An HPC-Accelerated Workflow for Efficient Identification of Anti-Asthma Compounds via Molecular Docking of Herbal Formula

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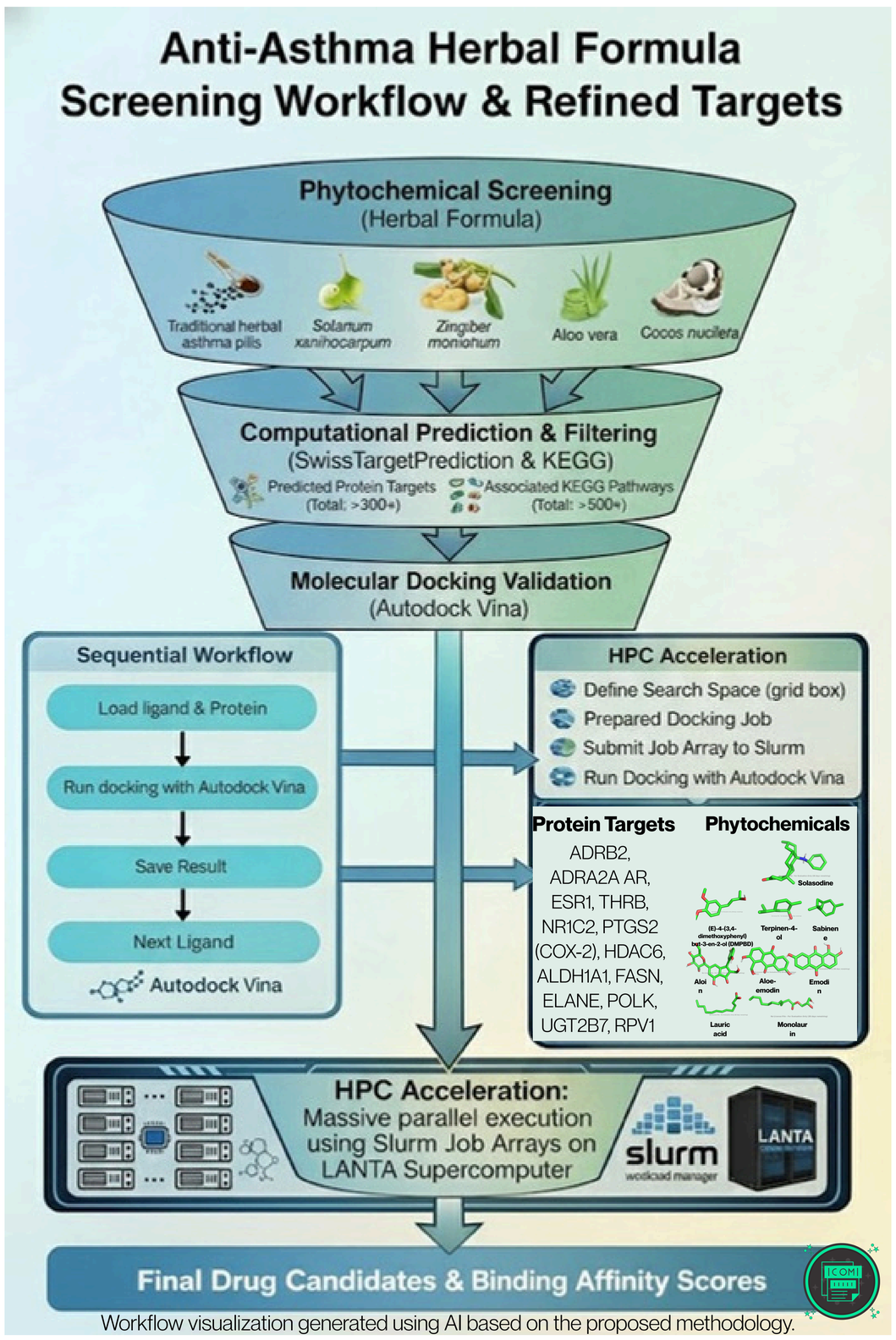
Background & Objectives

Asthma, a global chronic respiratory condition [1], has traditionally been treated in Thailand with multi-herbal bolus formulations containing *Aloe vera, Cocos nucifera*, *Solanum xanthocarpum*, and *Zingiber montanum*. Those plants were known to possess relevant anti-inflammatory phytochemicals [2,3]. However, the specific molecular pathways mediating their therapeutic effects remain unelucidated. This study therefore developed and evaluated a high performance computing (HPC) enhanced workflow to efficiently screen bioactive compounds from these traditional herbs, establishing a robust computational pipeline for future ethnopharmacology studies.

Methodology



Workflow visualization generated using AI based on the proposed methodology.

Results: sequential VS HPC workflow

Speedup Achieved

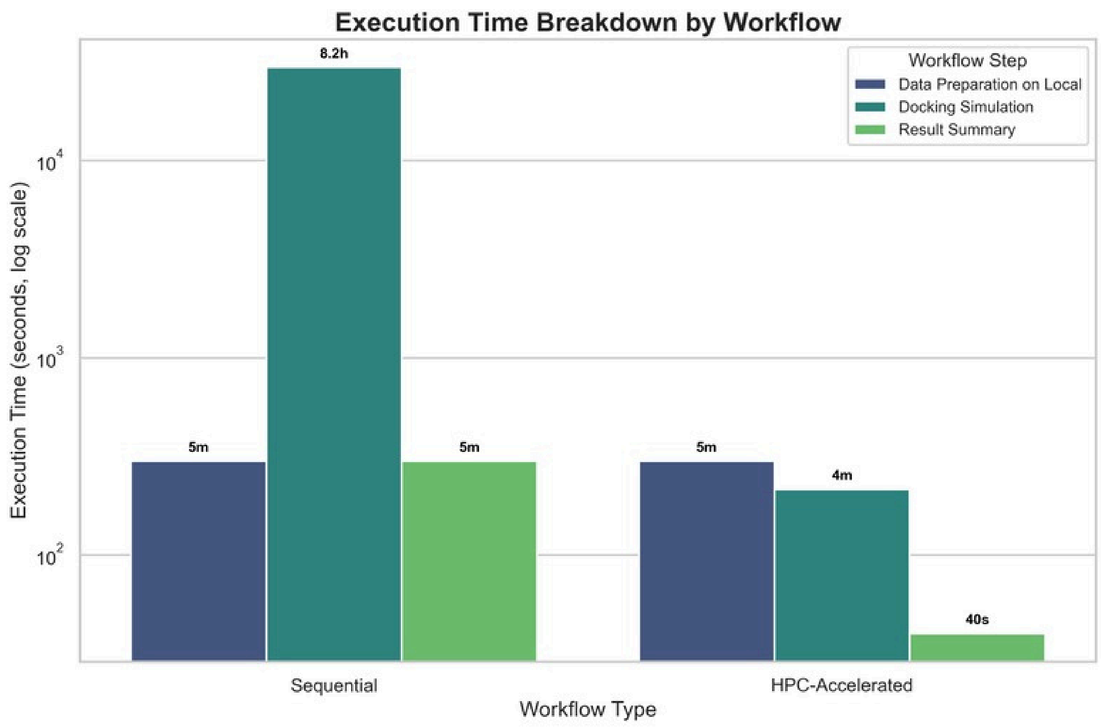
118-fold

Runtime Reduce

8.24 hours ➤ 4.25 minutes

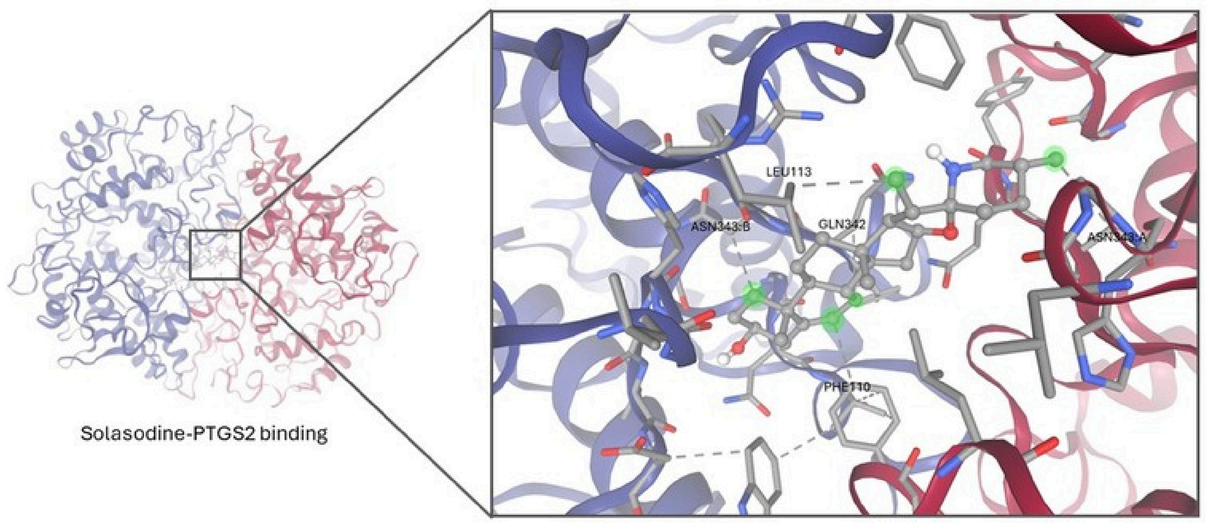
Parallel Efficiency

94.1%



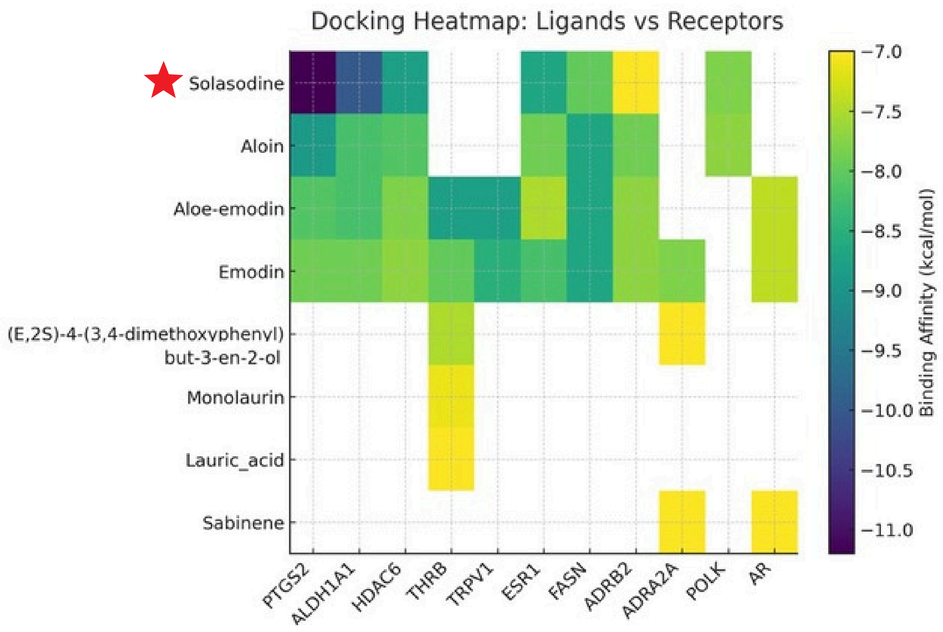
Performance metrics were obtained from a single deterministic benchmark run for 126 docking jobs.
Error bars are omitted as execution times remained consistent under controlled cluster conditions on LANTA.

Result: Example of docking result



Solasodine-PTGS2 binding

Result: Binding affinity



Conclusion

This study combined traditional Thai herbal knowledge with an HPC-accelerated computational workflow to identify multi-target anti-asthmatic phytochemicals, with solasodine, aloin, aloe-emodin, and emodin showing strong predicted binding to key asthma-related proteins [5] The workflow achieved ~118× speedup on the LANTA supercomputer, demonstrating high scalability and suitability for large-scale natural product screening. While the findings remain predictive, they provide mechanistic support for ethnomedicinal use and establish a foundation for further validation using advanced simulations and experimental assays.

References

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