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Identification of new pyridinium ionic liquids tagged with Schiff bases: Design, synthesis, *in silico* ADMET predictions and biological evaluations

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ABSTRACT

The discovery of a novel series of task-specific fluorinated pyridinium ionic liquids (TsILs) tagged with Schiff bases is reported using ultrasound-assisted and conventional syntheses. The synthesis required the quaternization of the appropriate pyridine Schiff base, followed by the metathesis of the resulting task-specific halogenated pyridinium ILs. The structures of the ILs were established by analytical and spectral data (IR, ¹H NMR, ¹³C NMR, ¹⁹F NMR and mass spectrometry). *In vitro* antimicrobial activities of the synthesized ILs on both gram-positive (*Bacillus cereus*, *Enterococcus faecalis*, and *Staphylococcus aureus*) and gram-negative (*Proteus mirabilis*, *Escherichia coli*, and *Pseudomonas aeruginosa*) bacterial strains and two fungal strains (*Candida albicans* and *Aspergillus brasiliensis*) were evaluated. Ionic liquids **8**, **18**, **19** and **20** appear to be the most active antimicrobials amongst the synthesized series. Preliminary studies were carried out to understand the relationship between the molecular structures and the inhibition activities of the synthesized ILs. In addition, the results of *in silico* studies revealed that all compounds exhibited good pharmacokinetic, bioavailability and toxicity profiles. Furthermore, drug likeness analysis suggests that the synthesized ILs might have appropriate oral absorption and brain penetration for application. *In vivo* computed LD₅₀ values (**2.59–2.78** mol/kg) were calculated for rat acute toxicity, and the compounds were found to be non-toxic and in a safe range for further study.

Keywords: Pyridinium ionic liquids; Schiff bases; Ultrasound irradiation; *In silico* analysis; Bioactivity of ILs.

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