Machine learning analyses on data including essential oil chemical composition and in vitro experimental antibiofilm activities from different bacterial belonging to either gram-positive or gram-negative species

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Microorganisms and opportunistic pathogens can cause persistent infections due to their peculiar antibiotic resistance mechanisms and to their ability to adhere and form biofilm. Biofilm resistance to antimicrobials is a complex phenomenon, not only driven by genetic mutation inducing resistance, but also by means of increased microbial cell density that supports horizontal gene transfer across cells. The interest in the development of new approaches for the prevention and treatment of bacterial biofilm (BB) formation has recently increased. Experimental data indicated that EOs are able to modulate biofilm production of different Gram-positive (*Pseudomonas aeruginosa*, PA) and Gram-negative (*Staphylococcus aureus* and *Staphylococcus epidermidis*, SA and SE) bacterial strains. In particular, EOs influenced biofilm production with unpredictable results leading to either BB inhibition or reduction depending both on EOs' chemical composition and on type of microorganism. Aim of this presentation is to demonstrate how application of machine learning (ML) application to complex matrix of data from 89 essential oils (EOs) chemical analysis and their related in vitro experimental antibiofilm potencies can lead to hypothesize on the mechanism of action of EOs' chemical components. To elucidate the obtained experimental results, ML algorithms were applied leading to statistically robust classification models. Analysis of the models in term of feature importance and partial dependence plots led to indicating those chemical components mainly responsible for biofilm production, inhibition or stimulation for each studied strain, respectively. Data from these investigations represent the basis for future experiments that could enable to produce blends of EOs specifically engineered to obtain more potent anti-biofilm efficacy applicable in many fields such as airborne decontamination, products for dermatological and respiratory tract infections, and others.

Speaker Biography

Rino Ragno is an Associate Professor of Medicinal Chemistry as Department of Dug Chemistry and Technology of Sapienza University of Rome. He is the coordinator of the Rome center for Molecular Design (RCMD) lab and has published more than 120 papers in peer-reviewed journals in English with more than 2700 citations (scopus.com accessed July 2019), an h-index of 31, 3 patents, four books or book chapters, presented his work at numerous conferences and symposia. In 2005 he was awarded by the Italian Chemistry Society's Medicinal Chemistry Division for his research in the medicinal chemistry field. His main research fields are focused on the application of computational methods to medicinal chemistry and extraction of essential oils aimed to characterize them chemically and microbiologically.

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