

Describing the Complex Chemistry of Benthic Seawater: from Exometabolite Sampling Strategies to MS-Based Metabolomics

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SUPPORTING INFORMATION

Table of all described marine exometabolites (EMs)

Organisms/ Ecosystems	Metabolites	Nº	MF	SMILES	R
<i>Sinularia Flexibilis</i> Eclipse Island Australia	flexibilide	4	C ₂₀ H ₃₀ O ₄	C/C1=C\CC[C@]([C@H]2[C@H](CC[C@]3([C@H](O3)CC1)C C(=C)C(=O)O2)(C)O	1,2
	dihydroflexibilide	5	C ₂₀ H ₃₂ O ₄	C[C@H]1[C@H]2CC[C@]3([C@H](O3)CC/C=C/CC[C@]([C@ @H](C2)OC1=O)(C)O)/C/C	
<i>Sarcophyton crassocaule</i> Eclipse Island Australia	sarcophine	6	C ₂₀ H ₂₈ O ₃	C/C1=C\CC[C@]2([C@H](O2)CC/C=C/[C@H]3C=C(C(=O)O3)C CC1)/C/C	1
	sarcophytoxide	7	C ₂₀ H ₃₀ O ₂	C/C1=C\CC[C@]2([C@H](O2)CC/C=C/[C@H]3C=C(CO3)C)CC1)/C/C	
<i>Aplysina fistularis</i> Casa Cove, La Jolla California &	aerothionin	1	C ₂₄ H ₂₆ Br ₄ N ₄ O ₈	COC1=C([C@H]([C@]2(CC(=NO2)C(=O)NCCCCN(=O)C3=NO[C @]4(C3)C=C(C=C([C@H]4O)Br)OC)Br)C=C1Br)O)Br	3,4
	homoaerothionin	2	C ₂₅ H ₂₈ Br ₄ N ₄ O ₈	COC1=C([C@H]([C@]2(CC(=NO2)C(=O)NCCCCN(=O)C3=NO[C @]4(C3)C=C(C=C([C@H]4O)Br)OC)Br)C=C1Br)O)Br	
<i>Aplysina cavernicola</i> Aquaria Mediterranean Sea	aerophobin 1	11	C ₁₅ H ₁₆ Br ₂ N ₄ O ₄	COC1=C([C@H]([C@]2(CC(=NO2)C(=O)NCCCC=CN=CN3)C=C1Br O)Br	4,5
	aplysine 1	12	C ₁₄ H ₁₉ Br ₂ N ₃ O ₄	O=C(C1=NO[C@]2([C@H](O)C(Br)=C(OC)C(Br)=C2)C1)NCCCC N	
	purealidin L	13	C ₁₅ H ₂₁ Br ₂ N ₅ O ₄	COC1=C([C@H]([C@]2(CC(=NO2)C(=O)NCCCCN=C(N)N)C=C1Br O)Br	
<i>Ircinia felix</i> Santa Marta Bay, Caribbean Coast of Colombia	thiobismethane	36	C ₂ H ₆ S	CSC	6
	methyl isocyanide	37	C ₂ H ₃ N	C[N+]#[C-]	
	methyl isothiocyanate	38	C ₂ H ₃ NS	CN=C=S	
<i>Geodia barretti</i> Koster Fjord area Sweden	barettin	8	C ₁₇ H ₁₉ BrN ₆ O ₂	C1=CC2=C(C=C1Br)NC=C2/C=C\3/C(=O)N([C@H](C(=O)N3)CCCN=C (N)N	7
	8,9-dihydrobarettin	9	C ₁₇ H ₂₁ BrN ₆ O ₂	C1=CC2=C(C=C1Br)NC=C2CC3C(=O)N(C(=O)N3)CCCN=C(N)N	
Sponge microorganisms Pacific Ocean/ South China	jasplakinolide	10	C ₃₆ H ₃₄ BrN ₄ O ₆	BrC1=C(C2=CC=CC=C2N1)C[C@H](N(C)C([C@H](C)NC([C@H](C)C/C(C)=C\([C@H](C)C3)=O)=O)C(N[C@H](C4=CC=C(O)C=C4) CC(O[C@H]3C)=O)=O	8
	jasplakinolide B jaspamide		C ₃₆ H ₄₃ BrN ₄ O ₇	BrC1=C(C2=CC=CC=C2N1)C[C@H](N(C)C([C@H](C)NC([C@H](C)C/C(C)=C\([C@H](C)C3)=O)=O)C(N[C@H](C4=CC=C(O)C=C4) CC(O[C@H]3C)=O)=O	
	jasplakinolide C		C ₃₆ H ₄₅ BrN ₄ O ₇	BrC1=C(C2=CC=CC=C2N1)C[C@H](N(C)C([C@H](C)NC([C@H](C)CC3=C(=O)C(N[C@H](C4=CC=C(O)C=C4)CC(O[C@H](C[C@ H](C)C3O)C)=O)=O	
<i>Crambe crambe</i> Mediterranean Sea	crambescidin 816	32	C ₄₅ H ₈₀ N ₆ O ₇	CCCC1=CCCC2(O1)CC3CCC4(N3C(=NC5(C4(=O)O)CCCCCCCCCCCC CCCC(=O)N(CCCN)CC(CCN)O)CCCC(O5)C)N2)O	9
	crambescidin A2 462	33	C ₂₅ H ₄₇ N ₆ O ₂	O=C(C1=C(CCC2)N2C(N)=NC1CCCCCCCCCCCC)OCCCC/N=C(N)/N	
	crambescidin 359		C ₂₁ H ₃₃ N ₃ O ₂	[H][C@]([CCC1C2)(N13)CC4(CCC=C[C@H](CC)O4)N=C3N[C@]52 CCC[C@H](C)O5	10
	crambescidin acid	34	C ₂₂ H ₃₃ N ₃ O ₄	[H][C@]([CCC1C2C(O)=O)(N13)CC4(CCC=C[C@H](CC)O4)N=C3N[C@]52CCC[C@H](C)O5	
	crambescidin 401		C ₂₂ H ₃₁ N ₃ O ₄	O=C(C1=C2CC[C@](N23)([H])C[C@]4(O[C@H](CC)C=CCC4)N=C3 N[C@]51O[C@H](C)CCC5)O	
	crambescidin B 281		C ₁₆ H ₃₁ N ₃ O	N=C(N1)N[C@H](CCCCCCCC)[C@]21OCCC2	
	crambescidin B 253	35	C ₁₄ H ₂₇ N ₃ O	CCCCCCC[C@H](N=C(N)N1)CC21CCCO2	
<i>Ircinia campana</i> & <i>Spheciospongia vesparium</i> Florida's coral reefs	xanthosine	26	C ₁₀ H ₁₂ N ₄ O ₆	C1=NC2=C(N1[C@H]3[C@H]([C@H]([C@H](O3)CO)O)O)NC(= O)NC2=O	11
	tyrosine	27	C ₉ H ₁₁ NO ₃	C1=CC(=CC=C1[C@H](C(=O)O)N)O	
<i>Ulva mutabilis</i> Cultivated, Aquaria	glycerol	28	C ₃ H ₈ O ₃	C(C(CO)O)O	12
	2,4,6-tribromophenol	29	C ₆ H ₃ Br ₃ O	C1=C(C=C(C=C1Br)O)Br)Br	

Organisms/ Ecosystems	Metabolites	Nº	MF	SMILES	R
<i>Callinectes sapidus</i> Urine, Aquaria <i>Gersemia antarctica</i> McMurdo Sound, Antartica	trigonelline	30	C ₇ H ₇ NO ₂	C[N+]=CC=CC(=C1)C(=O)[O-]	13, 14
	homarine	31	C ₇ H ₇ NO ₂	C[N+]=CC=CC=C1C(=O)[O-]	
Coral genus: <i>Acropora</i> , <i>Platygyra</i> Saadiyat Reef, Abu Dhabi, UAE	17-β estradiol	39	C ₁₈ H ₂₄ O ₂	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@H]2O)CCC4=C3C=CC(=C4)O	15
	coumaroyl-homoserine lactone	40	C ₁₃ H ₁₃ NO ₄	O=C(N[C@H]1C(OCC1=O)/C=C/C2=CC=C(O)C=C2	
	bromofuranone	41	C ₄ H ₃ BrO ₂	C1=COC(=O)C1Br	
	malabaricone C	42	C ₂₁ H ₂₆ O ₅	C1=CC(=C(C(=C1)O)C(=O)CCCCCCCCC2=CC(=C(C=C2)O)O)O	
<i>Diploria strigosa</i> & <i>Orbicella faveolata</i> , Coral-turf algae interface Caribbean island of Curaçao	ceramide 18:1/16:0	18	C ₃₄ H ₆₇ NO ₃	CCCCCCCCCCCCCCCC(=O)N[C@@H](CO)[C@@H](/C=C/CCCCCCC CCCCC)O	16
<i>Gorgonia ventalina</i> US Virgin Islands	indole-3-acetic acid	19	C ₁₀ H ₉ NO ₂	C1=CC=C2C(=C1)C(=CN2)CC(=O)O	17
<i>Plexaura homomalla</i> <i>Gorgonia ventalina</i> <i>Pseudodiploria strigosa</i> <i>Porites astreoides</i> US Virgin Islands	pantothenic acid	20	C ₉ H ₁₇ NO ₅	CC(C)(CO)C(C(=O)NCCC(=O)O)O	
<i>Ramicrusta textilis</i> US Virgin Islands	riboflavin	21	C ₁₇ H ₂₀ N ₄ O ₆	CC1=CC2=C(C=C1)N(C3=NC(=O)NC(=O)C3=N2)C[C@@H]([C@@ H])([C@@H](CO)O)O	
US Virgin Islands	caffeine	22	C ₈ H ₁₀ N ₄ O ₂	CN1C=NC2=C1C(=O)N(C(=O)N2)C	18
US Virgin Islands	tryptophan	23	C ₁₁ H ₁₂ N ₂ O ₂	C1=CC=C2C(=C1)C(=CN2)C[C@@H](C(=O)O)N	19
Florida's Coral Reef habitats, from Dry Tortugas to and North Key Largo/Biscayne Bay	taurocholic acid	24	C ₂₆ H ₄₅ NO ₇ S	C[C@H](CCC(=O)NCCS(=O)(=O)O)[C@H]1CC[C@@H]2[C@@]1([C @H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CC[C@H](C4)O C)O)C	
	5'-methylthioadenosine	25	C ₁₁ H ₁₅ N ₅ O ₃ S	CSC[C@H]1[C@H]([C@H]([C@@H]([C@@H](O1)N2C=NC3=C(N=CN=C32) N)O)O	
<i>Spongia officinalis</i> Mediterranean Sea	furospongine-1	16	C ₂₁ H ₃₀ O ₃	O[C@H](C[C@@H](C)CCCC1=COC=C1)C(C)C=C/C/C=C/C=C	5
	demethylfurospongine-4	15	C ₂₅ H ₃₄ O ₅	O=C(O)/C(C)=C/CC/C(C(=O)O)=C/CC/C(C)=C/CC/C(C)=C/CCC1=CO C=C1	
	12-epi-deoxoscalarin	17	C ₂₇ H ₄₂ O ₄	CC(O)[C@@H]1C[C@]2([H])[C@@]3(C)CCCC(C)(C)[C@]3([H])CC[C @@]2(C)[C@@]4([H])[C@@]1(C)[C@]5([H])C(CO[C@H]5O)=CC4 =O	
<i>Agelas oroides</i> Mediterranean Sea	longamide B methylester	14	C ₁₀ H ₁₀ Br ₂ N ₂ O ₃	O=C(OC)C[C@H]1CNC(C2=CC(Br)=C(Br)N21)=O	20
<i>Agelas conifera</i> Caribbean Sea	oroidin	3	C ₁₁ H ₁₁ Br ₂ N ₅ O	C1=C(NC(=C1Br)Br)C(=O)NC/C=C/C2=CN=C(N2)N	21
Benthic diatom <i>Seminavis robusta</i> (laboratory culture)	Sex-Inducing Pheromone SIP +	43	C ₂₉ H ₄₅ N ₇ O ₁₆ S ₃	O=C(N(C[C@H]1O)[C@H](C1)C(N[C@H](C)O)=O)[C@H](C(=O) O)OS(=O)(O)=O)[C@H](C[C@H]2O)N(C2)C([C@@H](NC3=O)C SSC[C@H](N)C(N[C@H](C(N[C@H]3CC(C)C)=O)C)=O)=O	
Microorganisms from marine sediments (sand slope) Mission Bay & Cabrillo state, Coast of California	chrysoeriol sulfate	46	C ₁₆ H ₁₂ O ₉ S	OC1=CC(OS(=O)(O)=O)=CC(OC(C2=CC=C(C(OC)=C2)O)=C3)=C1C3= O	22
	aplysiopsene A	47	C ₁₂ H ₁₆ O ₃	CC/C=C(/C)C1=CC(=C(C(=O)O1)C)OC	
	cabrillostatin	44	C ₁₈ H ₃₃ NO ₄	O=C(N[C@H]([C@H](C1)O)CC(C)CCCCCCC(OC1=O)C	
	cabrillospiral A	45	C ₂₉ H ₄₀ BrClO ₉	CC(CBr)[C@]1([H])C[C@H](O)[C@H](Cl)[C@]2(CCC(C(C3C=C C=C(O)C=C3)C)O)O2)O1)C[C@@](O/4)([H])[C@@H](O)CC4=C(CO /C([H])=O	

MF = molecular formula, N = attributed number in the manuscript, R = References as indicated below

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