MOLECULAR DOCKING STUDY OF SOME ACTIVE PRINCIPLES FROM *SILYBUM MARIANUM*, *CHELIDONIUM MAJUS*, *GINKGO BILOBA*, *GELSEMIUM SEMPERVIRENS*, *ARTEMISIA ANNUA*, AND *TARAXACUM OFFICINALE*

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Abstract. G protein-coupled receptors (GPCRs) play an important role in cancer progression and are therefore promising targets for the development of new anticancer compounds. In this study, we investigated by molecular docking, the interaction of fourteen natural compounds (artemisinin, bilobalide, bilobetin, chelerythrine, chelidonin, epicatechin, gelsemic acid, ginkgolide A, isosilybin, silicristin, silybin, taraxacin, taraxacoside, and taraxinic acid) from *Silbum marianum*, *Chelidonium majus*, *Ginkgo biloba*, *Gelsemium sempervirens*, *Artemisia annua*, and *Taraxacum officinale* with three cancer-related GPCRs: the apelin receptor, the *β*2-adrenoceptor, and the A2B adenosine receptor. QuickVina2 was used to determine the binding affinities and identify the nature of the strongest interactions. Several compounds (bilobetin, isosilybin, chelidonin, silicristin, and artemisinin) showed high binding affinities and interactions with key residues responsible for the receptor activity. These results highlight the potential of phytochemicals in modulating the activity of GPCRs and may form the basis for further experimental validation.

Keywords: molecular docking, natural compounds, apelin receptor, β2-adrenoceptor, A2B adenosine receptor.