

Supporting Information
for
Partial thioamide scan on the lipopeptaibiotic trichogin GA IV. Effects on
folding and bioactivity

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Chemical characterization data for the peptides reported in Schemes 1–3.

Table S-I: ROE constraints, deviations from idealized geometry, and mean energies for the NMR-based structures (energy < 144 kcal/mol) of ψ [CS-NH]⁹.

Number of NOEs	
total	69
intraresidue	24
sequential	23
$i, i+n, n = 2, 3, 4$	22
Mean rmsd ^(a) from ideality of accepted structures	
bonds (Å)	0.0086
angles (°)	1.05
impropers (°)	67.0
ROEs (Å)	0.118
Mean energies (kcal/mol) of accepted structures	
E _{overall}	140.8
E _{bond}	12.6
E _{angle}	46.7
E _{ROE}	44.3

(a) Root-mean-square deviation.

Table S-II: Average values (°) for the torsion angles ϕ_m and ψ_m and their relative standard deviations resulting from the 18 calculated structures (energy < 144 kcal/mol) of ψ [CS-NH]⁹ (400 MHz, 1 mM in CD₃CN solution, 298 K).

Residue	ϕ_m	$\Delta\phi$	ψ_m	$\Delta\psi$
Aib ¹	—	—	67.1	±1.0
Gly ²	146.8	±5.3	-33.5	±2.6
L-Leu ³	-46.2	±2.6	-45.1	±3.2
Aib ⁴	-79.5	±1.0	-24.6	±3.2
Gly ⁵	-130.2	±4.9	-22.2	±5.0
Gly ⁶	-71.8	±2.6	-25.3	±1.7
L-Leu ⁷	-74.5	±1.5	-28.1	±3.5
Aib ⁸	-62.2	±3.8	-28.3	±1.7
Gly ⁹ (CS)	-89.2	±4.9	-52.2	±1.1
L-Ile ¹⁰	-106.1	±2.8	-16.0	±3.1
L-Leu-OMe ¹¹	-49.1	±8.1	—	—

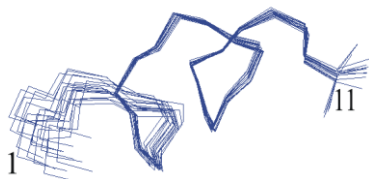


Figure S-I: Representation of the 18 3D structures with energy < 144 kcal/mol resulting from the MD calculations of ψ [CS-NH]⁹ with the backbone atoms of residues 4–11 superimposed.

Chemical characterization data for the peptides reported in Schemes 1–3 and not characterized elsewhere [1-5]

Boc-Aib-Gly-Ile-Leu-OMe: mp 170–172 °C; R_{f1} 0.40; R_{f2} 0.85; R_{f3} 0.30; $[\alpha]_D^{20}$: -91.1 (*c* 0.1, MeOH); $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 7.86 (d, 1H, Ile NH), 7.00 (t, 1H, Gly NH), 6.77 (d, 1H, Leu NH), 5.02 (s, 1H, Aib NH), 4.64–4.52 (m, 1H, Leu α -CH), 4.34–4.27 (m, 1H, Ile α -CH), 3.95–3.27 (d, 2H, Gly α -CH₂), 3.70 (s, 3H, OMe CH₃), 2.07 (m, 1H, Ile β -CH), 1.78–1.63 (m, 20H, Leu γ -CH, Boc 3 CH₃, Aib 2 β -CH₃, Leu β -CH₂, Ile γ -CH₂), 0.95–0.85 (m, 12H, Leu 2 δ -CH₃, Ile γ - and δ -CH₃); IR (KBr) 3288, 1756, 1652, 1526 cm^{-1} .

Boc-Gly-Leu-Aib-Gly-Ile-Leu-OMe: mp 82–84 °C; R_{f1} 0.40; R_{f2} 0.95; R_{f3} 0.30; $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 7.86–7.22 (d, 1H, Leu NH), 7.34–7.30 (m, 2H, Ile NH, Gly NH), 6.99 (s, 1H, Aib NH), 6.73–6.69 (d, 1H, Leu NH), 5.68–5.62 (t, 1H, Gly NH), 4.18–3.35 (m, 10H, 2 Leu α -CH, Ile α -CH, 2 Gly α -CH₂, OMe CH₃), 2.08 (m, 1H, Ile β -CH), 1.64–1.50 (m, 14H, 2 Leu β -CH₂, 2 Leu γ -CH, Aib 2 β -CH₃), 1.41 (s, 9H, Boc 3 CH₃, Ile γ -CH₂), 0.95–0.82 (m, 18H, 2 Leu 2 δ -CH₃, Ile γ - and δ -CH₃); IR (KBr): 3315, 1654, 1536 cm^{-1} .

Boc-Gly- ψ [CS-NH]-Leu-Aib-OMe: mp 79–82 °C; R_{f1} 0.90; R_{f2} 0.90; R_{f3} 0.45; $[\alpha]_D^{20}$ -58.8 (*c* 0.5, MeOH); $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 8.97 (d, 1H, Leu NH), 7.08 (s, 1H, Aib NH), 5.51 (m, 1H, Gly NH), 4.43 (m, 2H, Gly α -CH₂), 4.12 (m, 1H, Leu α -CH), 3.71 (s, 3H, OMe CH₃), 1.66 (m, 3H; Leu β -CH₂ and γ -CH), 1.51 (m, 6H, Aib 2 β -CH₃), 1.41 (s, 9H Boc 3 CH₃), 0.93 (d, 6H, Leu 2 δ -CH₃); IR (KBr): 3446, 3280, 1738, 1720, 1694, 1652, 1547, 1526 cm^{-1} .

Boc-Aib-Gly- ψ [CS-NH]-Leu-Aib-OMe: mp 175–178 °C; R_{f1} 0.85; R_{f2} 0.90; R_{f3} 0.20; $[\alpha]_D^{20}$ -40.9 (*c* 0.5, MeOH); $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 8.97 (d, 1H, Leu NH) 7.08 (s, 1H, Aib NH), 6.10 (s, 1H, Aib NH), 5.51 (m, 1H, Gly NH), 4.43 (m, 2H, Gly α -CH₂), 4.12 (m, 1H, Leu α -CH), 3.71 (s, 3H, OMe CH₃), 1.66 (m, 3H; 2H Leu β -CH₂ and γ -CH), 1.51 (m, 12H, 2 Aib 2 β -CH₃), 1.41 (s, 9H Boc 3 CH₃), 0.93 (d, 6H, Leu 2 δ -CH₃); IR (KBr): 3349, 3265, 1717, 1691, 1665, 1510 cm^{-1} .

***n*-Oct-Aib-Gly- ψ [CS-NH]-Leu-Aib-OMe:** oil; R_{f1} 0.81; R_{f2} 0.90; R_{f3} 0.15; $[\alpha]_D^{20}$ -5.68 (*c* 0.2, MeOH); $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 8.97 (d, 1H, Leu NH) 7.08 (s, 1H, Aib NH), 6.10 (s, 1H, Aib NH), 5.51 (m, 1H, Gly NH), 4.43 (m, 2H, Gly α -CH₂), 4.12 (m, 1H, Leu α -CH), 3.71 (s, 3H, OMe CH₃), 2.28 (m, 2H, *n*-Oct β -CH₂), 1.66 (m, 3H, Leu β -CH₂ and γ -CH), 1.51 (m, 12H, 2 Aib 2 β -CH₃), 1.26 (m, 10H, *n*-Oct 5 CH₂), 0.93–0.82 (m, 9H, Leu 2 δ -CH₃ and *n*-Oct ω -CH₃); IR (KBr): 3313, 3240, 1742, 1730, 1650, 1531 cm^{-1} .

***n*-Oct-Aib-Gly- ψ [CS-NH]-Leu-Aib-OH:** R_{f1} 0.10; R_{f2} 0.70; R_{f3} 0.00; $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 8.97 (d, 1H, Leu NH) 7.08 (s, 1H, Aib NH), 6.10 (s, 1H, Aib NH), 5.51 (m, 1H, Gly NH), 4.43 (m, 2H, Gly α -CH₂), 4.12 (m, 1H, Leu α -CH), 2.28 (m, 2H, *n*-Oct β -CH₂), 1.66 (m, 3H, Leu β -CH₂ and γ -CH), 1.51 (m, 12H, 2 Aib 2 β -CH₃), 1.26 (m, 10H, *n*-Oct 5 CH₂), 0.93–0.82 (m, 9H, Leu 2 δ -CH₃ and *n*-Oct ω -CH₃); IR (KBr): 3310, 3044, 1720, 1650, 1531 cm^{-1} .

***n*-Oct-Aib-Gly- ψ [CS-NH]-Leu-Aib-Gly-Gly-Leu-Aib-Gly-Ile-Leu-OMe:** mp 114–116 °C; R_{f1} 0.20; R_{f2} 0.85; R_{f3} 0.00; $[\alpha]_D^{20}$ -38.61 (*c* 0.5, MeOH); $^1\text{H NMR}$ (400 MHz, CD_3CN) δ 9.30 (d, 1H, NH Leu³), 7.77 (t, 1H, NH Gly⁶), 7.49 (t, 1H, NH Gly²), 7.47 (t, 1H, NH Gly⁵), 7.47 (s, 1H, NH Aib⁴), 7.42 (t, 1H, NH Gly⁹), 7.40 (d, 1H, NH Leu⁷), 7.37 (s, 1H, NH Aib⁸), 7.30 (d, 1H, NH Ile¹⁰), 7.22 (s, 1H, NH Aib¹), 7.12 (d, 1H, NH Leu¹¹), 4.21 (m, 1H, α -CH Leu¹¹), 4.20 (m, 1H, α -CH Leu⁷), 4.17 (m, 1H, α -CH Leu³), 4.05 (dd, 1H, α -CH Ile¹⁰), 3.78 (dd, 1H, 1 α -CH Gly⁶), 3.74 (dd, 1H, 1 α -CH Gly⁶), 3.71 (s, 3H, CH₃ OMe), 3.67 (dd, 1H, 1 α -CH Gly⁹), 3.65 (dd, 1H, 1 α -CH Gly²), 3.64 (m, 2H, α -CH₂ Gly⁵), 3.60 (dd, 1H, 1 α -CH Gly⁹), 3.58 (dd, 1H, 1 α -CH Gly²), 2.15 (t, 2H, β -CH₂ *n*-Oct), 1.50 (m, 2H, γ -CH₂ *n*-Oct), 2.15 (m, 2H, δ -CH₂ *n*-Oct), 1.84 (m, 1H, β -CH Ile¹⁰), 1.53 (m, 2H, β -CH₂ Leu⁷), 1.53 (m, 2H, β -CH₂ Leu³), 1.62 (m, 1H, γ -CH Leu³), 1.60 (m, 1H, γ -CH Leu⁷), 1.59 (m, 1H, γ -CH Leu¹¹), 1.48 (m, 1H, 1 β -CH Leu¹¹), 1.53 (m, 1H, 1 β -CH Leu¹¹), 1.45 (m, 1H, γ -CH Ile¹⁰), 1.36 (s, 6H, 2 β -CH₃ Aib⁴), 1.35 (s, 6H, 2 β -CH₃ Aib⁸), 1.32 (s, 6H, 2 β -CH₃ Aib¹), 1.17 (m, 1H, 1 γ -CH Ile¹⁰), 0.88 (m, 3H, δ -CH₃ Leu³), 0.87 (m, 3H, δ -CH₃ Leu¹¹), 0.86 (d, 3H, γ -CH₃ Ile¹⁰), 0.83 (m, 3H, δ -CH₃ Leu³), 0.81 (m, 3H, δ -CH₃ Ile¹⁰), 0.80 (t, 3H, ω -CH₃ *n*-Oct), 0.78 (m, 3H, δ -CH₃ Leu¹¹); IR (KBr): 3314, 3057, 1744, 1656, 1537 cm^{-1} .

Z-Gly-Leu-Aib-Ot-Bu: mp 112–114 °C; R_{f1} 0.80; R_{f2} 0.65; R_{f3} 0.50; $[\alpha]_D^{20}$ -39.0 (*c* 0.5, MeOH); $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 7.33 (m, 5H, Z Ph), 6.85 (s, 1H, Aib NH), 6.79 (d,

1H, Leu NH), 5.70 (t, 1H, Gly NH), 5.10 (s, 2H, Z CH₂), 4.40 (m, 1H, Leu α -CH), 3.86 (t, 2H, Gly α -CH₂), 1.58 (m, 3H; Leu β -CH₂ and γ -CH), 1.51 (2s, 6H, Aib 2 β -CH₃), 1.43 (s, 9H, *Ot*-Bu 3 CH₃), 0.91 (d, 6H, Leu 2 δ -CH₃); IR (KBr): 3324, 1731, 1705, 1659, 1546 cm⁻¹.

Z-Aib-Gly-Leu-Aib-*Ot*-Bu: mp 165–166 °C; *R*_{f1} 0.50; *R*_{f2} 0.80; *R*_{f3} 0.30; [α]_D²⁰ -3.2 (*c* 0.5, MeOH); ¹H NMR (200 MHz, CDCl₃) δ 7.36 (m, 6H, Z Ph and 1 NH), 6.93 (m, 1H, NH), 6.87 (s, 1H, Aib NH), 5.37 (s, 1H, Aib NH), 5.10 (2d, 2H, Z CH₂), 4.42 (m, 1H, Leu α -CH), 3.93 (d, 2H, Gly α -CH₂), 1.70–1.68 (m, 3H, Leu β -CH₂ and γ -CH), 1.50–1.48 (m, 12H, 2 Aib 2 β -CH₃), 1.42 (s, 9H, *Ot*-Bu 3 CH₃), 0.91 (m, 6H, 2 Leu δ -CH₃); IR (KBr): 3316, 1732, 1701, 1659, 1536 cm⁻¹.

***n*-Oct-Aib-Gly-Leu-Aib-*Ot*-Bu:** mp 169–171 °C; *R*_{f1} 0.45; *R*_{f2} 0.55; *R*_{f3} 0.30; [α]_D²⁰ -2.58 (*c* 0.5, MeOH); ¹H NMR (200 MHz, CDCl₃) δ 6.93 (m, 1H, NH), 6.87 (s, 1H, Aib NH), 5.37 (s, 1H, Aib NH), 4.42 (m, 1H, Leu α -CH), 3.93 (d, 2H, Gly α -CH₂), 2.23 (m, 2H *n*-Oct β -CH₂) 1.70–1.68 (m, 3H, Leu β -CH₂ and γ -CH), 1.50–1.48 (m, 12H, 2 Aib 2 β -CH₃), 1.42 (s, 9H, *Ot*-Bu 3 CH₃), 1.26 (m, 10H, *n*-Oct 5 CH₂), 0.95–0.82 (m, 6H, 2 Leu δ -CH₃, *n*-Oct ω -CH₃); IR (KBr): 3315, 1740, 1709, 1656, 1536 cm⁻¹.

Fmoc-Gly- ψ [CS-NH]-Gly-Leu-Aib-*Ot*-Bu: mp 108–111 °C; *R*_{f1} 0.72; *R*_{f2} 0.94; *R*_{f3} 0.22; [α]_D²⁰ -18.6 (*c* 0.5, MeOH); ¹H NMR (200 MHz, CDCl₃) δ 8.98 (t, 1H, Gly NH), 7.75 (d, 2H, Fmoc), 7.58 (t, 2H, Fmoc), 7.49 (m, 2H, Fmoc), 6.81 (s, 1H, Aib NH), 6.67 (t, 1H, Leu NH), 5.99 (t, 1H, Gly NH), 5.02 (m, H, Leu α -CH), 4.61–4.73(m,3H, Fmoc), 3.95–3.27 (d, 4H, 2Gly α -CH₂), 1.63–1.78(m, 9H, Leu β -CH₂ and γ -CH, Aib 2 β -CH₃), 1.43 (s, 9H, *Ot*-Bu 3 CH₃), 0.92 (m, 6H, Leu 2 δ -CH₃); IR (KBr): 3299, 1730, 1706, 1658, 1528 cm⁻¹.

Fmoc-Gly- ψ [CS-NH]-Gly-Leu-Aib-Gly-Ile-Leu-OMe: mp 126–128 °C; *R*_{f1} 0.74; *R*_{f2} 0.92; *R*_{f3} 0.15; [α]_D²⁰ -17.3 (*c* 0.5, MeOH); ¹H NMR (200 MHz, CDCl₃) δ 8.98 (t, 1H, Gly NH), 7.86 (d, 1H, Ile NH), 7.75 (d, 2H, Fmoc), 7.58 (t, 2H, Fmoc), 7.49 (m, 2H, Fmoc), 7.00 (t, 1H, Gly NH), 6.81 (s, 1H, Aib NH), 6.67 (m, 2H, 2 Leu NH), 5.99 (t, 1H, Gly NH), 5.02 (m, 2H, 2 Leu α -CH), 4.62–4.87 (m, 3H, Fmoc), 4.34–4.27 (m, 1H, Ile α -CH), 3.95–3.27 (d, 6H, 3Gly α -CH₂), 2.07 (m, 1H, Ile β -CH), 1.78–1.63 (m, 14H, 2 Leu β -CH₂ and γ -CH, Aib 2 β -CH₃, Ile γ -CH₂), 1.43 (s, 9H, *Ot*-Bu 3 CH₃), 0.95–0.85 (m, 24H, 2 Leu 2 δ -CH₃, Ile γ -CH₃ and δ -CH₃); IR (KBr): 3309, 3065, 1730, 1656, 1531cm⁻¹.

***n*-Oct-Aib-Gly-Leu-Aib-Gly-ψ[CS-NH]-Gly-Leu-Aib-Gly-Ile-Leu-OMe:** mp 125–128 °C; R_{f1} 0.20; R_{f2} 0.85; R_{f3} 0.00; $[\alpha]_D^{20}$ -21.3 (*c* 0.5, MeOH); $^1\text{H NMR}$ (200 MHz, CD_3CN) δ 9.42 (t, 1H, NH Gly⁶), 7.75 (t, 1H, NH Gly⁵), 7.67 (d, 1H, NH Leu³), 7.540 (s, 1H, NH Aib⁴), 7.40 (t, 1H, NH Gly²), 7.33 (t, 1H, NH Gly⁹), 7.29 (d, 1H, NH Ile¹⁰), 7.28 (d, 1H, NH Leu⁷), 7.27 (s, 1H, NH Aib⁸), 7.17 (s, 1H, NH Aib¹), 7.07 (d, 1H, NH Leu¹¹), 4.21 (m, 1H, α -CH Leu¹¹), 4.20 (m, 1H, α -CH Leu⁷), 4.17 (m, 1H, α -CH Leu³), 4.05 (dd, 1H, α -CH Ile¹⁰), 3.78 (dd, 1H, 1 α -CH Gly⁶), 3.74 (dd, 1H, 1 α -CH Gly⁶), 3.71 (s, 3H, CH₃ OMe), 3.67 (dd, 1H, 1 α -CH Gly⁹), 3.65 (dd, 1H, 1 α -CH Gly²), 3.64 (m, 2H, α -CH Gly⁵), 3.60 (dd, 1H, 1 α -CH Gly⁹), 3.58 (dd, 1H, 1 α -CH Gly²), 2.15 (t, 2H, β -CH₂ *n*-Oct), 2.15 (m, 2H, δ -CH₂ *n*-Oct), 1.84 (m, 1H, β -CH Ile¹⁰), 1.68 (m, 1H, γ -CH Leu³), 1.60 (m, 1H, γ -CH Leu⁷), 1.59 (m, 1H, γ -CH Leu¹¹), 1.53 (m, 1H, 1 β -CH Leu¹¹), 1.53 (m, 2H, β -CH₂ Leu⁷), 1.53 (m, 2H, β -CH₂ Leu³), 1.50 (m, 2H, γ -CH₂ *n*-Oct), 1.48 (m, 1H, 1 β -CH Leu¹¹), 1.47 (m, 1H, γ -CH₂ Ile¹⁰), 1.46 (s, 6H, 2 β -CH₃ Aib⁴), 1.35 (s, 6H, 2 β -CH₃ Aib⁸), 1.32 (s, 6H, 2 β -CH₃ Aib¹), 1.28 (m, 1H, 1 γ -CH₂ Ile¹⁰), 0.88 (m, 3H, δ -CH₃ Leu³), 0.87 (m, 3H, δ -CH₃ Leu¹¹), 0.86 (d, 3H, γ -CH₃ Ile¹⁰), 0.83 (m, 3H, δ -CH₃ Leu³), 0.81 (m, 3H, δ -CH₃ Ile¹⁰), 0.80 (t, 3H, ω -CH₃ *n*-Oct), 0.78 (m, 3H, δ -CH₃ Leu¹¹); IR (KBr): 3302, 1742, 1657, 1651, 1536 cm^{-1} .

Boc-Gly-ψ[CS-NH]-Ile-Leu-OMe: oil; R_{f1} 0.90; R_{f2} 0.92; R_{f3} 0.60; $[\alpha]_D^{20}$ -56.1 (*c* 0.5, MeOH); $^1\text{H NMR}$ (200 MHz, CDCl_3) δ 8.74 (d, 1H, Ile NH), 6.53–6.48 (d, 1H, Leu NH), 5.45–5.37 (t, 1H, Gly NH), 4.62–3.76 (m, 4H, Ile α CH, Leu α CH, Gly α CH₂), 3.71 (s, 3H, OMe CH₃), 2.20–1.46 (m, 6H, Ile β -CH and γ -CH₂, Leu β -CH₂ and γ -CH), 1.44 (s, 9H, Boc 3 CH₃), 1.00–0.74 (m, 12H, Leu 2 δ -CH₃, Ile γ -CH₃ and δ -CH₃); IR (KBr): 3313, 1747, 1721, 1659, 1594, 1524 cm^{-1} .

***n*-Oct-Aib-Gly-Leu-Aib-Gly-Gly-Leu-Aib-Gly-ψ[CS-NH]-Ile-Leu-OMe:** oil; R_{f1} 0.20; R_{f2} 0.87; R_{f3} 0.00; $[\alpha]_D^{20}$ -23.3 (*c* 0.2, MeOH); $^1\text{H NMR}$ (400 MHz, CD_3CN) δ 8.96 (d, 1H, NH Ile¹⁰), 7.91 (t, 1H, NH Gly⁶), 7.84 (t, 1H, NH Gly⁵), 7.74 (d, 1H, NH Leu³), 7.69 (t, 1H, NH Gly²), 7.66 (t, 1H, NH Gly⁹), 7.60 (d, 1H, NH Leu⁷), 7.540 (s, 1H, NH Aib⁴), 7.52 (s, 1H, NH Aib⁸), 7.35 (s, 1H, NH Aib¹), 7.13 (d, 1H, NH Leu¹¹), 4.21 (m, 1H, α -CH Leu¹¹), 4.20 (m, 1H, α -CH Leu⁷), 4.17 (m, 1H, α -CH Leu³), 4.05 (dd, 1H, α -CH Ile¹⁰), 3.78 (dd, 1H, 1 α -CH Gly⁶), 3.74 (dd, 1H, 1 α -CH Gly⁶), 3.71 (s, 3H, CH₃ OMe), 3.68 (dd, 1H, 1 α -CH Gly⁹), 3.66 (dd, 1H,

1 α -CH Gly²), 3.64 (m, 2H, α -CH₂ Gly⁵), 3.60 (dd, 1H, 1 α -CH Gly⁹), 3.58 (dd, 1H, 1 α -CH Gly²), 2.25 (t, 2H, β -CH₂ *n*-Oct), 1.57 (m, 2H, γ -CH₂ *n*-Oct), 2.15 (m, 2H, δ -CH₂ *n*-Oct), 1.84 (m, 1H, β -CH Ile¹⁰), 1.53 (m, 2H, β -CH₂ Leu⁷), 1.53 (m, 2H, β -CH₂ Leu³), 1.68 (m, 1H, γ -CH Leu³), 1.60 (m, 1H, γ -CH Leu⁷), 1.59 (m, 1H, γ -CH Leu¹¹), 1.48 (m, 1H, 1 β -CH Leu¹¹), 1.53 (m, 1H, 1 β -CH Leu¹¹), 1.47 (m, 1H, γ -CH Ile¹⁰), 1.46 (s, 6H, 2 β -CH₃ Aib⁴), 1.35 (s, 6H, 2 β -CH₃ Aib⁸), 1.32 (s, 6H, 2 β -CH₃ Aib¹), 1.28 (m, 1H, 1 γ -CH Ile¹⁰), 0.88 (m, 3H, δ -CH₃ Leu³), 0.86 (m, 3H, δ -CH₃ Leu¹¹), 0.84 (d, 3H, γ -CH₃ Ile¹⁰), 0.83 (m, 3H, δ -CH₃ Leu³), 0.82 (m, 3H, δ -CH₃ Ile¹⁰), 0.79 (t, 3H, ω -CH₃ *n*-Oct), 0.78 (m, 3H, δ -CH₃ Leu¹¹); IR (KBr): 3299, 1741, 1660, 1537 cm⁻¹.

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