第216回 創薬科学 セミナー
GTR セミナー / CIBoG セミナー

日時：2026年7月9日（木曜日）16：00～ 17：30

場所：創薬科学研究館2階　講義室

このセミナーは創薬科学研究科・先端薬科学特論の単位認定となります

Lecture title：

Accelerating the Discovery of High-Performance Ionic Liquids Using Machine Learning and COSMO-RS

Speaker：

Prof. Hsiang-Yu (Angie) Wang

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Abstract：

Ionic liquids (ILs) are highly tunable “designer solvents” with negligible vapor pressure, wide electrochemical windows, and excellent thermal stability, making them valuable for metal recovery, biopolymer dissolution, energy storage, catalysis, and pharmaceutical processing. However, the vast IL chemical space, estimated to exceed 10^{18} possible cation–anion combinations, makes conventional trial-and-error screening impractical. Early machine learning (ML) approaches were limited by scarce curated datasets, inadequate molecular featurization, poor interpretability, and weak transferability across chemically distinct IL families. The absence of physically grounded feature selection also restricted model extrapolation and prospective discovery.

To address these challenges, we developed an integrated ML and thermodynamic modeling framework combining rigorous feature engineering, interpretable regression, and transfer learning. The framework uses a Mutual Information–Decision Tree (MI-DT) hybrid strategy for feature selection, coupled with Elastic Net regularized Quantitative Structure–Property Relationship (QSPR) modeling, to identify physically meaningful molecular descriptors from heterogeneous datasets. COSMO-RS thermodynamic simulations are incorporated to augment limited experimental data and anchor predictions in thermochemical principles, improving accuracy while revealing mechanistic insights into IL solvation and coordination behavior.

For metal extraction, the framework was validated using 497 literature samples involving imidazolium-based ILs for extracting Ni^{2+}, Au^{3+}, and Cu^{2+}. The MI-DT/QSPR models achieved extrapolation R^2 values of 0.91, 0.95, and 0.89, respectively, demonstrating strong predictive performance and providing molecular guidance for designing selective ILs for hydrometallurgy and environmental remediation. The framework was further extended to fucoidan dissolution, where limited experimental data required transfer learning. A QSPR model trained on cellulose dissolution was fine-tuned for fucoidan using COSMO-RS simulations, enabling virtual screening of over 2,500 ILs. This process identified promising candidates and key structural features governing effective dissolution while preserving bioactivity. Overall, the platform offers a robust, data-efficient, and transferable strategy for accelerating IL discovery across diverse applications.

皆様奮ってご参加ください。

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