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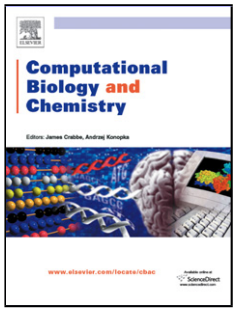

Title: Imidazolium ionic liquids as effective antiseptics and disinfectants against drug resistant *S. aureus*: *In silico* and *in vitro* studies

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Imidazolium ionic liquids as effective antiseptics and disinfectants against drug resistant *S. aureus*: *in silico* and *in vitro* studies

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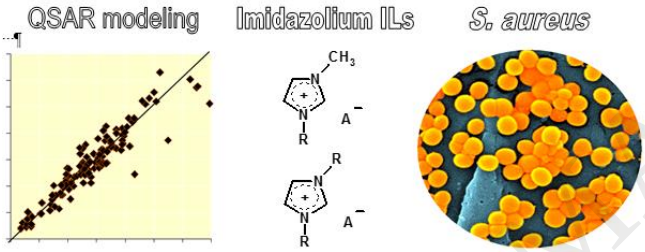
Graphical Abstract:



Highlights:

- Classification and regression QSAR models were created to predict the antibacterial activity of imidazolium ionic liquids.
- A series of synthesized 1,3-dialkylimidazolium ionic liquids with predicted activity were tested *in vitro* against *S. aureus* ATCC 25923 and its clinical isolate.
- The active imidazolium ILs with alkyl chain of 12 carbon atoms or with two identical alkyl chains C_8 or C_9 are effective anti-Staphylococcus aureus agents in particular against resistant *S. aureus* clinical isolate strains.
- The high activity of 7 ILs was analyzed by the molecular docking to prokaryotic homologue of a eukaryotic tubulin FtsZ.