Supporting Information

for

The chemical design of antimicrobial ionic liquids guided by machine learning: a review on balancing efficacy and toxicity

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Scope and literature search

To make the scope, we conducted a structured literature search in the Web of Science Core Collection (topic search; last accessed on 20 Dec 2025) using the keywords ionic liquid* AND toxicity AND machine learning, implemented as **TS=("ionic liquid*" AND (toxicity OR cytotoxicity OR hemolysis OR ecotoxicity) AND ("machine learning" OR "deep learning" OR "artificial intelligence" OR QSAR OR QSTR))**. To ensure coverage of antimicrobial endpoints and design workflows, we additionally used **TS=("ionic liquid*" AND (antimicrobial OR antibacterial OR biofilm) AND ("machine learning" OR QSAR OR QSTR OR "virtual screening" OR "multi-objective" OR "inverse design"))**.

We focused on studies published between 2000 and 2025 and complemented database search with backward/forward citation tracking of key resources (e.g., curated IL-toxicity datasets such as ILTox[1]) and representative ML/QSTR studies[2].

We included studies that (i) report well-defined cation/anion structures and quantitative antibacterial endpoints (e.g., MIC/pMIC) and/or toxicity endpoints (e.g., IC50/EC50/HC50) and (ii) provide mechanistic evidence, descriptors/representations, or modelling frameworks relevant to efficacy-toxicity trade-offs and rational design. Mixtures without clear ionic structures and reports lacking quantitative biological endpoints were excluded. Polymeric ionic liquids and ionogels were included when IL-derived motifs are the primary antimicrobial components and when quantitative efficacy/toxicity data enable meaningful structure-property and modelling discussions; otherwise, they are discussed only to contextualize application scenarios (e.g., coatings/hydrogels) rather than as the main modelling targets.

References

1 J. Yan, G. Liu, H. Chen, S. Hu, X. Wang, B. Yan and X. Yan, *Environ. Sci. Technol. Lett.*, 2023, **10**, 983–988.

2 I. Dasgupta, B. Das, Sk. A. Amin and S. Gayen, *J. Hazard. Mater.*, 2025, **496**, 139533.