# Thiazoline Peptides and a *Tris*–Phenethyl Urea from *Didemnum molle* with Anti–HIV Activity— Supporting Information

Zhenyu Lu,[†] Mary Kay Harper,[†] Christopher D. Pond,[‡] Louis R. Barrows,[‡] Chris M. Ireland,[†] Ryan M. Van Wagoner[*,†]

[†]*Department of Medicinal Chemistry and* [‡]*Department of Pharmacology and Toxicology, College of Pharmacy, University of Utah, Salt Lake City, UT 84112, USA.*

[*]To whom correspondence should be addressed. Tel: (801) 581-4932. Fax: (801) 585-6208. E-mail: r.m.vanwagoner@pharm.utah.edu.

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**Figure S1.** $^{1}$H-NMR spectrum of (**1**) in DMSO–$d_6$

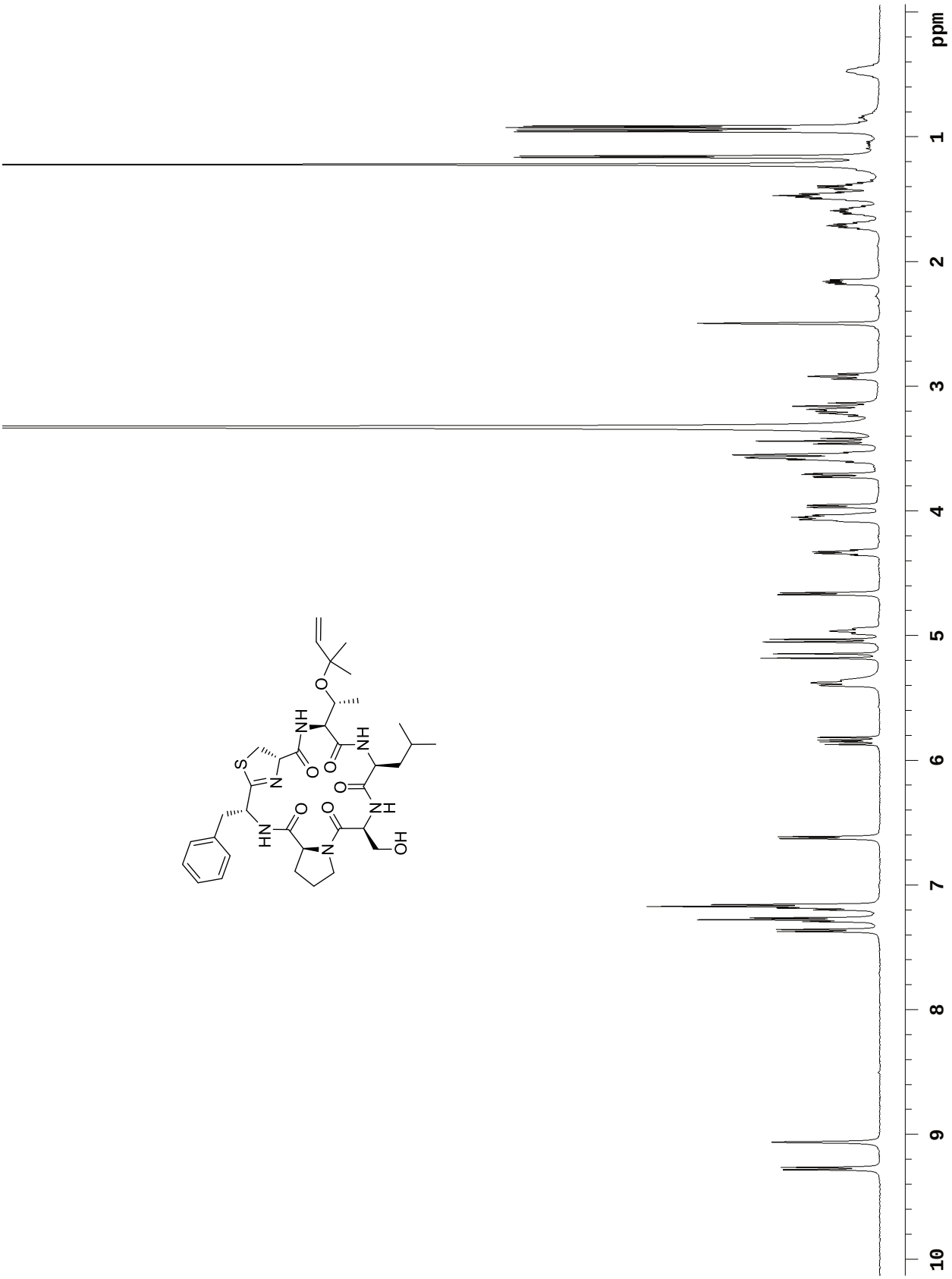


**Figure S2.** gCOSY spectrum of (**1**) in DMSO–$d_6$

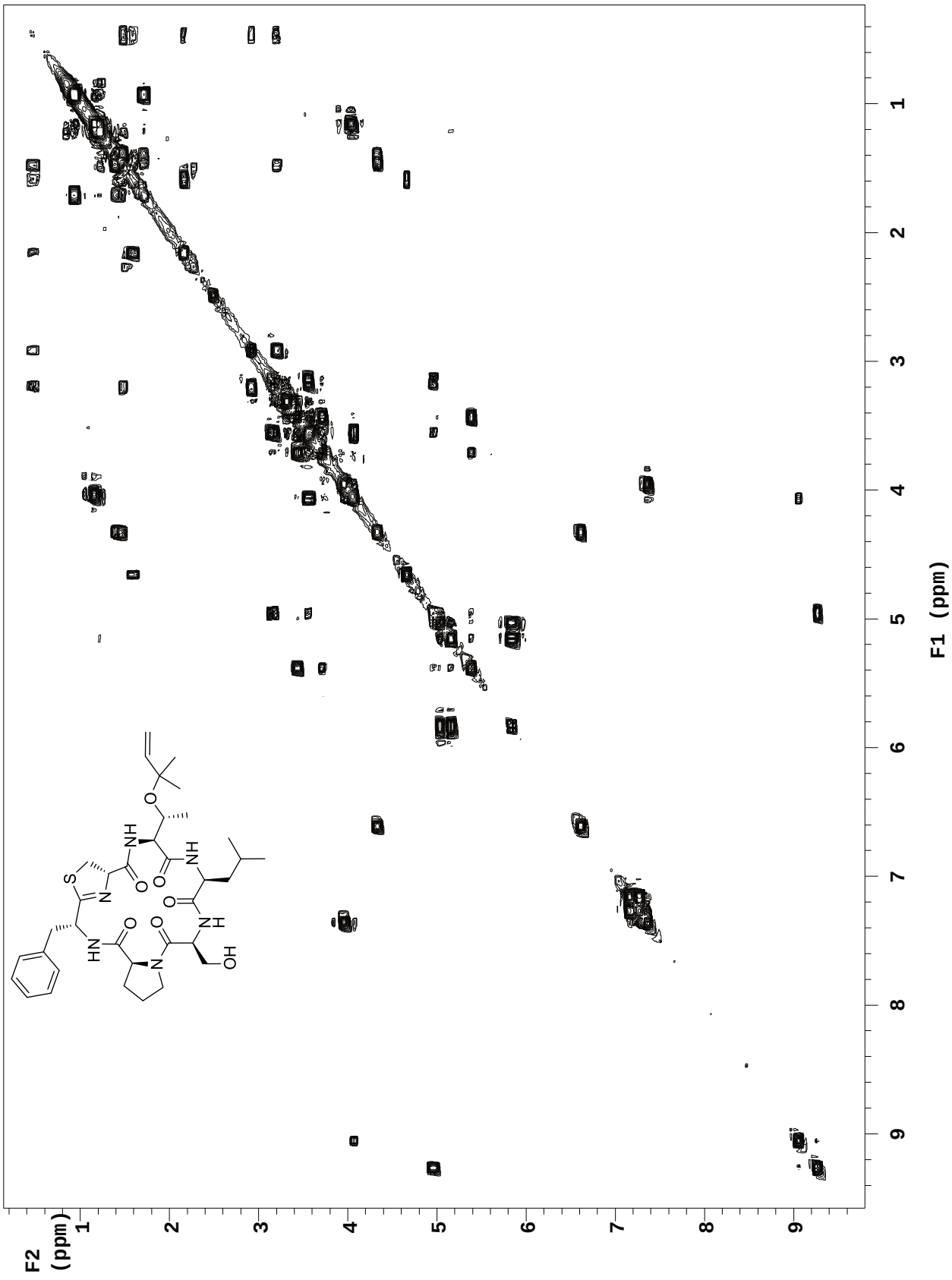


**Figure S3.** HMBC spectrum of (**1**) in DMSO–$d_6$

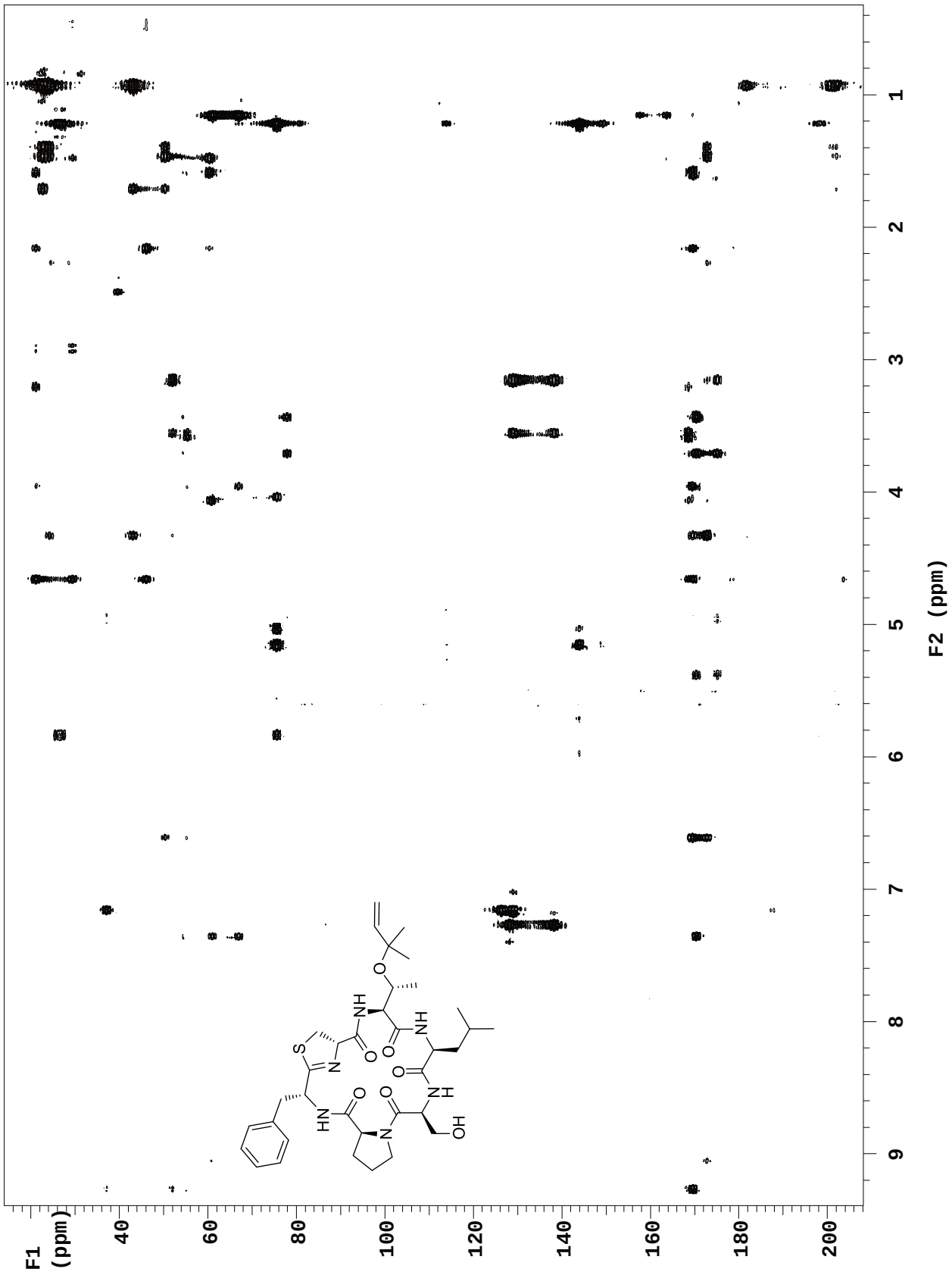


**Figure S4.** ROESY spectrum of (**1**) in DMSO–$d_6$

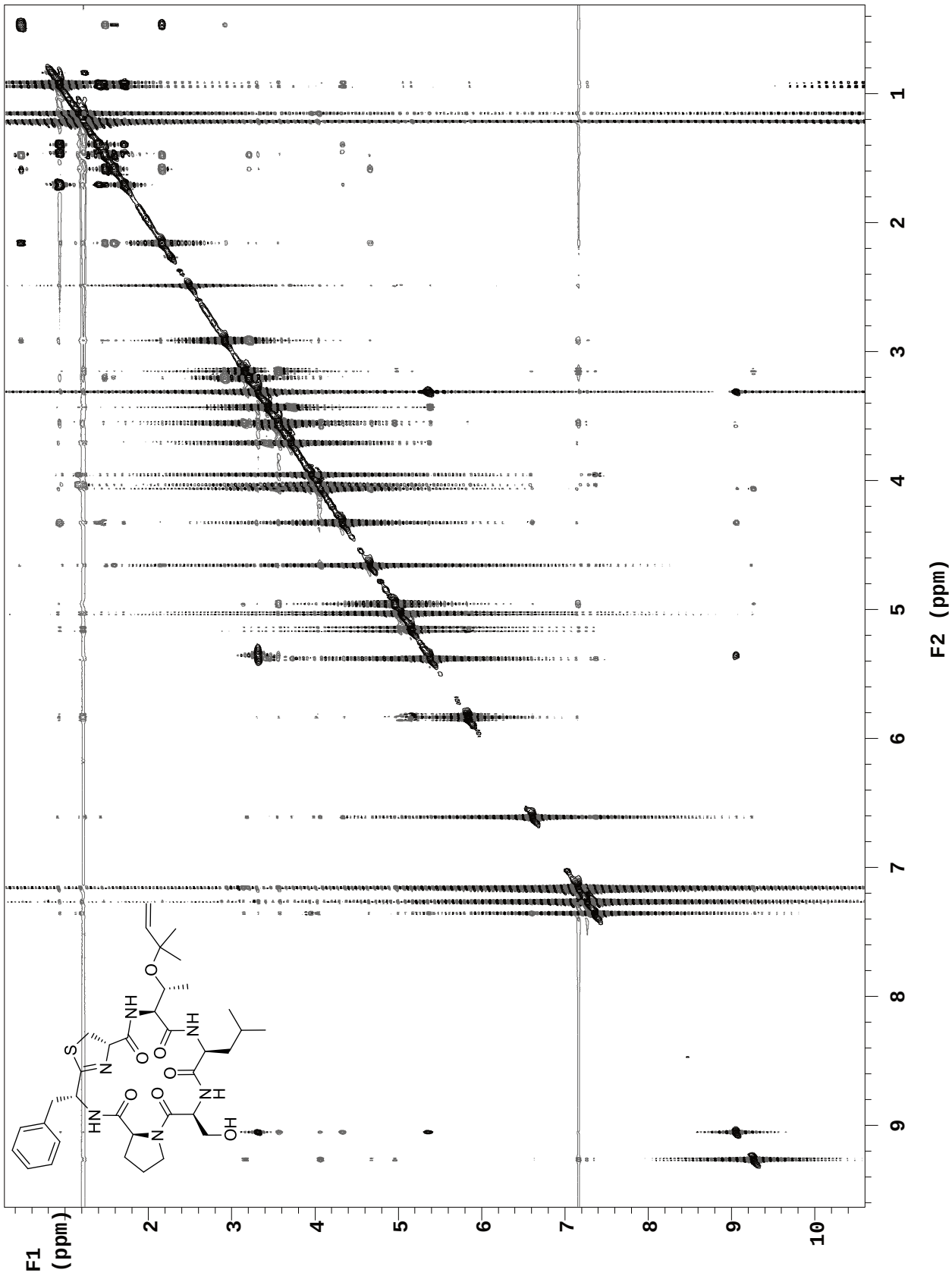


**Figure S5.** $^{1}$H-NMR spectrum of (**2**) in DMSO–$d_6$

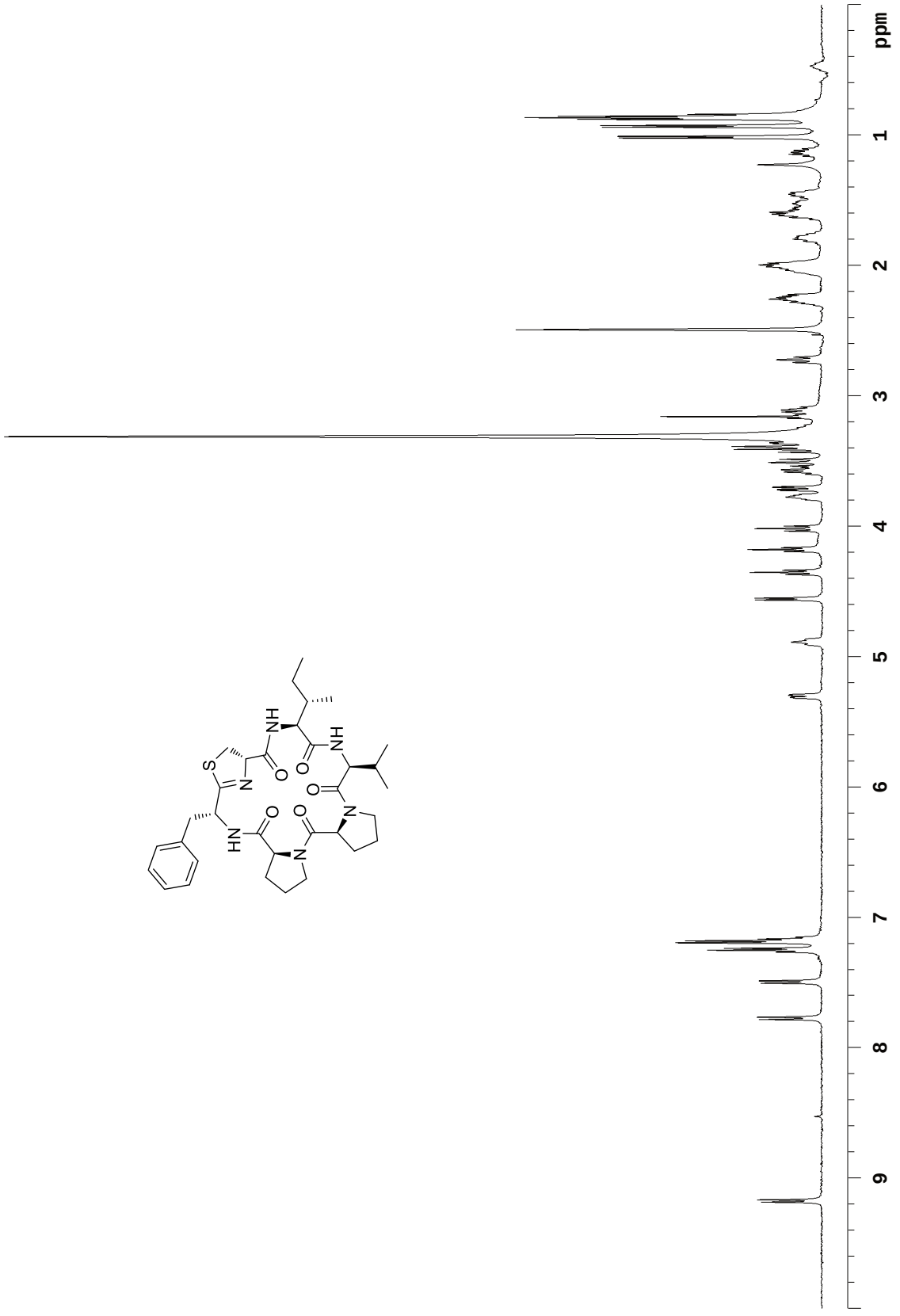


**Figure S6.** gCOSY spectrum of (**2**) in DMSO–$d_6$

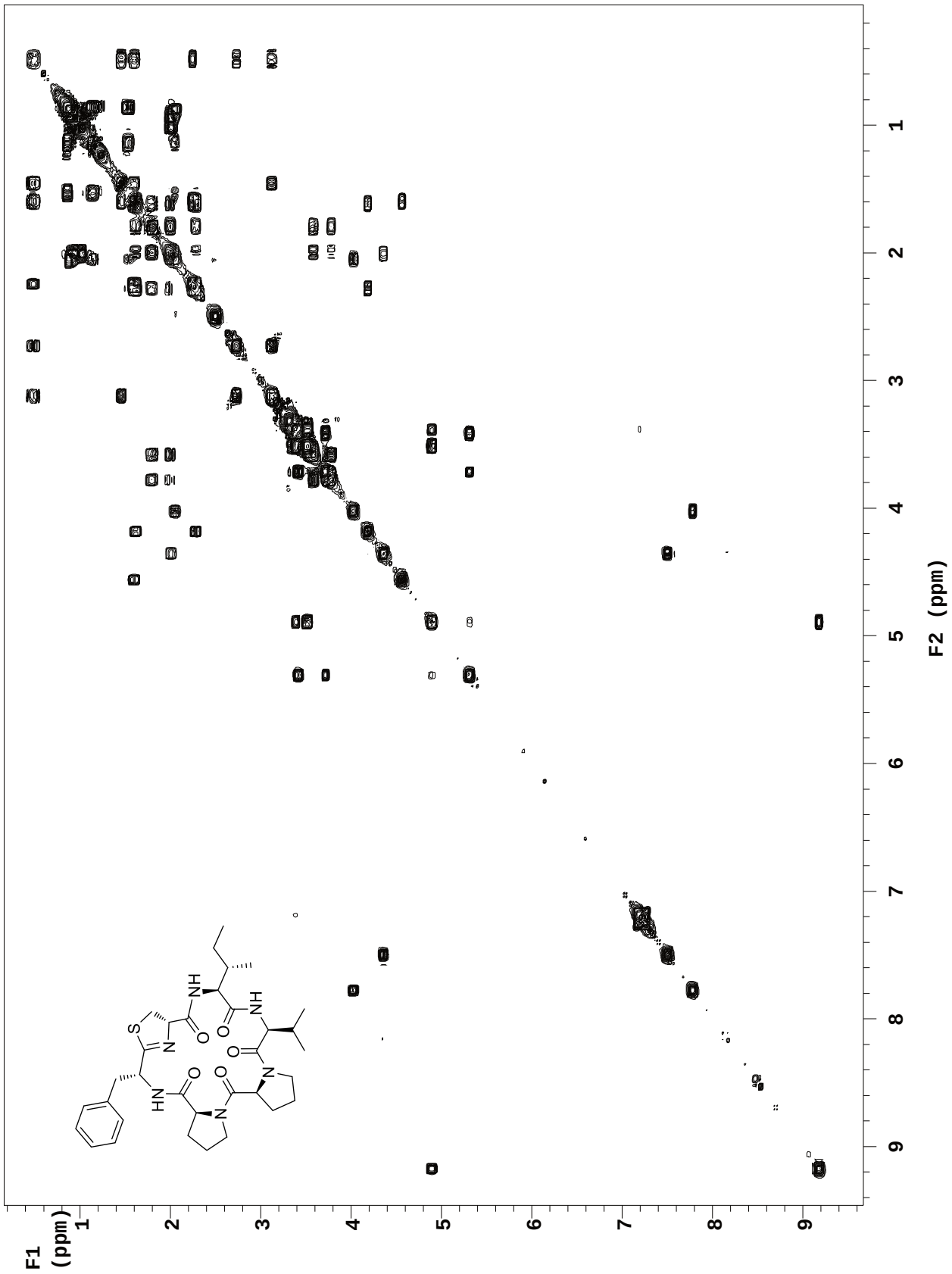


**Figure S7.** HMBC spectrum of (**2**) in DMSO–$d_6$

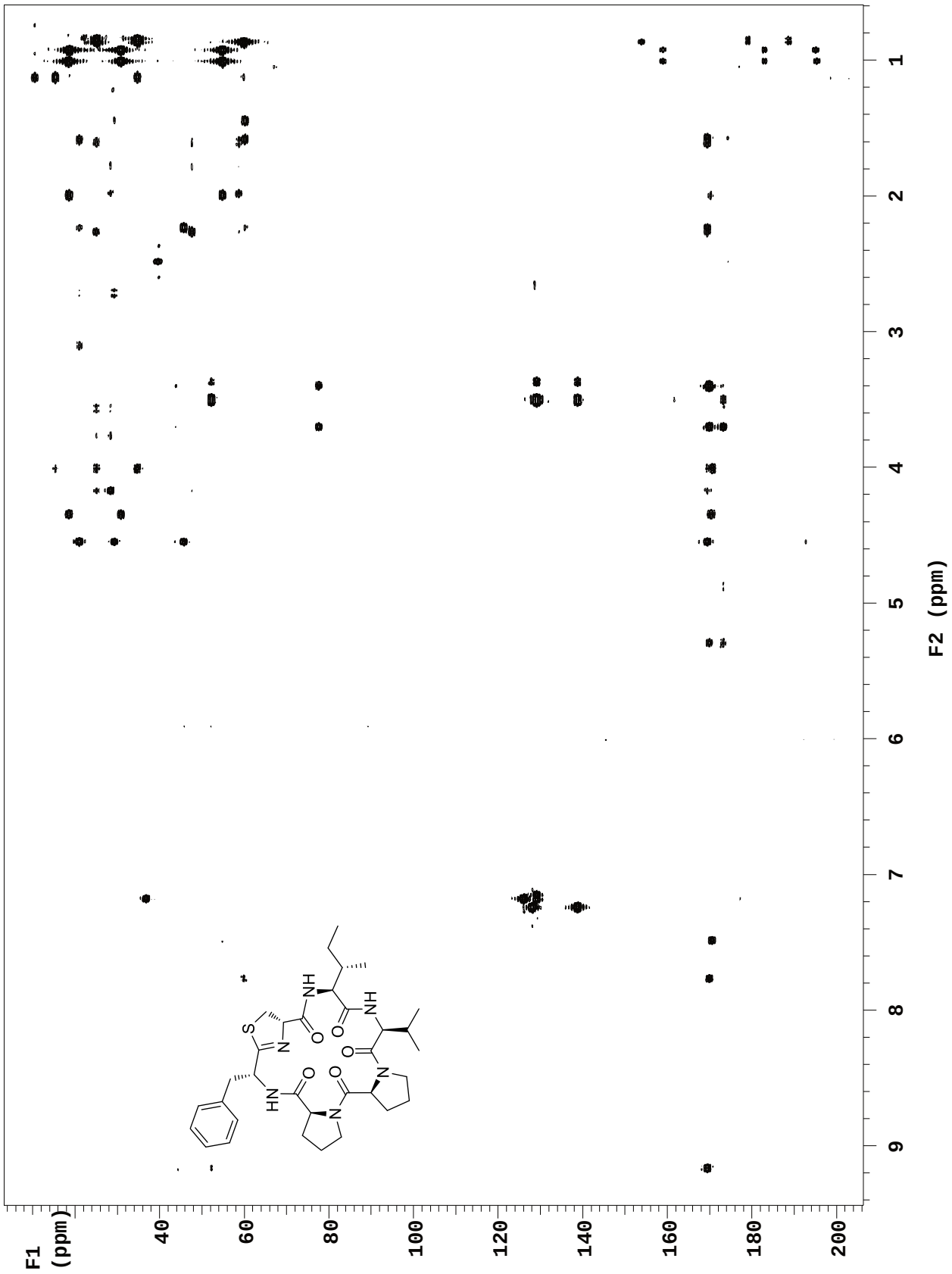


**Figure S8.** ROESY spectrum of (**2**) in DMSO–$d_6$

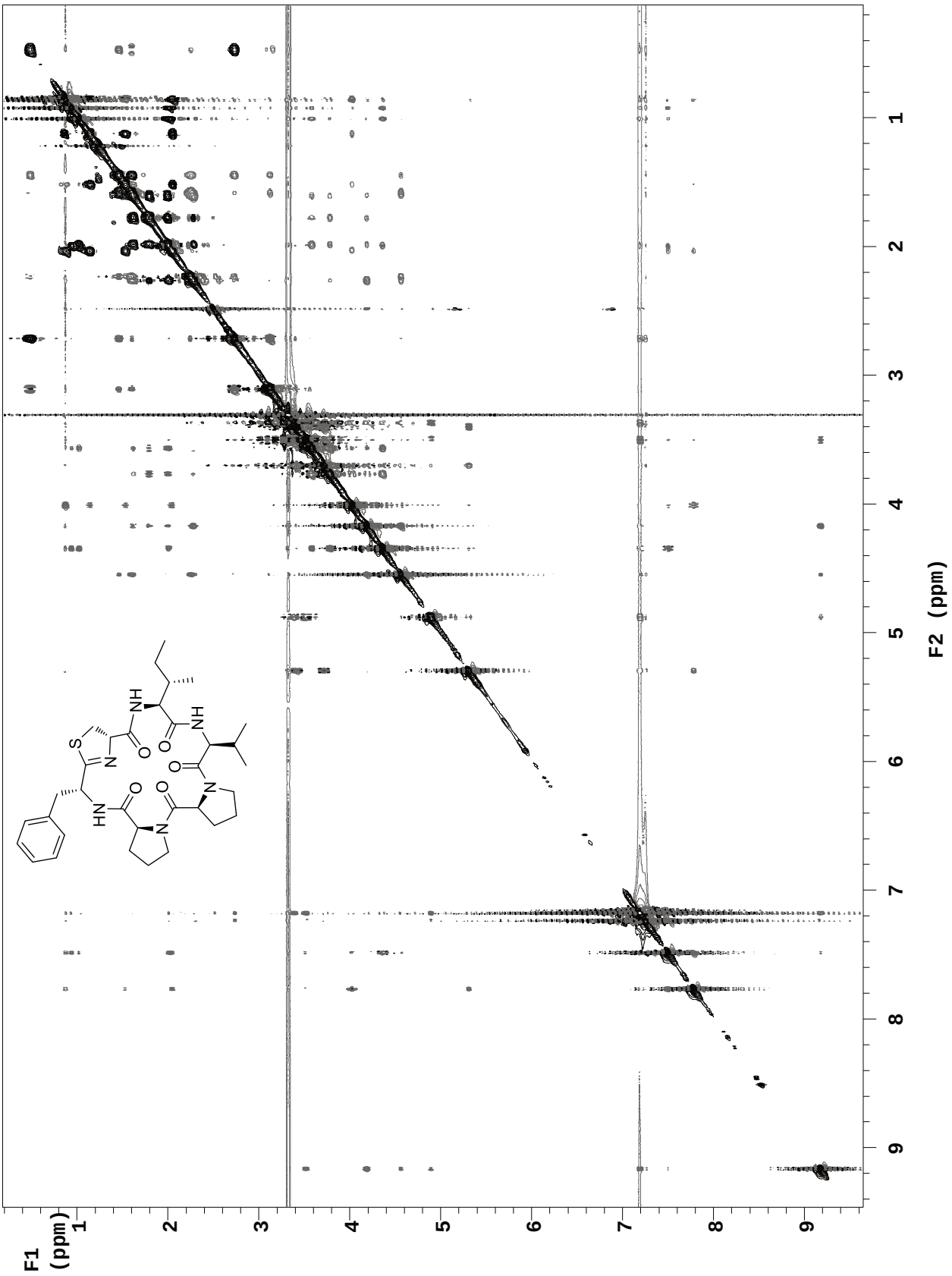


**Figure S9.** $^{1}$H-NMR spectrum of (**3**) in benzene–$d_6$

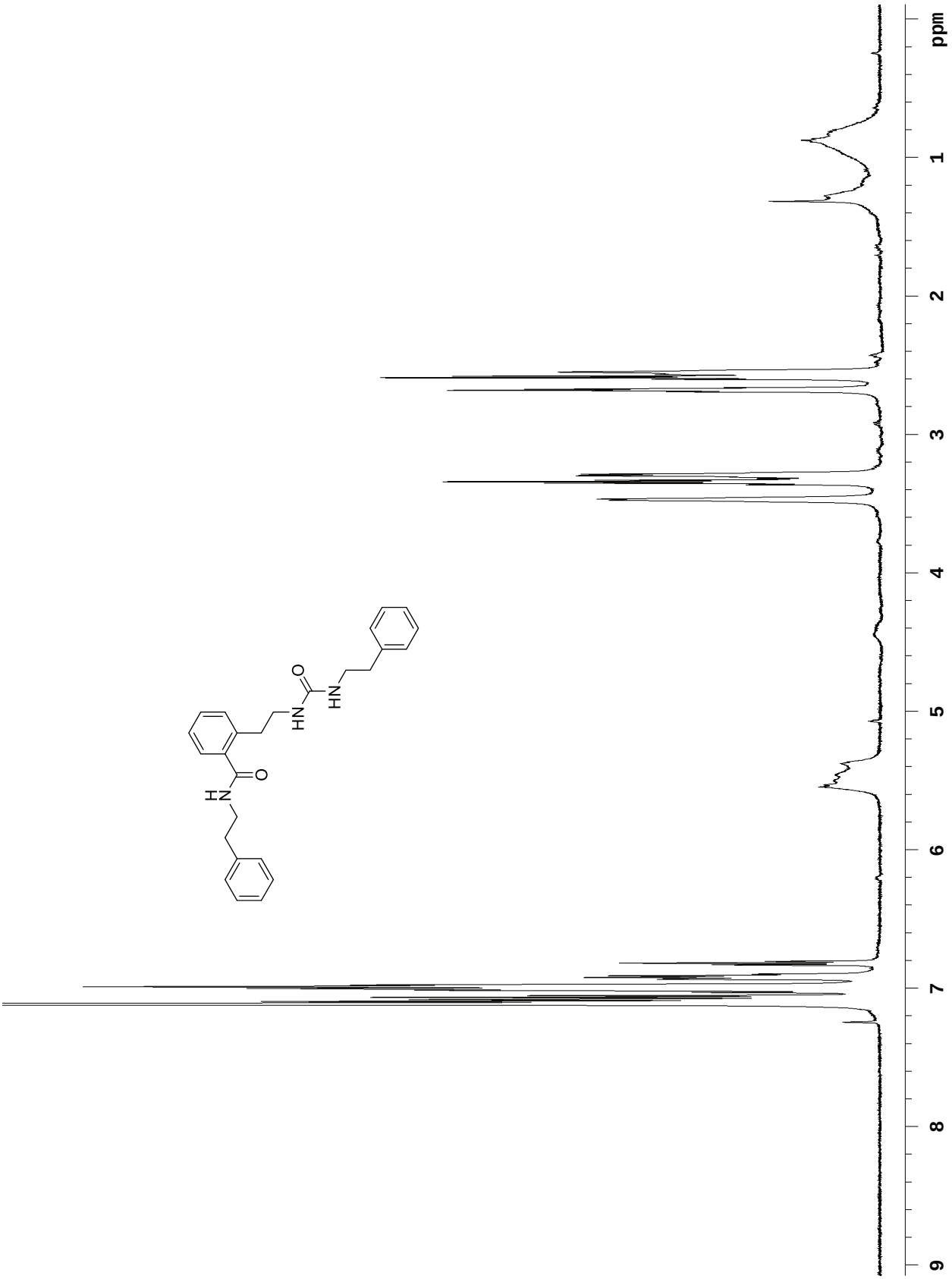


**Figure S10.** HMBC spectrum of (**3**) in benzene–$d_6$

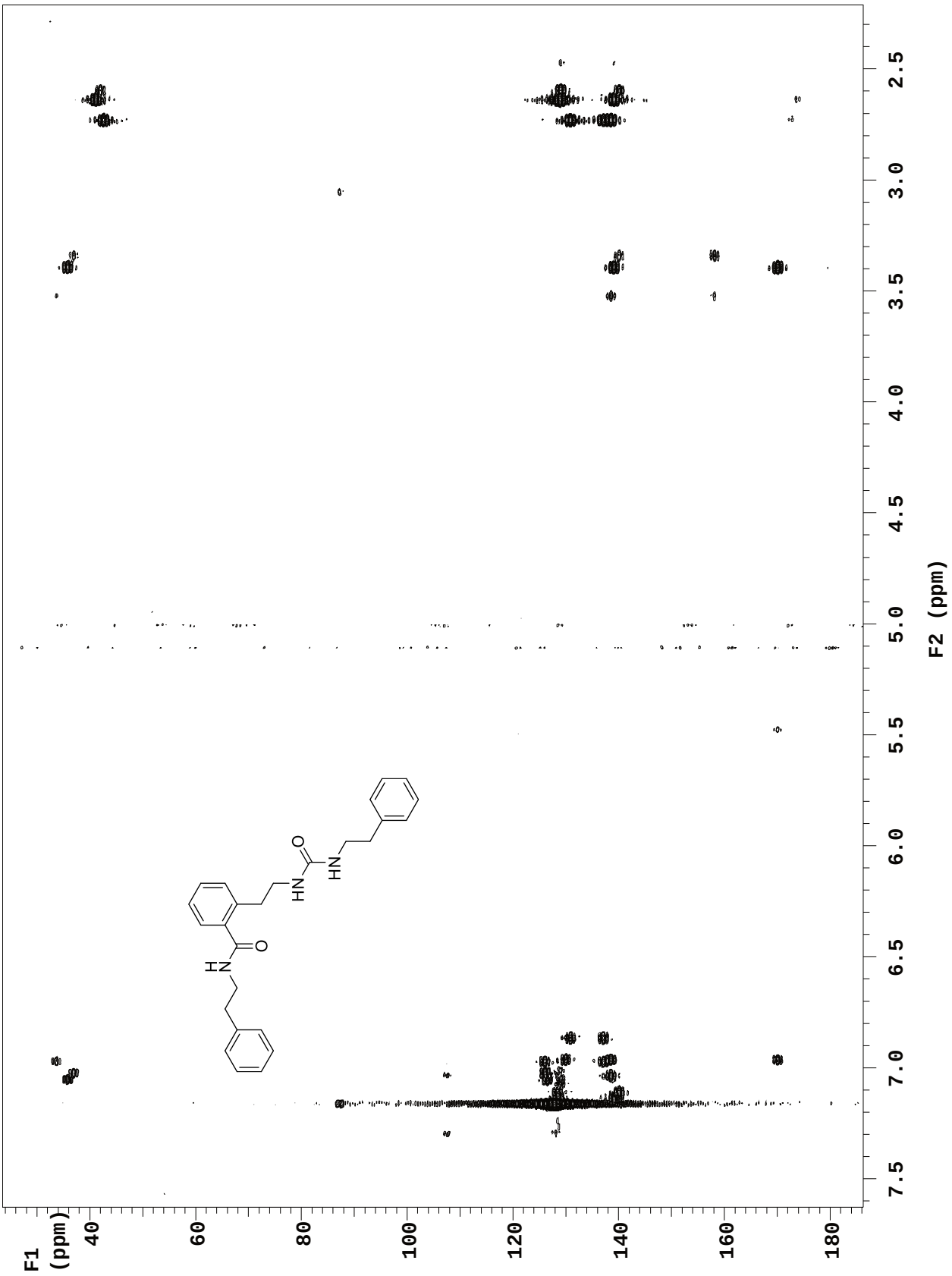


**Figure S11.** Ion chromatograms of co-injection of hydrolyzed compound **1** with L-Thr in negative ion mode monitoring at *m/z* 412.

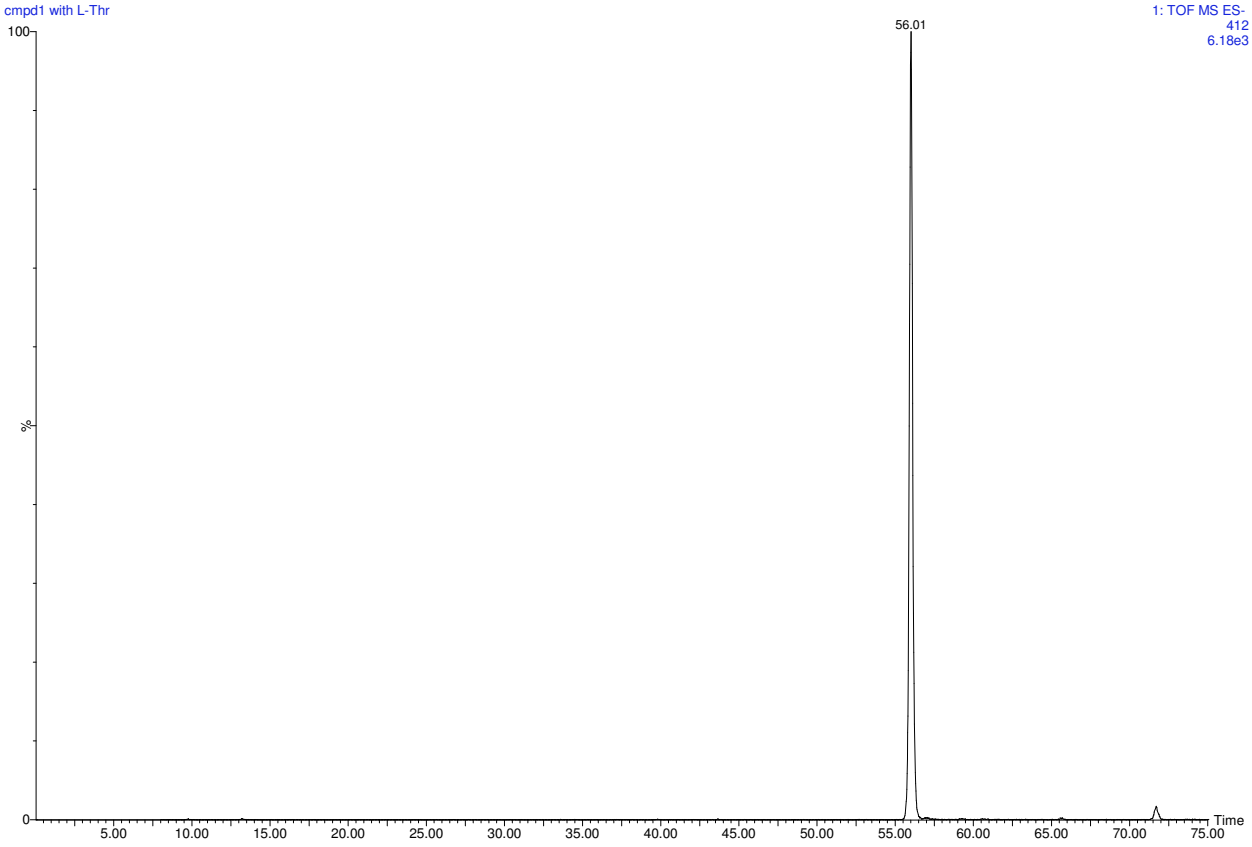


**Figure S12.** Ion chromatograms of co-injection of hydrolyzed compound **1** with D/L-*allo*-Thr in negative ion mode monitoring at *m/z* 412.

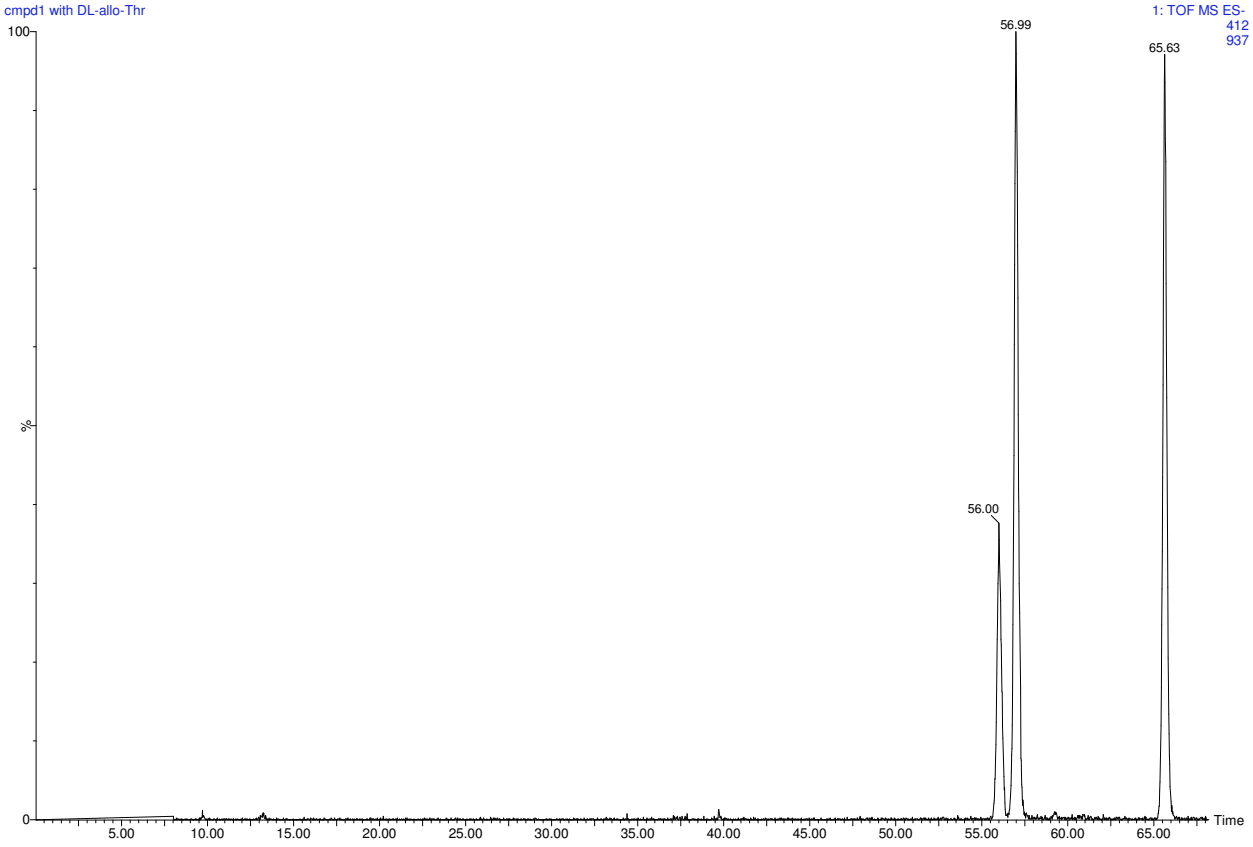


**Figure S13.** Ion chromatograms of co-injection of hydrolyzed compound **2** with L-Ile in negative ion mode monitoring at *m/z* 424.

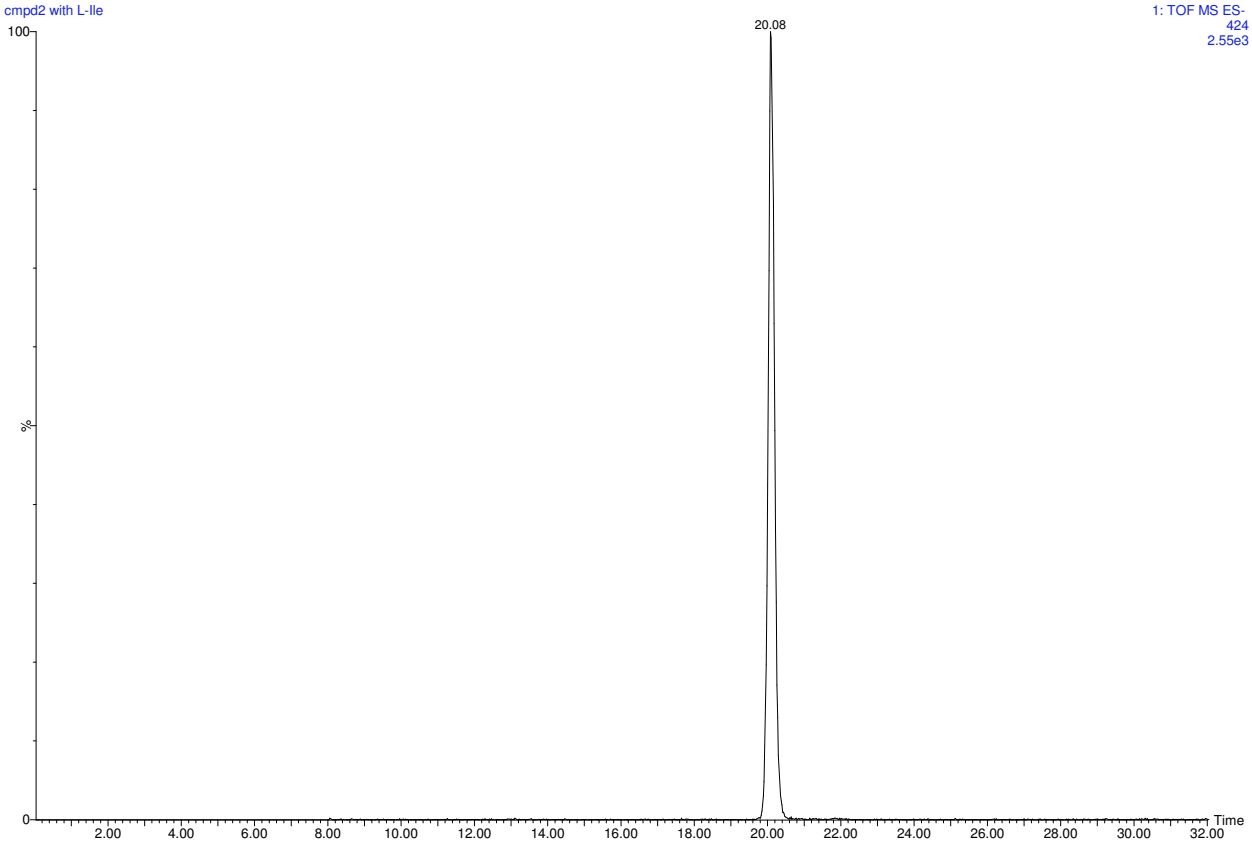


**Figure S14.** Ion chromatograms of co-injection of hydrolyzed compound **2** with L-*allo*-Ile in negative ion mode monitoring at *m/z* 424.

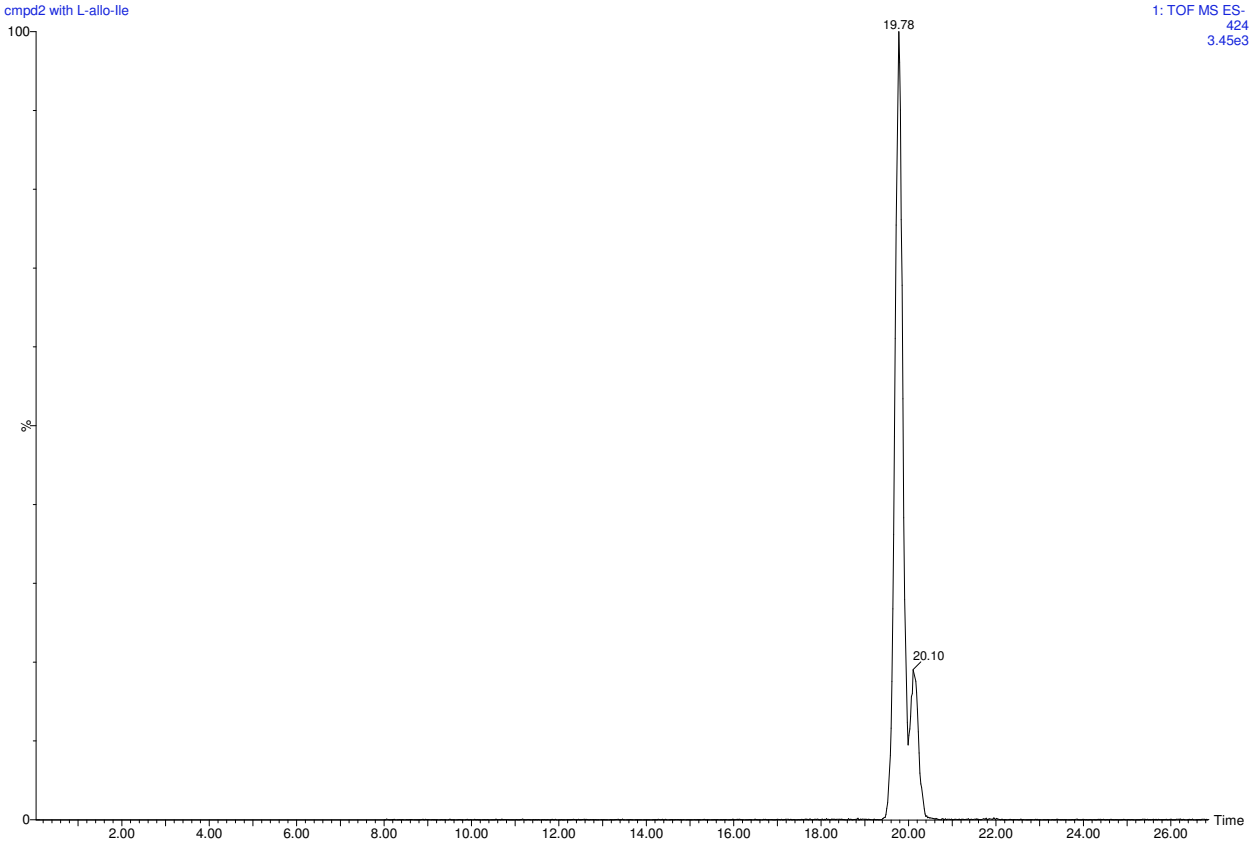


**Figure S15.** Ion chromatograms of hydrolyzed compounds **1**, **2**, L-Cys and D-Cys in negative ion mode monitoring at *m/z* 783 for 2-amino-3-((2-aminoethyl)disulfanyl)propanoic acid.

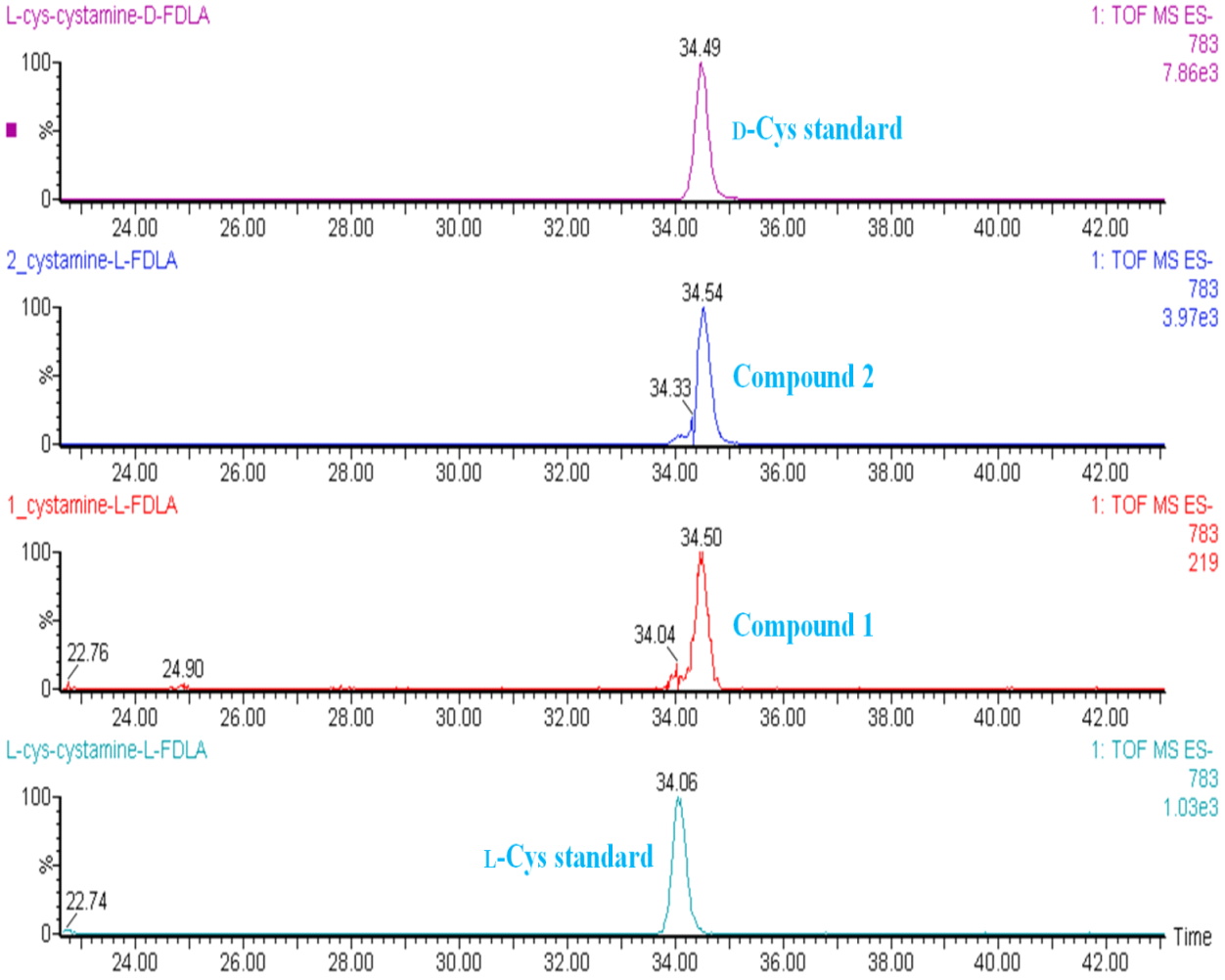


**Figure S16.** Selected ion chromatograms for $[M - H]^-$ of FDLA-Phe. A- L-FDLA derivative of D-Phe standard. B- L-FDLA derivative of L-Phe standard. C- L-FDLA derivative of mollamide E (**1**) hydrolysate. D- L-FDLA derivative of mollamide F (**2**) hydrolysate.

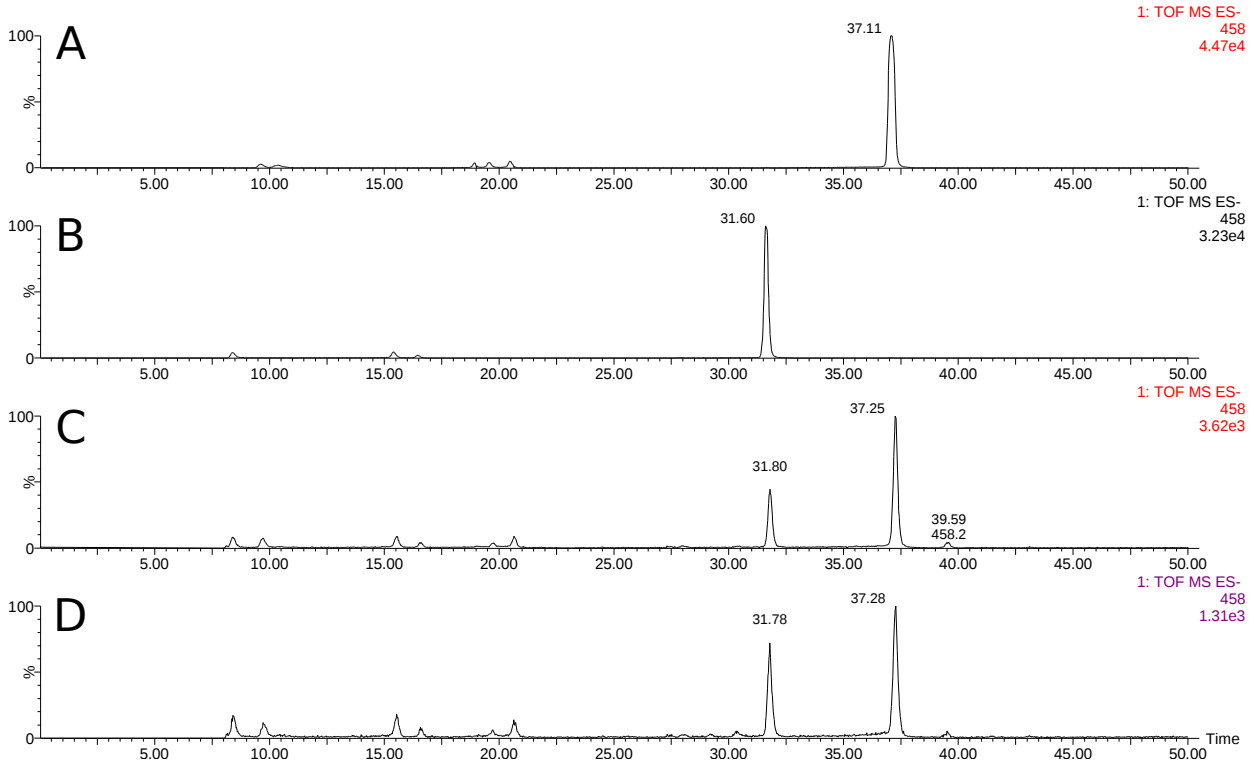


**Figure S17.** MS-MS spectrum for $[M + H]^+$ of **1**.

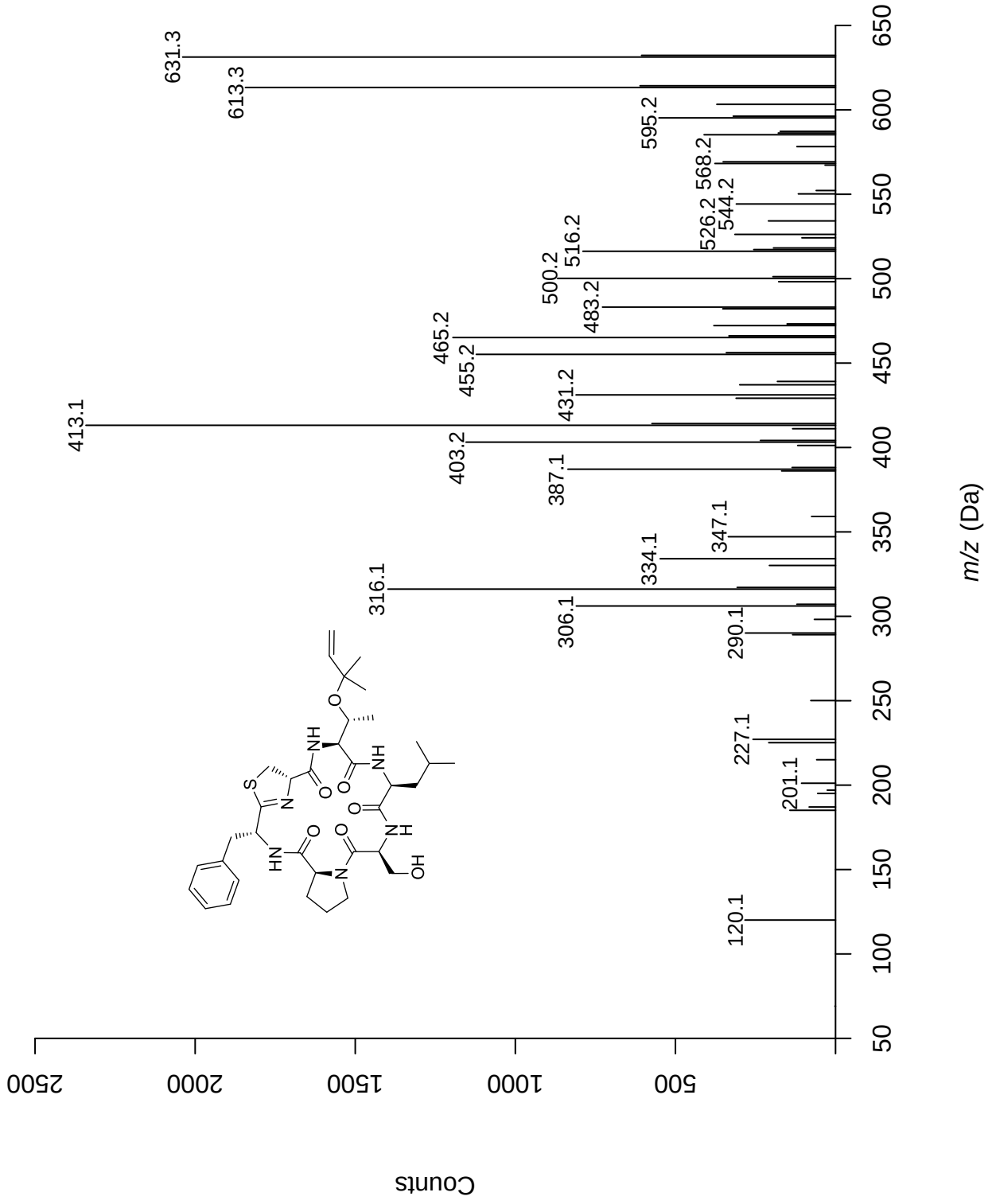
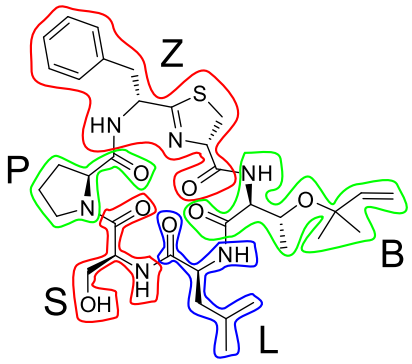


**Table S1.** Assignments for fragments observed in MS-MS of compound **1**.

| *m/z* | **Assignment**[a] |
|---|---|
| 631.3 | $[M + H]^+$ - isoprene |
| 613.3 | $[M + H]^+$ - isoprene - $H_2O$ |
| 603.3 | a5ZP - isoprene |
| 595.3 | b4PS - $H_2O$ + H? |
| 585.3 | b4ZP - $H_2O$ + H? |
| 568.3 | b4SL - $H_2O$ |
| 544.3 | b4PS - isoprene |
| 534.3 | b4ZP - isoprene |
| 526.2 | b4PS - isoprene - $H_2O$ |
| 516.2 | b4ZP - isoprene - $H_2O$ |
| 500.2 | b3SL - isoprene |
| 483.2 | –[b] |
| 465.2 | b4BZ - 2H? |
| 455.2 | –[b] |
| 439.1 | a4BZ |
| 431.2 | b3PS - isoprene |
| 413.2 | b3PS - isoprene - $H_2O$ |
| 403.2 | a3PS - isoprene |
| 387.1 | a3SL - 2H? |
| 347.1 | –[b] |
| 334.1 | b2ZP - isoprene |
| 330.1 | b2PS - isoprene |
| 316.1 | b2ZP - isoprene - $H_2O$ |
| 306.1 | a2ZP - isoprene |
| 290.1 | –[b] |
| 227.1 | –[b] |
| 201.1 | b2LB |
| 120.1 | –[b] |




[a] Assignments are given after the notation proposed in Ngoka, L.C.; Gross, M.L. **1999**, *J. Am. Soc. Mass Spectrom.*, *10*, 360–363.

[b] Not assigned.

**Figure S18.** MS-MS spectrum for $[M + H]^+$ of **2**.

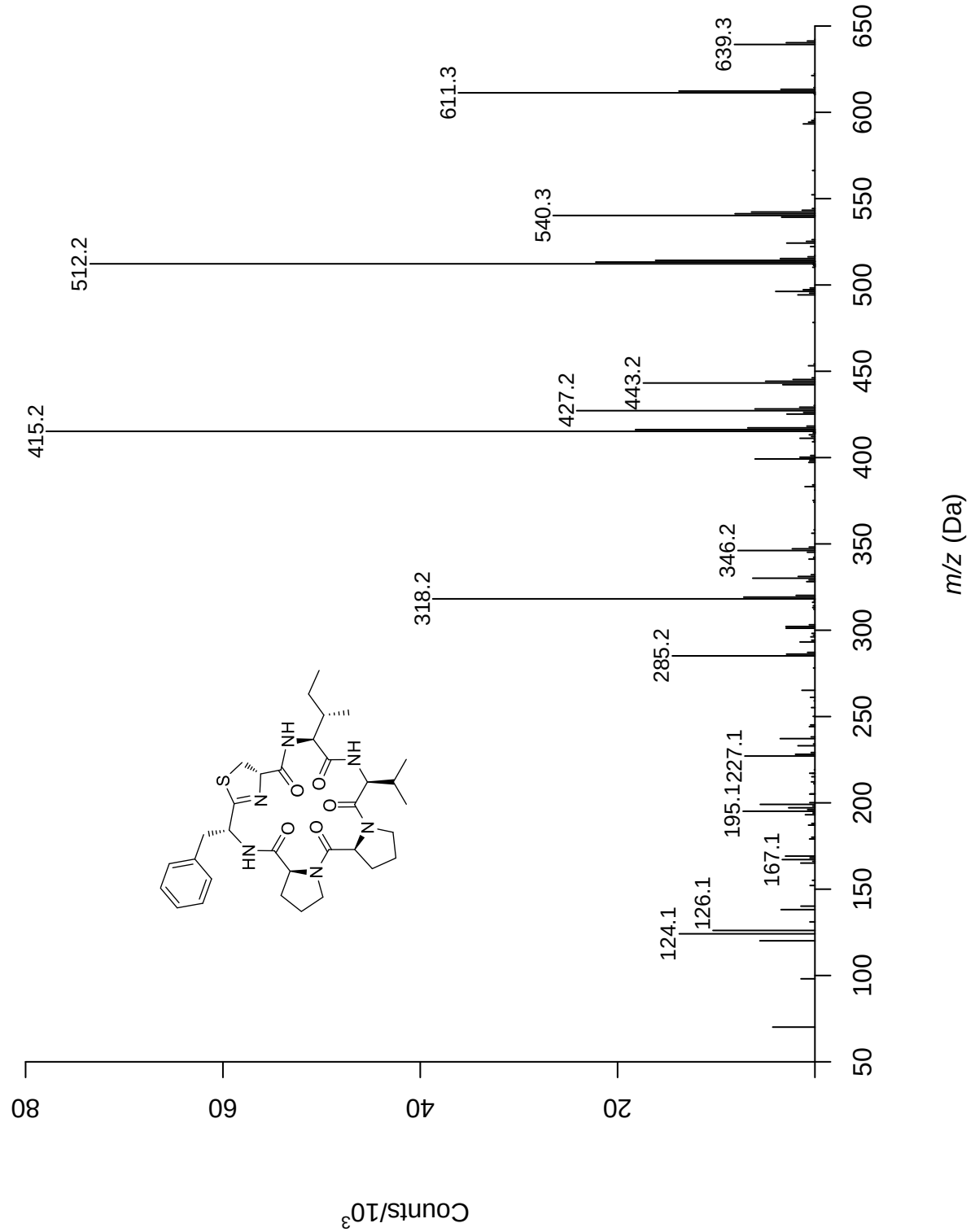
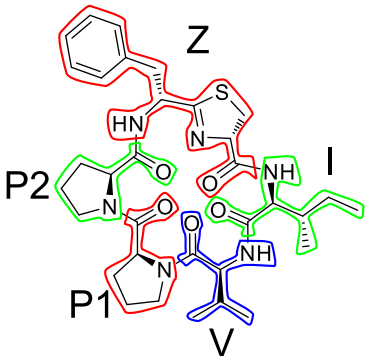


**Table S2.** Assignments for fragments observed in MS-MS of compound **2**.

| ***m/z*** | **Assignment**[a] |
|---|---|
| 639.2 | $[M + H]^+$ |
| 611.2 | a5ZP2 |
| 540.2 | b4P1V |
| 514.2 | a4ZP2 |
| 512.2 | a4P1V |
| 443.2 | b3P2P1 |
| 427.2 | b3P1V |
| 415.2 | a3P2P1 |
| 399.2 | a3P1V |
| 346.2 | b2ZP2 |
| 330.2 | b2P2P1 |
| 318.2 | a2ZP2 |
| 285.2 | –[b] |
| 227.1 | –[b] |
| 195.1 | b2P1V |
| 124.1 | –[b] |




[a] Assignments are given after the notation proposed in Ngoka, L.C.; Gross, M.L. **1999**, *J. Am. Soc. Mass Spectrom.*, *10*, 360–363.

[b] Not assigned.

**Figure S19.** Effect of weak base conditions on mollamide E (**1**) configuration. A- Selected ion chromatogram for $[M + H]^+$ of **1** after 24 h incubation in DMF at room temperature. B- Selected ion chromatogram for $[M + H]^+$ of **1** after 24 h incubation in 20% piperidine in DMF at room temperature.