# Prediction and Screening of Solubility of Pharmaceuticals in Single- and Mixed-Ionic Liquids using COSMO-SAC model

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The prediction of solubility (xd) of drug molecules in single- and mixed-ionic liquid (IL) solutions using the COSMO-SAC activity coefficient model is investigated. In particular, the effect of dissociation of IL on solubility is examined. The prediction accuracy is found to be 91% in xd (root-mean-square deviation in ln $x_d$ is 0.65) for a total of 442 data points with solubility ranging from 0.93 to $2.84 \times 10^{-4}$ (mole fraction) and temperature ranging from 248.92 K to 488.3 K. The solubility of drug is found not sensitive to the treatment of dissociation of IL in the calculations. The method is used to determine the solubility of paracetamol in 2,624 single IL made from combination of 82 cations and 32 anions. The solubility of a drug in binary IL solution can be significantly higher or lower than those in pure IL components. For the 3,441,376 binary IL mixtures, about 8% of the mixtures exhibit higher solubility for paracetamol and 6% exhibit lower solubility. Our results indicate that mixing ILs can be a viable approach for tuning drug solubility.