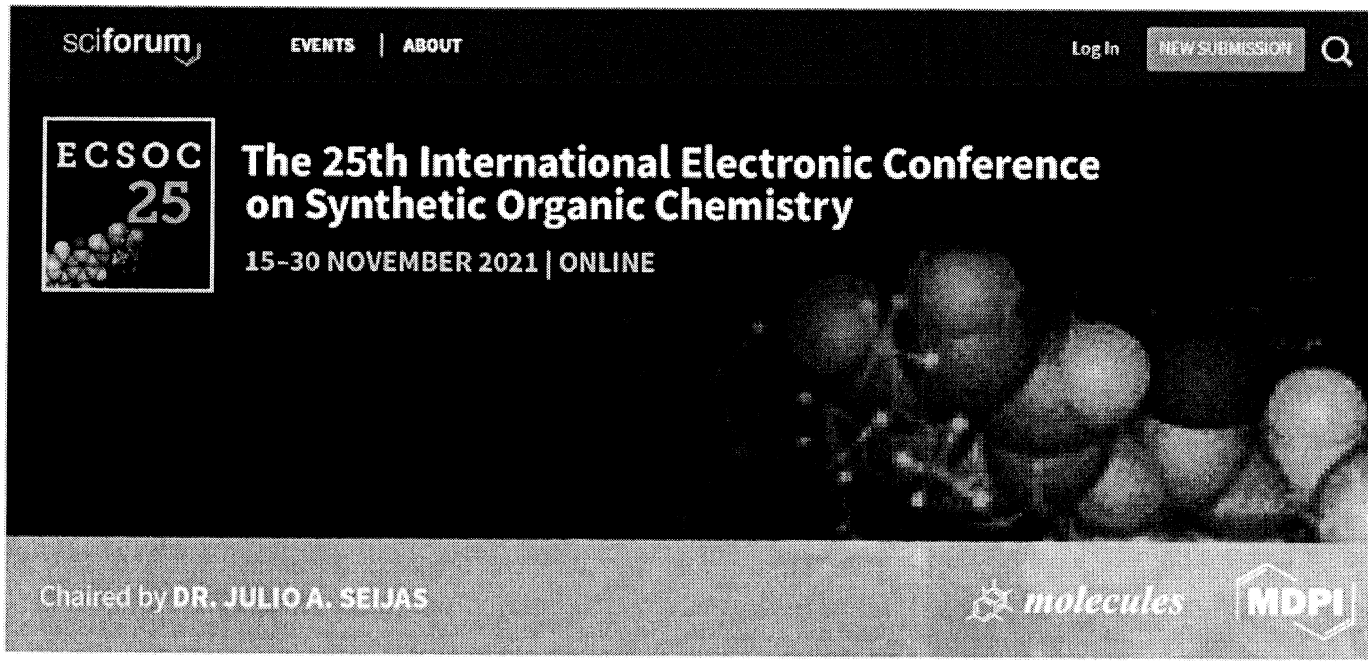

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sciforum-050781 | ***In silico* prediction of protein targets for volatile compounds of *Geranium* L. species** | N/A | N/A | Natalija Antić, Milan Ilić, Mirjana Marčetić, Milica Drobac, Mire Zloh | Hide Abstract

The *Geranium* L. species have significant use in traditional medicine. Previous studies showed that these plants are rich in phytochemicals, expecially in polyphenols and volatile compounds. The aim of this study was to determine potential target proteins for volatile compounds present in *Geranium* species and to provide a rationale for its current uses. The structures of identified volatile molecules were collated and their potential protein targets were predicted using PIDGIN software. The 2D and 3D structures of these compounds were generated using KingDraw software, while the 3D structures of selected target proteins were obtained from Protein Data Bank. All volatile compounds were docked against the whole surface of endothelial PAS domain-containing protein 1 (EPAS-1; PDBID: F310) and muscarinic receptors M1 (PDBID: 6WJC), M2 (PDBID: 3UON), M4 (PDBID: 5DG) and M5 (PDBID: 6OL9) using LeDock software. The study revealed several compounds with the potential to interact with target proteins. Hexahydrofarnesyl acetone and γ-curcumene formed the most favorable binding poses inside the binding sites of all muscarinic receptors. Linalool and δ-guaiene formed favorable interactions to EPAS-1 target protein. Predicted interaction energies are generally lower compared to ligands for these protein targets, mainly due to their size, hydrophobic properties, and the lack of H-bond forming groups. However, these compounds can fit the target site and form favorable interactions. It can be hypothesized that these plants and their extracts exert pharmacological activity via synergistic action of several components that can interact with multiple proteins *in vivo*. Additionally, new therapeutic applications of these plants may be proposed based on the other targets predicted by PIDGIN but not reported in this abstract. Further *in vitro* studies are required to confirm *in silico* prediction and gain further insights on potential interactions of tested compounds and target proteins.