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Molecular Docking Studies of Derivatives of *Majorana hortensis* Leaves against Anti Apoptotic Targets

Radha Palaniswamy[1] and Padma P.R.[2]

[1]Dept of Biotechnology, Dr. NGP Arts and Science College, Coimbatore – 641048, India
[2]Dept of Biochemistry, Biotechnology and Bioinformatics, Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore – 641045, India

Abstract : Objective: Cancer is one of the most devastating disease and development of anticancer drugs or targets is of paramount importance in the field of biomedicine. Methods: *Majorana hortensis* leaves were subjected phytochemical analysis and piperitol from saponin fraction and terpinene 4-ol and trans sabinene hydrate from terpene fraction showed significant anticancer properties. Hence the above 3 ligands were targeted against the apoptotic targets (Trail, Bax, Bcl2, MDM2, Bak). The study was carried out using Schrodinger (GLIDE) software and the results were documented based on glide score, glide energy, pose number, good contacts, confirmation, and H bonding. Results: Results showed that piperitol possessed good docking capacity with all 5 targets. However, for Terpene 4-ol docking was not seen with MDM2 and Bak proteins. For trans-sabinene hydrate, docking did not appear in Bax, MDM2 and Bak. Conclusion: This proved that piperitol was most potent for anticancer therapy with respect to molecular docking studies.
Keywords : piperitol, terpene 4–ol, trans-sabinene hydrate, docking, anti apoptotic proteins.

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