Drug Discovery: Depression, Alzheimer's Disease, Toxicity Prediction

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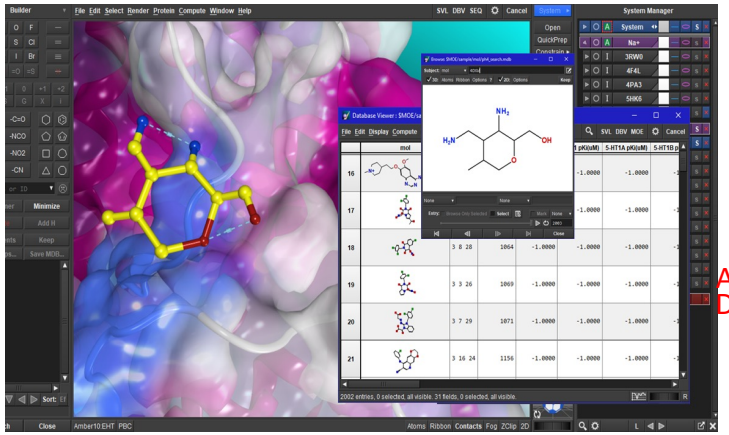
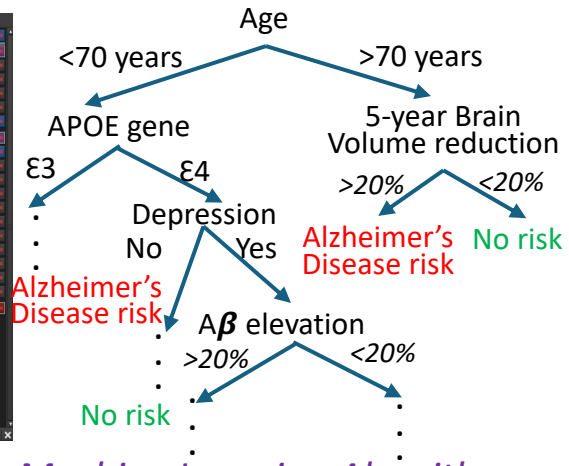


Molecular Modeling



Machine Learning Algorithms

Objectives

- Discover new applications for established drugs
- Find new biomarkers for Alzheimer's disease and depressive disorders using patients' brain images, biomedical and genetic data
- Predict toxicity and side effects of drugs and drug candidates
- Discover patterns in molecular structure of compounds that are associated with specific therapeutic or adverse effects
- Identify enzymes or receptors that specific compounds may bind to and the consequence of binding
- Build disease models to help identify pathophysiology of disease

Approach

Will use some of the skills below:

- Molecular modeling
- Protein-ligand docking
- Databases: cohort databases, clinical trials data, brain image data, biomedical data (e.g. inflammation biomarkers, etc.)
- Pathway analysis
- Machine learning
- Collaborations both internally (several NSU colleges) and internationally

Accomplishments

- Publications of 70+ research papers and book chapters, some of which involve undergraduate and PhD students
- Funded by Pharmaceutical industry and major UK research councils
- Student awards and research awards
- Mentored many successful students who later worked for prestigious organizations such as the FDA, University of Oxford (England), and major Pharmaceutical firms
- Associate editor of Springer Nature's journal, "Molecular Diversity", and editorial board member of several other renowned journals including Frontiers in Pharmacology and MDPI Biomedicines.