Supplementary Materials

Table S1. Patents on mycosporines and mycosporine-like amino acids.

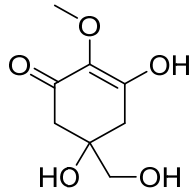
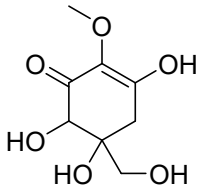
Year	Title	Patent n.º	Ref. [1]
1984	Mycosporine-like amino acid	JPS59137450	[1]
1987	Sunscreen compositions and compounds for use therein	WO1988002251 US5000946A	[2,3]
1990	UV-absorbing compounds and compositions	WO1990009995	[4]
2000	Solar radiation protection composition	WO2000024369 EP1123083 US6787147	[5–7]
2001	Algal extracts containing amino acid analogs of mycosporin are useful as dermatological protecting agents against ultraviolet radiation	FR2803201A1	[8]
2001	The utilization of natural pigments from lichens, cyanobacteria, fungi and plants for sun protection	WO2003020236 EP1424990A2 US20050129630 AU2002329025	[9–12]
2001	Topical cosmetic composition, useful for protecting skin and hair against sunlight, contains an extract from the red alga *Polysiphonia lanosa*	FR2803200	[13]
2002	Personal care compositions	WO2002039974 EP1341514A1	[14,15]
2002	Natural UV filters derived from pigments of lichens	IL0200725	[16]
2003	Extract having antioxidant activity and ultraviolet-absorbing activity, external preparation for skin, and food	JP2004238519A	[17]
2004	Cosmetic skin care products and cosmetic agents for protecting skin against premature aging	EP1473028	[18]
2004	Beta-glucuronidase inhibitors for use in deodorants and antiperspirants	US20040234466	[19]
2005	Amino-benzophenone UV filter formulations for the prevention of tanning	GB2412866	[20]
2005	Use of a mycosporin-type amino acid (porphyra 334) as an antioxidant	WO2007026035 ES2301293	[21,22]
2005	Use of a mycosporin-type amino acid (shinorine) as an antioxidant	WO2007026038 ES2301426	[23,24]
2005	Use of a mixture of mycosporin-type amino acids (asterin 330 + palythine) as an antioxidant	WO2007026037	[25]
2006	Use of a mycosporin-type amino acid (M-gly) as an antioxidant	WO2007026036	[26]
2006	Compositions comprising Porphyra and methods of making and using thereof	WO2007144779 EP2001311 US20070220806	[27–29]
2006	Sunscreen composition with extract of algae and lichens	ES2317741	[30]
2007	Extracts of Aphanizomenon flos-aquae and nutritional, cosmetic and pharmaceutical composition containing the same	WO2008000431 EP2032122 US20100021493	[31–33]
2007	Alphanizomenon flos aquae preparation, extracts and purified components thereof for the treatment of neurological, neurodegenerative and mood disorders	WO2008000430 EP2046354 US20090311286	[34–36]
2007	Mycosporin-like amino acid derivative having glycosyl group and method for producing the same	JP2009120562	[37]

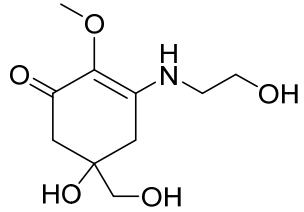
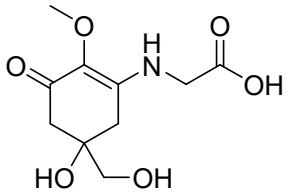
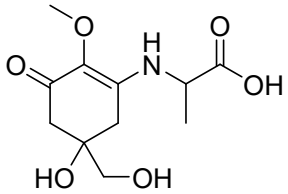
Year	Title	Patent n.º	Ref. [1]
2007	Cosmetic including natural substance having sun-screening function	CN101061995	[38]
2008	Antioxidant compound, antioxidant algae extract and method for producing the same	JP2008247901A	[39]
2009	Cosmetic sunscreen composition	GB2472021	[40]
2010	Method for preparing UV screening nontoxic extract from red algae, and nontoxic sunscreen using same	WO2011096628 KR100969325 CN102740869	[41]
2011	Topical composition	JP2013518871A WO2011158041	[42]
2012	Preparation method for laver mycosporine like amino acids porphyra-334	CN102659621	[43]
2012	Beauty product containing desert algae radiation-proof ingredient and natural medical whitening ingredient and preparation method thereof	CN102764206	[44]
2013	Imino compounds as protecting agents against ultraviolet radiations	WO2013181741 US20150152046	[45,46]
2013	Mycosporine-like amino acid and method for producing the same, UV protection agent, and antioxidant	JP6049200B2	[47]
2013	Mycosporin-like amino acids, production method thereof, UV protecting agents and antioxidants	JP2014227339	[48]
2013	Method for extracting mycosporine-like amino acid shinorine from microcystis	CN103755589	[49]
2013	Topical composition comprising transformed bacteria expressing a compound of interest	WO2014025938 US20140044677 US20160000701	[50,51]
2013	Synthesis of UV absorbing compounds	WO2014082124 US20150299124	[52,53]
2013	Anti-UV Composition for Skin External Application Comprising Peptide derivatives from Extract of Microalgae Comprising the Same	KR20150008238A	[54]
2014	UV absorbing compounds, compositions comprising same and uses thereof	WO2015006803 US20160244409	[55,56]
2015	Topical formulations for UV protection	WO2015195546	[57]
2015	Method for producing mycosporine-like amino acid using microbes	WO2015174427 US2017202762A1 EP3144392A1	[58–60]
2016	Novel mycosporine-like amino acid	WO2017082144A1	[61]
2016	Wound healing composition for skin external application comprising Mycosporine-like amino acid and Method for Preparing the Same	KR20170090690A	[62]
2016	Culture method capable of improving mycosporine-like amino acid content in umbilical laver	CN105684880B	[63]
2016	Extraction of mycosporine-like amino acids consisting of amino acid derivatives, separation and purification with chemically modified surface-modified activated carbon filler, and automation of their production	JP6058853B1	[64]
2017	Microorganism for producing a mycosporine-like amino acid method for producing a mycosporine-like amino acid using the same	CA3072748A1	[65]

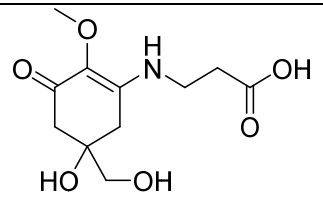
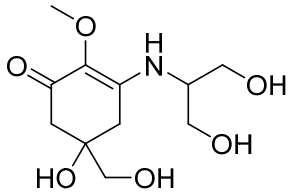
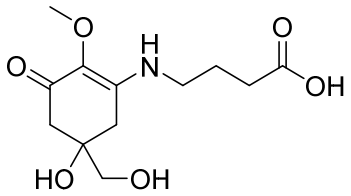
Year	Title	Patent n.º	Ref. [1]
2018	A microorganism for producing a Mycosporine-like amino acid and a method for preparing a Mycosporine-like amino acid using the same	KR102003911B1	[66]
2018	Production of mycosporine-like amino acids in cyanobacteria	WO2019094447A2	[67]
2020	Microorganism for producing a mycosporine-like amino acid and method for producing a mycosporine-like amino acid using the same	US20200283810A1	[68]
2020	Solution containing stabilized mycosporine-like amino acid and method for producing the same	JP2020114871A	[69]

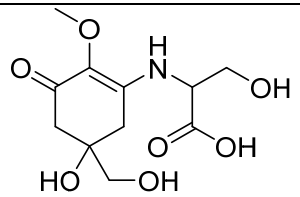
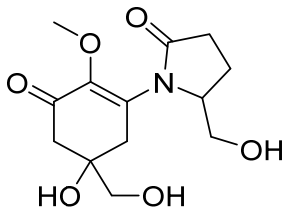
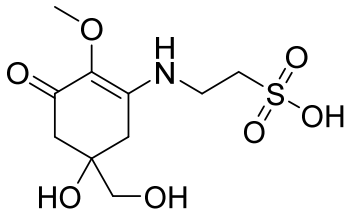
[1] Ref: References.

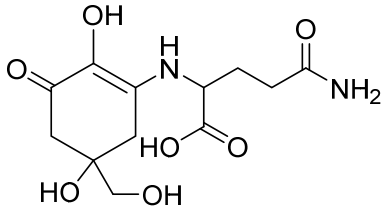
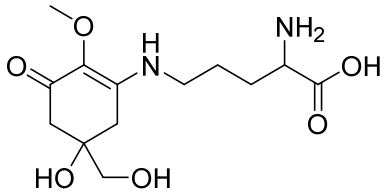
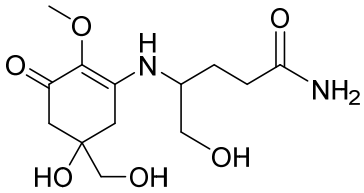
Table S2. Mycosporines and mycosporine-like amino acids (MAAs) with their corresponding absorption maxima (λmax), molar absorptivities (ε), molecular formula, exact mass, molecular structure, fragments (underline font represents $[M+H]^+$) and phylum, (-) no information available.

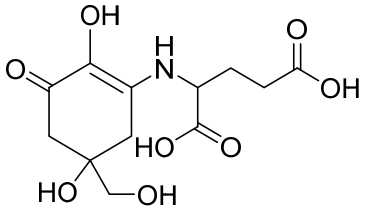
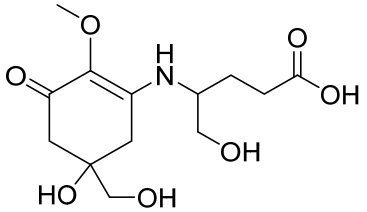
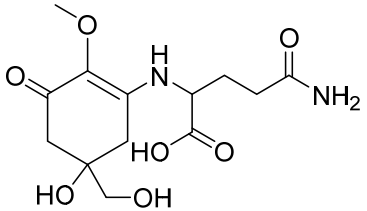
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-like amino-acids precursors						
4-Deoxygadusol (Cyclohexenone) 85926716	269 15,700	$C_8H_{12}O_5$ 188.07	 OC(CC(CO)(O)C1)=C(OC)C1=O	66.9, 70.0, 85.3, 95.0, 113.4, 160.0, 175.2, <u>189.2</u>	Cnidaria, Equinodermata, Lichen, Chordata	[70–73]
Gadusol 195955	268 12,400	$C_8H_{12}O_6$ 204.06	 OC(CC(CO)(O)C1O)=C(OC)C1=O	58.3, 84.8, 117.5, 145.2, 160.0, 175.1, 203.7, 204.9, <u>205.4</u>	Arthropoda, Chordata, Lichen	[70,72,74–76]
Oxo-mycosporines						

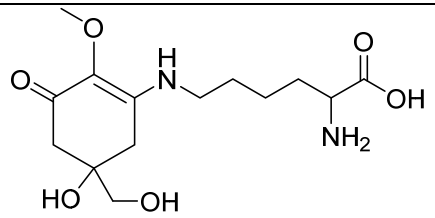
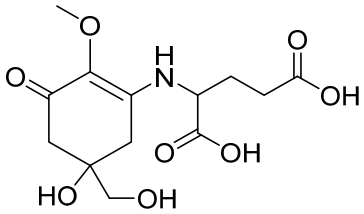
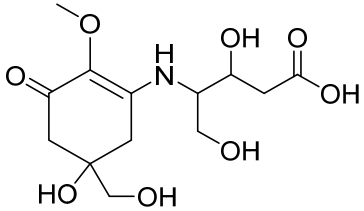
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-ethanolamine	310	$C_{10}H_{17}NO_5$ 231.11	 O=C1CC(CO)(O)CC(NCCO)=C1OC	-	Porifera	[77]
Mycosporine-glycine 14444486	310 28,100	$C_{10}H_{15}NO_6$ 245.09	 O=C1CC(CO)(O)CC(NCC(O)=O)=C1OC	57.1, 84.9, 100.1, 117.7, 143.9, 171.2, 231.7, 246.4	Arthropoda, Chlorophyta, Chordata, Cnidaria, Cyanobacteria, Dinoflagellata, Echinodermata, Lichen, Miozoa, Mollusca, Ochrophyta, Phaeophyta, Porifera, Rhodophyta	[70,71,78–83]
Mycosporine-alanine	310 640	$C_{11}H_{17}NO_6$ 259.11	 O=C1CC(CO)(O)CC(NC(C)C(O)=O)=C1OC	147, **171**, 42, 260,1	Fungi	[84]

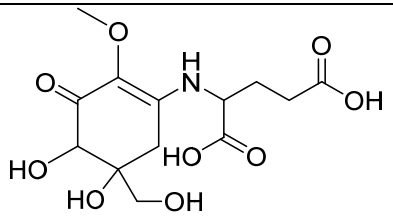
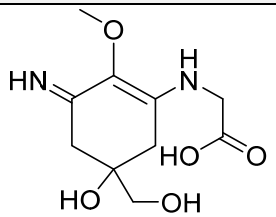
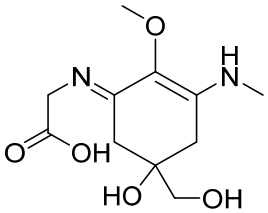
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-β-alanine	- -	$C_{11}H_{17}NO_6$ 259.11	 O=C1CC(CO)(O)CC(NCCC(O)=O)=C1OC	260,1	Cnidaria	[85,86]
Mycosporine-serinol 442866	310 27,270	$C_{11}H_{19}NO_6$ 261.12	 O=C1CC(CO)(O)CC(NC(CO)CO)=C1OC	184, 194, 212.1, 216, 243.1, 262.1	Fungi, Cyanobacteria	[87,88]
Mycosporine-GABA	310 28,900	$C_{12}H_{20}NO_6$ 273.12	 O=C1CC(CO)(O)CC(NCCCC(O)=O)=C1OC	87.1, 137.1, 186.2, 274.1	Cyanobacteria, Dinoflagellata	[81,89,90]

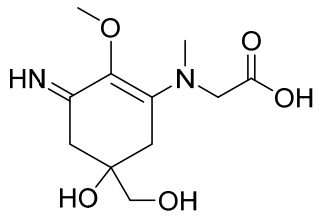
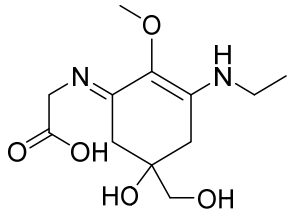
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-serine	310 -	$C_{11}H_{17}NO_7$ 275.10	 O=C1CC(CO)(O)CC(NC(C(O)=O)CO)=C1OC	228, 236, 258, 276.1	Fungi	[91,92]
Mycosporine-2 101324823	310 -	$C_{13}H_{19}NO_6$ 285.12	 O=C1CC(CO)(O)CC(N2C(CO)CCC2=O)=C1OC	286.1	Fungi	[93,94]
Mycosporine-taurine	309 28,100	$C_{10}H_{17}NO_7S$ 295.07	 O=C1CC(O)(CO)CC(NCCS(=O)(O)=O)=C1OC	57.1, 186.2, 236.1, 263.3, 277.2, 296.2	Cnidaria, Cyanobacteria, Lichen	[70,95–97]

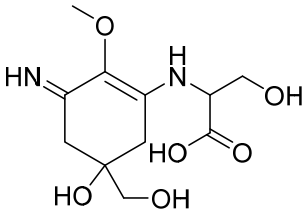
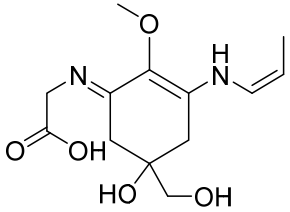
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Normycosporine-glutamine	320 -	$C_{12}H_{18}N_2O_7$ 302.11	 OC1=C(NC(C(O)=O)CCC(N)=O)CC(CO)(O)CC1=O	303.1	Fungi	[92,98]
Mycosporine-ornithine	310 -	$C_{13}H_{22}N_2O_6$ 302.15	 O=C1CC(O)(CO)CC(NCCCC(C(O)=O)N)=C1OC	191.1, 235.2, 267.0, 303.2	Cyanobacteria	[81,99]
Mycosporine-glutaminol 101835613	310 12,542	$C_{13}H_{22}N_2O_6$ 302.15	 O=C1CC(O)(CO)CC(NC(CO)CCC(N)=O)=C1OC	235, 267, 285, 303.2	Cyanobacteria, Fungi, Lichen	[100–102]

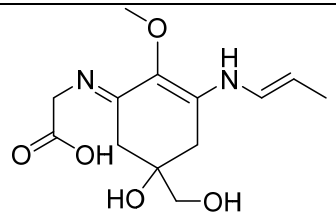
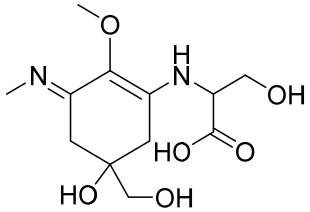
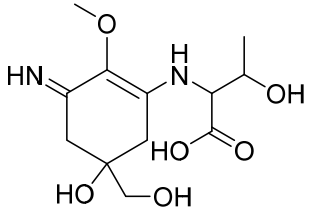
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Normycosporine-glutamic acid (artifact)	320 -	$C_{12}H_{17}NO_8$ 303.10	 OC1=C(NC(C(O)=O)CCC(O)=O)CC(CO)(O)CC1=O	304.1	Fungi	[98]
Mycosporine-glutamicol 9882880	310 17,248	$C_{13}H_{21}NO_7$ 303.13	 O=C1CC(CO)(O)CC(NC(CO)CCC(O)=O)=C1OC	178, 210, 236, 258, 268, 286, 304.1	Fungi, Lichen	[94,98,102,103]
Mycosporine-glutamine 101835612	310 -	$C_{13}H_{20}N_2O_7$ 316.13	 O=C1CC(CO)(O)CC(NC(C(O)=O)CCC(N)=O)=C1OC	317.1	Fungi	[98]

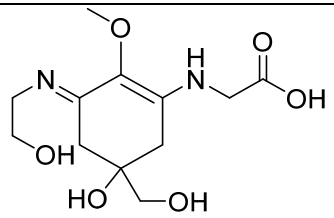
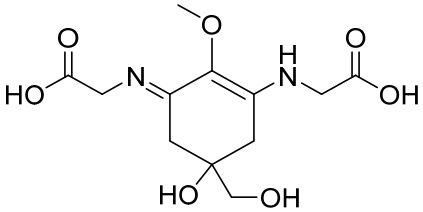
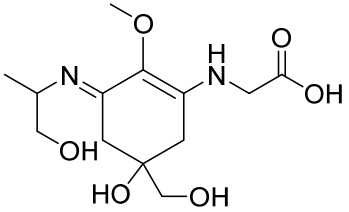
Compound **Pubchem CID**	**λmax (nm)** **ε ($M^{-1}.cm^{-1}$)**	**Molecular Formula** **Exact mass**	**Molecular structure** **Smiles**	**Fragments**	**Phylum**	**Ref.**
Mycosporine-lysine	310 -	$C_{14}H_{24}N_2O_6$ 316.16	 O=C1CC(CO)(O)CC(NCCCCC(N)C(O)=O)=C1OC	281.1, 317.2	Cyanobacteria	[99,104]
Mycosporine-glutamic acid 102095611	311 20,900	$C_{13}H_{19}NO_8$ 317.11	 O=C1CC(CO)(O)CC(NC(C(O)=O)CCC(O)=O)=C1OC	225, 281, 299, 318.1	Fungi	[78,98,105]
Mycosporine-hydroxyglutamicol 101805382	310 -	$C_{13}H_{21}NO_8$ 319.13	 O=C1CC(CO)(O)CC(NC(CO)C(O)CC(O)=O)=C1OC	320.1	Lichen	[103]

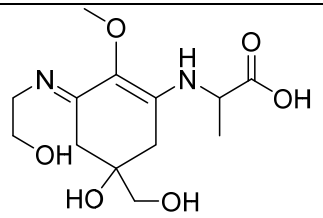
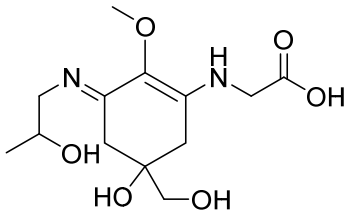
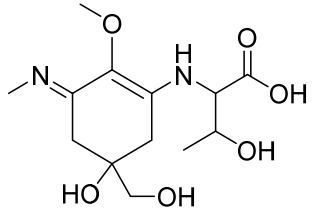
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Prasiolin 132581102	324 12,393	$C_{13}H_{19}NO_9$ 333.11	 O=C1C(O)C(CO)(O)CC(NC(CCC(O)=O)C(O)=O)=C1OC	334.1	Chlorophyta	[106]
Imino-mycosporines						
Palythine 16047608	320 35,500-36,200	$C_{10}H_{16}N_2O_5$ 244.11	 N=C1CC(CO)(O)CC(NCC(O)=O)=C1OC	137.2, 168.2, 185.9, 198.9, 209.2, 230.2, 245.1	Arthropoda, Bacillariophyta, Chlorophyta, Chordata, Cnidaria, Dinoflagellata, Echinodermata, Lichen, Miozoa, Mollusca, Ochrophyta, Phaeophyta, Porifera, Rhodophyta	[80–83,107–110]
N-methylpalythine = Aplysiapalythine C	330 -	$C_{11}H_{18}N_2O_5$ 258.12	 CNC1=C(OC)/C(CC(CO)(O)C1)=N/CC(O)=O	259.1	Cyanobacteria, Mollusca	[81,111]

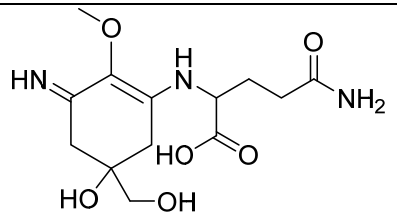
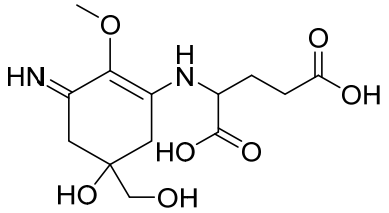
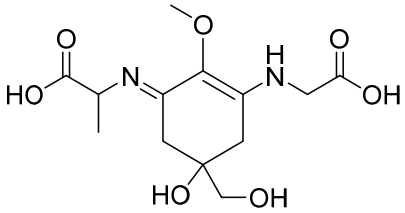
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Aplysiapalythine D	330 -	$C_{11}H_{18}N_2O_5$ 258.12	 N=C1CC(CO)(O)CC(N(C)CC(O)=O)=C1OC	259.1	Cyanobacteria	[112]
Dehydroxyl-usujirene	356 -	$C_{13}H_{19}N_2O_4$ 267.13	(a)	209, 224, 268.2	Cyanobacteria	[96]
N-ethylpalythine = Aplysiapalythine B	332 -	$C_{12}H_{20}N_2O_5$ 272.14	 OC(CC(NCC)=C/1OC)(CO)CC1=N/CC(O)=O	273.1	Mollusca, Rhodophyta	[80,111,113]

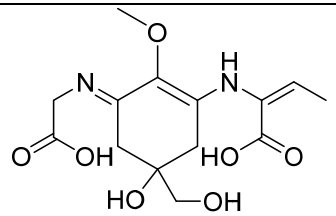
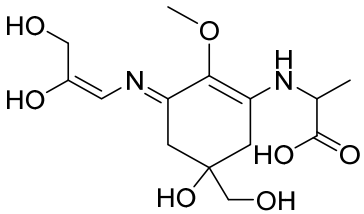
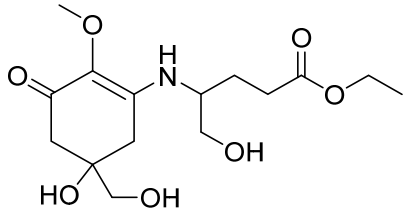
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Palythine-serine	320 10,500	$C_{11}H_{18}N_2O_6$ 274.12	 N=C1CC(CO)(O)CC(NC(CO)C(O)=O)=C1OC	260, 275.1	Cnidaria, Cyanobacteria	[81,114]
Usujirene (cis isomer) 15847474	357 -	$C_{13}H_{20}N_2O_5$ 284.14	 OC(CC(N/C=C\C)=C/1OC)(CO)CC1=N/CC(O)=O	197, 226, 241, 270, 285.1	Rhodophyta	[80,115,116]

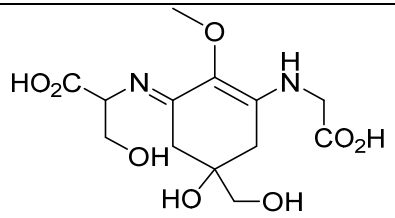
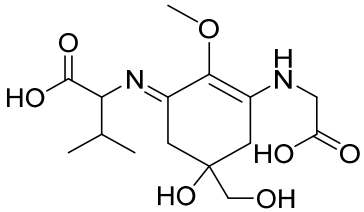
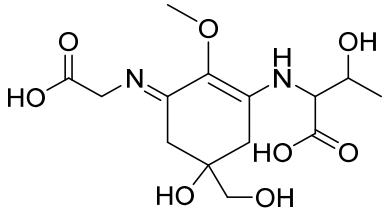
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Palythene (trans isomer) 21773785	360 50,000	$C_{13}H_{20}N_2O_5$ 284.14	 OC(CC(N/C=C/C)=C/1OC)(CO)CC1=N/CC(O)=O	139.1, 185.0, 197.3, 205.0, 223.0, 241.2, <u>285.0</u>	Arthropoda, Chlorophyta, Cnidaria, Lichen, Mollusca, Phaeophyta, Porifera, Rhodophyta	[70,80,83,110,117]
Mycosporine methylamine serine = N-methylmycosporine-serine	325 16,600	$C_{12}H_{20}N_2O_6$ 288.13	 OC(CC(NC(CO)C(O)=O)=C/1OC)(CO)CC1=N/C	274, <u>289.1</u>	Cnidaria	[114]
Palythine–threonine	320 -	$C_{12}H_{20}N_2O_6$ 288.13	 N=C1CC(CO)(O)CC(NC(C(C)O)C(O)=O)=C1OC	169, 172, 230, 245, 256, 274, <u>289.1</u>	Cnidaria, Cyanobacteria	[81,118,119]

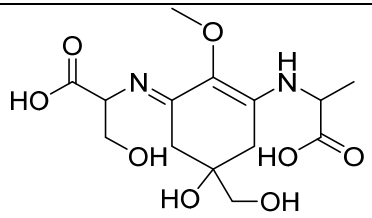
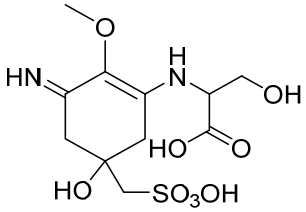
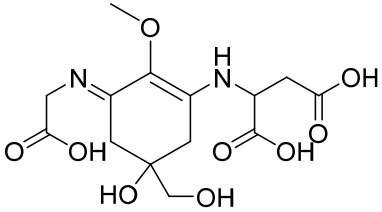
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Asterina-330 13194807	330 43,800	$C_{12}H_{20}N_2O_6$ 288.13	 OC(CC(NCC(O)=O)=C/1OC)(CO)CC1=N/CCO	137, 167.8, 186.0, 198.4, 230.2, 243.1, 273.1, <u>289.2</u>	Arthropoda, Chlorophyta, Chordata, Echinodermata, Lichen, Mollusca, Ochrophyta, Phaeophyta, Rhodophyta	[70,80,82,111,120,121]
Mycosporine-2-glycine 23427657	334	$C_{12}H_{18}N_2O_7$ 302.11	 OC(CC(NCC(O)=O)=C/1OC)(CO)CC1=N/CC(O)=O	151.1, 164.1, 185.1, 200.1, 244.1, 288.1, <u>303.1</u>	Bacillariophyta, Cnidaria, Cyanobacteria, Echinodermata, Mollusca, Rhodophyta	[80,95,122,123]
Palythinol 9948334	332 43,500	$C_{13}H_{22}N_2O_6$ 302.15	 OC(CC(NCC(O)=O)=C/1OC)(CO)CC1=N/C(CO)C	102.2, 150.0, 186.1, 199.2, 243.2, 288.0, <u>303.5</u>	Chlorophyta, Lichen, Phaeophyta, Porifera, Rhodophyta	[70,80,83,110,117]

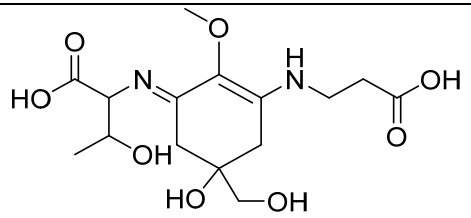
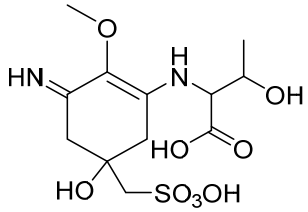
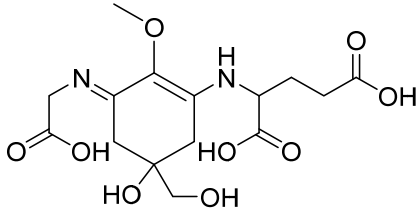
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Asterina-methyl ester	330	$C_{13}H_{22}N_2O_6$ 302.15	 OC(CC(NC(C)C(O)=O)=C/1OC)(CO)CC1=N/CCO	303.2	Dinoflagellata	[124]
N-isopropanolpalythine = Aplysiapalythine A	332	$C_{13}H_{22}N_2O_6$ 302.15	 OC(CC(NCC(O)=O)=C/1OC)(CO)CC1=N/CC(C)O	303.2	Mollusca, Rhodophyta	[80,111]
Mycosporine-methylamine-threonine	327 33,300	$C_{13}H_{22}N_2O_6$ 302.15	 OC(CC(NC(C(C)O)C(O)=O)=C/1OC)(CO)CC1=N/C	303.2	Cnidaria, Rhodophyta	[80,125]

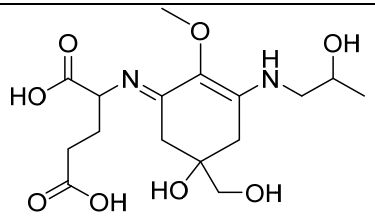
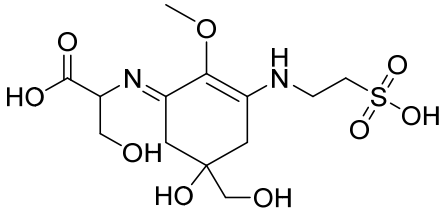
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Palythine-glutamine = Bostrychine-A	322	$C_{13}H_{21}N_3O_6$ 315.14	 N=C1CC(CO)(O)CC(NC(C(O)=O)CCC(N)=O)=C1OC	316.1	Rhodophyta	[126]
Palythine-glutamic acid = Bostrychine-C	322 22,351	$C_{13}H_{20}N_2O_7$ 316.13	 N=C1CC(CO)(O)CC(NC(C(O)=O)CCC(O)=O)=C1OC	317.1	Rhodophyta	[126]
Mycosporine-glycine-alanine 102110164	333 -	$C_{13}H_{20}N_2O_7$ 316.13	 OC(CC(NCC(O)=O)=C/1OC)(CO)CC1=N/C(C(O)=O)C	186, 214, 258, 302, 317.1	Cyanobacteria, Rhodophyta	[80,127]

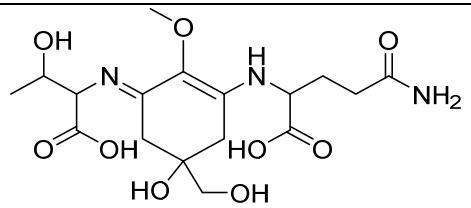
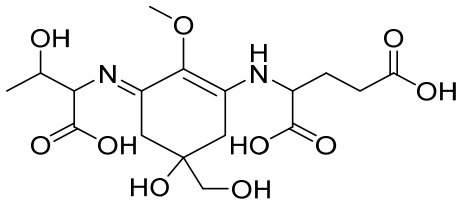
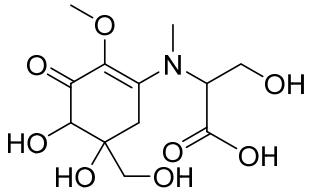
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Palythenic acid 101016648	337 29,200	$C_{14}H_{20}N_2O_7$ 328.13	 OC(CC(N/C(C(O)=O)=C/C)=C/1OC)(CO)CC1=N/CC(O)=O	138, 193, 197, 205, 237, 268, 283, 296, <u>329.1</u>	Dinoflagellata, Mollusca, Rhodophyta	[80,81,110]
Euhalothece-362 102182144	362 -	$C_{14}H_{22}N_2O_7$ 330.14	 OC(CC(NC(C)C(O)=O)=C/1OC)(CO)CC1=N/C=C(CO)/O	213.1, 228.1, 242.1, 272.1, 316.1, <u>331.1</u>	Cyanobacteria	[122,128]
Mycosporine-glutamicol ethyl ester	310 21,295	$C_{15}H_{25}NO_7$ 331.16	 O=C1CC(CO)(O)CC(NC(CO)CCC(OCC)=O)=C1OC	218, 264, 286, 314, <u>332.2</u>	Fungi, Lichen	[102]

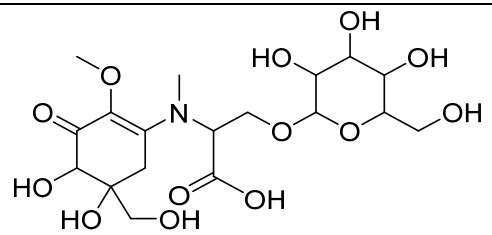
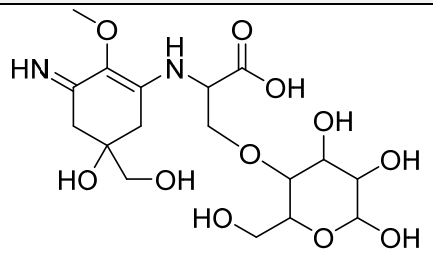
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Shinorine 101926676	334 44,668	$C_{13}H_{20}N_2O_8$ 332.12	 OC(CC(NCC(O)=O)=C/1OC)(CO)CC1=N/C(C(O)=O)CO	137.1, 186.2, 230.0, 241.3, 255.0, 298.0, 333.3	Arthropoda, Bacillariophyta, Chlorophyta, Chordata, Cyanobacteria, Dinoflagellata, Lichen, Miozoa, Mollusca, Ochrophyta, Phaeophyta, Porifera, Rhodophyta	[70,80–83,110,129]
Mycosporine-glycine-valine 101016647	335	$C_{15}H_{24}N_2O_7$ 344.16	 OC(CC(NCC(O)=O)=C/1OC)(CO)CC1=N/C(C(O)=O)C(C)C	116.0, 118.1, 130.6, 183.9, 198.1, 268.2, 295.0, 313.0	Arthropoda, Cnidaria, Chordata, Echinodermata, Lichen, Mollusca, Porifera	[70,83]
Porphyra-334 91864535	334 42,300	$C_{14}H_{22}N_2O_8$ 346.14	 OC(CC(NC(C(O)C)C(O)=O)=C/1OC)(CO)CC1=N/CC(O)=O	137, 151, 168, 186, 227, 243, 288, 303, 332, 347.1	Arthropoda, Bacillariophyta, Chlorophyta, Chordata, Cnidaria, Cyanobacteria, Dinoflagellata, Miozoa, Mollusca, Ochrophyta, Phaeophyta, Porifera, Rhodophyta	[80–83,110,130]

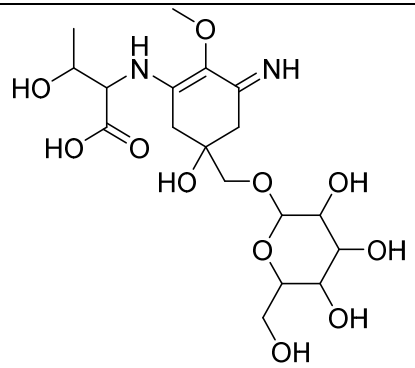
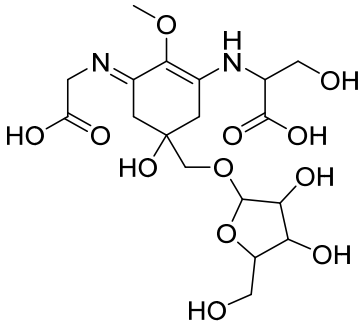
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-serine-glycine methyl ester = Shinorine methyl ester	332 -	$C_{14}H_{22}N_2O_8$ 346.14	 OC(CC(NC(C)C(O)=O)=C/1OC)(CO)CC1=N/C(C(O)=O)CO	244, 269, 288, 314, 332, 347.3	Dinoflagellata	[131]
Palythine-serine-sulfate	321 -	$C_{11}H_{18}N_2O_9S$ 354.07	 N=C1CC(CS(=O)(OO)=O)(O)CC(NC(CO)C(O)=O)=C1OC	355.1	Cnidaria	[120]
Mycosporine-glycine - aspartic acid	333 -	$C_{14}H_{20}N_2O_9$ 360.12	 OC(CC(NC(CC(O)=O)C(O)=O)=C/1OC)(CO)CC1=N/CC(O)=O	361.1	Arthropoda	[75]

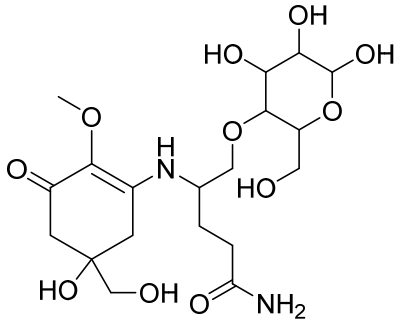
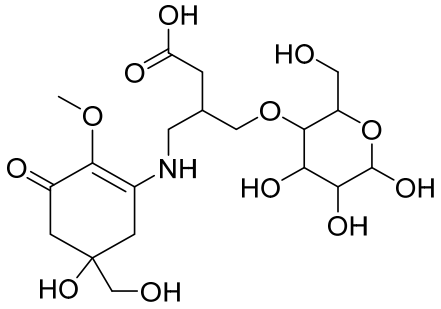
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-threonine-β-alanine = Bostrychine-F	332 44,994	$C_{15}H_{24}N_2O_8$ 360.15	 OC(CC(NCCC(O)=O)=C/1OC)(CO)CC1=N/C(C(C)O)C(O)=O	361.2	Rhodophyta	[126]
Palythine-threonine-sulfate	321 -	$C_{12}H_{20}N_2O_9S$ 368.09	 N=C1CC(CS(=O)(OO)=O)(O)CC(NC(C(C)O)C(O)=O)=C1OC	369.1	Cnidaria	[120]
Mycosporine-glycine - glutamic acid 102446627	330 43,900	$C_{15}H_{22}N_2O_9$ 374.13	 OC(CC(NC(CCC(O)=O)C(O)=O)=C/1OC)(CO)CC1=N/CC(O)=O	118.2, 176.0, 192.2, 228.3, 258.1, 297.1, 331.2, 375.3	Cnidaria, Lichen, Rhodophyta	[70,126,132]

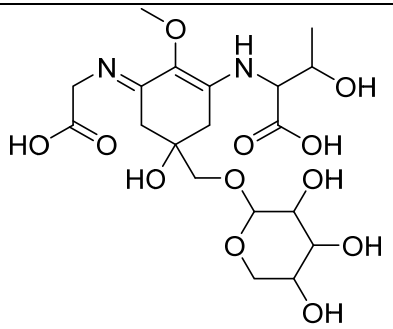
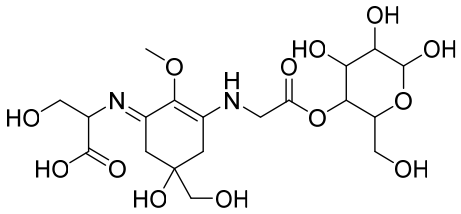
Compound **Pubchem CID**	**λmax (nm)** **ε ($M^{-1}.cm^{-1}$)**	**Molecular Formula** **Exact mass**	**Molecular structure** **Smiles**	**Fragments**	**Phylum**	**Ref.**
Mycosporine-threamine-glutamic acid = Bostrychine-E	333 21,618	$C_{16}H_{26}N_2O_8$ 374.17	 OC(CC(NCC(O)C)=C/1OC)(CO)CC1=N/C(CCC(O)=O)C(O)=O	375.2	Rhodophyta	[126]
Catenelline	320 -	$C_{13}H_{22}N_2O_9S$ 382.10	 OC(CC(NCCS(O)(=O)=O)=C/1OC)(CO)CC1=N/C(C(O)=O)CO	383.1	Rhodophyta	[80,133]
M-343	343 -	- 386	-	387	Cyanobacteria	[96]

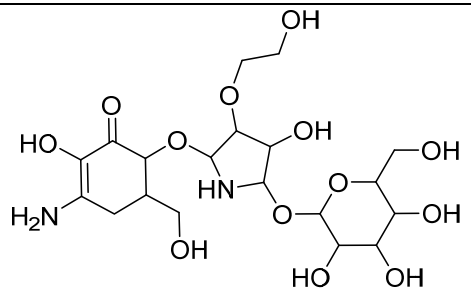
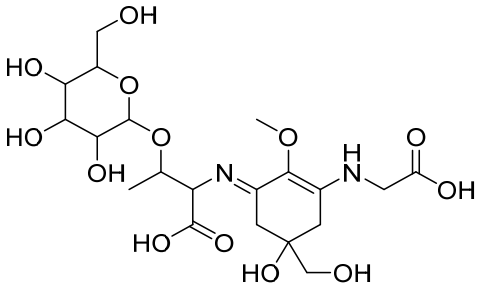
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-threonine-glutamine = Bostrychine-B	335 36,155	$C_{17}H_{27}N_3O_9$ 417.17	 OC(CC(NC(C(O)=O)CCC(N)=O)=C/1OC)(CO)CC1=N/C(C(O)=O)C(O)C	418.2	Rhodophyta	[126]
Mycosporine-threonine-glutamic acid = Bostrychine-D	337 31,956	$C_{17}H_{26}N_2O_{10}$ 418.16	 OC(CC(NC(C(O)=O)CCC(O)=O)=C/1OC)(CO)CC1=N/C(C(O)=O)C(O)C	419.1	Rhodophyta	[126]
Glycosylated Oxo-mycosporines						
Klebsormidin B	324 -	$C_{12}H_{19}NO_8$ 305.11	 O=C1C(O)C(O)(CO)CC(N(C)C(C(O)=O)CO)=C1OC	306.1	Charophyta	[134]

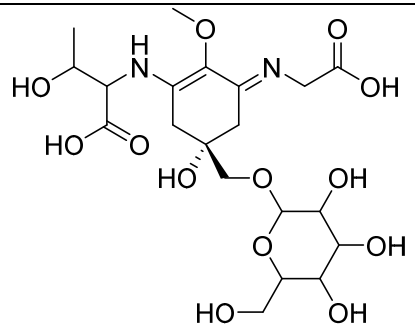
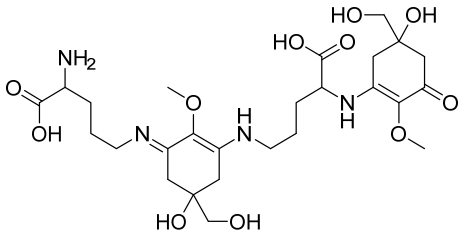
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Klebsormidin A	324 -	$C_{18}H_{29}NO_{13}$ 467.16	 O=C1C(O)C(O)(CO)CC(N(C)C(C(O)=O)COC2OC(CO)C(O)C(O)C2O)=C1OC	468.2	Charophyta	[134]
Glycosylated Imino-mycosporines						
Hexose-palythine-serine	320 -	$C_{17}H_{28}N_2O_{11}$ 436.17	 N=C1CC(O)(CO)CC(NC(COC2C(CO)OC(O)C(O)C2O)C(O)=O)=C1OC	142, 171, 207, 239, 241, 245, 257, 275, 378, 391, 407, 422, 437.2	Cyanobacteria	[81,135]

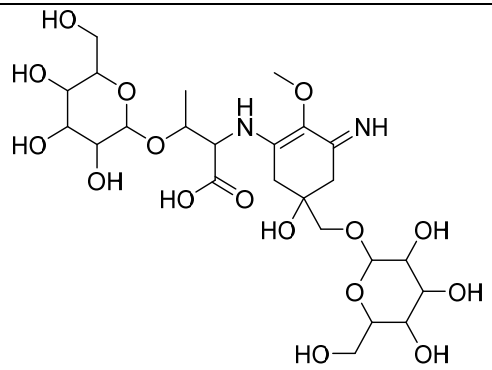
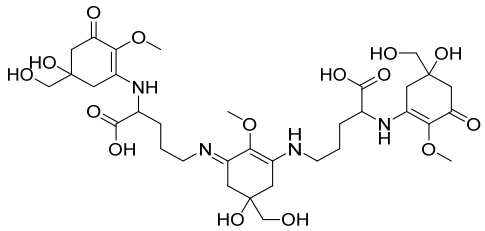
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Hexose-bound palythine-threonine	322 -	$C_{18}H_{30}N_2O_{11}$ 450.18	 OC(CC(NC(C(O)=O)C(C)O)=C1OC)(COC2OC(CO)C(O)C(O)C2O)CC1=N	185.2, 289.2, 349.2, 389.2, 407.2	Cyanobacteria	[81,119]
Pentose-bound shinorine	332 -	$C_{18}H_{28}N_2O_{12}$ 464.16	 OC(C/1)(COC2OC(CO)C(O)C2O)CC(NC(C(O)=O)CO)=C(OC)C1=N\CC(O)=O	211.3, 333.3, 377.1, 421.1, 465.1	Cyanobacteria	[89]

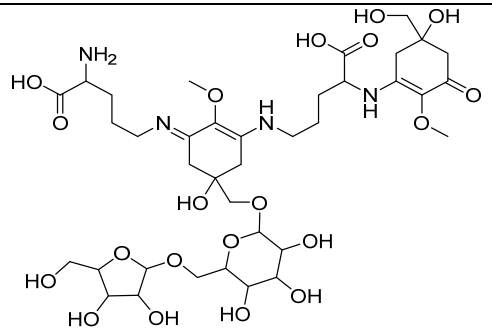
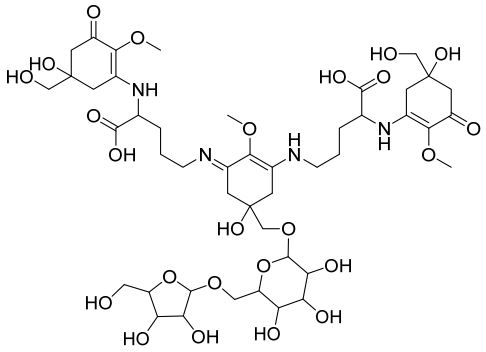
Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Mycosporine-glutaminol-*O*-glucoside	310 25,000	$C_{19}H_{32}N_2O_{11}$ 464.20	 OC(C/1)(COC2OC(CO)C(O)C2O)CC(NC(C(O)=O)CO)=C(OC)C1=N\CC(O)=O	303, 428, 446, <u>465.0</u>	Fungi	[98,136,137]
Mycosporine-glutamicol-*O*-glucoside	310 25,000	$C_{19}H_{31}NO_{12}$ 465.18	 O=C1CC(CO)(O)CC(NCC(COC2C(O)C(O)C(O)OC2CO)CC(O)=O)=C1OC	304, <u>466.2</u>	Fungi	[137,138]

Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Arabinose-bound porphyra-334 = 478 Da MAA	335 33,200	$C_{19}H_{30}N_2O_{12}$ 478.18	 OC(C/1)(COC2OCC(O)C(O)C2O)CC(NC(C(O)=O)C(C)O)=C(OC)C1=N\CC(O)=O	214.8, 273.0, 377.1, 435.1, 437.1, 479.2	Cyanobacteria	[139]
Hexose-shinorine	333 -	$C_{19}H_{30}N_2O_{13}$ 494.17	 OC(C/1)(CO)CC(NCC(OC2C(CO)OC(O)C(O)C2O)=O)=C(OC)C1=N\C(C(O)=O)CO	186, 230, 265, 274, 287, 300, 303, 318, 333, 392, 436, 365, 480, 495.2	Cyanobacteria	[135]

Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Collemin A 10074531	311 34,000	$C_{19}H_{32}N_2O_{13}$ 496.19	 OC(C(C(C(CO)O1)O)O)C1OC(C2O)NC(OC3C(C(O)=C(N)CC3CO)=O)C2OCCO	95.0, 198.1, 235.8, 300.2, 340.2, 409.1, 435.0, 497.2	Lichen	[70,140]
13-O-(β-galactosyl)-porphyra-334	334 -	$C_{20}H_{32}N_2O_{13}$ 508.19	 OC(C/1)(CO)CC(NCC(O)=O)=C(OC)C1=N\C(C(O)=O)C(OC2OC(CO)C(O)C(O)C2O)C	347.1, 509.2	Cyanobacteria	[141]

Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Hexose-bound porphyra-334	334 36,300	$C_{20}H_{32}N_2O_{13}$ 508.19	 O[C@@](CC(NC(C(O)=O)C(C)O)=C/1OC)(COC2OC(CO)C(O)C(O)C2O)CC1=N/CC(O)=O	303.2, 347.2, 361.2, 421.2, 465.2, 509.2	Cyanobacteria	[119]
586-Da MAA	332 -	$C_{26}H_{42}N_4O_{11}$ 586.29	 OC(C/1)(CO)CC(NCCCC(C(O)=O)NC2=C(OC)C(CC(CO)(O)C2)=O)=C(OC)C1=N\CCCC(N)C(O)=O	417.2, 428.2, 472.2, 499.3, 525.3, 543.3, 569.4, 587.3	Cyanobacteria	[142]

Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
Glycosylated Palythine-threonine = 612-Da MAA	324 28,200	$C_{24}H_{40}N_2O_{16}$ 612.24	 OC(CC(NC(C(O)=O)C(C)OC1OC(CO)C(O)C(O)C1O)=C2OC)(COC3OC(CO)C(O)C(O)C3O)CC2=N	187.2, 289.2, 349.1, 389.2, 407.2, 451.2, 569.2, <u>613.2</u>	Cyanobacteria	[119]
Nostoc-756 = 756-Da MAA 146683732	313 -	$C_{34}H_{52}N_4O_{15}$ 756.34	 OC(C/1)(CO)CC(NCCCC(C(O)=O)NC2=C(OC)C(CC(CO)(O)C2)=O)=C(OC)C1=N\CCCC(NC3=C(OC)C(CC(CO)(O)C3)=O)C(O)=O	454.1, 516.1, 552.1, 603.1, 639.1, 657.1, 694.9, <u>757.2</u>	Cyanobacteria	[142]

Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
880-Da MAA	331 49,800	$C_{37}H_{60}N_4O_{20}$ 880.38	 OC(C/1)(COC2OC(COC3OC(CO)C(O)C3O)C(O)C(O)C2O)CC(NCCCC(C(O)=O)NC4=C(OC)C(CC(CO)(O)C4)=O)=C(OC)C1=N\CCCC(N)C(O)=O	445.3, 489.3, 533.3, 737.4, 795.5, 837.5, <u>881.4</u>	Cyanobacteria	[89]
1050-Da MAA	312/ 340 58,800	$C_{45}H_{70}N_4O_{24}$ 1050.44	 OC(C/1)(COC2OC(COC3OC(CO)C(O)C3O)C(O)C(O)C2O)CC(NCCCC(C(O)	410.4, 437.1, 481.1, 501.0, 581.9, 722.3, 766.3, 963.4, <u>1051.4</u>	Cyanobacteria	[139]

Compound Pubchem CID	λmax (nm) ε ($M^{-1}.cm^{-1}$)	Molecular Formula Exact mass	Molecular structure Smiles	Fragments	Phylum	Ref.
			=O)NC4=C(OC)C(CC(CO)(O)C4)=O)=C(OC)C1=N\CCCC(NC5=C(OC)C(CC(CO)(O)C5)=O)C(O)=O			

[1] Ref: References. [a] although the correct molecular weight for dehidrousujerene is $C_{13}H_{20}N_2O_4$ (MW = 268.31) and $[M+H]^+$ might be m/z = 269, according to nitrogen rules and ionization in positive mode in ESI.

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