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Cover
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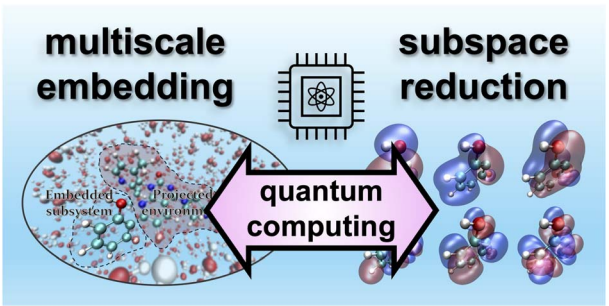
Inside cover
See Ge Lei and Samuel J. Cooper, pp. 3455–3465. Image reproduced by permission of Ge Lei and Samuel J. Cooper from *Digital Discovery*, 2025, **4**, 3455. Image created with the use of Google Gemini and Adobe Photoshop Generative Fill.

PERSPECTIVE



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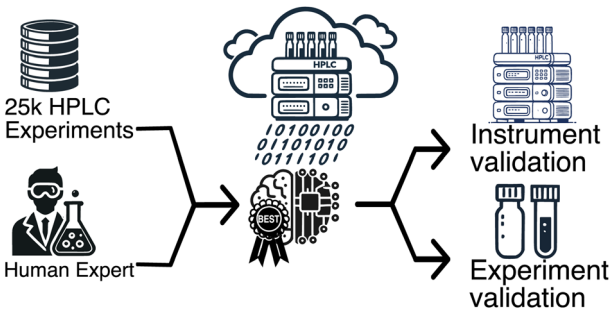

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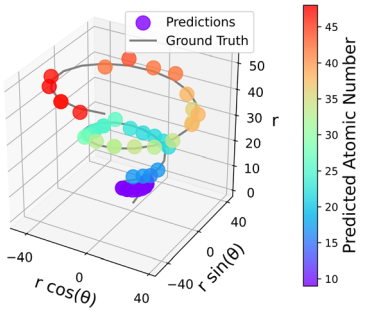

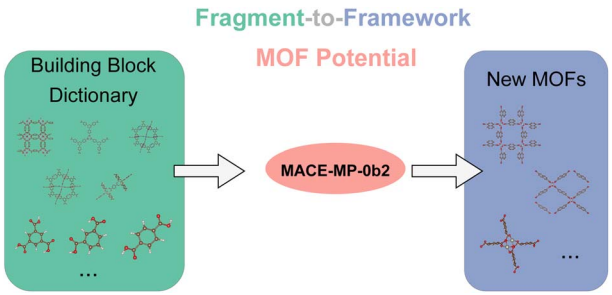

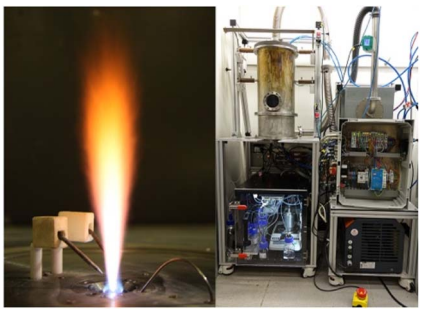

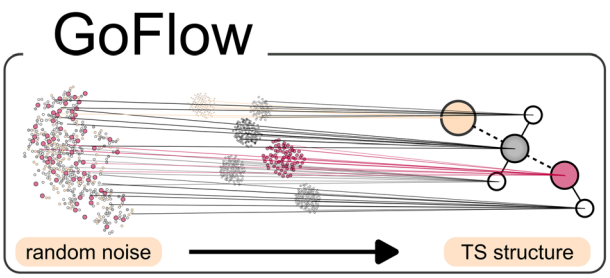

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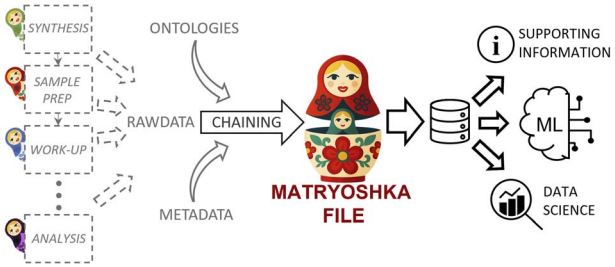

A FAIR research data infrastructure for high-throughput digital chemistry

Alice Gauthier, Laure Vancauwenberghe, Jean-Charles Cousty,* Cyril Matthey-Doret, Robin Franken, Sabine Maennel, Pascal Miéville and Oksana Riba Grognuz

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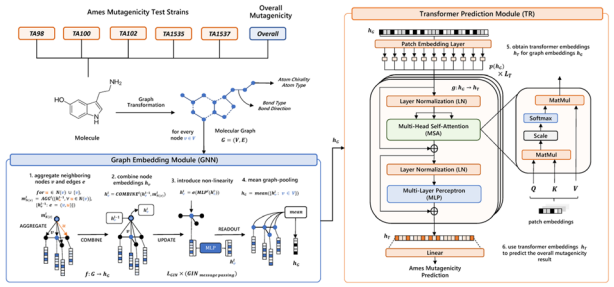

Advancing mutagenicity predictions in drug discovery with an explainable few-shot deep learning framework

Luis H. M. Torres,* Sofia M. da Silva, Joel P. Arrais, Catarina Pimentel and Bernardete Ribeiro

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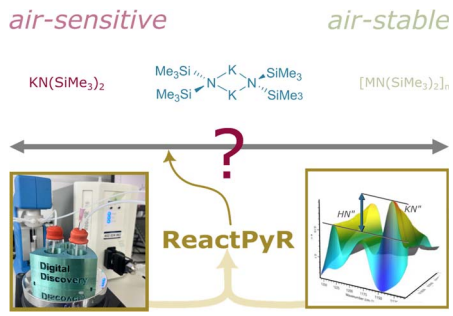

ReactPyR: a python workflow for ReactIR allows for quantification of the stability of sensitive compounds in air

Nicola L. Bell,* Emanuele Berardi, Marina Gladkikh, Richard Drummond Turnbull and Freya Turton

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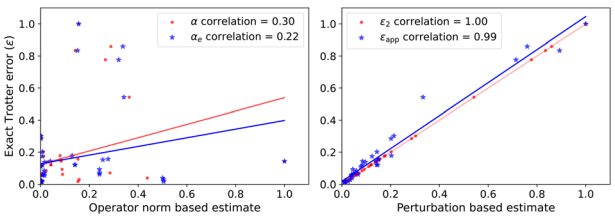

Estimating Trotter approximation errors to optimize Hamiltonian partitioning for lower eigenvalue errors

Shashank G. Mehendale, Luis A. Martínez-Martínez, Prathami Divakar Kamath and Artur F. Izmaylov*

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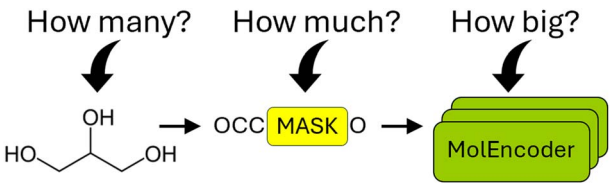

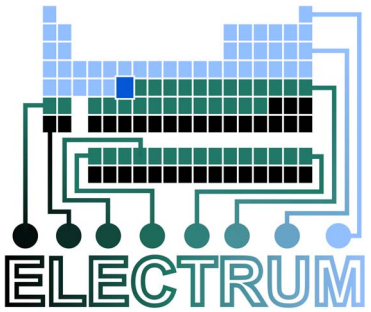

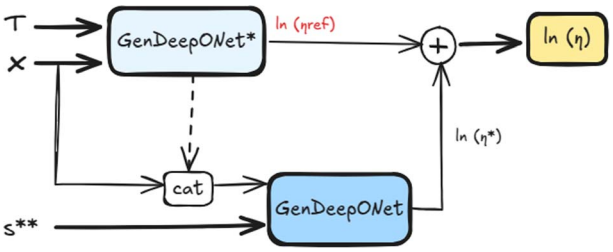

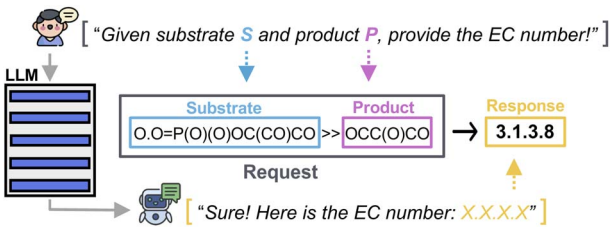

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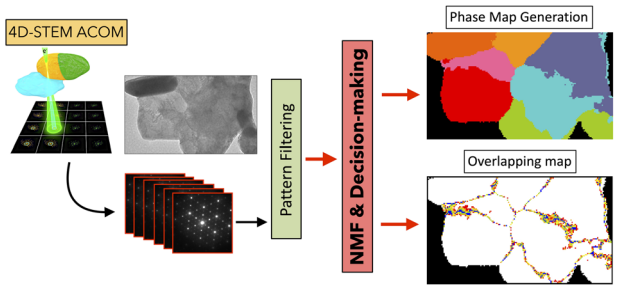

Unsupervised multi-clustering and decision-making strategies for 4D-STEM orientation mapping

Junhao Cao, Nicolas Folastre, Gozde Oney, Edgar Rauch, Stavros Nicolopoulos, Partha Pratim Das and Arnaud Demortière*

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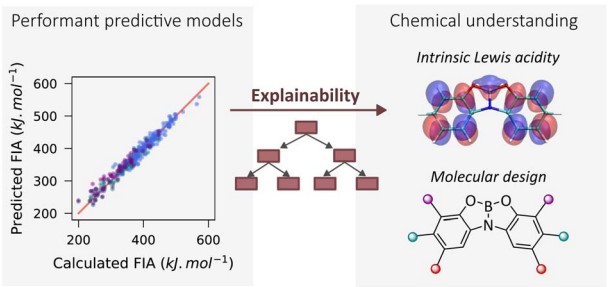

Constructing and explaining machine learning models for the exploration and design of boron-based Lewis acids

Juliette Fenogli,* Laurence Grimaud* and Rodolphe Vuilleumier*

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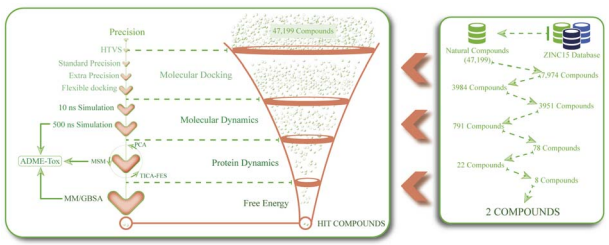

Database mining of ZINC15 natural compounds reveals potential thyroid receptor β agonists for NAFLD management: an *in silico* study

Ahmet Buğra Ortaakarsu,* Michel Hosny, Mansour Sobeh and Mohamed A. O. Abdelfattah

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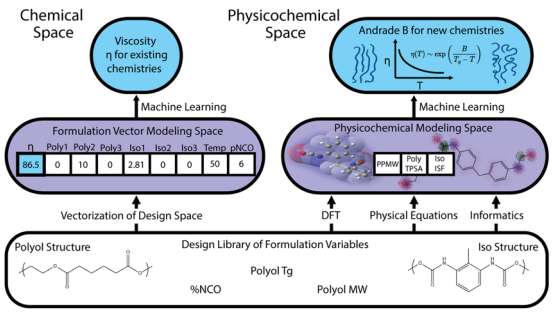

Machine learning of polyurethane prepolymer viscosity: a comparison of chemical and physicochemical approaches

Joseph A. Pugar, Calvin Gang, Isabelle Millan, Karl Haider and Newell R. Washburn*

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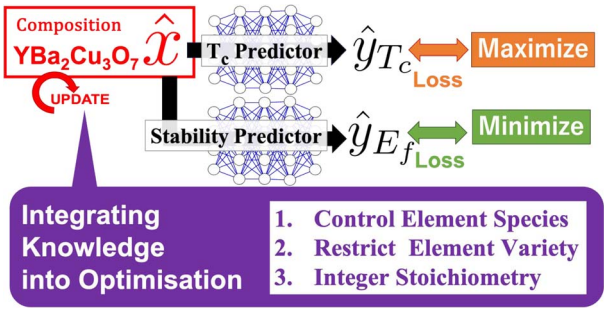

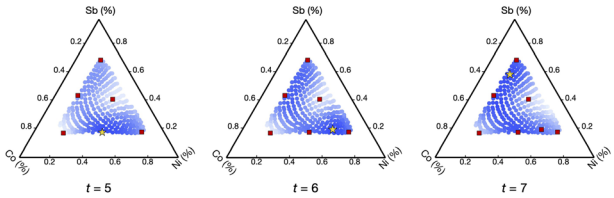

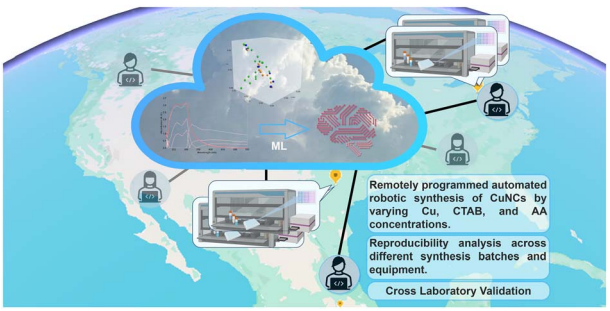

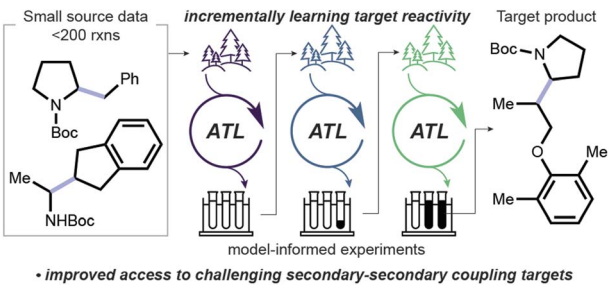

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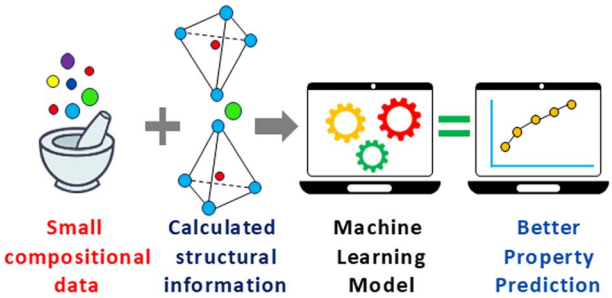

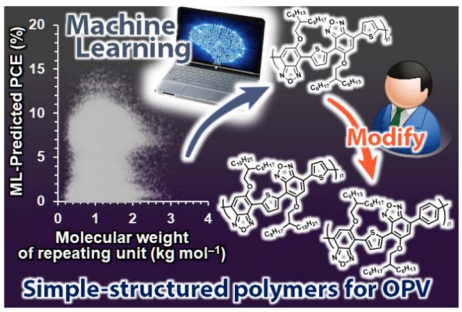

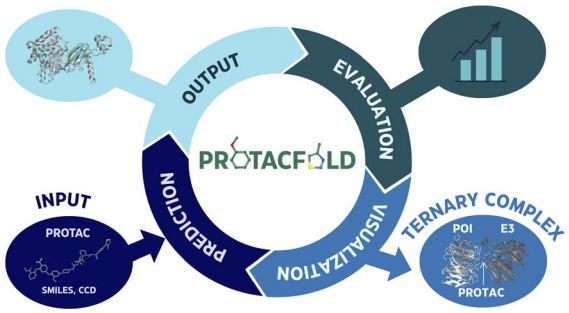

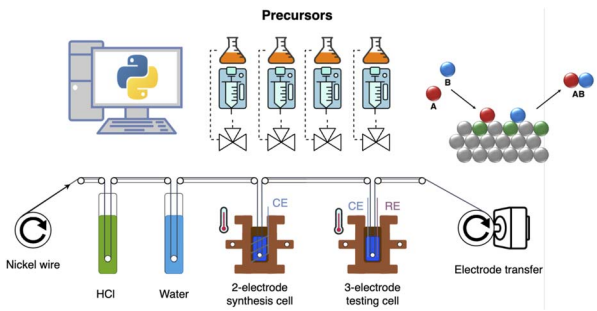

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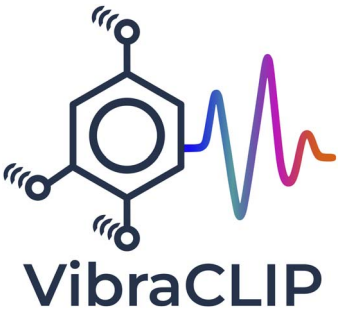

CORRECTION