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Abstract

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Discovery of Novel Enzyme Inhibitors from Nature *via in vitro* and *in silico* Methods

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Abstract: Natural products are always important in finding new drug candidates and natural product chemistry research has been a mainstay in drug discovery and development. Enzyme inhibitors are known as one of the strongest therapy strategies against a wide range of diseases. In other words, enzyme inhibitors are one of the vital classes of drugs clinically available. In search novel enzyme inhibitors from natural sources being mostly plants, we have been screening many medicinal plants and pure natural compounds using microplate assays against a number of enzymes including cholinesterase family, elastase, collagenase, tyrosinase, xanthine oxidase, phosphodiesterase-I, carbonic anhydrase-II, lipoxygenase, HMG CoA reductase, etc. Since some of these enzymes are related to cosmetics, we have been also studying developing new formulations for anti-aging cosmetics. The active inhibitors found by our group are further investigated by *in silico* methods using molecular docking experiments. During these studies, we found many promising compounds such as coumarins and other polyphenolics such as flavonoids have been identified as active inhibitors through our results. In this study, examples of natural products as promising inhibitors determined by our group against different enzymes will be underlined.

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