Review: Using Conformal Prediction to Prioritize Compound Synthesis in Drug Discovery

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1 Paper Profile

- Title: Using Conformal Prediction to Prioritize Compound Synthesis in Drug Discovery

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2. Method

    (a) Data
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3 Summary

This work illustrates how computational models can be more tightly coupled with experiments to generate decision data at lower cost without reducing the quality of the decision. The results show that there is a clear possibility to reduce the number of synthesized compounds with minimal reduction in the quality of data that decisions are taken on. And their motivation for this research was on finding how to efficiently detect the early stage drug discovery in terms of cost and under a limited budget.