Bioactivity Potential of Marine Natural Products from Scleractinia-Associated Microbes and *In Silico* Anti-SARS-COV-2 Evaluation

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Table S1: Marine natural products isolated from Scleractinia-associated organisms

No.	Name	Chemical category	Source organism	Host	Biological activity	Geographical location	Reference
1	12-Dimethoxy-pinselin	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
2	12-*O*-acetyl-AGI-B4	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
3	AGI-B4	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Cytotoxic	Red sea, Egypt, Africa	[1]
4	Hyperxanthone C	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
5	Pinselin	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Immuno-suppressive	Red sea, Egypt, Africa	[1,2]
6	Sydowinin B	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Immuno-suppressive	Red sea, Egypt, Africa	[1,3]
7	13-*O*-acetyl-sydowinin B	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Antioxidant	Red sea, Egypt, Africa	[1,4]
8	2,11-Dihydroxy-1-methoxycarbonyl-9-carboxyl-xanthone	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
9	Sydowinin A	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Immuno-suppressive	Red sea, Egypt, Africa	[1,3]

10	8-(Methoxycarbonyl)-1-hydroxy-9-oxo- 9H-xanthene-3-carboxylic acid	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
11	Methyl-3,8-dihydroxy-6-methyl-9-oxo-9H- xanthene-1-carboxylate	Xanthone	*Scopulariopsis* sp.	*Stylophora* sp.	Cytotoxic	Red sea, Egypt, Africa	[1,5]
12	Sydowic acid	Sesquiterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Anti-phytopathogenic	Red sea, Egypt, Africa	[1,6]
13	Sydonic acid	Sesquiterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Anti-phytopathogenic	Red sea, Egypt, Africa	[1,6]
14	11-Hydroxysydonic acid	Sesquiterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
15	11,12-Dihydroxysydonic acid	Sesquiterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
16	1-Hydroxyboivinianic acid	Sesquiterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
17	Violaceol I	Phenyl ether derivative	*Scopulariopsis* sp.	*Stylophora* sp.	Cytotoxic and antioxidant	Red sea, Egypt, Africa	[1,4]
18	Violaceol II	Phenyl ether derivative	*Scopulariopsis* sp.	*Stylophora* sp.	Cytotoxic and antioxidant	Red sea, Egypt, Africa	[1,4]
19	Diorcinol	Phenyl ether derivative	*Scopulariopsis* sp.	*Stylophora* sp.	Antioxidant	Red sea, Egypt, Africa	[1,4]

20	Rikuzenol	Phenyl ether derivative	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
21	Scopulamide	Alkaloid	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
22	Lumichrome	Alkaloid	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
23	WIN 64821	Alkaloid	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
24	Scopularide A	Cyclodepsi-peptide	*Scopulariopsis* sp.	*Stylophora* sp.	Cytotoxic	Red sea, Egypt, Africa	[1]
25	Scopularide B	Cyclodepsi-peptide	*Scopulariopsis* Sp.	*Stylophora* Sp.	Anticancer	Red sea, Egypt, Africa	[1,7]
26	Scopupyrone	α-Pyrone derivative	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
27	Pyrenochaetic acid	Benzoic acid derivative	*Scopulariopsis* sp.	*Stylophora* sp.	Cytotoxic	Red sea, Egypt, Africa	[1,8]
28	7-OH-2,5-Dimethyl-chromone	Chromone derivative	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
29	Ergosterol	Sterol	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red sea, Egypt, Africa	[1]
30	4-Methyl-candidusin A	Candidusin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
31	Aspetritone A	Anthraquinone derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]

32	Aspetritone B	Anthraquinone derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
33	3,4-Dimethyl-3''-prenylcandidusin A	Prenylcandidusin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
34	4-Methyl-3”-prenylcandidusin A	Prenylcandidusin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
35	3,4-Dimethylcandidusin A	Candidusin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Not mentioned	Malaysia, Asia	[9]
36	Candidusin A	Candidusin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic and antibacterial	Malaysia, Asia	[9]
37	4,4'-Deoxyterphenyllin	Terphenyllin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Not mentioned	Malaysia, Asia	[9]
38	4''-Deoxyterphenyllin	Terphenyllin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
39	3-Prenylterphenyllin	Terphenyllin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
40	Terphenyllin	Terphenyllin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
41	3-Hydroxyterphenyllin	Terphenyllin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]

42	3-Hydroxy-3''-deoxyterphenyllin	Terphenyllin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Not mentioned	Malaysia, Asia	[9]
43	3''-Prenylterphenyllin	Terphenyllin derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
44	Emodin	Anthraquinone derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
45	3-Hydroxy- 1,2,5,6-tetramethoxyanthracene-9,10-dione	Anthraquinone derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Cytotoxic Antibacterial	Malaysia, Asia	[9]
46	3-Hydroxy-2-hydroxymethyl-1-methoxyanthracene-9,10-dione	Anthraquinone derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Not mentioned	Malaysia, Asia	[9]
47	1,2,3-Trimethoxy-7-hydroxymethylanthracene-9,10-dione	Anthraquinone derivative	*Aspergillus tritici* SP2-8-1	*Galaxea fascicularis*	Not mentioned	Malaysia, Asia	[9]
48	3β,7β,15α,24-Tetrahydroxyolean-12-ene-11,22-dione	Triterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
49	15α,22β,24-Trihydroxyolean-11,13-diene-3-one	Triterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
50	7β,15α,24-Trihydroxyolean-12-ene-3,11,22-trione	Triterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]

51	15α,24-Dihydroxyolean-12-ene-3,11,22-trione	Triterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
52	Soyasapogenol B	Triterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Antimutagenic, antiviral and anti-inflammatory	Red Sea, Egypt, Africa	[10,11]
53	(2*E*, 4*E*)-4′-Dihydrophaseic acid	Sesquiterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
54	2*Z*, 4*E*)-4′-Dihydrophaseic acid	Sesquiterpene	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
55	6-Hydroxy-2,7-dimethyl-1,4-naphthoquinone	Polyketide	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
56	6-Hydroxy-2,2-dimethyl-2*H*-chromene	Polyketide	*Scopulariopsis* sp.	*Stylophora* sp.	Antioxidant and cancer protecting effects	Red Sea, Egypt, Africa	[10,12]
57	Scoparone	Polyketide	*Scopulariopsis* sp.	*Stylophora* sp.	Immuno-suppressive, antiproliferative and antioxidant	Red Sea, Egypt, Africa	[10,13-15]
58	5-Methyluracil	Nitrogenous compound	*Scopulariopsis* sp.	*Stylophora* sp.	Antitumor	Red Sea, Egypt, Africa	[10,16]

59	4-Hydroxy-3-methoxy-2(1*H*)-quinolinone	Nitrogenous compound	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
60	4-Hydroxyphenyl-glyoxylic acid amide	Nitrogenous compound	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
61	Indole-3-carboxaldehyde	Nitrogenous compound	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
62	Indole-3-carboxylic acid	Nitrogenous compound	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
63	(1*H*-Indol-3-yl)-oxo-acetamide	Nitrogenous compound	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
64	*N*-Acetyl-β-oxo-tryptamine	Nitrogenous compound	*Scopulariopsis* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[10]
65	Gliomastin A	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Cytotoxic	Red Sea, Egypt, Africa	[17]
66	Gliomastin B	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]
67	Gliomastin C	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Antitubercular	Red Sea, Egypt, Africa	[17]
68	Gliomastin D	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]
69	9-*O*-Methyl-gliomastin C	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]

70	Acremonin A 1-*O*-β-D-gluco- pyranoside	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]
71	Gliomastin E 1-*O*- β-D-gluco -pyranoside	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]
72	6′-*O*-Acetyl-isohomoarbutin	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]
73	Isohomoarbutin	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]
74	2-Methyl-1,4-benzenediol	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Cytotoxic Antitubercular Antibacterial	Red Sea, Egypt, Africa	[17]
75	Acremonin A	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Cytotoxic Antitubercular	Red Sea, Egypt, Africa	[17]
76	Prenylhydro-quinone	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Cytotoxic Antitubercular Antibacterial	Red Sea, Egypt, Africa	[17]
77	F-11334A$_1$	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Cytotoxic Antitubercular	Red Sea, Egypt, Africa	[17]
78	(R)-2-(2-Hydroxy-propan2-yl)-2,3-dihydro-5-hydroxybenzofuran	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]
79	2,2-Dimethyl-chroman-3,6-diol	Hydroquinone derivative	*Gliomastix* sp.	*Stylophora* sp.	Not mentioned	Red Sea, Egypt, Africa	[17]

80	Verruculosin A	Oligophen-alenone dimer	*Talaromyces verruculosus*	*Goniopora* sp.	Antitumor	South China Sea, China, Asia	[18]
81	Verruculosin B	Oligophen-alenone dimer	*Talaromyces verruculosus*	*Goniopora* sp.	Antitumor	South China Sea, China, Asia	[18]
82	Bacillisporin F	Oligophen-alenone dimer	*Talaromyces verruculosus*	*Goniopora* sp.	Antitumor	South China Sea, China, Asia	[18]
83	Duclauxin	Oligophen-alenone dimer	*Talaromyces verruculosus*	*Goniopora* sp.	Antitumor and antileukemia	South China Sea, China, Asia	[18]
84	Xenoclauxin	Oligophen-alenone dimers	*Talaromyces verruculosus*	*Goniopora* sp.	Antitumor	South China Sea, China, Asia	[18]
85	Erythroxanthin sulfate	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
86	Ketonostoxanthin	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
87	Nostoxanthin sulfate	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
88	Caloxanthin sulfate	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
89	Nostoxanthin	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
90	Zeaxanthin sulfate	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
91	Caloxanthin	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
92	Bacterio-rubixanthinal	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
93	Zeaxanthin	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Radioprotectant and antioxidant	Indonesia	[19-21]

94	β-Cryptoxanthin	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Antioxidant, anti-inflammatory, anticancer, homeostatic and anti-osteoporosis	Indonesia	[19,22]
95	Bacteriochlorophyll	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Not mentioned	Indonesia	[19]
96	β-Carotene	Carotenoid	*Erythrobacter flavus*	*Acropora nasuta*	Antioxidant and anticancer	Indonesia	[19,23]
97	Aranciamycin K	Anthracycline analogue	*Streptomyces* sp.	*Porites* sp.	Not mentioned	China	[24]
98	Isotirandamycin B	Tirandamycin analogue	*Streptomyces* sp.	*Porites* sp.	Bacteriostatic	China	[24]
99	γ-Rhodomycinone	Anthracycline derivative	*Streptomyces* sp.	*Porites* sp.	Not mentioned	China	[24]
100	β-Rhodomycinone	Anthracycline derivative	*Streptomyces* sp.	*Porites* sp.	Cytotoxic	China	[24]
101	262-6	Anthracycline derivative	*Streptomyces* sp.	*Porites* sp.	Antibacterial Cytotoxic	China	[24]
102	β-Rhodomycin-II	Anthracycline derivative	*Streptomyces* sp.	*Porites* sp.	Antibacterial Cytotoxic	China	[24]
103	Tirandamycin A	Tirandamycin derivative	*Streptomyces* sp.	*Porites* sp.	Antibacterial	China	[24]

104	Tirandamycin B	Tirandamycin derivative	*Streptomyces* sp.	*Porites* sp.	Antibacterial	China	[24]
105	Pelopuradazole	Imidazole alkaloid	*Pelomonas puraquae*	*Acropora* sp.	Not mentioned	South China Sea	[25]
106	3*H*-Imidazole-4-carboxylic acid	Imidazole alkaloid	*Pelomonas puraquae*	*Acropora* sp.	Not mentioned	South China Sea	[25]
107	2-Methyl-3H-imidazole-4-carboxylic acid	Imidazole alkaloid	*Pelomonas puraquae*	*Acropora* sp.	Not mentioned	South China Sea	[25]
108	1*H*-Pyrrole-2-carboxylic acid	Imidazole alkaloid	*Pelomonas puraquae*	*Acropora* sp.	Antibacterial	South China Sea	[25]
109	Pelopurin A	Cyclodipeptide	*Pelomonas puraquae*	*Acropora* sp.	Not mentioned	South China Sea	[25]
110	Pelopurin B	Cyclodipeptide	*Pelomonas puraquae*	*Acropora* sp.	Not mentioned	South China Sea	[25]
111	Unnamed	Hydroxy-quinaldic acid derivative	*Streptomyceces cyaneofuscatus*	Different corals belong to *Scleractinia*	Cytotoxic	Northeast Atlantic, Europe	[26]
112	Unnamed	Hydroxy-quinaldic acid derivative	*Streptomyceces cyaneofuscatus*	Different corals belong to *Scleractinia*	Not mentioned	Northeast Atlantic, Europe	[26]
113	Unnamed	Hydroxy-quinaldic acid derivative	*Streptomyceces cyaneofuscatus*	Different corals belong to *Scleractinia*	Not mentioned	Northeast Atlantic, Europe	[26]
114	3-Hydroxyquinaldic acid	Hydroxyquinaldic acid derivative	*Streptomyceces cyaneofuscatus*	Different corals belong to *Scleractinia*	Not mentioned	Northeast Atlantic, Europe	[26]

115	3- Hydroxyquinaldic acid amide	Hydroxyquinaldic acid derivative	*Streptomyceces cyaneofuscatus*	Different corals belong to *Scleractinia*	Cytotoxic	Northeast Atlantic, Europe	[26]
116	Nakienone A	Cyclic C-11	*Synechocystis* sp.	*Acropora* sp.	Cytotoxic	Okinawa, Japan, Asia	[27]
117	Nakitriol	Cyclic C-11	*Synechocystis* sp.	*Acropora* sp.	Cytotoxic	Okinawa, Japan, Asia	[27]
118	Nakienone B	Cyclic C-11	*Synechocystis* sp.	*Acropora* sp.	Not mentioned	Okinawa, Japan, Asia	[27]
119	Nakienone C	Cyclic C-11	*Synechocystis* sp.	*Acropora* sp.	Not mentioned	Okinawa, Japan, Asia	[27]
120	Pitiamide A	Fatty acid amide	*Phormidium corallyticum*	*Porites* sp.	Anti-proliferative	USA, North America	[28]
121	1*E*-Pitiamide B	Fatty acid amide	*Phormidium corallyticum*	*Porites* sp.	Anti-proliferative	USA, North America	[28]
122	Looekeyolide A	Macrolide	*Roseofilum reptotaenium*	*Montastraea* sp.	Not mentioned	Florida, North America	[29]
123	Looekeyolide B	Macrolide	*Roseofilum reptotaenium*	*Montastraea* sp.	Not mentioned	Florida, North America	[29]
124	Alteramide A	Tetracyclic alkaloid	*Pseudoalteromonas* sp.	*Montipora* sp.	Cytotoxic and antifungal	Japan, Asia	[30,31]
125	Alteramide B	Tetracyclic alkaloid	*Pseudoalteromonas* sp.	*Montipora* sp.	Antifungal	Japan, Asia	[30,31]
126	(2*Z*,4*E*)-3-Methyl-2,4-decadienoic acid	Fatty acid	*Microbulbifer* sp.	*Porites* sp.	Antibacterial	Japan, Asia	[32]

127	Nesteretal A	Polyhemiketal,	*Nesterenkonia* sp.	*Platygyra* sp.	RXR*α* activity	China Asia	[33]
128	Lobophorin K	Lobophorin	*Streptomyces* sp.	*Lophelia pertusa*	Cytotoxic Antibacterial	Cantabrian Sea, North America	[34]
129	Gorgosterol	Sterol	*Zooxanthellae*	*Oculina diffusa*	Not mentioned	Permuda, Europe	[35]
130	23-Desmethyl-gorgosterol	Sterol	*Zooxanthellae*	*Oculina diffusa*	Not mentioned	Permuda, Europe	[35]
131	Dinosterol	Sterol	*Zooxanthellae*	*Oculina diffusa*	Not mentioned	Permuda, Europe	[35]
132	Cholesterol	Sterol	*Zooxanthellae*	*Oculina diffusa*	Not mentioned	Permuda, Europe	[35]
133	4*α*-(24S)-Dimethyl-cholesta-3β-ol	Sterol	*Zooxanthellae*	*Oculina diffusa*	Not mentioned	Permuda, Europe	[35]
134	4*α*-(24R)-Dimethyl-cholesta-22-en-3β-ol	Sterol	*Zooxanthellae*	*Oculina diffusa*	Not mentioned	Permuda, Europe	[35]

Table S2: Docking energies (kcal/mol) of investigated compounds with different SARS-CoV-2 targets

Compound Number	**6LU7**	**6W4H, nsp16**	**7BV2, nsp12**	**6VW1**	**6M0J**
	Main protease, M^{pro}	**Methyl Transferase**	**RNA-dependent RNA polymerase**	**Human ACE2**	**Receptor-binding domain (RBD) of S-protein**
3	-7.4	-7.1	-6.3	-5.6	-6.1
7	-6.9	-7.9	-7	-6.4	-6.4
17	-6.6	-7.6	-6.2	-5.8	-6.4
18	-7.7	-8.2	-6.3	-7	-6.7
31	-7.1	-7.3	-6.3	-5.2	-5.6
32	-7.4	-7.2	-6.3	-5.9	-5.9
39	-7.9	-8.0	-6.3	-5.8	-6.7
53	-6.1	-6.3	-5.9	-6.1	-5.9
77	-5.8	-6.5	-5.4	-5.3	-5.6
98	-7.8	-8.4	-7.6	-5.9	-6.8
103	-7.9	-8.5	-8.1	-6.3	-6.8
104	-7.8	-8.3	-7.9	-5.9	-6.8
120	-5.8	-5.8	-5	-5	-5.1
121	-5.2	-6.3	-4.8	-5.2	-4.8
124	-7.1	-8.2	-9	-6.1	-7.4
Ligand	-7.9 (N3)	-8.1 (SAM)	-7.0 (RemdesivirTP)	----	---

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