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Essential oil composition and biological aspects of *Aconitum heterophyllum*

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Aconitum heterophyllum Wall. is consumed for its promising medicinal properties in several parts of the world. Present study consists of hydro distillation, antioxidant potential and *in-silico* antiapoptotic study of *A. heterophyllum* oil. Antioxidant activities were evaluated by *in-vitro* assays i.e., 2, 2-diphenyl-1-picrylhydrazyl (DPPH), Cupric Reducing Antioxidant Capacity (CUPRAC) and Superoxide inhibitor. It was found that the anti-oxidative effect of *A. heterophyllum* oil was dose dependent upto 200 µg/ml. For studying the apoptotic nature of the volatile constituents, *in silico* studies were carried out using BCL-2 anti-apoptotic receptors (BCL-2, BCL-XL and MCL-1). To understand the cascade of mechanisms leading to apoptosis, NF-κB was also considered. Docking score of various constituents with specific receptors were compared and it was found that β-fenchol binds best with NF-κB with the dock score of -4.36 kcal/ mol as compared to the selective inhibitors parthenolide (dock score was -3.04 kcal/mol). However, the constituents show favorable binding affinity for the receptors in the case of BCL-2 receptor, α-longipinene has a dock score of -4.26 kcal/mol as compared to that of standard inhibitor ABT 263 (-4.67 kcal/mol); Another constituent i.e., neryl acetate shows a dock score of -4.05 kcal/mol with BCL-XL as compared to stand inhibitor ABT 737 (-9.47 kcal/mol).

Biography

Yashika is a researcher at University institute of Pharmaceutical Sciences, Panjab University, India

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