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Predictive binding affinity of plant-derived natural products towards the protein kinase G enzyme of *Mycobacterium tuberculosis*

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Tuberculosis (TB) caused by *Mycobacterium tuberculosis* is a growing public health concern worldwide, especially with the emerging challenge of drug resistance to the current drugs. Efforts to discover and develop some novel, more effective and safer anti-TB drugs are urgently needed. Products from natural sources, such as medicinal plants have long played an important role in traditional medicine and continue to provide some inspiring templates for the design of new drugs. Protein kinase G, produced by *M. tuberculosis* (MtPKnG), is a eukaryotic-like serine/threonine kinase that has been reported to prevent phagosome-lysosome fusion and help prolong *M. tuberculosis* survival within the host's macrophages. Here, we used an in silico target-based approach (docking) to predict the interactions between MtPknG and 84 chemical constituents from two medicinal plants (*Pelargonium reniforme and Pelargonium sidoides*) that have a well-documented historical use as natural remedies for TB. Docking scores for ligands towards the target protein were calculated using AutoDock Vina as the predicted binding free energies, with the lowest score indicating the highest ligand/protein affinity. The scores obtained ranged between -5.8 and -13.2 kcal/mol. The flavonoid derivatives (isoorientin 2"-O-gallate and isovitexin 2"-O-gallate) present in *P. reniforme/sidoides* aerial parts displayed the best binding affinity towards MtPknG (-13.2 and -12.6 kcal/mol), with docking scores superior to the control inhibitor AX20017 (-7.9 kcal/mol). The observation of the predictive binding affinity of these natural products towards MtPknG warrants further in vitro investigations as they could represent some chemical scaffolds for the design of new MtPknG inhibitors.

Biography

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