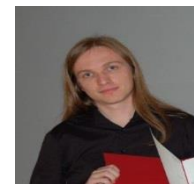


## *In-Silico Studies of Molecular Mechanisms Responsible for Rosemary Antimicrobial, Antioxidant and Anticancerogenic Properties*

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### **Abstract**

Rosemary (*Rosmarinus officinalis*) is a perennial, evergreen herb native to the Mediterranean region. Studies suggest that phytochemicals found in rosemary can exhibit a number of pharmacological properties – most notable are its antimicrobial, antioxidant and anticancerogenic effects. These properties are generally attributed to four distinct molecules: carnosol, carnosic acid, rosmarinic acid and rosmanol. While various *in-vitro* and *in-vivo* studies report the mentioned beneficial health effects, little is known of the specific molecular mechanisms that cause them. Here, we present an inverse molecular docking approach using a novel knowledge-based docking algorithm (ProBiS-Dock), where the four compounds were docked into all (approximately 60 000 protein structures) obtained from the Protein Data Bank. We report the highest scoring matches between protein targets and the four phytochemicals, thereby offering new insight into possible mechanistic insights behind the exhibited biological activity of rosemary compounds. Moreover, the same compounds were investigated using a series of *ab initio*, density functional theory and semiempirical quantum-chemical calculations to determine their ability to scavenge and subsequently deactivate known carcinogens, such as urethane or aflatoxin B<sub>1</sub> – both commonly found in everyday human food. In addition to the study offering insights for specific phytochemicals found in rosemary our work also presents new *in-silico* methods and their applications that can potentially be used with any naturally occurring or synthetic molecule.

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### **Biography:**

Samo Lešnik earned his PhD in 2017 at the University of Ljubljana, Faculty of Pharmacy. He gathered international experience working at the Department of Physics at the Free University of Berlin. Currently, he is positioned as a postdoctoral student at the Faculty of Chemistry and Chemical Engineering University of Maribor. To date, he has published more than 15 original papers on the topic of drug design in reputed scientific journals.