

Drug Discovery and Bioinformatics of Marine Natural Products

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Marine natural products covering 9% of biomedical compounds [1] have become a hot resource for drug discovery [2]. Interestingly, different extractions of natural products may yield different cellular functions. For example, algae have been reviewed [3] to be anti-cancer, anti-inflammation, and anti-oxidative stress. In the organic extracts of red algae (*Gracilaria tenuistipitata*), it is cytotoxic to oral cancer Ca9-22 cell lines, such as methanol extract of *G. tenuistipitata* (MEGT) [4] and ethanol extract of *G. tenuistipitata* (EEGT) [5]. Additionally, cultivation environment may also affect the bioactive metabolite content of marine algae [6].

In contrast, the aqueous extracts of *G. tenuistipitata* (AEGT) have some protective properties against cellular oxidative stress [7]. For example, H₂O₂-induced plasmid DNA damages, growth retardation, cellular DNA damage, and cell cycle G2/M arrest in H1299 cells is recovered by AEGT. This result suggests that AEGT is a helpful antioxidant and may protect against oxidative stress-related cell damages.

For the contribution of bioinformatics, a marine natural product database had been constructed in 2002 [8]. A database of natural products and chemical entities from marine habitat has been reported [9] although it is unreachable currently. SuperNatural is a searchable database of natural compounds [10]. Chem Spider (<http://www.chemspider.com/>) [11] is a comprehensive database of organic molecules from many different providers, including marine natural products database and others. Currently, the natural product domain seeker (NaPDoS) (http://www.biokepler.org/use_cases/napdos) is developed to provide the phylogeny information for studying secondary metabolite gene diversity [12]. Therefore, the bioinformatics has gradually progressing to the field of marine natural products.

Furthermore, bioinformatics may also help to analyze pharmacogenomics study [13] in terms of SNP-SNP interaction [14-18] to predict the effectiveness of drugs and disease susceptibility. In future, the bioinformatics and pharmacogenomics studies may become more popular in marine natural products.

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