

Peer Review

# Review of: "Strategies for Robust, Accurate, and Generalisable Benchmarking of Drug Discovery Platforms"

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This study presents a well-structured and highly relevant approach to improving benchmarking in computational drug discovery. The proposed optimizations to CANDO and the introduction of compbench, a head-to-head benchmarking framework, provide a notable contribution to the field. The methodology is thorough, the results are well-justified, and the conclusions are meaningful.

Overall, I recommend publication.

Some aspects may benefit from further refinement.

1) The study primarily compares two CANDO-based pipelines. Including additional external drug discovery methods and a real application would strengthen the generalizability of the findings. I understand that it would represent a high amount of work and is not mandatory for me to grant publication.

2) The presentation of compbench could be a bit clearer/simpler in order to be better understood by a non-technical audience.

## Declarations

**Potential competing interests:** No potential competing interests to declare.