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

By [Noor, NM](#) (Mohd Noor, Najihah) ^[1]; [Elgharbawy, AAM](#) (Elgharbawy, Amal A. M.) ^[2]; [Khan, HW](#) (Khan, Huma Warsi) ^[3]; [Salleh, HM](#) (Mohd Salleh, Hamzah) ^[4]; [Hashim, YZH](#) (Hashim, Yumi Zuhanis Has-Yun) ^[2]; [Darmawan, N](#) (Darmawan, Noviyani) ^[5]; [Hizaddin, HF](#) (Hizaddin, Hanee Farzana) ^[6], ^[7]

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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 (CO₃²⁻) and acetate (OAc⁻) formed strong hydrogen bonding networks with Arg. The ILs [TEA][CO₃²⁻] and [TeMA][CO₃²⁻] 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][CO₃²⁻] showed greater resistance to hydration-induced Arg loss than [TEA][CO₃²⁻], indicating better retention of antimicrobial functionality. These findings support the potential of IL-Arg systems as effective and safe next-generation food preservatives.

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Author Information Corresponding Address: Mohd Noor, (corresponding author) Najihah

▼ Int Islamic Univ Malaysia, Dept Chem Engn & Sustainabil, Kulliyyah Engn, Kuala Lumpur, Malaysia

Corresponding Address: Elgharbawy, Amal A. (corresponding author)
M.

▼ Int Islamic Univ Malaysia, Int Inst Halal Res & Training
INHART, Kuala Lumpur, Malaysia

E-mail Addresses :

Najihahmnoor@gmail.com; amalgh@iium.edu.my

Addresses :

▼ ¹ Int Islamic Univ Malaysia, Dept Chem Engn & Sustainabil,
Kulliyyah Engn, Kuala Lumpur, Malaysia

▼ ² Int Islamic Univ Malaysia, Int Inst Halal Res & Training
INHART, Kuala Lumpur, Malaysia

▼ ³ Univ Teknol PETRONAS, Chem Engn Dept, Seri Iskandar,
Malaysia

▼ ⁴ Sultan Sharif Ali Islamic Univ, Fac Halal Sci & Sustainable
Tourism, Halalan Thayyiban Res Ctr, Bandar Seri Begawan,
Brunei

▼ ⁵ IPB Univ, Fac Math & Nat Sci, Dept Chem, Bogor,
Indonesia

[...more addresses](#)

E-mail Addresses :

Najihahmnoor@gmail.com; amalgh@iium.edu.my

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The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflict of interest statement

The authors declare no conflicts of interest.

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