

Digital Discovery

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IN THIS ISSUE

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Cover

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

EDITORIAL

1659

Introduction to “Accelerate Conference 2022”

Keith A. Brown, Fadwa El Mellouhi and Claudiane Ouellet-Plamondon



PERSPECTIVES

1662

Bioprocessing 4.0: a pragmatic review and future perspectives

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



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PERSPECTIVES

1682

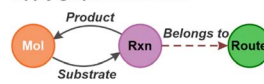
Chemistry in a graph: modern insights into commercial organic synthesis planning

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

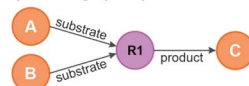
Chemical reaction:



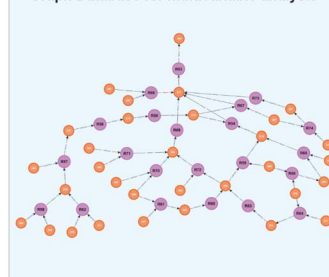
Apply graph data model:



Equivalent graph representation:



Graph Database for multivariable analysis

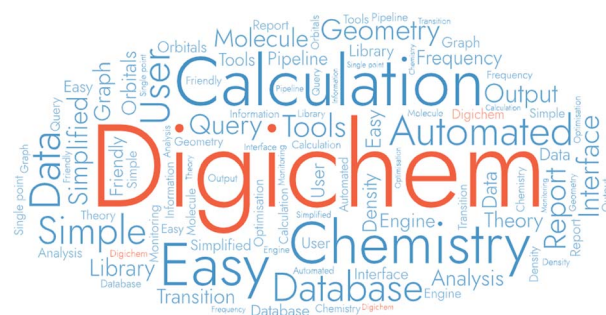


PAPERS

1695

Digichem: computational chemistry for everyone

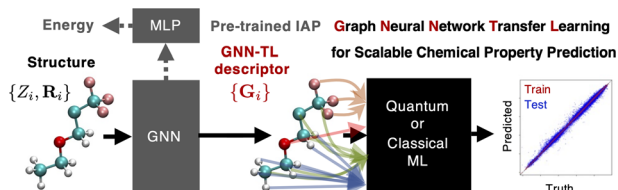
Oliver S. Lee, Malte C. Gather* and Eli Zysman-Colman*



1714

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

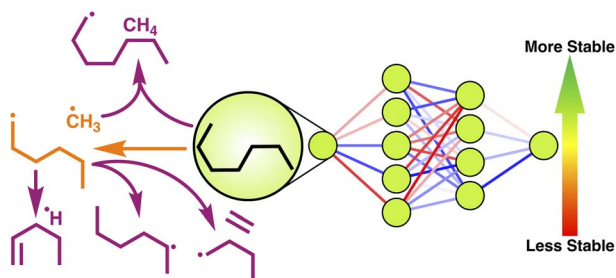
Tomoya Shiota,* Kenji Ishihara and Wataru Mizukami*



1729

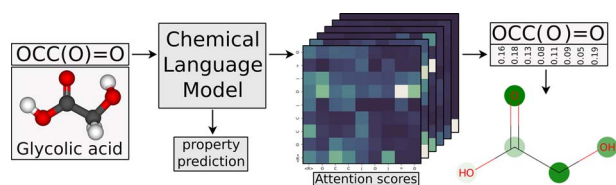
Machine learning of stability scores from kinetic data

Veerupaksh Singla, Qiyuan Zhao and Brett M. Savoie*



PAPERS

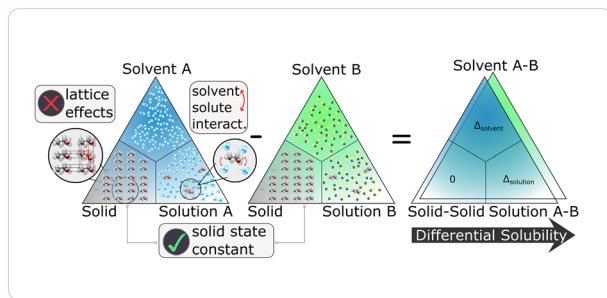
1738



What can attribution methods show us about chemical language models?

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

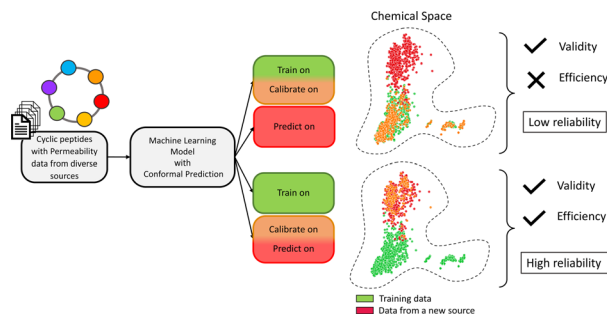
1749



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

Jan Wollschläger* and Floriane Montanari

1761

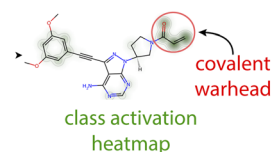


A methodology to correctly assess the applicability domain of cell membrane permeability predictors for cyclic peptides

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

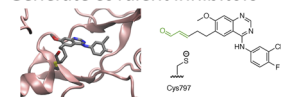
1776

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

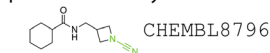


Uses:

Generate covalent inhibitors



Screen compound libraries for protein-reactivity



Graph neural networks for identifying protein-reactive compounds

Renee Gil and Christopher N. Rowley*

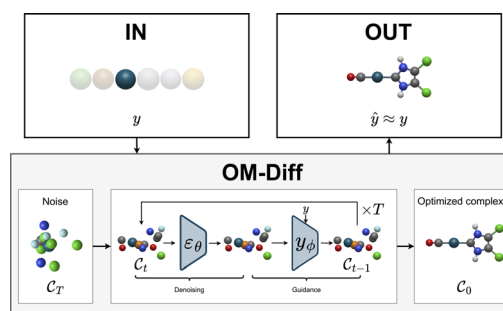


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1793

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

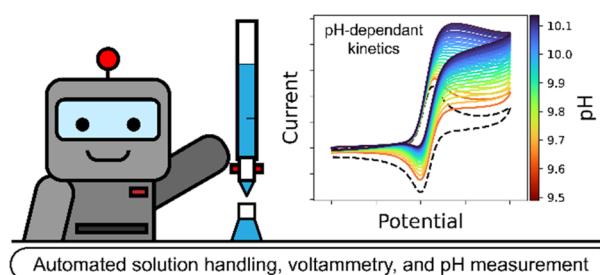
François Cornet, Bardi Benediktsson, Bjarke Hastrup, Mikkel N. Schmidt and Arghya Bhowmik*



1812

An automated electrochemistry platform for studying pH-dependent molecular electrocatalysis

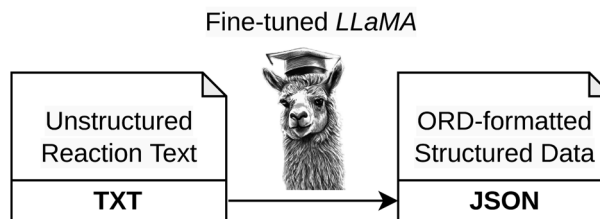
Michael A. Pence, Gavin Hazen and Joaquín Rodríguez-López*



1822

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

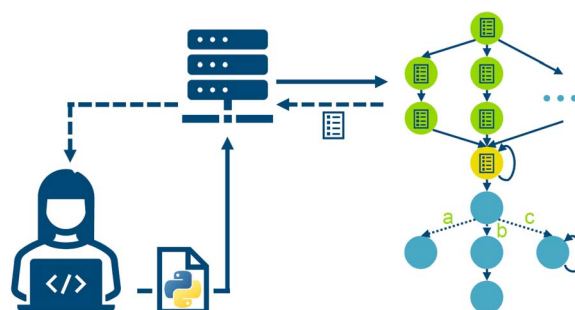
Qianxiang Ai, Fanwang Meng, Jiale Shi, Brenden Pelkie and Connor W. Coley*



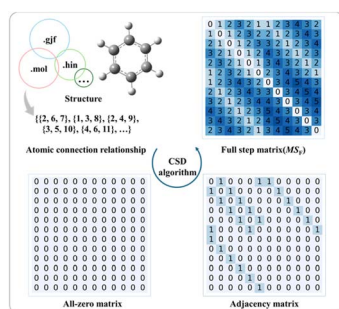
1832

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*



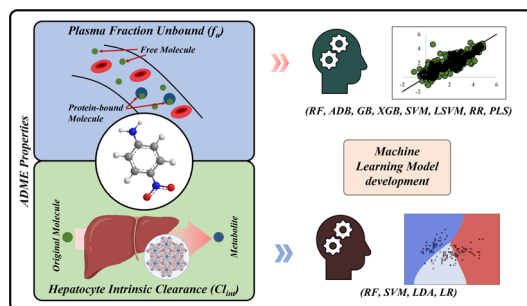
1842



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*

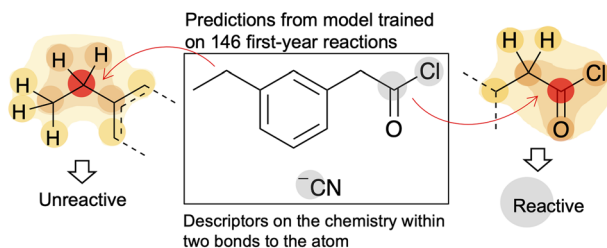
1852



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*

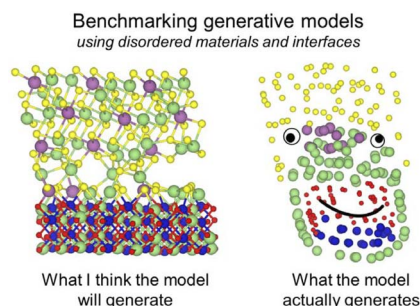
1878



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

Ching Ching Lam and Jonathan M. Goodman*

1889



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

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

