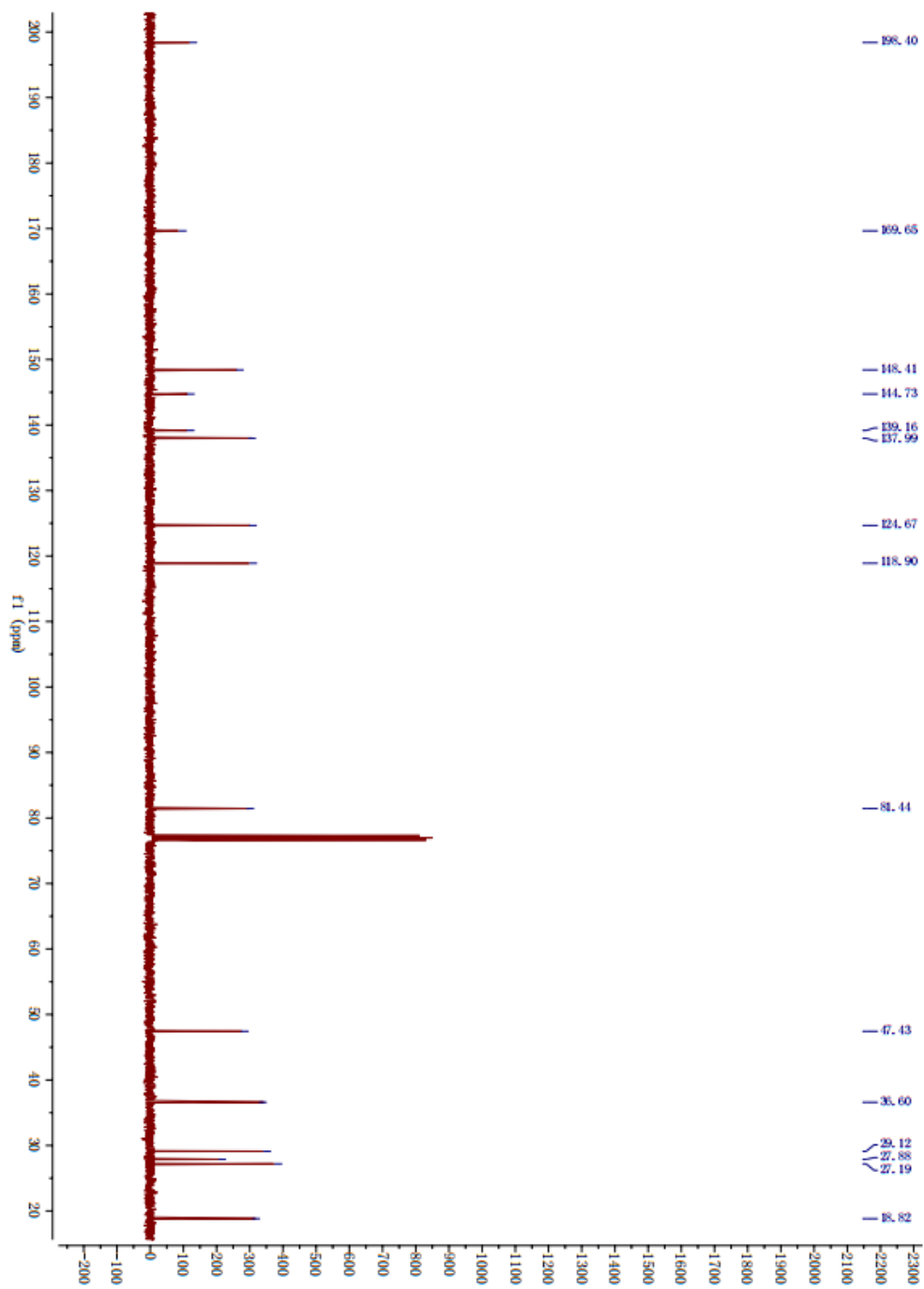
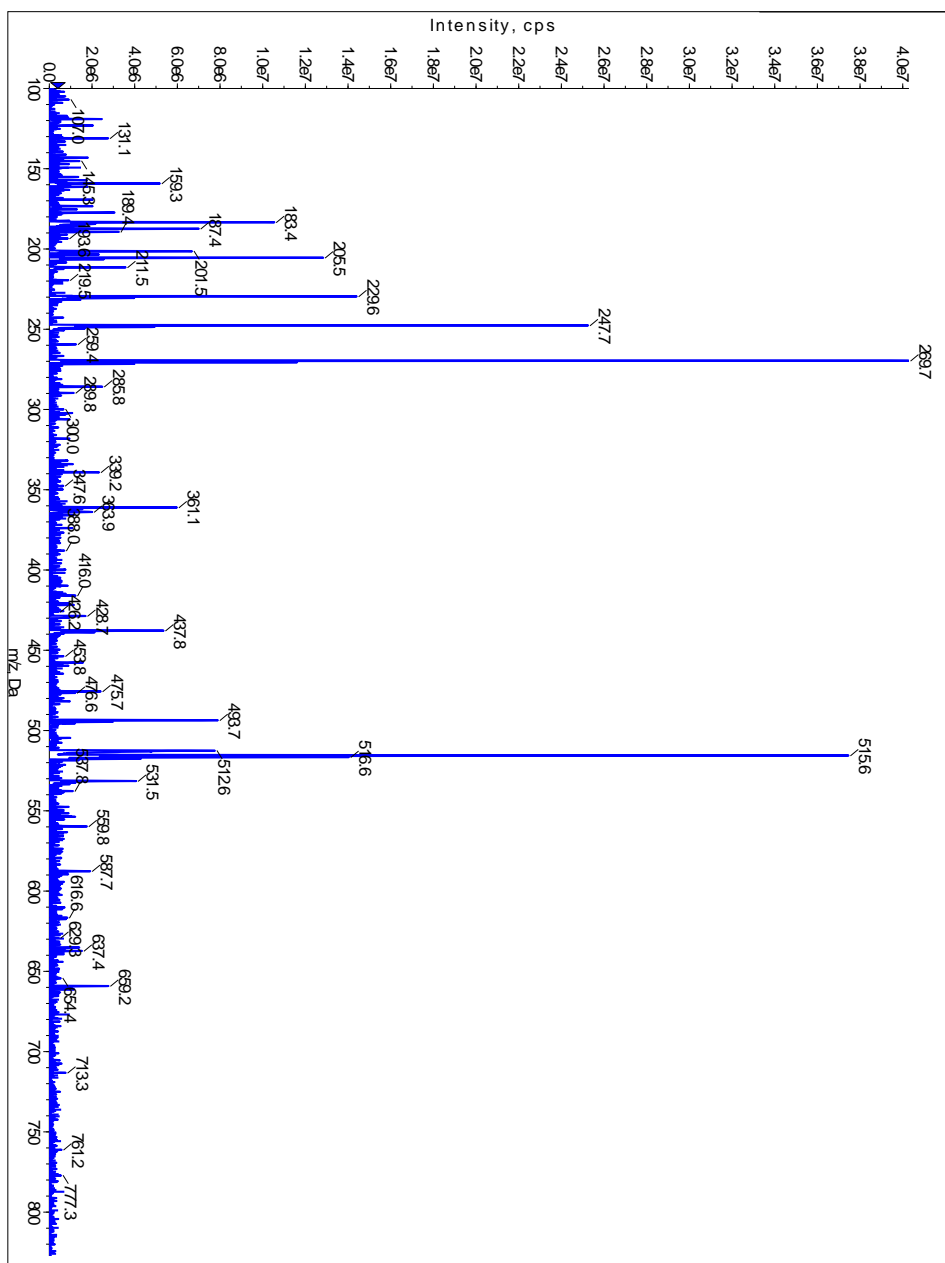


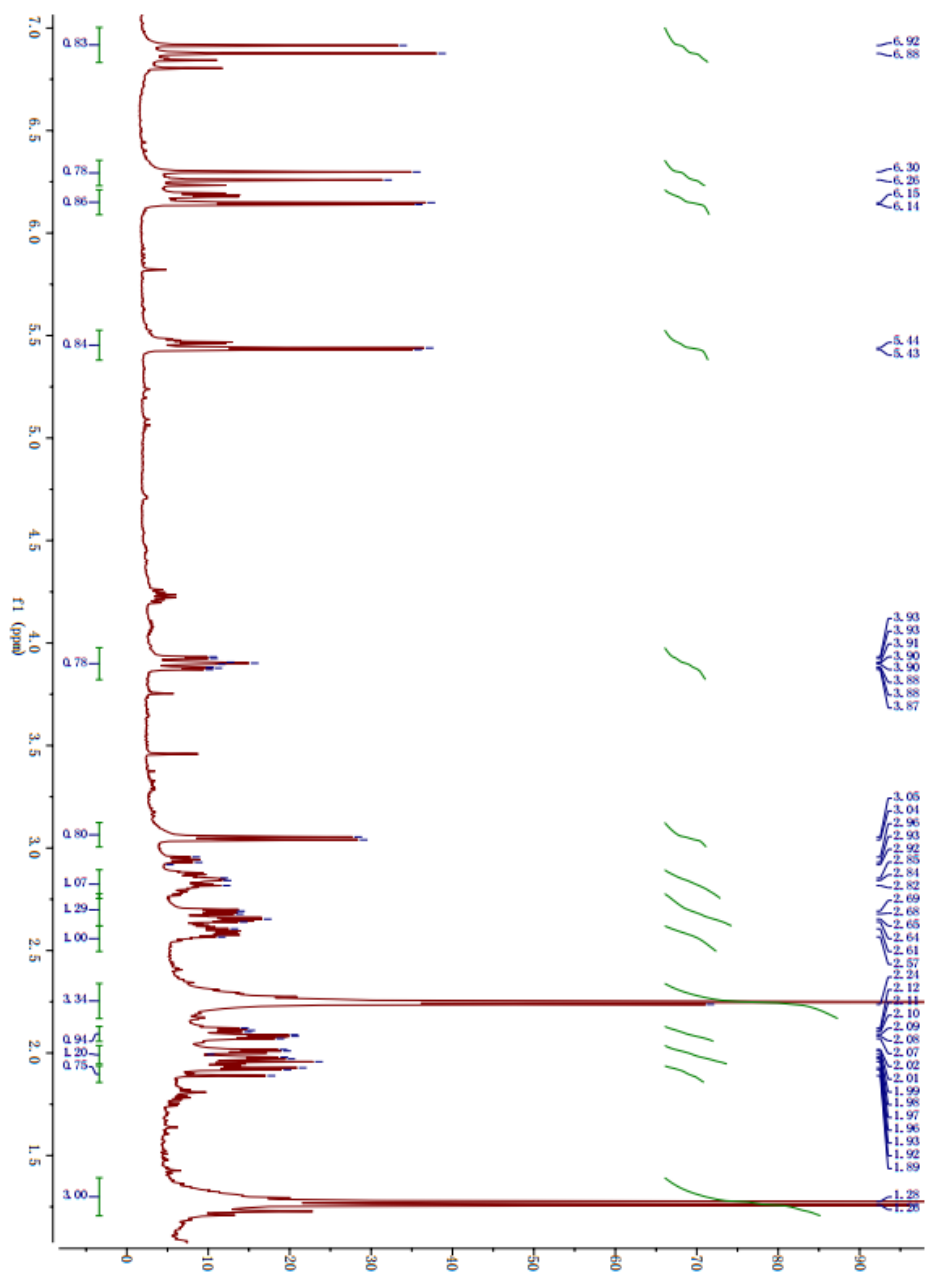
Figure S1.  $^1\text{H}$  NMR spectrum of xanthatin (1) ( $\text{CDCl}_3$ , 400 MHz).



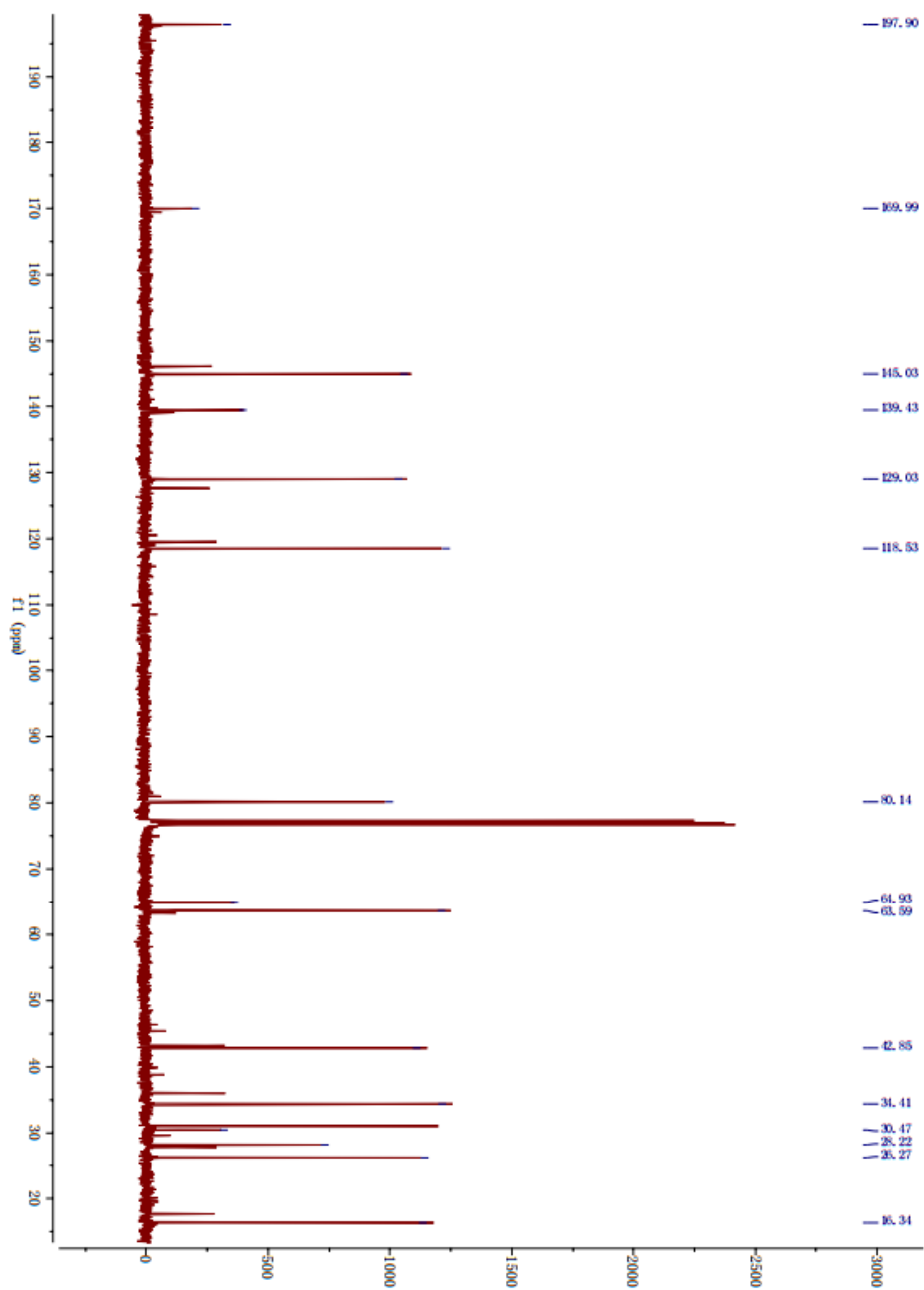
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of xanthatin (1) ( $\text{CDCl}_3$ , 100 MHz).



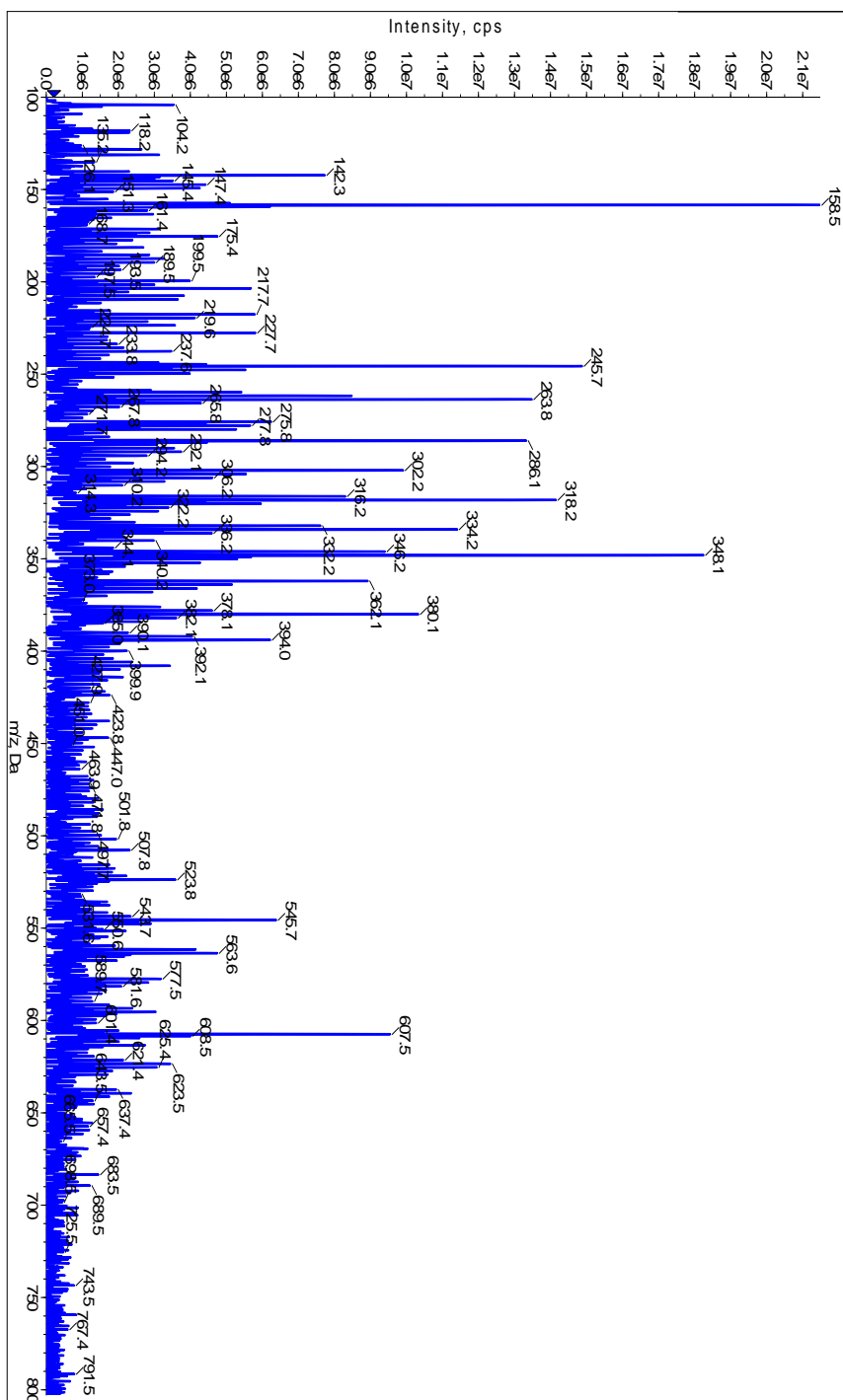
**Figure S3.** Mass spectrum of xanthatin (1).



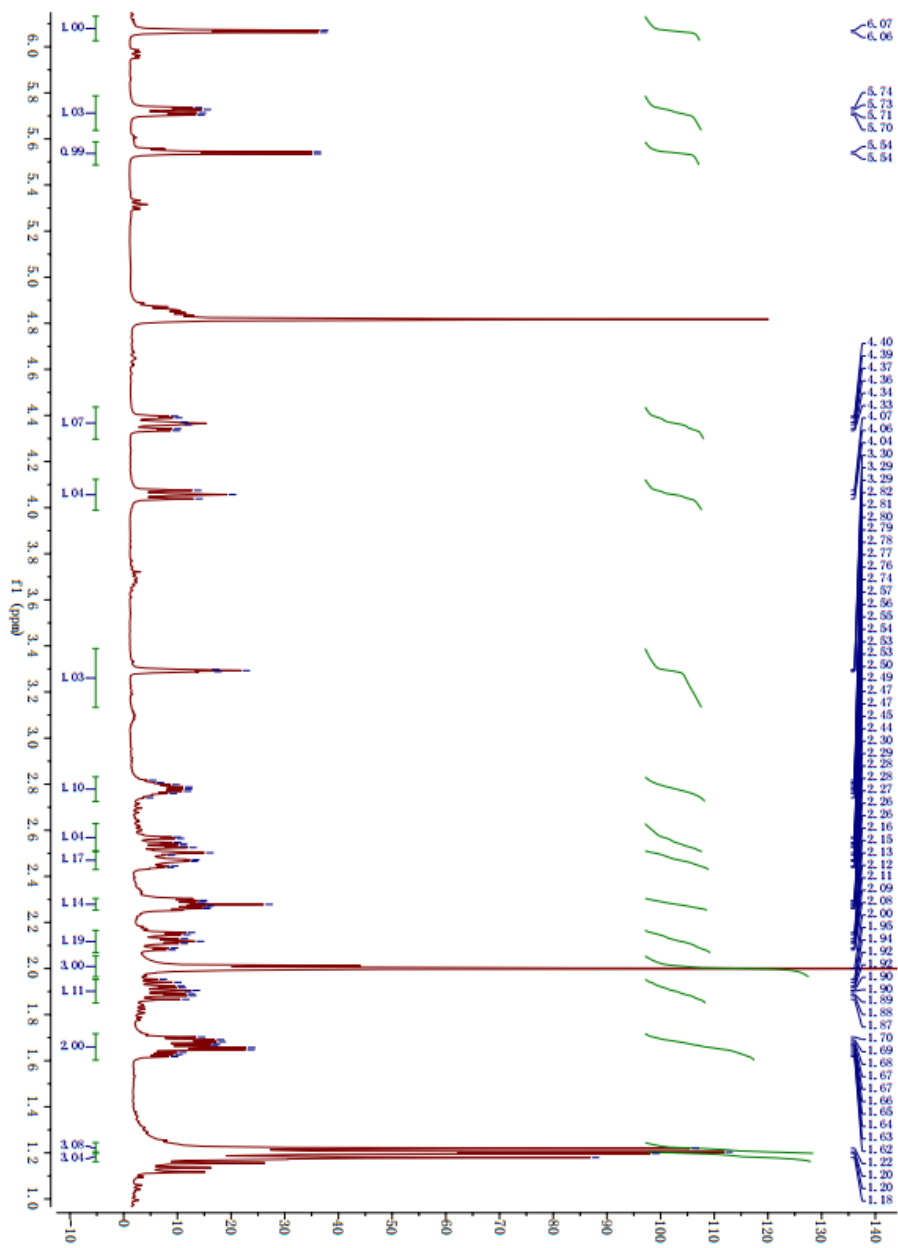
**Figure S4.**  $^1\text{H}$  NMR spectrum of  $1\alpha, 5\alpha$ -epoxyxanthatin (2) ( $\text{CDCl}_3$ , 400 MHz).



**Figure S5.**  $^{13}\text{C}$  NMR spectrum of 1 $\alpha$ , 5 $\alpha$ -epoxyxanthatin (**2**) ( $\text{CDCl}_3$ , 100 MHz).

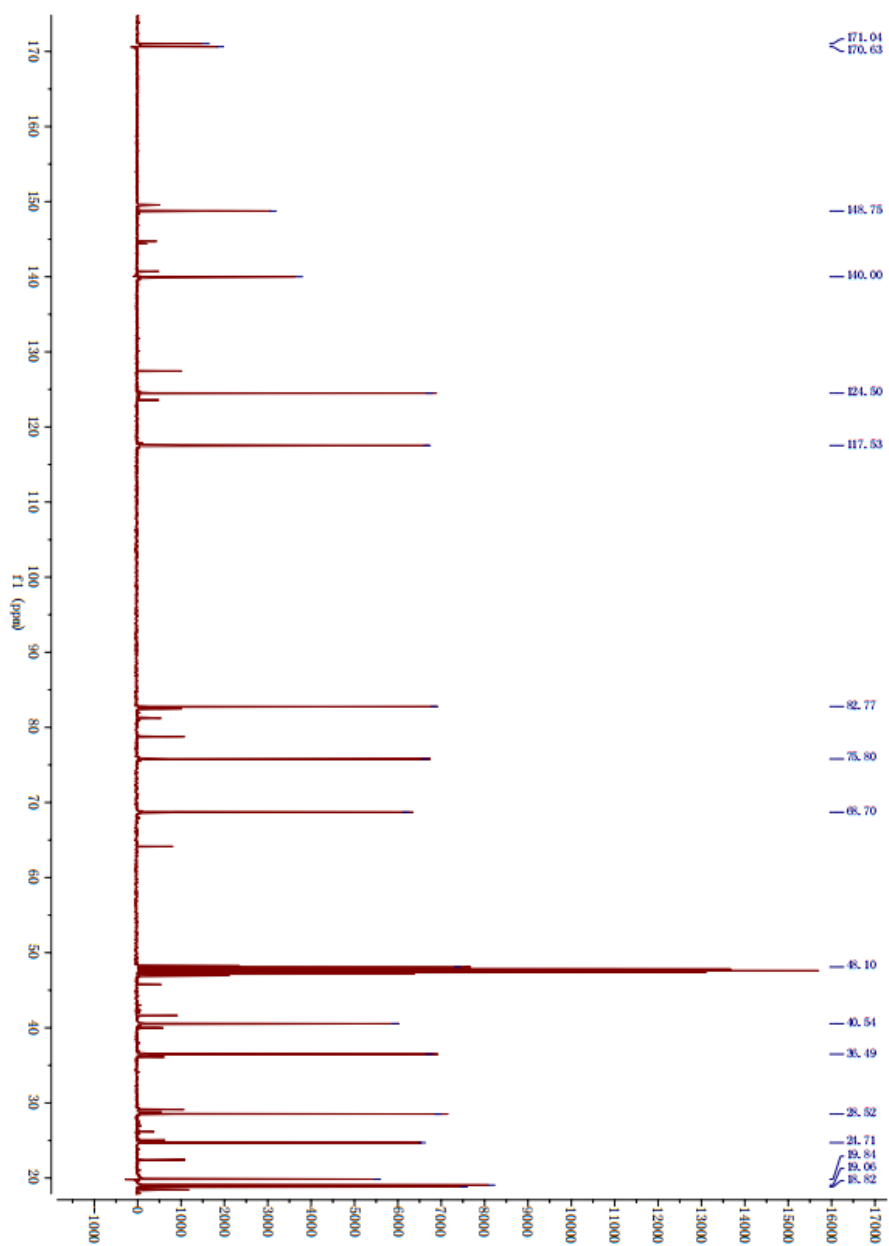


**Figure S6.** Mass spectrum of 1 $\alpha$ , 5 $\alpha$ -epoxyxanthatin (2).

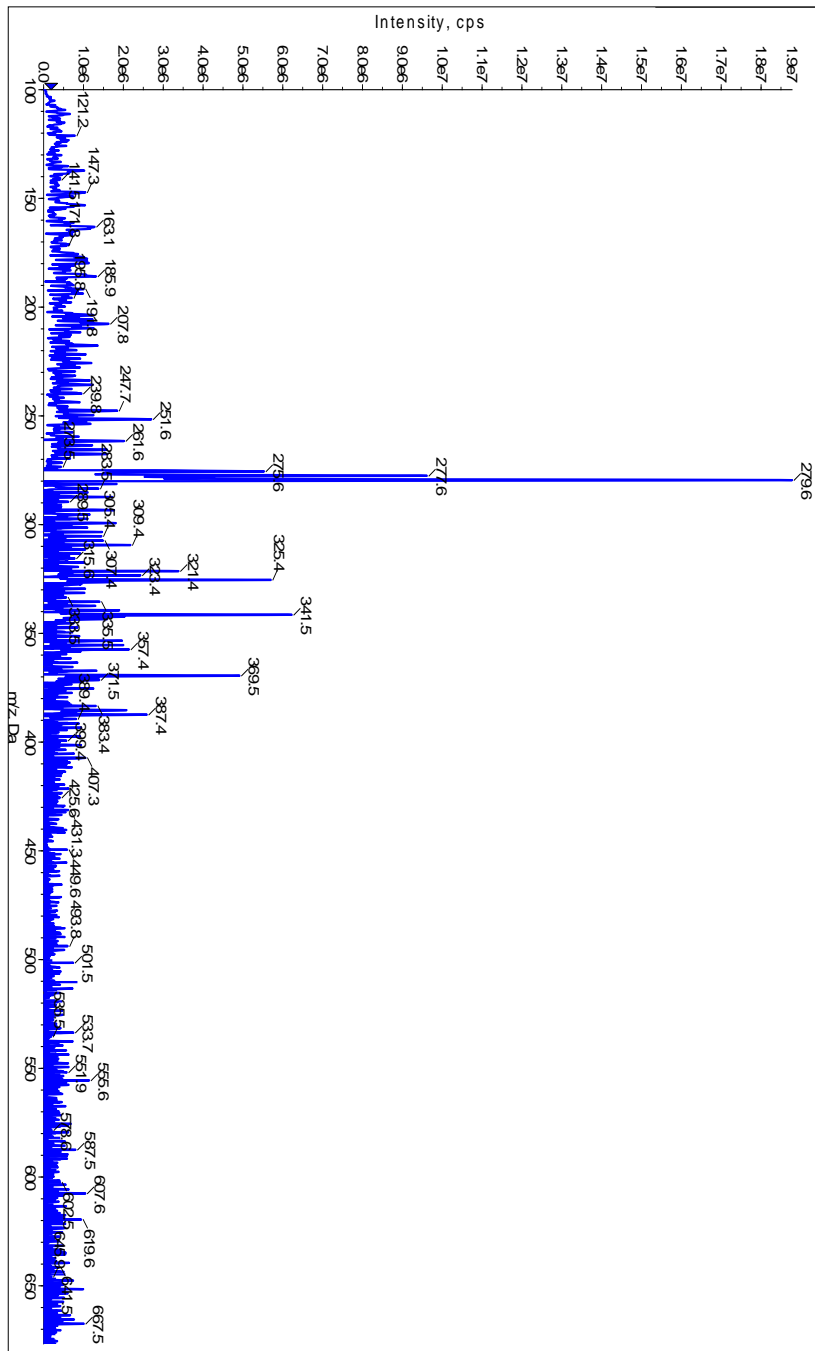


**Figure S7.** <sup>1</sup>H NMR spectrum of 4-epiisoxanthanol (**3**) (CD<sub>3</sub>OD, 400 MHz).

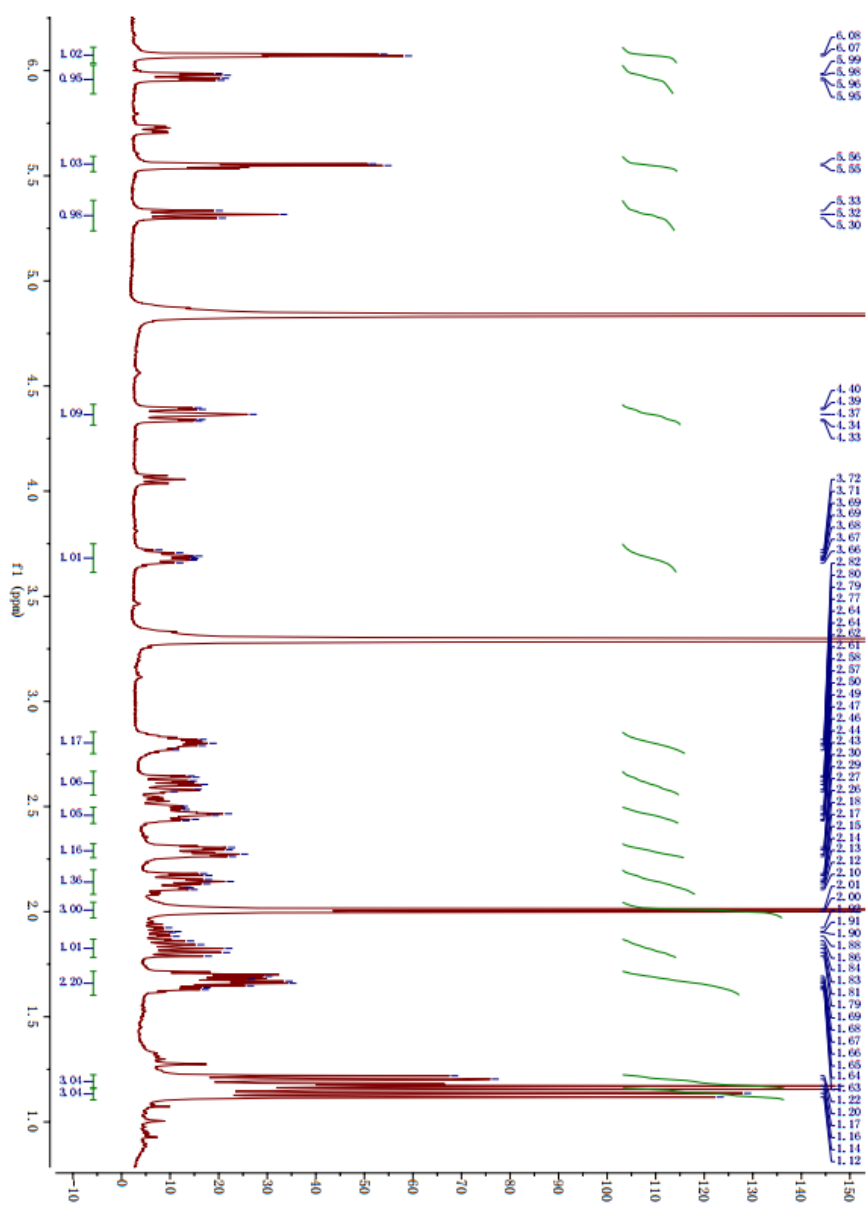




**Figure S8.**  $^{13}\text{C}$  NMR spectrum of 4-epiisoxanthanol (**3**) ( $\text{CD}_3\text{OD}$ , 100 MHz).



**Figure S9.** Mass spectrum of 4-epiisoxanthanol (**3**).



**Figure S10.**  $^1\text{H}$  NMR spectrum of 4-epixanthanol (**4**) ( $\text{CD}_3\text{OD}$ , 400 MHz).

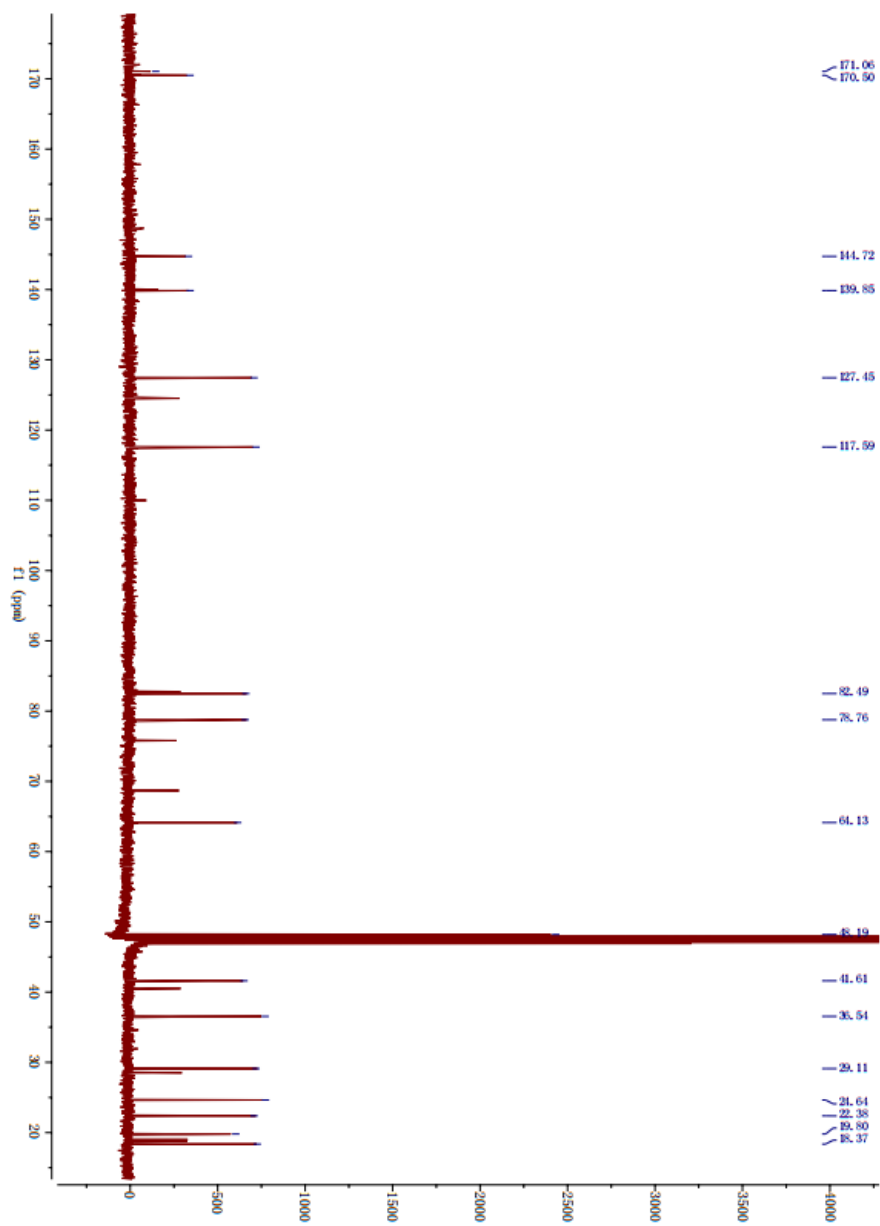
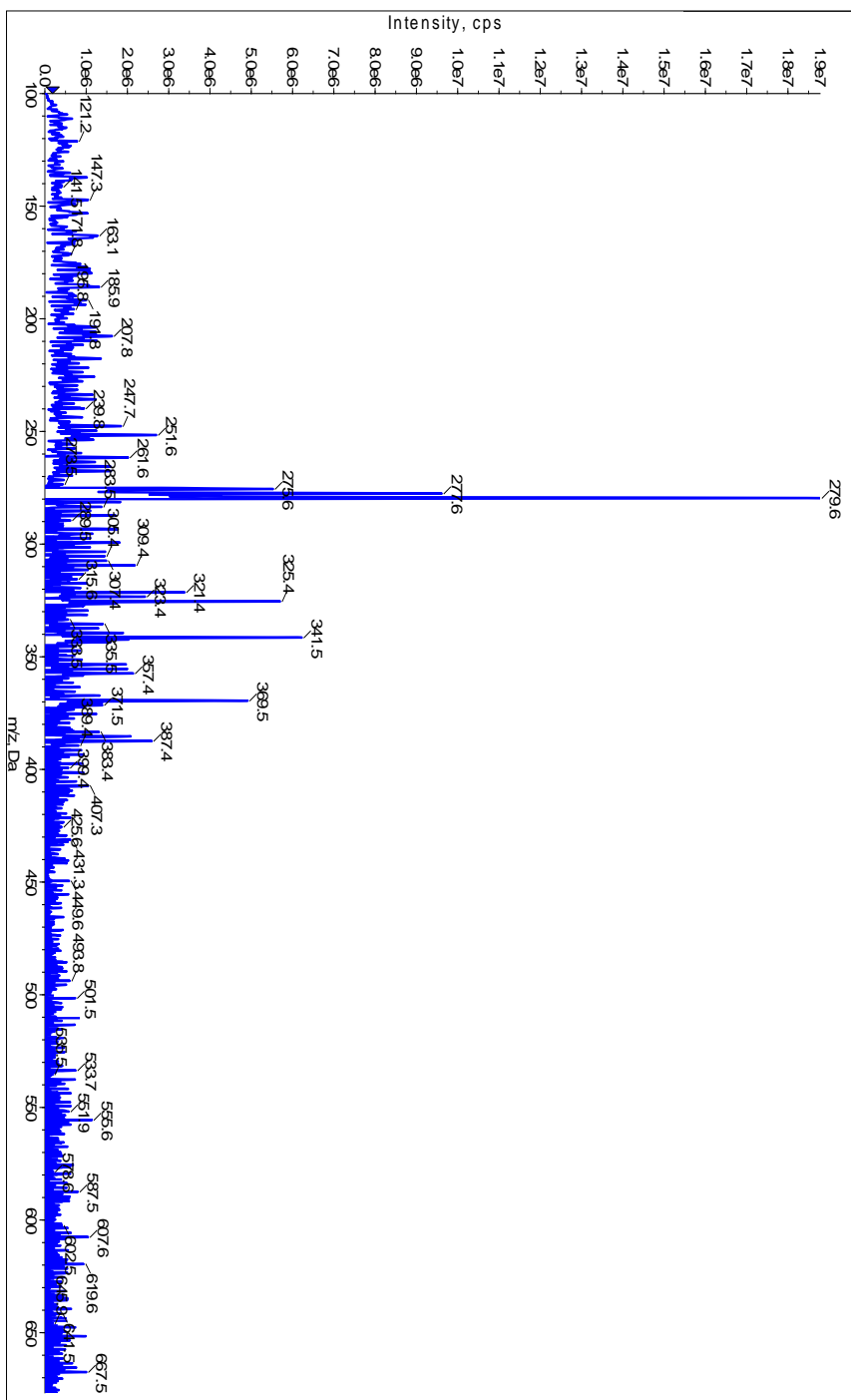
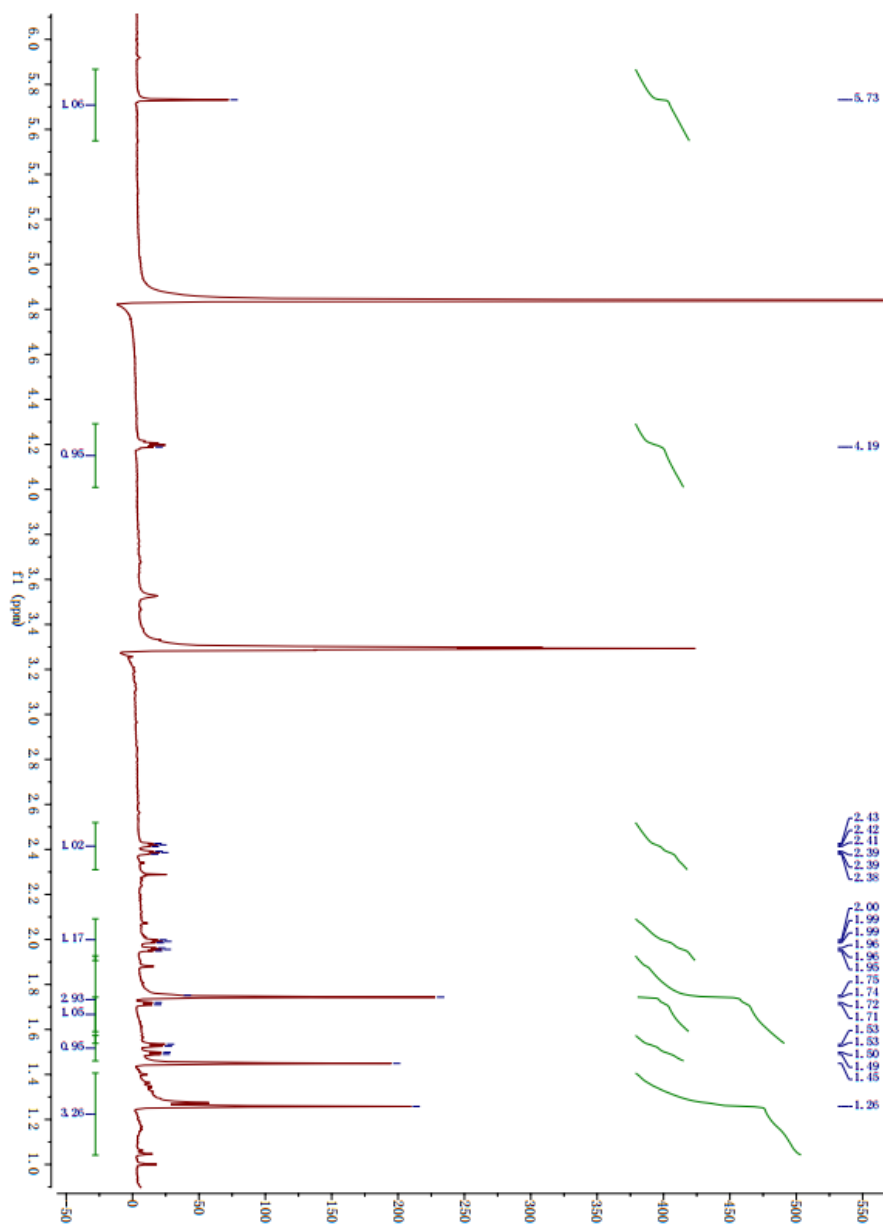


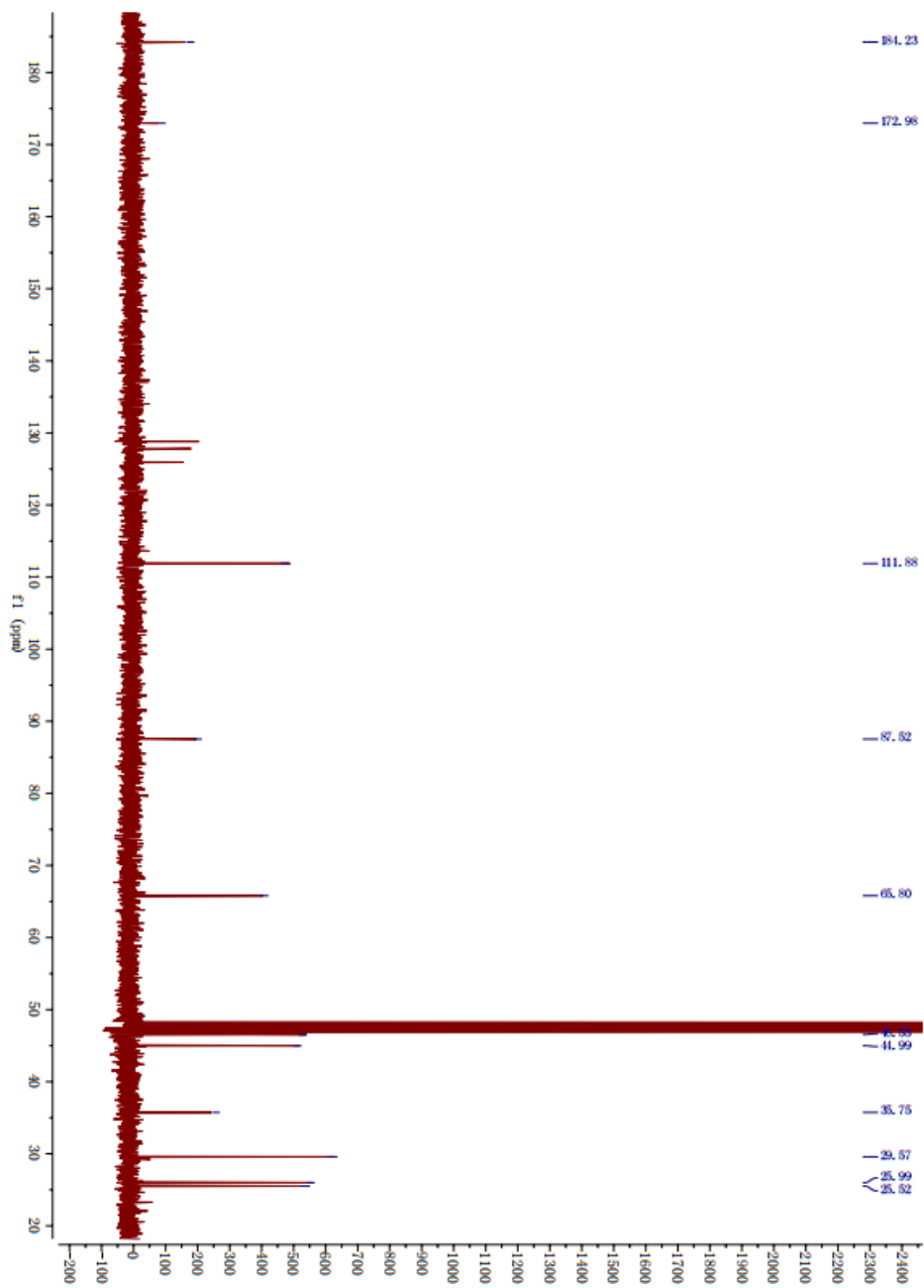
Figure S11.  $^{13}\text{C}$  NMR spectrum of 4-epixanthanol (**4**) ( $\text{CD}_3\text{OD}$ , 100 MHz).



**Figure S12.** Mass spectrum of 4-epixanthanol (**4**).



**Figure S13.** <sup>1</sup>H NMR spectrum of loliolide (**5**) (CD<sub>3</sub>OD, 400 MHz).



**Figure S14.**  $^{13}\text{C}$  NMR spectrum of loliolide (5) ( $\text{CD}_3\text{OD}$ , 100 MHz).

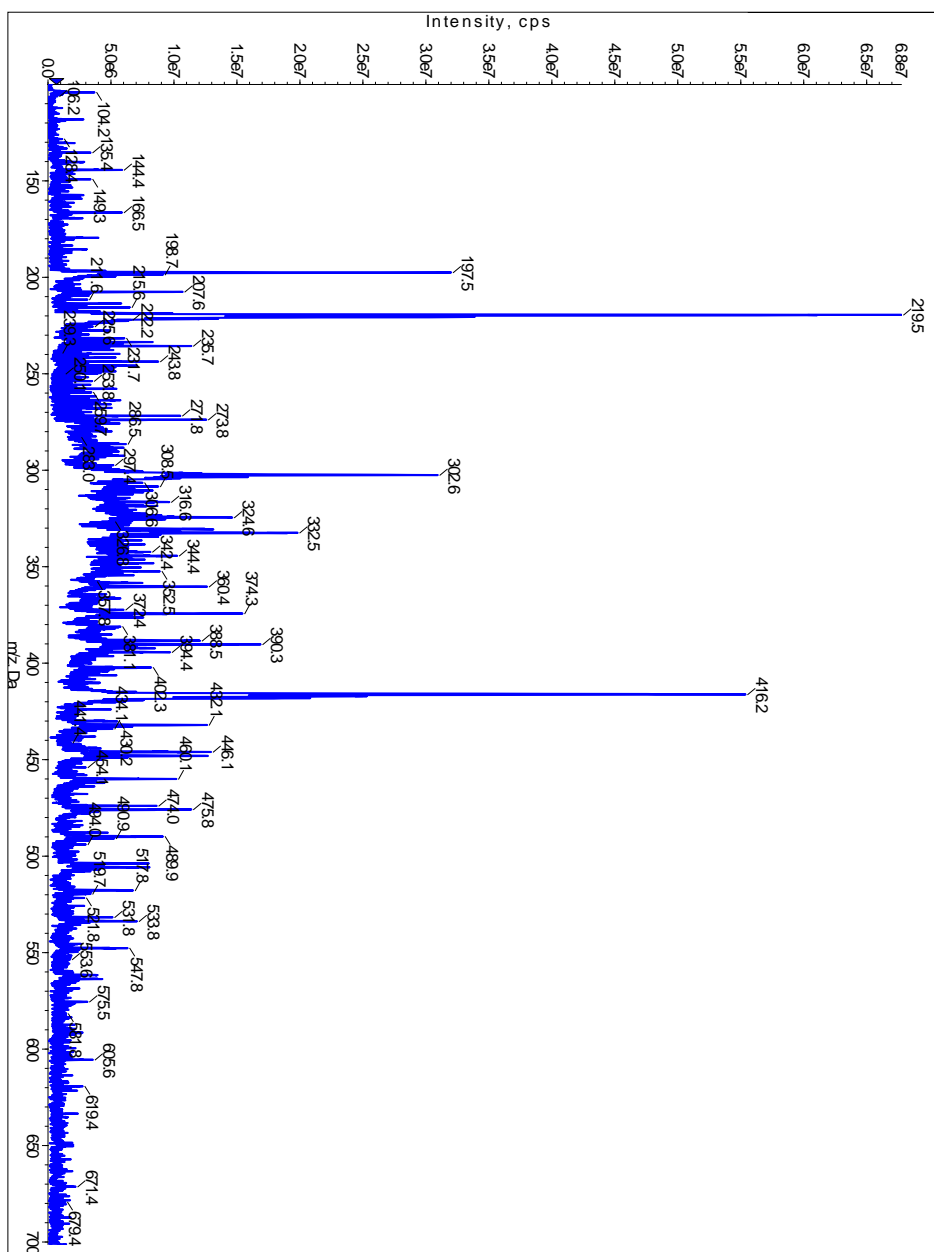
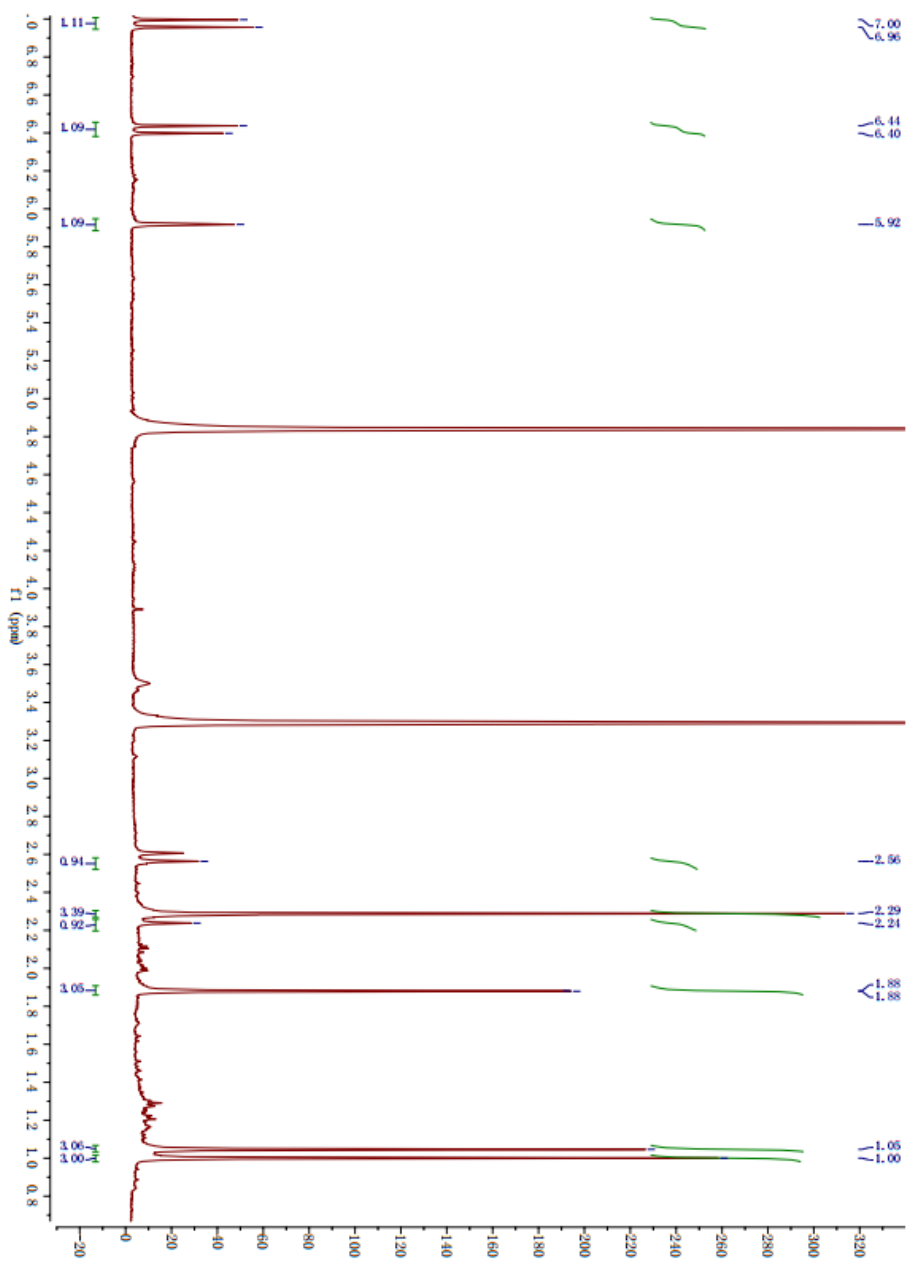
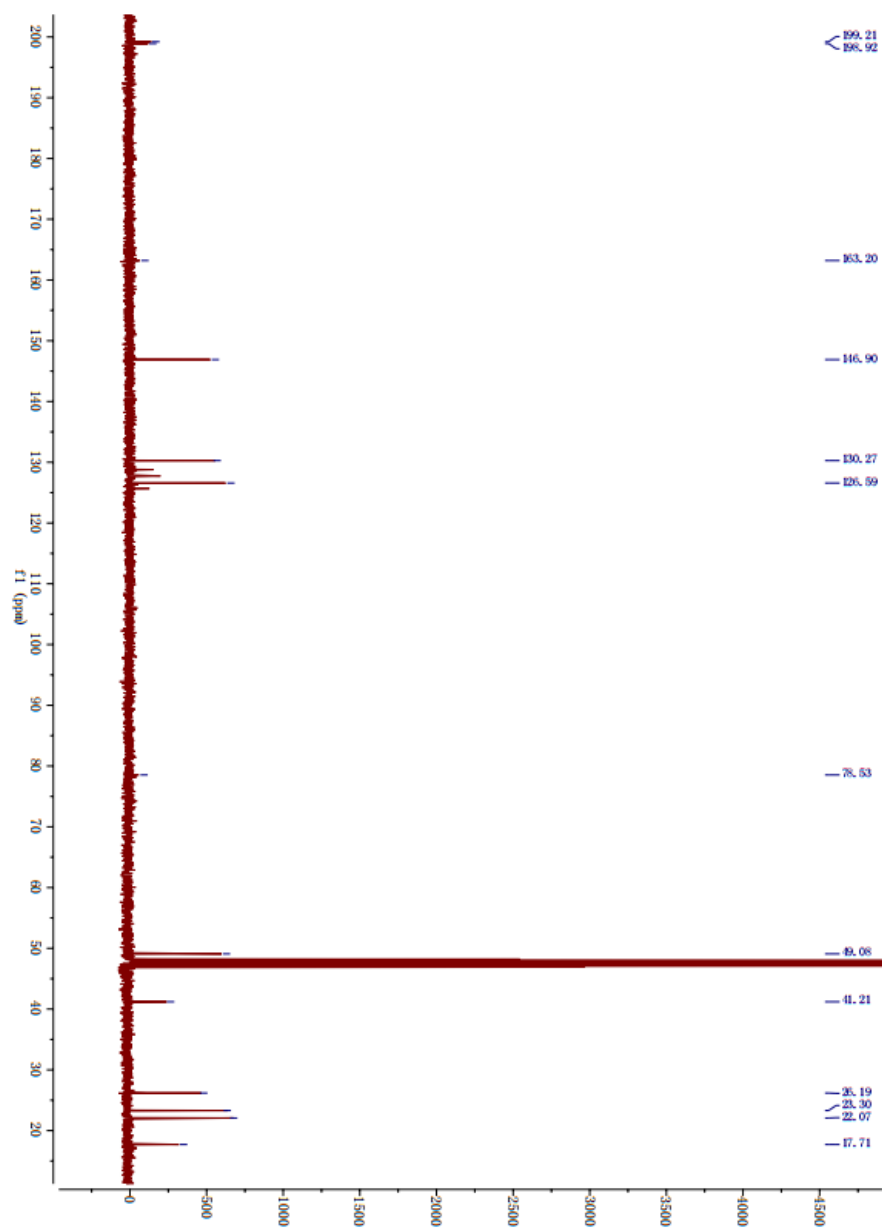


Figure S15. Mass spectrum of loliolide (5).





**Figure S16.**  $^1\text{H}$  NMR spectrum of dehydrovomifoliol (**6**) ( $\text{CD}_3\text{OD}$ , 400 MHz).



**Figure S17.**  $^{13}\text{C}$  NMR spectrum of dehydrovomifoliol (**6**) ( $\text{CD}_3\text{OD}$ , 100 MHz).

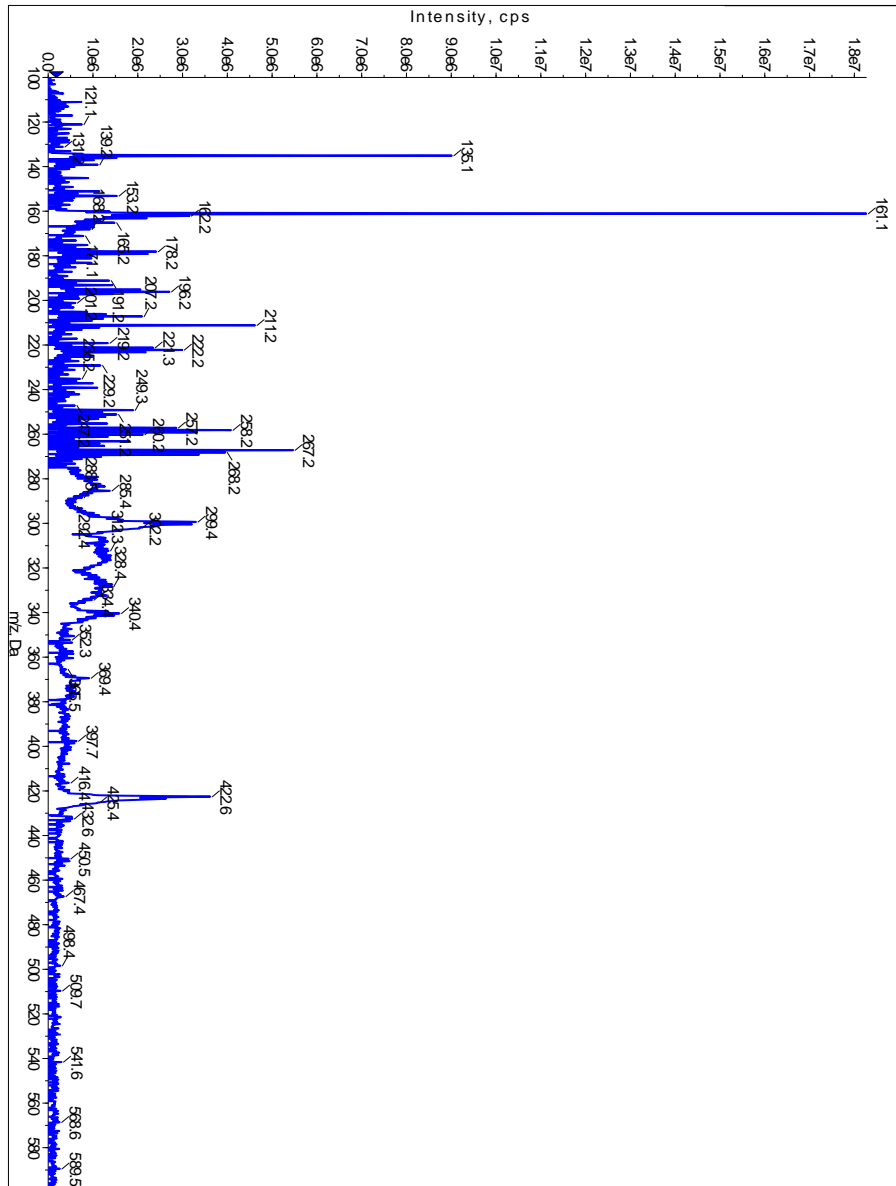


Figure S18. Mass spectrum of dehydrovomifoliol (6) .