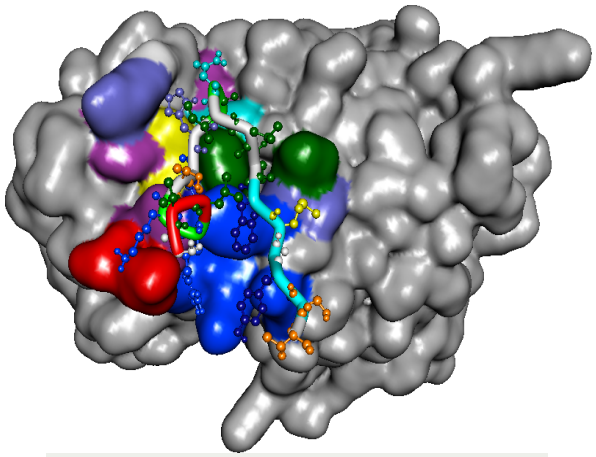
Protein and DNA Modeling

The SAMM Group has a great deal of experience with programs that examine protein-protein, or protein-peptide interactions; programs that perform protein-substrate docking simulations; and predict the activity of new compounds using pharmacophore modeling.
In collaboration with Dr. Morrison (CCR), the SAMM Group examined putative peptide inhibitors of BRAF and CRAF dimerization.



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ABCC
Simulation, Analysis and Mathematical Modeling

ISP, FNLCR

Advanced Data Analysis
- Biomarker Identification and Classification
- Machine Learning
- Numerical Simulations

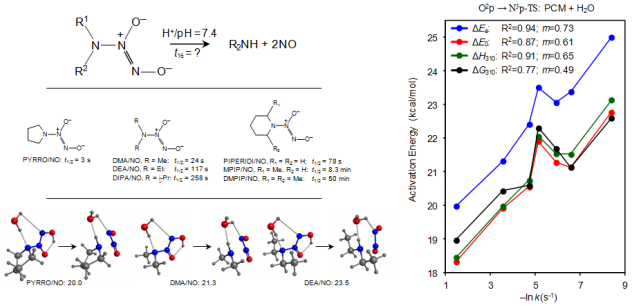
Protein and DNA Modeling
- Modeling the Impact of Protein Mutations
- Modeling Protein-Ligand and Protein-DNA Interactions
- Pharmacophore Modeling of Putative Drugs/ Screening

Electronic Structure of Proteins and Nanoparticles
- Predicting Absorption/Emission Spectra of Fluorescent Proteins
- Modeling Transition Structures of Enzymatic Reactions
- Calculating Properties of Nanoparticles

Accurate Calculations of Drug Molecules
- Determining Relative Energies of Drug Conformers
- Accurate Determination of Transition State Energies
- High Quality Predictions of Product Distributions

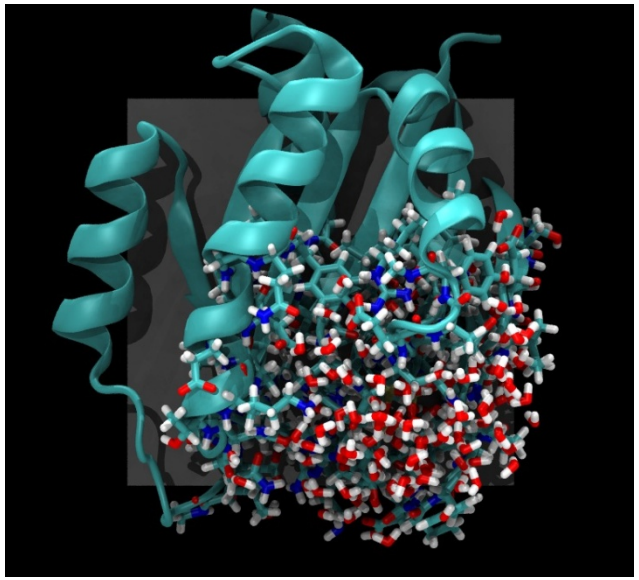
Quantum Chemical Modeling of Biomolecules

The SAMM Group can assist research efforts by performing mathematical analyses of virtually any dataset and can perform modeling simulations on molecules ranging from drugs to protein complexes to provide added insight.
In collaboration with Dr. Keefer (CCR) the SAMM Group is studying the NO and HNO releasing ability of various prodrugs.



Electronic Properties of Proteins and Nanoparticles

New quantum mechanical techniques can be used to model the electronic properties of proteins. Electronic modeling can now be performed on systems with over 18,000 atoms. The extended active site of RAS is shown to the left and covalently bound inhibitors can now be examined.



Mathematical Analysis of Data

The SAMM Group can develop custom codes and analytical procedures to answer questions related to virtually any dataset. Statistical significance of results can be determined through standard techniques, or by running large numbers of custom simulations. One example of this was assistance supplied to the GTEx program.

Multi-scale Modeling and Analysis

The SAMM Group is able to apply state-of-the-art techniques to treat problems at a multitude of scales. For example, in an analysis of mutation mechanisms within DNA, the analysis went from sequences to the removal of a single electron