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In Silico Recognition of Natural Products for Medical Care

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Natural products have been always using for several types of applications by humankind for so many years. Food and medical applications have been seen very much important for such products in their original forms or reproduction in new forms. As a main resource for generating so many other compounds, synthetic derivatives have been evaluated for the essential extractions of natural products for more specified applications especially for medical core with controlled dosage medication and compounds. Therefore, recognition of potency of natural products for such specified application have been always seen as a dominant factor for undergoing further improvements in this case. Besides the original extracted essentials, modifying chemical structures could help for lead optimization of such important compounds for possible efficient cares. Indeed, lead optimization could be provided very well by employing in silico approach for potent chemical compounds up to reaching them to specified medication (1). For this purpose, computer-based works could be performed for optimizing lead compound materials in two ways of structural features and activity behaviors to make sense the idea (2). Numerous molecular based methodologies, including density functional theory (DFT), have been developed to characterize structural features of chemical compounds for providing required descriptors of ligands for drug design purposes. Next, molecular docking (MD) simulations could be performed for target screening of desired ligand structures for evaluating medical care possibilities regarding the examination of ligand-target interactions. For natural products, the extracted essential materials could be very well recognized by in silico approach in order to perform lead optimization and activity examination (3). Indeed, such compounds could work very well for assigning as the lead compound component to evaluate appropriate medical care activity (4). Structural features could focus on the importance of addition of functional groups on the main physicochemical properties of chemical structure provided by a wide variety of descriptors. On the other hand, activity examination could focus on the bimolecular formations of ligand-target interacting complexes to evaluate features of binding strength and interacting quality to recognize a product useful for a specified application. In silico approach could make easy the investigation of complicated system of biology related problems to carefully examine all sides of such problem in the lowest scale of molecular and atomic levels (5). In this case, theoretical background, software development and problem-based phenomena could help all for reaching to a possible solution for the targeted problem. When knowing potency of a compound for medical care applications, its recognition at the lowest scale could help very much for reaching to a brighter knowledge about such important topic (6). To this time, numerous works have been developed to apply in silico approach for recognition of natural compounds for medical care, but the story has not been finalized yet and further works are required (7-10).

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