Docking Studies and High Throughput Virtual Screening for Breast Cancer Drug Discovery Using a Distributed Environment

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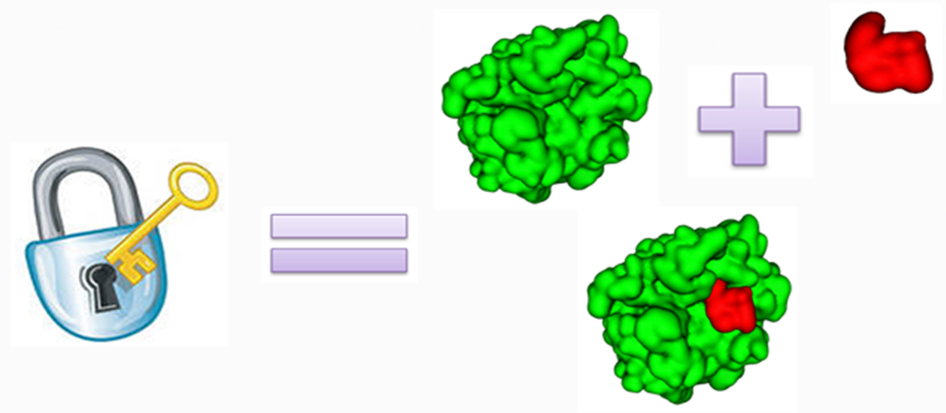
1) Abstract

- Breast Cancer is the second most common form of cancer
- Traditional drug designing method is time consuming and costly
- High Throughput environments are proprietary
- Indigenous Plants + Commercial Compounds need to be tested

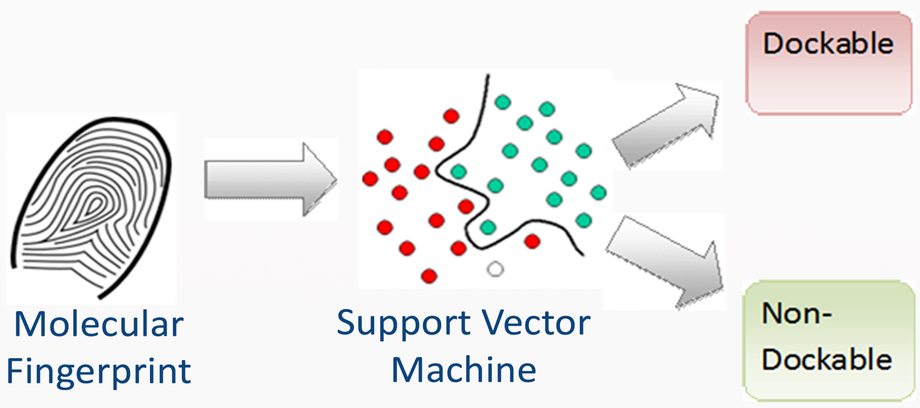
2) Molecular Docking

- This is like Lock & Key problem.
- Find most stable Receptor – Ligand complex

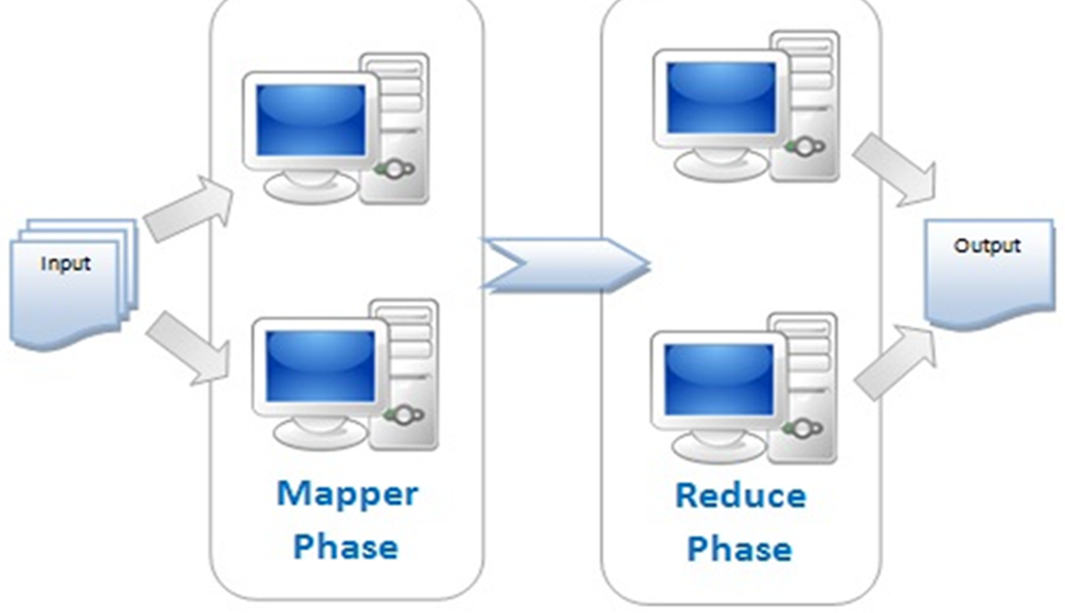


3) Search Space Optimization

- Molecular data converted to Molecular Fingerprint
- Support Vector Machine Active Learning
- Identify Dockable compounds prior to the docking process

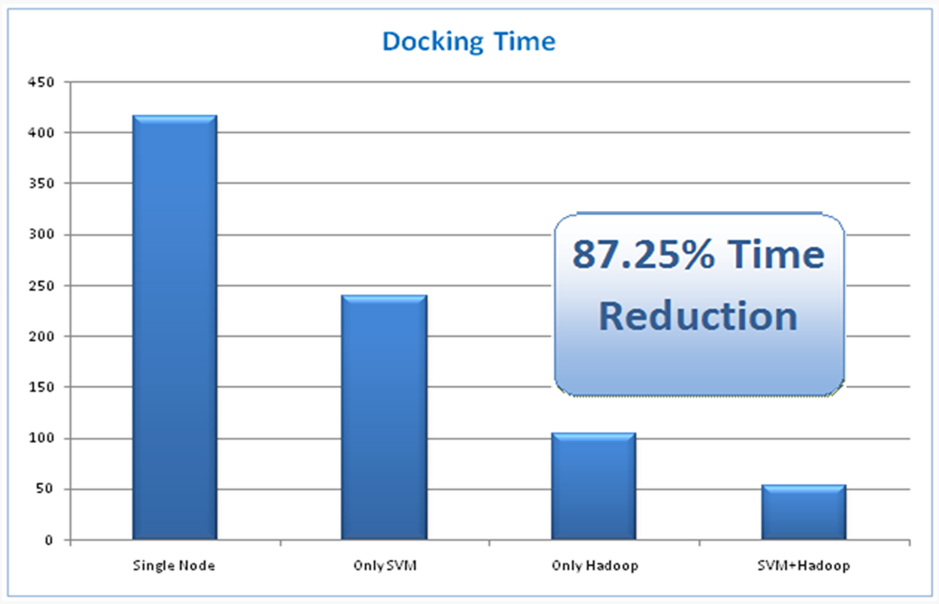


4) Docking on Hadoop Environment



- Novel MapReduce algorithm to run jobs in a parallel manner on the cluster environment

5) Docking Time Analysis



6) Conclusion

- Developing open source High Throughput environment
- 87.25% time reduction
- Found 2 commercial compounds and 6 indigenous plants as potential drugs