Supplementary materials

Biosynthesis and antimicrobial activity of pseudodesmin and viscosinamide cyclic lipopeptides produced by pseudomonads associated with the cocoyam rhizosphere

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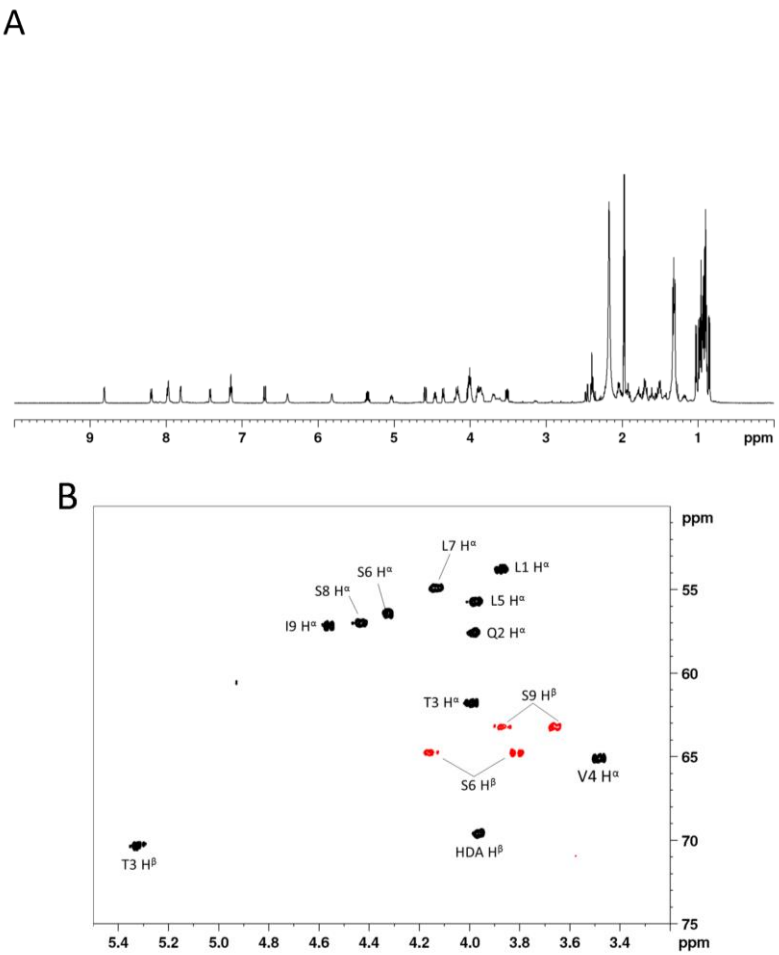

Figure S1. A) 1D ^{1}H NMR spectrum of major isolated CLP (N6, pseudodesmin A) (500 MHz, CD_3CN, 298K); **B)** The alpha region of a ^{1}H-^{13}C gHSQC spectrum of the isolated CLP shows the presence of 9 amino acids. The high chemical shift of the Thr3 CH^{β} indicates that the C-terminal ester bond is formed with this residue.

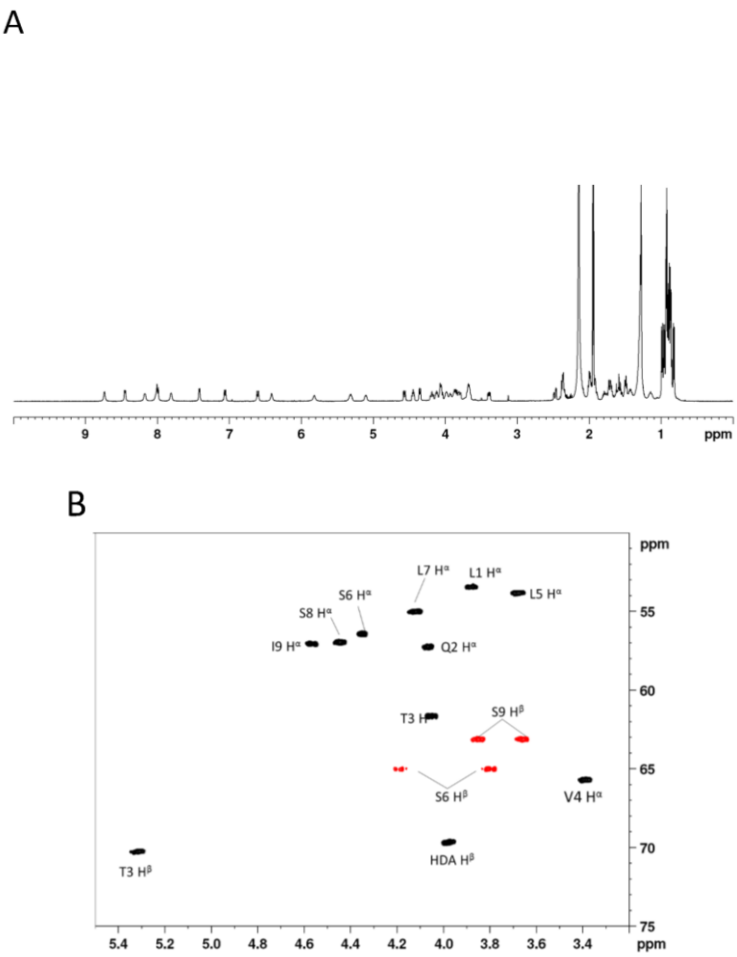

Figure S2. A) 1D ^{1}H NMR spectrum of viscosinamide A as extracted from A2W4.9 (500 MHz, CD_3CN, 298K); **B)** The alpha region of a ^{1}H-^{13}C gHSQC spectrum of the isolated CLP shows the presence of 9 amino acids. The high chemical shift of the Thr3 CH^{β} indicates that the C-terminal ester bond is formed with this residue.

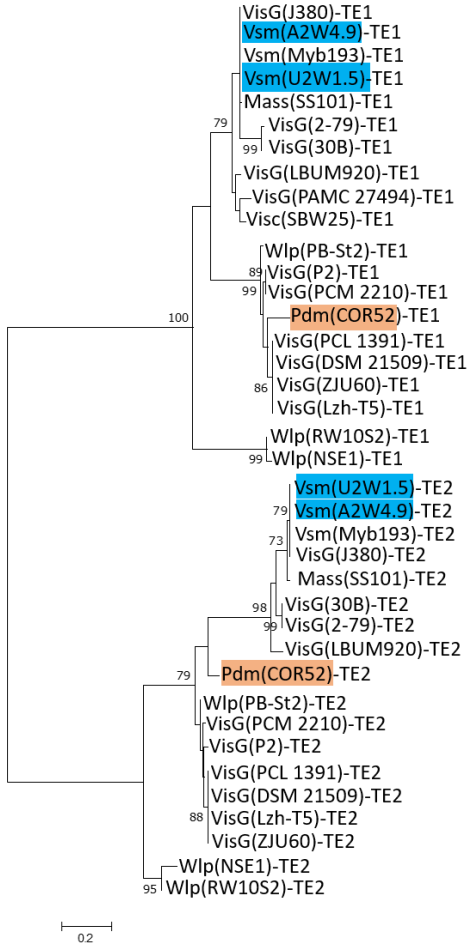

Figure S3. Phylogenetic analyses of the TE domains extracted from the modules of CLP gene clusters. Phylogenetic analyses of the Thioesterase (Te) domains extracted from functionally characterized and select putative *Pseudomonas* NRPSs. Lipopeptide-specific codes used for NRPS enzymes: Pdm (pseudodesmin, *Pseudomonas* sp. COR52, highlighted in blue); Vsm (viscosinamide, *Pseudomonas* sp. A2W4.9 and *Pseudomonas* sp. U2W1.5, highlighted in orange); Wlp (white line inducing principle, *Pseudomonas* sp. NSE1, *P. putida* RW10S2, *P. chlororaphis* Pb-St2); Mass (massetolide, *P. lactis* SS101); Visc (viscosin, *P. fluorescens* SBW25); VisG (viscosin group, not characterized: *Pseudomonas* sp. Myb193, *Pseudomonas* sp. J380, *P. synxantha* 30B, *P. synxantha* 2-79, *P. antarctica* PAMC 27494, *Pseudomonas* sp. LBUM920, *P. chlororaphis* subsp. *piscium* PCL1391, *P. chlororaphis* subsp. *aurantiaca* PCM 2210, *P. chlororaphis* subsp. *aureofaciens* P2, *P. chlororaphis* subsp. *piscium* DSM 21509, *P. chlororaphis* subsp. *piscium* ZJU60 and *P. chlororaphis* Lzh-T5). For each domain, the substrate specificity is indicated in parentheses, using the standard amino acid three-letter code. VisG represent NRPS enzymes for Viscosin Group CLPs that have been characterised based on genome mining only. Phylogenetic tree was drawn using the Geneious 11.1.5 software.

Table S1. ^{1}H and ^{13}C chemical shift values of the isolated compound (N6, pseudodesmin A) (500 MHz, CD_3CN, 298K).

		^{1}H δ	^{13}C δ
HDA			
	CO	-	175.61
	CH_2α1	2.44	44.75
	CH_2α2	2.35	44.75
	CHβ	3.96	69.58
	CH_2γ	1.48	38.23
	CH_2δ1	1.44	26.31
	CH_2δ2	1.30	26.31
	CH_2ε	1.30	30.11
	CH_2ζ	1.28	30.29
	CH_2η	1.28	32.62
	CH_2θ	1.29	23.39
	CH_2ι	0.88	14.46
	OH	n.d.	-
Leu1			
$^{3}J_{HNH\alpha}$ 4.1 Hz	NH	7.78	-
	CHα	3.87	53.70
	CO	-	175.64
	CH_2β1	1.75	39.29
	CH_2β2	1.66	39.29
	CHγ	1.67	25.42
	CH_3δ1	0.94	23.22
	CH_3δ2	0.90	22.08
Gln2			
$^{3}J_{HNH\alpha}$ 3.9 Hz	NH	8.78	-
	CHα	3.98	57.54
	CO	-	177.19
	CH_2β	2.02	26.42
	CH_2γ	2.37	31.96
	COδ	-	176.33
	OH	n.d.	-
Thr3			
$^{3}J_{HNH\alpha}$ 7.2 Hz	NH	8.16	-
	CHα	3.99	61.76
	CO	-	174.47
	CH_2β	5.32	70.32
	CHγ	1.30	18.50
Val4			
$^{3}J_{HNH\alpha}$ 6.2 Hz	NH	7.39	-
	CHα	3.48	65.09
	CO	-	174.78
	CHβ	2.18	29.89
	CH_1γ1	0.95	21.08
	CH_2γ2	0.92	19.50
Leu5			
$^{3}J_{HNH\alpha}$ n.d.	NH	7.94	-
	CHα	3.97	55.68
	CO	-	173.77
	CH_2β1	1.67	40.63
	CH_2β2	1.51	40.63
	CHγ	1.77	25.49
	CH_3δ1	0.88	21.29
	CH_3δ2	0.86	23.33
Ser6			
$^{3}J_{HNH\alpha}$ n.d.	NH	7.12	-
	CHα	4.33	56.40
	CO	-	172.26
	CH_2β1	4.15	64.72
	CH_2β2	3.81	64.72
	OH	5.00	-
Leu7			
$^{3}J_{HNH\alpha}$ n.d.	NH	7.11	-
	CHα	4.13	54.87
	CO	-	174.31
	CH_2β1	1.89	42.06
	CH_2β2	1.58	42.06
	CHγ	1.90	25.51
	CH_3δ1	0.99	23.47
	CH_3δ2	0.90	21.35
Ser8			
$^{3}J_{HNH\alpha}$ n.d.	NH	7.50	-
	CHα	4.43	56.97
	CO	-	172.36
	CH_2β1	3.87	63.17
	CH_2β2	3.66	63.17
	OH	3.81	-
Ile9			
$^{3}J_{HNH\alpha}$ 10.2 Hz	NH	6.67	-
	CHα	4.56	57.16
	CO	-	170.38
	CHβ	1.97	36.93
	CH_2γ1	1.16	25.22
	CH_2γ2	0.97	25.22
	CH_3γ	0.82	16.24
	CH_3δ2	0.86	12.29

n.d: not determined.

Table S2. ^{1}H and ^{13}C chemical shift values of viscosinamide A as extracted from *P.* sp. A2W4.9. (500 MHz, CD_3CN, 298K).

			^{1}H δ	^{13}C δ
HDA				
		CO	-	175.34
		$CH_2\alpha1$	2.47	44.73
		$CH_2\alpha2$	2.36	44.73
		CHβ	3.98	69.66
		$CH_2\gamma$	1.49	38.10
		$CH_2\delta1$	1.43	26.36
		$CH_2\delta2$	1.31	26.36
		$CH_2\varepsilon$	1.31	30.02
		$CH_2\zeta$	1.31	30.02
		$CH_2\eta$	1.28	32.60
		$CH_2\theta$	1.29	32.30
		$CH_2\iota$	0.88	14.33
		OH	n.d.	-
Leu1				
$^{3}J_{HNH\alpha}$	n.d.	NH	7.99	-
		CHα	3.87	53.41
		CO	-	n.d.
		$CH_2\beta1$	1.79	39.14
		$CH_2\beta2$	1.71	39.14
		CHγ	1.69	25.27
		$CH_3\delta1$	0.92	23.21
		$CH_3\delta2$	0.89	21.89
Gln2				
$^{3}J_{HNH\alpha}$	n.d.	NH	8.73	-
		CHα	4.07	57.24
		CO	-	n.d.
		$CH_2\beta$	1.99	26.39
		$CH_2\gamma$	2.36	32.00
		COδ	-	n.d.
		NH_2	6.41/5.81	-
Thr3				
$^{3}J_{HNH\alpha}$	n.d.	NH	8.17	-
		CHα	4.05	61.65
		CO	-	n.d.
		$CH_2\beta$	5.32	70.27
		CHγ	1.28	18.38
Val4				
$^{3}J_{HNH\alpha}$	n.d.	NH	7.81	-
		CHα	3.39	65.69
		CO	-	174.00
		CHβ	2.11	29.98
		$CH_1\gamma1$	0.95	20.76
		$CH_2\gamma2$	0.92	19.48
Leu5				
$^{3}J_{HNH\alpha}$	6.3 Hz	NH	8.45	-
		CHα	3.68	53.81
		CO	-	n.d.
		$CH_2\beta1$	1.94	37.35
		$CH_2\beta2$	1.73	37.35
		CHγ	1.61	25.50
		$CH_3\delta1$	0.83	23.92
		$CH_3\delta2$	0.86	21.28
Ser6				
$^{3}J_{HNH\alpha}$	8.1 Hz	NH	7.06	-
		CHα	4.35	56.42
		CO	-	172.30
		$CH_2\beta1$	4.18	65.03
		$CH_2\beta2$	3.80	65.03
		OH	5.10	-
Leu7				
$^{3}J_{HNH\alpha}$	5.6 Hz	NH	7.41	-
		CHα	4.12	54.99
		CO	-	n.d.
		$CH_2\beta1$	1.91	41.98
		$CH_2\beta2$	1.55	41.91
		CHγ	1.93	35.35
		$CH_3\delta1$	0.98	23.31
		$CH_3\delta2$	0.91	21.41
Ser8				
$^{3}J_{HNH\alpha}$	n.d.	NH	8.00	-
		CHα	4.45	56.94
		CO	-	n.d.
		$CH_2\beta1$	3.85	63.12
		$CH_2\beta2$	3.66	63.12
		OH	3.92	-
Ile9				
$^{3}J_{HNH\alpha}$	10.0 Hz	NH	6.60	-
		CHα	4.56	57.04
		CO	-	n.d.
		CHβ	1.99	36.75
		$CH_2\gamma1$	1.15	25.11
		$CH_2\gamma2$	0.95	25.11
		$CH_3\gamma$	0.82	16.13
		$CH_3\delta2$	0.86	12.21

n.d: not determined.