

# Digital Discovery

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## IN THIS ISSUE

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**Cover**  
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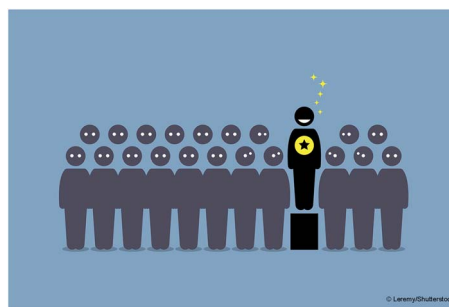


**Inside cover**  
See Maciej Haranczyk *et al.*, pp. 2001–2011. Image reproduced by permission of Alex Mascaraque León from *Digital Discovery*, 2025, 4, 2001. Created with the use of Google's Gemini model via Google Cloud Platform.

## EDITORIAL

1987

### Outstanding Reviewers for *Digital Discovery* in 2024

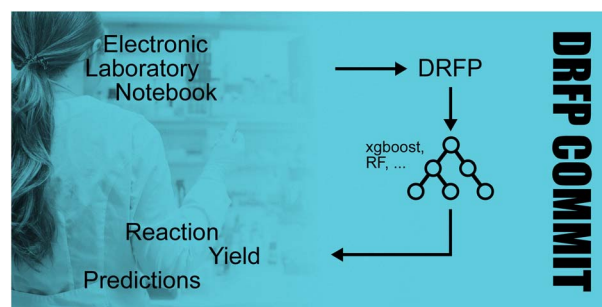


## COMMIT

1988

### Commit: Reaction classification and yield prediction using the differential reaction fingerprint DRFP

Daniel Probst



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1991

## BayBE: a Bayesian Back End for experimental planning in the low-to-no-data regime

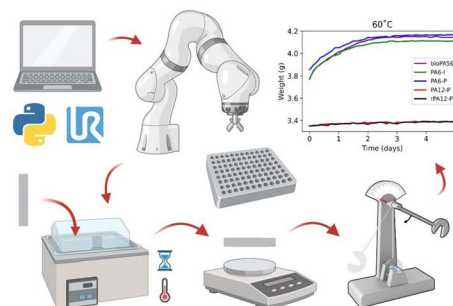
Martin Fitzner, Adrian Šošić, Alexander V. Hopp, Marcel Müller, Rim Rihana, Karin Hrovatin, Fabian Liebig, Mathias Winkel, Wolfgang Halter and Jan Gerit Brandenburg\*



2001

## Streamlining material degradation testing: collaborative robotics for specimen monitoring

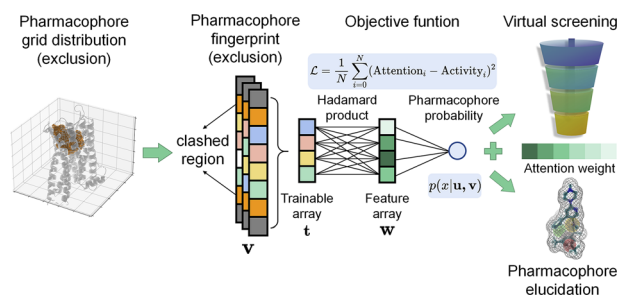
Brody Stack, Miguel Hernández-del-Valle, Alex Mascaraque-León, Petronela Chovancová, Loris Langeois, Jacob Porath, Juan P. Fernandez-Blazquez, Mónica Echeverry-Rendón and Maciej Haranczyk\*



2012

## Enhancing multifunctional drug screening via artificial intelligence

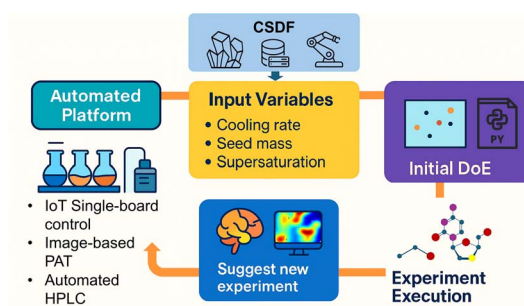
Junlin Dong,\* Chenyang Wu,\* Tianle Lu,\* Shiyu Wang,\* Wenjin Zhan, Marc Xu, Bing Wang, Zhenquan Hu, Horst Vogel and Shuguang Yuan



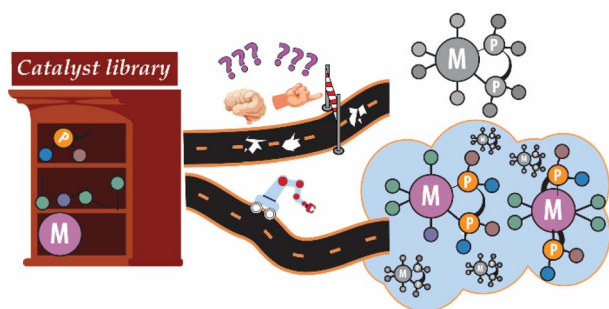
2025

## Automated scale-up crystallisation DataFactory for model-based pharmaceutical process development: a Bayesian case study

Thomas Pickles, Youcef Leghrib, Matt Weisshaar, Mikhail Goncharuk, Peter Timperman, Timothy Doherty, David D. Ford, Jonathan Moores, Alastair J. Florence and Cameron J. Brown\*



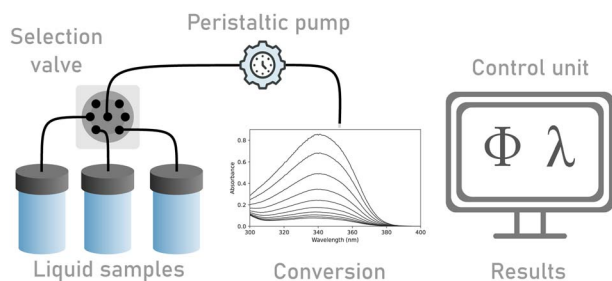
2033



### Unveiling the impact of ligand configurations and structural fluxionality on virtual screening of transition-metal complexes

Adarsh V. Kalikadien, Niels J. van der Lem, Cecile Valsecchi, Laurent Lefort and Evgeny A. Pidko\*

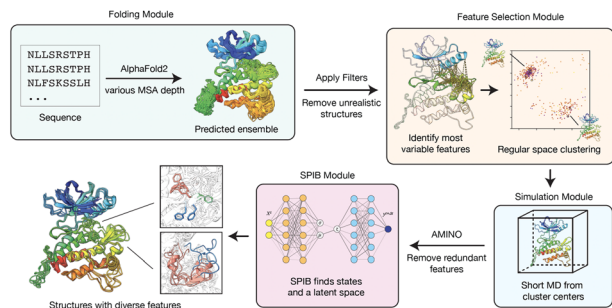
2045



### An automated photo-isomerisation and kinetics characterisation system for molecular photoswitches

Jacob Lyng Elholm, Paulius Baronas, Paul A. Gueben, Victoria Gneiting, Helen Hölzel and Kasper Moth-Poulsen\*

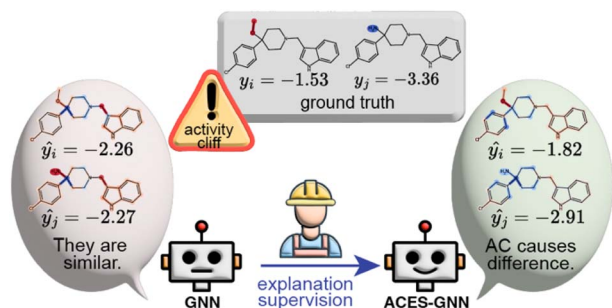
2052



### af2rave: protein ensemble generation with physics-based sampling

Da Teng, Vanessa J. Meraz, Akashnathan Aranganathan, Xinyu Gu and Pratyush Tiwary\*

2062



### ACES-GNN: can graph neural network learn to explain activity cliffs?

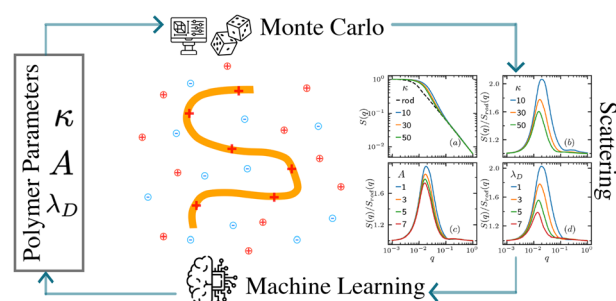
Xu Chen, Dazhou Yu, Liang Zhao and Fang Liu\*



2075

### Machine learning inversion from small-angle scattering for charged polymers

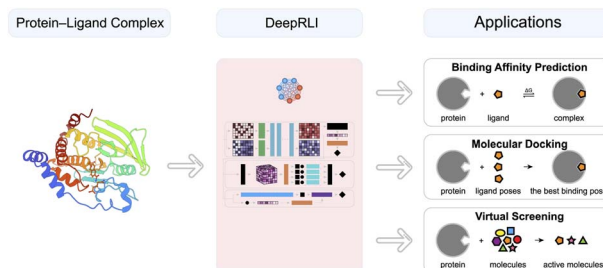
Lijie Ding, Chi-Huan Tung, Jan-Michael Y. Carrillo, Wei-Ren Chen and Changwoo Do\*



2083

### DeepRLI: a multi-objective framework for universal protein–ligand interaction prediction

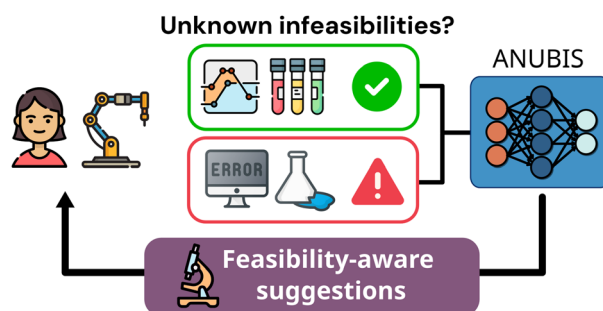
Haoyu Lin, Jintao Zhu, Shiwei Wang, Yibo Li, Jianfeng Pei\* and Luhua Lai\*



2104

### Anubis: Bayesian optimization with unknown feasibility constraints for scientific experimentation

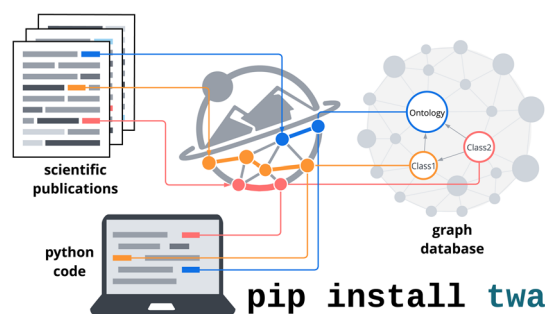
Riley J. Hickman,\* Gary Tom, Yunheng Zou, Matteo Aldeghi and Alán Aspuru-Guzik\*



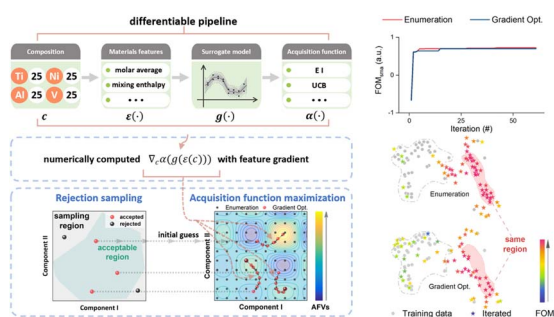
2123

### twa: The World Avatar Python package for dynamic knowledge graphs and its application in reticular chemistry

Jiaru Bai, Simon D. Rihm, Aleksandar Kondinski, Fabio Saluz, Xinhong Deng, George Brownbridge, Sebastian Mosbach, Jethro Akroyd and Markus Kraft\*



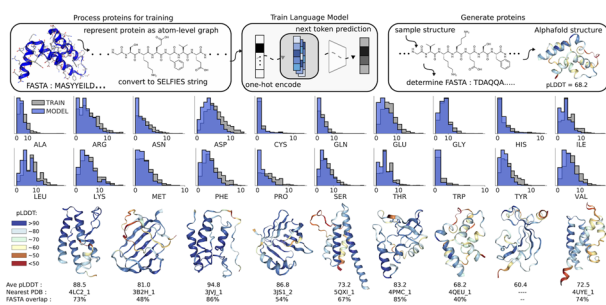
2136



## Leveraging feature gradient for efficient acquisition function maximization in material composition design

Yuehui Xian, Yunfan Wang, Pengfei Dang, Xinquan Wan, Yumei Zhou,\* Xiangdong Ding,\* Jun Sun and Dezhen Xue\*

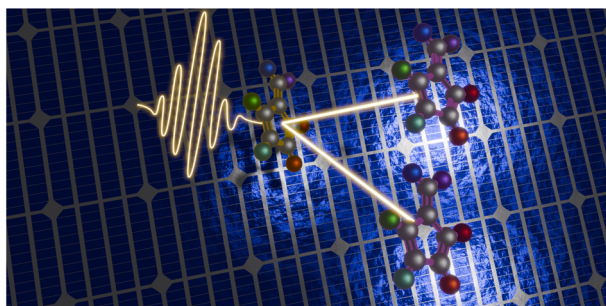
2150



## Chemical language models can generate biomolecules atom-by-atom

Kevin Zhu, Daniel Flam-Shepherd and Alán Aspuru-Guzik\*

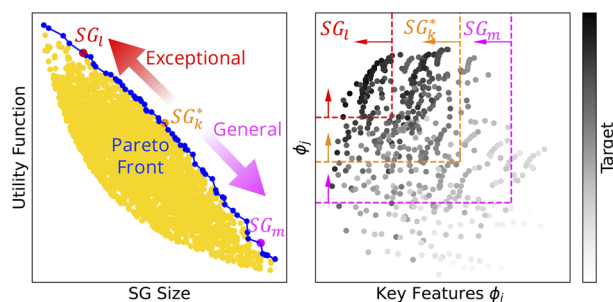
2156



## Pursuit of singlet fission fulvene candidates using inverse design

Irene Casademont-Reig,\* Roger Monreal-Corona, Eline Desmedt, Freija De Vleeschouwer\* and Mercedes Alonso\*

2175



## Coherent collections of rules describing exceptional materials identified with a multi-objective optimization of subgroups

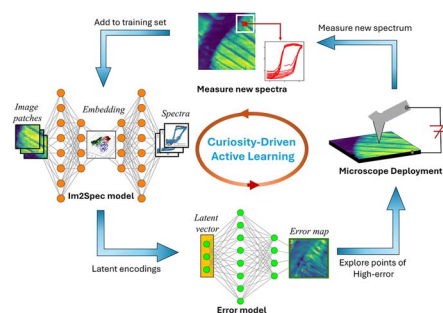
Lucas Foppa\* and Matthias Scheffler



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## Curiosity driven exploration to optimize structure–property learning in microscopy

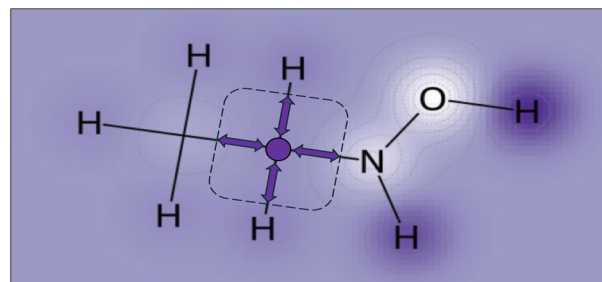
Aditya Vatsavai, Ganesh Narasimha, Yongtao Liu, Jawad Chowdhury, Jan-Chi Yang, Hiroshi Funakubo, Maxim Ziatdinov and Rama Vasudevan\*



2198

## PIL-Net: a physics-informed graph convolutional network for predicting atomic multipoles

Caitlin Whitter,\* Alex Pothen and Aurora Clark

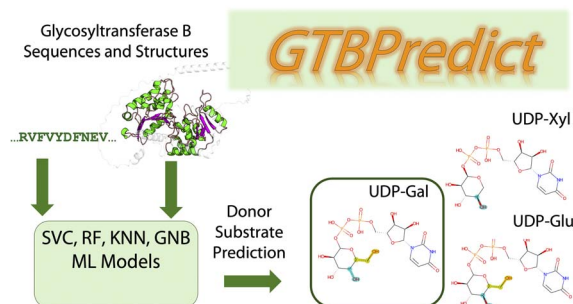


Depiction of the atomic charge distribution of  $C_2H_5NO$  with a graph convolution around a Carbon atom.

2214

## Decoding substrate specificity determining factors in glycosyltransferase-B enzymes – insights from machine learning models

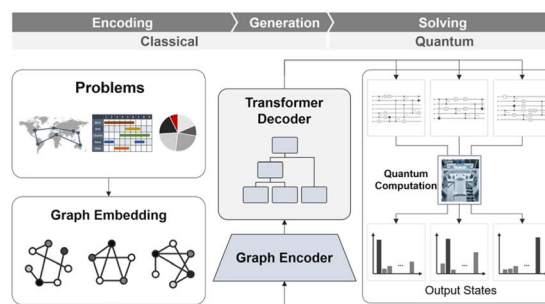
Samantha G. Hennen, Yannick J. Bomble, Breanna R. Urbanowicz and Vivek S. Bharadwaj\*



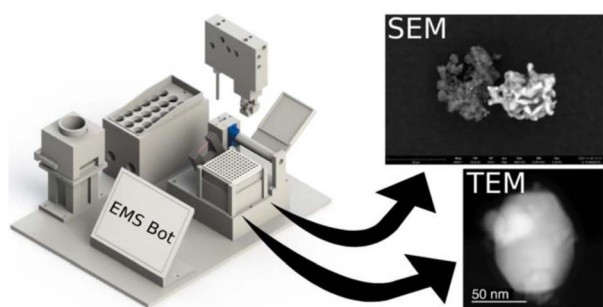
2229

## Generative quantum combinatorial optimization by means of a novel conditional generative quantum eigensolver

Shunya Minami,\* Kouhei Nakaji, Yohichi Suzuki, Alán Aspuru-Guzik and Tadashi Kadowaki



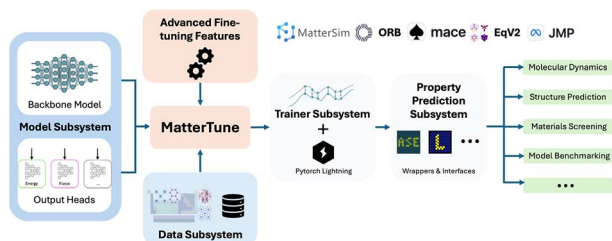
2244



### Automated electron microscopy sample preparation system

David Milsted, Tara P. Mishra, Lauren N. Walters, Yuxing Fei, Bernardus Rendy, Pragnay Nevatia, Haegyeom Kim and Gerbrand Ceder\*

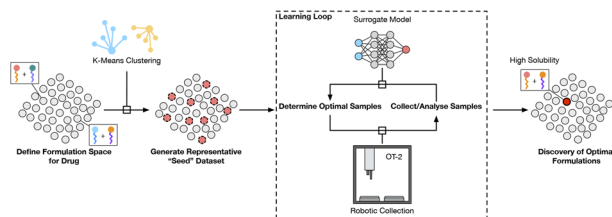
2253



### MatterTune: an integrated, user-friendly platform for fine-tuning atomistic foundation models to accelerate materials simulation and discovery

Lingyu Kong, Nima Shoghi, Guoxiang Hu, Pan Li and Victor Fung\*

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### Efficient discovery of new medicine formulations using a semi-self-driven robotic formulator

Helena Ros, Youssef Abdalla, Michael T. Cook\* and David Shorthouse\*

