ESSENCE-DOCK: A UNIFIED FRAMEWORK FOR INTEGRATING DOCKING METHODS AND ENHANCING HIT IDENTIFICATION

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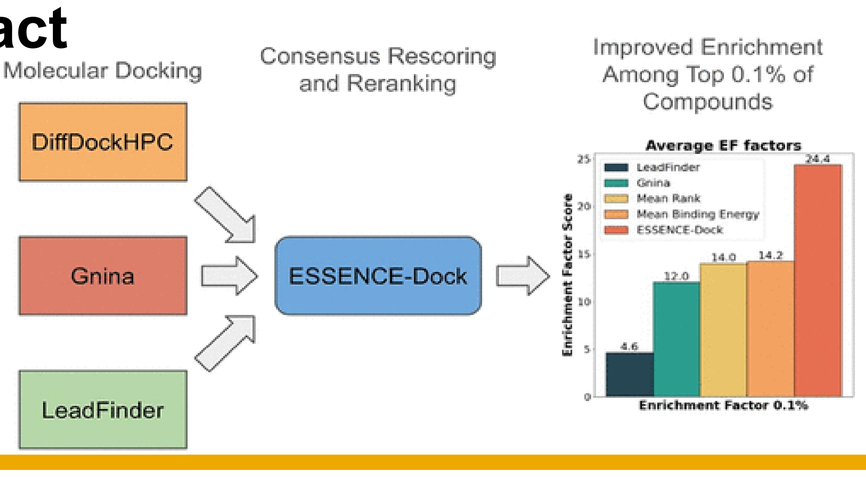
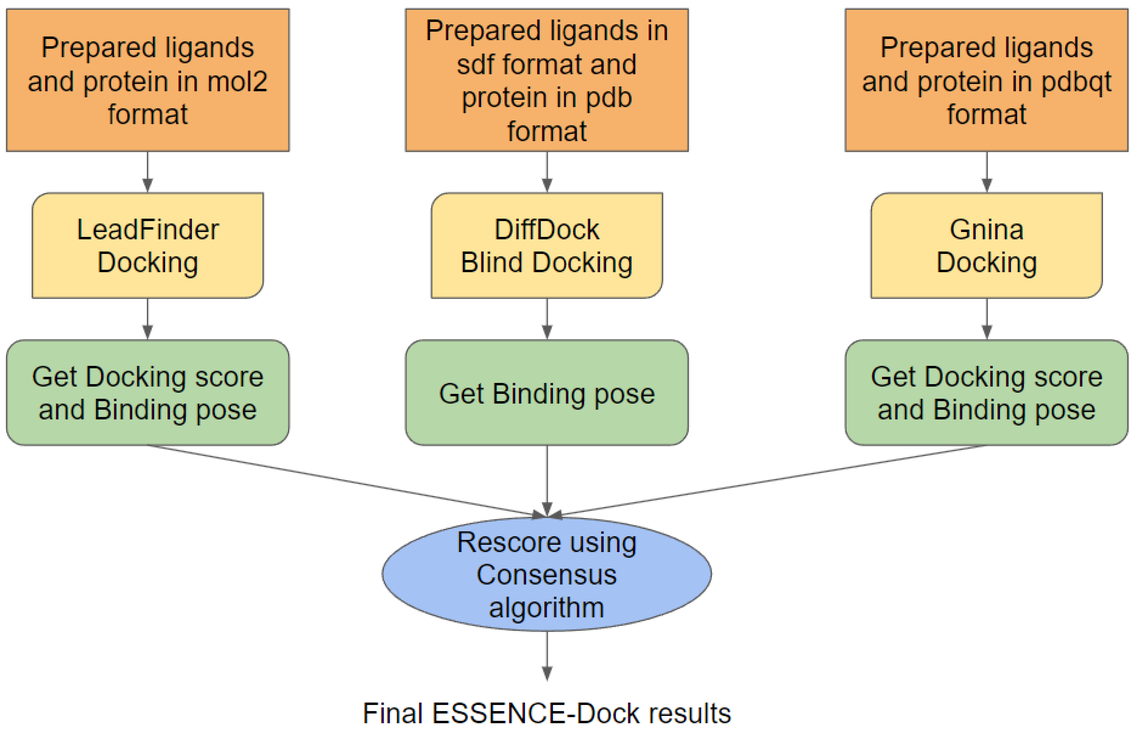
Abstract



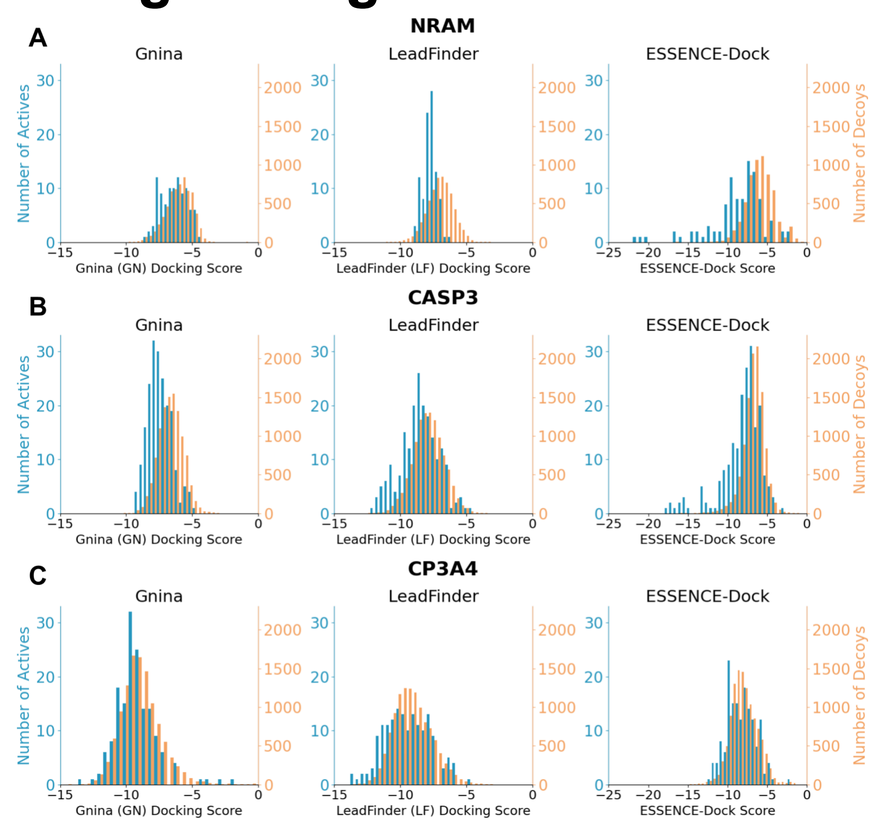
Virtual Screening

- Cheaper than experimental HTS screening
- Explore larger chemical space
- Molecular docking predicts pose and score, but not always accurate
- Combine docking methods in order to reduce false-positives

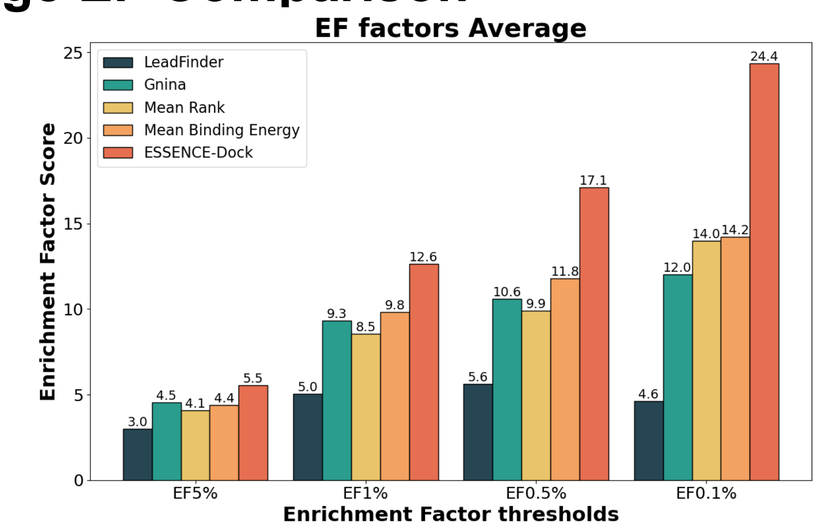
Workflow Overview



Distinguishing actives from decoys



Average EF Comparison



Key Takeaways and Outlook

- Great enrichment capabilities, excels at virtual screening
- Seamlessly integrates with High-Performance Computing (HPC) clusters
- Visualize top compounds with interactive PyMol session files, including predicted protein-ligand interactions via PLIP
- Future work: Improve re-scoring function by implementing a machine learning-based scoring function

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References

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