

# **Xylapeptide A, an Antibacterial Cyclopentapeptide with an Uncommon L-Pipecolinic Acid Moiety from the Associated Fungus *Xylaria* sp. (GDG-102)**

Wei-Feng Xu,<sup>†,‡,¶</sup> Xue-Mei Hou,<sup>‡,§,¶</sup> Fei-Hua Yao,<sup>†</sup> Na Zheng,<sup>†</sup> Jun Li,<sup>†</sup> Chang-Yun Wang,<sup>‡,§</sup> Rui-Yun Yang<sup>\*,†</sup> and Chang-Lun Shao<sup>\*,‡,§</sup>

<sup>†</sup>State Key Laboratory for the Chemistry and Molecular Engineering of Medicinal Resources, College of Chemistry and Pharmaceutical Sciences, Guangxi Normal University, Guilin 541004, The People's Republic of China

<sup>‡</sup>Key Laboratory of Marine Drugs, The Ministry of Education of China, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, The People's Republic of China

<sup>§</sup>Laboratory for Marine Drugs and Bioproducts, Qingdao National Laboratory for Marine Science and Technology, Qingdao 266200, The People's Republic of China

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

\* To whom correspondence should be addressed. Tel/Fax: +86-773-2120-958 (R.-Y.Y.); +86-532-8203-1503 (C.-L.S.). E-mails: yang\_rui\_yun@163.com (R.-Y.Y.); shaochanglun@163.com (C.-L.S.).

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**Figure S1.**  $^1\text{H}$  NMR spectra of the organic extracts, and xylapeptides A and B in  $\text{CDCl}_3$ .

**Figure S2.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**.

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**Figure S12.** HSQC ( $\text{CDCl}_3$ ) spectrum of compound **2**.

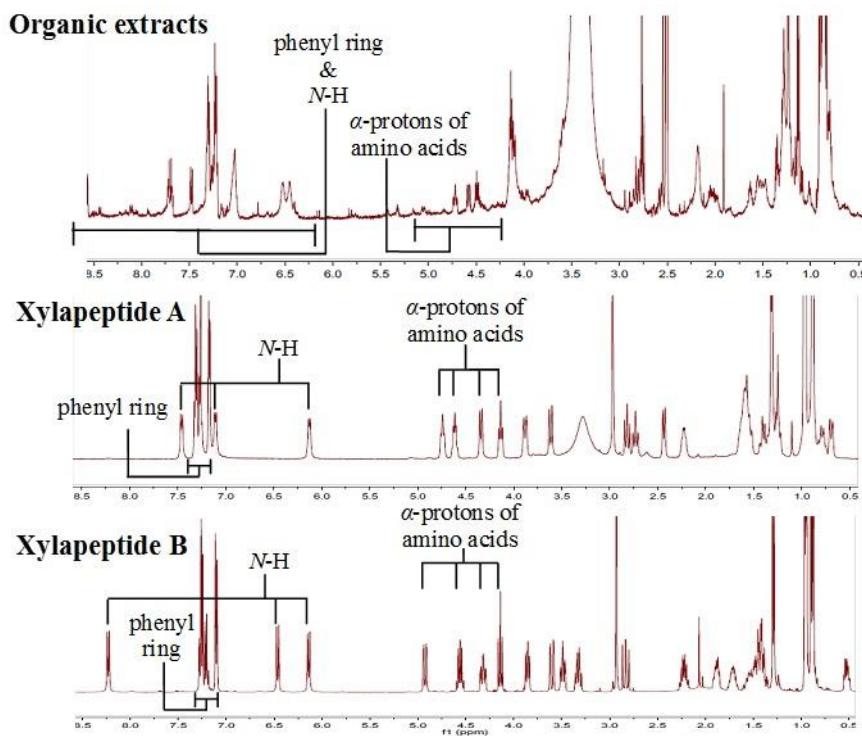
**Figure S13.** HMBC ( $\text{CDCl}_3$ ) spectrum of compound **2**.

**Figure S14.** HRESIMS spectrum of compound **2**.

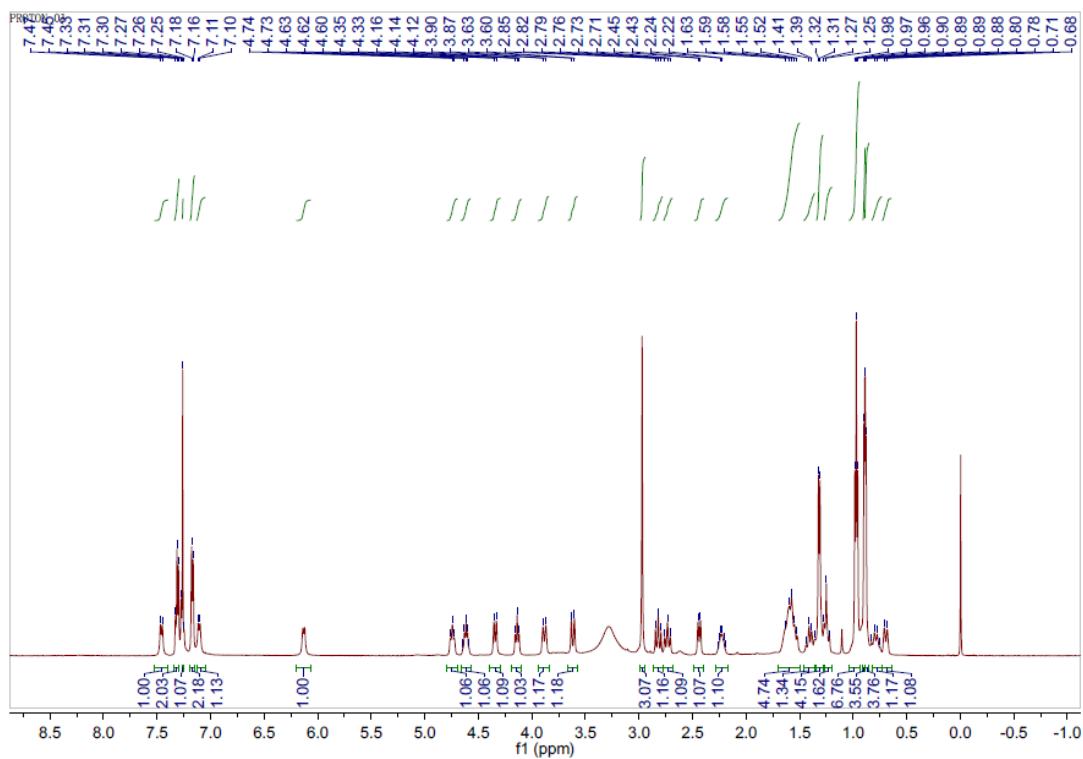
**Figure S15.** ESI MS<sup>2</sup> spectrum of compound **2**.

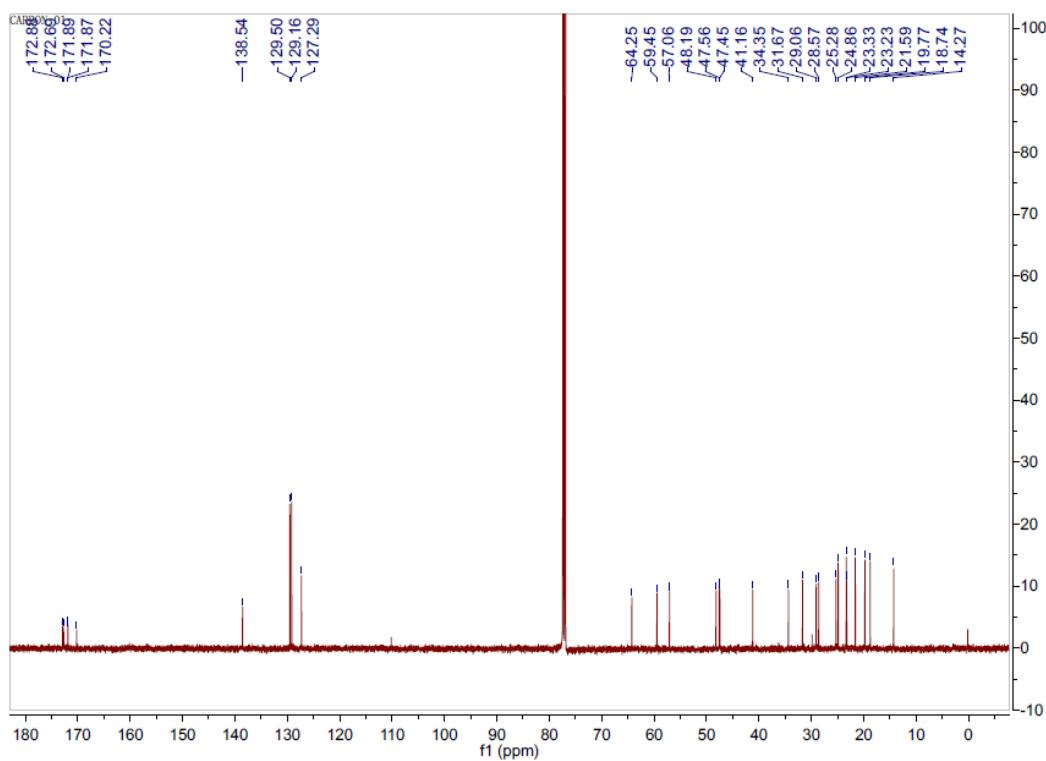
**Figure S16.** Assignments of ESI MS<sup>2</sup> fragmentation data for **1** and **2**.

**Figure S17.** Marfey's analysis of the amino acids in **1** and **2** on UPLC-MS.

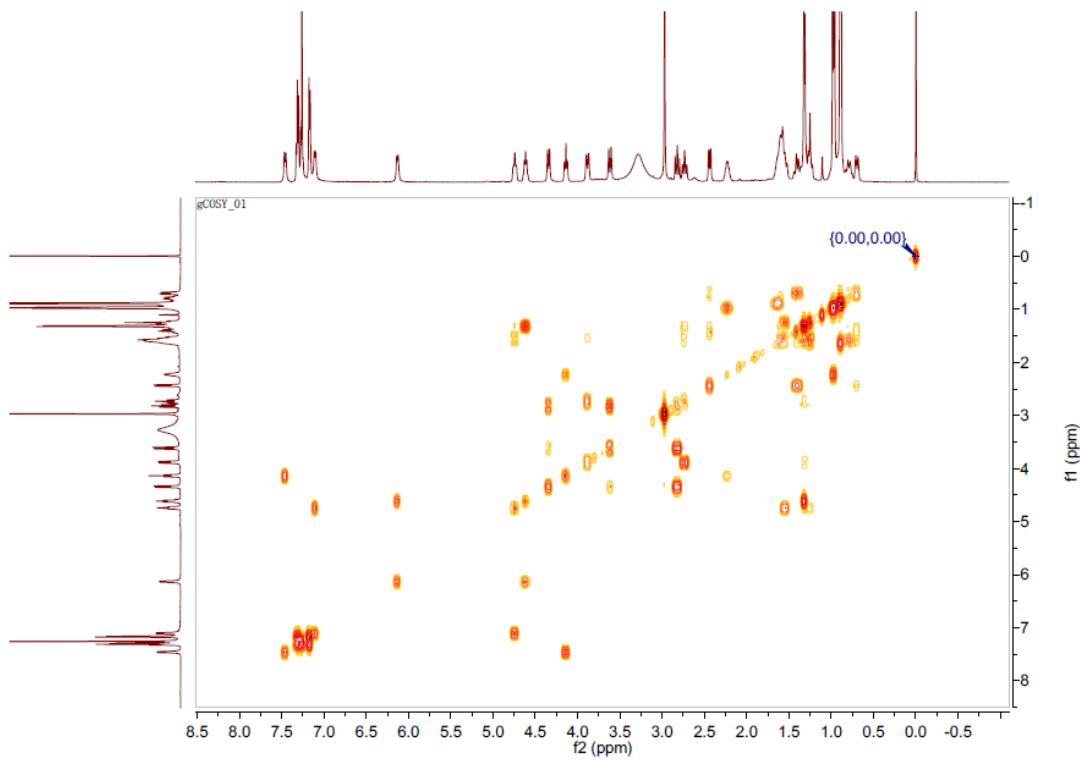


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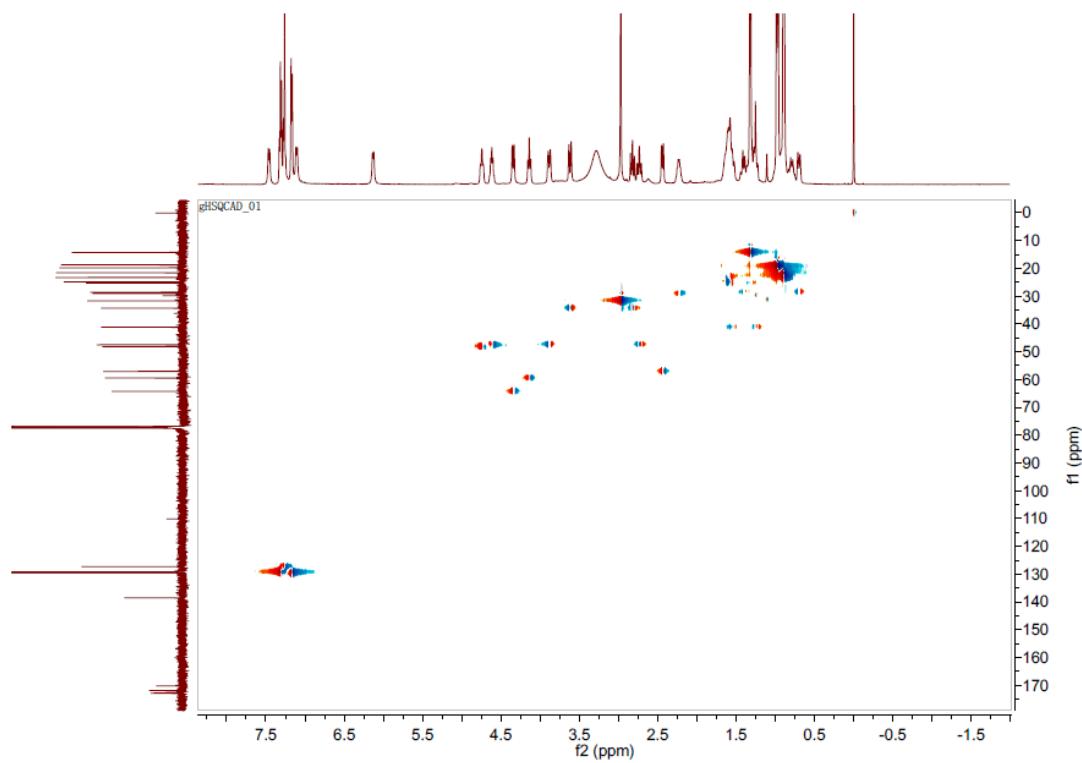




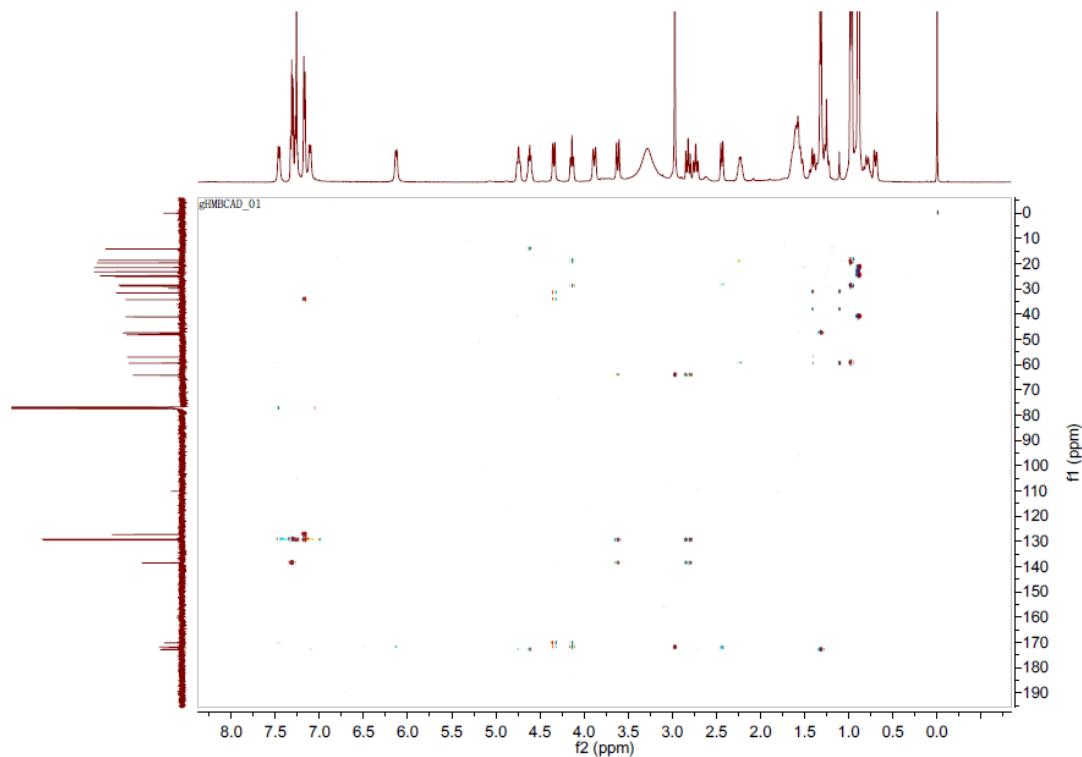
**Figure S3.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**.



**Figure S4.**  $^1\text{H}$ - $^1\text{H}$  COSY ( $\text{CDCl}_3$ ) spectrum of compound **1**.

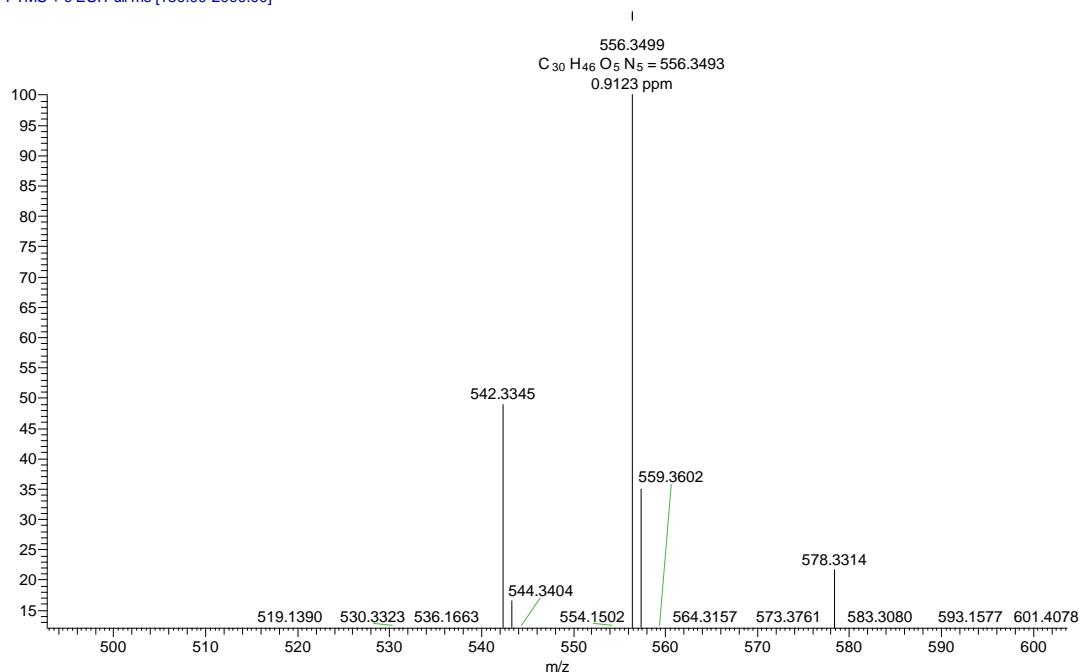


**Figure S5.** HSQC ( $\text{CDCl}_3$ ) spectrum of compound 1.



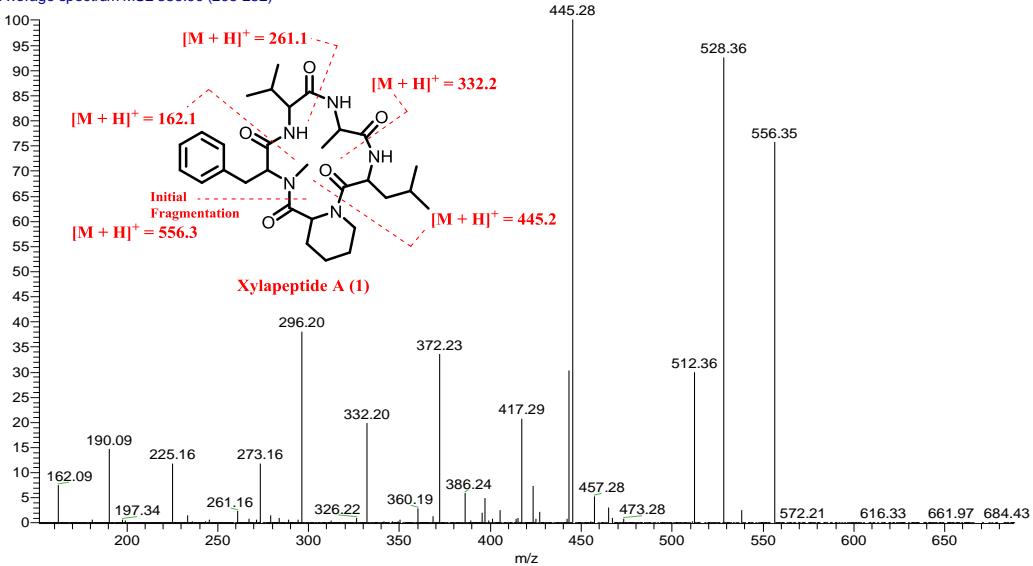
**Figure S6.** HMBC ( $\text{CDCl}_3$ ) spectrum of compound 1.

20160112-CY23\_160112104831 #91 RT: 0.79 AV: 1 NL: 1.51E7  
T: FTMS + c ESI Full ms [150.00-2000.00]

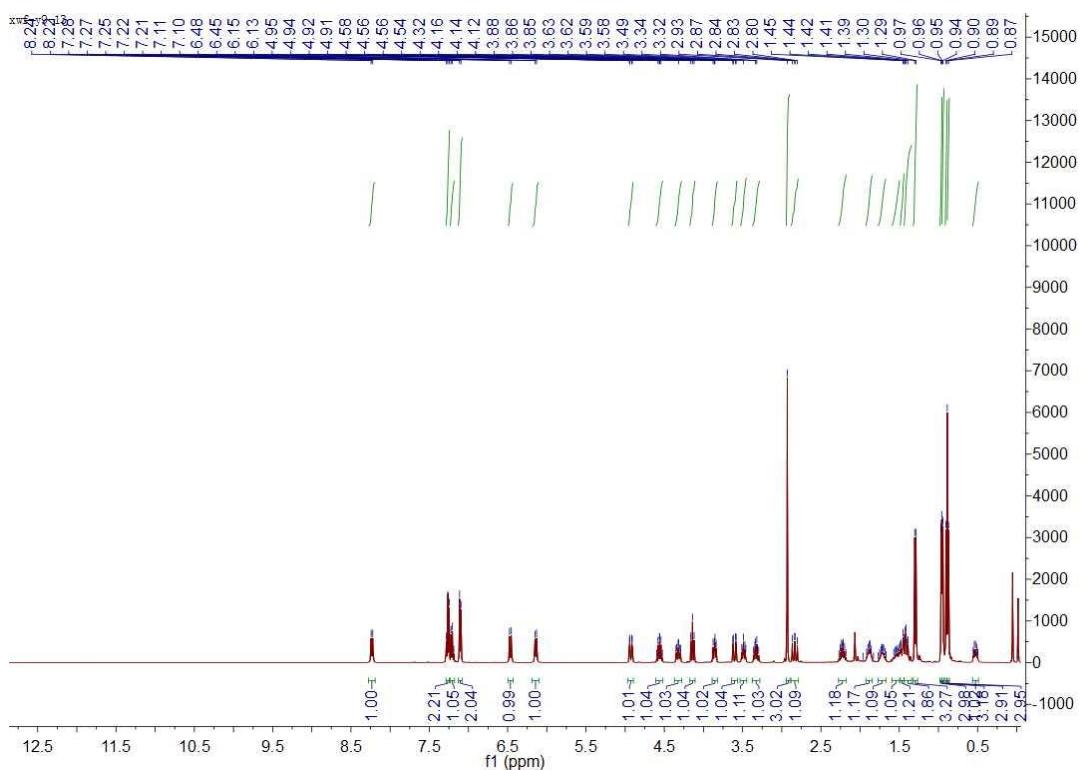


**Figure S7.** HRESIMS spectrum of compound 1.

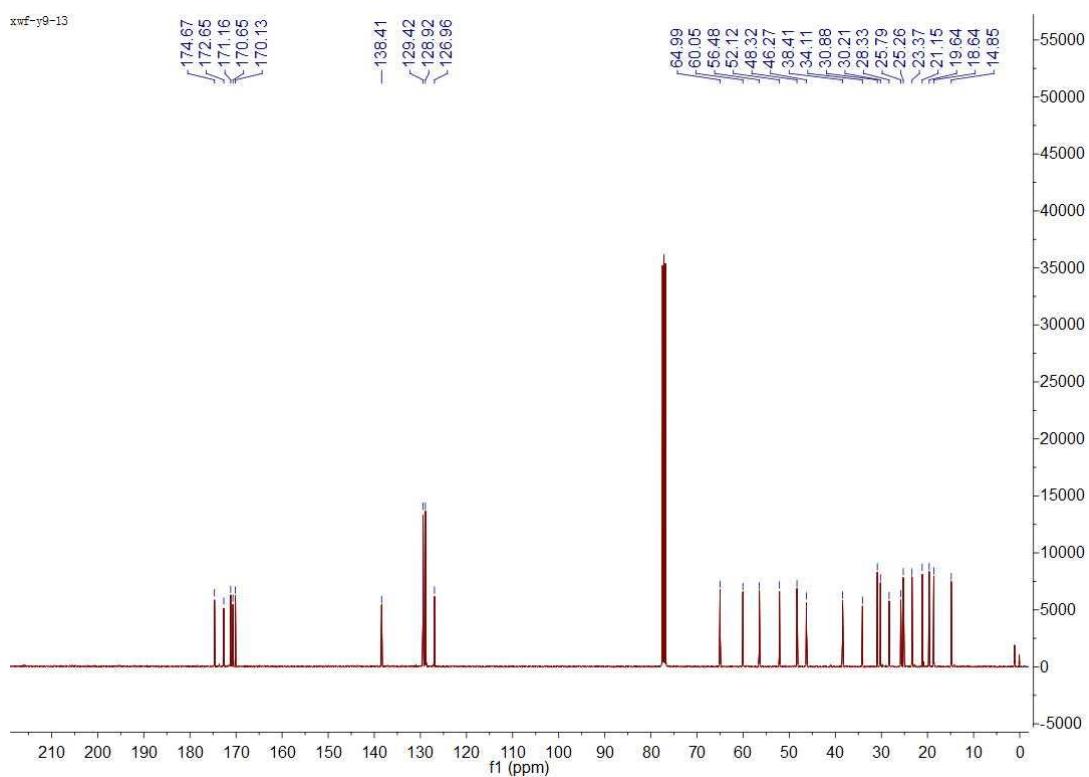
20160120-CY23\_160120102732 #206-252 RT: 1.67-2.32 AV: 47 NL: 1.66E6  
T: Average spectrum MS2 556.00 (206-252)



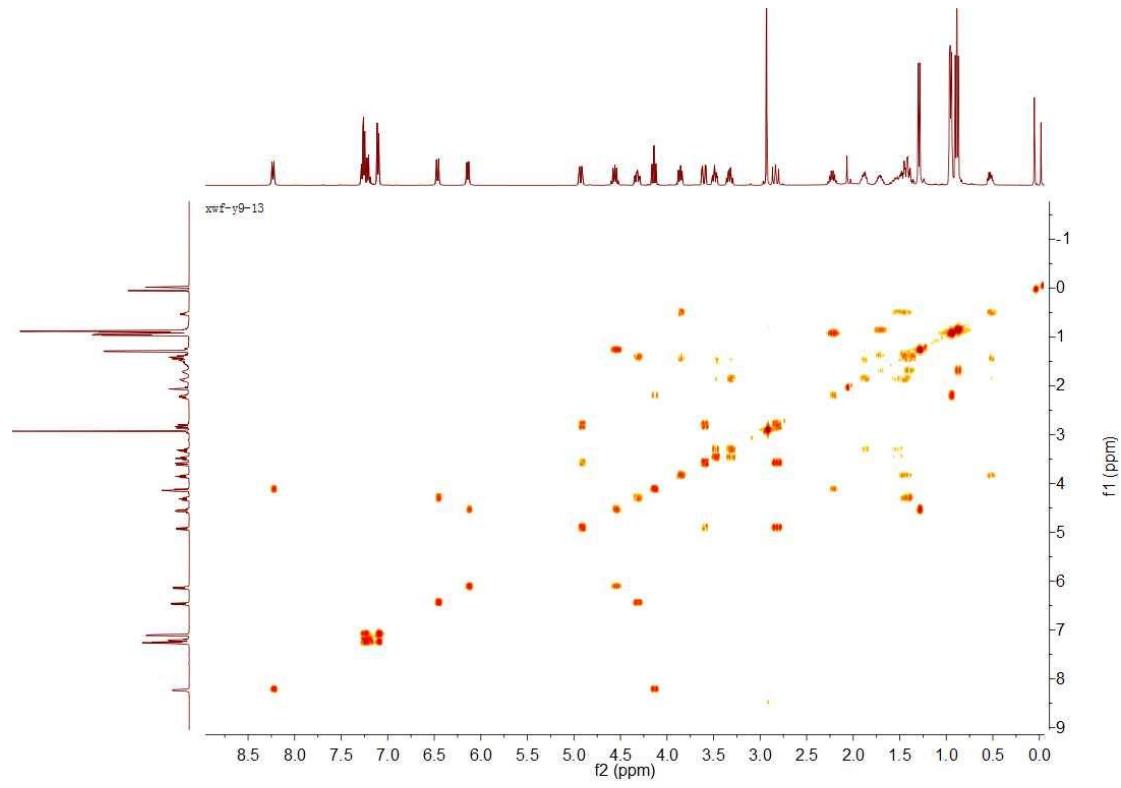
**Figure S8.** ESI MS<sup>2</sup> spectrum of compound 1.



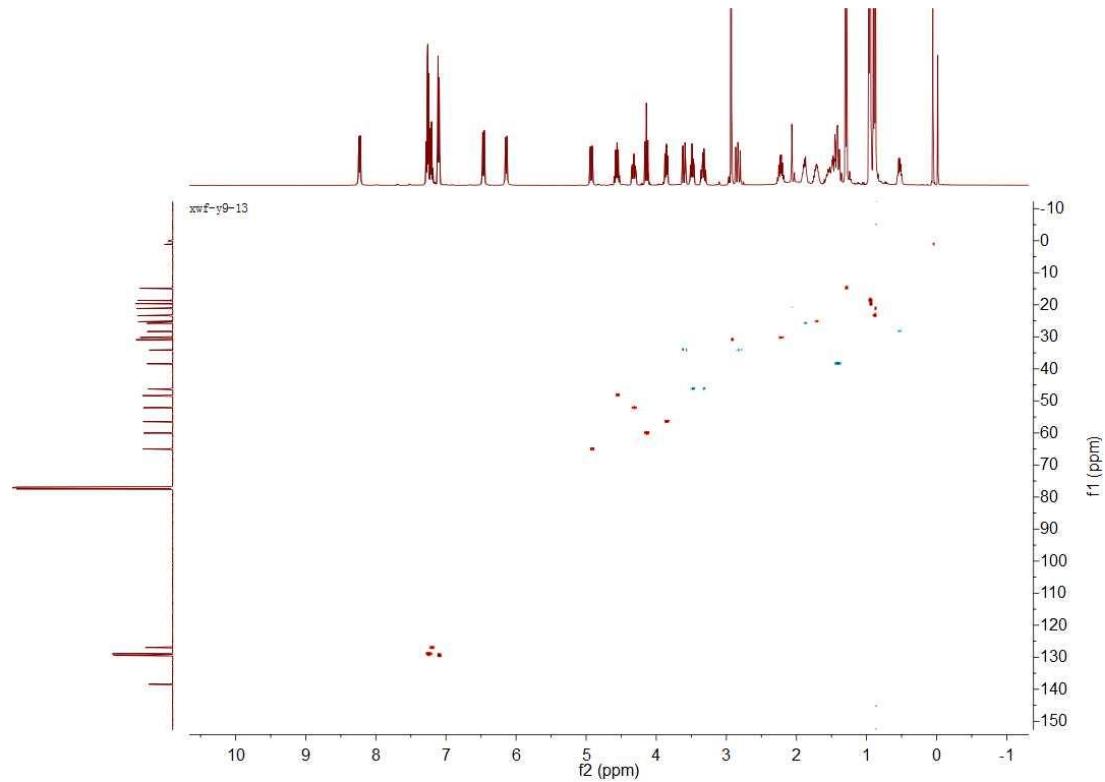
**Figure S9.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of compound **2**.



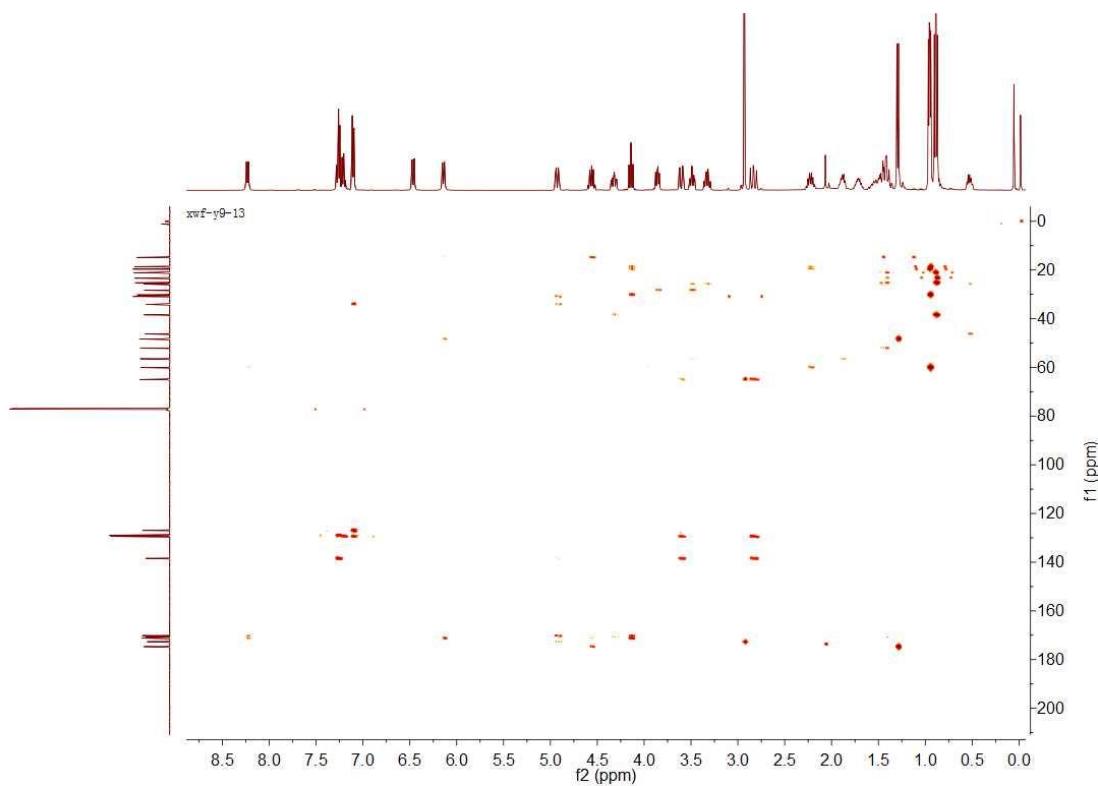
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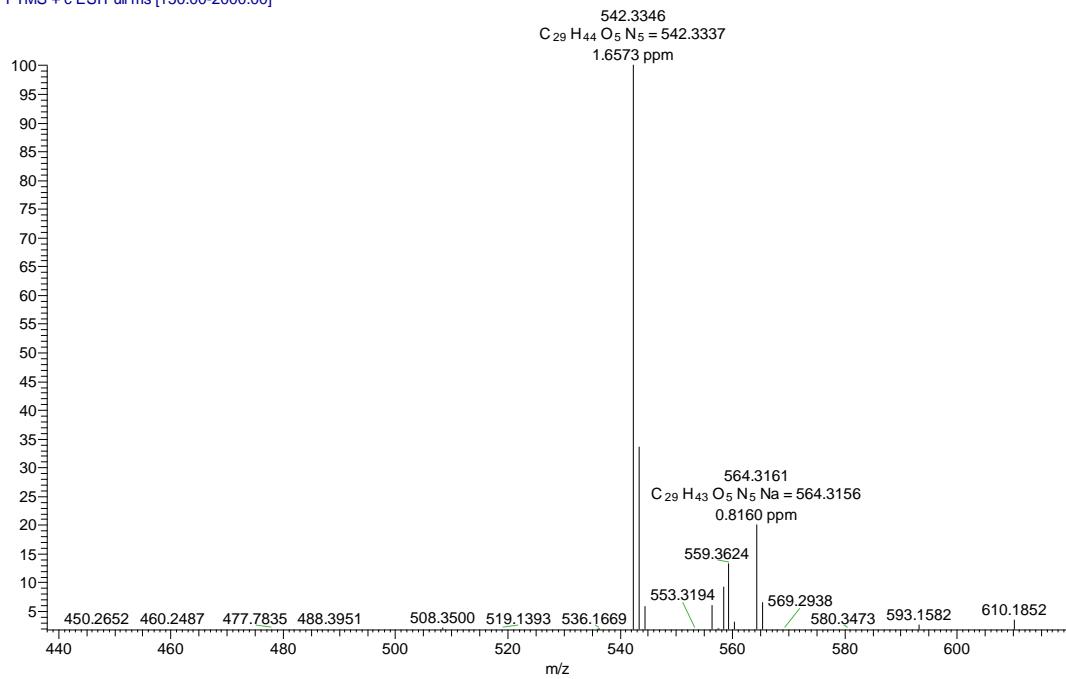


**Figure S12.** HSQC ( $\text{CDCl}_3$ ) spectrum of compound **2**.



**Figure S13.** HMBC ( $\text{CDCl}_3$ ) spectrum of compound 2.

20160112-Y9-13\_160112104831 #89 RT: 0.78 AV: 1 NL: 2.00E7  
T: FTMS + c ESI Full ms [150.00-2000.00]



**Figure S14.** HRESIMS spectrum of compound 2.

20160115-Y9-13\_160112143934 #53 RT: 0.48 AV: 1 NL: 7.11E6  
T: FTMS + c ESI Full ms2 542.00@cid20.00 [145.00-2000.0]

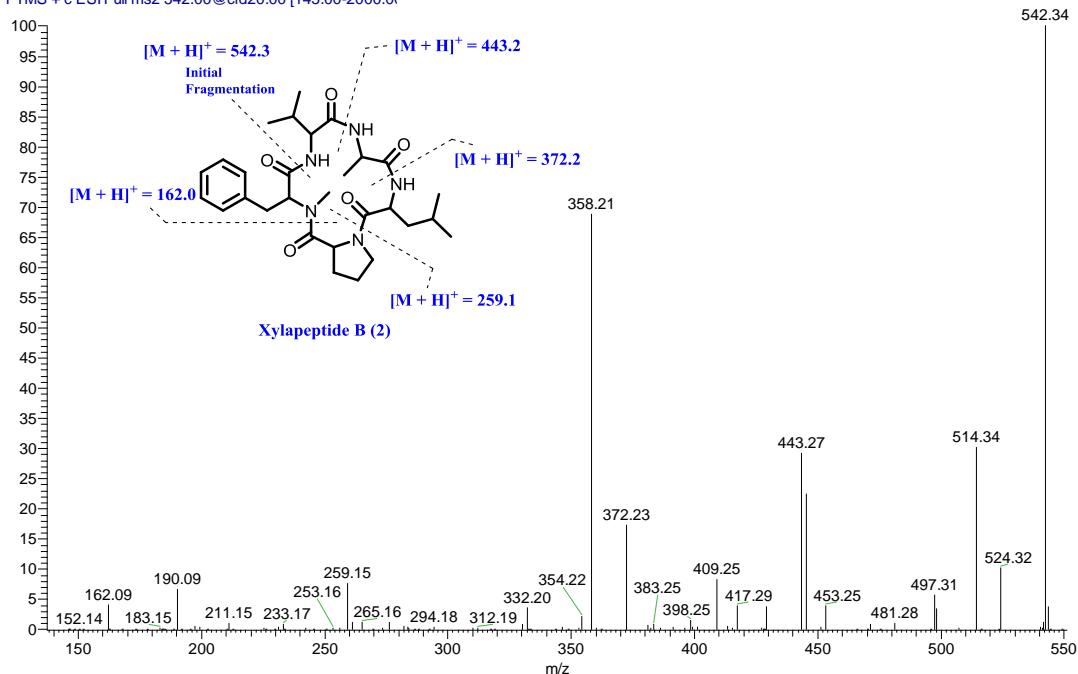


Figure S15. ESI MS<sup>2</sup> spectrum of compound 2.

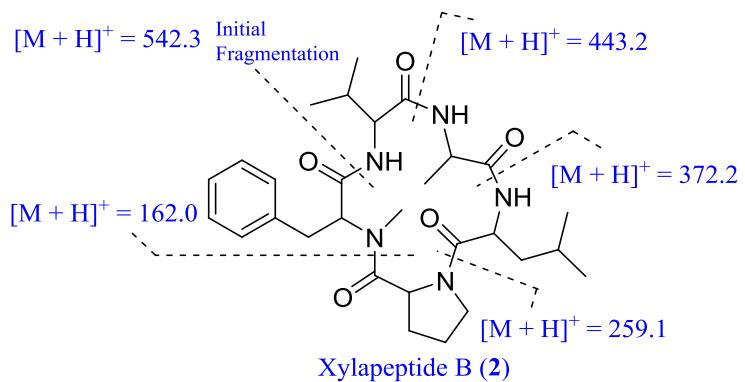
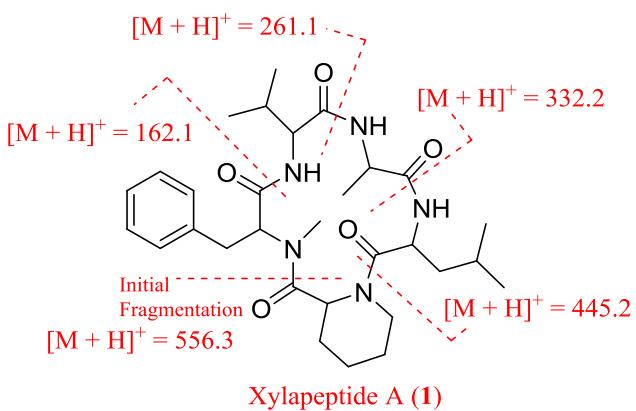
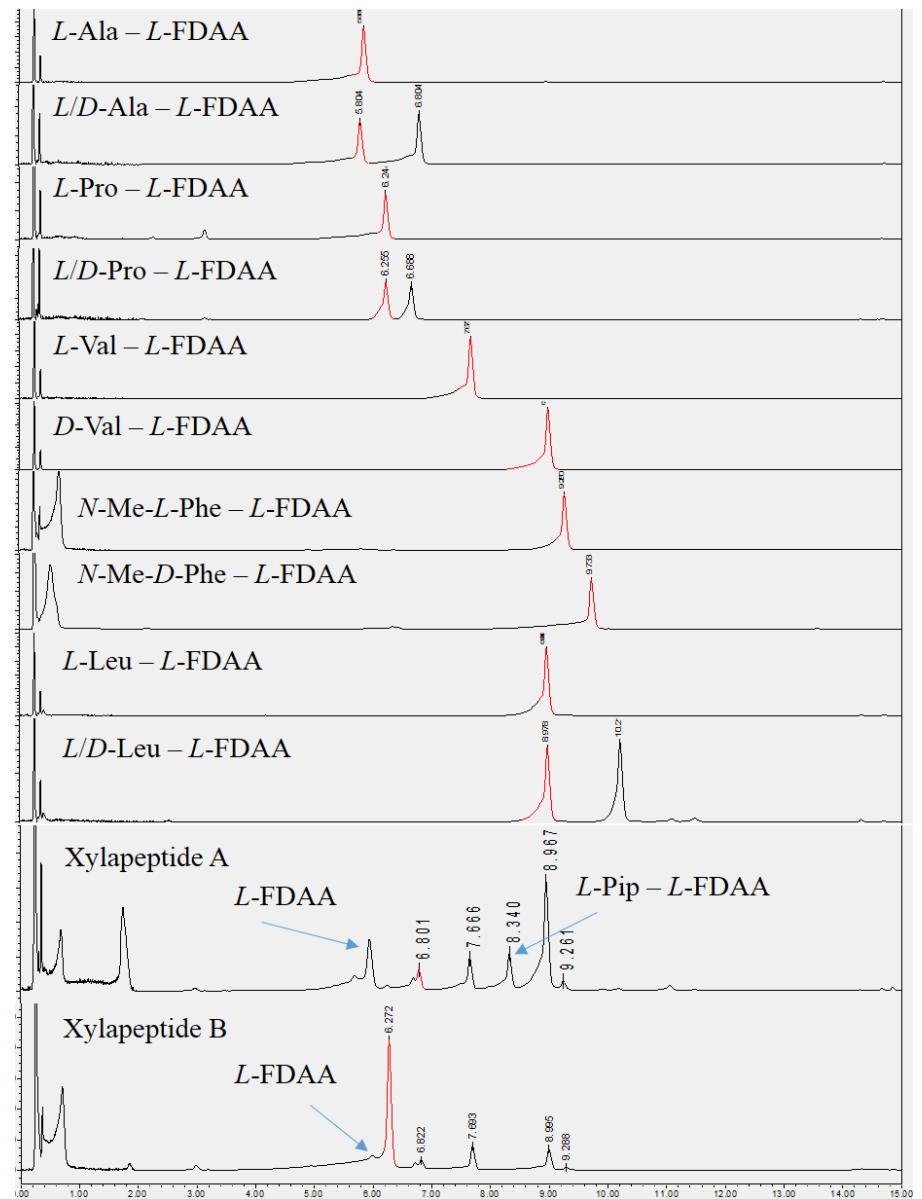


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