

Delfos: deep learning model for prediction of solvation free energies in generic organic solvents

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Prediction of aqueous solubilities or hydration free energies is an extensively studied area in machine learning applications in chemistry since water is the sole solvent in the living system. However, for non-aqueous solutions, few machine learning studies have been undertaken so far despite the fact that the solvation mechanism plays an important role in various chemical reactions. Here, we introduce Delfos (deep learning model for solvation free energies in generic organic solvents), which is a novel, machine-learning-based QSPR method which predicts solvation free energies for various organic solute and solvent systems. A novelty of Delfos involves two separate solvent and solute encoder networks that can quantify structural features of given compounds via word embedding and recurrent layers, augmented with the attention mechanism which extracts important substructures from outputs of recurrent neural networks. As a result, the predictor network calculates the solvation free energy of a given solvent-solute pair using features from encoders. With the results obtained from extensive calculations using 2495 solute-solvent pairs, we demonstrate that Delfos not only has great potential in showing accuracy comparable to that of the state-of-the-art computational chemistry methods, but also offers information about which substructures play a dominant role in the solvation process.

References:

1. Delfos: deep learning model for prediction of solvation free energies in generic organic solvents, Hyun-tae Lim and YounJoon Jung, Chemical Science 2019 DOI: 10.1039/C9SC02452B (2019)
2. Media

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