

CONSENSUS-ENHANCED VIRTUAL SCREENING UNVEILS NEW OPPORTUNITIES FOR ONCOLOGY DRUG DESIGN

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Abstract text

The discovery of selective and potent cancer inhibitors remains a major challenge due to the vastness of chemical space and the limitations of traditional virtual screening. Within the ULTRA project, we have developed and applied **MetaScreener** (<https://github.com/bio-hpc/metascreeener>), a scalable, consensus-enhanced virtual screening framework that integrates structure-based, ligand-based, and AI-driven methodologies. This adaptive workflow allows the exploration of ultra-large chemical libraries while maintaining high predictive accuracy through iterative benchmarking and feedback from experimental data. Using this approach, we identified promising inhibitors against key cancer-related targets such as **Wee1**, **DDR1**, **Fascin1**, and other cancer related proteins, which are currently under biochemical and biophysical validation. These results demonstrate the potential of consensus-based strategies to improve hit identification and reliability in oncology drug discovery. Our findings highlight the value of reproducible, open, and adaptive computational pipelines to accelerate the transition from in silico prediction to experimental success.

