



Showcasing research from Amit Kadan, Dr Kevin Ryczko and Dr Takeshi Yamazaki, SandboxAQ, California, USA.

Guided multi-objective generative AI to enhance structure-based drug design

In this work we present IDOLpro, a modular framework for guided diffusion which can generate molecules with a plurality of optimized properties for structure-based drug design, accelerating the drug discovery process.

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