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Findings of the Second Challenge to Predict Aqueous Solubili

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Journal of Chemical Information and Modeling, 2020,
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16	Machine learning in prediction of intrinsic aqueous solubility of drug-like compounds: Generalization, complexity, or predictive ability?. <i>Journal of Chemometrics</i> , 2021 , 35, e3349	1.6	9
15	SolTranNet-A Machine Learning Tool for Fast Aqueous Solubility Prediction. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2530-2536	6.1	5
14	Application of Artificial Neural Networks to Predict the Intrinsic Solubility of Drug-Like Molecules. <i>Pharmaceutics</i> , 2021 , 13,	6.4	0
13	ADME prediction with KNIME: A retrospective contribution to the second "Solubility Challenge".. <i>ADMET and DMPK</i> , 2021 , 9, 209-218	1.3	0
12	Salt solubility and disproportionation - uses and limitations of equations for pH and the in-silico prediction of pH. <i>Journal of Pharmaceutical Sciences</i> , 2021 ,	3.9	1
11	Predicting Solubility of Newly-Approved Drugs (2016-2020) with a Simple ABSOLV and GSE() Consensus Model Outperforming Random Forest Regression.. <i>Journal of Solution Chemistry</i> , 2022 , 1-36	1.8	1
10	Model agnostic generation of counterfactual explanations for molecules.. <i>Chemical Science</i> , 2022 , 13, 3697-3705	9.4	5
9	Evaluation of Deep Learning Architectures for Aqueous Solubility Prediction.. <i>ACS Omega</i> , 2022 , 7, 15695-15710	3.5	0
8	Solubility and Solvent Effect Analysis of Boc-L-glutamine in Different Solvents at Multiple Temperatures. <i>Journal of Chemical & Engineering Data</i> ,	2.8	0
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6	Leveraging genetic algorithms to maximise the predictive capabilities of the SOAP descriptor.		0
5	Intrinsic Aqueous Solubility: Mechanistically Transparent Data-Driven Modeling of Drug Substances. 2022 , 14, 2248		0
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2	A unified ML framework for solubility prediction across organic solvents.		0

- 1 Blinded Predictions and Post Hoc Analysis of the Second Solubility Challenge Data: Exploring Training Data and Feature Set Selection for Machine and Deep Learning Models. **2023**, 63, 1099-1113

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