Targeting poor solubility of docetaxel: Computational screening of ionic liquids using COSMO-RS

Journal of Ionic Liquids • Article • 2025 • DOI: 10.1016/j.jil.2025.100168

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Abstract

Docetaxel (DTX), a chemotherapeutic agent widely used in cancer treatment, has limited therapeutic efficacy owing to its poor oral absorption and low bioavailability. This study aims to improve DTX solubility by predicting its compatibility with ionic liquids (ILs) using conductor-like screening model for real solvents (COSMO-RS) computational modelling. A library of 340 ILs comprising 17 cations and 20 anions was screened for their potential to dissolve DTX, with a particular focus on imidazolium-based ILs that enhance its solubility and pertinence to cytotoxic applications. Computational analysis identifies ILs containing cations such as 1-methylimidazolium [MIM] and 1,3-dimethylimidazolium

[DMIM] and anions such as [CH_3COO^-], [Br^-], and [Cl^-], which have high solubility potential for DTX. Parameters such as the activity coefficient, solubility, capacity, selectivity, and performance index were evaluated. The σ-profile of DTX shows a predominantly nonpolar surface with limited hydrogen bond acceptor regions, indicating that its solubility in ILs is primarily driven by nonpolar (dispersion) interactions, with minor contributions from hydrogen bonding. Although these findings identify several promising IL candidates for improving the solubility of DTX, experimental validation is essential to confirm these computational predictions and assess the suitability of selected ILs in pharmaceutical formulations. This study demonstrates the value of COSMO-RS as a predictive tool for pharmaceutical formulation design and provides a pathway to enhance drug delivery for chemotherapeutics with poor solubility.

Author keywords

Active pharmaceutical ingredients; COSMO-RS; Docetaxel; Ionic liquids; Solubility; Therapeutic agent

Indexed keywords

Engineering controlled terms

Biochemistry; Computational methods; Drug discovery; Drug products; Hydrogen bonds; Positive ions; Targeted drug delivery

Engineering uncontrolled terms

Active pharmaceuticals ingredients; Chemotherapeutic agents; Computational modelling; Conductor-like screening model for real solvents; Docetaxel; Oral absorption; Pharmaceutical formulation; Poor solubilities; Therapeutic agents; Therapeutic efficacy

Engineering main heading

Ionic liquids; Solubility

Funding details

Details about financial support for research, including funding sources and grant numbers as provided in academic publications.

Funding sponsor	Funding number	Acronym
Ministry of Higher Education, Malaysia See opportunities by MOHE	FRGS/1/2021/STG02/UIAM/03/1	MOHE
Ministry of Higher Education, Malaysia See opportunities by MOHE		MOHE
Sultan Sharif Ali Islamic University	UNISSA/PPP/Grant/CRP0012 – 2023/2024	

Funding text

This work was supported by the Fundamental Research Grant Scheme of MoHE, Malaysia [grant number FRGS/1/2021/STG02/UIAM/03/1] and University Research Leave and Grant of Sultan Sharif Ali Islamic University [UNISSA/PPP/Grant/CRP0012 \u2013 2023/2024].

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