

Supplementary file S5. Predicted polyketide synthase, non-ribosomal peptide synthetase and terpenoid synthase assembly lines in *Clonostachys rosea*.

Table 1. Predicted polyketide synthases in the *Clonostachys rosea* genome.

PKS	Protein Id	Length (aa)	Domains	Type
PKS1	BN869_T00000928_1	1787	SAT KS AT PT T	NR
PKS2	BN869_T00010693_1	2622	SAT KS AT PT T MT R	NR
PKS3	BN869_T00000911_1	2417	SAT KS AT PT T MT TE	NR
PKS4	BN869_T00006898_1	2555	SAT KS AT PT T MT R	NR
PKS5	BN869_T00011525_1	2700	KS AT DH MT ER KR T	HR
PKS6	BN869_T00008325_1	2672	KS AT DH MT ER KR T	HR
PKS7	BN869_T00008884_1	2598	KS AT DH MT ER KR T	HR
PKS8	BN869_T00011033_1	2357	KS AT DH ER KR T	HR
PKS9	BN869_T00006567_1	2530	KS AT DH ER KR T	HR
PKS10	BN869_T00013077_1	2375	KS AT DH ER KR T	HR
PKS11	BN869_T00008198_1	2428	KS AT DH ER KR T	HR
PKS12	BN869_T00010694_1	2600	KS AT DH MT ER KR T	HR
PKS13	BN869_T00013279_1	2584	KS AT DH MT ER KR T	HR
PKS14	BN869_T00006415_1	2502	KS AT DH MT ER KR T	HR
PKS15	BN869_T00009642_1	2349	KS AT DH ER KR	HR
PKS16	BN869_T00013307_1	2403	KS AT DH MT ER KR T	HR
PKS17	BN869_T00012010_1	2238	KS AT DH ER KR T	HR
PKS18	BN869_T00007381_1	2505	KS AT DH MT ER KR T	HR
PKS19	BN869_T00013339_1	2346	KS AT DH ER KR T	HR
PKS20	BN869_T00010238_1	2411	KS AT DH MT ER KR T	HR
PKS21	BN869_T00007502_1	2544	KS AT DH MT ER KR T	HR
PKS22	BN869_T00009884_1	2490	KS AT DH MT ER KR T	HR
PKS23	BN869_T00010141_1	2614	KS AT DH MT ER KR T	HR

PKS24	BN869_T00005452_1	2561	KS AT DH MT ER KR T	HR
PKS25	BN869_T00012373_1	2707	KS AT DH MT ER KR T	HR
PKS26	BN869_T00013405_1	2418	KS AT DH MT ER KR	HR
PKS27	BN869_T00009545_1	2000	KS AT DH MT ER	HR
PKS28	BN869_T00005753_1	2345	KS AT DH ER KR T	HR
PKS29	BN869_T00010453_1	2378	KS AT DH MT ER KR T	HR
PKS30	BN869_T00008531_1	271	KS	fragment
PKS31	BN869_T00001420_1	430	KS	fragment
PKS32	BN869_T00013212_1	3889	KS AT DH ER KR T C A T R	hybrid

Abbreviations: AT=acyl transferase, DH=dehydratase, ER=enoyl reductase, KR=ketoreductase, KS=ketosynthase, PT=product template domain (first ring cyclase), R=reducatse, SAT=starter unit acyl transferase, TE=thioesterase HR=highly reducing, NR=nonreducing, hybrid=PKS-NRPS hybrid.

Table 2. Predicted non-ribosomal peptide synthetase gene clusters and their proposed domain structure in the *Clonostachys rosea* genome.

NRPS Gene cluster	Protein ID	Length (aa)	Domains	Proposed function/ comment
NPS1	BN869_T00013362_1	2206	A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ T ₃	putative ETP synthetase
NPS2	BN869_T00008995_1	1022	A ₁ X	paralog of BN869_T00008995_1
NPS3 (NPS3A, NPS3B)	BN869_T00006601_1	984	A ₁ X	paralog of BN869_T00008995_1
	BN869_T00006619_1	1285	A ₁ T ₂ R	
NPS4 (NPS4A, NPS4B)	BN869_T00007296_1	4331	AT T ₀ C ₁ A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ A ₃ T ₃ C ₃	putative peptaibol synthetase (11 modules)
	BN869_T00007295_1	8453	A ₄ T ₄ C ₄ A ₅ T ₅ C ₅ A ₆ T ₆ C ₆ A ₇ T ₇ C ₇ A ₈ T ₈ C ₈ A ₉ T ₉ C ₉ A ₁₀ T ₁₀ C ₁₀ A ₁₁ T ₁₁ R	
NPS5	BN869_T00010383_1	5443	A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ A ₃ T ₃ C ₃ A ₄ T ₄ C ₄ A ₅ T ₅ C ₅	
NPS6	BN869_T00000574_1	9406	A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ A ₃ T ₃ C ₃ A ₄ T ₄ C ₄ A ₅ T ₅ C ₅ A ₆ T ₆ C ₆ A ₇ T ₇ C ₇ A ₈ T ₈ C ₈	
NPS7	BN869_T00012973_1	6047	A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ A ₃ T ₃ C ₃ A ₄ T ₄ C ₄ A ₅ T ₅ C ₅ A ₆ T ₆ C ₆	
NPS8	BN869_T00008264_1	4858	A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ T ₃ C ₃ A ₄ T ₄ C ₄ T ₅ C ₅ T ₆ C ₆	putative ferricrocin siderophore synthetase
NPS9	BN869_T00013091_1	21815	A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ A ₃ T ₃ C ₃ A ₄ T ₄ C ₄ A ₅ T ₅ C ₅ A ₆ T ₆ C ₆ A ₇ T ₇ C ₇ A ₈ T ₈ C ₈ A ₉ T ₉ C ₉ A ₁₀ T ₁₀ C ₁₀ A ₁₁ T ₁₁ C ₁₁ A ₁₂ T ₁₂ C ₁₂ A ₁₃ T ₁₃ C ₁₃ A ₁₄ T ₁₄ C ₁₄ A ₁₅ T ₁₅ C ₁₅ A ₁₆ T ₁₆ C ₁₆ A ₁₇ T ₁₇ C ₁₇ A ₁₈ T ₁₈ C ₁₈ A ₁₉ T ₁₉ C ₁₉ A ₂₀ T ₂₀ C ₂₀	putative peptaibol synthetase (20 modules)
NPS10	BN869_T00012004_1	3381	A ₁ T ₁ C ₁ A ₂ T ₂ A ₃ T ₃ A ₄ T ₄ A ₅ T ₅ C ₅	
NPS11	BN869_T00006571_1	6728	C ₀ A ₁ T ₁ C ₁ A ₂ T ₂ A ₃ T ₃ A ₄ T ₄ A ₅ T ₅ C ₅ A ₆ T ₆ C _{6a} C _{6b} A ₇ T ₇ C ₇	
NPS12	BN869_T00013096_1	6368	C ₀ A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ A ₃ T ₃ C ₃ A ₄ T ₄ C ₄ A ₅ T ₅ C ₅ A ₆ T ₆	putative peptaibol synthetase
NPS13	BN869_T00012005_1	2433	A ₁ T ₁ C ₁ A ₂ T ₂ C ₂	

NPS14	BN869_T00012688_1	1588	T ₁ C ₁ A ₂ T ₂ R	Putative incomplete peptaibole synthetase (terminal portion)
NPS15	BN869_T00013464_1	6844	C ₀ A ₁ T ₁ C ₁ A ₂ T ₂ C ₂ A ₃ T ₃ C ₃ A ₄ T ₄ C ₄ A ₅ T ₅ C ₅ A ₆ T ₆ C ₆	putative peptaibol synthetase
NPS16	BN869_T00007957_1	12980	C A ₁ T ₁ C ₁ *A ₂ T ₂ C ₂ A ₃ T ₃ C ₃ A ₄ T ₄ C ₄ A ₅ T ₅ C ₅ A ₆ T ₆ C ₆ A ₇ T ₇ C ₇ A ₈ T ₈ C ₈ A ₉ T ₉ C ₉ A ₁₀ T ₁₀ C ₁₀ A ₁₁ T ₁₁ C ₁₁ A ₁₂ T ₁₂ C ₁₂	putative peptaibol synthetase
NPS17	BN869_T00006516_1	1178	A ₁ T ₁ R	2-aminoadipate reductase

Abbreviations: A=adenylation domain, AT=acyltransferase, C=condensation domain, T=thiolation domain, R=reductase, *=truncated.

Table 3. Adenylation domains of NRPS gene clusters, their non-ribosomal specificity code and predicted substrates. Predictions were performed manually or using the NRPSPredictor2 server.

NRPS Cluster	Protein Id	A-domain	Nonribosomal Code	Predicted substrate (NRPSPredictor2)
NPS1	BN869_T00013362_1	1	DACAIGASMK	Trp [#]
		2	DVMAYCAILK	Ala
NPS2	BN869_T00008995_1	1	DMWIAACIVK	hydrophobic-aliphatic
NPS3 (NPS3A, NPS3B)	BN869_T00006601_1	1	DMWIAACIVK	hydrophobic-aliphatic
	BN869_T00006619_1	2	--WLWNVEVK	hydrophobic-aliphatic
NPS4 (NPS4A, NPS4B)	BN869_T00007296_1	1	DFCFFAGVVK	Aib/Iva
		2	DLGIVAAVIK	hydrophobic-aliphatic
		3	DAMVIGAVIK	hydrophobic-aliphatic
	BN869_T00007295_1	4	DQLMLGAVIK	hydrophobic-aliphatic
		5	DIGWAAGLVK	Aib/Iva
		6	DLFFGGLSCK	Pro
		7	DLTYSGGVHK	Glu
		8	DFVCLGAVMK	Gly/Ala
		9	DGGMVGNYK	Gln
		10	DIGFLAH-DK	Ile
		11	DASVNGAISK	Leu
NPS5	BN869_T00010383_1	1	DVSNLSTFKK	Ala
		2	DVIGVAWVAK	hydrophobic-aliphatic
		3	DVVNVGWAAK	Ala
		4	DAWGYGMSTK	Phe,Trp
		5	DVSYAGIQAK	hydrophobic-aliphatic
NPS6	BN869_T00000574_1	1	DVSNIALIGK	Leu
		2	DVCILILTFK	hydrophobic-aliphatic

		3	DTNDIGCPTK	Orn, Lys, Arg
		4	DVSDLSTVKK	hydrophobic-aliphatic
		5	DTQEIGSPTK	Asp,Asn,Glu,Gln,Aad
		6	HIRNIDMTK [#]	unknown
		7	DQSDIGCPTK	Leu
		8	DISDVAMVKK	hydrophobic-aliphatic
NPS7	BN869_T00012973_1	1	DVLI IAGMCK	hydrophobic-aromatic
		2	DILIVVGLCK	hydrophobic-aromatic
		3	DLEEVGTPTK	Asp,Asn,Glu,Gln,Aad
		4	DVDEIGTPTK	Asp,Asn,Glu,Gln,Aad
		5	DVDH- -TPTK	Ala
		6	DLEEVGTPTK	Asp,Asn,Glu,Gln,Aad
NPS8	BN869_T00008264_1	1	DVFELIMIHK	Gly [#]
		2	DVFSVAGNIK	Ser [#]
		3	DVLDIGAIGK	Aho [#]
NPS9	BN869_T00013091_1	1	DVSMLVAIFK	Ala
		2	DLGYMAACFK	Aib/Iva
		3	DLGFLAGCFK	Aib/Iva
		4	DVGMVTSINK	Aad
		5	DFCFFAAVCK	Aib/Iva
		6	DMGWVAGCLK	Aib/Iva
		7	DVCMVAIFK	Aib/Iva
		8	DYCGIGAICK	Cys
		9	DFGFLAVFLK	Aib/Iva
		10	DWMFGGFINK	Pro
		11	DFGLQGAYAK	Aib/Iva
		12	DLGYLAGCFK	Aib/Iva
		13	DLGYVAACFK	Aib/Iva
		14	DIIFGGLICK	Pro
		15	DATLIGAVCK	Leu
		16	DFGYVGATIK	Aib/Iva

		17	DLGYLAGCFK	Aib/Iva
		18	DIIFGGLICK	Pro
		19	DFGMFAVFAK	Aib/Iva
		20	DFAFVALVGK	Aib/Iva
NPS10	BN869_T00012004_1	1	DMYFVASPGK	Leu
		2	DFSFGIVMK	Leu
		3	DMFLAAVPGK	aromatic
		4	DLYQVAVPCK	Pro
		5	DAMLIGAVIK	hydrophobic-aliphatic
NPS11	BN869_T00006571_1	1	DIHIVGAPHK	Leu
		2	DVSENGTPTK	hydrophilic
		3	DDFSLGGCTK	Lys
		4	DAMFLIAPLK	hydrophobic-aliphatic
		5	DVSATGSIQK	hydrophilic
		6	DVYLIVATNK	Cys
		7	DAFVLGAVIK	hydrophobic-aliphatic
NPS12	BN869_T00013096_1	1	DMGYVIACIK	hydrophobic-aliphatic
		2	DMYSVALCCK	Pro
		3	DFGLGGMFAK	Ala/Gly
		4	DFGFIGACFK	Aib/Iva
		5	DIIFGGLICK	Pro
		6	DFGFFAGVAK	Aib/Iva
NPS13	BN869_T00012005_1	1	DICHCSVIVK	hydrophobic-aliphatic
		2	DFSFAGVVIK	hydrophobic-aliphatic
NPS14	BN869_T00012688_1	3	DVYFVCGPFK	hydrophobic-aliphatic
NPS15	BN869_T00013464_1	1	DFGYMGAVFK	Aib/Iva
		2	DLFFGGLSCK	hydrophobic-aliphatic
		3	DFGLLGAFIK	hydrophobic-aliphatic
		4	DMGYAAGVFK	Aib/Iva
		5	DMLFGGINCK	hydrophobic-aliphatic

		6	DFGLGGFFAK	hydrophobic-aliphatic
NPS16	BN869_T00007957_1	1	DFMIFGAVCK	hydrophobic-aliphatic
		2	n . a .	
		3	DLGYLAACK	Aib/Iva
		4	DIIFGGLICK	Pro
		5	DFACIAIVAK	hydrophobic-aliphatic
		6	DAGMMTGVPK	Aib/Iva
		7	DIIFGGLICK	Pro
		8	DFGFIAGIVK	Aib/Iva
		9	DMGYVAAVLK	Pro
		10	DLGYLAGCFK	Iva
		11	DLGYLAGCFK	Iva
		12	DFAWVGLVAK	hydrophobic-aliphatic
NPS17	BN869_T00006516_1	1	DPRHFVLRK	Aad
PKS32 (PKS- NRPS hybrid)	BN869_T00013212_1	1	DVSYIAEVQK	hydrophobic-aliphatic

Abbreviations of non-proteinogenic substrates: Aad=2-amino adipic acid, Aho= N^5 -acyl- N^5 -hydroxyornithine, Aib=2-aminoisobutyric acid, Iva=isovaline, Orn=ornithine. n.a.=not applicable, #=manually extracted NRPS code.

Table 4. Predicted terpenoid synthases (TS)¹ in the *Clonostachys rosea* genome.

TS	Protein ID	Gene length (bp)	InterProScan/PFAM ID family domains	Description
TES1	BN869_T00002098_1	2283	IPR008949, IPR017446, IPR000092, PF00348, PF03936	Terpene synthase family, metal binding domain
TES2	BN869_T00006434_1	1068	IPR008949, PF03936	Terpene synthase family, metal binding domain
TES3	BN869_T00002452_1	963	IPR008949, PF03936, PF06330	Terpene synthase family, metal binding domain/Trichodiene synthase (TRI5)
TES4	BN869_T00004037_1	1299	IPR008949, IPR017446, IPR000092, PF00348	Polyprenyl synthase
TES5	BN869_T00011314_1	1029	IPR008949, IPR017446, IPR000092, PF00348	Polyprenyl synthase
TES6	BN869_T00002638_1	1098	IPR008949, IPR017446, IPR000092, 2 domains of PF00348	2 domains of polyprenyl synthase
TES7	BN869_T00000651_1	1389	IPR008949, IPR002060, IPR006449, PF00494	Squalene/phytoene synthase
TES8	BN869_T00005085_1	1743	IPR008949, IPR002060, IPR017825, PF00494	Squalene/phytoene synthase and lycopene cyclase

¹ The identification of predicted TS related proteins were based on domain searches using any of the following domains for either InterProScan: IPR008949 = terpenoid_synth, IPR017446 = polyprenyl_synth-rel, IPR000092 = polyprenyl_synth, IPR002060 = Squ/phyt_synthase, IPR006449 = Squal_synth, IPR017825 = Lycopene_cyclase_dom, or from Pfam v. 27.0 (by using E-value \leq 1.0): PF00348 = polyprenyl synth, PF03936 = Terpene synth C, PF06330 = TRI5, PF00494 = SQS PSY.