

Supporting Information

Opportunistic Sampling of Roadkill as an Entry Point to Accessing Natural Products Assembled by Bacteria Associated with Non-Anthropoidal Mammalian Microbiomes

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Contents

- Figure 1.** Thermal ellipsoid plot structure for viscosin (1).
- Figure 2.** Packing diagram for viscosin (1).
- Table 1.** Crystal data and structure refinement for viscosin (1).
- Table 2.** Atom coordinates for viscosin (1).
- Table 3.** Bond distances and angle for viscosin (1).
- Table 4.** Anisotropic displacement parameters for viscosin (1).
- Table 5.** Hydrogen atom parameters for viscosin (1).
- Table 6.** Torsion angles for viscosin (1).
- Table 7.** Hydrogen bond details for viscosin (1).
- Figure 3.** ^1H NMR spectrum of serrawettin W2 (2) (DMSO- d_6 , 600 MHz, 25°C).
- Figure 4.** ^{13}C NMR spectrum of serrawettin W2 (2) (DMSO- d_6 , 150 MHz, 25°C). Offsets from 169.0 to 173.0 ppm and 10.0 to 45.0 ppm are shown for ease of viewing.
- Figure 5.** ^1H - ^{13}C HSQCTOCSY spectrum of serrawettin W2 (2) (DMSO- d_6 , 25°C). CH/CH₃ groups are shown in red, CH₂ groups are shown in blue.
- Figure 6.** ^1H - ^{15}N HSQC spectrum of serrawettin W2 (2) (DMSO- d_6 , 25°C).
- Figure 7.** ^1H - ^{13}C HSQC spectrum of serrawettin W2 (2) (DMSO- d_6 , 25°C). CH/CH₃ groups are shown in red, CH₂ groups are shown in blue.
- Figure 8.** ^1H - ^1H dqfCOSY spectrum of serrawettin W2 (2) (DMSO- d_6 , 25°C).
- Figure 9.** ^1H - ^1H TOCSY spectrum of serrawettin W2 (2) (DMSO- d_6 , 25°C).
- Figure 10.** ^1H - ^{13}C HMBC spectrum of serrawettin W2 (2) (DMSO- d_6 , 25°C).
- Figure 11.** ^1H NMR spectrum of serrawettin W4 (3) (DMSO- d_6 , 600 MHz, 25°C).
- Figure 12.** ^{13}C NMR spectrum of serrawettin W4 (3) (DMSO- d_6 , 150 MHz, 25°C). Offsets from 168.0 to 173.0 ppm and 12.0 to 31.0 ppm are shown for ease of viewing.
- Figure 13.** ^1H - ^{13}C HSQC spectrum of serrawettin W4 (3) (DMSO- d_6 , 25°C). CH/CH₃ peaks are shown in red, CH₂ peaks are shown in blue.
- Figure 14.** ^1H - ^1H dqfCOSY spectrum of serrawettin W4 (3) (DMSO- d_6 , 25°C).
- Figure 15.** ^1H TOCSY spectrum of serrawettin W4 (3) (DMSO- d_6 , 25°C).
- Figure 16.** ^1H - ^{13}C HMBC spectrum of serrawettin W4 (3) (DMSO- d_6 , 25°C).

Figure 17. ^1H NMR Spectrum of serrawettin W5 (4) (DMSO- d_6 , 600 MHz, 25°C).

Figure 18. ^{13}C NMR Spectrum of serrawettin W5 (4) (DMSO- d_6 , 150 MHz, 25°C).

Figure 19. ^1H - ^{13}C HSQC Spectrum of serrawettin W5 (4) (DMSO- d_6 , 25°C). CH/CH₃ peaks are shown in red and CH₂ peaks are shown in blue.

Figure 20. ^1H - ^1H dqfCOSY Spectrum of serrawettin W5 (4) (DMSO- d_6 , 25°C).

Figure 21. ^1H - ^1H TOCSY Spectrum of serrawettin W5 (4) (DMSO- d_6 , 25°C).

Figure 22. ^1H - ^{13}C HMBC Spectrum of serrawettin W5 (4) (DMSO- d_6 , 25°C).

Figure 23. ^1H NMR Spectrum of serrawettin W6 (5) (DMSO- d_6 , 600 MHz, 25°C).

Figure 24. ^1H - ^{13}C HSQC Spectrum of serrawettin W6 (5) (DMSO- d_6 , 25°C). CH/CH₃ peaks are shown in red, CH₂ peaks are shown in blue.

Figure 25. ^1H - ^1H dqfCOSY Spectrum of serrawettin W6 (5) (DMSO- d_6 , 25°C).

Figure 26. ^1H - ^1H TOCSY Spectrum of serrawettin W6 (5) (DMSO- d_6 , 25°C).

Figure 27. ^1H - ^{13}C HMBC Spectrum of serrawettin W6 (5) (DMSO- d_6 , 25°C).

Table 8. Selected COSY & HMBC correlations (DMSO- d_6) for serrawettin W2 (2).

Table 9. Selected COSY and HMBC correlations (DMSO- d_6) for serrawettin W4 (3).

Table 10. Selected COSY and HMBC correlations (DMSO- d_6) for serrawettin W5 (4).

Table 11. Selected COSY and HMBC correlations (DMSO- d_6) for serrawettin W6 (5).

Figure 28. Selected ion trace for m/z 713-717 for serrawettin W2 (2) after FDAA derivatization.

Figure 29. Selected ion trace for m/z 741-745 for serrawettin W2 (2) after FDAA derivatization.

Figure 30. Selected ion trace for m/z 765-769 for serrawettin W2 (2) after FDAA derivatization.

Figure 31. Selected ion trace for m/z 833-837 for serrawettin W2 (2) after FDAA derivatization.

Figure 32. Selected ion trace for m/z 713-717 for serrawettin W2 (2) after FDAA derivatization.

Figure 33. Selected ion trace for m/z 737-740 for serrawettin W2 (2) after FDAA derivatization.

Figure 34. Selected ion trace for m/z 741-745 for serrawettin W4 (3) after FDAA derivatization.

Figure 35. Selected ion trace for m/z 765-769 for serrawettin W4 (3) after FDAA derivatization.

Figure 36. Selected ion trace for m/z 833-837 for serrawettin W4 (3) after FDAA derivatization.

Figure 37. Selected ion trace for m/z 765-769 for serrawettin W5 (4) after FDAA derivatization.

Figure 38. Selected Ion Trace for m/z 741-745 for serrawettin W5 (4) after FDAA derivatization

Figure 39. Selected Ion Trace for m/z 833-837 for serrawettin W5 (4) after FDAA derivatization

Figure 40. Selected Ion Trace for m/z 713-717 for serrawettin W5 (4) after FDAA derivatization

Figure 41. Selected Ion Trace for m/z 741-745 for serrawettin W6 (5) after FDAA derivatization

Figure 42. Selected Ion Trace for m/z 684-688 for serrawettin W6 (5) after FDAA derivatization

Figure 43. Selected Ion Trace for m/z 713-717 for serrawettin W6 (5) after FDAA derivatization

Figure 44. Selected Ion Trace for m/z 765-769 for serrawettin W6 (5) after FDAA derivatization

Figure 45. Selected Ion Trace for m/z 741-745 FDAA derivatized *D-allo* Threonine

Figure 46. Selected Ion Trace for m/z 741-745 FDAA derivatized *L-allo* Threonine

Figure 47. Selected Ion Trace for m/z 741-745 FDAA derivatized *L*-Threonine

Figure 48. Selected Ion Trace for m/z 737-740 FDAA derivatized *D*-Valine

Figure 49. Selected Ion Trace for m/z 737-740 FDAA derivatized *L*-Valine

Figure 50. Selected Ion Trace for m/z 765-769 FDAA derivatized *D*-Isoleucine

Figure 51. Selected Ion Trace for m/z 765-769 FDAA derivatized *L*-Isoleucine

Figure 52. Selected Ion Trace for m/z 765-769 FDAA derivatized *D-allo*-Isoleucine

Figure 53. Selected Ion Trace for m/z 765-769 FDAA derivatized *L-allo*-Isoleucine

Figure 54. Selected Ion Trace for m/z 765-769 FDAA derivatized D-Leucine
Figure 55. Selected Ion Trace for m/z 765-769 FDAA derivatized L-Leucine
Figure 56. Selected Ion Trace for m/z 713-717 FDAA derivatized D-Serine
Figure 57. Selected Ion Trace for m/z 713-717 FDAA derivatized L-Serine
Figure 58. Selected Ion Trace for m/z 833-837 FDAA derivatized D/L-Phenylalanine
Figure 59. Selected Ion Trace for m/z 833-837 FDAA derivatized L-Phenylalanine
Figure 60. Selected Ion Trace for m/z 684-688 FDAA derivatized D/L-Tyrosine
Figure 61. Selected Ion Trace for m/z 684-688 FDAA derivatized L-Tyrosine
Table 12. Summary of Marfey's analysis retention times and peak assignments
Table 13. Reported and observed optical rotation values for 3-hydroxy fatty acids.
Table 14. *Candida albicans* SC5314 biofilm inhibition and growth inhibition by compounds 1-5.

Figure 1. Thermal ellipsoid plot structure for viscisin (1).

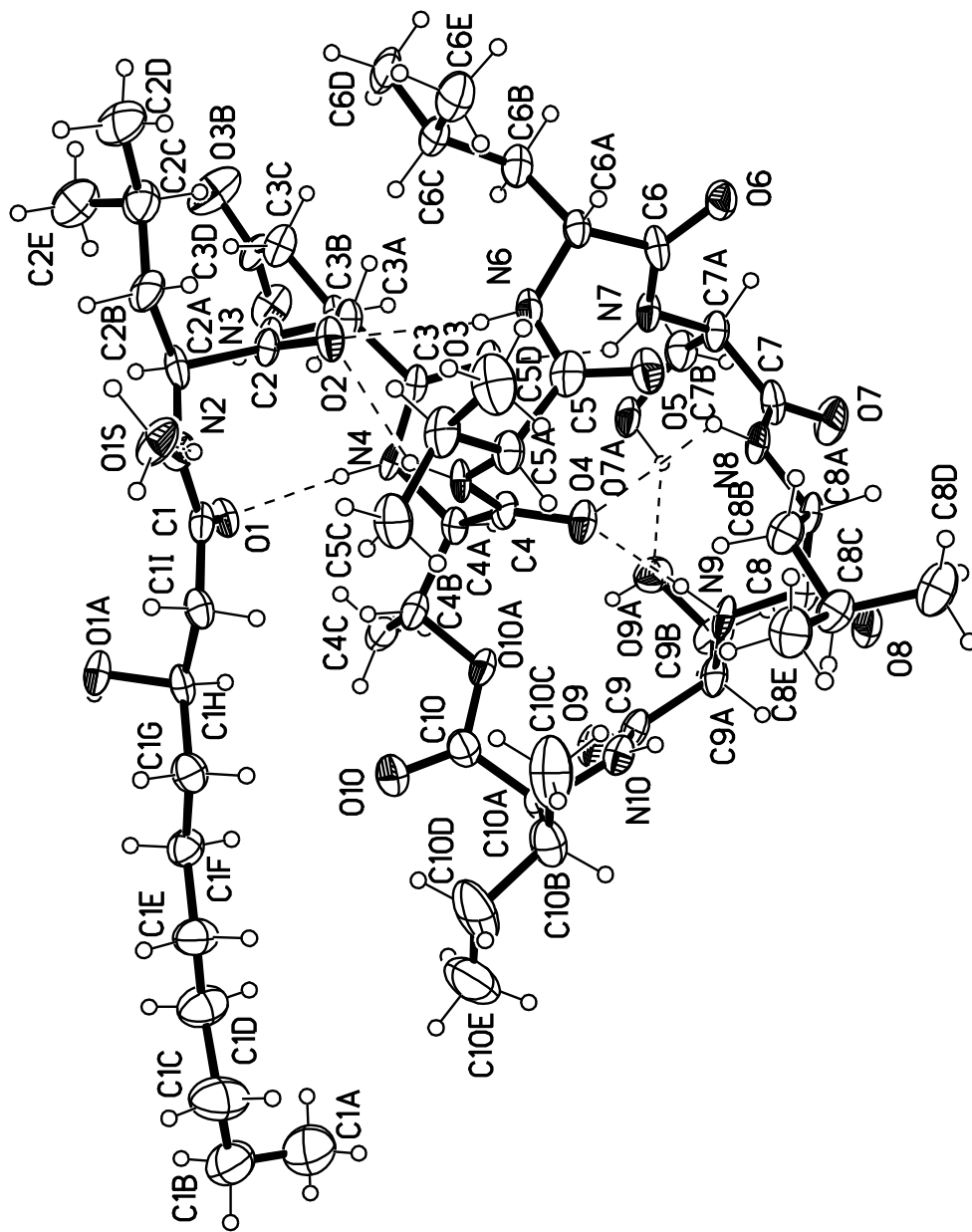


Figure 2. Packing diagram for viscosin (1).

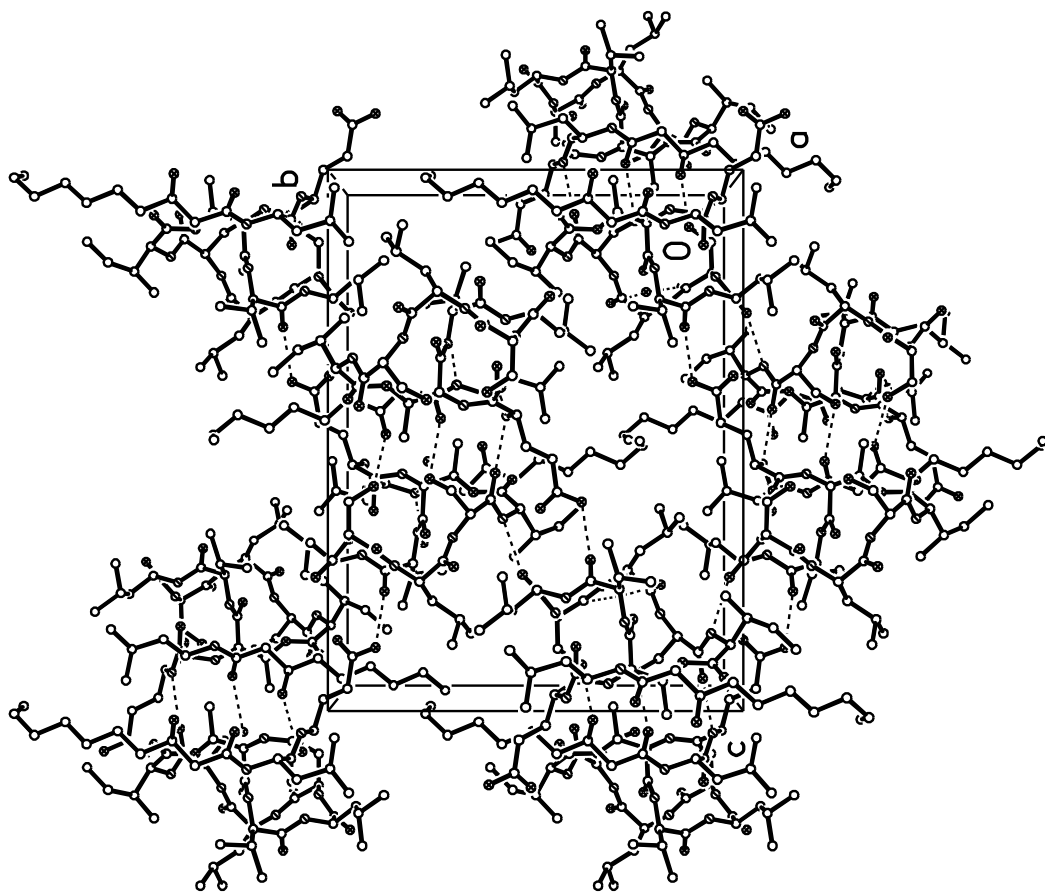


Table 1. Crystal data and structure refinement for viscosin (1).

Empirical formula	$C_{54} H_{95} N_9 O_{16} \cdot (H_2 O)$	
	$C_{54} H_{97} N_9 O_{17}$	
Formula weight	1144.40	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	$a = 14.152(3) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 18.712(4) \text{ \AA}$	$\beta = 90^\circ$
	$c = 24.381(5) \text{ \AA}$	$\gamma = 90^\circ$
Volume	$6456(2) \text{ \AA}^3$	
Z, Z'	4, 1	
Density (calculated)	1.177 Mg/m^3	
Wavelength	1.54178 \AA	
Temperature	100(2) K	
$F(000)$	2480	
Absorption coefficient	0.721 mm^{-1}	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.972 and 0.835	
Theta range for data collection	3.626 to 71.353°	
Reflections collected	39420	
Independent reflections	11566 [R(int) = 0.145]	
Data / restraints / parameters	11566 / 51 / 767	
$wR(F^2 \text{ all data})$	$wR2 = 0.3772$	
$R(F \text{ obsd data})$	$R1 = 0.1281$	
Goodness-of-fit on F^2	1.238	
Observed data [$I > 2\sigma(I)$]	11016	
Absolute structure parameter	-1.2(6)	
Extinction coefficient	0.0195(19)	
Largest and mean shift / s.u.	0.000 and 0.000	
Largest diff. peak and hole	0.783 and -0.891 e/\AA^3	

$$wR2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$$

$$R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for viscosin (1). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1A)	0.7023(17)	0.2418(11)	0.5010(12)	0.101(8)
C(1B)	0.5975(13)	0.2319(8)	0.5098(7)	0.062(4)
C(1C)	0.5515(15)	0.2866(8)	0.5470(6)	0.066(4)
C(1D)	0.5482(12)	0.3621(7)	0.5222(5)	0.052(3)
C(1E)	0.5068(11)	0.4182(6)	0.5610(5)	0.043(3)
C(1F)	0.5107(8)	0.4926(6)	0.5370(5)	0.035(2)
C(1G)	0.4812(8)	0.5506(6)	0.5775(4)	0.034(2)
C(1H)	0.4876(7)	0.6254(6)	0.5540(4)	0.029(2)
C(1I)	0.4702(7)	0.6821(6)	0.5984(4)	0.029(2)
O(1A)	0.4174(5)	0.6364(4)	0.5117(3)	0.0323(16)
C(1)	0.4861(7)	0.7571(6)	0.5781(4)	0.029(2)
O(1)	0.5432(5)	0.7718(4)	0.5405(3)	0.0287(15)
N(2)	0.4364(6)	0.8084(5)	0.6032(4)	0.0307(18)
C(2A)	0.4461(7)	0.8828(6)	0.5847(4)	0.032(2)
C(2B)	0.3831(8)	0.9319(6)	0.6182(4)	0.035(2)
C(2C)	0.3872(9)	1.0110(7)	0.5991(5)	0.040(3)
C(2D)	0.3319(10)	1.0577(8)	0.6394(6)	0.051(3)
C(2E)	0.3518(11)	1.0227(8)	0.5408(6)	0.054(3)
C(2)	0.5488(6)	0.9074(5)	0.5903(4)	0.026(2)
O(2)	0.5876(5)	0.9074(4)	0.6356(3)	0.0311(16)
N(3)	0.5896(6)	0.9302(5)	0.5452(3)	0.0279(18)
C(3A)	0.6880(7)	0.9555(6)	0.5462(4)	0.029(2)
C(3B)	0.7209(7)	0.9770(6)	0.4890(4)	0.030(2)
C(3C)	0.6641(8)	1.0389(6)	0.4663(4)	0.035(2)
C(3D)	0.6813(8)	1.0502(6)	0.4063(5)	0.034(2)
O(3A)	0.7287(7)	1.0111(5)	0.3775(4)	0.048(2)
O(3B)	0.6384(8)	1.1087(6)	0.3879(4)	0.062(3)
C(3)	0.7545(7)	0.8989(5)	0.5701(4)	0.025(2)
O(3)	0.8257(5)	0.9187(4)	0.5948(3)	0.0325(16)
N(4)	0.7319(6)	0.8303(5)	0.5633(3)	0.0258(17)
C(4A)	0.7938(6)	0.7750(5)	0.5862(4)	0.0242(19)
C(4B)	0.7621(7)	0.7021(6)	0.5666(4)	0.030(2)
C(4C)	0.7767(9)	0.6922(7)	0.5058(5)	0.041(3)
C(4)	0.7972(7)	0.7781(6)	0.6481(4)	0.028(2)
O(4)	0.8708(5)	0.7693(4)	0.6746(3)	0.0315(16)
N(5)	0.7156(6)	0.7923(5)	0.6745(3)	0.0256(17)
C(5A)	0.7156(7)	0.8046(6)	0.7337(4)	0.030(2)
C(5B)	0.6139(7)	0.8081(7)	0.7570(4)	0.036(2)

C(5C)	0.5649(8)	0.7359(7)	0.7507(5)	0.041(3)
C(5D)	0.6151(9)	0.8332(9)	0.8168(5)	0.051(3)
C(5)	0.7742(7)	0.8707(6)	0.7465(4)	0.031(2)
O(5)	0.8341(5)	0.8704(4)	0.7832(3)	0.0353(17)
N(6)	0.7551(6)	0.9291(5)	0.7169(3)	0.0286(18)
C(6A)	0.8006(7)	0.9972(5)	0.7295(4)	0.026(2)
C(6B)	0.7602(8)	1.0556(6)	0.6937(5)	0.035(2)
C(6C)	0.6513(8)	1.0666(6)	0.6991(5)	0.037(2)
C(6D)	0.6227(8)	1.1299(7)	0.6633(5)	0.046(3)
C(6E)	0.6201(9)	1.0770(8)	0.7580(6)	0.048(3)
C(6)	0.9097(7)	0.9942(6)	0.7234(4)	0.029(2)
O(6)	0.9593(5)	1.0318(4)	0.7534(3)	0.0328(16)
N(7)	0.9434(6)	0.9530(5)	0.6836(3)	0.0280(18)
C(7A)	1.0463(7)	0.9481(6)	0.6728(4)	0.029(2)
C(7B)	1.0676(8)	0.9467(7)	0.6126(5)	0.038(2)
O(7A)	1.0251(5)	0.8891(4)	0.5846(3)	0.0333(17)
C(7)	1.0921(7)	0.8838(6)	0.7017(4)	0.033(2)
O(7)	1.1790(5)	0.8759(5)	0.6965(4)	0.044(2)
N(8)	1.0377(6)	0.8388(5)	0.7301(3)	0.0283(18)
C(8A)	1.0753(6)	0.7772(6)	0.7588(4)	0.027(2)
C(8B)	0.9961(8)	0.7492(6)	0.7963(4)	0.034(2)
C(8C)	1.0197(8)	0.6823(6)	0.8300(4)	0.036(2)
C(8D)	1.0962(9)	0.6989(8)	0.8731(5)	0.047(3)
C(8E)	0.9282(9)	0.6568(7)	0.8588(5)	0.044(3)
C(8)	1.1123(7)	0.7201(6)	0.7200(4)	0.032(2)
O(8)	1.1904(5)	0.6934(4)	0.7283(3)	0.0375(18)
N(9)	1.0555(5)	0.6991(5)	0.6781(3)	0.0285(18)
C(9A)	1.0927(7)	0.6553(6)	0.6347(4)	0.031(2)
C(9B)	1.1418(9)	0.6998(6)	0.5912(5)	0.037(2)
O(9A)	1.0785(6)	0.7531(4)	0.5705(3)	0.0392(18)
C(9)	1.0140(7)	0.6084(6)	0.6090(4)	0.030(2)
O(9)	1.0099(5)	0.5977(5)	0.5602(3)	0.0364(17)
N(10)	0.9538(6)	0.5800(5)	0.6450(3)	0.0306(19)
C(10A)	0.8707(8)	0.5378(6)	0.6279(4)	0.030(2)
C(10B)	0.8298(9)	0.5002(7)	0.6779(5)	0.044(3)
C(10C)	0.7899(10)	0.5532(11)	0.7187(6)	0.066(4)
C(10D)	0.7560(12)	0.4429(10)	0.6626(7)	0.071(5)
C(10E)	0.7926(18)	0.3872(9)	0.6221(9)	0.092(7)
O(10A)	0.8225(5)	0.6532(4)	0.5974(3)	0.0288(15)
C(10)	0.8011(8)	0.5832(6)	0.5968(4)	0.033(2)
O(10)	0.7313(6)	0.5588(5)	0.5745(4)	0.050(2)
O(1S)	0.3374(5)	0.7889(4)	0.7021(4)	0.0414(19)

Table 3. Bond distances [\AA] and angles [$^\circ$] for viscosin (1).

C(1A)-C(1B)	1.51(3)	C(2E)-C(2C)-C(2B)	113.8(11)
C(1A)-H(1A1)	0.96	C(2D)-C(2C)-C(2B)	109.5(10)
C(1A)-H(1A2)	0.9599	C(2E)-C(2C)-H(2C)	107.6
C(1A)-H(1A3)	0.96	C(2D)-C(2C)-H(2C)	107.6
C(1B)-C(1C)	1.51(2)	C(2B)-C(2C)-H(2C)	107.6
C(1B)-H(1B1)	0.99	C(2C)-C(2D)-H(2D1)	109.4
C(1B)-H(1B2)	0.99	C(2C)-C(2D)-H(2D2)	108.7
C(1C)-C(1D)	1.54(2)	H(2D1)-C(2D)-H(2D2)	109.5
C(1C)-H(1C1)	0.99	C(2C)-C(2D)-H(2D3)	110.4
C(1C)-H(1C2)	0.99	H(2D1)-C(2D)-H(2D3)	109.5
C(1D)-C(1E)	1.529(17)	H(2D2)-C(2D)-H(2D3)	109.5
C(1D)-H(1D1)	0.99	C(2C)-C(2E)-H(2E1)	110.2
C(1D)-H(1D2)	0.99	C(2C)-C(2E)-H(2E2)	108.4
C(1E)-C(1F)	1.510(16)	H(2E1)-C(2E)-H(2E2)	109.5
C(1E)-H(1E1)	0.99	C(2C)-C(2E)-H(2E3)	109.8
C(1E)-H(1E2)	0.99	H(2E1)-C(2E)-H(2E3)	109.5
C(1F)-C(1G)	1.525(15)	H(2E2)-C(2E)-H(2E3)	109.5
C(1F)-H(1F1)	0.99	O(2)-C(2)-N(3)	123.6(9)
C(1F)-H(1F2)	0.99	O(2)-C(2)-C(2A)	120.1(9)
C(1G)-C(1H)	1.515(15)	N(3)-C(2)-C(2A)	116.2(9)
C(1G)-H(1G1)	0.99	C(2)-N(3)-C(3A)	120.5(8)
C(1G)-H(1G2)	0.99	C(2)-N(3)-H(3)	130(9)
C(1H)-O(1A)	1.447(12)	C(3A)-N(3)-H(3)	106(9)
C(1H)-C(1I)	1.537(14)	N(3)-C(3A)-C(3B)	111.1(8)
C(1H)-H(1H)	1	N(3)-C(3A)-C(3)	111.5(8)
C(1I)-C(1)	1.505(15)	C(3B)-C(3A)-C(3)	110.1(8)
C(1I)-H(1IA)	0.99	N(3)-C(3A)-H(3A)	108
C(1I)-H(1IB)	0.99	C(3B)-C(3A)-H(3A)	108
O(1A)-H(1AO)	0.99(6)	C(3)-C(3A)-H(3A)	108
C(1)-O(1)	1.252(13)	C(3C)-C(3B)-C(3A)	112.0(9)
C(1)-N(2)	1.338(14)	C(3C)-C(3B)-H(3B1)	109.2
N(2)-C(2A)	1.470(14)	C(3A)-C(3B)-H(3B1)	109.2
N(2)-H(2)	0.87(5)	C(3C)-C(3B)-H(3B2)	109.2
C(2A)-C(2B)	1.518(14)	C(3A)-C(3B)-H(3B2)	109.2
C(2A)-C(2)	1.531(13)	H(3B1)-C(3B)-H(3B2)	107.9
C(2A)-H(2A)	1	C(3D)-C(3C)-C(3B)	112.2(9)
C(2B)-C(2C)	1.554(17)	C(3D)-C(3C)-H(3C1)	109.2
C(2B)-H(2B1)	0.99	C(3B)-C(3C)-H(3C1)	109.2
C(2B)-H(2B2)	0.99	C(3D)-C(3C)-H(3C2)	109.2
C(2C)-C(2E)	1.524(18)	C(3B)-C(3C)-H(3C2)	109.2
C(2C)-C(2D)	1.529(16)	H(3C1)-C(3C)-H(3C2)	107.9

C(2C)-H(2C)	1	O(3A)-C(3D)-O(3B)	123.5(10)
C(2D)-H(2D1)	0.96	O(3A)-C(3D)-C(3C)	124.8(10)
C(2D)-H(2D2)	0.96	O(3B)-C(3D)-C(3C)	111.8(9)
C(2D)-H(2D3)	0.96	C(3D)-O(3B)-H(3BO)	113(10)
C(2E)-H(2E1)	0.9602	O(3)-C(3)-N(4)	123.2(9)
C(2E)-H(2E2)	0.9599	O(3)-C(3)-C(3A)	118.7(9)
C(2E)-H(2E3)	0.9599	N(4)-C(3)-C(3A)	118.1(8)
C(2)-O(2)	1.235(12)	C(3)-N(4)-C(4A)	119.2(8)
C(2)-N(3)	1.312(13)	C(3)-N(4)-H(4)	125(8)
N(3)-C(3A)	1.471(13)	C(4A)-N(4)-H(4)	115(8)
N(3)-H(3)	0.87(5)	N(4)-C(4A)-C(4)	111.8(8)
C(3A)-C(3B)	1.524(14)	N(4)-C(4A)-C(4B)	109.8(8)
C(3A)-C(3)	1.532(13)	C(4)-C(4A)-C(4B)	111.0(8)
C(3A)-H(3A)	1	N(4)-C(4A)-H(4A)	108
C(3B)-C(3C)	1.515(15)	C(4)-C(4A)-H(4A)	108
C(3B)-H(3B1)	0.99	C(4B)-C(4A)-H(4A)	108
C(3B)-H(3B2)	0.99	O(10A)-C(4B)-C(4C)	110.4(8)
C(3C)-C(3D)	1.497(15)	O(10A)-C(4B)-C(4A)	103.3(8)
C(3C)-H(3C1)	0.99	C(4C)-C(4B)-C(4A)	112.3(9)
C(3C)-H(3C2)	0.99	O(10A)-C(4B)-H(4B)	110.2
C(3D)-O(3A)	1.216(14)	C(4C)-C(4B)-H(4B)	110.2
C(3D)-O(3B)	1.329(14)	C(4A)-C(4B)-H(4B)	110.2
O(3B)-H(3BO)	0.99(6)	C(4B)-C(4C)-H(4C1)	108.3
C(3)-O(3)	1.230(12)	C(4B)-C(4C)-H(4C2)	110
C(3)-N(4)	1.332(13)	H(4C1)-C(4C)-H(4C2)	109.5
N(4)-C(4A)	1.467(12)	C(4B)-C(4C)-H(4C3)	110.1
N(4)-H(4)	0.86(5)	H(4C1)-C(4C)-H(4C3)	109.5
C(4A)-C(4)	1.512(14)	H(4C2)-C(4C)-H(4C3)	109.5
C(4A)-C(4B)	1.514(15)	O(4)-C(4)-N(5)	120.0(9)
C(4A)-H(4A)	1	O(4)-C(4)-C(4A)	122.8(9)
C(4B)-O(10A)	1.459(12)	N(5)-C(4)-C(4A)	117.2(8)
C(4B)-C(4C)	1.509(15)	C(4)-N(5)-C(5A)	120.2(8)
C(4B)-H(4B)	1	C(4)-N(5)-H(5)	109(8)
C(4C)-H(4C1)	0.96	C(5A)-N(5)-H(5)	126(8)
C(4C)-H(4C2)	0.96	N(5)-C(5A)-C(5)	109.4(8)
C(4C)-H(4C3)	0.9599	N(5)-C(5A)-C(5B)	111.6(8)
C(4)-O(4)	1.236(12)	C(5)-C(5A)-C(5B)	113.4(9)
C(4)-N(5)	1.348(13)	N(5)-C(5A)-H(5A)	107.4
N(5)-C(5A)	1.461(13)	C(5)-C(5A)-H(5A)	107.4
N(5)-H(5)	0.87(5)	C(5B)-C(5A)-H(5A)	107.4
C(5A)-C(5)	1.521(16)	C(5C)-C(5B)-C(5D)	111.8(10)
C(5A)-C(5B)	1.549(13)	C(5C)-C(5B)-C(5A)	110.4(10)
C(5A)-H(5A)	1	C(5D)-C(5B)-C(5A)	110.5(9)

C(5B)-C(5C)	1.527(17)	C(5C)-C(5B)-H(5B)	108
C(5B)-C(5D)	1.532(16)	C(5D)-C(5B)-H(5B)	108
C(5B)-H(5B)	1	C(5A)-C(5B)-H(5B)	108
C(5C)-H(5C1)	0.96	C(5B)-C(5C)-H(5C1)	109.4
C(5C)-H(5C2)	0.96	C(5B)-C(5C)-H(5C2)	109.4
C(5C)-H(5C3)	0.96	H(5C1)-C(5C)-H(5C2)	109.5
C(5D)-H(5D1)	0.9601	C(5B)-C(5C)-H(5C3)	109.5
C(5D)-H(5D2)	0.9599	H(5C1)-C(5C)-H(5C3)	109.5
C(5D)-H(5D3)	0.9599	H(5C2)-C(5C)-H(5C3)	109.5
C(5)-O(5)	1.233(13)	C(5B)-C(5D)-H(5D1)	109.7
C(5)-N(6)	1.337(15)	C(5B)-C(5D)-H(5D2)	108.7
N(6)-C(6A)	1.460(13)	H(5D1)-C(5D)-H(5D2)	109.5
N(6)-H(6)	0.87(5)	C(5B)-C(5D)-H(5D3)	109.9
C(6A)-C(6B)	1.512(15)	H(5D1)-C(5D)-H(5D3)	109.5
C(6A)-C(6)	1.552(13)	H(5D2)-C(5D)-H(5D3)	109.5
C(6A)-H(6A)	1	O(5)-C(5)-N(6)	122.3(10)
C(6B)-C(6C)	1.560(15)	O(5)-C(5)-C(5A)	121.3(10)
C(6B)-H(6B1)	0.99	N(6)-C(5)-C(5A)	116.4(9)
C(6B)-H(6B2)	0.99	C(5)-N(6)-C(6A)	120.7(8)
C(6C)-C(6E)	1.514(18)	C(5)-N(6)-H(6)	117(8)
C(6C)-C(6D)	1.526(17)	C(6A)-N(6)-H(6)	121(8)
C(6C)-H(6C)	1	N(6)-C(6A)-C(6B)	110.0(8)
C(6D)-H(6D1)	0.96	N(6)-C(6A)-C(6)	112.8(8)
C(6D)-H(6D2)	0.9601	C(6B)-C(6A)-C(6)	110.3(8)
C(6D)-H(6D3)	0.9601	N(6)-C(6A)-H(6A)	107.9
C(6E)-H(6E1)	0.96	C(6B)-C(6A)-H(6A)	107.9
C(6E)-H(6E2)	0.96	C(6)-C(6A)-H(6A)	107.9
C(6E)-H(6E3)	0.96	C(6A)-C(6B)-C(6C)	114.8(9)
C(6)-O(6)	1.234(12)	C(6A)-C(6B)-H(6B1)	108.6
C(6)-N(7)	1.328(14)	C(6C)-C(6B)-H(6B1)	108.6
N(7)-C(7A)	1.483(12)	C(6A)-C(6B)-H(6B2)	108.6
N(7)-H(7)	0.87(5)	C(6C)-C(6B)-H(6B2)	108.6
C(7A)-C(7B)	1.499(15)	H(6B1)-C(6B)-H(6B2)	107.5
C(7A)-C(7)	1.536(15)	C(6E)-C(6C)-C(6D)	111.4(10)
C(7A)-H(7A)	1	C(6E)-C(6C)-C(6B)	112.7(9)
C(7B)-O(7A)	1.411(14)	C(6D)-C(6C)-C(6B)	108.4(10)
C(7B)-H(7B1)	0.99	C(6E)-C(6C)-H(6C)	108.1
C(7B)-H(7B2)	0.99	C(6D)-C(6C)-H(6C)	108.1
O(7A)-H(7AO)	0.99(6)	C(6B)-C(6C)-H(6C)	108.1
C(7)-O(7)	1.246(14)	C(6C)-C(6D)-H(6D1)	109.1
C(7)-N(8)	1.335(14)	C(6C)-C(6D)-H(6D2)	109.8
N(8)-C(8A)	1.449(13)	H(6D1)-C(6D)-H(6D2)	109.5
N(8)-H(8)	0.87(5)	C(6C)-C(6D)-H(6D3)	109.5

C(8A)-C(8)	1.520(15)	H(6D1)-C(6D)-H(6D3)	109.5
C(8A)-C(8B)	1.540(14)	H(6D2)-C(6D)-H(6D3)	109.5
C(8A)-H(8A)	1	C(6C)-C(6E)-H(6E1)	110.2
C(8B)-C(8C)	1.533(15)	C(6C)-C(6E)-H(6E2)	109.5
C(8B)-H(8B1)	0.99	H(6E1)-C(6E)-H(6E2)	109.5
C(8B)-H(8B2)	0.99	C(6C)-C(6E)-H(6E3)	108.8
C(8C)-C(8D)	1.541(17)	H(6E1)-C(6E)-H(6E3)	109.5
C(8C)-C(8E)	1.548(16)	H(6E2)-C(6E)-H(6E3)	109.5
C(8C)-H(8C)	1	O(6)-C(6)-N(7)	124.1(9)
C(8D)-H(8D1)	0.9599	O(6)-C(6)-C(6A)	119.2(9)
C(8D)-H(8D2)	0.96	N(7)-C(6)-C(6A)	116.7(8)
C(8D)-H(8D3)	0.96	C(6)-N(7)-C(7A)	121.2(8)
C(8E)-H(8E1)	0.9599	C(6)-N(7)-H(7)	134(9)
C(8E)-H(8E2)	0.9599	C(7A)-N(7)-H(7)	105(9)
C(8E)-H(8E3)	0.9599	N(7)-C(7A)-C(7B)	111.8(8)
C(8)-O(8)	1.229(14)	N(7)-C(7A)-C(7)	112.5(8)
C(8)-N(9)	1.358(14)	C(7B)-C(7A)-C(7)	110.6(9)
N(9)-C(9A)	1.440(13)	N(7)-C(7A)-H(7A)	107.2
N(9)-H(9)	0.87(5)	C(7B)-C(7A)-H(7A)	107.2
C(9A)-C(9B)	1.515(15)	C(7)-C(7A)-H(7A)	107.2
C(9A)-C(9)	1.551(15)	O(7A)-C(7B)-C(7A)	113.6(10)
C(9A)-H(9A)	1	O(7A)-C(7B)-H(7B1)	108.8
C(9B)-O(9A)	1.432(13)	C(7A)-C(7B)-H(7B1)	108.8
C(9B)-H(9B1)	0.99	O(7A)-C(7B)-H(7B2)	108.8
C(9B)-H(9B2)	0.99	C(7A)-C(7B)-H(7B2)	108.8
O(9A)-H(9AO)	0.99(6)	H(7B1)-C(7B)-H(7B2)	107.7
C(9)-O(9)	1.208(13)	C(7B)-O(7A)-H(7AO)	103(8)
C(9)-N(10)	1.334(13)	O(7)-C(7)-N(8)	123.1(10)
N(10)-C(10A)	1.476(14)	O(7)-C(7)-C(7A)	117.6(9)
N(10)-H(10)	0.87(5)	N(8)-C(7)-C(7A)	119.2(9)
C(10A)-C(10)	1.505(15)	C(7)-N(8)-C(8A)	122.7(8)
C(10A)-C(10B)	1.522(15)	C(7)-N(8)-H(8)	115(8)
C(10A)-H(10A)	1	C(8A)-N(8)-H(8)	122(8)
C(10B)-C(10C)	1.52(2)	N(8)-C(8A)-C(8)	112.7(8)
C(10B)-C(10D)	1.542(18)	N(8)-C(8A)-C(8B)	106.9(8)
C(10B)-H(10B)	1	C(8)-C(8A)-C(8B)	112.3(9)
C(10C)-H(10C)	0.9601	N(8)-C(8A)-H(8A)	108.3
C(10C)-H(10D)	0.96	C(8)-C(8A)-H(8A)	108.3
C(10C)-H(10E)	0.96	C(8B)-C(8A)-H(8A)	108.3
C(10D)-C(10E)	1.53(3)	C(8C)-C(8B)-C(8A)	115.9(9)
C(10D)-H(10F)	0.99	C(8C)-C(8B)-H(8B1)	108.3
C(10D)-H(10G)	0.99	C(8A)-C(8B)-H(8B1)	108.3
C(10E)-H(10H)	0.96	C(8C)-C(8B)-H(8B2)	108.3

C(10E)-H(10I)	0.9599	C(8A)-C(8B)-H(8B2)	108.3
C(10E)-H(10J)	0.9601	H(8B1)-C(8B)-H(8B2)	107.4
O(10A)-C(10)	1.343(13)	C(8B)-C(8C)-C(8D)	110.7(10)
C(10)-O(10)	1.217(14)	C(8B)-C(8C)-C(8E)	108.1(9)
O(1S)-H(1SA)	0.99(6)	C(8D)-C(8C)-C(8E)	109.9(9)
O(1S)-H(1SB)	0.99(6)	C(8B)-C(8C)-H(8C)	109.4
C(1B)-C(1A)-H(1A1)	109.4	C(8D)-C(8C)-H(8C)	109.4
C(1B)-C(1A)-H(1A2)	108.6	C(8E)-C(8C)-H(8C)	109.4
H(1A1)-C(1A)-H(1A2)	109.5	C(8C)-C(8D)-H(8D1)	109.2
C(1B)-C(1A)-H(1A3)	110.4	C(8C)-C(8D)-H(8D2)	109.3
H(1A1)-C(1A)-H(1A3)	109.5	H(8D1)-C(8D)-H(8D2)	109.5
H(1A2)-C(1A)-H(1A3)	109.5	C(8C)-C(8D)-H(8D3)	109.9
C(1A)-C(1B)-C(1C)	115.1(16)	H(8D1)-C(8D)-H(8D3)	109.5
C(1A)-C(1B)-H(1B1)	108.5	H(8D2)-C(8D)-H(8D3)	109.5
C(1C)-C(1B)-H(1B1)	108.5	C(8C)-C(8E)-H(8E1)	109.5
C(1A)-C(1B)-H(1B2)	108.5	C(8C)-C(8E)-H(8E2)	108.8
C(1C)-C(1B)-H(1B2)	108.5	H(8E1)-C(8E)-H(8E2)	109.5
H(1B1)-C(1B)-H(1B2)	107.5	C(8C)-C(8E)-H(8E3)	110.1
C(1B)-C(1C)-C(1D)	113.5(13)	H(8E1)-C(8E)-H(8E3)	109.5
C(1B)-C(1C)-H(1C1)	108.9	H(8E2)-C(8E)-H(8E3)	109.5
C(1D)-C(1C)-H(1C1)	108.9	O(8)-C(8)-N(9)	122.6(11)
C(1B)-C(1C)-H(1C2)	108.9	O(8)-C(8)-C(8A)	119.5(9)
C(1D)-C(1C)-H(1C2)	108.9	N(9)-C(8)-C(8A)	117.8(9)
H(1C1)-C(1C)-H(1C2)	107.7	C(8)-N(9)-C(9A)	120.1(8)
C(1E)-C(1D)-C(1C)	113.5(11)	C(8)-N(9)-H(9)	119(8)
C(1E)-C(1D)-H(1D1)	108.9	C(9A)-N(9)-H(9)	117(8)
C(1C)-C(1D)-H(1D1)	108.9	N(9)-C(9A)-C(9B)	111.7(9)
C(1E)-C(1D)-H(1D2)	108.9	N(9)-C(9A)-C(9)	110.9(8)
C(1C)-C(1D)-H(1D2)	108.9	C(9B)-C(9A)-C(9)	111.0(9)
H(1D1)-C(1D)-H(1D2)	107.7	N(9)-C(9A)-H(9A)	107.7
C(1F)-C(1E)-C(1D)	112.3(10)	C(9B)-C(9A)-H(9A)	107.7
C(1F)-C(1E)-H(1E1)	109.2	C(9)-C(9A)-H(9A)	107.7
C(1D)-C(1E)-H(1E1)	109.2	O(9A)-C(9B)-C(9A)	110.1(9)
C(1F)-C(1E)-H(1E2)	109.2	O(9A)-C(9B)-H(9B1)	109.6
C(1D)-C(1E)-H(1E2)	109.2	C(9A)-C(9B)-H(9B1)	109.6
H(1E1)-C(1E)-H(1E2)	107.9	O(9A)-C(9B)-H(9B2)	109.6
C(1E)-C(1F)-C(1G)	113.2(9)	C(9A)-C(9B)-H(9B2)	109.6
C(1E)-C(1F)-H(1F1)	108.9	H(9B1)-C(9B)-H(9B2)	108.2
C(1G)-C(1F)-H(1F1)	108.9	C(9B)-O(9A)-H(9AO)	103(8)
C(1E)-C(1F)-H(1F2)	108.9	O(9)-C(9)-N(10)	123.5(10)
C(1G)-C(1F)-H(1F2)	108.9	O(9)-C(9)-C(9A)	121.7(9)
H(1F1)-C(1F)-H(1F2)	107.7	N(10)-C(9)-C(9A)	114.8(9)
C(1H)-C(1G)-C(1F)	113.3(9)	C(9)-N(10)-C(10A)	122.4(8)

C(1H)-C(1G)-H(1G1)	108.9	C(9)-N(10)-H(10)	119(9)
C(1F)-C(1G)-H(1G1)	108.9	C(10A)-N(10)-H(10)	119(9)
C(1H)-C(1G)-H(1G2)	108.9	N(10)-C(10A)-C(10)	111.2(8)
C(1F)-C(1G)-H(1G2)	108.9	N(10)-C(10A)-C(10B)	108.9(8)
H(1G1)-C(1G)-H(1G2)	107.7	C(10)-C(10A)-C(10B)	114.6(10)
O(1A)-C(1H)-C(1G)	111.2(8)	N(10)-C(10A)-H(10A)	107.3
O(1A)-C(1H)-C(1I)	107.1(8)	C(10)-C(10A)-H(10A)	107.3
C(1G)-C(1H)-C(1I)	111.2(8)	C(10B)-C(10A)-H(10A)	107.3
O(1A)-C(1H)-H(1H)	109.1	C(10C)-C(10B)-C(10A)	111.4(11)
C(1G)-C(1H)-H(1H)	109.1	C(10C)-C(10B)-C(10D)	111.2(13)
C(1I)-C(1H)-H(1H)	109.1	C(10A)-C(10B)-C(10D)	112.6(10)
C(1)-C(1D)-C(1H)	112.8(8)	C(10C)-C(10B)-H(10B)	107.1
C(1)-C(1D)-H(1IA)	109	C(10A)-C(10B)-H(10B)	107.1
C(1H)-C(1D)-H(1IA)	109	C(10D)-C(10B)-H(10B)	107.1
C(1)-C(1D)-H(1IB)	109	C(10B)-C(10C)-H(10C)	108.8
C(1H)-C(1D)-H(1IB)	109	C(10B)-C(10C)-H(10D)	109.9
H(1IA)-C(1D)-H(1IB)	107.8	H(10C)-C(10C)-H(10D)	109.5
C(1H)-O(1A)-H(1AO)	112(8)	C(10B)-C(10C)-H(10E)	109.8
O(1)-C(1)-N(2)	121.1(10)	H(10C)-C(10C)-H(10E)	109.5
O(1)-C(1)-C(1I)	122.9(9)	H(10D)-C(10C)-H(10E)	109.5
N(2)-C(1)-C(1I)	116.1(9)	C(10E)-C(10D)-C(10B)	113.6(15)
C(1)-N(2)-C(2A)	119.4(9)	C(10E)-C(10D)-H(10F)	108.8
C(1)-N(2)-H(2)	114(9)	C(10B)-C(10D)-H(10F)	108.8
C(2A)-N(2)-H(2)	118(9)	C(10E)-C(10D)-H(10G)	108.8
N(2)-C(2A)-C(2B)	110.7(9)	C(10B)-C(10D)-H(10G)	108.8
N(2)-C(2A)-C(2)	110.3(9)	H(10F)-C(10D)-H(10G)	107.7
C(2B)-C(2A)-C(2)	109.1(9)	C(10D)-C(10E)-H(10H)	109.7
N(2)-C(2A)-H(2A)	108.9	C(10D)-C(10E)-H(10I)	108
C(2B)-C(2A)-H(2A)	108.9	H(10H)-C(10E)-H(10I)	109.5
C(2)-C(2A)-H(2A)	108.9	C(10D)-C(10E)-H(10J)	110.8
C(2A)-C(2B)-C(2C)	113.2(9)	H(10H)-C(10E)-H(10J)	109.5
C(2A)-C(2B)-H(2B1)	108.9	H(10I)-C(10E)-H(10J)	109.5
C(2C)-C(2B)-H(2B1)	108.9	C(10)-O(10A)-C(4B)	118.2(8)
C(2A)-C(2B)-H(2B2)	108.9	O(10)-C(10)-O(10A)	123.7(10)
C(2C)-C(2B)-H(2B2)	108.9	O(10)-C(10)-C(10A)	122.9(10)
H(2B1)-C(2B)-H(2B2)	107.7	O(10A)-C(10)-C(10A)	113.4(9)
C(2E)-C(2C)-C(2D)	110.4(11)	H(1SA)-O(1S)-H(1SB)	112(10)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for viscosin (1). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1A)	95(16)	65(11)	140(20)	-27(12)	-39(15)	21(11)
C(1B)	66(10)	51(8)	69(9)	-3(7)	-7(8)	13(7)
C(1C)	97(13)	46(8)	55(8)	-9(6)	2(8)	5(8)
C(1D)	69(10)	45(7)	42(7)	-4(5)	2(6)	11(7)
C(1E)	60(8)	32(6)	36(6)	-1(5)	-7(5)	4(5)
C(1F)	34(6)	37(5)	34(5)	-3(4)	-1(5)	6(4)
C(1G)	34(6)	39(6)	29(5)	-1(4)	-2(4)	-3(5)
C(1H)	17(5)	40(5)	30(5)	0(4)	-5(4)	-8(4)
C(1I)	18(5)	38(5)	31(5)	-2(4)	1(4)	-6(4)
O(1A)	19(3)	51(4)	27(3)	0(3)	-4(3)	6(3)
C(1)	17(5)	45(6)	25(5)	-5(4)	-5(4)	3(4)
O(1)	21(3)	38(4)	27(3)	-3(3)	-1(3)	-7(3)
N(2)	23(4)	35(4)	34(4)	4(4)	4(4)	0(4)
C(2A)	17(5)	47(6)	31(5)	-6(4)	-6(4)	-8(4)
C(2B)	22(5)	46(6)	36(5)	-6(5)	5(4)	12(4)
C(2C)	31(6)	48(6)	41(6)	-3(5)	1(5)	3(5)
C(2D)	41(7)	54(7)	57(8)	-6(6)	17(6)	14(6)
C(2E)	48(8)	59(8)	55(8)	7(6)	9(6)	12(6)
C(2)	10(4)	35(5)	33(5)	1(4)	1(4)	-1(4)
O(2)	22(3)	51(4)	21(3)	-2(3)	-4(3)	-2(3)
N(3)	18(4)	44(5)	21(4)	-1(3)	-6(3)	3(3)
C(3A)	16(5)	39(5)	31(5)	2(4)	-1(4)	-3(4)
C(3B)	22(5)	38(5)	30(5)	-3(4)	-8(4)	-4(4)
C(3C)	27(5)	50(6)	28(5)	9(5)	3(4)	6(5)
C(3D)	22(5)	43(6)	37(6)	2(5)	6(4)	12(4)
O(3A)	45(5)	62(5)	38(4)	9(4)	6(4)	12(4)
O(3B)	78(7)	75(7)	34(4)	20(4)	16(5)	38(6)
C(3)	16(5)	37(5)	23(4)	6(4)	-4(4)	-1(4)
O(3)	15(3)	52(4)	30(4)	0(3)	-2(3)	1(3)
N(4)	14(4)	36(4)	27(4)	5(3)	-3(3)	7(3)
C(4A)	9(4)	35(5)	29(5)	2(4)	6(3)	-4(4)

C(4B)	22(5)	40(5)	28(5)	0(4)	-4(4)	10(4)
C(4C)	36(6)	42(6)	45(6)	-4(5)	-10(5)	14(5)
C(4)	8(4)	36(5)	41(5)	1(4)	2(4)	0(4)
O(4)	18(4)	49(4)	27(3)	0(3)	-2(3)	5(3)
N(5)	10(4)	44(5)	23(4)	2(3)	-4(3)	-4(3)
C(5A)	18(5)	42(6)	30(5)	1(4)	3(4)	-1(4)
C(5B)	16(5)	60(7)	34(5)	-2(5)	9(4)	2(5)
C(5C)	24(5)	62(7)	38(6)	6(5)	6(5)	-10(5)
C(5D)	34(7)	80(9)	38(6)	-3(6)	8(5)	-8(6)
C(5)	15(5)	51(6)	27(5)	-1(4)	11(4)	3(4)
O(5)	27(4)	51(4)	27(4)	-6(3)	-4(3)	-1(3)
N(6)	18(4)	42(5)	26(4)	-8(4)	-5(3)	2(3)
C(6A)	16(5)	35(5)	26(5)	-2(4)	-1(4)	-1(4)
C(6B)	24(5)	46(6)	35(5)	0(5)	-4(4)	1(5)
C(6C)	21(5)	42(6)	48(6)	-6(5)	-7(4)	8(4)
C(6D)	23(6)	61(8)	53(7)	-7(6)	-10(5)	17(5)
C(6E)	31(6)	57(7)	57(7)	3(6)	-4(6)	5(6)
C(6)	17(5)	50(6)	21(4)	-1(4)	-3(4)	-7(4)
O(6)	20(3)	39(4)	39(4)	-2(3)	-2(3)	0(3)
N(7)	15(4)	44(5)	25(4)	-2(3)	-4(3)	2(3)
C(7A)	14(4)	44(5)	29(5)	2(4)	1(4)	0(4)
C(7B)	28(6)	49(6)	38(6)	-1(5)	-2(5)	2(5)
O(7A)	18(3)	50(4)	32(4)	-5(3)	-6(3)	6(3)
C(7)	20(5)	49(6)	30(5)	4(4)	-9(4)	-10(4)
O(7)	16(4)	61(5)	55(5)	9(4)	1(3)	2(4)
N(8)	11(4)	42(5)	32(4)	6(4)	-3(3)	1(3)
C(8A)	8(4)	42(5)	33(5)	2(4)	-4(4)	2(4)
C(8B)	28(5)	42(6)	31(5)	5(4)	3(4)	4(4)
C(8C)	30(6)	42(6)	34(5)	4(5)	2(4)	7(5)
C(8D)	39(7)	66(8)	36(6)	13(5)	1(5)	11(6)
C(8E)	33(6)	56(7)	42(6)	4(5)	4(5)	-2(5)
C(8)	25(5)	48(6)	23(4)	11(4)	0(4)	-4(5)
O(8)	24(4)	47(4)	42(4)	7(3)	-8(3)	-1(3)
N(9)	8(4)	51(5)	27(4)	3(4)	0(3)	10(3)
C(9A)	14(5)	48(6)	30(5)	-2(4)	0(4)	5(4)
C(9B)	36(6)	41(6)	35(5)	12(5)	11(5)	8(5)

O(9A)	48(5)	36(4)	33(4)	4(3)	-1(4)	5(4)
C(9)	16(5)	42(5)	31(5)	5(4)	2(4)	8(4)
O(9)	25(4)	54(5)	30(4)	-2(3)	3(3)	9(3)
N(10)	26(4)	42(5)	24(4)	2(3)	-1(3)	6(4)
C(10A)	31(6)	33(5)	27(5)	1(4)	-3(4)	-5(4)
C(10B)	33(6)	55(7)	43(6)	4(5)	-2(5)	-13(6)
C(10C)	32(7)	123(14)	41(7)	8(8)	8(6)	-11(8)
C(10D)	60(10)	89(12)	64(9)	23(8)	-11(8)	-50(9)
C(10E)	129(19)	52(9)	94(13)	14(9)	-48(13)	-39(10)
O(10A)	19(3)	37(4)	30(3)	1(3)	-4(3)	8(3)
C(10)	30(6)	36(5)	34(5)	0(4)	-3(4)	-5(4)
O(10)	30(4)	45(5)	74(6)	-7(4)	-15(4)	-3(4)
O(1S)	21(4)	48(5)	56(5)	14(4)	12(3)	10(3)

Table 5. Hydrogen coordinates and isotropic displacement parameters for viscosin (1).

	x	y	z	U(eq)
H(1A1)	0.7134	0.2867	0.4831	0.152
H(1A2)	0.7249	0.2036	0.4782	0.152
H(1A3)	0.7351	0.2409	0.5355	0.152
H(1B1)	0.5867	0.1838	0.5255	0.074
H(1B2)	0.5656	0.2335	0.4737	0.074
H(1C1)	0.5868	0.2885	0.582	0.079
H(1C2)	0.4863	0.271	0.5553	0.079
H(1D1)	0.613	0.3766	0.5119	0.063
H(1D2)	0.5097	0.3608	0.4883	0.063
H(1E1)	0.4403	0.4059	0.5692	0.052
H(1E2)	0.5424	0.4175	0.5959	0.052
H(1F1)	0.4687	0.4947	0.5045	0.042
H(1F2)	0.5759	0.5023	0.5243	0.042
H(1G1)	0.4154	0.5415	0.5893	0.041
H(1G2)	0.5221	0.5475	0.6103	0.041
H(1H)	0.5519	0.6326	0.5379	0.035
H(1IA)	0.4044	0.6777	0.6118	0.035
H(1IB)	0.513	0.6729	0.6298	0.035
H(1AO)	0.441(9)	0.624(7)	0.475(3)	0.039
H(2)	0.428(10)	0.801(7)	0.638(2)	0.037
H(2A)	0.427	0.8859	0.5453	0.038
H(2B1)	0.4023	0.9292	0.6571	0.042
H(2B2)	0.317	0.9147	0.6155	0.042
H(2C)	0.4548	1.0265	0.6005	0.048
H(2D1)	0.354	1.0489	0.676	0.076
H(2D2)	0.2661	1.0456	0.6369	0.076
H(2D3)	0.3401	1.1074	0.6306	0.076
H(2E1)	0.3563	1.0723	0.5311	0.081
H(2E2)	0.287	1.0077	0.5389	0.081
H(2E3)	0.3888	0.9948	0.5156	0.081
H(3)	0.578(9)	0.919(6)	0.511(2)	0.033
H(3A)	0.6911	0.9987	0.5703	0.034
H(3B1)	0.7885	0.9907	0.4906	0.036
H(3B2)	0.715	0.9356	0.4641	0.036
H(3C1)	0.596	1.0296	0.4723	0.042
H(3C2)	0.6809	1.0831	0.4864	0.042
H(3BO)	0.648(13)	1.116(10)	0.348(3)	0.075
H(4)	0.677(5)	0.815(6)	0.552(5)	0.031
H(4A)	0.8592	0.7836	0.5721	0.029

H(4B)	0.6943	0.694	0.5764	0.036
H(4C1)	0.7378	0.7261	0.4868	0.062
H(4C2)	0.7589	0.6446	0.4952	0.062
H(4C3)	0.8418	0.7002	0.4965	0.062
H(5)	0.674(7)	0.808(6)	0.651(4)	0.031
H(5A)	0.7478	0.7629	0.7513	0.037
H(5B)	0.5777	0.844	0.735	0.044
H(5C1)	0.5954	0.7013	0.7738	0.062
H(5C2)	0.5687	0.7206	0.7132	0.062
H(5C3)	0.4997	0.7402	0.7612	0.062
H(5D1)	0.6487	0.7992	0.8389	0.076
H(5D2)	0.5512	0.837	0.8296	0.076
H(5D3)	0.6454	0.879	0.8193	0.076
H(6)	0.725(8)	0.923(7)	0.686(3)	0.034
H(6A)	0.786	1.0094	0.7685	0.031
H(6B1)	0.775	1.0444	0.6549	0.042
H(6B2)	0.7921	1.1012	0.7029	0.042
H(6C)	0.6193	1.0229	0.6845	0.044
H(6D1)	0.5553	1.1356	0.6648	0.069
H(6D2)	0.6417	1.1215	0.6261	0.069
H(6D3)	0.6527	1.1725	0.6767	0.069
H(6E1)	0.6542	1.1159	0.7743	0.073
H(6E2)	0.6317	1.034	0.7784	0.073
H(6E3)	0.5537	1.0875	0.7584	0.073
H(7)	0.918(9)	0.923(5)	0.661(4)	0.034
H(7A)	1.0761	0.9922	0.6882	0.035
H(7B1)	1.0456	0.992	0.596	0.046
H(7B2)	1.1369	0.944	0.6075	0.046
H(7AO)	1.054(9)	0.847(5)	0.602(5)	0.04
H(8)	0.978(4)	0.850(7)	0.731(5)	0.034
H(8A)	1.1288	0.7936	0.7825	0.033
H(8B1)	0.9781	0.7878	0.822	0.041
H(8B2)	0.9401	0.7386	0.7733	0.041
H(8C)	1.0429	0.6439	0.8048	0.043
H(8D1)	1.151	0.7179	0.855	0.07
H(8D2)	1.1129	0.6557	0.892	0.07
H(8D3)	1.0727	0.7333	0.8989	0.07
H(8E1)	0.9423	0.6169	0.882	0.065
H(8E2)	0.8834	0.6426	0.8313	0.065
H(8E3)	0.902	0.6949	0.8803	0.065
H(9)	1.005(6)	0.724(6)	0.671(5)	0.034
H(9A)	1.1409	0.6226	0.6511	0.037
H(9B1)	1.1982	0.7231	0.6072	0.045

H(9B2)	1.1629	0.6685	0.5609	0.045
H(9AO)	1.062(10)	0.735(7)	0.533(3)	0.047
H(10)	0.964(10)	0.586(7)	0.680(2)	0.037
H(10A)	0.8936	0.4999	0.6022	0.036
H(10B)	0.8833	0.4749	0.6964	0.052
H(10C)	0.7664	0.5275	0.75	0.099
H(10D)	0.7392	0.5796	0.7022	0.099
H(10E)	0.8386	0.5856	0.7302	0.099
H(10F)	0.7352	0.4183	0.6964	0.085
H(10G)	0.7002	0.4668	0.6464	0.085
H(10H)	0.7964	0.4078	0.5861	0.137
H(10I)	0.7489	0.348	0.6217	0.137
H(10J)	0.8539	0.3703	0.6329	0.137
H(1SA)	0.306(10)	0.746(5)	0.717(5)	0.05
H(1SB)	0.292(8)	0.828(6)	0.695(6)	0.05

Table 6. Torsion angles [°] for viscosin (1).

C(1A)-C(1B)-C(1C)-C(1D)	68(2)
C(1B)-C(1C)-C(1D)-C(1E)	-176.7(14)
C(1C)-C(1D)-C(1E)-C(1F)	176.0(13)
C(1D)-C(1E)-C(1F)-C(1G)	-172.9(11)
C(1E)-C(1F)-C(1G)-C(1H)	178.4(10)
C(1F)-C(1G)-C(1H)-O(1A)	68.4(12)
C(1F)-C(1G)-C(1H)-C(1I)	-172.3(9)
O(1A)-C(1H)-C(1I)-C(1)	-64.5(10)
C(1G)-C(1H)-C(1I)-C(1)	173.9(9)
C(1H)-C(1I)-C(1)-O(1)	-29.0(13)
C(1H)-C(1I)-C(1)-N(2)	152.1(9)
O(1)-C(1)-N(2)-C(2A)	2.7(14)
C(1I)-C(1)-N(2)-C(2A)	-178.4(8)
C(1)-N(2)-C(2A)-C(2B)	179.4(9)
C(1)-N(2)-C(2A)-C(2)	-59.7(12)
N(2)-C(2A)-C(2B)-C(2C)	-177.8(9)
C(2)-C(2A)-C(2B)-C(2C)	60.7(12)
C(2A)-C(2B)-C(2C)-C(2E)	63.0(13)
C(2A)-C(2B)-C(2C)-C(2D)	-172.8(10)
N(2)-C(2A)-C(2)-O(2)	-59.9(12)
C(2B)-C(2A)-C(2)-O(2)	61.9(13)
N(2)-C(2A)-C(2)-N(3)	122.6(10)
C(2B)-C(2A)-C(2)-N(3)	-115.6(10)
O(2)-C(2)-N(3)-C(3A)	2.2(15)
C(2A)-C(2)-N(3)-C(3A)	179.7(9)
C(2)-N(3)-C(3A)-C(3B)	178.2(9)
C(2)-N(3)-C(3A)-C(3)	55.1(12)
N(3)-C(3A)-C(3B)-C(3C)	62.6(11)
C(3)-C(3A)-C(3B)-C(3C)	-173.5(9)
C(3A)-C(3B)-C(3C)-C(3D)	-167.7(9)
C(3B)-C(3C)-C(3D)-O(3A)	6.0(17)
C(3B)-C(3C)-C(3D)-O(3B)	-173.9(11)
N(3)-C(3A)-C(3)-O(3)	-149.6(9)
C(3B)-C(3A)-C(3)-O(3)	86.6(11)
N(3)-C(3A)-C(3)-N(4)	30.0(12)
C(3B)-C(3A)-C(3)-N(4)	-93.7(10)
O(3)-C(3)-N(4)-C(4A)	0.1(14)
C(3A)-C(3)-N(4)-C(4A)	-179.5(8)
C(3)-N(4)-C(4A)-C(4)	64.5(11)
C(3)-N(4)-C(4A)-C(4B)	-171.9(8)
N(4)-C(4A)-C(4B)-O(10A)	-173.7(7)

C(4)-C(4A)-C(4B)-O(10A)	-49.5(10)
N(4)-C(4A)-C(4B)-C(4C)	67.4(10)
C(4)-C(4A)-C(4B)-C(4C)	-168.4(8)
N(4)-C(4A)-C(4)-O(4)	-139.7(10)
C(4B)-C(4A)-C(4)-O(4)	97.2(11)
N(4)-C(4A)-C(4)-N(5)	39.3(12)
C(4B)-C(4A)-C(4)-N(5)	-83.7(11)
O(4)-C(4)-N(5)-C(5A)	6.5(15)
C(4A)-C(4)-N(5)-C(5A)	-172.5(9)
C(4)-N(5)-C(5A)-C(5)	62.5(12)
C(4)-N(5)-C(5A)-C(5B)	-171.1(10)
N(5)-C(5A)-C(5B)-C(5C)	65.1(12)
C(5)-C(5A)-C(5B)-C(5C)	-170.9(9)
N(5)-C(5A)-C(5B)-C(5D)	-170.7(10)
C(5)-C(5A)-C(5B)-C(5D)	-46.6(14)
N(5)-C(5A)-C(5)-O(5)	-132.4(9)
C(5B)-C(5A)-C(5)-O(5)	102.4(11)
N(5)-C(5A)-C(5)-N(6)	49.4(12)
C(5B)-C(5A)-C(5)-N(6)	-75.9(11)
O(5)-C(5)-N(6)-C(6A)	-4.2(14)
C(5A)-C(5)-N(6)-C(6A)	174.0(8)
C(5)-N(6)-C(6A)-C(6B)	-174.7(9)
C(5)-N(6)-C(6A)-C(6)	61.7(12)
N(6)-C(6A)-C(6B)-C(6C)	58.4(12)
C(6)-C(6A)-C(6B)-C(6C)	-176.6(9)
C(6A)-C(6B)-C(6C)-C(6E)	52.8(14)
C(6A)-C(6B)-C(6C)-C(6D)	176.5(9)
N(6)-C(6A)-C(6)-O(6)	-148.2(9)
C(6B)-C(6A)-C(6)-O(6)	88.4(11)
N(6)-C(6A)-C(6)-N(7)	35.0(13)
C(6B)-C(6A)-C(6)-N(7)	-88.5(12)
O(6)-C(6)-N(7)-C(7A)	1.2(16)
C(6A)-C(6)-N(7)-C(7A)	177.9(9)
C(6)-N(7)-C(7A)-C(7B)	-139.7(10)
C(6)-N(7)-C(7A)-C(7)	95.3(12)
N(7)-C(7A)-C(7B)-O(7A)	-59.2(12)
C(7)-C(7A)-C(7B)-O(7A)	66.9(11)
N(7)-C(7A)-C(7)-O(7)	-178.1(10)
C(7B)-C(7A)-C(7)-O(7)	56.1(13)
N(7)-C(7A)-C(7)-N(8)	3.0(14)
C(7B)-C(7A)-C(7)-N(8)	-122.7(11)
O(7)-C(7)-N(8)-C(8A)	1.6(17)
C(7A)-C(7)-N(8)-C(8A)	-179.6(9)

C(7)-N(8)-C(8A)-C(8)	-68.4(12)
C(7)-N(8)-C(8A)-C(8B)	167.7(10)
N(8)-C(8A)-C(8B)-C(8C)	178.6(9)
C(8)-C(8A)-C(8B)-C(8C)	54.5(12)
C(8A)-C(8B)-C(8C)-C(8D)	66.9(12)
C(8A)-C(8B)-C(8C)-C(8E)	-172.6(10)
N(8)-C(8A)-C(8)-O(8)	132.4(10)
C(8B)-C(8A)-C(8)-O(8)	-106.8(11)
N(8)-C(8A)-C(8)-N(9)	-49.3(12)
C(8B)-C(8A)-C(8)-N(9)	71.5(11)
O(8)-C(8)-N(9)-C(9A)	-13.2(15)
C(8A)-C(8)-N(9)-C(9A)	168.6(9)
C(8)-N(9)-C(9A)-C(9B)	-83.7(12)
C(8)-N(9)-C(9A)-C(9)	152.0(9)
N(9)-C(9A)-C(9B)-O(9A)	-55.7(12)
C(9)-C(9A)-C(9B)-O(9A)	68.6(12)
N(9)-C(9A)-C(9)-O(9)	140.7(10)
C(9B)-C(9A)-C(9)-O(9)	15.9(14)
N(9)-C(9A)-C(9)-N(10)	-41.0(12)
C(9B)-C(9A)-C(9)-N(10)	-165.7(9)
O(9)-C(9)-N(10)-C(10A)	-5.9(16)
C(9A)-C(9)-N(10)-C(10A)	175.8(9)
C(9)-N(10)-C(10A)-C(10)	-64.9(12)
C(9)-N(10)-C(10A)-C(10B)	167.8(10)
N(10)-C(10A)-C(10B)-C(10C)	66.2(13)
C(10)-C(10A)-C(10B)-C(10C)	-59.1(13)
N(10)-C(10A)-C(10B)-C(10D)	-168.1(12)
C(10)-C(10A)-C(10B)-C(10D)	66.6(15)
C(10C)-C(10B)-C(10D)-C(10E)	-179.2(14)
C(10A)-C(10B)-C(10D)-C(10E)	55.0(18)
C(4C)-C(4B)-O(10A)-C(10)	-71.4(12)
C(4A)-C(4B)-O(10A)-C(10)	168.4(8)
C(4B)-O(10A)-C(10)-O(10)	-4.2(16)
C(4B)-O(10A)-C(10)-C(10A)	177.5(8)
N(10)-C(10A)-C(10)-O(10)	173.4(10)
C(10B)-C(10A)-C(10)-O(10)	-62.6(15)
N(10)-C(10A)-C(10)-O(10A)	-8.3(13)
C(10B)-C(10A)-C(10)-O(10A)	115.7(11)

Table 7. Hydrogen bonds for viscosin (1) [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O(1A)-H(1AO)...O(7A)#1	0.99(6)	1.89(7)	2.839(10)	160(12)
N(2)-H(2)...O(1S)	0.87(5)	2.04(8)	2.814(12)	149(13)
N(3)-H(3)...O(9)#1	0.87(5)	2.02(6)	2.856(11)	162(12)
O(3B)-H(3BO)...O(5)#2	0.99(6)	1.62(6)	2.612(11)	178(19)
N(4)-H(4)...O(1)	0.86(5)	2.08(5)	2.939(11)	169(11)
C(4C)-H(4C2)...O(10)	0.96	2.54	3.074(16)	114.9
N(5)-H(5)...O(2)	0.87(5)	2.26(9)	2.971(11)	140(10)
N(6)-H(6)...O(2)	0.87(5)	2.32(7)	3.117(10)	152(11)
C(6B)-H(6B2)...O(8)#3	0.99	2.42	3.280(14)	144.8
N(7)-H(7)...O(3)	0.87(5)	2.08(9)	2.807(11)	141(11)
O(7A)-H(7AO)...O(9A)	0.99(6)	1.94(11)	2.677(11)	129(10)
N(8)-H(8)...O(4)	0.87(5)	2.55(11)	3.018(11)	115(10)
N(8)-H(8)...O(5)	0.87(5)	2.43(8)	3.213(11)	150(11)
N(9)-H(9)...O(4)	0.87(5)	2.09(6)	2.926(10)	163(11)
O(9A)-H(9AO)...O(1)#4	0.99(6)	1.83(7)	2.791(10)	163(12)
N(10)-H(10)...O(6)#5	0.87(5)	2.21(9)	2.909(11)	138(11)
O(1S)-H(1SA)...O(8)#6	0.99(6)	1.93(9)	2.815(11)	148(13)
O(1S)-H(1SB)...O(7)#6	0.99(6)	1.83(8)	2.772(11)	157(13)

Symmetry transformations used to generate equivalent atoms:

#1 $x-1/2, -y+3/2, -z+1$ #2 $-x+3/2, -y+2, z-1/2$ #3 $-x+2, y+1/2, -z+3/2$

#4 $x+1/2, -y+3/2, -z+1$ #5 $-x+2, y-1/2, -z+3/2$ #6 $x-1, y, z$

Figure 3. ^1H NMR spectrum of serrawettin W2 (2) in $\text{DMSO-}d_6$ (600 MHz).

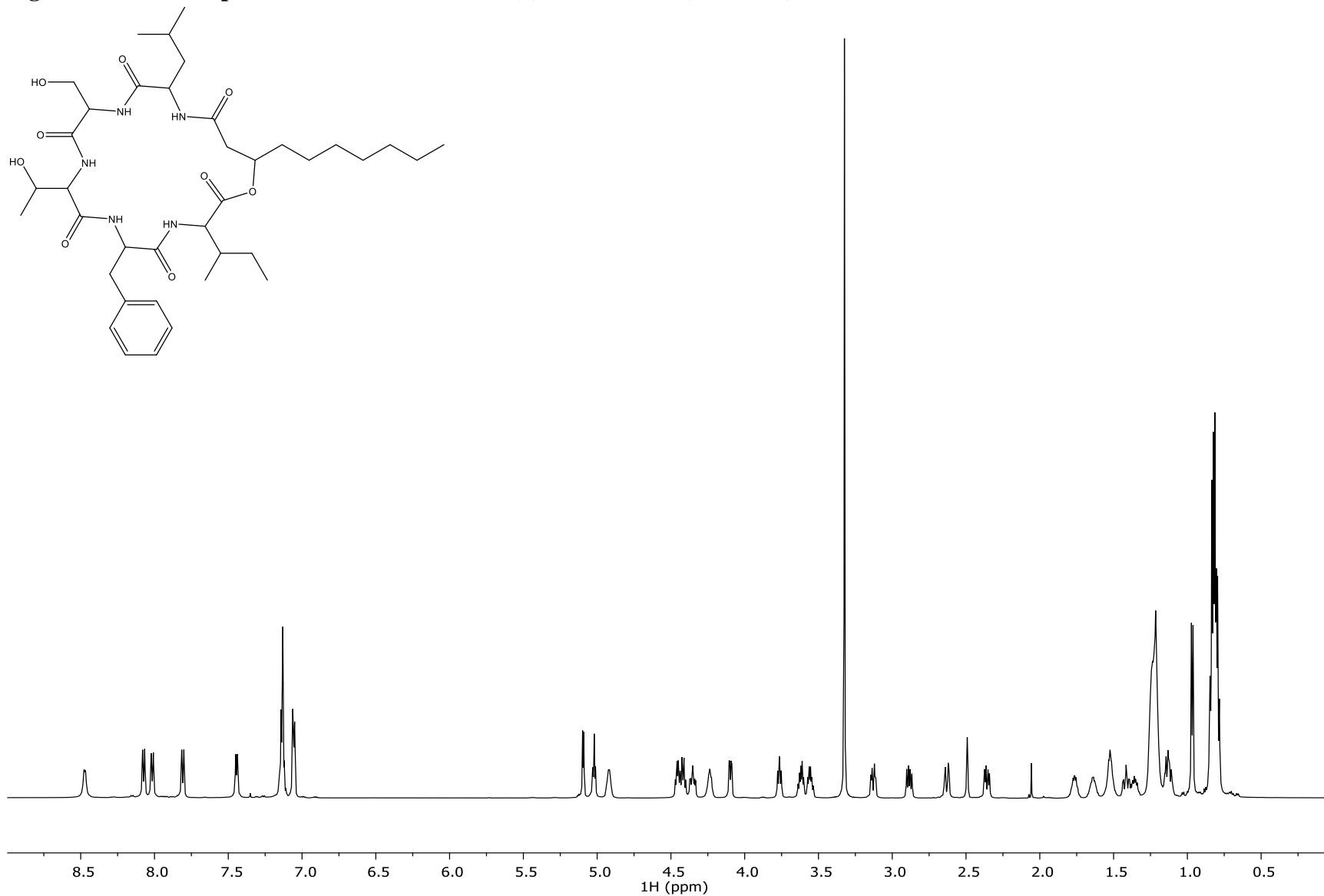


Figure 4. ^{13}C NMR spectrum of serrawettin W2 (2) in $\text{DMSO-}d_6$ (150 MHz).

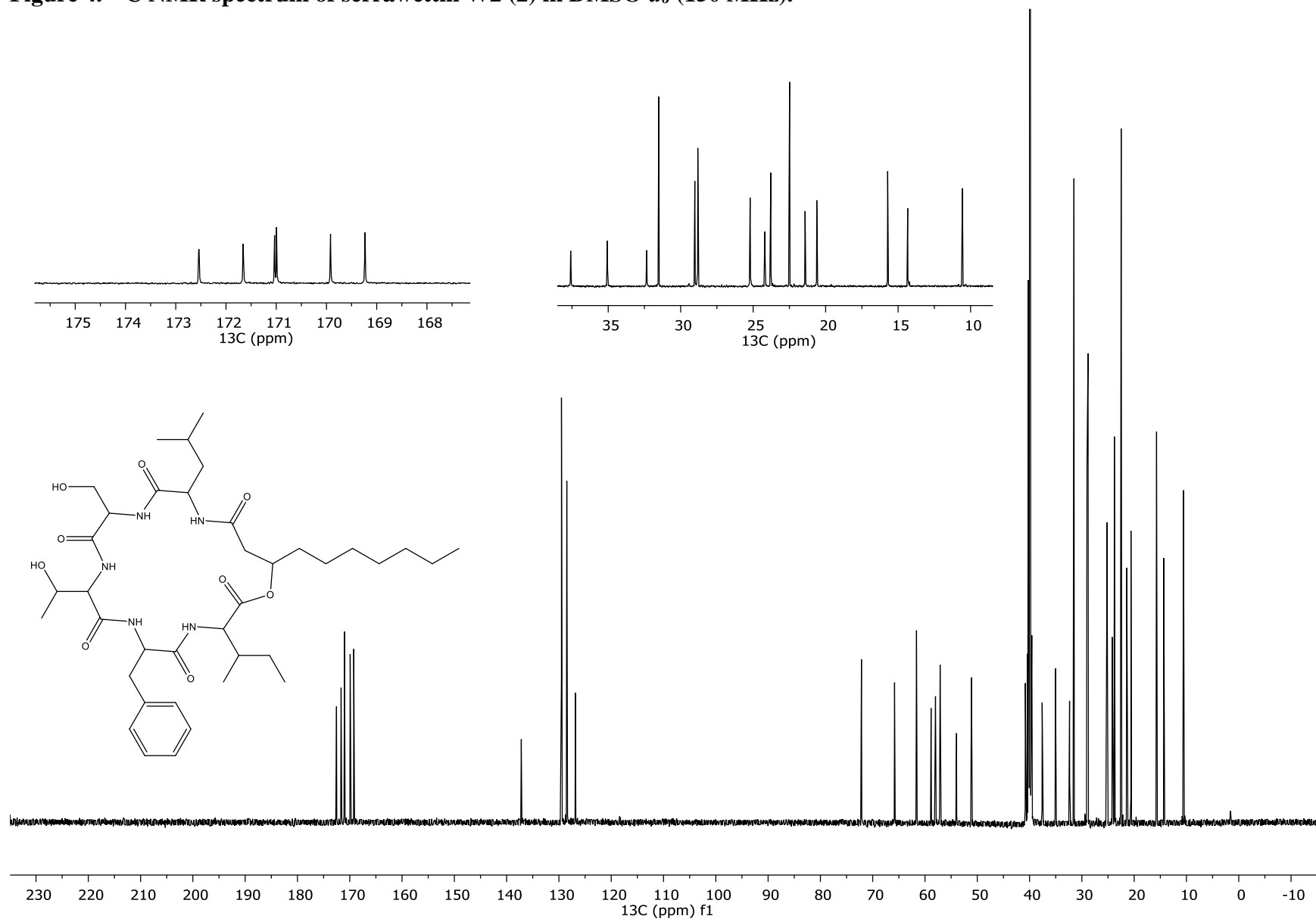


Figure 5. ^1H - ^{13}C HSQCTOCSY spectrum of serrawettin W2 (2) in $\text{DMSO-}d_6$.

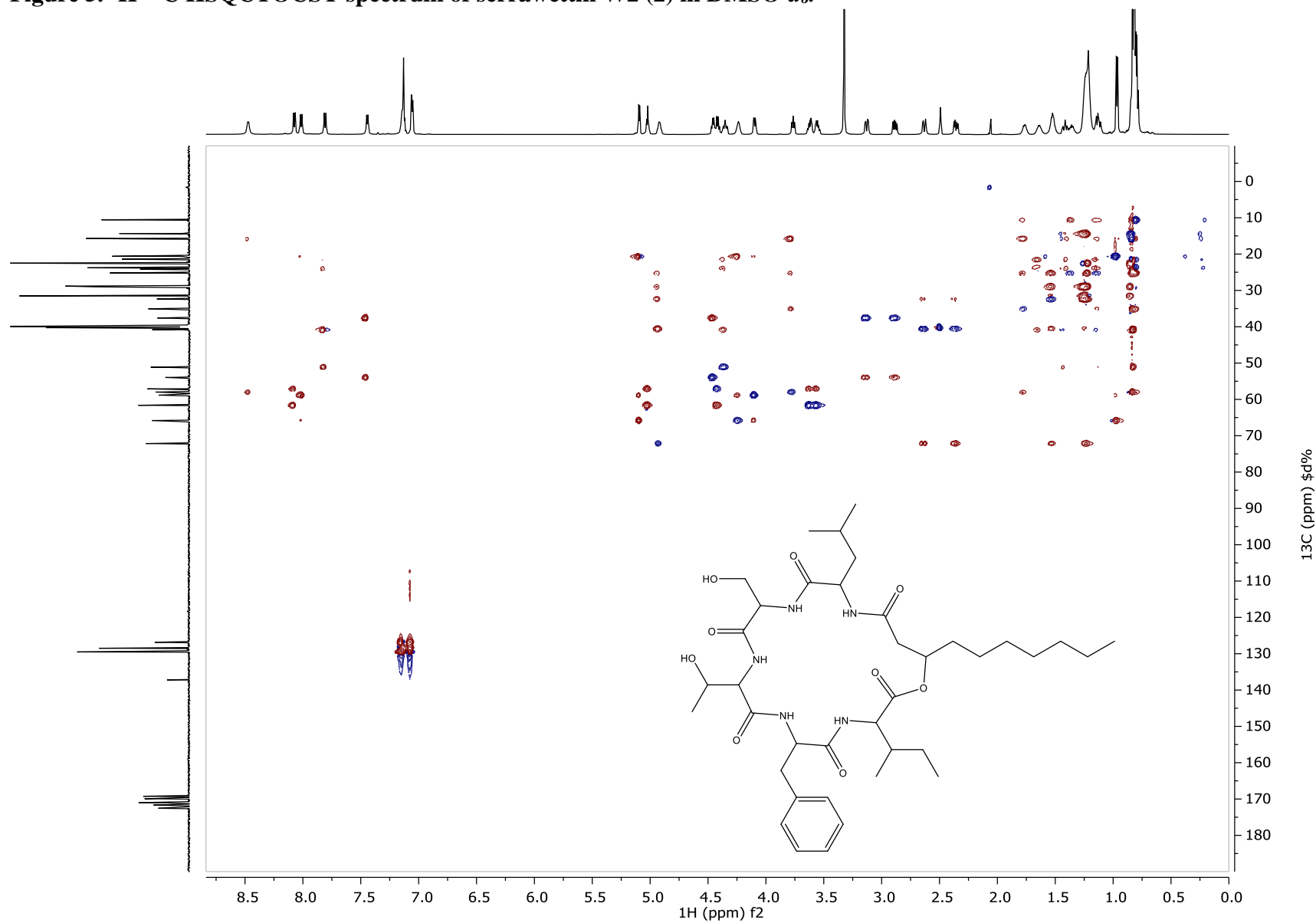


Figure 6. ^1H - ^{15}N HSQC spectrum of serrawettin W2 (2) in $\text{DMSO-}d_6$.

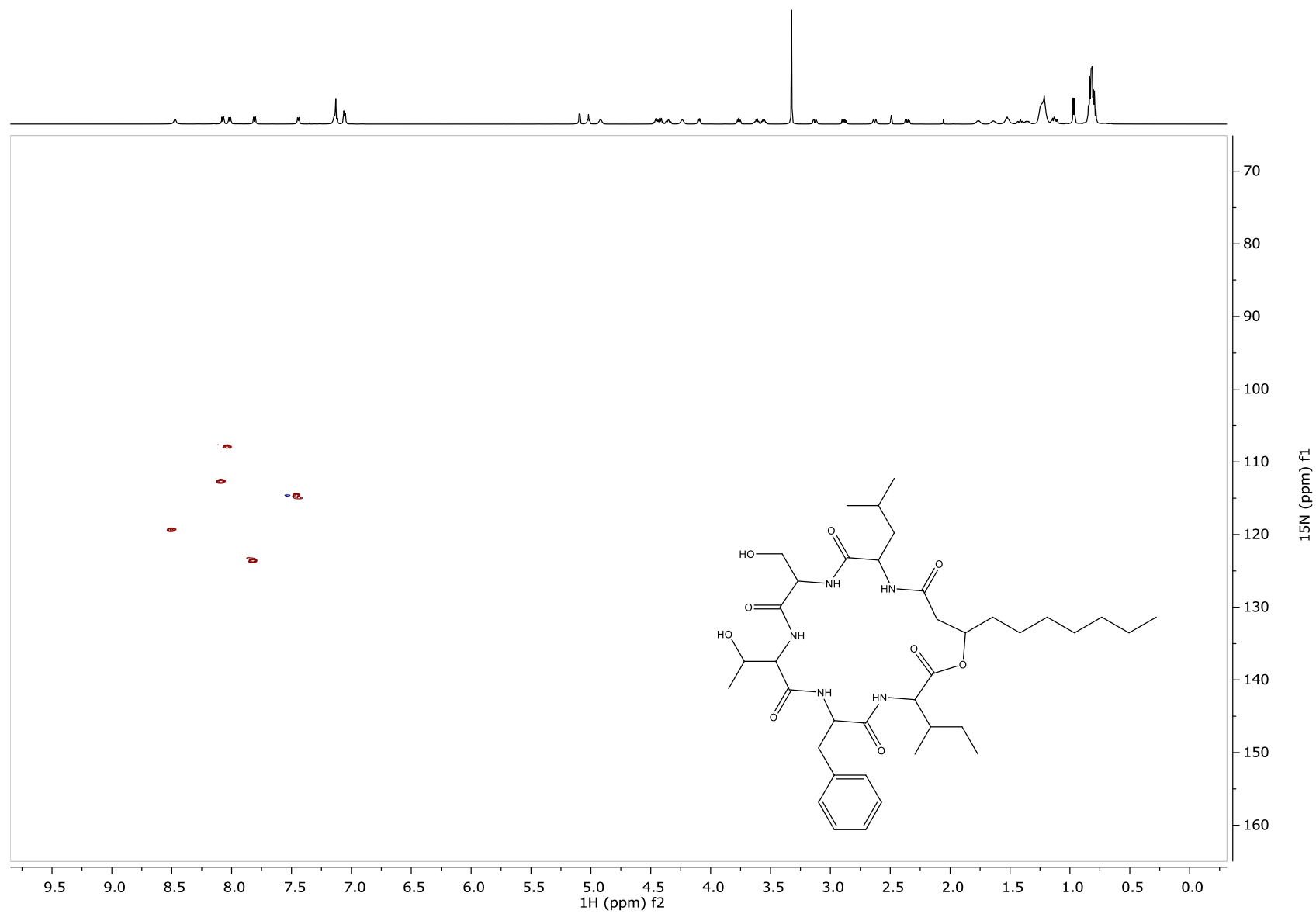


Figure 7. ^1H - ^{13}C HSQC spectrum of serrawettin W2 (2) in $\text{DMSO-}d_6$.

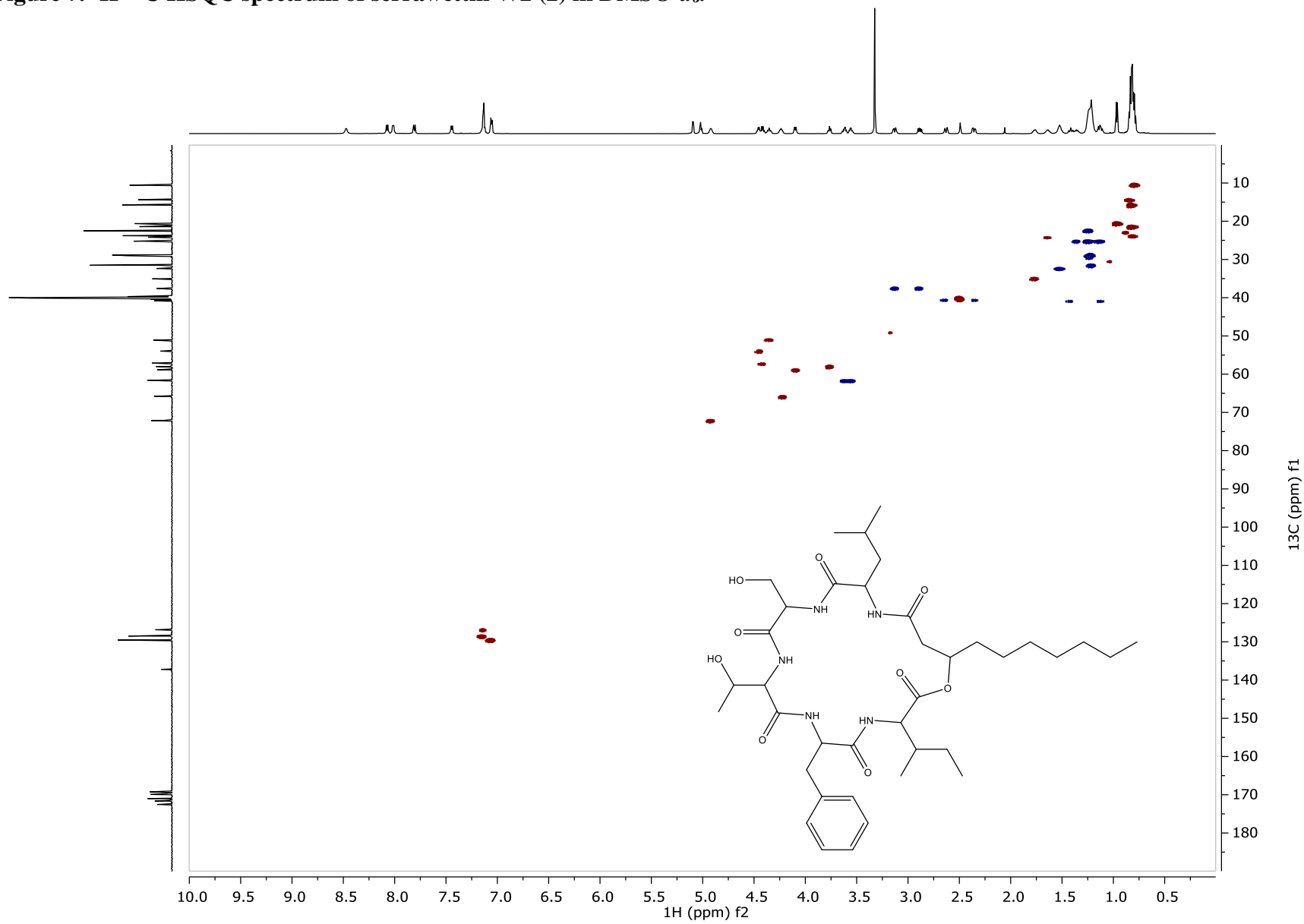


Figure 9. ^1H - ^1H TOCSY spectrum of serrawettin W2 (2) in $\text{DMSO-}d_6$.

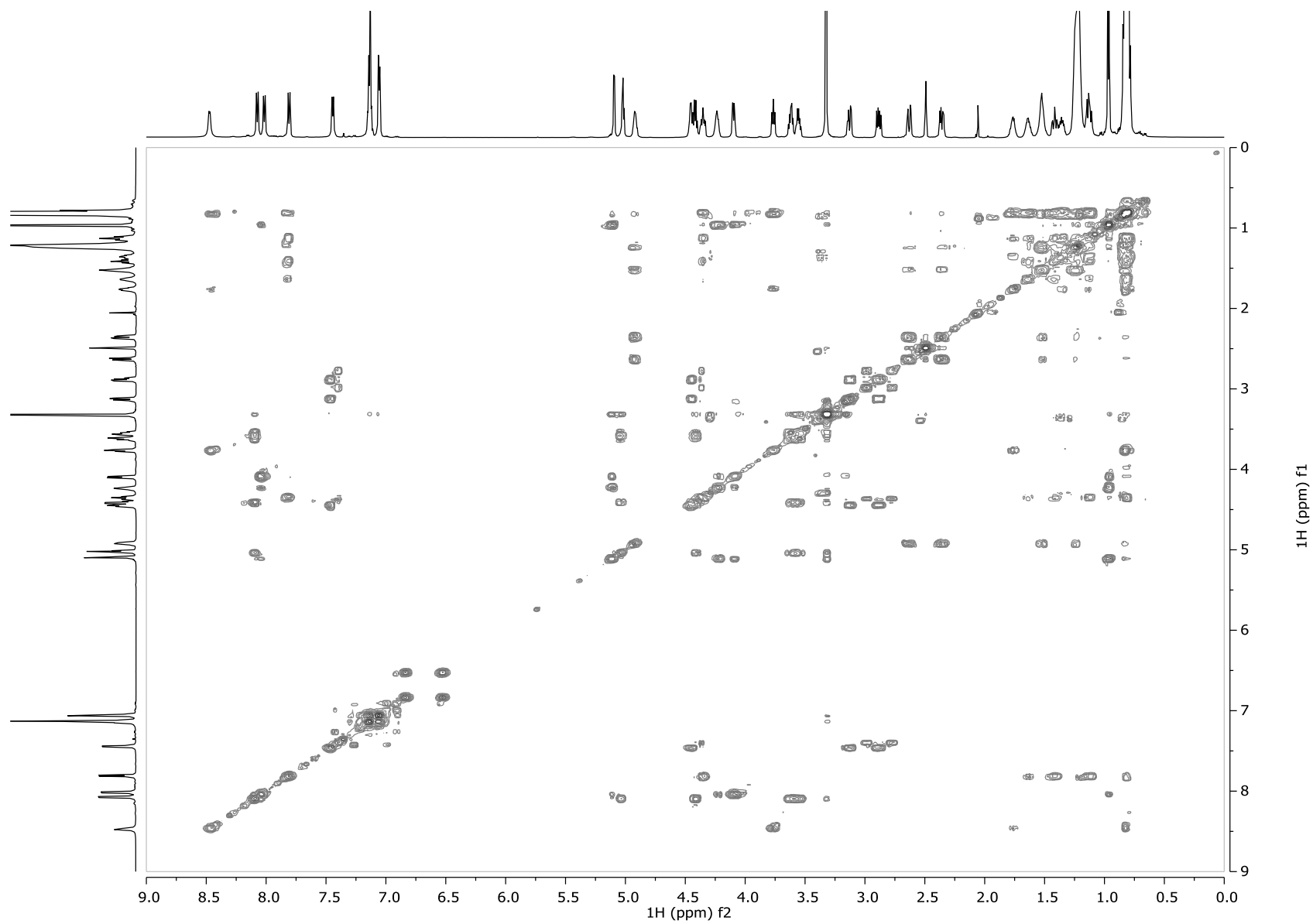


Figure 10. ^1H - ^{13}C HMBC spectrum of serrawettin W2 (2) in $\text{DMSO-}d_6$.

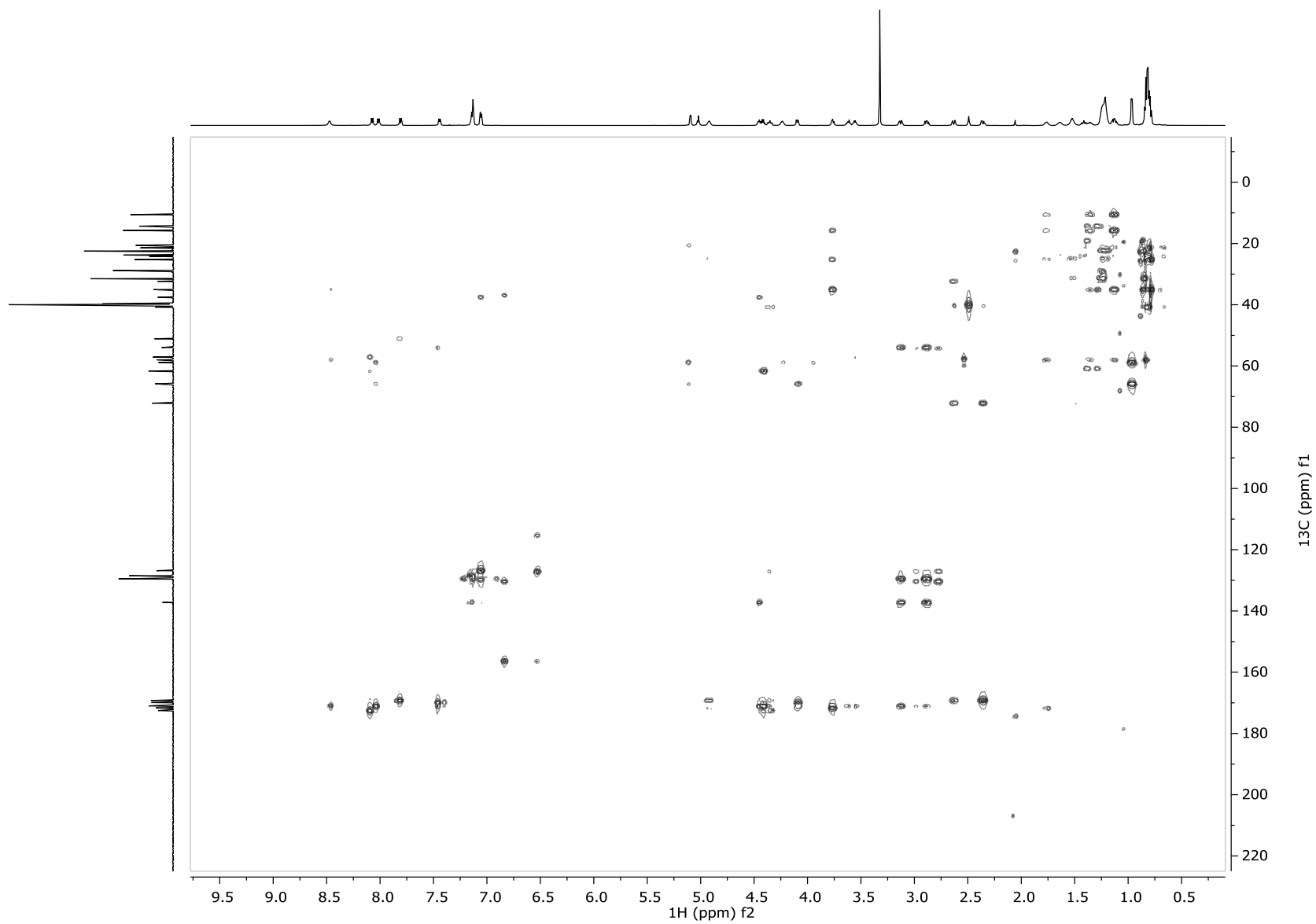


Figure 11. ^1H NMR spectrum of serrawettin W4 (3) in $\text{DMSO-}d_6$ (600 MHz).

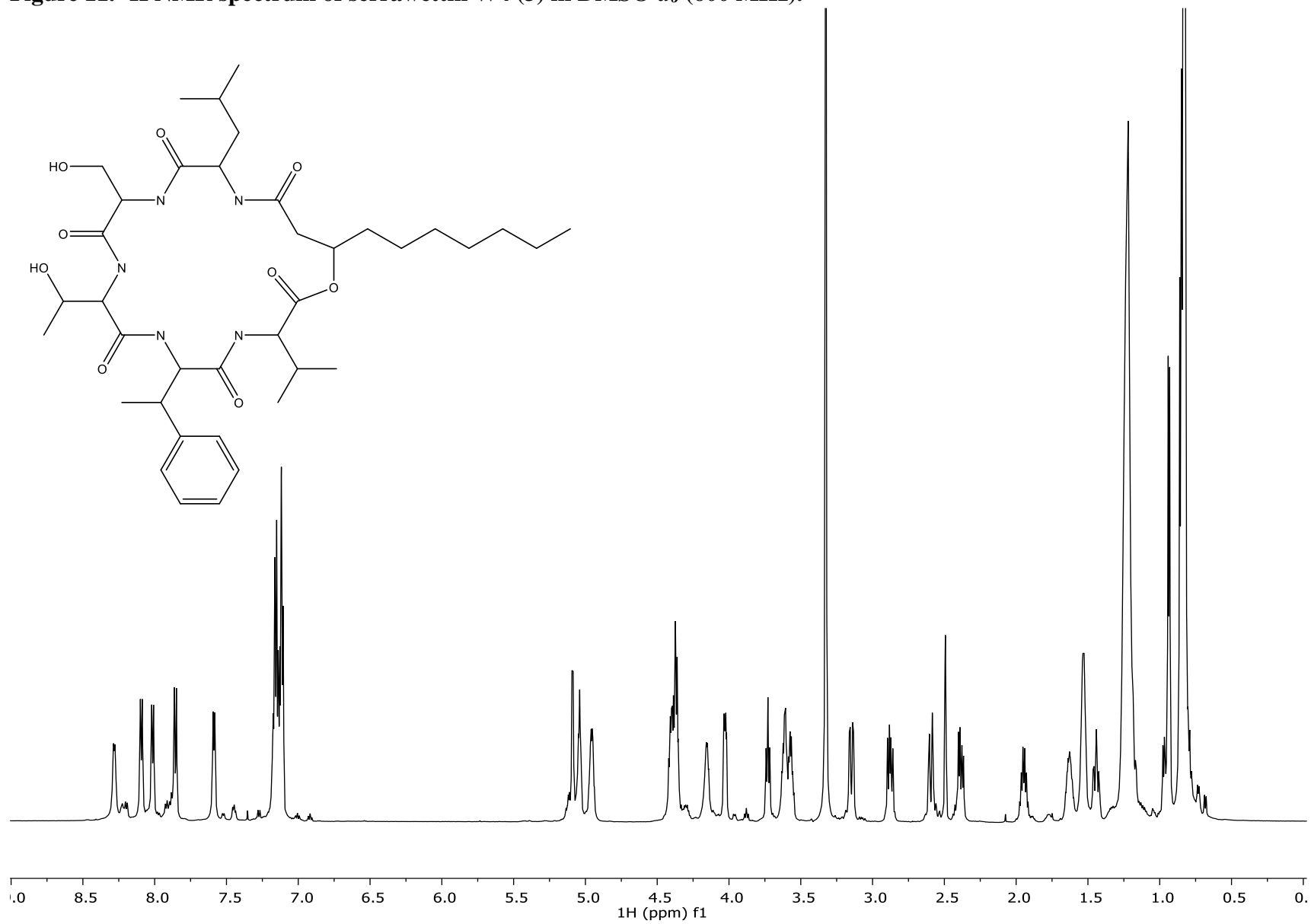


Figure 12. ^{13}C NMR spectrum of serrawettin W4 (3) in $\text{DMSO-}d_6$ (150 MHz).

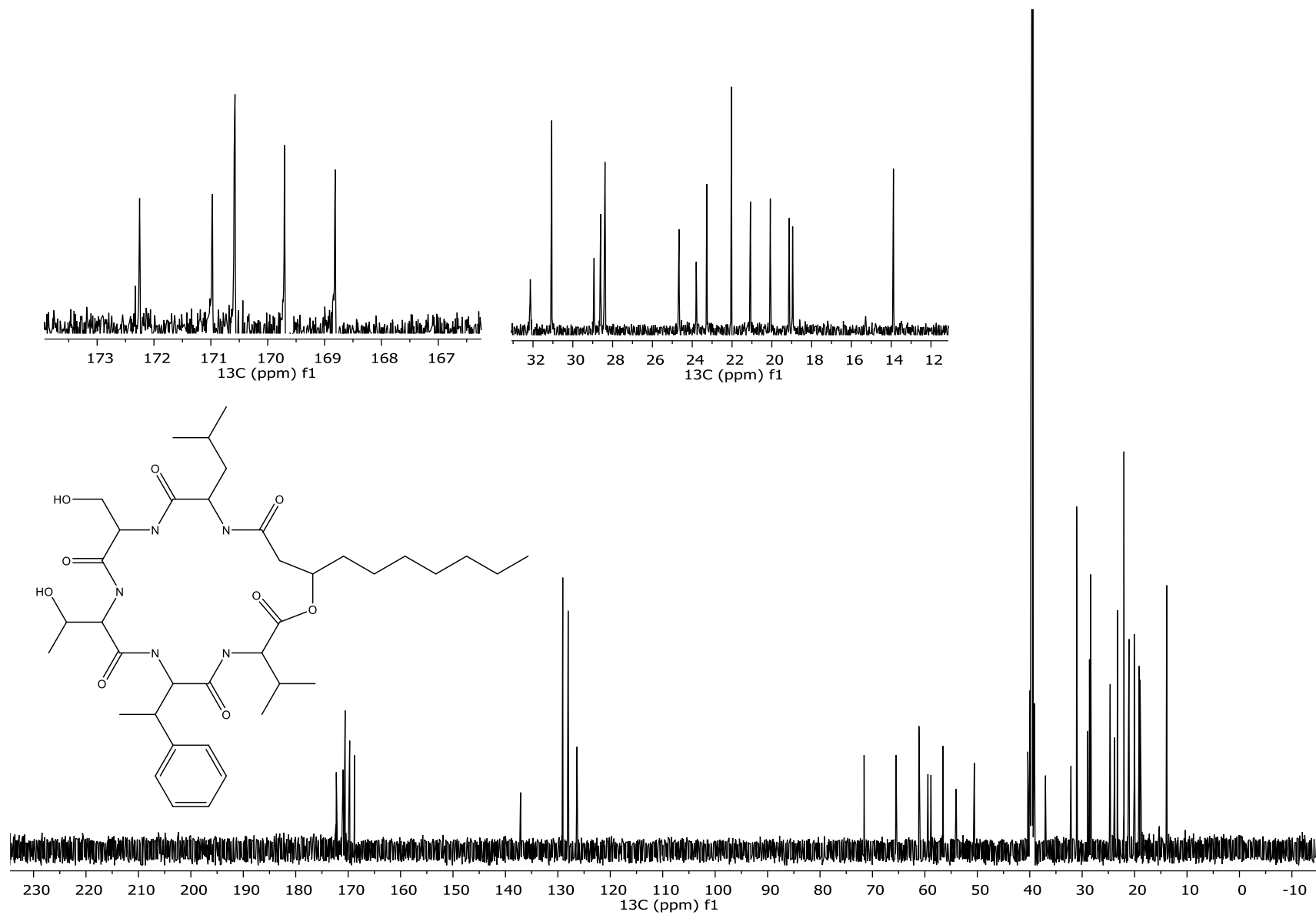


Figure 13. ^1H - ^{13}C HSQC spectrum of serrawettin W4 (3) in $\text{DMSO-}d_6$.

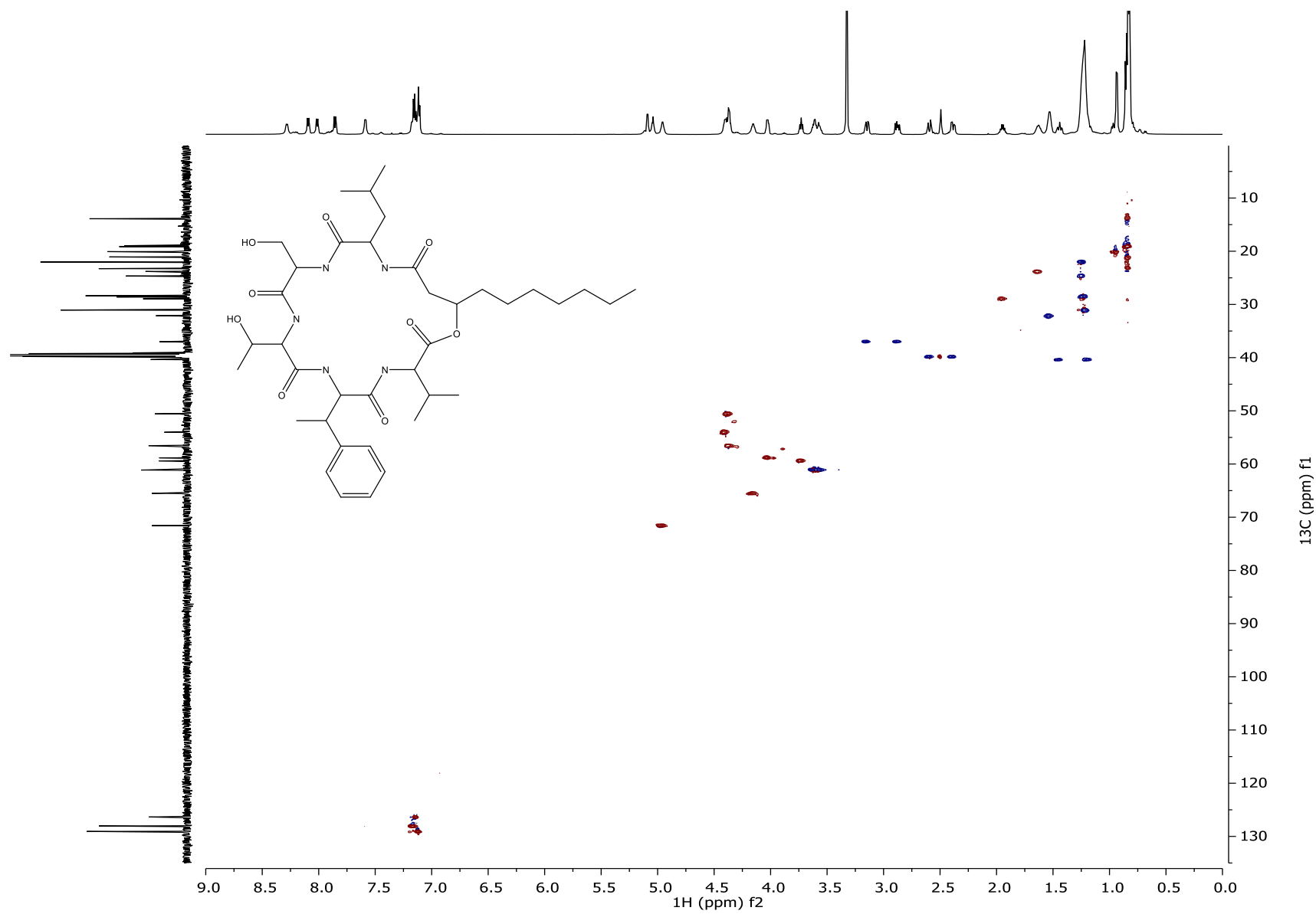


Figure 15. ^1H TOCSY spectrum of serrawettin W4 (3) in $\text{DMSO-}d_6$.

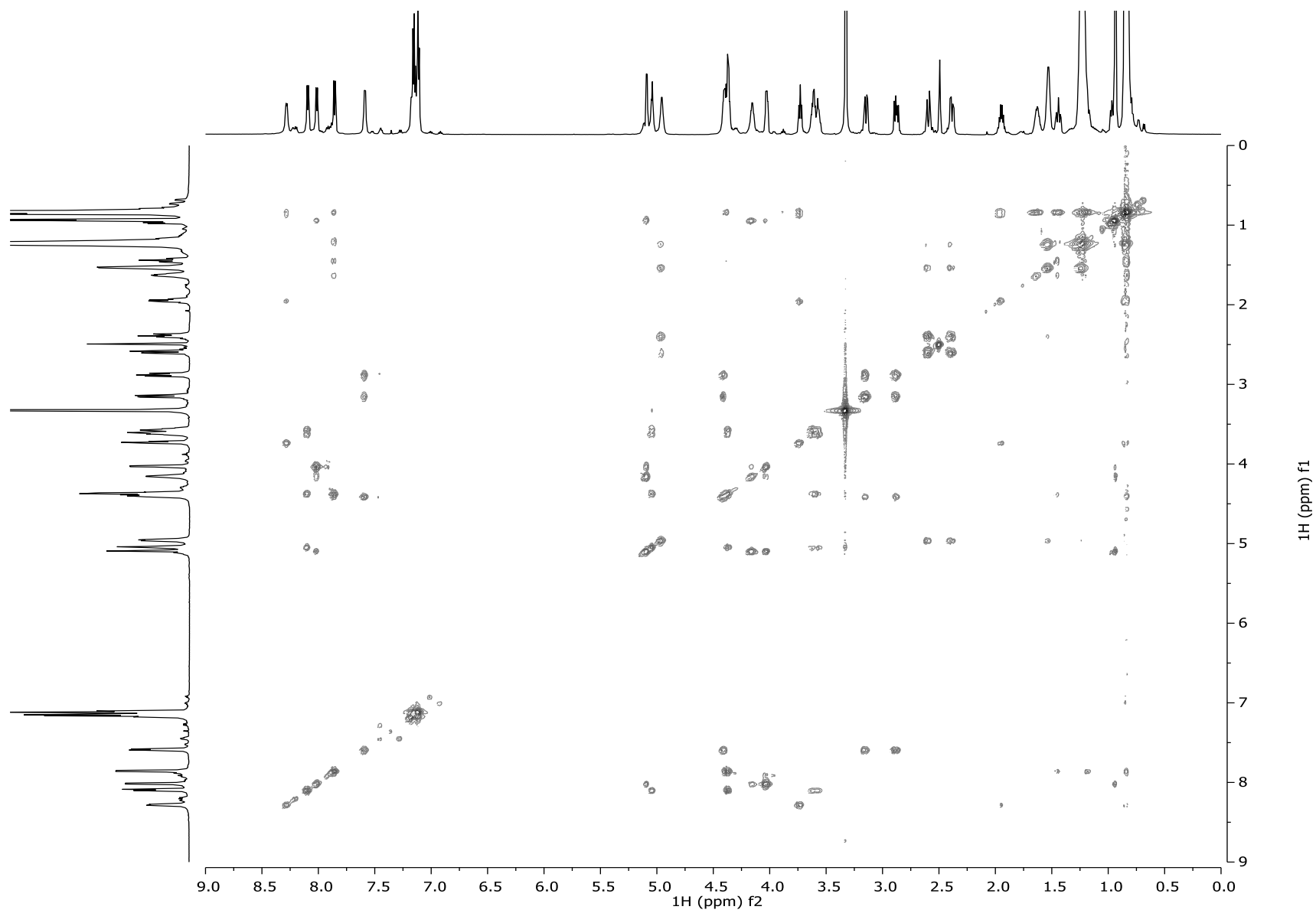


Figure 16. ^1H - ^{13}C HMBC spectrum of serrawettin W4 (3) in $\text{DMSO-}d_6$.

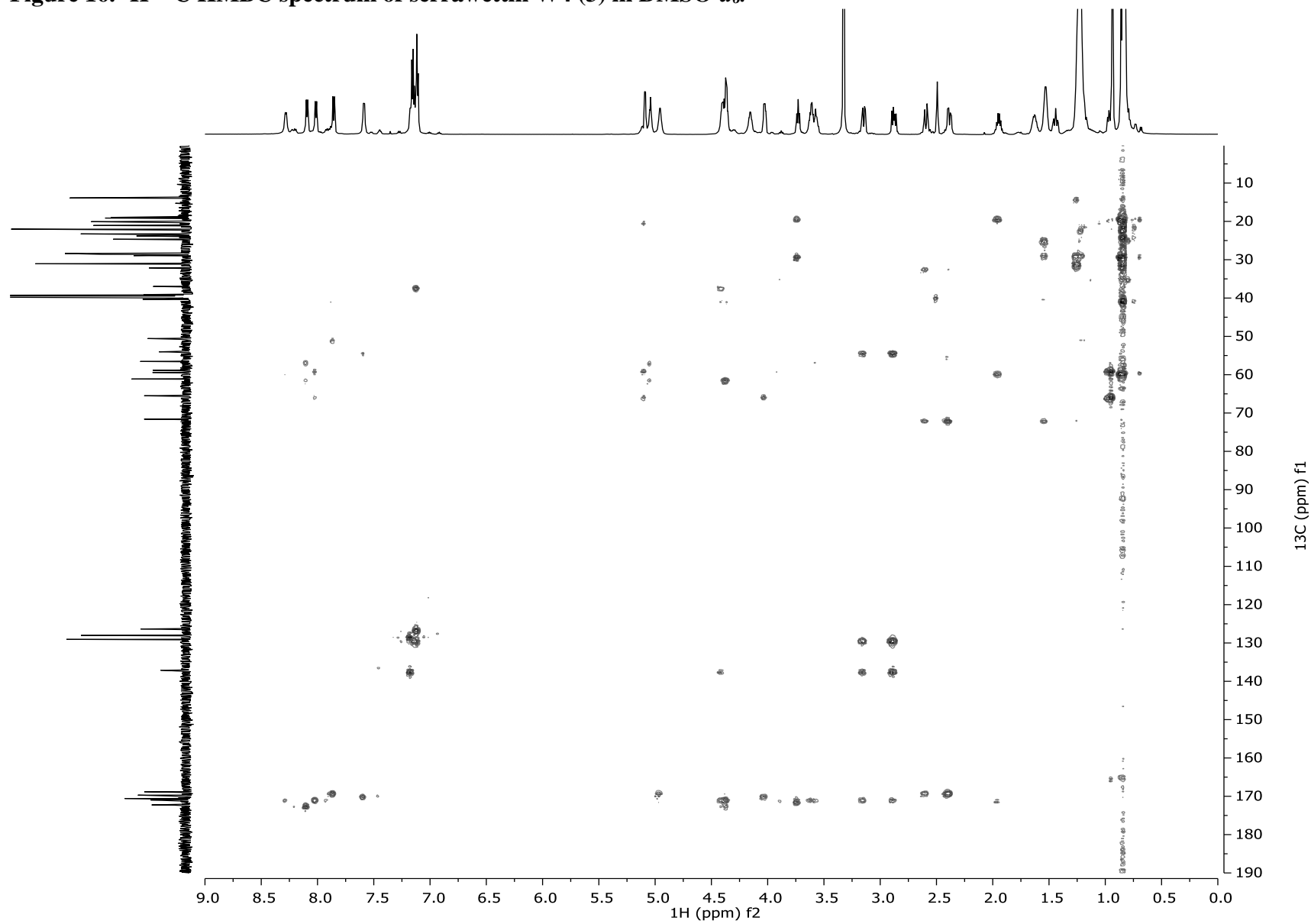


Figure 17. ^1H NMR spectrum of serrawettin W5 (4) in $\text{DMSO-}d_6$ (600 MHz).

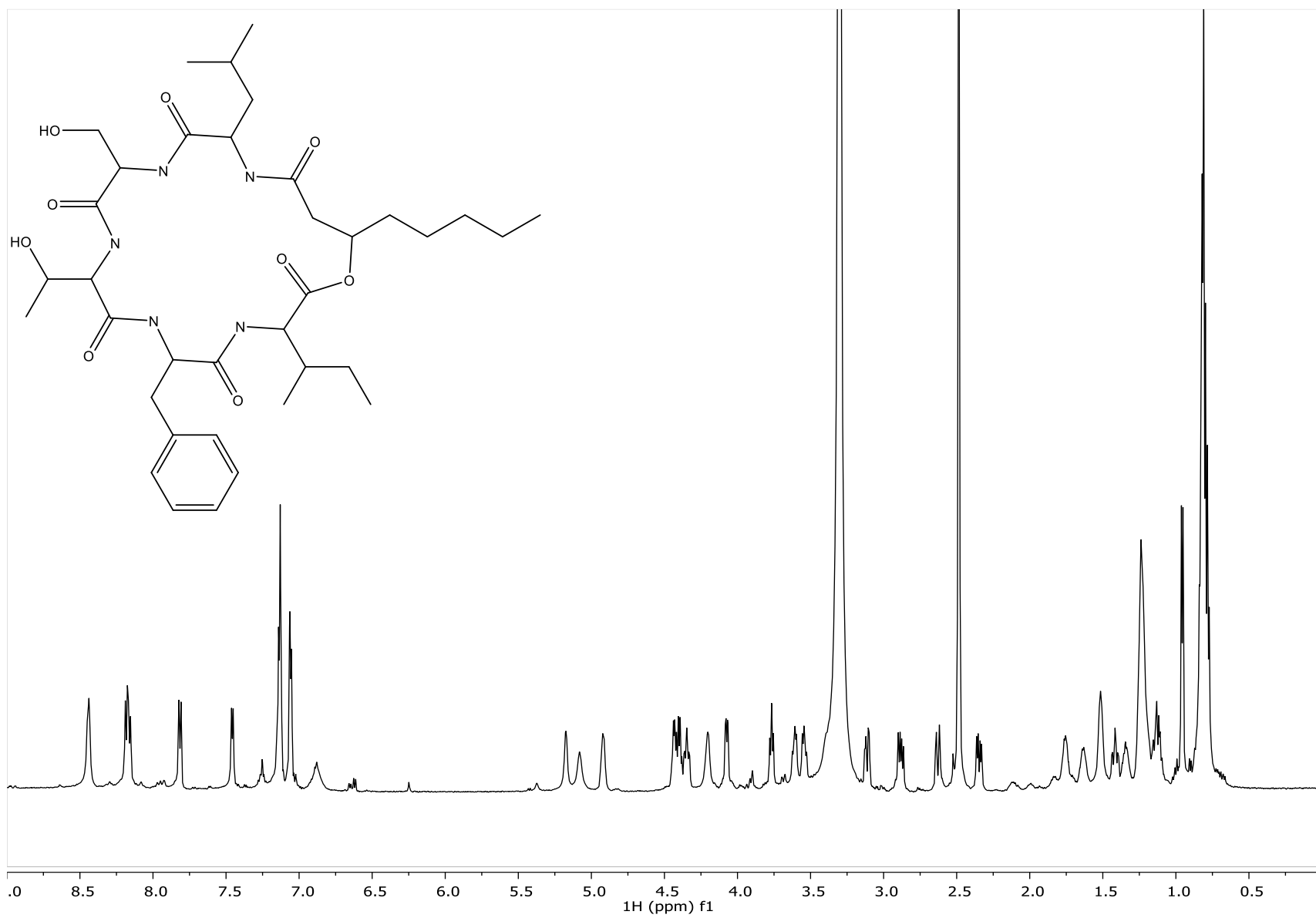


Figure 19. ^1H - ^{13}C HSQC spectrum of serrawettin W5 (4) in $\text{DMSO-}d_6$.

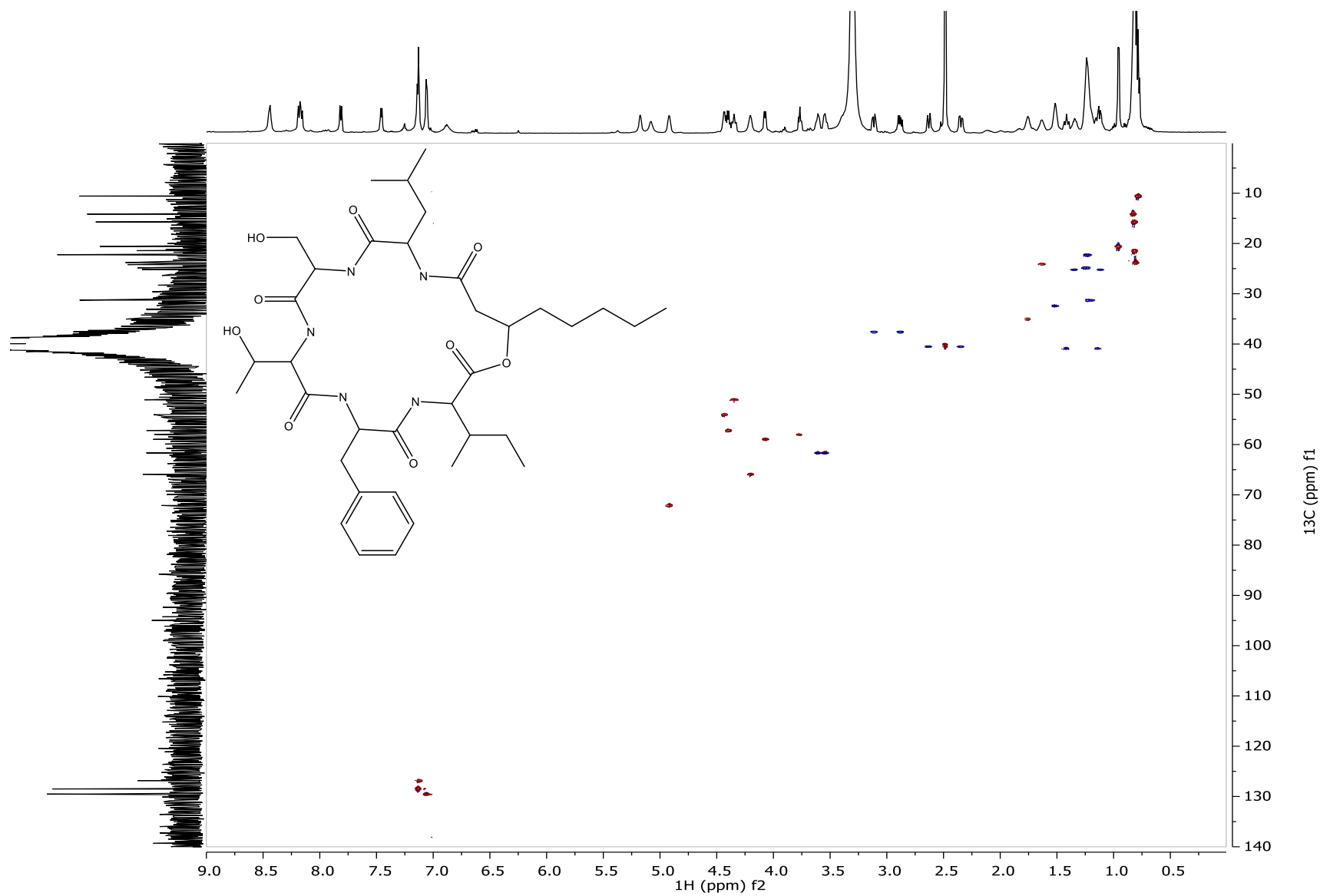


Figure 20. ^1H - ^1H dqfCOSY spectrum of serrawettin W5 (4) in $\text{DMSO-}d_6$.

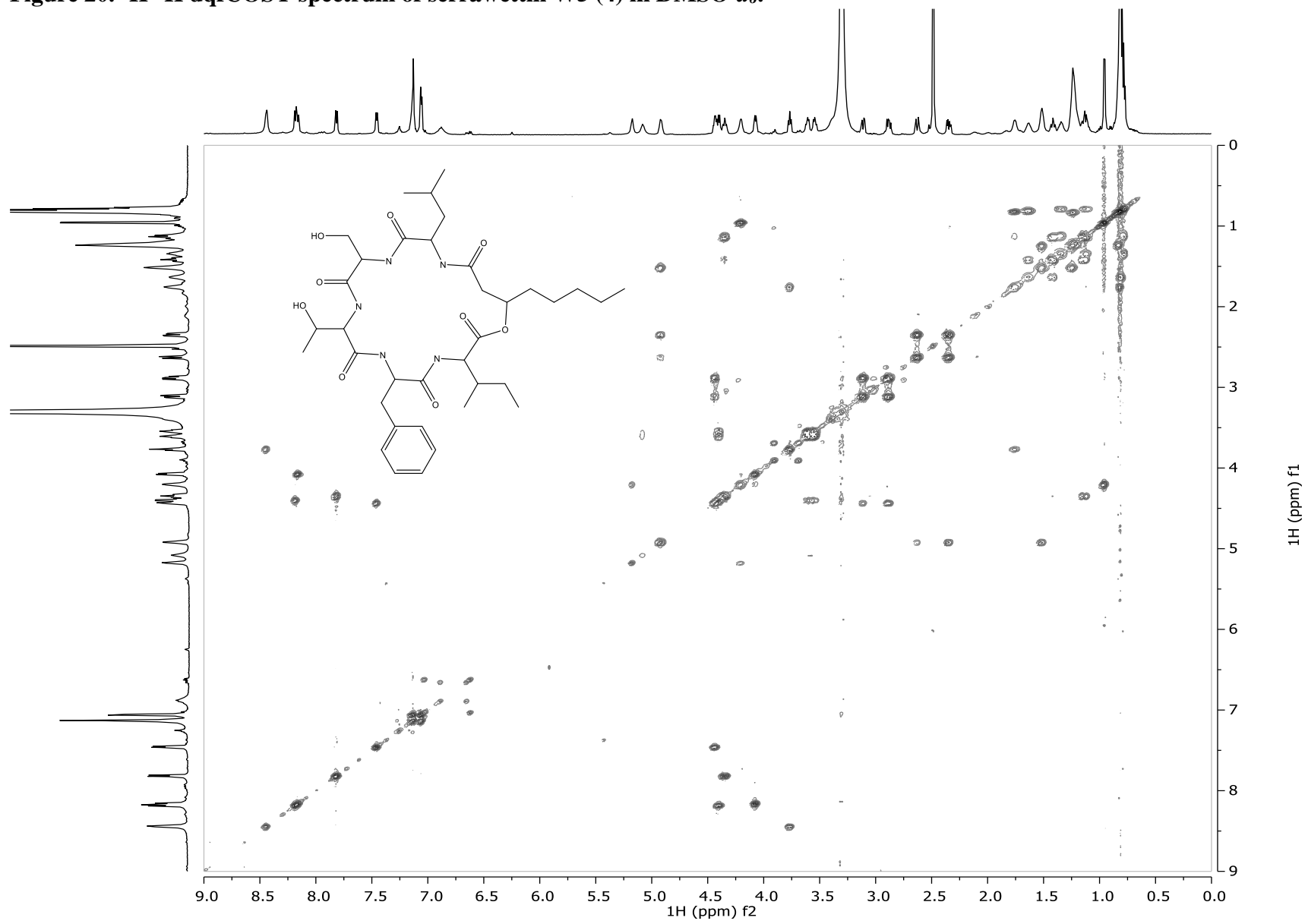


Figure 21. ^1H - ^1H TOCSY spectrum of serrawettin W5 (4) in $\text{DMSO-}d_6$.

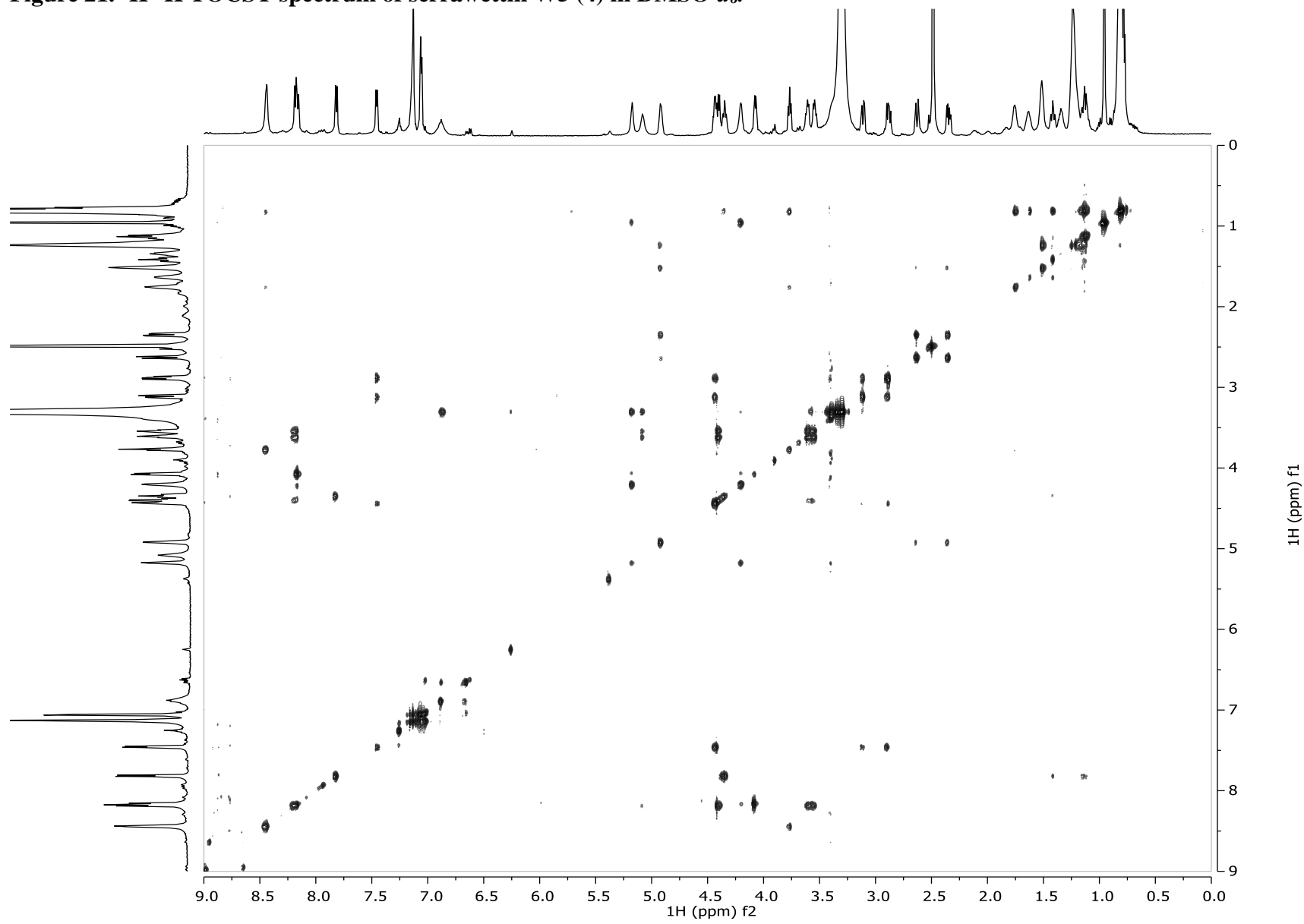


Figure 22. ^1H - ^{13}C HMBC spectrum of serrawettin W5 (4) in $\text{DMSO-}d_6$.

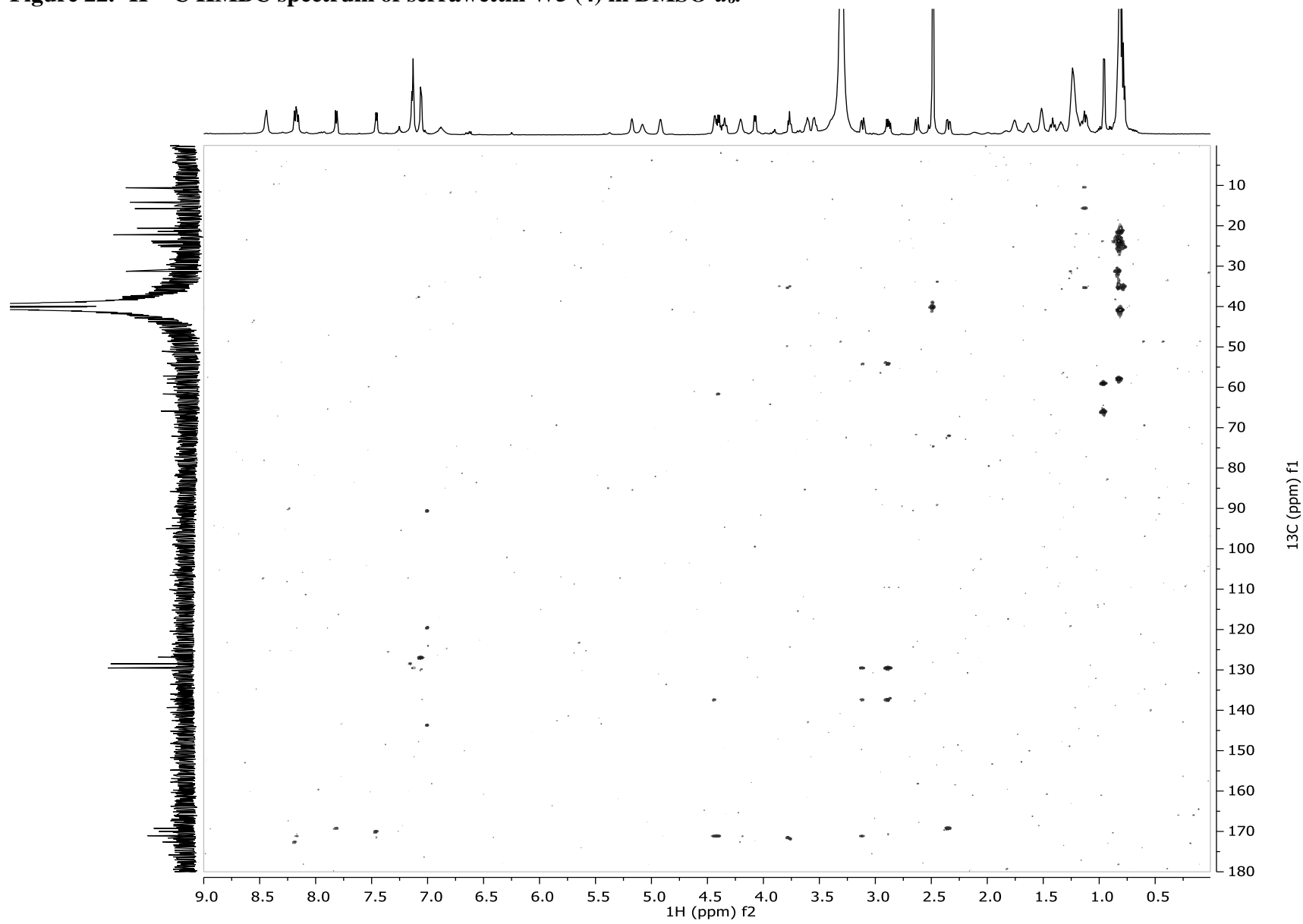


Figure 23. ^1H NMR spectrum of serrawettin W6 (5) in $\text{DMSO-}d_6$.

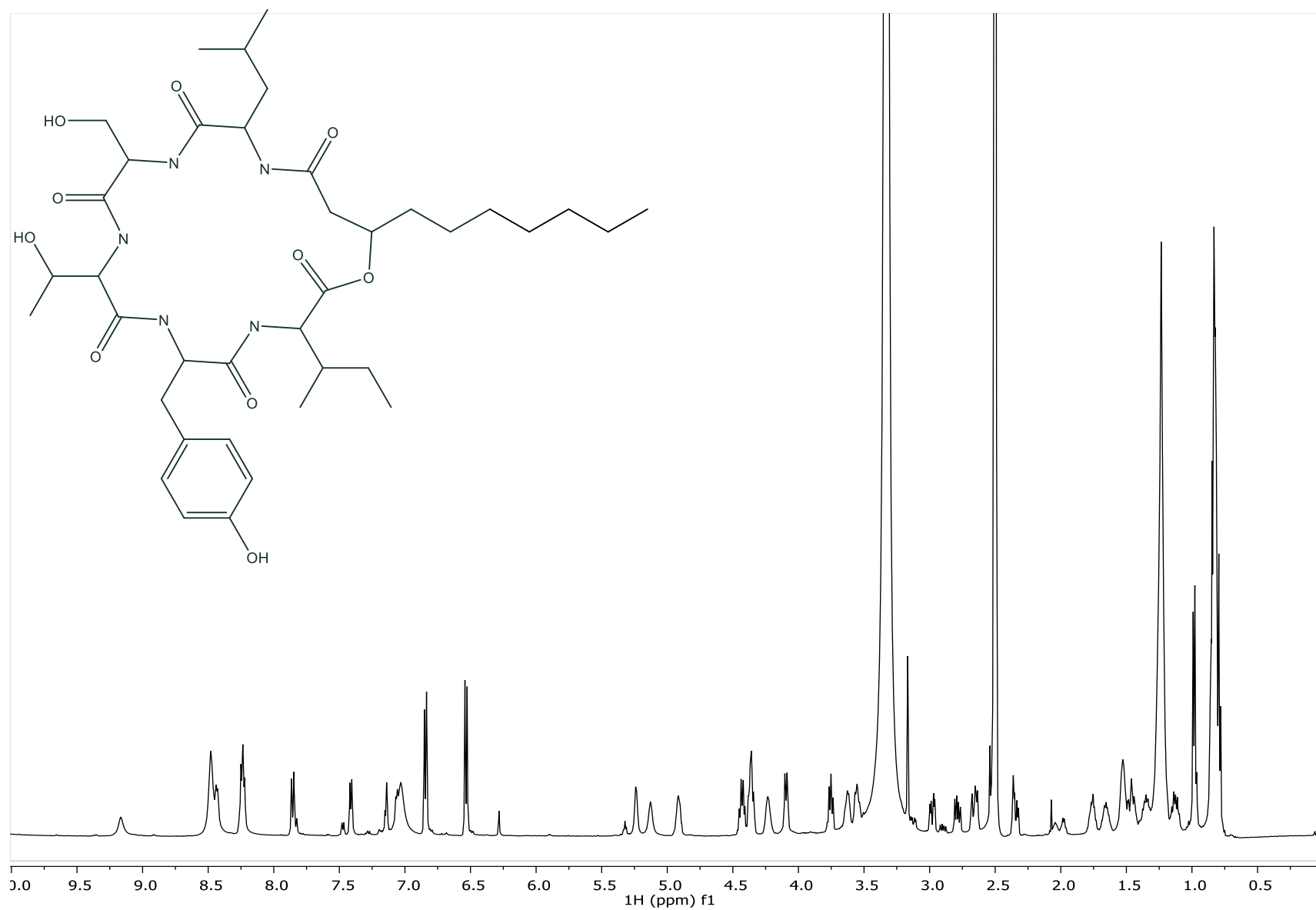


Figure 24. ^1H - ^{13}C HSQC spectrum of serrawettin W6 (5) in $\text{DMSO-}d_6$.

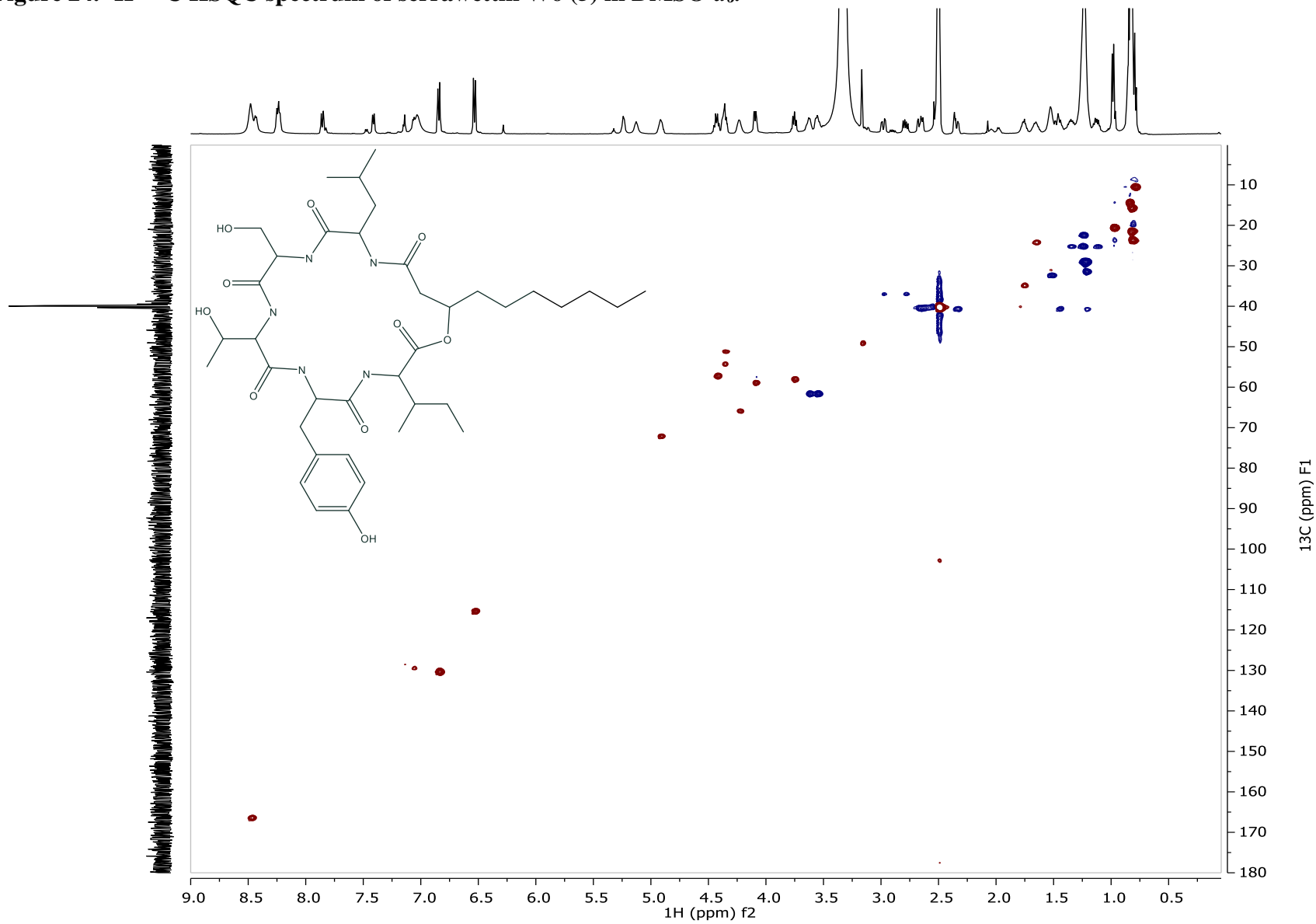


Figure 25. ^1H - ^1H dqfCOSY spectrum of serrawettin W6 (5) in $\text{DMSO-}d_6$.

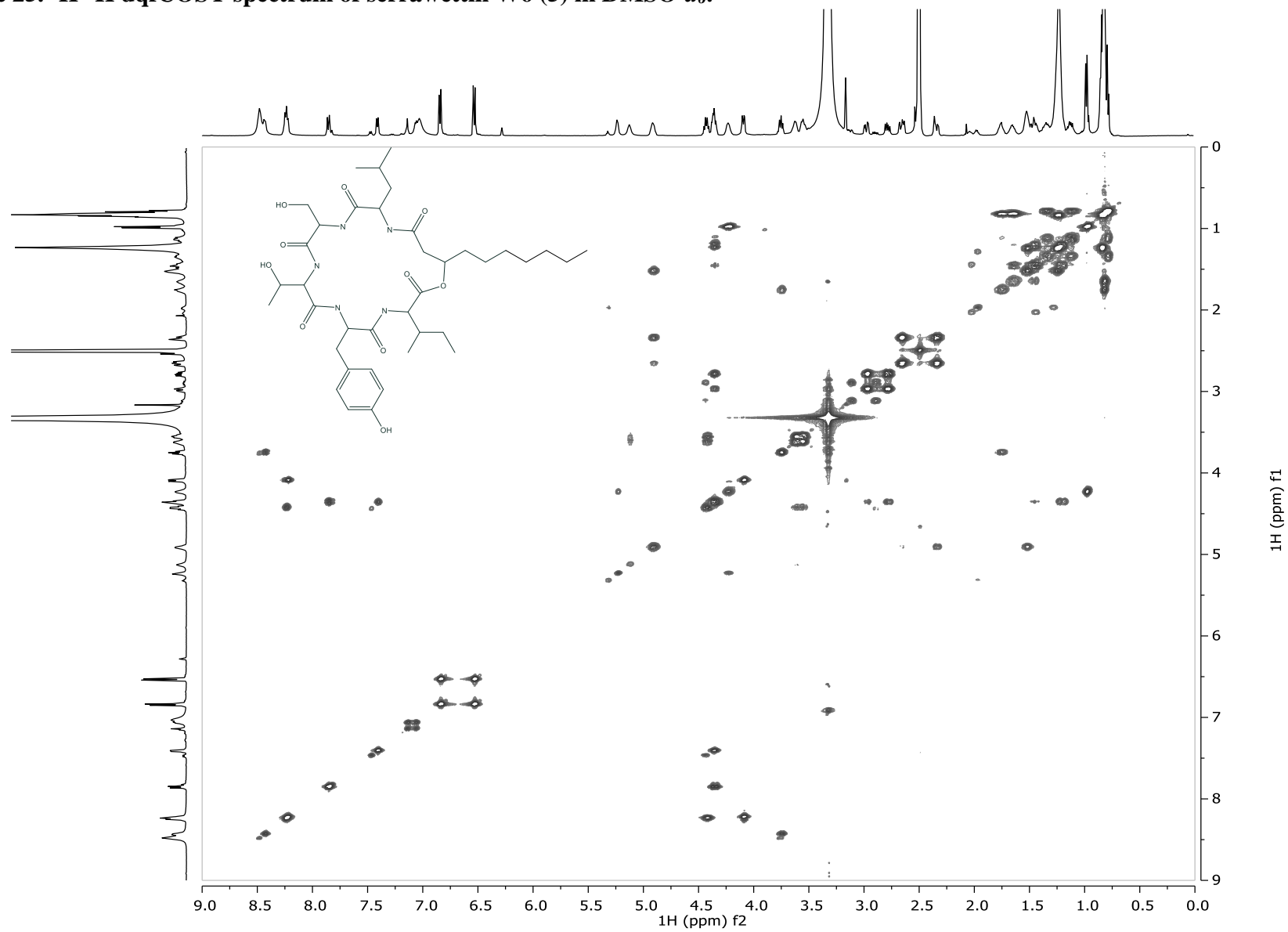


Figure 26. ^1H - ^1H TOCSY spectrum of serrawettin W6 (5) in $\text{DMSO-}d_6$.

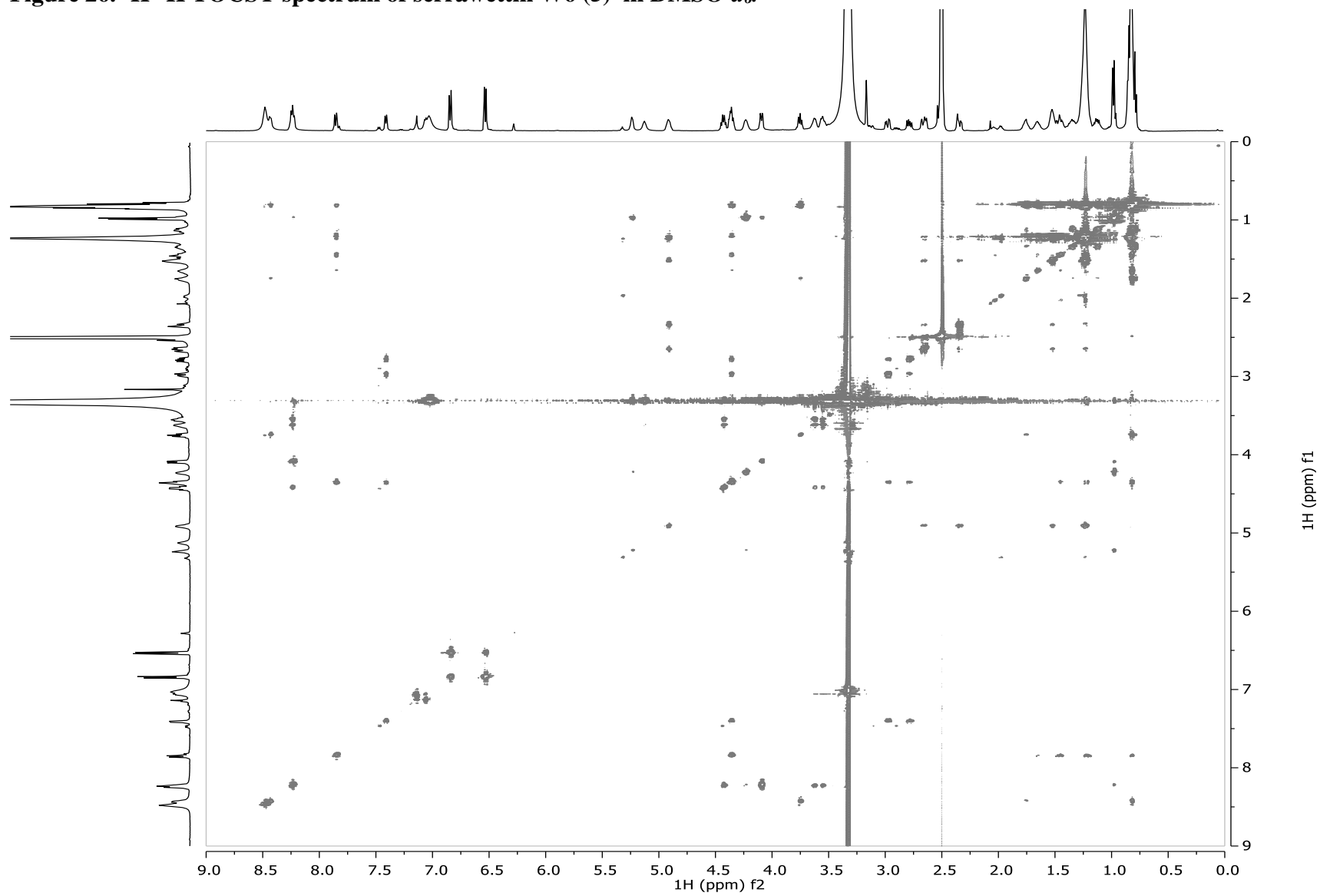


Figure 27. ^1H - ^{13}C HMBC spectrum of serrawettin W6 (5) in $\text{DMSO-}d_6$.

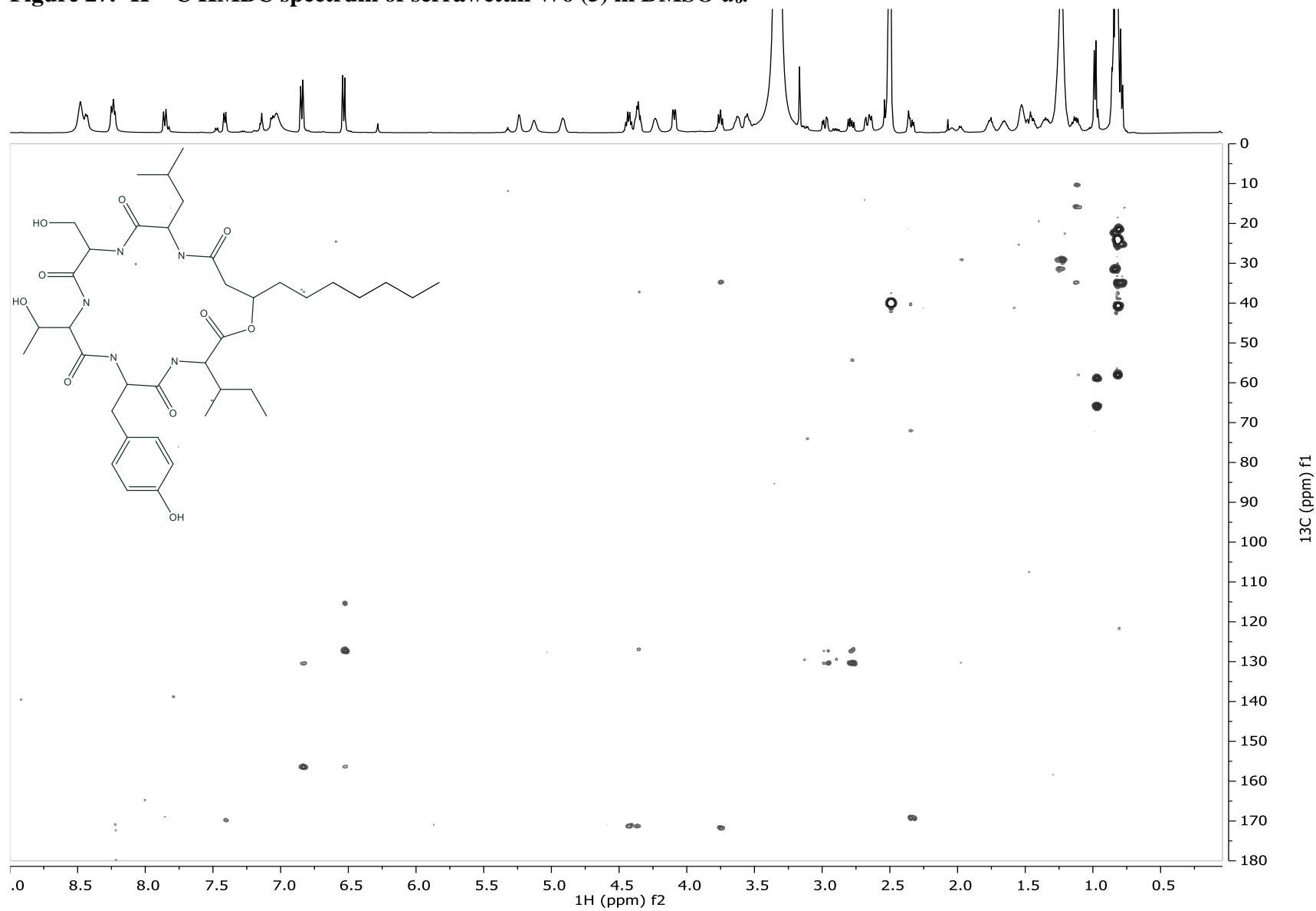


Table 8. Selected COSY and HMBC correlations (DMSO-*d*₆) for serrawettin W2 (2).

serrawettin W2 (2)		
position	COSY Correlations	HMBC Correlations
1		
2	3	1, 3, 4
3	2, 4	1
4	3	
5		
6		
7		
8		
9	10	
10	9	
11	12	1, 12
12	11, 13', 13''	13
13	12, 14	14, 15, 16
14	13', 13'', 15, 16	13, 15, 16
15	14	13, 14
16	14	13, 14
17		
18	19	19, 20, 22
19	18, 20', 20''	20, 22
20	19, 21	22
21	20', 20''	
22		
23	24	24, 25, 28
24	23, 25	25, 28
25	24, 26, 27	24
26	25	24, 25, 27
27	25	24, 25
28		
29	30	28, 30, 38
30	29, 31', 31''	28, 31, 32

31	30	28, 32, 34, 36, 30
32		
33	34	32
34	33, 35	31, 32, 33, 35, 36
35	34, 36	32, 33, 34, 36, 37
36	35, 37	31, 32, 33, 34, 37
37	36	32, 33, 34, 35, 37
38		
39	40	40, 45
40	39, 41	41, 42, 44, 45
41	40, 42', 42''	40, 43, 44, 45
42	41,43	40, 41, 42, 43, 44
43	42	41, 42, 44
44		40, 41, 42
45		

Table 9. Selected COSY and HMBC correlations (DMSO-*d*₆) for serrawettin W4 (3).

serrawettin W4 (3)		
position	COSY Correlations	HMBC Correlations
1		
2	3	1, 3, 4
3	2', 2'', 4	2', 2'', 4
4	3, 5	3, 6, 8
5	4, 6	
6	5, 7	
7	6, 8	
8	7, 9	
9	7, 10	
10	9	
11	12	1, 12
12	11, 13', 13''	13
13	12, 14	12, 17, 15, 16
14	13, 15, 16	
15	14	13, 16
16	14	13
17		
18	19	17, 19, 20
19	18, 20	17, 20, 22
20	19, 21	19, 22
21	20	19, 20
22		
23	24	22, 24, 25
24	23, 25	25, 28
25	24, 26, 27	
26	25	24, 25, 27
27	25	24, 25
28		
29	30	28, 30
30	29, 31', 31''	31, 32, 38
31	30	30, 32, 34, 36, 38
32		

33	34	31, 32, 34, 35, 36, 37
34	33, 35	31, 32, 33, 35, 36
35	34, 36	31, 32, 33, 34, 36, 37
36	35, 37	31, 32, 33, 34, 35, 37
37	36	31, 32, 33, 34, 35, 36
38		
39	40	38
40	39, 41	38, 41, 42, 45
41	40, 42, 44	38, 40
42		40, 41
43	N/A	N/A
44	41	40, 41, 42
45		

Table 10. Selected COSY and HMBC correlations (DMSO-*d*₆) for serrawettin W5 (4).

serrawettin W5 (4)		
position	COSY Correlations	HMBC Correlations
1		
2	3	1, 11
3	2', 2'', 4	
4	3, 5	
5	4, 6	
6	5, 7	
7	6, 8	
8	7	5, 7
9	N/A	N/A
10	N/A	N/A
11	12	
12	11, 13', 13''	
13	12, 14	
14	13', 15, 16	
15	14	13, 14, 16
16	14	13, 14
17		
18	19	17
19	18, 20	20, 22
20	19, 21	
21	20	
22		
23	24	22
24	23, 25	
25	24, 26, 27	22
26	25	
27	25	24, 25
28		
29	30	28
30	29, 31', 32''	31', 31''
31	30	30, 34, 36
32		

33	34	34, 36
34	33, 35	31, 35
35	34, 36	33, 37
36	35, 37	31, 35
37	38	34, 36
38		40
39	40	
40	39, 41	38, 41
41	40, 42', 44	40, 42
42	41, 43	40, 41, 43, 44
43	42', 42''	40, 42, 44
44	41	40, 41, 42
45		

Table 11. Selected COSY and HMBC correlations (DMSO-*d*₆) for serrawettin W6 (5).

serrawettin W5 (4)		
position	COSY Correlations	HMBC Correlations
1		
2	3	1
3	2', 2'', 4	
4	3, 4, 5	
5		
6		
7		
8		
9		
10	9	
11	12	1, 12, 17
12	11, 13', 13''	17
13	12, 14	16
14	13', 13'', 15, 16	
15	14	12, 13, 14, 16
16	14	12, 13, 14, 15
17		
18	19	17, 22
19	18, 20	20, 22
20	19, 21	
21	20	
22		18, 19, 23, 24
23	24	22
24	23, 25	22, 28
25	24, 26, 27	
26	25	
27	27	24, 25
28		
29	30	28
30	29, 31', 31''	31, 32
31	30	30, 32, 33
32		30, 31', 31'', 34, 36

33	34	35
34	33	32, 35
35		
36	37	28, 32, 33
37	36	33, 35
38		
39	40	
40	39, 41	42", 43', 44
41	40, 42, 44	40, 42", 43', 44
42	41, 43,	40, 41, 43, 44
43	42	40, 41,42
44	41	40, 41,42
45		

Figure 28. Selected ion trace for m/z 713-717 for serrawettin W2 (2) after FDAA derivatization.

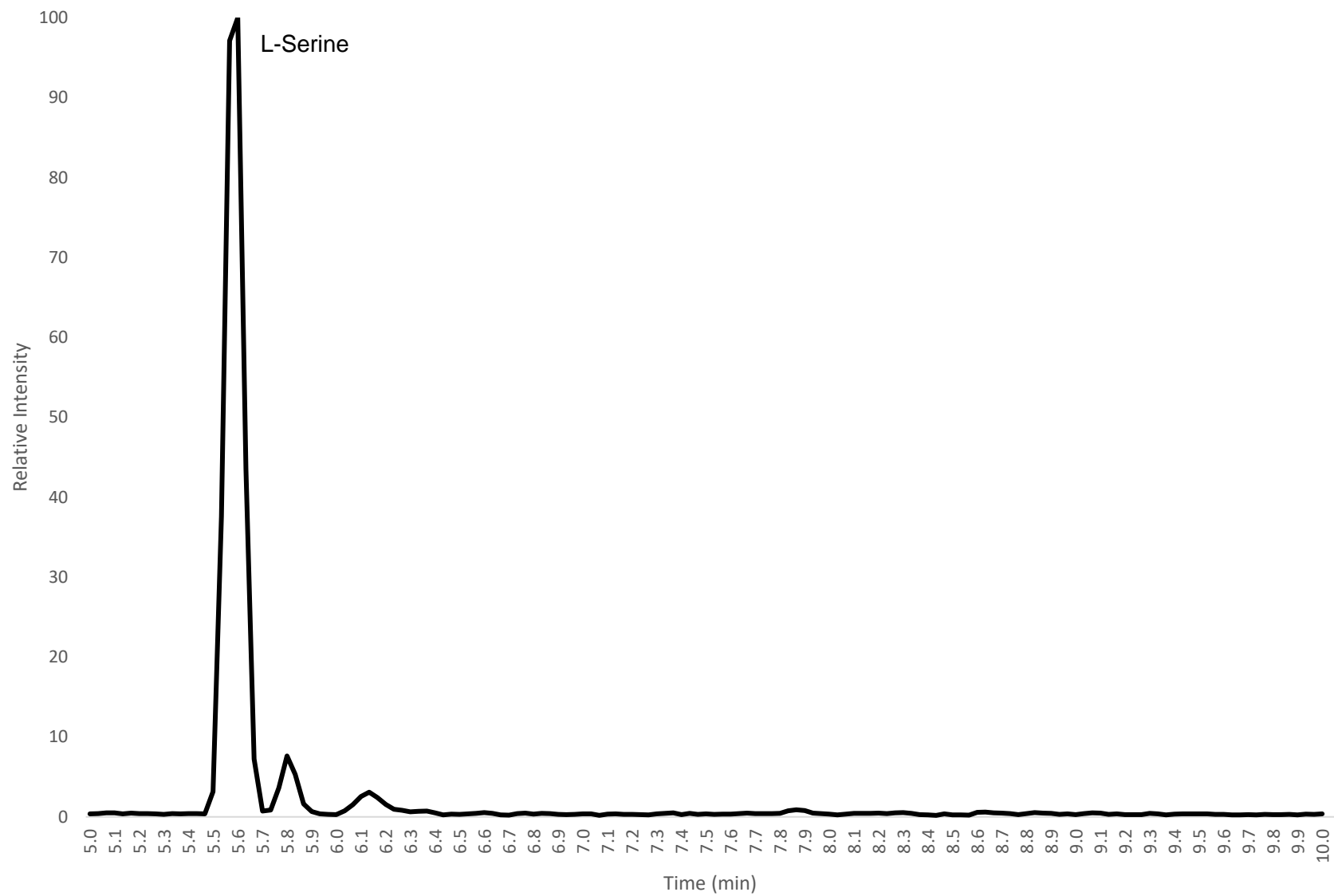


Figure 29. Selected ion trace for m/z 741-745 for serrawettin W2 (2) after FDAA derivatization.

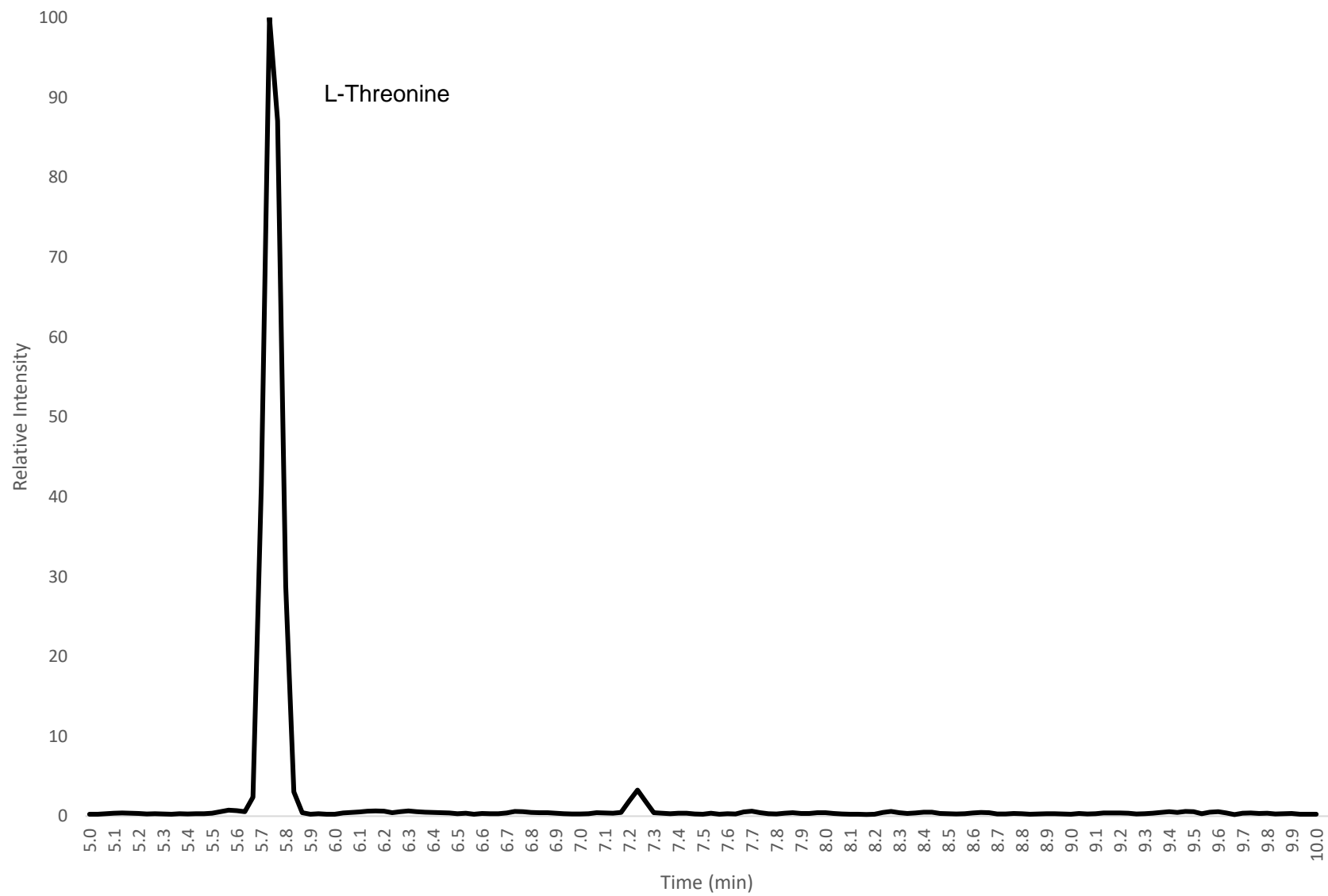


Figure 30. Selected ion trace for m/z 765-769 for serrawettin W2 (2) after FDAA derivatization.

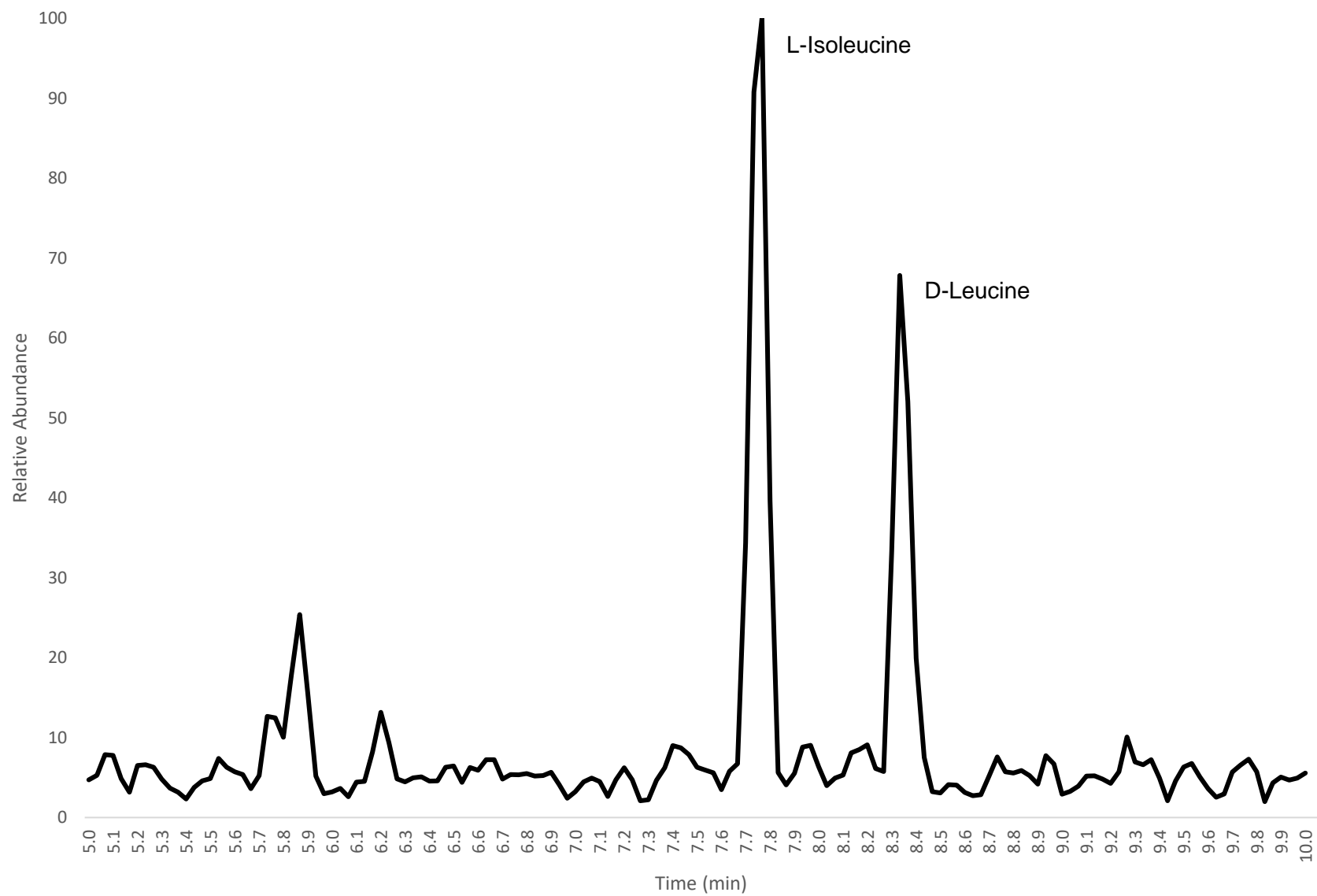


Figure 31. Selected ion trace for m/z 833-837 for serrawettin W2 (2) after FDAA derivatization.

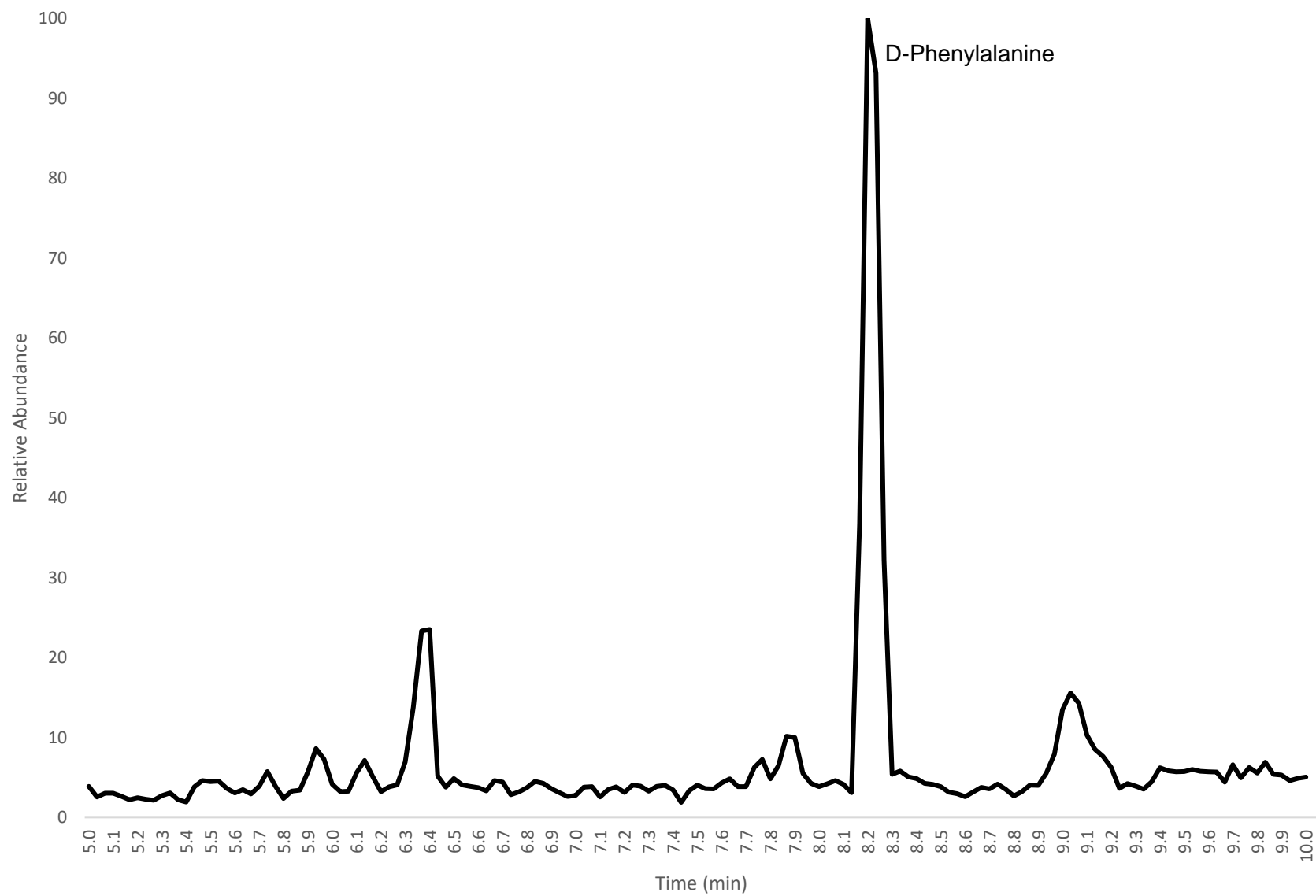


Figure 32. Selected ion trace for m/z 713-717 for serrawettin W4 (3) after FDAA derivatization.

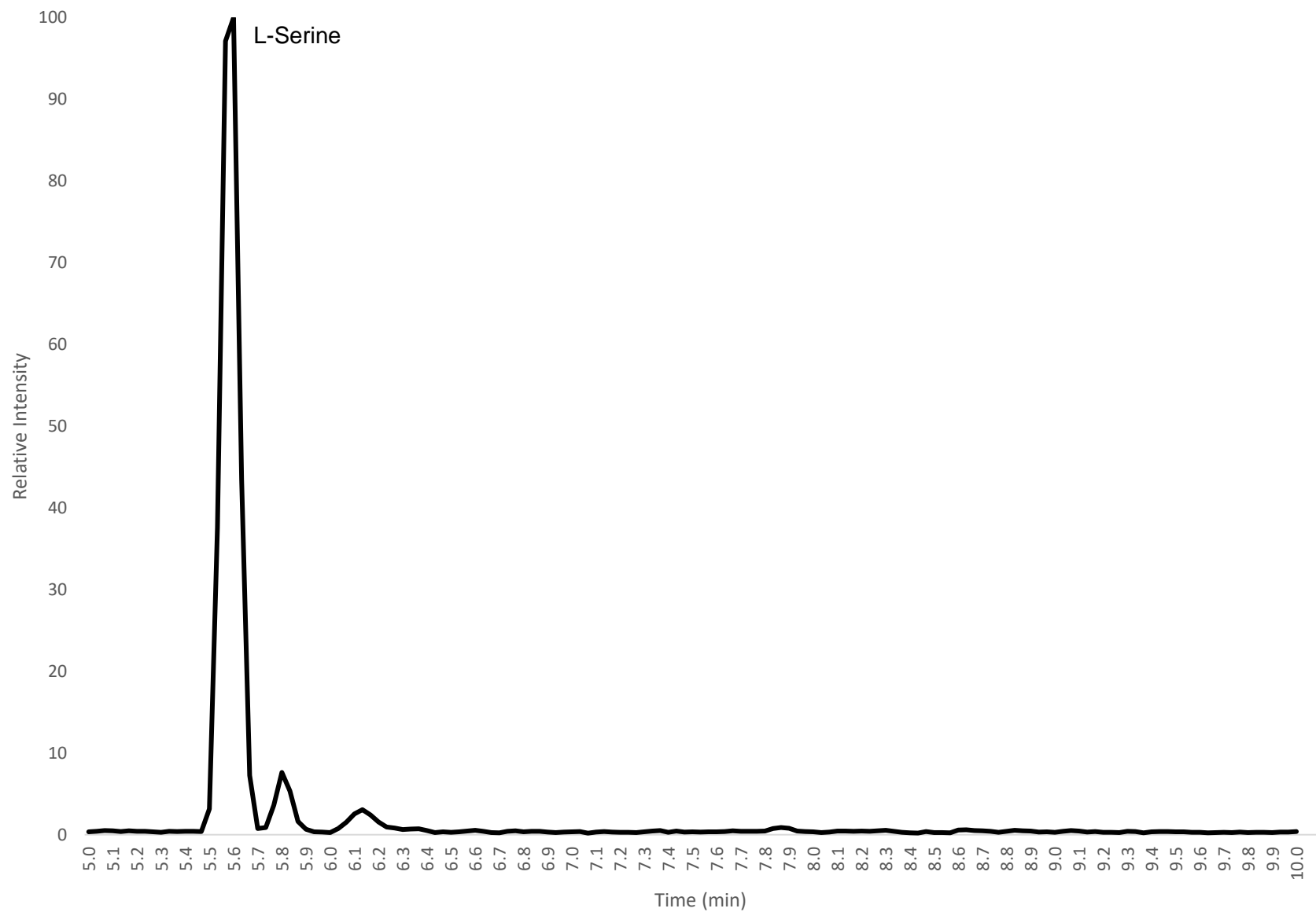


Figure 33. Selected ion trace for m/z 737-740 for serrawettin W4 (3) after FDAA derivatization.

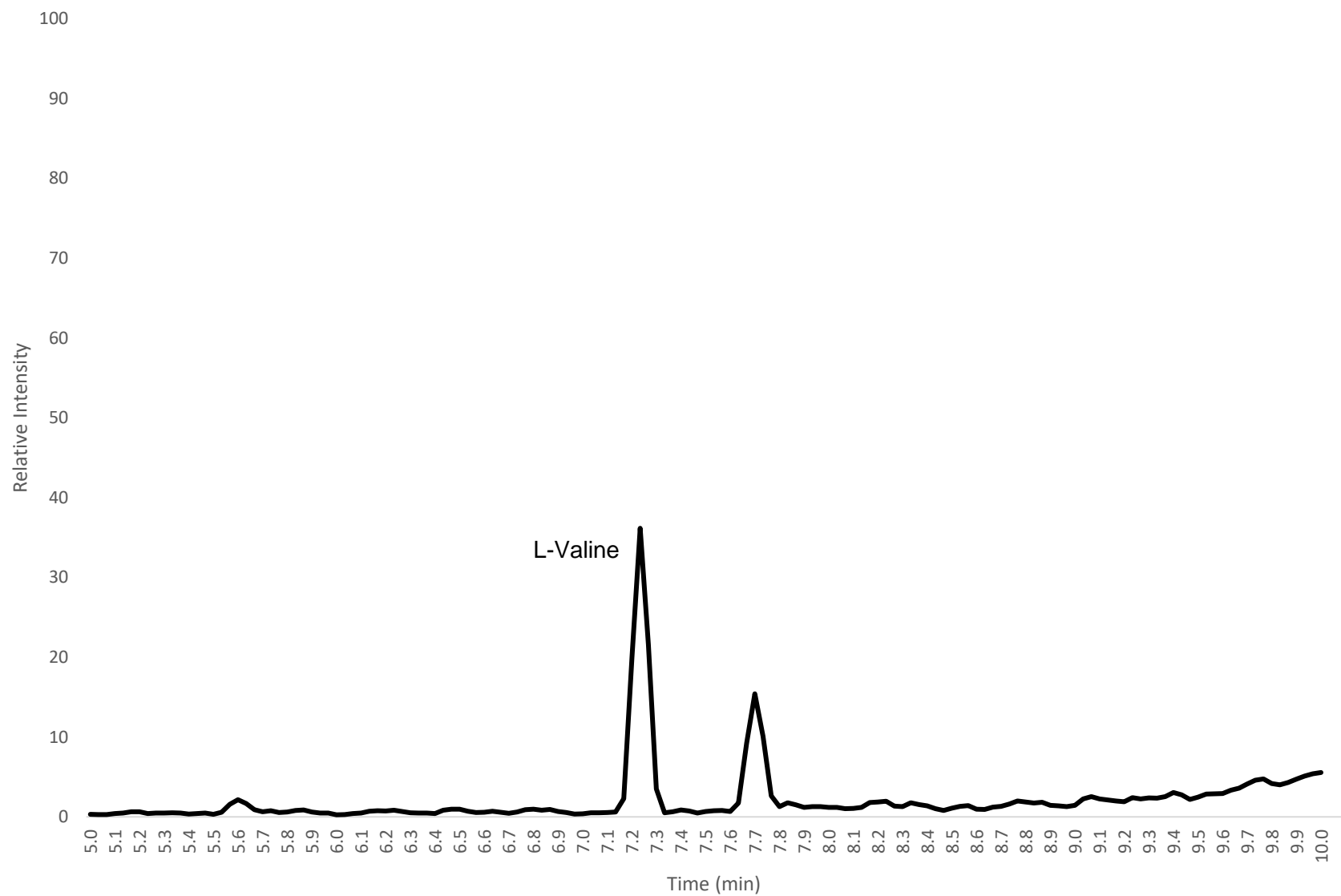


Figure 34. Selected ion trace for m/z 741-745 for serrawettin W4 (3) after FDAA derivatization.

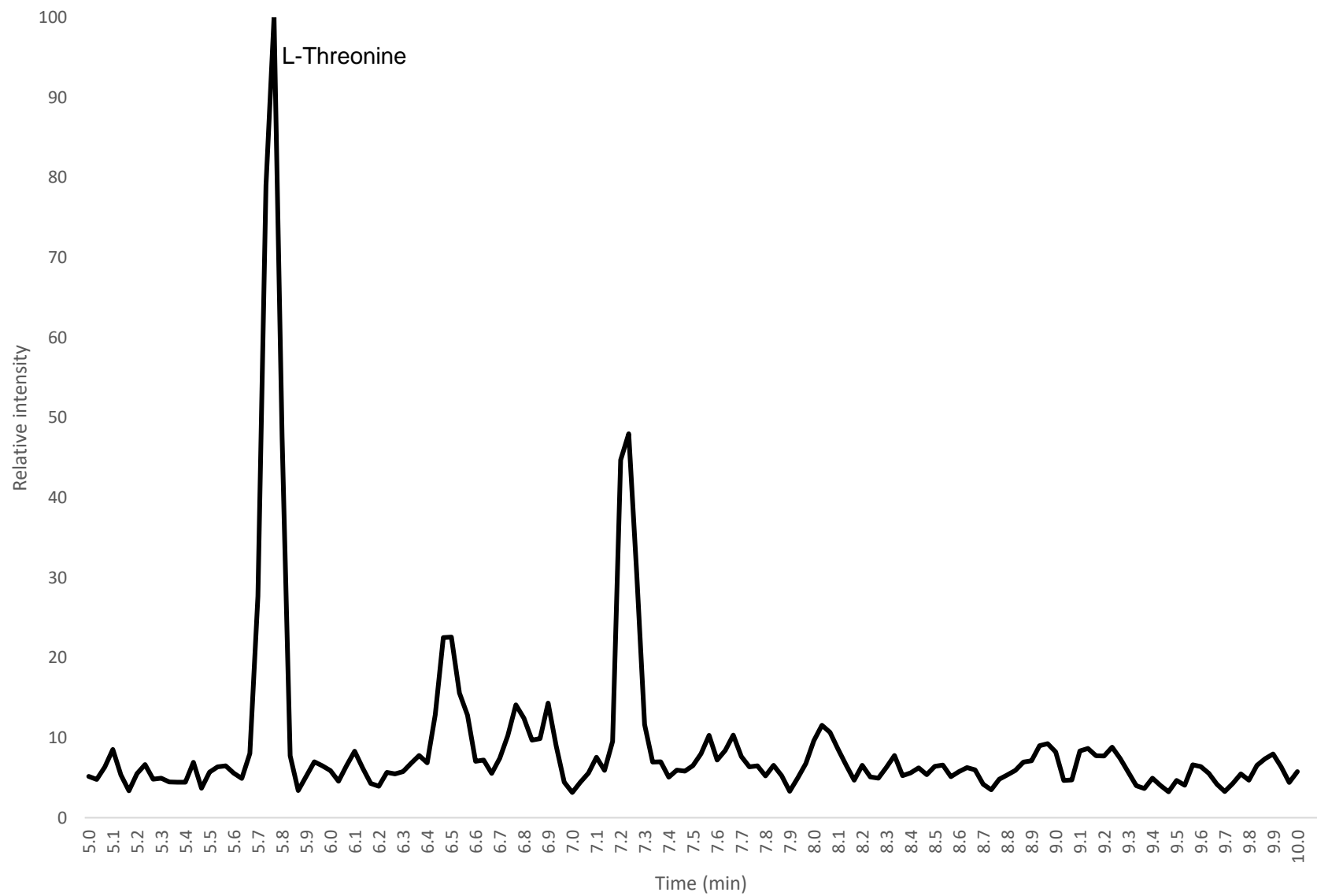


Figure 35. Selected ion trace for m/z 765-769 for serrawettin W4 (3) after FDAA derivatization.

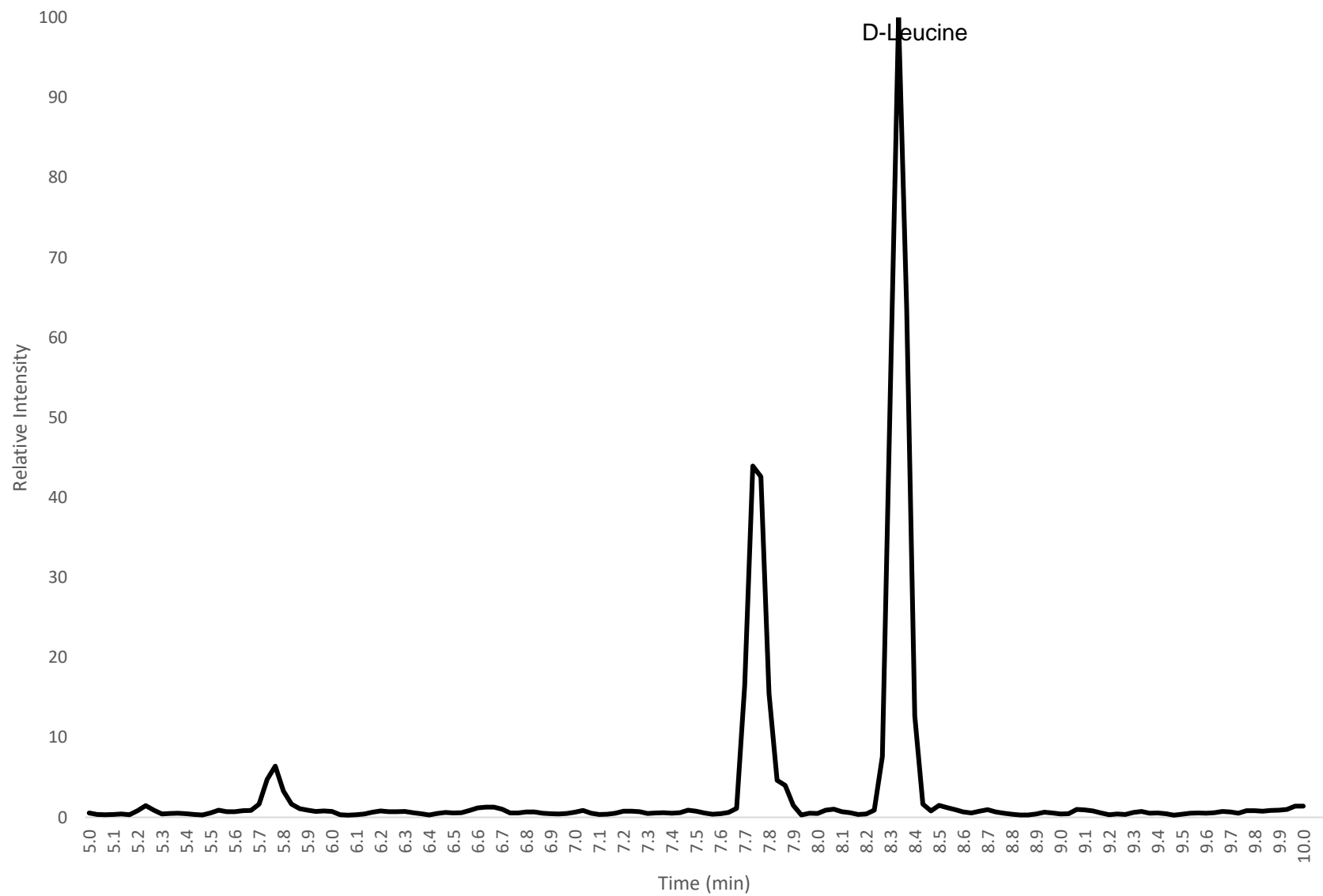


Figure 36. Selected ion trace for m/z 833-837 for serrawettin W4 (3) after FDAA derivatization.

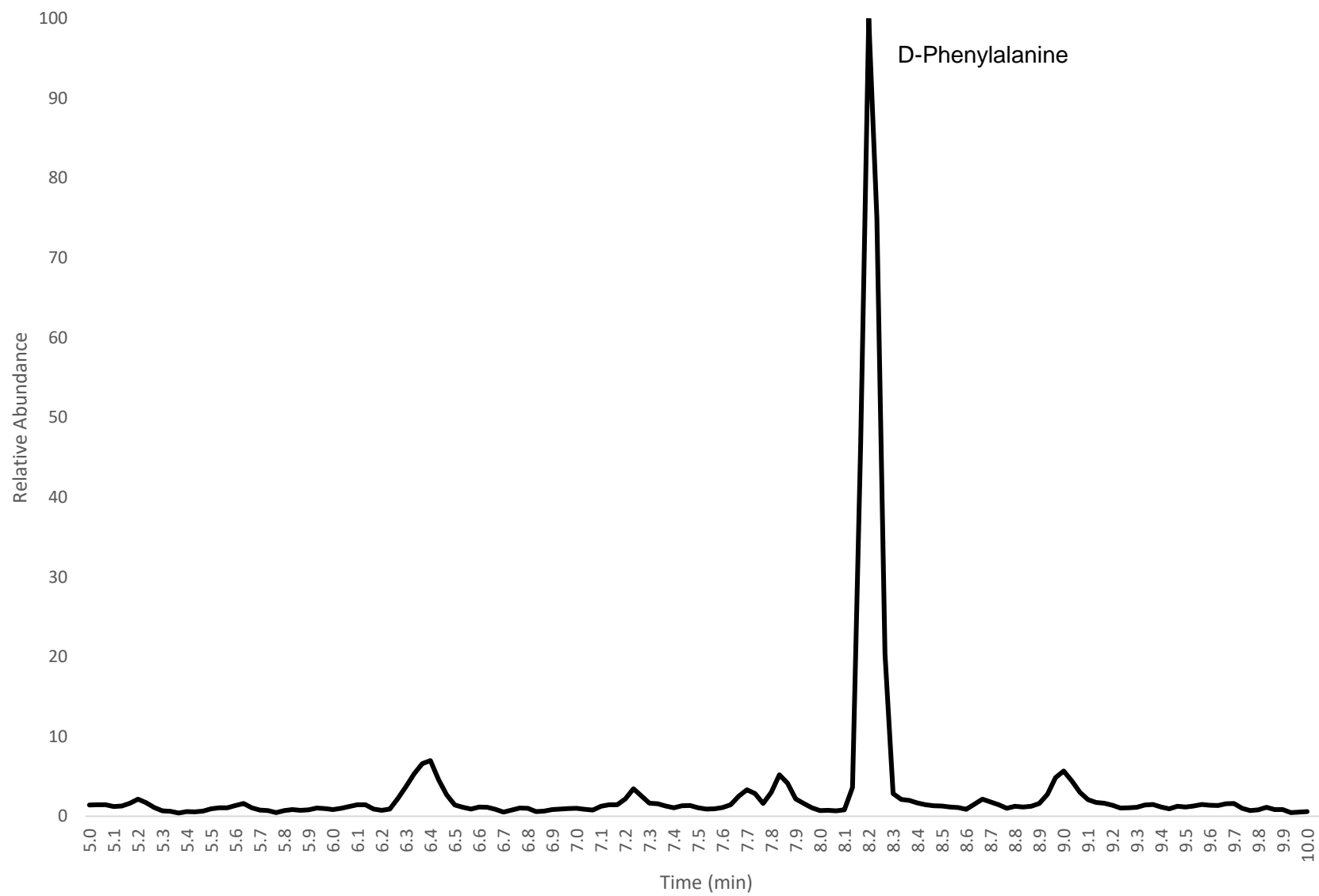


Figure 37. Selected ion trace for m/z 765-769 for serrawettin W5 (4) after FDAA derivatization.

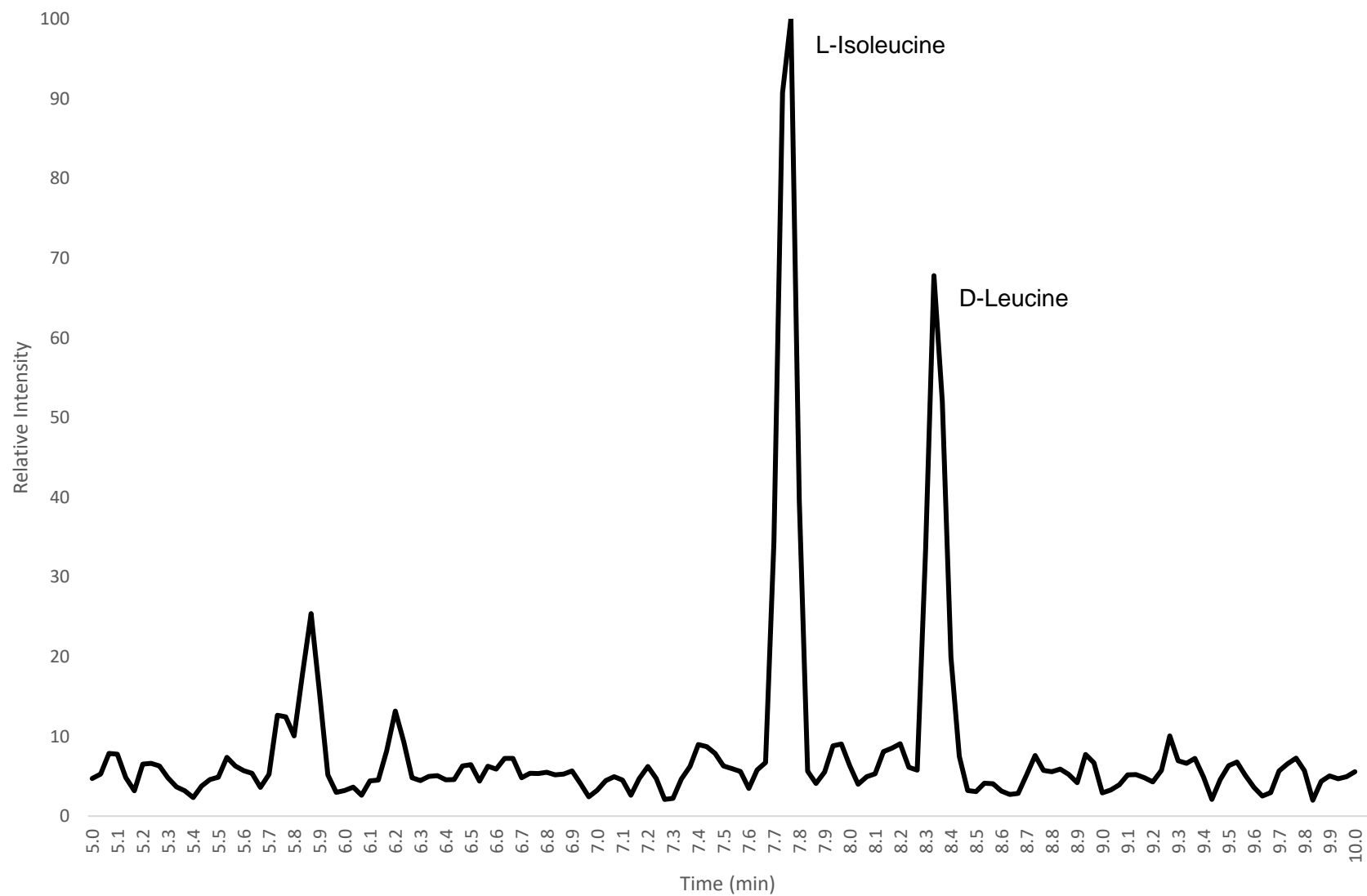


Figure 38. Selected ion trace for m/z 741-745 for serrawettin W5 (4) after FDAA derivatization.

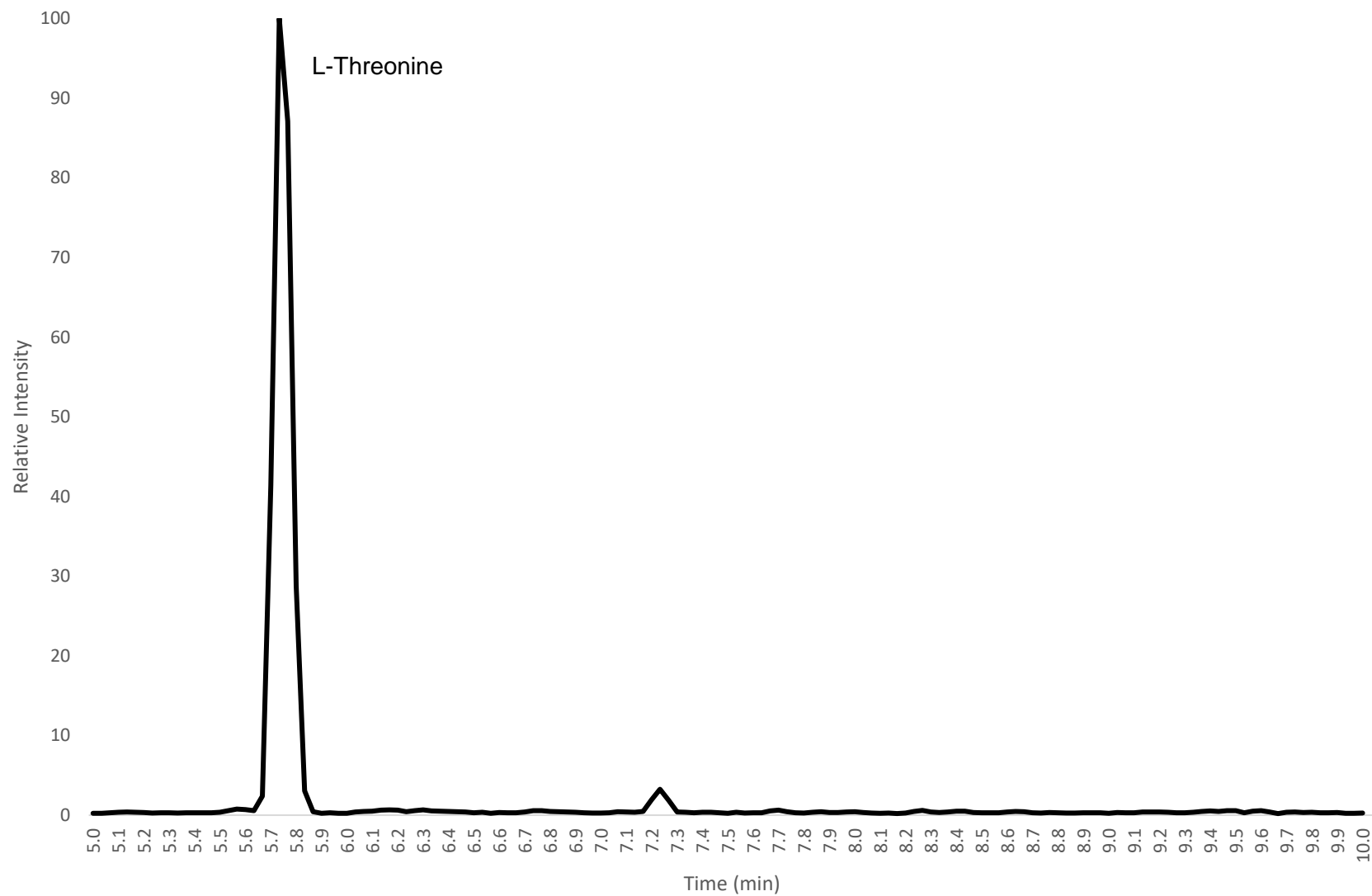


Figure 39. Selected ion trace for m/z 833-837 for serrawettin W5 (4) after FDAA derivatization.

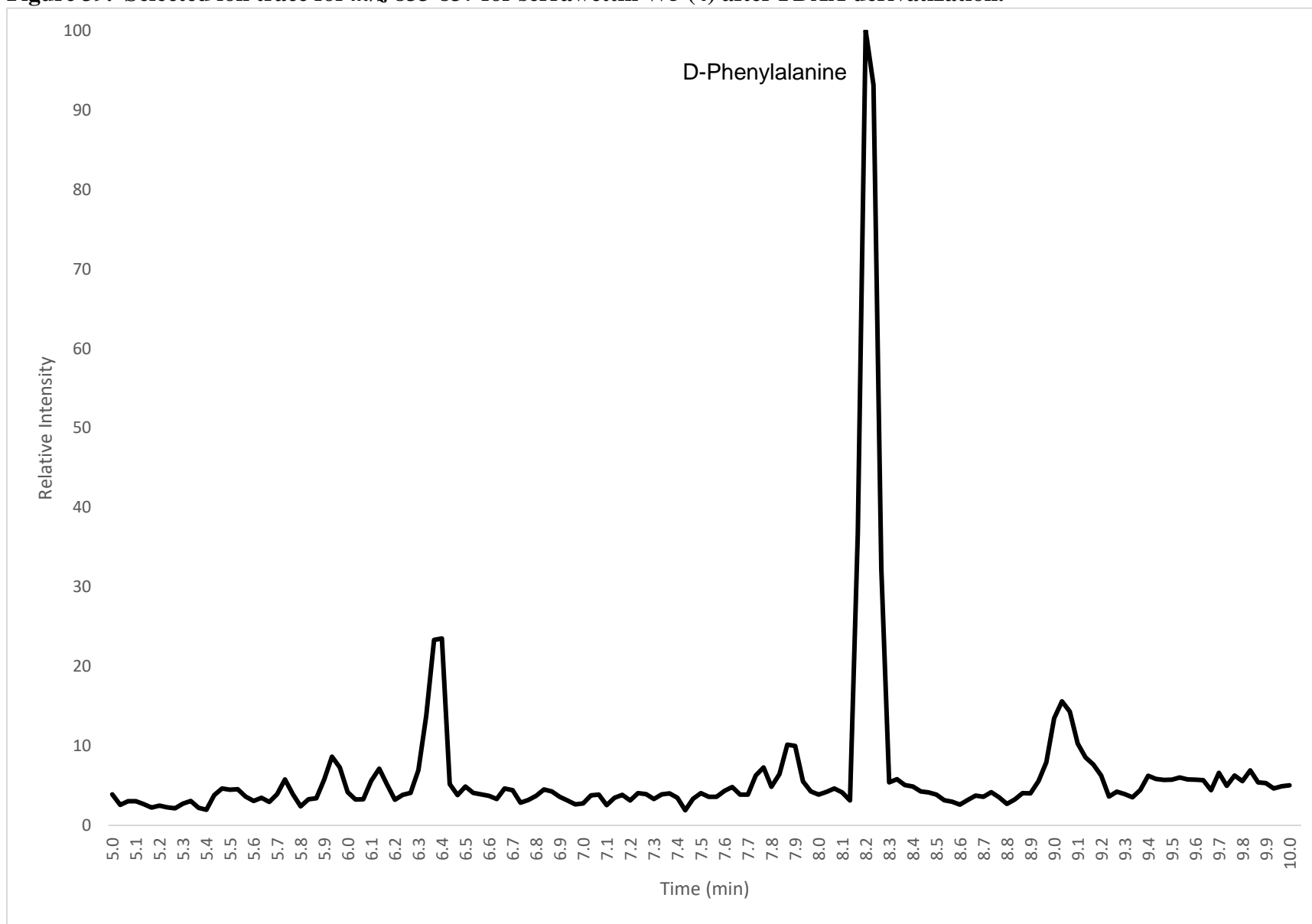


Figure 40. Selected ion trace for m/z 713-717 after serrawettin W5 (4) after FDAA derivatization.

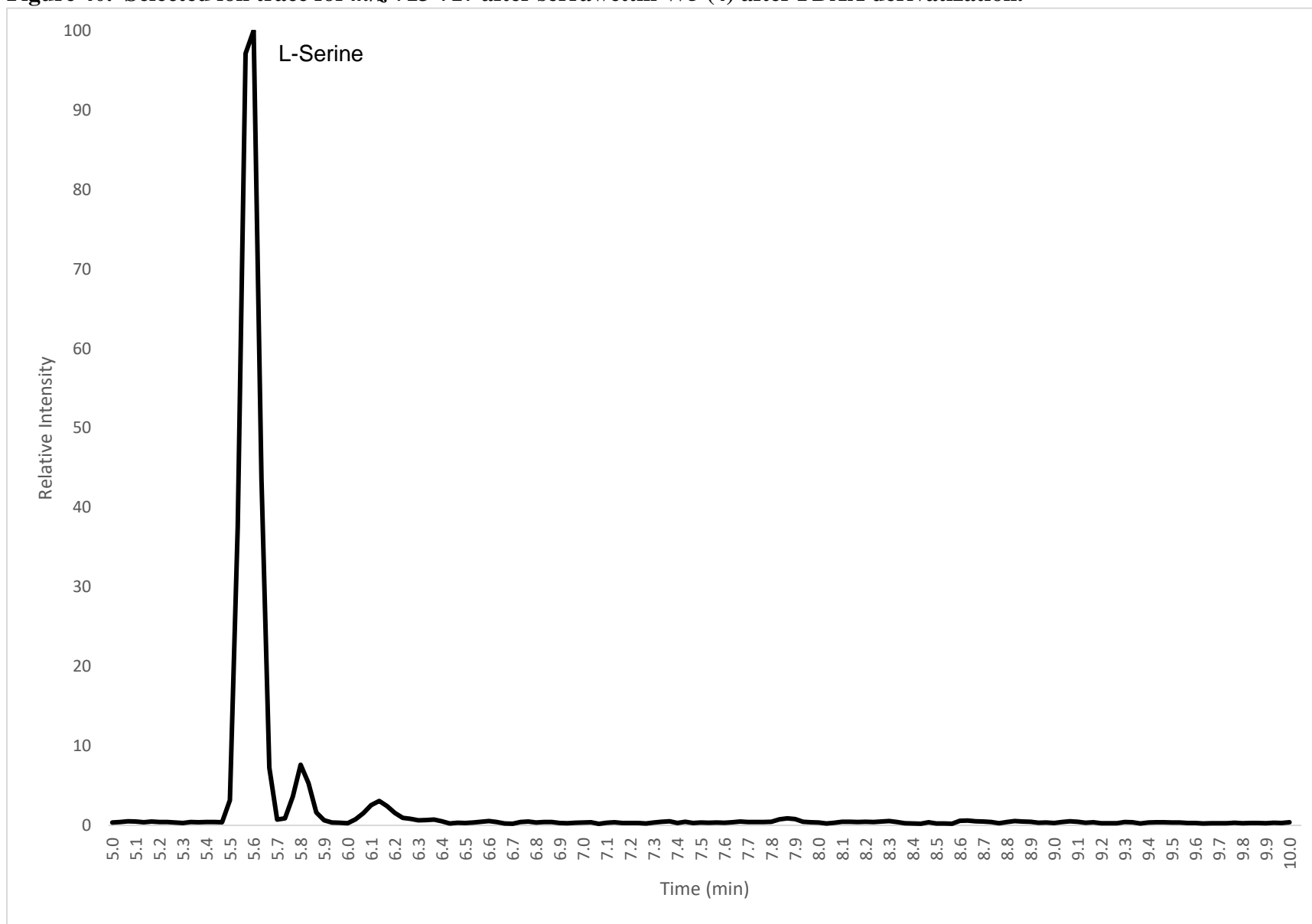


Figure 41. Selected ion trace for m/z 741-745 for serrawettin W6 (5) after FDAA derivatization.

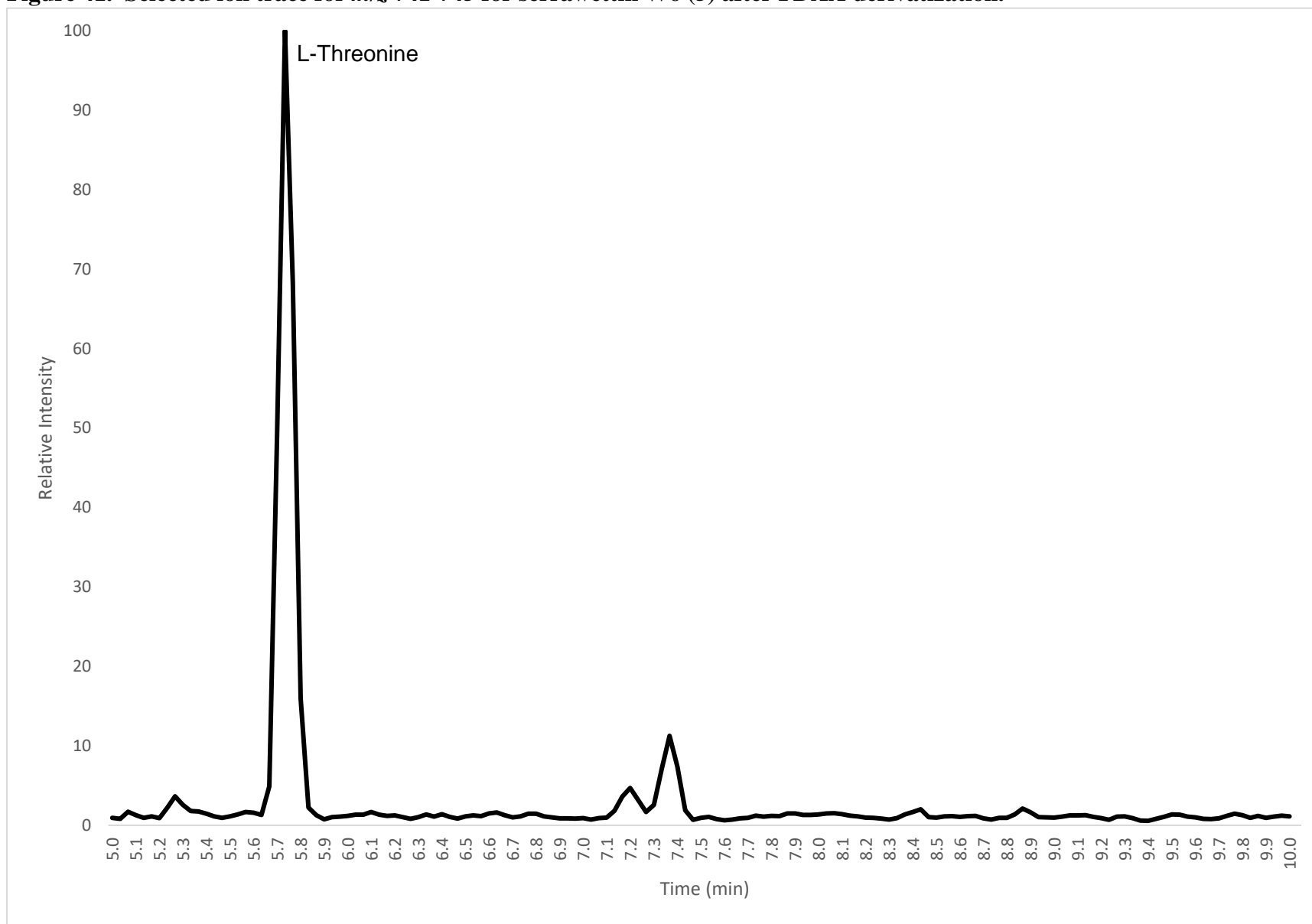


Figure 42. Selected ion trace for m/z 684-688 for serrawettin W6 (5) after FDAA derivatization.

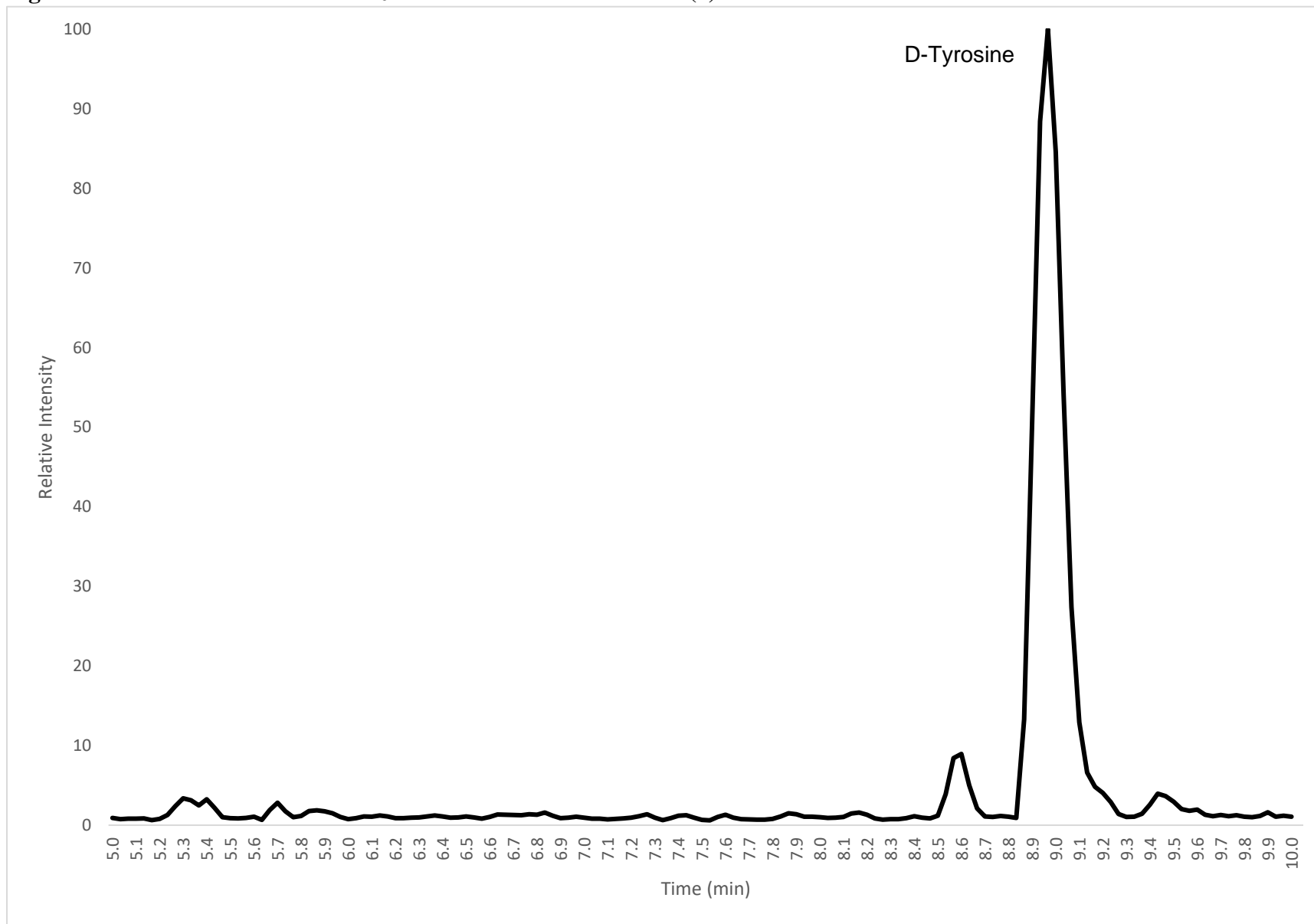


Figure 43. Selected ion trace for m/z 713-717 for serrawettin W6 (5) after FDAA derivatization.

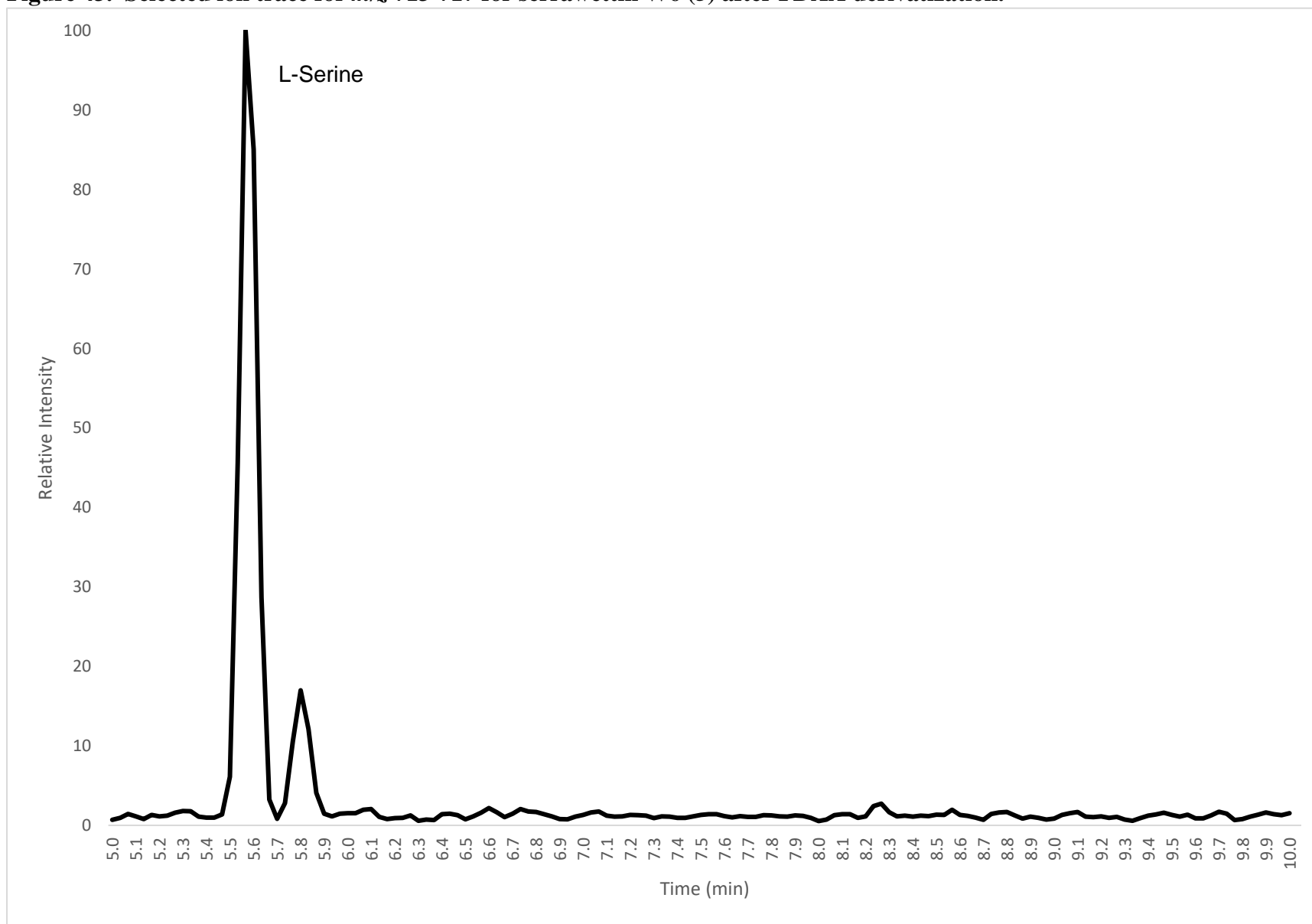


Figure 44. Selected ion trace for m/z 765-769 for serrawettin W6 (5) after FDAA derivatization.

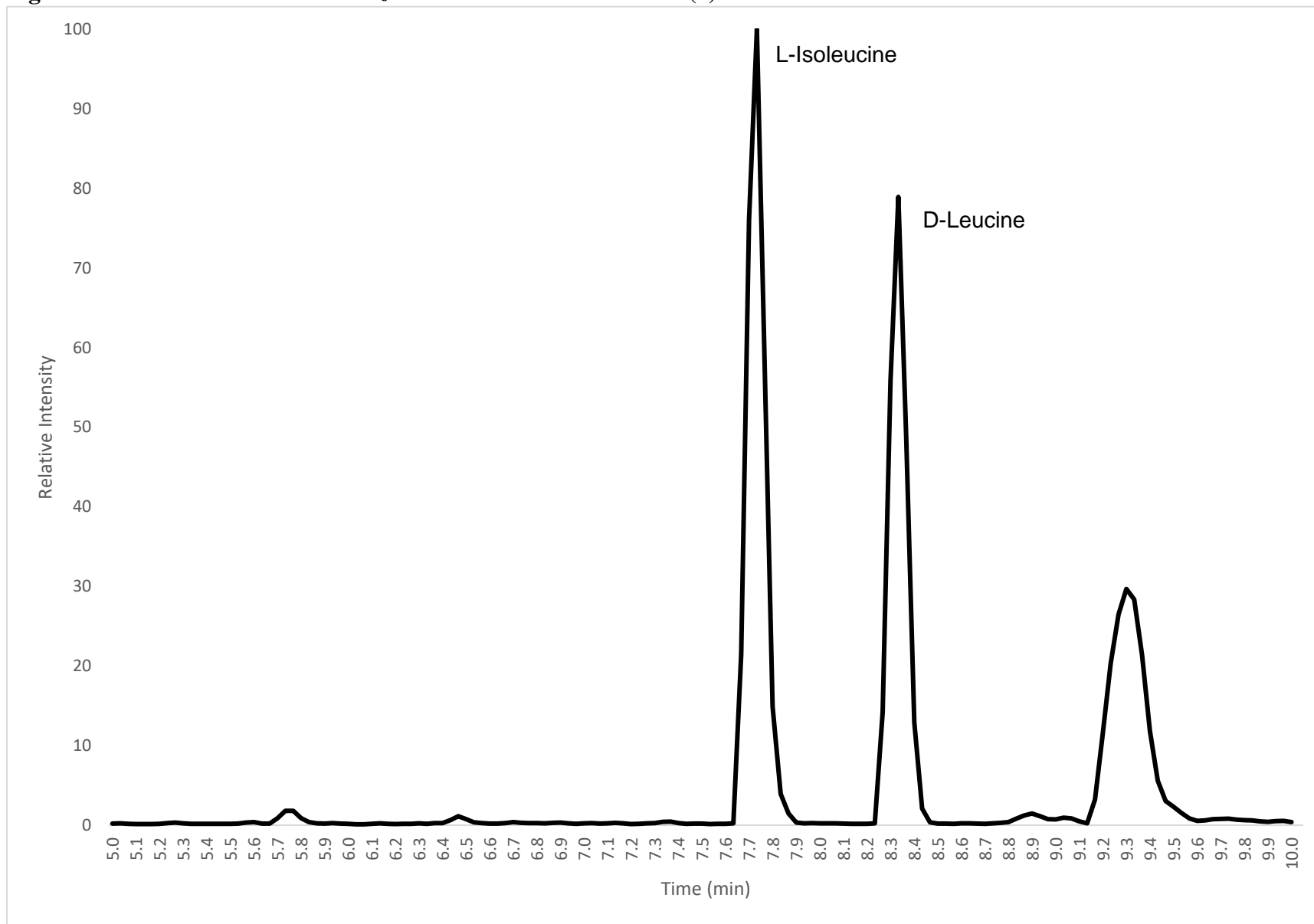


Figure 45. Selected ion trace for m/z 741-745 for FDAA derivatized D-allo threonine standard.

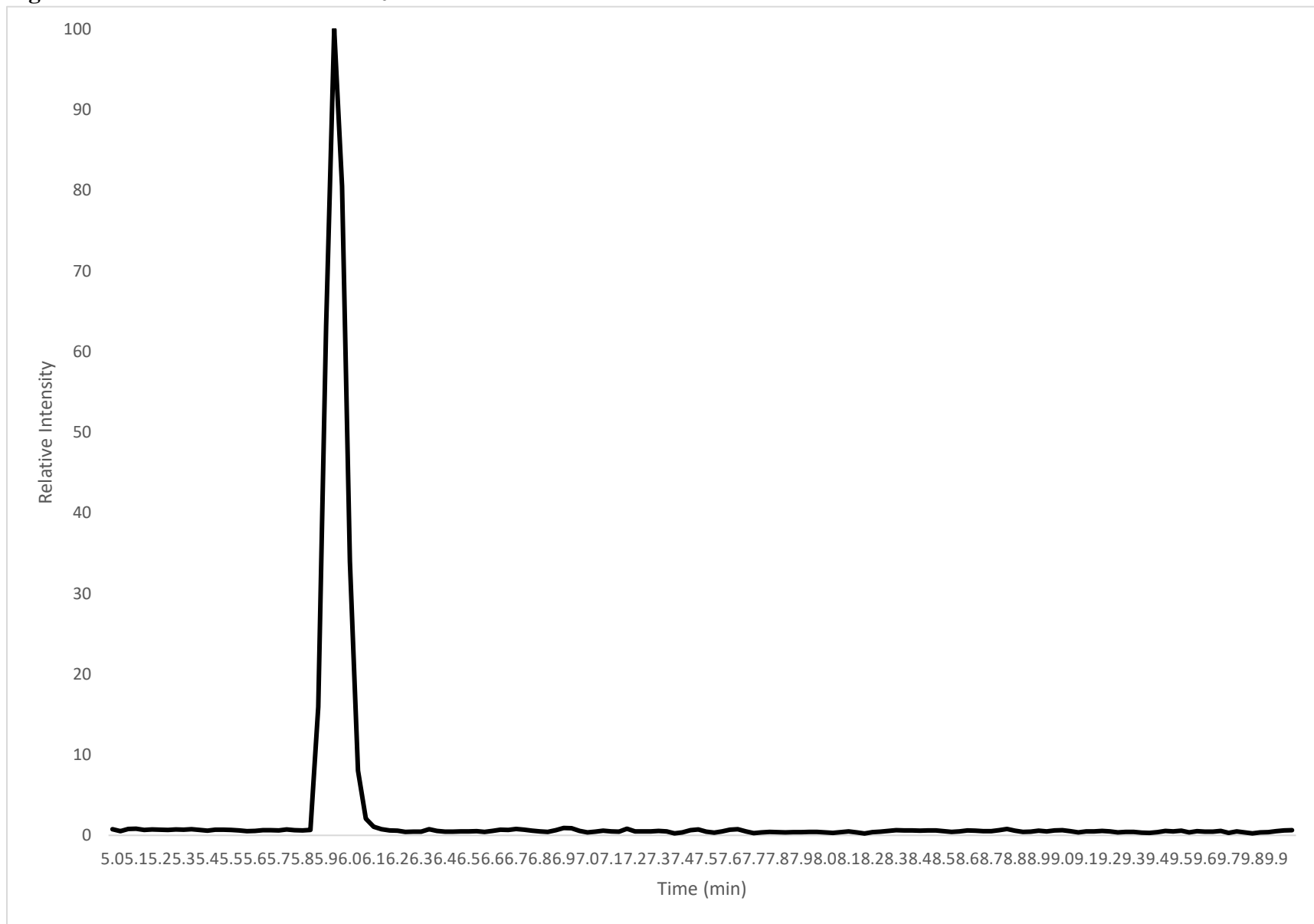


Figure 46. Selected ion trace for m/z 741-745 for FDAA derivatized L-allo threonine standard.

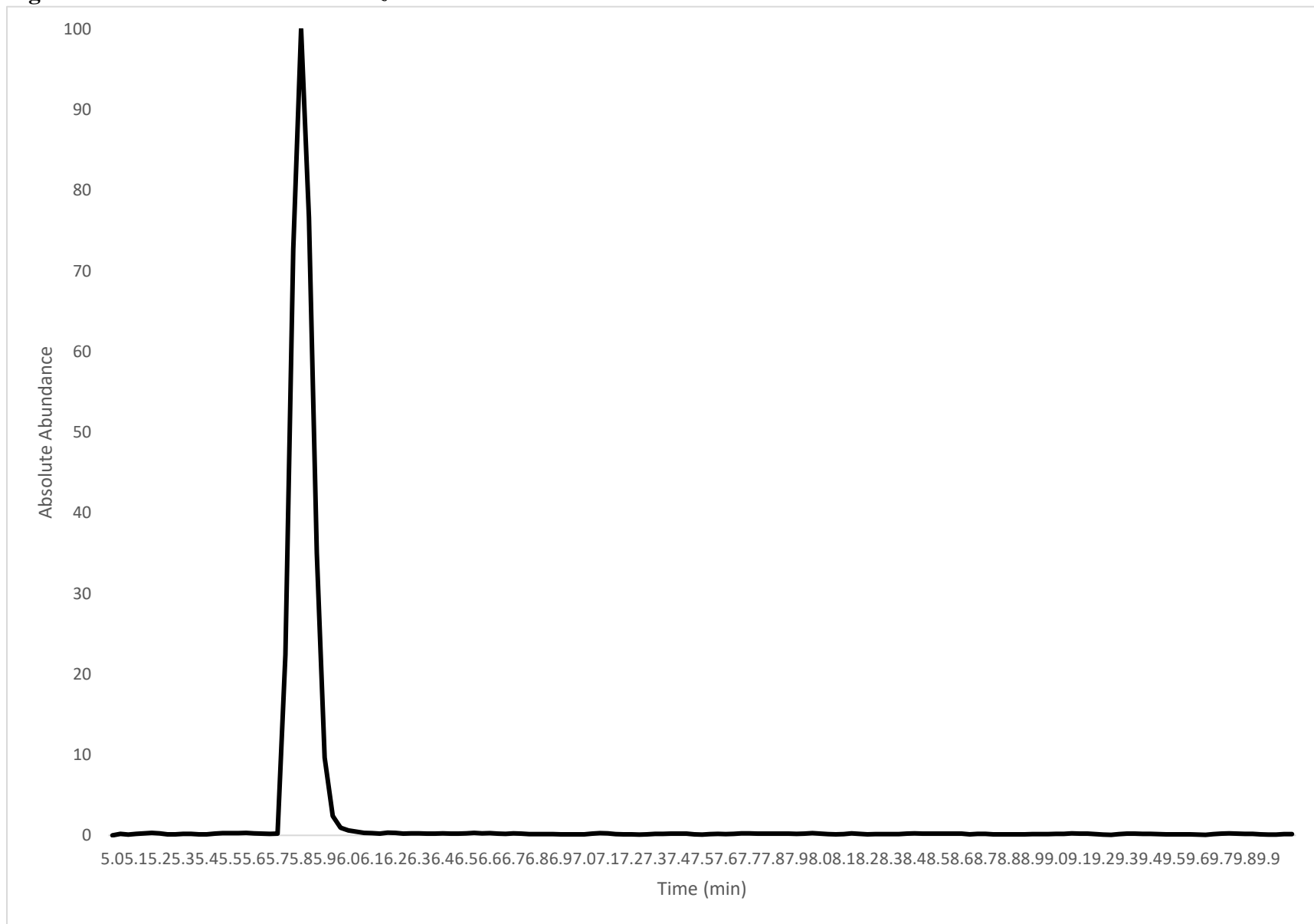


Figure 47. Selected ion trace for m/z z 741-745 for FDAA derivatized L-threonine standard.

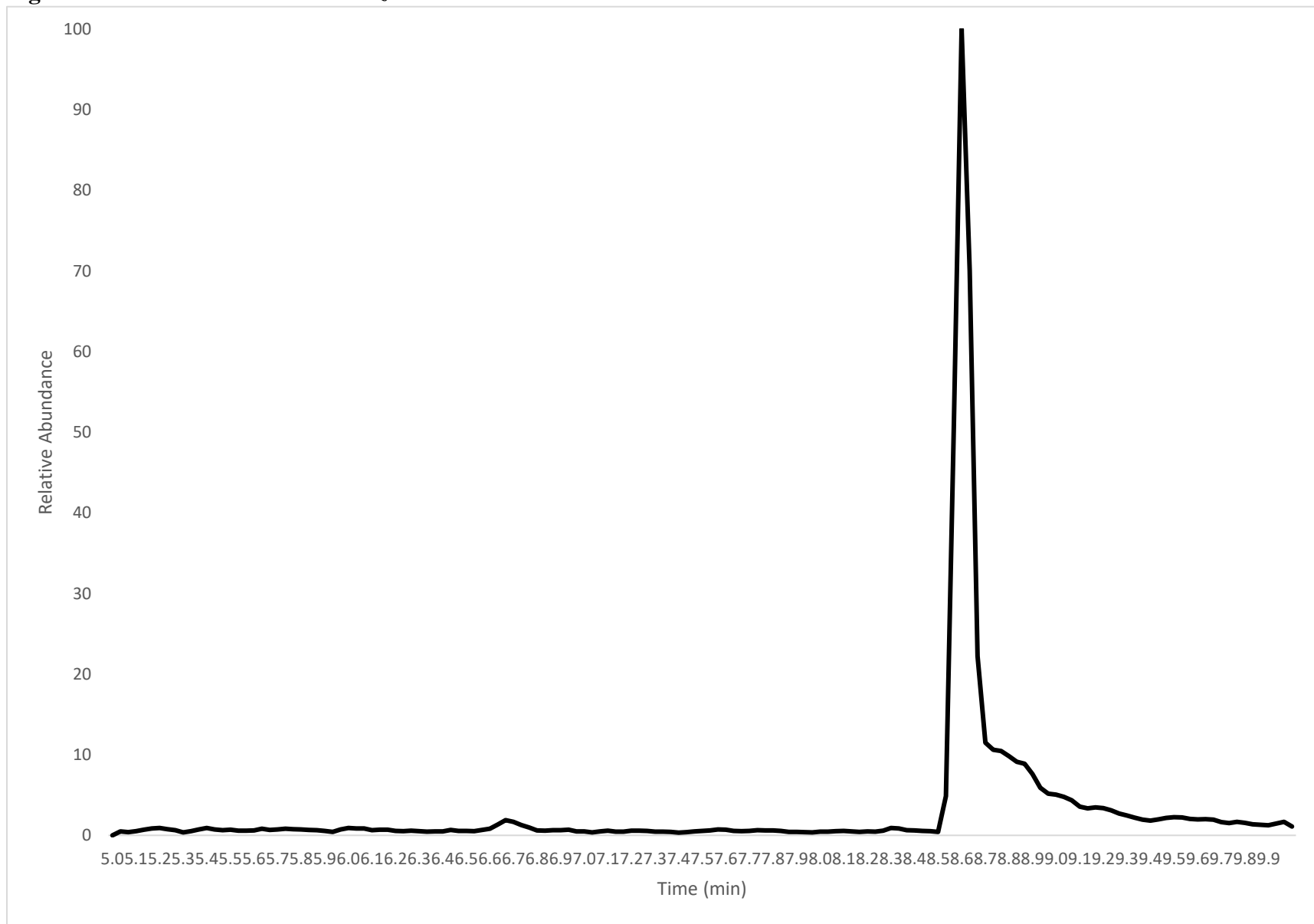


Figure 48. Selected ion trace for m/z 737-740 for FDAA derivatized D-valine standard.

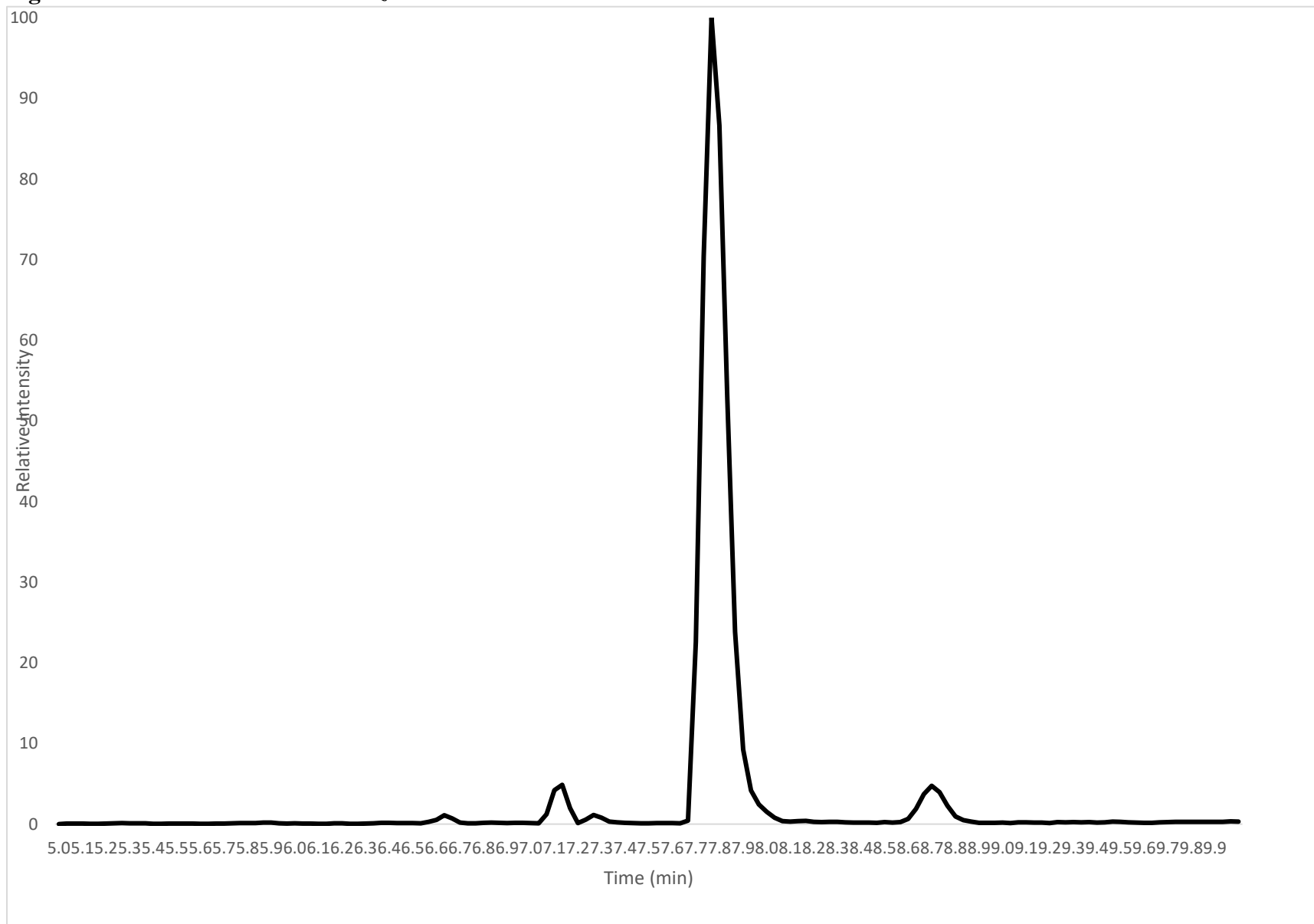


Figure 49. Selected ion trace for m/z 737-740 for FDAA derivatized L-valine standard.

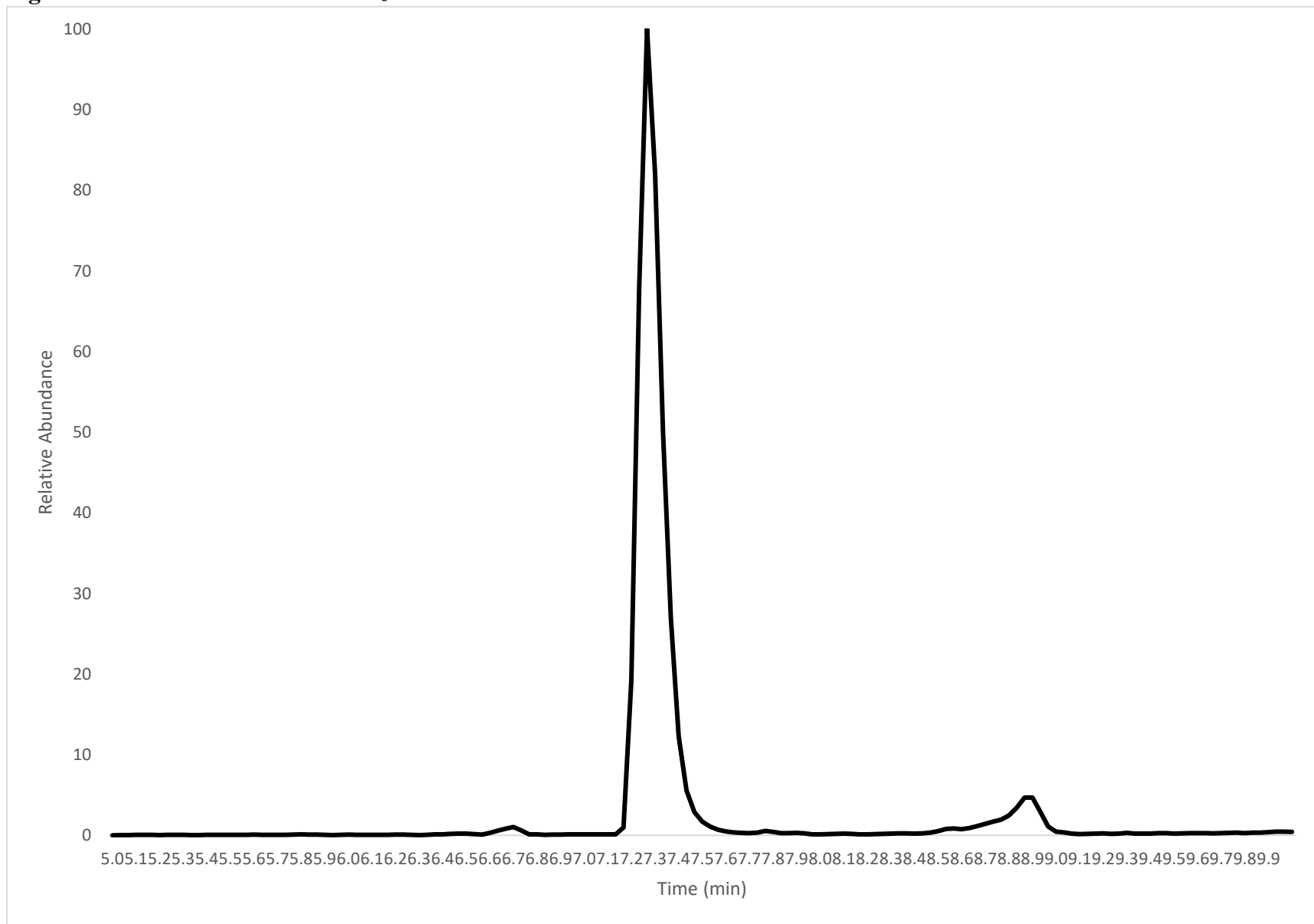


Figure 50. Selected ion trace for m/z 765-769 for FDAA derivatized D-isoleucine standard.

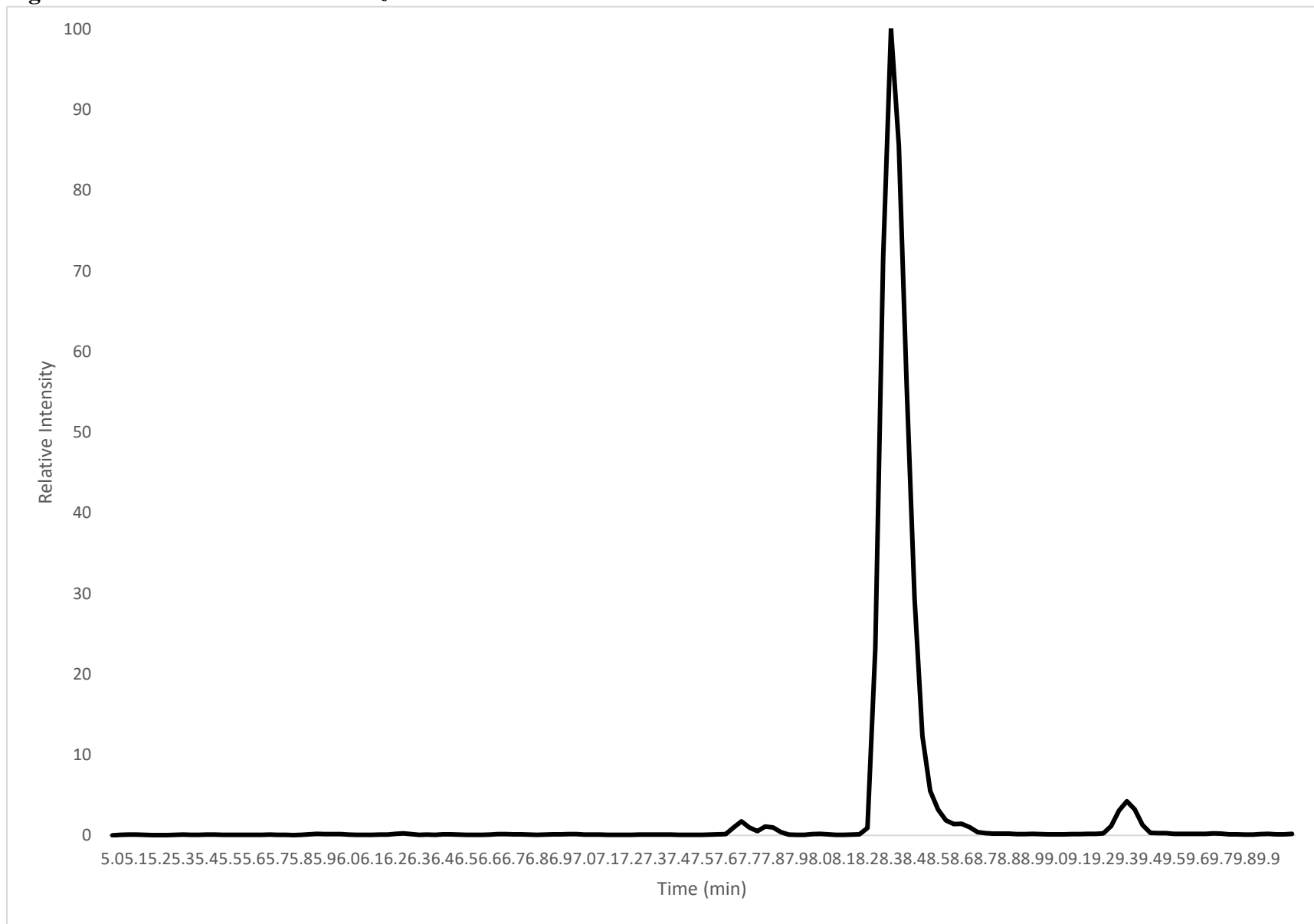


Figure 51. Selected ion trace for m/z 765-769 for FDAA derivatized L-isoleucine standard.

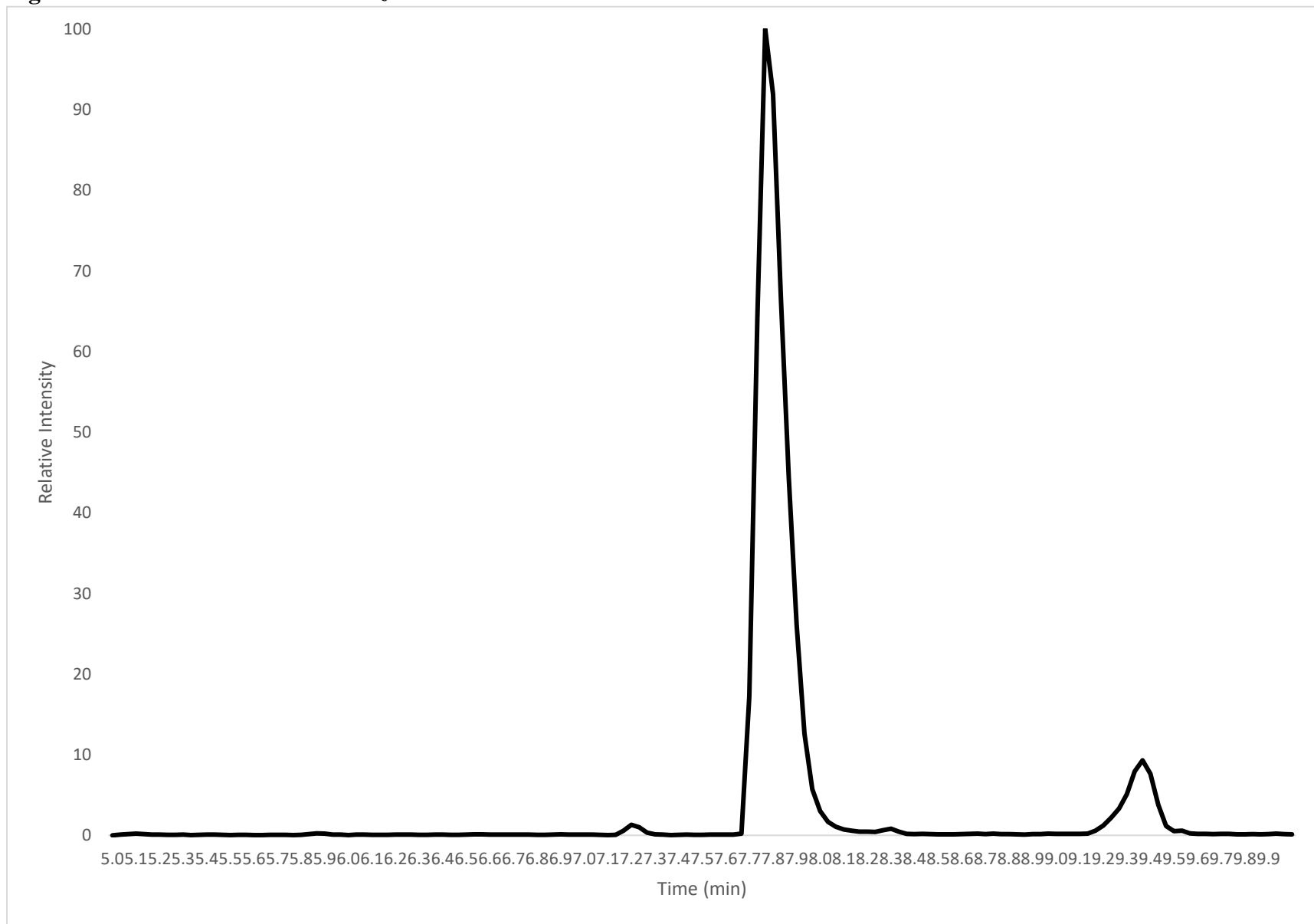


Figure 52. Selected ion trace for m/z 765-769 for FDAA derivatized D-allo-isoleucine standard.

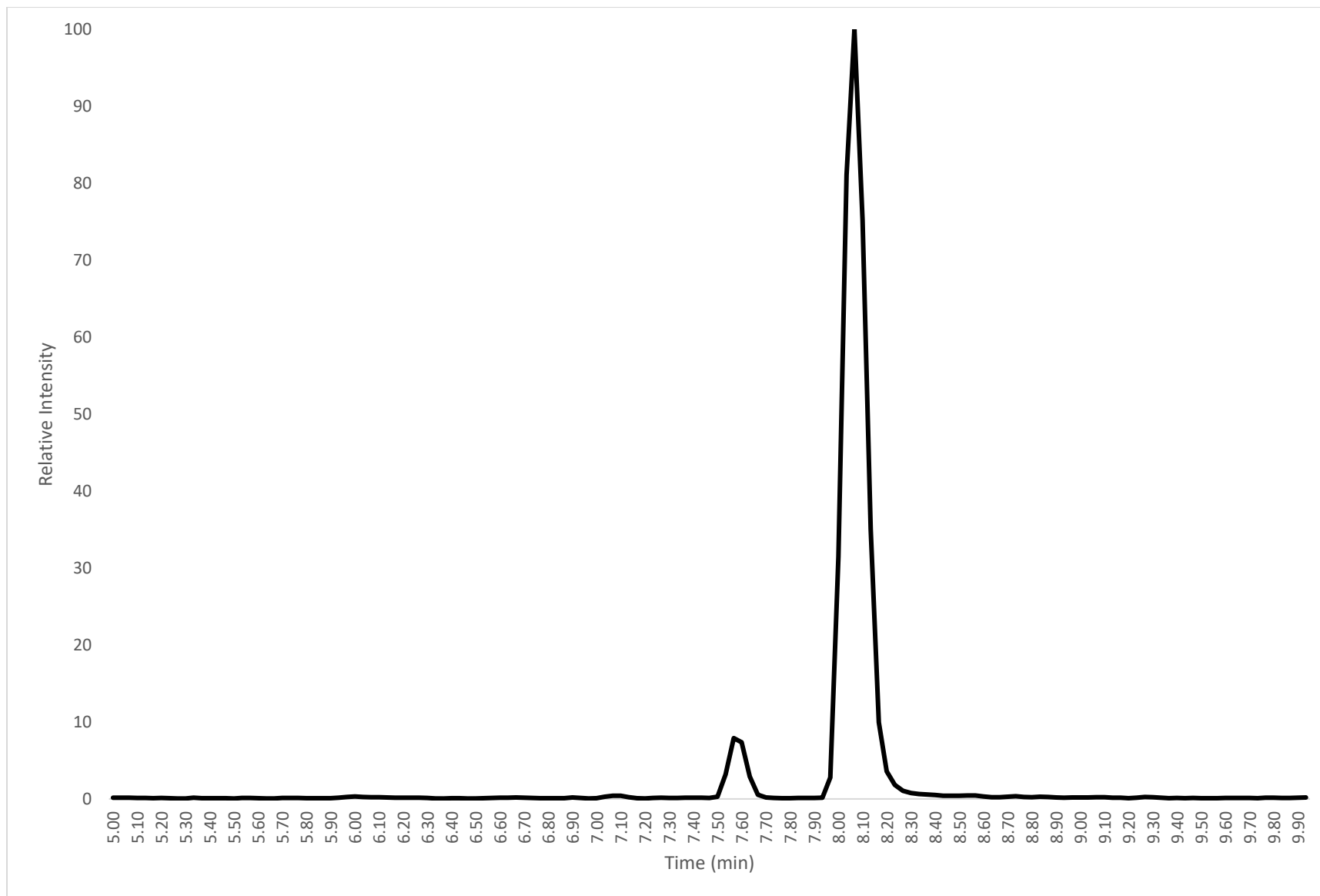


Figure 53. Selected ion trace for m/z 765-769 for FDAA derivatized L-allo-isoleucine standard.

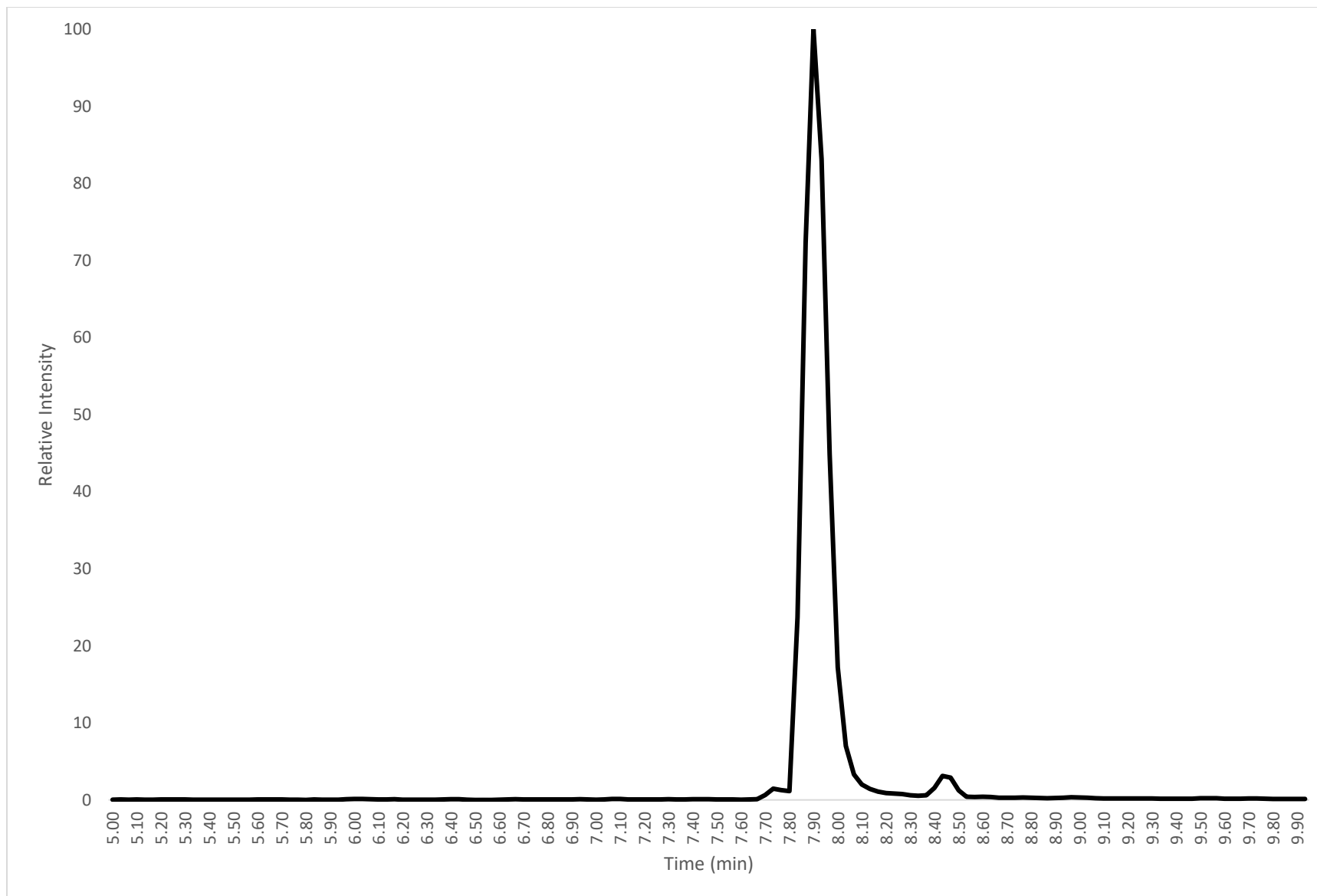


Figure 54. Selected ion trace for m/z 765-769 for FDAA derivatized D-leucine standard.

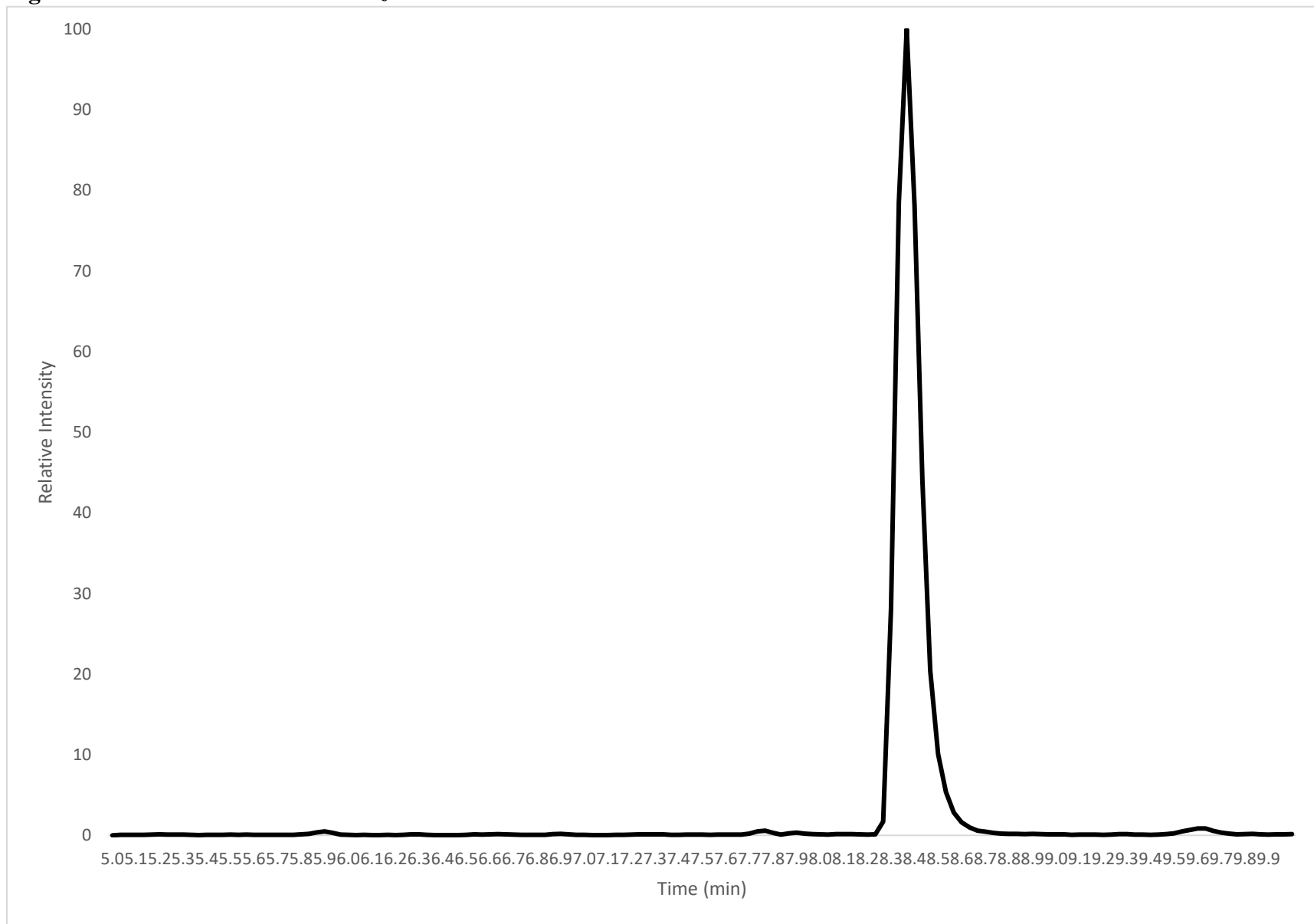


Figure 55. Selected ion trace for m/z 765-769 for FDAA derivatized L-leucine standard.

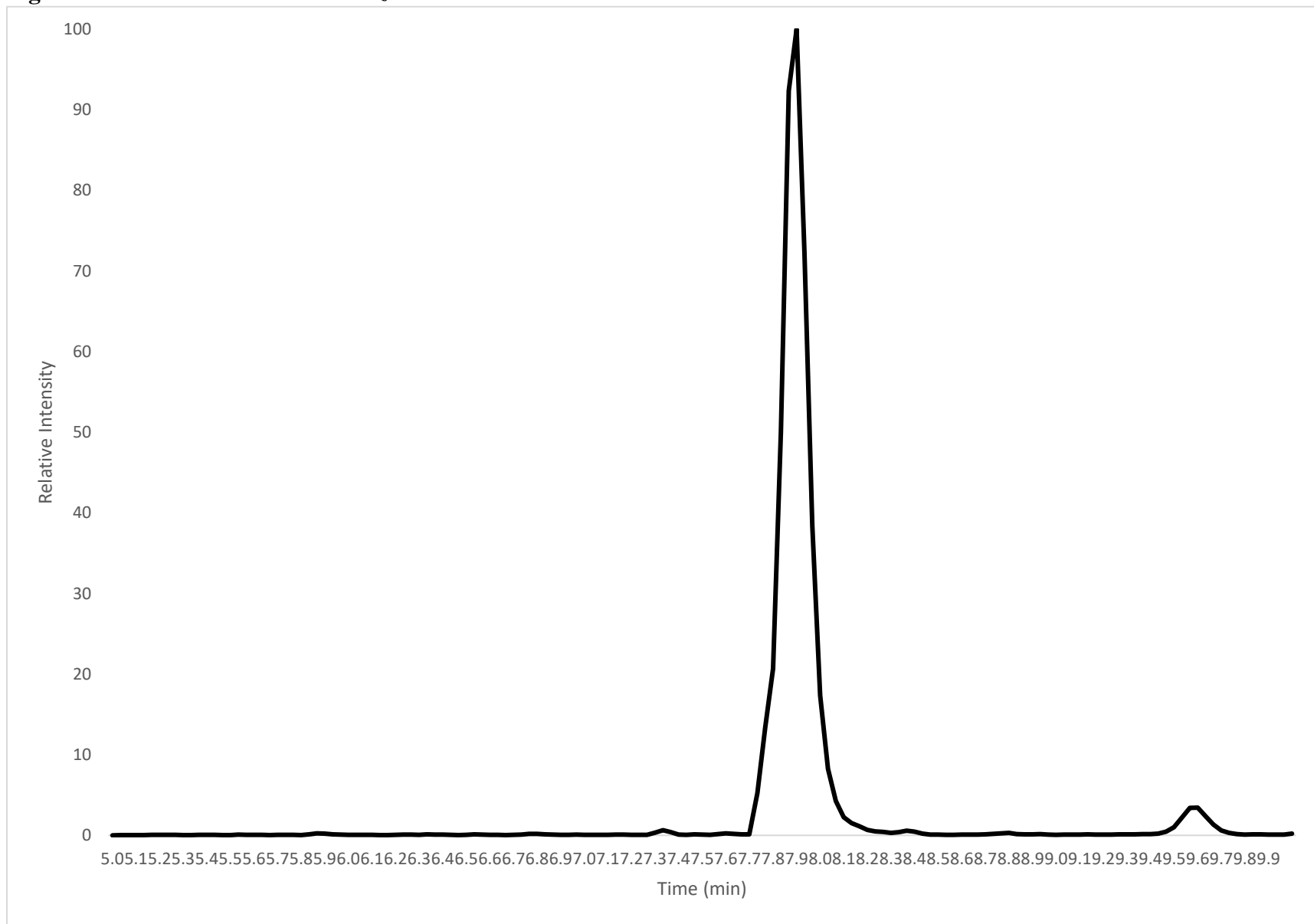


Figure 56. Selected ion trace for m/z 713-717 for FDAA derivatized D-serine standard.

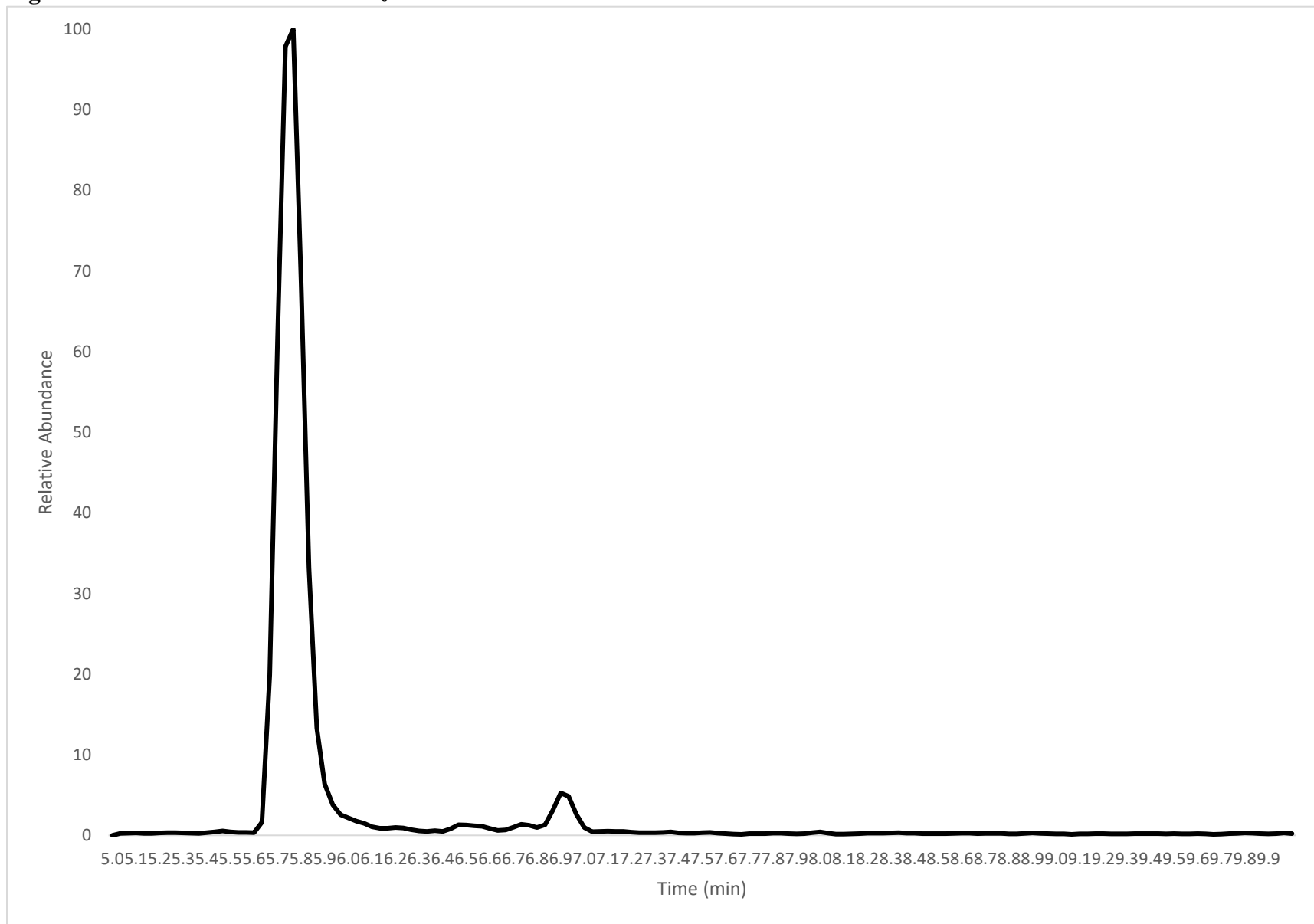


Figure 57. Selected ion trace for m/z 713-717 for FDAA derivatized L-serine standard.

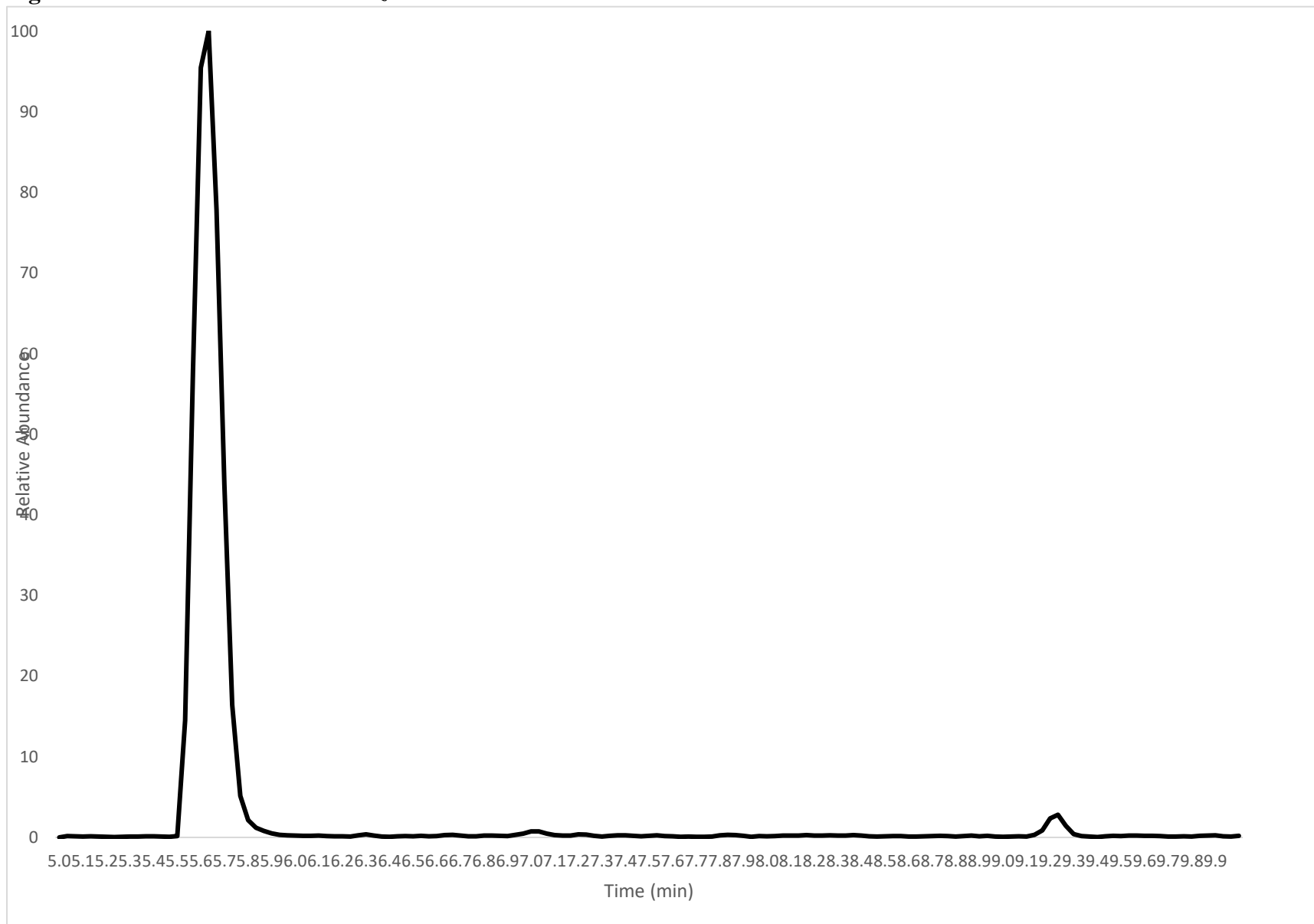


Figure 58. Selected ion trace for m/z 833-837 for FDAA derivatized D/L-phenylalanine mixture standard.

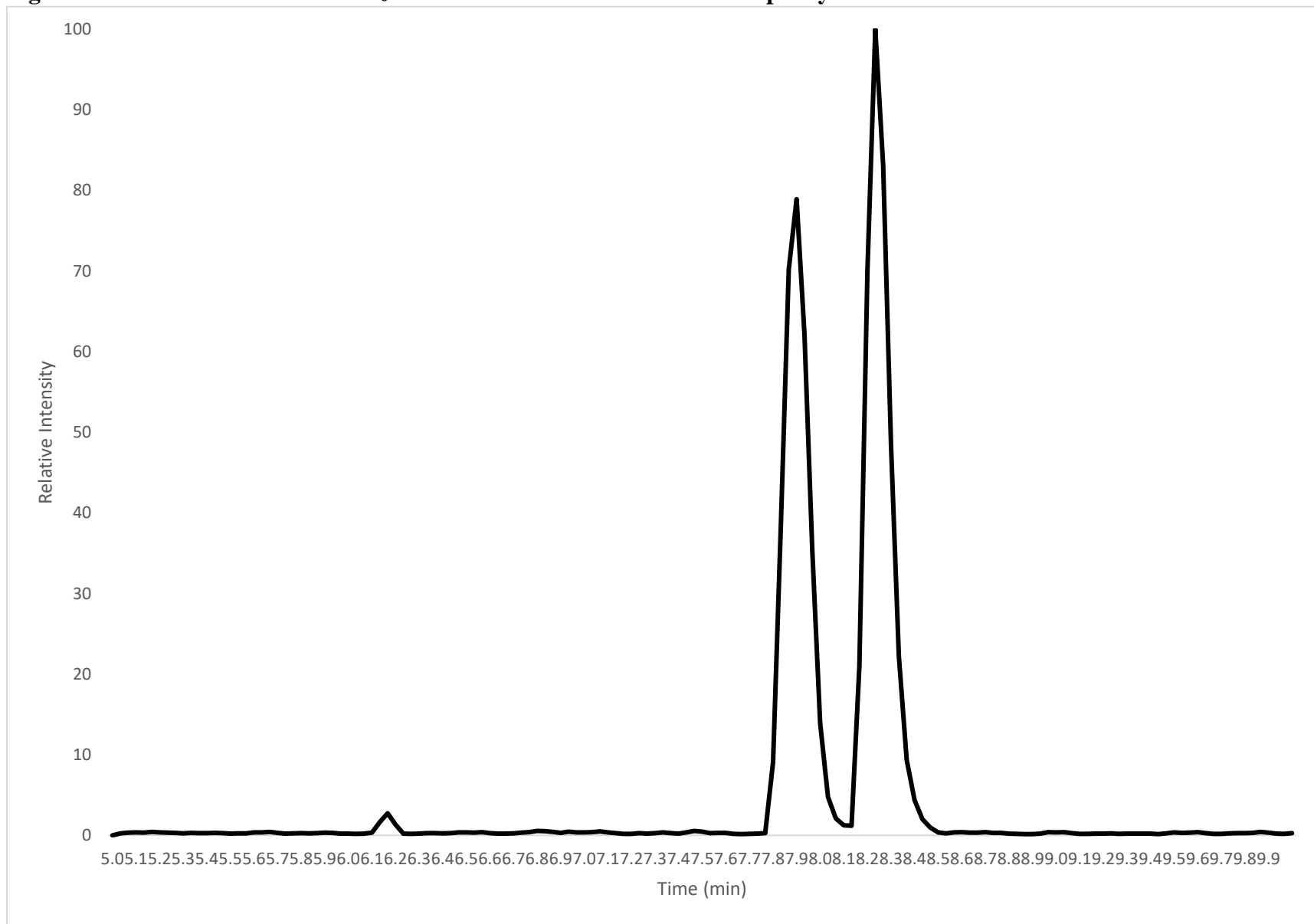


Figure 59. Selected ion trace for m/z 833-837 for FDAA derivatized L-phenylalanine standard.

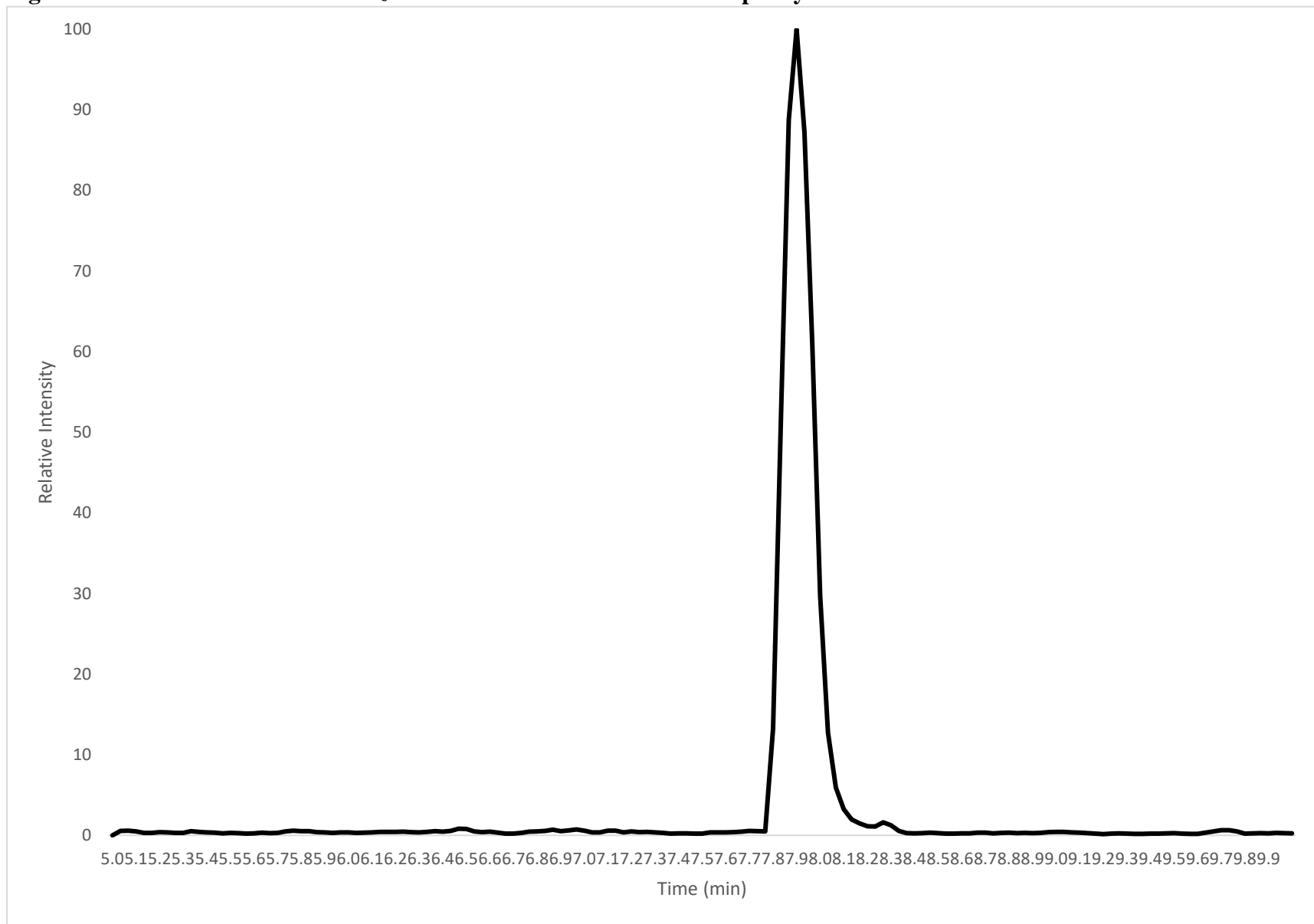


Figure 60. Selected ion trace for m/z 684-688 for FDAA derivatized D/L-tyrosine mixture standard.

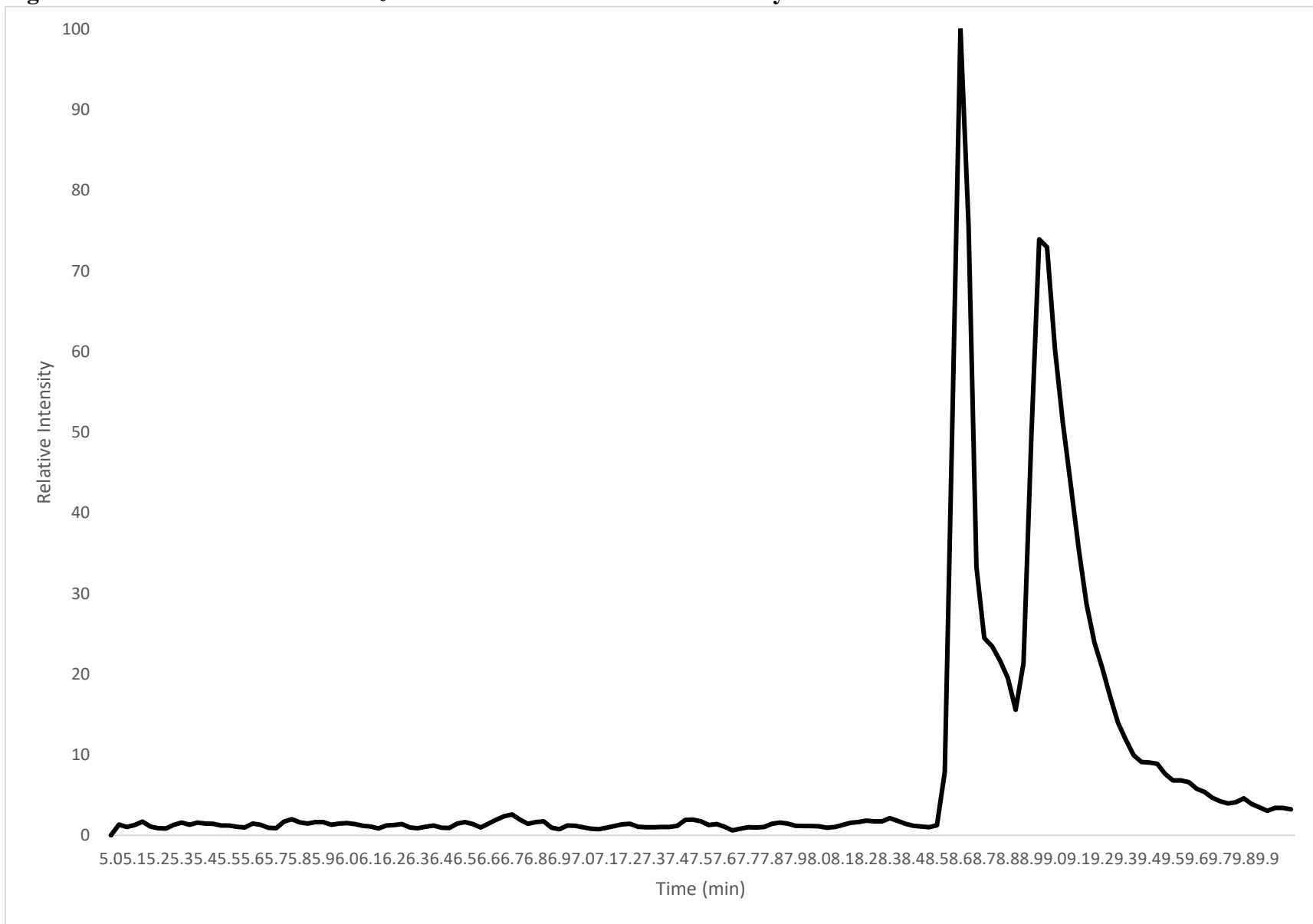


Figure 61. Selected ion trace for m/z 684-688 for FDAA derivatized L-tyrosine standard.

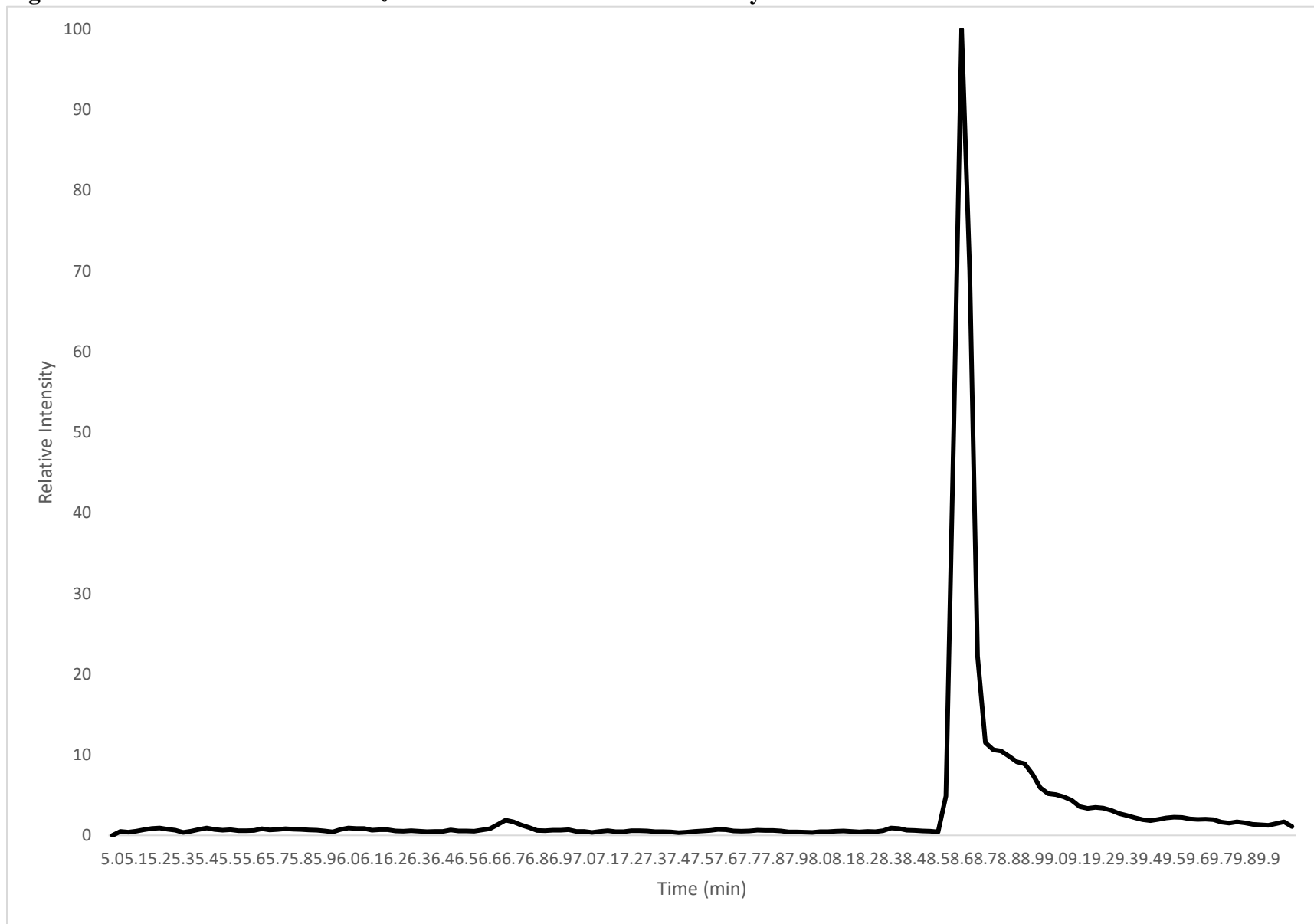


Table 12. Summary of Marfey's analysis retention times and peak assignments

	m/z	Retention Time (min)	2	3	4	5
D-Leucine	384	8.30	8.30	8.30	8.30	8.30
L-Leucine	384	7.83				
D-Serine	358	5.70				
L-Serine	358	5.57	5.57	5.57	5.57	5.53
L-Threonine	372	8.53				
D-allo-Threonine	372	5.90				
L-allo-Threonine	372	5.73	5.70	5.73	5.70	5.70
D-Phenylalanine	418	8.17	8.17	8.17	8.17	
L-Phenylalanine	418	7.83				
D-Tyrosine	434	8.87				8.93
L-Tyrosine	434	8.53				
D-Isoleucine	384	8.23				
L-Isoleucine	384	7.70	7.73		7.70	7.70
D-allo-Isoleucine	384	8.07				
L-allo-Isoleucine	384	7.90				
D-Valine	370	7.70				
L-Valine	370	7.20		7.17		

Table 13. Reported and observed optical rotation values ($[\alpha]_D^{20}$) for 3-hydroxy fatty acids.

Lipid	Literature Values		Serrawettin W2 (2)		Serrawettin W4 (3)		Serrawettin W5 (4)		Serrawettin W6 (5)	
	CHCl ₃	EtOH	CHCl ₃	EtOH	CHCl ₃	EtOH	CHCl ₃	EtOH	CHCl ₃	EtOH
R-3 hydroxy hexanoic acid	-20.0 (c. 3.0) ¹									
S-3-hydroxy hexanoic acid	26.8 (c. 1.1) ²									
R-3-hydroxy octanoic acid							-14.8 (c. 0.1)	4.9 (c. 0.1)		
S-3-hydroxy octanoic acid	14.2 (c. 0.5) ³									
R-3-hydroxy nonanoic acid	-20.5 (c. 1.14) ⁴									
R-3-hydroxy decanoic acid	-21 (2.5%) ⁵		-39.0 (c. 0.1)	5.0 (c. 0.1)	-20.0 (c. 0.1)	4.5 (c. 0.1)			-13.3 (c. 0.1)	4.2 (c. 0.1)
S-3-hydroxy decanoic acid	20 (c. 2.5) ⁶	Flip in sign noted but no value given								
R-3-hydroxy undecanoic acid	-12 (c. 1.0) ⁷									
R-3-hydroxy dodecanoic acid	-17.8 (c. 1.2) ⁸									

- (1) Le Sann, C.; Munoz, D. M.; Saunders, N.; Simpson, T. J.; Smith, D. I.; Soulas, F.; Watts, P.; Willis, C. L. *Org Biomol Chem* **2005**, *3*, 1719.
- (2) Wang, Y.-C.; Yan, T.-H. *The Journal of Organic Chemistry* **2000**, *65*, 6752.
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- (4) Kiho, T.; Nakayama, M.; Yasuda, K.; Miyakoshi, S.; Inukai, M.; Kogen, H. *Bioorganic & Medicinal Chemistry* **2004**, *12*, 337.
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- (6) Serck-Hanssen, K.; Stenhagen, E.; Hanshoff, G.; Prydz, H. *Acta Chemica Scandinavica* **1955**, *9*, 866.
- (7) Utaka, M.; Watabu, H.; Higashi, H.; Sakai, T.; Tsuboi, S.; Torii, S. *The Journal of Organic Chemistry* **1990**, *55*, 3917.
- (8) Guaragna, A.; Nisco, M. D.; Pedatella, S.; Palumbo, G. *Tetrahedron: Asymmetry* **2006**, *17*, 2839.

Table 14. *Candida albicans* SC5314 biofilm inhibition and growth inhibition properties of compound 1-5.

Compound	The IC ₅₀ ^a for Biofilm inhibition (μM)	The MIC ^b for growth inhibition (μM)
Viscosin (1)	4.63±1.02	>100
Serrawettin W2 (2)	7.73±0.70	>100
Serrawettin W4 (3)	59.75±5.69	>100
Serrawettin W5 (4)	13.41±0.17	>100
Serrawettin W6 (5)	29.17±0.42	>100

^aIC₅₀ expressed as the concentration corresponding to 50% of the yeast biofilm formation.

^bMIC were defined as the lowest concentration causing prominent growth reduction (in ≥80% reduction in the metabolic activity).