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3rd World Congress on

Microbiology & Applied Microbiology

February 11, 2022 | Webinar

Structure-Activity-Mechanism Studies for Various Natural Compounds: Phenol Group Is Crucial for the Antimicrobial Activity

Bengü Ergüden
Gebze Technical University, Turkey

Pandemic we are facing today increased our awareness about the antiviral, antibacterial and antifungal compounds. Bioactive molecules having antimicrobial properties are of special interest for the control of pathogens that cause infections in humans. We focus on the mode of action of these compounds and especially relation between structure-activity-mode of action trio.

Terpenoids, secondary metabolites abundantly found in plants, are known to possess antibacterial activity against both Gram-negative and Gram-positive bacteria, and antifungal activity against pathogenic fungi. Recently, we studied the structure-activity relation of various substituted diterpenes and showed that phenolic structures are superior to their relatives against both bacteria and fungi. We also analyzed effect of these compounds on the microbial cell wall structure and maintenance of homeostasis. Free hydroxyl group of the phenol moiety was essential for this effect, since neither the O-methyl derivatives nor the benzylic partners were as effective. We demonstrated that phenols increase membrane permeability and cause leakage of ions. We thus propose that perturbation of ion homeostasis upon increase in cell wall permeability is key for the action of terpenoids against bacteria cells.

On the other hand, chalcones, valuable precursors for flavonoids, have important antibacterial and antifungal activities against bacteria, pathogens, harmful fungi, and even antibiotic-resistant microorganisms that cause food spoilage and infectious diseases. It is widely known that chalcones target various vital metabolic pathways of the bacterial cells. We aimed to study their action on the cell wall architecture, and studies various substituted chalcones. Similar to the case for terpenoids, phenolic chalcones proved to be superior to other substituted derivatives against both Gram-negative and Gram-positive bacteria. We also demonstrate that the cell wall is the first barrier that the chalcone molecules face for their action, and that phenolic chalcones increase ionic cell wall permeability to a greater extent than the other substituted members. Especially, against Gram-positive bacteria ion leakage can be detected at lower concentrations than the minimum inhibitory levels. Even though, disruption of metabolic pathways may be the principal mode of action of chalcones; in accord with our observations, we propose that the ion leakage precedes other inhibitory effects and contribute to the antibacterial action of phenolic chalcones.

Since, plant derived active reagents can be used as food preservatives and pharmaceutical agents, it is very important to understand their mode of action and their main target sites in the cell. Thus, this research not only opens new perspectives to understand antimicrobial activity mechanisms of these compounds, but also help widen their use.

e: b.sezen@gtu.edu.tr