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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 they 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 explains the previously puzzling sigmoidal relationship between enzymatic rate and calcium concentration and provides a reason 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.