General. Spectrograde solvents were used without further purification with the exception of anhydrous methylene chloride, which was purchased from Aldrich. All ^{1}H and ^{13}C NMR spectra were recorded on Bruker spectrometers at the indicated frequency.

Data of staphyloferrin A

Diastereomer 1: Purity by HPLC 100%

^{1}H NMR (D_2O : CD_3COOD = 4:1; 500 MHz) δ 4.16 (m, 1H), 3.21 (t, J = 10 Hz, 2H), 2.80-2.70 (m, 4H), 2.70 (d, ^{2}J = 15 Hz, 1H), 2.66 (d, ^{2}J = 15 Hz, 1H), 2.62 ((d, ^{2}J = 15 Hz, 1H), 2.60 (d, ^{2}J = 15 Hz, 1H), 1.80 (m, 1H), 1.69 (m, 1H), 1.56 (m, 1H); **^{13}C NMR** (D_2O : CD_3COOD = 4:1; 500 MHz) δ 180.1, 179.9, 178.9, 178.0, 172.4, 172.0, 171.9, 74.8, 74.7, 54.9, 45.1, 44.9, 44.5, 44.2, 38.9, 29.1, 24.7; **HRMS (ESI)**: m/z calcd for $C_{17}H_{24}N_2O_{14}$ + Na^+ $[M+Na]^+$ 503.1125, found 503.1118.

$[\alpha]_D^{25}$ = - 4.8 (c 1.0, H_2O)

Diastereomer 2: Purity by HPLC 75.1%

^{1}H NMR (D_2O : CD_3COOD = 4:1; 500 MHz) δ 4.21 (m, 1H), 3.22 (t, J = 10 Hz, 2H), 2.92-2.87 (m, 2H), 2.82-2.75 (m, 2H), 2.75(d, ^{2}J = 15 Hz, 1H), 2.72 (d, ^{2}J = 15 Hz, 1H), 2.70 ((d, ^{2}J = 15 Hz, 1H), 2.66 (d, ^{2}J = 15 Hz, 1H), 1.84 (m, 1H), 1.73 (m, 1H), 1.59 (m, 1H); **^{13}C NMR** (D_2O : CD_3COOD = 4:1; 500 MHz) δ 179.0, 178.9, 178.4, 175.6, 171.9, 171.5, 74.3, 74.3, 54.0, 44.7, 44.4, 44.0, 44.9, 39.0, 29.1, 25.0; **HRMS (ESI)**: m/z calcd for $C_{17}H_{24}N_2O_{14}$ + Na^+ $[M+Na]^+$ 503.1125, found 503.1142.

$[\alpha]_D^{25}$ = - 4.8 (c 1.0, H_2O)

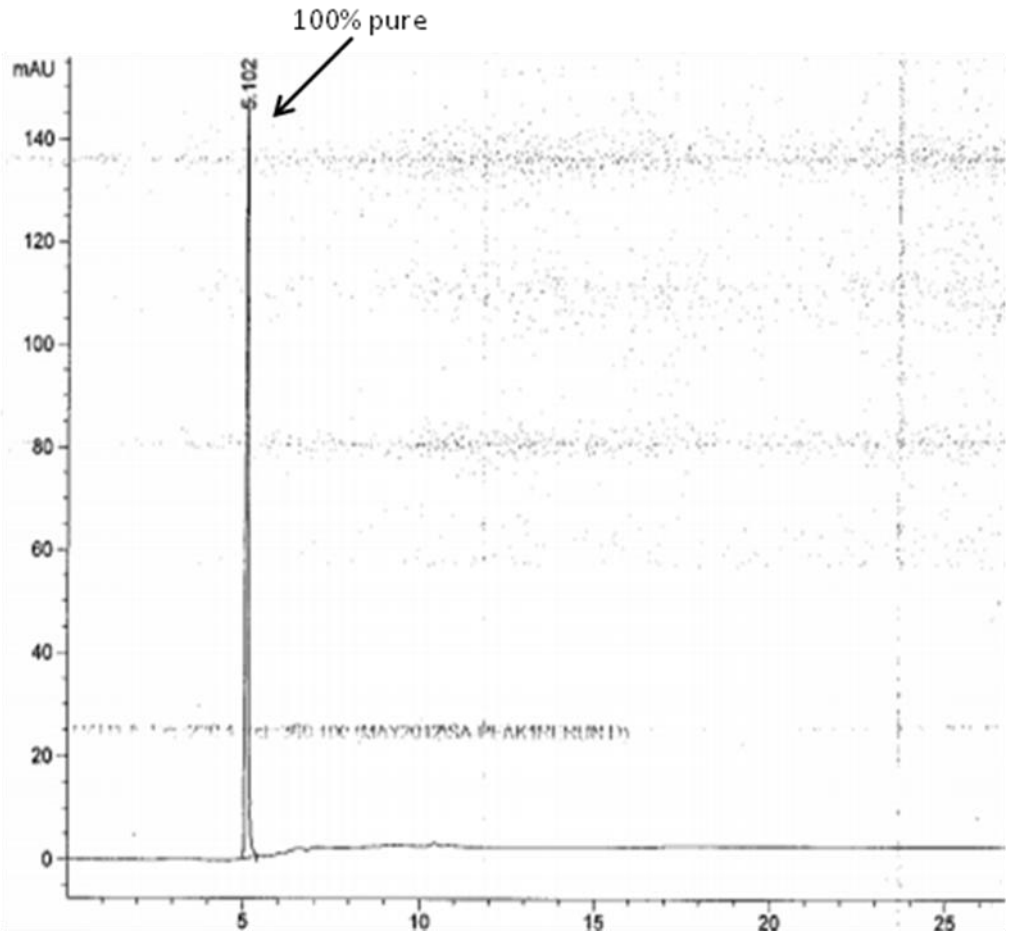

Figure S1. HPLC chromatogram of purified staphyloferrin A diastereomer 1

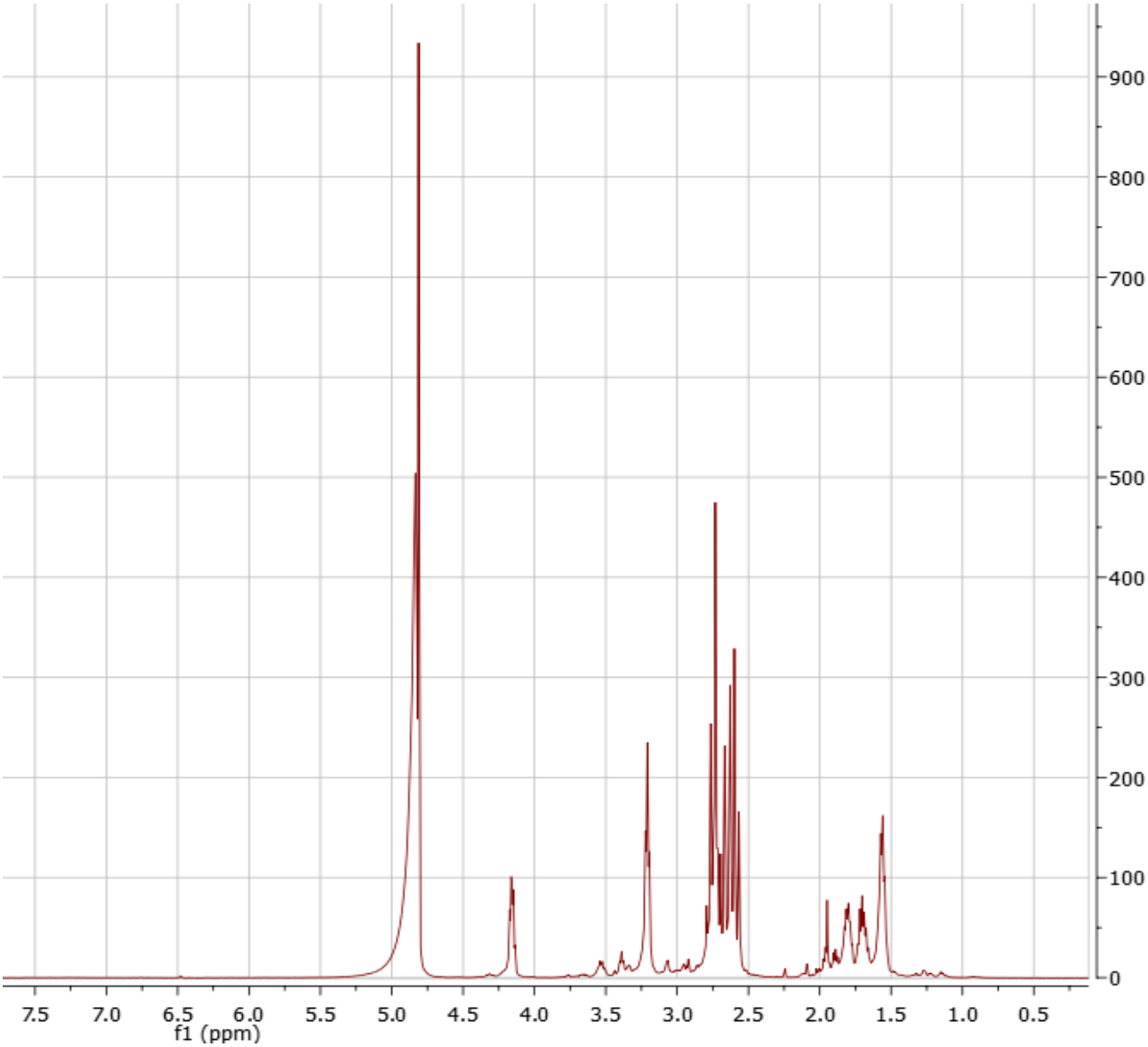

Figure S2. ^{1}H NMR spectrum of staphyloferrin A diastereomer 1. Bruker DRX500.

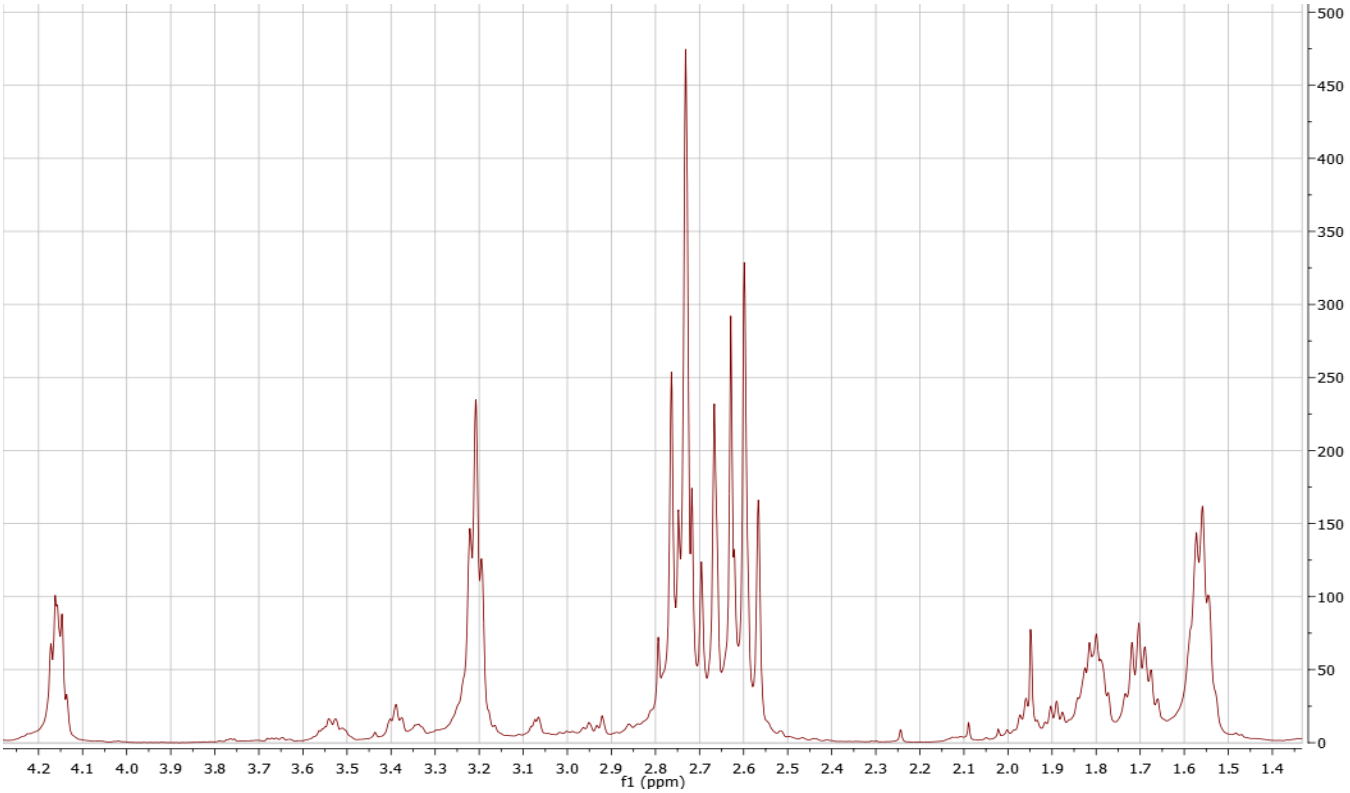

Figure S3. ^{1}H NMR spectrum of staphyloferrin A diastereomer 1 (expanded). Bruker DRX500.

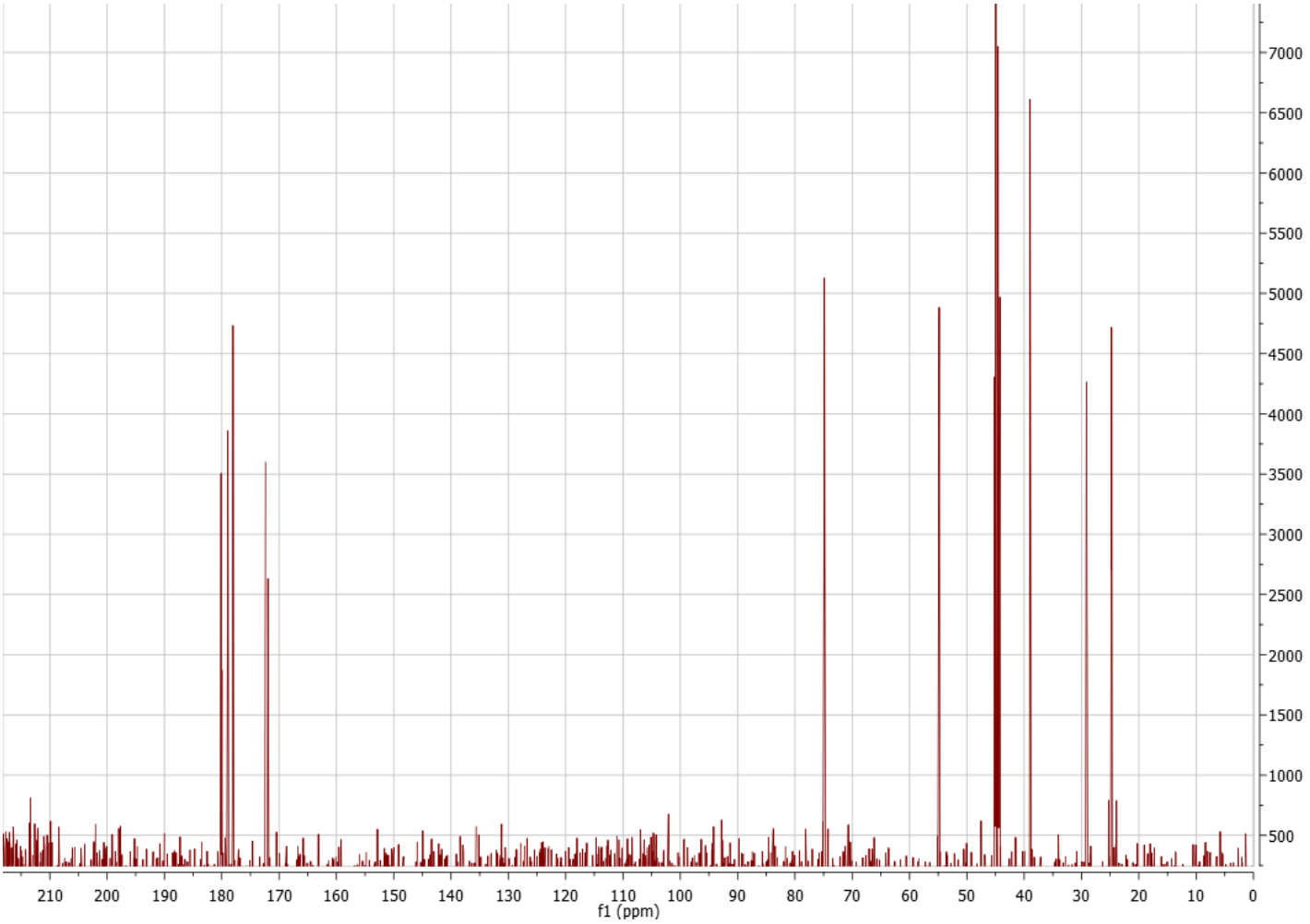

Figure S4. ^{13}C NMR spectrum of staphyloferrin A diastereomer 1. Bruker DRX500.

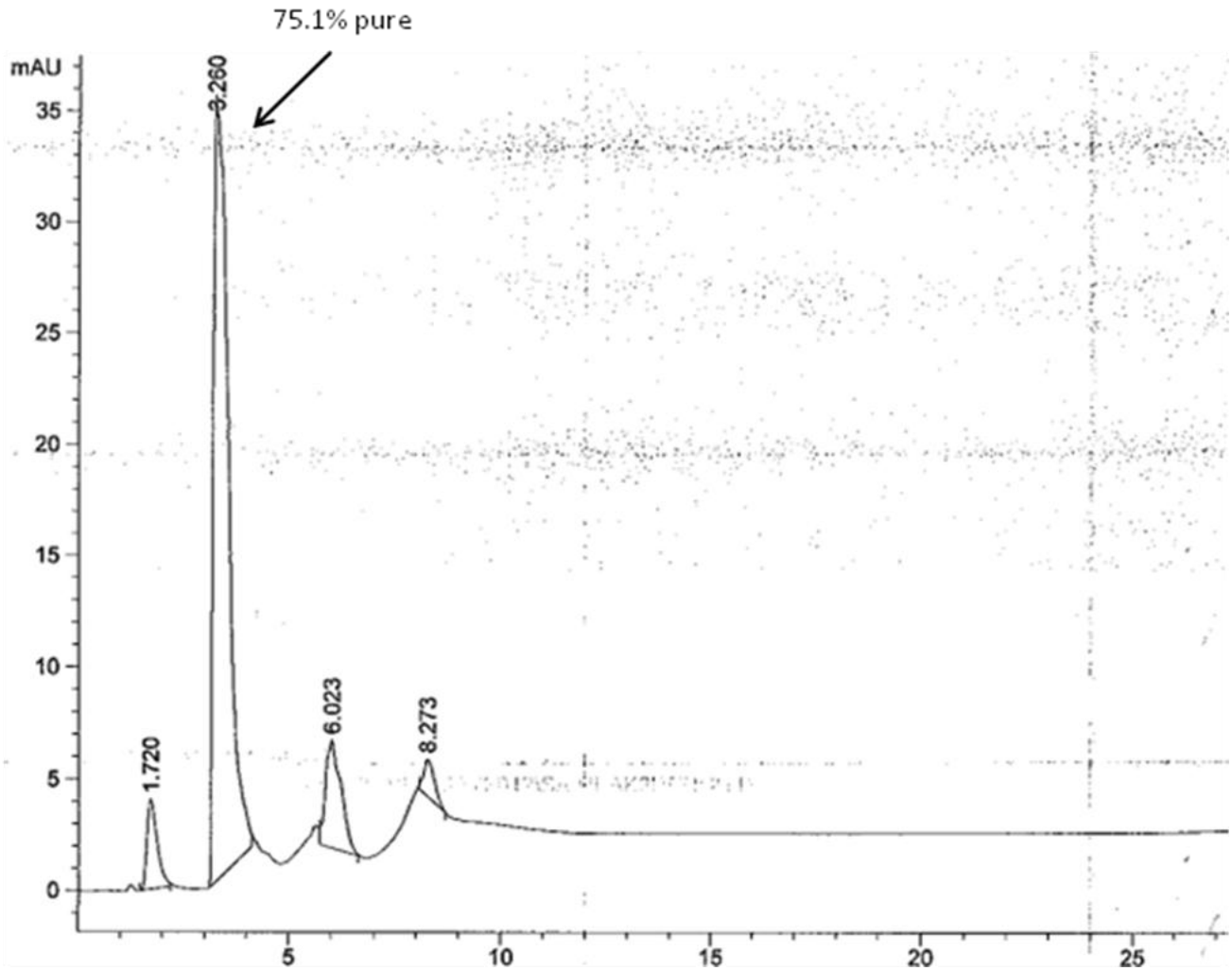

Figure S5. HPLC chromatogram of purified staphyloferrin A diastereomer 2.

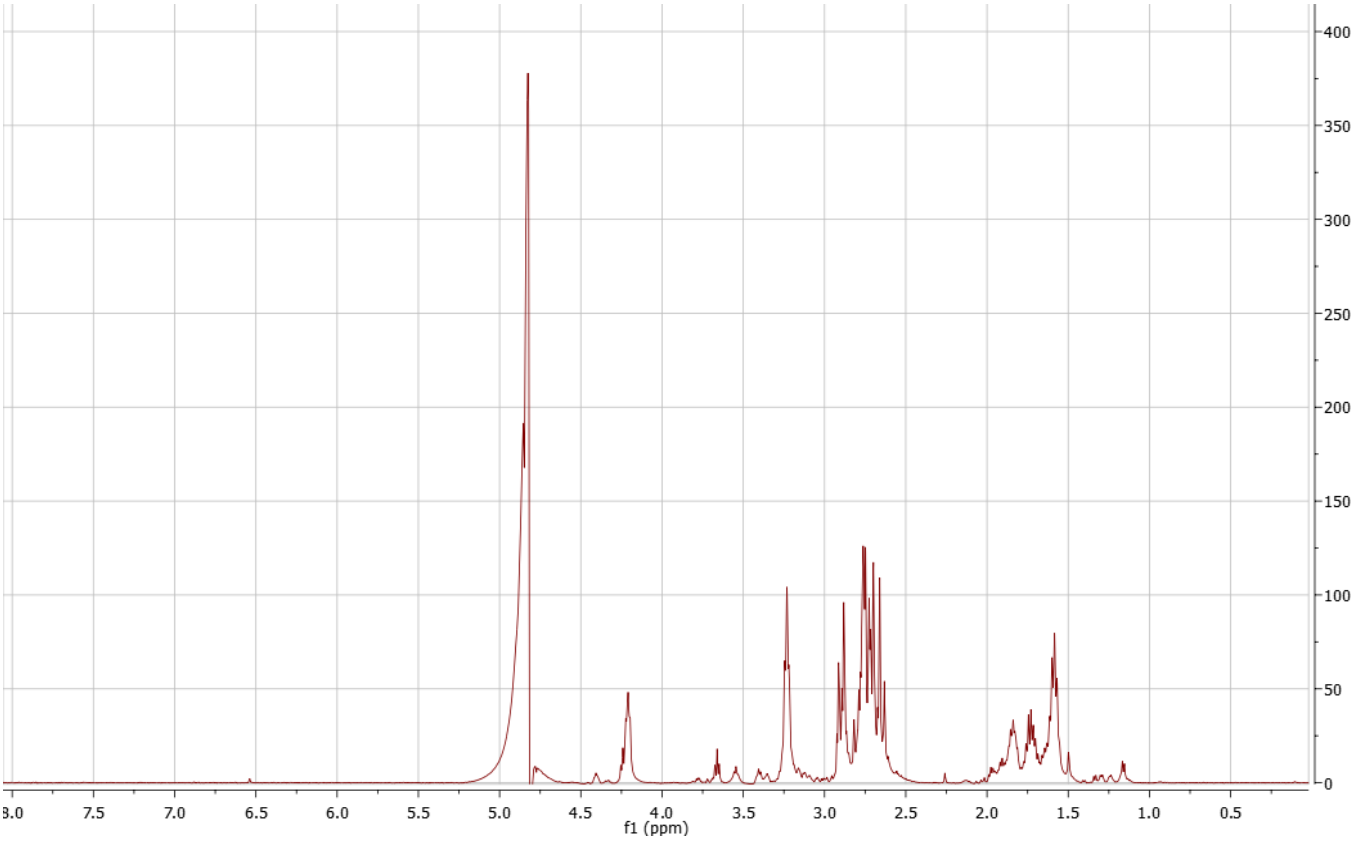

Figure S6. 1H NMR spectrum of staphyloferrin A diastereomer 2. Bruker DRX500.

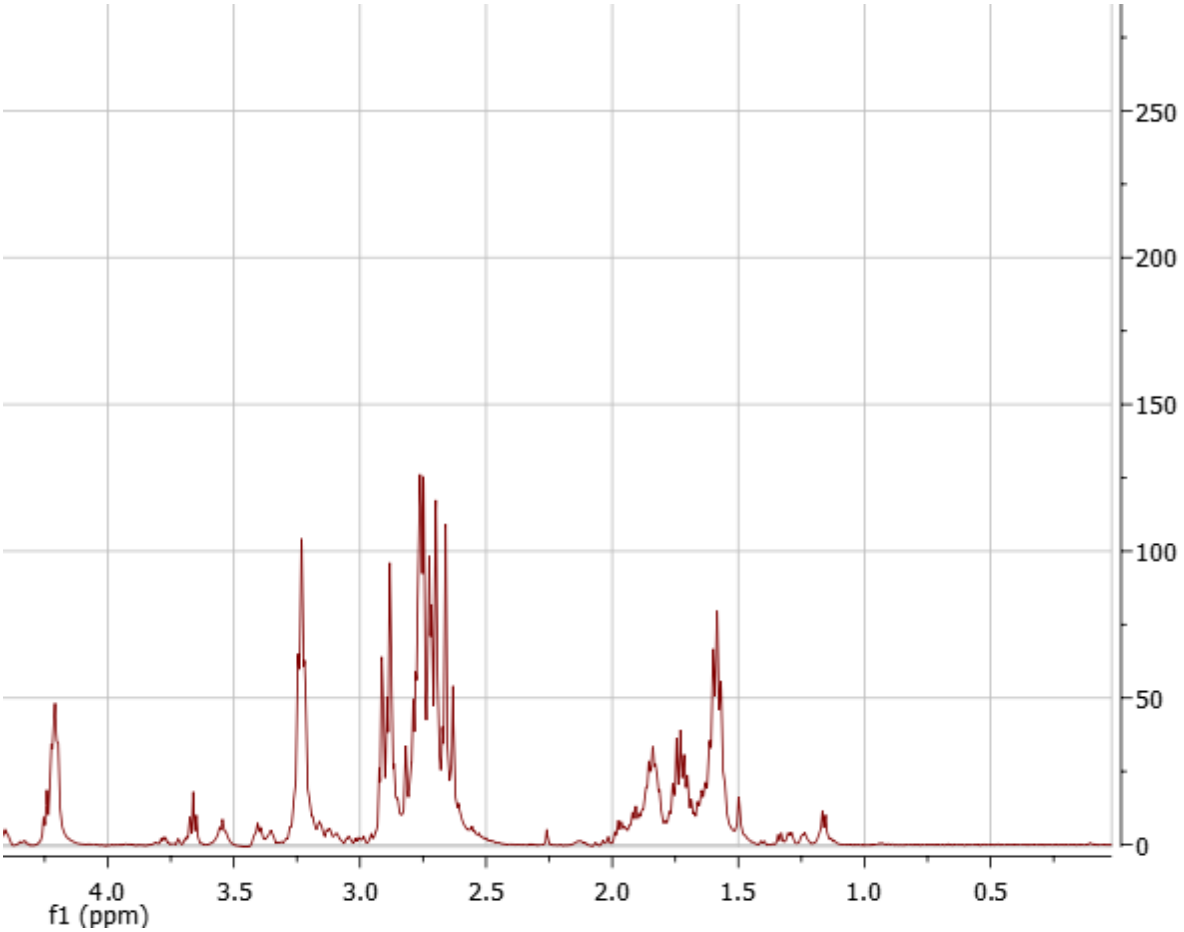

Figure S7. ^{1}H NMR spectrum of staphyloferrin A diastereomer 2 (expanded). Bruker DRX500.

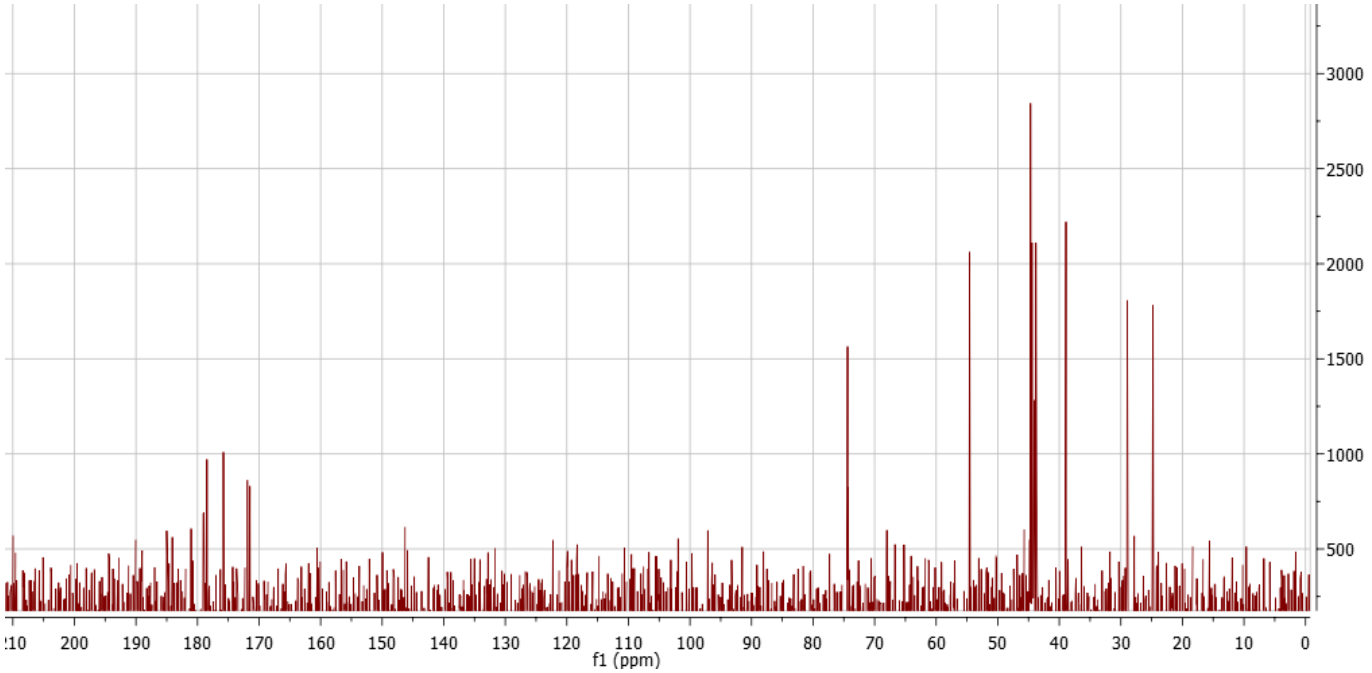

Figure S8. ^{13}C NMR spectrum of staphyloferrin A diastereomer 2. Bruker DRX500.