

# Digital Discovery

rsc.li/digitaldiscovery

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

## 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

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\*



# EES Catalysis

GOLD  
OPEN  
ACCESS

Exceptional research on energy  
and environmental catalysis

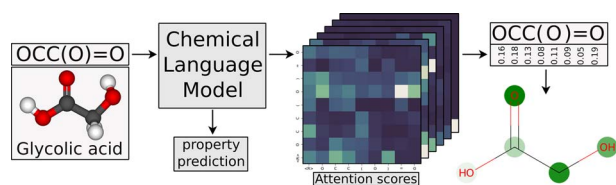
Open to everyone. Impactful for all

[rsc.li/EESCatalysis](https://rsc.li/EESCatalysis)

Fundamental questions  
Elemental answers



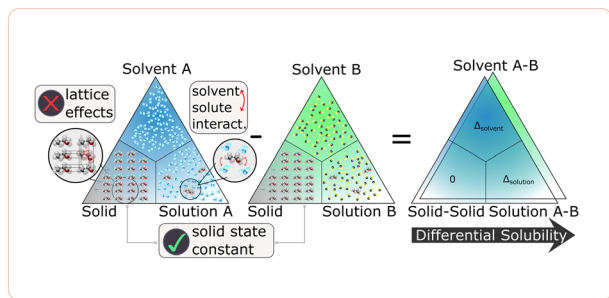
1738



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

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

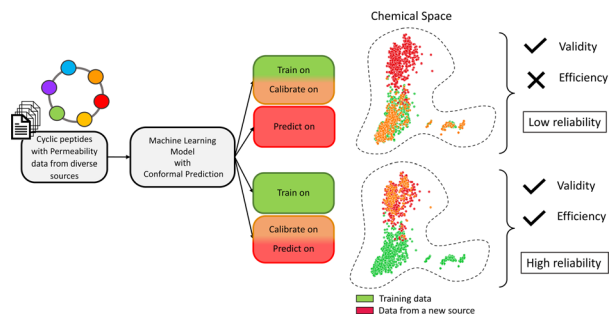
1749



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

Jan Wollschläger\* and Floriane Montanari

1761

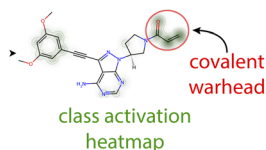


### A methodology to correctly assess the applicability domain of cell membrane permeability predictors for cyclic peptides

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

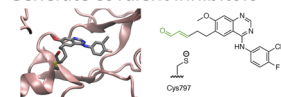
1776

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



#### Uses:

Generate covalent inhibitors



Screen compound libraries for protein-reactivity



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

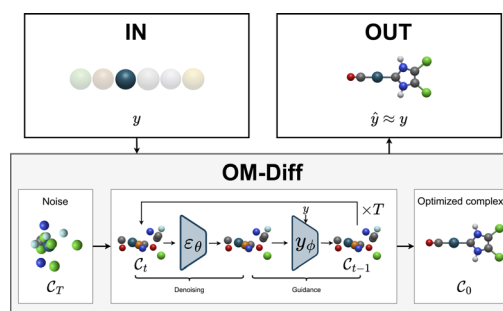
Renee Gil and Christopher N. Rowley\*



1793

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

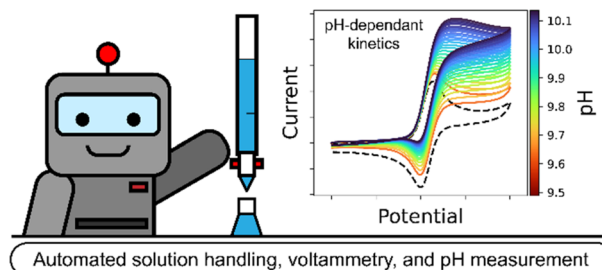
François Cornet, Bardi Benediktsson, Bjarke Hastrup, Mikkel N. Schmidt and Arghya Bhowmik\*



1812

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

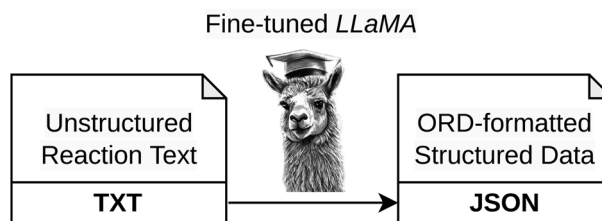
Michael A. Pence, Gavin Hazen and Joaquín Rodríguez-López\*



1822

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

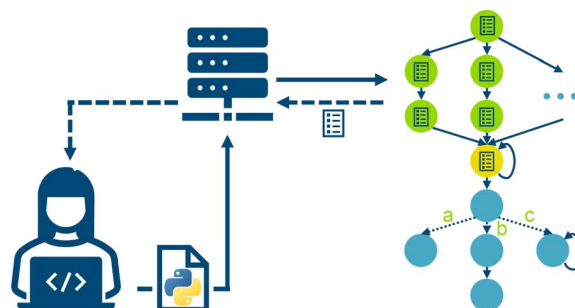
Qianxiang Ai, Fanwang Meng, Jiale Shi, Brenden Pelkie and Connor W. Coley\*



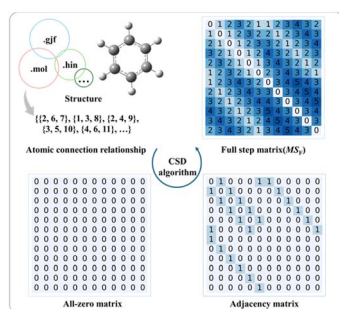
1832

### 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\*



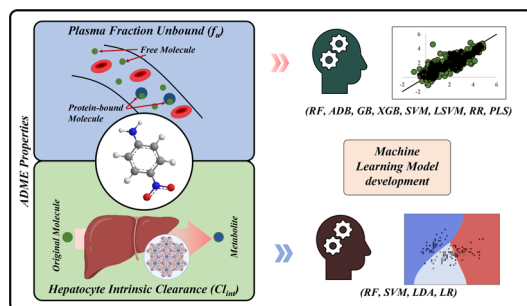
1842



### 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\*

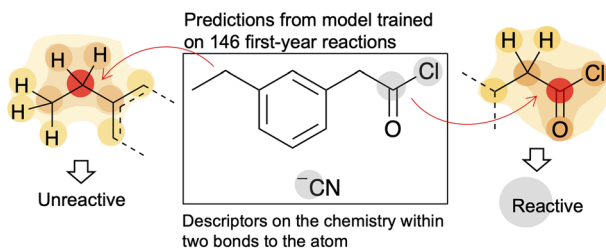
1852



### 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\*

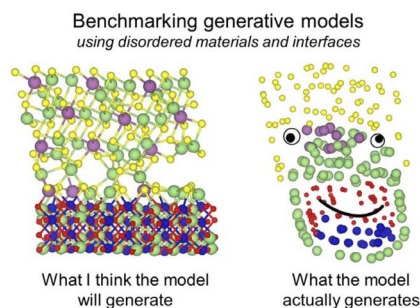
1878



### 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\*

