

Data-driven search for drug–membrane permeability models (12 min talk + 3 min discussion)

Wednesday, 14 April 2021 15:00 (15 minutes)

Passive drug–membrane permeability of a drug molecule quantifies its capacity to cross cell membranes on the way of reaching its target. In this contribution, I will present results from our work where we used sure-independence screening and sparsifying operator (SISSO) to find equations for the permeability coefficient that combine both hydrophobicity and acidity of the drugs. The predicted equations provide more accurate values of permeability, on average, than the existing models for a diverse and exhaustive class of small drug molecules. Analysis of the inhomogeneous solubility-diffusion model in several asymptotic acidity regimes further leads to a rationalization of the equations.

Poster title

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