

In Silico Study of the Biological and Pharmacological Activity of Nigella sativa

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Abstract : Background: Nigella sativa is an annual flowering plant, belongs to the Ranunculaceae family. It has many pharmacological activities such as anti-inflammatory; anti-bacterial; anti-hepatotoxic activities etc. Materials: In order to predict the pharmacological activity of Nigella Sativa's compounds, some web based servers were used, namely, PubChem, Molinspiration, ADMET-SAR, PASS online and PharMapper. In addition to that, AutoDOCK was used to investigate the different molecular interactions between the selected compounds and their target proteins. Results: All compounds displayed a stable interaction with their targets and satisfactory binding energies, which means that they are active on their targets. Conclusion: Nigella sativa is an effective medicinal plant that has several ethno-medical uses; the latter uses are proven herein via an in-silico study of their pharmacological activities.

Keywords : Nigella sativa, AutoDOCK, PubChem, Molinspiration, ADMET-SAR, PharMapper, PASS online server, docking

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