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* You should state whether an appropriate sample size was computed when the study was being designed
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* If no explicit power analysis was used, you should describe how you decided what sample (replicate) size (number) to use

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The submission introduces a computational method for drug discovery and it doesn’t include experimental setups. Therefore, the requested information doesn’t apply to our submission.

**Statistical reporting**

* Statistical analysis methods should be described and justified
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* Report exact p-values wherever possible alongside the summary statistics and 95% confidence intervals. These should be reported for all key questions and not only when the p-value is less than 0.05.

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(For large datasets, or papers with a very large number of statistical tests, you may upload a single table file with tests, Ns, etc., with reference to sections in the manuscript.)

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* We encourage you to upload relevant additional data files, such as numerical data that are represented as a graph in a figure, or as a summary table
* Where provided, these should be in the most useful format, and they can be uploaded as “Source data” files linked to a main figure or table
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The source data corresponding to all figures and analysis are provided in terms of supplementary files1 to 8, and linked appropriately to the text.