Supplementary Materials

Discovery of DNA topoisomerase I inhibitors with low-cytotoxicity based on virtual screening from natural products

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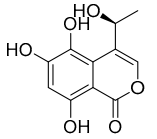
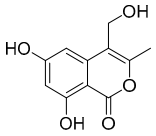
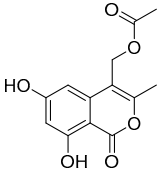
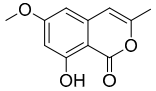
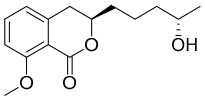
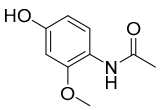
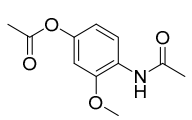
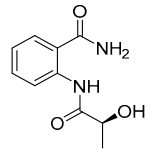
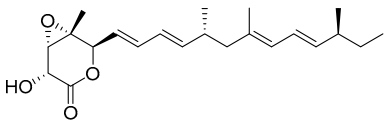
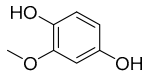
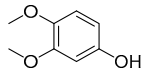
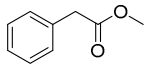
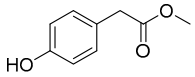
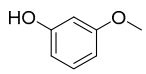
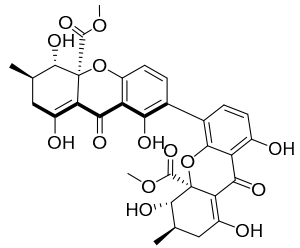
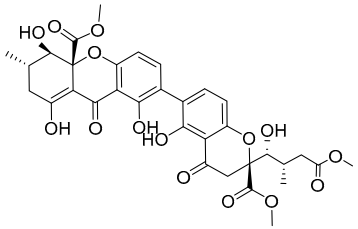
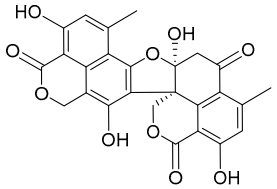
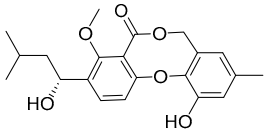
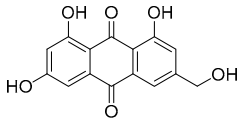
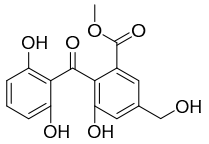
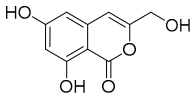
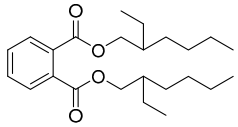
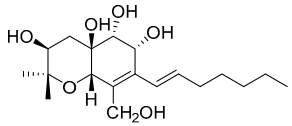
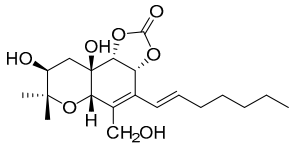
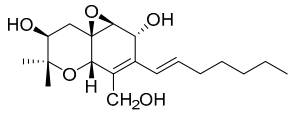
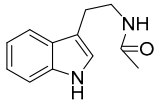
List of Supplementary Materials

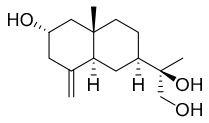
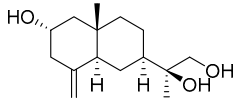
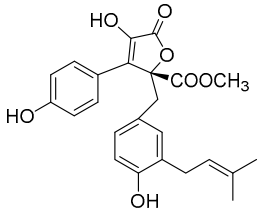
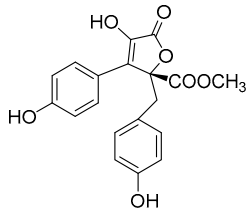
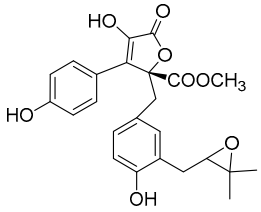
Table S1 138 compounds derived from coral-derived fungi and plants.

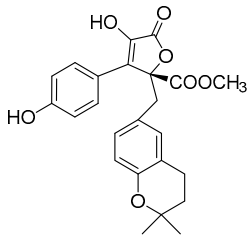
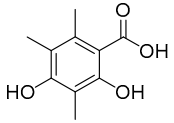
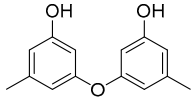
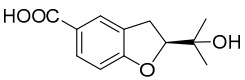
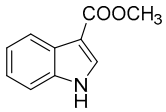
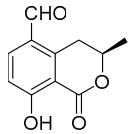
Compounds	Sources	Structures	Low/non-cytotoxicity[a]
S-(−)-5,6,8-Trihydroxy-4-(1′-hydroxyethyl)isocoumarin	Gorgonian-derivd fungi *Penicillium purpurogenum*		Ref. [1]: HL-60: no cytotoxicity; K562: no cytotoxicity; A549: no cytotoxicity.
Sescandelin B	Gorgonian-derivd fungi *Penicillium purpurogenum*		Ref. [2]: CF-1: weak cytotoxicity at 2 μg/ml.
Penicimarin E	Gorgonian-derivd fungi *Penicillium purpurogenum*		Ref. [1]: HL-60: no cytotoxicity; K562: no cytotoxicity; A549: no cytotoxicity.
8-Hydroxy-6-methoxy-3-methylisocoumarin	Gorgonian-derivd fungi *Penicillium purpurogenum*		Ref. [3]: HCT-8: IC_{50} > 25 μg/ml; MDA-MB-435: IC_{50} > 25 μg/ml; SF295: IC_{50} > 25 μg/ml; HL-60: IC_{50} > 25 μg/ml.
Penicimarin B	Gorgonian-derivd fungi *Penicillium purpurogenum*		Ref. [1]: HL-60: no cytotoxicity; K562: no cytotoxicity; A549: no cytotoxicity.
N-(4-Hydroxy-2-methoxyphenyl)acetamide	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.

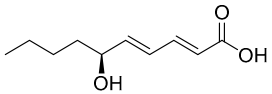
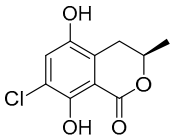
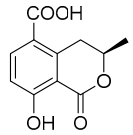
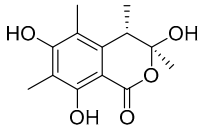
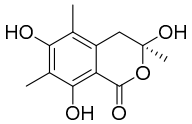
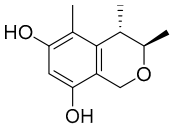
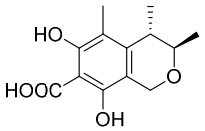
4-Acetoxy-2-methoxyacetanilide	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.
S-(−)-2-(2-Hydroxypropanamido)benzamide	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.
Nafuredin	Gorgonian-derivd fungi *Penicillium purpurogenum*		Ref. [4]: L5178Y: no cytotoxicity.
2-Methoxybenzene-1,4-diol	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: IC_{50} > 10 μM; RD: IC_{50} > 10 μM ; Hep-2: IC_{50} > 10 μM ; A549: IC_{50} > 10 μM.
3,4-Dimethoxyphenol	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.
Phenyl-acetic acid methyl ester	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.
Metyl *p*-hydroxy phenyl acetate	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.
3-Methoxy phenol	Gorgonian-derivd fungi *Penicillium purpurogenum*		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity;

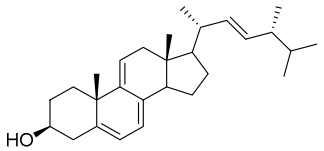
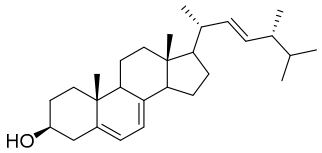
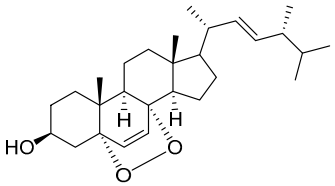
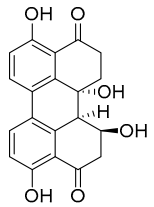
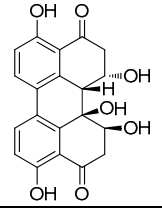
			A549: no cytotoxicity.
Penicillixanthone A	Gorgonian-derived fungi *Talaromyces stipitatus*		Our test: K562: IC_{50} > 10 μM; Vero: IC_{50} > 10 μM.
Versixanthone F	Gorgonian-derived fungi *Talaromyces stipitatus*		Ref. [5]: A549: IC_{50} = 10.6 μM; HO9810: IC_{50} = 20.8 μM.
Bacillosporin C	Gorgonian-derivd fungi *Talaromyces stipitatus*		Our test: HepG2: IC_{50} > 10 μM; HCT-116: IC_{50} > 10 μM; HL-60: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.
Vermixocin A	Gorgonian-derived fungi *Talaromyces stipitatus*		Ref. [6]: P388: no cytotoxicity at 25 μg/ml.
ω-Hydroxyemodin	Gorgonian-derived fungi *Talaromyces stipitatus*		Ref. [7]: MCF-7: IC_{50} = 22 μg/ml; NCI-H187: IC_{50} = 39 μg/ml; Vero: IC_{50} > 50 μg/ml.

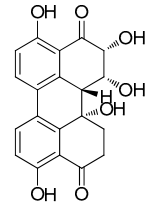
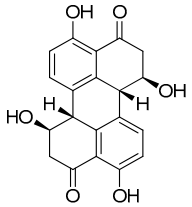
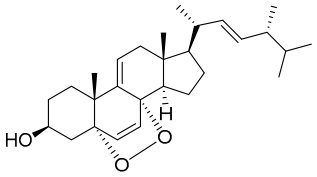
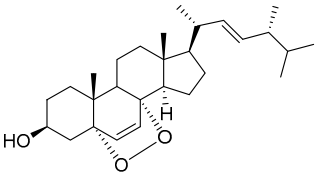
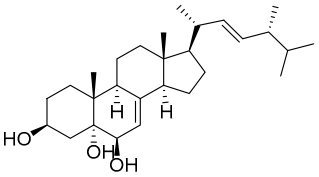
2-(2,6-Dihydroxybenzoyl)-3-hydroxy-5-hydroxymethylbenzoic acid methyl ester	Gorgonian-derived fungi *Talaromyces stipitatus*		Our test: K562: no cytotoxicity; Hela: IC_{50} > 10 μM; HCT-116: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.
3-Hydroxymethyl-6,8-dihydroxyisocoumarin	Gorgonian-derived fungi *Talaromyces stipitatus*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
Di-(2-ethyl)-hexylphthalate	Gorgonian-derived fungi *Talaromyces stipitatus*		Ref. [8]: NCI-H460: no cytotoxicity; MCF-7: no cytotoxicity; HepG2: no cytotoxicity; SF268: no cytotoxicity.
Cytosporin L	Gorgonian-derived fungi *Eutypella* sp.		Our test: K562: IC_{50} > 10 μM; MCF-7: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; Vero: IC_{50} > 10 μM.
Cytosporin E	Gorgonian-derived fungi *Eutypella* sp.		Our test: K562: IC_{50} > 10 μM; MCF-7: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; Vero: IC_{50} > 10 μM.
Cytosporin D	Gorgonian-derived fungi *Eutypella* sp.		Our test: K562: IC_{50} > 10 μM; MCF-7: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; Vero: IC_{50} > 10 μM.
N-Acetyltryptamine	Gorgonian-derived fungi *Eutypella* sp.		Our test: K562: IC_{50} > 10 μM; MCF-7: IC_{50} > 10 μM; A549: IC_{50} > 10 μM;

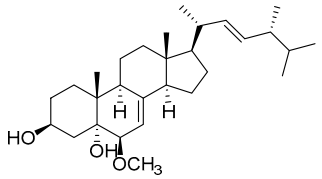
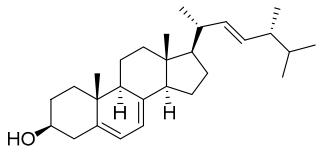
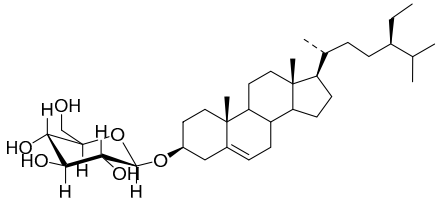
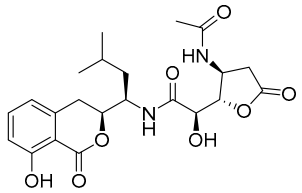
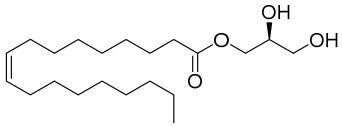
			Vero: IC_{50} > 10 μM.
(11*R*)-2,11,12-Trihydroxy-β-selinene	Gorgonian-derived fungi *Eutypella* sp.		Our test: K562: IC_{50} > 10 μM; MCF-7: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; Vero: IC_{50} > 10 μM.
(11*S*)-2,11,13-Trihydroxy-β-selinene	Gorgonian-derived fungi *Eutypella* sp.		Our test: K562: IC_{50} > 10 μM; MCF-7: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; Vero: IC_{50} > 10 μM.
Butyrolactone I	Gorgonian-derived fungi *Eutypella* sp.		Ref. [9]: MDA-MB-231: IC_{50} = 34.4 μM; MCF-7: IC_{50} = 17.4 μM.
Butyrolactone II	Gorgonian-derived fungi *Eutypella* sp.		Ref. [10]: HL-60: IC_{50} > 80 μM; ASPC1: IC_{50} > 80 μM; PC-3: IC_{50} > 80 μM; HCT-116: IC_{50} > 80 μM.
Butyrolactone III	Gorgonian-derived fungi *Eutypella* sp.		Ref. [10]: HL-60: IC_{50} > 80 μM; ASPC1: IC_{50} > 80 μM; PC-3: IC_{50} > 80 μM; HCT-116: IC_{50} > 80 μM.

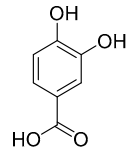
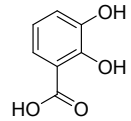
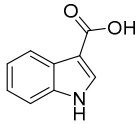
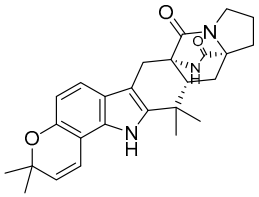
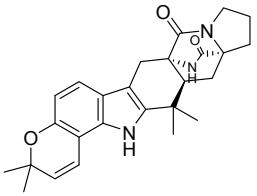
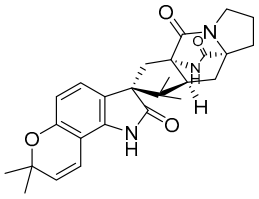
Butyrolactone V	Gorgonian-derived fungi *Eutypella* sp.		Ref. [9]: MDA-MB-231: IC_{50} = 22.2 μM; MCF-7: IC_{50} = 31.9 μM.
2,4-Dihydroxy-3,5,6-trimethylbenzoic acid	Gorgonian-derived fungi *Eutypella* sp.		Ref. [11]: HL-60: IC_{50} > 160 μM; HepG2: IC_{50} > 160 μM.
Diorcinol	Gorgonian-derived fungi *Eutypella* sp.		Ref. [12]: SK-MEL-28: IC_{50} = 40 μM; HCT-116: IC_{50} =22.8 μM.
Anodendroic acid	Gorgonian-derived fungi *Xylaria* sp.		Ref [13]: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
Methyl indole-3-carboxylate	Gorgonian-derived fungi *Xylaria* sp.		Ref [13]: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
5-Formylmellein	Gorgonian-derived fungi *Eutypella* sp.		Ref [14]: NUGC-3: no cytotoxicity; HONE-1: no cytotoxicity.

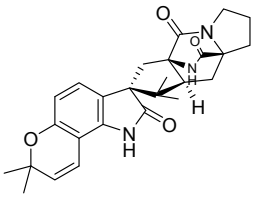
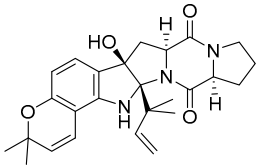
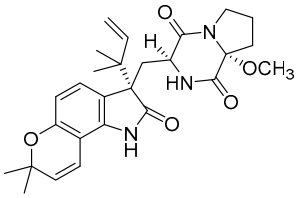
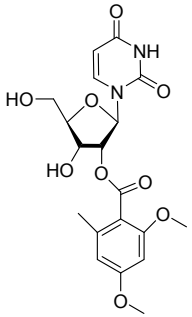
(2*E*,4*E*,6*S*)-6-Hydroxydeca-2,4-dienoic acid	Gorgonian-derived fungi *Eutypella* sp.		Ref [13]: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
7-Chloro-5-hydroxymellein	Gorgonian-derived fungi *Xylaria* sp.		Ref [13]: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
5-Carboxylmellein	Gorgonian-derived fungi *Xylaria* sp.		Ref [13]: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
Sclerotinin A	Gorgonian-derived fungi *Eutypella* sp.		Ref [15]: L5178Y: IC_{50} > 10 μg/ml.
Sclerotinin B	Gorgonian-derived fungi *Eutypella* sp.		Ref [15]: L5178Y: IC_{50} > 10 μg/ml.
Decarboxydihydrocitrinin	Gorgonian-derived fungi *Xylaria* sp.		Ref [16]: KB: no cytotoxicity; MCF-7: no cytotoxicity; Vero: no cytotoxicity.
Dihydrocitrinin	Gorgonian-derived fungi *Xylaria* sp.		Ref [16]: KB: no cytotoxicity; MCF-7: no cytotoxicity; Vero: no cytotoxicity.

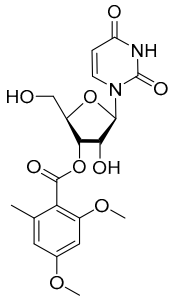
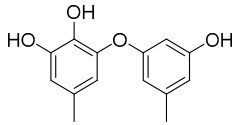
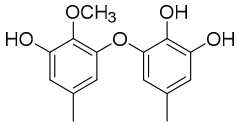
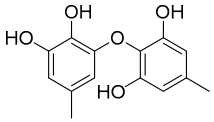
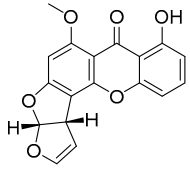
(22*E*)-Ergosta-5,7,9(11)22-tetraen-3β-ol	Gorgonian-derived fungi *Xylaria* sp.		Our test: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
Ergosta-5,7,22-triene-3β-ol	Gorgonian-derived fungi *Xylaria* sp.		Ref [17]: MCF-7: IC_{50} > 50 μg/ml; SF-268: IC_{50} > 50 μg/ml; NCI-H460: IC_{50} > 50 μg/ml.
5α,8α-Epidioxy-ergosta-6,22*E*-dien-3β-ol	Gorgonian-derived fungi *Xylaria* sp.		Ref [13]: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
Altertoxin I	Soft coral-derived fungi *Alternaria alternata*		Our test: HepG2: IC_{50} > 10 μM; HCT-116: IC_{50} > 10 μM; HL-60: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.
6-epi-Stemphytriol	Soft coral-derived fungi *Alternaria alternata*		Our test: Hela: IC_{50} > 10 μM; HL-60: IC_{50} > 10 μM; K562: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.

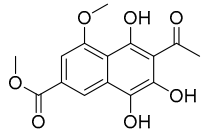
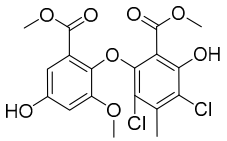
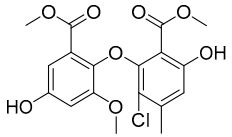
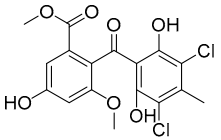
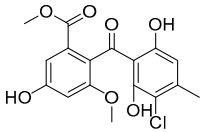
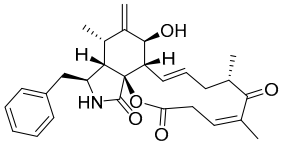
7-epi-8-Hydroxyaltertoxin I	Soft coral-derived fungi *Alternaria alternata*		Our test: Hela: IC_{50} > 10 μM; HL-60: IC_{50} > 10 μM; K562: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.
Stemphyperylenol	Soft coral-derived fungi *Alternaria alternata*		Ref [18]: KB: no cytotoxicity; KBv200: no cytotoxicity.
5α,8α-Epidioxy-ergosta-6,9,22*E*-trien-3β-ol	Gorgonian-derived fungi *Cladosporium* sp.		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.
5α,8α-Epidioxy-ergosta-6,22*E*-dien-3β-ol	Gorgonian-derived fungi *Cladosporium* sp.		Ref [13]: Hela: no cytotoxicity; Hep-2: no cytotoxicity; RD: no cytotoxicity; A549: no cytotoxicity.
Ergosta-7,22-diene-3β,5α,6β-triol	Gorgonian-derived fungi *Cladosporium* sp.		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; RD: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; Vero: IC_{50} > 10 μM.

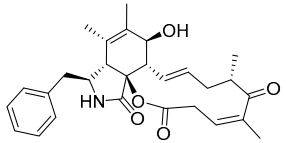
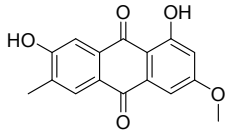
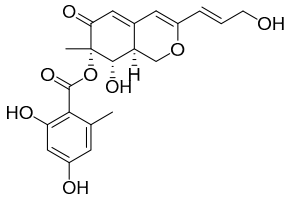
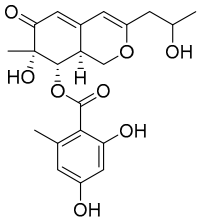
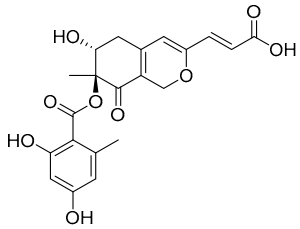
3β,5α-Dihydroxy-6β-methoxyer-gosta-7,22-diene	Gorgonian-derived fungi *Cladosporium* sp.		Ref [16]: SK-OV-3: IC_{50} > 30 μM; SK-MEL-2: IC_{50} > 30 μM; XF498: IC_{50} > 30 μM; HCT-115: IC_{50} > 30 μM; A549: IC_{50} > 30 μM.
Ergosterol	Gorgonian-derived fungi *Cladosporium* sp.		Ref [19]: SK-OV-3: IC_{50} = 12.03 μM; SK-MEL-2: IC_{50} = 12.36 μM; XF498: IC_{50} = 18.90 μM; HCT-115: IC_{50} = 16.04 μM; A549: IC_{50} = 23.11 μM.
β-Sitosterol glucoside	Gorgonian-derived fungi *Cladosporium* sp.		Ref [20]: HCT-116: IC_{50} = 8.52 μg/ml.
AI-77-C	Gorgonian-derived fungi *Cladosporium* sp.		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; RD: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.
9-Octadecenoic acid-2′,3′-dihydroxy propyl ester	Gorgonian-derived fungi *Cladosporium* sp.		Our test: Hela: no cytotoxicity; RD: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity.

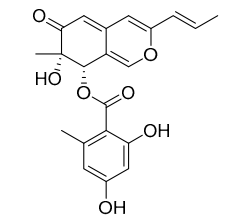
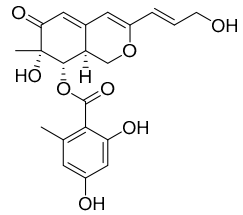
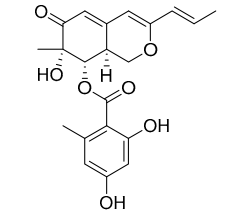
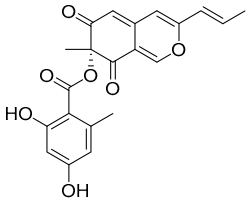
3,4-Dihydroxybenzoic acid	Gorgonian-derived fungi *Cladosporium* sp.		Ref [21]: HL-60: IC_{50} = 64.6 μM; Hel-299: IC_{50} > 100 μM.
2,3-Dihydroxybenzoic acid	Gorgonian-derived fungi *Cladosporium* sp.		Our test: Hela: no cytotoxicity; HL-60: no cytotoxicity;
Indole-3-carboxylic acid	Gorgonian-derived fungi *Cladosporium* sp.		Ref [22]: MCF-7: IC_{50} = 12.9 μm/ml.
6-epi-Stephacidin A	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [23]: HL-60: no cytotoxicity; A549: no cytotoxicity.
Stephacidin A	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [24]: Hela: no cytotoxicity.
Notoamide B	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [25]: Hela: IC_{50} > 22 μg/ml; L1210: IC_{50} >22 μg/ml.

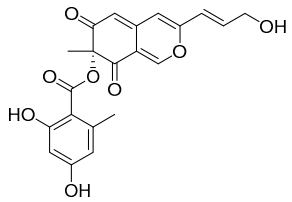
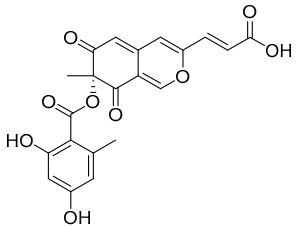
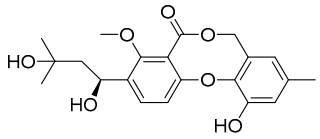
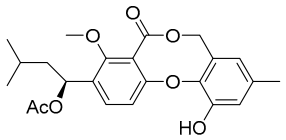
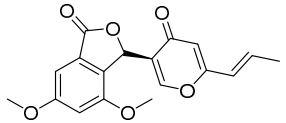
(−)-Versicolamide B	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [23]: HL-60: no cytotoxicity; A549: no cytotoxicity.
Notoamide D	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [25]: Hela: IC_{50} > 100 μg/ml; L1210: IC_{50} > 100 μg/ml.
Notoamide Q	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [26]: K562: IC_{50} > 100 μM; ASPC: IC_{50} > 100 μM; H460: IC_{50} > 100 μM; A549: IC_{50} > 100 μM.
Kipukasin E	Gorgonian-derived fungi *Aspergillus versicolor*		Our test: K562: IC_{50} > 10 μM; Hela: IC_{50} > 10 μM; HCT-116: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.

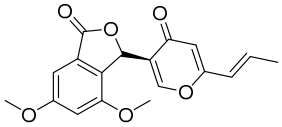
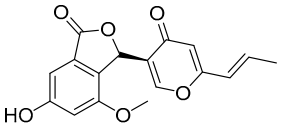
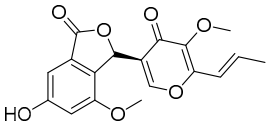
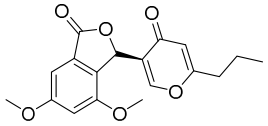
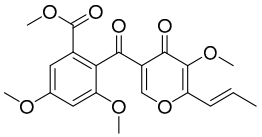
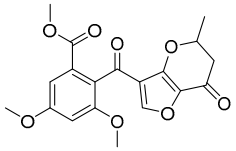
Kipukasin D	Gorgonian-derived fungi *Aspergillus versicolor*		Our test: K562: IC_{50} > 10 μM; Hela: IC_{50} > 100 μM; HCT-116: IC_{50} > 100 μM; A549: IC_{50} > 100 μM.
Cordyol C	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [27]: K562: IC_{50} > 10 μM; HL-60: IC_{50} > 10 μM.
Diorcinol F	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [28]: PC3: no cytotoxicity; A2780: no cytotoxicity; MDA-MB-231: no cytotoxicity; A549: no cytotoxicity.
Violaceol II	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [29]: KB: IC_{50} > 10 μm/ml; BC: IC_{50} = 5.50 μm/ml; NCI-H187: IC_{50} = 3.70 μm/ml.
Sterigmatocystin	Gorgonian-derived fungi *Aspergillus versicolor*		Ref [30]: L-929: IC_{50} = 163.3 μM; Neuro-2a: IC_{50} = 40.1 μM; HepG2: IC_{50} = 286.1 μM.

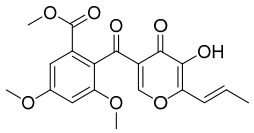
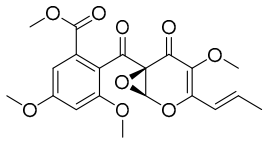
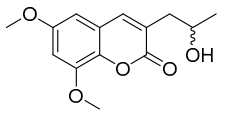
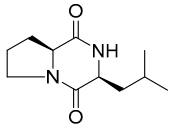
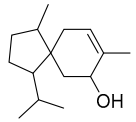
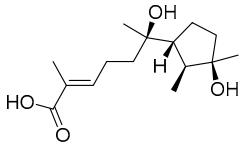
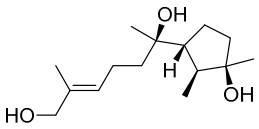
Methyl 6-acetyl-4-methoxy-5,7,8-trihydroxynaphthalene-2-carboxylate	Gorgonian-derived fungi *Aspergillus micronesiensis*		Ref [31]: K562: no cytotoxicity; Hun-7: no cytotoxicity; A549: no cytotoxicity.
3,5-Dichloroasterric acid	Gorgonian-derived fungi *Aspergillus micronesiensis*		Our test: Hela: IC_{50} > 10 μM; A549: IC_{50} > 10 μM.
Penicillither	Gorgonian-derived fungi *Aspergillus micronesiensis*		Ref [31]: KB: no cytotoxicity; MCF-7: no cytotoxicity; Vero: no cytotoxicity.
Dihydrogeodin	Gorgonian-derived fungi *Aspergillus micronesiensis*		Ref [32]: KB: no cytotoxicity; MCF-7: no cytotoxicity; Vero: no cytotoxicity.
2-(3-Chloro-4-methyl-γ-resorcyloyl)-5-hydroxy-*m*-anisic acid methyl ester	Gorgonian-derived fungi *Aspergillus micronesiensis*		Ref [32]: KB: no cytotoxicity; MCF-7: no cytotoxicity; Vero: no cytotoxicity.
Cytochalasin Z16	Gorgonian-derived fungi *Aspergillus micronesiensis*		Ref [33]: HL-60: no cytotoxicity; BEL-7402: no cytotoxicity; P388: no cytotoxicity.

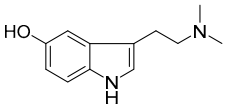
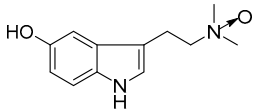
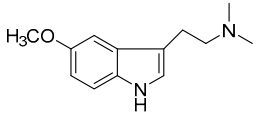
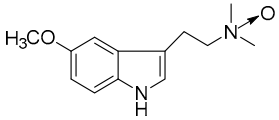
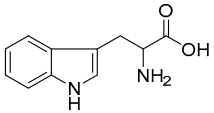
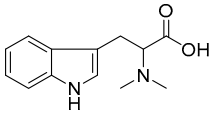
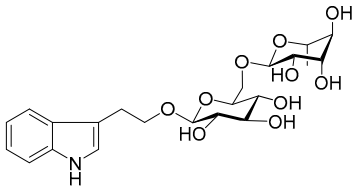
Cytochalasin Z17	Gorgonian-derived fungi *Aspergillus micronesiensis*		Ref [33]: HL-60: no cytotoxicity; BEL-7402: no cytotoxicity; P388: no cytotoxicity.
9,10-Anthracenedione	Gorgonian-derived fungi *Aspergillus micronesiensis*		Our test: L1210: IC_{50} > 100 μM; A549: IC_{50} > 100 μM.
Pinophilin D	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
Pinophilin E	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
Pinophilin F	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.

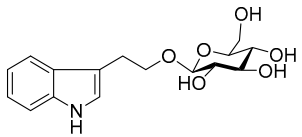
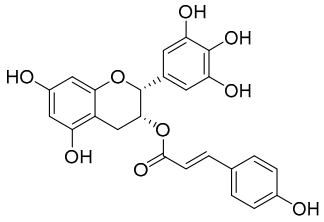
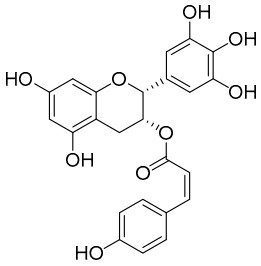
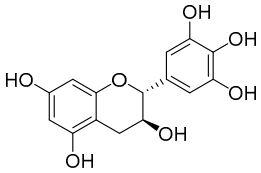
Sch 1385568	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
Pinophilin B	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
Sch 725680	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
(−)-Mitorubrin	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.

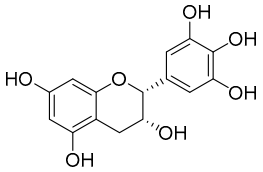
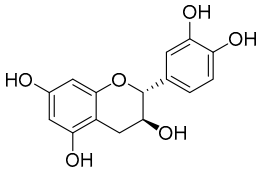
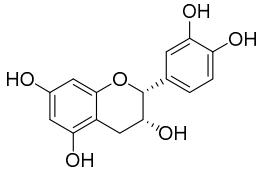
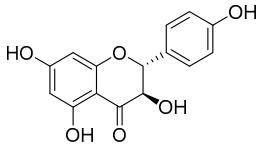
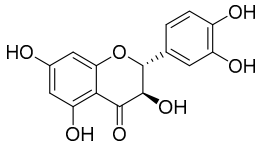
(−)-Mitorubrinol	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
(−)-Mitorubrinic acid	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
Isopenicillide	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
Purpactin A	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [34]: Hep-2: no cytotoxicity; RD: no cytotoxicity; Hela: no cytotoxicity.
Vermistatin	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [35]: KB: IC_{50} = 90.2 μm/ml; KBv200: no cytotoxicity.

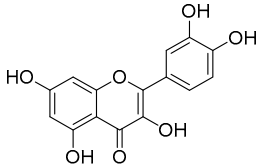
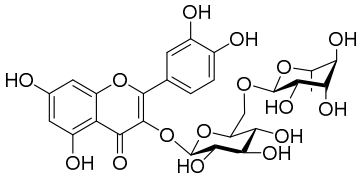
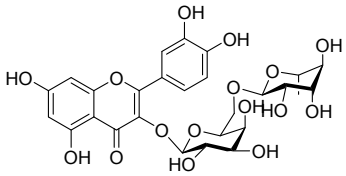
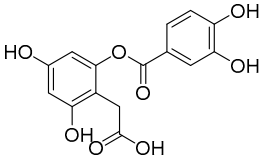
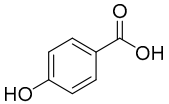
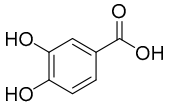
Methoxyvermistatin	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [35]: KB: IC_{50} = 20.0 μm/ml; KBv200: IC_{50} = 15.1 μm/ml
4-Demethylvermistatin	Gorgonian-derived fungi *Penicillium pinophilum*		Our test: Hela: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity; RD: no cytotoxicity.
4-Demethyl-11-methoxyvermistatin	Gorgonian-derived fungi *Penicillium pinophilum*		Our test: Hela: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity; RD: no cytotoxicity.
Dihydrovermistatin	Gorgonian-derived fungi *Penicillium pinophilum*		Our test: Hela: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity; RD: no cytotoxicity.
3-*O*-Methylfunicone	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [36]: KB: IC_{50} = 35.3 μM.
Penifupyrone	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [36]: KB: IC_{50} = 4.7 μM.

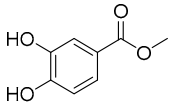
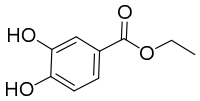
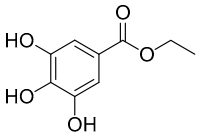
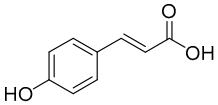
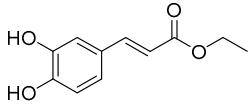
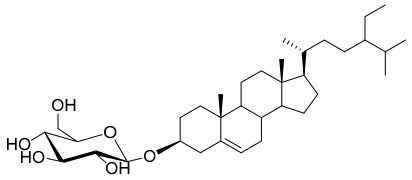
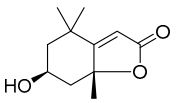
Funicone	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [36]: KB: IC_{50} = 13.2 μM.
3-*O*-Methyl-5,6-epoxyfunicone	Gorgonian-derived fungi *Penicillium pinophilum*		Our test: Hela: no cytotoxicity; Hep-2: no cytotoxicity; A549: no cytotoxicity; RD: no cytotoxicity.
Pestalasin A	Gorgonian-derived fungi *Penicillium pinophilum*		Ref [37]: L5178Y: no cytotoxicity; Hela: no cytotoxicity; PC12: no cytotoxicity.
Cyclo(L-Leu-L-Pro)	Soft coral-derived fungi *Trichoderma harzianum*		Ref [38]: Hep-2: IC_{50} = 242 mg/l.
Trichoacorenol	Soft coral-derived fungi *Trichoderma harzianum*		Our test: MCF-7: no cytotoxicity; HepG2: no cytotoxicity; A549: no cytotoxicity; HCT-116: no cytotoxicity.
Ascotrichic acid	Soft coral-derived fungi *Trichoderma harzianum*		Our test: MCF-7: no cytotoxicity; HepG2: no cytotoxicity; A549: no cytotoxicity; HCT-116: no cytotoxicity.
Cyclonerotriol	Soft coral-derived fungi *Trichoderma harzianum*		Our test: MCF-7: no cytotoxicity; HepG2: no cytotoxicity; A549: no cytotoxicity; HCT-116: no cytotoxicity.

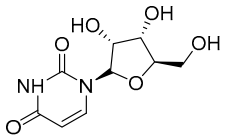
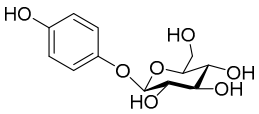
5-Hydroxy-*N*,*N*-dimethyltryptamine	*Phyllodium pulchellum*		Ref [39]: KB: IC_{50} > 100 mg/l; HepG2: IC_{50} > 100 mg/l .
5-Hydroxy-*N*,*N*-dimethyltryptamine-oxide	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
5-Methoxy-*N*,*N*-dimethyltryptamine	*Phyllodium pulchellum*		Ref [39]: KB: IC_{50} > 100 mg/l; HepG2: IC_{50} = 80.5 mg/l .
5-Methoxy-*N*,*N*-dimethyltryptamine-oxide	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
L-Tryptophan	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
N,*N*-Dimethyl-L-tryptophan	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
2-(Indol-3-yl)ethyl-α-L-rhamnopyra-nosyl-(1→6)-β-D-glu copyranoside	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.

2-(Indol-3-yl)ethyl-β-D-glucopyranoside	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
(−)-Epigallocatechin 3-*O*-(*E*)-*p*-coumaroate	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
(−)-Epigallocatechin 3-*O*-(*Z*)-*p*-coumaroate	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
(−)-Gallocatechin	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.

(−)-Epigallocatechin	*Phyllodium pulchellum*		Ref [40]: HSC-2: IC_{50} = 67 μM.
(+)-Catechin	*Phyllodium pulchellum*		Ref [40]: HSC-2: IC_{50} = 497 μM.
(−)-Epicatechin	*Phyllodium pulchellum*		Ref [40]: HSC-2: IC_{50} > 500 μM.
(+)-Dihydrokaempferol	*Phyllodium pulchellum*		Ref [41]: A-549: no cytotoxicity; BEL-7402: no cytotoxicity; HCT-8: no cytotoxicity; A2780: no cytotoxicity; BGC-823: no cytotoxicity.
Dihydroquercetin	*Phyllodium pulchellum*		Ref [42]: HCT-116: IC_{50} = 63.42 μM.

Quercetin	*Phyllodium pulchellum*		Ref [43]: HT-29: IC_{50} > 30 μM; Caco-2: IC_{50} > 15 μM.
Rutin	*Phyllodium pulchellum*		Ref [44]: SW480: IC_{50} = 125 μM.
Quercetin-3-*O*-α-L-rhamnopyranosyl-(1→6)-β-D-galactopyranoside	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
2-*O*-(3,4-Dihydroxybenzoyl)-2,4,6-trihydroxyphenylacetic acid	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 100 μM; Hep-2: IC_{50} > 100 μM; A549: IC_{50} > 100 μM; RD: IC_{50} > 100 μM.
p-Hydroxybenzoic acid	*Phyllodium pulchellum*		Ref [45]: HepG2: no cytotoxicity; Hep-3B: no cytotoxicity; MCF-7: no cytotoxicity; MDA-MB-231: no cytotoxicity; A-549: no cytotoxicity.
Protocatechuic acid	*Phyllodium pulchellum*		Ref [46]: HL-60: IC_{50} = 4.54 mM.

Protocaechuic acid methyl ester	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
Protocatechuic acid ethyl ester	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
Ethyl gallate	*Phyllodium pulchellum*		Ref [47]: Vero: IC_{50} > 100 μg/ml; Hela: IC_{50} > 72 μg/ml.
p-Coumaric acid	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
Caffeic acid ester	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
Daucosterol	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
Loliolide	*Phyllodium pulchellum*		Ref [48]: HL-60: IC_{50} > 100 μM; A-549: IC_{50} > 100 μM; SK-BR3: IC_{50} > 100 μM.

Uridine	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.
Arbutin	*Phyllodium pulchellum*		Our test: Hela: IC_{50} > 10 μM; Hep-2: IC_{50} > 10 μM; A549: IC_{50} > 10 μM; RD: IC_{50} > 10 μM.

[a] the cytotoxicity data of the 138 compounds derived from coral-derived fungi and plants.

HL-60 = promyelocytic leukemia cell line; K562 = chronic leukemia cell line; A549 = lung carcinoma cell line; CF-1: = spruce budworm cell line; HCT-8 = human colon carcinoma cell line; MDA-MB-435 = human breast cancer cell line; SF-295 = human glioblastoma cell line; Hela = human carcinoma cell line; RD = rhabdomyosarcoma cell line; Hep-2 = epider-moid carcinoma cell line; L5178Y = mouse lymphoma cell line; HepG2 = human hepatoma cell line; HCT-116 = human colon carcinoma cell line; P388 = mouse leukemia cell line; MCF-7 = human breast cancer cell line; NCI-H187 = human small-cell lung cancer cell line; Vero = african green monkey kidney fibroblasts; MDA-MB-231 = human breast cancer cell line; ASPC1 = pancreatic cancer cell line; PC-3 = prostate cancer cell line; SK-MEL-28 = human melanoma cell line; NUGC-3 = human gastric carcinoma cell line; HONE-1 = human nasopharyngeal carcinoma cell line; KB = human oral epidermoid carcinoma cell line; SF-268 = human glioblastoma cell line; NCI-H460 = human small-cell lung cancer cell line; SK-OV-3 = human ovarian cancer cell line; SK-MEL-2 = skin melanoma cell line; XF498 = human CNS tumor cell line; HCT-115 = human colon carcinoma cell line; Hel-299 = human embryonic lung cell line; L1210 = murine leukemia cell line; ASPC = human pancreatic tumor cell line; H460 = human lung cancer cell line; PC3 = prostate cancer cell line; A2780 = human ovarian carcinoma cell line; BC = human breast cancer cell line; L-929 = murine fibroblasts; Neuro-2a = neuronal cell line; Huh-7: human hepatoma cell line; BEL-7402 = human hepatocellular carcinoma cell line; KBv200 = human multidrug-resistant cell line; PC12 = rat pheochromocytoma cell line; HSC-2 = human oral tumor cell line; BGC-823 = stomach cancer cell line; HT-29 = human colon carcinoma cell line; Caco-2 = human colon carcinoma cell line; SW480 = human colon carcinoma cell line; Hep-3B = human hepatoma cell line.

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Table S2 The binding energy of 138 compounds bound with the crystal structure of the ternary complex of topotecan-DNA-Topo I (PDB ID: 1K4T).

Compounds	MOE Dock[a] (kcal/mol)	Ledock[b] (kcal/mol)
S-(−)-5,6,8-Trihydroxy-4-(1′-hydroxyethyl)isocoumarin	−7.7786	−4.16
Sescandelin B	−7.8138	−3.99
Penicimarin E	−8.8656	−4.34
8-Hydroxy-6-methoxy-3-methylisocoumarin	−7.5626	−3.21
Penicimarin B	−8.7150	−4.07
N-(4-Hydroxy-2-methoxyphenyl)acetamide	−7.1517	−3.53
4-Acetoxy-2-methoxyacetanilide	−8.7605	−3.8
S-(−)-2-(2-Hydroxypropanamido)benzamide	−7.4790	−5.01
Nafuredin	−10.5718	−5.05
2-Methoxybenzene-1,4-diol	−5.7260	−2.77
3,4-Dimethoxyphenol	−6.3581	−2.68
Phenyl-acetic acid methyl ester	−6.6832	−2.49
Metyl *p*-hydroxy phenyl acetate	−6.6527	−3.13
3-Methoxy phenol	−5.6058	−2.39
Penicillixanthone A	−11.5816	−6.61
Versixanthone F	−13.9518	−7.26
Bacillosporin C	−11.5710	−5.64
Vermixocin A	−9.0248	−5.34
ω-Hydroxyemodin	−8.9439	−4.97
2-(2,6-Dihydroxybenzoyl)-3-hydroxy-5-hydroxymethylbenzoic acid methyl ester	−9.3932	−5.37
3-Hydroxymethyl-6,8-dihydroxyisocoumarin	−7.1588	−3.72
Di-(2-ethyl)-hexylphthalate	−11.6068	−5.15
Cytosporin L	−8.0071	−5.76
Cytosporin E	−7.5546	−3.93
Cytosporin D	−8.7805	−5.11
N-Acetyltryptamine	−8.5530	−4.33
(11*R*)-2,11,12-Trihydroxy-β-selinene	−6.7288	−4.36
(11*S*)-2,11,13-Trihydroxy-β-selinene	−6.7383	−4.33
Butyrolactone I	−8.9953	−5.31
Butyrolactone II	−8.4991	−5.65
Butyrolactone III	−8.9402	−5.67
Butyrolactone V	−8.7235	−3.74
2,4-Dihydroxy-3,5,6-trimethylbenzoic acid	−7.2234	−3.54
Diorcinol	−8.4427	−4.33
Anodendroic acid	−7.4820	−3.94
Methyl indole-3-carboxylate	−7.1386	−3.82
5-Formylmellein	−7.2639	−3.91

(2*E*,4*E*,6*S*)-6-Hydroxydeca-2,4-dienoic acid	−11.1233	−5.18
7-Chloro-5-hydroxymellein	−7.1996	−3.21
5-Carboxylmellein	−7.2904	−3.64
Sclerotinin A	−8.0502	−3.83
Sclerotinin B	−8.1939	−3.99
Decarboxydihydrocitrinin	−7.5784	−3.83
Dihydrocitrinin	−8.3894	−3.6
(22*E*)-Ergosta-5,7,9(11)22-tetraen-3β-ol	−9.6860	−4.06
Ergosta-5,7,22-triene-3β-ol	−9.8870	−4.77
5α,8α-Epidioxy-ergosta-6,22*E*-dien-3β-ol	−9.8810	−4.96
Altertoxin I	−9.3041	−5.12
6-epi-Stemphytriol	−9.0633	−5.39
7-epi-8-Hydroxyaltertoxin I	−8.4352	−5.7
Stemphyperylenol	−9.3307	−4.99
5α,8α-Epidioxy-ergosta-6,9,22*E*-trien-3β-ol	−9.9299	−4.89
5α,8α-Epidioxy-ergosta-6,22*E*-dien-3β-ol	−10.2242	−4.95
Ergosta-7,22-diene-3β,5α,6β-triol	−11.0112	−5.69
3β,5α-Dihydroxy-6β-methoxyer-gosta-7,22-diene	−10.0029	−5.62
Ergosterol	−9.7855	−4.99
β-Sitosterol glucoside	−12.3521	−7.08
AI-77-C	−11.1595	−6.04
9-Octadecenoic acid-2′,3′-dihydroxy propyl ester	−12.1452	−5.08
3,4-Dihydroxybenzoic acid	−6.0901	−3.37
2,3-Dihydroxybenzoic acid	−5.5446	−3.13
Iindole-3-carboxylic acid	−6.3862	−4.09
6-epi-Stephacidin A	−10.4080	−5.92
Stephacidin A	−9.9812	−6.06
Notoamide B	−9.4178	−5.78
(−)-Versicolamide B	−9.5583	−5.61
Notoamide D	−9.5547	−5.06
Notoamide Q	−10.4351	−6.63
Kipukasin E	−10.4288	−6.02
Kipukasin D	−11.0463	−6.11
Cordyol C	−8.7782	−4.36
Diorcinol F	−8.6403	−4.35
Violaceol II	−8.7515	−4.84
Sterigmatocystin	−9.4854	−4.53
Methyl 6-acetyl-4-methoxy-5,7,8-trihydroxynaphthalene-2-carboxylate	−8.3894	−4.32
3,5-Dichloroasterric acid	−8.6927	−4.89
Penicillither	−8.5524	−4.78

Dihydrogeodin	–8.4534	–4.55
2-(3-Chloro-4-methyl-γ-resorcyloyl)-5-hydroxy-*m*-anisic acid methyl ester	–8.4576	–4.43
Cytochalasin Z16	–9.2543	–4.96
Cytochalasin Z17	–9.3522	–4.87
9,10-Anthracenedione	–9.05	–4.56
Pinophilin D	–10.5462	–6.24
Pinophilin E	–10.3545	–5.90
Pinophilin F	–10.6397	–6.08
Sch 1385568	–10.5149	–5.65
Pinophilin B	–9.6737	–6.07
Sch 725680	–9.5385	–5.56
(−)-Mitorubrin	–10.0119	–5.43
(−)-Mitorubrinol	–10.2443	–5.96
(−)-Mitorubrinic acid	–9.6060	–5.98
Isopenicillide	–8. 9541	–5.54
Purpactin A	–8.7728	–4.93
Vermistatin	–9.8455	–4.61
Methoxyvermistatin	–9.8457	–4.69
4-Demethylvermistatin	–8.9950	–4.57
4-Demethyl-11-methoxyvermistatin	–10.1777	–4.74
Dihydrovermistatin	–10.1114	–4.57
3-*O*-Methylfunicone	–10.5720	–4.8
Penifupyrone	–10.1709	–4.74
Funicone	–10.8324	–4.89
3-*O*-Methyl-5,6-epoxyfunicone	–11.6626	–4.75
Pestalasin A	–8.8730	–3.94
Cyclo(L-Leu-L-Pro)	–8.0535	–3.72
Trichoacorenol	–6.5643	–3.64
Ascotrichic acid	–8.3855	–4.29
Cyclonerotriol	–8.4226	–4.23
5-Hydroxy-*N*,*N*-dimethyltryptamine	–8.0560	–4.49
5-Hydroxy-*N*,*N*-dimethyltryptamine-oxide	–7.9782	–4.71
5-Methoxy-*N*,*N*-dimethyltryptamine	–8.7528	–4.24
5-Methoxy-*N*,*N*-dimethyltryptamine-oxide	–8.8962	–4.61
L-Tryptophan	–7.8726	–5.02
N,*N*-Dimethyl-L-tryptophan	–8.7611	–4.62
2-(Indol-3-yl)ethyl-α-L-rhamnopyra-nosyl-(1→6)-β-D-glucopyranoside	–11.9737	–6.98
2-(Indol-3-yl)ethyl-β-D-glucopyranoside	–9.7652	–5.77
(−)-Epigallocatechin 3-*O*-(*E*)-*p*-coumaroate	–10.9265	–7.15
(−)-Epigallocatechin 3-*O*-(*Z*)-*p*-coumaroate	–10.1798	–7.15

(−)-Gallocatechin	−9.4846	−5.48
(−)-Epigallocatechin	−9.0181	−5.51
(+)-Catechin	−8.2783	−5.24
(−)-Epicatechin	−8.2367	−5.21
(+)-Dihydrokaempferol	−7.9162	−4.76
Dihydroquercetin	−9.4265	−5.26
Quercetin	−9.2606	−5.39
Rutin	−14.1506	−7.7
Quercetin-3-*O*-α-L-rhamnopyranosyl-(1→6)-β-D-galactopyranoside	−14.2123	−8.4
2-*O*-(3,4-Dihydroxybenzoyl)-2,4,6-trihydroxyphenylacetic acid	−8.9730	−5.47
p-Hydroxybenzoic acid	−5.6547	−2.89
Protocatechuic acid	−5.9525	−3.45
Protocaechuic acid methyl ester	−6.6400	−3.36
Protocatechuic acid ethyl ester	−7.2568	−3.65
Ethyl gallate	−7.5169	−3.9
p-Coumaric acid	−6.5956	−3.22
Caffeic acid ester	−7.9648	−3.94
Daucosterol	−12.2041	−6.54
Loliolide	−6.1666	−3.01
Uridine	−7.5324	−4.36
Arbutin	−7.5324	−4.78

[a]MOE Dock: cutoff value at −9.0 kcal/mol. [b]Ledock: cutoff value at −5.0 kcal/mol

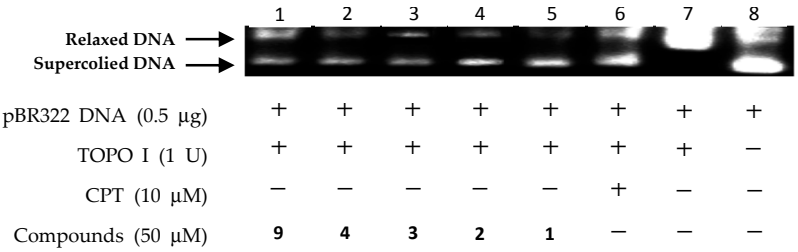

Figure S1 DNA Topo I inhibitory activities of (−)-epigallocatechin 3-*O*-(*E*)-*p*-coumaroate (**1**), (−)-epigallocatechin 3-*O*-(*Z*)-*p*-coumaroate (**2**), (−)-epigallocatechin (**3**), quercetin (**4**) and altertoxin I (**9**) at 50 μM. Lanes 1–5: DNA + Topo I + tested compounds; lane 6: DNA + Topo I + CPT; lane 7: DNA + Topo I; lane 8: DNA.

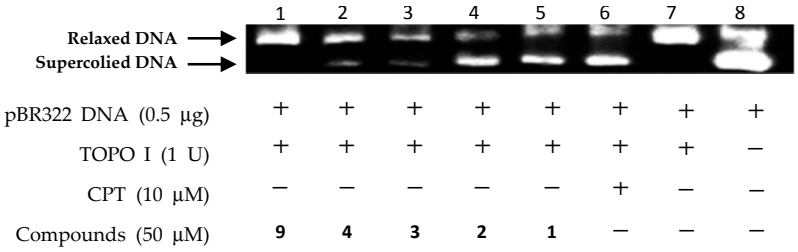

Figure S2 DNA Topo I inhibitory activities of (−)-epigallocatechin 3-*O*-(*E*)-*p*-coumaroate (**1**), (−)-epigallocatechin 3-*O*-(*Z*)-*p*-coumaroate (**2**), (−)-epigallocatechin (**3**), quercetin (**4**) and altertoxin I (**9**) at 25 μM. Lanes 1–5: DNA + Topo I + tested compounds; lane 6: DNA + Topo I + CPT; lane 7: DNA + Topo I; lane 8: DNA

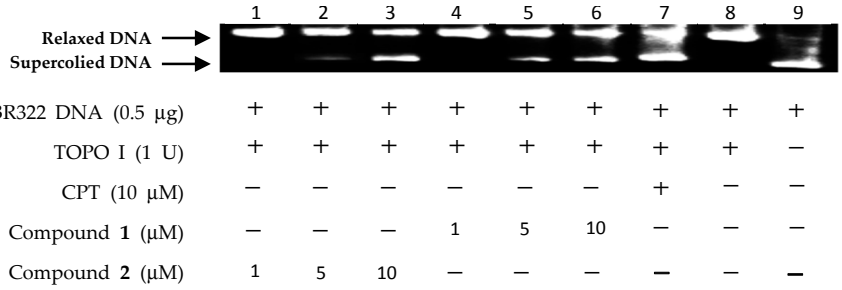

Figure S3 DNA Topo I inhibitory activities of (−)-epigallocatechin 3-*O*-(*E*)-*p*-coumaroate (**1**) and (−)-epigallocatechin 3-*O*-(*Z*)-*p*-coumaroate (**2**) at 1, 5, and 10 μM. Lanes 1–3: DNA + Topo I + compound **2** at various concentrations; Lanes 4–6: DNA + Topo I + compound **1** at various concentrations; lane 7: DNA + Topo I + CPT; lane 8: DNA + Topo I; lane 9: DNA.

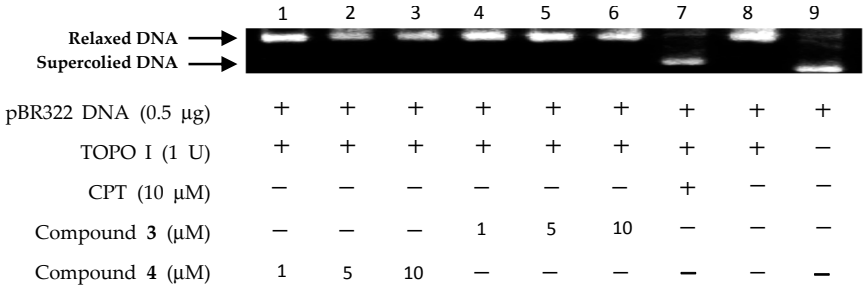

Figure S4 DNA Topo I inhibitory activities of (−)-epigallocatechin (**3**) and quercetin (**4**) at 1, 5, and 10 μM. Lanes 1–3: DNA + Topo I + compound **4** at various concentrations; Lanes 4–6: DNA + Topo I + compound **3** at various concentrations; lane 7: DNA + Topo I + CPT; lane 8: DNA + Topo I; lane 9: DNA.