

# Pocillastrin H, a Chondropsin-type Macrolide with a Conjugated Pentaene Moiety, from a *Characella* sp. Marine Sponge

Rei Suo,<sup>†</sup> Kentaro Takada,<sup>\*†</sup> Raku Irie,<sup>†</sup> Ryuichi Watanabe,<sup>§</sup> Toshiyuki Suzuki,<sup>§</sup> Yuji Ise,  
<sup>‡</sup> Susumu Ohtsuka,<sup>⊥</sup> Shigeru Okada,<sup>†</sup> and Shigeki Matsunaga<sup>\*†</sup>

<sup>†</sup>*Laboratory of Aquatic Natural Products Chemistry, Graduate School of Agricultural and Life Sciences, The University of Tokyo, Bunkyo-ku, Tokyo 113-8657, Japan*

<sup>§</sup>*National Research Institute of Fisheries Science, 2-12-4 Fukuura, Kanazawa, Yokohama 236-8648, Japan*

<sup>‡</sup>*Sugashima Marine Biological Laboratory, Graduate School of Science, Nagoya University, Toba, Mie 517-0004, Japan*

<sup>⊥</sup>*Takehara Marine Science Station, Hiroshima University, Takehara, Hiroshima 725-0024, Japan*

## Table of Contents

Figure S1-S7. NMR spectra of pocillastrin H (**1**) in CD<sub>3</sub>OD.

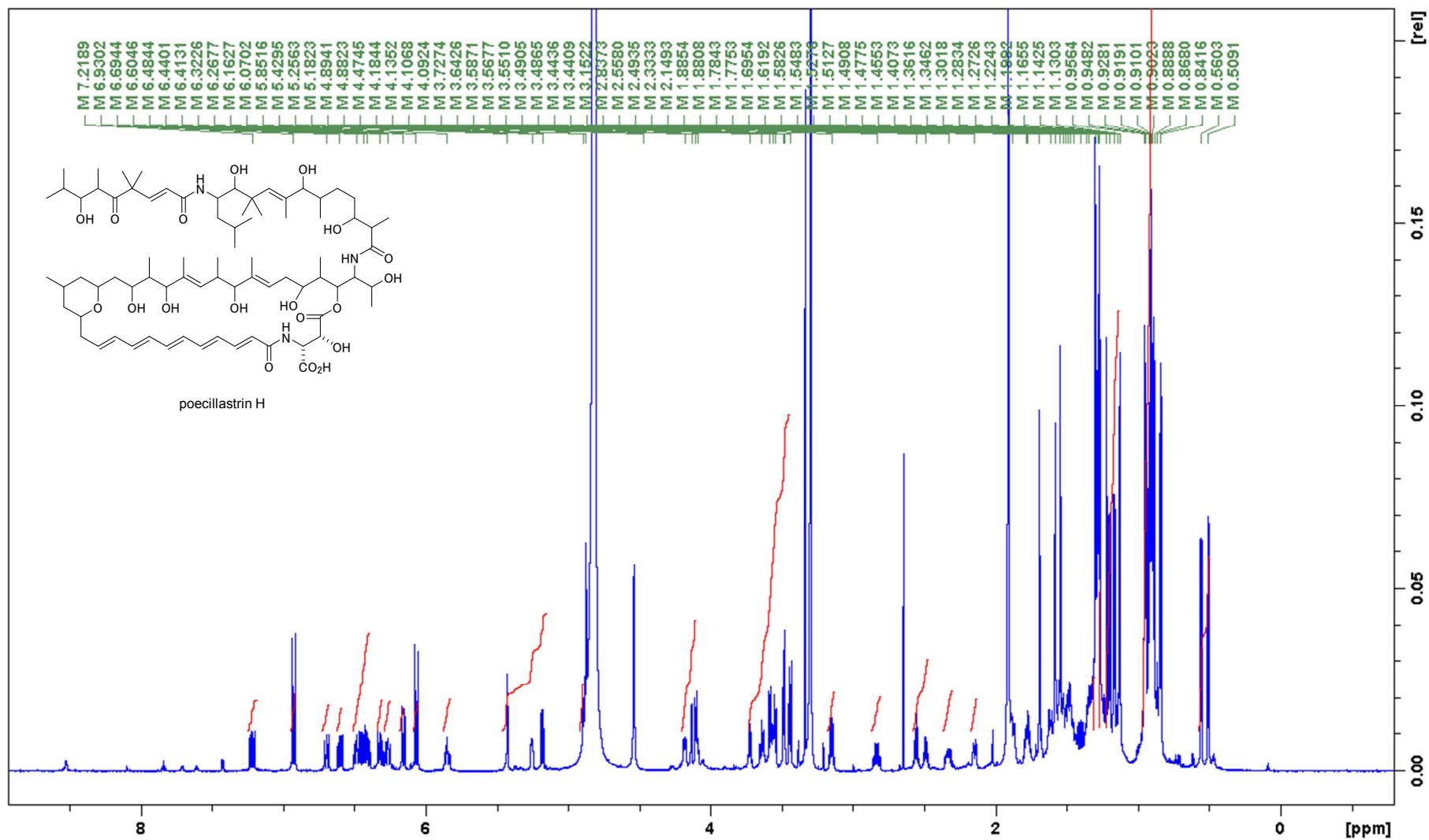
Figure S8. LC-MS chromatograms of Marfey's derivatives.

Figure S9. LC-MS chromatograms of Marfey's derivatives.

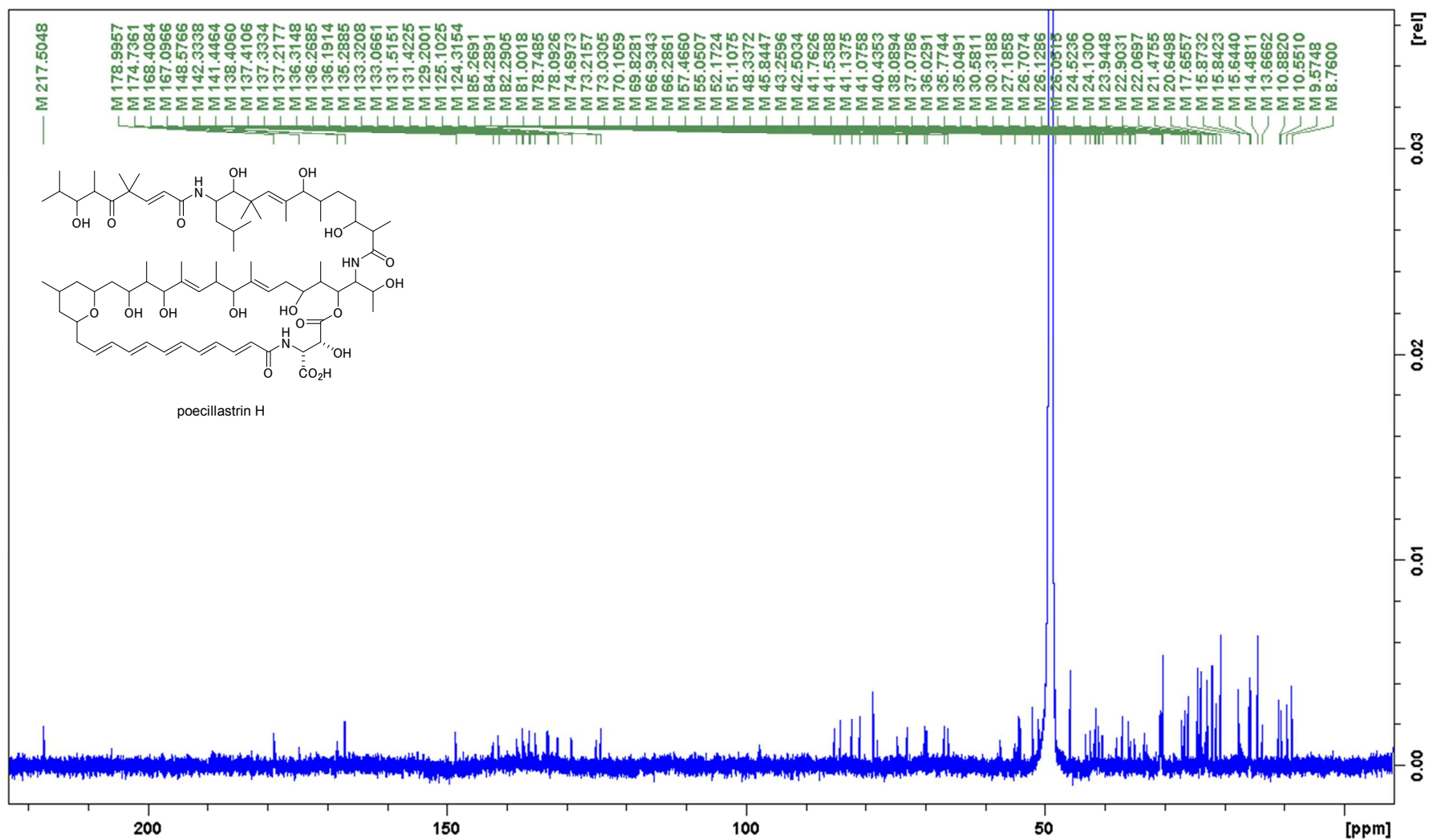
Figure S10. <sup>1</sup>H NMR spectrum of isomerized pocillastrin H (**1**) in CD<sub>3</sub>OD.

Figure S11. LC-MS chromatograms of photoisomerization of pocillastrin H.



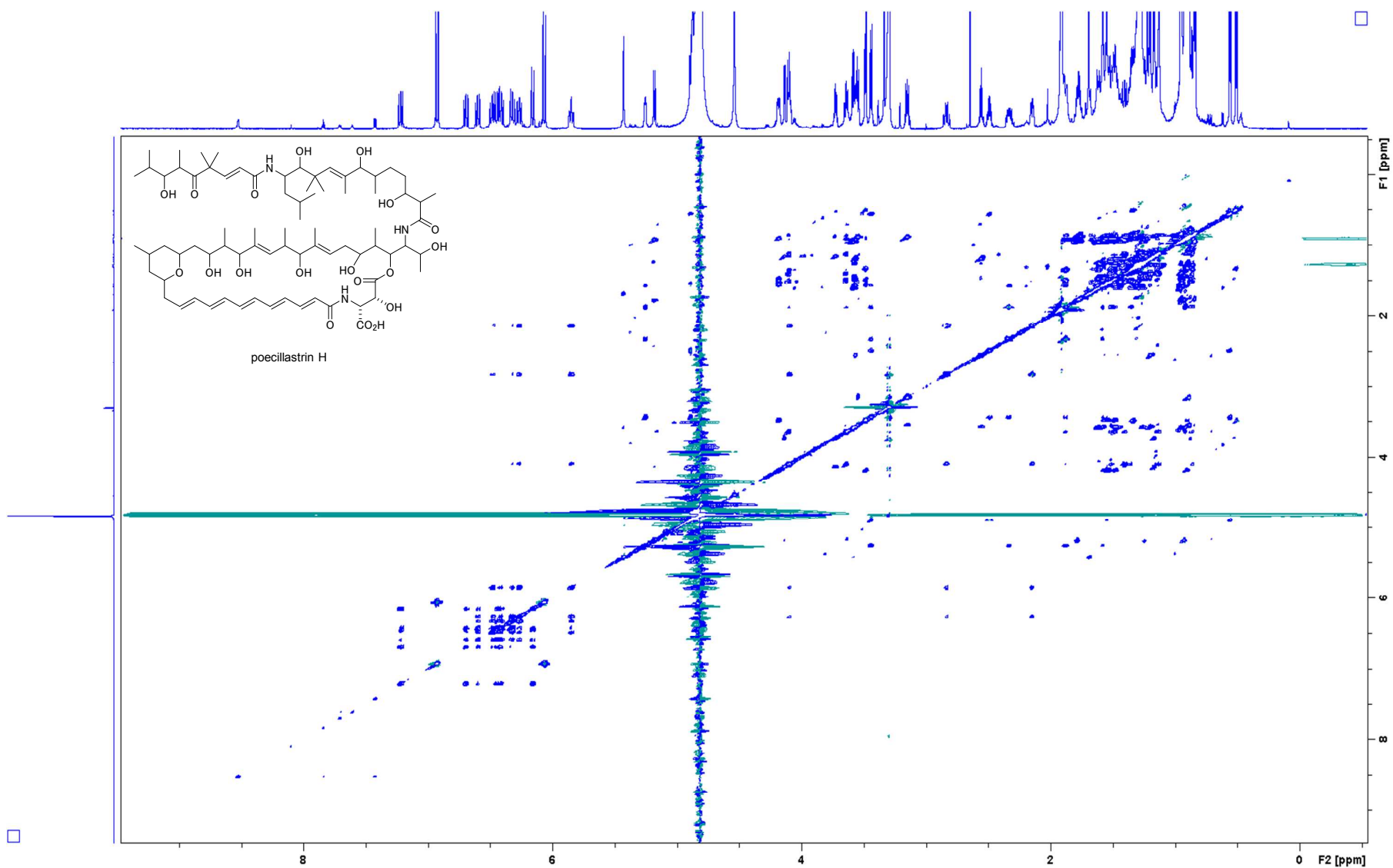


**Figure S1.**  $^1\text{H}$  NMR spectrum of poecillastrin H in  $\text{CD}_3\text{OD}$ .



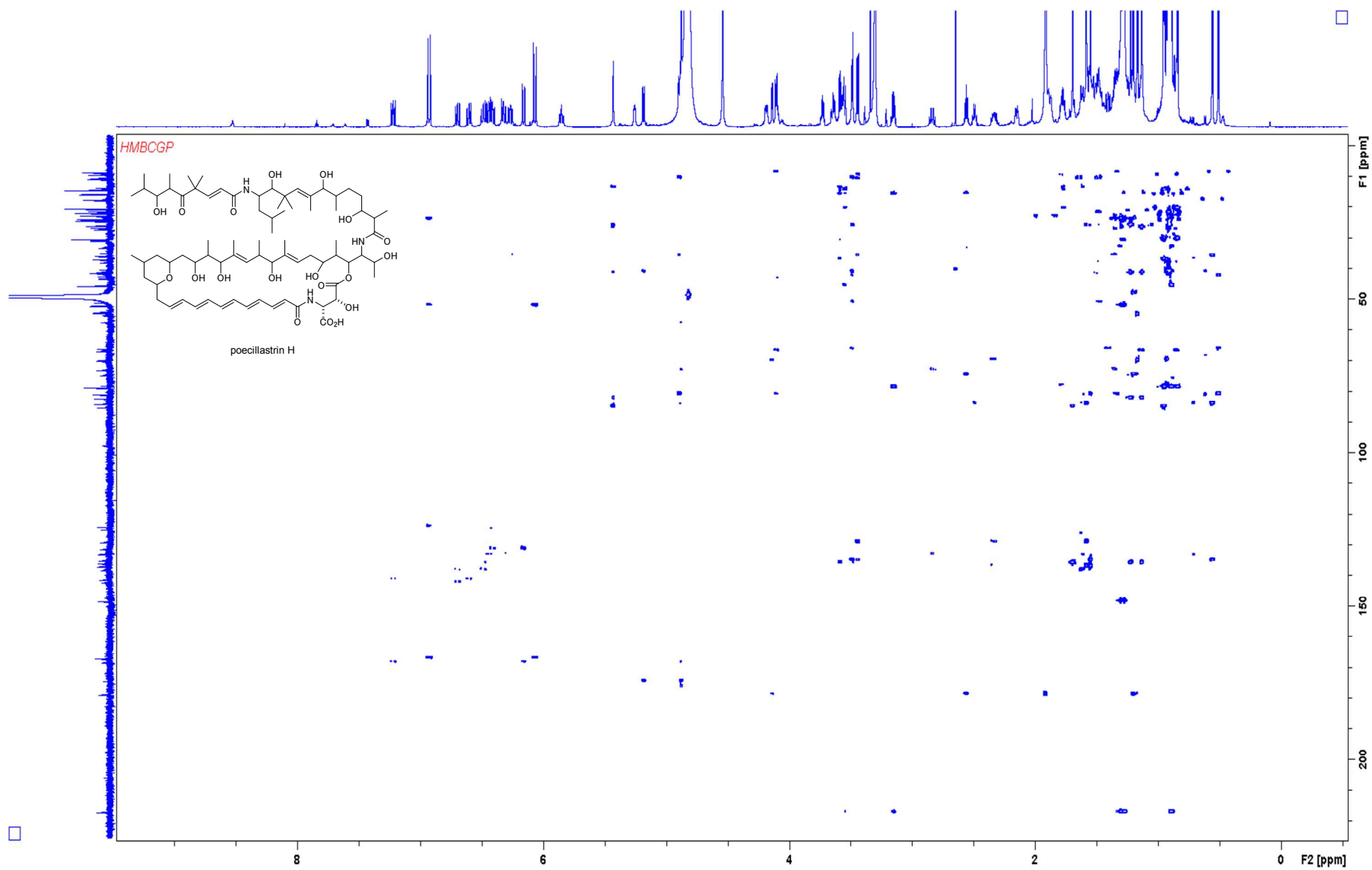
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of poecillastrin H in  $\text{CD}_3\text{OD}$ .





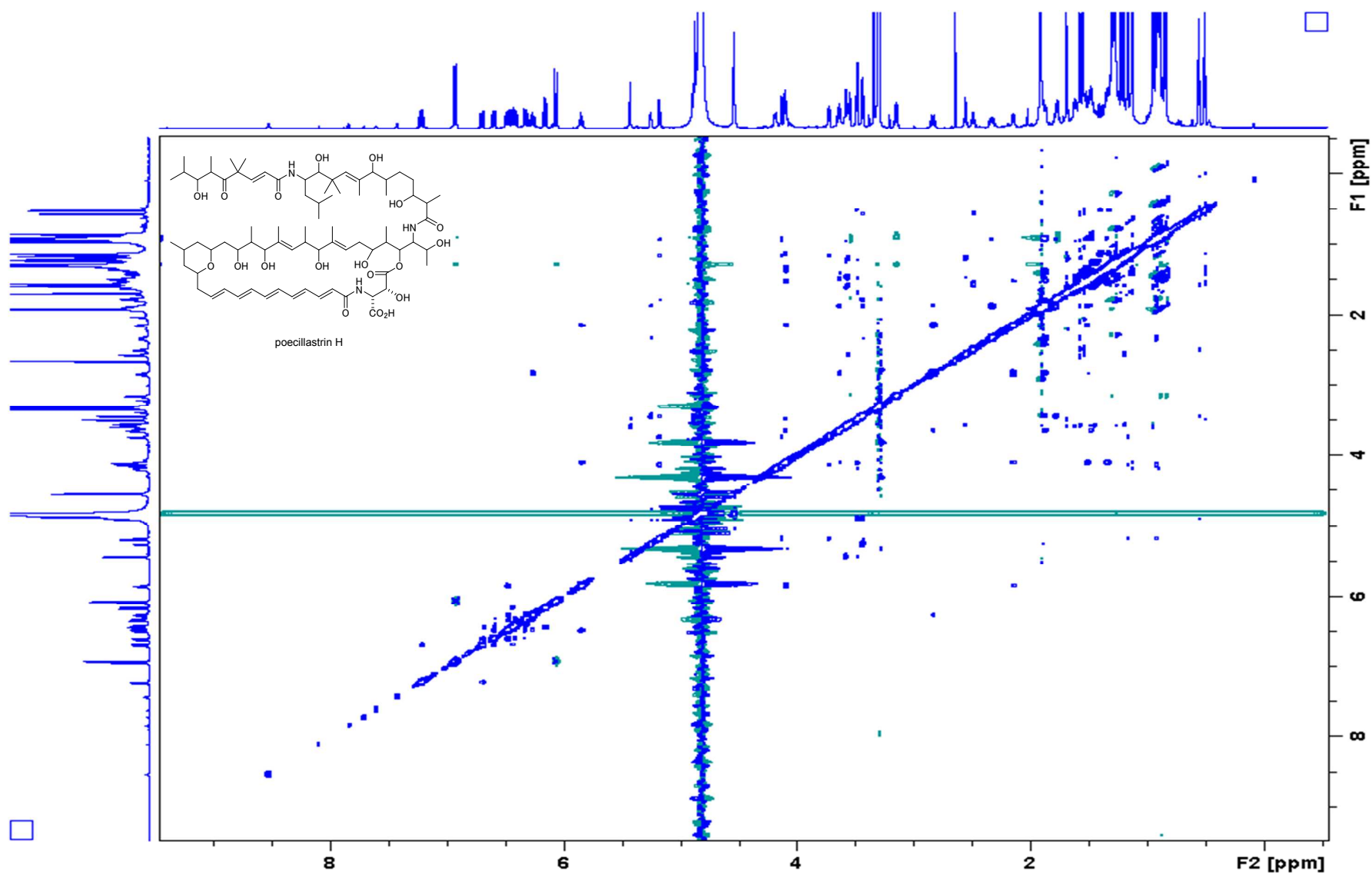
**Figure S4.** TOCSY spectrum of poecillastrin H in CD<sub>3</sub>OD.



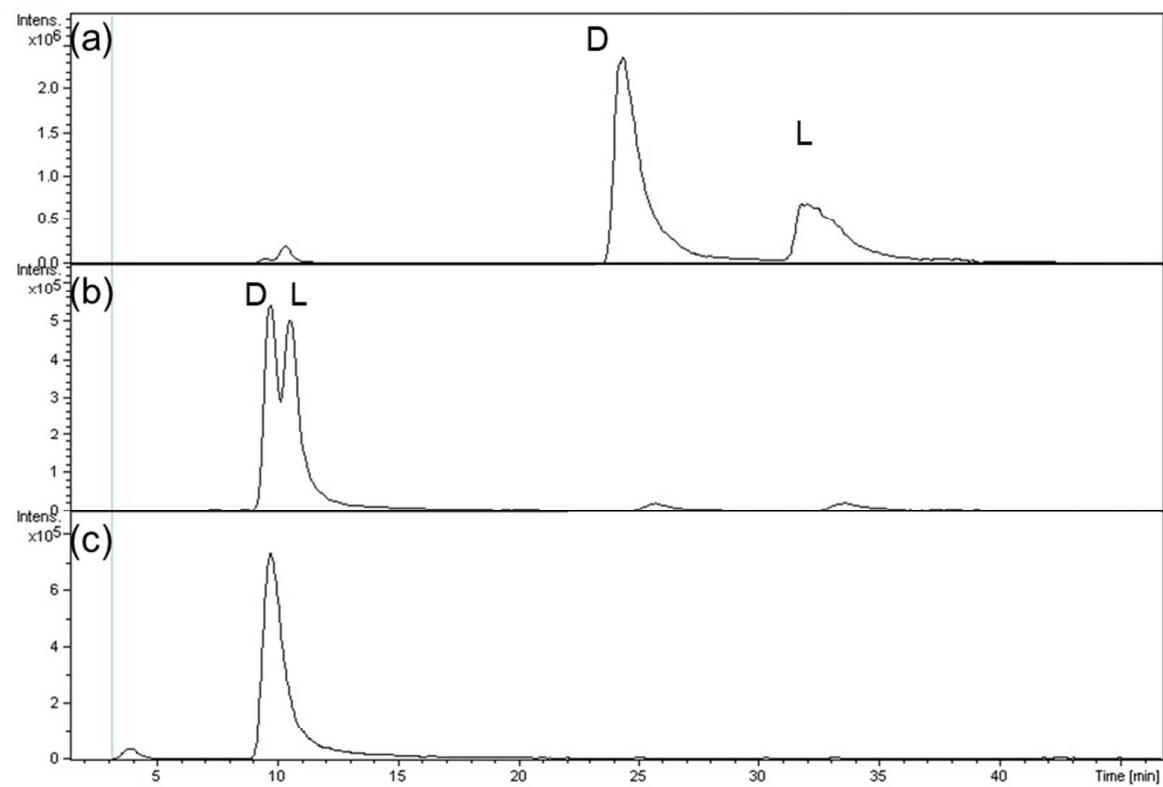


**Figure S6.** HMBC spectrum of poecillastrin H in CD<sub>3</sub>OD.



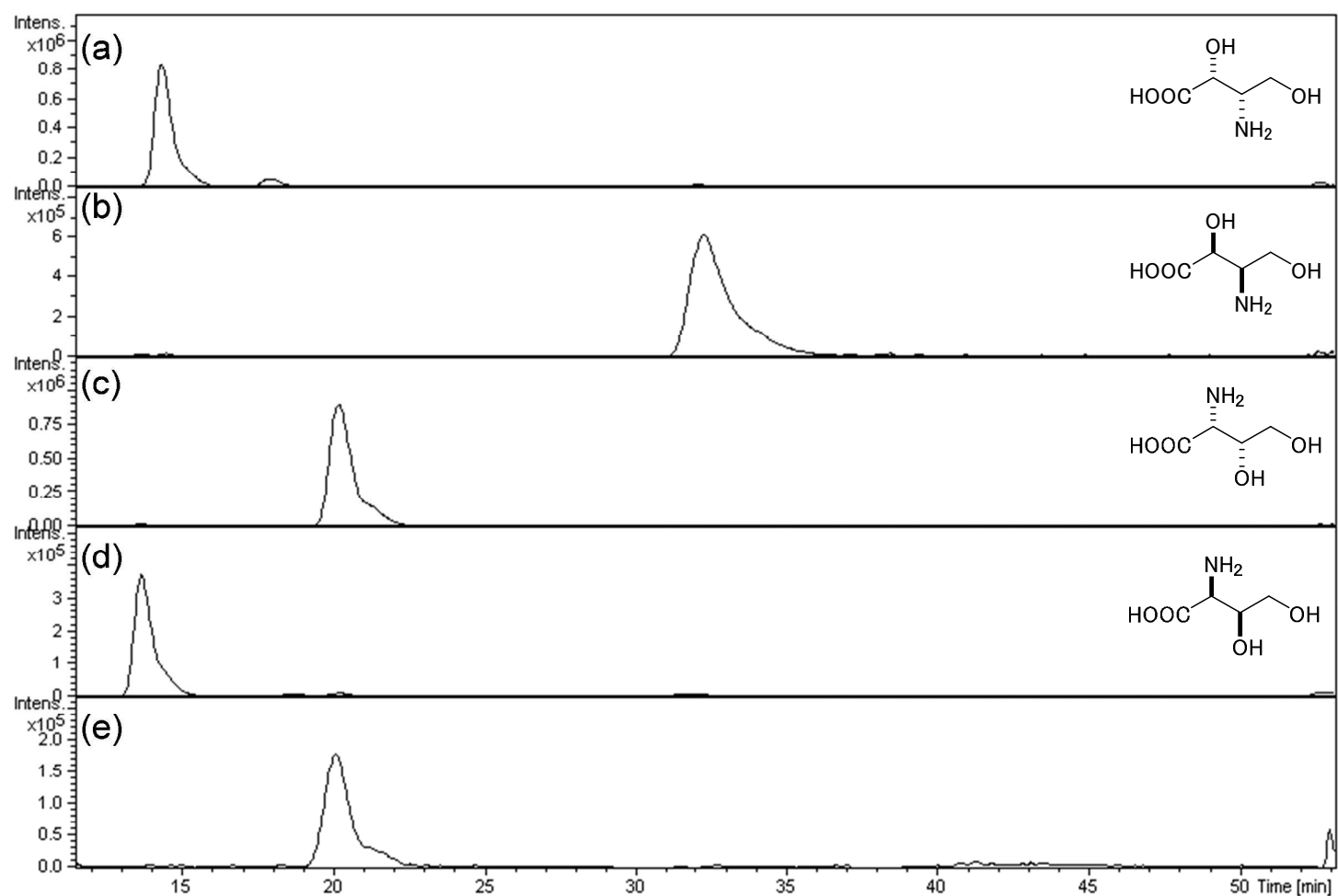


**Figure S7.** NOESY spectrum of poecillastrin H in  $\text{CD}_3\text{OD}$ .



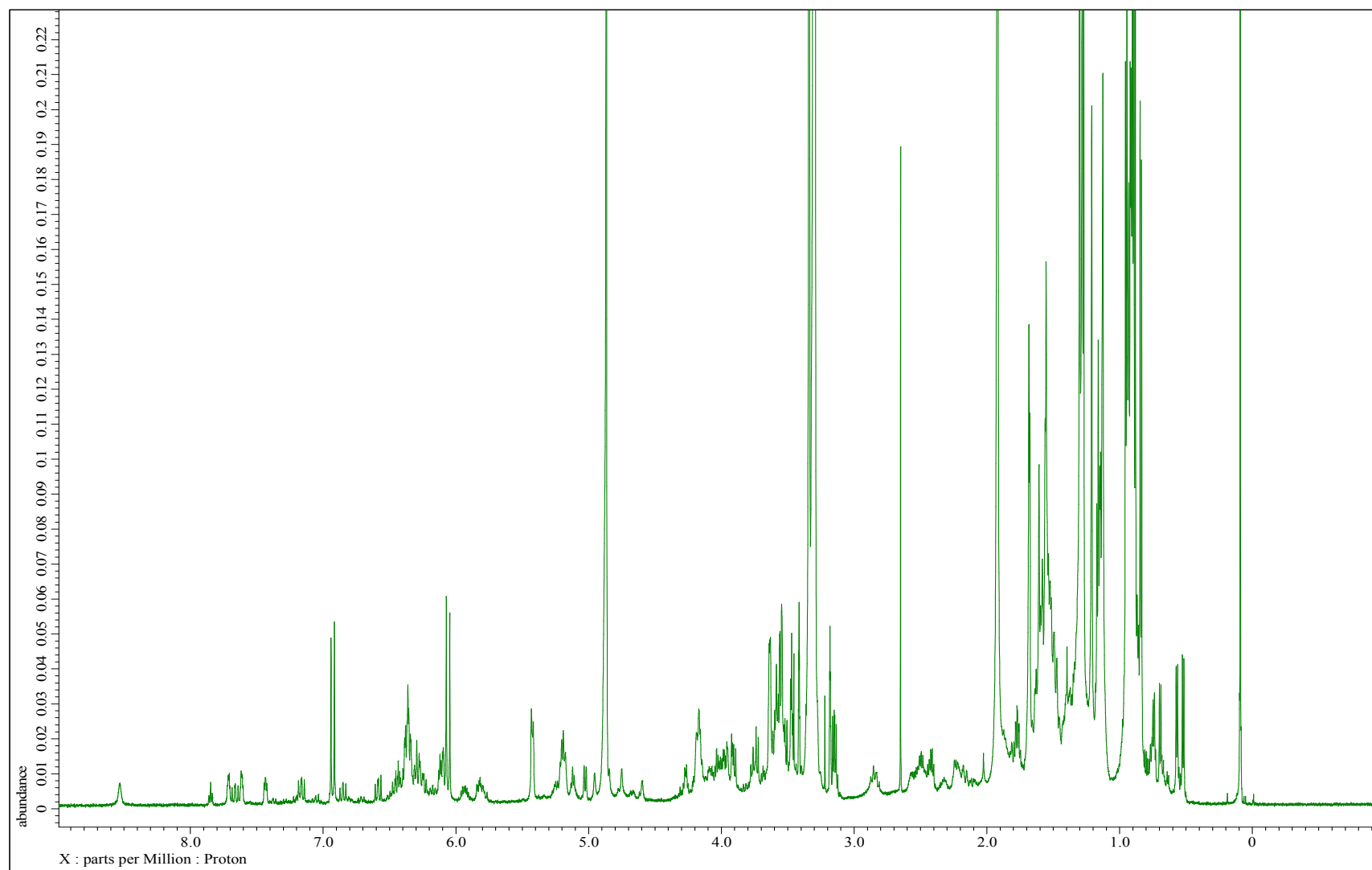
**Figure S8.** LC-MS chromatograms of Marfey's derivatives.

(a) *erythro*- $\beta$ -hydroxyaspartic acid, (b) *threo*- $\beta$ -hydroxyaspartic acid, (c) acid hydrolysate of poecillastrin H

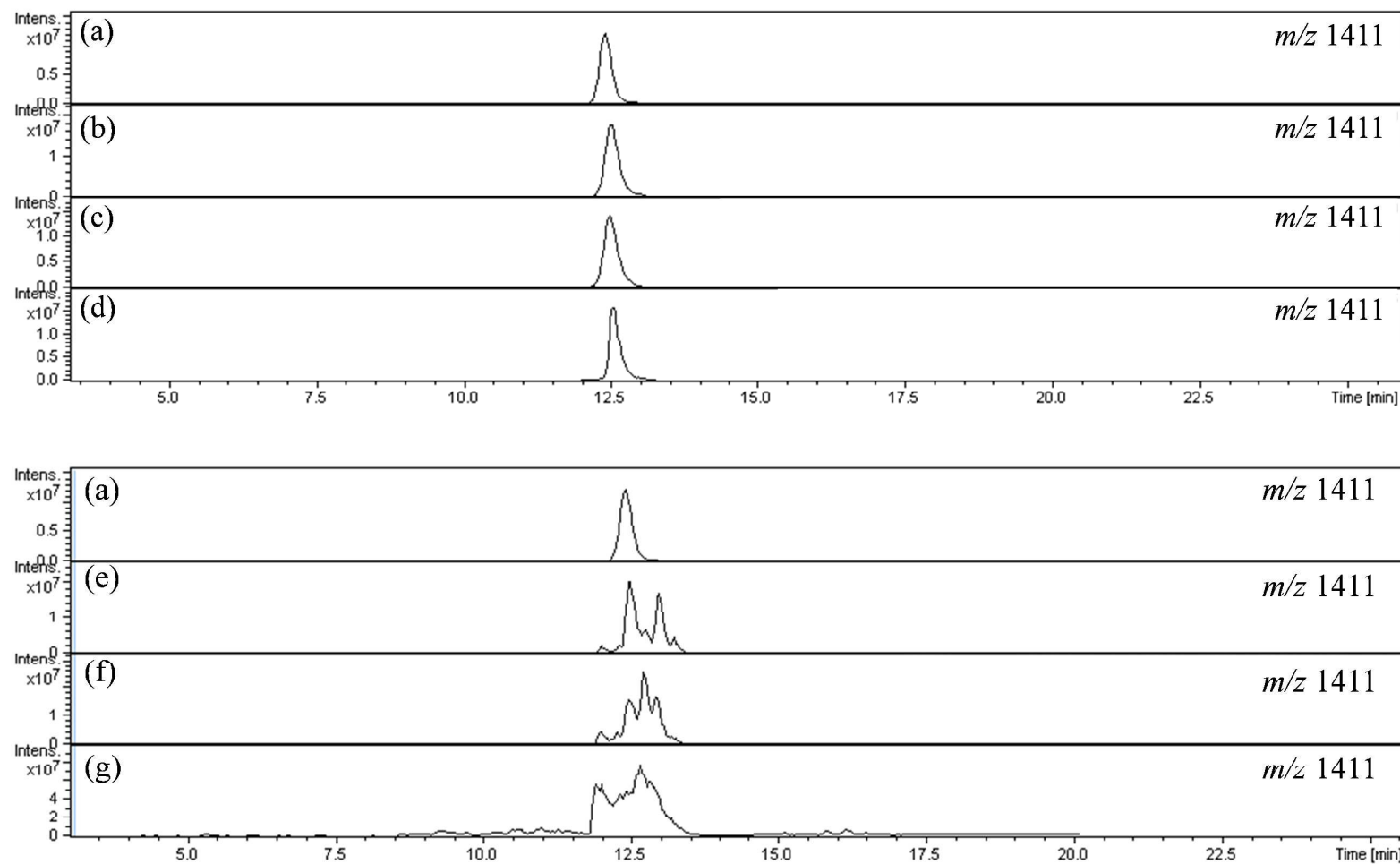


**Figure S9.** LC-MS chromatograms of Marfey's derivatives.

(a) (2R, 3S)-3-amino-2,4-dihydroxybutanoic acid, (b) (2S, 3R)-3-amino-2,4-dihydroxybutanoic acid, (c) (2R, 3R)-2-amino-3,4-dihydroxybutanoic acid, (d) (2S, 3S)-2-amino-3,4-dihydroxybutanoic acid (e) acid hydrolysate of reduction product of poecillastrin H



**Figure S10.**  $^1\text{H}$  NMR spectrum of isomerized poecillastrin H (**1**) in  $\text{CD}_3\text{OD}$ .



**Figure S11.** LC-MS chromatograms of poecillastrin H.

(a) poecillastrin H right after purification, (b) poecillastrin H which is not exposed to the room light for 30 min, (c) poecillastrin H which is not exposed to the room light for 2 day, (d) poecillastrin H which is not exposed to the room light for 3 day, (e) poecillastrin H which is exposed to the room light for 30 min, (f) poecillastrin H which is exposed to the room light for 2 day, (g) poecillastrin H which is exposed to the room light for 3 day.