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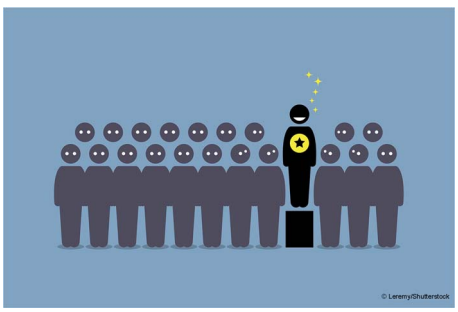
**Cover**
See Wenbo Yang, Jinzhe Cao, Shengyang Tao *et al.*, pp. 1958–1966. Image reproduced by permission of Wenbo Yang, Jinzhe Cao, and Shengyang Tao from *Digital Discovery*, 2024, **3**, 1958.


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

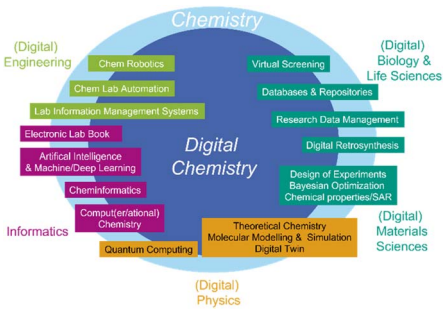
## EDITORIAL





## PERSPECTIVES





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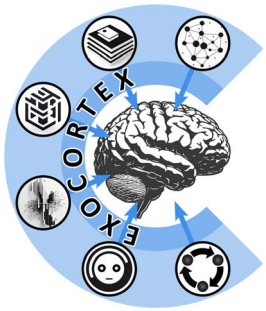
## PERSPECTIVES



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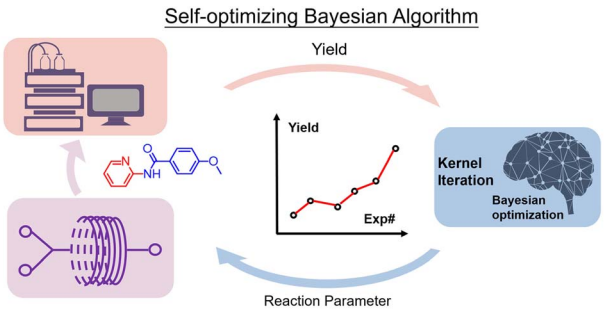




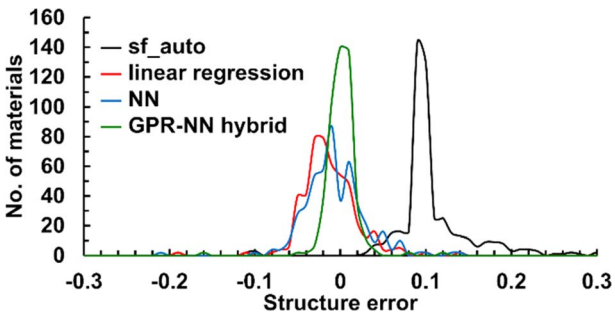




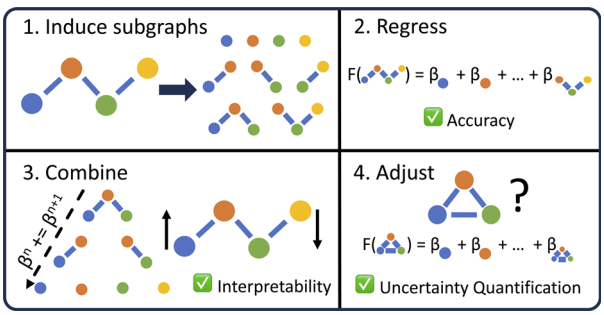

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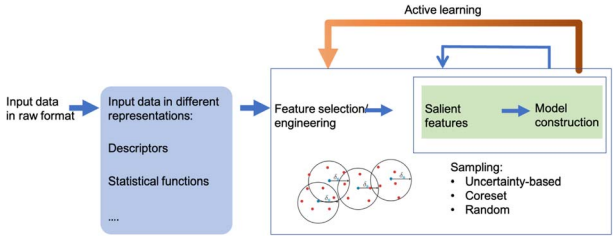
1997




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

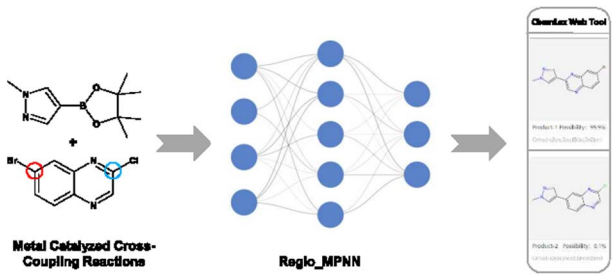
Hao Liu,* Berkay Yucel, Baskar Ganapathysubramanian, Surya R. Kalidindi, Daniel Wheeler and Olga Wodo

2010


## Application of machine learning for predicting G9a inhibitors

Mariya L. Ivanova,* 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*

2032

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

Miguel Hernández-del-Valle, Jorge Ilarraza-Zuazo, Enrique Dios-Lázaro, Javier Rubio, Joris Audoux and Maciej Haranczyk*

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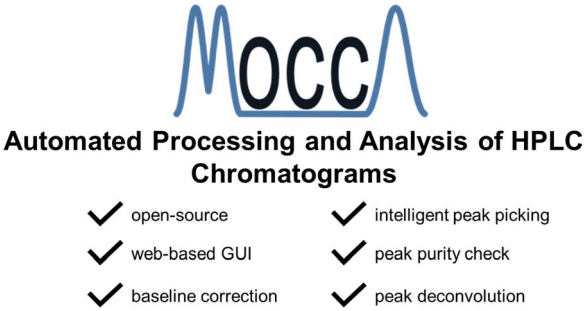




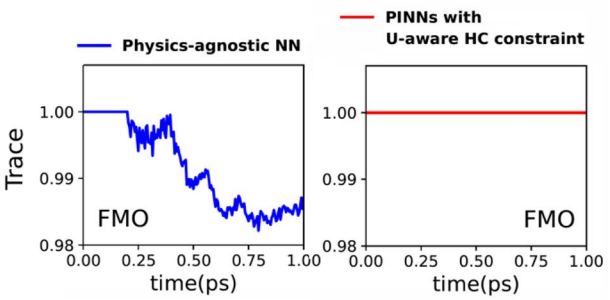




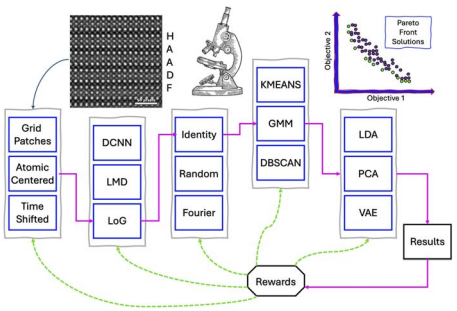




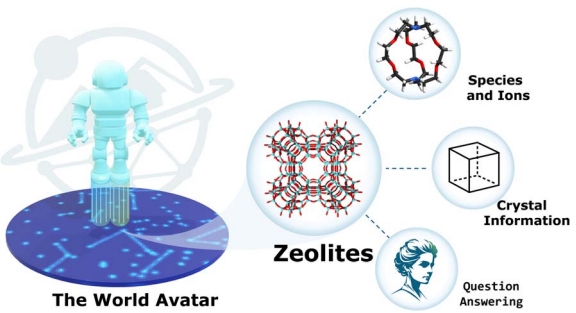

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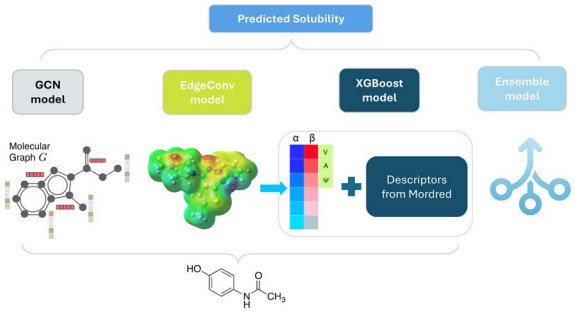
2085




## 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*

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## 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*

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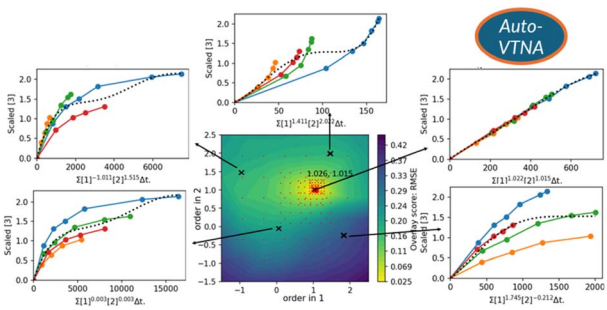


## Auto-VTNA: an automatic VTNA platform for determination of global rate laws

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

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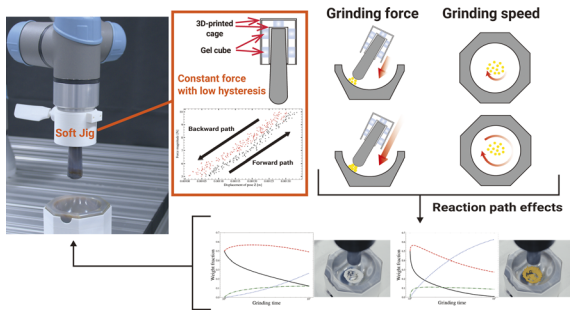


## Force-controlled robotic mechanochemical synthesis

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

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# Exploring inhomogeneous surfaces: Ti-rich $SrTiO_3$(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*