

Digital Discovery

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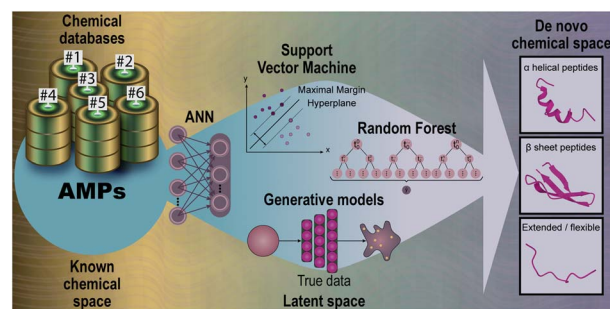
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See Miroslava Nedyalkova, Marco Lattuada *et al.*, pp. 9–22. Image reproduced by permission of Miroslava Alexandrova Nedyalkova from *Digital Discovery*, 2024, 3, 9.

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Progress and future of the computational design of antimicrobial peptides (AMPs): bio-inspired functional molecules

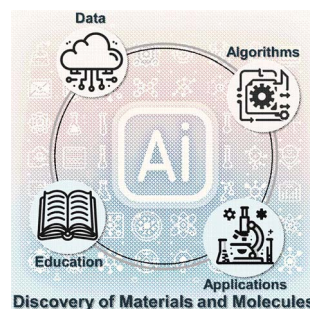
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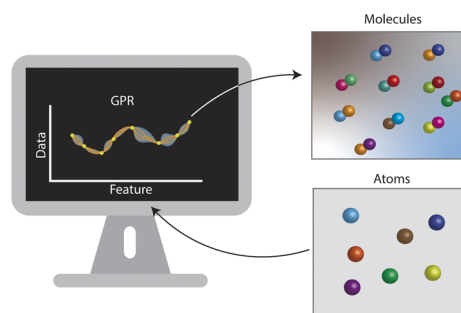


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Spectroscopic constants from atomic properties: a machine learning approach

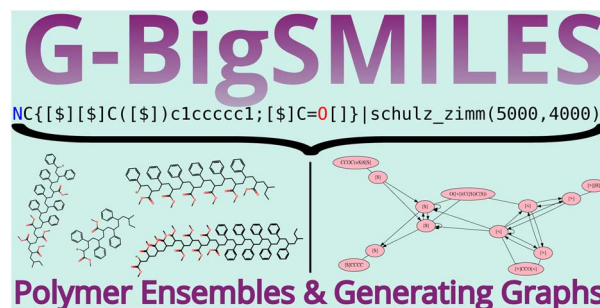
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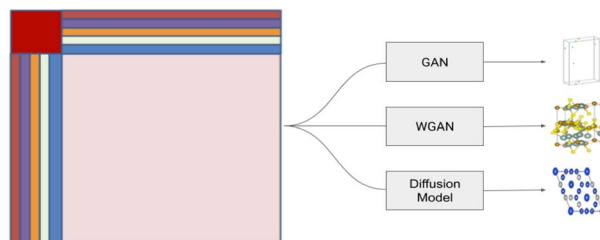
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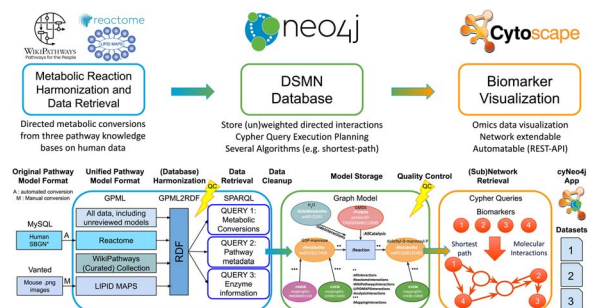
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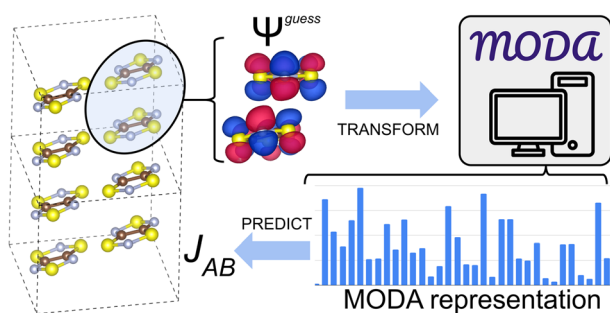
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Discovering life's directed metabolic (sub)paths to interpret human biochemical markers using the DSMN tool

Denise Slenter,* Martina Kutmon, Chris T. Evelo and Egon L. Willighagen



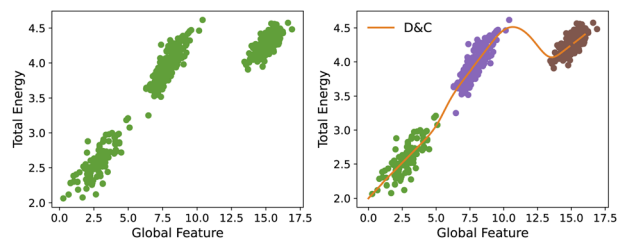
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Raul Santiago,* Sergi Vela, Mercè Deumal and Jordi Ribas-Arino

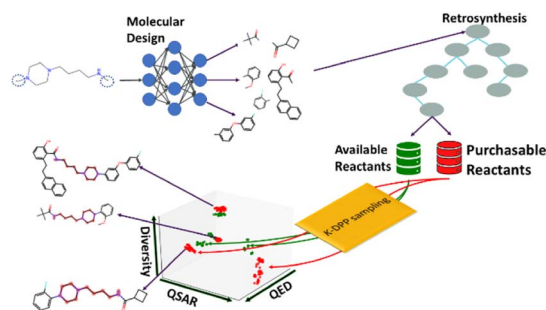
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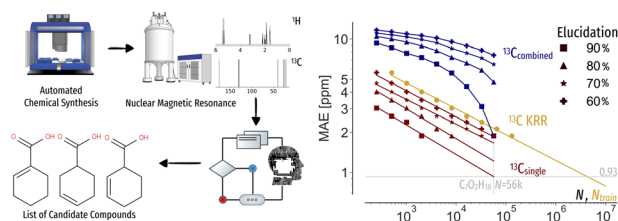
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Simon Viet Johansson,* Morteza Haghir Chehreghani, Ola Engkvist and Alexander Schliep

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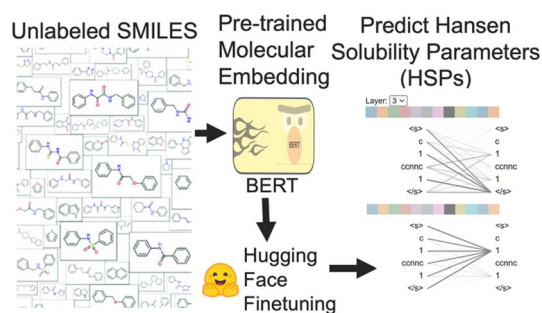
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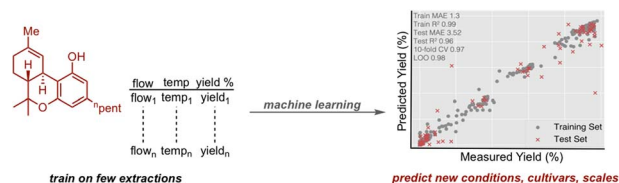
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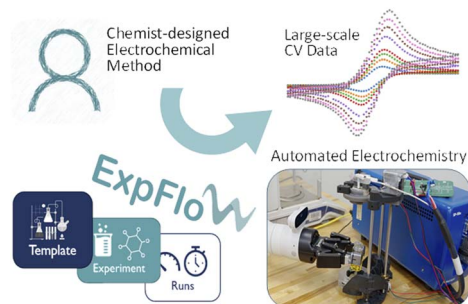
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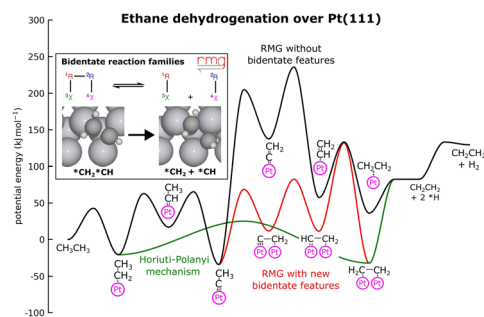
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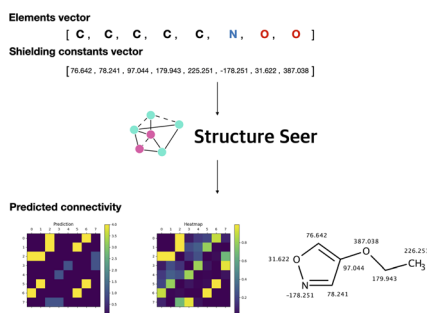
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Automatic mechanism generation involving kinetics of surface reactions with bidentate adsorbates

Bjarne Kreitz,* Katrín Blöndal, Kirk Badger, Richard H. West and C. Franklin Goldsmith*



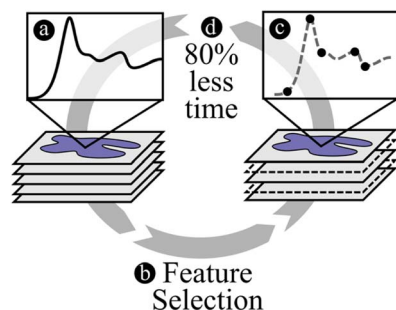
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Structure Seer – a machine learning model for chemical structure elucidation from node labelling of a molecular graph

Denis Andzhevich Sapegin* and Joseph C. Bear

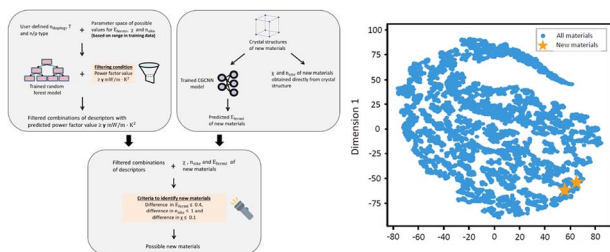
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