COSMO-RS-Guided Design of Arginine–Ionic Liquid Systems with Predicted Antibacterial Potential for Food Preservation

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Mohd Noor, Najihah [a] ; Elgharbawy, Amal A.M. [b] ; Khan, Huma Warsi [c] ; Mohd Salleh, Hamzah [d] ; Hashim, Yumi Zuhanis Has-Yun [b] ; +2 authors

[a] Department of Chemical Engineering and Sustainability, Kulliyyah of Engineering, International Islamic University Malaysia, Kuala Lumpur, Malaysia

Abstract

Food preservation is essential for maintaining product quality, safety, and shelf life. Ionic liquids (ILs) have emerged as promising alternatives to traditional preservatives due to their tunable physicochemical properties, allowing compatibility with diverse food matrices without compromising flavor, texture, or nutritional value. However, identifying IL systems that balance antimicrobial efficacy and food quality remains challenging. Computational screening using COSMO-RS offers a predictive approach to evaluate IL-solute interactions without extensive experimental trials. In this study, 40 ILs were systematically assessed for their interactions with L-Arginine (Arg). Tetramethylammonium [TeMA] and Triethylammonium [TEA] cations exhibited reduced steric hindrance, promoting stronger association with Arg. Among the anions, carbonate (CO_3^{2-}) and acetate (OAc^-) formed strong hydrogen bonding networks with Arg. The ILs [TEA][CO_3^{2-}]

and [TeMA][CO_3^{2-}] showed the strongest affinity toward bacterial cell wall components, including N-Acetylmuramic acid (MurNAc), N-Acetyl-D-glucosamine (GlcNAc), and N-Acetylneuraminic acid (NANA), suggesting disruption of the peptidoglycan layer. The effect of water content was evaluated across varying water mole fractions to simulate moisture-rich, spoilage-prone food matrices. At low to intermediate hydration levels, [TeMA][CO_3^{2-}] showed greater resistance to hydration-induced Arg loss than [TEA][CO_3^{2-}], indicating better retention of antimicrobial functionality. These findings support the potential of IL-Arg systems as effective and safe next-generation food preservatives. © 2026 Wiley-VCH GmbH.

Author keywords

cosmo-RS; food preservation; green solvents; ionic liquids

Corresponding authors

Corresponding author	N. Mohd Noor
Affiliation	Department of Chemical Engineering and Sustainability, Kulliyyah of Engineering, International Islamic University Malaysia, Kuala Lumpur, Malaysia
Email address	Najihahmnoor@gmail.com
Corresponding author	A.A.M. Elgharbawy
Affiliation	International Institute For Halal Research and Training (INHART), International Islamic University Malaysia, Kuala Lumpur, Malaysia
Email address	amalgh@iium.edu.my

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