3rd Global Experts Meeting on
Chemistry and Medicinal Chemistry
November 23, 2021 | Webinar

Piperine alkaloids and derivatives: Multistage extraction, structural optimization, DFT analysis, and biomedical application

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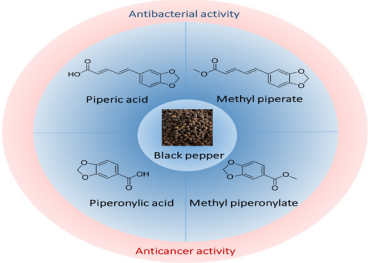
The natural product, black pepper, plays important roles in the food and pharmaceutical industries since it is rich in versatile bioactive molecules. To achieve the most medicinal value of piperine alkaloids from black pepper, we developed a variety of green and multistage extraction strategies. Encouragingly, these strategies display high extraction yields and purity for the refinement and separation of piperine alkaloids. Furthermore, four bioactive derivatives of piperine alkaloids (i.e., piperic acid, methyl piperate, piperonylic acid, and methyl piperonylate) were prepared through structural optimization. Among them, the formed piperic acid and piperonylic acid with ionizable carboxyl group are able to address the delivery barriers after intravenous injection, due to the improved aqueous solubility. The formed methyl piperate and methyl piperonylate show high membrane permeability for efficient oral absorption. The piperine alkaloids and their derivatives were characterized by 1H and 13C NMR, FTIR, UV-vis and fluorescence spectroscopy, as well as high-performance liquid chromatography (HPLC). Moreover, the density functional theory (DFT) was employed to explore the relationship of geometry structure, energy gap, thermodynamic equilibrium, electronic property, and bioactivity of the piperine alkaloids and derivatives. For biomedical applications, the antibacterial and anticancer activities of piperine alkaloids and derivatives were evaluated and compared. The piperine alkaloids and methyl piperate exhibited the potent antibacterial effect against some types of microorganisms such as S. aureus, S. pyogenes, E. coli, and S. typhi with the lowest MIC of 400 kg/ml, suggesting that piperine alkaloids and methyl piperate can be developed as the excellent antibacterial agents. Likewise, the anticancer effects of piperine alkaloids and derivatives were investigated on different cancer cell lines (e.g., B16, PANC, 4T1, and HeLa cells) using CCK-8 assay. The results revealed that piperine alkaloids possess the best anticancer activity (IC50 = 18.4 kg/mL) for 4T1 cells compared to other derivatives. In summary, our work provided a blueprint for the development and optimization of the next generation of highly effective phytomedicine.



Biography

Xin Li received his M.Sc. degree in Biochemical Engineering from Donghua University in 2017, and Ph.D. degree in Chemistry from RWTH Aachen University in 2021. Then he work as postdoctoral Research Fellow in DWI-Leibniz-Institute for Interactive Materials e.V. He has published more than 50 peer-reviewed SCI-indexed journal articles. His current research interests are focused on the development of phytomedicine, nanoprodrug, intelligent nanocarriers, organic/inorganic hybrid nanoplatforms for biomedical applications, in particular for precision cancer imaging and therapy.

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