

Supplementary Information

Automated structure prediction of *trans*-acyltransferase polyketide synthase products

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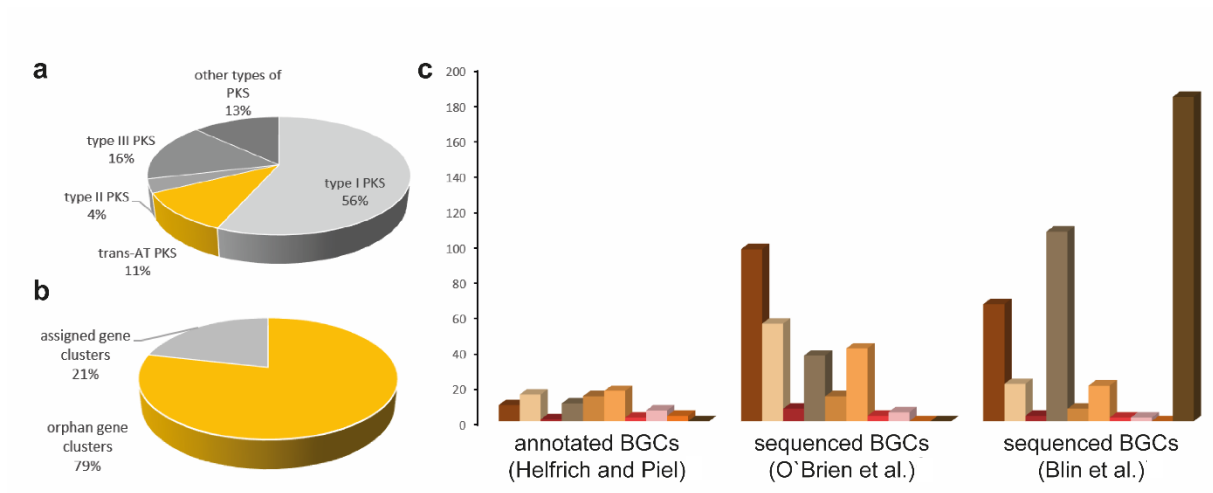
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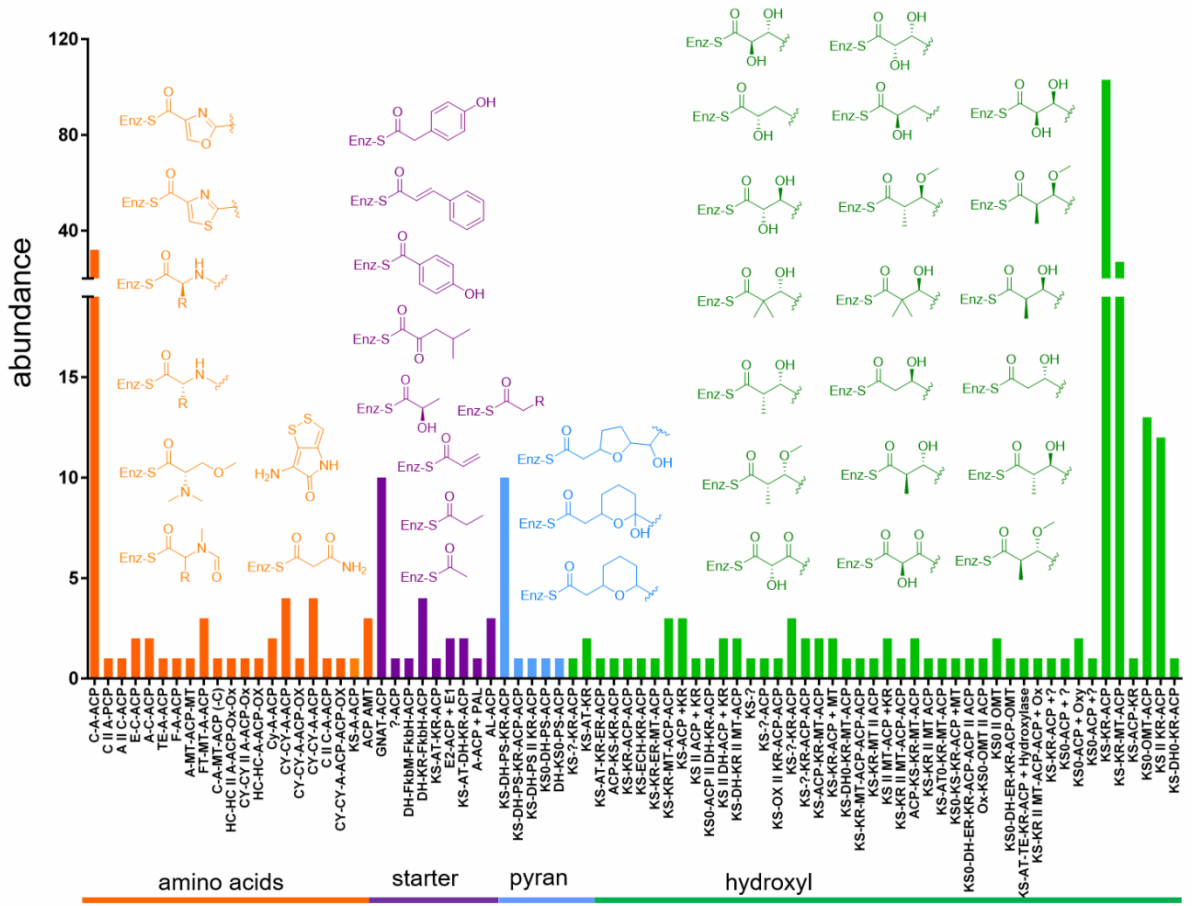
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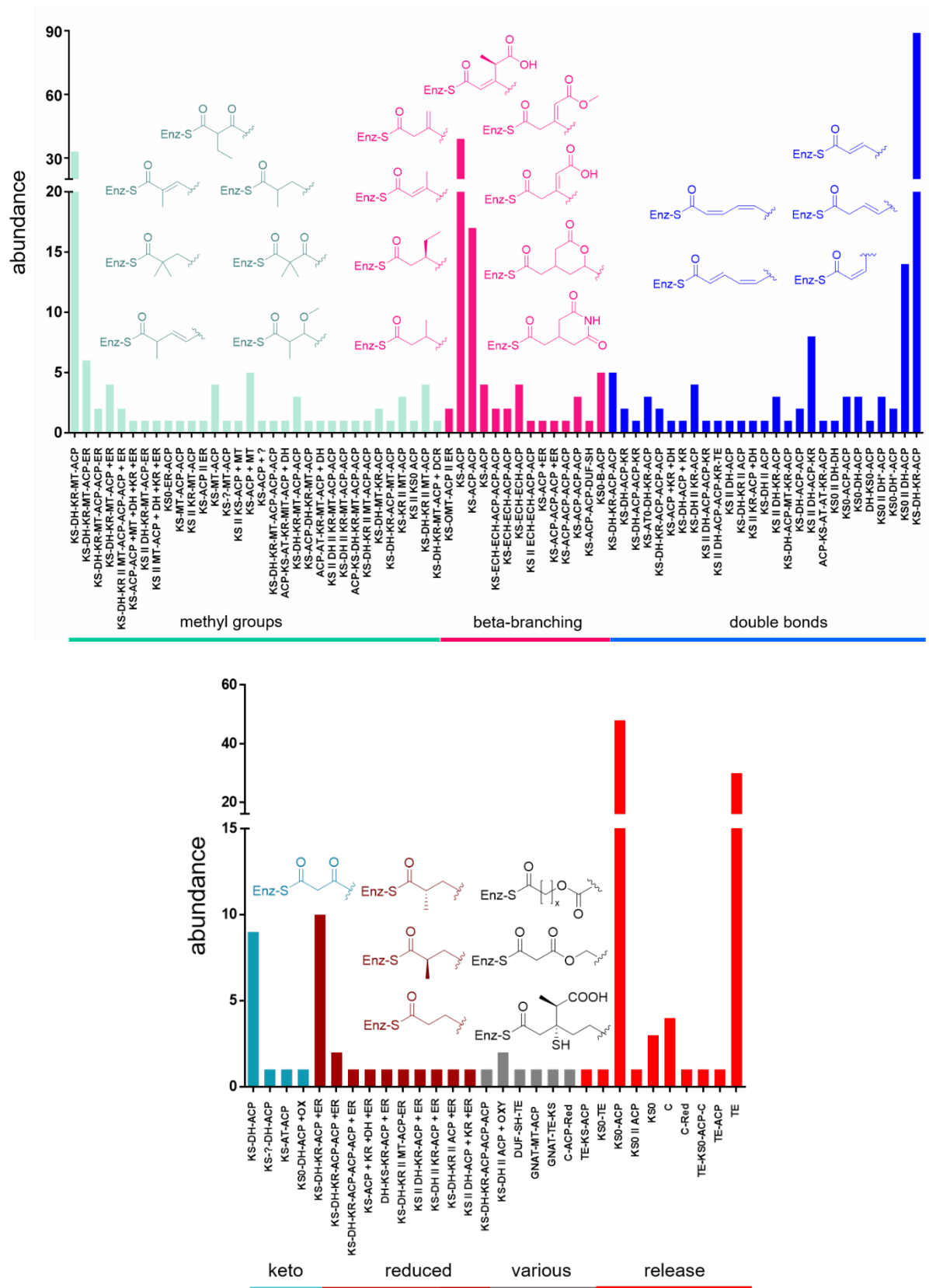
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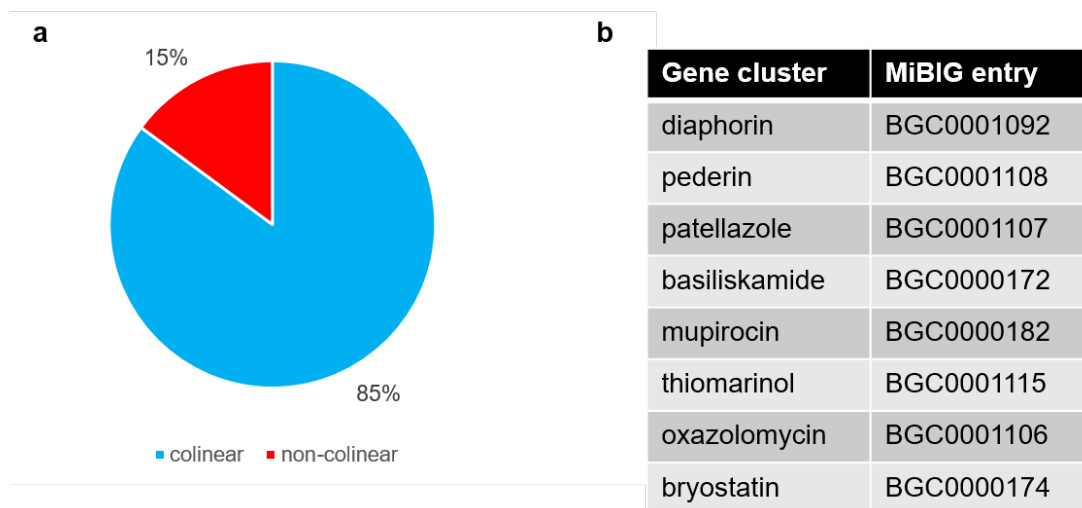


Supplementary Figure 1: Distribution of *trans*-AT PKS BGCs (a) Relative abundance of polyketide BGCs according to the antiSMASH database.¹ (b) Comparison between characterized and orphan *trans*-AT PKS BGCs. (c) Comparison of BGCs with characterized polyketides^{2,3} and published data^{1,4} on the occurrence of *trans*-AT PKS BGCs in published genomes.

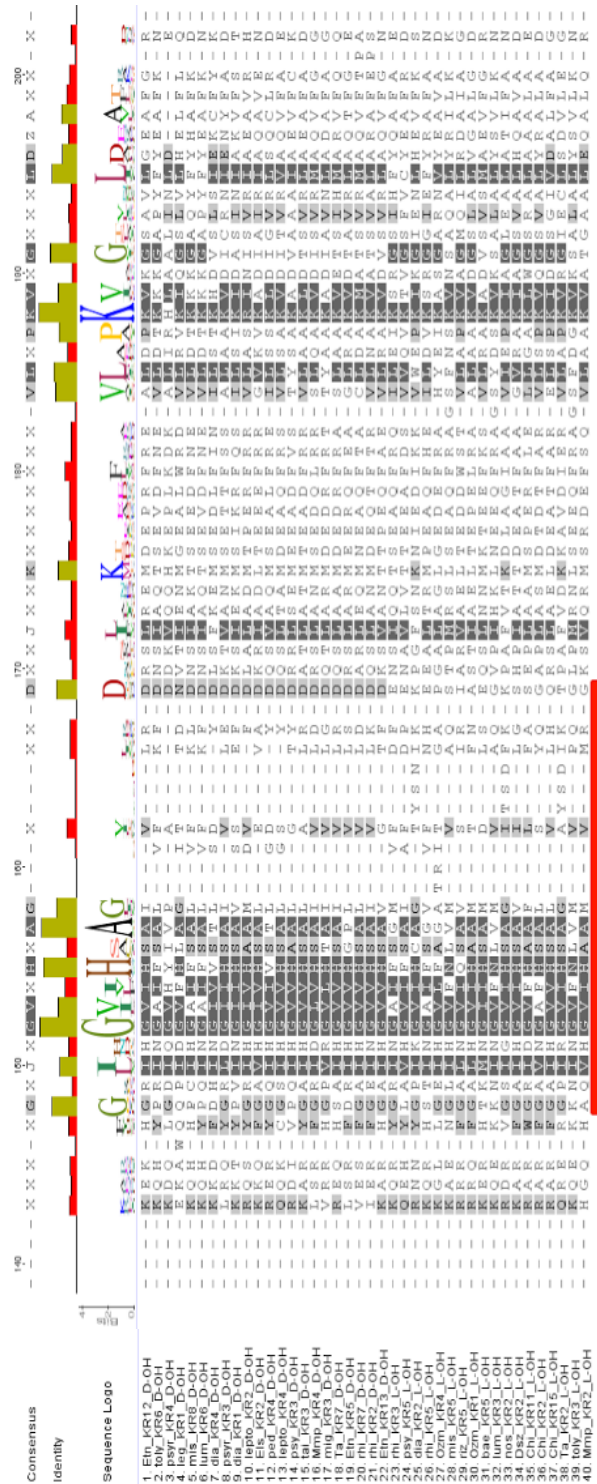




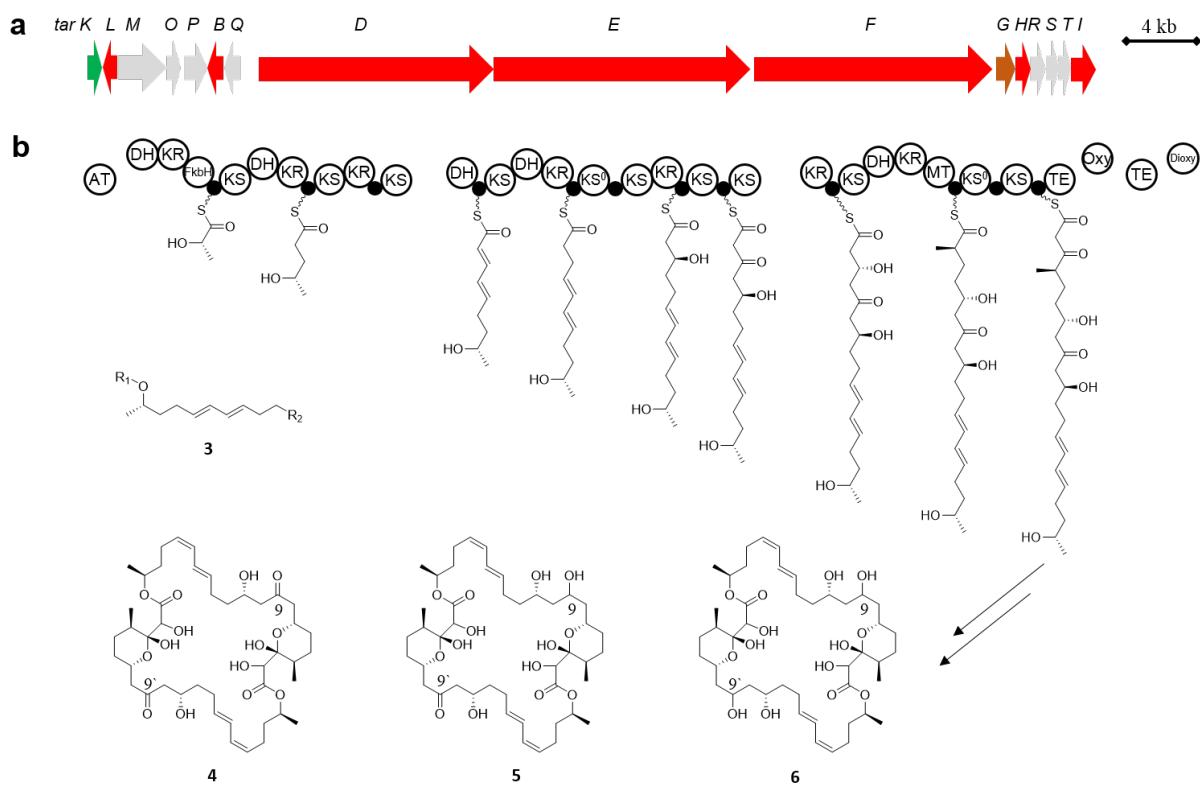
Supplementary Figure 2: Module variants encountered in *trans*-AT PKSs. Module variants were extracted and quantified from all annotated *trans*-AT PKS BGCs as described by Helfrich and Piel 2016⁵ and Piel 2010.² Module variants are grouped according to the modifications introduced into the polyketide backbone. "+" in module descriptors signifies non-covalent interactions with *trans*-acting enzymes. OXY: oxygenase, PAL: phenylalanine ammonia lyase, DUF: domain of unknown function, SH: cysteine lyase, DCR: 2,4-dienoyl-CoA reductase.



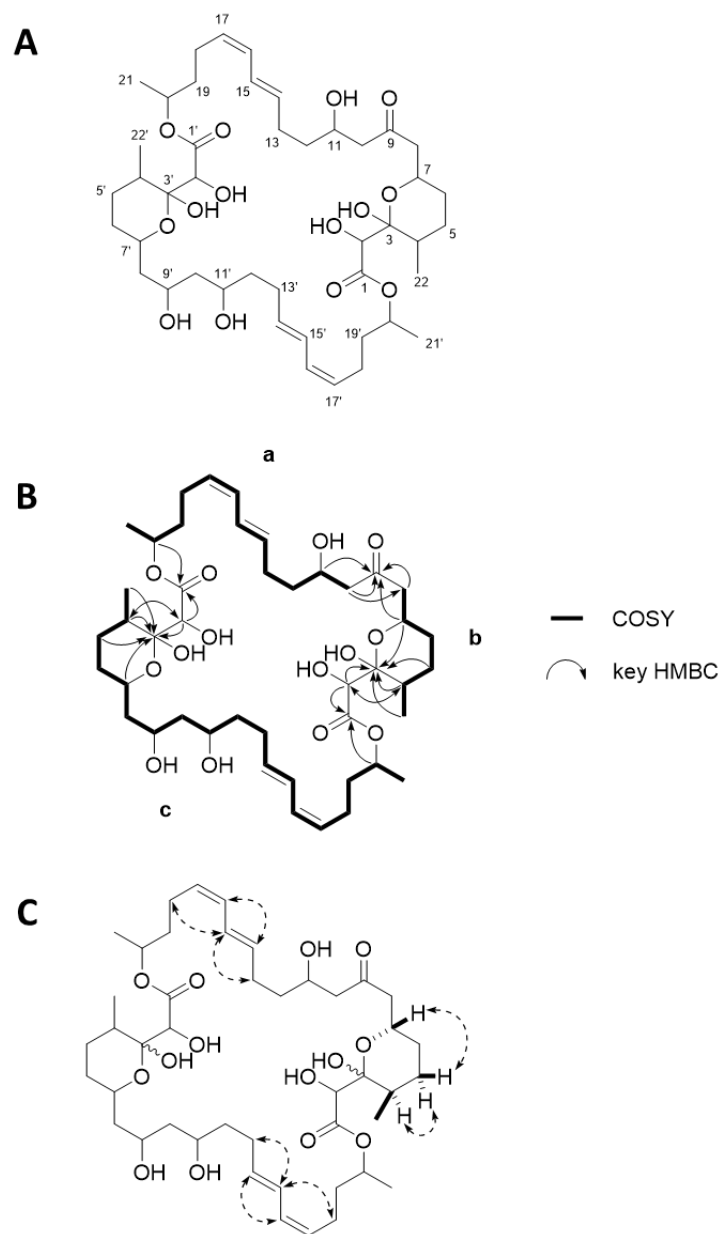
Supplementary Figure 3: Colinearity between gene order in the BGC and protein order during polyketide biosynthesis in 54 characterized *trans*-AT PKS clusters. (a) Colinearity between PKS genes and order at the protein level. **(b)** Table of all characterized *trans*-AT PKS BGCs that do not show a colinearity between gene order and order of the corresponding proteins in the PKS.



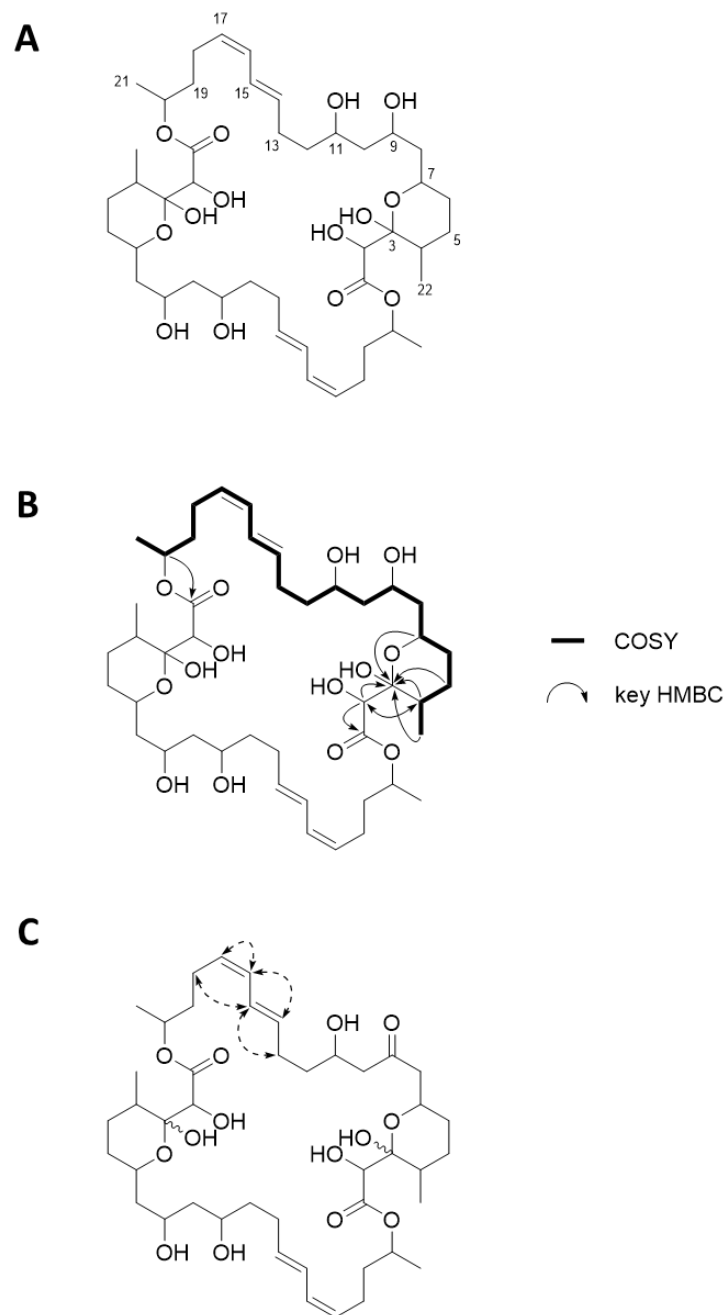
Supplementary Figure 4: KR alignment around the fuzzpro pattern used to distinguish between D-OH and L-OH groups. Red bar: KR Fuzzpro pattern used. Blue bar: Stereochemistry-determining residue with D (Asp) forming D-configured OH groups and all other amino acids giving rise to L-OH groups. Fuzzpro pattern: $[GDPSE RVIHK NAT]_x(3)[GVTA][IVAL][VHILF][HYFVQY][SIATGMLCFNV][AVTSP][GLIMRP]_x(3)D$.



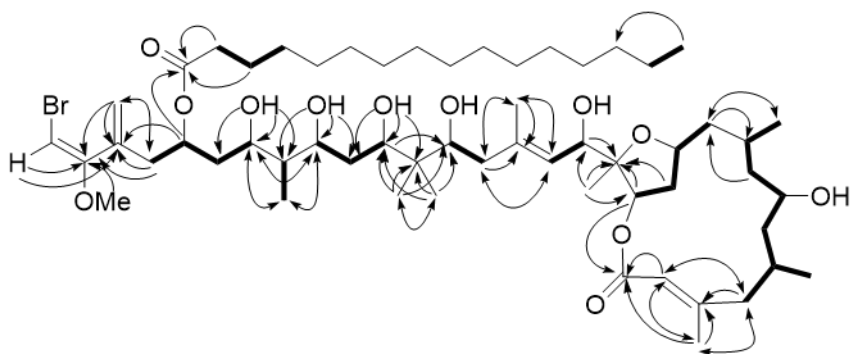
Supplementary Figure 5: Model for tartrolon biosynthesis. (a) *tar* BGC. Red: PKS genes, grey: hypothetical genes, brown: oxygenase genes, green: regulatory genes. **(b)** Proposed model for tartrolon biosynthesis, high-confidence part (3) of the structure generated by TransATor and used for MarinLit library search, and isolated homo- and heterodimeric tartrolon D, F and G (4-6).



Supplementary Figure 6: A: Structure of tartrolon F (5). B: COSY and key HMBC correlations of tartrolon F (5). C: Key NOESY correlation of tartrolon F (5).

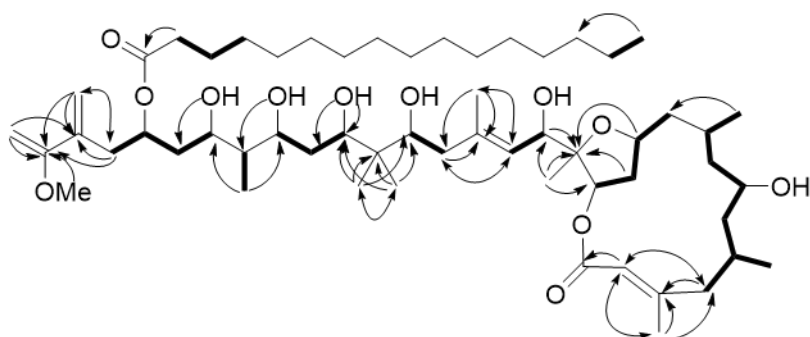
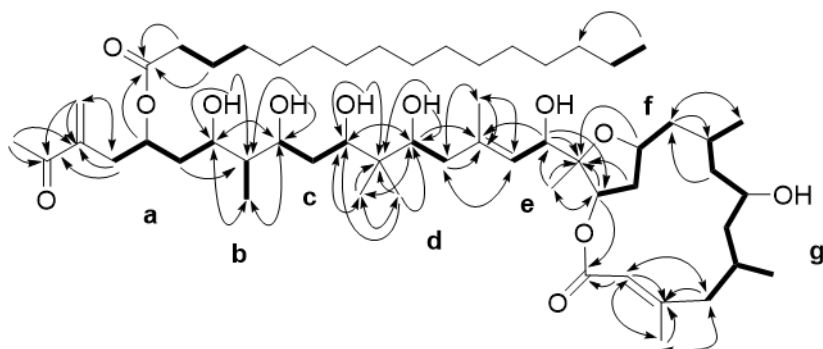


Supplementary Figure 7: A: Structure of tartrolon G (6). B: COSY and key HMBC correlations of tartrolon G (6). C: Key NOESY correlation of tartrolon G (6).

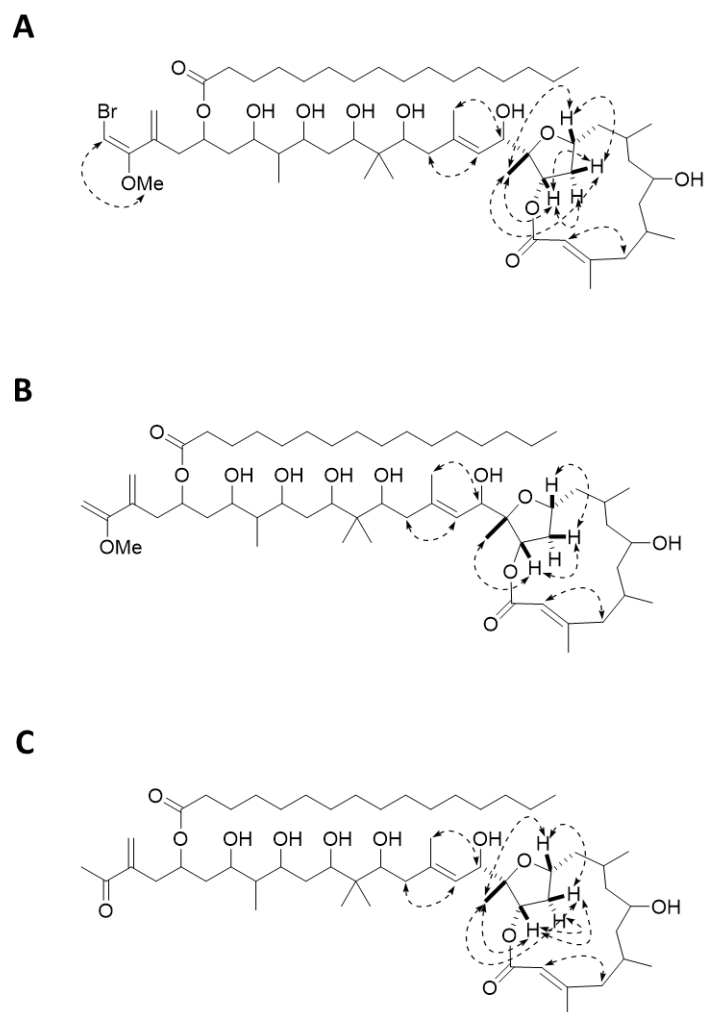
A

— COSY

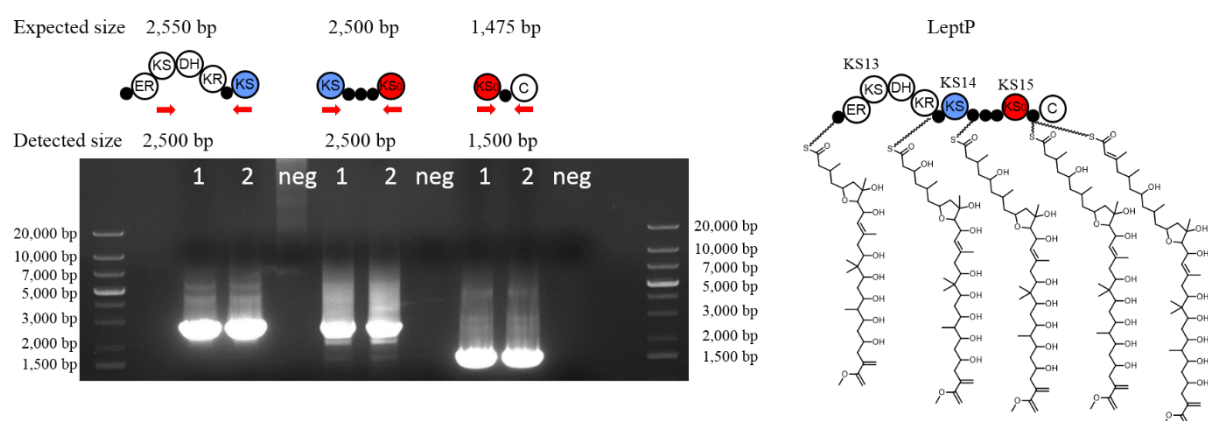
↷ key HMBC

B**C**

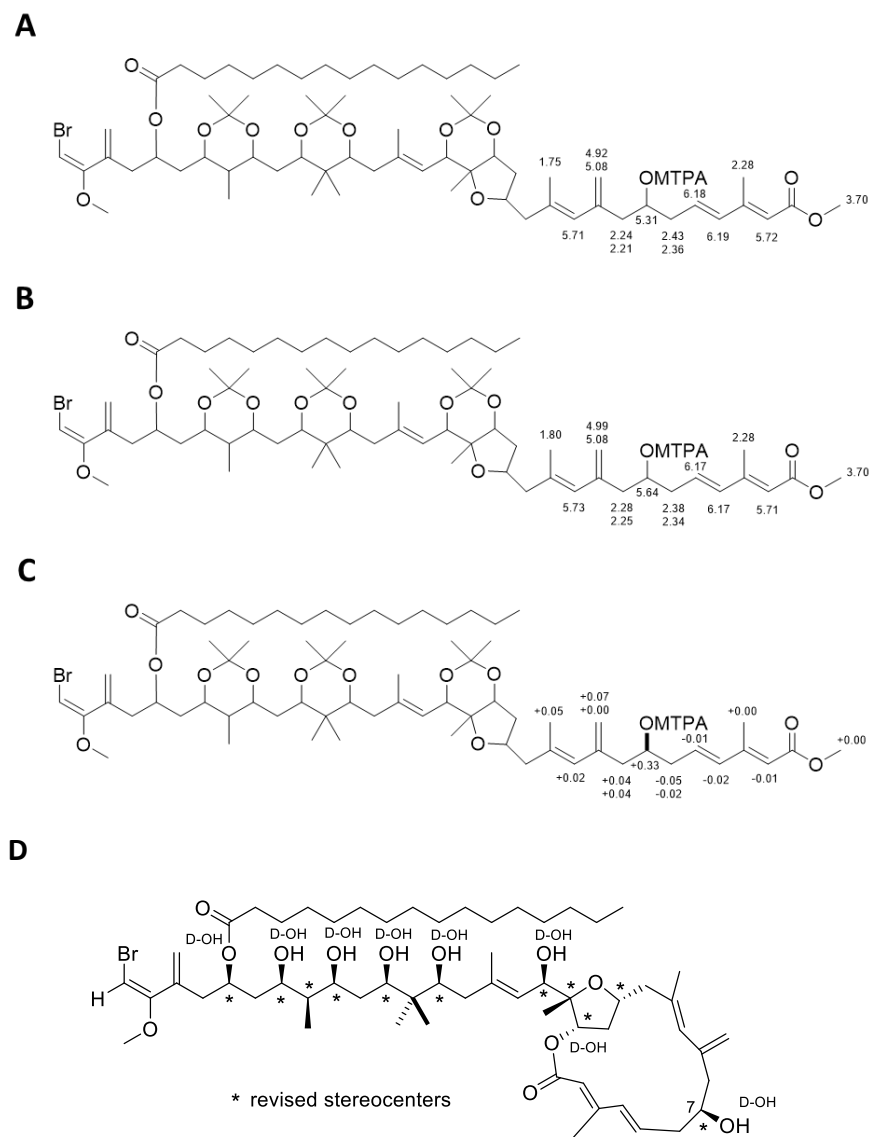
Supplementary Figure 8: Key NMR correlations of leptolyngbyalide A-C. A: leptolyngbyalide A (10), B: leptolyngbyalide B (11), and C: leptolyngbyalide C (12).



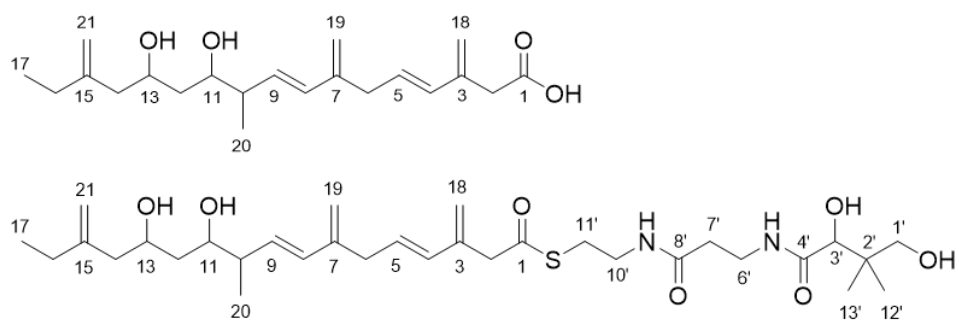
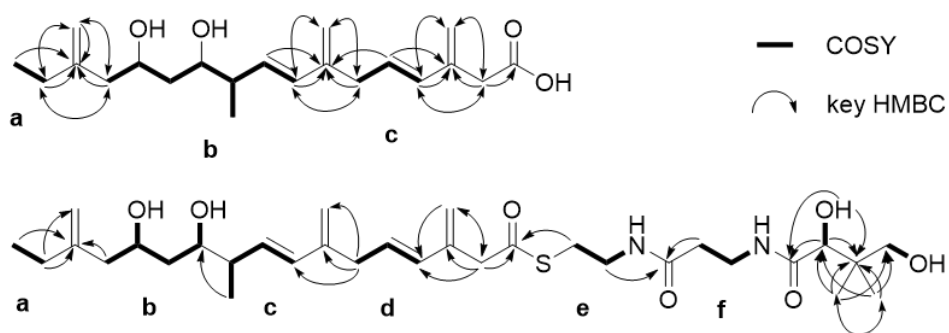
Supplementary Figure 9: Key NOESY correlations of leptolyngbyalides A-C. A: leptolyngbyalide A (10), B: leptolyngbyalide B (11), and C: leptolyngbyalide C (12).



Supplementary Figure 10: PCR-based verification of the correct assembly of the last PKS gene (*leptP*). Module 14 is putatively used iteratively and installs two beta branches. PCRs were conducted in duplicates (1-2). Neg: negative control. The detection of PCR fragments of the expected size indicates correct sequence assembly of the *lept* locus. Red arrows indicate translated primer annealing sites on the PKS level for the visualization of the corresponding PKS section and its assigned biosynthetic functions.



Supplementary Figure 11: Absolute stereochemistry of phormidolide. ^1H NMR chemical shifts of **A**: phormidolide triacetonide methyl ester (*R*)-MTPA ester and **B**: (*S*)-MTPA ester from the literature. **C**: $\Delta\delta_{S-R}$ values of phormidolide triacetonide methyl ester MTPA ester. **D**: Proposed revised absolute stereochemistry based on TransATor analysis and reexamination of published primary data.^{6,7}

A**B**

Supplementary Figure 12: A: Structures of cuniculene 6A (14) and cuniculene 6B (15). B: COSY and key HMBC correlations of cuniculene 6A (14) and 6B (15).

Supplementary Table 1: Ubiquitous distribution of *trans*-AT PKS BGCs across bacterial phyla. Distribution of functionally assigned *trans*-AT PKS BGCs^{2,5} for which the corresponding metabolite is characterized versus the distribution of sequenced BGCs as reported by O'Brien *et al.*⁴ and based on the AntiSMASH database.⁸ This discrepancy between annotated *trans*-AT PKS BGCs and the studies by O'Brien *et al.*⁴ and Blin *et al.*⁸ is either due to a higher abundance of *trans*-AT PKS BGCs in certain phyla, or due to a general overrepresentation of these genomes in GenBank. Firmicutes, Actinobacteria, β -Proteobacteria and γ -Proteobacteria as well as bacterial phyla not traditionally studied for natural product discovery show a huge potential for the isolation of novel *trans*-AT PKS-derived polyketides.

Phylum/Class	Annotated BGCs	Sequenced BGCs (O'Brien <i>et al.</i>)	Sequenced BGCs (AntiSMASH database)
Firmicutes	9	97	66
Actinobacteria	15	55	21
α -Proteobacteria	1	7	3
β -Proteobacteria	10	37	107
δ -Proteobacteria	14	14	7
γ -Proteobacteria	17	41	20
Bacteroidetes	2	3	2
Cyanobacteria	6	5	2
Other	3	0	183
total	77	259	411

Supplementary Table 2: *trans*-AT PKS ketide clades. HMMs were trained for each clade and used for TransATor predictions.

Clade ID	Clade Description
Clade_1	GNAT starter
Clade_2	α -Me shifted double bond or OH
Clade_5	amino acids (oxa/thia)
Clade_7	β D-OH
Clade_8	unusual starter (AMT/succinate)
Clade_9	aromatic starter
Clade_10	amino acids (glycine)
Clade_11	shifted double bonds
Clade_12	vinyllogous chain branching
Clade_13	lactate starter
Clade_14	exomethyl/exoester
Clade_21	α -Me red or keto
Clade_23	α -Me
Clade_25	completely reduced
Clade_26	pyran/furan rings
Clade_27	acetyl starter
Clade_28	amino acids
Clade_30	bimodule β D-OH
Clade_31	non-elongating (bimodule β D-OH)
Clade_32	cis-AT PKS
Clade_33	various starters
Clade_34	methoxycarbonyl starter
Clade_35	oxidative rearrangement
Clade_36	non-elongating (oxazole/thiazole rings)
Clade_38	non-elongating (pyran/furan rings)
Clade_39	amino acids (glycine)
Clade_40	β D-OH or β keto
Clade_42	shifted double bonds
Clade_43	α D-Me shifted double bonds
Clade_44	non-elongating (α -Me completely reduced or shifted double bond)

Clade ID	Clade Description
Clade_81	non-elongating (β D-OH)
Clade_82	double bonds (mostly <i>E</i> -configured)
Clade_83	non-elongating (mostly α -Me double bonds)
Clade_84	non-elongating
Clade_85	non-elongating (bimodule β D-OH)
Clade_86	α -L-Me red or OH
Clade_88	non-elongating
Clade_89	α -Me β -OH
Clade_90	β -keto or double bonds
Clade_92	non-elongating (α D-OH β -L-OH)
Clade_93	non elongating (β -OH)
Clade_94	non-elongating (various)
Clade_95	various specificities
Clade_96	various specificities (mainly α -Me)
Clade_97	β D-OH
Clade_98	non-elongating (various)
Clade_99	double bonds (<i>E</i> -configured)
Clade_100	mainly double bonds
Clade_101	double bonds
Clade_102	β D-OH
Clade_103	β OMe
Clade_104	β OMe or β Me double bond
Clade_106	lactate starter
Clade_107	mainly reduced
Clade_108	shifted double bonds
Clade_109	completely reduced
Clade_110	β D-OH or double bonds (<i>e</i> -configured)
Clade_111	α L-(di)Me β OH
Clade_112	α L-(di)Me β OH
Clade_113	double bonds (<i>e</i> -configured) (some with α -Me)

Clade_45	non-elongating (β -keto)
Clade_46	non-elongating (hemiacetal)
Clade_47	amino acids (oxazole/thiazole rings)
Clade_49	shifted double bonds (some with α -Me)
Clade_51	double bonds (<i>Z</i> -configured)
Clade_52	α -Me double bond
Clade_53	β D-OH
Clade_54	lactate starter
Clade_55	α -Me double bonds (<i>E</i> -configured)
Clade_56	α -Me double bonds (<i>Z</i> -configured)
Clade_57	double bonds (<i>E</i> -configured) (some with α -Me)
Clade_60	double bonds (<i>Z</i> -configured)
Clade_61	α L-Me β D-OH
Clade_62	β D-OH (some with α L-Me)
Clade_64	non-elongating (double bonds (mostly <i>Z</i> -configured))
Clade_65	double bonds
Clade_66	β L-OH
Clade_67	phosphoglycerate-derived starters
Clade_68	α L-OH/Me β D-OH
Clade_70	α OH β D-OH
Clade_72	α L-(di)Me β OH
Clade_73	Exomethylene
Clade_74	α Me β OH
Clade_75	non-elongating (β L-OH)
Clade_76	non-elongating (double bonds)
Clade_77	vinylous chain branching
Clade_78	non-elongating (mostly β OH)
Clade_79	starters or β OH
Clade_80	non-elongating (β OH)
Clade_114	β L-OH
Clade_115	β -keto or double bonds
Clade_116	β -keto or double bonds
Clade_117	α -Me red or keto
Clade_118	mainly double bonds
Clade_119	non elongating (β -OH)
Clade_120	non-elongating (various)
Clade_121	α D-OH β D-OH
Clade_122	double bonds (<i>E</i> -configured) (some with α -Me)
Clade_123	β D-OH
Clade_124	β D-OH
Clade_125	double bonds (<i>E</i> -configured)
Clade_126	double bonds (<i>E</i> -configured)
Clade_127	double bonds (<i>E</i> -configured)
Clade_128	double bonds (<i>E</i> -configured)
Clade_129	double bonds (<i>E</i> -configured)
Clade_130	double bonds (<i>E</i> -configured)
Clade_131	α -Me double bonds (<i>Z</i> -configured)
Clade_132	α -Me double bonds (<i>E</i> -configured)
Clade_133	α -Me double bonds (<i>E</i> -configured)
Clade_134	double bonds (<i>E</i> -configured)
Clade_135	β D-OH
Clade_136	β D-OH
Clade_137	β D-OH
Clade_138	α L-Me β OH
Clade_139	β OH
Clade_140	β D-OH
Clade_141	α -Me double bonds
Clade_142	non-elongating (various)

Supplementary Table 3: Annotation of KS sequences based on their respective ketide clades. Sequence names contain the following descriptors: name of the corresponding polyketide_protein harboring the respective KS_number of KS on the respective protein_KS number when counting from first KS of the pathway_substrate specificity.

Sequence	Clade
>basiliskamides_P615_14890_KS5_eDB	Clade_1
>kalimantacin_batumin_Bat1_1_KS1_AcStarter	Clade_1
>diaphorin_DipP_1_KS1_GNATstarter	Clade_1
>nosperin_NspA_1_KS1_GNATstarter	Clade_1
>onnamide_OnnB_1_KS1_GNATstarter	Clade_1
>pederin_PedI_1_KS1_GNATstarter	Clade_1
>psymberin_PsyA_1_KS1_GNATstarter	Clade_1
>bryostatin_BryX_1_KS14_GNATstarter	Clade_1
>oxazolomycin_OzmH_2_KS6_AAgly	Clade_10
>luminaolid_LumA_1_KS1_AAgly	Clade_10
>tolytoxin_TtoC_1_KS1_AAgly	Clade_10
>griseoviridin_SgvE2_2_KS4_eDB	Clade_100
>virginiamycin_VirA_4_KS4_eDB	Clade_100
>tartrolon_TrtF_1_KS9_b_D_OH	Clade_100
>oxazolomycin_OzmN_2_KS3_eDB	Clade_101
>kirromycin_KirAIV_1_KS7_eDB	Clade_101
>kirromycin_KirAIV_2_KS8_aMeeDB	Clade_101
>leinamycin_LnmI_2_KS2_AAoxz	Clade_101
>rhizopodin_RizD_5_KS15_bimod_bOH	Clade_101
>luminaolid_LumD_3_KS13_b_D_OH	Clade_102
>tolytoxin_TtoE_7_KS13_b_D_OH.	Clade_102
>misakinolide_MisE_3_KS13_b_D_OH	Clade_102
>luminaolid_LumE_3_KS17_b_D_OH	Clade_102
>tolytoxin_TtoF_3_KS17_b_D_OH	Clade_102
>misakinolide_MisF_3_KS17_b_D_OH	Clade_102
>bryostatin_BryD_2_KS13_0b_D_OH	Clade_102
>onnamide_OnnI_3_KS6_b_D_OH	Clade_102
>bryostatin_BryA_KS3_3_b_D_OH	Clade_102
>phormidolide_EKU96423_PhorL_1_KS4_aMeb_D_OH	Clade_102
>etnangien_EtnG_3_KS13_b_L_OMe	Clade_103
>luminaolid_LumD_2_KS12_b_D_OMe	Clade_103
>misakinolide_MisE_2_KS12_b_D_OMe	Clade_103
>tolytoxin_TtoE_6_KS12_b_D_OMe.	Clade_103
>calyculin_CalE_7_KS15_b_L_OH.	Clade_103
>calyculin_CalF_4_KS19_b_D_OMe.	Clade_103
>sorangicin_SorG_2_KS19_b_L_OH	Clade_103
>oxazolomycin_OzmK_1_KS12_a_L_OMe	Clade_103
>corallopyronin_CorL_3_KS12_bMeDB	Clade_104
>myxopyronin_MxnK_4_KS10_bMeDB	Clade_104
>luminaolid_LumB_1_KS4_a_D_Meb_D_OMe	Clade_104
>tolytoxin_TtoD_1_KS4_a_D_Meb_D_OMe	Clade_104
>misakinolide_MisC_4_KS4_bOMe	Clade_104
>rhizopodin_RizD_4_KS14_b_D_OMe	Clade_104
>rhizopodin_RizB_4_KS4_a_D_Meb_D_OMe	Clade_104
>rhizopodin_RizB_8_KS8_b_D_OMe	Clade_104
>rhizopodin_RizE_2_KS18_b_L_OMe	Clade_104
>etnangien_EtnI_1_KS17_reda_L_Me	Clade_104
>griseoviridin_SgvE3_1_KS5_eDB	Clade_104
>virginiamycin_VirF_1_KS5_bMeeDB	Clade_104
>paenimacrolidin_KS2_DB	Clade_108
>oocydin_Smar_OocR_2_KS12_shDB	Clade_108
>oocydin_Ddad_OocR_2_KS12_shDB	Clade_108
>rhizoxins_RhiD_2_KS10_shD	Clade_108

>corallopyronin_CorL_2_KS11_red	Clade_109
>myxopyronin_MxnK_3_KS9_red	Clade_109
>macrolactin_MlnB_3_KS3_red	Clade_109
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>bacillaene_Bamy_BaeN_3_KS12_shDB	Clade_11
>bacillaene_Bsub_PksN_3_KS13_shDB	Clade_11
>9methylstreptimidone_Smdl_4_KS4_eDB	Clade_110
>cycloheximide_ChxE_4_KS4_b_D_OH	Clade_110
>dorrigocin_migrastatin_MgsF_1_KS4_b_D_OH_eDB	Clade_110
>onnamide_OnnI_4_KS7_adiMeb_D_OH	Clade_111
>psymberin_PsyD_4_KS6_adiMeb_D_OH	Clade_111
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>elansolid_Cpin_ElsP_2_KS12_b_L_OH	Clade_114
>thailandamide_TaiD_2_KS2_b_L_OH	Clade_114
>disorazole_DszB_1_KS5_zDB	Clade_115
>disorazole_DszB_2_KS6_zDB	Clade_115
>SIA7248_SiaF_2_KS5_b_D_OH	Clade_115
>rhizopodin_RizB_5_KS5_bketo	Clade_115
>chlorotonil_CtoD_2_KS6_eDB	Clade_115
>SIA7248_SiaG_2_KS9_eDB	Clade_115
>legioliulin_LglD_4_KS4_bketo	Clade_115
>SIA7248_SiaH_KS12_bketo	Clade_115
>thailandamide_TaiL_2_KS10_bketo	Clade_116
>psymberin_PsyD_8_KS10_aMebketo	Clade_116
>dorrigocin_migrastatin_MgsF_3_KS6_aMeeDB	Clade_116
>basiliskamides_P615_BasF_1_KS1_GNATstarter	Clade_117
>basiliskamides_P615_BasE_1_KS2_a_L_Me_red	Clade_117
>elansolid_Csan_ElaK_2_KS4_aMe	Clade_117
>elansolid_Cpin_ElsJ_2_KS4_aMe	Clade_117
>elansolid_Csan_ElaK_1_KS3_adiMeb_D_OH	Clade_117
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>difficidin_DifL_1_KS14_redaMe	Clade_117
>calyculin_CalE_6_KS16_adiMbketo	Clade_117
>sorangicin_SorA_3_KS3_reda_D_Me	Clade_117
>myxovirescin_TaP_1_KS1_reda_D_Me	Clade_117
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>corallopyronin_CorK_2_KS8_eDB	Clade_118
>myxopyronin_MxnK_2_KS8_0red	Clade_118
>disorazole_DszA_2_KS2_eDB	Clade_118
>disorazole_DszB_4_KS8_0zDB	Clade_118
>difficidin_DifF_1_KS1_unusualStarters_acryloyl	Clade_118

>calyculin_CalE_2_KS11_aketo	Clade_118
>9methylstreptimidone_Smdl_3_KS3_vinylogous	Clade_12
>cycloheximide_ChxE_3_KS3_vinylogous	Clade_12
>dorrigin_migrastatin_MgsE_3_KS3_vinylogous	Clade_12
>tartrolon_TrtrF_2_KS10_0reda_D_Me	Clade_120
>griseoviridin_SgvE4_1_KS7_b_D_OH	Clade_120
>virginiamycin_VirH_1_KS7_0AAoxz	Clade_120
>mupirocin_MmpA_2_KS6_a_D_OHb_D_OH	Clade_121
>thiomarinol_TmpA_2_KS6_a_D_OHb_D_OH	Clade_121
>calyculin_CalF_2_KS17_a_D_OHb_D_OH	Clade_121
>myxovirescin_Ta1_4_KS4_b_L_OH	Clade_121
>chivosazole_ChiC_4_KS7_eDB	Clade_122
>lankacidin_LkcC_1_KS2_aMeeDB	Clade_122
>leinamycin_LnmJ_3_KS6_aMeDB	Clade_122
>diaphorin_DipT_3_KS6_b_D_OH	Clade_123
>pederin_PedF_3_KS6_b_D_OH	Clade_123
>thiomarinol_TmpA_3_KS7_bOH	Clade_124
>mupirocin_MmpA_3_KS7_b_D_OH	Clade_124
>SIA7248_SiaG_3_KS10_eDB	Clade_125
>myxovirescin_Ta1_7_KS7_eDB	Clade_125
>thailandamide_TaiL_4_KS12_eDB	Clade_125
>legioliulin_LglD_2_KS2_eDB	Clade_126
>chlorotonil_CtoE_1_KS9_DB_DA	Clade_126
>rhizopodin_RizD_6_KS16_eDB	Clade_126
>mupirocin_MmpB_1_KS8_esterification	Clade_126
>chivosazole_ChiC_3_KS6_eDB_zDB	Clade_127
>disorazole_DszB_3_KS7_eDB	Clade_127
>chlorotonil_CtoD_1_KS5_eDB	Clade_127
>chivosazole_ChiF_3_KS17_eDB_zDB	Clade_127
>kirromycin_KirAV_1_KS12_eDB	Clade_128
>anthracimycin_AtcE_KS6_eDB	Clade_128
>anthracimycin_AtcE_KS5_eDB	Clade_128
>lankacidin_LkcF_1_KS3_b_D_OH.	Clade_128
>oxazolomycin_OzmH_3_KS7_eDB	Clade_128
>anthracimycin_AtcF_2_KS9_eDB_DA	Clade_128
>thiomarinol_TmpB_1_KS8_eDBbMe	Clade_129
>thiomarinol_TmpD_3_KS3_eDB	Clade_129
>mupirocin_MmpD_3_KS3_eDB	Clade_129
>tartrolon_TrtrD_1_KS1_unusualStarter_lactate	Clade_13
>SIA7248_SiaD_1_KS1_unusualStarter_lactate	Clade_13
>FR901464_Fr9C_1_KS1_unusualstarter_lactate	Clade_13
>thailanstatin_TstC_1_KS1_lactateStarter	Clade_13
>bryostatin_BryA_1_KS1_lactateStarter	Clade_13
>etnangien_EtnH_2_KS16_eDB	Clade_130
>kirromycin_KirAll_1_KS3_eDB	Clade_130
>bacillaene_Bamy_BaeM_2_KS9_zDBaMe	Clade_131
>bacillaene_Bsub_PksM_2_KS9_zDBaMe	Clade_131
>difficidin_DifI_1_KS7_aMezDB	Clade_131
>calyculin_CalG_2_KS22_aMeDB	Clade_132
>albicidin_Albi_2_KS2_aMeeDB	Clade_132
>FR901464_Fr9F_4_KS7_aMeeDB	Clade_133
>thailanstatin_TstDEF_4_KS7_aMeeDB	Clade_133
>malleilactone_burkholderic_acid_BurF_2_KS2_aMeeDB	Clade_133
>thailandamide_TaiM_3_KS15_aMeeDB	Clade_133
>chlorotonil_CtoC_3_KS3_eDB	Clade_134
>anthracimycin_AtcD_3_KS3_eDB	Clade_134
>FR901464_Fr9H_3_KS9_b_D_OH	Clade_135
>thailanstatin_TstGH_2_KS9_b_D_OH	Clade_135
>rhizopodin_RizB_1_KS1_AAgly	Clade_136

>disorazole_DszA_4_KS4_b_D_OH	Clade_136
>chivosazole_ChiB_2_KS2_b_D_OH	Clade_136
>kirromycin_KirAll_3_KS5_b_D_OH	Clade_136
>thailandamide_TaiL_3_KS11_b_D_OH	Clade_137
>psymberin_PsyD_3_KS5_b_D_OH	Clade_137
>basiliskamides_P615_BasE_2_KS3_a_D_Meb_D_OH	Clade_137
>oocydin_Smar_OocS_1_KS13_aMebOH	Clade_138
>oocydin_Ddad_OocS_1_KS13_aMebOH	Clade_138
>diaphorin_DipT_4_KS7_adiMebOH	Clade_138
>pederin_PedF_4_KS7_adiMeb_D_OH	Clade_138
>luminaolid_LumC_1_KS7_a_L_Meb_L_OME_a_L_Meb_L_OH	Clade_138
>tolytoxin_TtoE_1_KS7_a_D_Meb_D_OH	Clade_138
>mupirocin_MmpA_KS2_b_D_OH	Clade_138
>thiomarinol_TmpD_2_KS2_a_L_Meb_L_OH	Clade_138
>onnamide_OnnI_4_KS7_adiMeb_D_OH	Clade_138
>luminaolid_LumC_4_KS10_a_L_Meb_L_OH	Clade_138
>tolytoxin_TtoE_4_KS10_a_L_Meb_L_OH	Clade_138
>misakinolide_MisD_4_KS10_a_L_Meb_L_OH	Clade_138
>psymberin_PsyD_4_KS6_adiMeb_D_OH	Clade_138
>phormidolide_EKU96423_PhorL_3_KS6_adiMeb_D_OH	Clade_138
>calyculin_CalE_4_KS13_b_L_OH	Clade_138
>rhizoxins_RhiC_2_KS7_a_D_Meb_L_OH	Clade_138
>rhizoxins_RhiD_1_K9_aMeb_D_OH	Clade_138
>psymberin_PsyD_6_KS8_a_D_Meb_L_OH	Clade_138
>calyculin_CalF_5_KS20_a_L_Meb_L_OH	Clade_138
>calyculin_CalG_1_KS21_a_L_Meb_L_OH	Clade_138
>bacillaene_Bsub_PksM_3_KS10_bOH	Clade_139
>oocydin_Smar_OocS_3_KS15_0b_L_OH	Clade_139
>oocydin_Ddad_OocS_3_KS15_0b_L_OH	Clade_139
>elansolid_Csan_ElaP_2_KS9_0bimod_bOH	Clade_139
>elansolid_Cpin_ElsO_2_KS9_0bimod_bOH	Clade_139
>etnangien_EtnF_3_KS10_b_L_OH	Clade_139
>etnangien_EtnG_2_KS12_0b_L_OH	Clade_139
>etnangien_EtnI_4_KS20_0b_L_OH	Clade_139
>bongkrekcic_acid_BonA_4_KS4_b_L_OH	Clade_139
>bryostatin_BryA_2_KS2_b_L_OH	Clade_139
>bryostatin_BryD_1_KS12_b_L_OH	Clade_139
>bryostatin_BryB_4_KS7_b_L_OH	Clade_139
>phormidolide_EKU96420_PhorO_3_KS11_b_L_OH	Clade_139
>rhizoxins_RhiE_2_KS13_b_L_OH	Clade_139
>diaphorin_DipT_6_KS9_b_L_OH	Clade_139
>pederin_PedF_6_KS9_b_L_OH	Clade_139
>luminaolid_LumC_3_KS9_b_L_OH	Clade_139
>tolytoxin_TtoE_3_KS9_b_L_OH	Clade_139
>misakinolide_MisD_3_KS9_b_L_OH	Clade_139
>onnamide_OnnI_6_KS9_b_L_OH	Clade_139
>kalimantacin_batumin_Bat2_2_KS3_bOH	Clade_139
>sorangicin_SorA_5_KS5_a_L_OHb_L_OH	Clade_139
>sorangicin_SorD_2_KS14_b_L_OH	Clade_139
>difficidin_DifI_2_KS8_bOH	Clade_139
>oocydin_Smar_OocN_3_KS7_b_L_OH	Clade_139
>oocydin_Ddad_OocN_3_KS7_b_L_OH	Clade_139
>psymberin_PsyD_7_KS9_b_L_OH	Clade_139
>elansolid_Csan_ElaQ_2_KS12_b_L_OH	Clade_139
>elansolid_Cpin_ElsP_2_KS12_b_L_OH	Clade_139
>thailandamide_TaiD_2_KS2_b_L_OH	Clade_139
>SIA7248_SiaF_1_KS4_b_D_OH	Clade_139
>SIA7248_SiaF_3_KS6_b_D_OH	Clade_139
>SIA7248_SiaF_4_KS7_b_D_OH	Clade_139

>SIA7248_SiaE_2_KS3_b_L_OH	Clade_139
>SIA7248_SiaE_1_KS2_b_D_OH	Clade_139
>FR901464_Fr9H_2_KS10_exometh	Clade_14
>thailanstatin_TstGH_3_KS10_exometh	Clade_14
>bryostatin_BryB_1_KS4_exoester	Clade_14
>bryostatin_BryC_1_KS8_exoester	Clade_14
>kalimantacin_batumin_Bat2_4_KS5_redbMe	Clade_14
>kalimantacin_batumin_Bat3_4_KS11_redbMe	Clade_14
>psymberin_PsyA_2_KS2_exometh	Clade_14
>oocydin_Smar_OocJ_2_KS2_exometh	Clade_14
>oocydin_Ddad_OocJ_2_KS2_exometh	Clade_14
>phormidolide_EKU96419_PhorP_1_KS13_redbMe	Clade_14
>phormidolide_EKU96424_PhorK_2_KS2_exometh	Clade_14
>nosperin_NspA_3_KS3_exometh	Clade_14
>onnamide_OnnB_3_KS3_exometh	Clade_14
>etnangien_EtnD_2_KS2_eDBbMe	Clade_14
>myxovirescin_TaO_1_KS8_redbethyl	Clade_14
>kalimantacin_batumin_Bat3_3_KS10_exometh	Clade_14
>paenimacrolidin_KS5_bMe	Clade_14
>diaphorin_DipP_3_KS3_exometh	Clade_14
>pederin_PedI_3_KS3_exometh	Clade_14
>9methylstreptimidone_Smdl_4_KS4_eDB	Clade_140
>cycloheximide_ChxE_4_KS4_b_D_OH	Clade_140
>dorrigocin_migrastatin_MgsF_1_KS4_b_D_OH_eDB	Clade_140
>nosperin_NspA_2_KS2_a_L_Meb_D_OH	Clade_140
>diaphorin_DipP_2_KS2_a_L_Meb_D_OH	Clade_140
>onnamide_OnnB_2_KS2_a_L_Me_D_OH	Clade_140
>pederin_PedI_2_KS2_a_L_Meb_D_OH	Clade_140
>etnangien_EtnD_3_KS3_b_D_OH	Clade_140
>etnangien_EtnI_2_KS18_a_L_Meb_D_OH	Clade_140
>etnangien_EtnI_3_KS19_a_L_Meb_D_OH	Clade_140
>kalimantacin_batumin_Bat2_3_KS4_bOH	Clade_140
>etnangien_EtnF_2_KS9_b_D_OH	Clade_140
>elansolid_Csan_ElaQ_1_KS11_a_L_Meb_D_OH	Clade_140
>elansolid_Cpin_ElsP_1_KS11_a_L_Meb_D_OH	Clade_140
>myxovirescin_TaI_2_KS2_b_L_OH	Clade_140
>difficidin_DifG_1_KS4_OH	Clade_140
>luminaolid_LumD_3_KS13_b_D_OH	Clade_140
>tolytoxin_TtoE_7_KS13_b_D_OH	Clade_140
>misakinolide_MisE_3_KS13_b_D_OH	Clade_140
>luminaolid_LumE_3_KS17_b_D_OH	Clade_140
>tolytoxin_TtoF_3_KS17_b_D_OH	Clade_140
>misakinolide_MisF_3_KS17_b_D_OH	Clade_140
>bryostatin_BryD_2_KS13_0b_D_OH	Clade_140
>onnamide_OnnI_3_KS6_b_D_OH	Clade_140
>bryostatin_BryA_KS3_3_b_D_OH	Clade_140
>phormidolide_EKU96423_PhorL_1_KS4_aMeb_D_OH	Clade_140
>diaphorin_DipT_3_KS6_b_D_OH	Clade_140
>pederin_PedF_3_KS6_b_D_OH	Clade_140
>thailandamide_TaiL_3_KS11_b_D_OH	Clade_140
>psymberin_PsyD_3_KS5_b_D_OH	Clade_140
>basiliskamides_P615_BasE_2_KS3_a_D_Meb_D_OH	Clade_140
>elansolid_Csan_ElaJ_2_KS2_eDB	Clade_141
>elansolid_Cpin_ElsI_2_KS2_eDB	Clade_141
>elansolid_Csan_ElaQ_3_KS13_aMeDB	Clade_141
>elansolid_Cpin_ElsP_3_KS13_aMeDB	Clade_141
>sorangicin_SorA_4_KS4_aMeDB	Clade_141
>sorangicin_SorC_1_KS12_eDB	Clade_141
>misakinolide_MisF_4_KS18_aMeDB	Clade_141

>tolytoxin_TtoF_4_KS18_aMeeDB	Clade_141
>difficidin_DifF_2_KS2_aMeeDB	Clade_141
>rhizoxins_RhiB_3_KS4_aMeeDB	Clade_141
>chivosazole_ChiF_1_KS15_aMeeDB	Clade_141
>oxazolomycin_OzmH_1_KS5_aMezDB	Clade_141
>corallopyronin_CorL_4_KS13_aMeDB	Clade_141
>myxopyronin_MxnK_5_KS11_aMeDB	Clade_141
>calyculin_CalG_2_KS22_aMeDB	Clade_141
>albicidin_Albi_2_KS2_aMeeDB	Clade_141
>FR901464_Fr9F_4_KS7_aMeeDB	Clade_141
>thailanstatin_TstDEF_4_KS7_aMeeDB	Clade_141
>malleilactone_burkholderic_acid_BurF_2_KS2_aMeeDB	Clade_141
>thailandamide_TaiM_3_KS15_aMeeDB	Clade_141
>bacillaene_Bamy_BaeM_2_KS9_zDBaMe	Clade_141
>bacillaene_Bsub_PksM_2_KS9_zDBaMe	Clade_141
>difficidin_DifI_1_KS7_aMezDB	Clade_141
>elansolid_Csan_ElaR_1_KS14_0eDB	Clade_142
>elansolid_ElsQ_1_KS14_0eDB	Clade_142
>luminaolid_LumE_4_KS18_0b_D_OH	Clade_142
>tolytoxin_TtoF_5_KS19_0eDB	Clade_142
>misakinolide_MisF_5_KS19_0eDB	Clade_142
>pederin_PedH_4_KS13_0eDB	Clade_142
>rhizoxins_RhiF_2_KS16_0eDB	Clade_142
>sorangicin_SorB_1_KS8_0zDB	Clade_142
>enacyloxin_Bamb_5919_2_KS11_0eDB	Clade_142
>bacillaene_Bamy_BaeR_1_KS13_0aMeDB	Clade_142
>bacillaene_Bsub_PksR_1_KS14_0aMeDB	Clade_142
>onnamide_OnnI_7_KS10_0red	Clade_142
>calyculin_CalH_3_KS27_eDB	Clade_142
>nosperin_NspC_3_KS6_0biomod_aMeeDB	Clade_142
>rhizoxins_RhiD_3_KS11_0biomod_aMeeDB	Clade_142
>chivosazole_ChiF_4_KS18_0zDB	Clade_142
>luminaolid_LumA_3_KS3_0biomod_a_D_Meb_D_OH	Clade_142
>tolytoxin_TtoC_3_KS3_0a_D_Meb_D_OH	Clade_142
>misakinolide_MisC_3_KS3_0biomod_b_D_OME	Clade_142
>chivosazole_ChiD_1_KS10_0AAoxz	Clade_142
>disorazole_DszC_1_KS9_0AAoxz	Clade_142
>rhizopodin_RizD_1_KS11_0AAoxa	Clade_142
>calyculin_CalC_1_KS7_KS0oxa	Clade_142
>rhizoxins_RhiB_1_KS2_0AAoxa	Clade_142
>leinamycin_LnmI_1_KS1_0AAoxz	Clade_142
>rhizopodin_RizB_7_KS7_0biomod_b_D_OH	Clade_142
>rhizopodin_RizD_3_KS13_0biomod_b_D_OH	Clade_142
>rhizopodin_RizB_3_KS3_0biomod_a_D_Meb_D_OH	Clade_142
>rhizopodin_RizE_1_KS17_0biomod_b_L_OH	Clade_142
>tartrolon_TrtrF_2_KS10_0reda_D_Me	Clade_142
>griseoviridin_SgvE4_1_KS7_b_D_OH	Clade_142
>virginiamycin_VirH_1_KS7_0AAoxz	Clade_142
>disorazole_DszC_1_KS2_0AAoxz	Clade_142
>corallopyronin_CorJ_2_KS5_0aMe	Clade_142
>myxopyronin_MxnJ_2_KS5_0reda_L_Me	Clade_142
>chlorotonil_CtoC_4_KS4_aMezshDB	Clade_2
>chlorotonil_CtoD_4_aMeshDB	Clade_2
>anthracimycin_AtcE_KS7_redaMe	Clade_2
>disorazole_DszA_3_KS3_adiMeb_L_OH	Clade_2
>corallopyronin_CorL_1_KS10_bMeDB	Clade_2
>chivosazole_ChiC_1_KS4_a_D_Meb_D_OH	Clade_2
>luminaolid_LumC_2_KS8_a_D_Meb_D_OH_b_D_OH	Clade_2
>tolytoxin_TtoE_2_KS8_a_D_Me_D_OH	Clade_2

>misakinolide_MisD_2_KS8_b_L_OH	Clade_2
>9methylstreptimidone_Smdl_KS5_5_a_D_Mebketo	Clade_21
>cycloheximide_ChxE_5_KS5_a_D_Mebketo	Clade_21
>FR901464_Fr9F_2_KS5_reda_L_Me	Clade_21
>thailanstatin_TstDEF_2_KS5_reda_L_Me	Clade_21
>calyculin_CalB_3_KS5_0reda_L_Me	Clade_21
>dorrigocin_migrastatin_MgsF_2_KS5_a_D_MebketodH	Clade_21
>dorrigocin_migrastatin_MgsF_5_KS8_b_L_OH	Clade_21
>bongkreki acid_BonA_3_KS3_aMeDB	Clade_23
>bongkreki acid_BonD_1_KS10_a_L_Me	Clade_23
>chlorotonil_CtoD_3_KS7_redaMe	Clade_23
>bacillaene_Bamy_BaeJ_2_KS2_red	Clade_25
>bacillaene_Bsub_PksJ_2_KS2_red	Clade_25
>bacillaene_Bamy_BaeN_2_KS11_shDB	Clade_25
>bacillaene_Bsub_PksN_2_KS12_shDB	Clade_25
>bacillaene_Bamy_BaeN_3_KS12_shDB	Clade_25
>bacillaene_Bsub_PksN_3_KS13_shDB	Clade_25
>difficidin_DifI_3_KS9_red	Clade_25
>paenimacrolidin_KS2_DB	Clade_25
>kalimantacin_batumin_Bat3_2_KS9_eDB	Clade_25
>diaphorin_DipO_2_KS11_DB	Clade_25
>pederin_PedH_2_KS11_red	Clade_25
>oocydin_Smar_OocR_2_KS12_shDB	Clade_25
>oocydin_Ddad_OocR_2_KS12_shDB	Clade_25
>rhizoxins_RhiD_2_KS10_shD	Clade_25
>myxovirescin_TaO_4_KS11_red	Clade_25
>myxovirescin_TaO_2_KS9_red	Clade_25
>calyculin_CalE_3_KS12_a_D_Meb_L_OH	Clade_25
>dorrigocin_migrastatin_MgsF_6_KS9_eDB	Clade_25
>dorrigocin_migrastatin_MgsG_1_KS10_red	Clade_25
>difficidin_DifF_3_KS3_red	Clade_25
>oocydin_Smar_OocN_5_KS9_red	Clade_25
>oocydin_Ddad_OocN_5_KS9_red	Clade_25
>sorangicin_SorA_2_KS2_red	Clade_25
>sorangicin_SorB_4_KS11_red	Clade_25
>myxovirescin_TaO_3_KS10_bketo	Clade_25
>phormidolide_EKU96424_PhorK_3_KS3_b_D_OH	Clade_25
>myxovirescin_Ta1_5_KS5_red	Clade_25
>calyculin_CalA_2_KS2_AAser	Clade_25
>bongkreki acid_BonB_2_KS8_red	Clade_25
>bryostatin_BryC_2_KS9_pyran	Clade_26
>diaphorin_DipT_5_KS8_pyran	Clade_26
>pederin_PedF_5_KS8_pyran	Clade_26
>luminaolid_LumE_2_KS16_pyran	Clade_26
>tolytoxin_TtoF_2_KS16_pyran	Clade_26
>misakinolide_MisF_2_KS16_pyran	Clade_26
>onnamide_OnnI_5_KS8_pyran	Clade_26
>psymberin_PsyD_5_KS7_pyran	Clade_26
>oocydin_Smar_OocN_4_KS8_furan	Clade_26
>oocydin_Ddad_OocN_4_KS8_furan	Clade_26
>phormidolide_EKU96420_PhorO_4_KS12_furan	Clade_26
>sorangicin_SorH_1_KS20_pyran	Clade_26
>sorangicin_SorE_2_KS16_pyran	Clade_26
>sorangicin_SorB_2_KS9_pyran	Clade_26s
>corallopyronin_CorK_1_KS7_acetyl	Clade_27
>myxopyronin_MxnK_1_KS7_starter	Clade_27
>disorazole_DszA_1_KS1_acetylStarter	Clade_27
>macrolactin_MlnB_1_KS1_acetylStarter	Clade_27
>anthracimycin_AtcD_1_KS1_acetylStarter	Clade_27

>chlorotonil_CtoC_1_KS1_acetylStarter	Clade_27
>misakinolide_MisC_1_KS1_acetylStarter	Clade_27
>calyculin_CalA_KS1_KSOAAser	Clade_28
>bacillaene_Bamy_BaeJ_1_KS1_Agly	Clade_28
>bacillaene_Bsub_PksJ_1_KS1_AAgly	Clade_28
>bacillaene_Bamy_BaeN_1_KS10_AAala	Clade_28
>bacillaene_Bsub_PksN_1_KS11_AAala	Clade_28
>diaphorin_DipT_2_KS5_AAgly	Clade_28
>pederin_PedF_2_KS5_AAgly	Clade_28
>onnamide_OnnI_2_KS5_AAgly	Clade_28
>psymberin_PsyD_2_KS4_AAgly	Clade_28
>calyculin_CalH_2_KS26_AAala	Clade_28
>nosperin_NspC_2_KS5_AAgly	Clade_28
>calyculin_CalB_2_KS4_AAgly	Clade_28
>kalimantacin_batumin_Bat2_1_KS2_AAGly	Clade_28
>myxovirescin_TaI_1_KS1_AAgly	Clade_28
>FR901464_Fr9D_1_KS4_AAthr	Clade_28
>thailandstatin_TstDEF_1_KS4_AAthr	Clade_28
>thailandamide_TaiE_1_KS5_AAala	Clade_28
>griseoviridin_SgvE2_1_KS3_AAgly	Clade_28
>virginiamycin_VirA_3_KS3_AAgly	Clade_28
>oxazolomycin_OzmN_1_KS2_AAoxa.	Clade_28
>oxazolomycin_OzmQ_1_KS1_AAgly	Clade_28
>malleilactone_burkholderic_acid_BurA_1_KS1_unusualStarter	Clade_28
>basiliskamides_P615_BasE_3_KS3_bOH	Clade_30
>elansolid_Csan_ElaO_2_KS7_bimod_b_D_OH	Clade_30
>elansolid_Cpin_ElsN_2_KS7_bimod_b_D_OH	Clade_30
>difficidin_DifI_4_KS10_bimod_bOH	Clade_30
>etnangien_EtnG_4_KS14_0bOH	Clade_30
>chivosazole_ChiC_2_KS5_bimod_bOH	Clade_30
>chivosazole_ChiD_3_KS12_bimod_bOH	Clade_30
>chivosazole_ChiF_2_KS16_bimod_bOH	Clade_30
>macrolactin_MlnE_2_KS8_bimod_bOH	Clade_30
>macrolactin_MlnG_1_KS11_bimod_bOH	Clade_30
>kirromycin_KirAIV_5_KS11_b_D_OH	Clade_30
>leinamycin_Lnml_3_KS3_zDB	Clade_30
>kirromycin_KirAI_2_KS2_zcrotonyl	Clade_30
>tartrolon_Trtd_KS3_3_bimod_bOH	Clade_30
>bacillaene_Bamy_BaeJ_3_KS3_0Hbimod_bOH	Clade_31
>bacillaene_Bsub_PksJ_3_KS3_0Hbimod_OH	Clade_31
>bacillaene_Bamy_BaeL_4_KS7_0Hbimod_bOH	Clade_31
>bacillaene_Bsub_PksL_4_KS7_0bimod_bOH	Clade_31
>difficidin_DifG_2_KS5_0Hbimod_bOH	Clade_31
>luminaolid_LumD_4_KS14_0bimod_b_D_OH	Clade_31
>tolytoxin_TtoE_8_KS14_0bimod_b_D_OH	Clade_31
>misakinolide_MisE_4_KS14_0b_L_OH	Clade_31
>bongkrekiac_acid_BonA_6_KS6_0bimod_bOH	Clade_31
>kalimantacin_batuminBat2_6_KS7_0bimod_bOH	Clade_31
>sorangicin_SorA_7_KS7_0bimod_bOH	Clade_31
>sorangicin_SorH_3_KS22_0bimod_bOH	Clade_31
>oxazolomycin_OzmH_4_KS8_0eDB	Clade_31
>thailandamide_TaiK_2_KS8_0bOH	Clade_31
>difficidin_DifJ_2_KS12_0bimod_bOH	Clade_31
>bongkrekiac_acid_BonA_KS1_1_GNATstarter	Clade_32
>enacyloxin_Bamb_5921_2_KS7_b_D_OH	Clade_32
>enacyloxin_Bamb_5924_3_KS3_b_D_OH	Clade_32
>enacyloxin_Bamb_5924_2_KS2_eDB	Clade_32
>enacyloxin_Bamb_5920_2_KS9_aMeDB	Clade_32
>psymberin_PsyD_9_KS11_bketo	Clade_32

>SIA7248_Sial_1_KS13_2biMod_OH	Clade_32
>2qo3_chainA_EryKS3_OUTGROUP	Clade_32
>2hg4_chainA_EryKS5_OUTGROUP	Clade_32
>enacyloxin_Bamb_5922_1_KS5_b_D_OH.	Clade_32
>enacyloxin_Bamb_5920_1_KS8_eDB	Clade_32
>enacyloxin_Bamb_5919_1_KS10_bketo	Clade_32
>enacyloxin_Bamb_5923_1_KS4_b_L_OH	Clade_32
>thiomarinol_TmpD_1_KS1_acetylStarter	Clade_33
>mupirocin_MmpD_1_KS1_acetylStarter	Clade_33
>thailandamide_TaiD_1_KS1_aromaticStarter	Clade_33
>corallopyronin_CorI_1_KS1_unusualStarter_methoxycarbonyl	Clade_34
>myxopyronin_MxnI_1_KS1_unusualstarter	Clade_34
>diaphorin_DipO_1_KS10_rearrangement	Clade_35
>pederin_PedH_1_KS10_rearrangement	Clade_35
>oocydin_Smar_OocL_1_KS3_rearrangement	Clade_35
>oocydin_Ddad_OocL_1_KS3_rearrangement	Clade_35
>chivosazole_ChiD_1_KS10_0AAoxz	Clade_36
>disorazole_DszC_1_KS9_0AAoxz	Clade_36
>rhizopodin_RizD_1_KS11_0AAoxa	Clade_36
>calyculin_CalC_1_KS7_KS0oxa	Clade_36
>rhizoxins_RhiB_1_KS2_0AAoxa	Clade_36
>leinamycin_LnmI_1_KS1_0AAoxa	Clade_36
>FR901464_Fr9I_2_KS12_0pyran	Clade_38
>thailanstatin_TstI_2_KS12_0pyran	Clade_38
>corallopyronin_CorI_2_KS2_AAgly	Clade_39
>myxopyronin_MxnI_2_KS2_AAgly	Clade_39
>lankacidin_LkcA_1_KS1_AAgly	Clade_39
>chivosazole_ChiC_5_KS8_b_L_OH	Clade_40
>anthracimycin_AtcF_3_KS10_bketo	Clade_40
>chlorotonil_CtoE_2_KS10_bketo	Clade_40
>kirromycin_KirAIV_4_KS10_b_L_OH	Clade_40
>macrolactin_MlnD_2_KS6_b_D_OH	Clade_40
>corallopyronin_CorJ_1_KS4_shDB	Clade_42
>myxopyronin_MxnJ_1_KS4_shDB	Clade_42
>luminaolid_LumA_2_KS2_a_D_MeshDB	Clade_43
>tolytoxin_TtoC_2_KS2_a_D_MeshDB	Clade_43
>bacillaene_Bamy_BaeR_2_KS14_0shDBMe	Clade_44
>bacillaene_Bsub_PksR_2_KS15_0shDBaMe	Clade_44
>calyculin_CalH_1_KS25_bMeDB	Clade_44
>calyculin_CalB_4_KS6_0reda_L_Me	Clade_44
>thailandamide_TaiD_4_KS4_0reda_D_Me	Clade_44
>oocydin_Smar_OocN_6_KS10_0bketo	Clade_45
>oocydin_Ddad_OocN_6_KS10_0bketo	Clade_45
>diaphorin_DipT_1_KS4_0acetal	Clade_46
>pederin_PedF_1_KS4_0acetal	Clade_46
>nosperin_NspC_1_KS4_0acetal	Clade_46
>onnamide_OnnI_1_KS4_0acetal	Clade_46
>nosperin_NspC_4_KS7_aMeshDB	Clade_49
>rhizoxins_RhiE_1_KS1_aMeshDB	Clade_49
>onnamide_OnnJ_1_KS11_bOH	Clade_49
>calyculin_CalI_1_KS24_shDB	Clade_49
>chivosazole_ChiD_2_KS11_AAoxa	Clade_5
>rhizopodin_RizD_2_KS12_AAoxa	Clade_5
>rhizoxins_RhiB_2_KS3_AAoxa	Clade_5
>calyculin_CalC_2_KS8_AAoxa	Clade_5
>bacillaene_Bamy_BaeL_1_KS4_zDB	Clade_51
>bacillaene_Bsub_PksL_1_KS4_zDB	Clade_51
>bacillaene_Bamy_BaeM_1_KS8_zDB	Clade_51
>bacillaene_Bsub_PksM_1_KS8_zDB	Clade_51

>difficidin_DifH_1_KS6_zDB	Clade_51
>chivosazole_ChiF_1_KS15_aMeeDB	Clade_52
>oxazolomycin_OzmH_1_KS5_aMezDB	Clade_52
>corallopyronin_CorL_4_KS13_aMeDB	Clade_52
>myxopyronin_MxnK_5_KS11_aMeDB	Clade_52
>macrolactin_MlnB_2_KS2_b_D_OH	Clade_53
>chlorotonil_CtoC_2_KS2_bOH	Clade_53
>anthracimycin_AtcD_2_KS2_bOH	Clade_53
>griseoviridin_SgvE1_2_KS2_b_D_OH	Clade_53
>virginiamycin_VirA_2_KS2_a_L_Meb_D_OH	Clade_53
>griseoviridin_SgvE3_2_KS6_b_L_OH	Clade_53
>virginiamycin_VirG_1_KS6_b_D_OH	Clade_53
>misakinolide_MisF_4_KS18_aMeeDB	Clade_55
>tolytoxin_TtoF_4_KS18_aMeeDB	Clade_55
>difficidin_DifF_2_KS2_aMeeDB	Clade_55
>rhizoxins_RhiB_3_KS4_aMeeDB	Clade_55
>oocydin_Smar_OocS_2_KS14_aMezDB	Clade_56
>oocydin_Ddad_OocS_2_KS14_aMezDB	Clade_56
>elansolid_Csan_ElaJ_2_KS2_eDB	Clade_57
>elansolid_Cpin_ElsI_2_KS2_eDB	Clade_57
>elansolid_Csan_ElaQ_3_KS13_aMeDB	Clade_57
>elansolid_Cpin_ElsP_3_KS13_aMeDB	Clade_57
>luminaolid_LumE_1_KS15_zDB	Clade_60
>tolytoxin_TtoF_1_KS15_zDB	Clade_60
>misakinolide_MisF_1_KS15_zDB	Clade_60
>nosperin_NspA_2_KS2_a_L_Meb_D_OH	Clade_61
>diaphorin_DipP_2_KS2_a_L_Meb_D_OH	Clade_61
>onnamide_OnnB_2_KS2_a_L_Me_D_OH	Clade_61
>pederin_PedI_2_KS2_a_L_Meb_D_OH	Clade_61
>etnangien_EtnD_3_KS3_b_D_OH	Clade_62
>etnangien_EtnI_2_KS18_a_L_Meb_D_OH	Clade_62
>etnangien_EtnI_3_KS19_a_L_Meb_D_OH	Clade_62
>kalimantacin_batumin_Bat2_3_KS4_bOH	Clade_62
>etnangien_EtnF_2_KS9_b_D_OH	Clade_62
>elansolid_Csan_ElaQ_1_KS11_a_L_Meb_D_OH	Clade_62
>elansolid_Cpin_ElsP_1_KS11_a_L_Meb_D_OH	Clade_62
>myxovirescin_Ta1_2_KS2_b_L_OH	Clade_62
>difficidin_DifG_1_KS4_OH	Clade_62
>9methylstreptimidone_Smdl_2_KS2_ozDB	Clade_64
>cycloheximide_ChxE_2_KS2_ozDB	Clade_64
>dorrigocin_migrastatin_MgsE_2_KS2_ozDB	Clade_64
>rhizoxins_RhiE_3_KS14_0eDB	Clade_64
>bacillaene_Bamy_BaeL_1_KS4_zD	Clade_65
>bacillaene_Bsub_PksL_1_KS4_zD	Clade_65
>bacillaene_Bamy_BaeM_1_KS8_zDB	Clade_65
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>difficidin_DifH_1_KS6_zDB	Clade_65
>luminaolid_LumE_1_KS15_zDB	Clade_65
>tolytoxin_TtoF_1_KS15_zDB	Clade_65
>misakinolide_MisF_1_KS15_zDB	Clade_65
>oocydin_Smar_OocS_2_KS14_aMezDB	Clade_65
>oocydin_Ddad_OocS_2_KS14_aMezDB	Clade_65
>difficidin_DifJ_1_KS11_zDB_zDB	Clade_65
>elansolid_Csan_ElaP_1_KS8_eDB	Clade_65
>elansolid_Cpin_ElsO_1_KS8_eDB	Clade_65
>oxazolomycin_OzmN_3_KS4_zDB	Clade_65
>kalimantacin_batumin_Bat3_1_KS8_eDB	Clade_65
>oxazolomycin_OzmH_5_KS9_eDB	Clade_65
>thailandamide_TaiL_1_KS9_eDB	Clade_65

>leinamycin_LnmJ_1_KS4_eDB	Clade_65
>SIA7248_SiaH_KS11_eDB	Clade_65
>bongkrekiac_acid_BonA_4_KS4_b_L_OH	Clade_66
>bryostatin_BryA_2_KS2_b_L_OH	Clade_66
>bryostatin_BryD_1_KS12_b_L_OH	Clade_66
>bryostatin_BryB_4_KS7_b_L_OH	Clade_66
>phormidolide_EKU96420_PhorO_3_KS11_b_L_OH	Clade_66
>rhizoxins_RhiE_2_KS13_b_L_OH	Clade_66
>diaphorin_DipT_6_KS9_b_L_OH	Clade_66
>pederin_PedF_6_KS9_b_L_OH	Clade_66
>luminaolid_LumC_3_KS9_b_L_OH	Clade_66
>tolytoxin_TtoE_3_KS9_b_L_OH	Clade_66
>misakinolide_MisD_3_KS9_b_L_OH	Clade_66
>onnamide_OnnI_6_KS9_b_L_OH	Clade_66
>kalimantacin_batumin_Bat2_2_KS3_bOH	Clade_66
>sorangicin_SorA_5_KS5_a_L_OHb_L_OH	Clade_66
>sorangicin_SorD_2_KS14_b_L_OH	Clade_66
>difficidin_DifI_2_KS8_bOH	Clade_66
>oocydin_Smar_OocN_3_KS7_b_L_OH	Clade_66
>oocydin_Ddad_OocN_3_KS7_b_L_OH	Clade_66
>psymberin_PsyD_7_KS9_b_L_OH	Clade_66
>oocydin_Smar_OocJ_1_KS1_unusualStarter	Clade_67
>oocydin_Ddad_OocJ_1_KS1_unusualStarter	Clade_67
>phormidolide_EKU96424_PhorK_1_KS1_unusualStarter	Clade_67
>sorangicin_SorD_1_KS13_a_L_OHb_L_OH	Clade_68
>sorangicin_SorG_1_KS18_a_L_Mb_L_OH	Clade_68
>chivosazole_ChiE_2_KS14_a_L_Meb_L_OH	Clade_68
>phormidolide_EKU96423_PhorL_2_KS5_b_D_OH	Clade_7
>phormidolide_EKU96423_PhorL_4_KS7_b_D_OH	Clade_7
>rhizoxins_RhiC_3_KS8_b_D_OH	Clade_7
>oocydin_Smar_OocN_2_KS6_a_D_OHb_L_OH	Clade_70
>oocydin_Ddad_OocN_2_KS6_a_D_OHb_L_OH	Clade_70
>phormidolide_EKU96420_PhorO_2_KS10_0aOHaMeb_D_OH	Clade_70
>bacillaene_Bamy_BaeL_3_KS6_bMeeDB	Clade_73
>bacillaene_Bsub_PksL_3_KS6_bMeeDB	Clade_73
>elansolid_Csan_ElaO_1_KS6_bMeeDB	Clade_73
>elansolid_Cpin_ElsN_1_KS6_bMeeDB	Clade_73
>oocydin_Smar_OocL_2_KS4_eDBbMe	Clade_73
>oocydin_Ddad_OocL_2_KS4_eDBbMe	Clade_73
>phormidolide_EKU96423PhorL_5_KS8_eDBbMe	Clade_73
>bongkrekiac_acid_BonA_2_KS2_bMeeDB	Clade_73
>sorangicin_SorA_6_KS6_zDB	Clade_73
>etnangien_EtnE_3_KS3_eDBbMe	Clade_73
>calyculin_CalG_3_KS23_bMeeDB	Clade_73
>thailandamide_TaiM_1_KS13_bMeeDB	Clade_73
>myxovirescin_Ta1_6_KS6_eDBbMe	Clade_73
>SIA7248_SiaG_1_KS8_bMeeDB	Clade_73
>thailandamide_TaiK_1_KS7_bMeeDB	Clade_73
>basiliskamides_P615_BasF_1_KS1_GNATstarter	Clade_74
>basiliskamides_P615_BasE_1_KS2_a_L_Me_red	Clade_74
>elansolid_Csan_ElaK_2_KS4_aMe	Clade_74
>elansolid_Cpin_ElsJ_2_KS4_aMe	Clade_74
>elansolid_Csan_ElaK_1_KS3_adiMeb_D_OH	Clade_74
>elansolid_Cpin_ElsJ_1_KS3_adiMeb_D_OH	Clade_74
>difficidin_DifI_1_KS14_redaMe	Clade_74
>calyculin_CalE_6_KS16_adiMbketo	Clade_74
>sorangicin_SorA_3_KS3_reda_D_Me	Clade_74
>myxovirescin_TaP_1_KS1_reda_D_Me	Clade_74
>paenimacrolidin_KS3_bMe	Clade_74

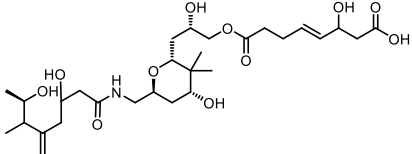
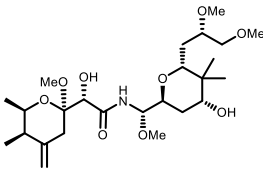
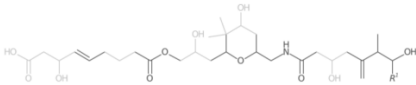
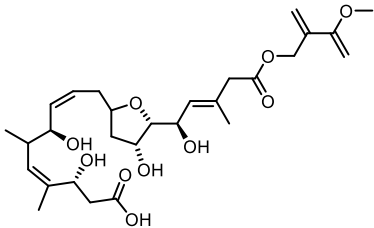
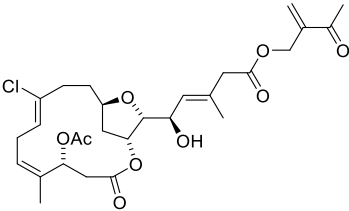
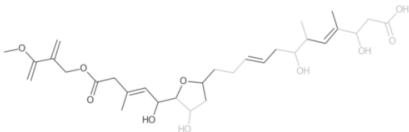
>paenimacrolidin_KS4_bMe	Clade_74
>bryostatin_BryB_2_KS5_adiMebketo	Clade_74
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>thiomarinol_TmpD_4_KS4_a_D_OH	Clade_74
>sorangicin_SorE_1_KS15_a_D_Mb_L_OH	Clade_74
>etnangien_EtnF_1_KS8_a_D_Meb_D_OH	Clade_74
>mupirocin_MmpD_4_KS4_a_D_Me	Clade_74
>mupirocin_MmpD_2_KS2_a_L_Meb_L_OH	Clade_74
>dorriginicin_migrastatin_MgsF_4_KS7_a_D_Meb_L_OH	Clade_74
>bacillaene_Bsub_PksM_3_KS10_bOH	Clade_75
>oocydin_Smar_OocS_3_KS15_0b_L_OH	Clade_75
>oocydin_Ddad_OocS_3_KS15_0b_L_OH	Clade_75
>elansolid_Csan_ElaP_2_KS9_0bimod_bOH	Clade_75
>elansolid_Cpin_ElsO_2_KS9_0bimod_bOH	Clade_75
>etnangien_EtnF_3_KS10_b_L_OH	Clade_75
>etnangien_EtnG_2_KS12_0b_L_OH	Clade_75
>etnangien_EtnI_4_KS20_0b_L_OH	Clade_75
>elansolid_Csan_ElaR_1_KS14_0eDB	Clade_76
>elansolid_ElsQ_1_KS14_0eDB	Clade_76
>luminaolid_LumE_4_KS18_0b_D_OH	Clade_76
>tolytoxin_TtoF_5_KS19_0eDB	Clade_76
>misakinolide_MisF_5_KS19_0eDB	Clade_76
>pederin_PedH_4_KS13_0eDB	Clade_76
>rhizoxins_RhiF_2_KS16_0eDB	Clade_76
>sorangicin_SorB_1_KS8_0zDB	Clade_76
>enacyloxin_Bamb_5919_2_KS11_0eDB	Clade_76
>bongkrekiic_acid_BonD_3_KS12_0vinylbranch	Clade_76
>sorangicin_SorI_2_KS24_0zDB	Clade_76
>oocydin_Smar_OocR_1_KS11_0bimod_bOH	Clade_78
>oocydin_Ddad_OocR_1_KS11_0bimod_bOH	Clade_78
>tartrolon_TrtE_2_KS5_0red	Clade_78
>griseoviridin_SgvE1_1_KS1_acetylStarter	Clade_79
>virginiamycin_VirA_1_KS1_unusualstarter	Clade_79
>FR901464_Fr9I_1_KS11_0b_D_OH	Clade_79
>thailanstatin_TstI_1_KS11_0b_D_OH	Clade_79
>lankacidin_LkcG_1_KS5_aMebketo	Clade_79
>kirromycin_KirAI_1_KS1_AcStarter	Clade_79
>9methylstreptimidone_Smdl_1_KS1_unusualstarter_AMT	Clade_8
>cycloheximide_ChxE_1_KS1_unusualStarter_AMT	Clade_8
>dorriginicin_migrastatin_MgsE_1_KS1_unusualStarter_AMT	Clade_8
>sorangicin_SorA_1_KS1_unusualStarter	Clade_8
>etnangien_EtnD_1_KS1_unusualStarters_Succ	Clade_8
>FR901464_Fr9C_2_KS2_0bOH	Clade_80
>thailanstatin_TstC_2_KS2_0bOH	Clade_80
>bryostatin_BryC_4_KS11_0b_D_OH	Clade_81
>nosperin_NspC_5_KS5_aMebOH	Clade_81
>luminaolid_LumD_1_KS11_0bimod_b_D_OH	Clade_81
>misakinolide_MisE_1_KS11_0b_D_OH	Clade_81
>tolytoxin_TtoE_5_KS11_0b_D_OH	Clade_81
>calyculin_CaE_5_KS14_0b_L_OH	Clade_81
>calyculin_CaF_3_KS18_0b_D_OH	Clade_81
>oxazolomycin_OzmJ_2_KS11_0a_L_OMebketo	Clade_81
>thailandamide_TaiN_1_KS16_0a_D_Meb_D_OH	Clade_81
>bacillaene_Bamy_Bael_2_KS5_eDB	Clade_82
>bacillaene_Bsub_PksL_2_KS5_eDB	Clade_82
>elansolid_Csan_ElaK_3_KS5_eDB	Clade_82
>elansolid_Cpin_ElsJ_3_KS5_eDB	Clade_82
>elansolid_Csan_ElaP_3_KS10_zDB	Clade_82
>elansolid_Cpin_ElsO_3_KS10_zDB	Clade_82

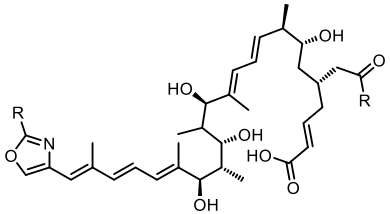
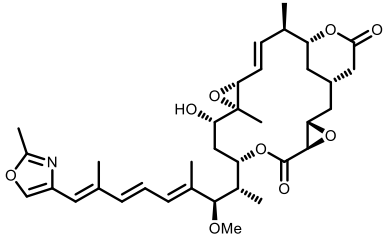
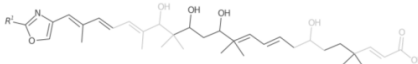
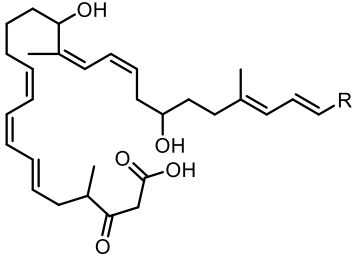
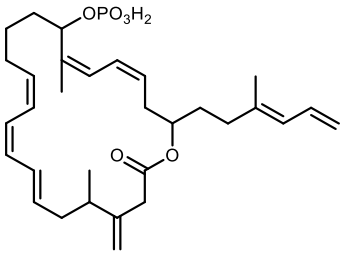
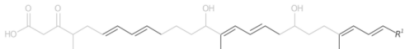
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>sorangicin_SorH_2_KS21_eDB	Clade_82
>sorangicin_SorE_3_KS17_eDB	Clade_82
>sorangicin_SorI_1_KS23_zDB	Clade_82
>etnangien_EtnE_1_KS5_eDB	Clade_82
>etnangien_EtnE_2_KS6_eDB	Clade_82
>bongkrekiac_acid_BonA_5_KS5_DB	Clade_82
>bongkrekiac_acid_BonC_1_KS9_eDB	Clade_82
>bongkrekiac_acid_BonB_1_KS7_DB	Clade_82
>bongkrekiac_acid_BonD_2_KS11_eDB	Clade_82
>bacillaene_Bamy_BaeR_1_KS13_0aMeDB	Clade_83
>bacillaene_Bsub_PksR_1_KS14_0aMeDB	Clade_83
>onnamide_OnnI_7_KS10_0red	Clade_83
>calyculin_CalH_3_KS27_eDB	Clade_83
>nosperin_NspC_3_KS6_0biomod_aMeeDB	Clade_83
>rhizoxins_RhiD_3_KS11_0biomod_aMeeDB	Clade_83
>chivosazole_ChiF_4_KS18_0zDB	Clade_83
>disorazole_DszC_1_KS2_0AAoxa	Clade_84
>corallopyronin_CorJ_2_KS5_0aMe	Clade_84
>myxopyronin_MxnJ_2_KS5_0reda_L_Me	Clade_84
>rhizopodin_RizB_7_KS7_0bimodb_D_OH	Clade_85
>rhizopodin_RizD_3_KS13_0bimod_b_D_OH	Clade_85
>rhizopodin_RizB_3_KS3_0bimod_a_D_Meb_D_OH	Clade_85
>rhizopodin_RizE_1_KS17_0bimod_b_L_OH	Clade_85
>chivosazole_ChiB_3_KS3_a_L_Meb_L_OH	Clade_86
>anthracimycin_AtcD_4_KS4_aMezshDB	Clade_86
>luminaolid_LumB_3_KS6_reda_L_Me	Clade_86
>tolytoxin_TtoD_3_KS6_reda_L_Me	Clade_86
>misakinolide_MisD_1_KS6_reda_L_Me	Clade_86
>rhizopodin_RizB_6_KS6_reda_L_Me	Clade_86
>rhizopodin_RizC_1_KS9_adiMeb_L_OH	Clade_86
>FR901464_Fr9C_3_KS3_0eDB	Clade_88
>thailanstatin_TstC_3_KS3_0eDB	Clade_88
>oocydin_Smar_OocS_4_KS16_0	Clade_88
>oocydin_Ddad_OocS_4_KS16_0	Clade_88
>phormidolide_EKU96419_PhorP_3_KS15_0eDBbMe	Clade_88
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>mupirocin_MmpA_KS2_b_D_OH	Clade_89
>thiomarinol_TmpD_2_KS2_a_L_Meb_L_OH	Clade_89
>albicidin_Albi_1_KS1_aromaticStarter_AL	Clade_9
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>elansolid_Cpin_ElsI_1_KS1_aromaticstarter	Clade_9
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>tolytoxin_TtoD_2_KS5_bketo	Clade_90
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>oocydin_Ddad_OocN_1_KS5_0a_D_OHb_L_OH	Clade_92
>diaphorin_DipT_1_KS4_0hacetal	Clade_93
>pederin_PedF_1_KS4_0hacetal	Clade_93
>nosperin_NspC_1_KS4_0hacetal	Clade_93
>onnamide_OnnI_1_KS4_0hacetales	Clade_93

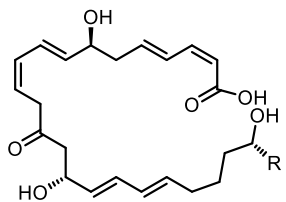
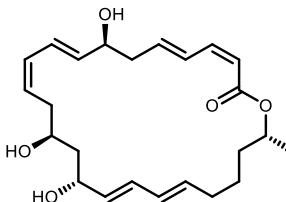
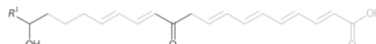
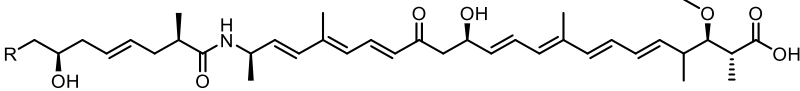
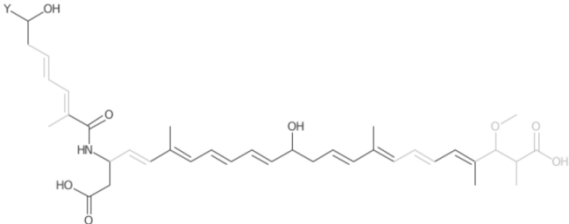
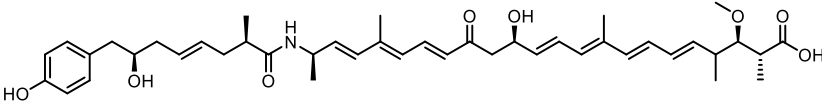
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>calyculin_CalF_1_KS16_0_b_L_OH_a_L_Meb_L_OH	Clade_93
>mupirocin_MmpA_1_KS5_0b_D_OH	Clade_93
>thiomarinol_TmpA_1_KS5_0b_D_OH	Clade_93
>myxovirescin_Ta1_3_KS3_0b_L_OH	Clade_93
>oocydin_Smar_OocN_1_KS5_0a_D_OHb_L_OH	Clade_93
>oocydin_Ddad_OocN_1_KS5_0a_D_OHb_L_OH	Clade_93
>oocydin_Smar_OocN_1_KS5_0a_D_OHb_L_OH	Clade_93
>oocydin_Ddad_OocN_1_KS5_0a_D_OHb_L_OH	Clade_93
>phormidolide_EKU96420_PhorO_1_KS9_aMe_D_OH	Clade_93
>luminaolid_LumA_3_KS3_0bimod_a_D_Meb_D_OH	Clade_94
>tolytoxin_TtoC_3_KS3_0a_D_Meb_D_OH	Clade_94
>misakinolide_MisC_3_KS3_0bimod_b_D_OMe	Clade_94
>rhizopodin_RizB_7_KS7_0bimodb_D_OH	Clade_94
>rhizopodin_RizD_3_KS13_0bimod_b_D_OH	Clade_94
>rhizopodin_RizB_3_KS3_0bimod_a_D_Meb_D_OH	Clade_94
>rhizopodin_RizE_1_KS17_0bimod_b_L_OH	Clade_94
>chivosazole_ChiC_6_KS9_0a_D_Meb_D_OH	Clade_94
>corallopyronin_CorL_2_KS11_red	Clade_95
>myxopyronin_MxnK_3_KS9_red	Clade_95
>macrolactin_MlnB_3_KS3_red	Clade_95
>corallopyronin_CorK_3_KS9_red	Clade_95
>rhizopodin_RizB_2_KS2_eDB	Clade_95
>misakinolide_MisC_5_KS5_L_OH_or_D_Py	Clade_95
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>cycloheximide_ChxE_3_KS3_vinylogous	Clade_96
>dorrigocin_migrastatin_MgsE_3_KS3_vinylogous	Clade_96
>kirromycin_KirAII_2_KS4_diMb_L_OH	Clade_96
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>kirromycin_KirAIII_4_KS6_AAgly	Clade_96
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>myxopyronin_MxnJ_3_KS6_reda_L_Me	Clade_96
>rhizoxins_RhiF_1_KS15_vinylogous	Clade_96
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>SIA7248_SiaF_3_KS6_b_D_OH	Clade_97
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>bacillaene_Bsub_PksR_2_KS15_OshDBaMe	Clade_98
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>thailandamide_TaiD_4_KS4_0reda_D_Me	Clade_98
>diaphorin_DipT_1_KS4_0acetal	Clade_98
>pederin_PedF_1_KS4_0acetal	Clade_98
>nosperin_NspC_1_KS4_0acetal	Clade_98
>onnamide_OnnI_1_KS4_0acetale	Clade_98
>psymberin_PsyD_1_KS3_bimod_0b_L_OH	Clade_98
>calyculin_CalB_1_KS3_KS0_b_L_OH	Clade_98
>calyculin_CalF_1_KS16_0_b_L_OH_a_L_Meb_L_OH	Clade_98
>mupirocin_MmpA_1_KS5_0b_D_OH	Clade_98
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>oocydin_Smar_OocR_1_KS11_0bimod_bOH	Clade_98

>oocydin_Ddad_OocR_1_KS11_0bimod_bOH	Clade_98
>phormidolide_EKU96420_PhorO_1_KS9_aMe_D_OH	Clade_98
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>tartrolon_Trte_2_KS5_0red	Clade_98
>bryostatin_BryB_3_KS6_eDB	Clade_99
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>difficidin_DifK_1_KS13_eDB	Clade_99
>FR901464_Fr9G_1_KS8_eDB	Clade_99
>thailanstatin_TstGH_1_KS8_eDB	Clade_99
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>thailandamide_TaiM_2_KS14_eDB	Clade_99

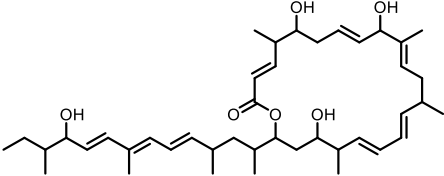
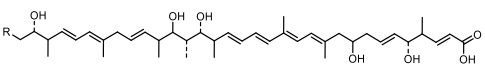
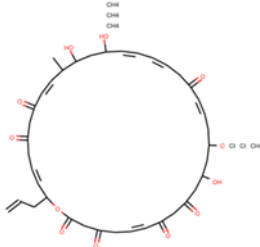
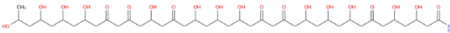
Supplementary Table 4: Selection of TransATor-based structure predictions of known metabolites and structures of the actual polyketides. Accuracy: number of correctly assigned KS substrate specificities (only top hits; as determined by comparison with published biosynthetic proposals) divided by total number of KSs present in a PKS. Hydroxyl group stereochemistry shown in the TransATor-based prediction panel, but missing in the original TransATor output representation are based on KR Fuzzpro patterns.

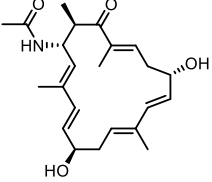
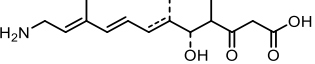
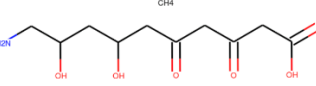
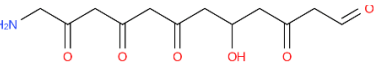
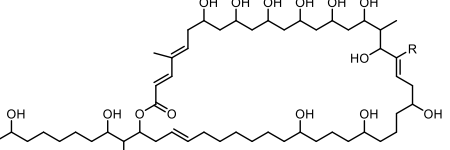
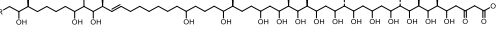
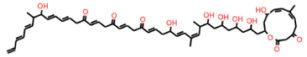
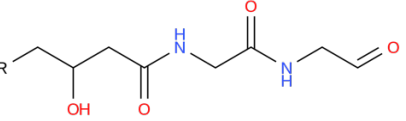
Polyketide	TransATor-based prediction	Actual polyketide	KS substrates	Original TransATor output	Accuracy
Pederin			KS1: GNAT starter KS2: α L-Me β D-OH KS3: exomethyl/exoester KS4: non-elongating (hemiacetal) KS5: amino acids KS6: β D-OH KS7: α L-(di)Me β OH KS8: pyran/furan rings KS9: β L-OH KS10: oxidative rearrangement KS11: completely reduced KS12: double bonds (<i>E</i> -configured) KS13: non-elongating (double bonds)		13/13 100%
Oocydin			KS1: phosphoglycerate-derived straters KS2: exomethylene KS3: oxidative rearrangement KS4: beta-branch KS5: non-elongating (α D-OH β L-OH) KS6: α OH β D-OH KS7: β L-OH KS8: pyran/furan rings KS9: completely reduced KS10: non-elongating (various) KS11: non-elongating (mostly β OH) KS12: shifted double bonds KS13: α L-Me β OH KS14: α Me double bonds (<i>Z</i> -configured) KS15: non-elongating (β L-OH) KS16: non-elongating		14/16 87.5%

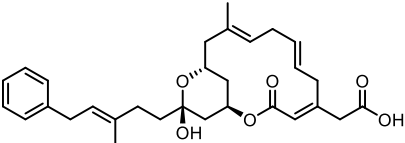
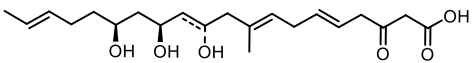
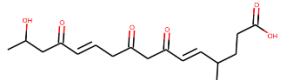
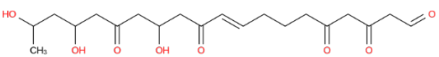
Rhizoxin			<p>KS1: non-elongating (various specificities) KS2: non-elongating (oxazole/thiazole rings) KS3: amino acids (oxazole/thiazole rings) KS4: α Me double bonds (<i>E</i>-configured) KS5: double bonds (<i>E</i>-configured) KS6: α Me double bonds KS7: α L-(di)Me β OH KS8: β D-OH KS9: α L-(di)Me β OH KS10: shifted double bonds KS11: non-elongating (mostly α-Me double bonds) KS12: shifted double bonds (some with α-Me) KS13: β L-OH KS14: non-elongating (double bonds (mostly <i>Z</i>-configured)) KS15: vinylogous chain branching/ (di)-methyl reduced KS16: non-elongating (double bonds)</p>		13/16 81%
Difficidin			<p>KS1: mainly double bonds KS2: α Me double bonds (<i>E</i>-configured) KS3: completely reduced KS4: β D-OH (some with α L-Me) KS5: non-elongating (bimodule β D-OH) KS6: double bonds (<i>Z</i>-configured) KS7: α Me double bonds (<i>Z</i>-configured) KS8: β L-OH KS9: completely reduced KS10: bimodule β D-OH KS11: double bonds KS12: non-elongating (bimodule β D-OH) KS13: double bonds (<i>E</i>-configured) KS14: α Me reduced/keto/D-OH</p>		14/14 100%

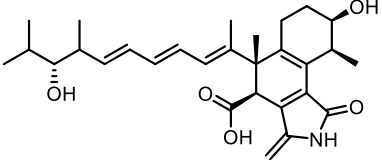
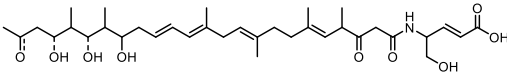
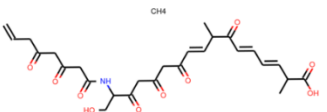
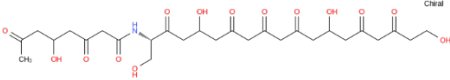
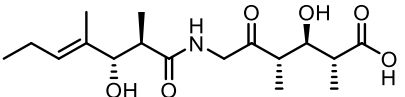
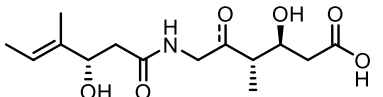
Macrolactin			<p>KS1: acetyl starter KS2: β D-OH KS3: completely reduced KS4: β-keto or double bonds KS5: β-keto or double bonds KS6: β D-OH or β keto KS7: β-keto or double bonds KS8: bimodule β D-OH KS9: β-keto or double bonds KS10: β-keto or double bonds KS11: bimodule β D-OH</p>		10/11 90%
Predicted thailandamide structure					
Actual structure of thailandamide			<p>KS1: various starters KS2: β L-OH KS3: double bonds (<i>E</i>-configured) KS4: non-elongating (α-Me completely reduced or shifted double bond) KS5: amino acids KS6: double bonds (mostly <i>E</i>-configured) KS7: beta branch KS8: non-elongating (bimodule β D-OH) KS9: double bonds KS10: β-keto or double bonds KS11: β D-OH KS12: double bonds (<i>E</i>-configured) KS13: beta branch KS14: double bonds (<i>E</i>-configured) KS15: a Me double bonds (<i>E</i>-configured) KS16: non-elongating (β D-OH)</p>		15/16 94%

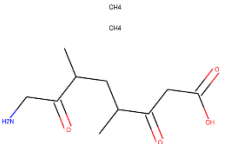
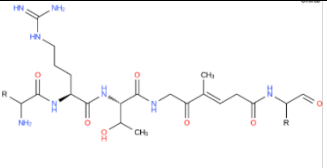
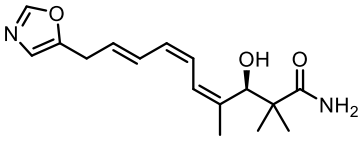
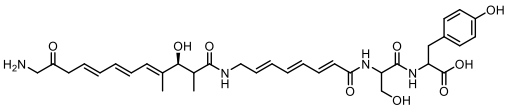
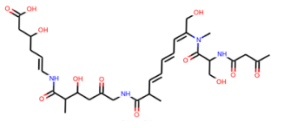
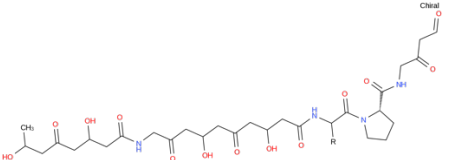
Supplementary Table 5: Comparison between TransATor, PRISM3, and antiSMASH4.0-based structural predictions of *trans*-AT PKS-derived polyketides that were not part of the initial training set used to generate HMMs for TransATor and that were deposited to GenBank. No accuracy predictions could be made for PRISM3-based predictions, as predicted structures differ too much from isolated compounds and no monomers are predicted. Accuracy: the provided ratio values signify the number of correctly assigned KS and A domain substrates (only top hits; as determined by comparison with published biosynthetic proposals) divided by the total number of KSs and A domains present in a PKS. The percentage value denotes the number of correctly assigned substrate specificities divided by total number of KS and A domains. The shown structures are outputs of the respective prediction tools (for TransATor predictions structures are derived from predictions in “Viewer” window). antiSMASH nomenclature: mal: β keto; ohmal: β hydroxyl. For monomer predictions in antiSMASH and TransATor, KSs were sorted according to their location in the proposed biosynthetic pathway. Green: correct prediction; red: incorrect prediction.

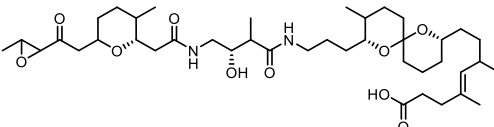
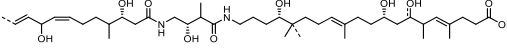
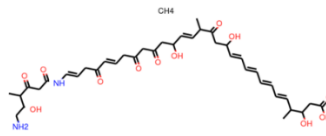
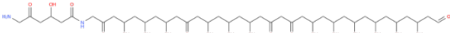
Actual polyketide	TransATor prediction	PRISM3 prediction	antiSMASH4.0 prediction
 Macrobrevin ⁹ (<i>Brevibacillus</i> sp. Leaf 182)	 Accuracy: 15/19 79%	 No monomers predicted	
KS1: acetyl starters KS2: α Me reduced KS3: β OH KS4: α Me shifted double bonds KS5: non-elongating (double bonds) KS6: shifted double bonds KS7: α -Me shifted double bonds KS8: α -Me reduced KS9: β OH KS10: α Me OH KS11: double bonds KS12: double bonds KS13: beta-branch KS14: α Me double bonds (<i>E</i> -configured)	KS1: various starters KS2: α Me reduced/keto/D-OH KS3: double bonds (mostly <i>e</i> -configured) KS4: α Me reduced/keto/D-OH KS5: non-elongating (α -Me double bonds) KS6: shifted double bonds (with α -Me) KS7: α Me reduced/keto/D-OH KS8: α Me reduced/keto/D-OH KS9: β D-OH (some with α L-Me) KS10: α Me reduced/keto/D-OH KS11: double bonds (mostly <i>E</i> -configured)	KS1: ohmal KS2: ohmal KS3: ohmal KS4: ohmal KS5: mal KS6: mal KS7: ohmal KS8: mal KS9: ohmal KS10: ohmal KS11: ohmal KS12: mal KS13: ohmal KS14: ohmal	

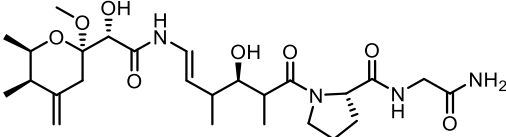
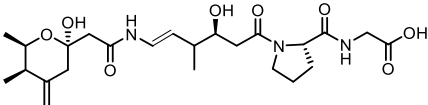
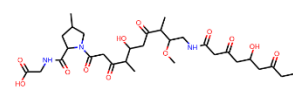
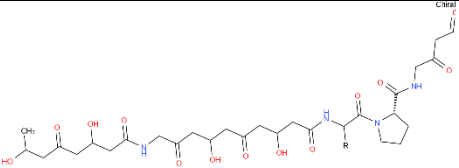
<p>KS15: β OH KS16: non-elongating (bimodule β D-OH) KS17: shifted double bonds KS18: α Me D-OH KS19: non-elongating (double bonds)</p>	<p>KS12: double bonds (mostly <i>E</i>-configured) KS13: beta-branch KS14: α Me double bonds (<i>E</i>-configured) KS15: β L-OH KS16: non-elongating (bimodule β D-OH) KS17: double bonds (<i>E</i>-configured) KS18: α Me reduced/keto/D-OH KS19: non-elongating (double bonds)</p>		<p>KS15: ohmal KS16: mal KS17: ohmal KS18: ohmal KS19: mal</p>
 <p>Chejuenolide¹⁰ (<i>Hahella chejuensis</i> MB-1084) PKS contains iterative modules</p> <p>A1: gly KS1: amino acids (glycine) KS2: α Me double bonds (<i>E</i>-configured) KS3: double bonds (<i>E</i>-configured) KS4: β -OH KS5: α Me b-OH</p>	 <p>Accuracy: 5/6 83%</p> <p>A1: gly KS1: amino acids (glycine) KS2: double bonds (<i>E</i>-configured) (some with α Me) KS3: double bonds (<i>E</i>-configured) KS4: various specificities (mainly α-Me) KS5: α Me reduced/keto/D-OH</p>	 <p>No monomers predicted</p>	 <p>A1: Gly KS1: mal KS2: mal KS3: ohmal KS4: mal KS5: mal</p>
 <p>Lacunalide¹¹ (<i>Gyvuella sunshinyii</i>)</p>	 <p>Accuracy: 21/25 84%</p>		

<p>KS1: acetyl starters KS2: β D-OH KS3: completely reduced KS4: completely reduced KS5: β D-OH with α L-Me KS6: β D-OH with α L-Me KS7: double bonds <i>E</i>-configured KS8: completely reduced KS9: completely reduced KS10: completely reduced KS11: β D-OH KS12: completely reduced KS13: β D-OH KS14: completely reduced KS15: β D-OH KS16: double bond with a Me KS17: a Me D-OH KS18: β L-OH KS19: β D-OH KS20: β L-OH KS21: β D-OH KS22: β L-OH KS23: β D-OH KS24: double bond e-configured KS25: non-elongating (double bonds e-configured)</p>	<p>KS1: various starters KS2: β D-OH (some with α L-Me) KS3: completely reduced KS4: completely reduced KS5: β D-OH (some with α L-Me) KS6: β D-OH (some with α L-Me) KS7: double bonds (mostly <i>E</i>-configured) KS8: completely reduced KS9: completely reduced KS10: completely reduced KS11: β D-OH KS12: completely reduced KS13: β D-OH (some with α L-Me) KS14: completely reduced KS15: D-OH KS16: β D-OH (some with α L-Me) KS17: β D-OH (some with α L-Me) KS18: β L-OH KS19: β D-OH (some with α L-Me) KS20: β L-OH KS21: β D-OH KS22: β L-OH KS23: β D-OH (some with α L-Me) KS24: β D-OH (some with α L-Me) KS25: : β D-OH (some with α L-Me)</p>	<p>No monomers predicted</p>	<p>No monomers predicted</p>
<p> Ripostatin¹² (<i>Sorangium cellulosum</i>)</p> <p>KS1: cis-AT PKS KS2: α Me double bond</p>	<p> Accuracy: 5/9 56%</p> <p>KS1: cis-AT PKS</p>	<p> No monomers predicted</p>	<p> KS1: ccmal KS2: redmal</p>

<p>KS3: reduced KS4: β keto KS5: β D-OH KS6: β D-OH KS7: β Me double bond KS8: completely reduced KS9: shifted double bonds (some with α-Me)</p>	<p>KS2: cis-AT PKS KS3: cis-AT PKS KS4: β D-OH or β keto KS5: β D-OH or β keto KS6: various specificities KS7: β OMe or β Me double bond KS8: bimodule β D-OH KS9: shifted double bonds (some with α-Me)</p>		<p>KS3: mal KS4: ohmal KS5: ohmal KS6: mal KS7: ohmal KS8: mal KS9: ccmal</p>
 <p>Pyxipyrrolone¹³ (<i>Pyxidicoccus</i> sp.)</p> <p>KS0: loading KS1: isobutyl starter KS2: skipped? KS3: α-Me b-OH KS4: double bond (e-configured) KS5: double bond (e-configured) KS6: α-Me double bond KS7: β Me double bond KS8: double bond (e-configured) KS9: α-L-Me b-keto A1: ser KS10: amino acids</p>	 <p>Accuracy: 6/11 55%</p> <p>KS1: acetyl starter KS2: β D-OH or β keto KS2: α-L-Me red or OH KS4: α-L-Me red or OH KS4: β D-OH KS5: double bonds (e-configured) KS6: α-Me double bond KS7: β OMe or β Me double bond KS8: α-L-Me red or OH KS9: α-Me shifted double bond or OH A1: ser KS10: amino acids</p>	 <p>No monomer predicted</p>	 <p>KS1: mal KS2: mal KS3: ohmal KS4: mal KS5: mal KS6: ohmal KS7: mal KS8: ohmal KS9: mal KS10: mal A1: ser KS11: ohmal</p>
			

<p>Alpiniamide¹⁴ (<i>Streptomyces</i> sp. IB2014/011-12)</p> <p>KS1: cis-AT PKS loading KS2: double bond (<i>E</i>-configured) KS3: non-elongating (α-Me β-OH) A1: gly KS4: amino acids KS5: α Me keto</p>	<p>Accuracy: 5/6 83%</p> <p>KS1: cis-AT PKS KS2: cis-AT PKS KS3: non-elongating (α-Me completely reduced or shifted double bond) A1: gly KS4: amino acids KS5: α Me reduced/keto/D-OH</p>	 <p>No monomer predicted</p>	 <p>KS1: mal A1: gly KS2: ccmal</p>
 <p>Phthoxazolin A¹⁵ (<i>Streptomyces avermitilis</i>) The PKS has additional modules that suggest phthoxazolin A is a cleavage product of a larger polyketide</p> <p>A1: gly KS1: amino acids KS2: amino acids KS3: double bonds (<i>E</i>-configured) KS4: double bonds (<i>Z</i>-configured) KS5: α-Me double bond A2: gly KS6: amino acids (glycine) KS7: double bonds (<i>E</i>-configured) KS8: non-elongating (bimodule β D-OH) KS9: double bonds (mostly <i>E</i>-configured) KS10: non-elongating (double bonds) A3: ser A4: tyr</p>	 <p>Accuracy: 14/14 100%</p> <p>A1: gly KS1: amino acids KS2: amino acids KS3: double bonds KS4: double bonds KS5: α-Me double bond A2: gly KS6: amino acids (glycine) KS7: double bonds (<i>E</i>-configured) KS8: non-elongating (bimodule β D-OH) KS9: double bonds (mostly <i>E</i>-configured) KS10: non-elongating (double bonds) A3: ser A4: tyr</p>	 <p>No monomer predicted</p>	 <p>A1: gly KS1: mal KS2: ohmal KS3: ohmal KS4: ohmal KS5: ohmal A2: gly KS6: ohmal KS7: ohmal KS8: mal KS9: ohmal KS10: mal A3: ser</p>

 <p>Lagriamide¹⁶ (<i>Burkholderia gladioli</i> Lv-StB)</p> <p>KS1: GNAT starter KS2: double bond <i>E</i>-configured KS3: L-OH KS4: double bond <i>E</i>-configured KS5: α-Me KS6: non-elongating (double bonds) A1: gly KS7: amino acids KS8: α L-Me β OH A1: gly KS9: amino acids KS10: completely reduced KS11: α L-Me β OH KS12: completely reduced KS13: skipped KS14: D-OH KS15: completely reduced KS16: β L-OH KS17: α Me DB KS18: reduced</p>	 <p>Accuracy: 17/20 85%</p> <p>KS1: <i>cis</i>-AT PKS KS2: double bonds (mostly <i>E</i>-configured) KS3: L-OH KS4: double bonds (mostly <i>E</i>-configured) KS5: α-Me KS6: non-elongating (double bonds) A1: gly KS7: amino acids KS8: α L-Me β OH A2: gly KS9: amino acids KS10: completely reduced KS11: α L-(di)Me β OH KS12: completely reduced KS13: α Me double bonds KS14: D-OH KS15: completely reduced KS16: β L-OH KS17: α Me reduced/keto/D-OH KS18: α Me double bonds</p>	 <p>No monomers predicted</p>	<p>A4: ala</p>  <p>KS1: ohmal KS2: ohmal KS3: ohmal KS4: ohmal KS5: ohmal KS6: mal A1: gly KS7: ohmal KS8: mal A2: gly KS9: ohmal KS10: ohmal KS11: ohmal KS12: mal KS13: ohmal KS14: ohmal KS15: ohmal KS16: ohmal KS16: mal KS17: mal</p>
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 <p>Cusperin¹⁷ (<i>Cuspidothrix issatschenkoi</i>)</p> <p>KS1: GNAT starter KS2: α L-Me β D-OH KS3: exomethyl/exoester KS4: non-elongating (hemiacetale) A1: gly KS5: amino acids KS6: non-elongating (double bonds) KS7: shifted double bonds with α-Me KS8: non-elongating (α-Me β D-OH) A2: pro A3: gly</p>	 <p>Accuracy: 11/11 100%</p> <p>KS1: GNAT starter KS2: α L-Me β D-OH KS3: exomethyl/exoester KS4: non-elongating (hemiacetale) A1: gly KS5: amino acids KS6: non-elongating (α-Me double bonds) KS7: shifted double bonds (with α-Me) KS8: non-elongating (β D-OH) A2: pro A3: gly</p>	 <p>No monomers predicted</p>	 <p>KS1: ohmal KS2: mal KS3: ohmal KS4: mal A1: gly KS5: ohmal KS6: mal KS7: ohmal KS8: mal A2: pro A3: gly KS9: mal</p>
<p>Total accuracy of TransATor (absolute/relativ)</p>	<p>99/121 82%</p>		<p>21/96 22%</p>

Supplementary Table 6: Proteins encoded in the tartrolon (*tar*) BGC and their putative functions.

Protein	Amino acids	Proposed function	Closest homolog	Identity (%)	Accession number ⁷
TarK	211	TetR/AcrR family transcriptional regulator	<i>Saccharospirillum impatiens</i> (WP_037337596.1)	57	WP_044617971.1
TarL	259	enoyl-CoA hydratase	<i>Rheinheimera nanhaiensis</i> (WP_008218131.1)	41	WP_044617970.1
TarM	959	peptidase M16	<i>Motiliproteus</i> sp. MSK22-1 (WP_076719499.1)	56	WP_076719499.1
TarO	193	thymidine kinase	<i>Vibrio</i> sp. S234-5 (WP_045571983.1)	65	WP_044617968.1
TarP	407	Cyclic di-GMP phosphodiesterase	<i>Marinimicrobium</i> sp. LS-A18 (WP_024461494.1)	42	WP_052830363.1
TarB	289	AT	<i>Teredinibacter</i> (WP_018276260.1)	74	WP_044617967.1
TarQ	236	hypothetical protein	<i>Teredinibacter turnerae</i> (WP_018416731.1)	65	WP_044620136.1
TarD	4388	PKS (DH*-KR*-FkbH-ACP-KS-DH-KR-ACP-KS-KR-ACP-KS)	<i>Teredinibacter turnerae</i> (WP_018416727.1)	51	AJQ95776.1
TarE	4856	PKS (KR-ACP-KS-DH-KR-MT-ACP-KS-ACP-KS-ACP)	<i>Teredinibacter</i> sp. 991H.S.0a.06 (WP_045825587.1)	52	WP_044620134.1
TarF	4540	PKS (KR-ACP-KS-DH-KR-MT-ACP-KS-ACP-KS-ACP)	<i>Teredinibacter turnerae</i> (WP_028876839.1)	54	AJQ95774.1
TarG	372	Flavin-dependent oxidoreductase	<i>Teredinibacter turnerae</i> (WP_028886452.1)	82	WP_044617966.1
TarH	262	TE	<i>Teredinibacter turnerae</i> (WP_028886452.1)	50	WP_082070762.1
TarR	283	ABC transporter ATP-binding protein	<i>Enterovibrio pacificus</i> (WP_068904725.1)	70	WP_044617965.1
TarS	227	hypothetical protein	<i>Enterovibrio pacificus</i> (WP_068904723.1)	55	WP_044617964.1
TarT	241	hypothetical protein	<i>Enterovibrio pacificus</i> (WP_068904723.1)	64	WP_044617963.1
TarI	452	dioxygenase	<i>Teredinibacter turnerae</i> (WP_028886454.1)	77	WP_044617962.1

Supplementary Table 7: Deduced proteins encoded on the *lept* BGC and their putative functions.

Gene	Protein	Protein size	Proposed function	Closest homolog*	Identity	Accession number
431	LeptA	532	ABC transporter permease/secreted hydrolase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40428.1)	38%	WP_006512961.1
430	LeptB	417	hypothetical protein	delta proteobacterium NaphS2 (EFK06465.1)	45%	WP_006512960.1
429	LeptC	84	hypothetical protein	<i>Desulfobacter hydrogenophilus</i> (WP_111956780.1)	46%	WP_006512959.1
428	LeptD	476	class III lipase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40431.1)	52%	WP_006512958.1
427	LeptE	292	alpha/beta hydrolase/AT	Planctomycetes bacterium (REK15718.1)	37%	WP_006512957.1
426	LeptF	477	class III lipase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40431.1)	62%	WP_006512956.1
425	LeptG	407	class III lipase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40431.1)	94%	WP_006512955.1
424	LeptH	417	3-oxoacyl-acyl-carrier protein synthase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40432.1)	96%	WP_006512954.1
423	LeptI	85	ACP	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40442.1)	99%	WP_006512953.1
422	LeptJ	315	AT (malonyl-CoA)	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40435.1)	94%	WP_006512952.1
421	LeptK	326	malonyl CoA-acyl carrier protein transacylase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40436.1)	99%	WP_006512951.1
420	LeptL	5057	PKS (DH-FkbM-FkbH-ACP-KS-ECH-ECH-ACP-ACP-KS-KR-ACP-KS-KR)	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40422.1)	93%	WP_006512950.1
419	LeptM	7161	PKS (MT-ACP-KS-KR-ACP-KS-KR-MT-ACP-KS-KR-ACP-KS-ACP-ACP-KS-MT-KR-ACP)	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40421.1)	92%	WP_006512949.1
418	LeptN	589	Ser/Thr protein kinase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40427.1)	95%	WP_006512948.1
417	LeptO	384	Flavin dependent mono-oxygenase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40433.1)	99%	WP_006512947.1
416	LeptP	4430	PKS (KS-ACP-KS-KR-ACP-KS-DH-PS-KR-ACP-KS-ACP)	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40423.1)	89%	WP_006512946.1
415	LeptQ	4309	PKS (ACP-KS-KR-ACP-KS-ACP-ACP-ACP-KS-ACP-C)	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40443.1)	61%	WP_006512945.1
414	LeptR	634	FAD-dependent halogenase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40426.1)	96%	WP_006512944.1
413	LeptS	559	hydrolase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40428.1)	93%	WP_006512943.1
412	LeptT	115	hypothetical protein	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40441.1)	95%	WP_006512942.1
411	LeptU	237	PPTase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40439.1)	89%	WP_006512941.1
410	LeptV	486	long-chain fatty acid CoA-ligase	<i>Leptolyngbya</i> sp. ISBN3-Nov-94-8 (AMH40429.1)	95%	WP_006512940.1

409	LeptW	255	enoyl-CoA hydratase	<i>Leptolyngbya</i> ISBN3-Nov-94-8 (AMH40437.1)	sp.	97%	WP_006512939.1
408	LeptX	255	enoyl-CoA hydratase	<i>Leptolyngbya</i> ISBN3-Nov-94-8 (AMH40438.1)	sp.	98%	WP_006512938.1
407	LeptY	440	HMG-CoA synthase	<i>Leptolyngbya</i> ISBN3-Nov-94-8 (AMH40430.1)	sp.	99%	WP_006512937.1
406	LeptZ	357	type IV secretion protein Rhs/WD40 repeat containing protein	<i>Leptolyngbya</i> ISBN3-Nov-94-8 (AMH40434.1)	sp.	96%	WP_006512936.1
405	LeptAA	1395	type IV secretion protein Rhs/WD40 repeat containing protein	<i>Leptolyngbya</i> ISBN3-Nov-94-8 (AMH40424.1)	sp.	98%	WP_006512935.1

Supplementary Table 8: Predicted stereochemistry for phormidolide and leptolyngbyalide A.

KR	Predicted stereochemistry of phormidolide	Predicted stereochemistry of leptolyngbyalide	Stereochemistry assigned by Williamson <i>et al.</i> ⁷	Suggested correct stereochemistry
Module 3	D-OH	D-OH	L-OH	D-OH
Module 4	D-OH	D-OH	L-OH	D-OH
Module 5	D-OH	D-OH	L-OH	D-OH
Module 6	D-OH	D-OH	L-OH	D-OH
Module 7	D-OH	D-OH	L-OH	D-OH
Module 9	D-OH	D-OH	L-OH	D-OH
Module 11	L-OH	L-OH	D-OH	L-OH
Module 12	D-OH	D-OH	L-OH	D-OH
Module 15	D-OH	D-OH	L-OH	D-OH
Module 16	D-OH	D-OH	L-OH	D-OH

Supplementary Table 9: deduced proteins encoded in the *cun* BGC and their putative functions.

Aq349 protein	# amino acids	Proposed function	Closest homolog (NCBI Ref. Seq.)	Identity (%)	Accession number
CunA	195	transcriptional activator	<i>Aquimarina megaterium</i> EL33 (WP_074405477.1)	100	WP_074405477.1
CunB	3516	PKS (ACP-DUF-PLP-KS-DH-KR-ACP-KS-DH)	<i>Aquimarina megaterium</i> EL33 (WP_074405476.1)	99	WP_108807999.1
CunC	589	Aminotransferase/aminomutase	<i>Aquimarina megaterium</i> EL33 (WP_074405475.1)	100	WP_074405475.1
CunD	1265	PKS (ACP-KS ⁰ -ACP-TE)	<i>Aquimarina megaterium</i> EL33 (WP_074405474.1)	99	WP_108807998.1
CunE	813	transporter	<i>Aquimarina megaterium</i> EL33 (WP_074405473.1)	100	WP_074405473.1
CunF	295	hypothetical protein	<i>Aquimarina megaterium</i> (WP_074405472.1)	100	WP_074405472.1
CunG	421	oxidoreductase	<i>Aquimarina megaterium</i> EL33 (WP_074405471.1)	98	WP_108807997.1
CunH	204	hypothetical protein	<i>Aquimarina megaterium</i> EL33 (WP_074405470.1)	100	WP_074405470.1
CunI*	1482	PKS (GNAT-ACP-KS-ECH-ECH-ECH)	<i>Aquimarina</i> sp. AU58 (WP_109851288.1)	93	*
CunJ	4377	PKS (ACP-KS-KR-ACP-KS-DH ⁰ -KR-cMT-ACP-KS-DH)	<i>Aquimarina</i> sp. AU58 (WP_109851288.1)	93	WP_108809475.1
CunK	1550	PKS (KR-ACP-KS-DH ⁰)	<i>Aquimarina</i> sp. AU58 (WP_109851289.1)	93	WP_132066262.1
CunL*	1373	PKS (ECH-ECH-ECH-ACP-ACP-KS-DH)	<i>Aquimarina</i> sp. AU58 (WP_109851289.1)	94	*
CunM	4745	PKS (KR-ACP-KS-DH ⁰ -ECH-ECH-ECH-ACP-ACP-KS-DH ⁰ -KR-ACP-KS)	<i>Aquimarina</i> sp. AU58 (WP_109851290.1)	93	WP_108807996.1
CunN	411	hypothetical protein	<i>Aquimarina megaterium</i> EL33 (WP_074409437.1)	99	WP_108807995.1
CunO	4617	PKS (DH-KR-ACP-KS-DH ⁰ -KR-ACP-KS-KR-ACP-KS-DH)	<i>Aquimarina</i> sp. AU58 (WP_109851292.1)	94	WP_108807994.1
CunP	273	hypothetical protein	<i>Aquimarina megaterium</i> EL33 (WP_074409439.1)	100	WP_074409439.1
CunQ	403	cysteine desulfurase	<i>Aquimarina megaterium</i> EL33 (WP_082994979.1)	100	WP_082994979.1
CunR	206	methyltransferase	<i>Aquimarina megaterium</i> EL33 (WP_074409440.1)	100	WP_074409440.1
CunS	664	aminotransferase	<i>Aquimarina megaterium</i> EL33 (WP_025666766.1)	99	WP_108807993.1
CunT	419	HMG-CoA synthase homolog	<i>Aquimarina megaterium</i> EL33 (WP_074409442.1)	100	WP_074409442.1
CunU	263	enoyl-CoA hydratase	<i>Aquimarina megaterium</i> EL33 (WP_074409443.1)	100	WP_074409443.1
CunV	450	hypothetical protein	<i>Aquimarina megaterium</i> (WP_074409444.1) EL33	100	WP_074409444.1
CunW	316	AT	<i>Aquimarina megaterium</i> EL33 (WP_074409445.1)	100	WP_074409445.1
CunX	241	hydroxyaxylglutathione hydrolase-like enzyme	<i>Aquimarina megaterium</i> EL33 (WP_082994980.1)	100	WP_082994980.1
CunY	86	ACP	<i>Aquimarina megaterium</i> EL33 (WP_074409446.1)	100	WP_074409446.1
CunZ	426	KS	<i>Aquimarina megaterium</i> EL33 (WP_074409447.1)	99	WP_108808230.1
CunAa	396	AT	<i>Aquimarina megaterium</i> EL33 (WP_074409448.1)	99	WP_108807992.1

* putatively split genes at contig borders. No accession numbers available.

Supplementary Dataset 1: Maximum likelihood phylogenetic tree from a MUSCLE alignment of 655 KS sequences of all 54 characterized *trans*-AT PKS BGCs (as of December 2016). Legend: aMe: α -methyl, bOH: β -hydroxyl, aOH: α -hydroxyl, 0: non elongating KS: hactal: hemiacetal, DB: double bond, shDB: shifted double bond, red: completely reduced, vinylogous: vinylogous chain branching, Oxa: oxazole, Thia: thiazole, eDB: *E*-configured DB, zDB: *Z*-configured DB, D_OH: D-configured hydroxyl group, L_OH: L-configured hydroxyl group, rearrangement: oxygen insertion. Branch nomenclature: polyketide name_protein name_number of KS on the respective protein_number of KS in the PKS_substrate specificity. Numbers on tree nodes indicate bootstrap values.

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