

**Table S2.** List of 54 candidate structures, which are consistent with previously identified peptides using DEREPLICATOR algorithm.

Compound	Producer	Phylum	Activity	Ref	Found in strain PMC*	Score	P-value	PepMass	SpecMass
Stylissamide C	<i>Stylissa caribica</i>	Porifera		1	1069, 1070, 1050, 1052, 1057	14	$6.5 \cdot 10^{-20}$	861.44	829.49
Sanguinamide_A	<i>Hexabranhus sanguineus</i>	Mollusca (Nudibranch)		2	1069, 1070, 1050, 1052, 1057	13	$1.0 \cdot 10^{-17}$	721.36	767.48
E'Champacyclin'	<i>Streptomyces</i> C42	Bacteria	Antibacterial	3	1069, 1070, 1050, 1052, 1057	13	$4.4 \cdot 10^{-17}$	897.61	910.57
B_12489_B_12489C	Unknown			-	1092	15	$5.7 \cdot 10^{-18}$	1114.64	989.57
Gramicidin S2	<i>Aneurinibacillus migulanus</i>	Bacteria	Antibacterial	4	1050, 1074, 1066, 1080, 1056, 1069, 1057	13	$1.1 \cdot 10^{-15}$	1126.69	1098.63
Viequeamide A	<i>Rivularia</i> sp	Cyanobacteria	Cytotoxic	5	1050, 1052, 1069,	12	$2.8 \cdot 10^{-17}$	803.50	892.55

					1057				
Dominicin	<i>Eurypon laughlini</i>	Porifera		6	1052, 1050, 1069, 1057	12	$2.1 \cdot 10^{-15}$	844.54	901.57
Wewakamide A	<i>Lyngbya semiplena</i> <i>Lyngbya majuscula</i>	Cyanobacteria	Cytotoxic	7	1057, 1069, 1050, 1052,	12	$4.4 \cdot 10^{-15}$	994.65	891.59
Wewakazole	<i>Lyngbya majuscula</i>	Cyanobacteria		8	1092, 1056	12	$6.7 \cdot 10^{-12}$	1140.54	1058.54
Nostophycin	<i>Nostoc</i> 152	Cyanobacteria	Cytotoxic	9	1092	11	$2.1 \cdot 10^{-15}$	888.48	943.55
Phakellistatin 2	<i>Phakellia carteri</i>	Porifera	Cytotoxic	10	1052, 1050, 1064, 1056, 1069, 1057, 1068	11	$1.2 \cdot 10^{-14}$	827.46	811.50
Rolloamide A	<i>Eurypon laughlini</i>	Porifera	Cytotoxic	11	1057, 1069, 1056, 1080, 1064, 1051, 1050	11	$1.5 \cdot 10^{-14}$	763.46	795.47
Majusculamide C_Demethoxy	<i>Lyngbya majuscula</i>	Cyanobacteria	Cytotoxic	12	1057, 1069, 1050, 1075	11	$4.6 \cdot 10^{-13}$	954.58	892.49
Callyaerin H	<i>Callyspongia</i> <i>aerizusa</i>	Porifera	Cytotoxic	13	1070, 1052, 1050, 1069, 1057	10	$1.8 \cdot 10^{-13}$	1043.62	938.57
Hymenamide B	<i>Hymeniacidon</i>	Porifera		14	1092	10	$4.0 \cdot 10^{-13}$	830.40	830.39

Haliclona B	Marine sponges	Porifera		15	1092	10	$5.4 \times 10^{-12}$	788.39	846.40
Empedopeptin	<i>Empedobacter haloabium</i> nov. sp. (ATCC 31962).	Bacteria	Antibacterial	16	1092	10	$7.5 \times 10^{-12}$	1125.56	1051.51
Anacyclamide A10	<i>Anabaena</i> sp. 90	Cyanobacteria	Cytotoxic	17	1092	10	$9.6 \times 10^{-11}$	1052.53	1009.49
Micropeptin_SD944	<i>Microcystis aeruginosa</i>	Cyanobacteria		18-	1092	9	$1.4 \times 10^{-14}$	944.52	929.53
Destruixins 2-Valine analogue5'-hydroxy,	<i>Beauveria felina</i>	Fungus	Insecticid Cytotoxic	19	1057	9	$1.6 \times 10^{-11}$	595.36	593.29
Cycloamanide_D	<i>Amanita phalloides</i>	Fungus	Immunosuppressive	20	1052, 1050, 1069, 1057,	9	$1.5 \times 10^{-10}$	884.48	857.49
Myriastramide_A	<i>Myriastria clavosa</i>	Porifera		21	1052, 1050, 1069, 1057	9	$1.6 \times 10^{-10}$	854.43	839.50
Myriastramide_A_?3''-Isomer,_2''?-chloro	Unknown			-	1092	9	$1.6 \times 10^{-10}$	888.39	846.38
Aureobasidin N	<i>Aureobasidium pullulans</i>	Marine-Derived Fungus	Antifungal	22	1092	9	$4.2 \times 10^{-10}$	1082.68	975.55
Sanguinamide B	<i>Hexabanchus sanguineus</i>	Mollusca (Nudibranch)		2	1092	9	$1.1 \times 10^{-9}$	710.27	677.22
Deoxy Mozamide B	<i>Theonella</i> sp.	Porifera		23	1071	8	$6.7 \times 10^{-12}$	844.49	832.52
Stylissamide E	<i>Stylissa caribica</i>	Porifera		24	1092	8	$6.5 \times 10^{-11}$	782.43	681.30
Ceratospongamide	Red alga <i>Ceratodictyon spongiosum</i> & symbiotic sponge <i>Sigmatocia</i> .	Algae and Porifera		25	1069, 1057, 1050	8	$8.3 \times 10^{-11}$	767.35	799.44
Xentrivalpeptide P	<i>Xenorhabdus</i> sp.	Bacteria		26	1050,	8	$9.8 \times 10^{-11}$	797.47	782.48

					1069, 1057				
Lissoclinamide 1	<i>Lissoclinum patella</i>	Chordata (Ascidian)	Cytotoxic	27	1076, 1071, 1052, 1050, 1069, 1057, 1068	8	$4.9 \cdot 10^{-10}$	705.28	659.39
Kulokekahilide 1	<i>Cephalaspidean mollusc Philinopsis speciosa</i>	Mollusca	Cytotoxic	28	1092	8	$7.1 \cdot 10^{-10}$	954.55	1069.53
Iturin A_Iturin A3	<i>Bacillus subtilis</i>	Bacteria	Antibacterial	29	1092	8	$8.7 \cdot 10^{-10}$	1056.56	1041.52
Iturin A_Iturin A2	<i>Bacillus subtilis</i>	Bacteria	Antibacterial	29	1092	8	$1.0 \cdot 10^{-9}$	1042.54	1023.50
Haliclonamide_B_O-(2-Hydroxy-3-methyl-3-butenyl)	<i>Haliclona</i> sp	Porifera		30-	1092	8	$1.6 \cdot 10^{-9}$	872.44	947.54
Citrusin VIII	<i>Citrus medica</i>	Plant, fruit peel		31	1070, 1069	8	$5.9 \cdot 10^{-9}$	821.48	782.41
Pteratide III	<i>Basidiomycete Pterula</i>	Fungus	Cytotoxic	32	1070, 1052, 1050, 1074, 1080, 1069, 1057, 1072	7	$5.9 \cdot 10^{-10}$	818.49	812.49
Vioprolide C	<i>Myxobacterium Cystobacter violaceus</i>	Bacteria	Antifungal Antibacterial	33	1071, 1052	7	$4.3 \cdot 10^{-9}$	848.41	896.57
Etamycin_A_2-(N-Methyl-L-leucine)_analogue	<i>Streptomyces</i> sp.	Bacteria	Antibacterial	34	1057, 1069, 1050, 1052	7	$4.6 \cdot 10^{-9}$	858.49	806.50
Xentrivalpeptide B	<i>Xenorhabdus</i> sp.	Bacteria		26	1050,	7	$4.7 \cdot 10^{-9}$	783.45	810.47

					1069, 1057				
Daitocidin B2	<i>Bacillus pumilus</i>	Bacteria	Antibacterial	35-	1050, 1069, 1057	7	$5.9 \cdot 10^{-9}$	895.53	893.53
Dolastatin I	<i>Dolabella auricularia</i>	Mollusca (Sea hare)	Cytotoxic	36	1092	7	$6.3 \cdot 10^{-9}$	516.22	577.24
Tunicyclin D	<i>Psammosilene tunicoides</i>	Plant	Antifungal	37	1052, 1050, 1069, 1057	7	$7.0 \cdot 10^{-9}$	900.46	823.50
Hymenamide F	<i>Hymeniacidon</i> sp.	Porifera		38	1057, 1069, 1050, 1052, 1070	7	$8.8 \cdot 10^{-9}$	764.44	768.47
Aerucyclamide C	<i>Microcystis aeruginosa</i>	Cyanobacteria		39	1092	7	$9.5 \cdot 10^{-9}$	516.22	645.28
[D-Asp3,(E)-Dhb7]Microcystin LR_ [D-Asp3,(E)-Dhb7]Microcystin LR	<i>Microcystis bloom</i>	Cyanobacteria	Cytotoxic	40	1092	7	$1.5 \cdot 10^{-8}$	980.53	846.91
Pitipeptolide A	<i>Lyngbya majuscula</i>	Cyanobacteria		41	1057, 1069, 1050	7	$1.6 \cdot 10^{-8}$	807.48	795.51
Microcystin RA	<i>Microcystis</i>	Cyanobacteria		40	1092	7	$1.7 \cdot 10^{-8}$	952.50	825.38
Prepatellamide A	<i>Lissoclinum patella</i>	Chordata, (Ascidian)		42	1052, 1056, 1064, 1051, 1050	7	$2.7 \cdot 10^{-8}$	760.34	657.29
Cyclonellin	<i>Axinella carteri</i>	Porifera		43	1080, 1069, 1072, 1074,	6	$1.8 \cdot 10^{-8}$	962.46	960.59

					1051, 1070, 1092				
Lissoclinamide 9	<i>Lissoclinum patella</i>	Ascidian	Cytotox	27	1056, 1057	6	$2.1 \cdot 10^{-8}$	707.29	593.29
Kailuin D	A marine-derived bacterium	Marine bacteria	Cytotox	44	1071,	6	$4.9 \cdot 10^{-8}$	751.51	804.52
Raocyclamide B	<i>Oscillatoria raoi</i>	Cyanobacteria		45	1056, 1057	6	$6.5 \cdot 10^{-8}$	568.21	581.17
Viomycin,_BAN,_INN_4'- Hydroxy	<i>Streptomyces</i>	Bacteria	Antibacterial, Antituberculosis	46	1050, 1051	6	$6.8 \cdot 10^{-8}$	701.32	602.26
Sclerotide A	<i>Aspergillus sclerotiorum PT06-1</i>	Marine- Derived Fungus	Antifungal	47	1052,	6	$7.3 \cdot 10^{-8}$	709.29	705.31

\* : Code strain : for all strains, read PMC XXXX.18 except for PMC 1092.19

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