

Anti Carcinogenic Potential of Xanthohumol by Inverse Molecular Docking and Quantum Mechanics Approach

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Abstract

Xanthohumol is a flavonoid, isolated from cones of the female inflorescences of the hop plant (*Humulus lupulus* L.). Hop is largely used in the brewing industry as a preservative and flavoring agent. In the scientific literature one finds ever reports indicating that xanthohumol possesses chemopreventive properties and protects cells against DNA damage caused by chemical carcinogens. Furthermore, it was found that xanthohumol inhibits DNA damage, proliferation of cancer cells (*in vitro*), inactivates free radicals and induces apoptosis. As xanthohumol could act as an anticarcinogenic agent, a novel inverse molecular docking approach was used to find its new potential human protein targets. Inverse docking was performed using an in-house docking algorithm and xanthohumol was docked into the predicted binding sites of all protein structures from the Protein Data Bank. A number of novel potential targets, into which xanthohumol was docked successfully, were found. These could explain known actions or predict new effects of xanthohumol. Furthermore, quantum mechanics (QM) simulation were applied as an alternative approach to inverse docking. Using the Hartree-Fock level of theory and flexible basis set 6-311++G(d,p) we were able to predict activation free energies of xanthohumol towards several chemical carcinogens of the epoxy type. To better model the biological environment in the cell, different solvation models were incorporated in the calculations as well. In a poster the results of both methods used in our computational experiments will be presented.

scientific journals (2 additional papers are in progress) and she is a co-author of new hop variety named *Styrian Kolibri*.

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Biography:

Zala Kolenc completed her PhD in the 2017 at University of Ljubljana and has now started her postdoctoral studies. The researcher was active in the field of drought stress on hop using proteomics and physiological approaches, as the main topics during PhD studies. In addition to drought stress her research field was sex determination in hop using multiplex PCR reactions in the breeding process and fingerprinting of hop cultivars with fluorescent labelled microsatellite markers. Now she started studying the antioxidant, antimicrobial and anticarcinogenic potential of hop extracts, as the main topic of her postdoctoral studies. She has published 6 original papers in