

# Digital Discovery

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## IN THIS ISSUE

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### Cover

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### Inside cover

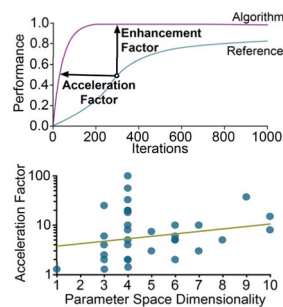
See Connor Forster and Carolin Müller, pp. 98–107. Image reproduced by permission of C. Forster and C. Müller from *Digital Discovery*, 2026, 5, 98.

## REVIEWS

14

### Benchmarking self-driving labs

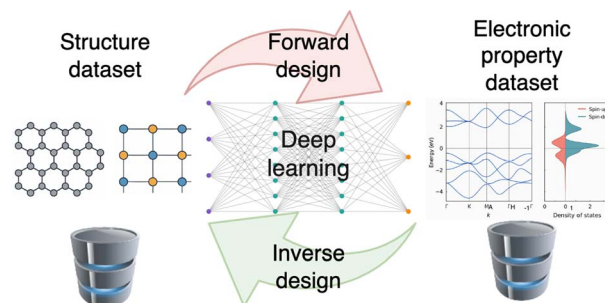
Adedire D. Adesiji, Jiashuo Wang, Cheng-Shu Kuo and Keith A. Brown\*



28

### Deep learning methods for 2D material electronic properties

Artem Mishchenko,\* Anupam Bhattacharya,\* Xiangwen Wang, Henry Kelbrick Pentz, Yihao Wei and Qian Yang



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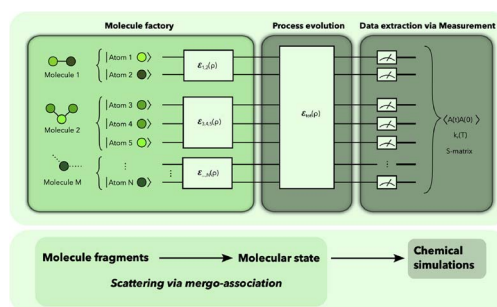


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64

## Chemically motivated simulation problems are efficiently solvable on a quantum computer

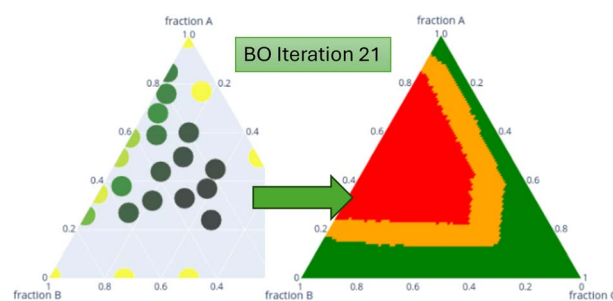
Philipp Schleich,\* Lasse Bjørn Kristensen, Jorge A. Campos-Gonzalez-Angulo, Abdulrahman Aldossary, Davide Avagliano, Mohsen Bagherimehrab, Christoph Gorgulla, Joe Fitzsimons and Alán Aspuru-Guzik



88

## Efficient simulation of complex fluid phase diagrams with Bayesian optimization

Steven G. Arturo, Clyde Fare, Kaoru Aou, Dan Dermody, Will Edsall, Jillian Emerson, Kathryn Grzesiak, Arjita Kulshreshtha, Paul Mwasame, Edward O. Pyzer-Knapp and Jed Pitera\*



93

## Commit: Digital pipette: open hardware for liquid transfer in self-driving laboratories

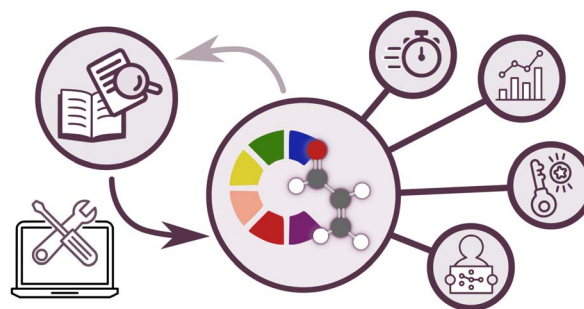
Naruki Yoshikawa,\* Kevin Angers, Kourosh Darvish, Sargol Okhovatian, Dawn Bannerman, Ilya Yakavets, Milica Radisic\* and Alán Aspuru-Guzik\*



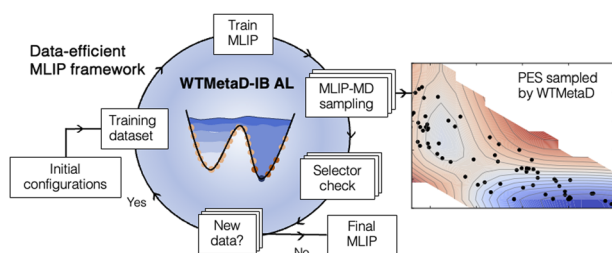
98

## From handbooks to high-throughput: rule-based prediction of electronic absorption maxima from SMILES with ChromoPredict

Connor Forster and Carolin Müller\*



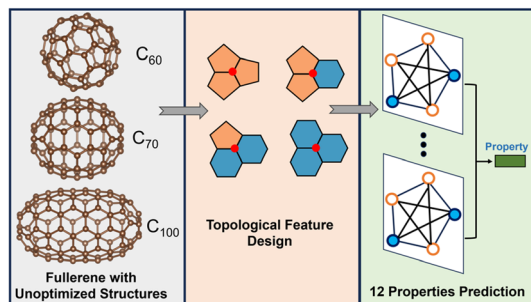
108



### Active learning meets metadynamics: automated workflow for reactive machine learning interatomic potentials

Valdas Vitartas, Hanwen Zhang, Veronika Juraskova, Tristan Johnston-Wood and Fernanda Duarte\*

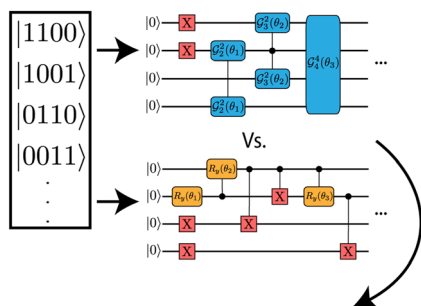
123



### Extrapolating beyond C<sub>60</sub>: advancing prediction of fullerene isomers with FullereneNet

Bin Liu, Jirui Jin and Mingjie Liu\*

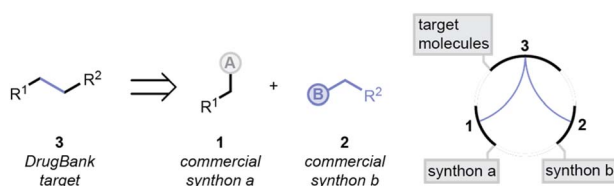
134



### Quantum state preparation of multiconfigurational states for quantum chemistry

Gabriel Greene-Diniz,\* Georgia Prokopiou, David Zsolt Manrique and David Muñoz Ramo

153



### One step retrosynthesis of drugs from commercially available chemical building blocks and conceivable coupling reactions

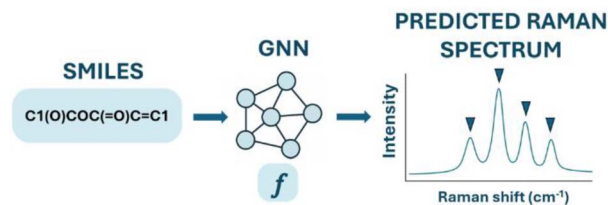
Babak Mahjour, Felix Katzenburg, Emil Lammi and Tim Cernak\*



161

### Mol2Raman: a graph neural network model for predicting Raman spectra from SMILES representations

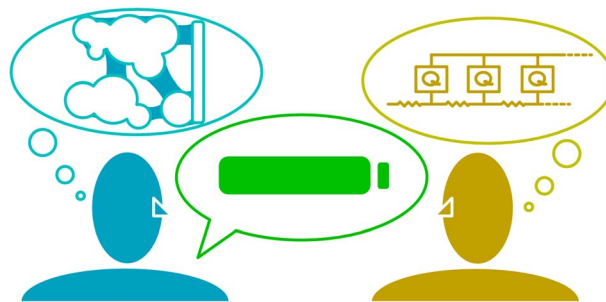
Salvatore Sorrentino,\* Alessandro Gussoni, Francesco Calcagno, Gioele Pasotti, Davide Avagliano, Ivan Rivalta, Marco Garavelli and Dario Polli\*



177

### Workflows and principles for collaboration and communication in battery research

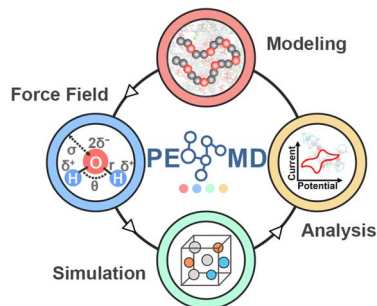
Yannick Kuhn, Bhawna Rana, Micha Philipp, Christina Schmitt, Roberto Scipioni, Eibar Flores, Dennis Kopljar, Simon Clark, Arnulf Latz and Birger Horstmann\*



193

### PEMD: a high-throughput simulation and analysis framework for solid polymer electrolytes

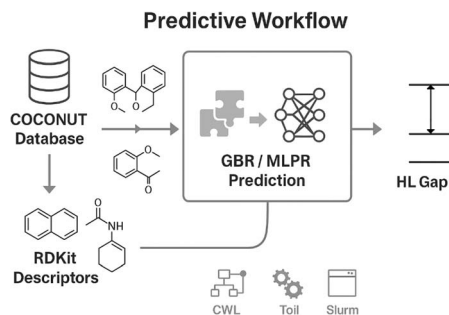
Shendong Tan, Bochun Liang, Dexin Lu, Chaoyuan Ji, Wenke Ji, Zihui Li and Tingzheng Hou\*



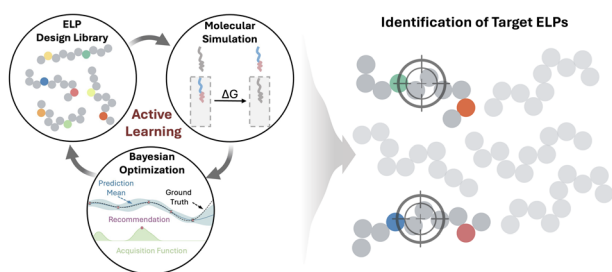
203

### High throughput tight binding calculation of electronic HOMO–LUMO gaps and its prediction for natural compounds

Sascha Thinius



214



### Computational design of polypeptide-based compartments for synthetic cells

Jianming Mao, Yongkang Xi, Armin Shayesteh Zadeh, Allen P. Liu and Andrew L. Ferguson\*

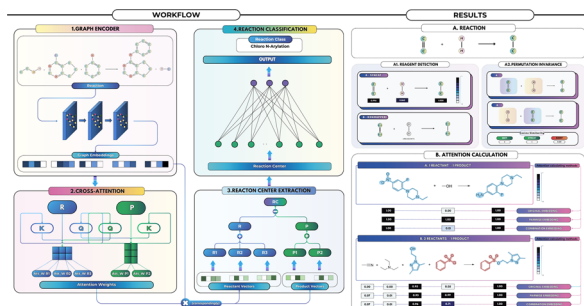
231



### An automated evaluation agent for Q&A pairs and reticular synthesis conditions

Nakul Rampal, Dongrong Joe Fu, Chengbin Zhao, Hanan S. Murayshid, Albatool A. Abaalkhail, Nahla E. Alhazmi, Majed O. Alawad, Christian Borgs,\* Jennifer T. Chayes\* and Omar M. Yaghi\*

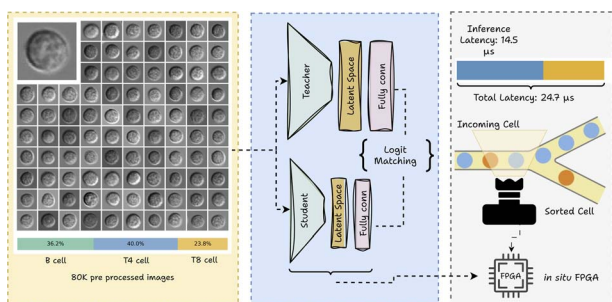
241



### SynCat: molecule-level attention graph neural network for precise reaction classification

Phuoc-Chung Van Nguyen, Van-Thinh To, Ngoc-Vi Nguyen Tran, Tieu-Long Phan,\* Tuyen Ngoc Truong, Thomas Gärtner, Daniel Merkle and Peter F. Stadler

254



### Real-time cell sorting with scalable *in situ* FPGA-accelerated deep learning

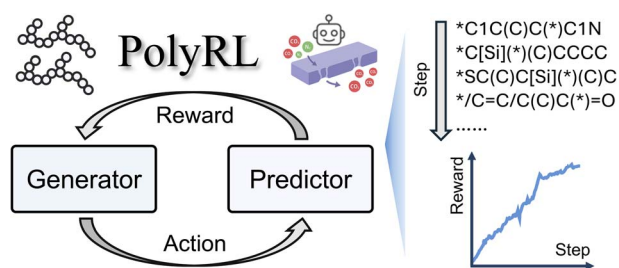
Khayrul Islam, Ryan F. Forelli, Jianzhong Han, Deven Bhadane, Jian Huang, Joshua C. Agar, Nhan Tran, Seda Ogrenci and Yaling Liu\*



266

### PolyRL: reinforcement learning-guided polymer generation for multi-objective polymer discovery

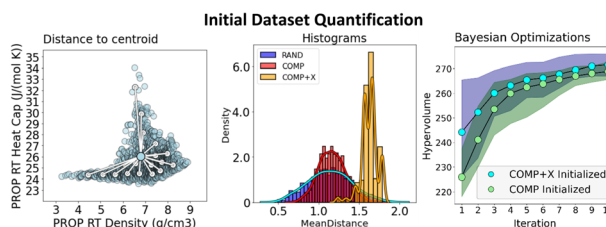
Wentao Li, Yijun Li, Qi Lei, Zemeng Wang and Xiaonan Wang\*



277

### Leveraging domain knowledge for optimal initialization in Bayesian materials optimization

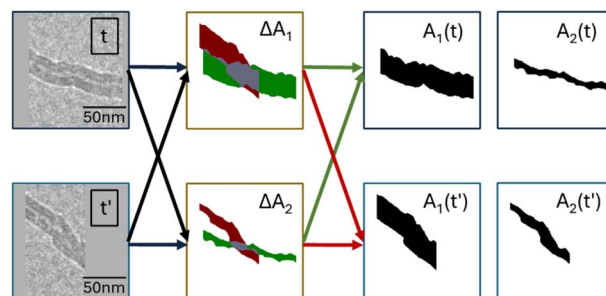
Trevor Hastings,\* James Paramore, Brady Butler and Raymundo Arróyave



290

### MultiTaskDeltaNet: change detection-based image segmentation for *operando* ETEM with application to carbon gasification kinetics

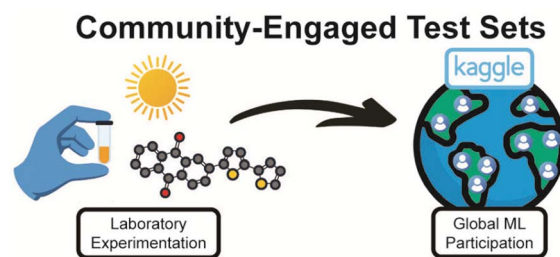
Yushuo Niu, Tianyu Li, Yuanyuan Zhu and Qian Yang\*



304

### Democratizing machine learning in chemistry with community-engaged test sets

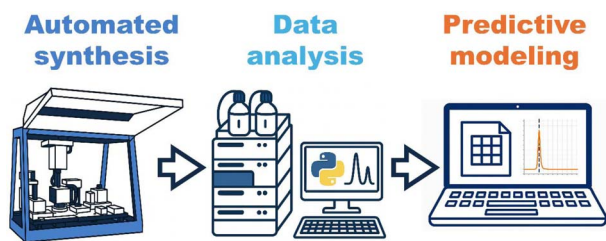
Jason L. Wu, David M. Friday, Changyun Hwang, Seungjoo Yi, Tiara C. Torres-Flores, Martin D. Burke, Ying Diao, Charles M. Schroeder and Nicholas E. Jackson\*



Democratizing Chemical Discovery



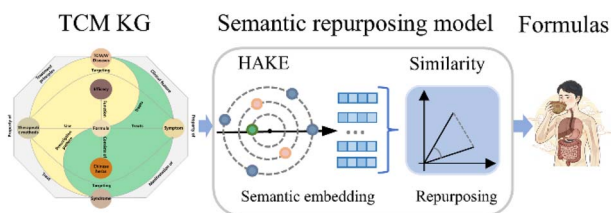
310



### Automated synthesis and fragment descriptor-based machine learning for retention time prediction in supercritical fluid chromatography

Sitanan Sartyoungkul, Balasubramaniyan Sakthivel, Pavel Sidorov\* and Yuuya Nagata\*

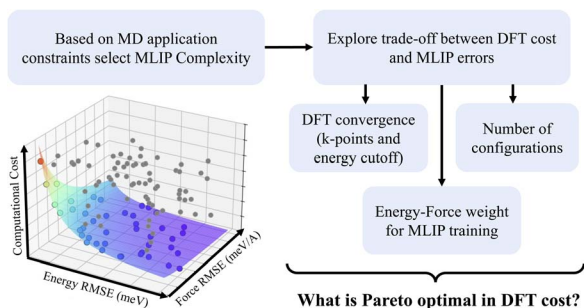
317



### Semantic repurposing model for traditional Chinese ancient formulas based on a knowledge graph

Xu Dong, Wenyan Zhao, Feifei Li, LiHong Hu,\* Hongzhi Li and Guangzhe Li\*

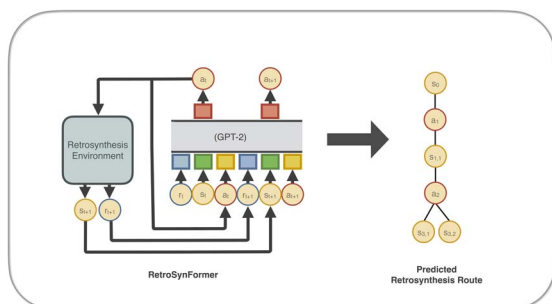
332



### Application-specific machine-learned interatomic potentials: exploring the trade-off between DFT convergence, MLIP expressivity, and computational cost

Ilgar Baghishov,\* Jan Janssen, Graeme Henkelman and Danny Perez\*

348



### RetroSynformer: planning multi-step chemical synthesis routes via a decision transformer

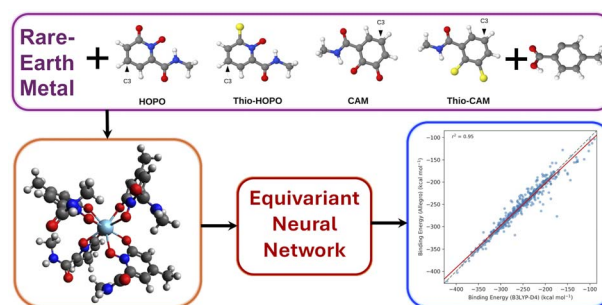
Emma Granqvist, Rocío Mercado and Samuel Genheden



363

### Toward accelerating rare-earth metal extraction using equivariant neural networks

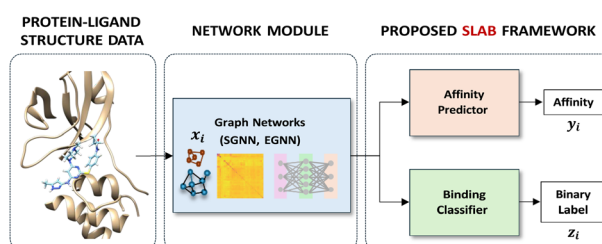
Ankur K. Gupta,\* Caitlin V. Hetherington and Wibe A. de Jong\*



375

### SLAB: simultaneous labeling and binding affinity prediction for protein–ligand structures

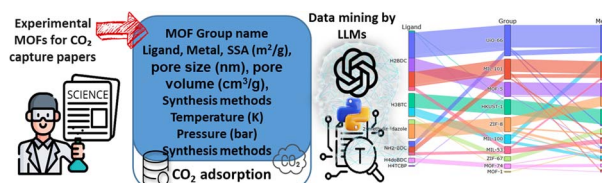
Aditya Ranganath,\* Hyojin Kim, Heesung Shim and Jonathan E. Allen



384

### Toward smart CO<sub>2</sub> capture by the synthesis of metal organic frameworks using large language models

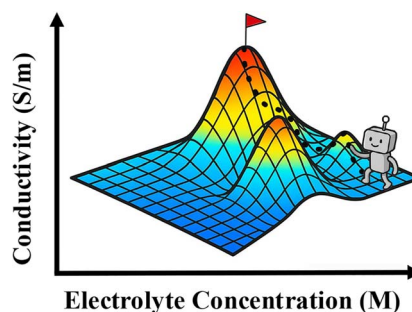
Hossein Mashhadimoslem,\* Mohammad Ali Abdol, Kourosh Zanganeh, Ahmed Shafeen, Encheng Liu, Sohrab Zendejboudi, Ali Elkamel and Aiping Yu\*



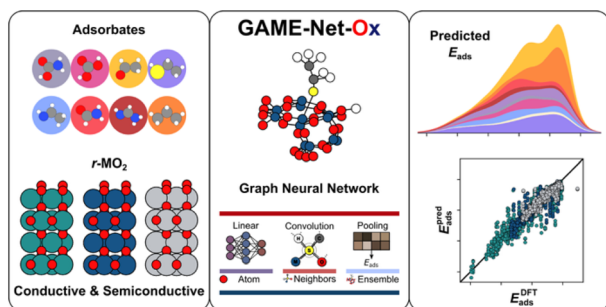
397

### BRINE: a cost-effective electrochemical self-driving laboratory for accelerated discovery of high-performance electrolytes

Mohamadreza Ramezani, Poulomi Nandi, Pablo Antonio De La Fuente-Moreno and Majid Beidaghi\*



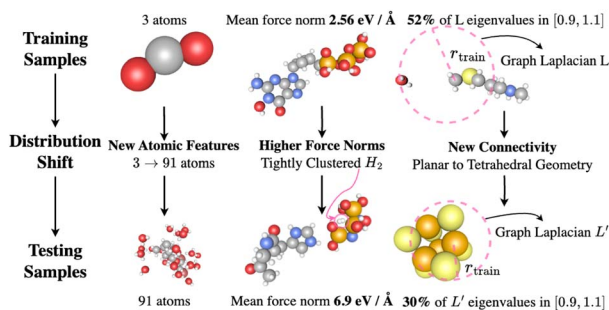
407



### Evaluating the transfer learning from metals to oxides with GAME-Net-Ox

Thomas Van Hout, Oliver Loveday, Jordi Morales-Vidal, Santiago Morandi and Núria López\*

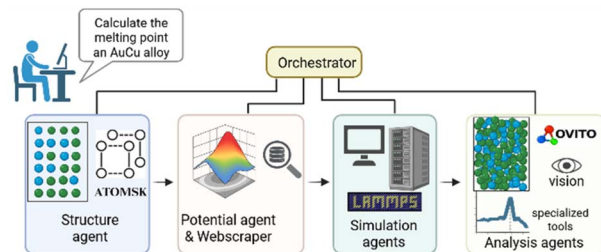
415



### Understanding and mitigating distribution shifts for universal machine learning interatomic potentials

Tobias Kreiman\* and Aditi S. Krishnapriyan

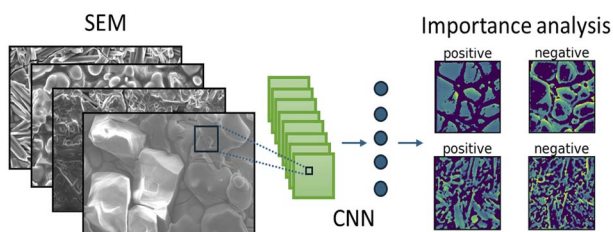
440



### Multi-agentic AI framework for end-to-end atomistic simulations

Aikaterini Vriza,\* Uma Kornu,\* Aditya Koneru, Henry Chan\* and Subramanian K. R. S. Sankaranarayanan\*

453



### Deep learning based SEM image analysis for predicting ionic conductivity in $\text{LiZr}_2(\text{PO}_4)_3$ -based solid electrolytes

Kento Murakami, Yudai Yamaguchi, Yo Kato, Kazuki Ishikawa, Naoto Tanibata, Hayami Takeda,\* Masanobu Nakayama\* and Masayuki Karasuyama



463

**Correction: Advancing mutagenicity predictions in drug discovery with an explainable few-shot deep learning framework**Luis H. M. Torres,<sup>\*</sup> Sofia M. da Silva, Joel P. Arrais, Catarina Pimentel and Bernardete Ribeiro