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Kesler Isoko, Joan L. Cordiner, Zoltan Kis and Peyman Z. Moghadam*

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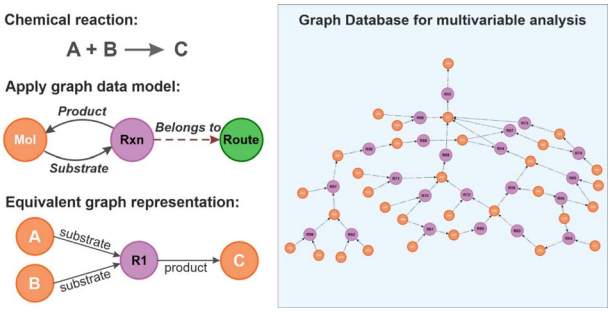
Claudio Avila,* Adam West, Anna C. Vicini, William Waddington, Christopher Brearley, James Clarke and Andrew M. Derrick



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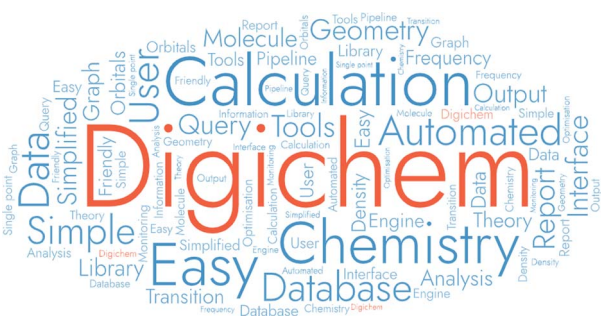
Digichem: computational chemistry for everyone

Oliver S. Lee, Malte C. Gather* and Eli Zysman-Colman*



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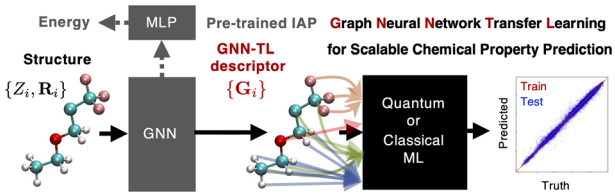
Universal neural network potentials as descriptors: towards scalable chemical property prediction using quantum and classical computers

Tomoya Shiota,* Kenji Ishihara and Wataru Mizukami*



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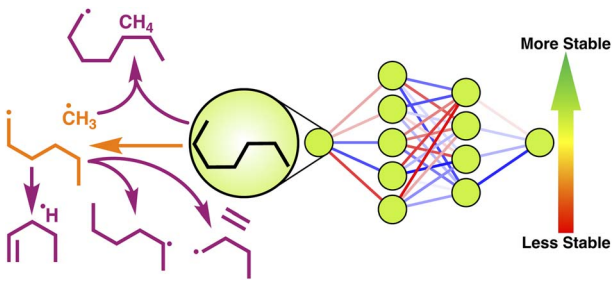
Machine learning of stability scores from kinetic data

Veerupaksh Singla, Qiyuan Zhao and Brett M. Savoie*



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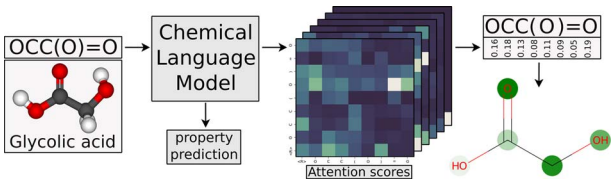

What can attribution methods show us about chemical language models?

Stefan Hödl, Tal Kachman, Yoram Bachrach, Wilhelm T. S. Huck and William E. Robinson*

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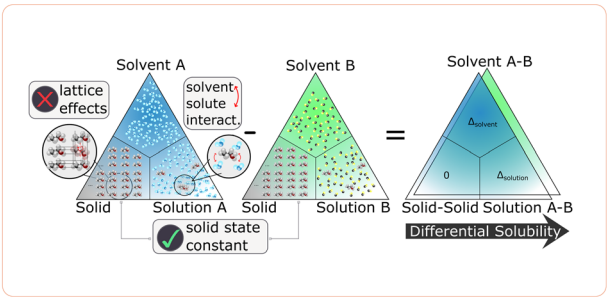

Solvmate – a hybrid physical/ML approach to solvent recommendation leveraging a rank-based problem framework

Jan Wollschläger* and Floriane Montanari

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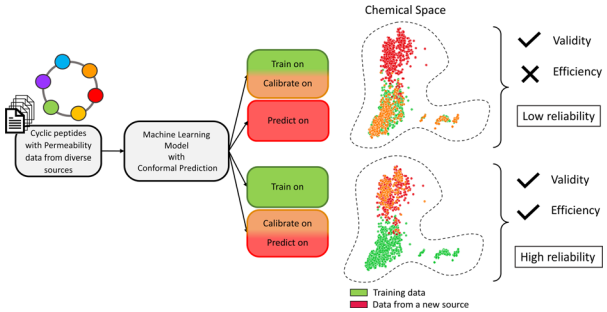

A methodology to correctly assess the applicability domain of cell membrane permeability predictors for cyclic peptides

Gökçe Geylan,* Leonardo De Maria, Ola Engkvist, Florian David and Ulf Norinder

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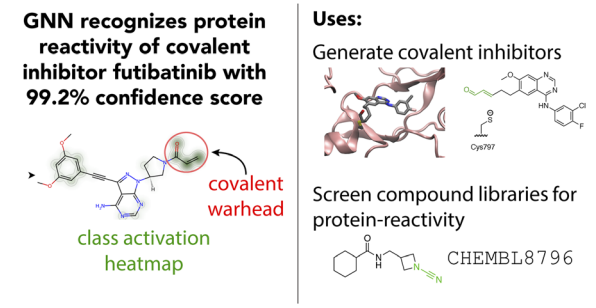

Graph neural networks for identifying protein-reactive compounds

Victor Hugo Cano Gil and Christopher N. Rowley*

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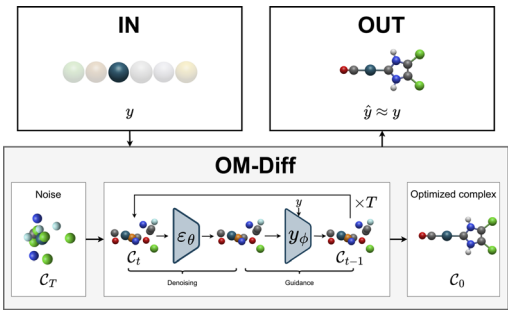
OM-Diff: inverse-design of organometallic catalysts with guided equivariant denoising diffusion

François Cornet, Bardi Benediktsson, Bjarke Hastrup, Mikkel N. Schmidt and Arghya Bhowmik*



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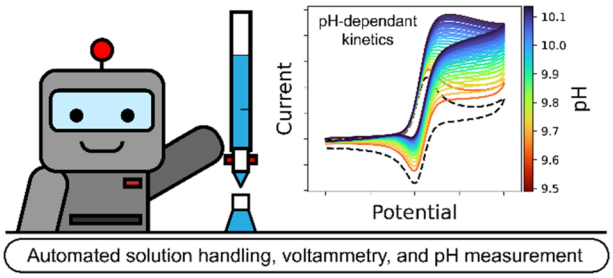
An automated electrochemistry platform for studying pH-dependent molecular electrocatalysis

Michael A. Pence, Gavin Hazen and Joaquín Rodríguez-López*



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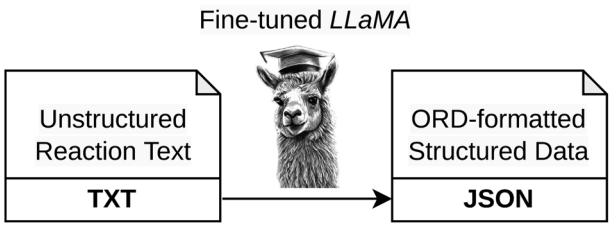
Extracting structured data from organic synthesis procedures using a fine-tuned large language model

Qianxiang Ai, Fanwang Meng, Jiale Shi, Brenden Pelkie and Connor W. Coley*



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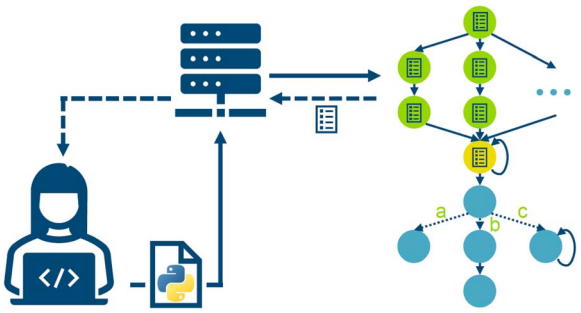
PerQueue: managing complex and dynamic workflows

Benjamin Heckscher Sjølin, William Sandholt Hansen, Armando Antonio Morin-Martinez, Martin Hoffmann Petersen, Laura Hannemose Rieger, Tejs Vegge, Juan Maria García-Lastra and Ivano E. Castelli*



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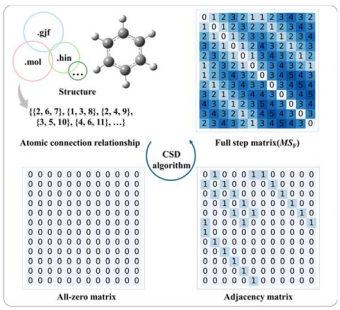

Connectivity stepwise derivation (CSD) method: a generic chemical structure information extraction method for the full step matrix

Jialiang Xiong, Xiaojie Feng, Jingxuan Xue, Yueji Wang, Haoren Niu, Yu Gu, Qingzhu Jia, Qiang Wang and Fangyou Yan*

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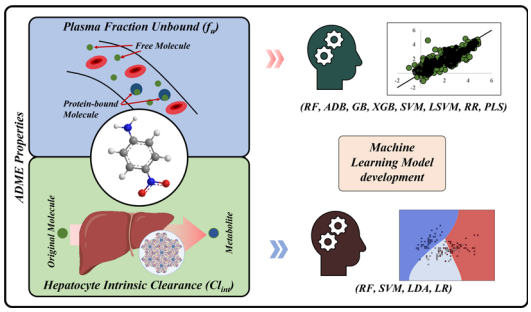

Insights into pharmacokinetic properties for exposure chemicals: predictive modelling of human plasma fraction unbound (f_u) and hepatocyte intrinsic clearance (Cl_{int}) data using machine learning

Souvik Pore and Kunal Roy*

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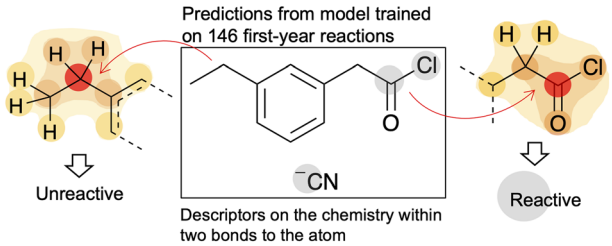

Every atom counts: predicting sites of reaction based on chemistry within two bonds

Ching Ching Lam and Jonathan M. Goodman*

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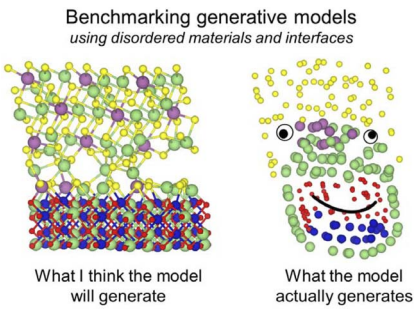

Dismai-Bench: benchmarking and designing generative models using disordered materials and interfaces

Adrian Xiao Bin Yong,* Tianyu Su and Elif Ertekin*

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