

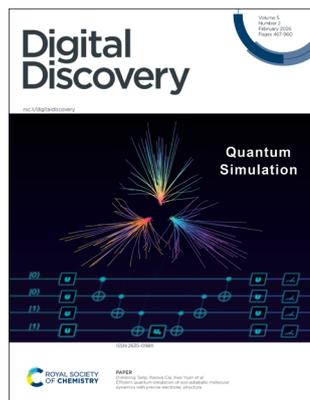
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IN THIS ISSUE

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Cover
See Diandong Tang, Xiaoxia Cai, Xiao Yuan *et al.*, pp. 548–570. Image reproduced by permission of Tianyi Li from *Digital Discovery*, 2026, 5, 548.



Inside cover
See Wei Zhou, Xiao Wang, Xing Lu *et al.*, pp. 523–547. Image reproduced by permission of Wei Zhou from *Digital Discovery*, 2026, 5, 523.

EDITORIAL

480

Introduction to the “Accelerate Conference 2023–2024” themed collection

Janine George, Claudiane Ouellet-Plamondon and Kristofer Reyes



PERSPECTIVE

482

The PPP model – a minimum viable parametrisation of conjugated chemistry for modern computing applications

Marcel D. Fabian,* Nina Glaser and Gemma C. Solomon



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OPINION

497

Accelerating catalytic advancements through the precision of high-throughput experiments & calculations

Jenny G. Vitillo,* Alán Aspuru-Guzik, Eric Dorskocil, Omar K. Farha, Timur Islamoglu, Heather J. Kulik, Peter M. Margl, Stuart Miller, Jordan Reddel, Aayush R. Singh and Varinia Bernales*



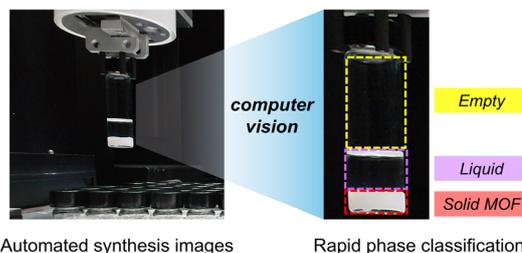
TUTORIAL REVIEW

510

Computer vision for high-throughput materials synthesis: a tutorial for experimentalists

Madeleine A. Gaidimas, Abhijoy Mandal, Pan Chen, Shi Xuan Leong, Gyu-Hee Kim, Akshay Talekar, Kent O. Kirlikovali, Kourosh Darvish, Omar K. Farha,* Varinia Bernales* and Alán Aspuru-Guzik*

Image-based characterization for high-throughput materials discovery

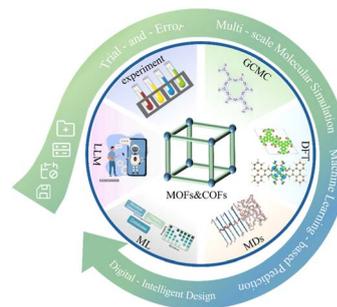


REVIEW

523

Advancing metal organic framework and covalent organic framework design via the digital-intelligent paradigm

Bing Ma, Na Qin, Qianqian Yan, Wei Zhou,* Sheng Zhang, Xiao Wang,* Lipiao Bao and Xing Lu*

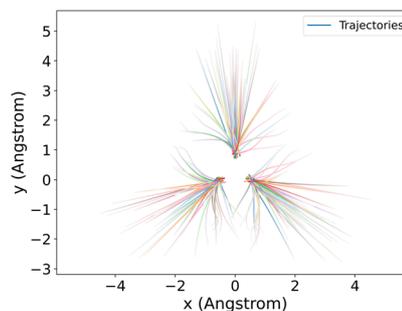


PAPERS

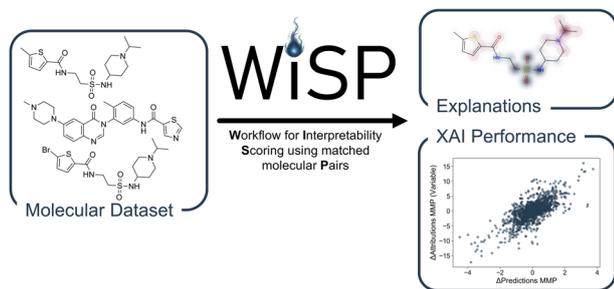
548

Efficient quantum simulation of non-adiabatic molecular dynamics with precise electronic structure

Tianyi Li, Yumeng Zeng, Qiming Ding, Zixuan Huo, Xiaosi Xu, Jiajun Ren, Diandong Tang,* Xiaoxia Cai* and Xiao Yuan*



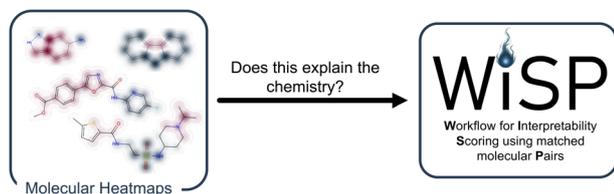
571



When machine learning models learn chemistry I: quantifying explainability with matched molecular pairs

Kerrin Janssen, Jan M. Wollschläger, Jonny Proppe* and Andreas H. Göller*

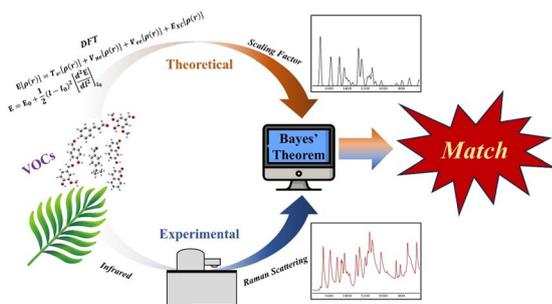
583



When machine learning models learn chemistry II: applying WISP to real-world examples

Kerrin Janssen, Jan M. Wollschläger, Jonny Proppe* and Andreas H. Göller*

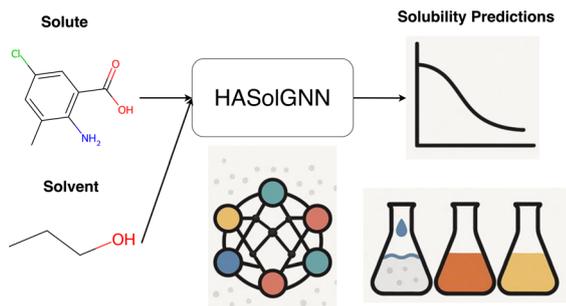
592



DFT meets Bayesian inference: creating a framework for the assignment of calculated vibrational frequencies

Michael Nicolaou, Hans M. Senn, Emma Gibson,* Mario González-Jiménez and Laia Vilà-Nadal*

603



Hierarchical attention graph learning with LLM enhancement for molecular solubility prediction

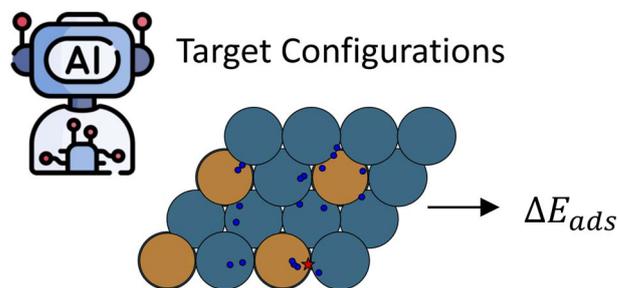
Yangxin Fan, Yinghui Wu, Roger H. French, Danny Perez, Michael G. Taylor and Ping Yang*



617

Adsorb-Agent: autonomous identification of stable adsorption configurations via a large language model agent

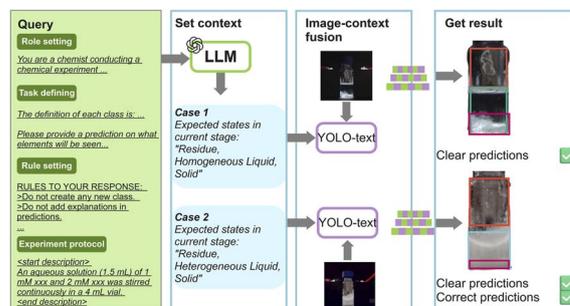
Janghoon Ock, Radheesh Sharma Meda, Tirtha Vinchurkar, Yayati Jadhav and Amir Barati Farimani*



630

Context-aware computer vision for chemical reaction state detection

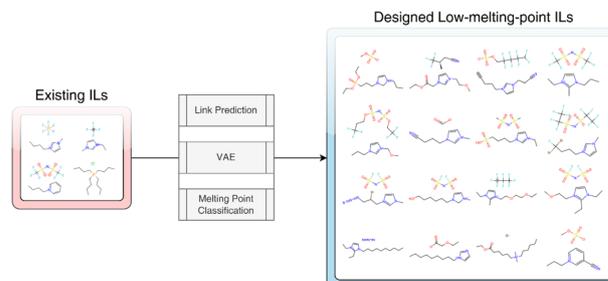
Junru Ren, Abhijoy Mandal, Rama El-khawaldeh, Shi Xuan Leong, Jason Hein, Alán Aspuru-Guzik, Lazaros Nalpantidis and Kourosh Darvish*



643

Deep learning-enabled discovery of low-melting-point ionic liquids

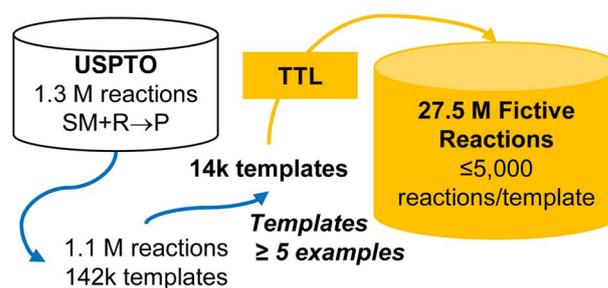
Gaopeng Ren, Austin M. Mroz, Frederik Philippi, Tom Welton and Kim E. Jelfs*



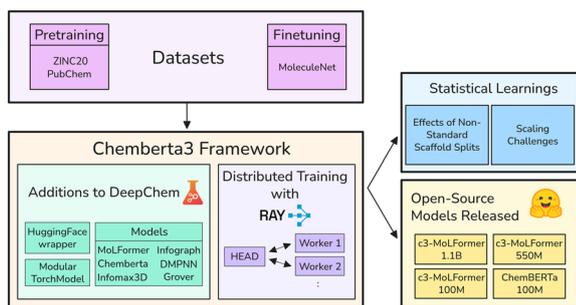
653

Data augmentation in a triple transformer loop retrosynthesis model

Yves Grandjean, David Kreutter and Jean-Louis Reymond*



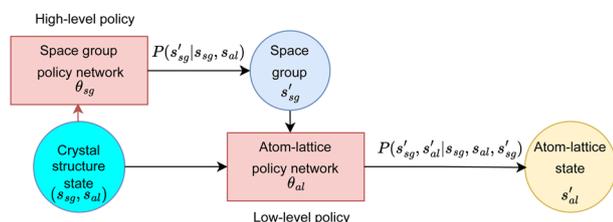
662



ChemBERTa-3: an open source training framework for chemical foundation models

Riya Singh, Aryan Amit Barsainyan, Rida Irfan, Connor Joseph Amorin, Stewart He, Tony Davis, Arun Thiagarajan, Shiva Sankaran, Seyone Chithrananda, Walid Ahmad, Derek Jones, Kevin McLoughlin, Hyojin Kim, Anoushka Bhutani, Shreyas Vinaya Sathyanarayana, Venkat Viswanathan, Jonathan E. Allen and Bharath Ramsundar*

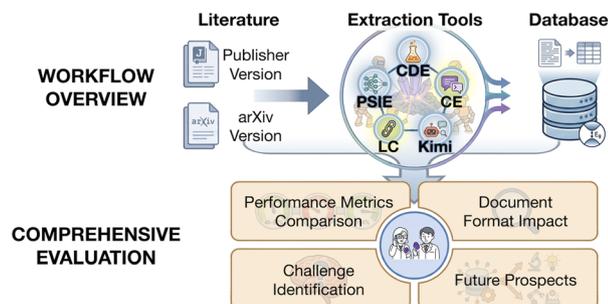
686



Efficient symmetry-aware materials generation via hierarchical generative flow networks

Tri Minh Nguyen,* Sherif Abdulkader Tawfik, Truyen Tran, Sunil Gupta, Santu Rana and Svetha Venkatesh

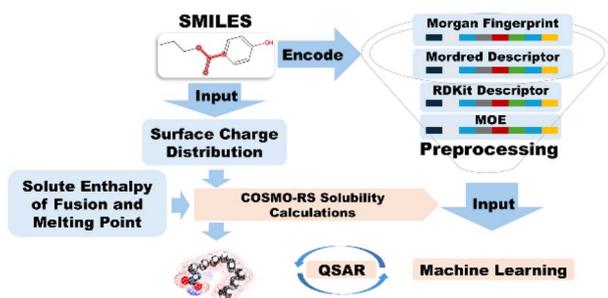
698



Optimizing data extraction from materials science literature: a study of tools using large language models

Wenkai Ning, Musen Li,* Jeffrey R. Reimers* and Rika Kobayashi*

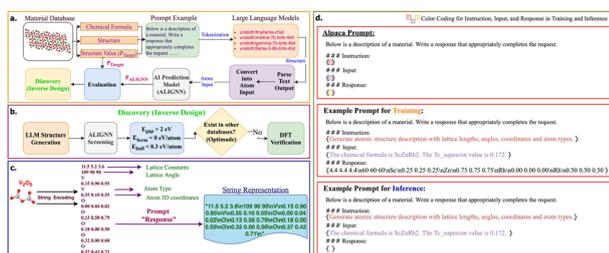
716



A case study on hybrid machine learning and quantum-informed modelling for solubility prediction of drug compounds in organic solvents

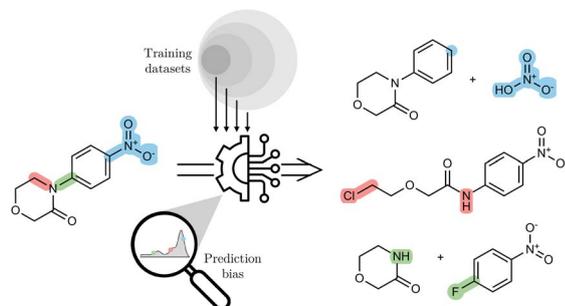
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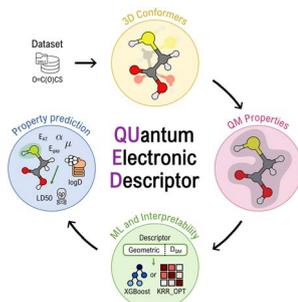
Evaluating large language models for inverse semiconductor design

Muhammed Nur Talha Kilic, Daniel Wines,*
Kamal Choudhary,* Vishu Gupta, Youjia Li,
Sayak Chakrabarty, Wei-Keng Liao, Alok Choudhary
and Ankit Agrawal*



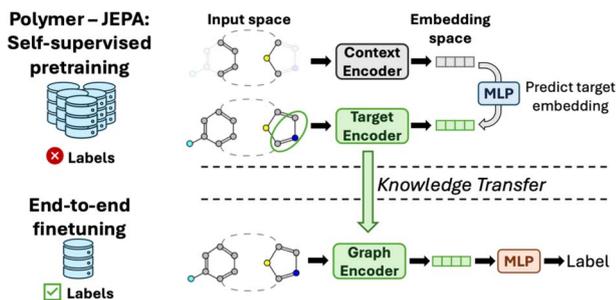
An exploration of dataset bias in single-step retrosynthesis prediction

Sara Tanovic, Ewa Wiczorek and Fernanda Duarte*



Assessing the performance of quantum-mechanical descriptors in physicochemical and biological property prediction

Alejandra Hinojosa Caldas, Artem Kokorin,
Alexandre Tkatchenko* and Leonardo Medrano
Sandona*

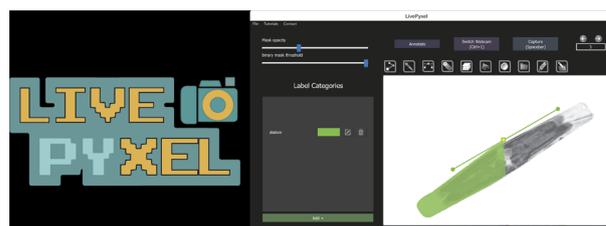


Joint embedding predictive architecture for self-supervised pretraining on polymer molecular graphs

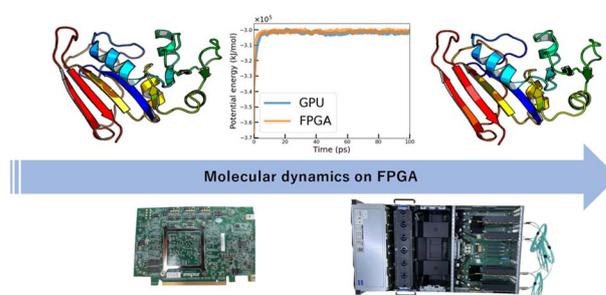
Francesco Piccoli, Gabriel Vogel and Jana M. Weber*



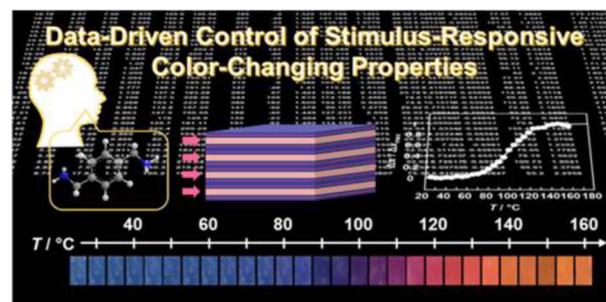
835

LivePyxel: accelerating image annotations with a Python-integrated webcam live streamingUriel Garcilazo-Cruz,^{*} Joseph O. Okeme and Rodrigo A. Vargas-Hernández^{*}

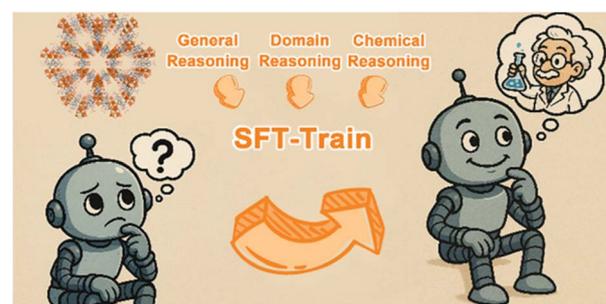
844

Molecular dynamics simulations accelerated on FPGA with high-bandwidth memoryJing Xiao, Jinfeng Chen, Ye Ding, You Xu and Jing Huang^{*}

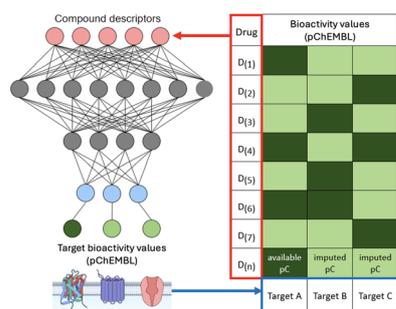
862

A data-driven approach to control stimulus responsivity of functional polymer materials: predicting thermoresponsive color-changing properties of polydiacetyleneRisako Shibata, Nano Shioda, Hiroaki Imai, Yasuhiko Igarashi and Yuya Oaki^{*}

869

MOFReasoner: think like a scientist—a reasoning large language model via knowledge distillationXuefeng Bai, Zhiling Zheng, Xin Zhang,^{*} Hao-Tian Wang, Rui Yang and Jian-Rong Li^{*}

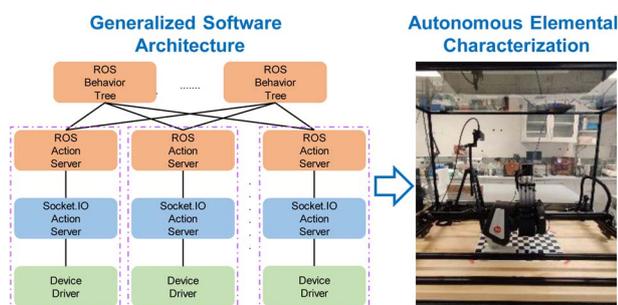
878



A multi-task learning approach for prediction of missing bioactivity values of compounds for the SLC transporter superfamily

Tarik Ćerimagić, Sergey Sosnin and Gerhard F. Ecker*

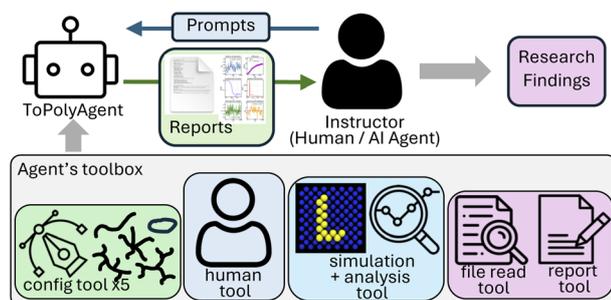
891



Autonomous elemental characterization enabled by a low cost robotic platform built upon a generalized software architecture

Xuan Cao,* Yuxin Wu and Michael L. Whittaker*

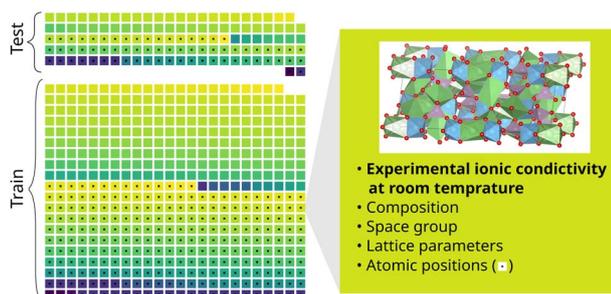
901



ToPolyAgent: AI agents for coarse-grained bead-spring topological polymer simulations

Lijie Ding,* Jan-Michael Carrillo and Changwoo Do*

910



OBELiX: a curated dataset of crystal structures and experimentally measured ionic conductivities for lithium solid-state electrolytes

Félix Therrien,* Jamal Abou Haibeh, Divya Sharma, Rhiannon Hendley, Leah Wairimu Mungai, Sun Sun, Alain Tchagang, Jiang Su, Samuel Huberman, Yoshua Bengio, Hongyu Guo,* Alex Hernández-García* and Homin Shin*

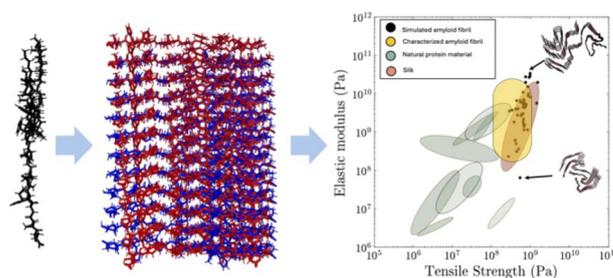


PAPERS

919

FiberForge: enabling high-throughput simulations of the mechanical properties of helical fibrils

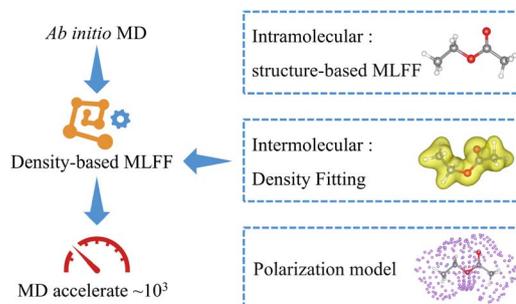
Kieran Nehil-Puleo and Zhongyue John Yang*



931

DBMLFF: linear scaling machine learning force fields via electron density decomposition for molecular electrolytes

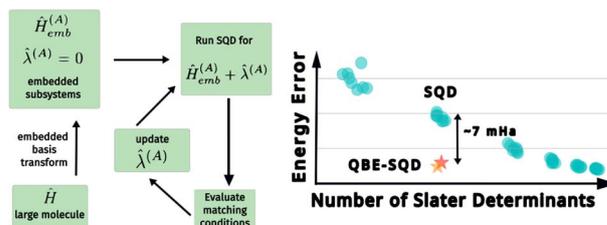
Jie Shen, Chenyu Wang, Libin Chen, Shaoqin Jiang,* Jianhui Chen, Cuilian Wen, Bo Wu, Baisheng Sa* and Lin-Wang Wang*



945

Towards utility-scale electronic structure with sample-based quantum bootstrap embedding

Joel Bierman and Yuan Liu*



CORRECTION

957

Correction: A case study on hybrid machine learning and quantum-informed modelling for solubility prediction of drug compounds in organic solvents

Weiling Wang, Isabel Cooley, Morgan R. Alexander, Ricky D. Wildman, Anna K. Croft and Blair F. Johnston*

