Anticancer compound found in monsoon-season delicacy

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Justicia wynaadensis - Wayanad Justicia from Periya. Credit: Vinayaraj

A small-branched shrub found in India known locally as Moddu Soppu (Justicia wynaadensis) is used to make a sweet dish during the monsoon season by the inhabitants of Kodagu district in Karanataka exclusively during the monsoons. Research published in the *International Journal of Computational Biology and Drug Design* has looked at phytochemicals present in extracts from the plant that may have putative anticancer agent properties.

C.D. Vandana and K.N. Shanti of PES University in Bangalore, Karnataka and Vivek Chandramohan of the Siddaganga Institute of Technology also in Tumkur, Karnataka, investigated several phytochemicals that had been reported in the scientific literature as having anticancer activity. They used a computer model to look at how well twelve different compounds "docked" with the relevant enzyme thymidylate synthase and compared this activity with a reference drug, capecitabine, which targets this enzyme.

Thymidylate synthase is involved in making DNA for cell replication. In cancer, uncontrolled cell replication is the underlying problem. If this enzyme can be blocked it will lead to DNA damage in the cancer cells and potentially halt the cancer growth.

Two compounds had comparable activity and greater binding to the enzyme than capecitabine. The first, campesterol, is a well-known plant chemical with a structure similar to cholesterol, the second stigmasterol is another well-known phytochemical involved in the structural integrity of plant cells. The former proved itself to be more stable than the latter and represents a possible lead for further investigation and testing as an anticancer drug, the team reports.

More information: C.D. Vandana et al. In silico studies of bioactive phytocompounds with anticancer activity from in vivo and in vitro extracts of Justicia wynaadensis (Nees) T. Anderson, *International Journal of Computational Biology and Drug Design* (2021). DOI: 10.1504/IJCBDD.2020.113836

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