

Supporting Information

Mirabamides E-H, HIV-Inhibitory Depsipeptides from the Sponge *Stelletta clavosa*

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Figure S1. $^1\text{H-NMR}$ spectrum of mirabamide E (**1**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1) with 0.1% TFA-d

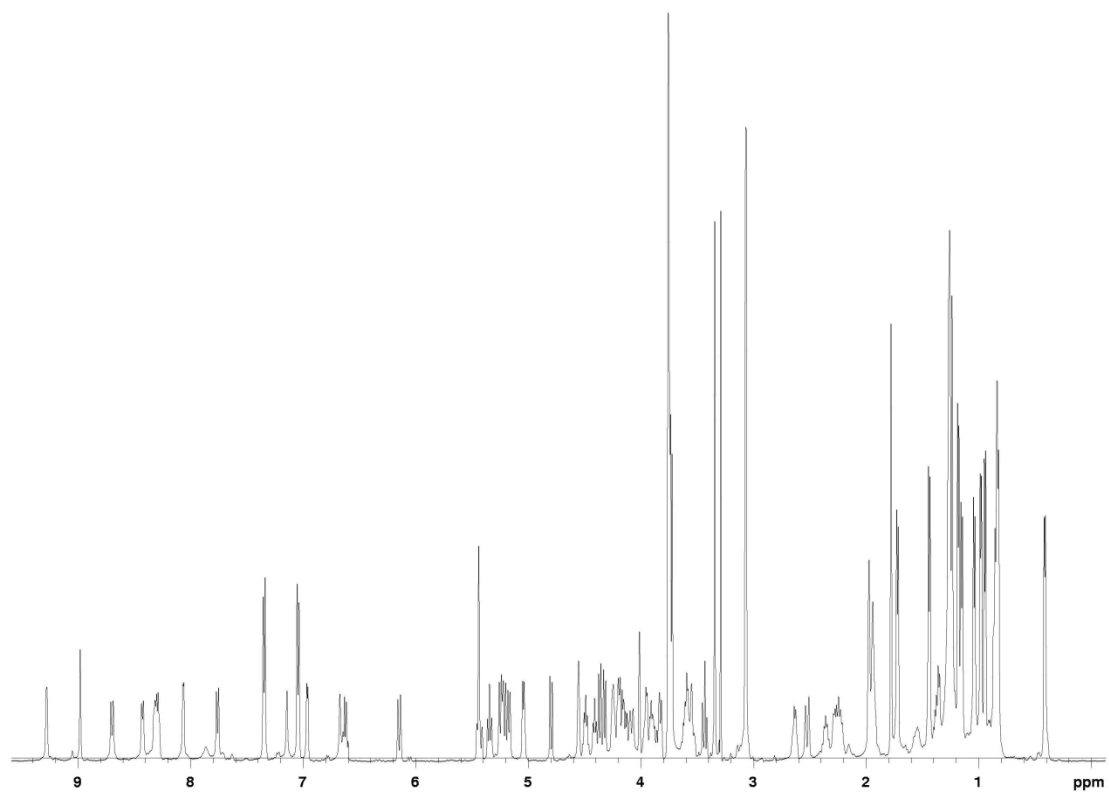


Figure S2. ^{13}C -NMR spectrum of mirabamide E (**1**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1)

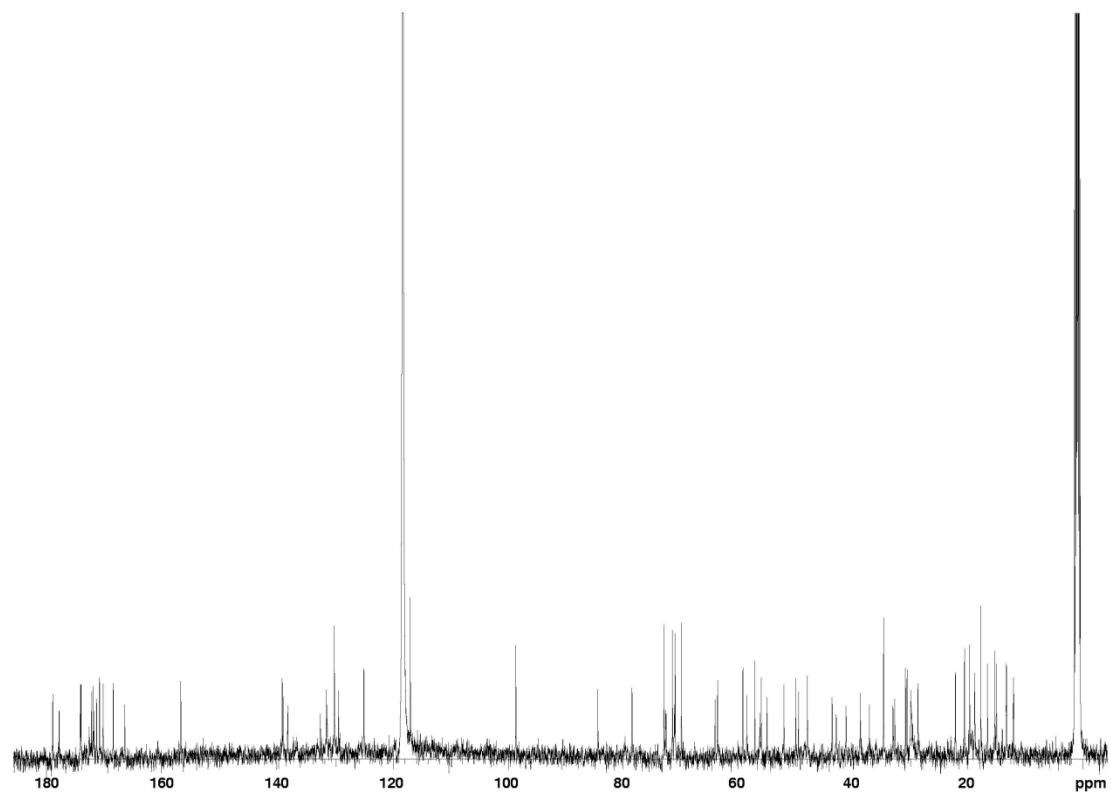


Figure S3. HMBC spectrum of mirabamide E (**1**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

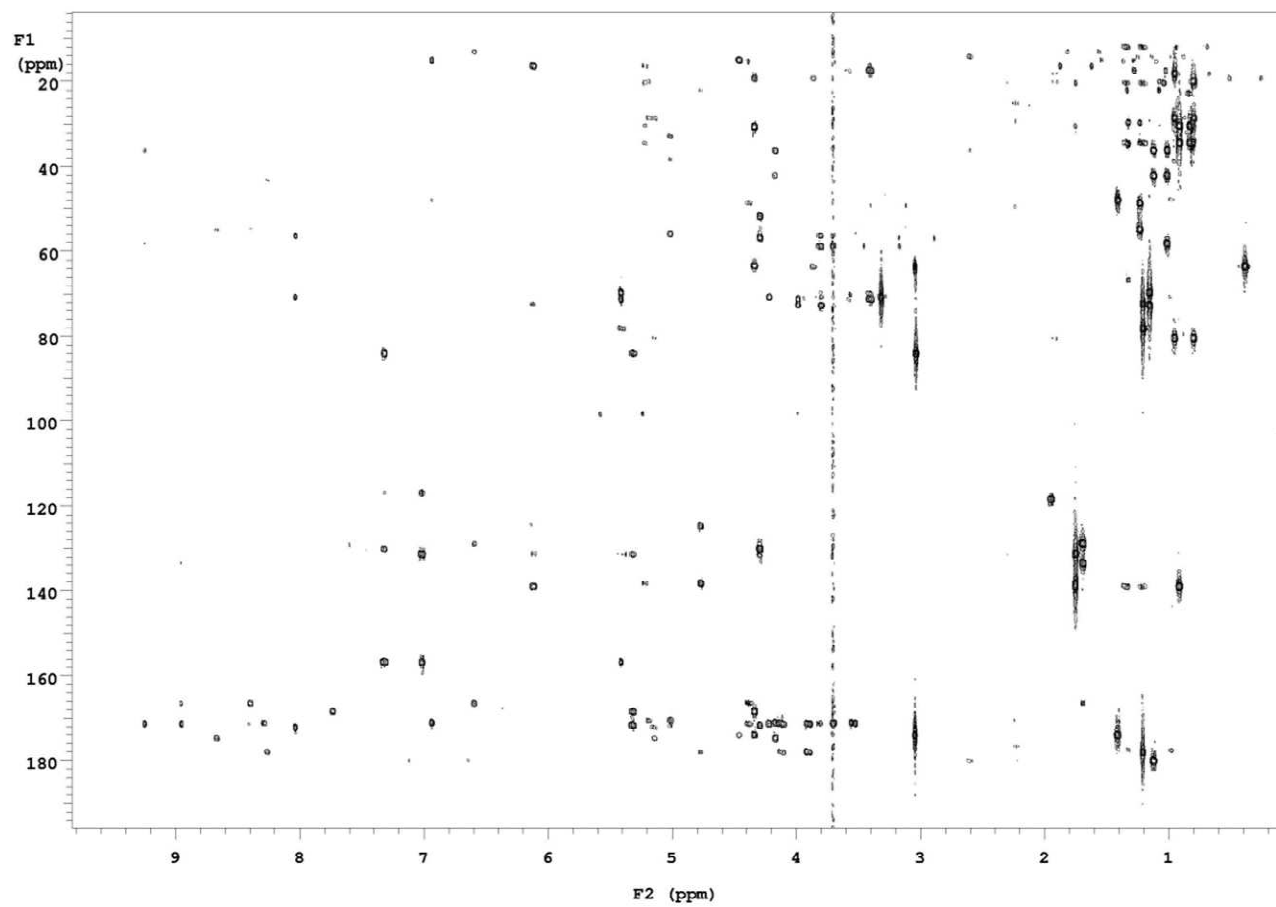


Figure S4. wgNOESY spectrum of mirabamide E (**1**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

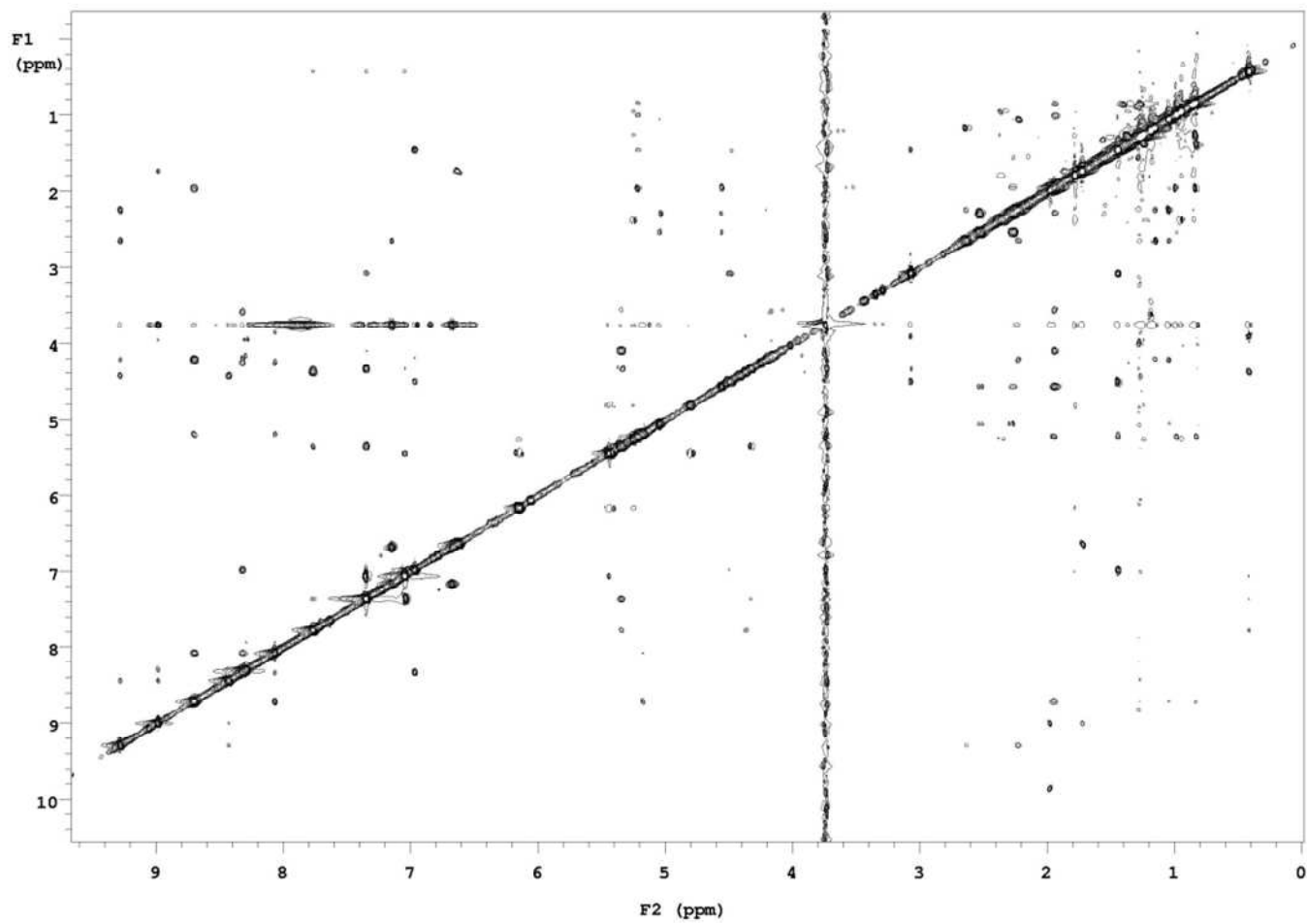


Figure S5. $^1\text{H-NMR}$ spectrum of mirabamide F (**2**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1) with 0.1% TFA-d

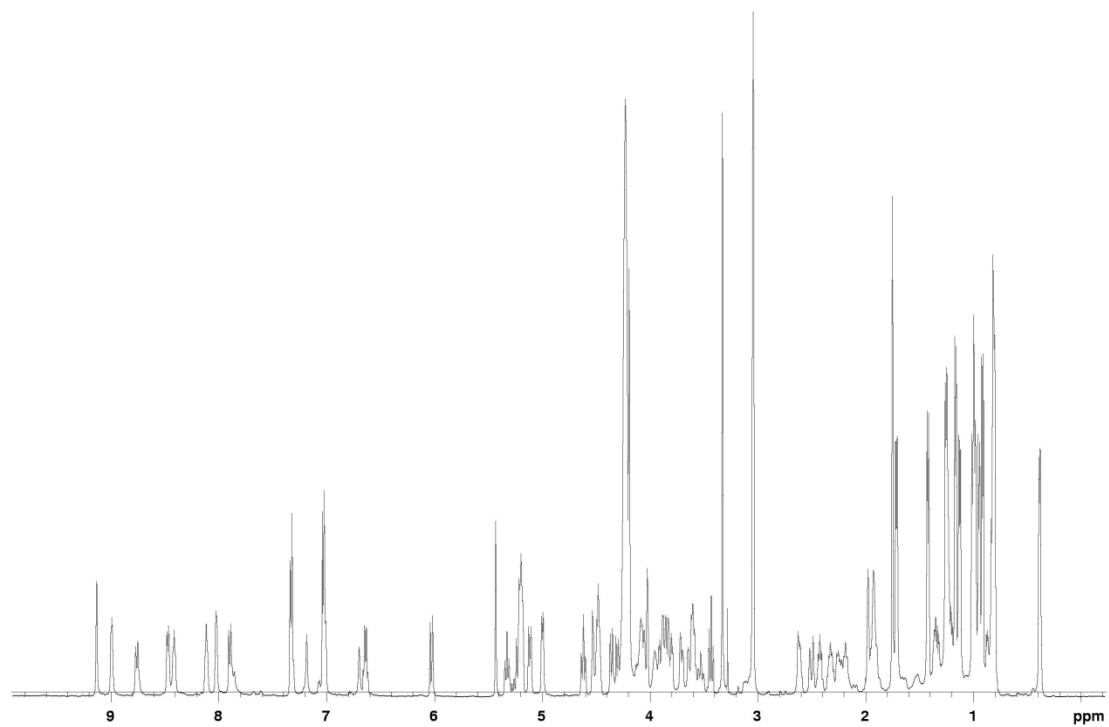


Figure S6. ^{13}C -NMR spectrum of mirabamide F (**2**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1)

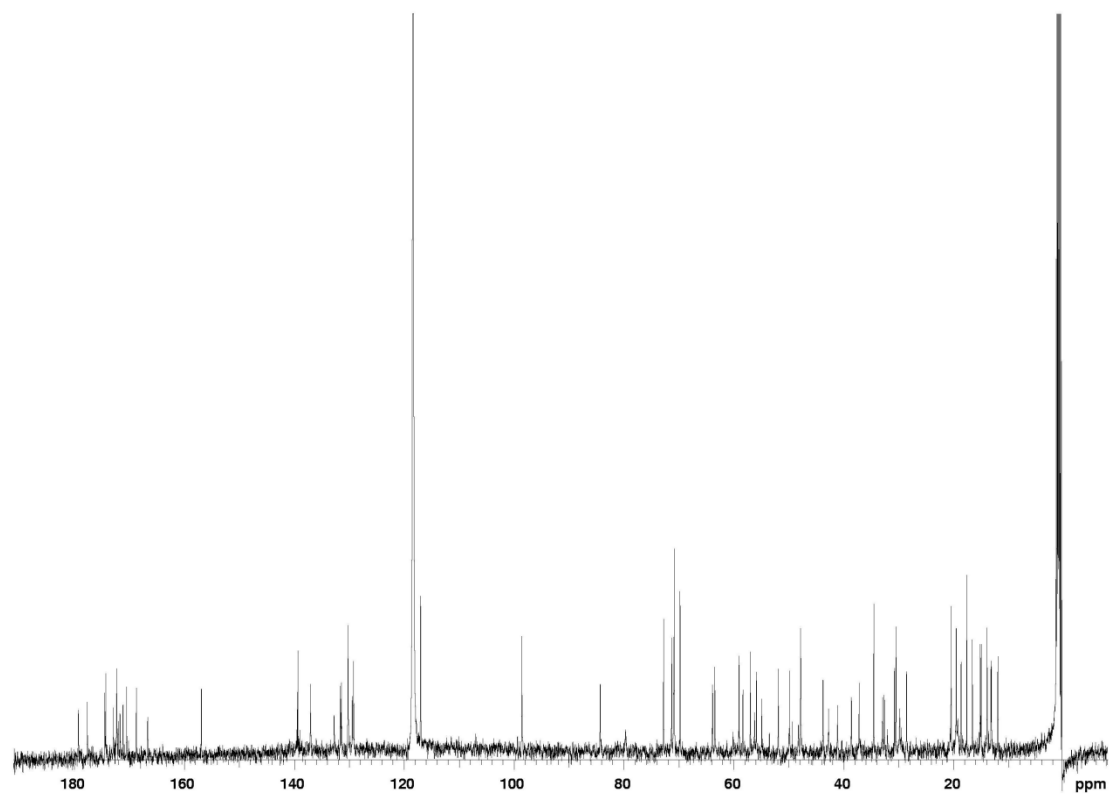


Figure S7. HMBC spectrum of mirabamide F (**2**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

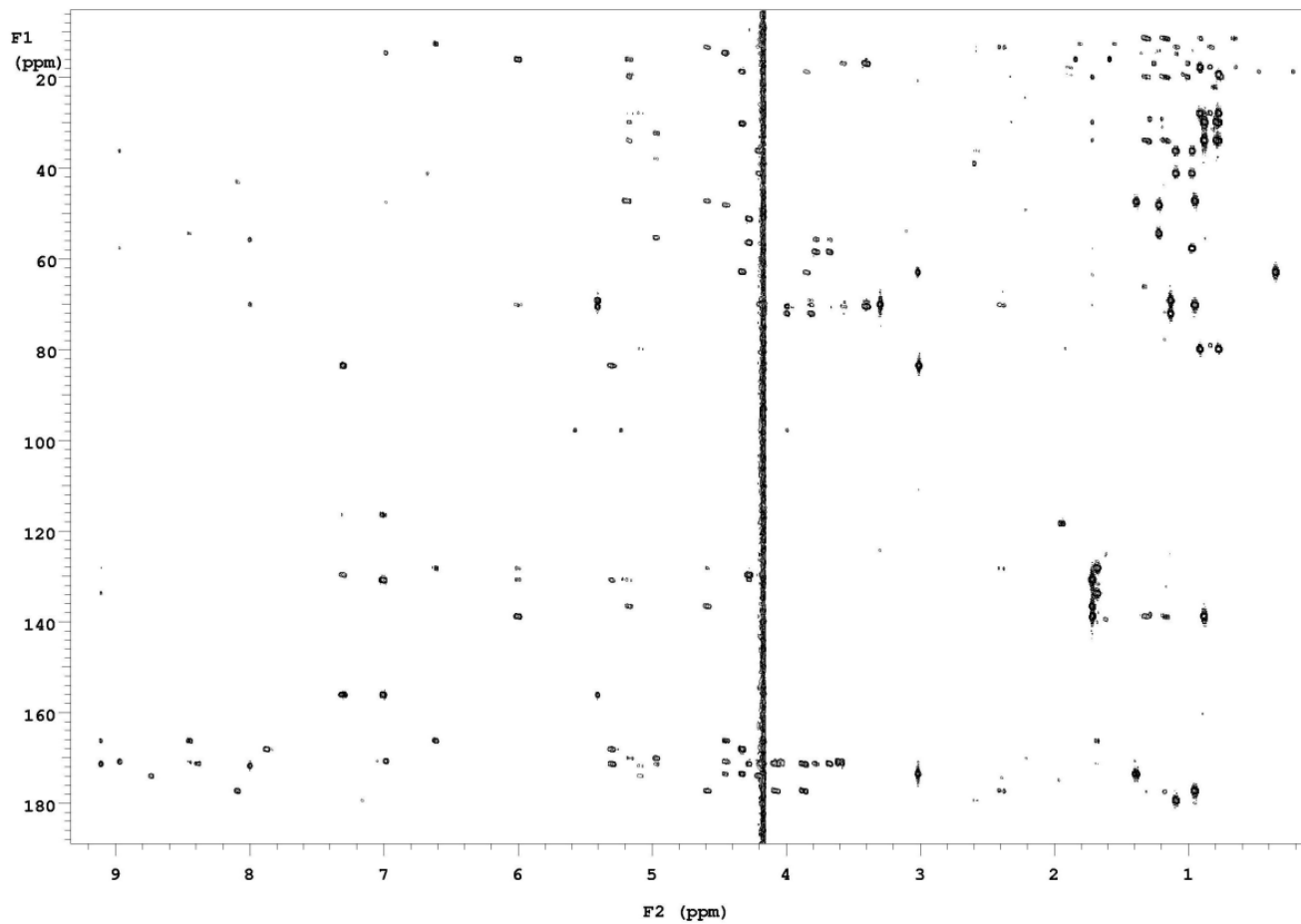


Figure S8. wgNOESY spectrum of mirabamide F (**2**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

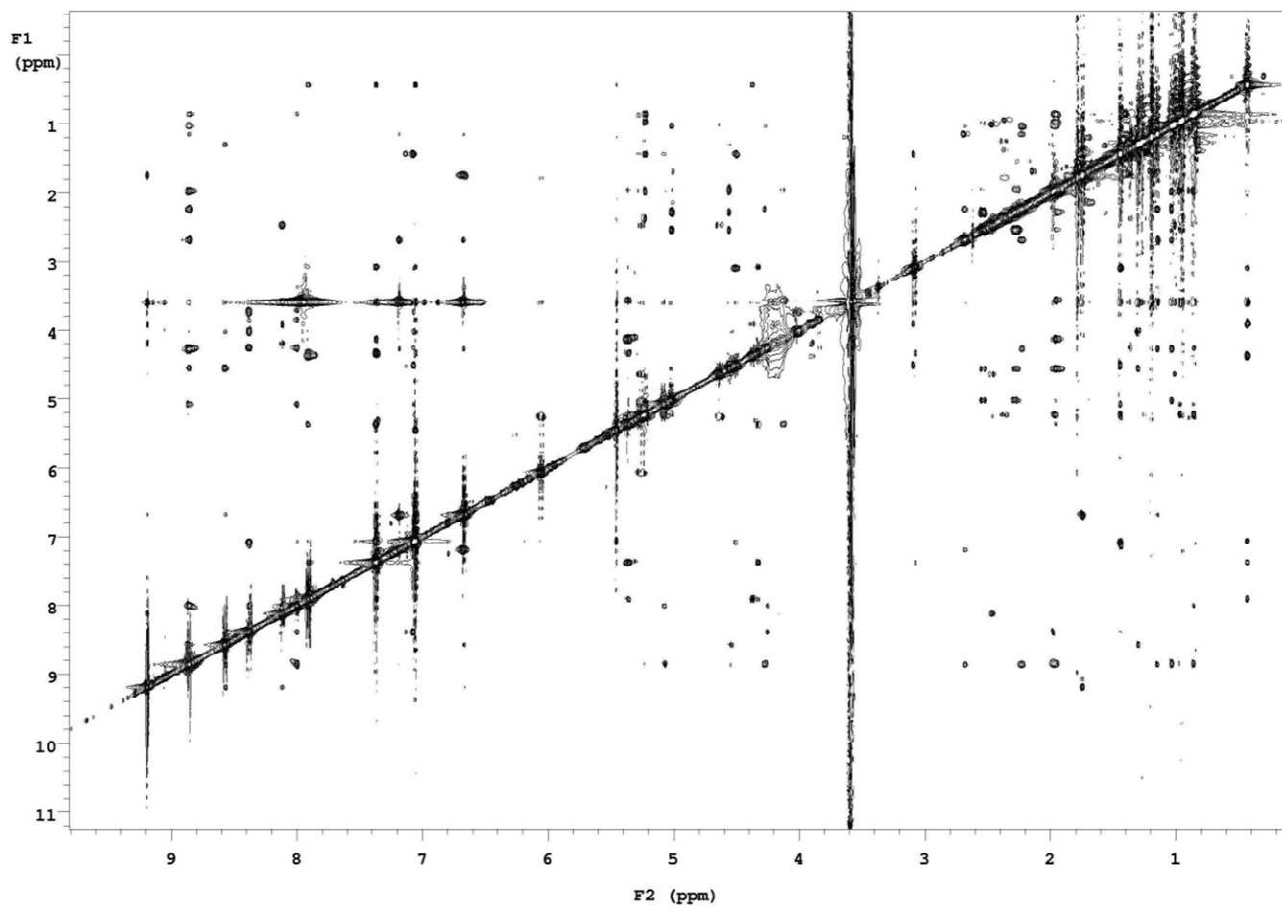


Figure S9. $^1\text{H-NMR}$ spectrum of mirabamide G (**3**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1) with 0.1% TFA-*d*

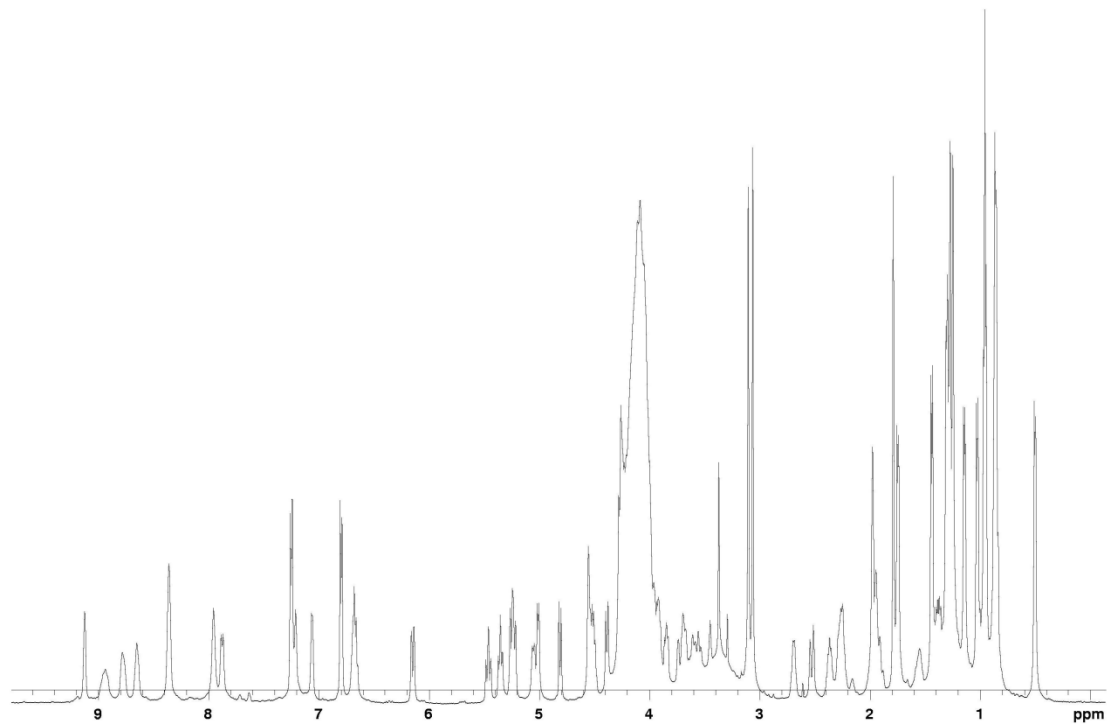


Figure S10. ^{13}C -NMR spectrum of mirabamide G (**3**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1)

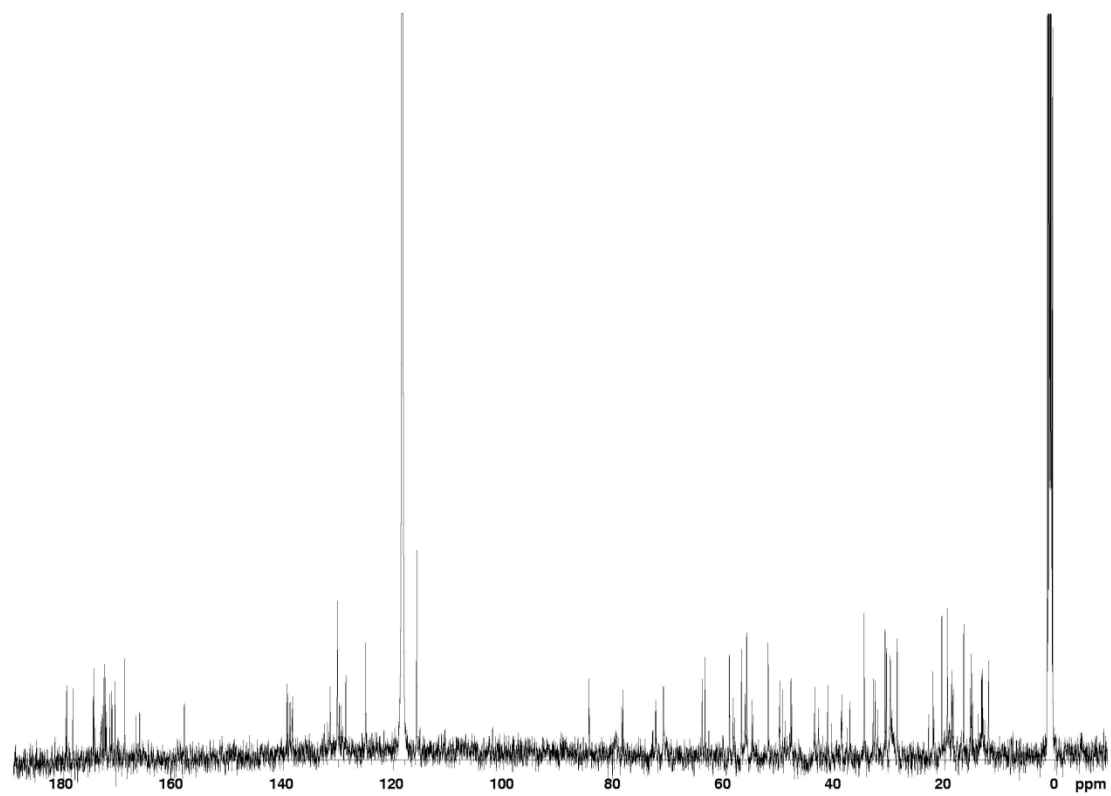


Figure S11. HMBC spectrum of mirabamide G (**3**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

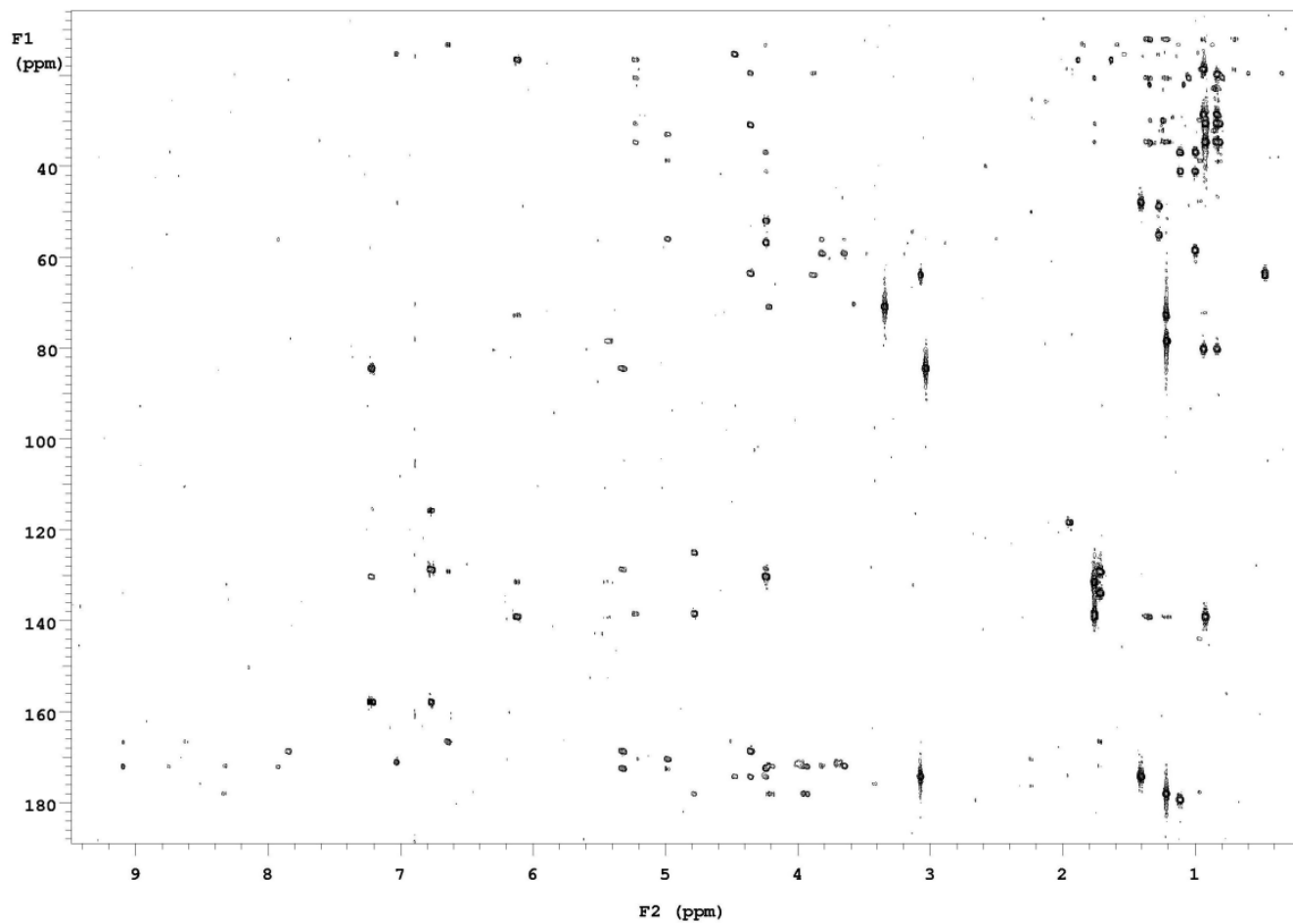


Figure S12. wgNOESY spectrum of mirabamide G (**3**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

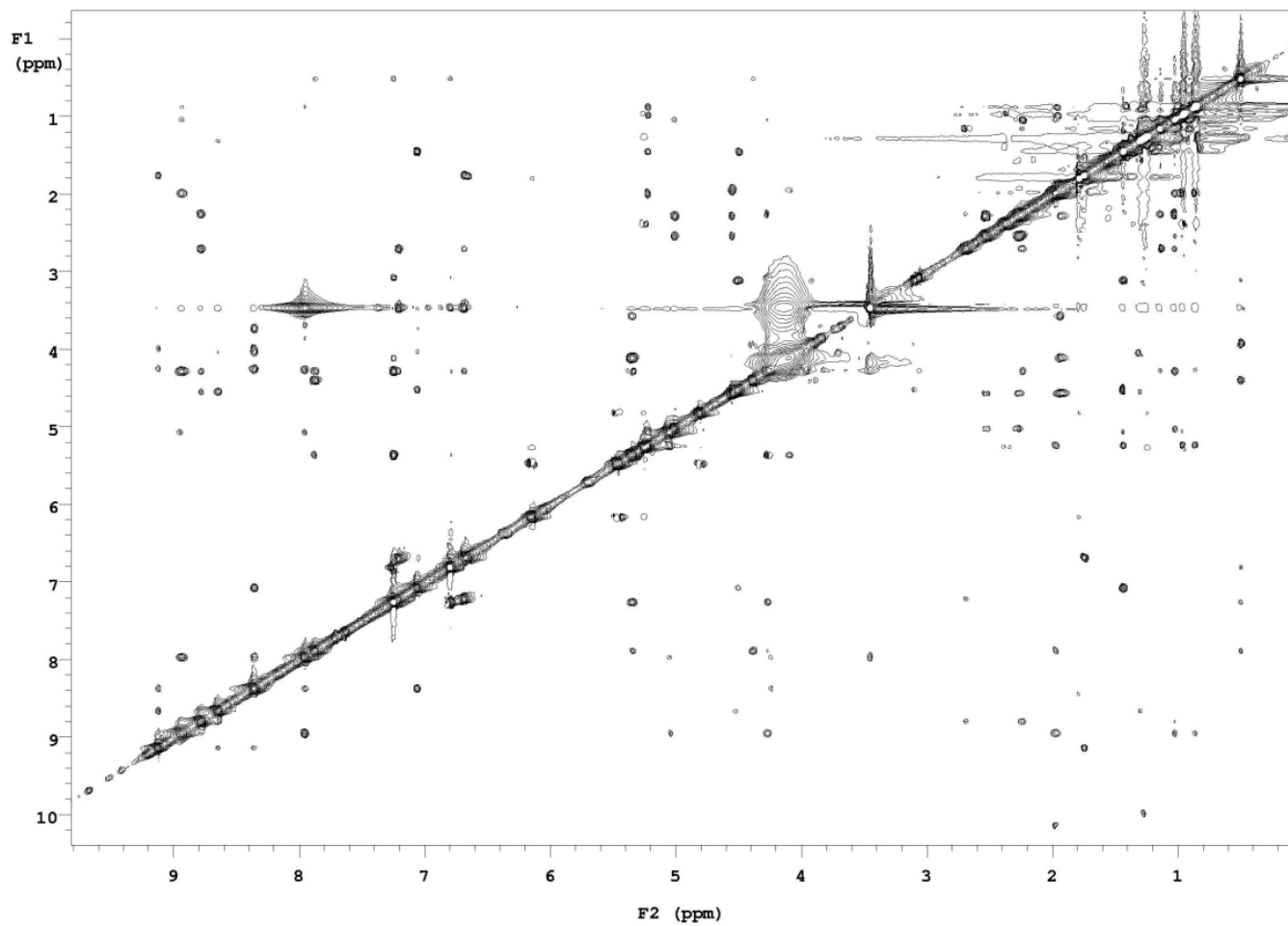


Figure S13. $^1\text{H-NMR}$ spectrum of mirabamide H (**4**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1) with 0.1% TFA-d

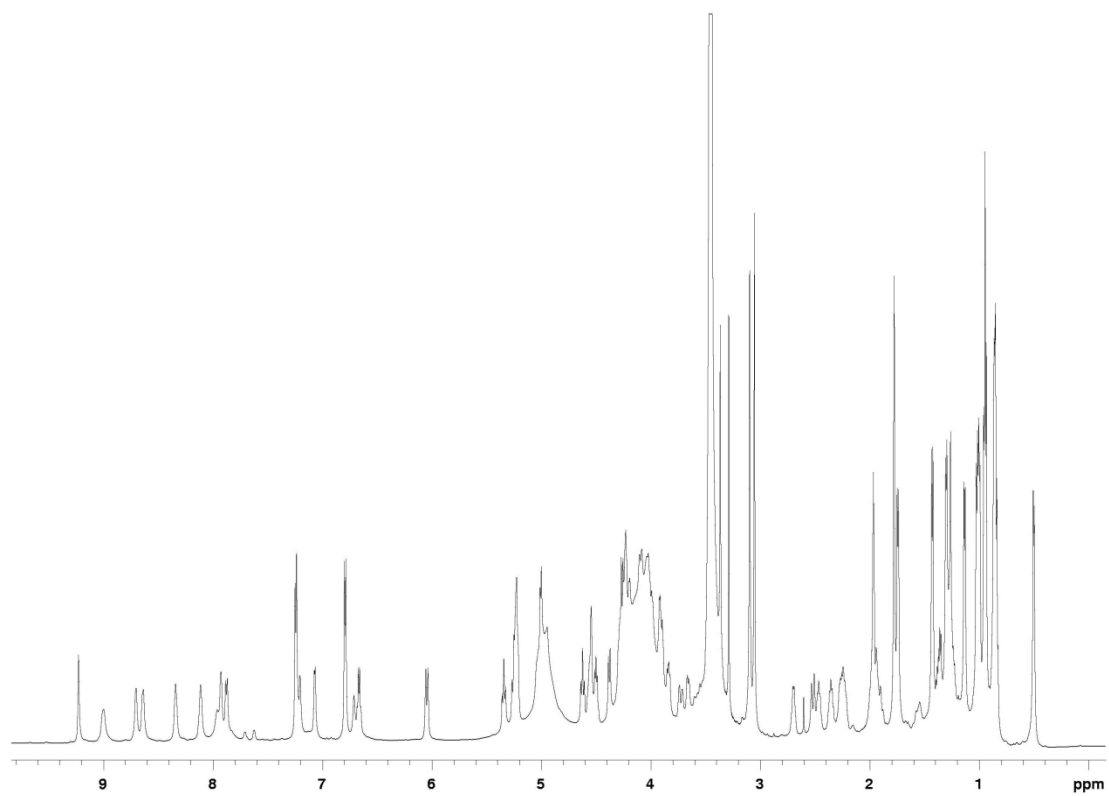


Figure S14. ^{13}C -NMR spectrum of mirabamide H (**4**) in $\text{CD}_3\text{CN-H}_2\text{O}$ (4:1)

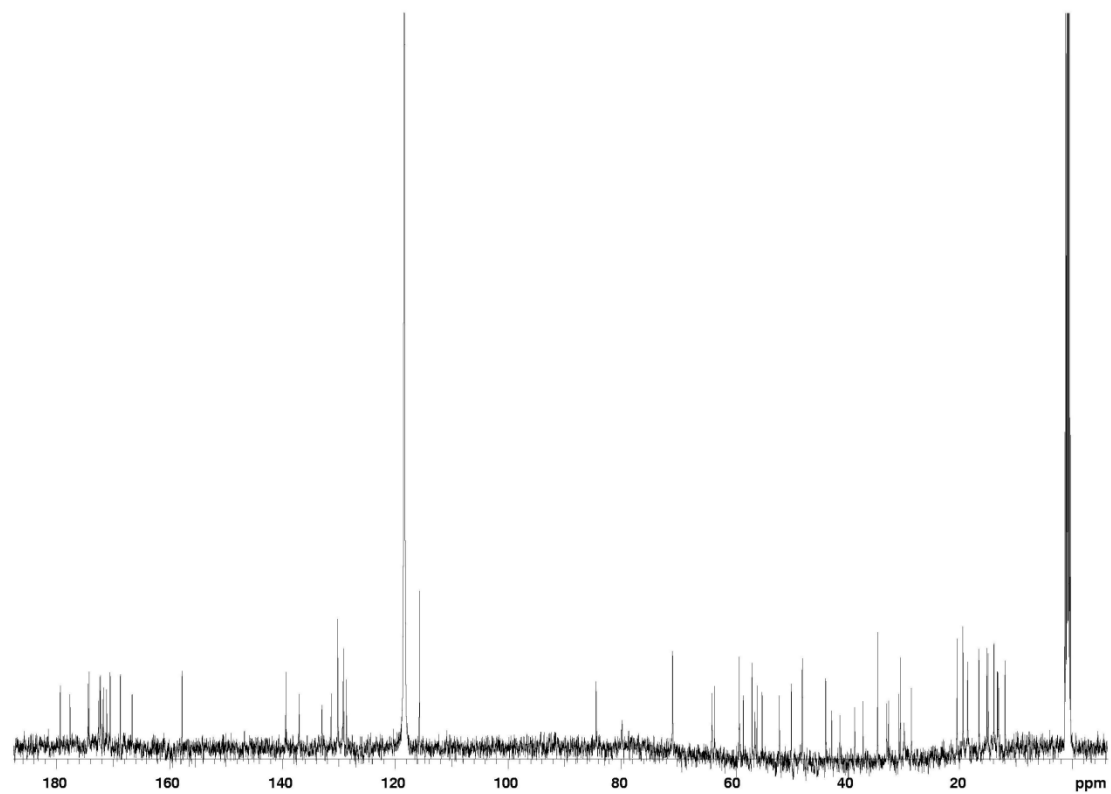


Figure S15. HMBC spectrum of mirabamide H (**4**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

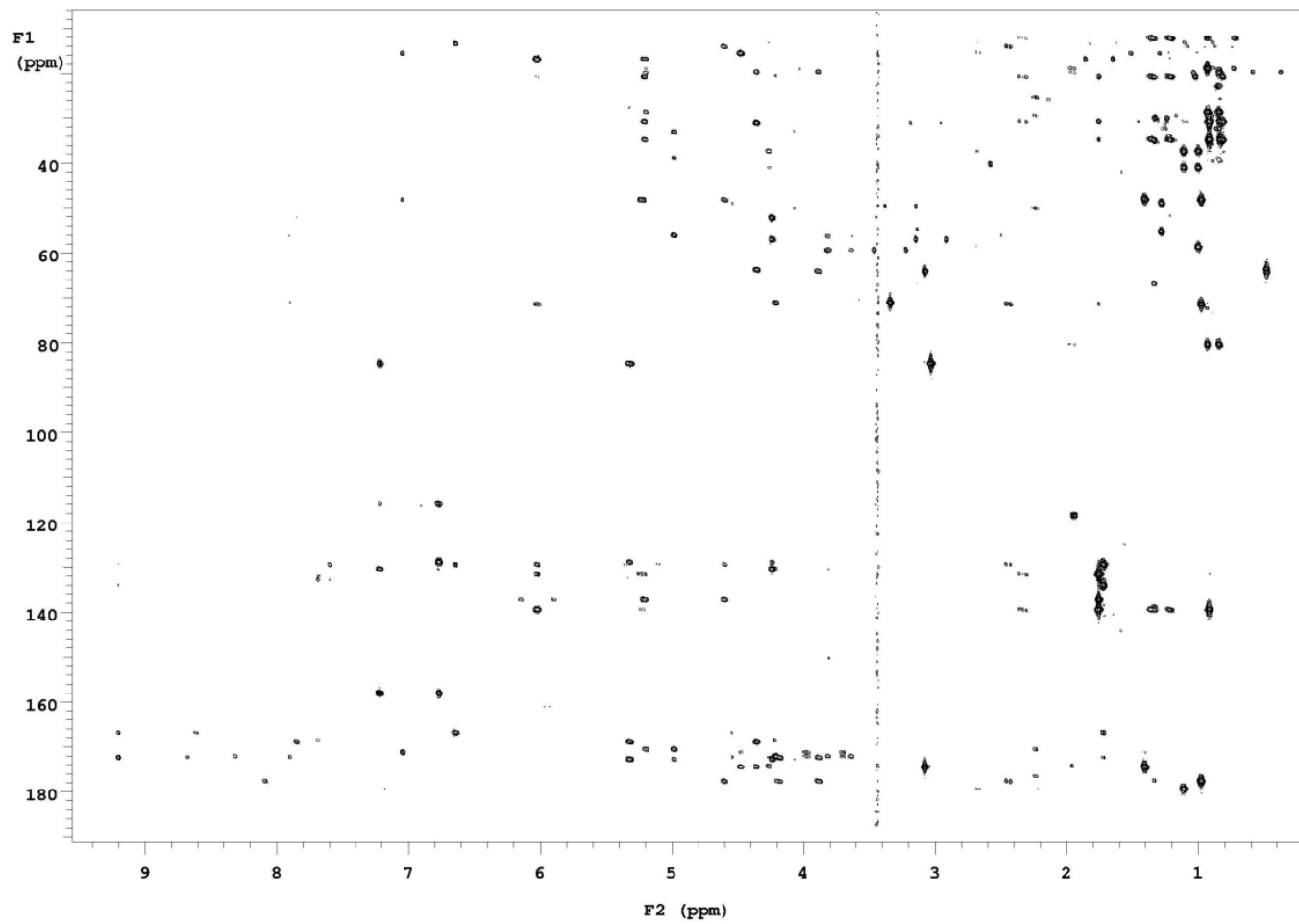


Figure S16. wgNOESY spectrum of mirabamide H (**4**) in CD₃CN-H₂O (4:1) with 0.1% TFA-*d*

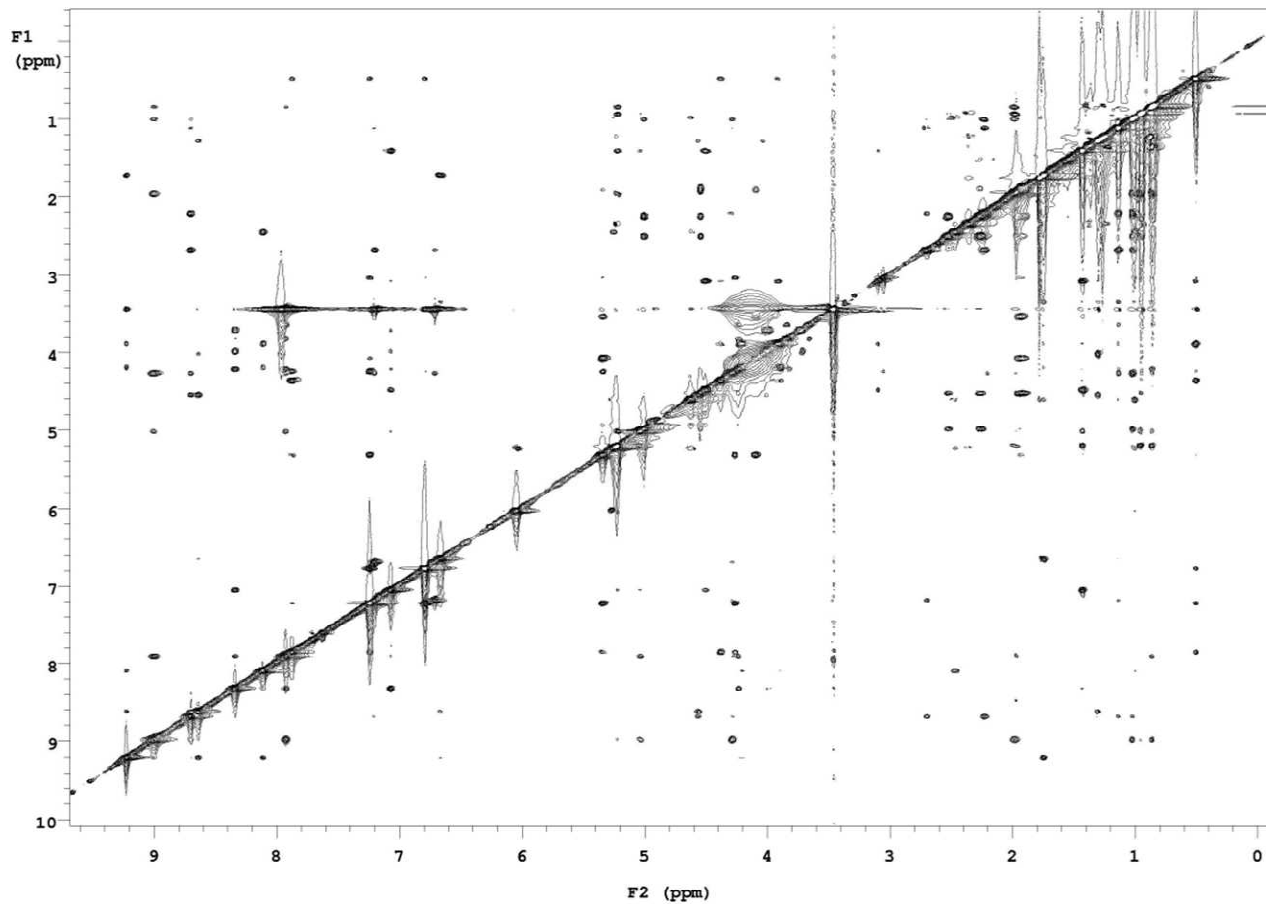


Figure S17-A. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (bottom) of the hydrolysis product of **1** in negative ion mode monitoring at 440 for 3-OHLeu residue.

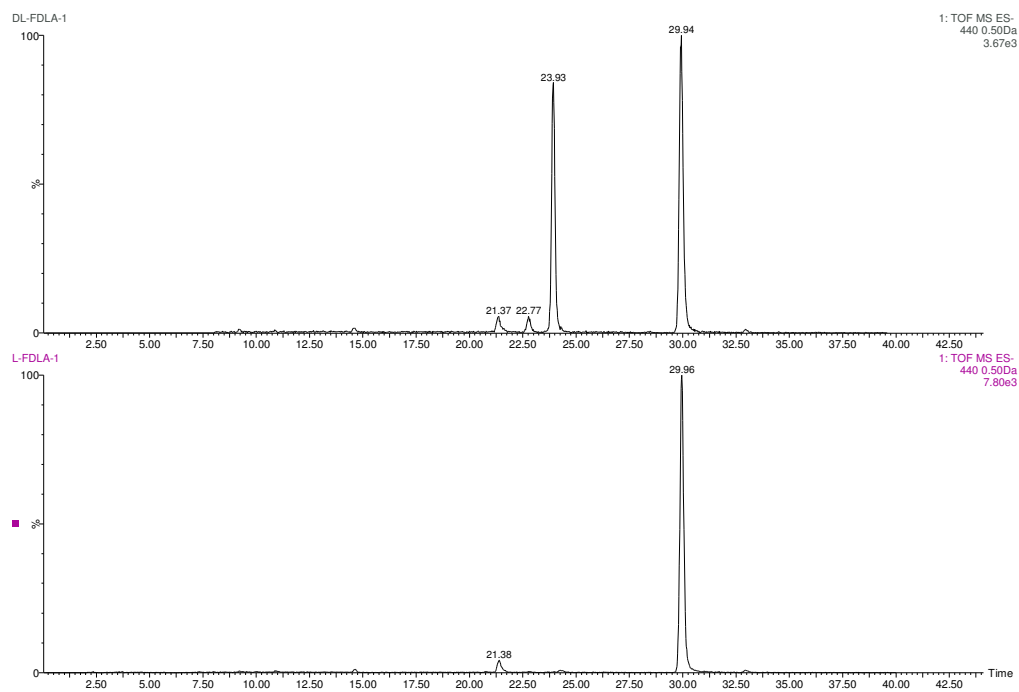


Figure S17-B. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (bottom) of the hydrolysis product of **1** in negative ion mode monitoring at 382 for Ala residue.

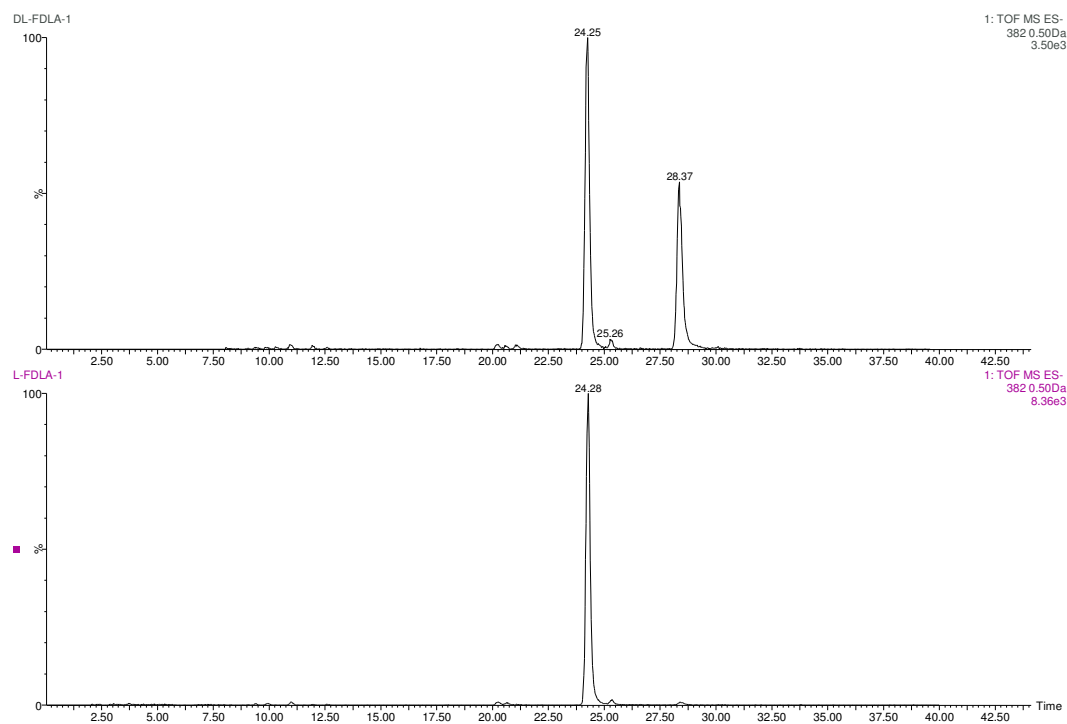


Figure S17-C. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (bottom) of the hydrolysis product of **1** in negative ion mode monitoring at 426 for NMeThr residue.

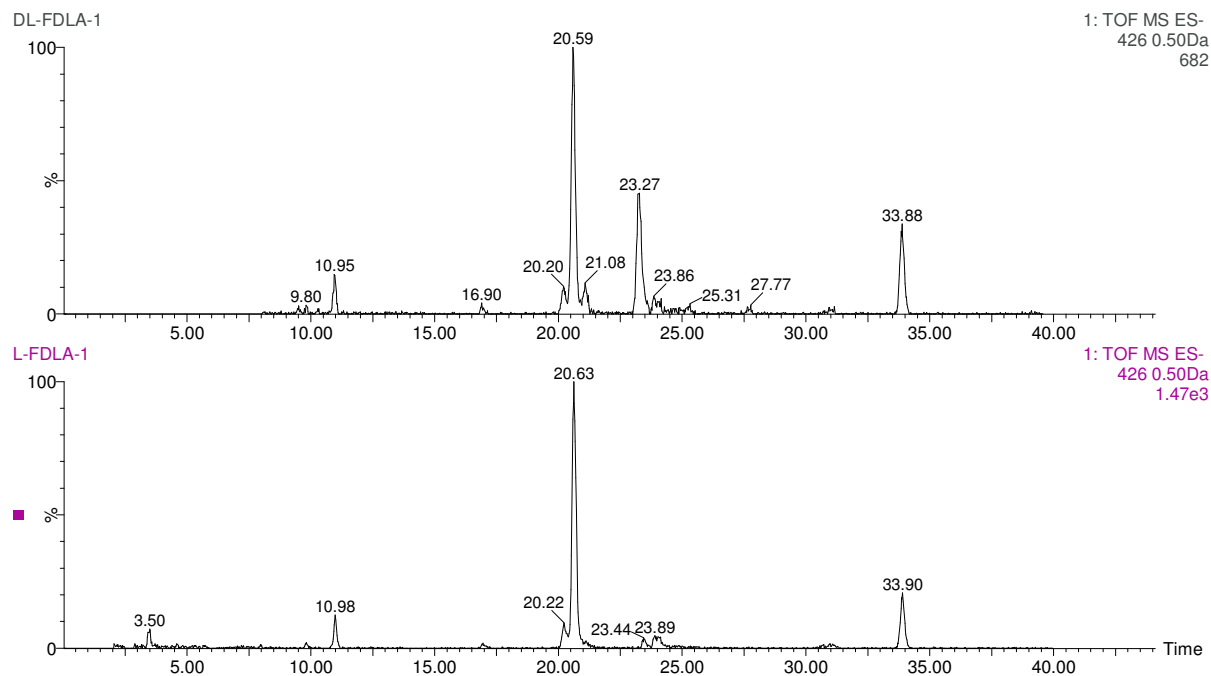


Figure S17-D. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (bottom) of the hydrolysis product of **1** in negative ion mode monitoring at 412 for 3-OMeAla residue.

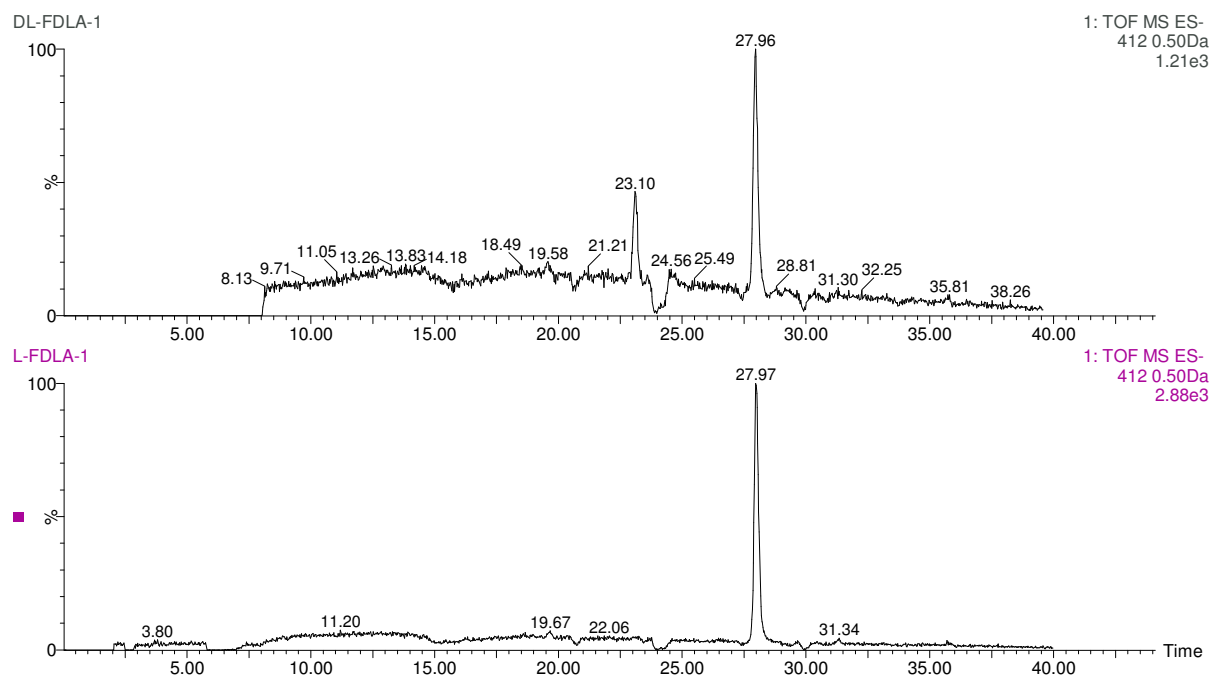


Figure S17-E. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (bottom) of the hydrolysis product of **1** in negative ion mode monitoring at 456 for ClHpr residue.

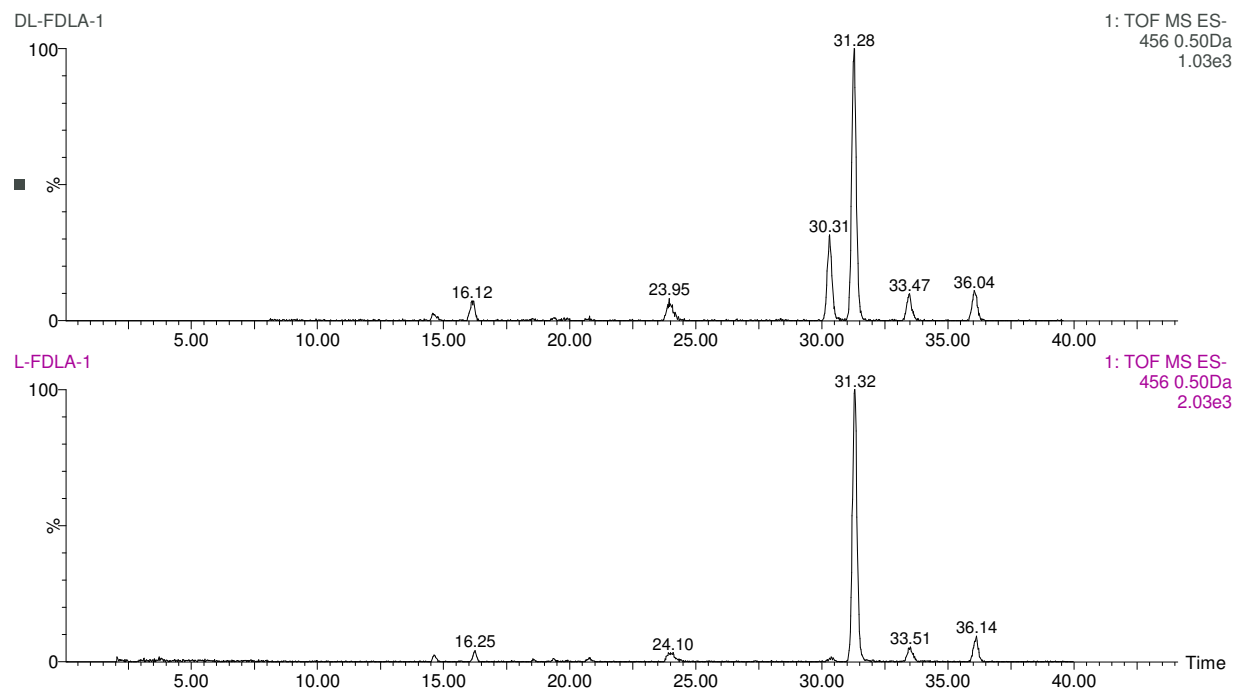


Figure S17-F. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (bottom) of the hydrolysis product of **1** in negative ion mode monitoring at 468 for 3,4-DiMeGln residue.

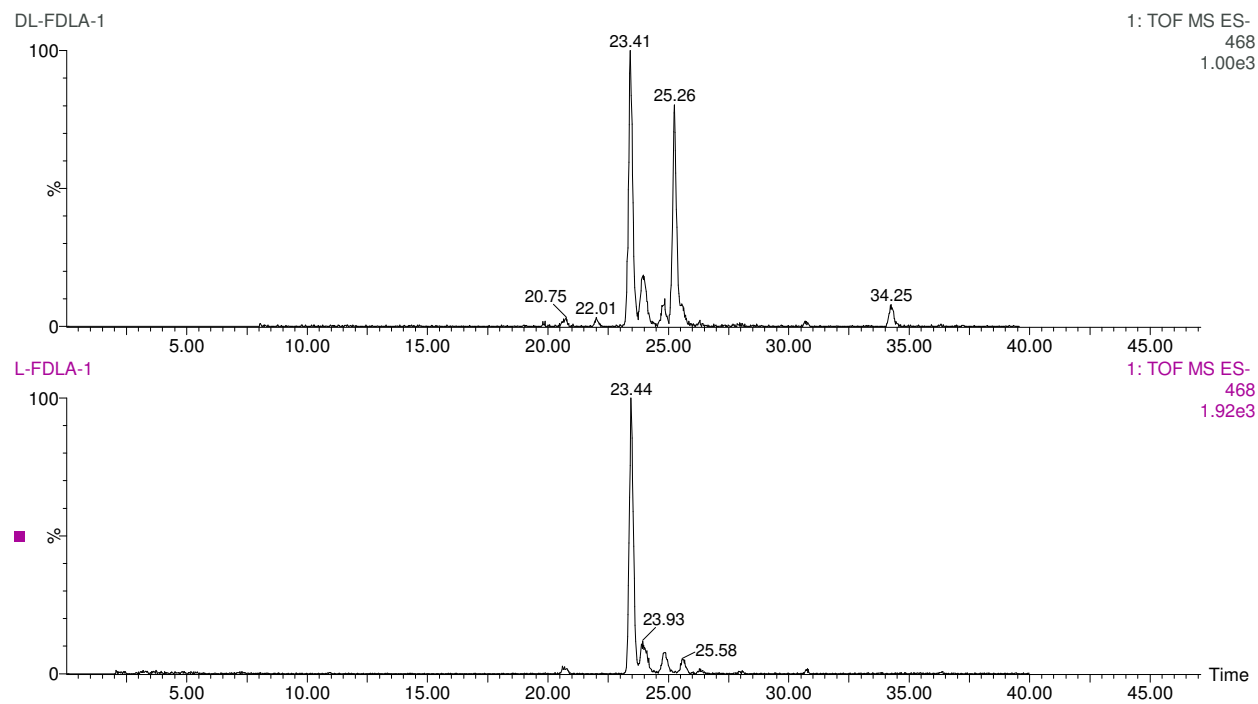


Figure S17-G. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (bottom) of the hydrolysis product of **1** in negative ion mode monitoring at 705 for Dab residue.

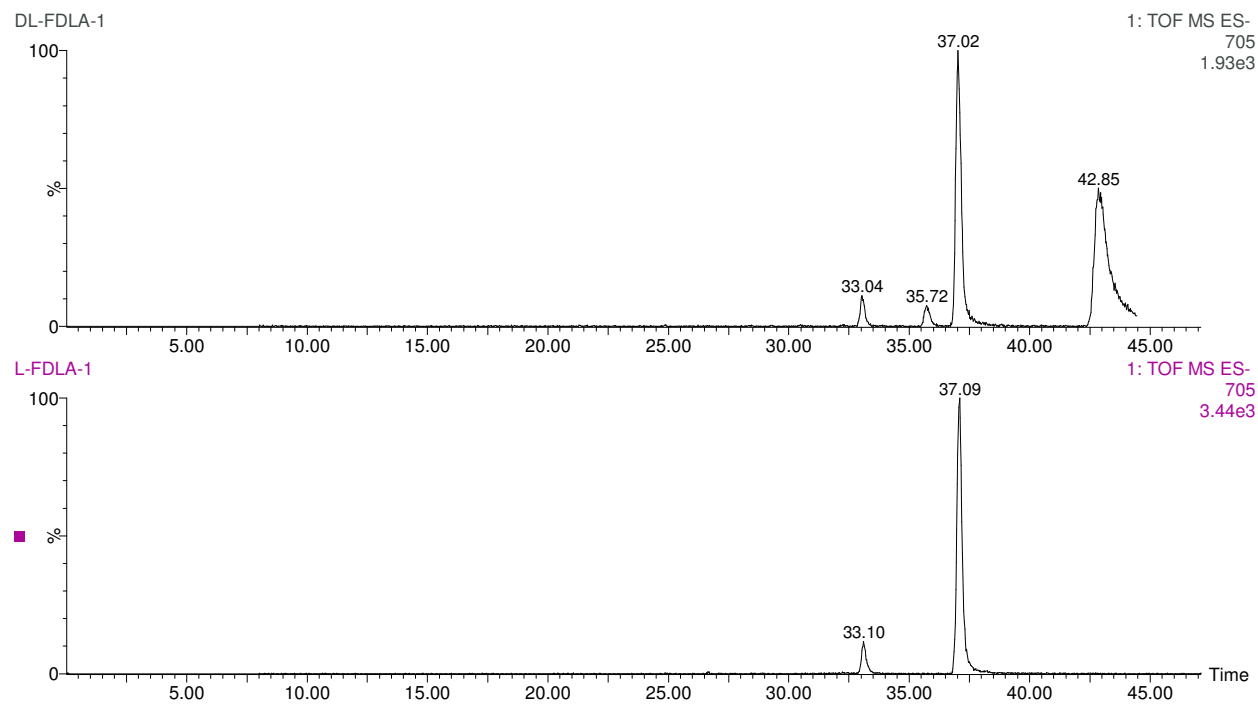


Figure S18. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (middle) of the hydrolysis product of **1** and the L-FDLA derivatives from the hydrolysates of papuamide A (bottom) in negative ion mode monitoring at 440 for 3-OHLeu residue and Newman projections analysis.

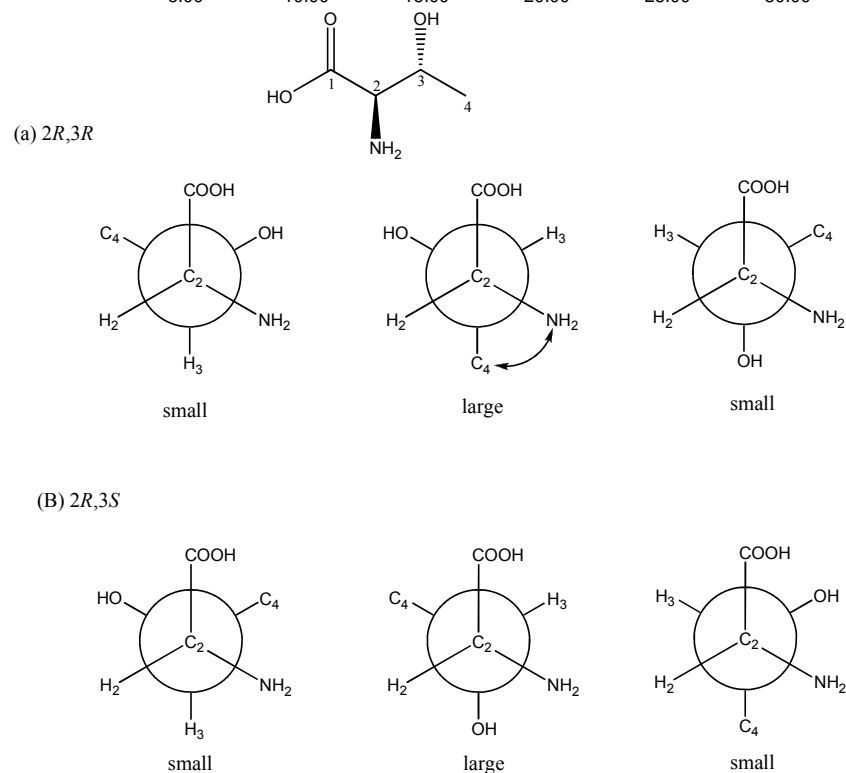
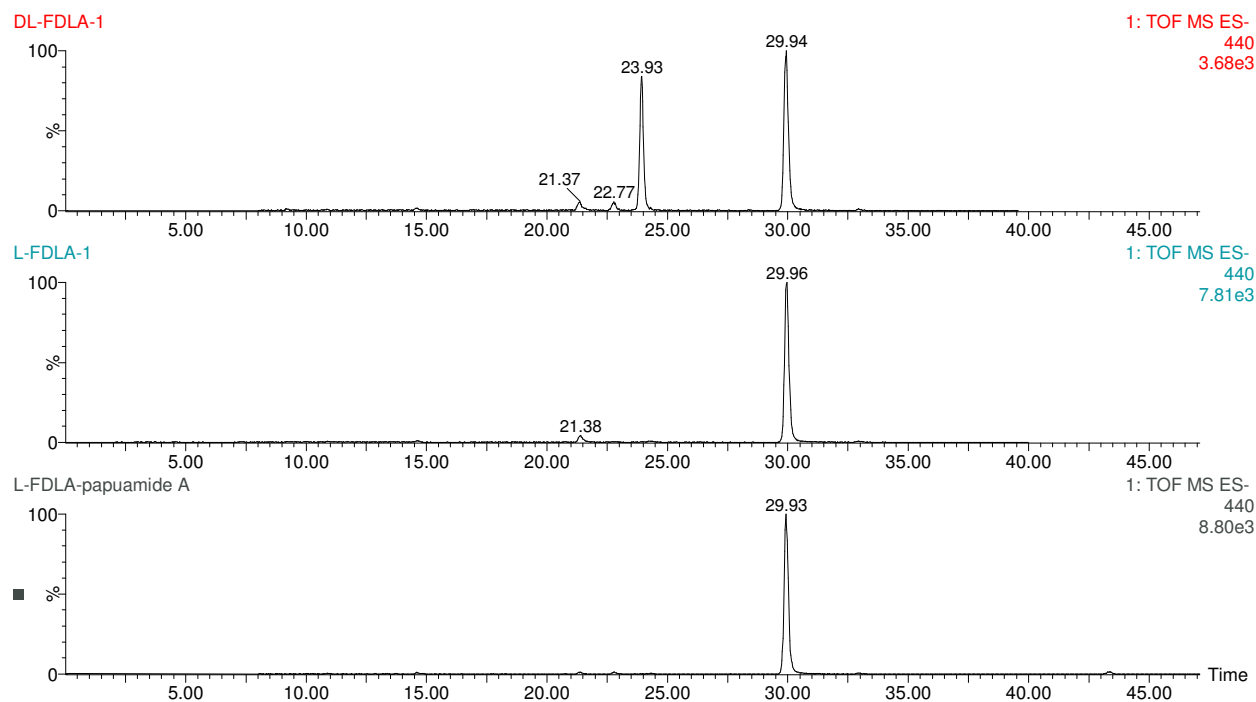
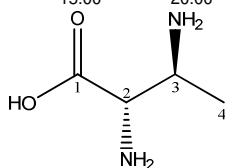
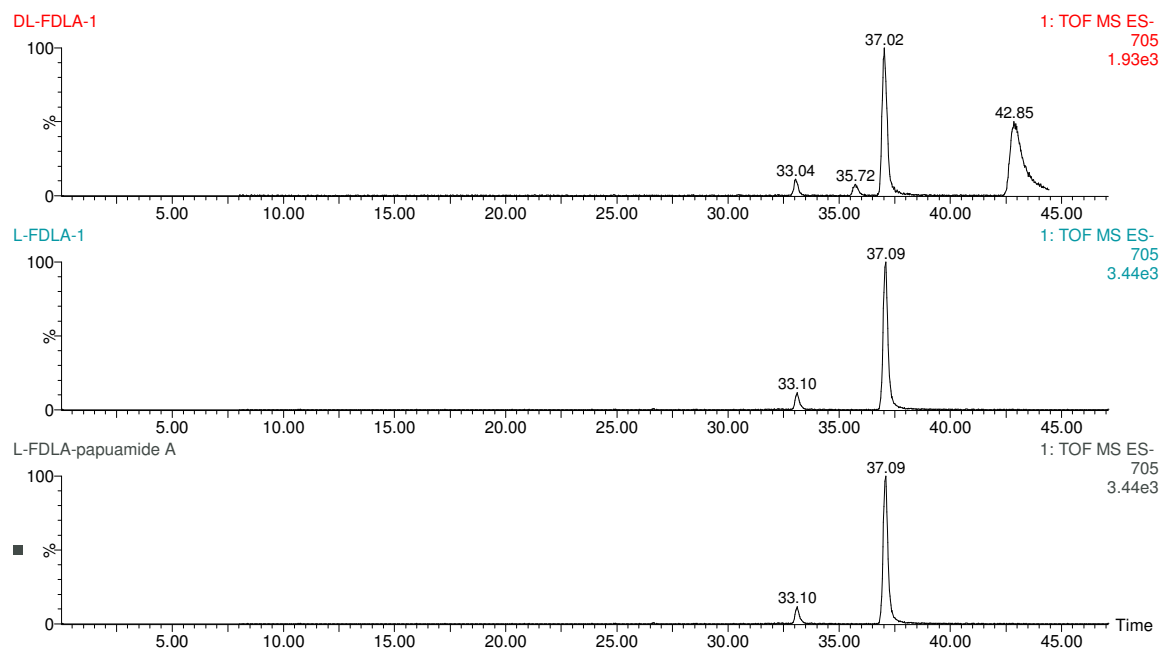
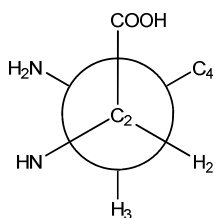


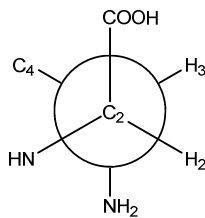
Figure S19. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (middle) of the hydrolysis product of **1** and the L-FDLA derivatives from the hydrolysates of papuamide A (bottom) in negative ion mode monitoring at 705 for Dab residue and Newman projections analysis.



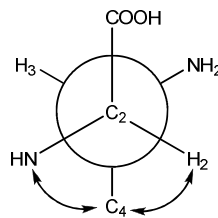
(a) $2S,3S$



small

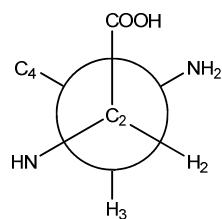


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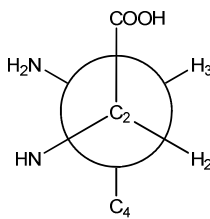


large

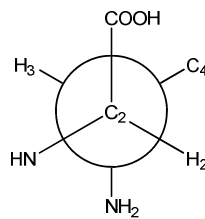
(b) $2S,3R$



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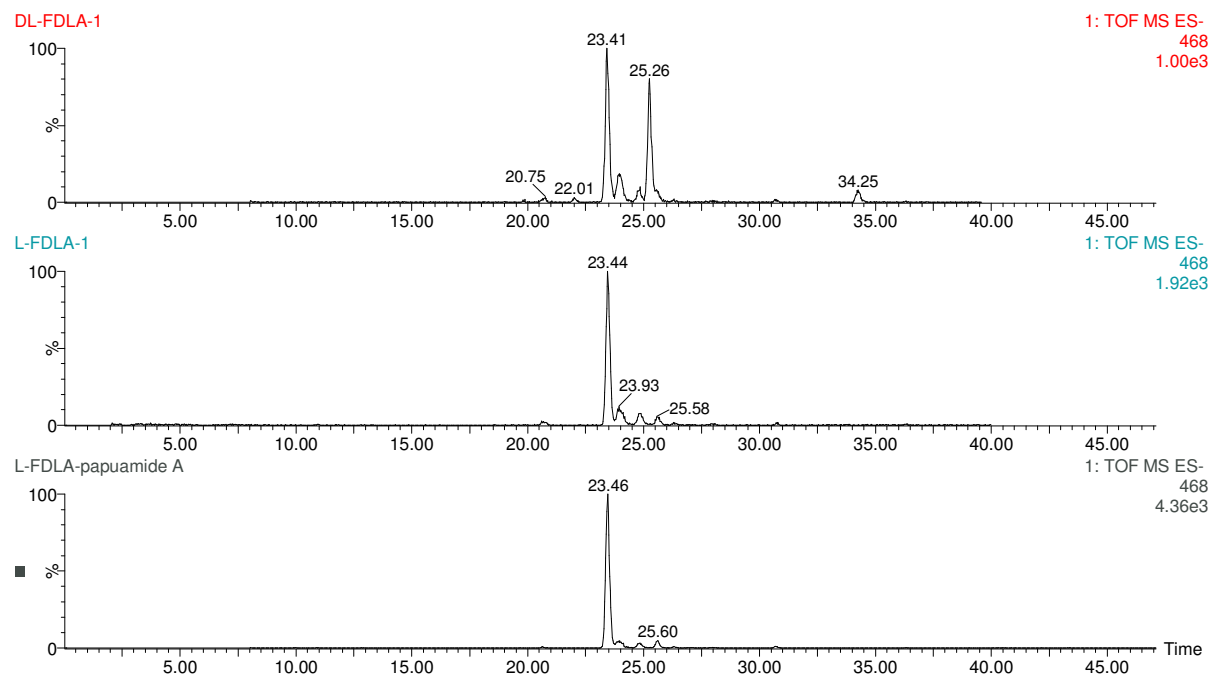


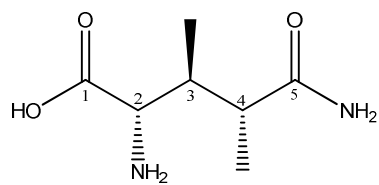
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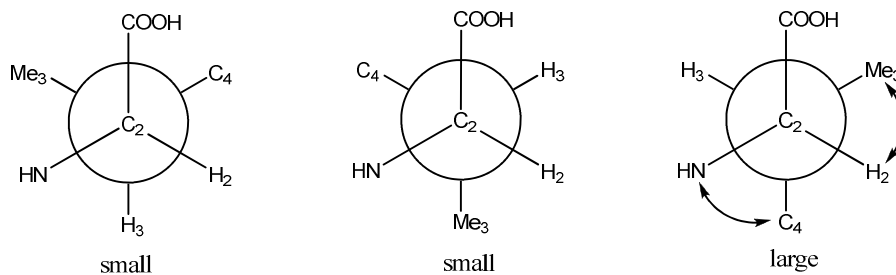
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Figure S20-A. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (middle) of the hydrolysis product of **1** and the L-FDLA derivatives from the hydrolysates of papuamide A (bottom) in negative ion mode monitoring at 468 for 3,4-DiMeGln residue and Newman projections analysis .

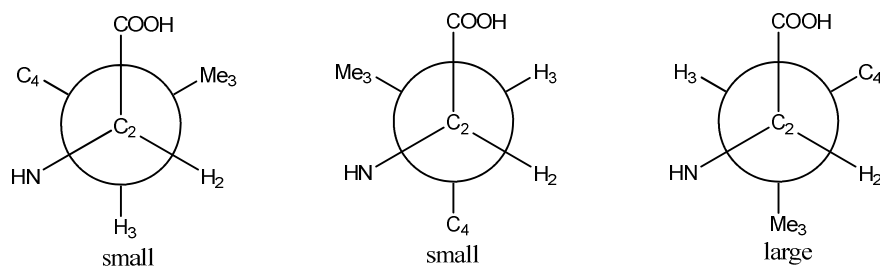




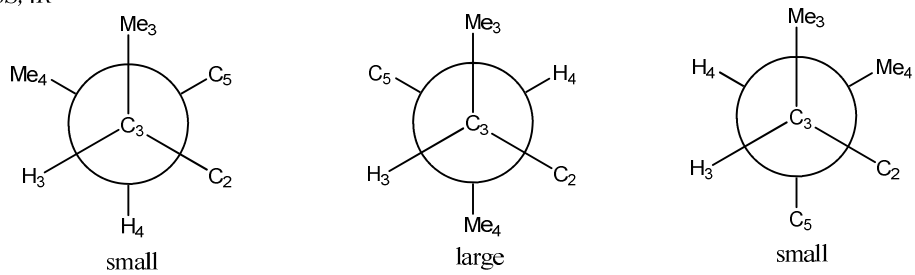
(a) $2S,3S$



(b) $2S,3R$



(c) $3S,4R$



(d) $3S,4S$

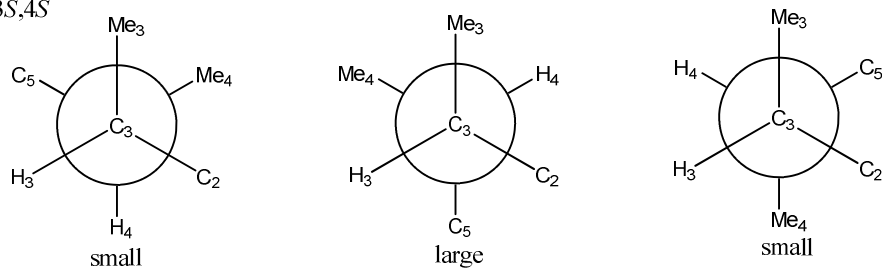


Figure S20-B. Ion chromatograms of the L-FDLA derivatives of the hydrolysis product of **1** (top) and the L-FDLA derivatives of the standard 2*S*, 3*S*, 4*R*-dimethylglutamine (middle) and 2*S*, 3*S*, 4*S*-dimethylglutamine (bottom) in negative ion mode monitoring at 468 for 3,4-DiMeGln residue

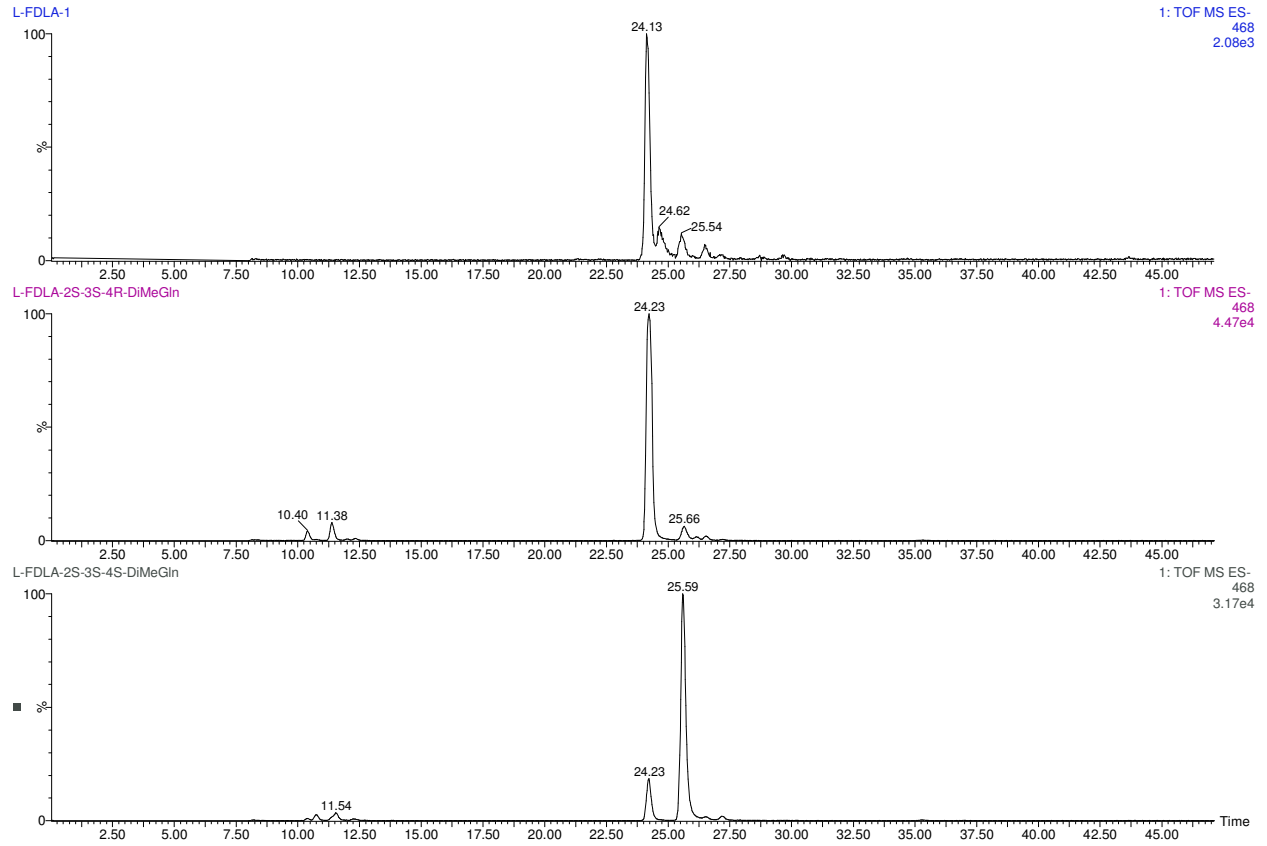
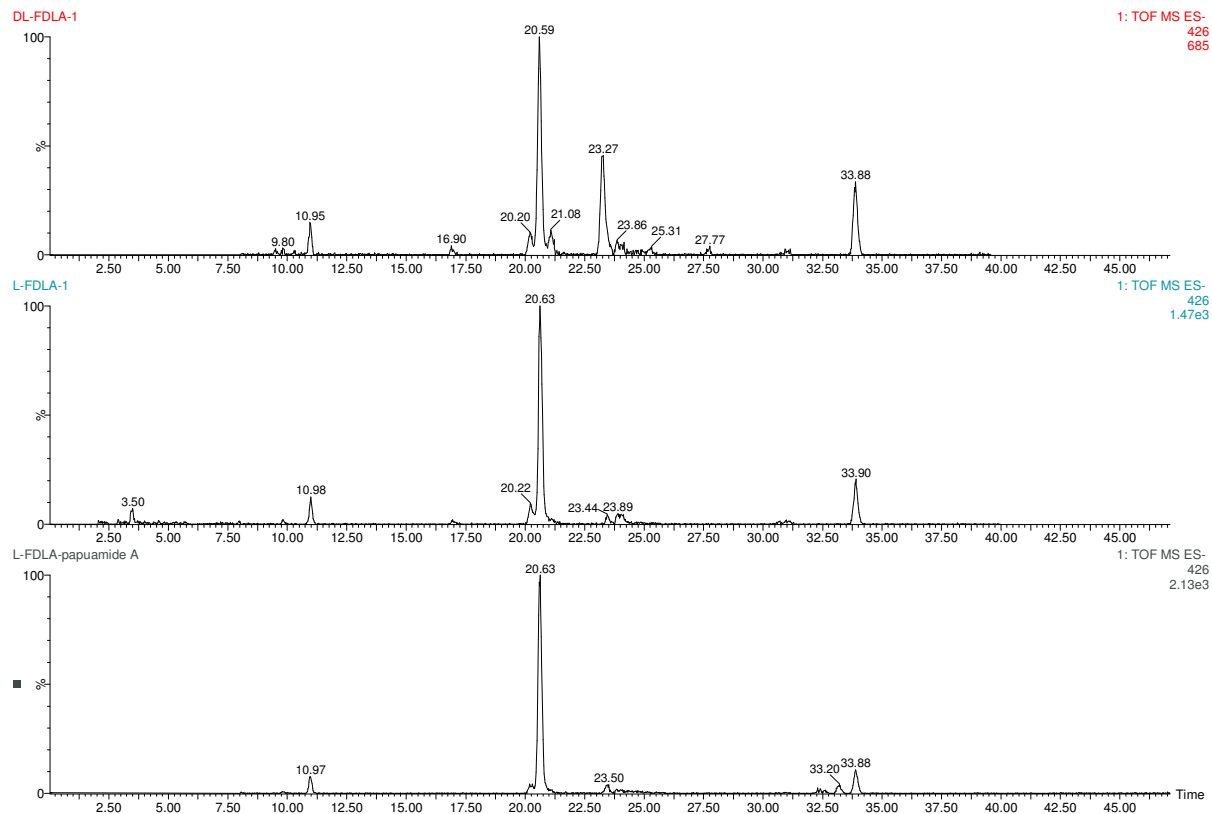
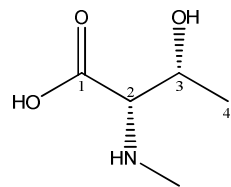
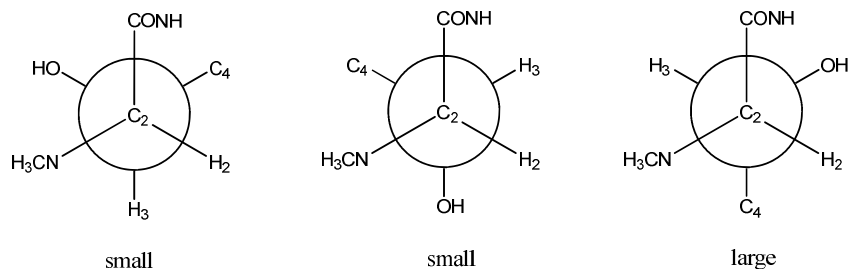


Figure S21. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (middle) of the hydrolysis product of **1** and the L-FDLA derivatives from the hydrolysates of papuamide A (bottom) in negative ion mode monitoring at 426 for NMeThr residue and Newman projections analysis





(a) 2*S*,3*S*



(b) 2*S*,3*R*

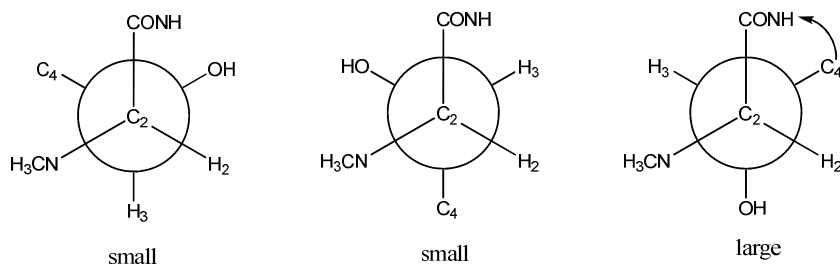


Figure S22. Ion chromatograms of the D/L-FDLA derivatives (top) and the L-FDLA derivatives (middle) of the hydrolysis product of **1** and the L-FDLA derivatives from the hydrolysates of mirabamide C (bottom) in negative ion mode monitoring at 456 for ClHpr residue.

