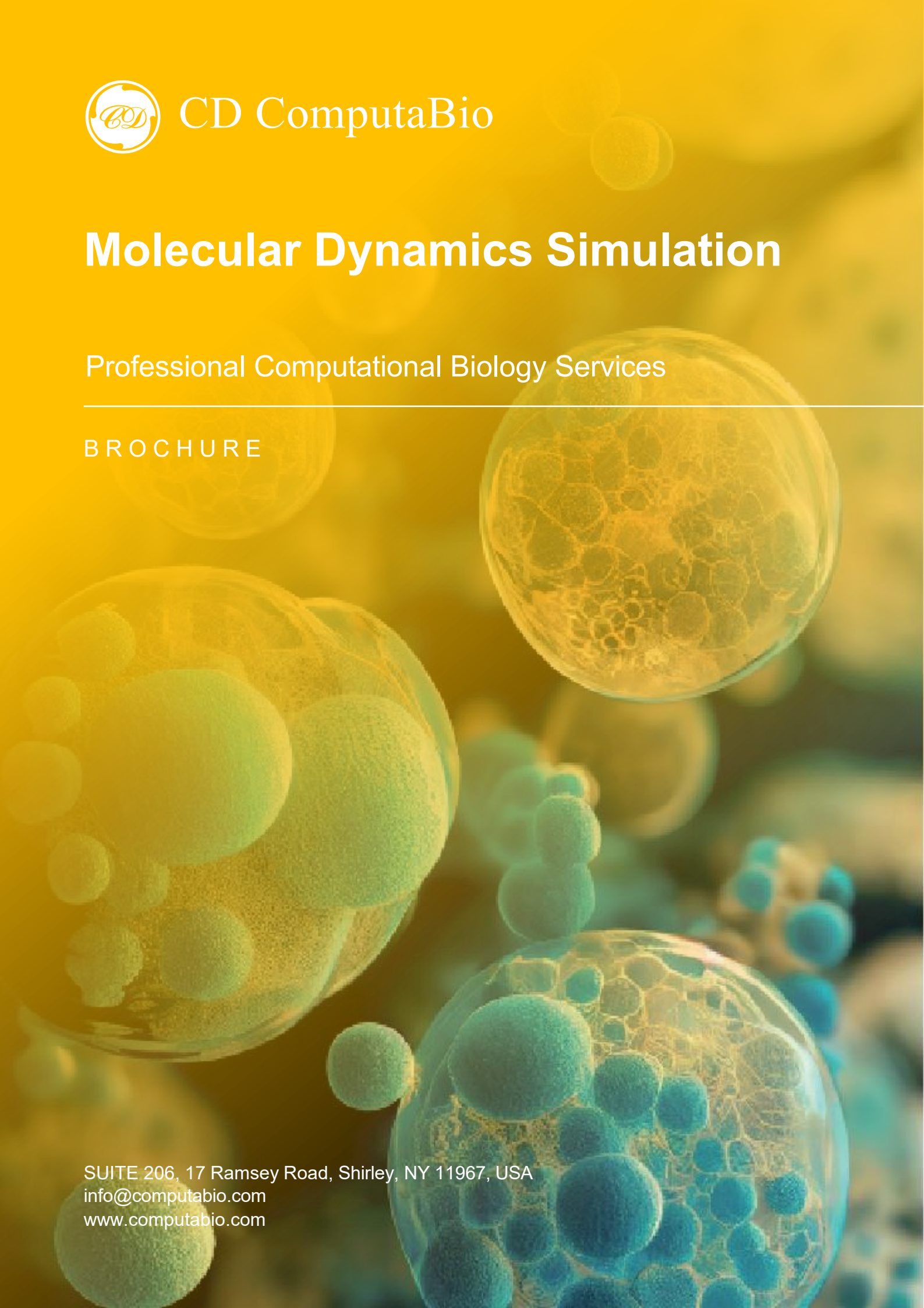
CD ComputaBio

# Molecular Dynamics Simulation

## Professional Computational Biology Services

BROCHURE



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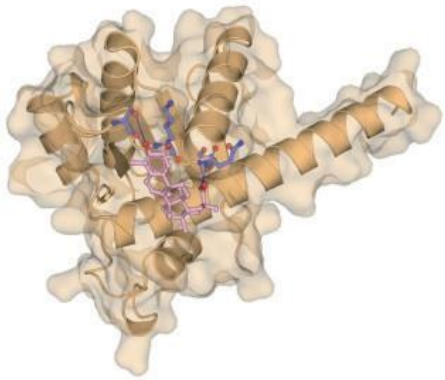
# About Us

CD ComputaBio specializes in offering computational biology services, with a particular emphasis on molecular dynamics simulations. This service enables our clients to investigate the structure and function of biomolecules by simulating their atomic-level movements and interactions. With a wealth of experience and expertise, our team is committed to providing high-quality, customised computational biology solutions to our clients.

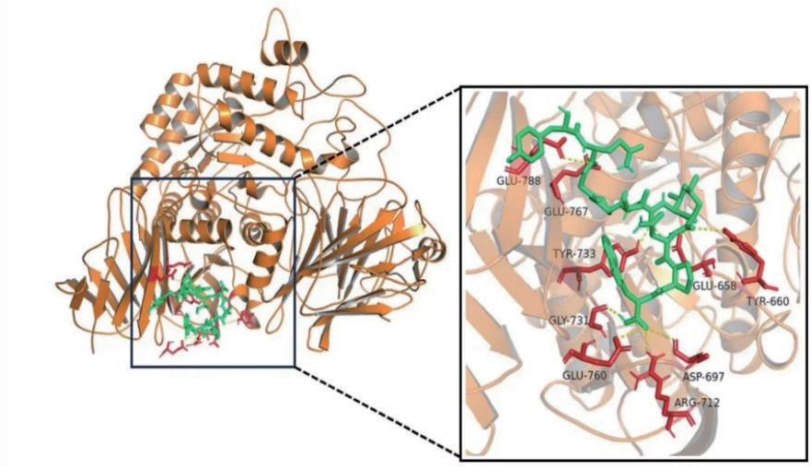
# Molecular Dynamics (MD) Simulation



Molecular Dynamics (MD) simulation is a collection of molecular simulation techniques and a powerful tool for studying condensed matter systems. By utilizing MD simulations, researchers can obtain the trajectories of atoms within the system, allowing them to observe a wide range of microscopic details related to atomic movements and interactions.

## Features of Molecular Dynamics (MD) Simulation

- MD provides detailed insights into the behavior of complex systems at the molecular level.
- MD enables the prediction of physical and chemical properties of materials.
- MD can be used to optimize the design of molecules and materials for specific applications.

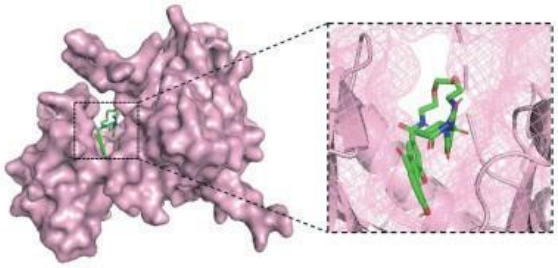


# Our Molecular Dynamics (MD) Simulation Services

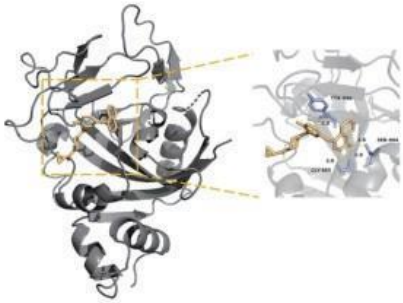
CD ComputaBio offers comprehensive molecular dynamics simulation services,

encompassing a variety of systems such as proteins, enzymes, lipids, membranes, peptides, and DNA/RNA.

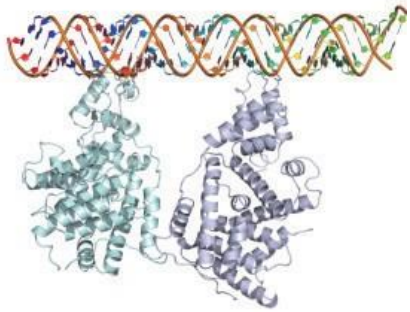
## Protein Molecular Dynamics Simulation Service



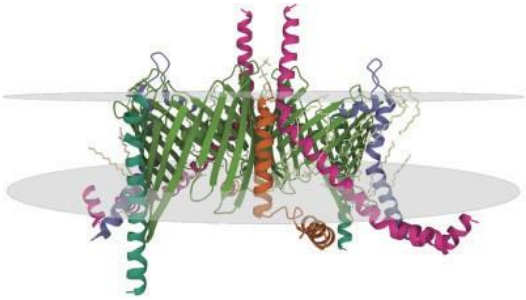
## Enzyme Molecular Dynamics Simulation Service



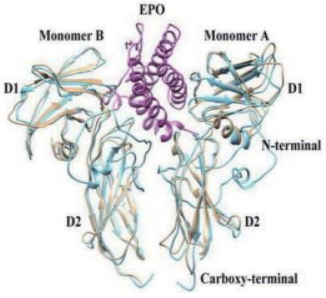
## DNA Molecular Dynamics simulation Service



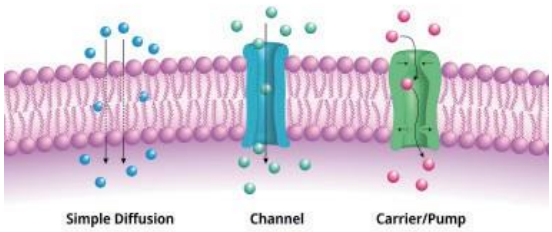
## Membrane Protein Molecular Dynamics Simulation Service



## Peptide Molecular Dynamics simulation

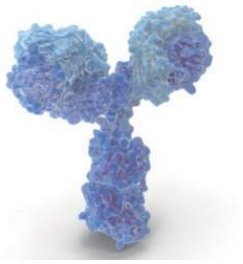



## Lipid Molecular Dynamics simulation Service



# Antibody Molecular Dynamics (MD) Simulation Services

Light chain and heavy chain sequences → Define framework regions by sequence alignment → Choose loop templates in the antibody database → Structure modeling by copying framework coordinates → H3 loop refinement → Final optimization model generation



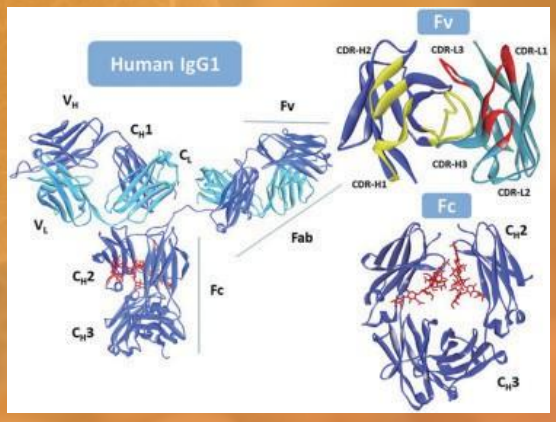
CD ComputaBio offers antibody molecular dynamics simulation services following the modeling process.

## Antibody Modeling Services

CD ComputaBio utilizes computer-aided structural simulation design to humanize antibodies from various species.

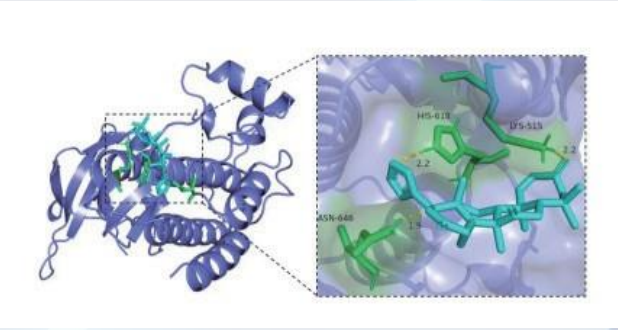
Related Service

- Antibody Docking Service
- Antibody Molecular Dynamics Service
- Antibody De Novo Design
- Antibody Structure Prediction



# Antibody Molecular Dynamics (MD) Simulation Services

CD ComputaBio's Molecular Dynamics offers a comprehensive solution to the complexities and challenges of interpreting MD simulation results. With our expertise, meticulous attention to detail, and commitment to innovative methodologies, we are the ideal partner to support your drug design efforts.



### Software We Use

- Amber
- Gromacs
- NAMD

## Force Field in Molecular Dynamics

### CHARMM Force Field

By incorporating CHARMM parameters, we enhance the predictive power of our simulations and refine the structural modeling of proteins.

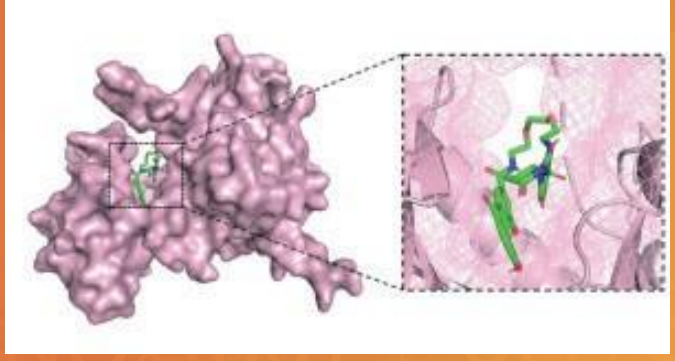
### AMBER Force Field

By utilizing AMBER parameters, we ensure the accuracy and consistency of our simulations, enabling comprehensive analyses of protein-ligand interactions.

### GROMACS Force Field

By utilizing the GROMACS algorithm, we have accelerated our simulations and deepened our understanding of proteins. environments.

## Sample Requirements in Molecular Dynamics Result Analysis

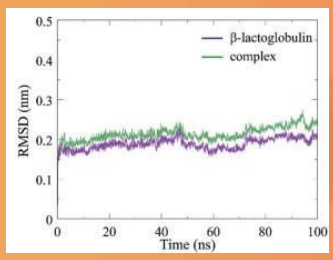


- Molecular dynamics simulation trajectories (in standard formats such as DCD, XTC, or TRR)
- Protein and ligand coordinate files (PDB or PDBQT format)
- Any additional parameters or constraints used in the simulations

# Molecular Dynamics (MD) Simulation

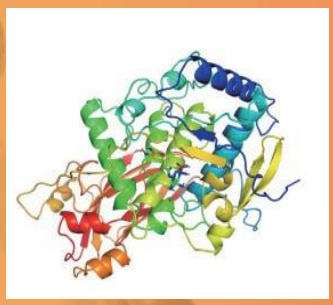
## 01 Structural Stability Assessment

- RMSD, RMSF Analysis Service
- Salt-Bridge Analysis
- Protein-ligand center of mass distance
- Contact Frequency Analysis or Contact Area Analysis
- Radius of Gyration (Rg) Analysis



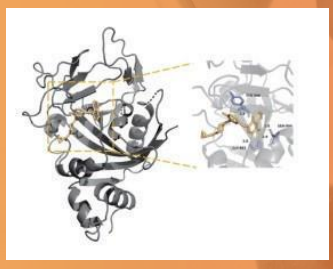

## 02 Interaction Force Assessment

- Interaction Force Assessment
- Hydrogen Bond Analysis Service
- Hydrophobic Interaction Analysis Service
- Electrostatic Interaction Analysis Service
- Macromolecular-macromolecule interaction
- Macromolecular-molecule interaction



## 03 Binding Affinity Prediction

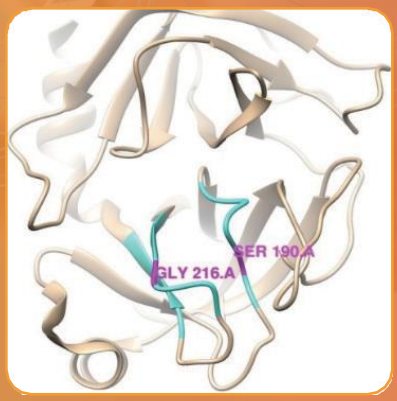
- Binding Free Energy (MMGBSA) Analysis Service
- Binding Free Energy Decomposition Analysis Services
- Binding Mode Analysis Services
- SASA (Solvent Accessible Surface Area) Analysis
- Principal Component Analysis Service



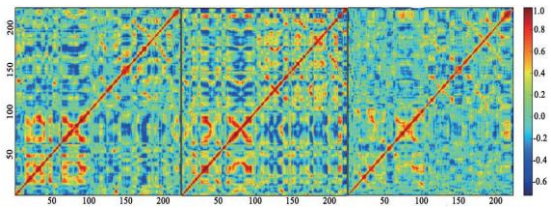
# Project: Molecular dynamics simulations to study the effect of ions on the free radical scavenging ability of specific proteases

## Workflow

- Structural Modelling — Protease structures were constructed using software based on unloaded trypsin structures. Gromacs was used to perform 50ns molecular dynamics simulations.
- Result Analysis — RMSD / radius of gyration / secondary structure / principal components (PCA)/ hydrogen bonding analysis

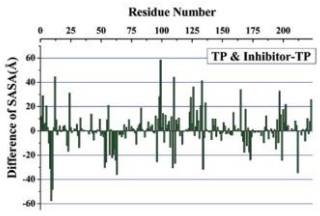


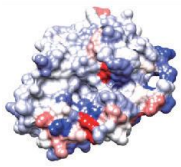

## PCA Analysis



The system as a whole has the most positive correlations, resulting in a more stable conformation of Protease.

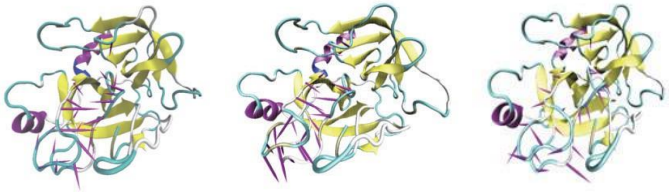
## SASA Analysis



The amino acids with the most pronounced SASA difference values in the system are mainly around the S1 binding pocket in domain A.

## Eigenvector Motion Analysis



The eigenvector motion in the system is more regular and the ions internalise the S1 pocket of the active centre of trypsin.

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Contact Us

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