

Digital Discovery

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See J. Pérez-Ríos *et al.*, pp. 34–50. Image reproduced by permission of Jesús Pérez-Ríos from *Digital Discovery*, 2024, 3, 34.



Inside cover

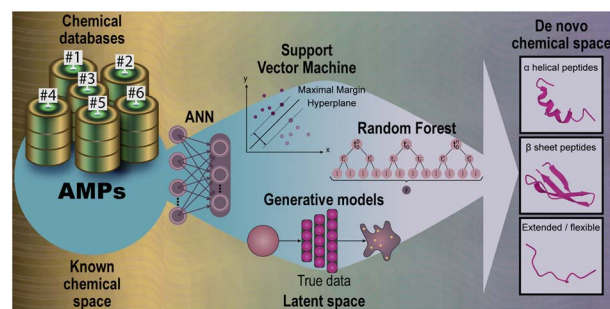
See Miroslava Nedyalkova, Marco Lattuada *et al.*, pp. 9–22. Image reproduced by permission of Miroslava Alexandrova Nedyalkova from *Digital Discovery*, 2024, 3, 9.

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

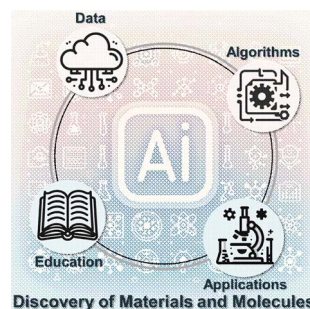
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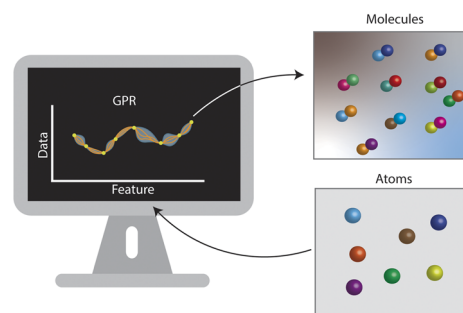


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Spectroscopic constants from atomic properties: a machine learning approach

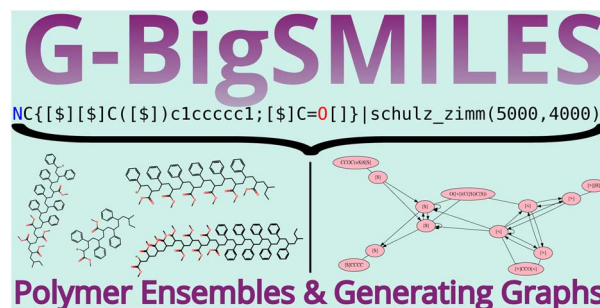
Mahmoud A. E. Ibrahim, X. Liu and J. Pérez-Ríos*



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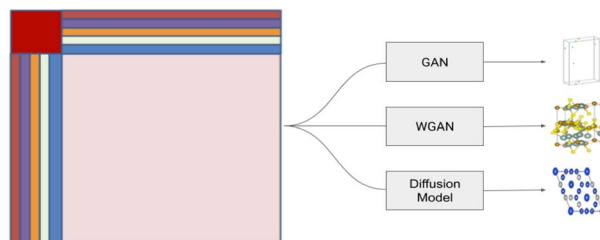
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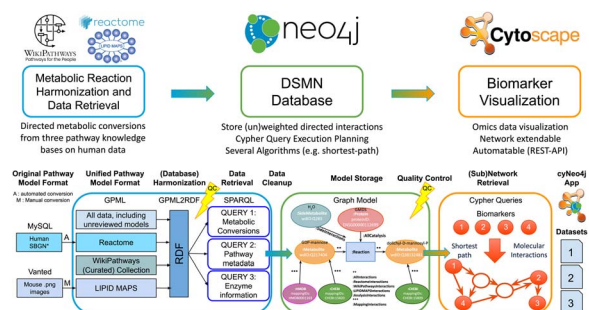
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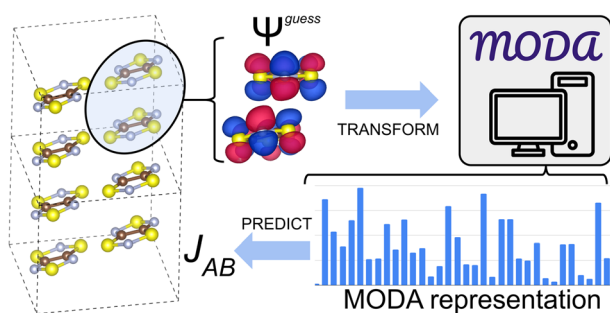
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Denise Slenter,* Martina Kutmon, Chris T. Evelo and Egon L. Willighagen



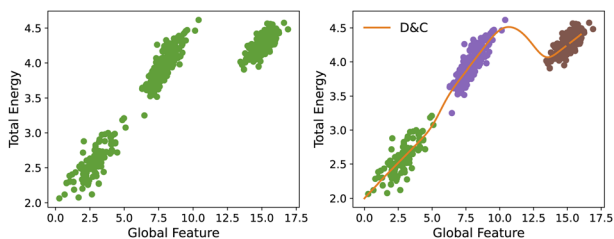
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Raul Santiago,* Sergi Vela, Mercè Deumal and Jordi Ribas-Arino

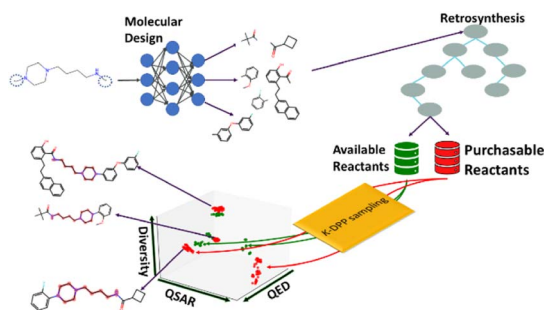
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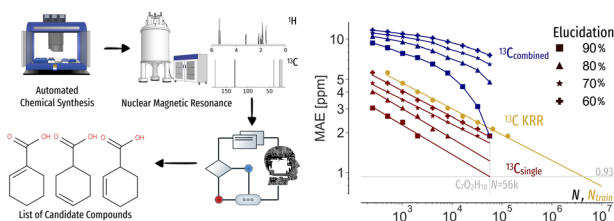
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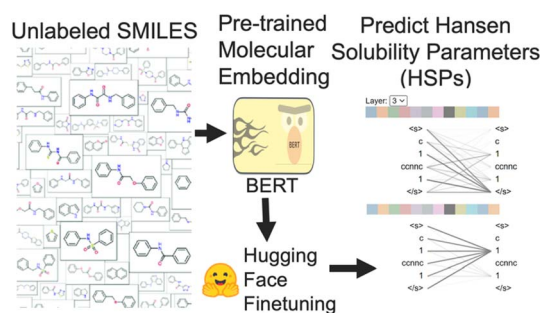
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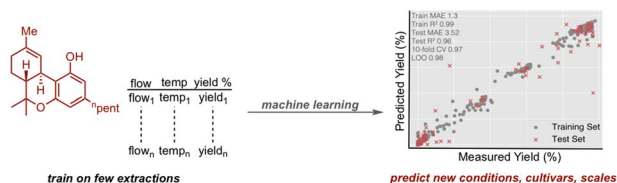
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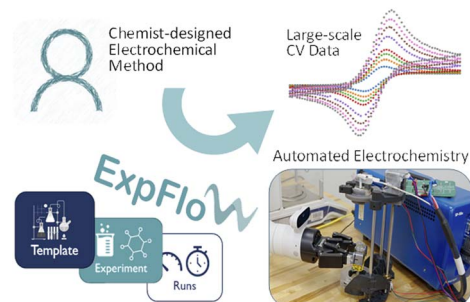
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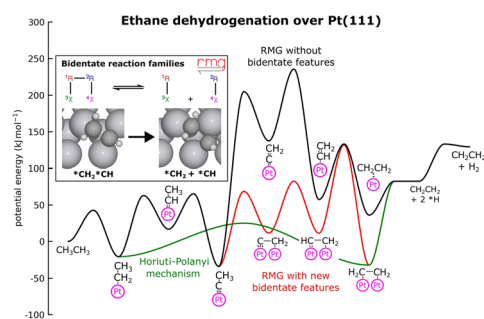
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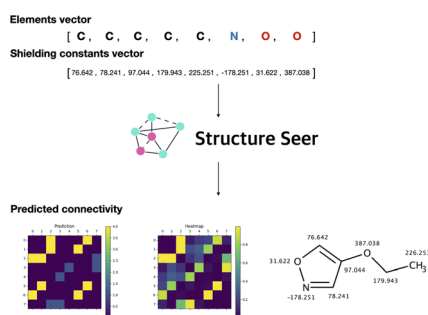
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Automatic mechanism generation involving kinetics of surface reactions with bidentate adsorbates

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



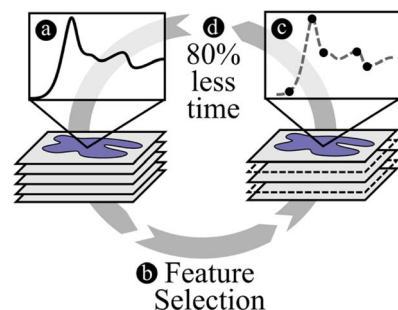
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Denis Andzhevich Sapegin* and Joseph C. Bear

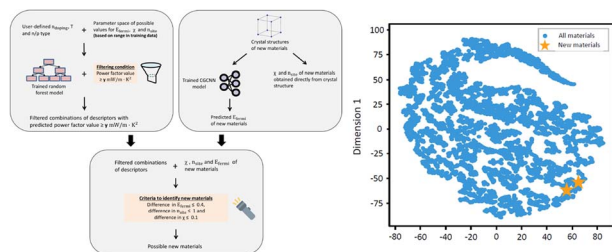
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