

# Supplementary Information

## Targeted Isolation of a Cytotoxic Cyclic Hexadepsipeptide from the Mesophotic Zone Sponge-Associated Fungus *Cymostachys* sp. NBUF082

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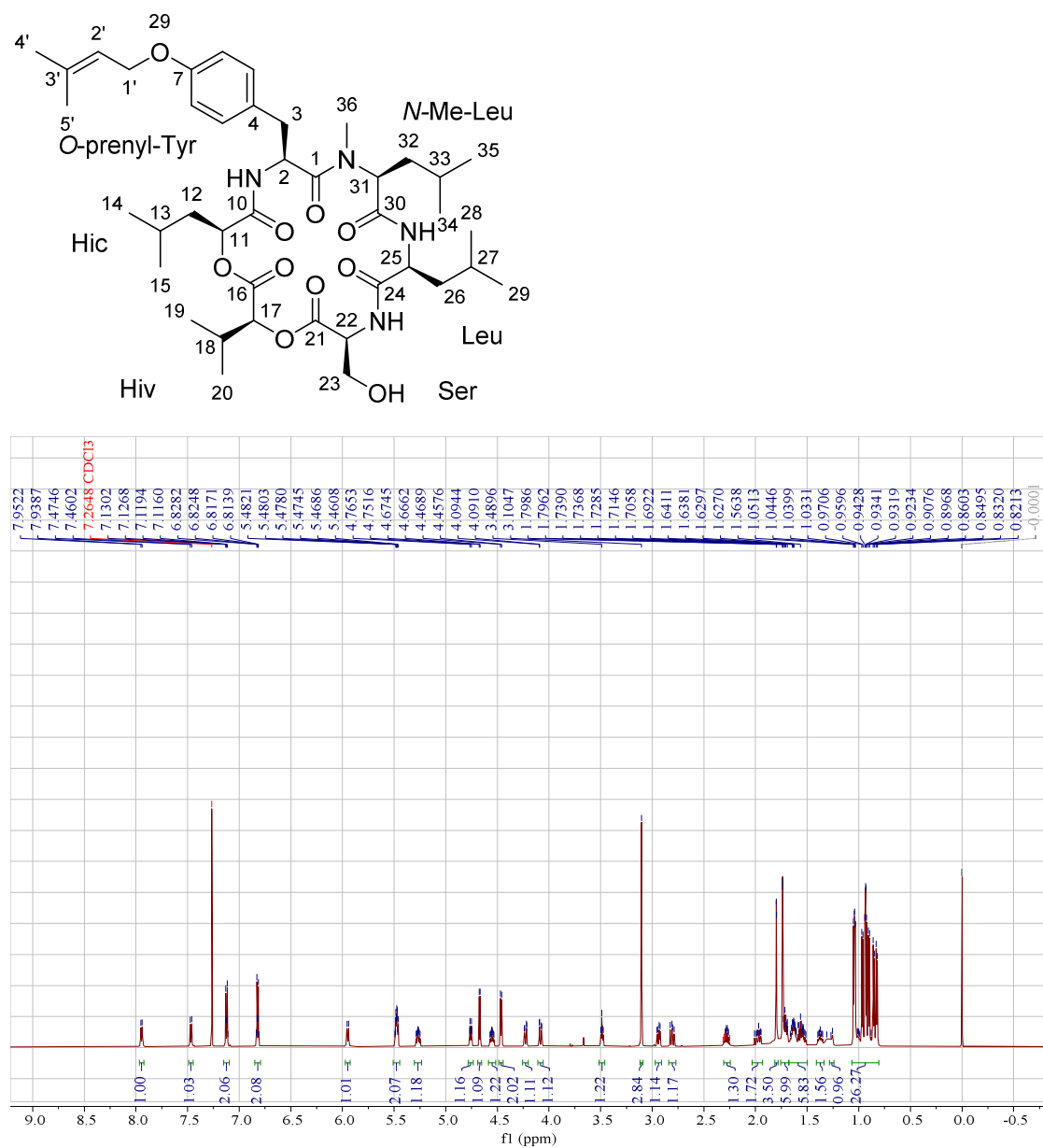
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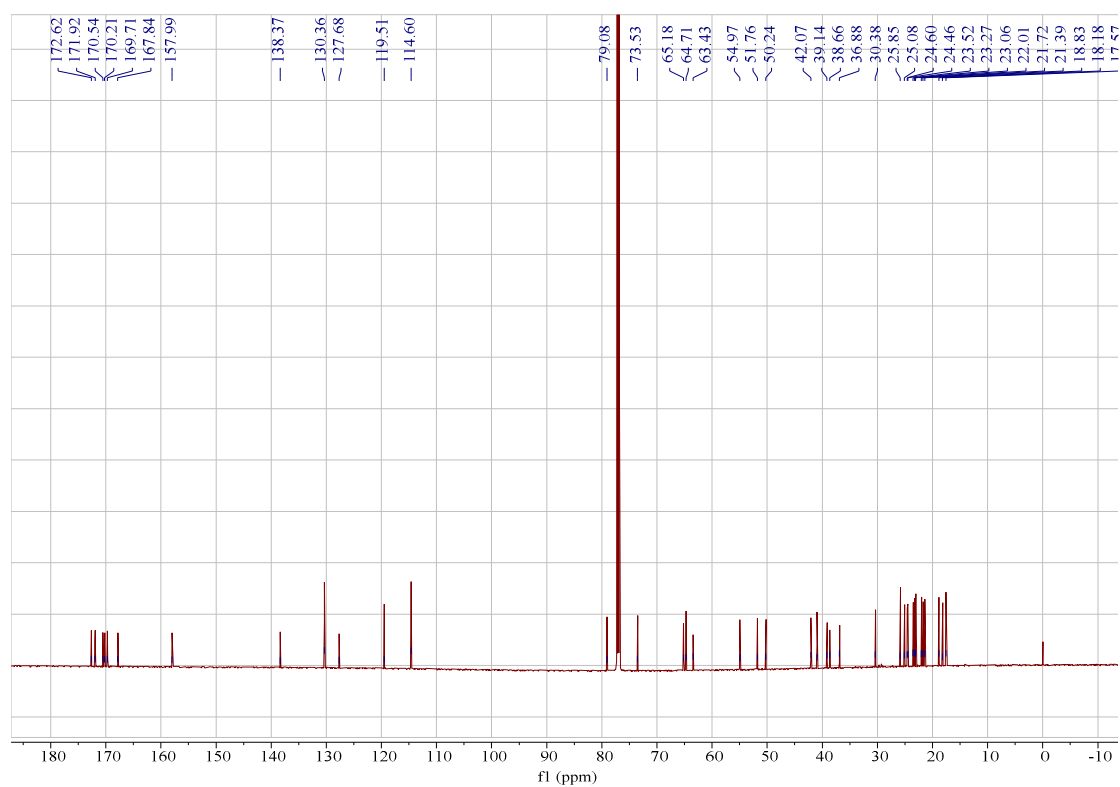
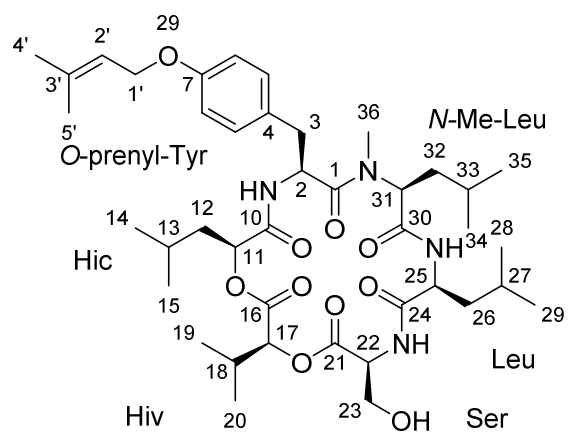
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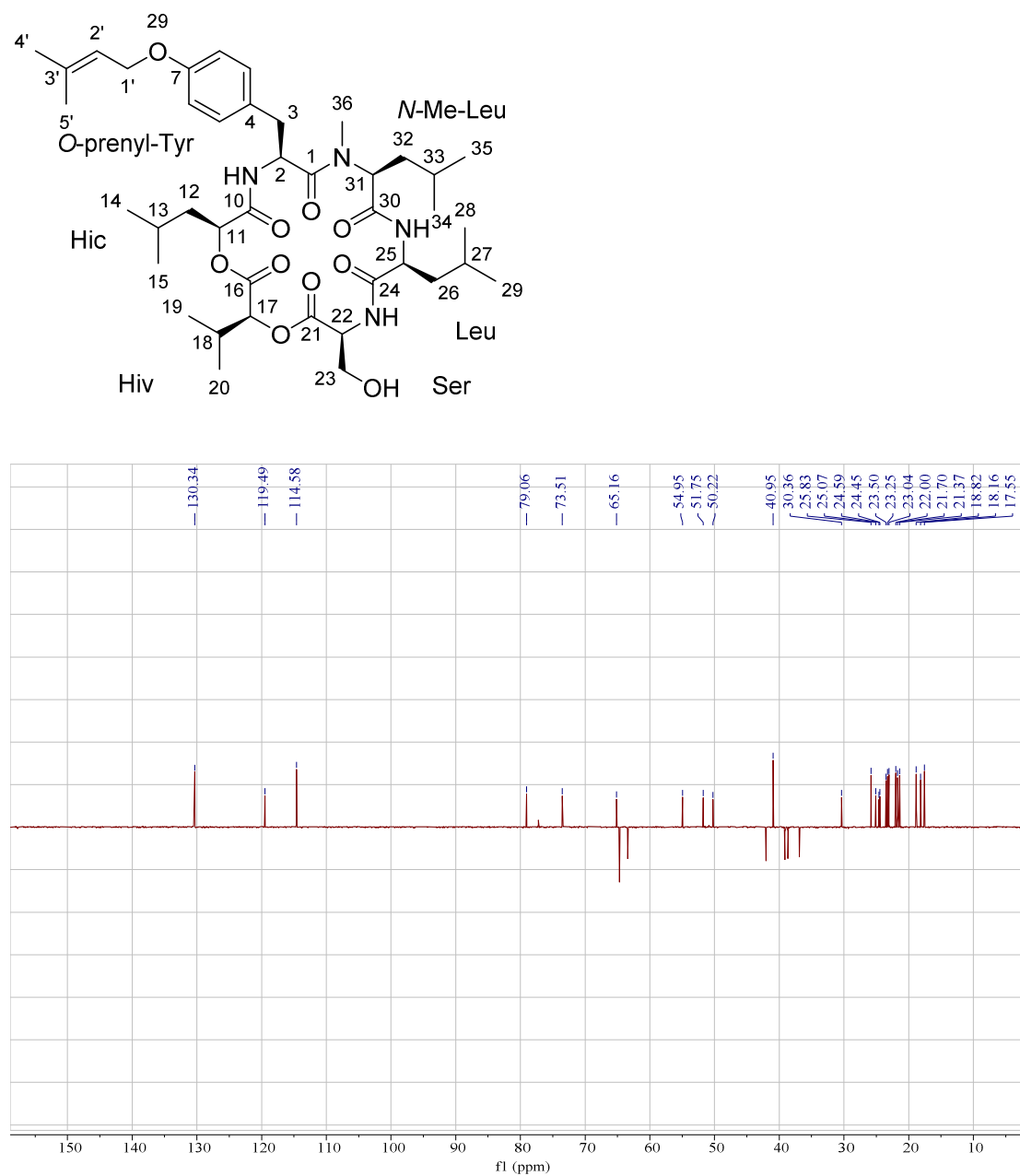
**Figure S1.** LC-MS/MS-derived molecular network of extracts from the fungus *Cymostachys* sp. NBUF082. The targeted nodes correlating to cyclic hexadepsipeptides were involved in the framed cluster.



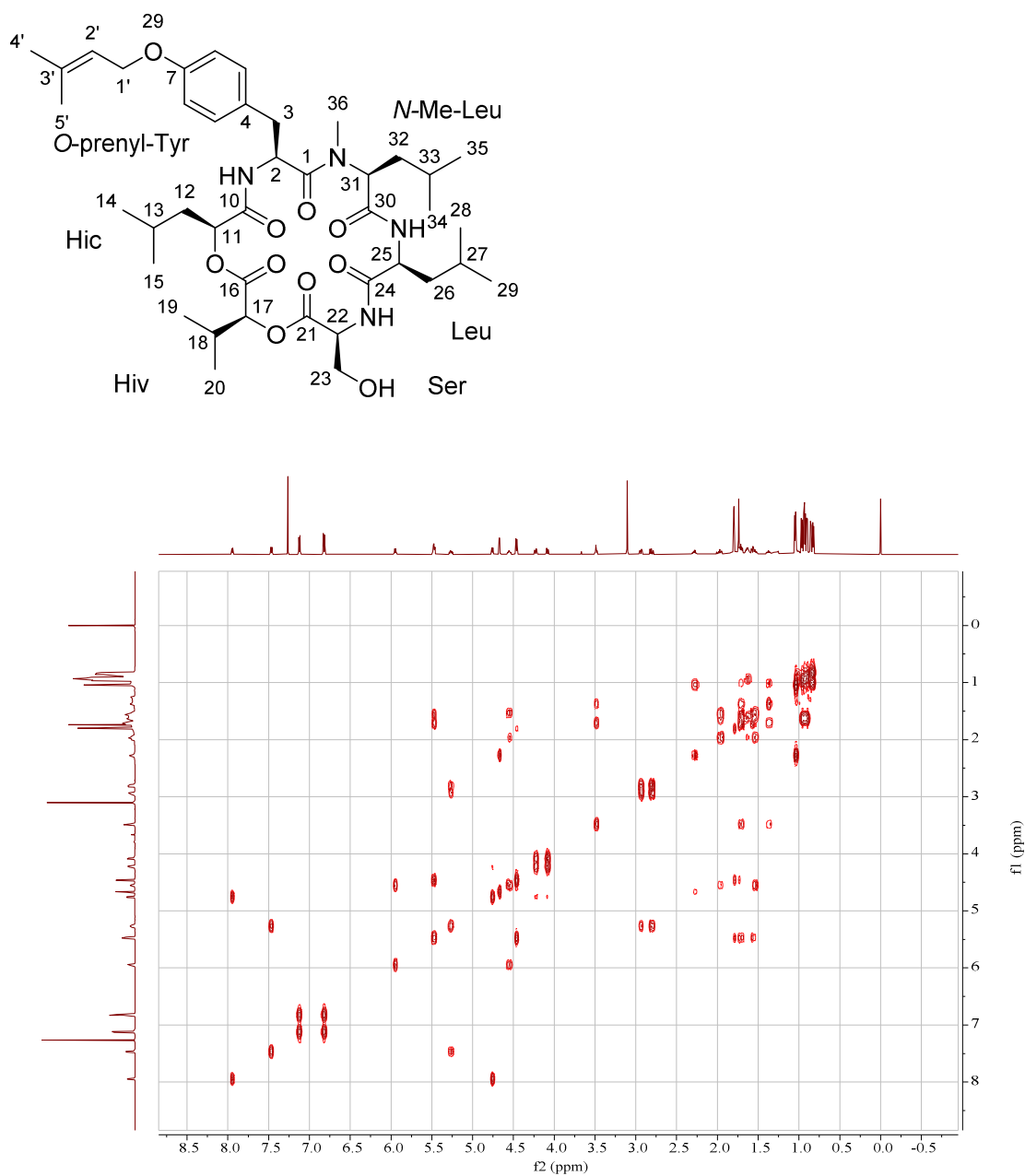
**Figure S2.**  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$  (600 MHz).



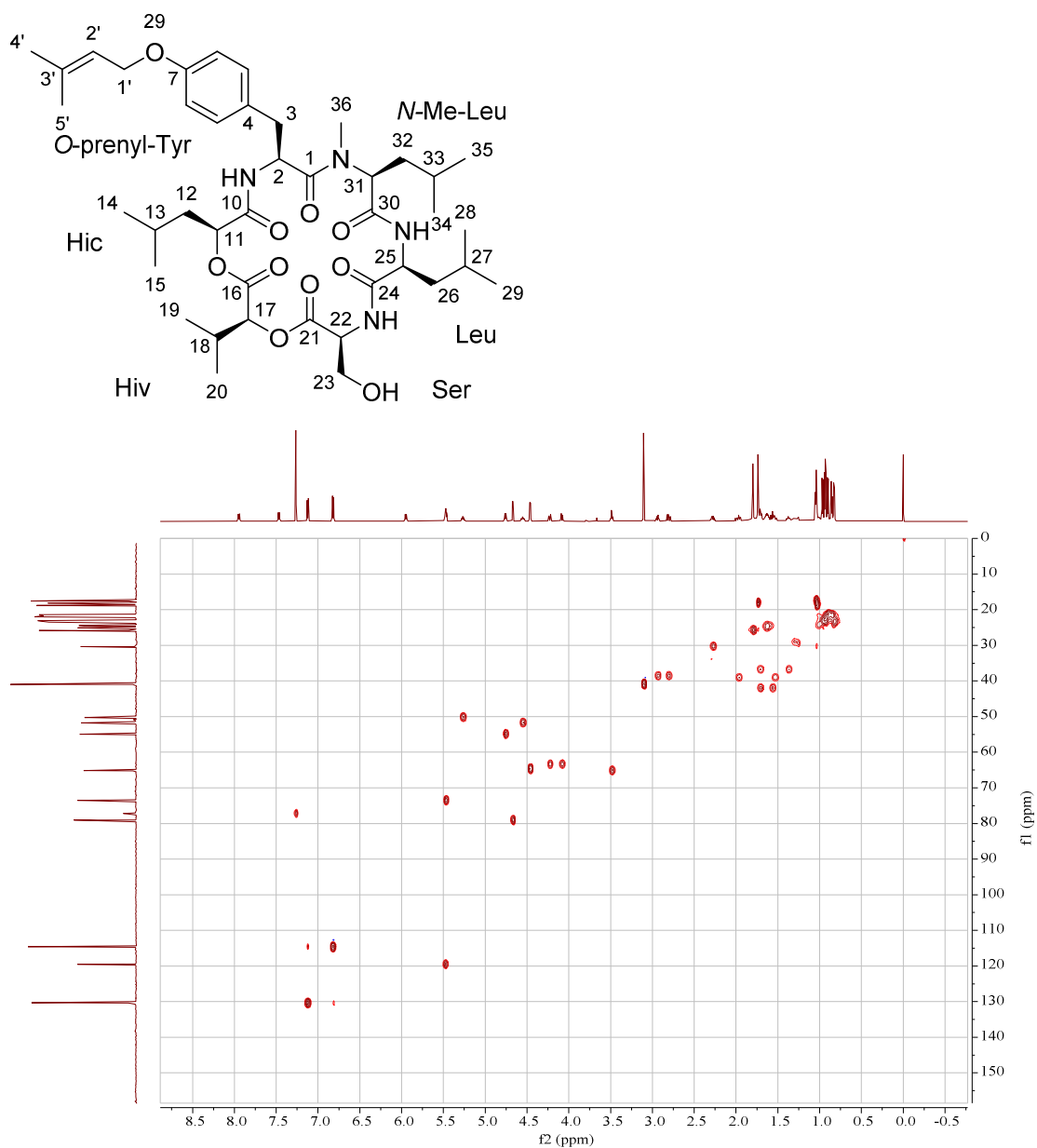
**Figure S3.**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  (150 MHz).



**Figure S4.** DEPT135 spectrum of **1** in CDCl<sub>3</sub> (150 MHz).

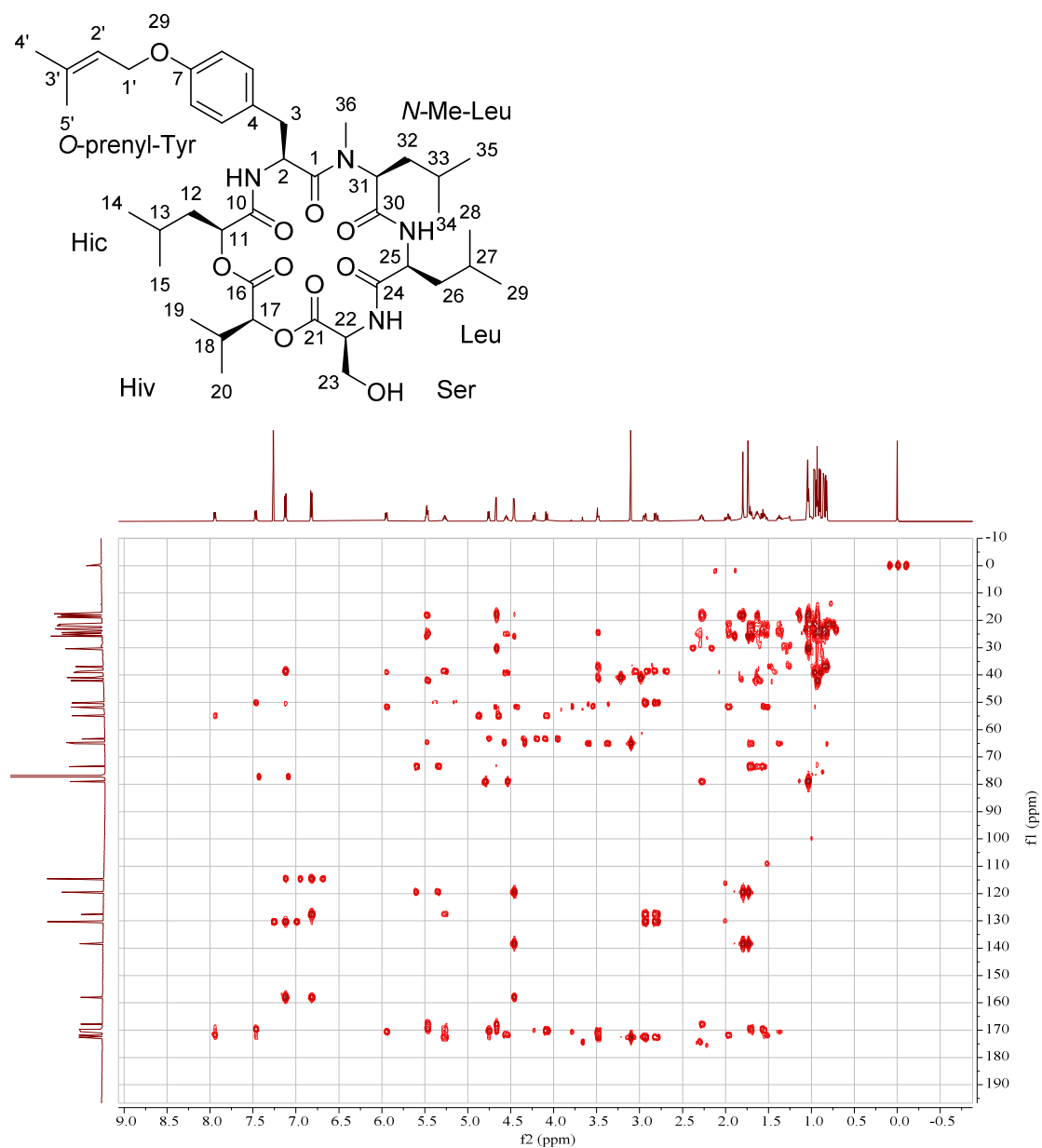


**Figure S5.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{CDCl}_3$ .

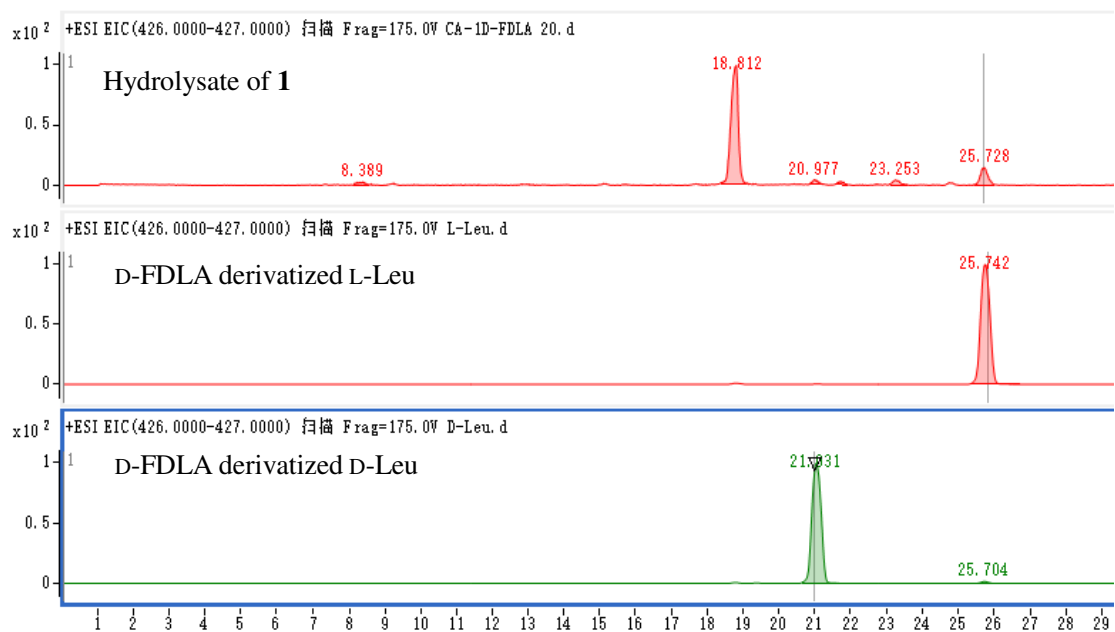
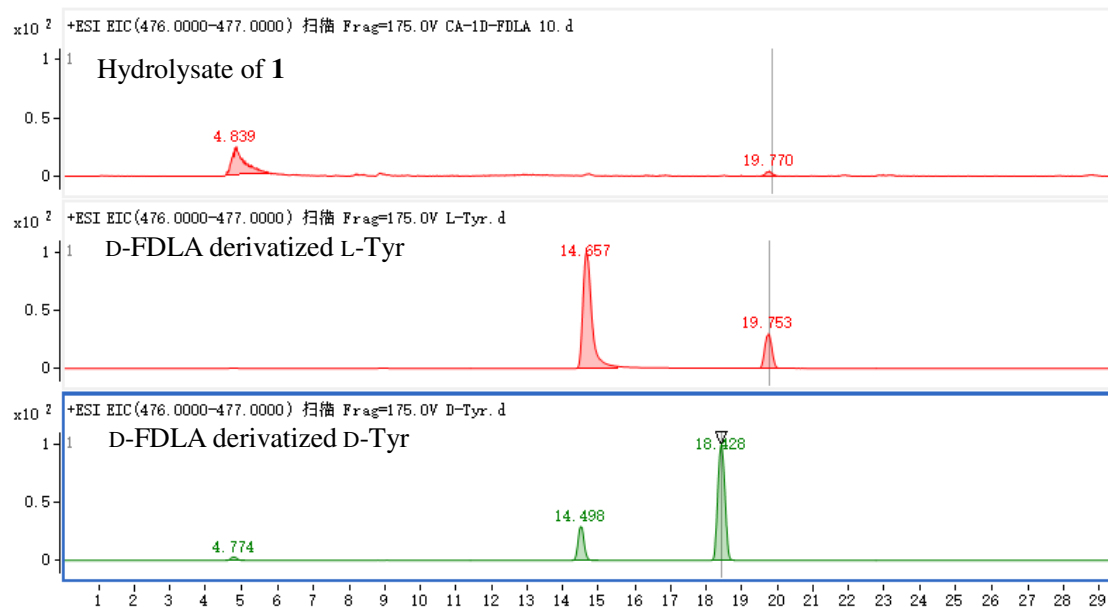


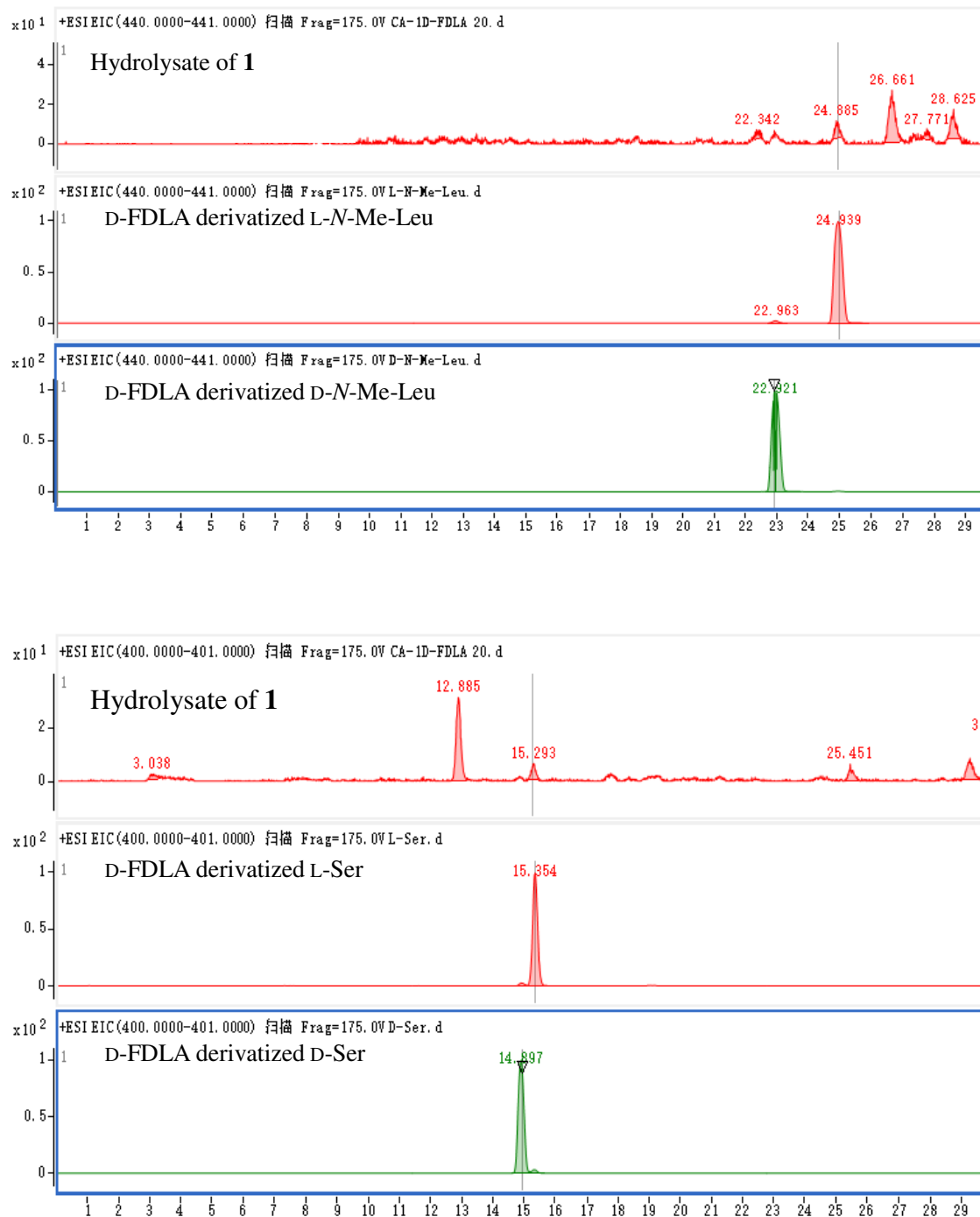
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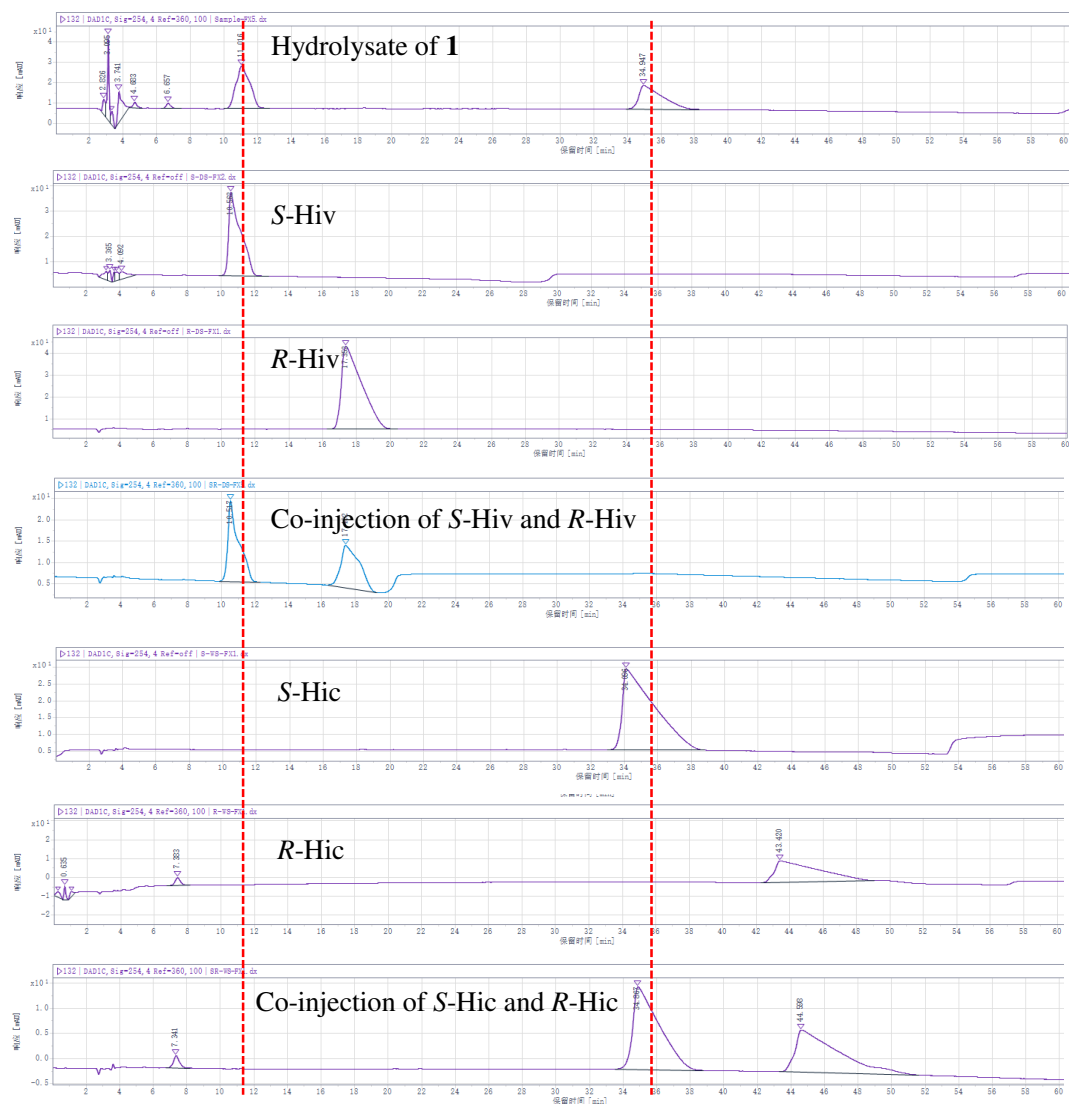


**Figure S7.** HMBC spectrum of **1** in CDCl<sub>3</sub>.





**Figure S8.** Chromatographic profiles of amino acids from compound **1** acid hydrolysis products



**Figure S9.** Chiral HPLC analysis performed on hydrolysis products of **1**.