

RSC Sustainability

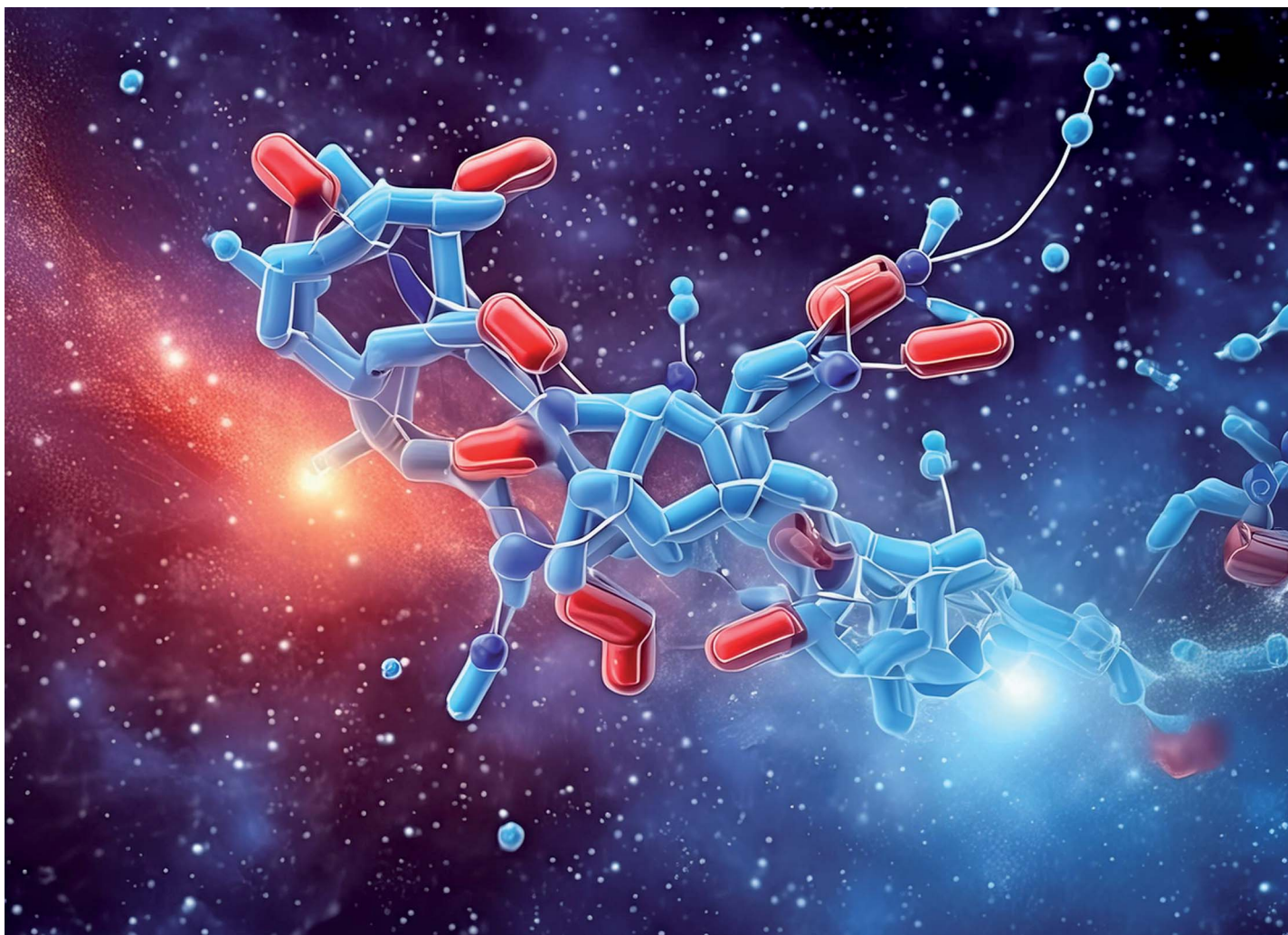
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Fundamental questions
Elemental answers



Showcasing research from Professor Kate Farrahi's laboratory, School of Electronics and Computer Science, University of Southampton, United Kingdom.

DrugPose: benchmarking 3D generative methods for early stage drug discovery

DrugPose introduces a novel benchmark framework to evaluate 3D molecule generation models. By leveraging Simbind, it assesses the coherence of generated molecules with initial hypotheses. DrugPose enhances insights into synthesizability by cross-referencing with commercial databases and applying the Ghose filter for drug-likeness. Current methods show 4.7% to 15.9% success in intended binding modes, 23.6% to 38.8% commercial accessibility, and 10% to 40% compliance with the Ghose filter, highlighting the need for more reliable 3D molecule generation techniques.

Image generated with Adobe Firefly.

As featured in:



See Zygimantas Jocyas *et al.*, *Digital Discovery*, 2024, **3**, 1308.