MOLECULAR DOCKING AND VIRTUAL SCREENING OF NATURAL PRODUCTS: APPROACHES FOR NEWER DRUG DISCOVERY

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Abstract

Natural products have been one of the converged targets of drug discovery due to their biocompatibility and safety upon *in vivo* administration. However, due to myriads of natural products available from millions of flora and fauna across the globe, it is a challenging job to realm in potential leads from this huge subset of natural products. Various approaches for virtual screening have evolved, however molecular docking has been one of the most reliable, quick and time economic approach in this sort. For example, Lanatoside B and Diadzen have been reported to exhibit significant inhibition score onAcrBand MexBwhich are efflux pumps for bacteria and thus contribute in bacterial antibiotic resistance. Hence the above compounds have the promising potential to relieve the current global problem of antibiotic resistance. Furthermore, docking guided virtual screening of 57 plant metabolites yielded Hesperidin and Narirutin as potential anti-influenza drugs. New promising lead for anti-inflammatory or anticancer drug has also been reported from ZINC database which comprises of more than 90,000 natural products in their characterized form.

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