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See Peyman Z. Moghadam *et al.*, pp. 1662–1681. Image reproduced by permission of Peyman Z. Moghadam from *Digital Discovery*, 2024, 3, 1662.

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



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Fundamental questions
Elemental answers

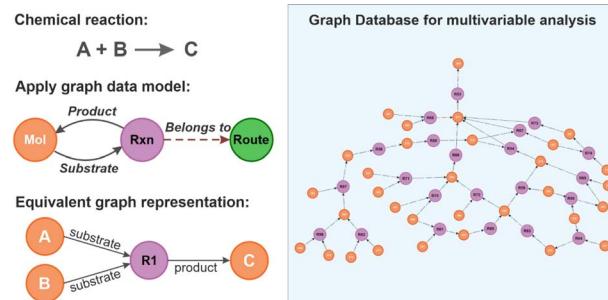
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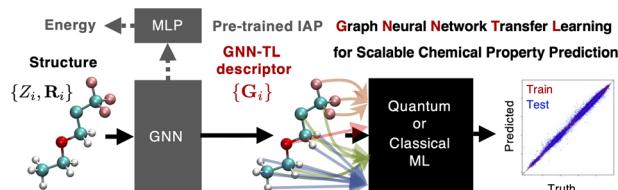
Oliver S. Lee, Malte C. Gather* and Eli Zysman-Colman*



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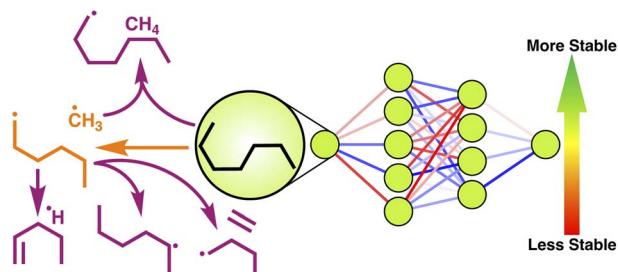
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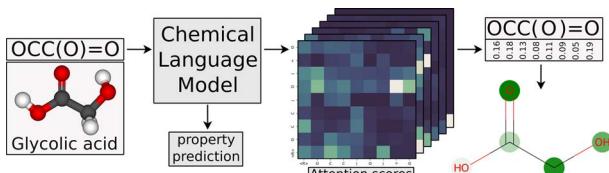
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Veerupaksh Singla, Qiyuan Zhao and Brett M. Savoie*



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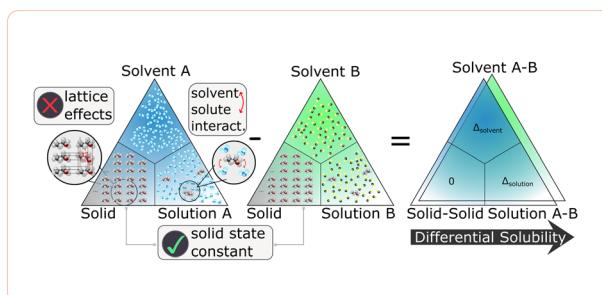
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What can attribution methods show us about chemical language models?

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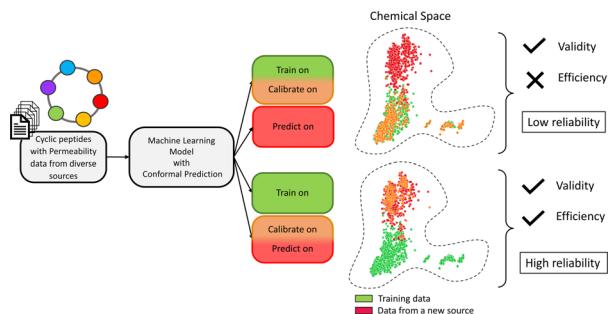
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Jan Wollschläger* and Floriane Montanari

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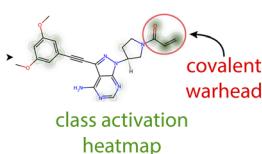


A methodology to correctly assess the applicability domain of cell membrane permeability predictors for cyclic peptides

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

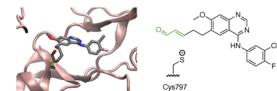
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GNN recognizes protein reactivity of covalent inhibitor futibatinib with 99.2% confidence score



Uses:

Generate covalent inhibitors



Screen compound libraries for protein-reactivity



Graph neural networks for identifying protein-reactive compounds

Renee Gil and Christopher N. Rowley*

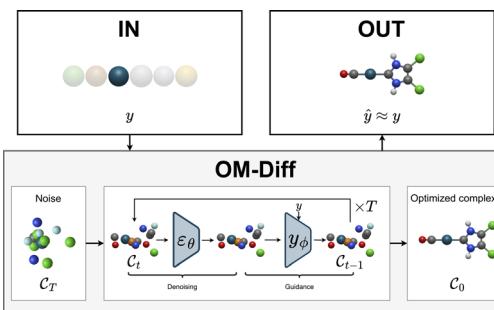


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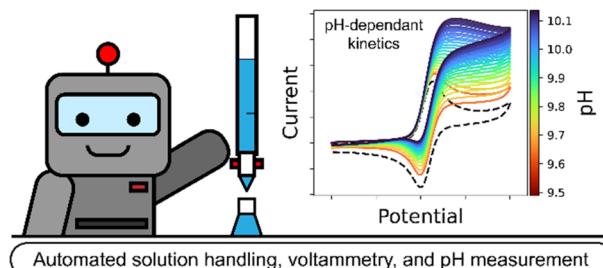
François Cornet, Bardi Benediktsson, Bjarke Hastrup, Mikkel N. Schmidt and Arghya Bhowmik*



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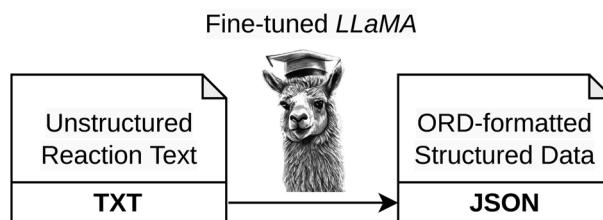
Michael A. Pence, Gavin Hazen and Joaquín Rodríguez-López*



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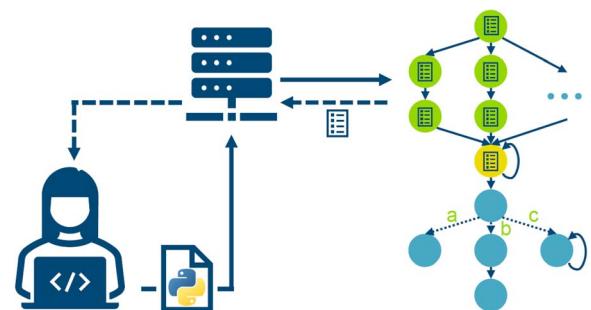
Qianxiang Ai, Fanwang Meng, Jiale Shi, Brenden Pelkie and Connor W. Coley*



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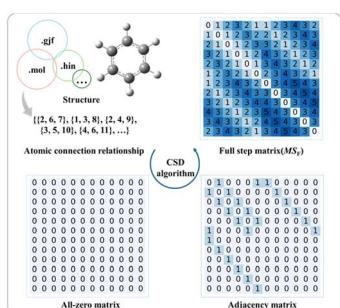
PerQueue: managing complex and dynamic workflows

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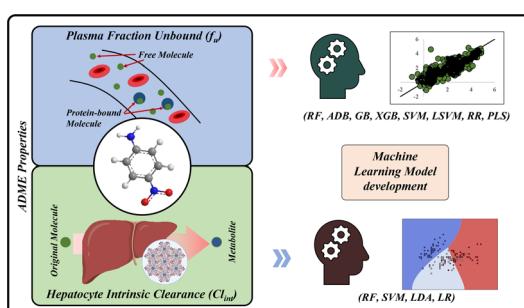
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Connectivity stepwise derivation (CSD) method: a generic chemical structure information extraction method for the full step matrix

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

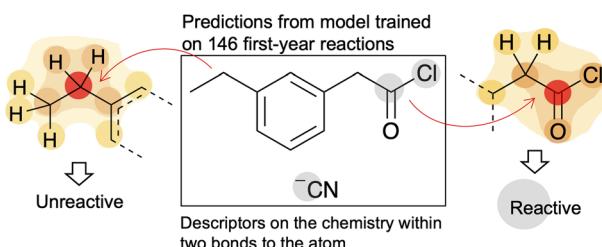
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Insights into pharmacokinetic properties for exposure chemicals: predictive modelling of human plasma fraction unbound (f_u) and hepatocyte intrinsic clearance (Cl_{int}) data using machine learning

Souvik Pore and Kunal Roy*

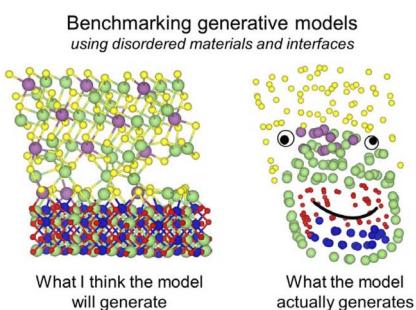
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Every atom counts: predicting sites of reaction based on chemistry within two bonds

Ching Ching Lam and Jonathan M. Goodman*

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

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

