

# Digital Discovery

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## IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 3(9) 1651–1912 (2024)



### 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

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### 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\*



# EES Catalysis

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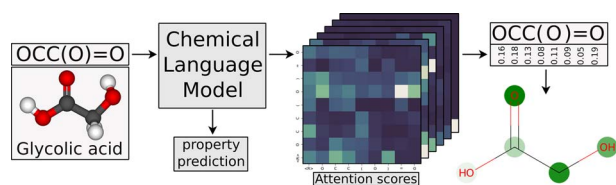
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Fundamental questions  
Elemental answers



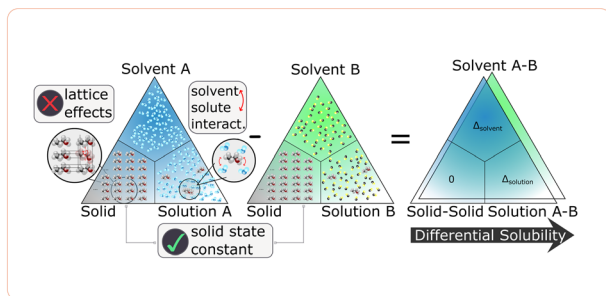
1738



### What can attribution methods show us about chemical language models?

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

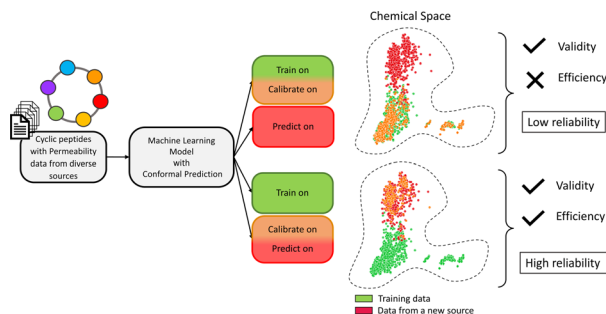
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### Solvmate – a hybrid physical/ML approach to solvent recommendation leveraging a rank-based problem framework

Jan Wollschläger\* and Floriane Montanari

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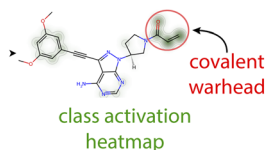


### A methodology to correctly assess the applicability domain of cell membrane permeability predictors for cyclic peptides

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

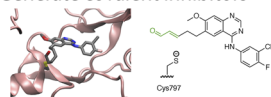
1776

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



#### Uses:

Generate covalent inhibitors



Screen compound libraries for protein-reactivity



### Graph neural networks for identifying protein-reactive compounds

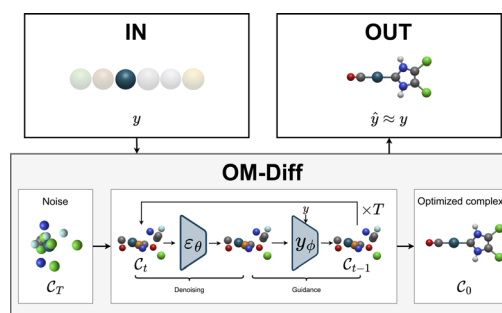
Victor Hugo Cano Gil and Christopher N. Rowley\*



1793

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

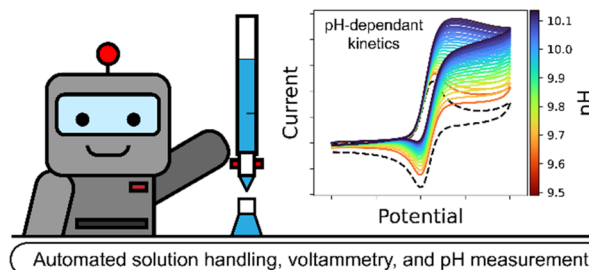
François Cornet, Bardi Benediktsson, Bjarke Hastrup, Mikkel N. Schmidt and Arghya Bhowmik\*



1812

### An automated electrochemistry platform for studying pH-dependent molecular electrocatalysis

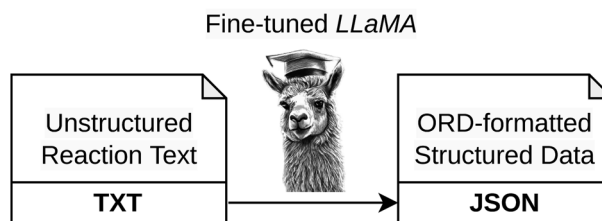
Michael A. Pence, Gavin Hazen and Joaquín Rodríguez-López\*



1822

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

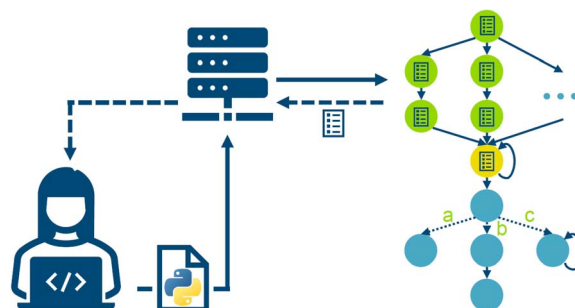
Qianxiang Ai, Fanwang Meng, Jiale Shi, Brenden Pelkie and Connor W. Coley\*



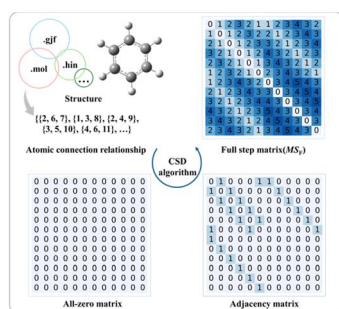
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### PerQueue: managing complex and dynamic workflows

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\*



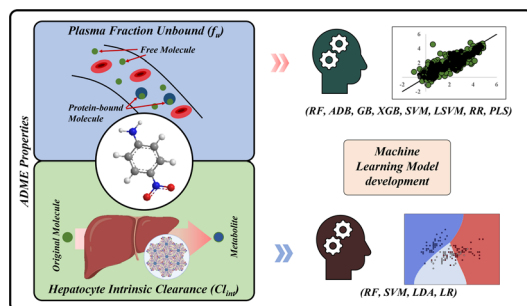
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### Connectivity stepwise derivation (CSD) method: a generic chemical structure information extraction method for the full step matrix

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

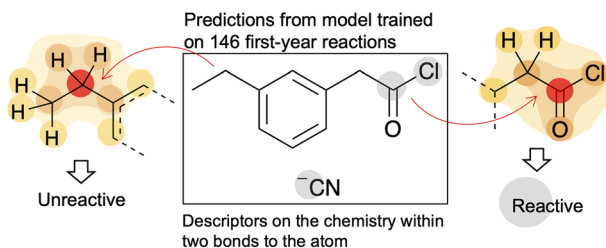
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### Insights into pharmacokinetic properties for exposure chemicals: predictive modelling of human plasma fraction unbound ( $f_u$ ) and hepatocyte intrinsic clearance ( $Cl_{int}$ ) data using machine learning

Souvik Pore and Kunal Roy\*

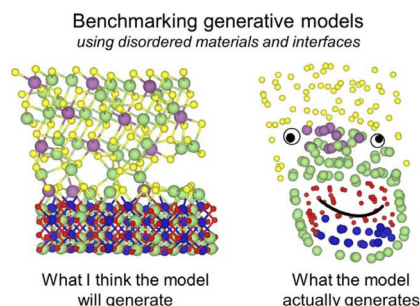
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### Every atom counts: predicting sites of reaction based on chemistry within two bonds

Ching Ching Lam and Jonathan M. Goodman\*

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

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

