Drug design for treatment of heart attack and stroke - How the hSCAN-1 enzyme is activated
Dalm a
(NYU
Abu
Dhab i)

Transferri ng data
to/from
the
clusters

Transferri ng data
to/from
Prince
ccluster
using
Globus

Submittin g jobs
with
sbatch

Available
software

Licensed
Software
Available
on the
HPC
Cluster

Building
Software

Slurm
Tutorial

Tutorials

FAQs

Scratch
Area
Cleanup

Programming for
Biologist s
The Brooklyn Research Cluster provides flexible computing, including for NYU Tandon's Visualization, Imaging, and Data Analytics research center.
• An app that translates sign language into spoken English using Brooklyn Research Cluster Platform

• An Event-Driven Model for Estimation of Phase-Amplitude Coupling at Time Scales of Cognitive Phenomena

• Drug design for treatment of heart attack and stroke - How the hSCA N-1 enzyme is activated

• How carcinogenic chemicals slip past DNA repair mechanisms
Recently it was discovered that saliva of certain blood-sucking insects contains an enzyme which indirectly prevents the blood from clotting, and that humans have an homologous protein, named hSCAN-1. Drs. David Rooklin and Yingkai Zhang from NYU's Department of Chemistry, with Dr. Min Lu from UMDNJ, set out to find how it might be modified for use in heart attack and stroke treatments. The key lay in developing an understanding of how the protein is activated, and the group ran hundreds of molecular simulations at quantum mechanical and atomistic scales. With any one simulation using up to 64 processors and running sometimes for weeks, the group used NYU's HPC resources to complete the workload. From the results the trio elucidated the detailed enzymatic mechanism of the human protein.

Their identification of a previously uncharacterized catalytic calcium-binding site (the magenta ion in the figure) reconciles an incongruous connection between acidic side chains and phosphate binding, explains the previously puzzling sigmoidal relationship between enzymatic rate and calcium concentration and provides a ... why hSCAN-1 is exclusively dependent on calcium and, in general, how catalytic calcium-activation is achieved.

Zhang, Rooklin, and Lu published "Revelation of a Catalytic Calcium-Binding Site Elucidates Unusual Metal Dependence of a Human Apyrase" in the Journal Of The American Chemical Society (published August 28, 2012) and have laid out a plan for interested experimental mutagenesis researchers to collaborate to support our understanding and push forward the redesign of hSCAN-1.

An article about their work can be found here, and more about the research undertaken by Dr. Zhang's group can be found at this page.