

Supplementary Material: Structural diversity and biological activity of cyanopeptolins produced by *Nostoc edaphicum* CCNP1411

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Table S1. Cyanopeptolin variants described so far.

Name	Mass	Cyanobacterium	strain	1	2	3	4	5	6	Side chain	References
Tasipeptin B	770.5	<i>Symploca</i>	NIH304	O-Thr	Leu	Ahp	Leu	N-MePhe	Val	BA	[30]
Micropeptin MZ771	771.5	<i>Microcystis</i>	TAU IL-361	O-Thr	Arg	O-MeAhp	Ile	N-MePhe	Ile		[47]
Micropeptin MM836	836.4	<i>Microcystis</i>	TAU IL-36	O-Thr	Leu	Ahp	Phe	N-MePhe	Ile	GA	[42]
		<i>Oscillatoria/ Planktothrix</i>									
Planktopeptin BL843	843.4	<i>rubescens</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Thr	N-MeTyr	Ile	GA-gamma-lactam	[45]
Micropeptin MZ845	845.5	<i>Microcystis</i>	TAU IL-361	O-Thr	Arg	Ahp	Ile	N-MePhe	Ile	GA	[47, 72]
Micropeptin MM850	850.4	<i>Microcystis</i>	TAU IL-36	O-Thr	Leu	Ahp	Phe	N-MePhe	Ile	GA	[42]
Micropeptin MZ859	859.5	<i>Microcystis</i>	TAU IL-361	O-Thr	Arg	O-MeAhp	Ile	N-MePhe	Ile	GA	[47]
Tasipeptin A	869.5	<i>Symploca</i>	NIH304	O-Thr	Leu	Ahp	Leu	N-MePhe	Val	Val-BA	[30]
		<i>Oscillatoria/ Planktothrix</i>									
Cyanopeptolin 880	880.5	<i>agardhii</i>	CYA 126/8	O-Thr	Hty	Ahp	Ile	N-MePhe	Ile	2-O-MeGa	[25]
		<i>Microcystis</i>									
Micropeptin 88A	883.5	<i>aeruginosa</i>	NIES-88	O-Thr	H4Tyr	Ahp	Val	N-MePhe	Ile	Glu	[63]
Micropeptin HU895B	895.4	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	Ahp	Ile	N-MeTyr	Ile	GA	[73]
Micropeptin HU895A	895.4	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	Ahp	Ile	N,O-diMe-Cl-Tyr	Val	GA	[73]
		<i>Dolabella</i>									
Dolastatin 13	905.5	<i>auricularia</i>	<i>n.a.</i>	O-Thr	Dhb	Ahp	Phe	N-MePhe	Val	Val-O-Me_Ga	[32]
Micropeptin HU909	909.4	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	O-MeAhp	Ile	N-Me-Cl-Tyr	Val	GA	[73]
Micropeptin SF909	909.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Gln	Ahp	Leu	N-MeTyr	Ile	Hpla	[21, 74]
Micropeptin LH911B	911.4	<i>Microcystis</i>	TAU IL-37	O-Thr	Arg	Ahp	Val	N-MePhe	Ile	SuGA	[75]
Micropeptin LH911A	911.4	<i>Microcystis</i>	TAU IL-37	O-Thr	Arg	Ahp	Ile	N-MePhe	Val	SuGA	[72, 75]
Cyanopeptolin 911	911.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Leu	N-MeTyr	Val	SuGA	[76]
Micropeptin LH911C	911.4	<i>Microcystis</i>	TAU IL-37	O-Thr	Me-Lys	Ahp	Ile	N-MePhe	Ile	SuGA	[75]
Micropeptin MM916	916.4	<i>Microcystis</i>	TAU IL-36	O-Thr	Leu	Ahp	Phe	N-MePhe	Ile	SuGA	[42]
Somamide B	918.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Dhb	Ahp	Phe	N-MeTyr	Val	Gln-BA	[69]
			TAU IL-								
		<i>Nostoc/Microcysti</i>	235/NIVA								
Nostopeptin BN920	920.5	<i>s aeruginosa</i>	Cya 43	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	GlnAc	[10, 40]
Micropeptin LH920	920.5	<i>Microcystis</i>	TAU IL-37	O-Thr	Gln	Ahp	Phe	N-MeTyr	Val	Gly-HA	[75]
Cyanopeptolin 920	920.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Phe	N-MeTyr	Val	Leu-Ac	[76]
Micropeptin MZ925	925.4	<i>Microcystis</i>	TAU IL-361	O-Thr	Arg	Ahp	Ile	N-MePhe	Ile	SuGA	[47, 72]
Cyanopeptolin S	925.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Ile	N-MeTyr	Val	SuGa	[42, 77]
					di-Me-						
Micropeptin LH925	925.4	<i>Microcystis</i>	TAU IL-37	O-Thr	Lys	Ahp	Ile	N-MePhe	Ile	SuGA	[75]
Nostopeptin B	926.5	<i>Nostoc minutum</i>	NIES-26	O-Hmp	Leu	Ahp	Ile	N-MeTyr	Ile	Gln-AC	[9]
Micropeptin KB928	928.5	<i>Microcystis</i>	TAU IL-381	O-Thr	Asp	Ahp	Val	N-MePhe	Ile	Asp-BA	[22]

Cyanopeptolin B	928.5	<i>Microcystis aeruginosa</i>	PCC7806	O-Thr	Lys	Ahp	Leu	N-MePhe	Val	Asp-HA	[3]
Cyanopeptolin 930	930.5	<i>Microcystis</i>		O-Thr	Lys	Ahp	Leu	N-MeTyr	Val	Glu-BA	[72]
Micropeptin MM932	932.4	<i>Microcystis Lyngbya semiplena</i>	TAU IL-36	O-Thr	Leu	Ahp	Phe	N-MeTyr	Ile	SuGA	[42]
Lyngbyastatin 8	932.5	<i>Chondromyces crocatus</i>		O-Thr	Abu	Ahp	Phe	N-MeTyr	Val	Val-Ac	[57]
precrocapeptin A2	933.5	<i>Chondromyces crocatus</i>	Cm c5	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Gln-Ibu	[33]
crocapeptin A1	935.5	<i>Microcystis</i>	Cm c5	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Gln-Propionate	[33]
Micropeptin MZ939B	939.4	<i>Microcystis</i>	TAU IL-361	O-Thr	Arg	O-MeAhp	Ile	N-MePhe	Ile	2-SuGA	[47]
Micropeptin MZ939A	939.4	<i>Microcystis</i>	TAU IL-361	O-Thr	Arg	O-MeAhp	Ile	N-MePhe	Ile	1-SuGA	[47]
Insulapeptolide A	941.5	<i>Nostoc insulare</i>	SAG 54.79	O-Hmp	Leu	Ahp	Ile	N-MeTyr	Val	Ac-Cit	[49]
Cyanopeptolin C	942.5	<i>Microcystis aeruginosa</i>	PCC7806	O-Thr	Me-Lys	Ahp	Leu	N-MePhe	Val	Asp-HA	[3]
Micropeptin SD944	944.5	<i>Microcystis aeruginosa</i>	TAU IL-215	O-Thr	Lys	Ahp	Ile	N-MeTyr	Val	Asp-HA	[78]
Micropeptin KT946	946.4	<i>Microcystis</i>	MB-K	O-Thr	Hty	Ahp	Ile	N-MePhe	Ile	Su-GA	[24]
Lyngbyastatin 7	946.5	<i>Lyngbya semiplena</i>	<i>n.a.</i>	O-Thr	Abu	Ahp	Phe	N-MeTyr	Val	Gln-Ha	[58]
Streptopectolin	947.4	<i>Streptomyces olivochromogene</i>									
Kempopeptin C	948.5	<i>s</i>	NBRC 3561	O-Thr	Gln	Ahp	Phe	N-MeTyr	Ala	Gln-Mba	[34]
		<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Leu	N,O-diMe-Cl-Tyr	Val	Val-BA	[52]
crocapeptin A2	949.5	<i>Chondromyces crocatus</i>	Cm c5	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Gln-Ibu	[33]
Anabaenopeptilide 90A	952.5	<i>Anabaena</i>	strain 90	O-Thr	Hty	Ahp	Thr	N,O-diMeTyr	Ile	N-formyl-Gln	[5]
Cyanopeptolin 954	954.4	<i>Microcystis aeruginosa</i>	NIVA Cya 43	O-Thr	Leu	Ahp	Phe	N-Me-Cl-Tyr	Val	GlnAc	[40]
Nostopeptin A	954.5	<i>Nostoc minutum</i>	NIES-26	O-Hmp	Leu	Ahp	Ile	N-MeTyr	Ile	Gln-BA	[9]
Insulapeptolide B	955.5	<i>Nostoc insulare</i>	SAG 54.79	O-Hmp	Leu	Ahp	Ile	N-MeTyr	Leu	Ac-Cit	[49]
Insulapeptolide C	955.5	<i>Nostoc insulare</i>	SAG 54.79	O-Hmp	Leu	Ahp	Ile	N,O-diMeTyr	Val	Ac-Cit	[49]
Micropeptin KB956	956.5	<i>Microcystis</i>	TAU IL-381	O-Thr	Asp	O-MeAhp	Val	N-MePhe	Ile	O-Me-Asp-BA	[22]
Cyanopeptolin A	956.5	<i>Microcystis aeruginosa</i>	PCC7806	O-Thr	Arg	Ahp	Leu	N-MePhe	Val	Asp-HA	[3]
Cyanopeptolin D	956.6	<i>Microcystis aeruginosa</i>	PCC7806	O-Thr	Lys	Ahp	Leu	N-MePhe	Val	Asp-HA	[3]
Cyanopeptolin 958	958.5	<i>Microcystis</i>		O-Thr	Arg	Ahp	Leu	N-MeTyr	Val	Glu-BA	[72]
Micropeptin B	958.5	<i>Microcystis aeruginosa</i>	NIES-100	O-Thr	Lys	Ahp	Leu	N-MeTyr	Val	Glu-HA	[37]
Cyanopeptolin 959	959.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Phe	N-MeTyr	Ile	SuGA	[76]

Cyanopeptolin 960	960.4	<i>Oscillatoria/ Planktothrix agardhii</i>	CYA 126/8	O-Thr	Hty	Ahp	Ile	N-MePhe	Ile	2-O-MeSuGa	[25]
Lyngbyastatin 9	960.5	Lyngbya sempilena		O-Thr	Abu	Ahp	Phe	N-MeTyr	Val	Val-BA	[57]
Bouillomide A	960.5	<i>Lyngbya bouillonii</i>	<i>n.a.</i>	O-Thr	Dhb	Ahp	Phe	N-MeTyr	Val	Leu-Ala-BA	[19]
Micropeptin HH960	960.5	<i>Microcystis aeruginosa</i>	TAU IL-347	O-Thr	Leu	Ahp	Leu	N-MePhe	Val	Asn-Hpla	[79]
Micropeptin 90	961.4	<i>Microcystis aeruginosa</i>	NIES-90	O-Thr	Arg	Ahp	Phe	N-MeTyr	Val	SuGA	[61]
Molassamide	962.5	<i>Leptolyngbya sp./Dichothrix utahensis</i>	DRTO-73	O-Thr	Abu	Ahp	Phe	N-MeTyr	Val	Thr-Ala-BA	[6, 52]
Cyanopeptolin CP962	962.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Arg	Ahp	Phe	N-MePhe	Val	Asp-BA	[8]
Cyanopeptolin 963A	963.5	<i>Microcystis aeruginosa</i>	PCC 7806	O-Thr	Tyr	Ahp	Leu	N-MePhe	Val	Glu-HA	[80]
crocapeptin A3	963.5	<i>Chondromyces crocatus</i>	Cm c5	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Gln-2-Me-Ibu	[33]
Micropeptin EI964	964.5	<i>Microcystis aeruginosa</i>	TAU IL-217; TAU IL-231	O-Thr	Arg	Ahp	Phe	N-MeTyr	Ile	Asp-AC	[10]
Somamide A	965.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Dhb	Ahp	Phe	N-MeTyr	Val	Met-O-HA	[69]
Cyanopeptolin CP969	969.4	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Tyr	Ahp	Phe	N-MePhe	Val	Asp-BA	[8]
Micropeptin KB970B	970.5	<i>Microcystis</i>	TAU IL-381	O-Thr	Asp	O-MeAhp	Val	N-MePhe	Ile	Asp-HA	[22]
Micropeptin KB970A	970.5	<i>Microcystis</i>	TAU IL-381	O-Thr	Asp	Ahp	Val	N-MePhe	Ile	O-Me-Asp-HA	[22]
Micropeptin KB970C	970.5	<i>Microcystis</i>	TAU IL-381	O-Thr	Asp	O-MeAhp	Val	N-MePhe	Val	O-Me-Asp-HA	[22]
Anabaenopeptilide 90B	972.4	<i>Anabaena</i>	strain 90	O-Thr	Hty	Ahp	Thr	N-Me-Cl-Tyr	Ile	N-formyl-Gln	[5]
Micropeptin 973	972.5	<i>Microcystis panniformis</i>	MIRS-04	O-Thr	Arg	Ahp	Ile	N-MePhe	Val	Gln-BA	[65]
Cyanopeptolin 972	972.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Leu	N-MeTyr	Val	Asp-HA	[72, 81]
Stigonemapeptin	973.5	<i>Stigonema</i>		O-Thr	Abu	Ahp	Phe	N-MeTyr	Val	Gln-N-formyl-Pro	[15]
Loggerpeptin C	974.5	<i>Leptolyngbya</i>	DRTO-73	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Abu-Ala-BA	[52]
Micropeptin 478A	975.4	<i>Microcystis aeruginosa</i>	NIES-478	O-Thr	Arg	Ahp	Ile	N-Me-Cl-Tyr	Ile	SuGA	[62]
Micropeptin HU975	975.4	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	Ahp	Ile	N-Me-Cl-Tyr	Ile	SuGA	[73]
Insulapeptolide D	976.6	<i>Nostoc insulare</i>	SAG 54.79	O-Hmp	Leu	Ahp	Ile	N,O-diMeTyr	Leu	Ac-Cit	[49]
Cyanopeptolin CP978	977.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Arg	Ahp	Phe	N-MeTyr	Val	Asp-BA	[8]
Micropeptin MM978	978.5	<i>Microcystis</i>	TAU IL-36	O-Thr	Gln	Ahp	Phe	N-MeTyr	Ile	Glu-HA	[42]
Micropeptin HM978	978.5	<i>Microcystis</i>	TAU IL-33	O-Thr	Leu	Ahp	Ile	N-MePhe	Val	Asn-Hpla	[82]
Micropeptin HH978	978.5	<i>Microcystis aeruginosa</i>	TAU IL-347	O-Thr	Leu	Ahp	Leu	N-MePhe	Val	Asn-Hpla	[79]
Micropeptin SD979	979.5	<i>Microcystis aeruginosa</i>	TAU IL-215	O-Thr	Tyr	Ahp	Ile	N-MeTyr	Val	Asp-HA	[78]

Micropeptin GH979	979.5	<i>Microcystis Scytonema</i>	TAU IL-33	O-Thr	Leu	Ahp	Ile	N-MePhe	Val	Asp-Hpla	[82]
Scyptolin A	980.5	<i>hofmannii</i>	PCC 7110	O-Thr	Leu	Ahp	Thr	N-Me-Cl-Tyr	Val	Thr-Ala-BA	[13]
Cyanopeptolin 984	983.4	<i>Microcystis wesenbergii</i>	NIVA-CYA 172/5	O-Thr	Leu	Ahp	Phe	N-Me-Cl-Tyr	Gln	GlnAC	[83]
Micropeptin HA983	983.4	<i>Microcystis</i>	TAU IL-33	O-Thr	Glu	Ahp	Phe	N-Me-Cl-Tyr	Ile	GlnAC	[82]
Cyanopeptolin 983	983.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Val	N,O-diMeTyr	Val	Gln-ProAc	[84]
Micropeptin KB984	984.6	<i>Microcystis</i>	TAU IL-381	O-Thr	Asp	O-MeAhp	Val	N-MePhe	Ile	O-Me-Asp-HA	[22]
Cyanopeptolin CP985	985.4	<i>Nostoc edaphicum Radiocystis</i>	CCNP1411	O-Thr	Tyr	Ahp	Phe	N-MeTyr	Val	Asp-BA	[8]
Micropeptin K139	986.5	<i>feernandoi</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Ile	N-MeTyr	Ile	Asp-HA	[29]
Cyanopeptolin 986	986.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Leu	N-MeTyr	Val	Glu-HA	[72]
Micropeptin A	986.6	<i>Microcystis aeruginosa</i>	NIES-100	O-Thr	Lys	Ahp	Leu	N-MeTyr	Val	Glu-OA	[37, 72]
Micropeptin HU989	989.4	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	Ahp	Ile	N,O-diMe-Cl-Tyr	Ile	SuGA	[73]
Insulapeptolide G	990.5	<i>Nostoc insulare</i>	SAG 54.79	O-Thr	Phe	Ahp	Thr	N-MePhe	Val	Ser-Pro-BA	[49]
Kempopeptin A	990.5	<i>Lyngbya</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Thr-Pro	[28]
Cyanopeptolin CP990	990.5	<i>Nostoc edaphicum Chondromyces</i>	CCNP1411	O-Thr	Arg	Ahp	Phe	N-MePhe	Val	Asp-HA	[8]
crocapeptin B	990.5	<i>crocatus</i>	Cm c5	O-Thr	Leu	Ahp	Phe	N-MeTyr	Ile	Cit-Ibu	[33]
Cyanopeptolin 991	991.4	<i>Microcystis</i>		O-Thr	Arg	Ahp	Leu	N-MePhe	Val	diSuGA	[72]
Kempopeptin B	992.5	<i>Lyngbya</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Ile	N,O-diMe-Br-Tyr	Val	Val-BA	[28]
Micropeptin EI992	992.5	<i>Microcystis aeruginosa</i>	TAU IL-217;	O-Thr	Arg	Ahp	Phe	N-MeTyr	Ile	Asp-BA	[10]
Cyanopeptolin 992	992.5	<i>Microcystis</i>	TAU IL-231	O-Thr	Lys	Ahp	Phe	N-MeTyr	Val	Glu-HA	[72]
Cyanopeptolin CP992	992.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Arg	Ahp	Phe	N,O-diMeTyr	Val	Asp-BA	[8]
Loggerpeptin A	992.5	<i>Leptolyngbya</i>	DRTO-73	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Thr-Ala-BA	[52]
Micropeptin KB992	992.5	<i>Microcystis</i>	TAU IL-381	O-Thr	Leu	O-MeAhp	Ile	N-MePhe	Val	Asn-Hpla	[22]
Micropeptin HH992	992.5	<i>Microcystis aeruginosa</i>	TAU IL-347	O-Thr	Leu	Ahp	Leu	N-MePhe	Val	Asn-Hpla	[79]
Micropeptin E	993.5	<i>Microcystis aeruginosa</i>	NIES-100	O-Thr	Tyr	Ahp	Leu	N-MeTyr	Val	Glu-HA	[20, 72]
Micropeptin SF995	995.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Ile	N-MeTrp	Val	Asp-HA	[74]
Micropeptin 996	996.5	<i>Microcystis aeruginosa</i>	UTEX LB2386	O-Thr	Hty	Ahp	Phe	N-MePhe	Val	Gln-BA	66
Cyanopeptolin 997 B	997.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Val	N,O-diMeTyr	Leu	Gln-ProAc	[84]
Cyanopeptolin 997 A	997.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Leu	N-MeTyr	Leu	Gln-ProAc	[84]
Cyanopeptolin 997 C	997.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Leu	N,O-diMeTyr	Val	Gln-ProAc	[84]
Micropeptin KR998	998.5	<i>Microcystis aeruginosa</i>	TAU IL-40	O-Thr	Tyr	Ahp	Phe	N-MeTyr	Val	Gln-BA	[85]
Cyanopeptolin CP999	999.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Tyr	Ahp	Phe	N,O-diMeTyr	Val	Asp-BA	[8]

Micropeptin SD999	999.5	<i>Microcystis aeruginosa</i>	TAU IL-215	O-Thr	Arg	Ahp	Ile	N-Me-Kyn	Val	Asp-HA	[78]
Kyanamide	1000.2	<i>Caldora penicillata</i>		O-Thr	Leu	Ahp	Phe	N-MeTrp	Val	Gln-HA	[4]
Cyanopeptolin 1000A	1000.6	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Leu	N-MeTyr	Ile	Glu-OA	[76]
Cyanopeptolin 1001	1001.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Leu	N-Me-O-Cl-Tyr	Leu	Gln-Mdhp	[84]
Micropeptin KR 1002	1002.5	<i>Microcystis aeruginosa</i>	TAU IL-40	O-Thr	H4Tyr	Ahp	Phe	N-MeTyr	Val	Gln-BA	[85]
Micropeptin SD1002	1002.5	<i>Microcystis aeruginosa</i>	TAU IL-215	O-Thr	Tyr	Ahp	Ile	N-MeTrp	Val	Asp-HA	[78]
Cyanopeptolin 1003	1003.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Val	N-Me-O-Cl-Tyr	Val	Gln-ProAc	[84]
Insulapeptolide H	1004.5	<i>Nostoc insulare</i>	SAG 54.79	O-Thr	Phe	Ahp	Thr	N-MePhe	Leu	Ser-Pro-BA	[49]
Cyanopeptolin SS	1005.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	??	Ahp	??	N-MeTyr	??	??	[42, 49]
Insulapeptolide F	1006.5	<i>Nostoc insulare</i>	SAG 54.79	O-Thr	Phe	Ahp	Thr	N-MeTyr	Val	Ser-Pro-BA	[49]
Cyanopeptolin 1007 MB2	1006.5	<i>Microcystis n.a./Nostoc edaphicum</i>	n.a./CCNP141	O-Thr	Lys	Ahp	Leu	N-Me-Cl-Tyr	Ile	Glu-HA	[86]
Cyanopeptolin CP1006	1006.5	<i>n.a.</i>	1	O-Thr	Arg	Ahp	Phe	N-MeTyr	Val	Asp-HA	[8, 72, 81]
Cyanopeptolin 1006D	1006.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Phe	N-MeTyr	Ile	Glu-HA	[76]
Micropeptin DR1006	1006.5	<i>Microcystis aeruginosa</i>	TAU IL-237	O-Thr	Leu	Ahp	Leu	N-MePhe	Ile	Gln-Hpla	[21]
Cyanopeptolin 1009	1009.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Cl-Phe	N-MeTyr	Ile	SuGA	[81]
Micropeptin T20	1010.3	<i>Microcystis aeruginosa</i>	<i>n.a.</i>	O-Thr	Phe	Ahp	Phe	N-MeTyr	Ile	GA-Na2H2PO3	[39]
Cyanopeptolin 1011	1011.6	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Leu	N,O-diMeTyr	Leu	Gln-ProAc	[84]
Cl-Cyanopeptolin W	1012.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Phe	N-Me-Cl-Tyr	Ile	GluAc	[81]
Cyanopeptolin CP1013	1013.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Tyr	Ahp	Phe	N-MeTyr	Val	Asp-HA	[8]
Cyanopeptolin 1014	1014.6	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Leu	N-MeTyr	Val	Glu-OA	[72]
Micropeptin T2	1015.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Phe	N-MeTrp	Val	Glu-HA	[38]
Cyanopeptolin 1017	1017.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Val	N-Me-O-Cl-Tyr	Leu	Gln-ProAc	[84]
Cyanopeptolin CP1018	1018.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Arg	Ahp	Phe	N-MePhe	Val	Asp-OA	[8]
Micropeptin MZ1019	1019.4	<i>Microcystis</i>	TAU IL-361	O-Thr	Arg	O-MeAhp	Ile	N-MePhe	Ile	1,2-SuGA	47
Cyanopeptolin 1020B	1020.5	<i>Microcystis</i>		O-Thr	Lys	Ahp	Leu	N-MeTyr	Val	Glu-OA	[72]
Insulapeptolide E	1020.5	<i>Nostoc insulare</i>	SAG 54.79	O-Thr	Phe	Ahp	Thr	N-MeTyr	Leu	Ser-Pro-BA	[49]
Cyanopeptolin 1020	1020.5	<i>Microcystis aeruginosa</i>	UV006	O-Thr	Arg	Ahp	Phe	N-MeTyr	Val	Glu-HA	[35, 72]
Cyanopeptolin CP1020	1020.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Arg	Ahp	Phe	N,O-diMeTyr	Val	Asp-HA	[8]
Micropeptin HU1021	1021.4	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	Ahp	Ile	N-MeTyr	Ile	diSuGA	[73]
Micropeptin LH1021	1021.5	<i>Microcystis</i>	TAU IL-37	O-Thr	Gln	Ahp	Phe	N-MeTyr	Val	Thr-Gly-HA	[75]
Micropeptin F	1021.5	<i>Microcystis aeruginosa</i>	NIES-100	O-Thr	Tyr	Ahp	Leu	N-MeTyr	Val	Glu-OA	[20, 72]
Aeruginopeptin 917SC	1022.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Leu	N-MeTyr	Ile	Hpla-Gln	[55]

Cyanopeptolin 1025	1025.6	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Leu	N,O-diMeTyr	Leu	Gln-PrPro	[84]
Cyanopeptolin CP1027	1027.5	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Tyr	Ahp	Phe	N,O-diMeTyr	Val	Asp-HA	[8]
Micropeptin C	1027.5	<i>Microcystis aeruginosa</i>	NIES-100	O-Thr	Tyr	Ahp	Phe	N-MeTyr	Val	Glu-HA	[20]
Micropeptin KR1030	1030.5	<i>aeruginosa</i>	TAU IL-40	O-Thr	H4Tyr	Ahp	Phe	N-MeTyr	Val	Gln-HA	[85]
Cyanopeptolin 1032	1031.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Leu	N,O-diMeTyr	Leu	Gln-PrPro	[84]
Oscillapeptilide 97B	1031.5	<i>Oscillatoria/agardhii</i>	strain 97	O-Thr	Leu	Ahp	Phe	N-MeTyr	Ile	Gln-N-AcPro	[27]
Cyanopeptolin CB071	1034.5	<i>Aphanocapsa</i>	1001	O-Thr	Arg	Ahp	Ile	N,O-diMe-Cl-Tyr	Val	Glu-HA	[16]
Cyanopeptolin 1034	1034.6	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Phe	N-MeTyr	Ile	Glu-OA	[76]
Lyngbyastatin 10	1038.4	Lyngbya semiplena		O-Thr	Abu	Ahp	Phe	N-Me-Br-Tyr	Val	Val-BA	[57]
Bouillomide B	10384	<i>Lyngbya bouillonii</i>	<i>n.a.</i>	O-Thr	Dhb	Ahp	Phe	N-Me-Br-Tyr	Val	Leu-Ala-BA	[19]
Cyanopeptolin 1041	1040.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Phe	N-MeTyr	Val	Glu-HA	[87]
A90720A	1040.5	<i>Microchaete loktakensis</i>	IC-39-2	O-Thr	Arg	Ahp	Leu	N-MeTyr	Val	Leu-SuGA	[7, 36]
Micropeptin HU1041	1041.3	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	Ahp	Ile	N-Me-Cl-Tyr	Val	diSuGA	[73]
Ichthyopeptin A	1042.5	<i>Microcystis ichthyoblade</i>	BM Mi/13	O-Thr	Tyr	Ahp	Val	N-MePhe	Ile	Gln-Hpla	[54]
Micropeptin KT1042	1042.5	<i>Microcystis aeruginosa</i>	TAU IL-347	O-Thr	Tyr	Ahp	allo-Ile	N-MePhe	Val	Gln-Hpla	[41]
Aeruginopeptin 228A	1044.5	<i>Microcystis</i>	TAC 954;	O-Thr	H4Tyr	Ahp	Thr	N-MePhe	Ile	Gln-Hpla	[23]
Micropeptin 103	1044.5	<i>aeruginosa</i>	M2285	O-Thr	H4Tyr	Ahp	Thr	N-MePhe	Ile	Gln-Hpla	[23]
		<i>Microcystis viridis</i>	NIES-103	O-Thr	Gln	Ahp	Phe	N-MeTrp	Val	Thr-Gly-HA	[43]
Oscillapeptilide 97A	1045.5	<i>Oscillatoria/agardhii</i>	strain 97	O-Thr	Leu	Ahp	Phe	N,O-diMeTyr	Ile	Gln-N-AcPro	[27]
Micropeptin KB1046	1046.5	<i>Microcystis</i>	TAU IL-381	O-Thr	H4Tyr	Ahp	Val	N-MePhe	Ile	Gln-Hpla	[22]
Aeruginopeptin 228B	1048.5	<i>Microcystis aeruginosa</i>	TAC 954;	O-Thr	H4Tyr	Ahp	Thr	N-MePhe	Ile	Gln-Hpla	[23]
Micropeptin KB1048	1048.5	<i>aeruginosa</i>	M2285	O-Thr	H4Tyr	Ahp	Thr	N-MePhe	Ile	Gln-Hpla	[23]
Cyanopeptolin CP1048	1048.6	<i>Microcystis</i>	TAU IL-381	O-Thr	Asp	O-MeAhp	Ile	N-Me-Cl-Tyr	Ile	O-Me-Asp-HA	[22]
Micropeptin LH1048	1048.6	<i>Nostoc edaphicum</i>	CCNP1411	O-Thr	Arg	Ahp	Phe	N,O-diMeTyr	Val	Asp-OA	[8]
Anabaenopeptilide 202A	1048.6	<i>Microcystis</i>	TAU IL-37	O-Thr	Arg	Ahp	Phe	N-MeTyr	Val	Glu-OA	[72, 75]
	1049.5	<i>Anabaena</i>	strain 202A2	O-Thr	Hty	Ahp	Thr	N-MeTyr	Ile	Gln-N-formyl-Pro	[5]
Symplocamide A	1050.4	<i>Symploca</i>	PNG-	O-Thr	Hty	Ahp	Thr	N-MeTyr	Ile	Gln-N-formyl-Pro	[5]
Micropeptin T1	1050.5	<i>Symploca</i>	12/15/03-5	O-Thr	Arg	Ahp	Ile	N,O-diMeTyr	Val	Gln-BA	[31]
Cyanopeptolin 1054	1050.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Tyr	Ahp	Phe	N-MeTrp	Val	Glu-HA	[38]
MB1	1054.5	<i>n.a.</i>		O-Thr	Arg	Ahp	Phe	N-Me-Cl-Tyr	Ile	Glu-HA	[86]

Cyanopeptolin 1054 MB2	1054.5	<i>n.a.</i>		O-Thr	Me-Lys	Ahp	Phe	N-Me-Cl-Tyr	Ile	Glu-HA	[86]
Micropeptin 478B	1055.3	<i>Microcystis aeruginosa</i>	NIES-478	O-Thr	Arg	Ahp	Ile	N-Me-Cl-Tyr	Ile	diSuGA	[62]
Micropeptin D	1055.5	<i>Microcystis aeruginosa</i>	NIES-100	O-Thr	Tyr	Ahp	Phe	N-MeTyr	Val	Glu-OA	[20]
Lyngbyastatin 5	1056.5	<i>Lyngbya</i>	<i>n.a.</i>	O-Thr	Abu	Ahp	Phe	N-MeTyr	Val	Hty-Ala-Ga	[58]
Micropeptin DR1056	1056.5	<i>Microcystis aeruginosa</i>	TAU IL-237 and IL-23	O-Thr	Tyr	Ahp	Leu	N-MePhe	Ile	Gln-Hpla	[21]
Hofmannolin	1057.5	<i>Scytonema hofmannii</i>	PCC 7110	O-Thr	Phe	Ahp	O-MeTyr	N-MeTyr	Val	Glu-Hmv	[14]
Micropeptin TR1058	1058.5	<i>Microcystis</i>	TAU IL-428	O-Thr	Gln	Ahp	Ile	N-MePhe	Val	Tyr-Hpla	[88]
Micropeptin DR1060	1060.5	<i>Microcystis aeruginosa</i>	TAU IL-237 and IL-23	O-Thr	H4Tyr	Ahp	Leu	N-MePhe	Ile	Gln-Hpla	[21]
Planktopeptin BL1061	1061.6	<i>Oscillatoria/Planktothrix rubescens</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Thr	N-MeTyr	Ile	Gln-Leu-GA	[45]
Oscillapeptin C	1061.6	<i>Oscillatoria/Planktothrix agardhii</i>	NIES-205	O-Thr	H4Tyr	Ahp	Ile	N-MePhe	Ile	Hty-OMeGa	[28]
Micropeptin 88N	1062.6	<i>Microcystis aeruginosa</i>	NIES-88	O-Thr	Tyr	Ahp	Val	N-MePhe	Ile	Glu-Leu-BA	[64]
Micropeptin 88E	1062.6	<i>Microcystis aeruginosa</i>	NIES-88	O-Thr	Leu	Ahp	Val	N-MePhe	Ile	Glu-Tyr-BA	[63]
Micropeptin LH1062	1062.6	<i>Microcystis</i>	TAU IL-37	O-Thr	Arg	Ahp	Phe	N-MeTyr	Val	MeO-Glu-OA	[75]
Cyanopeptolin 1063	1063.6	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Tyr	Ahp	Ile	N-MeTyr	Ile	Gln-LeuAc	[76]
Pompanopeptin A	1068.4	<i>Lyngbya confervoides</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Ile	N,O-diMe-Br-Tyr	Val	Met(O)-Ba	[68]
Cyanopeptolin 1068	1068.5	<i>Microcystis aeruginosa</i>	<i>n.a.</i>	O-Thr	di-Me-Lys	Ahp	Phe	N-Me-Cl-Tyr	Ile	Glu-HA	[86]
Micropeptin HU1069	1069.4	<i>Microcystis</i>	TAU IL-342	O-Thr	Arg	Ahp	Ile	N,O-diMe-Cl-Tyr	Ile	diSuGA	[73]
Anabaenopeptilide 202B	1069.5	<i>Anabaena</i>	strain 202A2	O-Thr	Hty	Ahp	Thr	N-Me-Cl-Tyr	Ile	Gln-N-formyl-Pro	[5]
Aeruginopeptin 917SA	1072.5	<i>Microcystis</i>	<i>n.a.</i>	O-Thr	Tyr	Ahp	Leu	N-MeTyr	Ile	Gln-Hpla	[55]
Microcystilide A	1072.5	<i>Microcystis aeruginosa</i>	NO-15-1840	O-Thr	Tyr	Ahp	Leu	N-MeTyr	Ile	Gln-Hpla	[59]
Aeruginopeptin 917SB	1076.5	<i>n.a.</i>	<i>n.a.</i>	O-Thr	H4Tyr	Ahp	Leu	N-MeTyr	Ile	Hpla-Gln	[55]
Micropeptin 88B	1078.5	<i>Microcystis aeruginosa</i>	NIES-88	O-Thr	Glu	Ahp	Val	N-MePhe	Ile	Glu-Tyr-BA	[63]
Micropeptin 88Y	1084.5	<i>Microcystis aeruginosa</i>	NIES-88	O-Thr	Tyr	Ahp	Val	N-MePhe	Ile	Glu-TyrAc	[64]

Oscillapeptin F	1088.5	<i>Oscillatoria/ Planktothrix agardhii</i>	NIES-596	O-Thr	Lys	Ahp	Ile	N-MePhe	Ile	Hty-O-Me-SuGA	[28]
Oscillapeptin J	1092.4	<i>Oscillatoria/ Planktothrix rubescens</i>		O-Thr	Arg	Ahp	Thr	N-MeTyr	Ile	Tyr-SuGA	[67]
Jizanpeptin A	1104.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Ile	N,O-diMe-Br-Tyr	Ile	Val-SuGA	[56]
Micropeptin 1106	1105.6	<i>Microcystis aeruginosa</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Val	N-MeTyr	Ile	Glu-Tyr-BA	[60]
Oscillapeptin G	1111.5	<i>Oscillatoria/ Planktothrix agardhii</i>		O-Thr	Leu	Ahp	Thr	N-MeTyr	Ile	Gln-Hty-GA	[35]
Micropeptin 88C	1112.5	<i>Microcystis aeruginosa</i>	NIES-88	O-Thr	Tyr	Ahp	Val	N-MePhe	Ile	Glu-Tyr-BA	[63]
Micropeptin 88F	1112.5	<i>Microcystis aeruginosa</i>	NIES-88	O-Thr	Tyr	Ahp	Val	N-MePhe	Ile	O-Me-Glu-Tyr-BA	[63]
Nostocyclin	1116.5	<i>Nostoc</i>	DUN901	O-Thr	Hse	Ahp	Phe	N-MePhe	Val	Hse-Ile-Hpla	[11]
Micropeptin 88D	1116.6	<i>Microcystis aeruginosa</i>	NIES-88	O-Thr	H4Tyr	Ahp	Val	N-MePhe	Ile	Glu-Tyr-BA	[63]
Jizanpeptin B	1118.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Ile	N,O-diMe-Br-Tyr	Ile	(R)Val-O-Me-SuGA	[56]
Jizanpeptin C	1118.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Ile	N,O-diMe-Br-Tyr	Ile	(S)Val-O-Me-SuGA	[56]
Micropeptin 1120	1119.6	<i>Microcystis aeruginosa</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Val	N-MeTyr	Ile	OMeGlu-Tyr-BA	[60]
Scyptolin B	1121.5	<i>Scytonema hofmannii</i>	PCC 7110	O-Thr	Leu	Ahp	Thr	N-Me-Cl-Tyr	Val	Ala-BA-Thr-Ala-BA	[13]
Planktopeptin BL1125	1125.6	<i>Oscillatoria/ Planktothrix rubescens</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	Thr	N-MeTyr	Ile	Gln-Hty-GA	[45]
Oscillapeptin D	1127.5	<i>Oscillatoria/ Planktothrix agardhii</i>	NIES-205	O-Thr	Hty	Ahp	Ile	N-MePhe	Ile	Hty-O-Me-SuGA	[28]
Jizanpeptin D	1132.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Lys	Ahp	Ile	N,O-diMe-Br-Tyr	Ile	Ile-O-Me-SuGA	[56]
Loggerpeptin B	1133.6	<i>Leptolyngbya Lyngbya</i>	DRTO-73	O-Thr	Leu	Ahp	Phe	N-MeTyr	Val	Thr-Ala-BA-O-Ala-BA	[52]
Lyngbyastatin 4	1136.4	<i>confervoides</i>	<i>n.a.</i>	O-Thr	Abu	Ahp	Phe	N-Me-Tyr	Val	Htyr-Ala-SuGa	[44]
Oscillapeptin E	1137.5	<i>Oscillatoria/ Planktothrix agardhii</i>	NIES-205	O-Thr	H4Tyr	Ahp	Ile	N-MePhe	Ile	Hty-O-Me-SuGA	[28, 89]
Aeruginopeptin 95A	1145.5	<i>Microcystis aeruginosa</i>	TAC 954; M2285	O-Thr	Tyr	Ahp	Thr	N-MePhe	Ile	Gln-Thr-Hpla	[23]
Jizanpeptin E	1146.4	<i>n.a.</i>	<i>n.a.</i>	O-Thr	Arg	Ahp	Ile	N,O-diMe-Br-Tyr	Ile	Val-O-Me-SuGA	[56]

Aeruginopeptin 95B	1149.6	<i>Microcystis aeruginosa</i>	TAC 954; M2285	O-Thr	H4Tyr	Ahp	Thr	N-MePhe	Ile	Gln-Thr-Hpla	[23]
Lyngbyastatin 6	1150.5	<i>Lyngbya</i>	<i>n.a.</i>	O-Thr	Abu	Ahp	Phe	N-MeTyr	Val	Hty-Ala-Na-SuGa	[58]
Oscillapeptin A	1167.5	<i>Oscillatoria/Planktothrix agardhii</i>	NIES-204	O-Thr	Hty	Ahp	Ile	N,O-diMeTyr	Ile	Hty-OMeSuGa	[46]
Oscillapeptin B	1181.5	<i>Oscillatoria/Planktothrix agardhii</i>	NIES-204	O-Thr	Me-Tyr	Ahp	Ile	N,O-diMeTyr	Ile	Hty-O-Me-SuGA	[28]
Largamide E	1187.6	<i>Planktothrix</i>	FL31-01	O-Thr	Tyr	Ahp	Thr	N-Me-Cl-Tyr	Val	Val-Ala-Ahppa-GA	[26]
Largamide D	1213.5	<i>Lyngbya confervoides</i>	<i>n.a.</i>	O-Thr	Leu	Ahp	allo-Thr	N-Me-Br-Tyr	Val	Val-Ala-Ahppa-GA	[90]
Largamide D	1231.5	<i>Oscillatoria/Planktothrix</i>	FL31-01	O-Thr	Hty	Ahp	Thr	N-Me-Br-Tyr	Val	Val-Ala-Ahppa-GA	[26]
Largamide F	1281.5	<i>Oscillatoria/Planktothrix</i>	FL31-01	O-Thr	Leu	Ahp	Thr	N-Me-Br-Tyr	Val	Val-Ala-Ahppa-GA	[26]
Largamide G	1295.5	<i>Oscillatoria/Planktothrix</i>	FL31-01	O-Thr	Leu	Ahp	Thr	N-Me-Br-Tyr	Val	Val-Ala-Ahppa-GA	[26]

Table S2. Cyanopeptolin variants produced by the *Nostoc edaphicum* CCNP1411.

Group	Name	Exact mass	(m/z) calc	(m/z) [M+H] ⁺	Error mass	Retention time	Structure	Mass of isolated CP [mg]	References
CP-Arg ²	CP 777	777.4174	778.4252	778.43			[Thr+Arg+Ahp+Phe+MePhe+Val]	0.3	
CP-Arg ²	CP 807	807.4279	808.4357	808.44			[Thr+Arg+Ahp+Phe+diMeTyr+Val]	0.5	
CP-Arg ²	CP 892	892.4443	893.4521	893.4521	0.0000	5.45	[Thr+Arg+Ahp+Phe+MePhe+Val]Asp		
CP-Arg ²	CP 922	922.4549	923.4627	923.4635	0.0008	5.02	[Thr+Arg+Ahp+Phe+diMeTyr+Val]Asp		
CP-Arg ²	CP 934	934.4549	935.4627	935.4626	0.0001	6.84	[Thr+Arg+Ahp+Phe+MePhe+Val]Asp+Ac	0.3	
CP-Arg ²	CP 944	944.4967	945.5046	945.5050	0.0005	5.81	[Thr+Arg+Ahp+Leu+MeTyr+Val]Asp+BA		
CP-Arg ²	CP 950	950.4498	951.4576	951.4577	0.0001	4.40	[Thr+Arg+Ahp+Phe+MeTyr+Val]Asp+Ac	0.4	
CP-Arg ²	CP 962	962.4862	963.4940	963.4939	0.0001	7.54	[Thr+Arg+Ahp+Phe+MePhe+Val]Asp+BA	1.2	[8]
CP-Arg ²	CP 964	964.4654	965.4733	965.4731	0.0001	6.69	[Thr+Arg+Ahp+Phe+diMeTyr+Val]Asp+Ac		
CP-Arg ²	CP 976	976.5018	977.5096	977.5074	0.0022	8.06	[Thr+Arg+Ahp+Phe+MePhe+Leu]Asp+BA		
CP-Arg ²	CP 978	978.4811	979.4889	979.4889	0.0000	6.04	[Thr+Arg+Ahp+Phe+MeTyr+Val]Asp+BA	4.4	[8]
CP-Arg ²	CP 990	990.5175	991.5253	991.5246	0.0007	8.51	[Thr+Arg+Ahp+Phe+MePhe+Val]Asp+HA	3.9	[8]
CP-Arg ²	CP 992	992.4967	993.5046	993.5043	0.0003	7.43	[Thr+Arg+Ahp+Phe+diMeTyr+Val]Asp+BA	0.3	[8]
CP-Arg ²	CP 992b	992.4967	993.5046	993.5047	0.0001	6.70	[Thr+Arg+Ahp+Phe+MeTyr+Leu]Asp+BA		
CP-Arg ²	CP 992c	992.4967	993.5046	993.50			[Thr+Arg+Ahp+Phe+MeTyr+Val]Glu+BA		
CP-Arg ²	CP 1006	1006.5124	1007.5202	1007.5198	0.0004	7.33	[Thr+Arg+Ahp+Phe+MeTyr+Val]Asp+HA		[76, 8]
CP-Arg ²	CP 1008	1008.4917	1009.4995	1009.50			[Thr+Arg+Ahp+Phe+diMe,OTyr+Val]Asp+BA		
CP-Arg ²	CP 1018	1018.5488	1019.5566	1019.5568	0.0002	9.58	[Thr+Arg+Ahp+Phe+MePhe+Val]Asp+OA	1.7	[8]
CP-Arg ²	CP 1020b	1020.5280	1021.5359	1021.5350	0.0009	8.41	[Thr+Arg+Ahp+Phe+diMeTyr+Val]Asp+HA	1.2	[8]
CP-Arg ²	CP 1020	1020.5280	1021.5359	1021.54			[Thr+Arg+Ahp+Phe+MeTyr+Val]Glu+HA		[35]
CP-Arg ²	CP 1034	1034.5437	1035.5515	1035.5509	0.0006	8.51	[Thr+Arg+Ahp+Phe+MeTyr+Val]Asp+OA	0.5	
CP-Arg ²	CP 1036	1036.5230	1037.5308	1037.5279	0.0029	7.48	[Thr+Arg+Ahp+Phe+diMe,OTyr+Val]Asp+HA		
CP-Arg ²	CP 1046	1046.5801	1047.5879	1047.5870	0.0009	10.69	[Thr+Arg+Ahp+Phe+MePhe+Val]Asp+DA	0.2	
CP-Arg ²	CP 1048	1048.5593	1049.5672	1049.5671	0.0001	9.47	[Thr+Arg+Ahp+Phe+diMeTyr+Val]Asp+OA	1.1	[8]
CP-Arg ²	CP 1076	1076.5906	1077.5985	1077.5988	0.0004	10.60	[Thr+Arg+Ahp+Phe+diMeTyr+Val]Asp+DA		

Group	Name	Exact mass	(m/z) calc	(m/z) [M+H-H ₂ O] ⁺	Error mass	Retention time	Structure	Mass of isolated CP [mg]	References
CP-Leu ²	CP 891	891.4378	874.4351	874.4342	0.0009	10.24	[Thr+Leu+Ahp+Phe+MePhe+Val]Asp+Ac		
CP-Leu ²	CP 907	907.4327	890.4300	890.4299	0.0001	8.26	[Thr+Leu+Ahp+Phe+MeTyr+Val]Asp+Ac		
CP-Leu ²	CP 919	919.4691	902.4664	902.4663	0.0001	11.35	[Thr+Leu+Ahp+Phe+MePhe+Val]Asp+BA	5.1	
CP-Leu ²	CP 921	921.4484	904.4457	904.4441	0.0015	10.00	[Thr+Leu+Ahp+Phe+diMeTyr+Val]Asp+Ac		
CP-Leu ²	CP 933	933.4848	916.4820	916.48			[Thr+Leu+Ahp+Phe+MePhe+Val]Glu+BA		
CP-Leu ²	CP 935	935.4640	918.4613	918.4610	0.0003	9.40	[Thr+Leu+Ahp+Phe+MeTyr+Val]Asp+BA	2.1	
CP-Leu ²	CP 947	947.5004	930.4977	930.4974	0.0003	12.69	[Thr+Leu+Ahp+Phe+MePhe+Val]Asp+HA		
CP-Leu ²	CP 949	949.4797	932.4770	932.4764	0.0005	11.11	[Thr+Leu+Ahp+Phe+diMeTyr+Val]Asp+BA	4.6	
CP-Leu ²	CP 963b	963.4953	946.4926	946.4920	0.0006	11.79	[Thr+Leu+Ahp+Phe+diMeTyr+Val]Glu+BA		
CP-Leu ²	CP 963	963.4953	946.4926	946.4916	0.0010	10.85	[Thr+Leu+Ahp+Phe+MeTyr+Val]Asp+HA		
CP-Leu ²	CP 965b	965.4746	948.4719	948.47			[Thr+Leu+Ahp+Phe+diMe,OTyr+Val]Asp+BA		
CP-Leu ²	CP 975	975.5317	958.5290	958.5276	0.0014	14.08	[Thr+Leu+Ahp+Phe+MePhe+Val]Asp+OA		
CP-Leu ²	CP 977	977.5110	960.5083	960.5083	0.0000	12.45	[Thr+Leu+Ahp+Phe+diMeTyr+Val]Asp+HA		
CP-Leu ²	CP 991	991.5266	974.5239	974.5215	0.0024	12.29	[Thr+Leu+Ahp+Phe+MeTyr+Val]Asp+OA		
CP-Leu ²	CP 1005	1005.5423	988.5396	988.5394	0.0001	13.84	[Thr+Leu+Ahp+Phe+diMeTyr+Val]Asp+OA		
CP-MeLeu ²	CP 933b	933.4848	916.4820	916.48			[Thr+MeLeu+Ahp+Phe+MePhe+Val]Asp+BA		
CP-MeLeu ²	CP 949b	949.4797	932.4770	932.48			[Thr+MeLeu+Ahp+Phe+MeTyr+Val]Asp+BA		
CP-MePhe ²	CP 939b	939.4378	922.4351	922.44			[Thr+MePhe+Ahp+Phe+MePhe+Val]Asp+Ac		
CP-MePhe ²	CP 967b	967.4691	950.4664	950.47			[Thr+MePhe+Ahp+Phe+MePhe+Val]Asp+BA		
CP-MePhe ²	CP 1011c	1011.4953	994.4926	994.49			[Thr+MePhe+Ahp+Phe+MeTyr+Val]Asp+HA		
CP-Met ²	CP 937	937.4255	920.4228	920.42			[Thr+Met+Ahp+Phe+MePhe+Val]Asp+BA		
CP-Met ²	CP 939	939.4048	922.4021	922.40			[Thr+Met+Ahp+Phe+diMeTyr+Val]Asp+Ac		
CP-Met ²	CP 953b	953.4205	936.4177	936.42			[Thr+Met+Ahp+Phe+MeTyr+Val]Asp+BA		
CP-Met ²	CP 995	995.4674	978.4647	978.47			[Thr+Met+Ahp+Phe+diMeTyr+Val]Asp+HA		
CP-Met ²	CP 1023	1023.4987	1006.4960	1006.50			[Thr+Met+Ahp+Phe+diMeTyr+Val]Asp+OA		
CP-MeTyr ²	CP 999d	999.4590	982.4562	982.46			[Thr+MeTyr+Ahp+Phe+MeTyr+Val]Asp+BA		

CP-MeTyr ²	CP 1014	1014.1269	997.1241	997.1572	0.0331	16.64	[Thr+MeTyr+Ahp+Phe+diMeTyr+Val]Asp+BA	
CP-Phe ²	CP 925	925.4222	908.4194	908.4189	0.0005	10.58	[Thr+Phe+Ahp+Phe+MePhe+Val]Asp+Ac	0.5
CP-Phe ²	CP 953	953.4535	936.4507	936.4500	0.0007	11.61	[Thr+Phe+Ahp+Phe+MePhe+Val]Asp+BA	0.8
CP-Phe ²	CP 955	955.4327	938.4300	938.4276	0.0024	10.35	[Thr+Phe+Ahp+Phe+diMeTyr+Val]Asp+Ac	0.7
CP-Phe ²	CP 967	967.4691	950.4664	950.4644	0.0020	12.16	[Thr+Phe+Ahp+Phe+MePhe+Leu]Asp+BA	
CP-Phe ²	CP 969b	969.4484	952.4457	952.4449	0.0008	10.60	[Thr+Phe+Ahp+Phe+MeTyr+Val]Asp+BA	0.8
CP-Phe ²	CP 981	981.4848	964.4820	964.4816	0.0004	12.89	[Thr+Phe+Ahp+Phe+MePhe+Val]Asp+HA	1.5
CP-Phe ²	CP 983	983.4640	966.4613	966.4612	0.0001	11.35	[Thr+Phe+Ahp+Phe+diMeTyr+Val]Asp+BA	4.6
CP-Phe ²	CP 997	997.4797	980.4770	980.4766	0.0004	11.08	[Thr+Phe+Ahp+Phe+MeTyr+Val]Asp+HA	1.1
CP-Phe ²	CP 1011	1011.4953	994.4926	994.4933	0.0007	12.64	[Thr+Phe+Ahp+Phe+diMeTyr+Val]Asp+HA	0.3
CP-Phe ²	CP 1025b	1025.5110	1008.5083	1998.51			[Thr+Phe+Ahp+Phe+MeTyr+Val]Asp+OA	
CP-Trp ²	CP 992d	992.4644	975.4616	975.4594	0.0022	11.88	[Thr+Trp+Ahp+Phe+MePhe+Val]Asp+BA	
CP-Trp ²	CP 1036c	1036.4906	1019.4878	1019.49			[Thr+Trp+Ahp+Phe+MeTyr+Val]Asp+HA	
CP-Trp ²	CP 1050	1050.5062	1033.5035	1033.50			[Thr+Trp+Ahp+Phe+diMeTyr+Val]Asp+HA	
CP-Tyr ²	CP 929	929.4171	912.4144	912.4266	0.0122	4.84	[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Asp	
CP-Tyr ²	CP 941	941.4171	924.4144	924.4140	0.0004	9.68	[Thr+Tyr+Ahp+Phe+MePhe+Val]Asp+Ac	3.4
CP-Tyr ²	CP 957	957.4120	940.4093	940.4080	0.0013	7.63	[Thr+Tyr+Ahp+Phe+MeTyr+Val]Asp+Ac	0.6
CP-Tyr ²	CP 965	965.4746	948.4719	948.4693	0.0026	2.56	[Thr+Tyr+Ahp+Leu+diMeTyr+Val]Asp+BA	
CP-Tyr ²	CP 969	969.4484	952.4457	952.4449	0.0008	10.60	[Thr+Tyr+Ahp+Phe+MePhe+Val]Asp+BA	1.6 [8]
CP-Tyr ²	CP 971	971.4277	954.4249	954.4252	0.0003	9.44	[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Asp+Ac	0.7
CP-Tyr ²	CP 983b	983.4640	966.4613	966.46			[Thr+Tyr+Ahp+Phe+MePhe+Leu]Asp+BA	
CP-Tyr ²	CP 983c	983.4640	966.4613	966.46			[Thr+Tyr+Ahp+Phe+MePhe+Val]Glu+BA	
CP-Tyr ²	CP 985	985.4433	968.4406	968.4396	0.0010	8.65	[Thr+Tyr+Ahp+Phe+MeTyr+Val]Asp+BA	3.1 [8]
CP-Tyr ²	CP 993	993.5059	976.5032	976.50			[Thr+Tyr+Ahp+Leu+diMeTyr+Val]Asp+HA	
CP-Tyr ²	CP 997b	997.4797	980.4770	980.4764	0.0005	11.84	[Thr+Tyr+Ahp+Phe+MePhe+Val]Asp+HA	2.6
CP-Tyr ²	CP 999	999.4590	982.4562	982.4555	0.0007	10.36	[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Asp+BA	8.1 [8]
CP-Tyr ²	CP 999b	999.4590	982.4562	982.4537	0.0025	9.22	[Thr+Tyr+Ahp+Phe+MeTyr+Leu]Asp+BA	
CP-Tyr ²	CP 999c	999.4590	982.4562	982.46			[Thr+Tyr+Ahp+Phe+MeTyr+Val]Glu+HA	
CP-Tyr ²	CP 1011b	1011.4953	994.4926	994.4917	0.0009	7.30	[Thr+Tyr+Ahp+Phe+MePhe+Leu]Asp+HA	
CP-Tyr ²	CP 1013b	1013.3746	996.3719	996.37			[Thr+Tyr+Ahp+Phe+diMeTyr+Leu]Asp+BA	
CP-Tyr ²	CP 1013	1013.4746	996.4719	996.4699	0.0020	10.04	[Thr+Tyr+Ahp+Phe+MeTyr+Val]Asp+HA	2.8 [8]
CP-Tyr ²	CP 1013c	1013.4746	996.4719	996.4702	0.0017	11.35	[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Glu+BA	
CP-Tyr ²	CP 1016	1016.0100	999.0072	999.0346	0.0274	12.72	[Thr+Tyr+Ahp+Phe+diMe,OTyr+Val]Asp+BA	

CP-Tyr ²	CP 1025	1025.5110	1008.5083	1008.5080	0.0002	13.24	[Thr+Tyr+Ahp+Phe+MePhe+Val]Asp+OA	0.2	[8]
CP-Tyr ²	CP 1027	1027.4903	1010.4875	1010.4869	0.0006	11.61	[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Asp+HA	1.3	
CP-Tyr ²	CP 1036b	1036.4906	1019.4878	1019.4445	0.0433	8.64	[Thr+Tyr+Ahp+Phe+MeTrp+Val]Asp+HA		
CP-Tyr ²	CP 1041	1041.5059	1024.5032	1024.5038	0.0006	11.53	[Thr+Tyr+Ahp+Phe+MeTyr+Val]Asp+OA		
CP-Tyr ²	CP 1053	1053.5423	1036.5396	1036.54			[Thr+Tyr+Ahp+Phe+MePhe+Val]Asp+DA		
CP-Tyr ²	CP 1055	1055.5216	1038.5188	1038.5183	0.0005	12.99	[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Asp+OA	1.4	
CP-Tyr ²	CP 1069	1069.5372	1052.5345	1052.5350	0.0005	13.09	[Thr+Tyr+Ahp+Phe+MeTyr+Val]Asp+DA		
CP-Tyr ²	CP 1083	1083.5529	1066.5501	1066.5454	0.0047	8.47	[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Asp+DA		
CP-Tyr ²	CP 1097	1097.5685	1080.5658	1082.57			[Thr+Tyr+Ahp+Phe+diMeTyr+Val]Glu+DA		

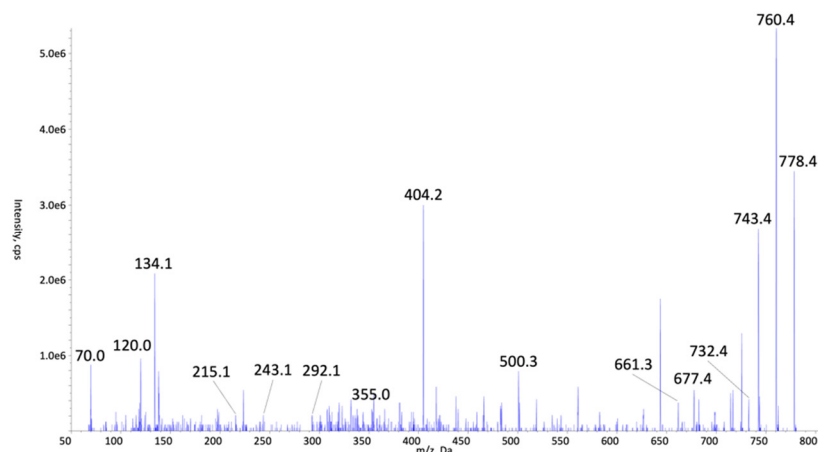
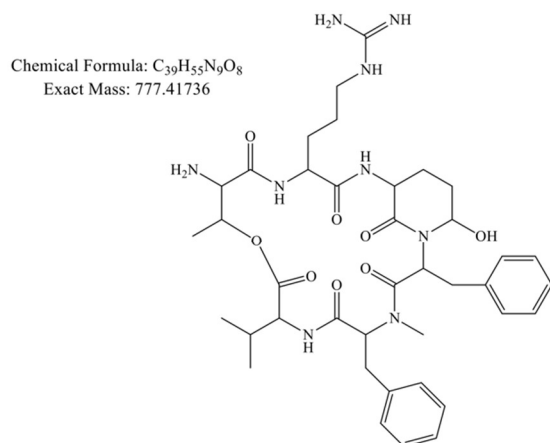


Figure S1. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 777.

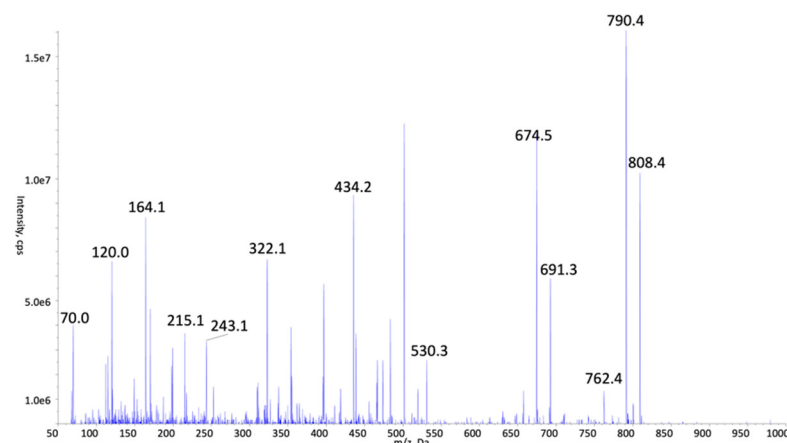
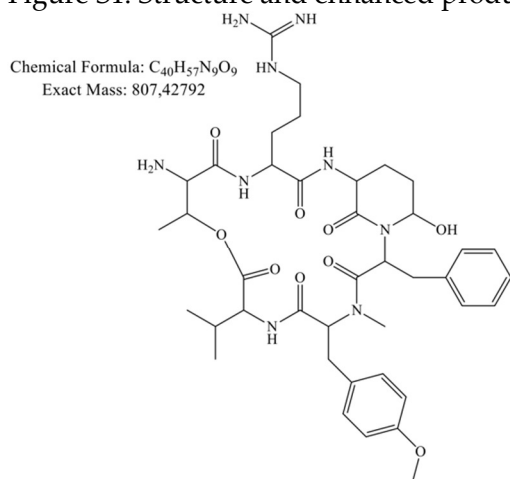


Figure S2. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 807.

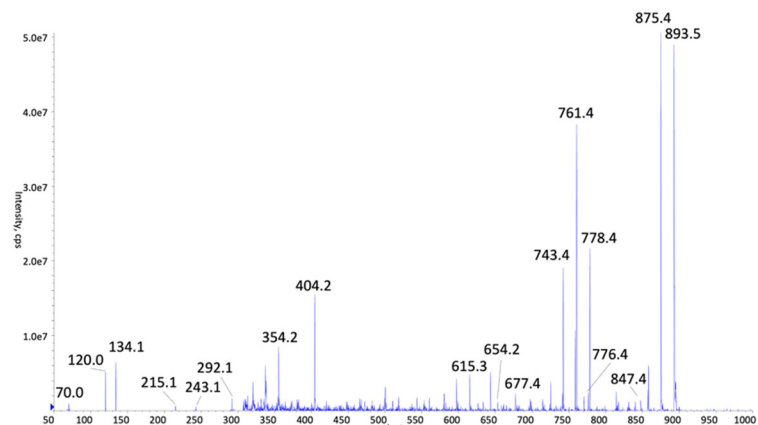
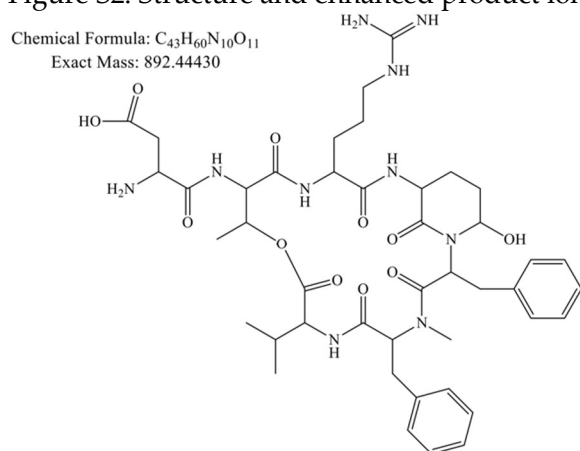


Figure S3. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 892.

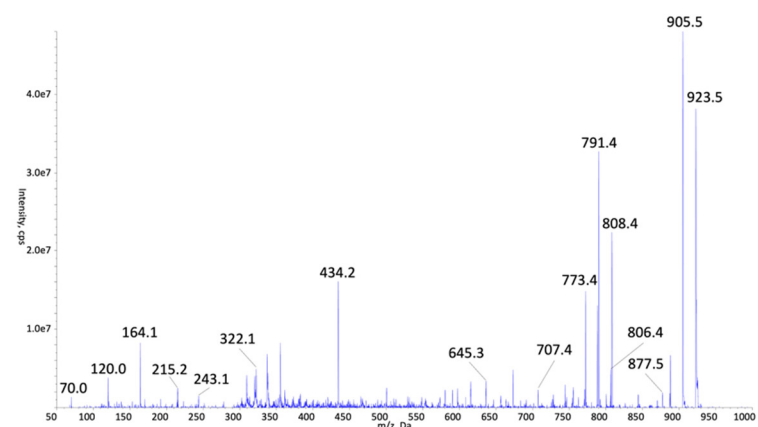
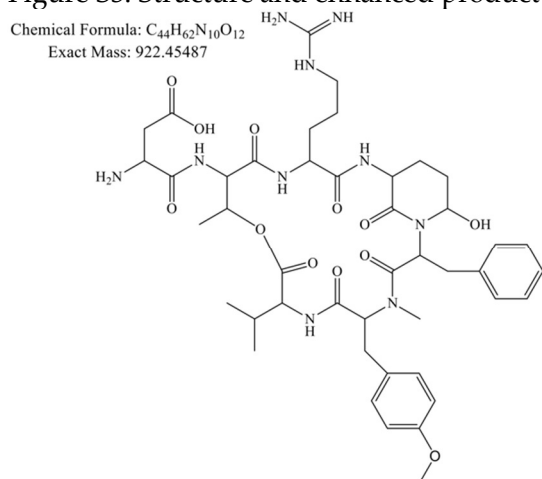


Figure S4. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 922.

Chemical Formula: $C_{46}H_{63}N_9O_{12}$
Molecular Weight: 934.04552

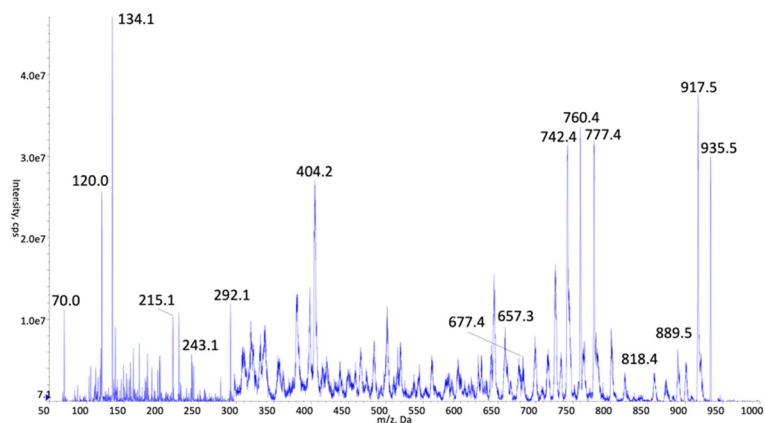
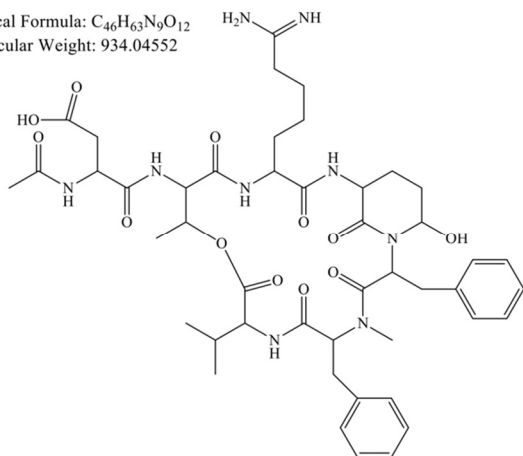


Figure S5. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 934.

Chemical Formula: $C_{44}H_{68}N_{10}O_{13}$
Exact Mass: 944.49673

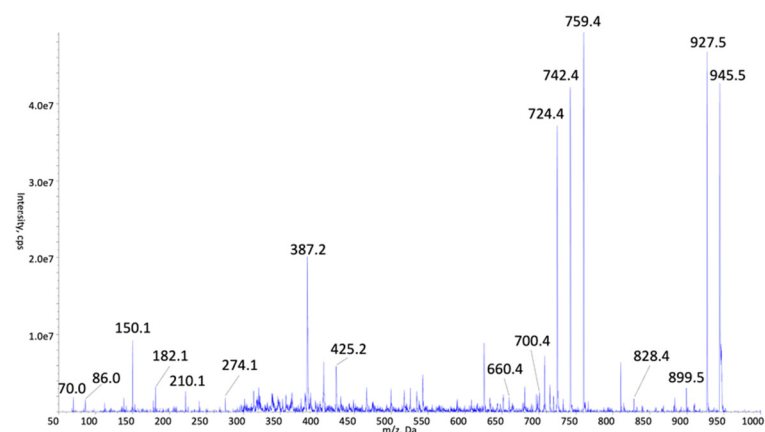
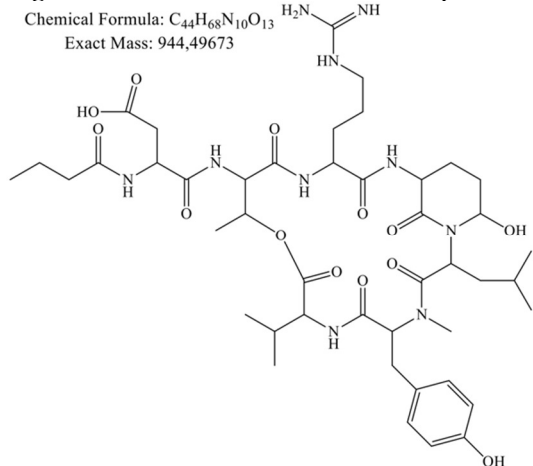


Figure S6. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 944.

Chemical Formula: $C_{45}H_{62}N_{10}O_{13}$
Exact Mass: 950.44978

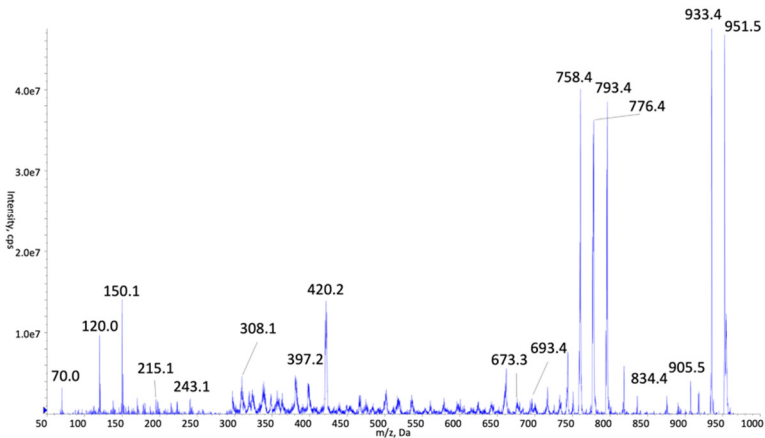
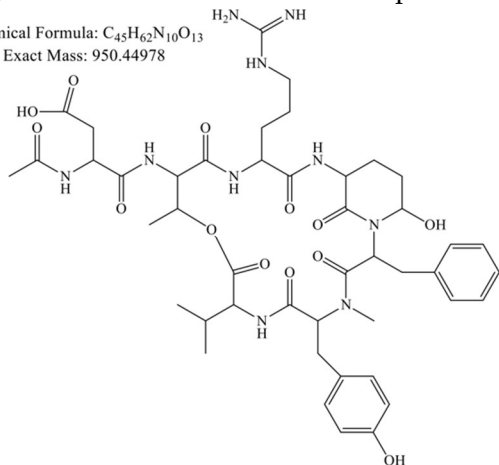


Figure S7. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 950.

Chemical Formula: $C_{47}H_{66}N_{10}O_{12}$
Exact Mass: 962.48617

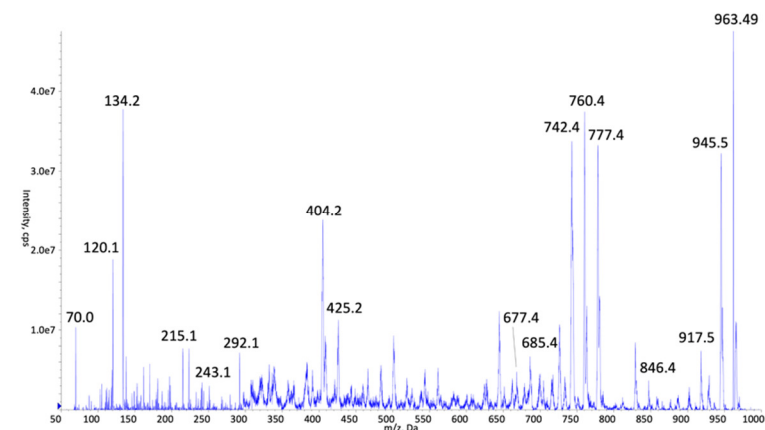
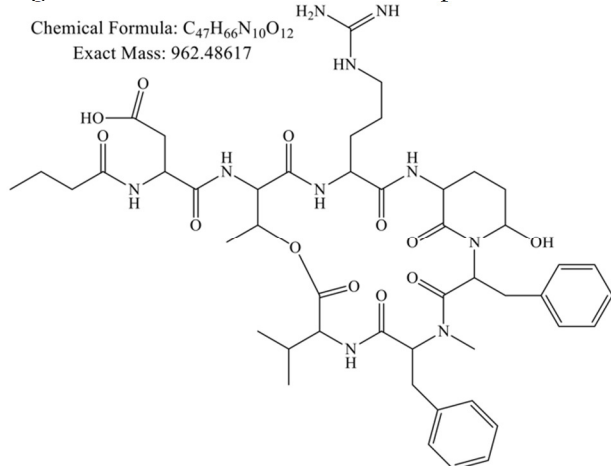


Figure S8. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 962 [8].

Chemical Formula: $C_{46}H_{64}N_{10}O_{13}$
Exact Mass: 964.46543

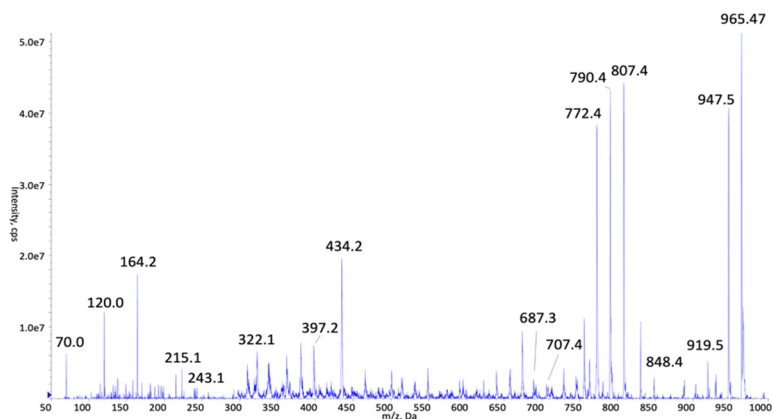
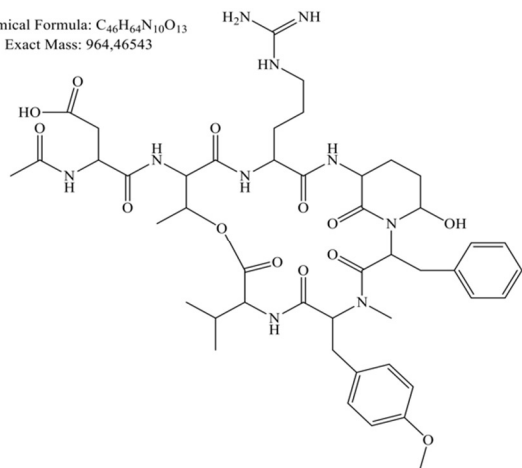


Figure S9. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 964.

Chemical Formula: $C_{48}H_{68}N_{10}O_{12}$
Exact Mass: 976.50182

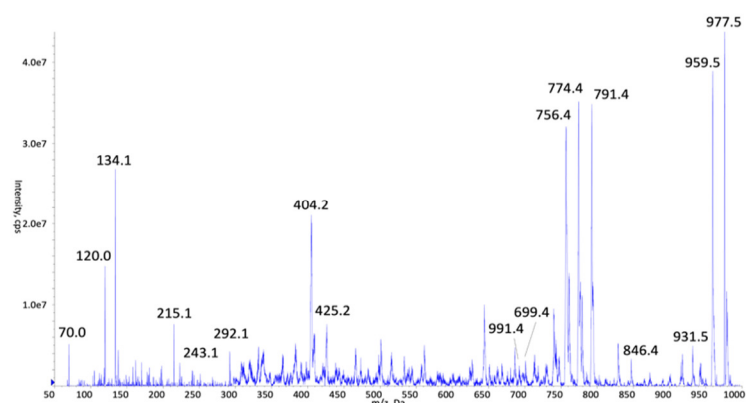
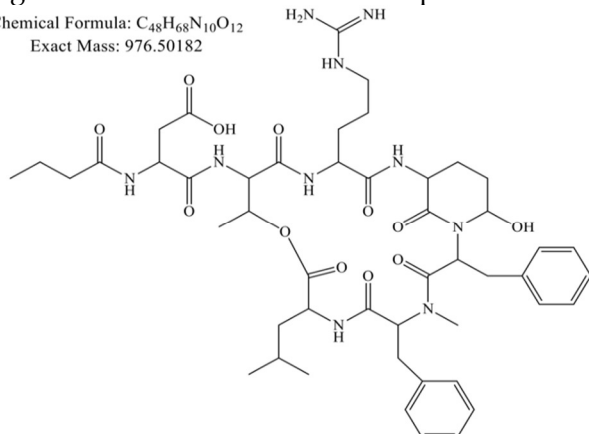


Figure S10. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 976.

Chemical Formula: $C_{47}H_{66}N_{10}O_{13}$
Exact Mass: 978.48108

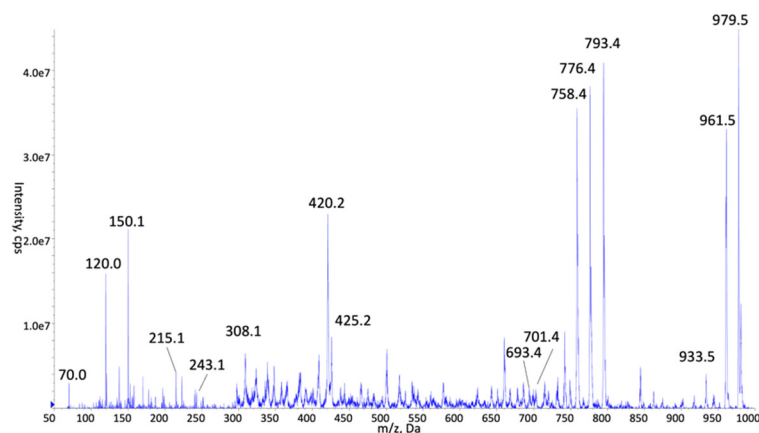
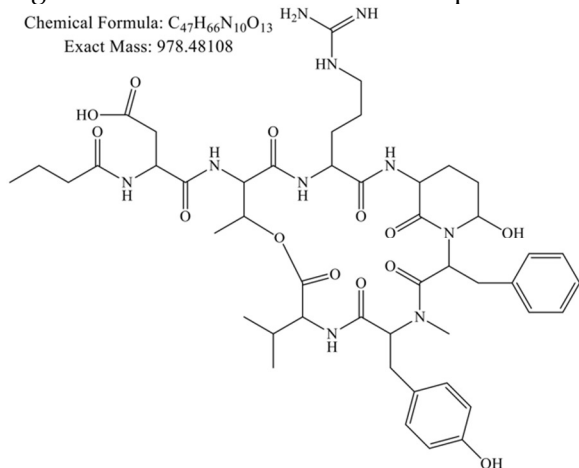


Figure S11. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 978 [8].

Chemical Formula: $C_{48}H_{68}N_{10}O_{13}$
Exact Mass: 992.49673

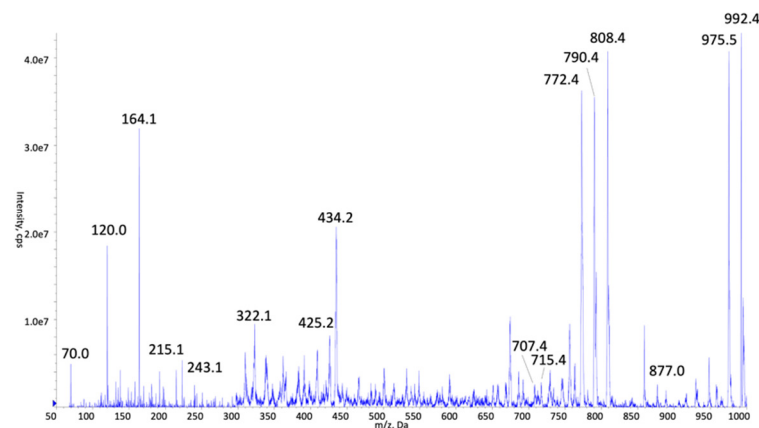
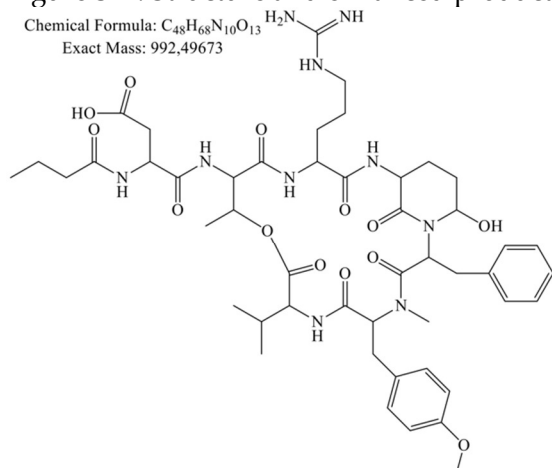


Figure S12. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 992 [8].

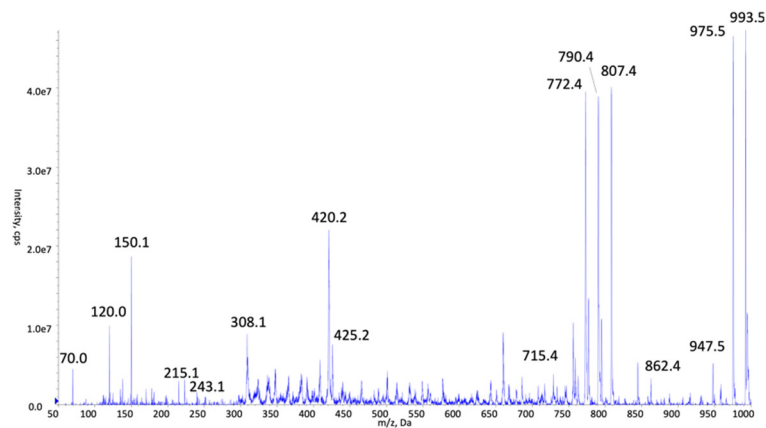
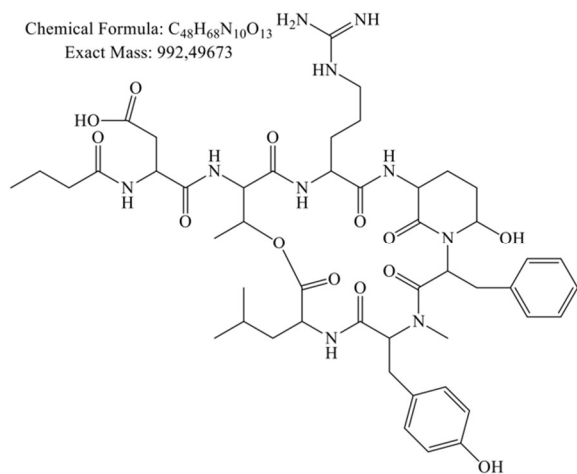


Figure S13. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 992b.

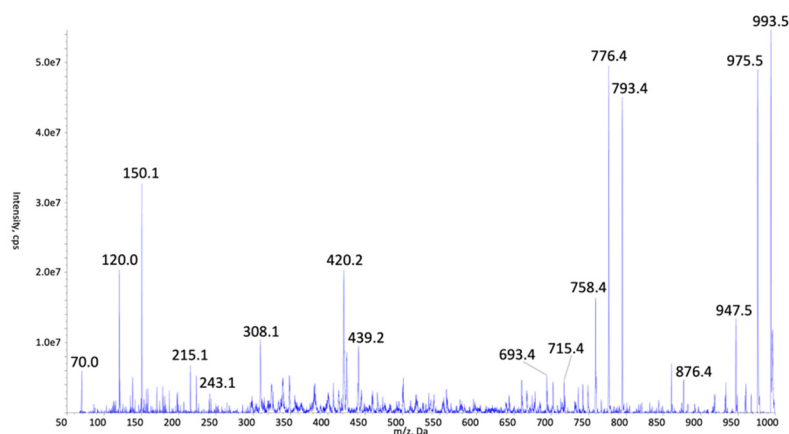
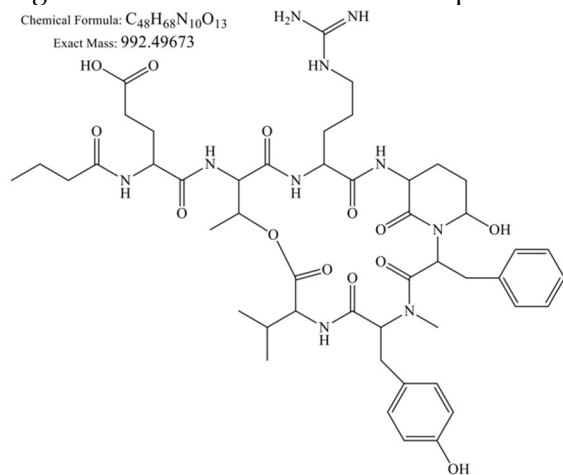


Figure S14. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 992c.

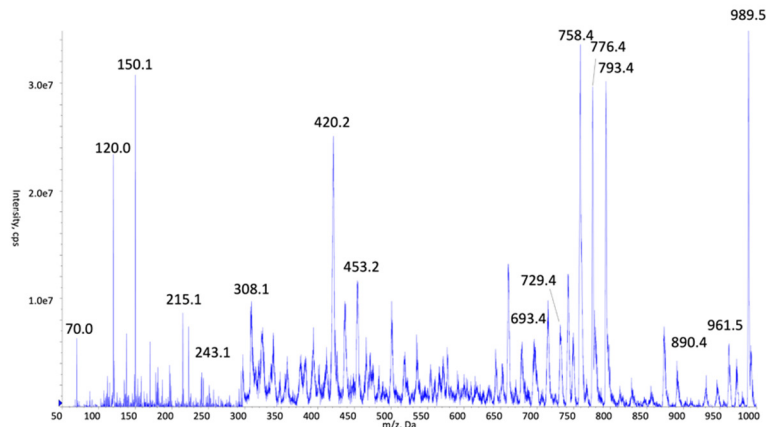
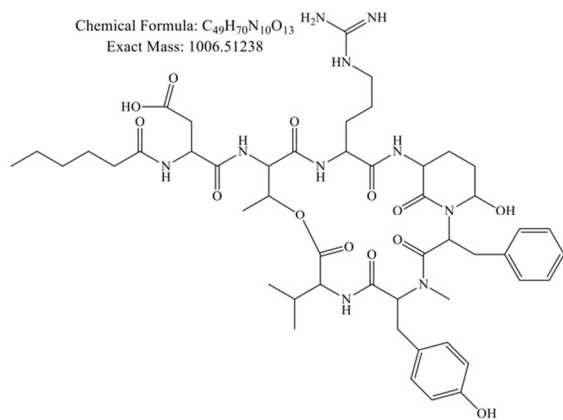


Figure S15. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1006[8].

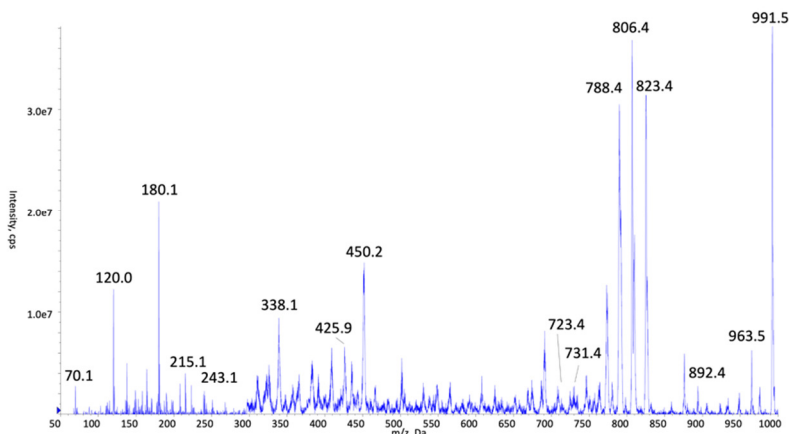
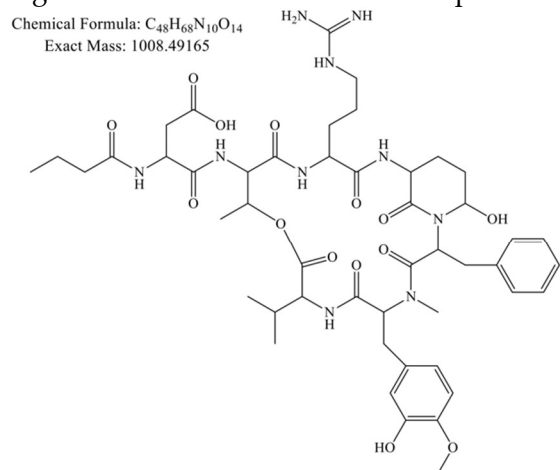


Figure S16. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1008.

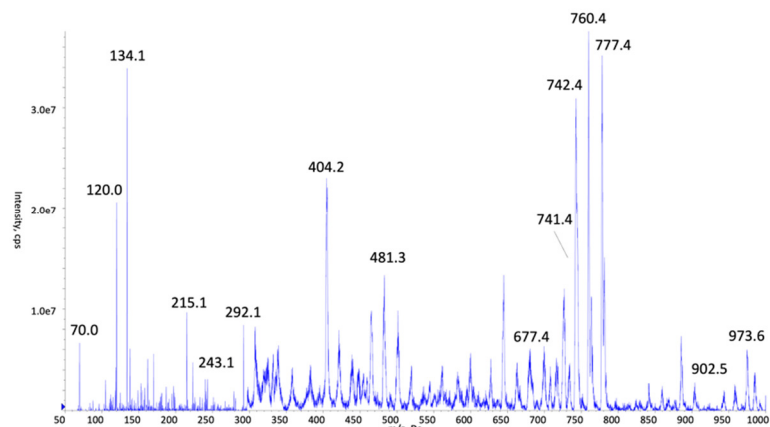
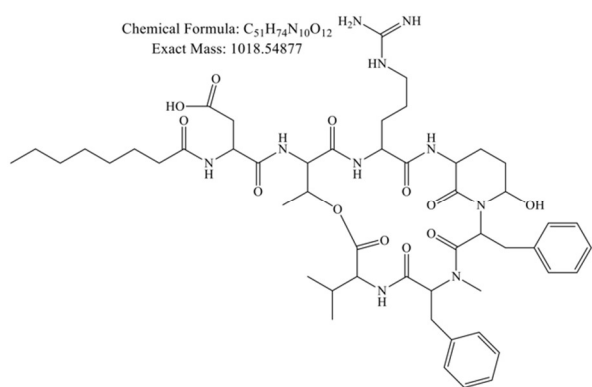


Figure S17. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1018 [8].

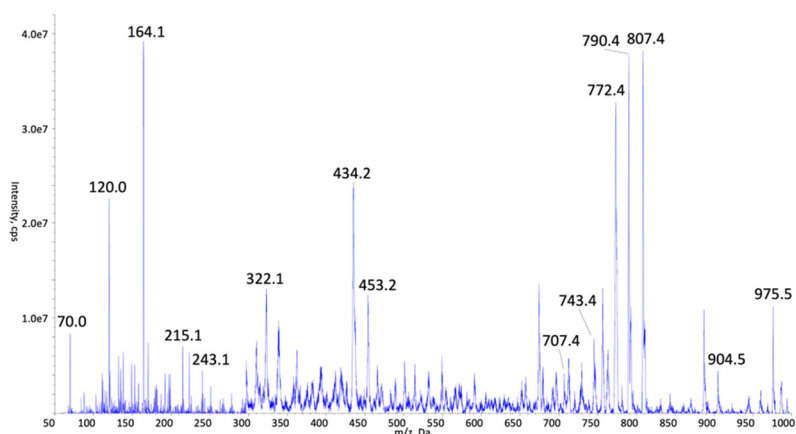
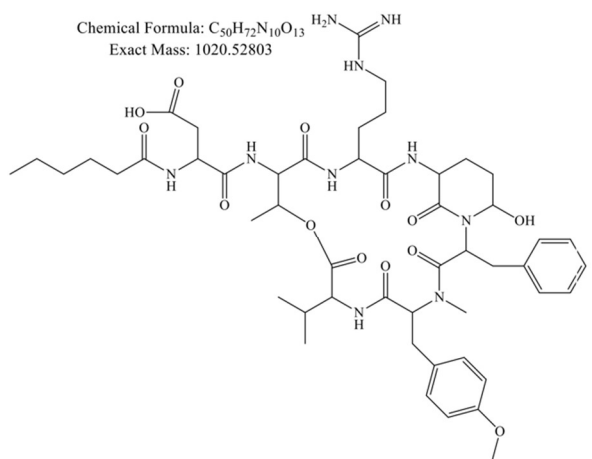


Figure S18. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1020b [8].

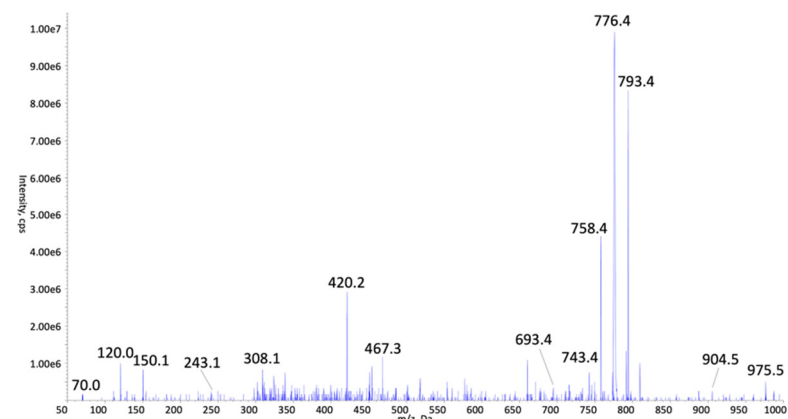
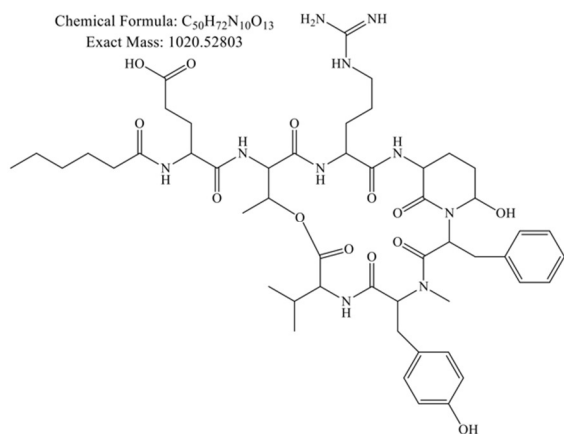


Figure S19. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1020.

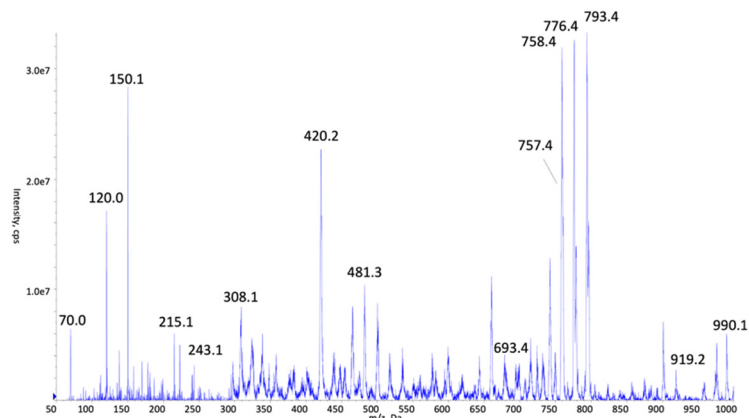
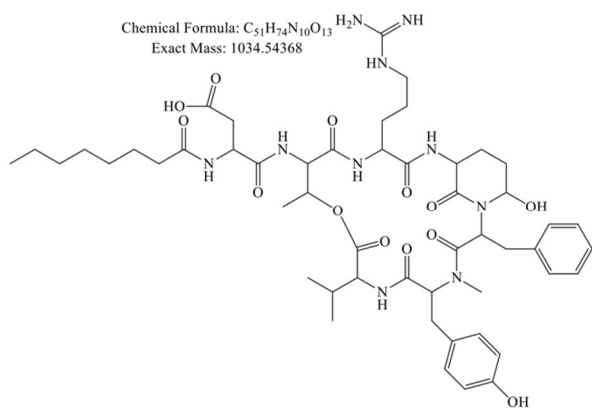


Figure S20. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1034.

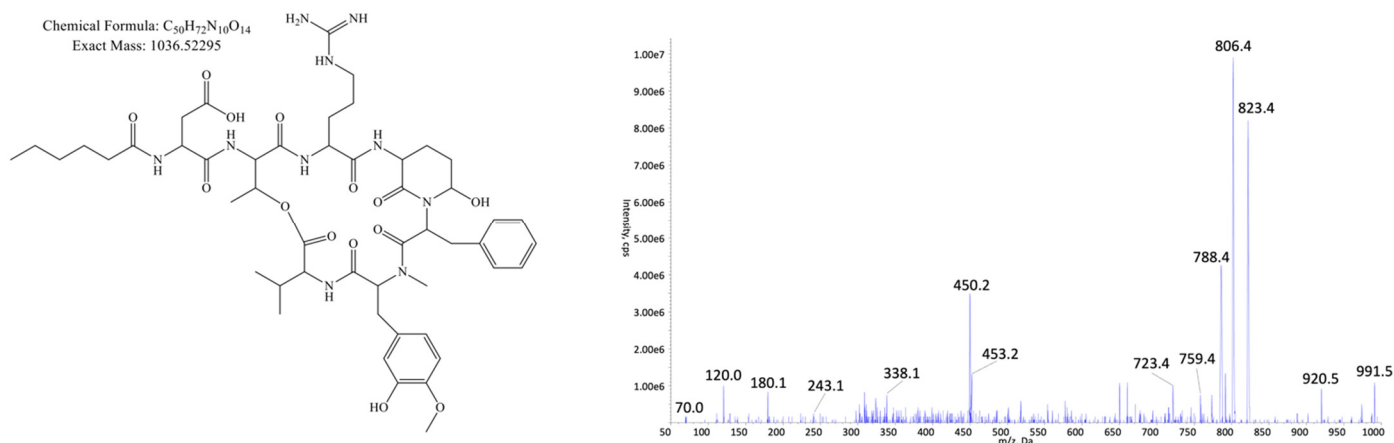


Figure S21. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1036.

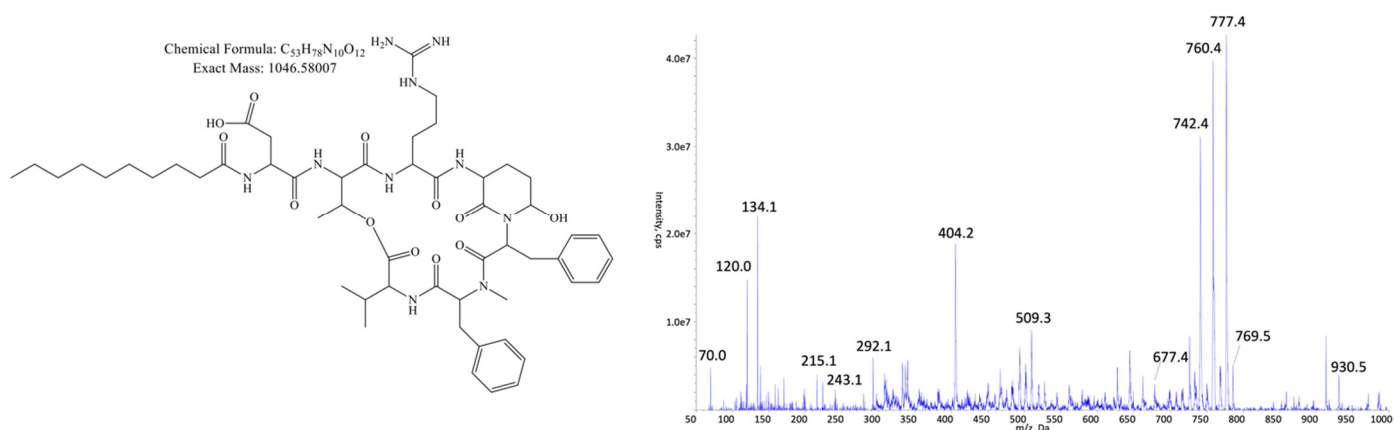


Figure S22. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1046.

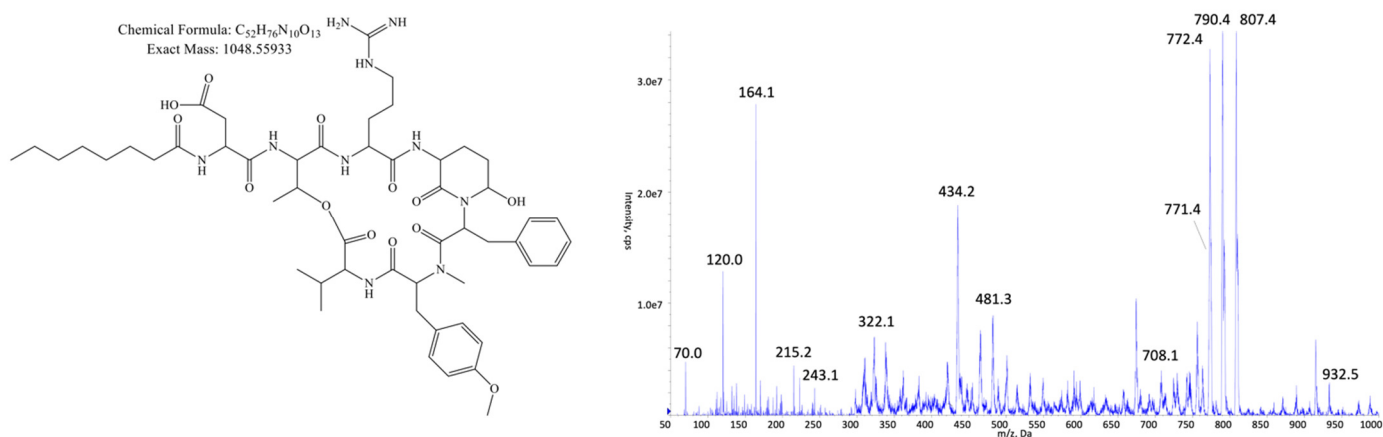


Figure S23. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1048 [8].

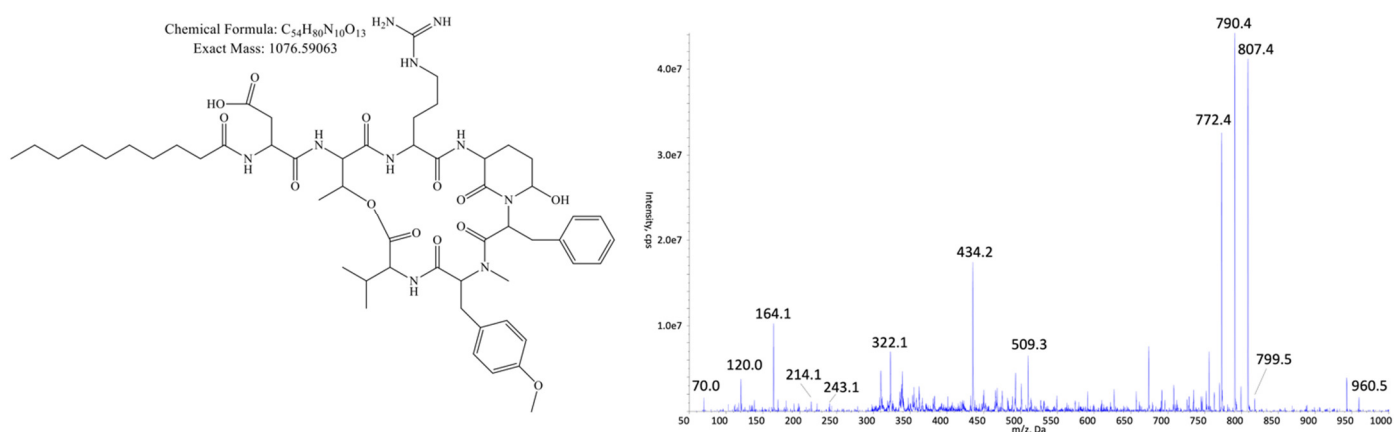


Figure S24. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1076.

Chemical Formula: $C_{45}H_{61}N_7O_{12}$
Exact Mass: 891.43782

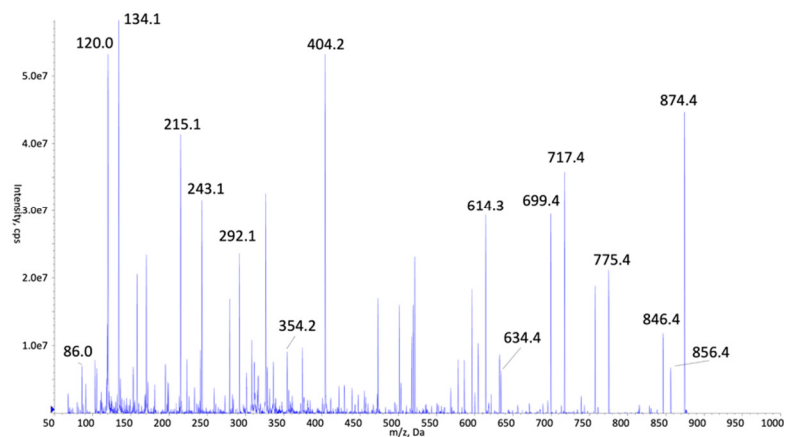
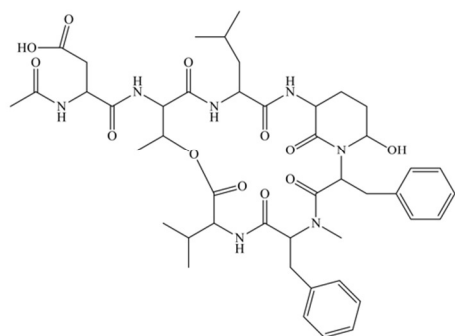


Figure S25. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 891.

Chemical Formula: $C_{45}H_{61}N_7O_{13}$
Exact Mass: 907.43274

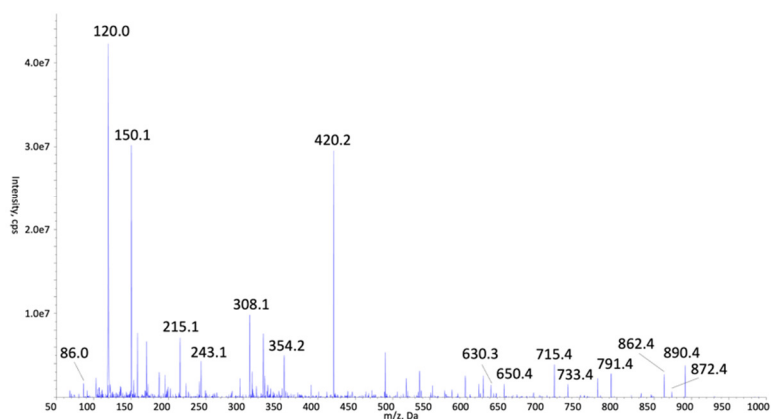
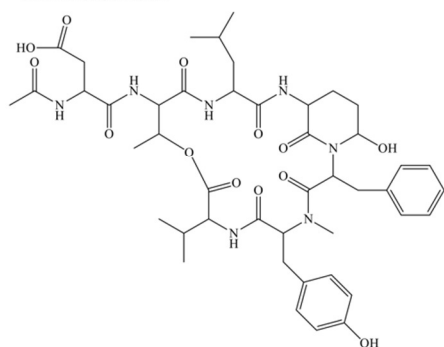


Figure S26. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 907.

Chemical Formula: $C_{46}H_{63}N_7O_{13}$
Exact Mass: 921.44839

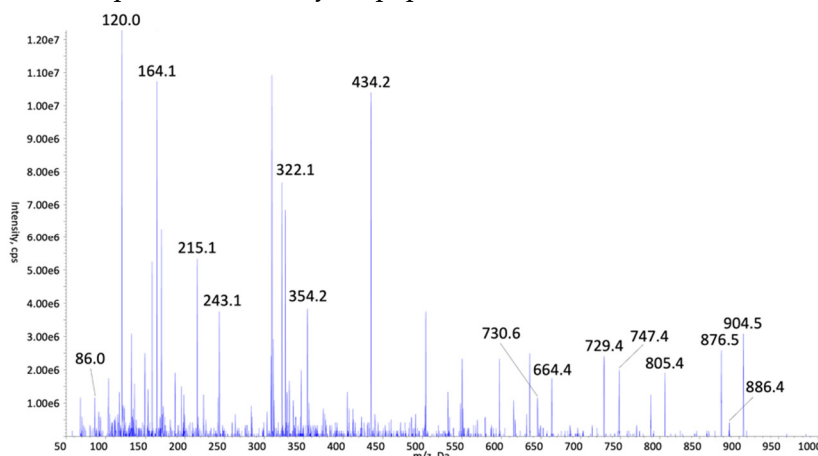
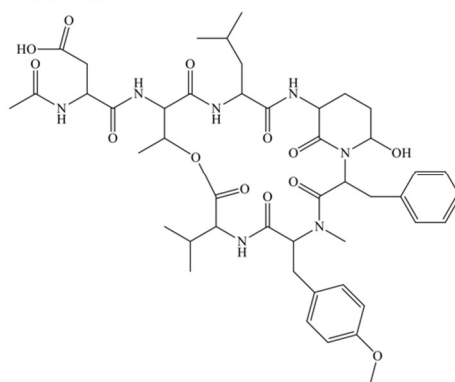


Figure S27. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 921.

Chemical Formula: $C_{48}H_{67}N_7O_{12}$
Exact Mass: 933.48477

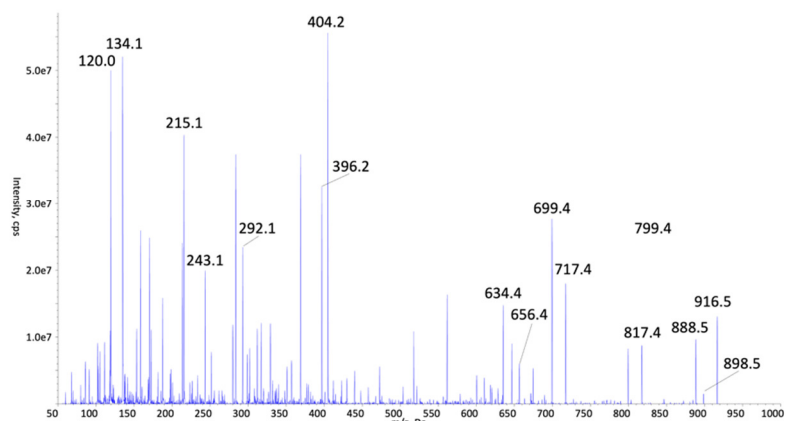
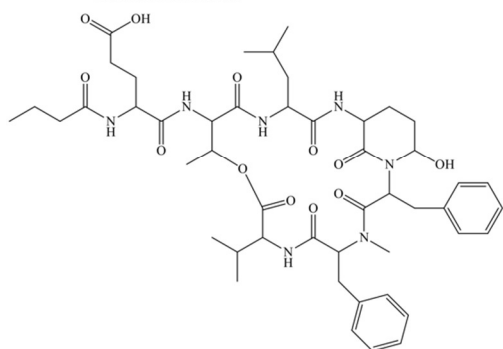


Figure S28. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 933.

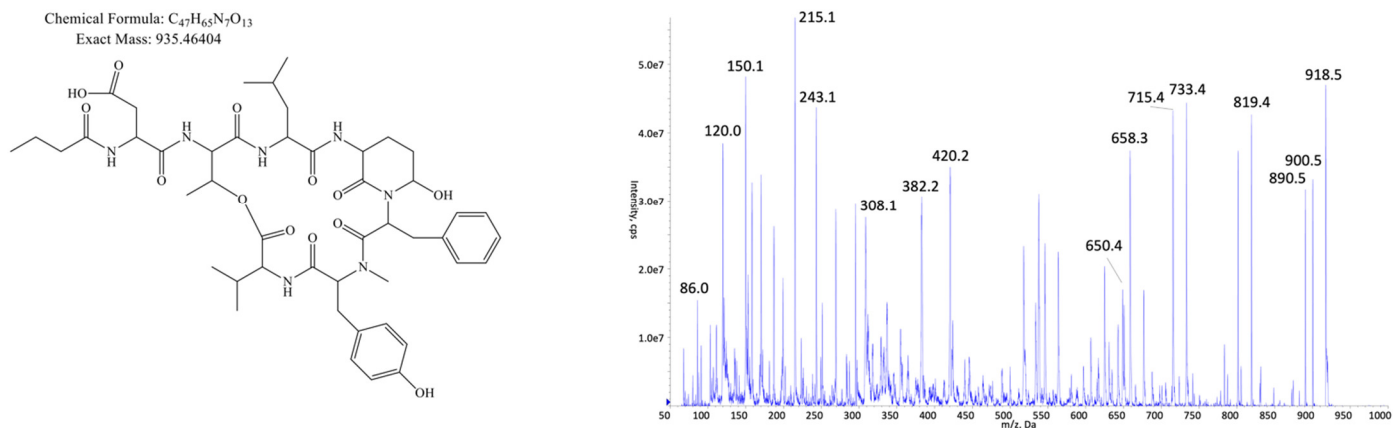


Figure S29. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 935.

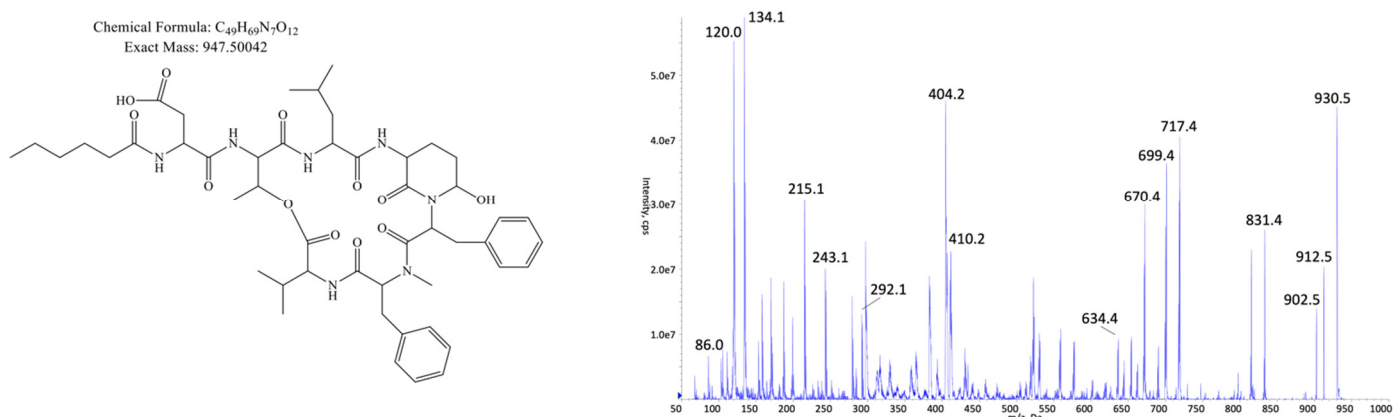


Figure S30. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 947.

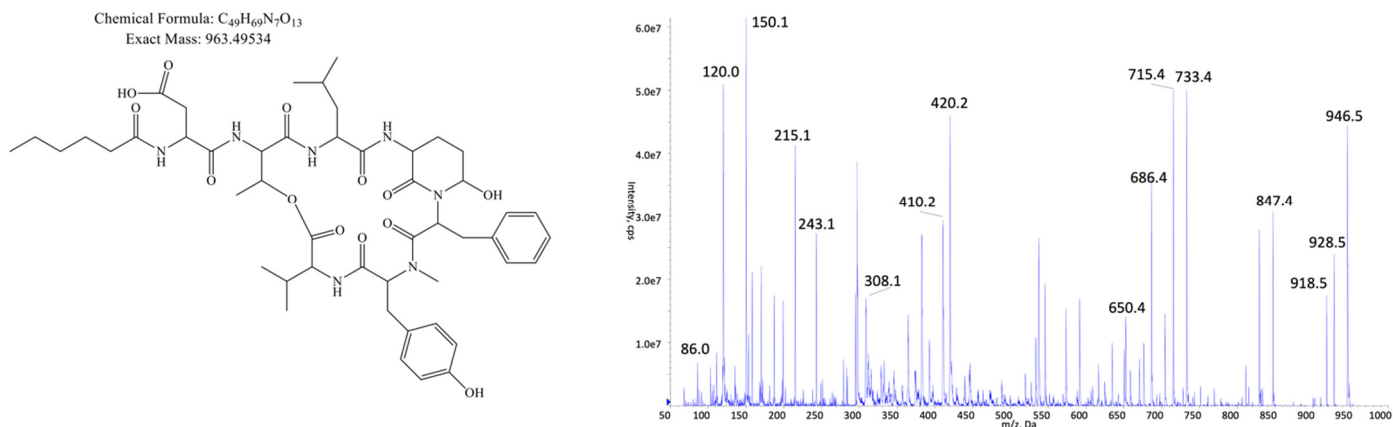


Figure S31. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 963.

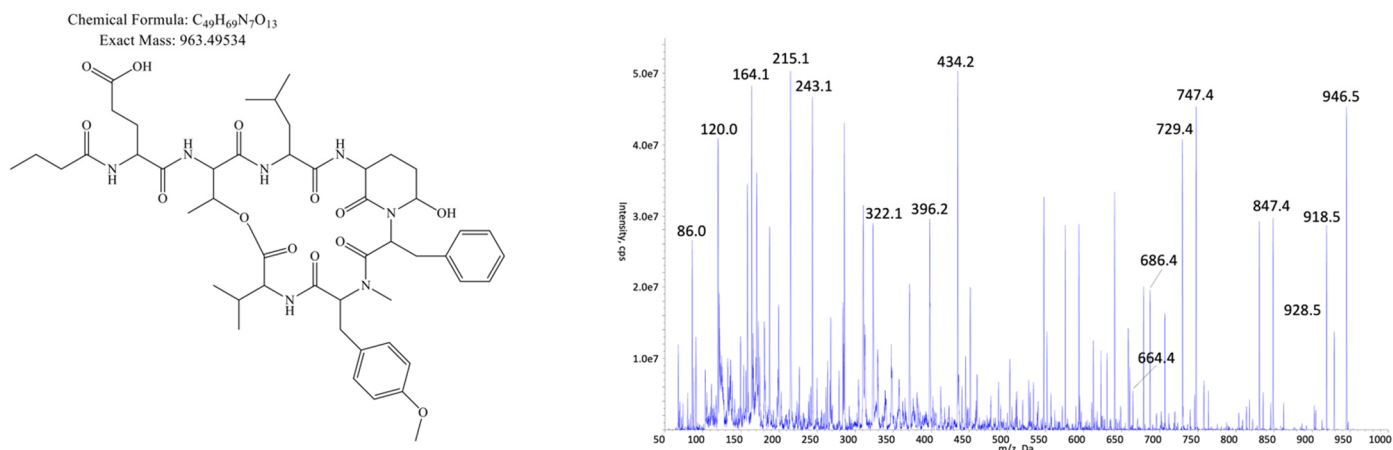


Figure S32. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 963b.

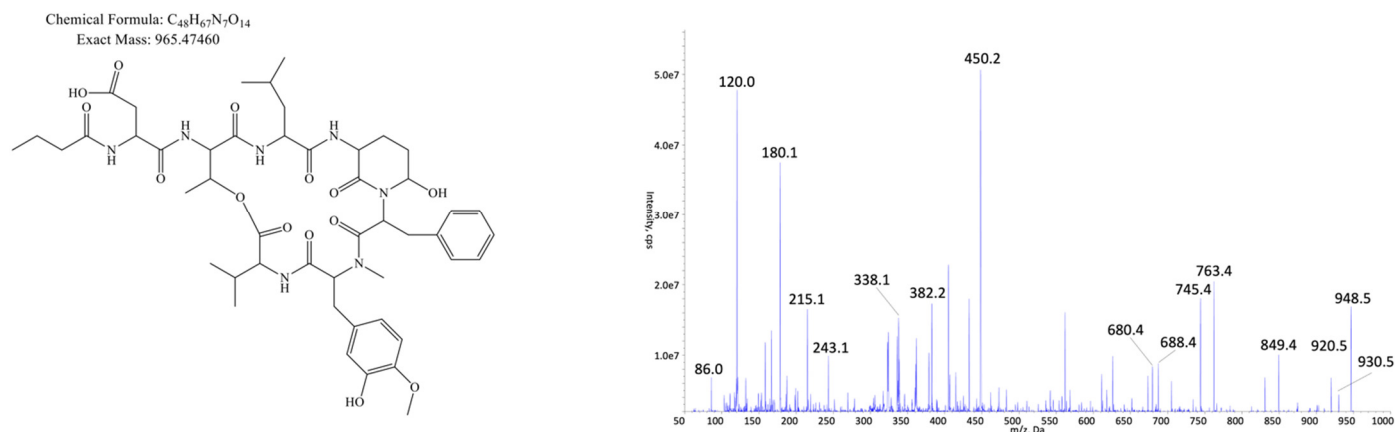


Figure S33. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 965b.

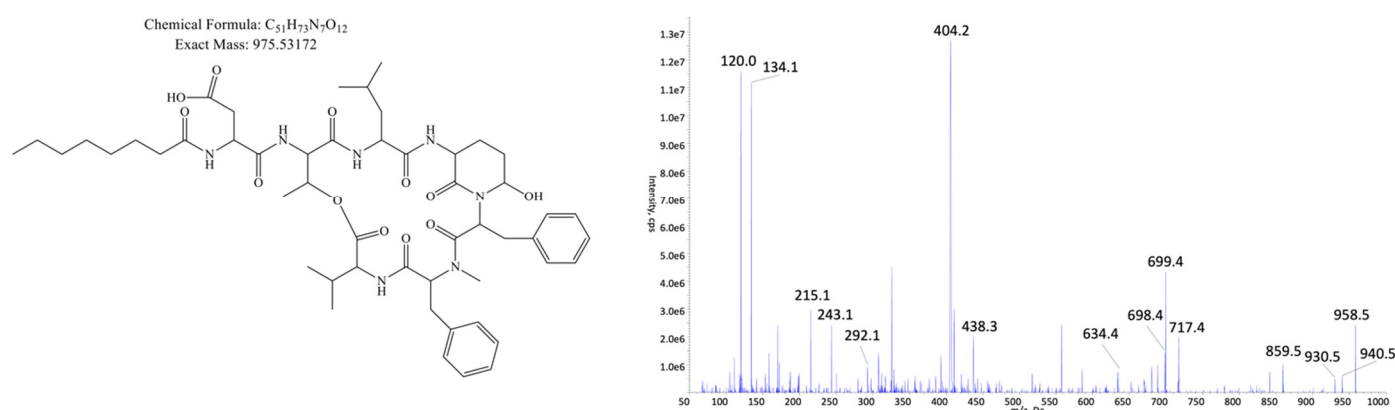


Figure S34. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 975.

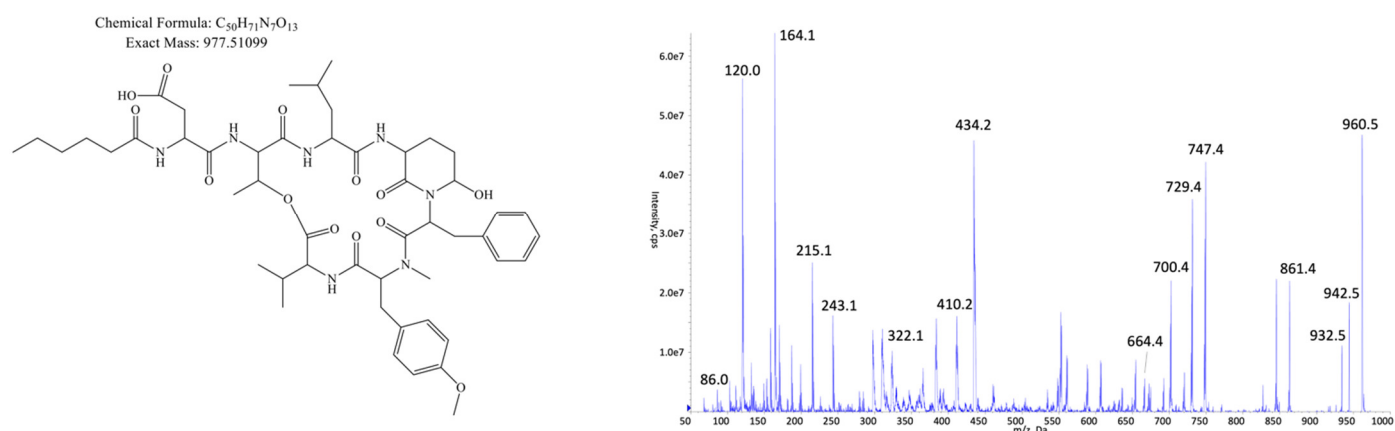


Figure S35. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 977.

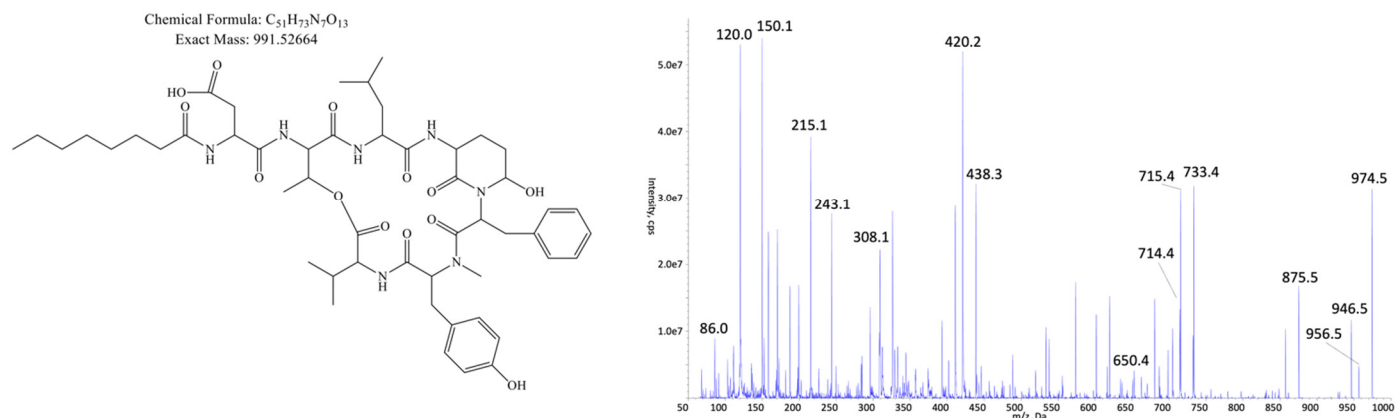


Figure S36. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 991.

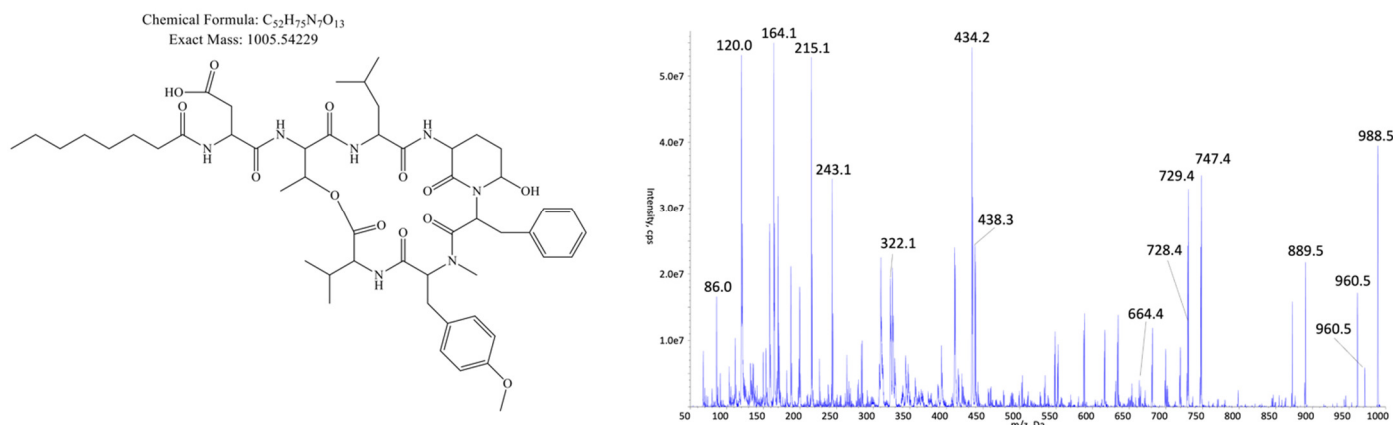


Figure S37. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1005.

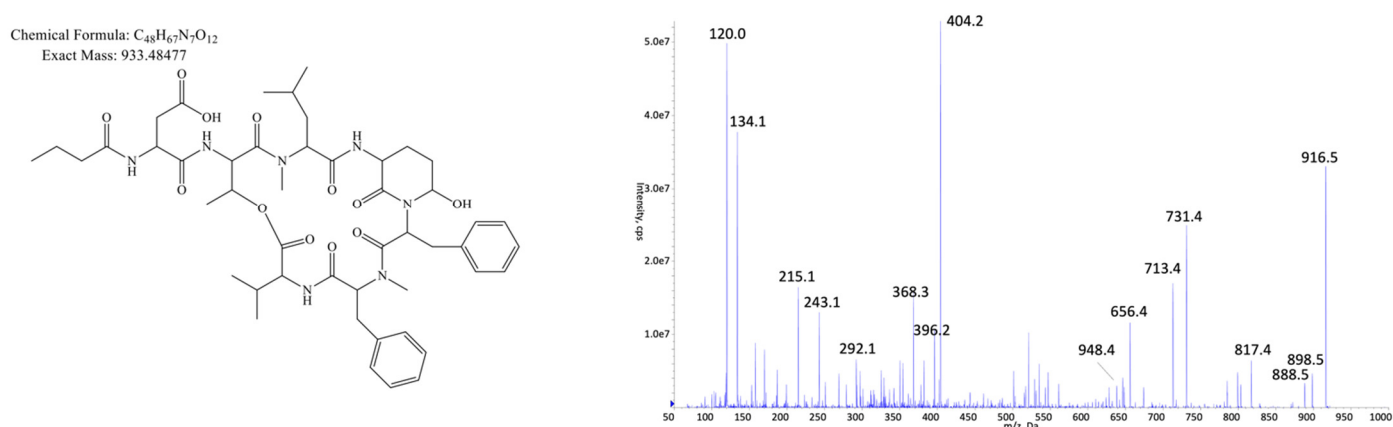


Figure S38. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 933b.

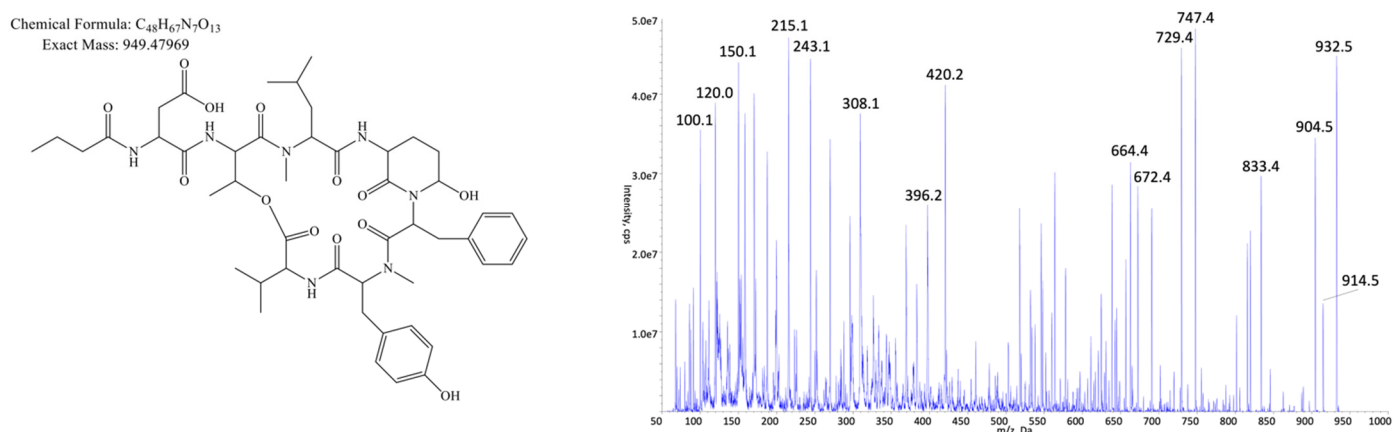


Figure S39. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 949b.

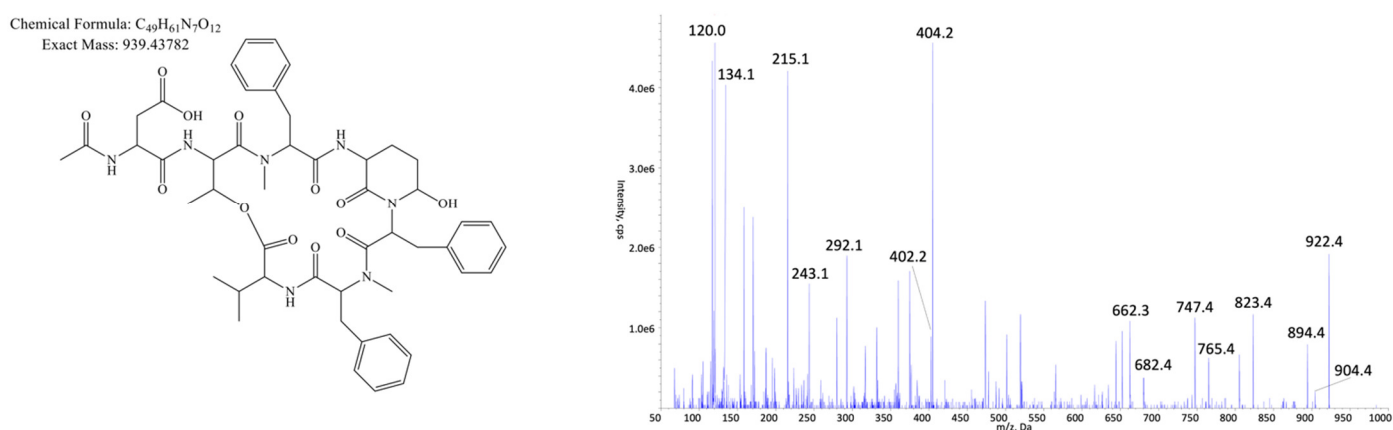


Figure S40. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 939b.

Chemical Formula: $C_{51}H_{65}N_7O_{12}$
Exact Mass: 967.46912

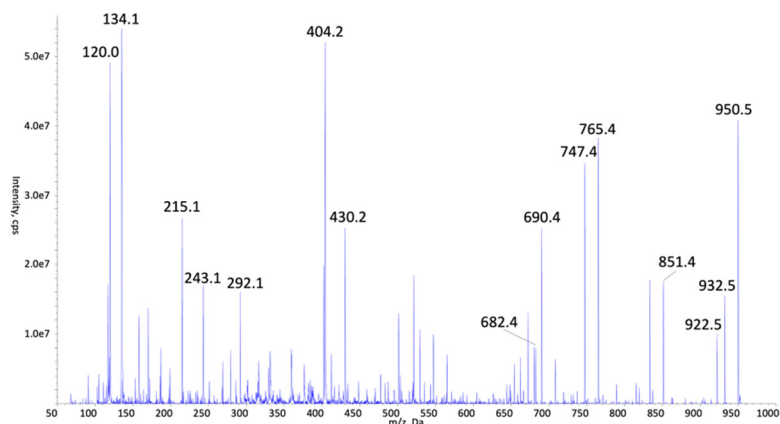
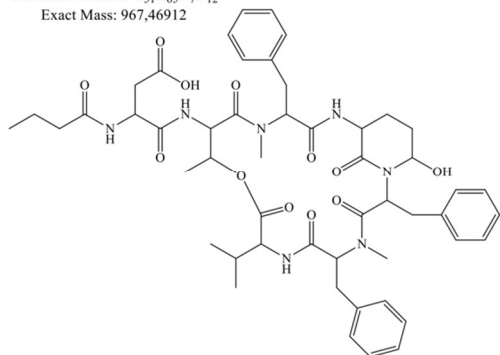


Figure S41. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 967b.

Chemical Formula: $C_{53}H_{69}N_7O_{13}$
Exact Mass: 1011.49534

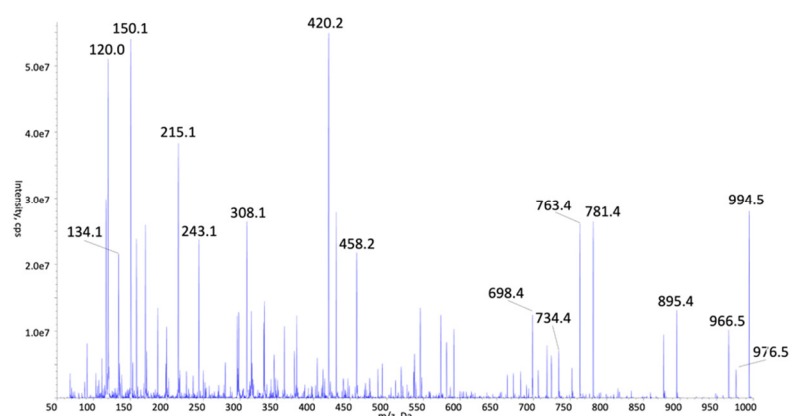
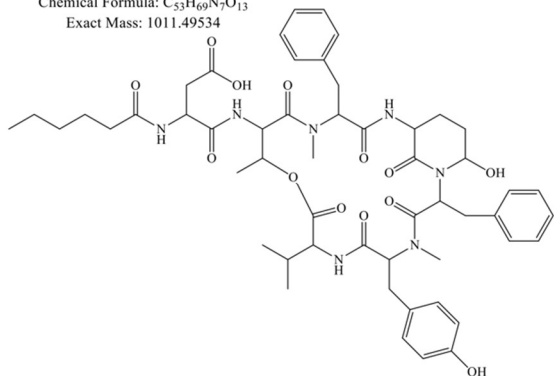


Figure S42. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1011c.

Chemical Formula: $C_{46}H_{63}N_7O_{12}S$
Exact Mass: 937.42554

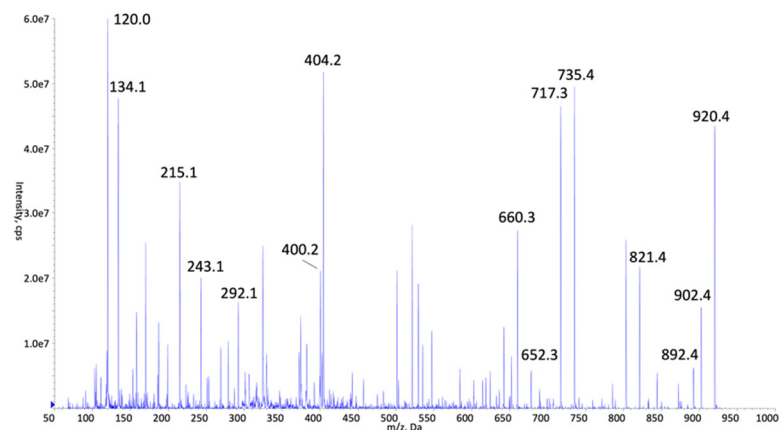
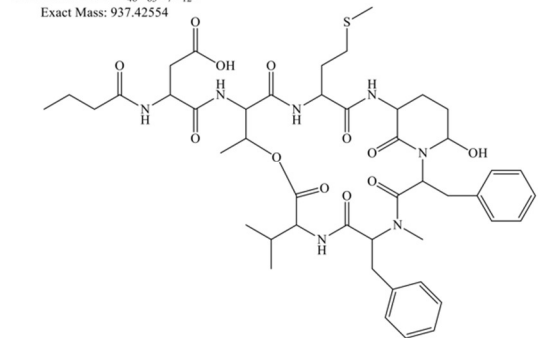


Figure S43. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 937.

Chemical Formula: $C_{45}H_{61}N_7O_{13}S$
Exact Mass: 939.40481

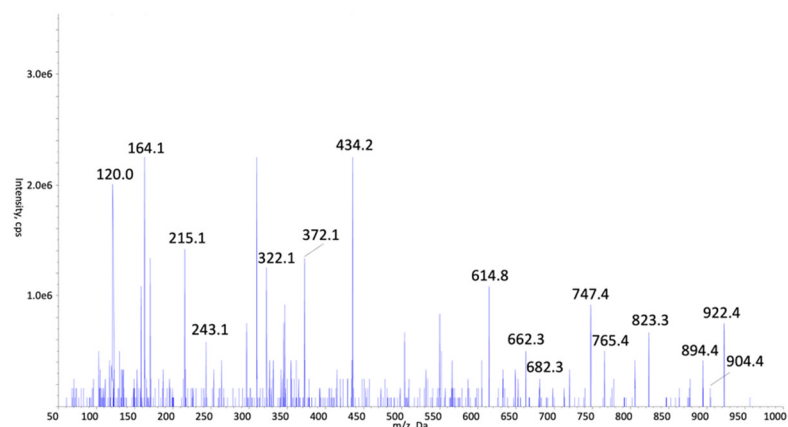
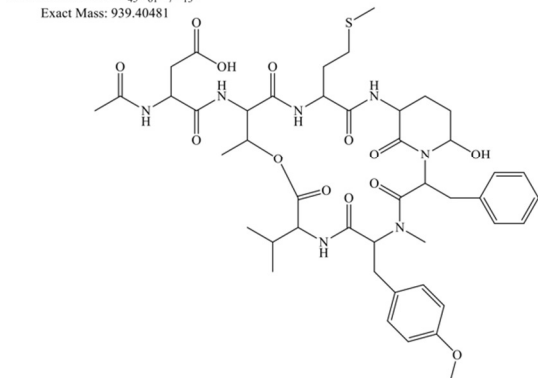


Figure S44. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 939.

Chemical Formula: $C_{48}H_{63}N_7O_{13}S$
Exact Mass: 953.42046

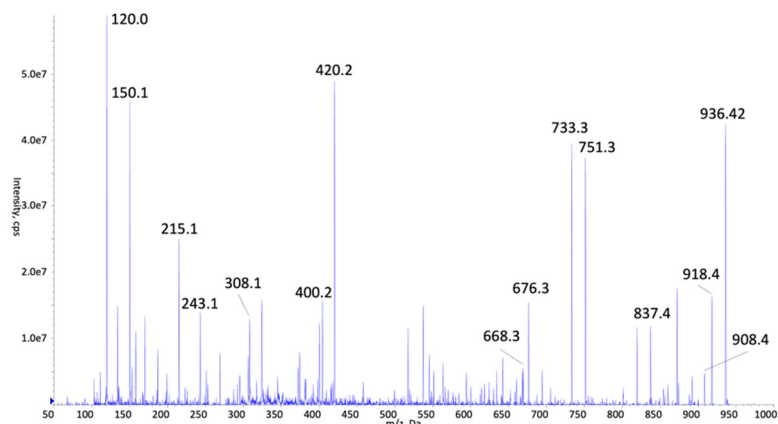
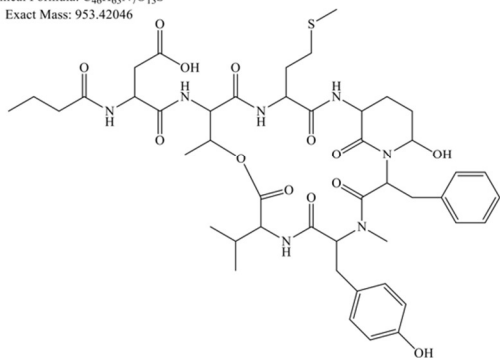


Figure S45. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 953b.

Chemical Formula: $C_{49}H_{69}N_7O_{13}S$
Exact Mass: 995.46741

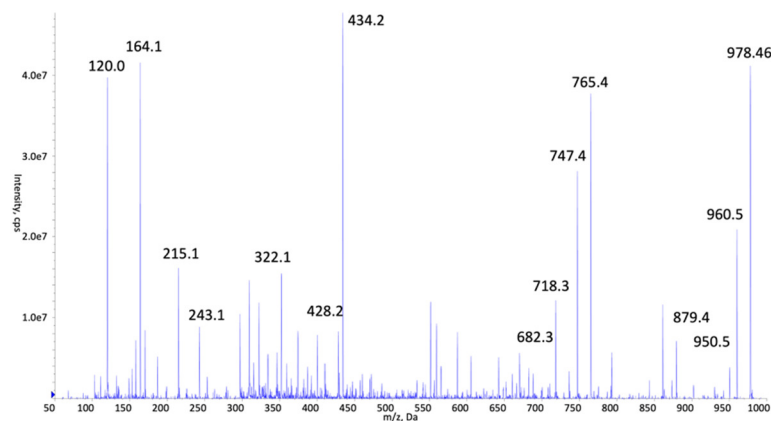
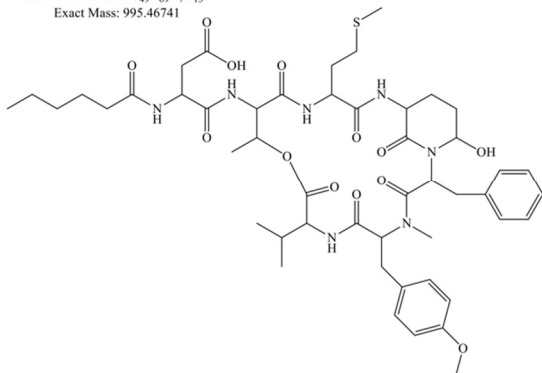


Figure S46. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 995.

Chemical Formula: $C_{51}H_{73}N_7O_{13}S$
Exact Mass: 1023.49871

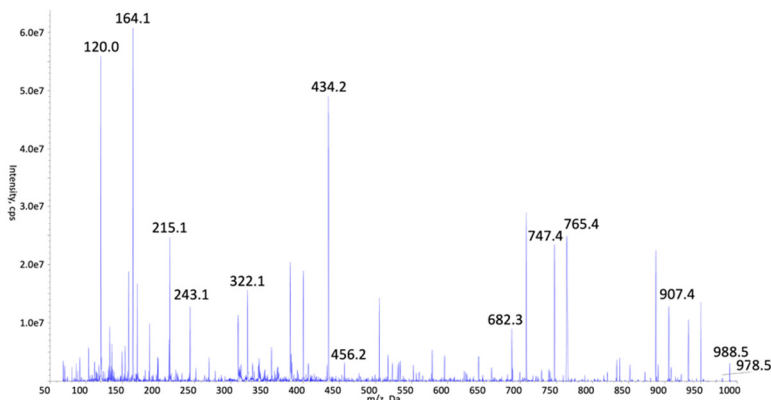
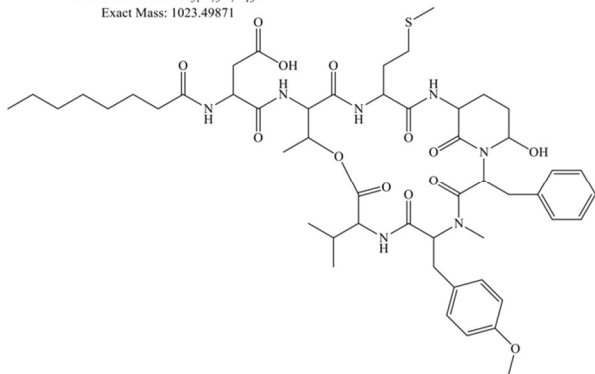


Figure S47. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1023.

Chemical Formula: $C_{51}H_{65}N_7O_{14}$
Exact Mass: 999.45895

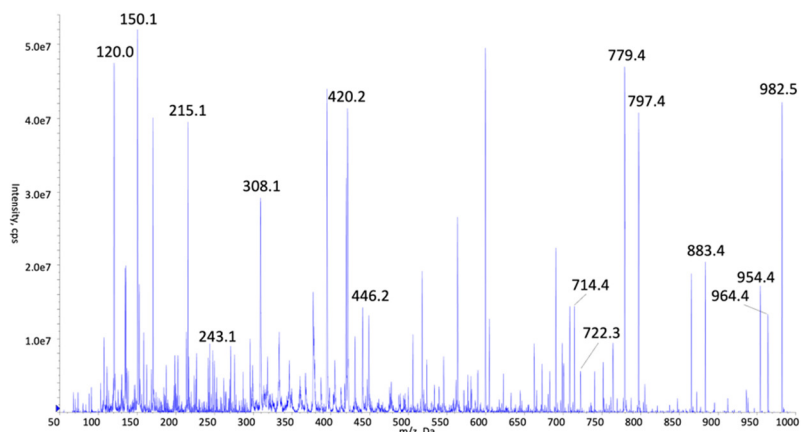
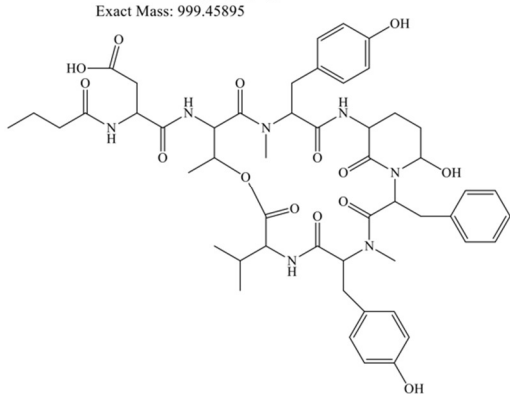


Figure S48. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 999d.

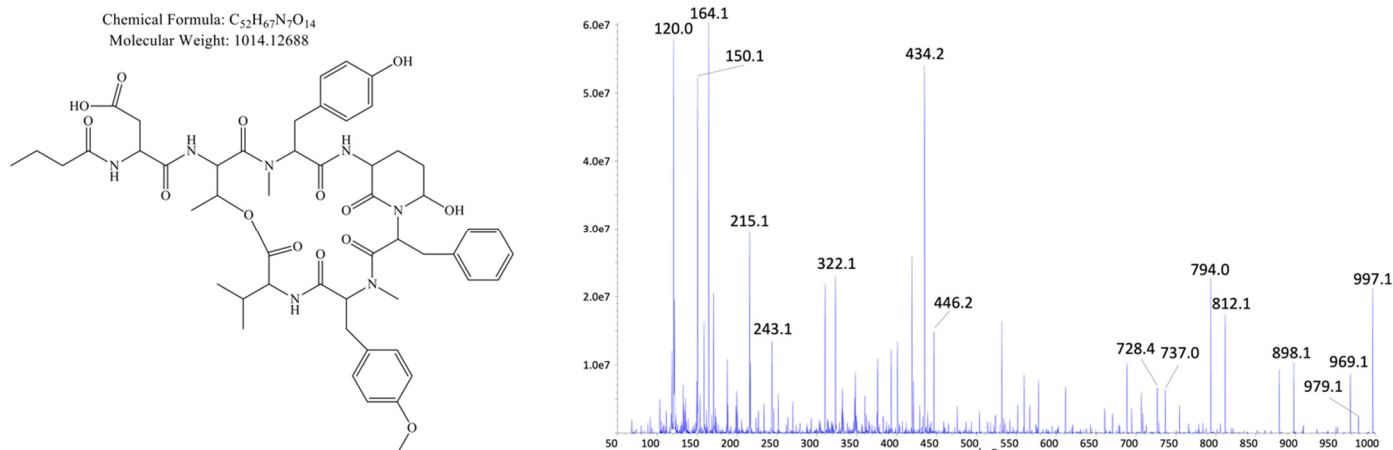


Figure S49. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1014.

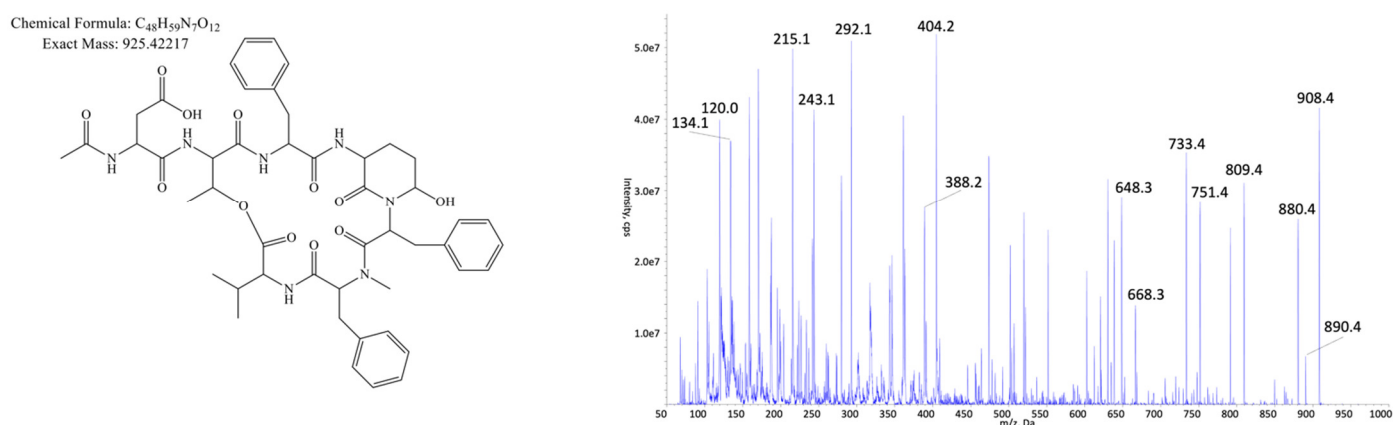


Figure S50. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 925.

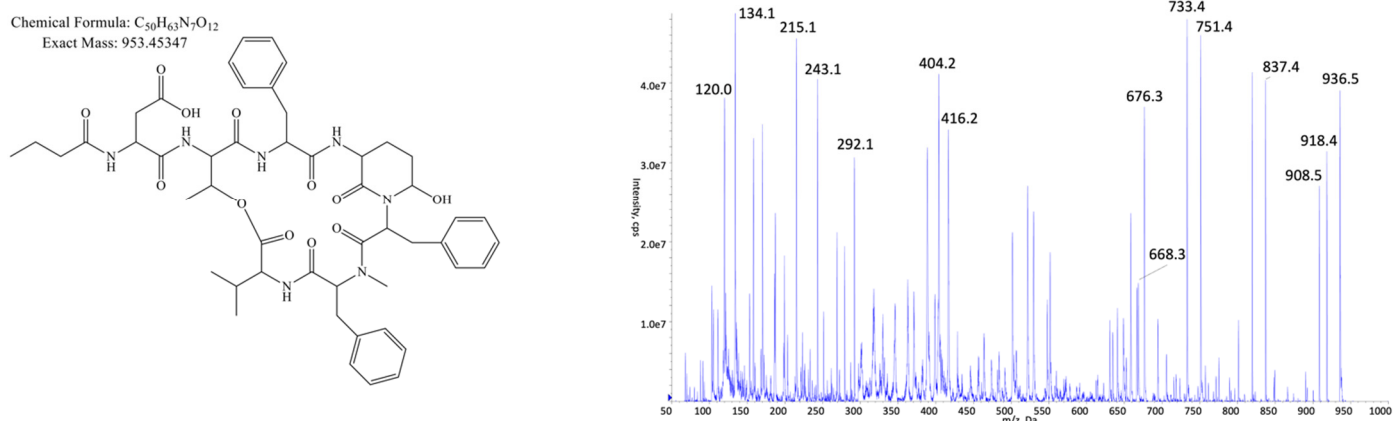


Figure S51. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 953.

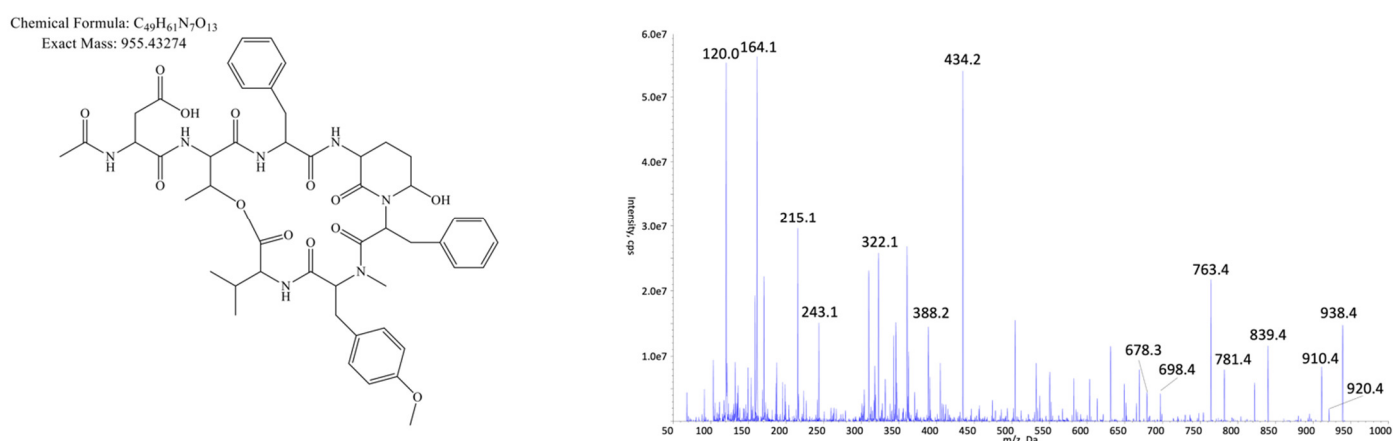


Figure S52. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 955.

Chemical Formula: $C_{51}H_{65}N_7O_{12}$
Exact Mass: 967.46912

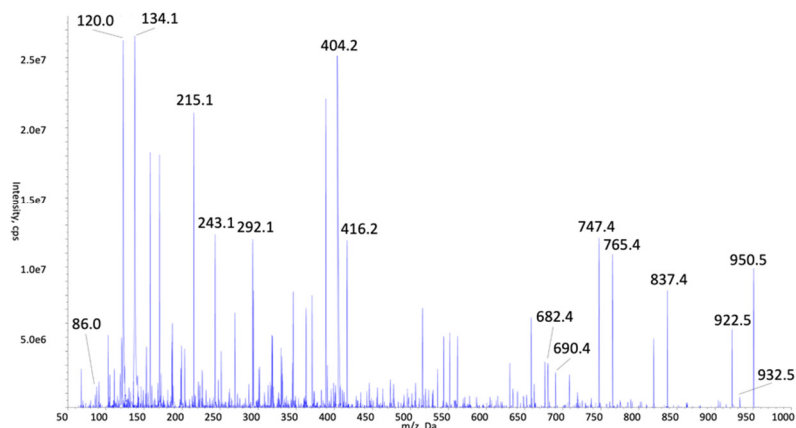
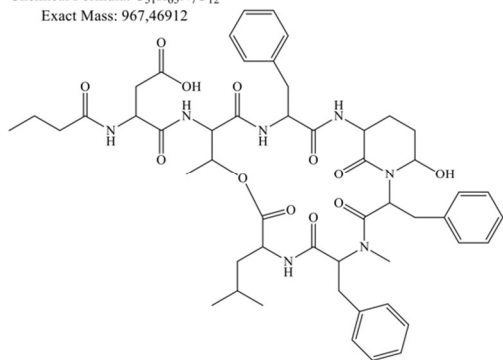


Figure S53. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 967.

Chemical Formula: $C_{50}H_{63}N_7O_{13}$
Exact Mass: 969.44839

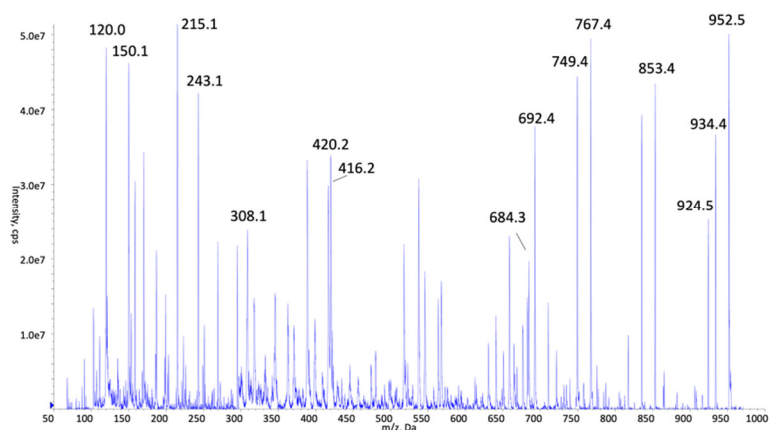
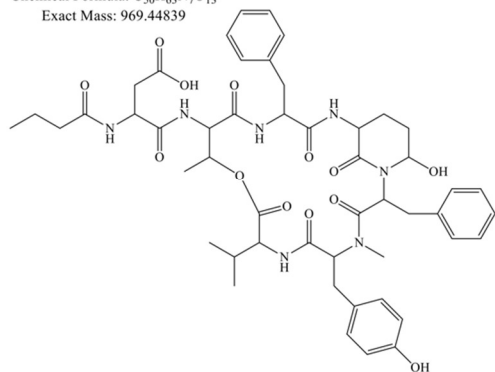


Figure S54. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 969b.

Chemical Formula: $C_{52}H_{67}N_7O_{12}$
Exact Mass: 981.48477

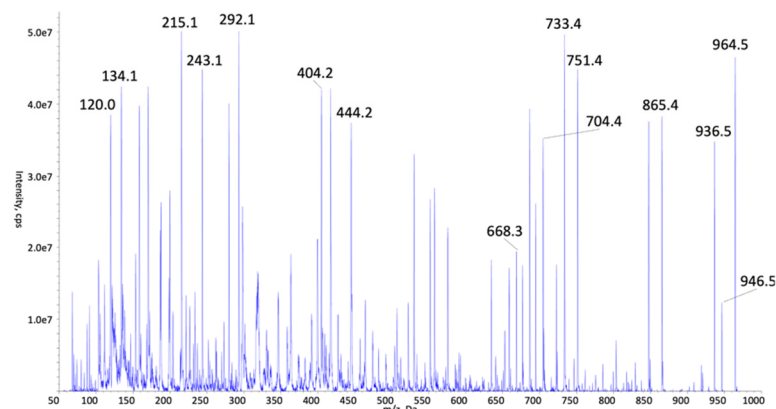
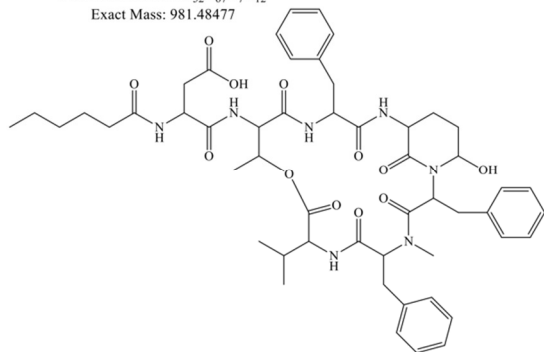


Figure S55. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 981.

Chemical Formula: $C_{52}H_{67}N_7O_{13}$
Exact Mass: 997.47969

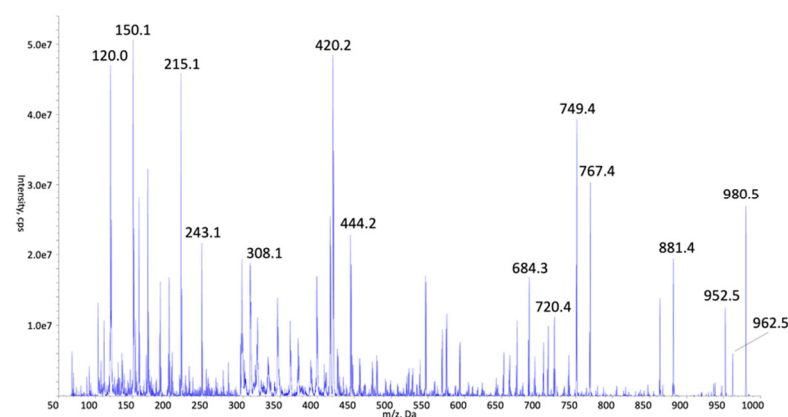
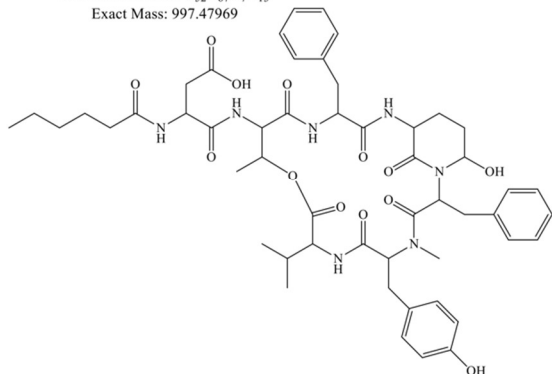


Figure S56. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 997.

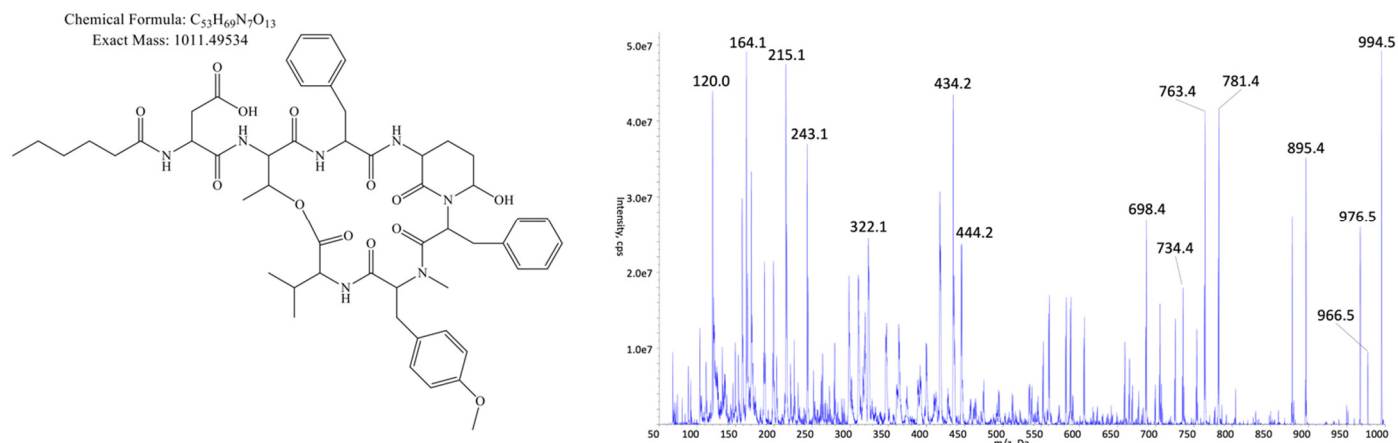


Figure S57. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1011.

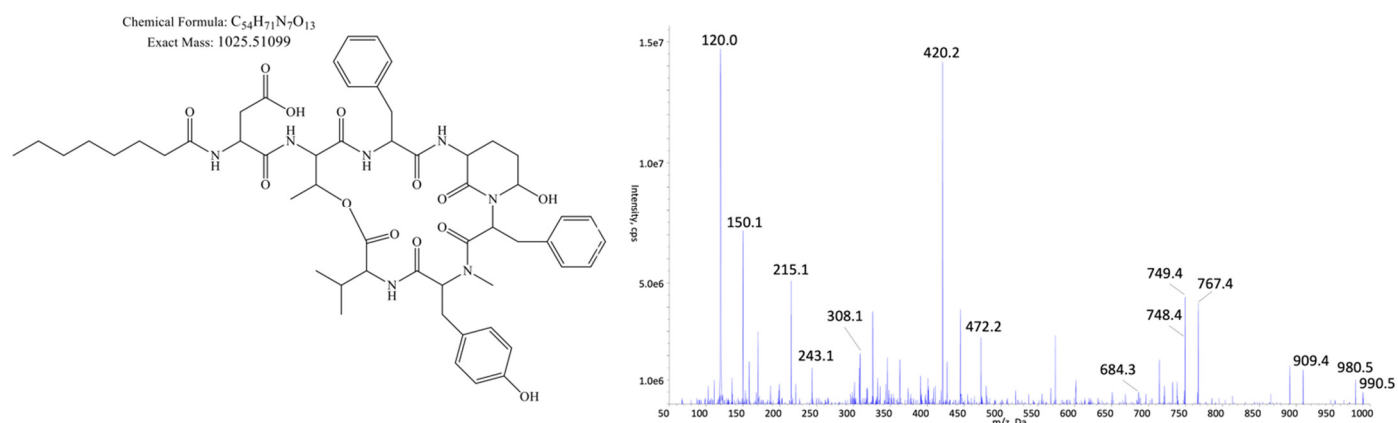


Figure S58. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1025b.

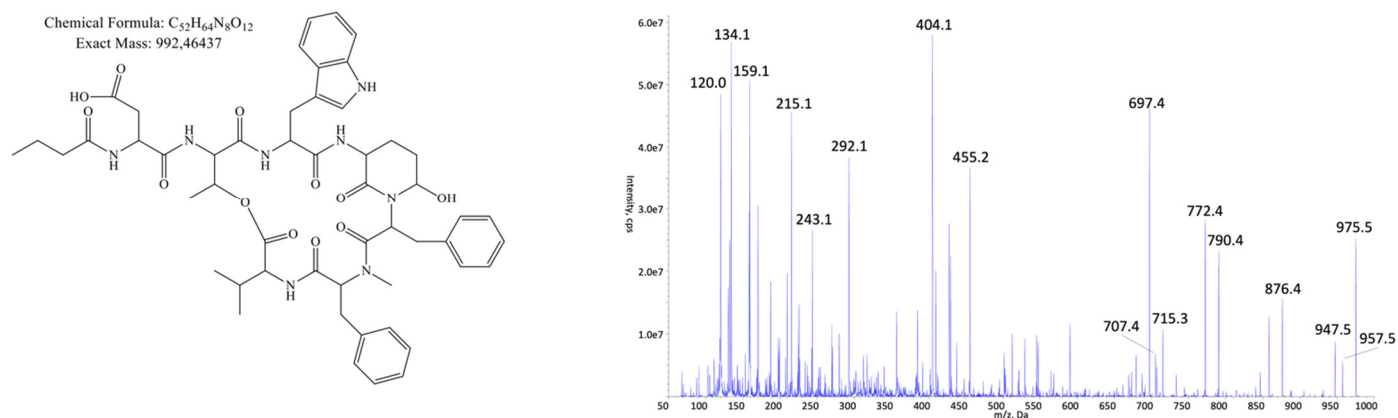


Figure S59. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 992d.

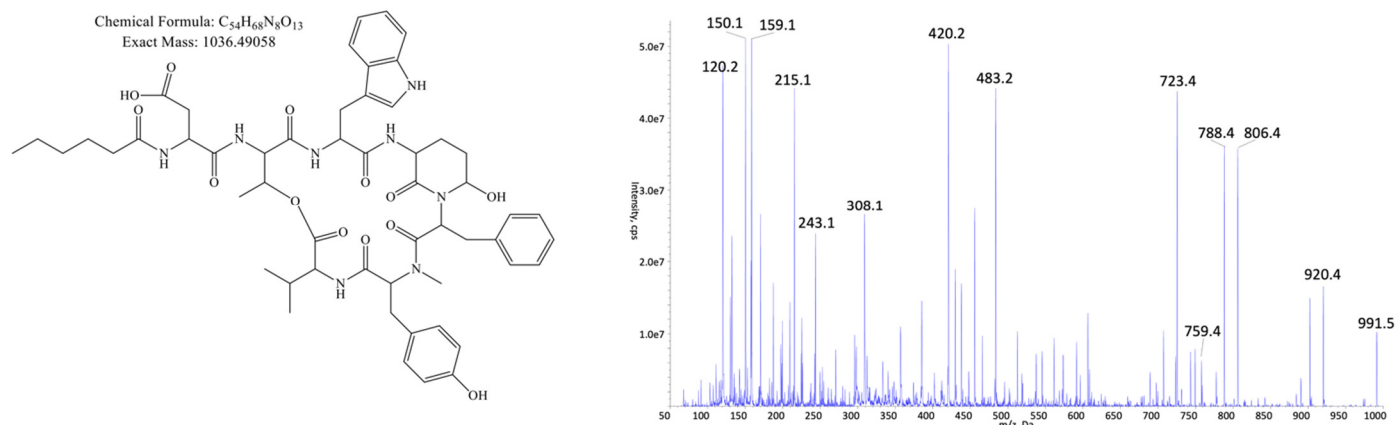


Figure S60. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1036c.

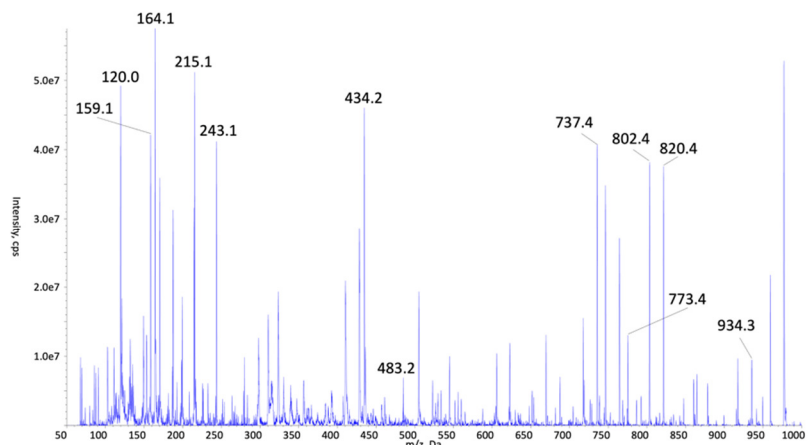
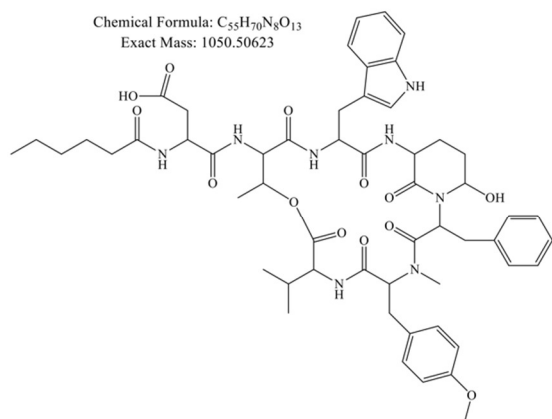


Figure S61. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1050.

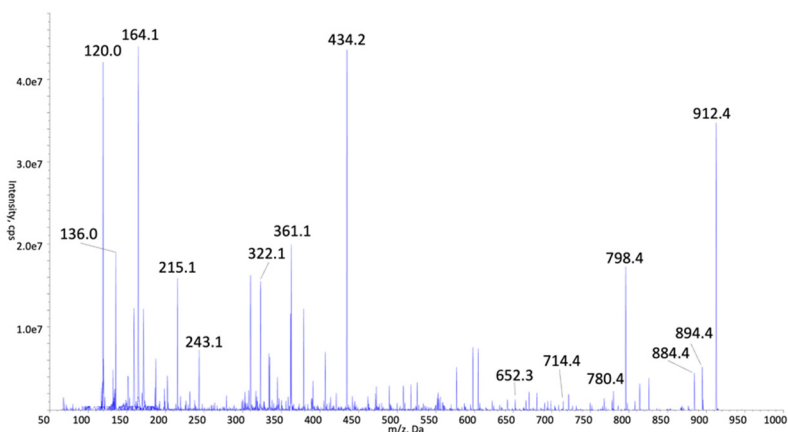
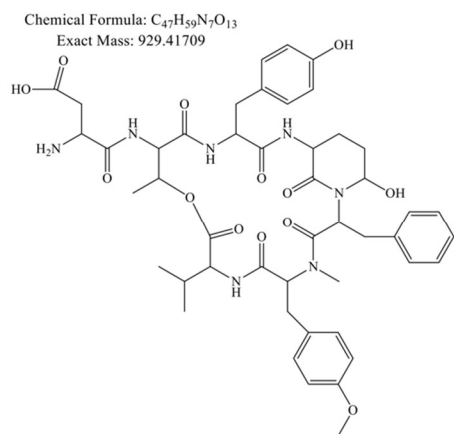


Figure S62. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 929.

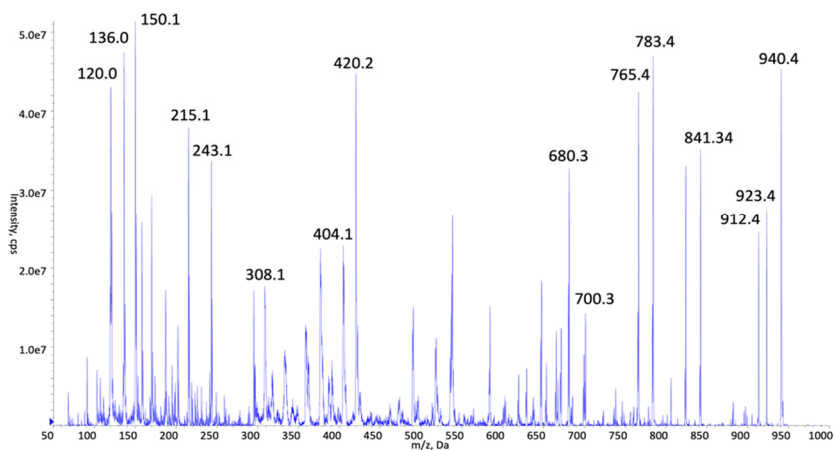
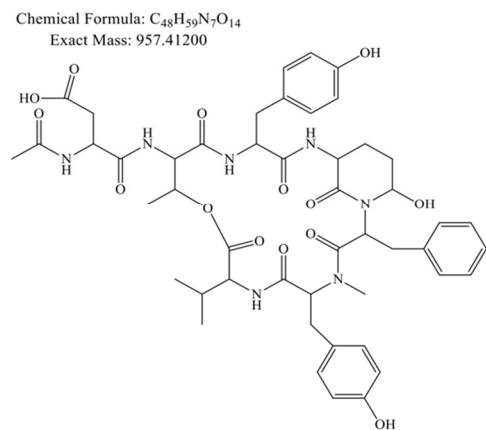


Figure S63. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 957.

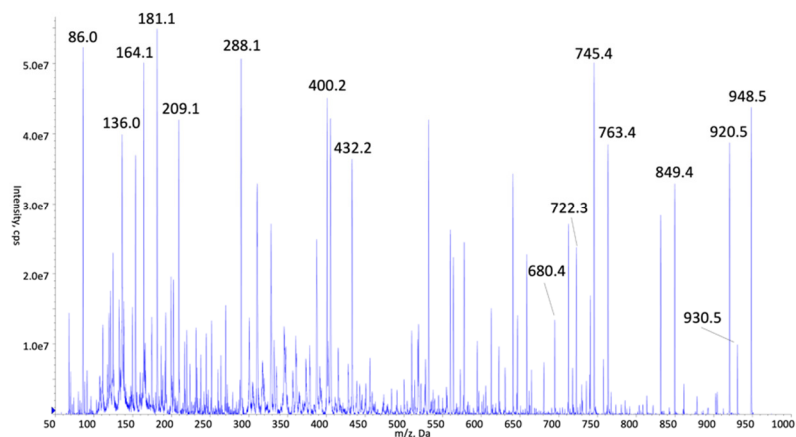
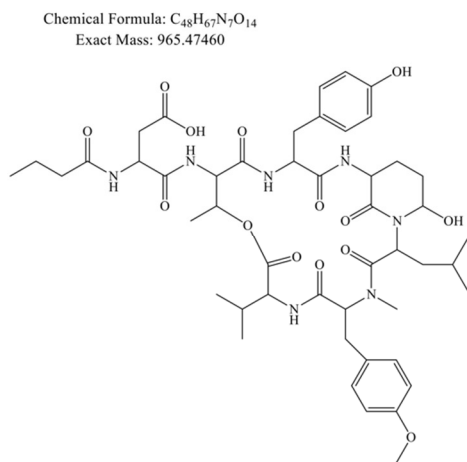


Figure S64. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 965.

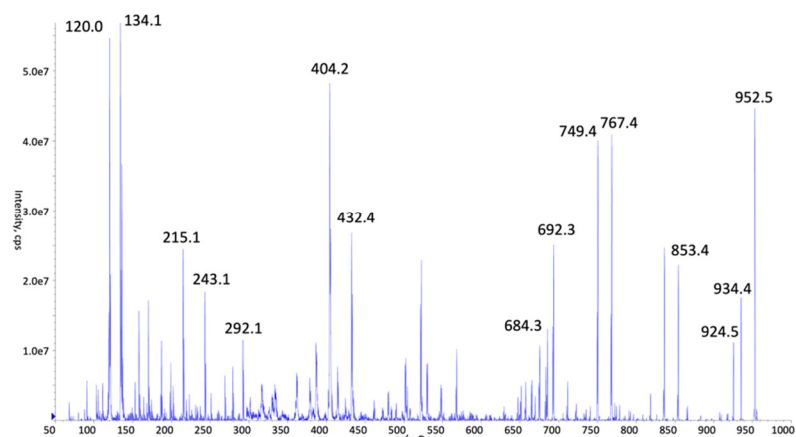
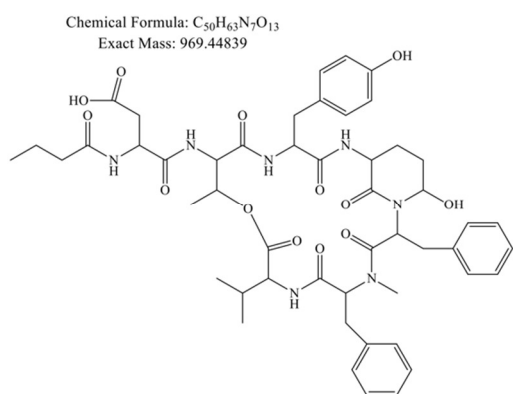


Figure S65. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 969 [8].

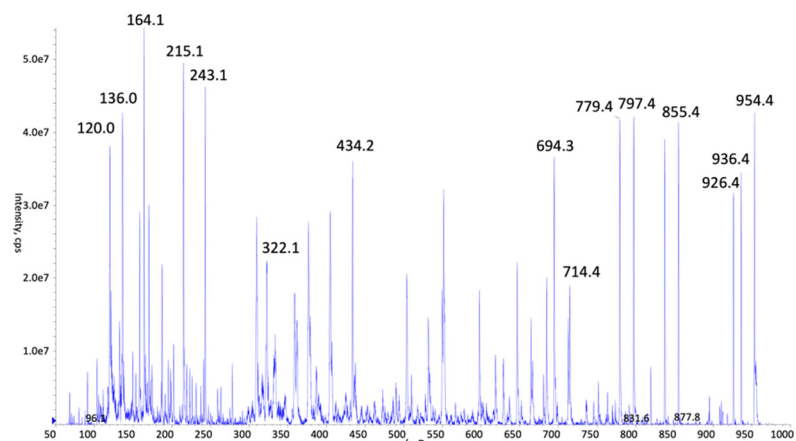
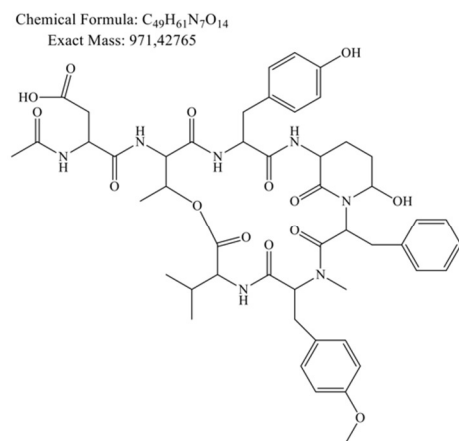


Figure S66. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 971.

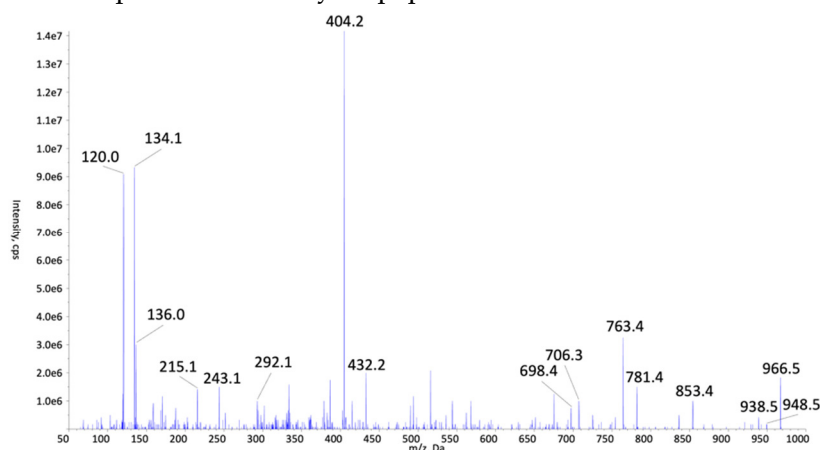
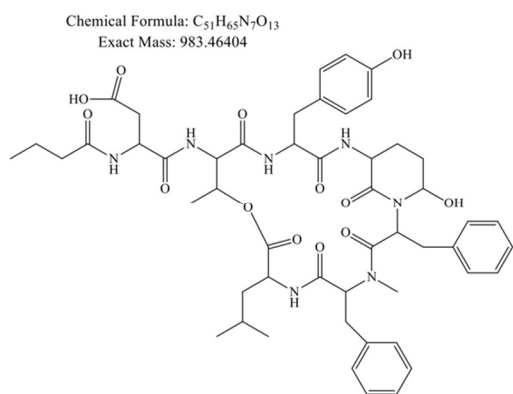
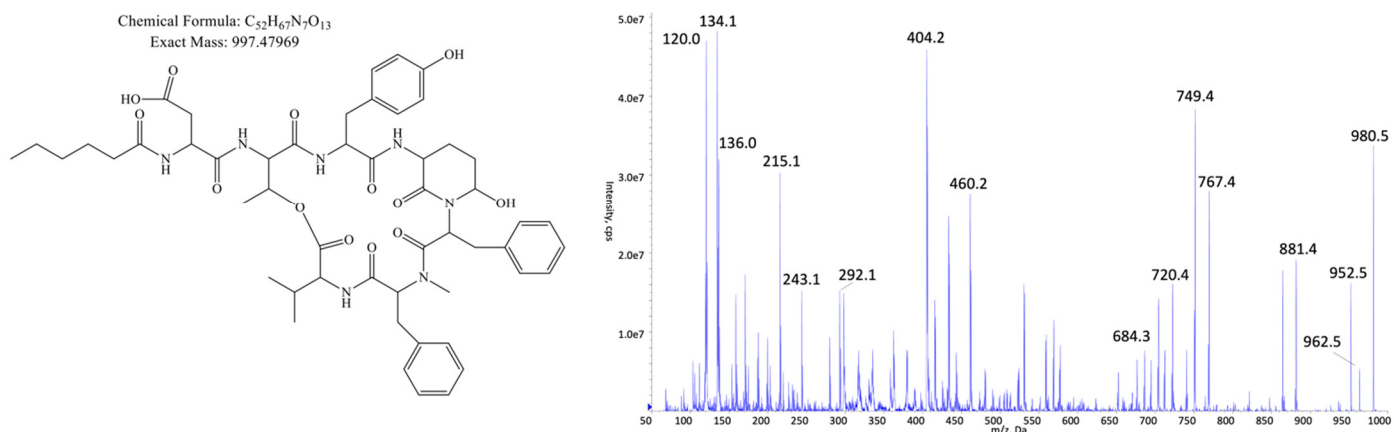
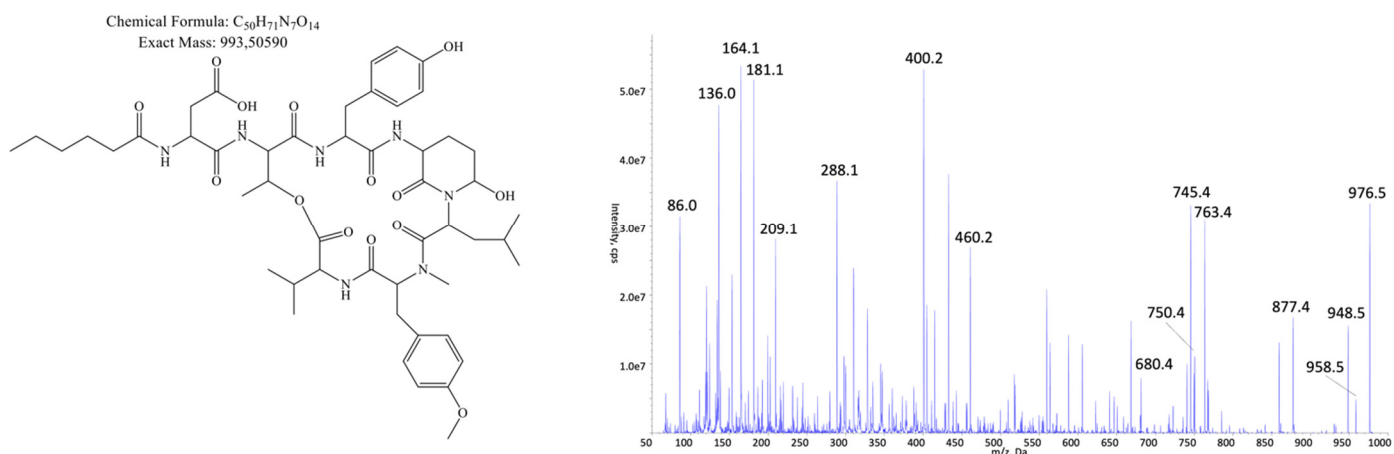
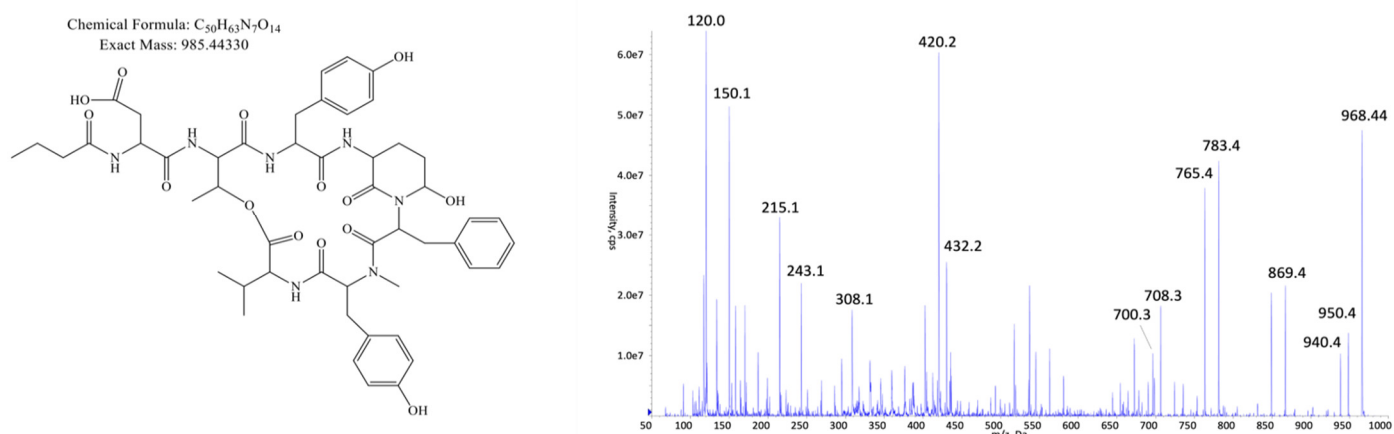
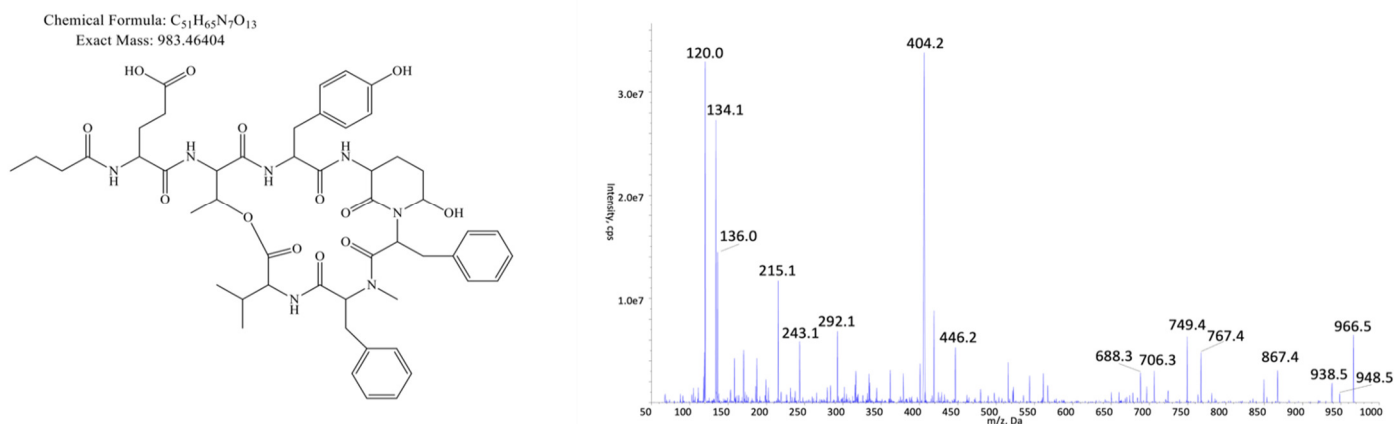


Figure S67. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 983b.



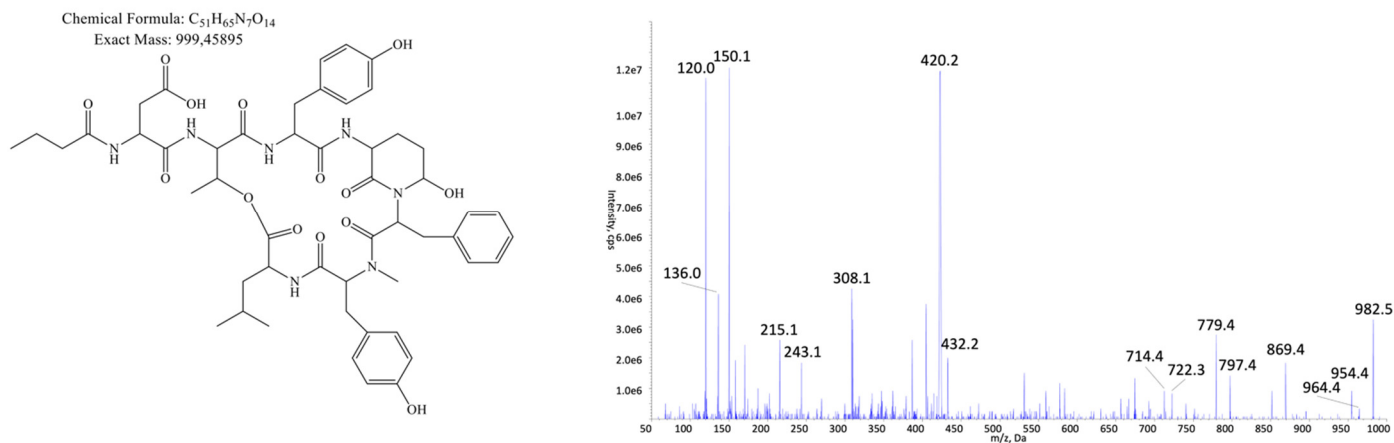


Figure S72. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 999b.

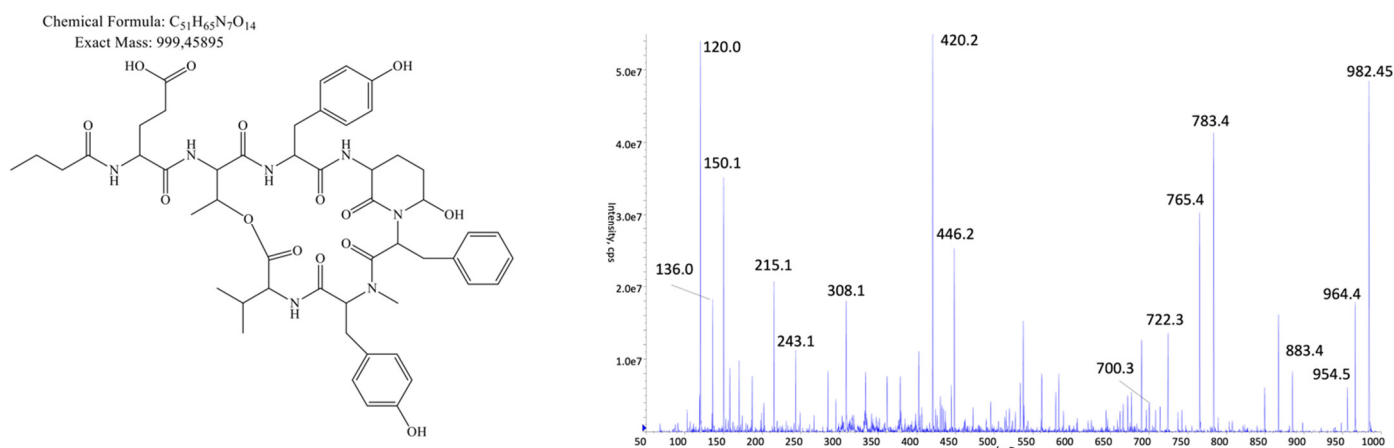


Figure S73. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 999c.

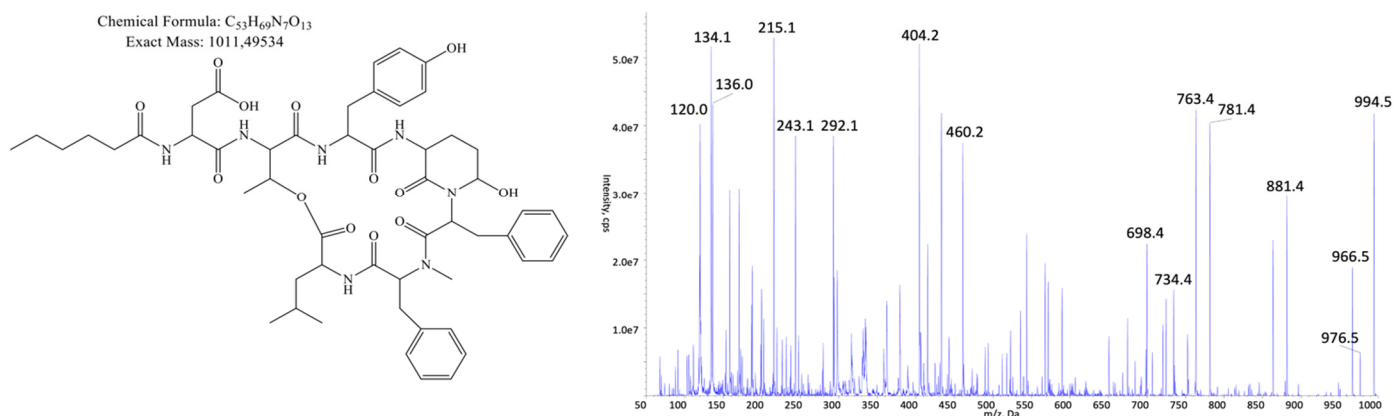


Figure S74. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1011b.

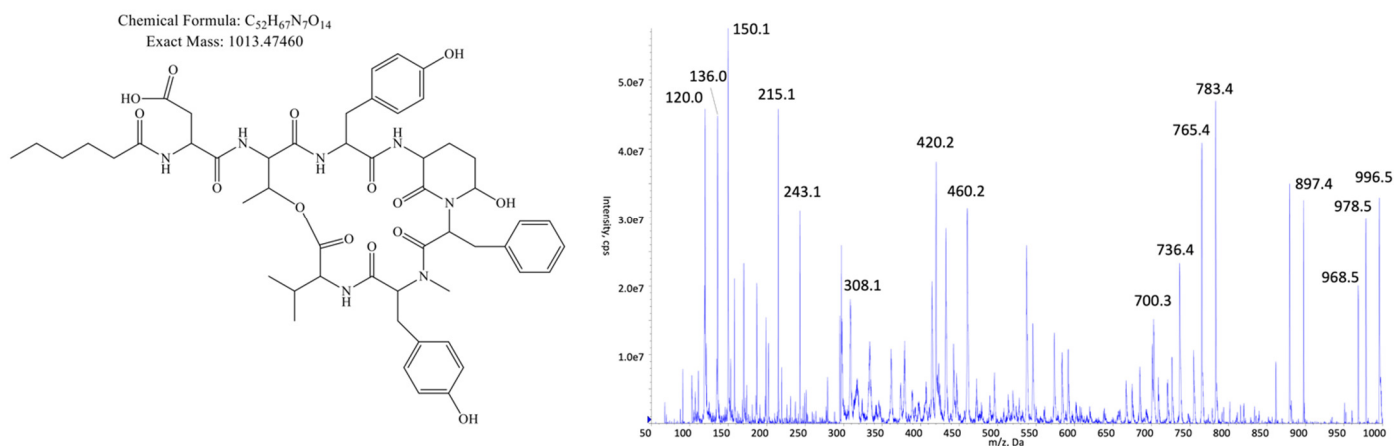


Figure S75. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1013 [8].

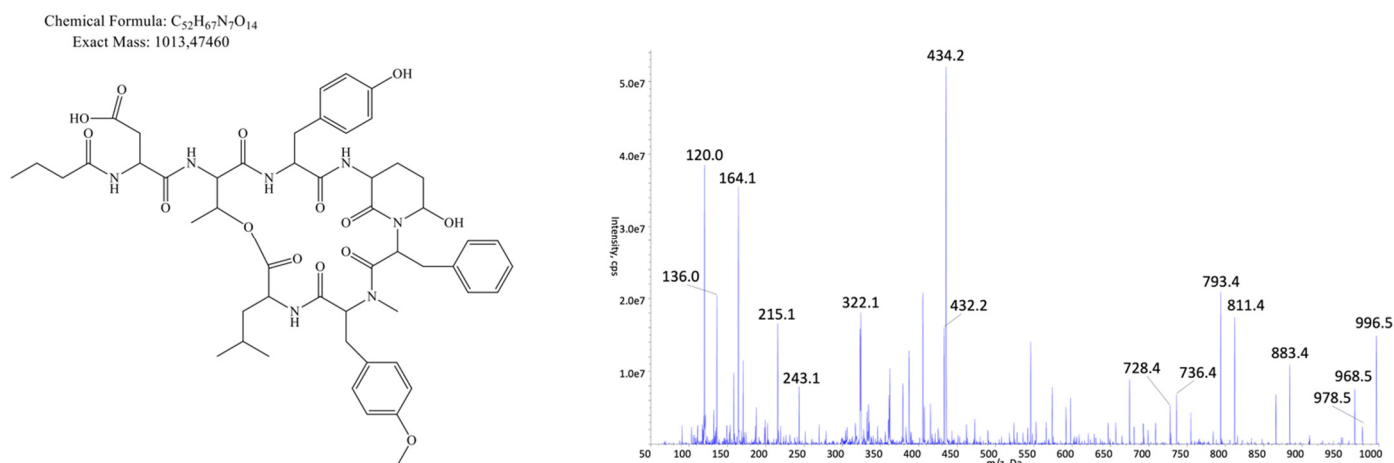


Figure S76. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1013b.

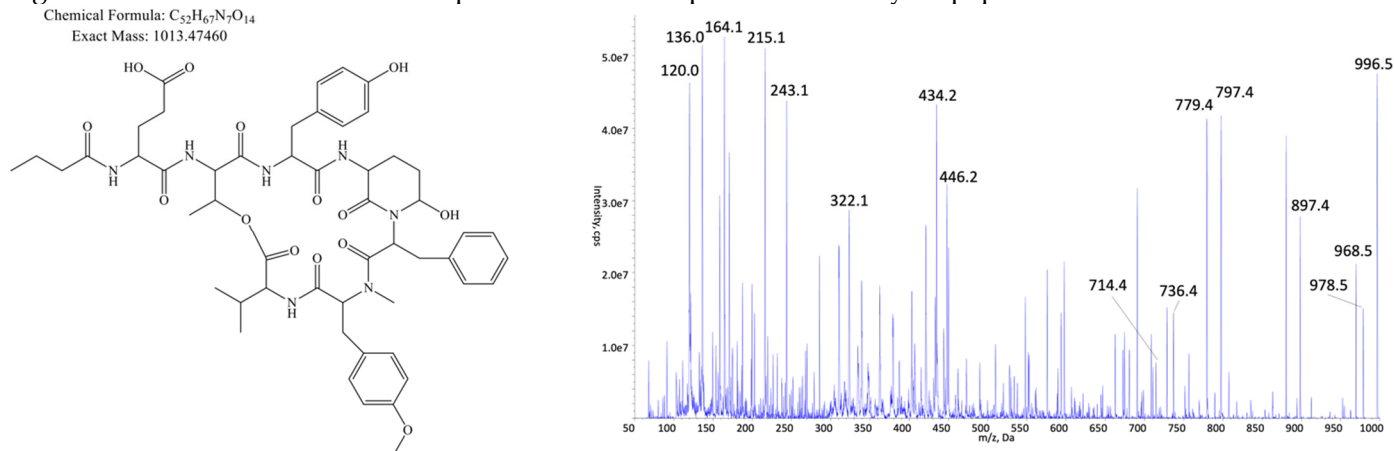


Figure S77. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1013c.

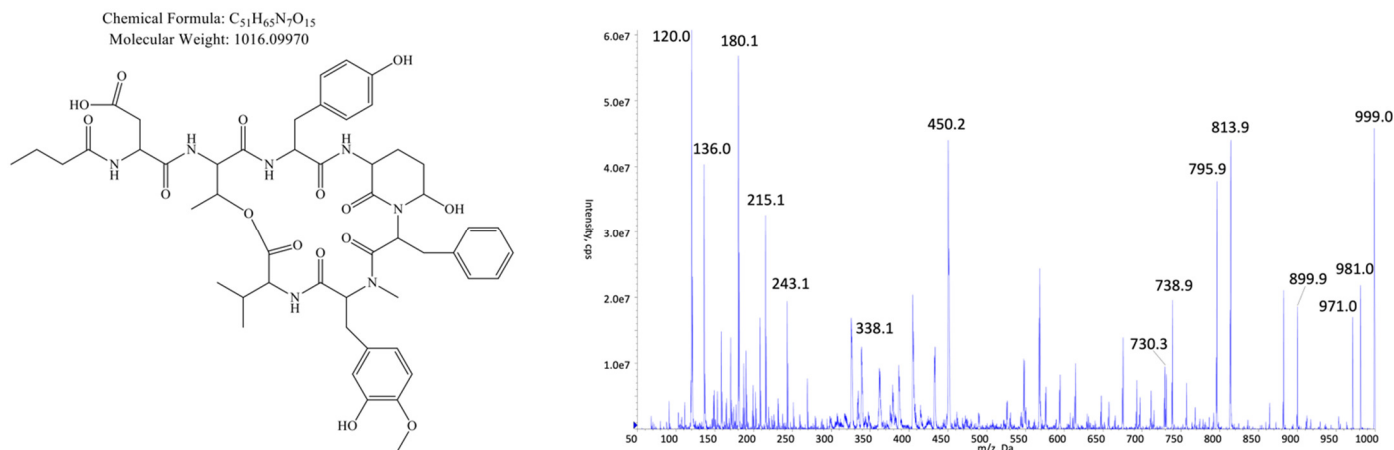


Figure S78. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1016.

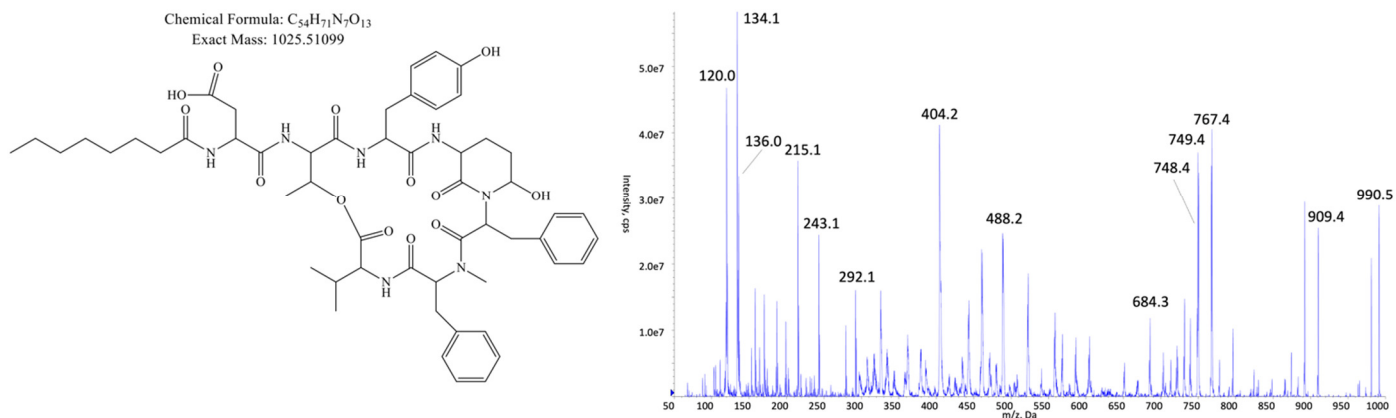


Figure S79. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1025.

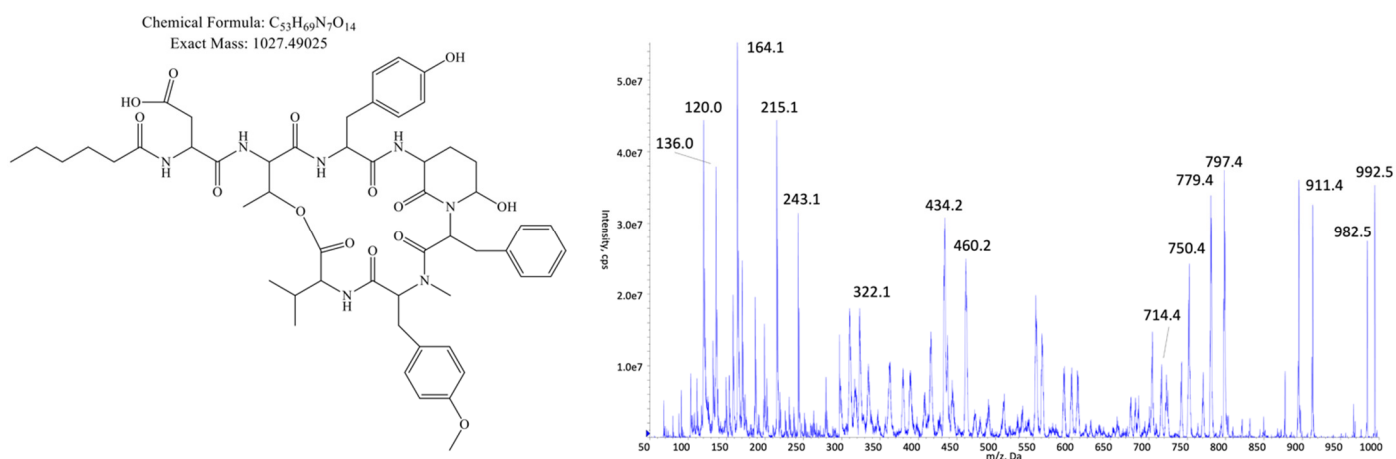


Figure S80. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1027 [8].

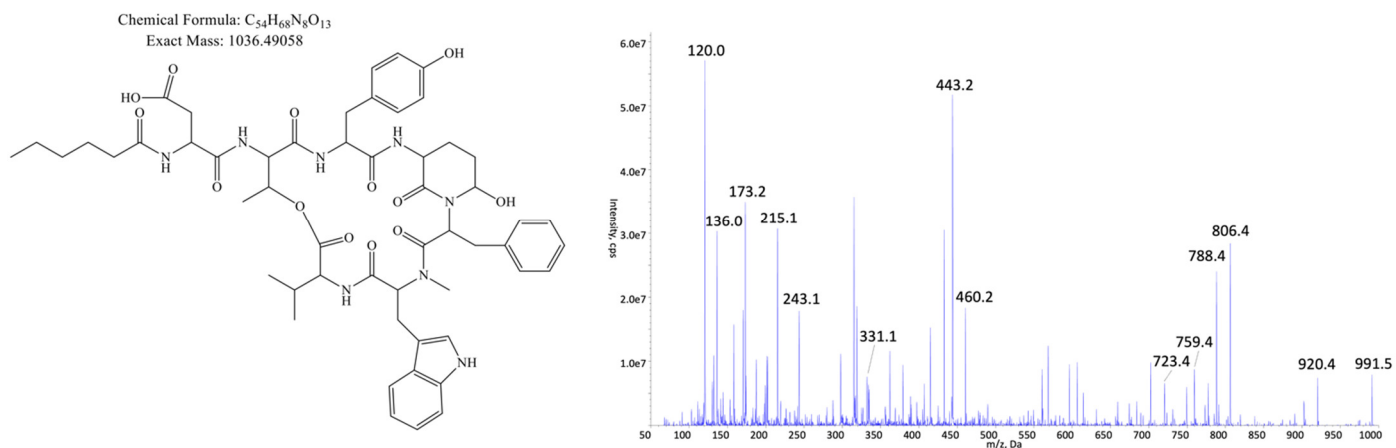


Figure S81. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1036b.

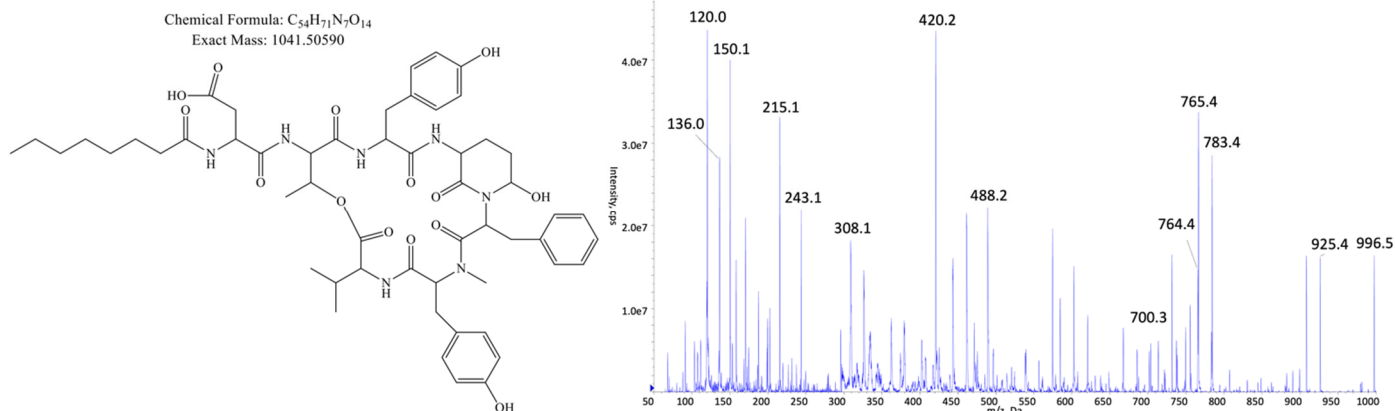


Figure S82. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1041.

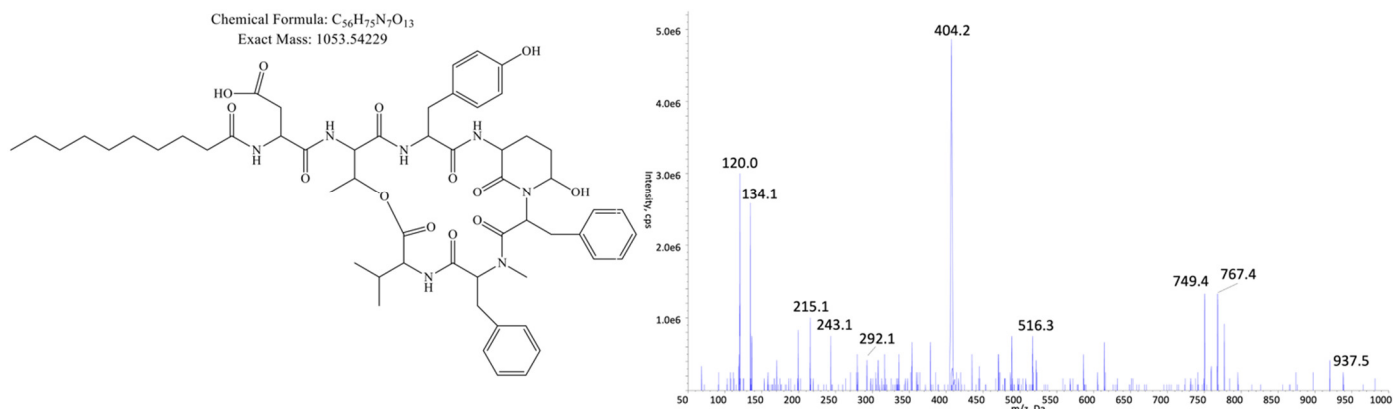


Figure S83. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1053.

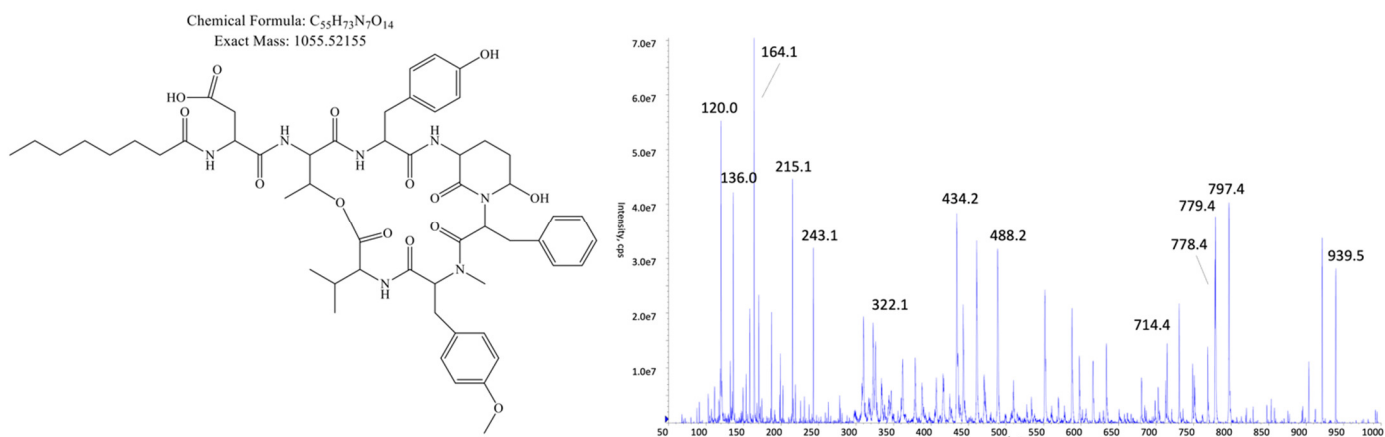


Figure S84. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1055.

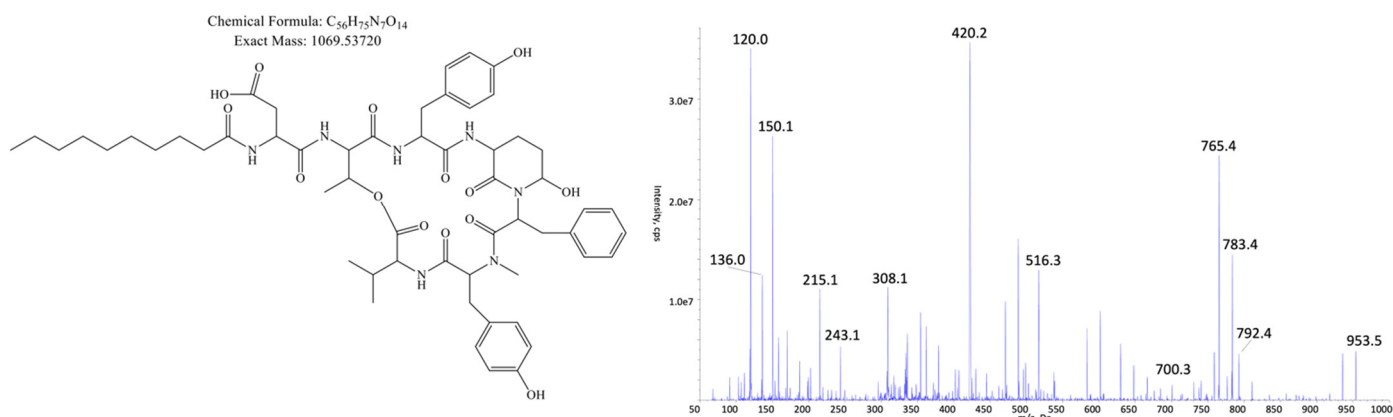


Figure S85. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1069.

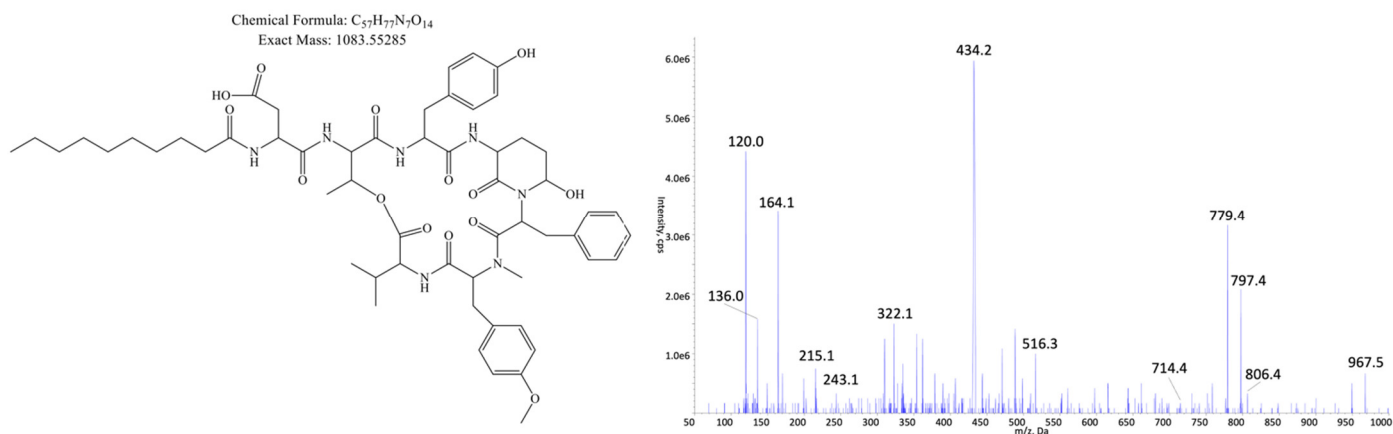


Figure S86. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1083.

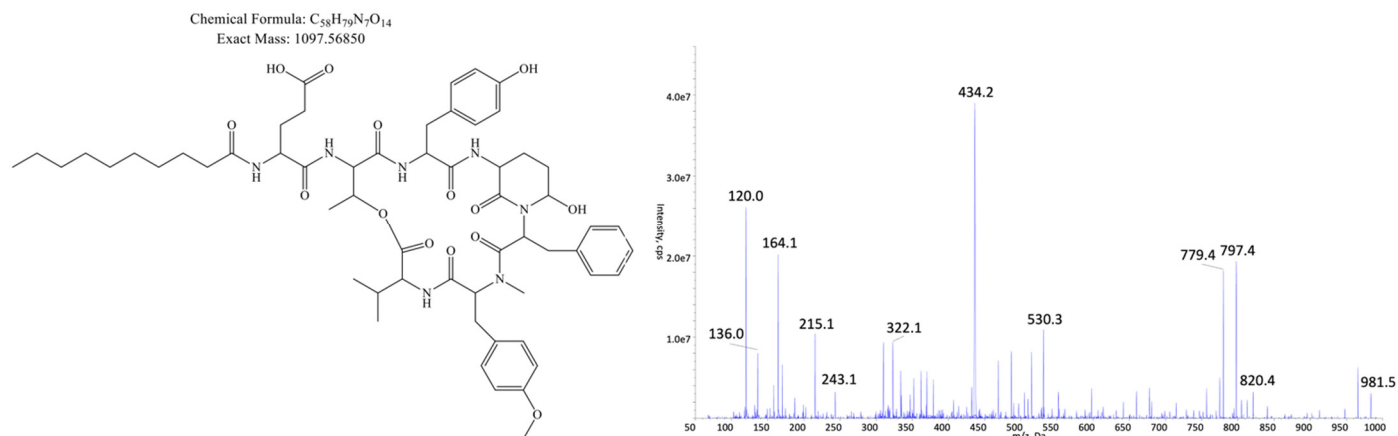


Figure S87. Structure and enhanced product ion mass spectrum of the cyanopeptolin CP 1097.

Table S3. Diagnostic ions for cyanopeptolins produced by *Nostoc edaphicum* CCNP1411.

Group	Name	(<i>m/z</i>) [M+H] ⁺	[M+H-H ₂ O] ⁺	[M+H-H ₂ O-CO] ⁺	[M+H-X ⁶ -H ₂ O] ⁺	[M+H-SC] ⁺	[M+2H-SC-H ₂ O] ⁺	[M+2H-SC-2H ₂ O] ⁺	[M+H-(Ahp+X ⁴)-H ₂ O] ⁺	[X ₂ +Ahp+X ⁴ +X ⁵ +X ⁶ +H] ⁺	[SC+Thr+X ² +H-H ₂ O] ⁺	[Ahp+X ⁴ +X ⁵ +H-H ₂ O] ⁺	[Ahp+X ⁴ +H-H ₂ O] ⁺	[X ⁴ +X ⁵ +2H-H ₂ O] ⁺	[Ahp+X ⁴ +H-CO-H ₂ O] ⁺
CP-Arg	CP 777	778.43	760.4	732.4	661.3				500.3	677.4		404.2	243.1	292.1	215.1
CP-Arg	CP 807	808.44	790.4	762.4	691.4				530.3	707.4		434.2	243.1	322.1	215.1
CP-Arg	CP 892	893.45	875.4	847.4	776.4	778.4	761.4	743.4	615.3	677.4	354.2	404.2	243.1	292.1	215.1
CP-Arg	CP 922	923.46	905.5	877.5	806.4	808.4	791.4	773.4	645.3	707.4	354.2	434.2	243.1	322.1	215.1
CP-Arg	CP 934	935.46	917.5	889.5	818.4	777.4	760.4	742.4	657.3	677.4	397.2	404.2	243.1	292.1	215.1
CP-Arg	CP 944	945.51	927.5	899.5	828.4	759.4	742.4	724.4	700.4	660.4	425.2	387.2	210.1	274.1	182.1
CP-Arg	CP 950	951.46	933.4	905.5	834.4	793.4	776.4	758.4	673.3	693.4	397.2	420.2	243.1	308.1	215.1
CP-Arg	CP 962	963.49	945.5	917.5	846.4	777.4	760.4	742.4	685.4	677.4	425.2	404.2	243.1	292.1	215.1
CP-Arg	CP 964	965.47	947.5	919.5	848.4	807.4	790.4	772.4	687.3	707.4	397.2	434.2	243.1	322.1	215.1
CP-Arg	CP 976	977.51	959.5	931.5	846.4	791.4	774.4	756.4	699.4	691.4	425.2	404.2	243.1	292.1	215.1
CP-Arg	CP 978	979.49	961.5	933.5	862.4	793.4	776.4	758.4	701.4	693.4	425.2	420.2	243.1	308.1	215.1
CP-Arg	CP 990	991.52	973.5	945.5	874.4	777.4	760.4	742.4	713.4	677.4	453.2	404.2	243.1	292.1	215.1
CP-Arg	CP 992	993.50	975.5	947.5	876.4	807.4	790.4	772.4	715.4	707.4	425.2	434.2	243.1	322.1	215.1
CP-Arg	CP 992b	993.50	975.5	947.5	862.4	807.4	790.4	772.4	715.4	707.4	425.2	420.2	243.1	308.1	215.1
CP-Arg	CP 992c	993.50	975.5	947.5	876.4	793.4	776.4	758.4	715.4	693.4	439.2	420.2	243.1	308.1	215.1
CP-Arg	CP 1006	1007.52	989.5	961.5	890.4	793.4	776.4	758.4	729.4	693.4	453.2	420.2	243.1	308.1	215.1
CP-Arg	CP 1008	1009.40	991.5	963.5	892.4	823.4	806.4	788.4	731.4	723.4	425.2	450.2	243.1	338.1	215.1
CP-Arg	CP 1018	1019.56		973.6	902.5	777.4	760.4	742.4	741.4	677.4	481.3	404.2	243.1	292.1	215.1
CP-Arg	CP 1020b	1021.54		975.5	904.5	807.4	790.4	772.4	743.4	707.4	453.2	434.2	243.1	322.1	215.1
CP-Arg	CP 1020	1021.54		975.5	904.5	793.4	776.4	758.4	743.4	693.4	467.3	420.2	243.1	308.1	215.1
CP-Arg	CP 1034	1035.55		989.5	918.5	793.4	776.4	758.4	757.4	693.4	481.3	420.2	243.1	308.1	215.1
CP-Arg	CP 1036	1037.53		991.5	920.5	823.4	806.4	788.4	759.4	723.4	453.2	450.2	243.1	338.1	215.1
CP-Arg	CP 1046	1047.59			930.5	777.4	760.4	742.4	769.5	677.4	509.3	404.2	243.1	292.1	215.1
CP-Arg	CP 1048	1049.57			932.5	807.4	790.4	772.4	771.4	707.4	481.3	434.2	243.1	322.1	215.1
CP-Arg	CP 1076	1077.60			960.5	807.4	790.4	772.4	799.5	707.4	509.3	434.2	243.1	322.1	215.1

Group	Name	(<i>m/z</i>) [M+H] ⁺	[M+H-H ₂ O] ⁺	[M+H-H ₂ O-CO] ⁺	[M+H-X ⁶ -H ₂ O] ⁺	[M+H-SC] ⁺	[M+2H-SC-H ₂ O] ⁺	[M+2H-SC-2H ₂ O] ⁺	[M+H-(Ahp+X ⁴)-H ₂ O] ⁺	[X ₂ +Ahp+X ⁴ +X ⁵ +X ⁶ +H] ⁺	[SC+Thr+X ² +H-H ₂ O] ⁺	[Ahp+X ⁴ +X ⁵ +H-H ₂ O] ⁺	[Ahp+X ⁴ +H-H ₂ O] ⁺	[X ⁴ +X ⁵ +2H-H ₂ O] ⁺	[Ahp+X ⁴ +H-CO-H ₂ O] ⁺
CP-Arg	CP 777	778.43	760.4	732.4	661.3				500.3	677.4		404.2	243.1	292.1	215.1
CP-Arg	CP 807	808.44	790.4	762.4	691.4				530.3	707.4		434.2	243.1	322.1	215.1
CP-Arg	CP 892	893.45	875.4	847.4	776.4	778.4	761.4	743.4	615.3	677.4	354.2	404.2	243.1	292.1	215.1
CP-Arg	CP 922	923.46	905.5	877.5	806.4	808.4	791.4	773.4	645.3	707.4	354.2	434.2	243.1	322.1	215.1
CP-Arg	CP 934	935.46	917.5	889.5	818.4	777.4	760.4	742.4	657.3	677.4	397.2	404.2	243.1	292.1	215.1
CP-Arg	CP 944	945.51	927.5	899.5	828.4	759.4	742.4	724.4	700.4	660.4	425.2	387.2	210.1	274.1	182.1
CP-Arg	CP 950	951.46	933.4	905.5	834.4	793.4	776.4	758.4	673.3	693.4	397.2	420.2	243.1	308.1	215.1
CP-Arg	CP 962	963.49	945.5	917.5	846.4	777.4	760.4	742.4	685.4	677.4	425.2	404.2	243.1	292.1	215.1
CP-Arg	CP 964	965.47	947.5	919.5	848.4	807.4	790.4	772.4	687.3	707.4	397.2	434.2	243.1	322.1	215.1
CP-Arg	CP 976	977.51	959.5	931.5	846.4	791.4	774.4	756.4	699.4	691.4	425.2	404.2	243.1	292.1	215.1
CP-Arg	CP 978	979.49	961.5	933.5	862.4	793.4	776.4	758.4	701.4	693.4	425.2	420.2	243.1	308.1	215.1
CP-Arg	CP 990	991.52	973.5	945.5	874.4	777.4	760.4	742.4	713.4	677.4	453.2	404.2	243.1	292.1	215.1
CP-Arg	CP 992	993.50	975.5	947.5	876.4	807.4	790.4	772.4	715.4	707.4	425.2	434.2	243.1	322.1	215.1
CP-Arg	CP 992b	993.50	975.5	947.5	862.4	807.4	790.4	772.4	715.4	707.4	425.2	420.2	243.1	308.1	215.1
CP-Arg	CP 992c	993.50	975.5	947.5	876.4	793.4	776.4	758.4	715.4	693.4	439.2	420.2	243.1	308.1	215.1
CP-Arg	CP 1006	1007.52	989.5	961.5	890.4	793.4	776.4	758.4	729.4	693.4	453.2	420.2	243.1	308.1	215.1
CP-Arg	CP 1008	1009.40	991.5	963.5	892.4	823.4	806.4	788.4	731.4	723.4	425.2	450.2	243.1	338.1	215.1
CP-Arg	CP 1018	1019.56		973.6	902.5	777.4	760.4	742.4	741.4	677.4	481.3	404.2	243.1	292.1	215.1
CP-Arg	CP 1020b	1021.54		975.5	904.5	807.4	790.4	772.4	743.4	707.4	453.2	434.2	243.1	322.1	215.1
CP-Arg	CP 1020	1021.54		975.5	904.5	793.4	776.4	758.4	743.4	693.4	467.3	420.2	243.1	308.1	215.1
CP-Arg	CP 1034	1035.55		989.5	918.5	793.4	776.4	758.4	757.4	693.4	481.3	420.2	243.1	308.1	215.1
CP-Arg	CP 1036	1037.53		991.5	920.5	823.4	806.4	788.4	759.4	723.4	453.2	450.2	243.1	338.1	215.1
CP-Arg	CP 1046	1047.59			930.5	777.4	760.4	742.4	769.5	677.4	509.3	404.2	243.1	292.1	215.1
CP-Arg	CP 1048	1049.57			932.5	807.4	790.4	772.4	771.4	707.4	481.3	434.2	243.1	322.1	215.1
CP-Arg	CP 1076	1077.60			960.5	807.4	790.4	772.4	799.5	707.4	509.3	434.2	243.1	322.1	215.1

Group	Name	(<i>m/z</i>) [M+H] ⁺	[M+H-H ₂ O] ⁺	[M+H-H ₂ O-CO] ⁺	[M+H-X ⁶ -H ₂ O] ⁺	[M+2H-SC-H ₂ O] ⁺	[M+2H-SC-2H ₂ O] ⁺	[M+H-(Ahp+X ⁴)-H ₂ O] ⁺	[X ² +Ahp+X ⁴ +X ⁵ +X ⁶ +H] ⁺	[SC+Thr+X ² +H-H ₂ O] ⁺	[Ahp+X ⁴ +X ⁵ +H-H ₂ O] ⁺	[Ahp+X ⁴ +H-H ₂ O] ⁺	[X ⁴ +X ⁵ +2H-H ₂ O] ⁺	[Ahp+X ⁴ +H-CO-H ₂ O] ⁺
CP-Leu	CP 891	874.44	856.4	846.4	775.4	717.4	699.4	614.3	634.4	354.2	404.2	243.1	292.1	215.1
CP-Leu	CP 907	890.43	872.4	862.4	791.4	733.4	715.4	630.3	650.4	354.2	420.2	243.1	308.1	215.1
CP-Leu	CP 919	902.47	884.5	874.5	803.4	717.4	699.4	642.4	634.4	382.2	404.2	243.1	292.1	215.1
CP-Leu	CP 921	904.45	886.4	876.5	805.4	747.4	729.4	644.3	664.4	354.2	434.2	243.1	322.1	215.1
CP-Leu	CP 933	916.48	898.5	888.5	817.4	717.4	699.4	656.4	634.4	396.2	404.2	243.1	292.1	215.1
CP-Leu	CP 935	918.46	900.5	890.5	819.4	733.4	715.4	658.3	650.4	382.2	420.2	243.1	308.1	215.1
CP-Leu	CP 947	930.50	912.5	902.5	831.4	717.4	699.4	670.4	634.4	410.2	404.2	243.1	292.1	215.1
CP-Leu	CP 949	932.48	914.5	904.5	833.4	747.4	729.4	672.4	664.4	382.2	434.2	243.1	322.1	215.1
CP-Leu	CP 963b	946.49	928.5	918.5	847.4	747.4	729.4	686.4	664.4	396.2	434.2	243.1	322.1	215.1
CP-Leu	CP 963	946.49	928.5	918.5	847.4	733.4	715.4	686.4	650.4	410.2	420.2	243.1	308.1	215.1
CP-Leu	CP 965b	948.47	930.5	920.5	849.4	763.4	745.4	688.4	680.4	382.2	450.2	243.1	338.1	215.1
CP-Leu	CP 975	958.53	940.5	930.5	859.5	717.4	699.4	698.4	634.4	438.3	404.2	243.1	292.1	215.1
CP-Leu	CP 977	960.51	942.5	932.5	861.4	747.4	729.4	700.4	664.4	410.2	434.2	243.1	322.1	215.1
CP-Leu	CP 991	974.52	956.5	946.5	875.5	733.4	715.4	714.4	650.4	438.3	420.2	243.1	308.1	215.1
CP-Leu	CP 1005	988.54	970.5	960.5	889.5	747.4	729.4	728.4	664.4	438.3	434.2	243.1	322.1	215.1
CP-MeLeu	CP 933b	916.48	898.5	888.5	817.4	731.4	713.4	656.4	648.4	396.2	404.2	243.1	292.1	215.1
CP-MeLeu	CP 949b	932.48	914.5	904.5	833.4	747.4	729.4	672.4	664.4	396.2	420.2	243.1	308.1	215.1
CP-MePhe	CP 939b	922.44	904.4	894.4	823.4	765.4	747.4	662.3	682.4	402.2	404.2	243.1	292.1	215.1
CP-MePhe	CP 967b	950.47	932.5	922.5	851.4	765.4	747.4	690.4	682.4	430.2	404.2	243.1	292.1	215.1
CP-MePhe	CP 1011c	994.49	976.5	966.5	895.4	781.4	763.4	734.4	698.4	458.2	420.2	243.1	308.1	215.1
CP-Met	CP 937	920.42	902.4	892.4	821.4	735.4	717.3	660.3	652.3	400.2	404.2	243.1	292.1	215.1
CP-Met	CP 939	922.40	904.4	894.4	823.3	765.4	747.4	662.3	682.3	372.1	434.2	243.1	322.1	215.1
CP-Met	CP 953b	936.42	918.4	908.4	837.3	751.3	733.3	676.3	668.3	400.2	420.2	243.1	308.1	215.1
CP-Met	CP 995	978.46	960.5	950.5	879.4	765.4	747.4	718.3	682.3	428.2	434.2	243.1	322.1	215.1
CP-Met	CP 1023	1006.50	988.5	978.5	907.4	765.4	747.4	746.4	682.3	456.2	434.2	243.1	322.1	215.1

CP-MeTyr	CP 999d	982.46	964.4	954.5	883.4	797.4	779.4	722.3	714.4	446.2	420.2	243.1	308.1	215.1
CP-MeTyr	CP 1014	997.12	979.1	969.1	898.1	812.1	794.0	737.0	728.4	446.2	434.2	243.1	322.1	215.1
CP-Phe	CP 925	908.42	890.4	880.4	809.4	751.4	733.4	648.3	668.3	388.2	404.2	243.1	292.1	215.1
CP-Phe	CP 953	936.45	918.4	908.5	837.4	751.4	733.4	676.3	668.3	416.2	404.2	243.1	292.1	215.1
CP-Phe	CP 955	938.43	920.4	910.4	839.4	781.4	763.4	678.3	698.4	388.2	434.2	243.1	322.1	215.1
CP-Phe	CP 967	950.47	932.5	922.5	837.4	765.4	747.4	690.4	682.4	416.2	404.2	243.1	292.1	215.1
CP-Phe	CP 969b	952.45	934.4	924.5	853.4	767.4	749.4	692.3	684.3	416.2	420.2	243.1	308.1	215.1
CP-Phe	CP 981	964.48	946.5	936.5	865.4	751.4	733.4	704.4	668.3	444.2	404.2	243.1	292.1	215.1
CP-Phe	CP 983	966.46	948.5	938.5	867.4	781.4	763.4	706.3	698.4	416.2	434.2	243.1	322.1	215.1
CP-Phe	CP 997	980.48	962.5	952.5	881.4	767.4	749.4	720.4	684.3	444.2	420.2	243.1	308.1	215.1
CP-Phe	CP 1011	994.49	976.5	966.5	895.4	781.4	763.4	734.4	698.4	444.2	434.2	243.1	322.1	215.1
CP-Phe	CP 1025b	1008.51	990.5	980.5	909.4	767.4	749.4	748.4	684.3	472.2	420.2	243.1	308.1	215.1
CP-Trp	CP 992d	975.46	957.5	947.5	876.4	790.4	772.4	715.3	707.4	455.2	404.2	243.1	292.1	215.1
CP-Trp	CP 1036c	1019.49		991.5	920.4	806.4	788.4	759.4	723.4	483.2	420.2	243.1	308.1	215.1
CP-Trp	CP 1050	1033.50			934.4	820.4	802.4	773.4	737.4	483.2	434.2	243.1	322.1	215.1
CP-Tyr	CP 929	912.41	894.4	884.4	813.3	798.4	780.4	652.3	714.4	361.1	434.2	243.1	322.1	215.1
CP-Tyr	CP 941	924.41	906.4	896.4	825.3	767.4	749.4	664.3	684.3	404.1	404.2	243.1	292.1	215.1
CP-Tyr	CP 957	940.41	922.4	912.4	841.3	783.4	765.4	680.3	700.3	404.1	420.2	243.1	308.1	215.1
CP-Tyr	CP 965	948.47	930.5	920.5	849.4	763.4	745.4	722.3	680.4	432.2	400.2	209.1	288.1	181.1
CP-Tyr	CP 969	952.45	934.4	924.5	853.4	767.4	749.4	692.3	684.3	432.2	404.2	243.1	292.1	215.1
CP-Tyr	CP 971	954.42	936.4	926.4	855.4	797.4	779.4	694.3	714.4	404.1	434.2	243.1	322.1	215.1
CP-Tyr	CP 983b	966.46	948.5	938.5	853.4	781.4	763.4	706.3	698.4	432.2	404.2	243.1	292.1	215.1
CP-Tyr	CP 983c	966.46	948.5	938.5	867.4	767.4	749.4	706.3	684.3	446.2	404.2	243.1	292.1	215.1
CP-Tyr	CP 985	968.44	950.4	940.4	869.4	783.4	765.4	708.3	700.3	432.2	420.2	243.1	308.1	215.1
CP-Tyr	CP 993	976.50	958.5	948.5	877.4	763.4	745.4	750.4	680.4	460.2	400.2	209.1	288.1	181.1
CP-Tyr	CP 997b	980.48	962.5	952.5	881.4	767.4	749.4	720.4	684.3	460.2	404.2	243.1	292.1	215.1
CP-Tyr	CP 999	982.46	964.4	954.5	883.4	797.4	779.4	722.3	714.4	432.2	434.2	243.1	322.1	215.1
CP-Tyr	CP 999b	982.46	964.4	954.5	869.4	797.4	779.4	722.3	714.4	432.2	420.2	243.1	308.1	215.1
CP-Tyr	CP 999c	982.46	964.4	954.5	883.4	783.4	765.4	722.3	700.3	446.2	420.2	243.1	308.1	215.1
CP-Tyr	CP 1011b	994.49	976.5	966.5	881.4	781.4	763.4	734.4	698.4	460.2	404.2	243.1	292.1	215.1
CP-Tyr	CP 1013b	996.37	978.5	968.5	883.4	811.4	793.4	736.4	728.4	432.2	434.2	243.1	322.1	215.1
CP-Tyr	CP 1013	996.47	978.5	968.5	897.4	783.4	765.4	736.4	700.3	460.2	420.2	243.1	308.1	215.1
CP-Tyr	CP 1013c	996.47	978.5	968.5	897.4	797.4	779.4	736.4	714.4	446.2	434.2	243.1	322.1	215.1

CP-Tyr	CP 1016	999.01	981.0	971.0	899.9	813.9	795.9	738.9	730.3	432.2	450.2	243.1	338.1	215.1
CP-Tyr	CP 1025	1008.51	990.5	980.5	909.4	767.4	749.4	748.4	684.3	488.2	404.2	243.1	292.1	215.1
CP-Tyr	CP 1027	1010.49	992.5	982.5	911.4	797.4	779.4	750.4	714.4	460.2	434.2	243.1	322.1	215.1
CP-Tyr	CP 1036b	1019.49		991.5	920.4	806.4	788.4	759.4	723.4	460.2	443.2	243.1	331.1	215.1
CP-Tyr	CP 1041	1024.50		996.5	925.4	783.4	765.4	764.4	700.3	488.2	420.2	243.1	308.1	215.1
CP-Tyr	CP 1053	1036.54			937.5	767.4	749.4	776.4	684.3	516.3	404.2	243.1	292.1	215.1
CP-Tyr	CP 1055	1038.52			939.5	797.4	779.4	778.4	714.4	488.2	434.2	243.1	322.1	215.1
CP-Tyr	CP 1069	1052.53			953.5	783.4	765.4	792.4	700.3	516.3	420.2	243.1	308.1	215.1
CP-Tyr	CP 1083	1066.55			967.5	797.4	779.4	806.4	714.4	516.3	434.2	243.1	322.1	215.1
CP-Tyr	CP 1097	1080.57			981.5	797.4	779.4	820.4	700.3	530.3	420.2	243.1	308.1	215.1

Table S4. NMR Spectroscopic Data for cyanopeptolin CP 941 – AC-Asp-[Thr-Tyr-Ahp-Phe-MePhe-Val].

Residue	Position	δ_C	δ_H (J in Hz)	ROESY	HMBC ^a
Ac	1	169.4			
	2	23.1	1.84, s		Ac-1
Asp	1	<i>nd</i>			
	2	50.5	4.48, m	Thr-NH	
	3a	37.7	2.35, m		
	3b		2.22, m		
	4	<i>nd</i>			
	NH		8.63, m		
Thr	1	169.3			
	2	54.8	4.51, d (9.9)	Tyr-NH	Thr-1
	3	72.8	5.35, q (6.8)	Tyr-NH	
	4	17.8	1.11, d (6.6)		Thr-2, Thr-3
	NH		7.68, d (9.6)	Asp-2	
Tyr	1	<i>nd</i>			
	2	54.5	4.26, m	Asp-NH	
	3a	35.4	3.13, dd (10.2, 3.7)	Tyr-2'/6'	
	3b		2.43 ^b , m	Tyr-2'/6'	
	1'	128.2			
	2'/6'	130.0	6.86, d (8.2)	Tyr-3a, Tyr-3b	Tyr-4'
	3'/5'	115.8	6.54, d (8.2)		Tyr-1'
	4'	156.7			
	NH		8.41, d (8.9)	Thr-2, Thr-3	
Ahp	1	<i>nd</i>			
	2	49.2	3.63, m		
	3a	21.9	2.41 ^b , m		
	3b		1.60, m		
	4a	29.7	1.69 ^c , m	Phe-2'/6'	
	4b		1.50, m	Phe-2'/6'	
	5	74.2	5.04, brs		
	NH		7.05, d (9.2)	Tyr-2	
	OH		5.98		
Phe	1	170.7			
	2	50.5	4.74, dd (6.9, 4.4)	Phe-2'/6'	
	3a	35.7	2.84 ^d , m	Phe-2'/6'	
	3b		1.69 ^c , m		
	1'	137.2			
	2'/6'	129.8	6.78, d (7.3)	Phe-2, Phe-3a,	Phe-3, Phe-4'
	3'/5'	128.2	7.19, t (7.4)	Ahp-4a, Ahp-4b	Phe-1'
	4'	126.7	7.14, t (7.3)		Phe-2'/6'
MePhe	1	<i>nd</i>			
	2	61.0	5.00, dd (9.1, 2.2)	MePhe-2'/6',	
	3a	34.3	3.23, m	Val-NH	
	3b		2.83 ^d , m	MePhe-2'/6'	
	1'	138.3		MePhe-2'/6'	
	2'/6'	130.0	7.25, d (7.3)		MePhe-4', MePhe-3
	3'/5'	129.1	7.41, t (7.7)	MePhe-2,	MePhe-1'
	4'	127.1	7.31, t (7.4)	MePhe-3a,	MePhe-2'/6'
	NCH ₃	30.9	2.79, s	MePhe-3b	MePhe-2, Phe-1
Val	1	<i>nd</i>			
	2	56.4	4.63, dd (4.9, 4.3)		
	3	31.4	2.03, m		
	4	19.7	0.86, d (6.8)		Val-2, Val-3, Val-5
	5	17.8	0.73, d (6.8)		Val-2, Val-3, Val-4
	NH		7.39, d (9.6)	MePhe-2	

^a HMBC correlations are given from proton(s) stated to the indicated carbon atom; ^{b-d} assignments with the same superscript are overlapping; *nd* – resonances not detected

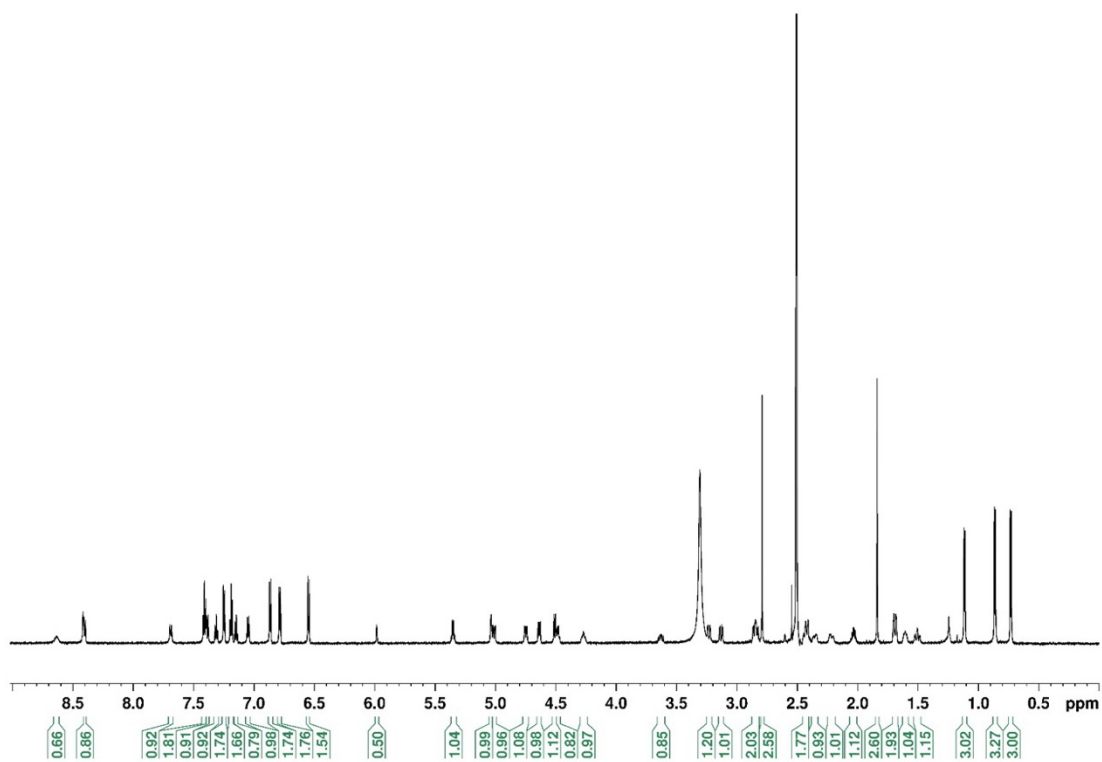


Figure S88. ¹H NMR spectrum of cyanopeptolin CP 941 in DMSO-d₆.

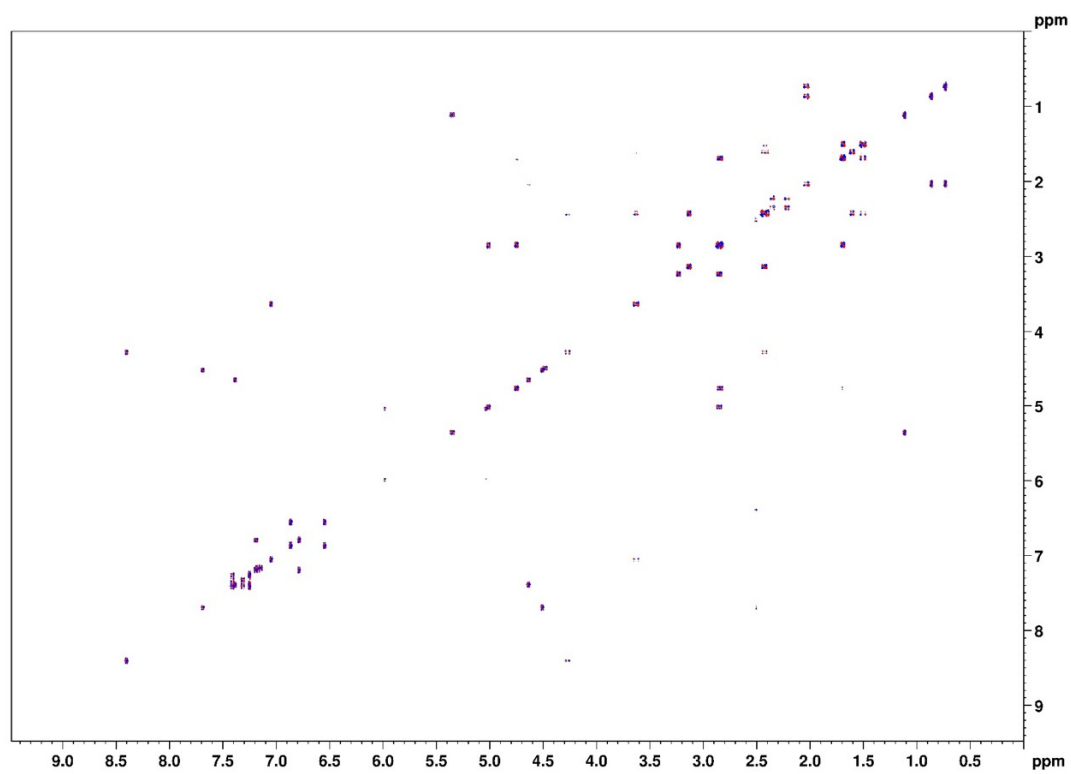


Figure S89. DQF-COSY spectrum of cyanopeptolin CP 941 in DMSO-d₆.

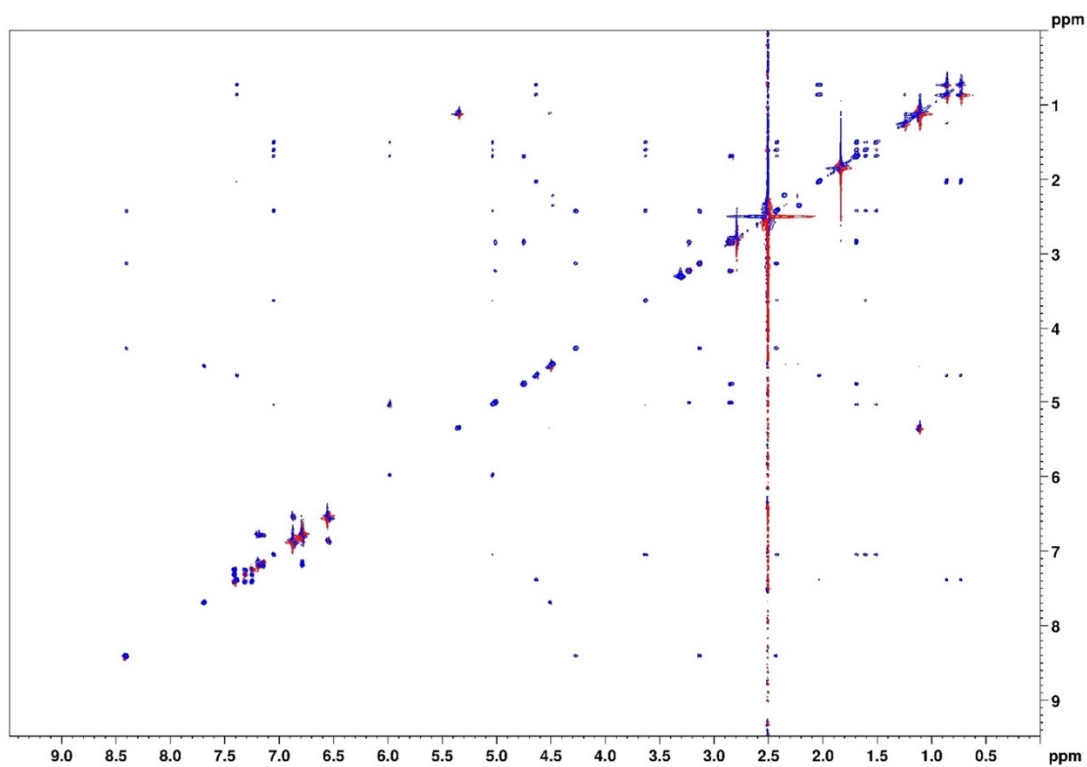


Figure S90. TOCSY spectrum of cyanopeptolin CP 941 in DMSO-d₆.

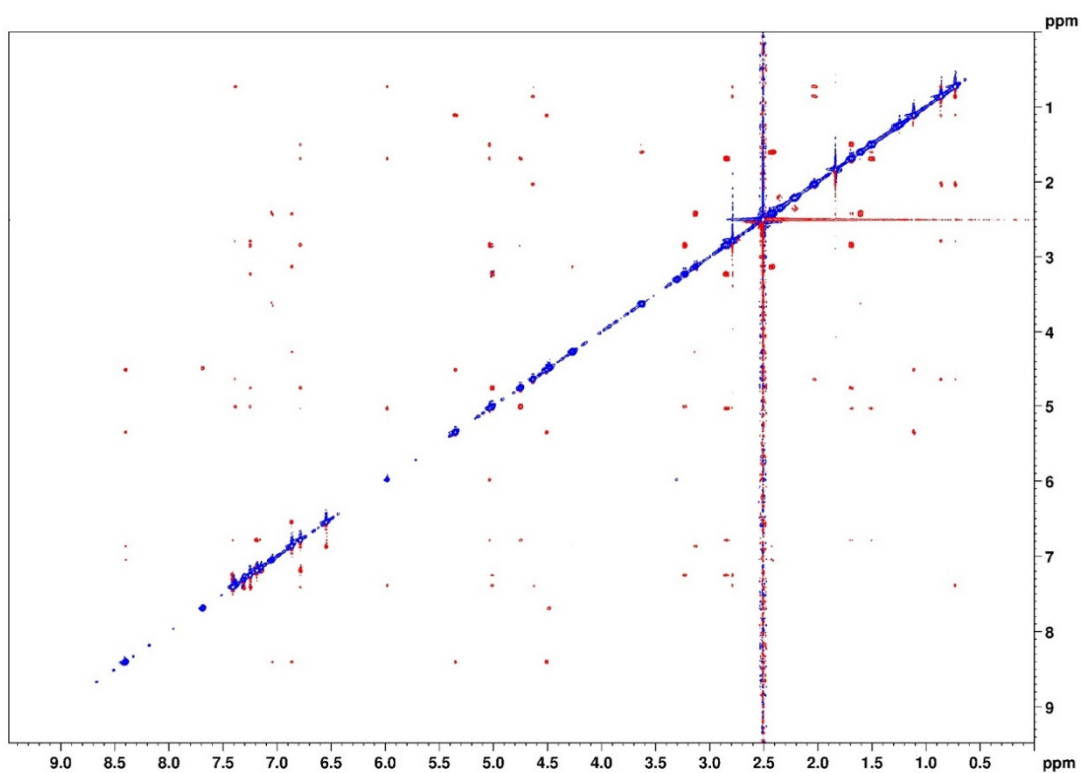


Figure S91. ROESY spectrum of cyanopeptolin CP 941 in DMSO-d₆.

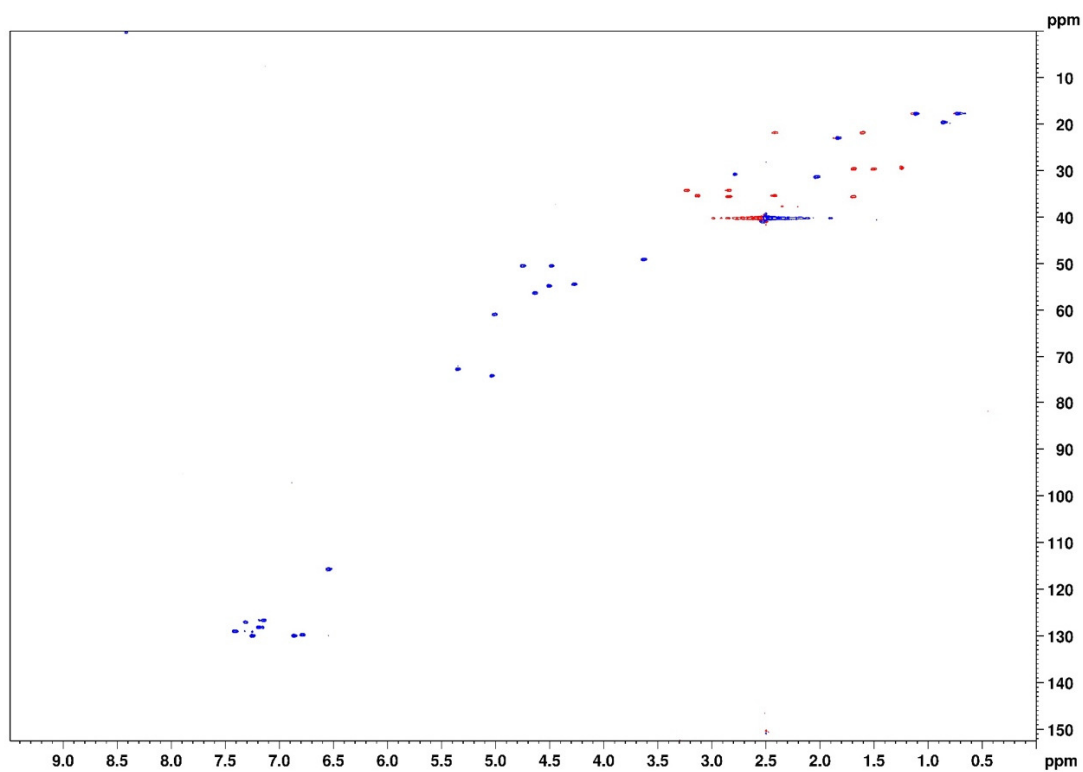


Figure S92. HSQC spectrum of cyanopeptolin CP 941 in DMSO-d₆.

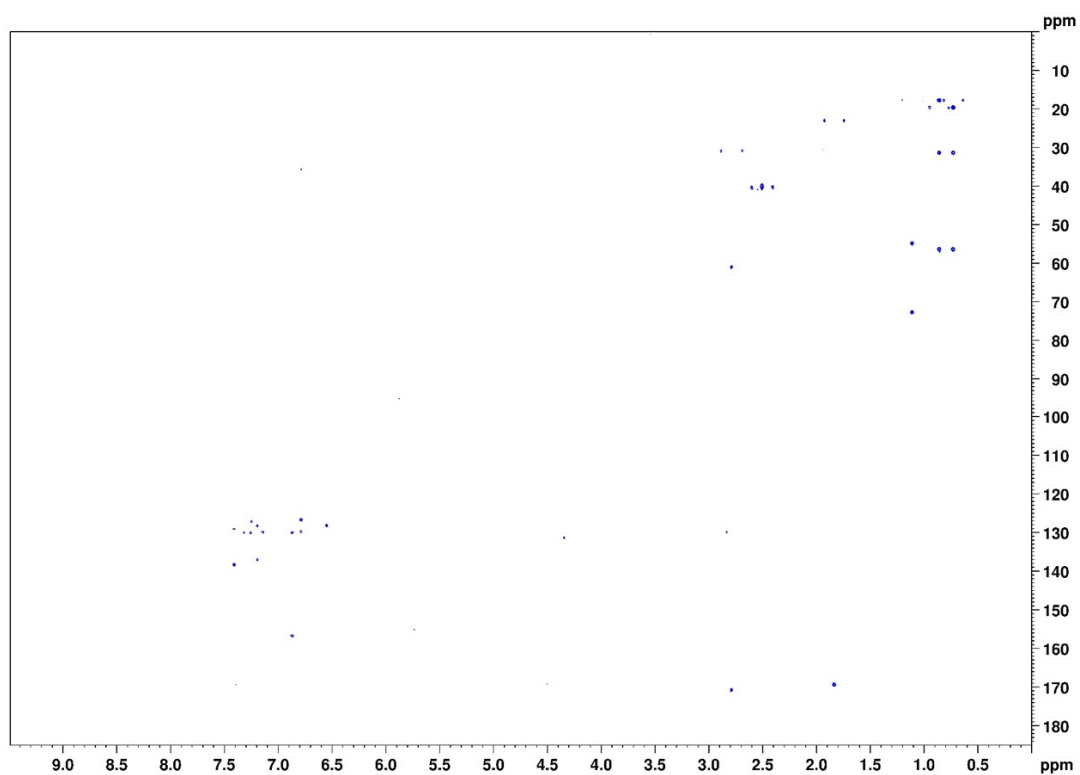


Figure S93. HMBC spectrum of cyanopeptolin CP 941 in DMSO-d₆.

Table S5. NMR Spectroscopic Data for cyanopeptolin CP 999 – BA-Asp-[Thr-Tyr-Ahp-Phe-MeTyr(OMe)-Val].

Residue	Position	δ_C	δ_H (J in Hz)	ROESY	HMBC ^a
BA	1	172			
	2	37.9	2.05, t (7.0)		BA-1, BA-3, BA-4
	3	19.2	1.53, q (7.3)		BA-1, BA-2, BA-4
	4	14.1	0.88, t (7.3)		BA-2, BA-3
Asp	1	<i>nd</i>			
	2	50.6	4.47, m	Thr-NH	
	3a	38.7	2.30, m		
	3b		2.12, m		
	4	<i>nd</i>			
Thr	NH		8.77, m		
	1	<i>nd</i>			
	2	54.7	4.54, d (9.9)	Tyr-NH	
	3	72.8	5.35, m	Tyr-NH	
	4	17.6	1.11, d (6.5)		Thr-2, Thr-3
Tyr	NH		7.68, d (8.5)	Asp-2	
	1	<i>nd</i>			
	2	54.7	4.22, m	Ahp-NH	
	3a	35.6	3.13, dd (10.4, 3.6)	Tyr-2'/6'	
	3b		2.38, m	Tyr-2'/6'	
Ahp	1'	128.0			
	2'/6'	129.9	6.84, d (8.5)	Tyr-3a, Tyr-3b	Tyr-3, Tyr-4'
	3'/5'	115.9	6.53, d (8.0)		Tyr-1'
	4'	156.9			
	NH		8.42, d (9.3)	Thr-2, Thr-3	
Phe	1	<i>nd</i>			
	2	49.1	3.67, m		
	3a	21.9	2.44, m		
	3b		1.61, m		
	4a	29.7	1.71, m		
	4b		1.54, m	Phe-2'/6'	
	5	74.2	5.06, brs	Phe-3a	
	NH		7.03, d (9.3)	Tyr-2	
N,O-MeTyr	OH		6.01		
	1	170.9			
	2	50.7	4.70, dd (6.8, 4.5)	MeTyr(OMe)-2	
	3a	35.8	2.87, dd (2.3, 11.8)	Ahp-5, Phe-2'/6'	Phe-2'/6'
	3b		1.79, dd (10.5, 3.8)	Phe-2'/6'	
	1'	137.2			
	2'/6'	129.7	6.79, d (7.2)	Phe-3a, Phe-3b, Ahp-4b	Phe-3, Phe-4'
	3'/5'	128.2	7.19, t (7.5)		Phe-1', Phe-2'/6'
Val	4'	126.7	7.15 ^b		Phe-2'/6'
	1	169.5			
	2	61.3	4.91, dd (8.9, 2.4)	Phe-2, Val-NH	
	3a	33.3	3.18, m	MeTyr(OMe)-2'/6'	
	3b		2.76, m	MeTyr(OMe)-2'/6'	
	1'	129.9			
	2'/6'	131.0	7.14 ^b	MeTyr(OMe)-3a,	MeTyr(OMe)-3, MeTyr(OMe)-4'
	3'/5'	114.5	6.97, d (8.8)	MeTyr(OMe)-3b	MeTyr(OMe)-1'
Val	4'	158.6			
	OCH ₃	55.5	3.71, s		MeTyr(OMe)-4'
	NCH ₃	30.8	2.77, s		MeTyr(OMe)-2, Phe-1
	1	<i>nd</i>			
	2	56.2	4.61, dd (5.0, 4.5)		
	3	31.3	2.02, m		
	4	19.8	0.86, d (6.8)		Val-2, Val-3, Val-5
	5	17.7	0.73, d (6.8)		Val-2, Val-3, Val-4
	NH		7.37, d (9.5)		MeTyr(OMe)-1

^a HMBC correlations are given from proton(s) stated to the indicated carbon atom; ^b assignments with the same superscript are overlapping; *nd* – resonances not detected

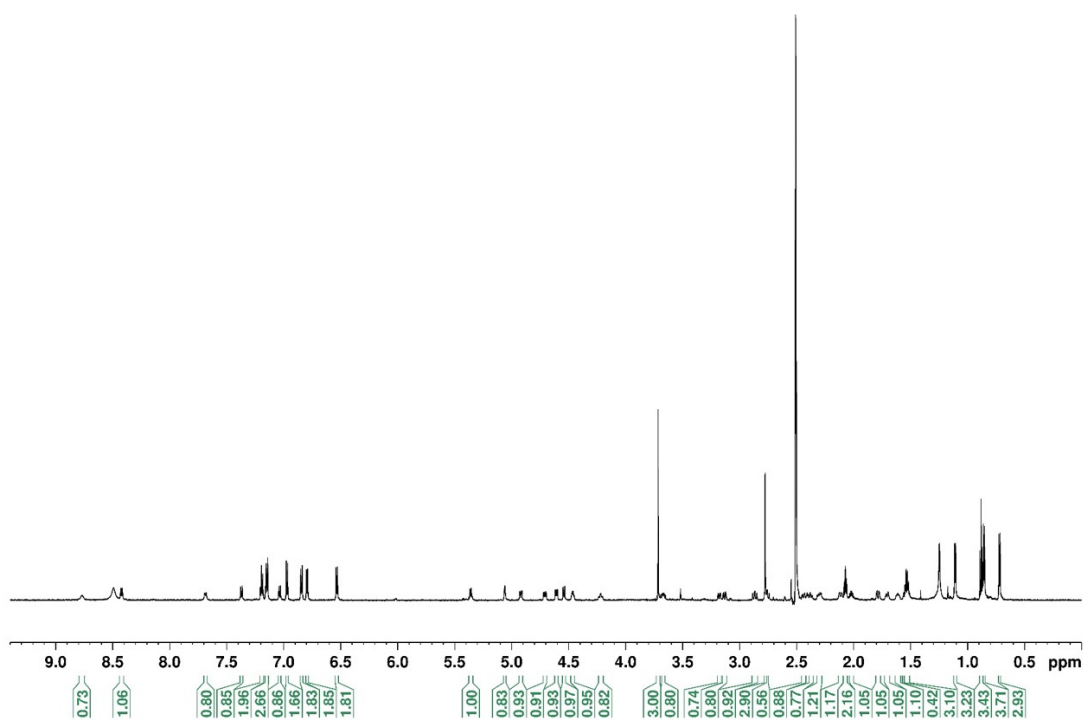


Figure S94. ^1H NMR spectrum of cyanopeptolin CP 999 in DMSO-d_6 .

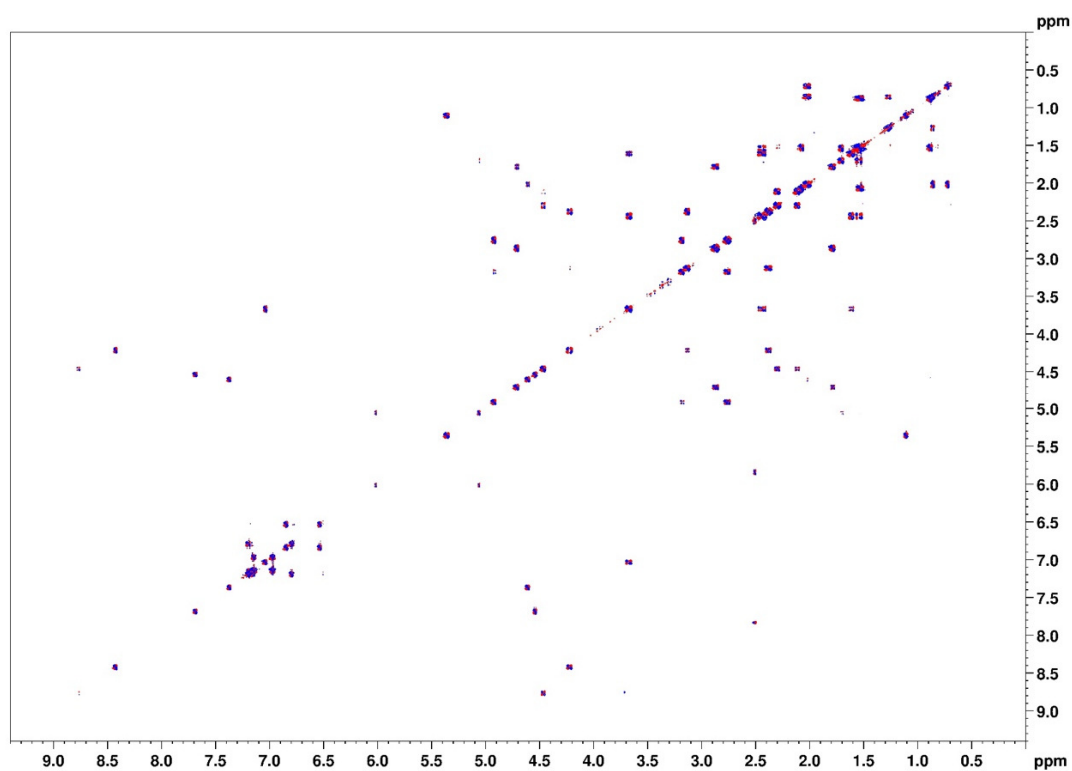


Figure S95. DQF-COSY spectrum of cyanopeptolin CP 999 in DMSO-d_6 .

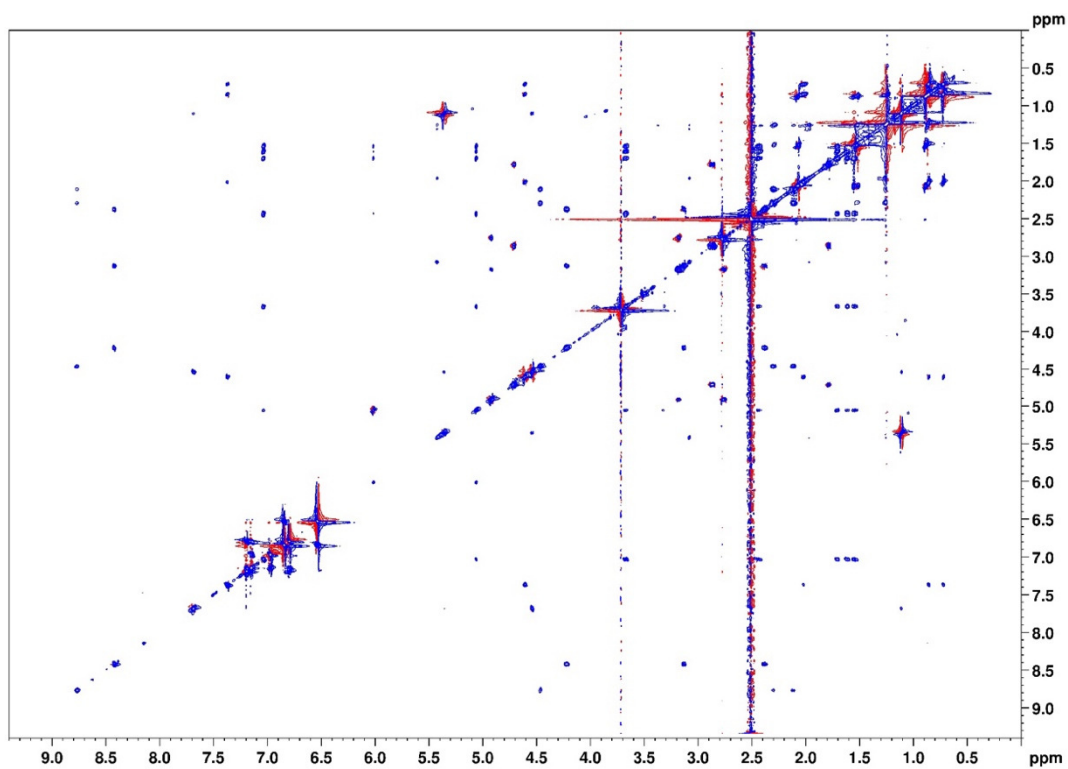


Figure S96. TOCSY spectrum of cyanopeptolin CP 999 in DMSO-d₆.

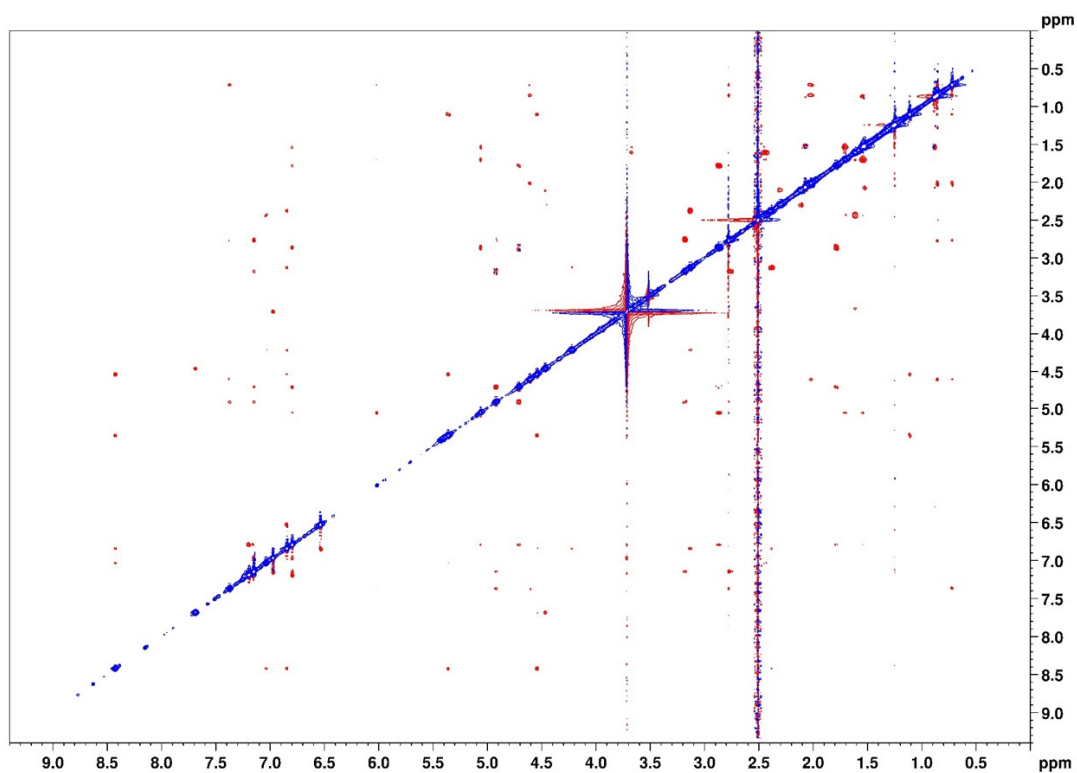


Figure S97. ROESY spectrum of cyanopeptolin CP 999 in DMSO-d₆.

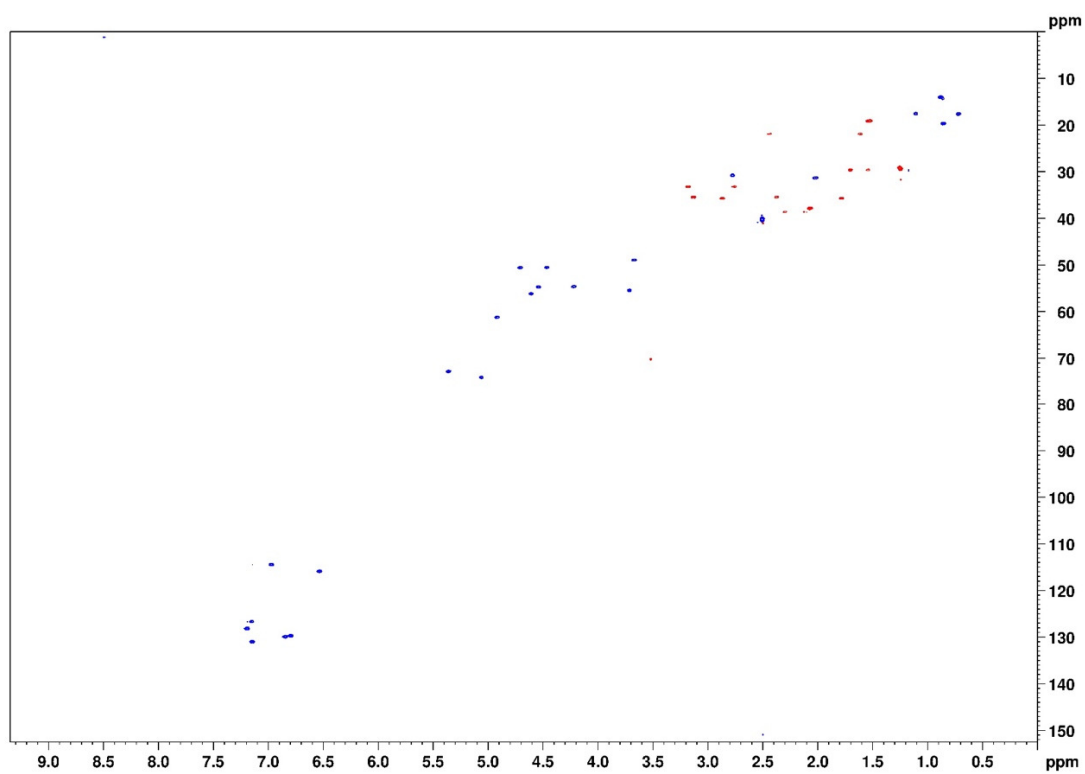


Figure S98. HSQC spectrum of cyanopeptolin CP 999 in DMSO-d₆.

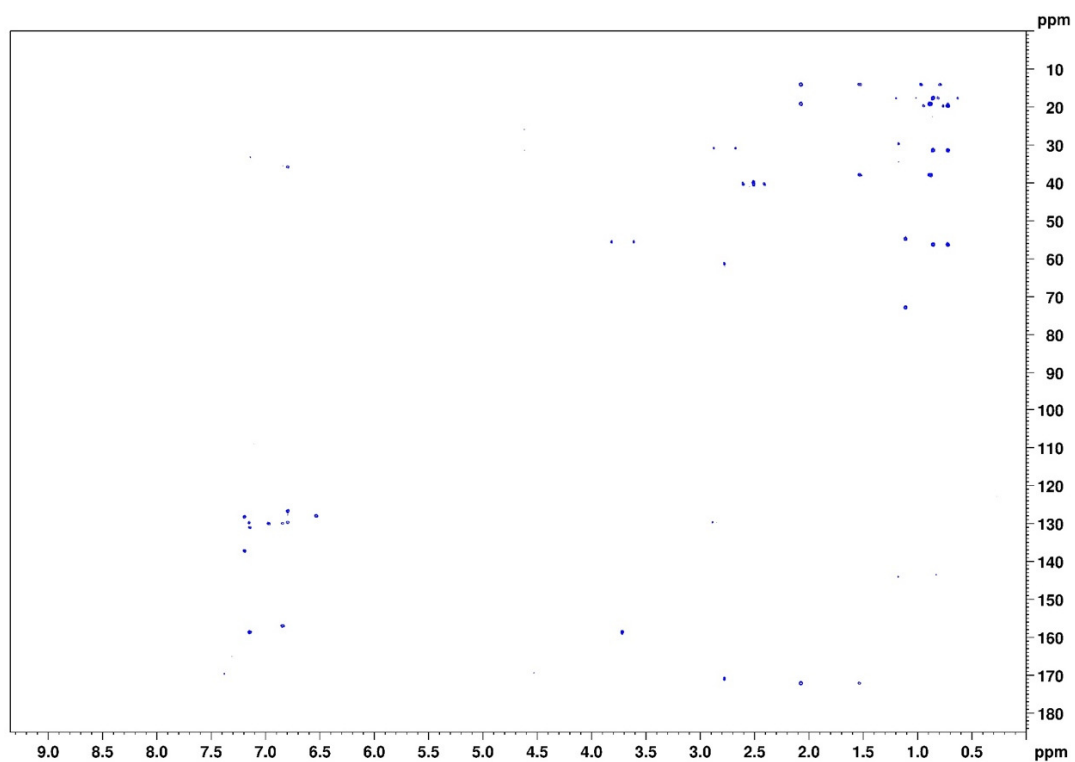


Figure S99. HMBC spectrum of cyanopeptolin CP 999 in DMSO-d₆.

Table S6. NMR Spectroscopic Data for cyanopeptolin CP 990 – HA-Asp-[Thr-Arg-Ahp-Phe-MePhe-Val]

Residue	Position	δ_c	δ_H (J in Hz)	ROESY	HMBC ^a
HA	1	172.3			
	2	35.5	2.09, t (7.3)		HA-1, HA-3, HA-4
	3	25.5	1.50, m		HA-1, HA-4, HA-5
	4	31.2	1.23, m		
	5	22.4	1.27, m		HA-4
	6	14.3	0.88 ^b , t		HA-4, HA-5
Asp	1	<i>nd</i>			
	2	50.8	4.52, m		
	3a	39.9	2.53, m		Asp-2
	3b		2.11, m		
	4	<i>nd</i>			
Thr	NH		8.00, d (8.1)		HA-1
	1	169.9			
	2	55.0	4.58, d (9.0)	Arg-NH	Thr-1
	3	72.2	5.31, q (6.6)	Arg-NH	Val-1
	4	17.9	1.14, d (6.6)		Thr-2, Thr-3
Arg	NH		7.23 ^c , d		
	1	170.3			
	2	50.9	4.15, m		
	3a	26.4	1.88, m		
	3b		1.45, m		
	4a	24.6	1.47, m		
	4b		1.17, m		
	5a	39.7	2.95, m		
	5b		2.89, m		
	6	<i>nd</i>		Thr-2, Thr-3	Thr-1
Ahp	NH		8.51, d (9.0)		
	1	<i>nd</i>			
	2	48.9	3.65, m		
	3a	21.9	2.42, m		
	3b		1.55, m		
	4a	29.6	1.69		
	4b		1.49, m	Phe-2'/6'	
	5	74.1	5.04	Phe-2'/6'	
Phe	NH		6.96, d (9.5)		Arg-1
	OH		6.01		
	1	170.7			
	2	50.6	4.74, dd (7.3, 4.4)	Phe-2'/6', MePhe-2	Phe-1
	3a	35.7	2.85, m	Phe-2'/6'	Phe-2'/6'
	3b		1.69, m	Phe-2'/6'	Phe-2'/6'
	1'	137.0			
	2'/6'	129.8	6.78, d (7.3)	Ahp-4b, Ahp-5, Phe-2, Phe-3a, Phe-3b	Phe-3, Phe-4'
MePhe	3'/5'	128.2	7.18, t (7.4)		Phe-1'
	4'	126.7	7.13, t (7.3)		Phe-2'/6'
	1	169.3			
	2	60.9	5.02	Phe-2, MePhe-2'/6', Val-NH	
	3a	34.4	3.23, dd (11.7, 2.7)	MePhe-2'/6'	
	3b		2.88, m	MePhe-2'/6'	
	1'	138.3			
	2'/6'	130.1	7.24 ^c , d	MePhe-2, MePhe-3a, MePhe-3b	MePhe-3, MePhe-4'
Val	3'/5'	129.1	7.42 ^d , t		MePhe-1'
	4'	127.1	7.32, t (7.4)		MePhe-2'/6'
	NCH ₃	30.9	2.80, s		MePhe-2, Phe-1
	1	172.6			
	2	56.3	4.71, dd (5.0, 4.3)		Val-1
	3	31.6	2.05, m		
	4	19.7	0.87 ^b , d		Val-2, Val-3, Val-5,
	5	17.9	0.74, d (6.8)		Thr-4
	NH		7.41 ^d , d	MePhe-2	Val-2, Val-3, Val-4
					MePhe-1

^a HMBC correlations are given from proton(s) stated to the indicated carbon atom; ^{b-d} assignments with the same superscript are overlapping; *nd* – resonances not detected

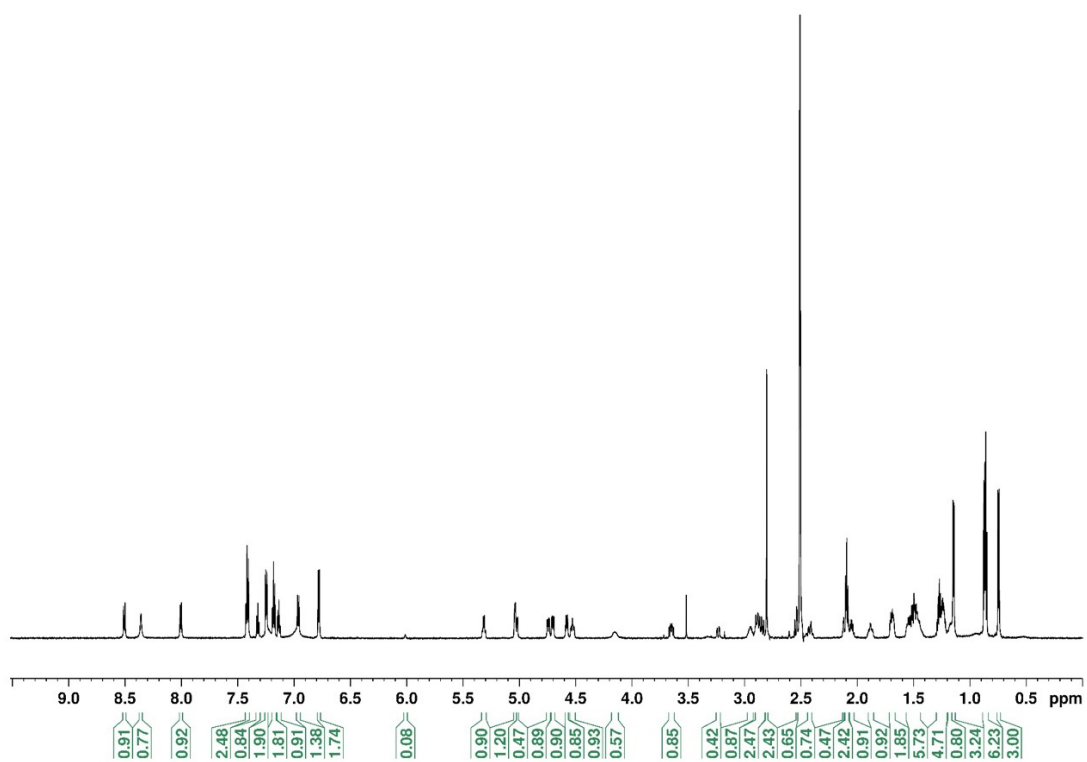


Figure S100. ^1H NMR spectrum of cyanopeptolin CP 990 in DMSO-d_6 .

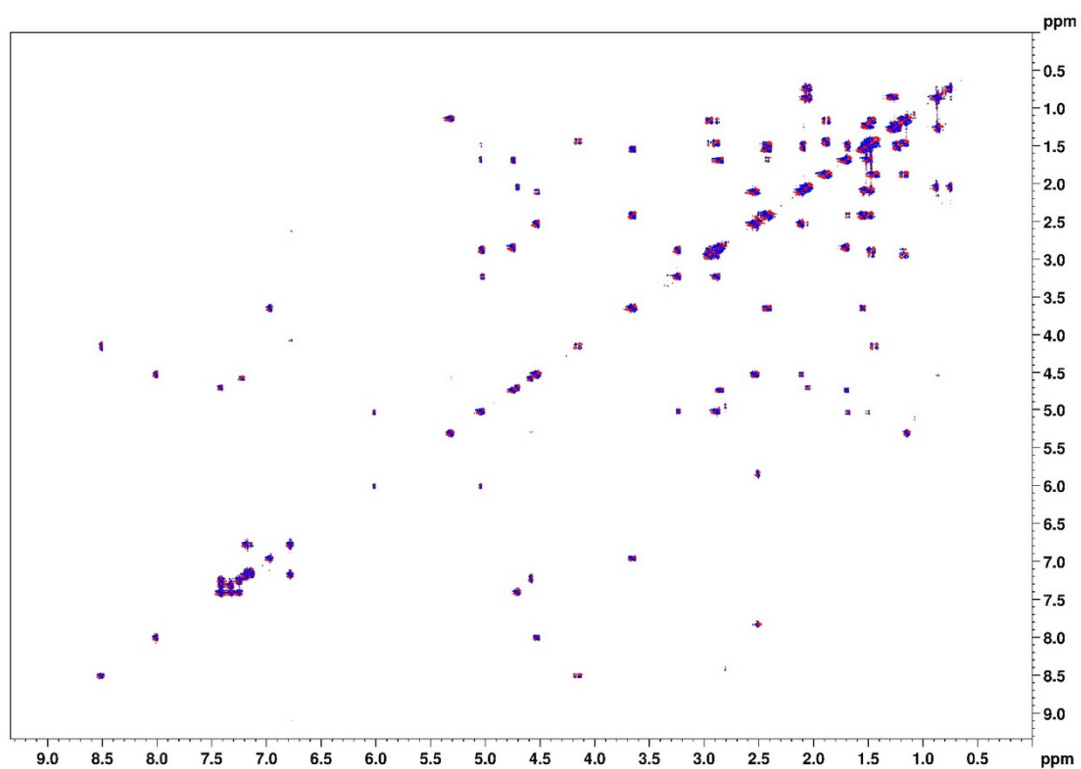


Figure S101. DQF-COSY spectrum of cyanopeptolin CP 990 in DMSO-d_6 .

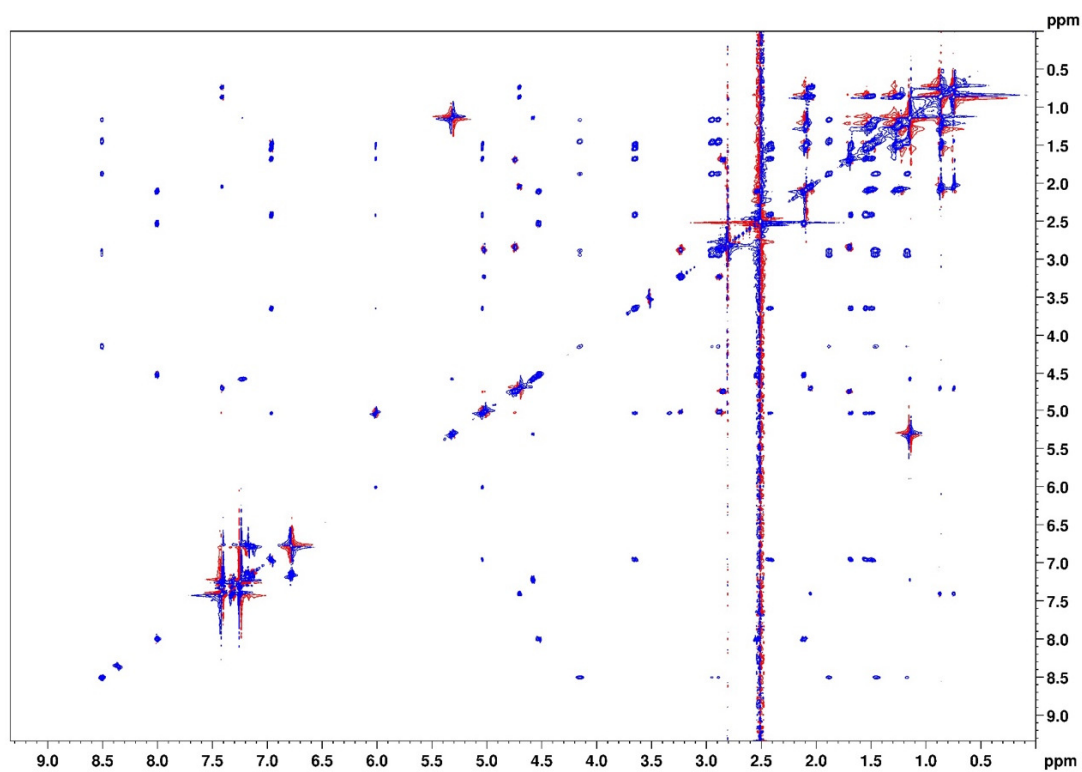


Figure S102. TOCSY spectrum of cyanopeptolin CP 990 in DMSO-d₆.

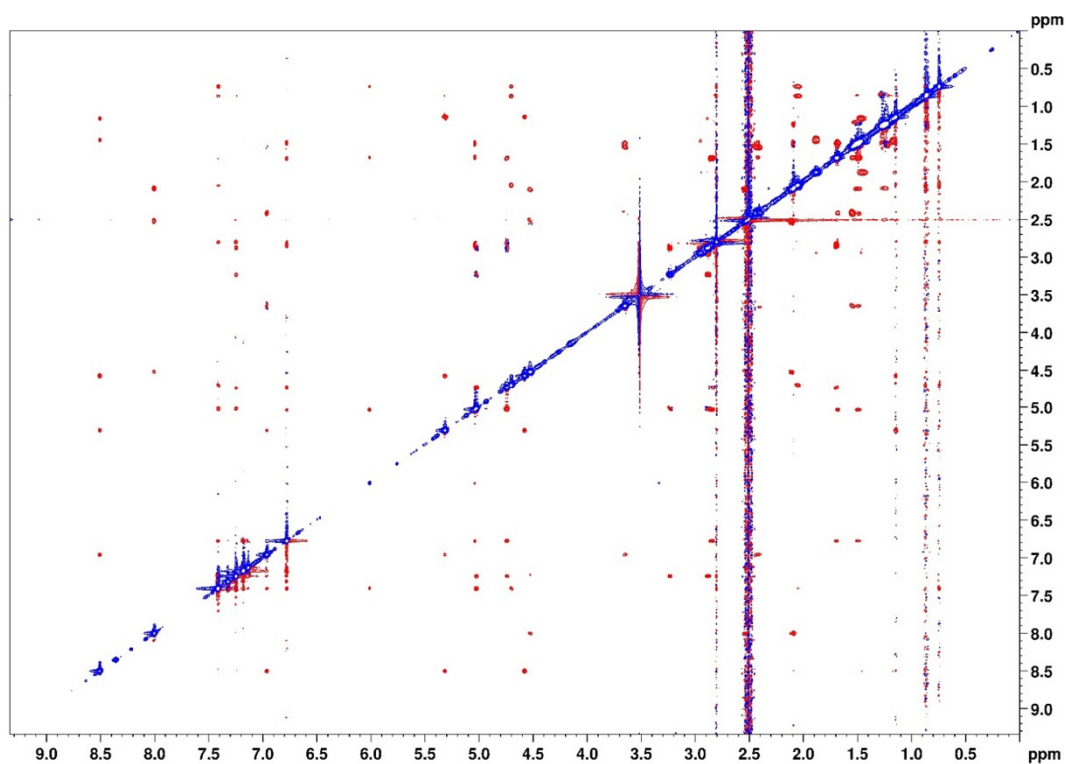


Figure S103. ROESY spectrum of cyanopeptolin CP 990 in DMSO-d₆.

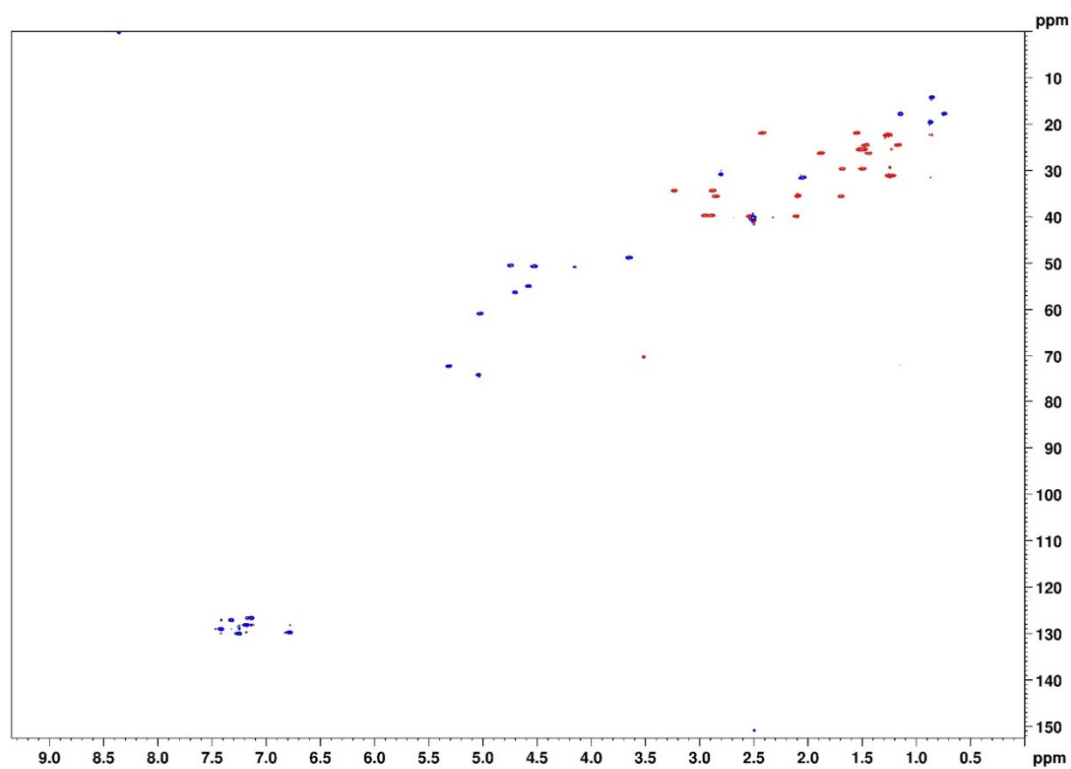


Figure S104. HSQC spectrum of cyanopeptolin CP 990 in DMSO-d₆.

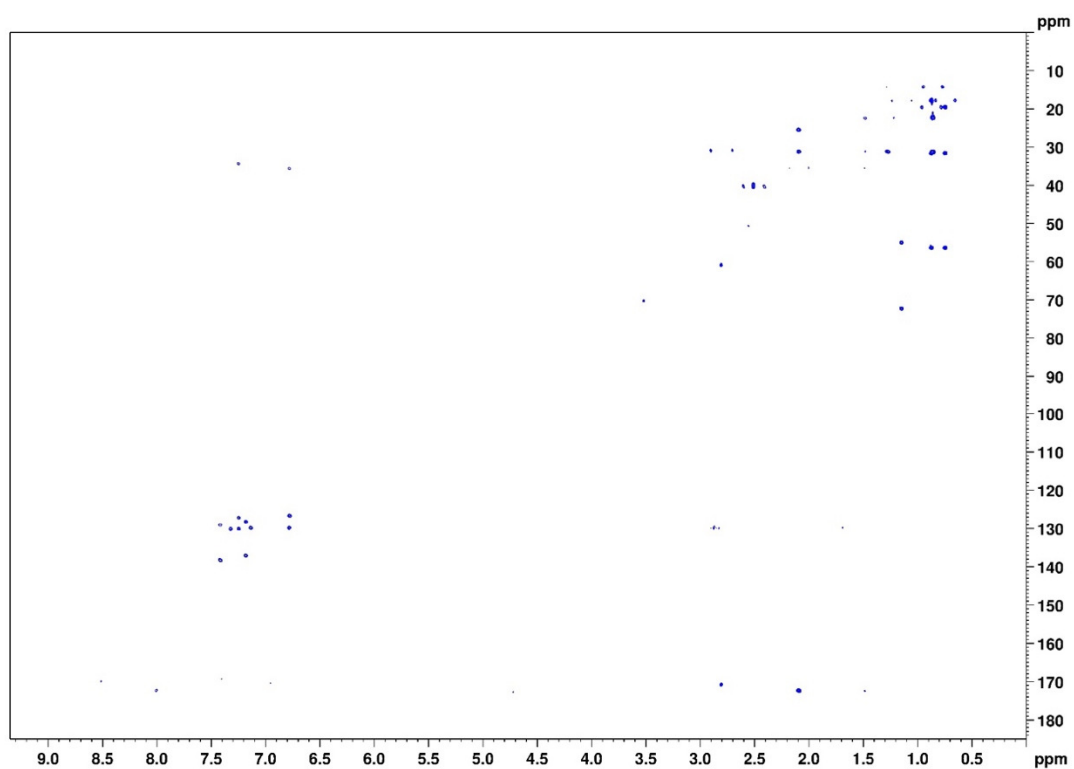


Figure S105. HMBC spectrum of cyanopeptolin CP 990 in DMSO-d₆.

Table S7. NMR Spectroscopic Data for cyanopeptolin CP 983 – BA-Asp-[Thr-Phe-Ahp-Phe-MeTyr(OMe)-Val].

Residue	Position	δ_c	δ_H (J in Hz)	ROESY	HMBC ^a
BA	1	172.7			
	2	37.8	2.11, t (6.9)	Asp-NH	BA-1, BA-3, BA-4
	3	19.2	1.54 ^e , m		BA-2, BA-4
	4	14.1	0.89, t (7.5)		BA-2, BA-3
Asp	1	<i>nd</i>			
	2	50.2	4.52, m		
	3a	<i>nd</i>	2.46, m		
	3b		2.36, m		
	4	<i>nd</i>			
Thr	NH		8.23, d (7.6)	BA-2	
	1	<i>nd</i>			
	2	54.8	4.48, m	Phe4-NH	
	3	72.6	5.35, m	Phe4-NH	
	4	18.0	1.13, d (6.7)		Thr-2, Thr-3
Phe4	NH		7.70, m		
	1	<i>nd</i>			
	2	53.9	4.39, m		
	3a	36.3	3.25, m	Phe4-2'/6'	
	3b		2.62, m	Phe4-2'/6'	
	1'	137.7/138.6 ^b			
	2'/6'	126.6-131.0 ^c	7.11-7.14 ^c	Phe4-3a, Phe4-3b	
	3'/5'	126.5/128.3 ^d	7.17-7.19 ^d		
	4'	126.6-131.0 ^c	7.11-7.14 ^c		
	NH		8.55, d (8.4)	Thr-2, Thr-3	
Ahp	1	<i>nd</i>			
	2	49.4	3.64, m		
	3a	21.9	2.41, m		
	3b		1.64, m		
	4a	29.7	1.71, m		
	4b		1.56 ^e , m	Phe6-2'/6'	
	5	74.2	5.06, brs	Phe6-3a, Phe6-2'/6'	
	NH		7.08, d (9.2)		
	OH		6.02		
Phe6	1	170.8			
	2	50.7	4.70, m	Phe6-2'/6'	
	3a	35.8	2.87, m	Ahp-5, Phe6-2'/6'	
	3b		1.79, m	Phe6-2'/6'	
	1'	137.7/138.6 ^b			
	2'/6'	129.8	6.79, d (7.1)	Phe6-2, Phe6-3a, Phe6-3b, Ahp-4b, Ahp-5	
	3'/5'	126.5/128.3 ^d	7.17-7.19 ^d		
	4'	126.6-131.0 ^c	7.11-7.14 ^c		
MeTyr(OMe)	1	<i>nd</i>			
	2	61.3	4.92, m	Val-NH	
	3a	33.3	3.17, m		
	3b		2.77, m		MeTyr(OMe)-2
	1'	<i>nd</i>			
	2'/6'	126.6-131.0 ^c	7.11-7.14 ^c	MeTyr(OMe)-3a, MeTyr(OMe)-3b	MeTyr(OMe)-3
	3'/5'	114.5	6.96, d (8.6)	MeTyr(OMe)-OCH ₃	
	4'	158.6			
	OCH ₃	55.5	3.71, s		MeTyr(OMe)-4'
	NCH ₃	30.8	2.78, s	MeTyr(OMe)-3'/5'	Phe6-1
Val	1	<i>nd</i>			
	2	56.3	4.63, m		
	3	31.4	2.03, m		
	4	19.7	0.86, d (6.9)		Val-2, Val-3, Val-5
	5	17.8	0.72, d (6.9)		Val-2, Val-3, Val-4
	NH		7.42, d (9.4)	MeTyr(OMe)-2	

^a HMBC correlations are given from proton(s) stated to the indicated carbon atom; ^{c,d} low amount of the sample made the unambiguous assignments of the aromatic signals impossible; ^e assignments are overlapping; *nd* – resonances not detected

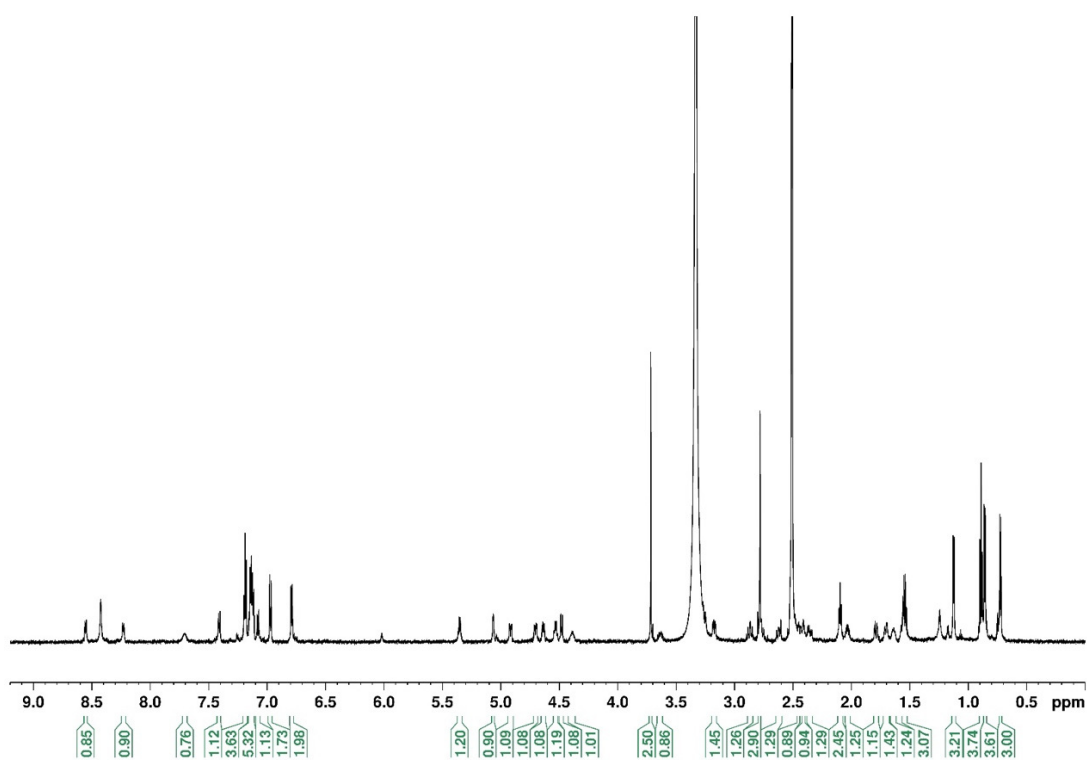


Figure S106. ^1H NMR spectrum of cyanopeptolin CP 983 in DMSO-d_6 .

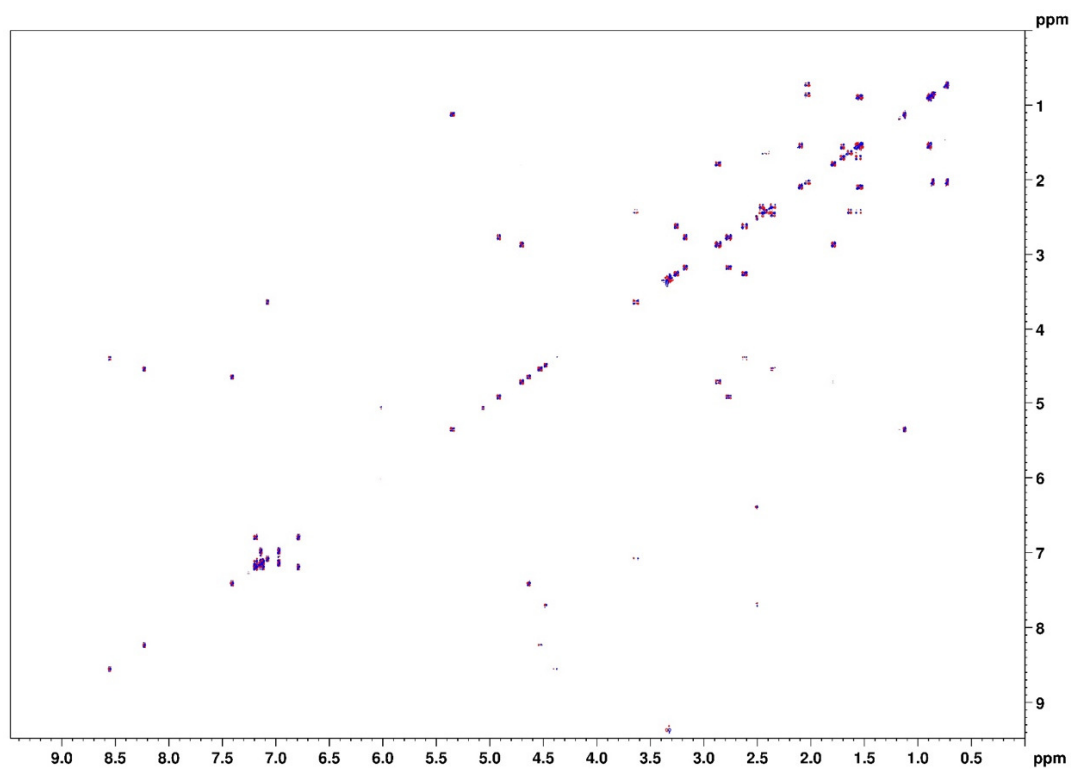


Figure S107. DQF-COSY spectrum of cyanopeptolin CP 983 in DMSO-d_6 .

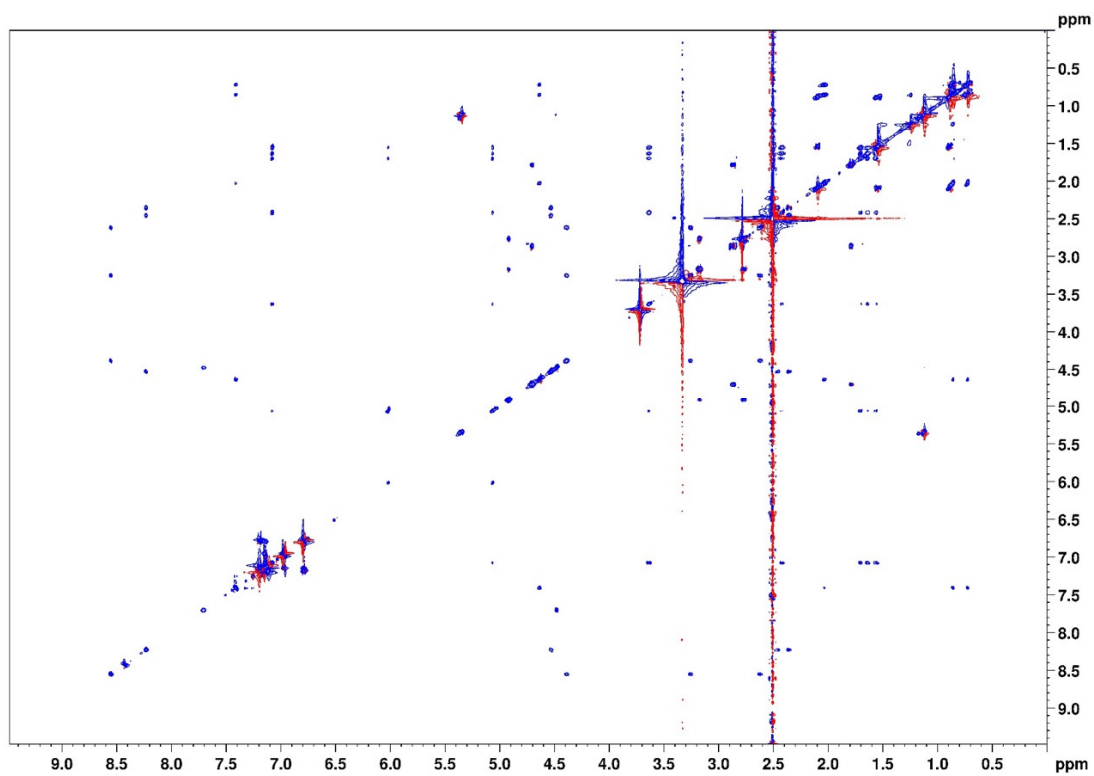


Figure S108. TOCSY spectrum of cyanopeptolin CP 983 in DMSO-d₆.

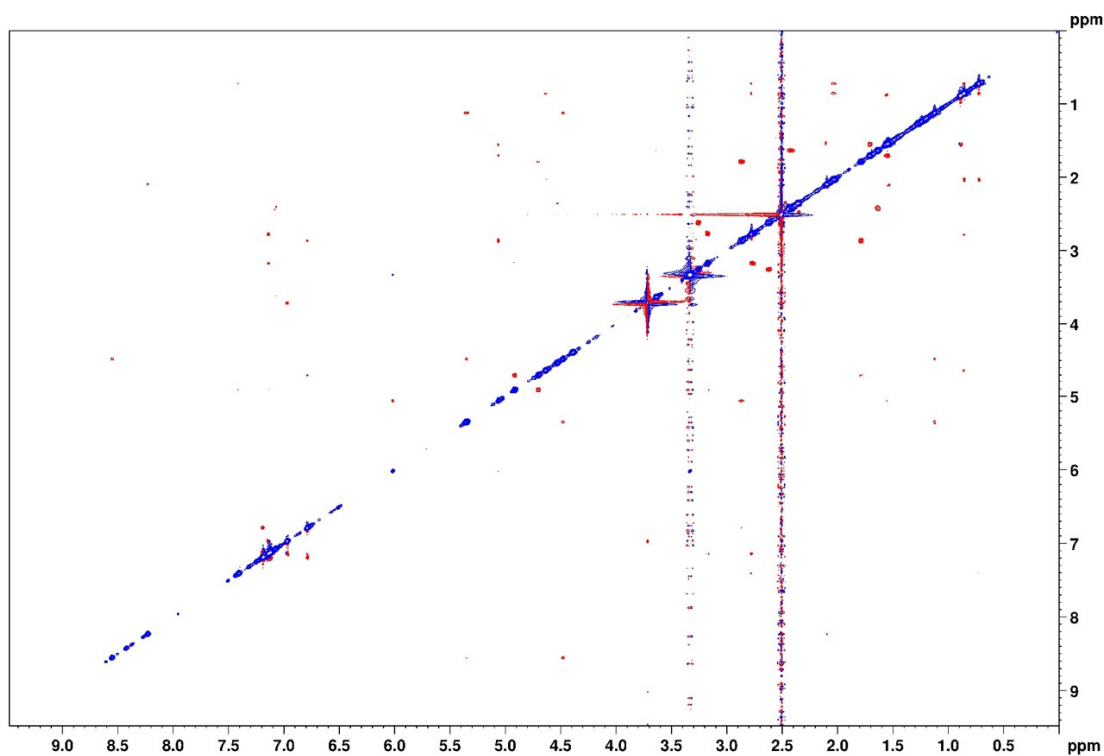


Figure S109. ROESY spectrum of cyanopeptolin CP 983 in DMSO-d₆.

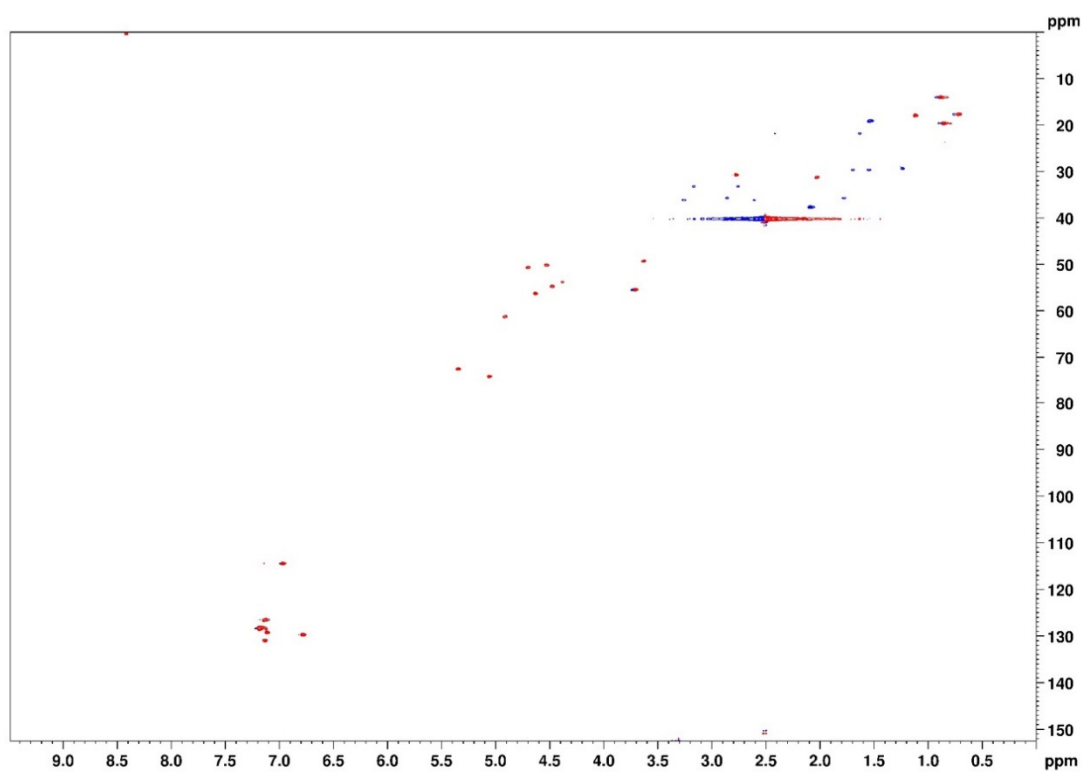


Figure S110. HSQC spectrum of cyanopeptolin CP 983 in DMSO-d₆.

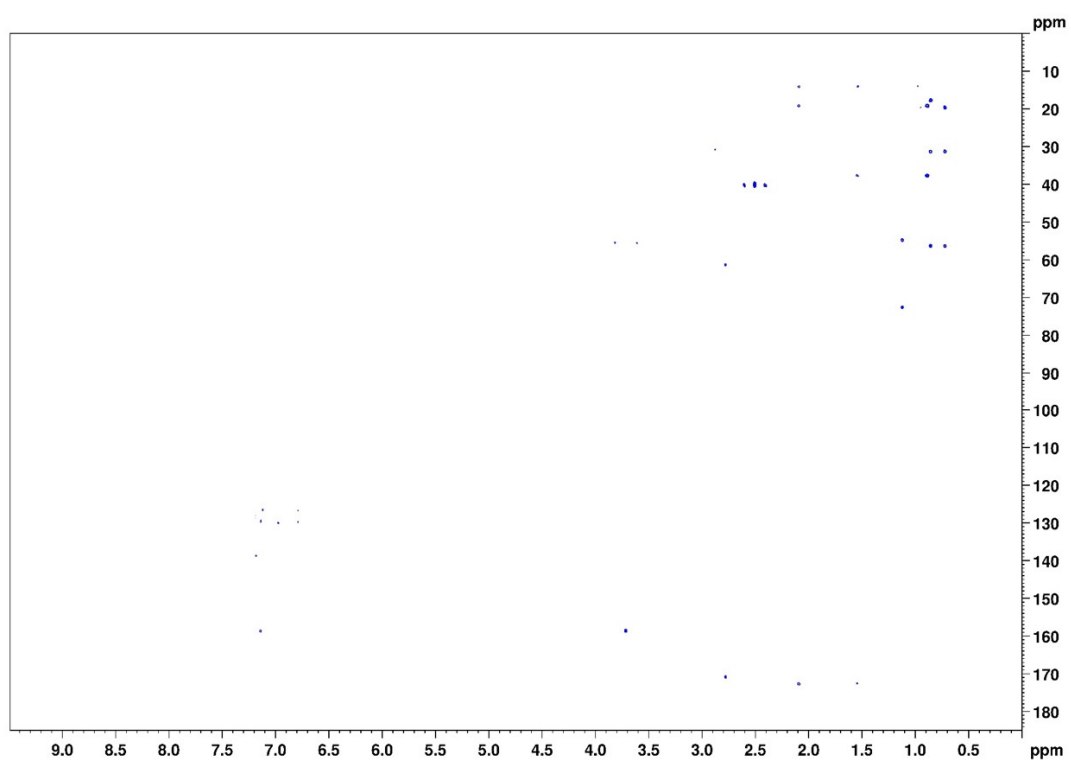


Figure S111. HMBC spectrum of cyanopeptolin CP 983 in DMSO-d₆.

Table S8. NMR Spectroscopic Data for cyanopeptolin CP 949 – BA-Asp-[Thr-Leu-Ahp-Phe-MeTyr(OMe)-Val]

Residue	Position	δ_C	δ_H	ROESY	HMBC ^a
BA	1	172.8			
	2	37.7	2.11		BA-1
	3	19.2	1.55		BA-1, BA-2
	4	14.1	0.90		BA-2, BA-3
Asp	1	<i>nd</i>			
	2	50.1	4.64	Thr-NH	
	3a	36.9	2.66		
	3b		2.45		
	4	<i>nd</i>			
Thr	NH		8.25		
	1	<i>nd</i>			
	2	55.0	4.55	Leu-NH	
	3	72.5	5.37	Leu-NH	
	4	18.2	1.17		
Leu	NH		7.71	Asp-2	
	1	<i>nd</i>			
	2	50.9	4.18		
	3a	39.5	1.71		
	3b		1.31		
Ahp	4	24.6	1.45		
	5	23.7	0.84		Leu-4
	6	21.5	0.75		
	NH		8.39	Thr-2, Thr-3	
	1	<i>nd</i>			
	2	49.1	3.63		
	3a	22.0	2.41		
	3b		1.58		
	4a	29.8	1.70		
	4b		1.52		
Phe	5	74.2	5.07	Phe-3a	
	NH		7.07		
	OH				
	1	170.8			
	2	50.7	4.71	Phe-2'/6'	
	3a	35.8	2.86	Ahp-5, Phe-2'/6'	
	3b		1.78	Phe-2'/6'	
	1'	<i>nd</i>			
	2'/6'	129.7	6.78	Phe-2, Phe-3a, Phe-3b	
	3'/5'	128.2	7.17		
MeTyr(OMe)	4'	126.7	7.13		
	1				
	2	61.3	4.94	Val-NH	
	3a	33.2	3.20	MeTyr(OMe)-2'/6'	
	3b		2.78	MeTyr(OMe)-2'/6'	
	1'	<i>nd</i>			
	2'/6'	131.0	7.15	MeTyr(OMe)-3a, MeTyr(OMe)-3b	MeTyr(OMe)-4'
	3'/5'	114.5	6.98	MeTyr(OMe)-OCH ₃	
	4'	158.6			
	OCH ₃	55.6	3.72	MeTyr(OMe)-3'/5'	MeTyr(OMe)-4'
Val	NCH ₃	30.8	2.78		Phe-1
	1	<i>nd</i>			
	2	56.3	4.67		
	3	31.3	2.05		
	4	19.7	0.88		Val-2, Val-3, Val-5
	5	17.8	0.74		Val-2, Val-3, Val-4
	NH		7.43	MeTyr(OMe)-2	

^a HMBC correlations are given from proton(s) stated to the indicated carbon atom; *nd* – resonances not detected

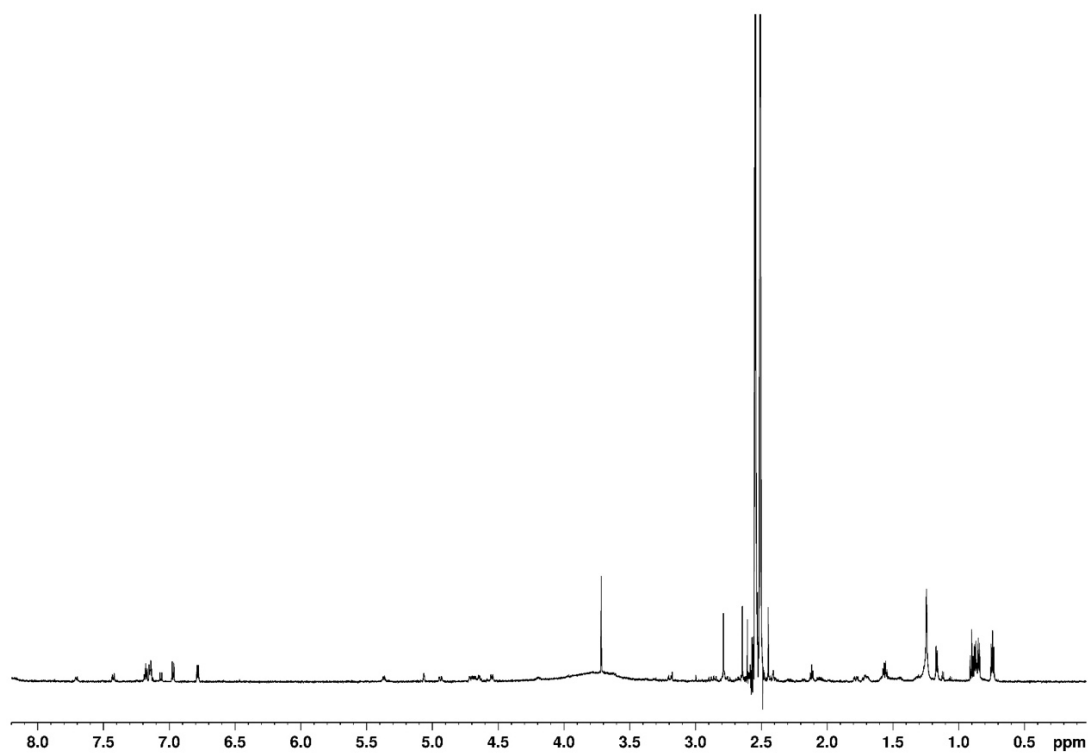


Figure S112. ^1H NMR spectrum of cyanopeptolin CP 949 in DMSO-d_6 .

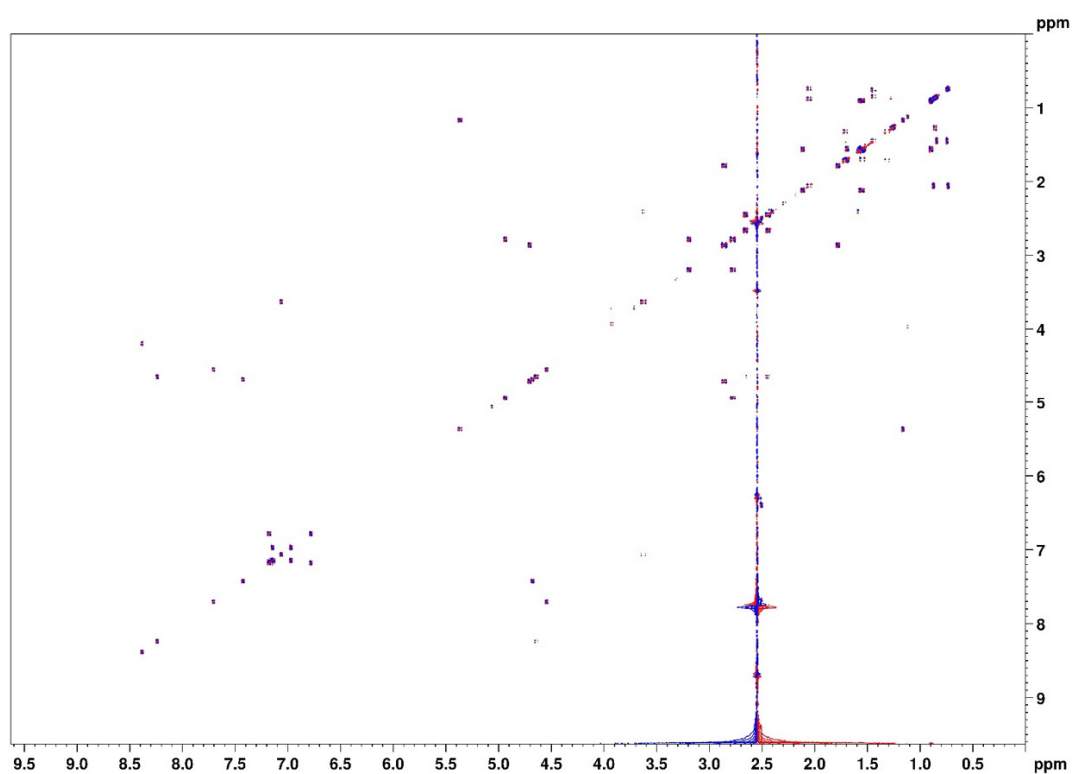


Figure S113. DQF-COSY spectrum of cyanopeptolin CP 949 in DMSO-d_6 .

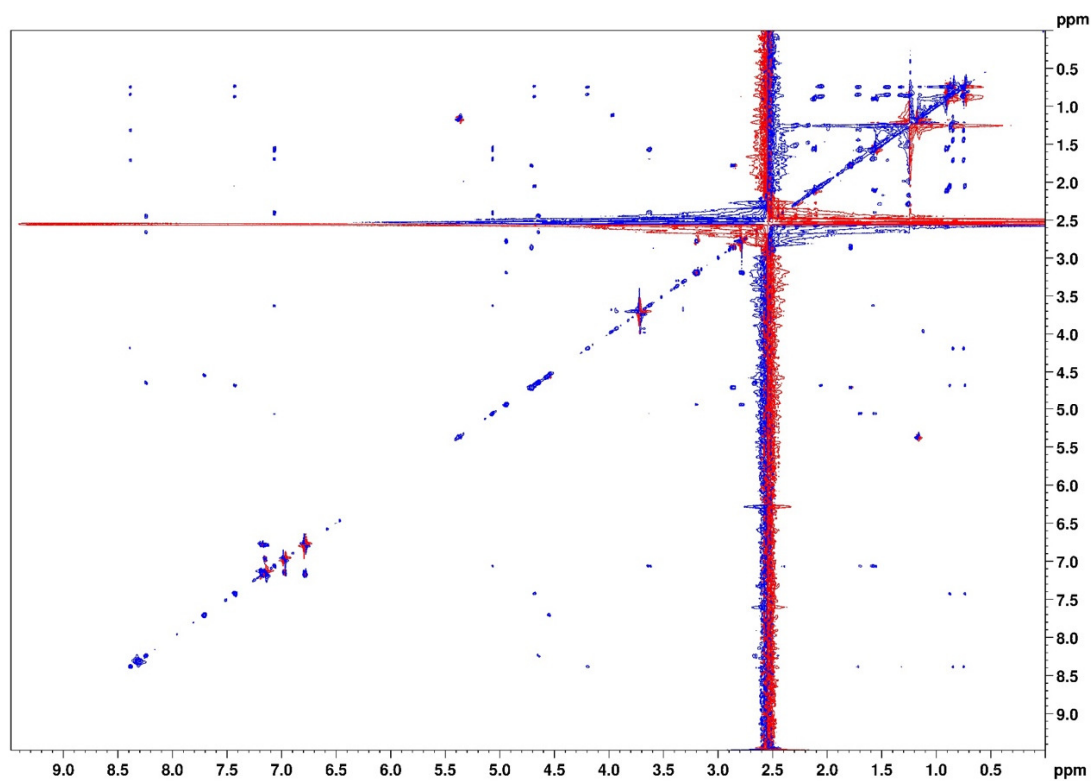


Figure S114. TOCSY spectrum of cyanopeptolin CP 949 in DMSO-d₆.

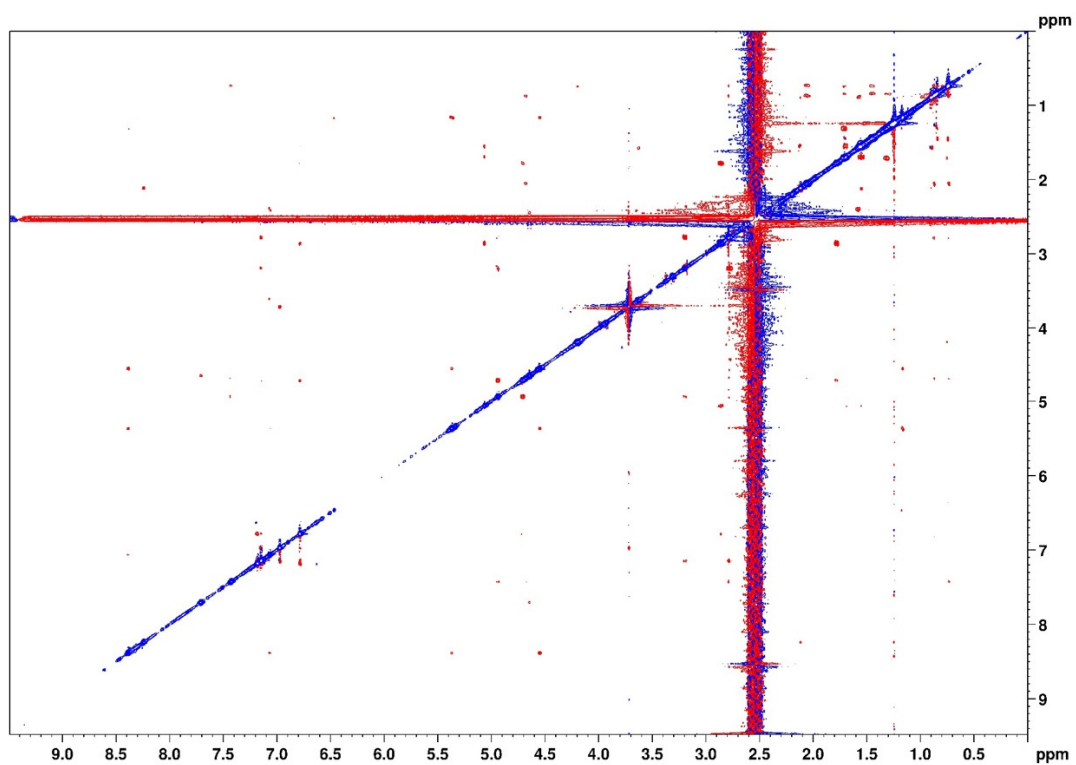


Figure S115. ROESY spectrum of cyanopeptolin CP 949 in DMSO-d₆.

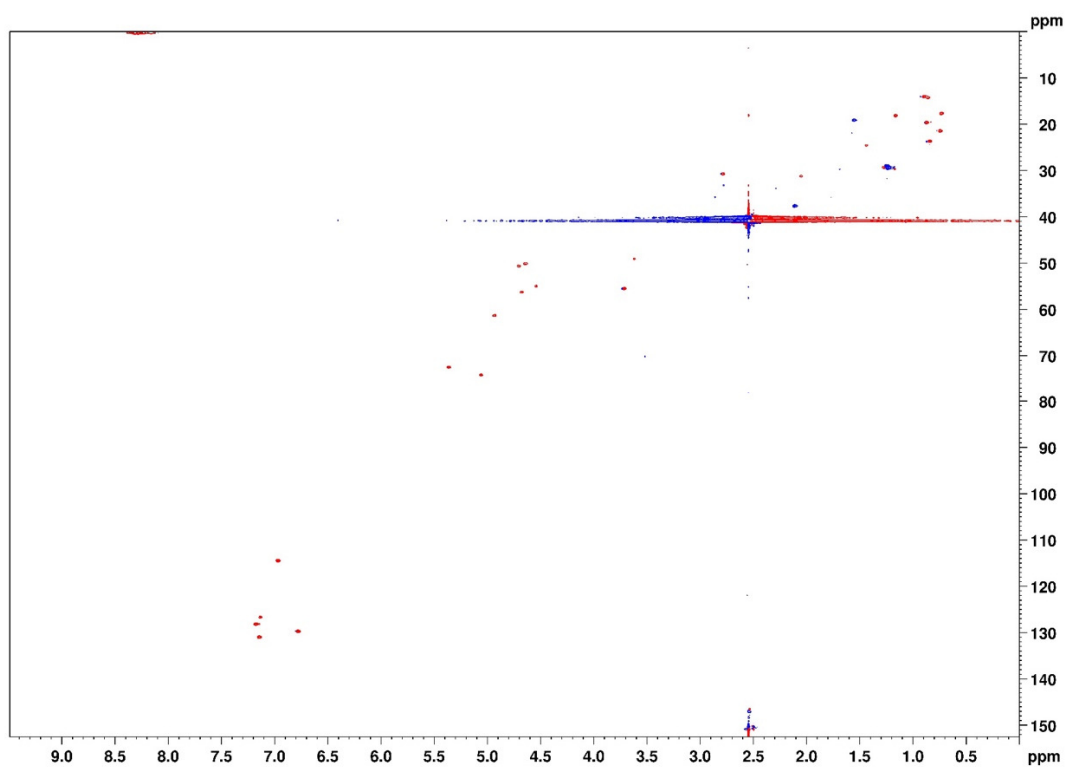


Figure S116. HSQC spectrum of cyanopectolin CP 949 in DMSO-d₆.

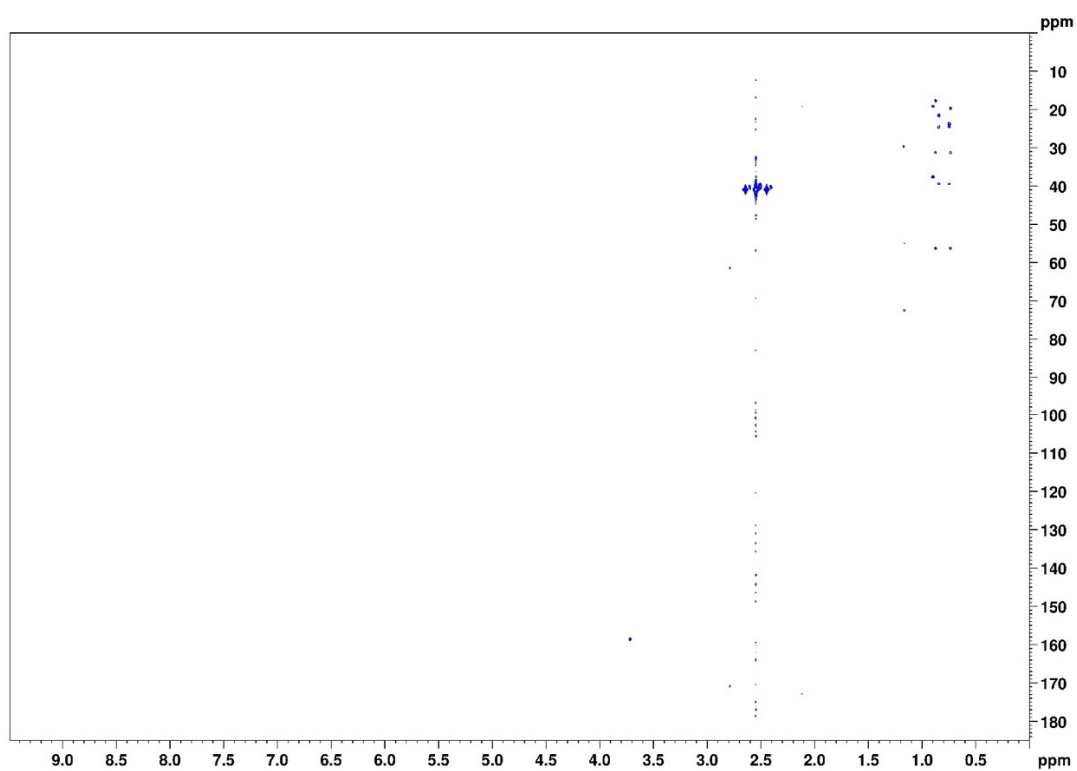


Figure S117. HMBC spectrum of cyanopectolin CP 949 in DMSO-d₆.

Table S9. NMR Spectroscopic Data for cyanopeptolin CP 919 – BA-Asp-[Thr-Leu-Ahp-Phe-MePhe-Val].

Residue	Position	δ_c	δ_H (J in Hz)	ROESY	HMBC ^a
BA	1	172.2			
	2	37.9	2.11, t (7.2)	Asp-NH	BA-1, BA-3, BA-4
	3	19.4	1.54, q (7.3)		BA-1, BA-2, BA-4
	4	14.1	0.89 ^b , t		BA-2, BA-3
Asp	1	<i>nd</i>			
	2	50.6	4.58, m		
	3a	40.9	2.35, m		
	3b		2.27, m		
	4	<i>nd</i>			
Thr	NH		8.19, m	BA-2	
	1	<i>nd</i>			
	2	55.1	4.53, d (8.7)	Leu-NH	
	3	72.7	5.36, m	Leu-NH	
	4	18.4	1.19, d (6.5)		Thr-2, Thr-3
Leu	NH		<i>nd</i>		
	1	<i>nd</i>			
	2	51.1	4.16, m		
	3a	39.3	1.71 ^c , m		
	3b		1.35, m		
	4	24.6	1.45, m		
	5	23.8	0.84, d (6.7)		Leu-6
	6	21.5	0.75 ^d , d		Leu-5
Ahp	NH		8.40, m	Thr-2, Thr-3	
	1	<i>nd</i>			
	2	49.1	3.62, m		
	3a	22.3	2.39, m		
	3b		1.56, m		
	4a	29.5	1.69, m		
	4b		1.51, m		
	5	74.1	5.04 ^e , m		
	NH		7.07, d (9.4)		
	OH		6.09		
Phe	1	170.9			
	2	50.3	4.75, m	MePhe-2	
	3a	35.8	2.84 ^f , m	Phe-2'/6'	
	3b		1.71 ^c , m	Phe-2'/6'	
	1'	137.2			
	2'/6'	129.8	6.78, d (6.9)	Phe-3a, Phe-3b	Phe-3, Phe-4'
	3'/5'	128.2	7.18, t (7.3)		Phe-1'
	4'	126.8	7.14, t (7.2)		Phe-2'/6'
MePhe	1	<i>nd</i>			
	2	61.1	5.03 ^e , m	Phe-2, MePhe-2'/6', NH-Val	
	3a	34.0	3.35, m		
	3b		2.84 ^f , m		
	1'	138.4			
	2'/6'	130.0	7.26, d (7.5)	MePhe-2	MePhe-3, MePhe-4'
	3'/5'	129.1	7.41, t (7.5)		MePhe-1', MePhe-2'/6'
	4'	127.2	7.31, t (7.3)		MePhe-2'/6'
Val	NCH ₃	30.8	2.81, s		MePhe-2, Phe-1
	1	<i>nd</i>			
	2	56.5	4.66, m		
	3	31.2	2.06, m		
	4	19.9	0.89 ^b , d		Val-2, Val-3, Val-5
	5	18.0	0.76 ^d , d		Val-2, Val-3, Val-4
	NH		7.52, d (9.4)	MePhe-2	

^a HMBC correlations are given from proton(s) stated to the indicated carbon atom; ^{b-g} assignments with the same superscript are overlapping; *nd* – resonances not detected

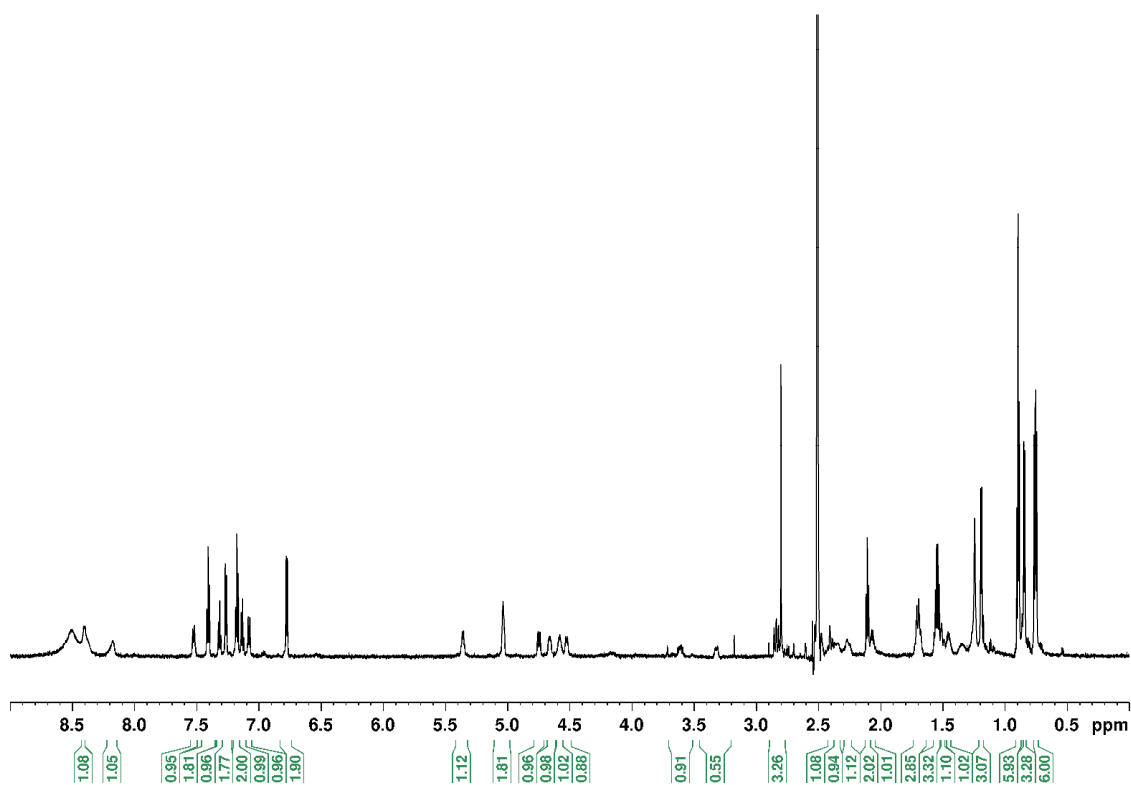


Figure S118. ¹H NMR spectrum of cyanopeptolin CP 919 in DMSO-d₆.

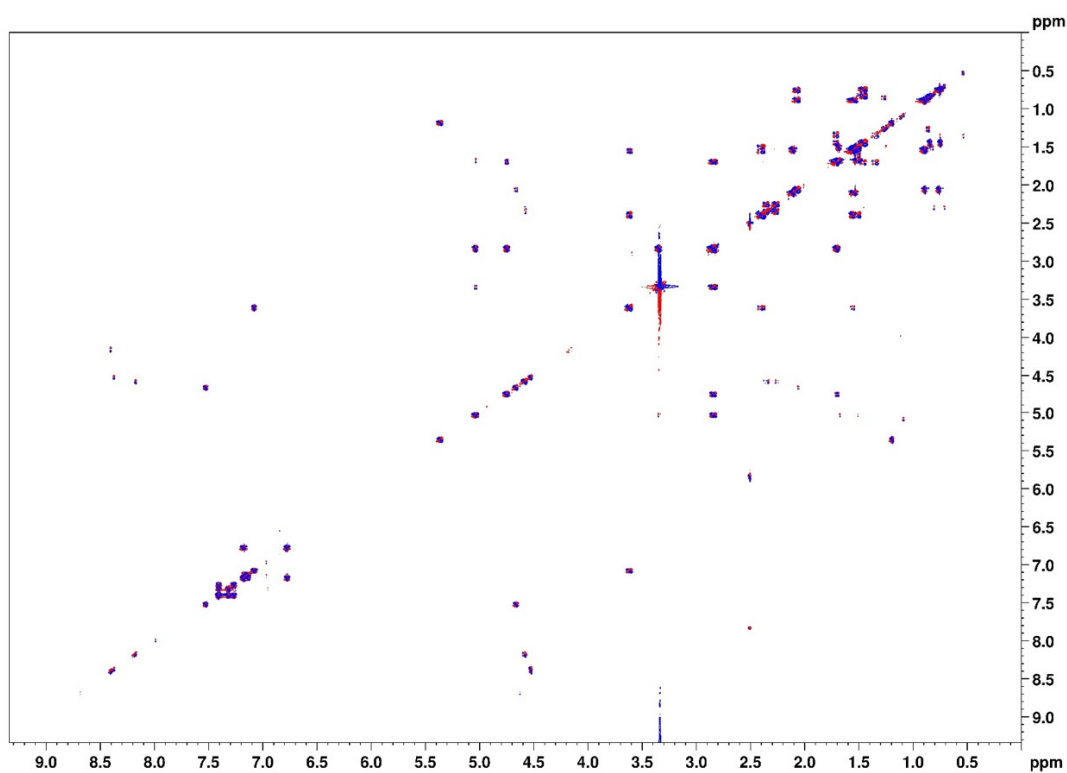


Figure S119. DQF-COSY spectrum of cyanopeptolin CP 919 in DMSO-d₆.

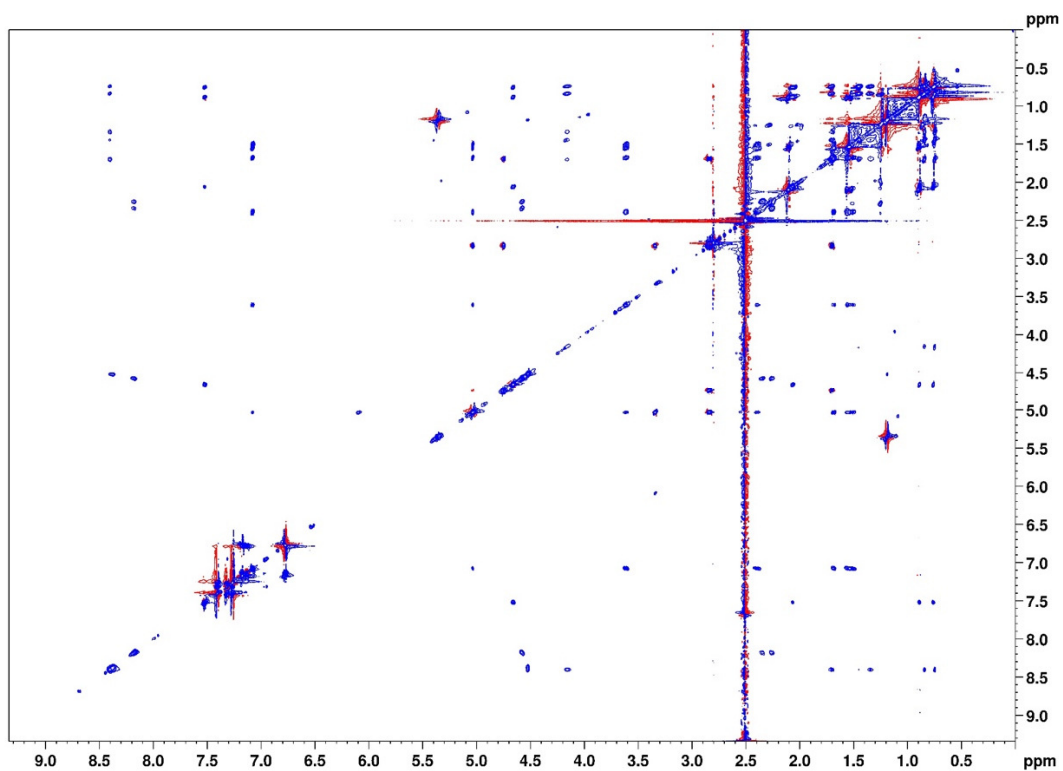


Figure S120. TOCSY spectrum of cyanopeptolin CP 919 in DMSO-d₆.

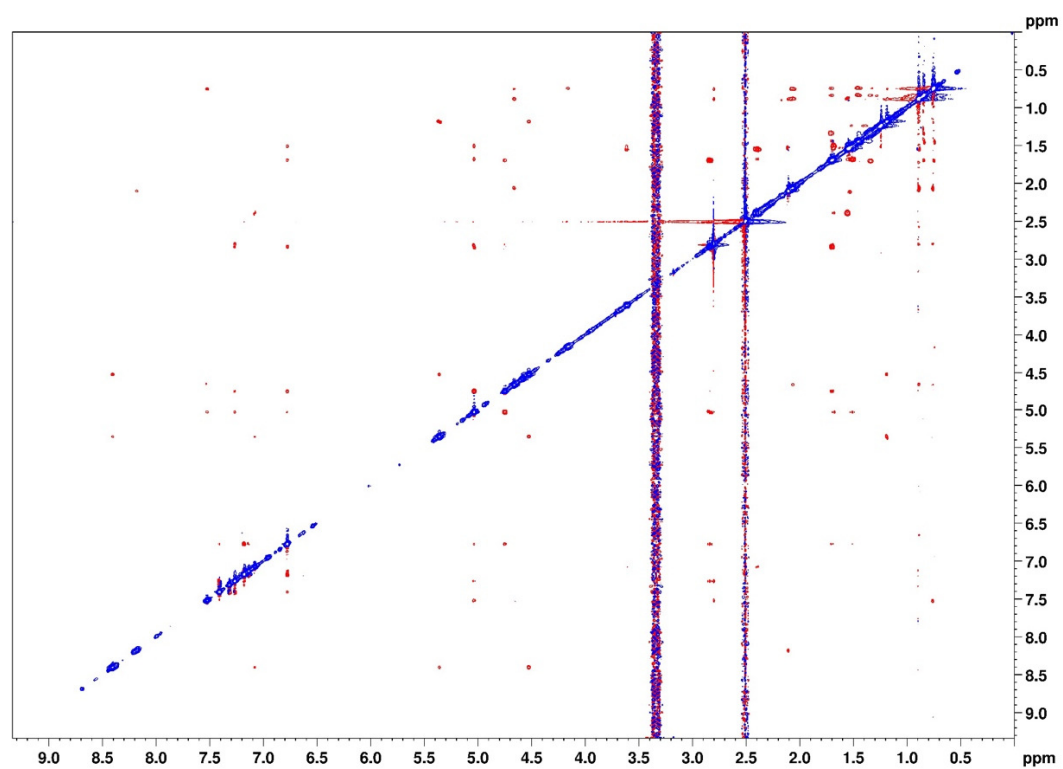


Figure S121. ROESY spectrum of cyanopeptolin CP 919 in DMSO-d₆.

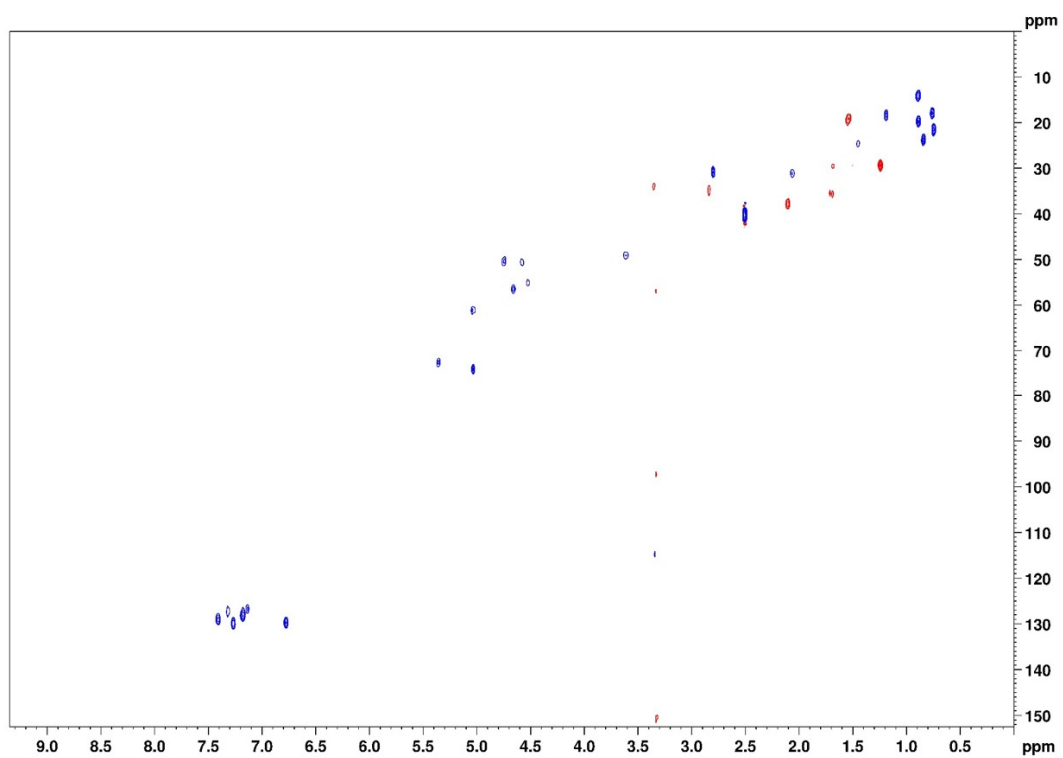


Figure S122. HSQC spectrum of cyanopeptolin CP 919 in DMSO-d₆.

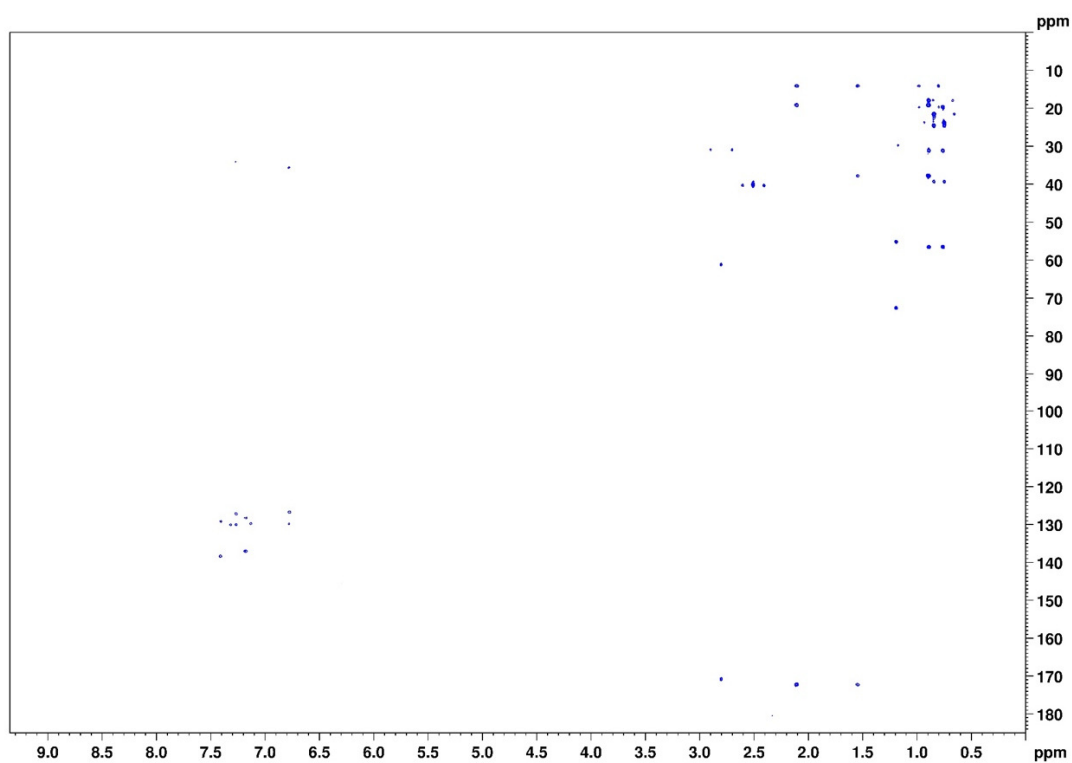


Figure S123. HMBC spectrum of cyanopeptolin CP 919 in DMSO-d₆.

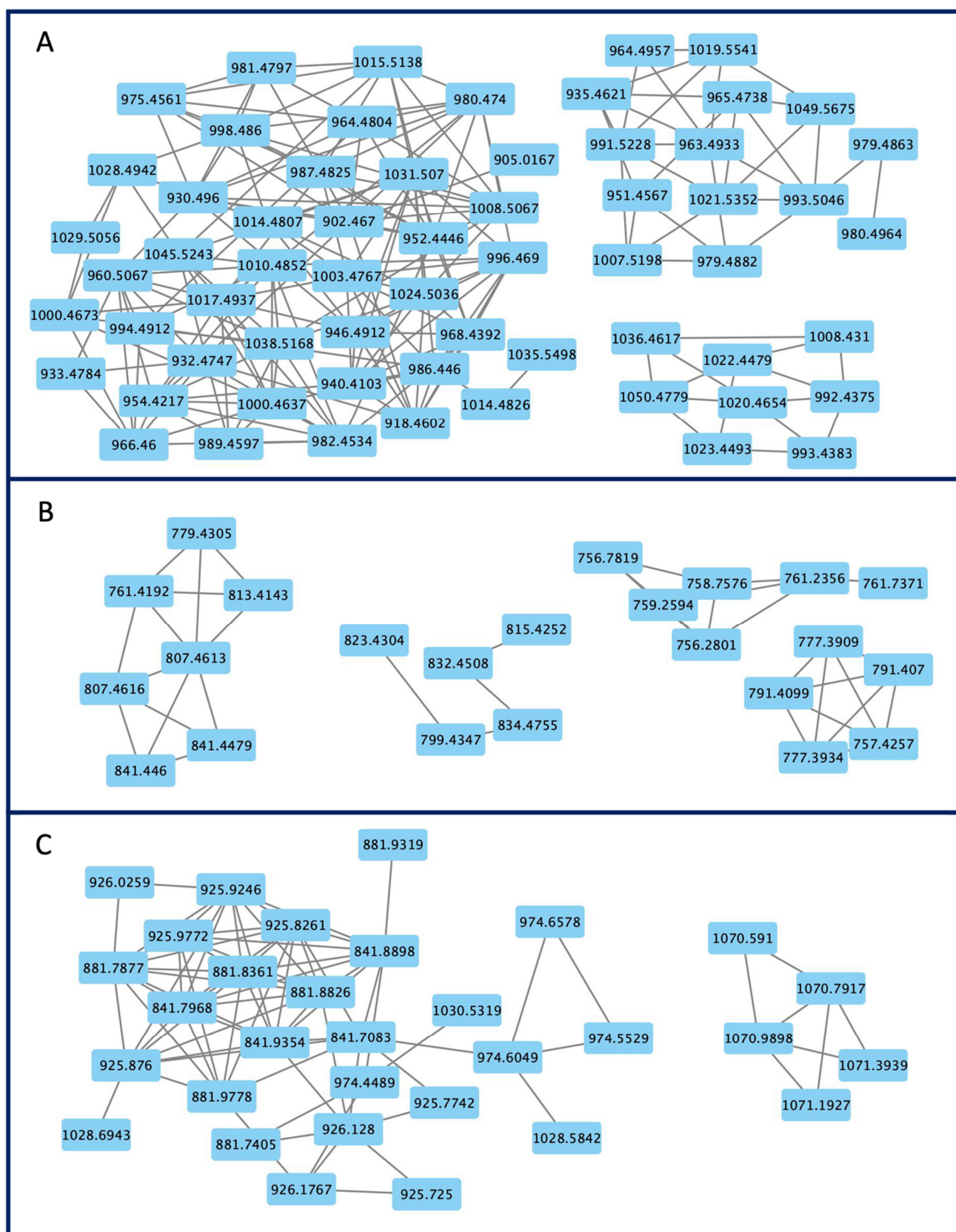


Figure S124. A CCNP1411 clusters formed by the GNPS analysis based on the HRMS/MS fragmentation spectra obtain from *Nostoc edaphicum* CCNP1411 extract. Clusters are separate as: A – nodes containing CPs features; B – nodes containing Nostocyclopeptides features C – nodes containing unknow features.