Transforming molecular optimization using collective intelligence

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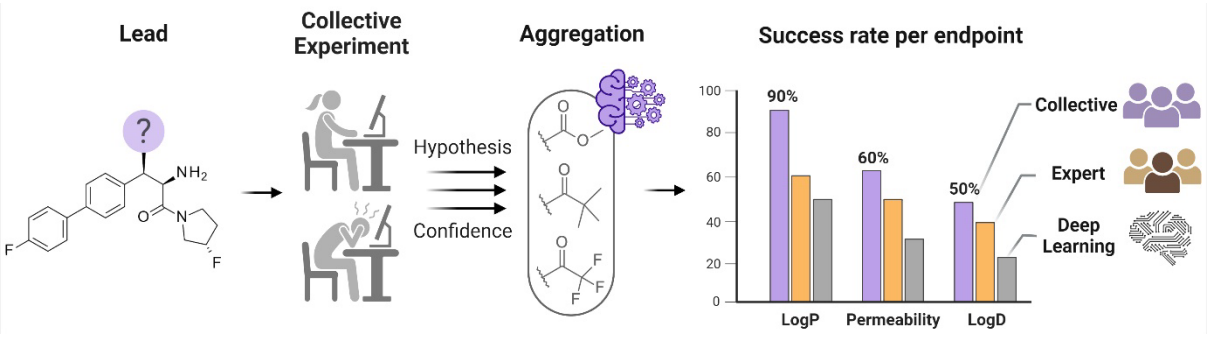
In drug discovery, molecular optimization is guided by the medicinal chemistry intuition, grounded in theoretical knowledge, personal experience, and inherent biases. The principle of collective intelligence stands as a promising complement, streamlining individual decision-making processes by emphasizing the wisdom of the collective over individual judgments and biases. Over the last decade, the application of collective intelligence alongside computational methods has significantly reshaped complex problem-solving, e.g., Foldit and Eterna. In the present study, we evaluate the application of collective intelligence in the lead optimization phase of drug discovery, featuring an experiment with 92 Sanofi researchers from varied scientific disciplines. By developing a collective intelligence framework and comparing its efficacy against an artificial intelligence model created simultaneously, we uncover three pivotal insights: the enhanced capability of collective decisions to improve ADMET endpoints over individual efforts, the superior performance of collective intelligence over artificial intelligence across nearly all endpoints, and the notable synergy achieved by merging collective intelligence with machine learning to address complex challenges. This study highlights the potential of collective intelligence, promoting strategic integration throughout the drug discovery process.



Lead optimization strategies for the proposition of molecular structures with enhanced ADMET properties in an industrial context