

Supplementary Materials

Novel Marine Secondary Metabolites Worthy of Development as Anticancer Agents: A Review

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Table S1. The IC₅₀ of marine derived alkaloids with anticancer activity

S/N	Isolated Compounds	Class	Status	Source	Year	Cancer cell line	Cancer Source	IC ₅₀ (μM)	Ref.
1.	Subereumoline D (Cpd. 1)	Bromotyrosine-derived alkaloids	Novel	Sea sponge <i>Fascaplysinopsis reticulata</i> from Xisha Islands in the south China	2019	Jurkat cell (T-cell leukaemia)	Human	0.88	³⁷
2.	N-glutarylchaetoviridin A (Cpd. 2) N-glutarylchaetoviridin C (Cpd. 4) Chaetomugilin A (Cpd. 5)	Glutamine-containing Azaphilone Alkaloids	Novel (Cpds. 2, 4) Known (Cpds. 5, 6)	Deep-Sea-Derived Fungus <i>Chaetomium globosum</i> HDN151398, a fungus isolated from a deep-sea sediment sample collected in South China Sea.	2019	HL-60 (leukaemia) HL-60 (leukaemia) K562 rhabdomyoma BEL-7402 (hepatoma) HCT-116 (colon) L-02 (hepatic) MGC-803 (gastric) HO8910 (ovary) (neuroblastoma) NCI-H1975 (lung adenocarcinoma) U87 (glioblastoma) MDA-MB-231(breast) HL-60 (lukaemia) K562 rhabdomyoma BEL-7402 (hepatoma) HCT-116 (colon) L-02 (hepatic) MGC-803 (gastric) HO8910 (ovary)	All human	10.3 11.1 11.7 10.9 11.3 18.2 6.6 9.7 11.2 18.3 13.2 6.4 11.1 17.9 6.1 15.2 15.3 12.1 18.3	³⁸

	Chaetomugilin C (Cpd. 6)				NCI-H1975 (<i>lung</i>)		6.6	
					HL-60 (<i>leukaemia</i>)		12.3	
					K562 (<i>rhabdomyoma</i>)		16.8	
					BEL-7402 (<i>hepatoma</i>)		5.7	
					HCT-116 (<i>colon</i>)		13.2	
					HeLa (<i>cervical</i>)		9.1	
					L-02 (<i>hepatic</i>)		9.6	
					MGC-803 (<i>gastric</i>)		8.8	
					HO8910 (<i>ovary</i>)		19.4	
					SHSY5Y (<i>neuroblastoma</i>)			
					NCI-H1975 (<i>lung</i>)		12.1	
					U87 (<i>glioblastoma</i>)		17.6	
3.	Monanchoxymycalin C (Cpd. 12)	Pentaacyclic guanidine alkaloid	Novel	Marine sponge <i>Monanchora pulchra</i> collected off the coast of Chirpoi Island	2019	HELa (<i>cervical</i>)	Human	3.5
4.	Araguspongine C (Cpd. 14)	Macrocyclic bis-quinolizidine alkaloid	Novel (Cpd. 15) others known	Marine sponge <i>Xestospongia muta</i> collected at the coral reef of Vinh Moc, Quang Tri, Vietnam	2019	HepG-2 (<i>liver</i>) HL-60 (<i>leukaemia</i>) LU-1 (<i>lung</i>) MCF-7 (<i>breast</i>) SK-MEL-2 (<i>Skin</i>)	All human	0.75 0.88 0.96 0.79 1.02
	Meso-araguspongine C (Cpd. 15)				HepG-2 (<i>liver</i>) HL-60 (<i>leukaemia</i>) LU-1 (<i>lung</i>) MCF-7 (<i>breast</i>) SK-MEL-2 (<i>Skin</i>)		0.43 0.62 0.76 0.44 0.77	
	Araguspongine N (Cpd. 18)				HepG-2 (<i>liver</i>) HL-60 (<i>leukaemia</i>) LU-1 (<i>lung</i>) MCF-7 (<i>breast</i>) SK-MEL-2 (<i>Skin</i>)		6.58 7.84 9.20 7.36 11.23	
	Araguspongines O (Cpd. 19)				HepG-2 (<i>liver</i>) HL-60 (<i>leukaemia</i>) LU-1 (<i>lung</i>) MCF-7 (<i>breast</i>) SK-MEL-2 (<i>Skin</i>)		5.06 5.65 5.63 5.32 5.45	
	Araguspongine P (Cpd. 20)				HepG-2 (<i>liver</i>) HL-60 (<i>leukaemia</i>) LU-1 (<i>lung</i>) MCF-7 (<i>breast</i>) SK-MEL-2 (<i>Skin</i>)		5.55 6.58 5.84 5.68 6.24	
	Araguspongine A (Cpd. 13)				HepG-2 (<i>liver</i>) HL-60 (<i>leukaemia</i>) LU-1 (<i>lung</i>)		6.85 9.19 9.88	

						MCF-7 (<i>breast</i>) SK-MEL-2 (<i>Skin</i>)		7.82 7.51	
5.	Ascomylactam A (Cpd. 23)	Macrocyclic alkaloids	All novel	Fungus CYSK-4 isolated from a marine semi mangrove <i>Pluchea indica</i> collected from Shankou Mangrove Nature Reserve in Guangxi Province, China	2019	MDA-MB-435 (<i>melanoma</i>)	All human	4.9	⁴¹
	Ascomylactam B (Cpd. 24)					MDA-MB-231 (<i>breast</i>)		5.9	
	Ascomylactam C (Cpd. 25)					SNB19 (<i>glioblastoma</i>)		6.8	
6.	Chaetoglobosins E (Cpd. 33)	Alkaloids	Known	<i>Chaetomium globosum</i> C2F17 isolated from a coral <i>Pocillopora damicornis</i> collected from the seashore near Sanya Bay, Hainan Province, China	2020	HCT116 (<i>colon</i>)	All human	5.5	⁴²
						NCI-H460 (<i>lung</i>)		4.4	
						PC-3 (<i>prostate</i>)		5.7	
						MDA-MB-435 (<i>melanoma</i>)		12	
						MDA-MB-231 (<i>breast</i>)		6.6	
						SNB19 (<i>glioblastoma</i>)		18	
						HCT116 (<i>colon</i>)		4.5	
						NCI-H460 (<i>lung</i>)		13	
						PC-3 (<i>prostate</i>)		20	
						MDA-MB-435 (<i>melanoma</i>)		7.8	
6.						MDA-MB-231 (<i>breast</i>)		5.1	
						SNB19 (<i>glioblastoma</i>)		7.8	
						HCT116 (<i>colon</i>)		4.2	
						NCI-H460 (<i>lung</i>)		4.4	
						PC-3 (<i>prostate</i>)		7.5	
						K562 (<i>chronic myelogenous leukemia</i>)	All human	8.9	⁴²
						A549 (<i>lung adenocarcinoma</i>)		5.9	
						Huh7 (<i>hepatocarcinoma</i>)		1.4	
						H1975 (<i>lung adenocarcinoma</i>)		9.2	
						MCF-7 (<i>breast carcinoma</i>)		2.1	
						U937 (<i>lymphocytic leukemia</i>)		1.4	
						BGC823 (<i>gastric adenocarcinoma</i>)		8.2	
						HL60 (<i>promyelocytic leukemia</i>)		2.5	
						Hela (<i>cervical carcinoma</i>)		2.8	

	Fex (Cpd. 38)				MOLT-4 (<i>acute T lymphoblastic leukaemia</i>) Huh7 (<i>hepatocarcinoma</i>) MCF-7 (<i>breast carcinoma</i>) U937 (<i>lymphocytic leukemia</i>) MOLT-4 (<i>acute T lymphoblastic leukaemia</i>)		1.4	
7.	Tridiscorhabdin (Cpd. 45)	Alkaloid	Novel	Sponge <i>Latrunculia biformis</i> Collected from southern Weddell deep sea (Antarctica)	2020	HCT-116 (colon)	Human	0.31 ⁴³
8.	7'-demethoxyrostratin C (Cpd. 50) Rostratin C (Cpd. 57)	Thiodiketopiperazine alkaloids	Novel Known	Fungal strain <i>Epicoccum nigrum</i> SD-388 was isolated from the deep-sea sediment collected in the West Pacific	2020	Huh7.5 (<i>Liver cancer</i>)	Human	9.52 ⁴⁴ 4.88
9.	Streptogltutarimide H (Cpd. 65) Streptovitacin A (Cpd. 68)	Glutarimide (Alkaloids)	Novel Known	Marine-derived actinomycete, Streptomyces sp. ZZ741 from the coastal area of Jintang Island in Zhoushan, China	2019	U87MG (<i>glioma</i>) U251 (<i>glioma</i>) U87MG (<i>glioma</i>) U251 (<i>glioma</i>)	All Human	3.8 1.5 0.22 0.05 ⁴⁵
10.	N-(3-Hydroxyphenethyl)-1-(1H-indole-3-carbonyl)-9Hpyrido[3,4-b]indole-3-carboxamide, 9e (Cpd. 73) N-(4-hydroxy-3-methoxybenzyl)-1-(1H-indole-3-carbonyl)-9H-pyrido[3,4-b]indole-3-carboxamid, 9l (Cpd. 80) Pityriacitrin - 1-(1H-indole-3-carbonyl)eN-(2-(methylsulfonyl)ethyl)-9Hpyrido[3,4-b]indole-3-carboxamide 9o (Cpd. 83) Methyl 2-(1-(1H-indole-3-carbonyl)-9H-pyrido[3,4-b] indole-3-carboxamido)-3-hydroxypropanoate 9p (Cpd. 84)	β- carboline derivative of Pityriacitrin Indole Alkaloid	All novel	Marine <i>Burkholderia</i> sp. NBF227 from China	2019	SGC-7901 (<i>gastric</i>) A875 (<i>melanoma</i>) HepG2 (<i>liver</i>) MARC145 (<i>Kidney</i>) SGC-7901 (<i>gastric</i>) A875 (<i>melanoma</i>) HepG2 (<i>liver</i>) MARC145 (<i>Kidney</i>) SGC-7901 (<i>gastric</i>) A875 (<i>melanoma</i>) HepG2 (<i>liver</i>) MARC145 (<i>Kidney</i>) SGC-7901 (<i>gastric</i>) A875 (<i>melanoma</i>) HepG2 (<i>liver</i>)	Human Human Human African green monkey	17.65 11.91 8.63 13.77 16.18 8.47 11.08 6.80 8.43 7.69 7.19 14.30 10.46 9.99 16.27 ⁴⁶
11.	Ochrazepine A (Cpd. 85)	Circumdatins derivatives alkaloid	Novel (Cpds. 84-87) Known (Cpds. 88,89)	Fungus <i>Aspergillus ochraceus</i> LCJ11-102 isolated from the coral <i>Dichotella gemmacea</i> (Valenciennes) collected in Lingao, Hainan province, China	2019	MV-4-11 (<i>biphenotypic B myelomonocytic leukemia</i>) K562 (<i>erythroleukemic cell line</i>)	All human except B16F10 which is from mouse	3.94 ⁴⁷ 6.05 3.10

				A673 (<i>rhabdomyoma cell line</i>)	8.67
				U87 (<i>glioblastoma cell line</i>)	9.62
				A549 (<i>lung carcinoma</i>)	6.10
				N87 (<i>gastric carcinoma</i>)	7.14
				H1299 (<i>non-small cell lung carcinoma</i>)	11.32
				HUCCT1 (<i>bile duct carcinoma</i>)	11.22
				B16F10 (<i>highly metastatic mouse melanoma cell line</i>)	
				Karpass299 (<i>T cell lymphoma</i>)	5.89
Ochrazepine B (Cpd. 86)				<u>U251 (<i>glioblastoma cell line</i>)</u>	<u>9.91</u>
Ochrazepine C (Cpd. 87)				A673 (<i>rhabdomyoma cell line</i>)	8.24
				U87 (<i>glioblastoma cell line</i>)	9.04
				Hep3B (<i>liver cancer</i>)	10.28
Ochrazepine D (Cpd. 88)				<u>U251 (<i>glioblastoma cell line</i>)</u>	<u>8.26</u>
2-hydroxycircumdatin C (Cpd. 89)				U251 (<i>glioblastoma cell line</i>)	8.95
Aspyrone (Cpd. 90)				<u>U251 (<i>glioblastoma cell line</i>)</u>	<u>2.54</u>
				MV-4-11 (<i>biphenotypic B myelomonocytic leukemia</i>)	5.22
				K562 (<i>erythroleukemic cell line</i>)	8.55
				A673 (<i>rhabdomyoma cell line</i>)	4.57
				N87 (<i>gastric carcinoma</i>)	5.83
				H1299 (<i>non-small cell lung carcinoma</i>)	9.79
				HUCCT1 (<i>bile duct carcinoma</i>)	5.89
				B16F10 (<i>highly metastatic mouse melanoma cell line</i>)	2.57
				Karpass299 (<i>T cell lymphoma</i>)	5.48
					5.92

					Hep3B (<i>liver cancer</i>) A431 (<i>Epidermoid carcinoma cell line</i>) 143B (<i>bone osteosarcoma</i>) MKN-45 (<i>gastric cancer</i>) H1975 (<i>non-small cell lung carcinoma with L858R and T790M mutation</i>) HL-60 (<i>promyelocytic leukemia</i>) DU145 (<i>prostate cancer</i>) SPC-A1 (<i>lung cancer over expressing maspin cell line</i>)		6.32 5.79 2.99 6.89 5.61 9.31
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Table S2. The IC₅₀ of marine-derived terpenes and terpenoids with anticancer activity

S/N	Isolated Compounds	Class	Status (Known /Novel)	Source	Year	Cancer cell line	Source	IC ₅₀ (μM)	Ref
1.	Eutypellacytosporin A, C ₄₀ H ₅₈ O ₁₁ (Cpd. 91) Eutypellacytosporin B, C ₄₀ H ₅₈ O ₁₁ (Cpd. 92) Eutypellacytosporin C, C ₄₀ H ₅₈ O ₁₁ (Cpd. 93) Eutypellacytosporin D, C ₄₀ H ₅₈ O ₁₁ (Cpd. 94)	Meroterpenoids	All Novel	Arctic fungus Eutypella sp. D-1 from soil of London Island of ongsfjorden of Ny-Ålesund District in the Arctic.	2019	DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>) DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>) DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>) DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>)	All human	17.1 7.3 8.4 9.7 11.0 4.9 4.9 7.9 13.5 9.6 11.2 10.2 13.4 8.2 9.6 7.5	⁴⁸

2.	Diorecinol (Cpd. 97) Versicolorin B (Cpd. 101)	Indoloditerpenes	Both Known	Marine-derived fungus <i>Aspergillus versicolor</i> ZZ761	2019	U87MG (<i>glioma</i>) U251(<i>glioma</i>) U87MG (<i>glioma</i>)	Both human	4.4 6.2 11.3	⁴⁹
3.	Insuliclide A (Cpd. 114)	Drimane sesquiterpenoid derivatives	Known	<i>Aspergillus. Flocculosus</i> obtained from marine sediment sample (Nha Trang Bay, South ChinanSea,Vietnam)	2019	22Rv1 (<i>prostate</i>) Neuro-2a (<i>neuron</i>)	Human Murine	3.0 4.9	⁵⁰
4.	19-methoxy-dictyoceratin-A (Cpd. 123) Smenospongianine (Cpd. 125)	?	Novel Known (Cpds. 125-128)	Marine sponge <i>Dactylospongia elegans</i> was collected off Yongxing Island in the South China Sea	2019	Huh7 (<i>liver</i>) DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>) DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>) DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>) DU145 (<i>prostate</i>) SW1990 (<i>pancreas</i>) Huh7 (<i>liver</i>) Panc-1 (<i>pancreas</i>)	All human	17.4 6.1 5.9 3.7 8.7 4.2 4.4 3.0 7.7 3.5 4.2 2.3 5.8 8.3 7.9 6.9 9.2	⁵¹
	Smenospongiorine (C. 126)								
	Smenospongimine (Cpd. 127)								
	Dictyoceratin-C (Cpd. 128)								
5.	Andrastone A (Cpd. 129)	Meroterpenoids	Novel	Deep-Sea-Derived Fungus <i>Penicillium allii-sativi</i> from the deep-sea water of the western Pacific	2019	HepG2 (<i>liver</i>)	Human	7.8	⁵²
6.	Sakurasosaponin (Cpd. 133)	Triterpene saponin	Both known	Leaves of the mangrove <i>Aegiceras corniculatum</i> were collected from Bai Tu Long bay, Quang Ninh Province, Vietnam	2019	MCF-7 (<i>breast</i>) A549 (<i>lung adenocarcinoma</i>) B16F10 (<i>melanoma</i>) HCT116 (<i>colon</i>) MCF-7 (<i>breast</i>) A549 (<i>lung adenocarcinoma</i>) B16F10 (<i>melanoma</i>) HCT116 (<i>colon</i>)	All human	9.85 2.89 4.96 3.40 9.86 5.45 18.27 2.21	⁵³
	Sakurasosaponin methyl ester (Cpd. 134)								
7.	Flaccidenol A (Cpd. 149)	Capnosane (Cpd.149) cembranoids (Cpd 151) -based diterpenoids	Novel (149, 151)	From marine soft coral <i>Klyxum flaccidum</i> , collected off the coast of the island of Pratas	2019	A549 (<i>lung adenocarcinoma</i>) DLD-1 (<i>colorectal adenocarcinoma</i>)	Human Human Mouse	9.7 6.0 7.2	⁵⁴

	Flaccidodioxide (Cpd. 151) 14-Oacetyl sarcophytol B (Cpd. 155)		Known		P388D1 (<i>mouse lymphocytic leukaemia</i>) P388D1 (<i>mouse lymphocytic leukaemia</i>) A549 (<i>lung adenocarcinoma</i>) DLD-1 (<i>colorectal adenocarcinoma</i>) P388D1 (<i>mouse lymphocytic leukemia</i>)		19.6 10.8 11.7 8.9		
8.	Asterolaurin N (Cpd. 156) 13-epi-9-desacetylxenicin (Cpd. 157) Xeniolide-B 9-acetate (Cpd. 158) Asterolaurin I (Cpd. 159)	Diterpenes	Novel (Cpd. 156) Known (Cpds. 157-159)	Taiwanese soft coral <i>Asterospicularia laurae</i> , southern coast of Taiwan	2019	Molt 4 (<i>T lymphoblast; acute lymphoblastic leukaemia</i>) Molt 4 (<i>T lymphoblast; acute lymphoblastic leukaemia</i>) K562 (<i>blood chronic myelogenous leukaemia</i>) Sup-T1 (<i>T cell lymphoblastic lymphoma</i>) U937 (<i>Caucasian histiocytic lymphoma</i>) Molt 4 T (<i>lymphoblast; acute lymphoblastic leukaemia</i>) Molt 4 T (<i>lymphoblast; acute lymphoblastic leukaemia</i>)	All human	19.41 1.30 1.19 3.17 2.45 15.13 18.75	⁵⁵
9.	Cembranolide diterpene derivative 1 (Cpd. 160)	Diterpenoid	Novel	Soft coral, <i>Lobophytum</i> sp. from the coast of Irabu Island, Okinawa, Japan	2019	HeLa (<i>cervix</i>) A549 (<i>lung</i>) B16-F10 (<i>melanoma</i>) RAW 264.7 (<i>murine macrophage</i>)	Human (First 3) Murine	7.81 9.30 10.83 5.99	⁵⁶
10.	Ambliol C (Cpd. 174)	Furanoditerpenes	Known	Sponge <i>Spongia tubulifera</i> collected from the coast of the Mexican Caribbean	2019	MCF-7 (<i>breast</i>) MiaPaca-2 (<i>pancreas</i>)	Both human	19.9 11.7	⁵⁷
11.	Aphidicolin A (Gpd. 183)	Diterpenoids	Novel	Deep-Sea-Derived Fungus <i>Botryotinia fuckeliana</i> MCCC 3A00494 western Pacific Ocean	2019	T24 (<i>Kidney</i>) HL-60 (<i>Leukaemia</i>)	Both human	2.5 6.1	⁵⁸

12.	Ilimaquinone (Cpd. 255)	Sesquiterpene quinones and quinols	All known	Marine Sponge <i>Dactylospongia elegans</i> Sheraton Caverns, Kauai, Hawaiian	2019	U251MG (glioblastoma)	Both human	19.3	59
	5- <i>epi</i> -iliamaquinone (Cpd. 256)					U251MG (glioblastoma)		19.4	
	Smenosponge (Cpd. 257)					Panc-1 (pancreatic carcinoma)		16.2	
	Smenospongoline (Cpd. 258)					U251MG (glioblastoma)		2.4	
	Smenospongianine (Cpd. 259)					U251MG (glioblastoma)		19.4	
	Smenospongidine (Cpd. 260)					U251MG (glioblastoma)		4.5	
	Dictyoceratin A (Cpd. 261)					Panc-1 (pancreatic carcinoma)		15.1	
	Dictyoceratin B (Cpd. 262)					U251MG (glioblastoma)		4.0	
	Dictyoceratin C (Cpd. 263)					Panc-1 (pancreatic carcinoma)		12.6	
	Erythrolide D (Cpd. 268)	Chlorinated briarane diterpenoids	All known	<i>Erythropodium caribaeorum</i> from soft coral collected from Caribbean sea in Colombia	2019	U251MG (glioblastoma)	All human	2.8	60
13.	Erythrolide A (Cpd. 275)					A549 (lung)		18.41	
	Erythrolide B (Cpd. 276)					A549 (lung)		6.77	
	Henridilactone A (Cpd. 281)	Nortriterpenoids (Cpd. 281) Lignan (Cpds. 287, 289)	Novel (Cpd. 281) Known (Cpds. 287, 289)	<i>Schisandra sphenanthera</i> collected in KonTum province, Vietnam	2019	MCF-7 (breast)	Both human	2.45	61
14.	Schisandrathera C (Cpd. 287)					PC3 (prostate)		15.21	
	Schirubrisin B (Cpd. 289)					MCF-7 (breast)		6.46	
	(+)-19-methylaminoavarone (Cpd. 290)					PC3 (prostate)		3.21	
15.	(-)-20-methoxyneavarone (Cpd. 291)	Sesquiterpenoid quinones	Novel (Gpd. 290) Known (Cpds. 292-296)	Marine sponge <i>Dysidea</i> sp from Xisha Islands, South China	2019	MCF-7 (breast)	All human	13.30	62
	(<i>b</i>)-20-methoxyavarone (Cpd. 292)					PC3 (prostate)		19.11	
	(-)-20-phenethylaminoavarone (Cpd. 294)					MCF-7 (breast)		13.30	
						PC3 (prostate)		3.21	
						MCF-7 (breast)		17.82	
						HCT-116 (colon)		5.48	
						A549 (lung)		4.61	
						HeLa (cervix)		0.93	
						HCT-116		1.31	
						Jurkat cell (<i>T-lymphocyte</i>)		2.29	
						K562 (leukaemia)		3.07	
						BEL-7402 (hepatoma)		4.02	
						HCT-116 (colon)		5.19	
						Jurkat cell (<i>T-lymphocyte</i>)		2.69	
						K562 (leukaemia)		13.35	
						A549 (lung)		7.66	
						HeLa (cervix)		4.88	
						HCT-116		3.52	
						Jurkat cell (<i>T-lymphocyte</i>)		12.58	

	(-)-20-methylaminoavarone (Cpd. 296)					K562 (<i>leukaemia</i>) <u>BEL-7402 (<i>hepatoma</i>)</u> A549 (<i>lung</i>) HeLa (<i>cervix</i>) Jurkat cell (<i>T-lymphocyte</i>)		9.81 9.40	
16.	Penicindopene A (Cpd. 297)	Andole diterpene	Novel	Deep-sea fungus <i>Penicillium</i> sp. YPCM4C1 from Yap Trench in West Pacific Ocean	2019	A549 (<i>lung</i>)	human	15.2	⁶³
17.	14,15-dehydro-6- <i>epi</i> -ophiobolin K (Cpd. 305) 14,15-dehydroophiobolin K (Cpd. 306) 14,15-dehydro-6- <i>epi</i> -ophiobolin G (Cpd. 307) 14,15-dehydro-ophiobolin G (Cpd. 308) 14,15-dehydro-(Z)-14-ophiobolin G (Cpd. 309) 6- <i>epi</i> -ophiobolin C (Cpd. 310)	Sesterterpenes	Novel (Cpd. 305-309), Known (Cpd. 310-313)	Fungus <i>Aspergillus flocculosus</i> 168ST-16.1 was isolated from the algae <i>Padina</i> sp., collected at a depth of 10 m in SonTra peninsular, Da Nang, Vietnam	2019	HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u>	All human	0.21 0.19 0.18 0.24 0.24 0.14 0.44 0.50 0.61 0.53 0.47 0.63 0.96 0.88 1.40 1.14 1.00 1.05 1.24 1.07 1.50 1.40 1.38 1.35 1.67 1.53 1.84 2.01 1.60 1.75 0.24 0.22 0.24 0.43 0.27	⁶⁴

	Ophiobolin C (Cpd. 311) 6- <i>epi</i> -ophiobolin N (Cpd. 312) Ophiobolin N (Cpd. 313)				PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u> HCT-15(<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>) <u>MDA-MB-231 (<i>breast</i>)</u>		0.19	
18.	12-O-acetyl-nardosinan-6-en-1-one (Cpd. 314) 6b-acetyl-1(10)-a-13-nornardosin-7-one (Cpd. 315) 6,7-seco-13-nornardosinane (Cpd. 316) 6a-acetyl-1(10)-a-13-nornardosin-7-one (Cpd. 317) 12-Acetoxy-l(10)-aristolene (Cpd. 318) 4-Acetoxy-2,8-neolemnadien-5-one (Cpd. 319) Cembranoid-diterpene Nephthalenol (Cpd. 320) 24-Methylcholesterol (Cpd. 321)	Sesquiterpenes (Cpds. 314 - 320) Steroid (Cpd. 321)	Novel (Cpds. 314 - 316) Known (Cpds 317 - 321)	Soft coral <i>Rhytisma. fulvum fulvum</i> collected from the Red Sea Coast at Jeddah, Saudi Arabia	2019	NCI-H1299 (<i>lung</i>) <u>HepG-2 (<i>liver</i>)</u> NCI-H1299 (<i>lung</i>) <u>MCF-7 (<i>breast</i>)</u> MCF-7 (<i>breast</i>)	All human	0.036 0.083 0.097 0.370 0.088 0.246 0.097 0.370 0.036 0.072 0.036 0.083 0.035 0.034 0.133

Table S3. The IC₅₀ of marine-derived amino acids, peptides, and polyketides with anticancer activity

S/N	Isolated Compounds	Class	Status (Known /Novel)	Source	Year	Cancer	Cell line	Source	IC ₅₀ (μM)	Ref.
1.	C ₃₁ H ₃₇ NO ₇ (Cpd. 323)	Ansamycins (Divergolide) – Macrolides (polyketides)	All Novel	<i>Streptomyces</i> sp. KFD18 from Danzhou, Hainan province, China	2019	SGC-7901 (<i>gastric</i>) K562 (<i>leukaemia</i>) Hela (<i>cervix</i>) A549 (<i>lung carcinoma</i>)	All Human		2.8	66
	C ₃₁ H ₃₇ NO ₈ (Cpd. 324)								6.6	
	C ₃₁ H ₃₇ NO ₇ (Cpd. 325)								9.6	
	C ₃₁ H ₃₇ NO ₇ (Cpd. 326)								14.9	
2.	Microcolin E (Cpd. 329)	Lipopeptides (Cpds. 329-335 and 337) Microcolins deriv. (342, 343)	Novel (Cpds. 329-335 and 337) Known (338-341)	The cyanobacteria (<i>Moorea producens</i>) samples were collected off Playa Kalki, Curacao	2019	H-460 (<i>lung</i>)	Human	1.0 0.037 0.16 0.047 0.55 0.069 0.20 0.51 0.91 0.65 0.075 2.80 5.0 2.0	67	
	Microcolin F (Cpd. 330)									
	Microcolin G (Cpd. 331)									
	Microcolin H (Cpd. 332)									
	Microcolin I (Cpd. 333)									
	Microcolin J (Cpd. 334)									
	Microcolin K (Cpd. 335)									
	Microcolin M (Cpd. 337)									
	Microcolin A (Cpd. 338)									
	Microcolin B (Cpd. 339)									
	Microcolin C (Cpd. 340)									
	Microcolin D (Cpd. 341)									
	3,4-dihydromicrocolins C (Cpd. 342)									
	3,4-dihydromicrocolins D (Cpd. 343)									
3.	Akazamicin (Cpd. 346)	Aromatic polyketide	Novel Known	Nonomuraea sp. AKA32, marine-derived actinomycetes isolated from deep-sea water in Sagami Bay, Japan	2019	B16 (<i>melanoma</i>)	Murine	1.7 1.2	69	
	Actinofuranone C (Cpd. 347)									
4.	Cytosaminomycin E (Cpd. 359)	Pyrimidine nucleoside (Cpd. 361) and derivatives (Cpds. 360-364)	Novel Known (360-364)	Marine-derived <i>Streptomyces</i> sp. SSA28 from Shengsi Archipelago (Zhejiang Province, China)	2019	HCT-116 (<i>colon</i>)	Human	0.39 0.78 6.45 6.63 2.14 0.89	70	
	40551-L (Cpd. 360)									
	40551-K (Cpd. 361)									
	40551-F (Cpd. 362)									
	40551-D (Cpd. 363)									
	40551-G (Cpd. 364)									
5.	Fuscasins A (Cpd. 372)	Cycloheptapeptides	Novel	Marine Sponge Phakellia fusca from the South China Sea	2019	HepG2 (<i>liver</i>)	Human	4.6	71	

6.	Julichrome Q6.6 (Cpd. 378)	Julichrome derivative Aromatic hydrocarbon	Both known	<i>Streptomyces</i> sp., NH1835 isolated from soil samples at the suburb of Wanning, Hainan province, China,	2019	HepG-2 (<i>hepatic</i>) SMMC-7721 (<i>liver</i>) MCF-7 (<i>breast</i>) MDA-MB-231 (<i>breast</i>)	All Human	1.45 0.11 0.37 0.26	72
	Gliotoxin (Cpd. 382)	Diketopiperazine Amino acid				HepG-2 (<i>hepatic</i>) SMMC-7721 (<i>liver</i>) MCF-7 (<i>breast</i>) MDA-MB-231 (<i>breast</i>)		13.18 1.89 0.99 0.92	
7.	Boshramycinones A (Cpd. 383)	Anthracyclinones. Polyketides	Novel	Marine-derived <i>Streptomyces</i> sp. Mei 16-1,2 from soil sample of Caeciliengroden salty marshland Wadden Sea at Jade Bay, North Sea coast of Germany)	2019	1218L(<i>bladder</i>) T24 (<i>bladder</i>) 498N (<i>CNS</i>) SF 268 (<i>CNS</i>) HCT-116(<i>Colorectal</i>) HT 29 (<i>Colorectal</i>) 251L (<i>Gastric</i>) 1121L (<i>Lung</i>) 289L (<i>Lung</i>) 526L (<i>Lung</i>) 529L (<i>Lung</i>) 629L (<i>Lung</i>) H460 (<i>Lung</i>) 401NL (<i>Breast</i>) MCF-7 (<i>Breast</i>) 276L (<i>melanoma</i>) 394NL (<i>melanoma</i>) 462NL (<i>melanoma</i>) 514L (<i>Melanoma</i>) 520L (<i>Melanoma</i>) 1619L (<i>Ovary</i>) 899L (<i>Ovary</i>) OVCAR (<i>Ovary</i>) Panc-1 (<i>Pancreas</i>) 22RV1 (<i>Prostate</i>) DU145(<i>Prostate</i>) LNCap (<i>Prostate</i>) PC3M (<i>Prostate</i>) 1752L (<i>Pleuromesothelioma</i>) 393NL (<i>Kidney</i>) 486L (<i>Kidney</i>) 944L (<i>Kidney</i>) 1718L (<i>Kidney</i>) 1138L (<i>Uterus</i>)	All Human	1.11 1.14 0.86 0.95 1.47 0.95 1.31 1.09 2.76 2.56 1.18 1.64 1.35 1.34 1.26 1.46 0.90 1.29 0.97 3.29 1.20 4.87 0.66 1.06 0.51 1.66 1.04 0.99 6.75 1.06 12.18 1.63 2.62 0.93	74

	Boshramycinones B (Cpd. 384)					MCF-7 (<i>breast</i>) 394NL (<i>Melanoma</i>) 22RV1 (<i>Prostate</i>)		14.30 17.27 12.91	
8.	16a-methylpregna-17a,19-dihydroxy-(9,11)-epoxy-4-ene-3,18-dione-20-acetoxy (Cpd. 392) Penicitrinone A (Cpd. 396)	Steroid Polyketide	Known Novel	Fungus <i>Penicillium citrinum</i> SCSIO 41017 associated with the sponge <i>Callryspongia</i> sp. from the sea area near Xuwen County, Guangdong Province, China	2019	MCF-7 (<i>breast</i>) SF-268 (<i>brain</i>) MCF-7 (<i>breast</i>) HepG-2 (<i>liver</i>) A549 (<i>lung</i>)	All human	1.3 13.7 17.2 13.5 18.0	⁷⁵
9.	Peniciversiol A (Cpd. 404) Penilactone A (Cpd. 407) Penilactone B (Cpd. 408) 3,3'-dihydroxy-5,5'-dimethyldiphenyl ether (Cpd. 411) Violaceol-II (Cpd. 415) 3,8-dihydroxy-4-(2,3-dihydroxy-1-hydroxymethylpropyl)-1-methoxyxanthone (Cpd. 416) Asperdemin (Cpd. 417) Cyclopenol (Cpd. 418) Radiclonic acid (Cpd. 419)	Polyketides	Novel (404, 407) Known (408-419)	Deep-Sea Derived Fungus <i>Penicillium chrysogenum</i> MCCC 3A00292	2019	BIU-87 (<i>liver</i>) ECA109 (<i>oesophagus</i>) ECA109 (<i>oesophagus</i>) BIU-87 (<i>liver</i>) ECA109 (<i>oesophagus</i>) BEL-7402 (<i>hepatoma</i>) BEL-7402 (<i>hepatoma</i>) BIU-87 (<i>liver</i>) BEL-7402 (<i>hepatoma</i>) BIU-87 (<i>liver</i>) ECA109 (<i>oesophagus</i>) BEL-7402 (<i>hepatoma</i>)	All human	10.21 12.41 15.60 16.41 8.95 15.94 12.75 8.34 7.81 12.47 7.70 13.75	⁷⁶
10.	Sekgranaticin (Cpd. 420) Granaticins A (Cpd. 421) Granaticins B (Cpd. 422) Methyl granaticinate (Cpd. 423)	Polyketide	Novel (Cpd. 420) Known (Cpds. 421-423)	<i>Streptomyces</i> sp. 166# isolated from clayey cold saline soil collected at County Naqu District, Tibet, China.	2019	MCF-7 (<i>breast</i>) A549 (<i>lung</i>) P6C (<i>colorectal</i>) HCT-116 (<i>colon</i>) MCF-7 (<i>breast</i>) A549 (<i>lung</i>) P6C (<i>colorectal</i>) HCT-116 (<i>colon</i>) MCF-7 (<i>breast</i>) A549 (<i>lung</i>) P6C (<i>colorectal</i>) HCT-116 (<i>colon</i>) MCF-7 (<i>breast</i>)	All human	1.26 4.84 4.45 6.77 0.28 1.55 2.12 1.55 0.37 3.57 0.28 0.01 0.23	⁷⁷

						A549 (<i>lung</i>) P6C (<i>colorectal</i>) HCT-116 (<i>colon</i>)		1.39 0.88 0.02	
11.	Fusaperazine F (Cpd. 425)	Diketopiperazine Cyclic dipeptides formed from N-terminal amino acid	Novel	Marine derived fungus <i>Penicillium crustosum</i> HDN153086 from Antarctic sediment from Prydz Bay	2019	K562 (<i>leukaemia</i>)	Human	12.7	⁷⁸
12.	K41 A (Cpd. 430)	Polyether polyketide	known	<i>Streptomyces species</i> Actinobacteria isolated from sediment sample obtained from Mersin Coastline (Turkey)	2019	CaCo-2 (<i>colorectal</i>) PC-3 (<i>prostate</i>)	Both human	7.4 11.8	⁷⁹
13.	Auxarthrol D (Cpd. 432) Auxarthrol F (Cpd. 434)	Anthraquinone derivatives (Polyketides)	Both novel	Fungal strain HDN16-802 isolated from the sediment sample of Zhangzi Island, from Dalian, Liaoning Province, China	2019	HL-60 (<i>leukaemia</i>) HCT-116 (<i>colorectal</i>) MDA-MB-231(<i>Breast</i>) BEL-7402 (<i>hepatoma</i>) HL-60 (<i>leukaemia</i>) Hela (<i>cervix</i>) HCT-116 (<i>colorectal</i>) MGC-803 (<i>gastric</i>) HO8910 (<i>ovary</i>) MDA-MB-231(<i>breast</i>) SH-SY5Y (<i>Neuroblastoma</i>) PC-3 (<i>prostate</i>) K562 (<i>chronic myeloid leukemia</i>)	All human	7.5 14.5 19.1 16.6 4.5 10.7 7.8 17.7 18.7 10.1 17.2 20.0 16.5	⁸⁰
14.	Jasplakinolide (Cpd 437) (+)-Jasplakinolide Z6 (Cpd. 440) (+)-Jasplakinolide Z4 (Cpd. 442) (+)-Jasplakinolide V (Cpd. 443)	Cyclodepsipeptide	Novel (Cpd. 440) Known (Cpds. 441, 442, 443)	Marine sponge <i>Jaspis splendens</i> Samama, Panjang and Shoal islands of East Kalimantan (Indonesia)	2019	L5178Y (<i>melanoma</i>)	Mouse	< 0.01 3.2 < 0.01 < 0.01	⁸²
15.	N-(3,7-dimethyl-2,6-octadienyl)-2-aza-2-deoxychaetoviridin A (Cpd. 445) 4'-epi-N-(3,7-dimethyl-2,6-octadienyl)-2-aza-2-deoxychaetoviridin A (Cpd. 446) N-(3-methyl-2-butenyl)-2-aza-2-deoxychaetoviridin A (Cpd. 447)	Nitrogenated azaphilone polyketide	All novel	Deep-sea-derived fungus <i>Chaetomium globosum</i> MP4-S01-7 obtained from a water sample collected in the West Pacific Ocean	2020	MGC803 (<i>gastric</i>) AGS (<i>gastric</i>) MGC803 AGS MGC803 AGS	Both human	0.78 0.12 0.46 0.62 2.7 6.5	⁸³

	<u>4'-epi-N-(3-methyl-2-butenyl)-2-aza-2-deoxychaetoviridin A (Cpd. 448)</u> <u>N-(3,7-dimethyl-2,6-octadienyl)-2-aza-2-deoxychaetoviridin E (Cpd. 449)</u> <u>N-(3-methyl-2-butenyl)-2-aza-2-deoxychaetoviridin E (Cpd. 450)</u> <u>4',5'-dinor-5'-deoxy-N-(3,7-dimethyl-2,6-octadienyl)-2-aza-2-deoxychaetoviridin A (Cpd. 451)</u> <u>4',5'-dinor-5'-deoxy-N-(3-methyl-2-butenyl)-2-aza-2-deoxychaetoviridin A (Cpd. 452)</u>					MGC803 AGS MGC803 AGS MGC803 AGS MGC803 AGS MGC803 AGS MGC803	3.0 2.9 0.72 0.12 6.8 2.0 2.2 1.2 5.8	
16.	Epidithiodiketopiperazine · DC1149B (Cpd. 455)	Piperazine	Novel	<i>Trichoderma lixii</i> isolated from an unidentified marine sponge collected at Mentawai, Indonesia	2020	PANC-1 (<i>pancreas</i>)	Human	0.02 ⁸⁴
17.	<u>Siphonellamides A (Cpd. 456)</u> <u>Siphonellamides B (Cpd. 457)</u>	Acetylene amides	Both novel	Marine sponge, <i>Siphonochalina. siphonella</i> collected from the reefs southwest of Magawish Island, Hurghada, Egypt	2020	HeLa (<i>cervix</i>) MCF-7 (<i>breast</i>) HeLa (<i>cervix</i>)	Both human	9.4 18.0 17.4 ⁸⁵
18.	<u>Bulbimidazoles A (Cpd. 453)</u> <u>Bulbimidazoles B (Cpd. 454)</u> <u>Bulbimidazoles C (Cpd. 465)</u>	Alkanoyl imidazole	All novel	Coral sample <i>Tubastraea</i> sp., collected as fishery waste near the coast of Minami-Ise, Mie, Japan,	2020	P388 (<i>murine leukemia</i>)	Murine	5.0 5.8 7.0 ⁸⁶
19.	<u>Shellmycin A (Cpd. 466)</u> <u>Shellmycin B (Cpd. 467)</u>	Polyketides	All novel	<i>Streptomyces</i> sp. shell-016 isolated from the shell sediment of the Binzhou Shell Dike Island and Wetland National Nature Reserve, China	2020	A375 (<i>malignant melanoma</i>) H1299 (<i>non-small cell lung cancer</i>) HepG2 (<i>Hepatocellular carcinoma</i>) HT29 (<i>colorectal adenocarcinoma</i>) HCC1937 (<i>breast cancer</i>) A375 (<i>malignant melanoma</i>) H1299 (<i>non-small cell lung cancer</i>) HepG2 (<i>Hepatocellular carcinoma</i>) HT29 (<i>colorectal adenocarcinoma</i>)	All human	0.69 1.32 0.89 0.85 2.62 0.95 2.62 1.35 1.12 ⁸⁷

	<p><u>Shellmycin C (Cpd. 468)</u></p>					HCC1937 (<i>breast cancer</i>)	3.11	
						A375 (<i>malignant melanoma</i>)	11.3	
						HepG2 (<i>Hepatocellular carcinoma</i>)	5.03	
						HT29 (<i>colorectal adenocarcinoma</i>)	4.33	
						HCC1937 (<i>breast cancer</i>)	12.6	
	<p><u>Shellmycin D (Cpd. 469)</u></p>					A375 (<i>malignant melanoma</i>)	0.78	
						H1299 (<i>non-small cell lung cancer</i>)	2.15	
						HepG2 (<i>Hepatocellular carcinoma</i>)	1.11	
						HT29 (<i>colorectal adenocarcinoma</i>)	1.02	
						HCC1937 (<i>breast cancer</i>)	2.89	

Table S4. The IC₅₀ of marine-derived lipids, sterols and steroids with anticancer activity

S/N	Isolated Compounds	Class	Status (Known /Novel)	Source	Year	Cancer cell line	Source	IC ₅₀ (μM)	Ref.
1.	16β-acetoxy-3β,7β,11β-trihydroxyergost-5,22-diene and named penicisteroid E (Cpd. 470) 16β-acetoxy-3β,5α,6β,7β-tetrahydroxyergost-22E-ene, and named penicisteroid G (Cpd. 473) 16β-acetoxy-3β,6β,7β-trihydroxyergost-22E-ene (Penicisteroid H) (Cpd. 474) Penicisteroid A (Cpd. 475) Penicisteroid C (Cpd. 476) Anicequol (Cpd. 477)	Steroids (470, 483) Steroids derivatives (474-488)	Novel (470-474) Known (475-488)	Deep-sea-derived fungus <i>Penicillium granulatum</i> MCCC 3A00475 Antarctic Ocean.	2019	SHG-44 (glioma) A549 (non-small cell lung) SHG-44 (glioma) Hep-G2 (liver) A549 (non-small cell lung) BIU-87 (liver) BEL-7402 (hepatoma) ECA-109 (oesophagus) Hela-S3 (cervix) Panc-1 (pancreas) Hep-G2 (liver) A549 (non-small cell lung) BIU-87 (liver) ECA-109 (oesophagus) Hela-S3 (cervix) SHG-44 (glioma) Hep-G2 (liver) A549 (non-small cell lung) BIU-87 (liver) BEL-7402 (hepatoma) ECA-109 (oesophagus) Hela-S3 (cervix) Panc-1 (pancreas) SHG-44 (glioma) HepG2 (liver) ECA-109 (oesophagus) Hela-S3 (cervix) Panc-1 (pancreas) A549 (non-small cell lung)	All human	8.3 5.5 4.8 6.7 8.0 14.4 8.5 8.3 10.0 5.6 7.0 4.4 8.5 9.2 7.2 12.5 6.2 4.5 7.7 8.8 4.1 4.8 4.2 7.8 4.4 6.6 9.9 7.0	88

	$3\beta,5\alpha,6\beta,22E$ -6-methoxyergosta-7,22-diene-3,5-diol (Cpd. 481) $5\alpha,6\alpha,8\alpha,9\alpha$ -diepoxy-(22E,24R)-ergox-22-ene-3 β ,7 β -diol (Cpd. 482) Incisterol A2 (Cpd. 488)					ECA-109 <i>(oesophagus)</i> <hr/> A549 (<i>non-small cell lung</i>) BIU-87 (<i>liver</i>) BEL-7402 (<i>bladder</i>) Panc-1 (<i>pancreas</i>) <hr/> ECA-109 <i>(oesophagus)</i> Hela-S3 (<i>cervix</i>) <hr/> HepG2 (<i>liver</i>) BEL-7402 (<i>bladder</i>) ECA-109 <i>(oesophagus)</i> Hela-S3 (<i>cervix</i>)		5.9
2.	2-hydroxyl-3-pyrenocine-thio propanoic acid (Cpd. 503) <hr/> 5,5-dichloro-1-(3,5-dimethoxyphenyl)-1,4-dihydroxypentan-2-one (Cpd. 506)	Polysulfated steroids	Both novel	<i>Penicillium citreonigrum</i> XT20-134 (MCCC 3A00956) isolated from southeast Indian Ocean sediments	2019	Bel7402 (<i>Hepatoma tumor cell</i>) HT1080 (<i>Fibrosarcoma tumor cell</i>) <hr/> Bel-7402 (<i>hepatoma</i>) HT1080 (<i>Fibrosarcoma tumor cell</i>)	All Human	7.63 13.14 <hr/> 10.22 16.53
3.	(24S)-ergosta-5,25-diene-3 β ,20,24,28-tetra 1 (Cpd. 526) <hr/> 1 α ,3 β -dihydroxyergosta-5,24(28)-dien-7 β -yl acetate (Cpd. 528)	Oxygenated ergostane-type sterols	Novel	Isolated from the soft coral <i>Sinularia</i> sp. collected from the water area near the Xisha Islands, South China Sea	2019	MDA-MB-436 (<i>breast</i>) H157 (<i>buccal mucosa</i>) <hr/> MDA-MB-436 Hep3B (<i>hepatic</i>) HT-29 (<i>colorectal</i>)	Both human	17.5 10.17 <hr/> 18.14 19.30 10.38
4.	Eburicol (Cpd. 529)	Steroid	known	Marine-derived fungi <i>Rhizopus</i> sp isolated from shellfish farming areas of the French Atlantic west coast	2019	MCF-7 (<i>breast</i>) MDA-MB-231 (<i>breast</i>)	Both human	2.0 15.7
5.	Dokdolipid B (Cpd. 531)	Hydroxylated rhamnolipids	Novel	Bacterial strain 179DD-027 (<i>Actinoalloteichus hymeniacidonis</i>) isolated from a sediment sample, collected off the coasts of Dokdo island, Republic of Korea	2019	HCT-15 (<i>colon</i>) NUGC-3 (<i>stomach</i>) NCI-H23 (<i>lung</i>) ACHN (<i>renal</i>) PC-3(<i>prostate</i>)	All human	16.7 19.3 13.7 14.1 18.2

Table S5. The IC₅₀ of marine-derived ketones, quinines, quinolones and xanthones with anticancer activity

S/N	Isolated Compounds	Class	Status (Known /Novel)	Source	Year	Cancer cell line	Source	IC ₅₀ (μM)	Ref.
1.	3-methyl-antibiotic G-15F (Cpd. 535)	Medermycin derivative	Known	<i>Streptomyces</i> sp. SS17A (from marine sediments of Shengsi Island (Zhejiang province, China)	2019	PC-3 (prostate) HCT-116 (colorectal)	Human Human	0.02 0.04	⁹³
2.	Peniquinone A (Cpd. 541) Peniquinone B (Cpd. 543)	1,4-benzoquinone (Aromatic)	Novel	Marine-derived fungus <i>Penicillium</i> sp. L129 from rhizosphere-soil of <i>Limonium sinense</i> (Girald) Kuntze collected in Yangkou Beach in Qingdao, China	2019	MCF-7 (breast) U87 (glioma) PC3 (prostate) U87 (glioma) PC3 (prostate)	All Human	12.39 9.01 14.59 13.45 19.93	⁹⁴
3.	Lithocarol A (Cpd. 558) Lithocarol B (Cpd. 559) Lithocarol D (Cpd. 561)	Poly-ketal derivatives in tenellone family ketones	Novel	Marine-derived fungus <i>Phomopsis lithocarpus</i> FS508 Deep-sea sediment from Indian Ocean	2019	MCF-7 (breast) A549 (lung) MCF-7m (breast) HepG2 (liver) A549 (lung)	Human	19.2 10.5 14.8 18.5 15.1	⁹⁵
4.	Suberosanone B (Cpd. 567)	Bicyclic lactone	Known	Octocoral <i>Dendronephthya mucronata</i> collected near Phu Quoc Island, Kiengiang, Vietnam	2019	HeLa (cervical adenocarcinoma)	Human	14.45	⁹⁶
5.	O-Demethylsterigmatocystin (Cpd. 586) Sterigmatocystin (Cpd. 587) Sterigmatin (Cpd. 588) AGI-B4 (Cpd. 589) Stephacidin A (Cpd. 594)	Xanthone derivatives (Cpds. 586-589) Alkaloid (Cpd. 594)	Known	Marine-derived fungus <i>Aspergillus versicolor</i> (code F8.1.3a) isolated from the sponge <i>Agelas oroides</i> , which was collected from Aliağa-İzmir, Turkey co-cultured with <i>Bacillus subtilis</i> lab strain 168 trpC2.	2019	L5178Y (lymphoma)	Mouse	5.8 2.2 2.3 2.0 16.7	⁹⁷
6.	ULDF4 (kigamicin) (Cpd. 603) ULDF5 (staurosporine) (Cpd. 604)	Xanthone Indolocarbazole	Both known	<i>Streptomyces bingchengensis</i> sediment samples collected from Folawiyo, Iddo in Lagos Lagoon, Nigeria	2019	HeLa (cervical adenocarcinoma)	Human	0.11 0.24	⁹⁸

Table S6. The IC₅₀ of other marine-derived compounds with anticancer activity

S/N	Isolated Compounds	Class	Status	Source	Year	Cancer Cell line	Source	IC ₅₀ (μM)	Ref.
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			(Known /Novel)					
1.	7-oxo-holyrin A (Cpd. 605)	Staurosporine derivatives Indolocarbazoles	Novel (Cpds 605-610)	<i>Streptomyces</i> sp. NB-A13 (from marine sediments of Ningbo City, Zhejiang province, China)	2019	PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)	Both human	4.03 2.14
	4'-N-formyl-7-oxo-holyrin A (Cpd. 606)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		2.05 0.74
	3'-(hydroxyl(oxiran-2-yl)methoxy)-holyrine A (Cpd. 607)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		2.45 2.00
	3'-epi-5'-methoxy-K252d (Cpd. 608)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		16.60 9.54
	7-oxo-MLR-52 (Cpd. 609)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		0.55 0.16
	RK-1409 (Cpd. 611)					SW-620 (<i>colon</i>)		0.010
	Holyrine A (Cpd. 612)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		2.06 0.76
	3'-N-formyl-holyrin A (Cpd. 613)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		2.50 0.73
	MLR-52 (Cpd. 614)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		0.56 0.18
	k252d (Cpd. 615)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		1.87 1.04
	7-oxo-k252d (Cpd. 616)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		2.27 0.81
	3'-demethyl-RK-1409 (Cpd. 617)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		0.67 0.49
	252a-Me (Cpd. 619)					PC-3 (<i>prostate</i>) SW-620 (<i>colon</i>)		0.77 0.02
2.	Altercrasin B (Cpd. 621)	Decalin derivatives	All novel	<i>Alternaria</i> sp. OUPS-117D-1 was isolated from the sea urchin <i>Anthocidaris Ccrassispina</i> , collected in Osaka bay, Japan	2019	P388 (<i>lukaemia</i>) HL-60 (<i>lukaemia</i>) L1210I (<i>leukaemia</i>)	Murine Human Murine	20.0 12.1 8.0
	Altercrasin D (Cpd. 623)					P388 (<i>lukaemia</i>) HL-60 (<i>lukaemia</i>) L1210I (<i>leukaemia</i>)		9.7 6.1 8.4
	Altercrasin E (Cpd. 624)					P388 (<i>lukaemia</i>) HL-60 (<i>lukaemia</i>) L1210I (<i>leukaemia</i>)		15.5 6.2 10.3
	Nocarterphenyl A (Cpd. 625)					HL60 (<i>leukaemia</i>) HCC1954 (<i>ductal carcinoma of the breast cells</i>) MDA-MB-468 (<i>triple negative breast cancer</i>)		All Human 0.38 0.10 2.8
3.		Benzothiazole containing - (Cpd. 630 only) p-terphenyls and its derivatives (Cpds. 633 – 635) aromatic hydrocarbon	Novel	Marine-Derived actinobacterial strain <i>Nocardiopsis</i> Sp. OUCMDZ-4936 from Dongzhaigang Mangrove Reserve, Hainan Province of China	2019			101

					H2228 (<i>lung</i>) MV4-11 ((<i>TLT3-activated AML cells</i>) K562 (<i>chronic myelogenous leukaemia</i>) A549 (<i>lung</i>) BT474 (<i>hormone sensitive breast cancer</i>) A431(<i>epidermoid</i>) MCF-7 (<i>breast</i>) 143B (<i>epidermoid carcinoma</i>)	1.7 4.0 9.0 7.8 6.0 4.6 18.0 5.5 0.77
	5-methoxy-4,7-bis(4-methoxyphenyl)benzo[d]thiazol-6-ol (Cpd. 628)		Known (Cpds 628-630)		K562 (<i>chronic myelogenous leukaemia</i>) 549 (<i>lung</i>) MCF-7 (<i>breast</i>) P6C (<i>CD44+ colorectal stem cell line</i>)	5.1 6.0 9.4
	2,4',4''-trimethoxyp-terphenyl-3,6-dione (Cpd. 629)				MV4-11 ((<i>TLT3-activated AML cells</i>) A549 (<i>lung</i>) HL60 (<i>leukaemia</i>) MKN-45 (<i>gastric</i>) N-87 (<i>gastric carcinoma</i>) A673 (<i>rhabdomyoma cell line</i>) K562 (<i>chronic myelogenous leukaemia</i>) BT474 (<i>hormone sensitive breast cancer</i>) H1229 (<i>non-small cell lung carcinoma</i>) HUCCT1(<i>bile duct carcinoma</i>) B16F10 (<i>highly metastatic mouse melanoma cell line</i>)	0.16 0.48 0.17 0.49 1.0 0.76 4.8 3.6 0.72 0.20 0.76 1.1

						MDB-MB-231 (breast)		5.0 2.0	
4.	Terrosamycins A (Cpd. 631)	Polycyclic polyether	Both novel	<i>Streptomyces</i> sp. RKND004 isolated from Prince Edward Island sediment	2019	HTB-26 (breast adenocarcinoma) MCF-7 (breast)	Both human	10.1 6.0	¹⁰²
	Terrosamycins B (Cpd. 632)					HTB-26 (breast adenocarcinoma) MCF-7 (breast)		6.0 3.9	
5.	Oxadiazine Nocuolin A (Cpd. 633)	Azoles	known	Cyanobacterial strain LEGE 06071 from the LEGE CC culture (26) of CIIMAR, Porto, Portugal	2019	HCT116 (colon) hTERT RPE-1 (immortalized epithelial cell line)	Both human	1.35 1.20	¹⁰⁴
6.	Psolusoside L (Cpd. 638)	Glycoside	Both novel	Sea cucumber <i>Psolus fabricii</i> (family Psolidae; order Dendrochirotid) were collected in the Sea of Okhotsk near Onekotan Island (Kurile Islands).	2019	Ehrlich ascites carcinoma (liver) Neuro-2A (neuroblastoma)	All mouse	9.73 10.60	¹⁰⁶
	Psolusoside N (Cpd. 640)					Neuro-2A		13.52	
7.	Terphenyllin (Cpd. 646)	<i>p</i> -terphenyls	Both known	Deep-sea-derived fungus <i>Aspergillus candidus</i> isolated from Atlantic Ocean	2019	HeLa (cervix) ECA-109 (oesophagus) Bel-7402 (hepatoma) Panc-1 (pancreas)	All human	9.2 7.0	¹⁰⁷
	Prenylterphenyllin (Cpd. 647)					HeLa (cervix) ECA-109 (oesophagus) Bel-7402 (hepatoma) Panc-1 (pancreas)		9.4 7.8 5.6 5.5 8.5 7.7	
8.	Oxalicumone A (Cpd. 656)	Dihydrothiophene	Known	Fungus <i>Aspergillus</i> sp. LS34 isolated from sponge <i>Haliclona</i> sp. collected at Lingshui, Hainan Province, China	2019	CCRF-CEM (human acute lymphoblastic leukemia T lymphocyte) K562 (chronic myeloid leukemia)	Both human	1.22 10.58	¹⁰⁸
9.	Holothurin A ₂ (Cpd. 659)	Triterpene Glycoside	All known	Sea cucumber <i>Holothuria (Halodeima) edulis</i> Lesson, 1830 collected from Cu Lao Cham Island, Quangnam, Vietnam	2019	LNCaP (prostate) HepG2 (liver) KB (epidermoid carcinoma) MCF-7 (breast) SK-MEL-2 (skin)	All human	0.96 0.76 0.75 0.81 0.84 1.30 2.03 1.79 2.29	¹⁰⁹
	Holothurin A (Cpd. 663)					LNCaP (prostate) HepG2 (liver) KB (epidermoid carcinoma) MCF-7 (breast)			

	Holothurin B (Cpd. 664)					SK-MEL-2 (<i>skin</i>) LNCaP (<i>prostate</i>) HepG2 (<i>liver</i>) KB (<i>epidermoid carcinoma</i>) MCF-7 (<i>breast</i>) SK-MEL-2 (<i>skin</i>)		2.49 2.74 2.63 2.75 3.35 3.66	
10.	Dragocin A (Cpd. 666)	Ribofuranose	Novel	Marine <i>cyanobacterium</i> collected in Boca del Drago, Panama	2019	H-460 (<i>lung</i>)	Human	7.6	¹¹⁰
11.	Terrein (Cpd. 670)	Not available	Known	<i>Aspergillus terreus</i> Strain S020 isolated from deep-sea sediment marine sponge collected from the Red Sea at Obhur, Jeddah, Saudi Arabia	2019	HCT-116 (<i>colorectal</i>)	Human	12.13	¹¹¹
12.	Prenylterphenyllin F (Cpd. 671) Prenylterphenyllin G (Cpd. 672) Prenylterphenyllin H (Cpd. 673) Prenylterphenyllins J (Cpd. 675)	Prenylterphenyllins	All novel	Endophytic fungus, <i>Aspergillus candidus</i> LDJ-5 isolated from the root of <i>Rhizophora apiculata</i> Blume collected from Sanya Bailu Park of Hainan Province, China	2020	MGC-803 (<i>Gastric</i>) HCT-116 (<i>colorectal</i>) BEL7402 (<i>hepatoma</i>) A549 (<i>Lung</i>) SH-SY5Y (<i>Neuroblast</i>) HeLa (<i>cervix</i>) HL-60 (<i>lukaemia</i>) MGC-803 (<i>Gastric</i>) HCT-116 (<i>colorectal</i>) BEL7402 (<i>hepatoma</i>) A549 (<i>Lung</i>) SH-SY5Y (<i>Neuroblast</i>) HeLa (<i>cervix</i>) MGC-803 (<i>Gastric</i>) HCT-116 (<i>colorectal</i>) A549 (<i>Lung</i>) SH-SY5Y (<i>Neuroblast</i>) HeLa (<i>cervix</i>) U87 MGC-803 (<i>Gastric</i>) HCT-116 (<i>colorectal</i>) A549 (<i>Lung</i>) SH-SY5Y (<i>Neuroblast</i>)	All human	11.0 9.3 12.4 10.2 10.4 8.3 7.1 12.5 16.9 12.6 16.3 12.4 11.5 0.7 0.5 0.4 0.6 2.0 13.8 8.1 6.2 7.6 15.6	¹¹²

	Prenylcandidusin G (Cpd. 679)					HeLa (<i>cervix</i>) K562 (<i>leukemic</i>) MGC-803 (<i>Gastric</i>) HCT-116 (<i>colorectal</i>) BEL7402 (<i>hepatoma</i>) A549 (<i>lung</i>) SH-SY5Y (<i>Neuroblast</i>) HeLa (<i>cervix</i>) HL-60 (<i>lukaemia</i>)		8.5 15.9	
13.	Monarubin B (Cpd. 683) Lunatinin (Cpd. 686)	Isocoumarin	Novel Known	Marine fungus <i>Monascus ruber</i> BB5 isolated from <i>Meretrix meretrix</i> collected from Hailing Island, Yangjiang, China	2020	HepG-2 (<i>liver</i>) QGY77011(<i>liver</i>) HepG-2 (<i>liver</i>) QGY77011(<i>liver</i>)	Both human	1.72 0.71 9.60 7.12	¹¹³
14.	Meleagrin (Cpd. 693)	Unknown	Novel	Fungal strain <i>Emericella dentata</i> Nq45 was isolated from sediment sample obtained from the sea water of Nabq bay, Red Sea, Egypt	2020	KB-3-1 (<i>cervix carcinoma</i>) KB-V1 (<i>multidrug resistant sub-clone of KB-3-1</i>)	Both human	3.07 6.07	¹¹⁴
15.	5,5'-oxybis(1-methoxy-3-methylbenzene) (Cpd. 711) 4'-(2-Hydroxy-1,3-propanediyloxy-4,1-phenylene(1-methylethyldene))]bisphenol (Cpd. 722)	Aromatic compounds	Both Known	Marine fungus <i>Trichoderma erinaceum</i> F1-1 isolated from inner tissue of the sea star <i>Acanthaster planci</i> collected from Hainan Sanya National Coral Reef Reserve, China		MDA-MB-435 (<i>melanocyte</i>) A549 (<i>lung</i>)	Both human	12.5 18.4	¹¹⁵
16.	Pyrenosetins A (Cpd. 725) Pyrenosetins B (Cpd. 726)	Decalinoylspirotetramic acid derivatives	Both novel	Fungal strain isolated from brown alga <i>Fucus vesiculosus</i> specimens collected in Falckenstein Beach Kiel Fjord, Baltic Sea, Germany	2020	A-375 (<i>malignant melanoma</i>)	Human	2.8 6.3	¹¹⁶
17.	Donghaecyclinones C (Cpd. 731)	Angucyclinone	Novel	<i>Streptomyces</i> sp. strain SUD119, which was isolated from a marine sediment sample collected from a volcanic island in Korea	2020	HCT116 (<i>colorectal</i>) MDA-MB231 (<i>breast</i>) SNU638 (<i>gastric</i>) A549 (<i>lung</i>) SK-HEP1(<i>liver</i>)	All human	8.0 6.7 9.5 9.6 6.0	¹¹⁷