

# Digital Discovery

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## IN THIS ISSUE

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**Cover**  
See Wenbo Yang, Jinzhe Cao, Shengyang Tao *et al.*, pp. 1958–1966. Image reproduced by permission of Wenbo Yang, Jinzhe Cao, and Shengyang Tao from *Digital Discovery*, 2024, 3, 1958.

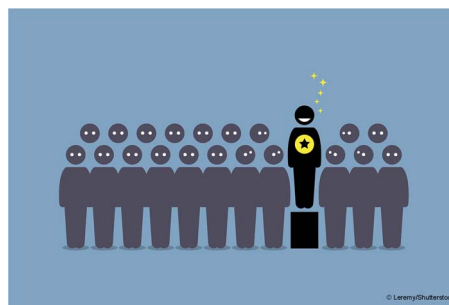


**Inside cover**  
See Stefan Bräse, pp. 1923–1932. Image reproduced by permission of Stefan Bräse and Vincenzo Pani from *Digital Discovery*, 2024, 3, 1923.

## EDITORIAL

1922

Outstanding Reviewers for *Digital Discovery* in 2023

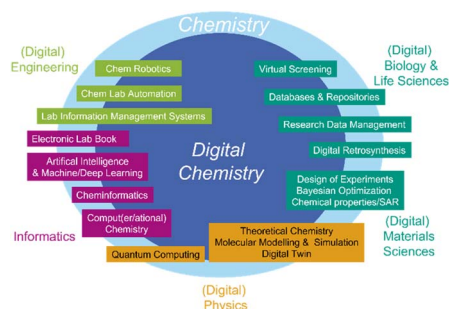


## PERSPECTIVES

1923

**Digital chemistry: navigating the confluence of computation and experimentation – definition, status quo, and future perspective**

Stefan Bräse\*



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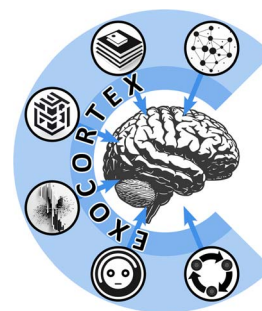
Fundamental questions  
Elemental answers

## PERSPECTIVES

1933

## Towards a science exocortex

Kevin G. Yager\*

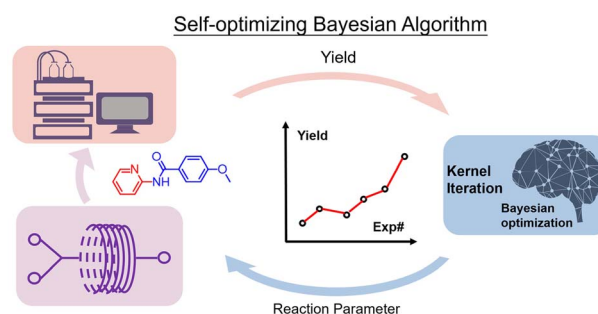


## PAPERS

1958

## Self-optimizing Bayesian for continuous flow synthesis process

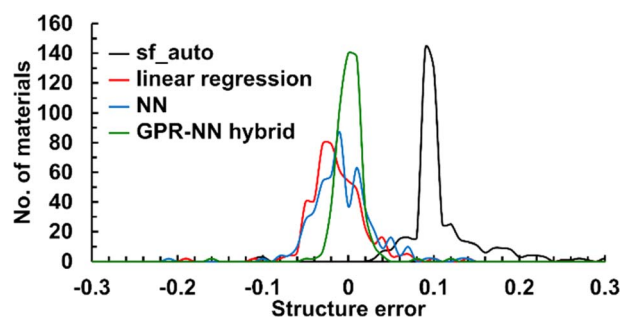
Runzhe Liu, Zihao Wang, Wenbo Yang,\* Jinzhe Cao\* and Shengyang Tao\*



1967

## Machine learning the screening factor in the soft bond valence approach for rapid crystal structure estimation

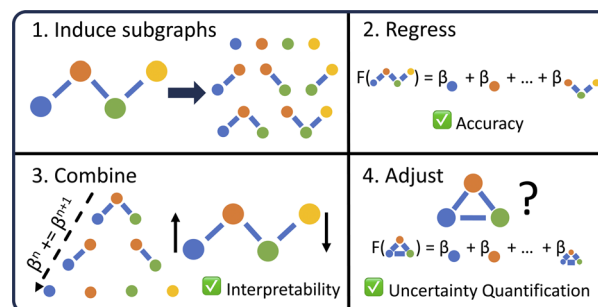
Keisuke Kameda,\* Takaaki Ariga, Kazuma Ito, Manabu Ihara\* and Sergei Manzhos\*



1980

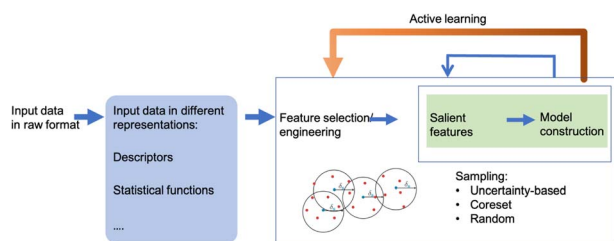
## Linear graphlet models for accurate and interpretable cheminformatics

Michael Tynes,\* Michael G. Taylor, Jan Janssen, Daniel J. Burrill, Danny Perez, Ping Yang\* and Nicholas Lubbers\*



## PAPERS

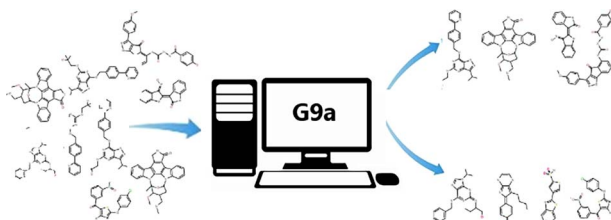
1997



### Active learning for regression of structure–property mapping: the importance of sampling and representation

Hao Liu,<sup>\*</sup> Berkay Yucel, Baskar Ganapathysubramanian, Surya R. Kalidindi, Daniel Wheeler and Olga Wodo

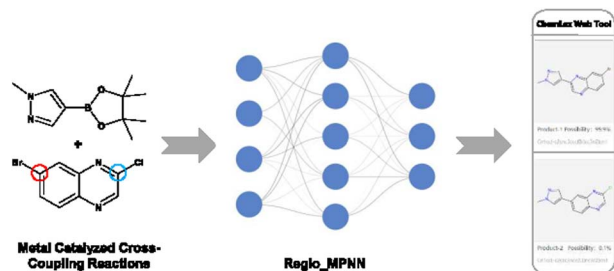
2010



### Application of machine learning for predicting G9a inhibitors

Mariya L. Ivanova,<sup>\*</sup> Nicola Russo, Nadia Djaid and Konstantin Nikolic

2019



### Regio-MPNN: predicting regioselectivity for general metal-catalyzed cross-coupling reactions using a chemical knowledge informed message passing neural network

Baochen Li, Yuru Liu, Haibin Sun, Rentao Zhang, Yongli Xie, Klement Foo, Frankie S. Mak, Ruimao Zhang, Tianshu Yu, Sen Lin, Peng Wang and Xiaoxue Wang<sup>\*</sup>

2032



### Pellet dispensomixer and pellet distributor: open hardware for nanocomposite space exploration via automated material compounding

Miguel Hernández-del-Valle, Jorge Ibarra-Zuazo, Enrique Dios-Lázaro, Javier Rubio, Joris Audoux and Maciej Haranczyk<sup>\*</sup>



2041

### Automated processing of chromatograms: a comprehensive python package with a GUI for intelligent peak identification and deconvolution in chemical reaction analysis

Jan Obořil, Christian P. Haas, Maximilian Lübbsmeyer, Rachel Nicholls, Thorsten Gressling, Klavs F. Jensen,\* Giulio Volpin\* and Julius Hillenbrand\*



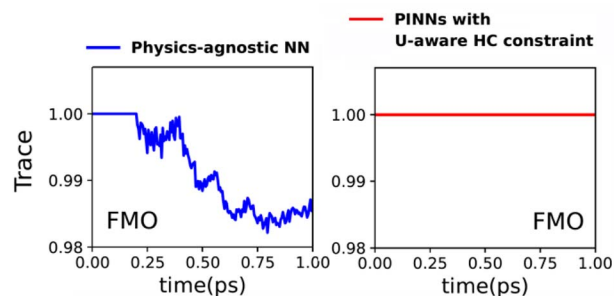
#### Automated Processing and Analysis of HPLC Chromatograms

- ✓ open-source
- ✓ intelligent peak picking
- ✓ web-based GUI
- ✓ peak purity check
- ✓ baseline correction
- ✓ peak deconvolution

2052

### Physics-informed neural networks and beyond: enforcing physical constraints in quantum dissipative dynamics

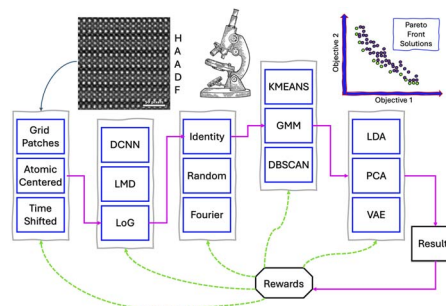
Arif Ullah,\* Yu Huang, Ming Yang and Pavlo O. Drat\*



2061

### Physics-based reward driven image analysis in microscopy

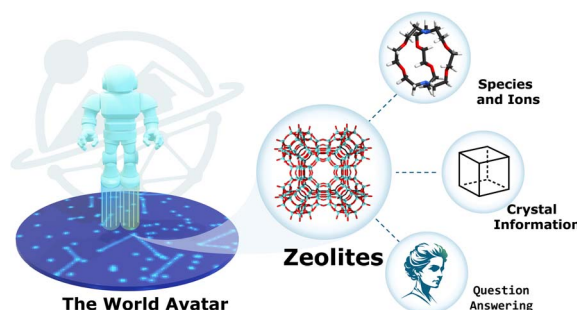
K. Barakati,\* Hui Yuan, Amit Goyal and S. V. Kalinin\*



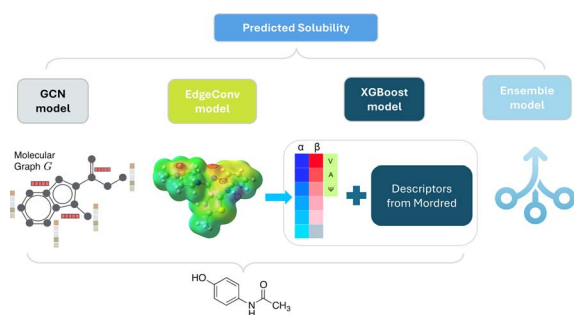
2070

### Knowledge graph representation of zeolitic crystalline materials

Aleksandar Kondinski, Pavlo Rutkevych, Laura Pascazio, Dan N. Tran, Feroz Farazi, Srishti Ganguly and Markus Kraft\*



2085



## A machine learning approach for the prediction of aqueous solubility of pharmaceuticals: a comparative model and dataset analysis

Mohammad Amin Ghanavati, Soroush Ahmadi and Sohrab Rohani\*

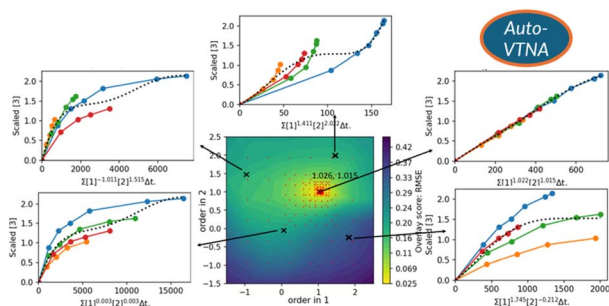
2105



## Extracting recalcitrant redox data on fluorophores to pair with optical data for predicting small-molecule, ionic isolation lattices

Michaela K. Loveless, Minwei Che, Alec J. Sanchez, Vikrant Tripathy, Bo W. Laursen, Sudhakar Pamidighantam, Krishnan Raghavachari and Amar H. Flood\*

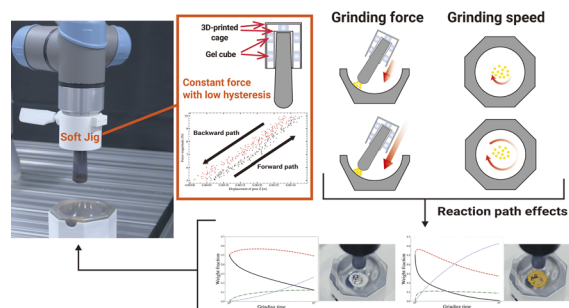
2118



## Auto-VTNA: an automatic VTNA platform for determination of global rate laws

Daniel Dalland, Linden Schrecker\* and King Kuok (Mimi) Hii

2130



## Force-controlled robotic mechanochemical synthesis

Yusaku Nakajima, Kai Kawasaki, Yasuo Takeichi, Masashi Hamaya, Yoshitaka Ushiku and Kanta Ono\*



2137

## Exploring inhomogeneous surfaces: Ti-rich SrTiO<sub>3</sub>(110) reconstructions *via* active learning

Ralf Wanzenböck, Esther Heid, Michele Riva, Giada Franceschi, Alexander M. Imre, Jesús Carrete, Ulrike Diebold and Georg K. H. Madsen\*

