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Topic of Research: **A multidisciplinary approach to investigate the chemotherapeutic potential of ethnomedicinal plants *Elaeocarpus ganitrus* and *Cyperus scariosus***

Keywords: ***Phytochemicals, STAT3, Cellular studies, Chemoinformatics, Bioavailability, Bioinformatics.***

Findings

This study explores the medicinal potential of *Elaeocarpus ganitrus* (Rudraksha) and *Cyperus scariosus* (Nagarmotha), particularly their anticancer effects and their influence on STAT3, a protein involved in various cancer-related processes like growth, invasion, and immune evasion. Both plants have traditional uses in medicine, but their effects on cancer and STAT3 have not been extensively studied.

Elaeocarpus ganitrus contains a variety of bioactive compounds, including alkaloids, flavonoids, and phenolic compounds, which are responsible for its broad therapeutic effects. This study explores its potential as a STAT3 inhibitor using both in vitro and computational methods. Different extracts of the plant's leaves were tested for cytotoxicity against HeLa cells, antioxidant properties, and anticancer activity. The active extracts were then subjected to GC-MS analysis to identify the phytochemicals they contained. These identified compounds were then subjected to molecular docking studies to determine promising candidates with strong binding affinity to the STAT3 receptor, suggesting their potential as anticancer agents. The study also highlighted the importance of these compounds in drug development, with favorable ADMET properties and stability in protein-ligand complexes.

The study highlighted six promising compounds, which showed superior binding and better bioavailability compared to known inhibitors.

Similarly, the anticancer potential of *Cyperus scariosus* was investigated. Different solvent extracts of the plant's root were evaluated for their cytotoxicity against HeLa cells, antioxidant properties, and anticancer effects. GC-MS analysis identified a number of phytochemicals, which were then tested for their interaction with the STAT3 receptor and assessed for their ADMET properties. The study identified six promising compounds that demonstrated stronger binding and better bioavailability compared to known inhibitors.

Both plants' compounds were selected for further evaluation through computational studies, including molecular dynamics simulations and bioinformatics tools. Three compounds from *E. ganitrus*- Butanoic acid, 3-methyl-, hexahydro-4-methylspiro, 7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione, and 3',4',7-trimethoxyflavone were found to have strong binding affinities and more stability in protein-ligand complexes with the STAT3 protein. These compounds also showed promising drug-like characteristics, including good bioavailability, and low toxicity.

Additionally, the study explored the chemotherapeutic potential of 7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione, one of the promising compounds from *E. ganitrus*, for cervical cancer treatment. This compound exhibited significant antioxidant and anticancer properties in vitro, further supported by molecular docking results, which confirmed its potential as a potent anticancer agent.

In conclusion, this study emphasizes the therapeutic potential of *Elaeocarpus ganitrus* and *Cyperus scariosus*, especially their capacity to inhibit STAT3, a crucial target in cancer treatment. The results indicate that continued research on these promising compounds could pave the way for the development of new anticancer agents with fewer side effects than traditional chemotherapy.