

A molecular dynamics simulation of a protein pocket. The protein surface is shown as a semi-transparent, multi-colored mesh (teal, yellow, and grey) with a complex, irregular shape. A small molecule, represented by a stick model with red, white, and blue atoms, is positioned within the pocket. The background is dark, making the protein and molecule stand out.

POCKET P.

SIMULATING MOLECULAR DYNAMICS OF POTENTIAL DRUG TARGET REGIONS

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DEFINING THE PROBLEM

RAS FAMILY OF G-PROTEINS

- UNDRUGGABLE
- LACK OF BINDING POCKETS
- UNEXPLORED DYNAMIC STRUCTURE

GOAL

IDENTIFY THE SHAPE & LOCATION
OF TRANSIENT POCKETS

SCOPE



DATA ANALYSIS

LOCATE POCKET

FIND VOLUME OF POCKET

TRACK POCKET STABILITY
OVER TIME



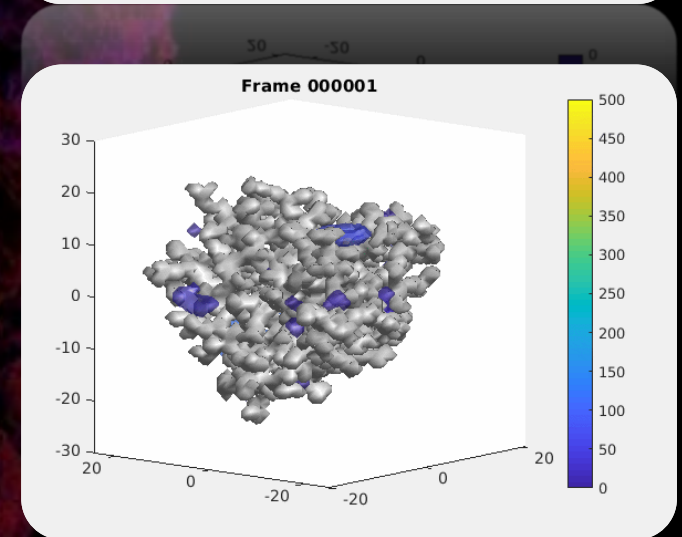
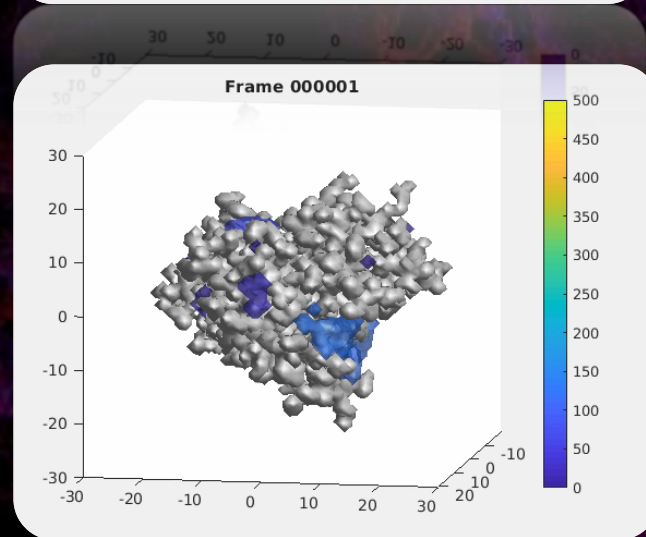
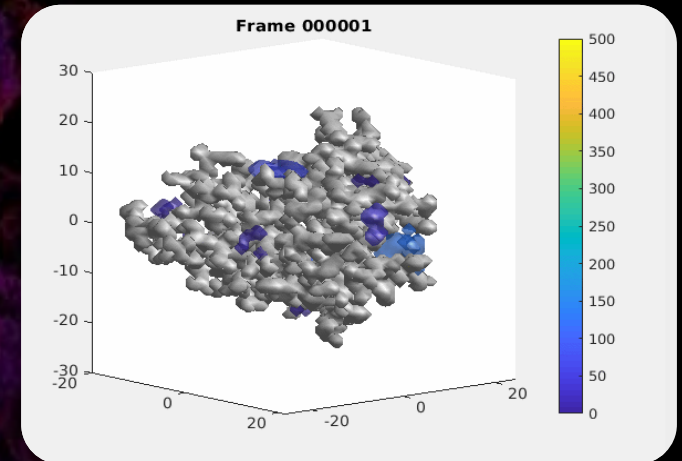
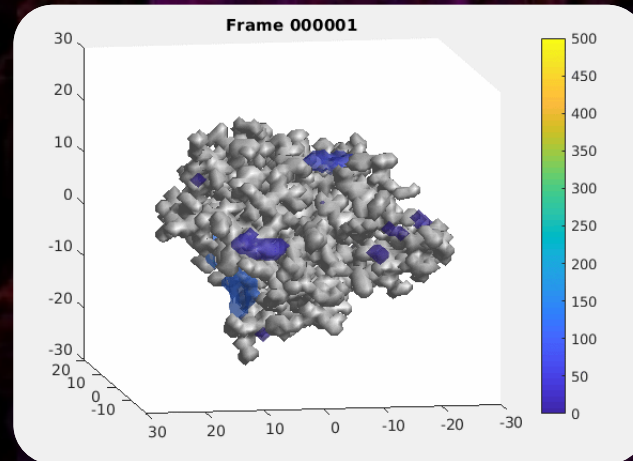
VISUALIZATION

3D IMAGE OF EACH FRAME

REAL TIME VIDEO MODUEL

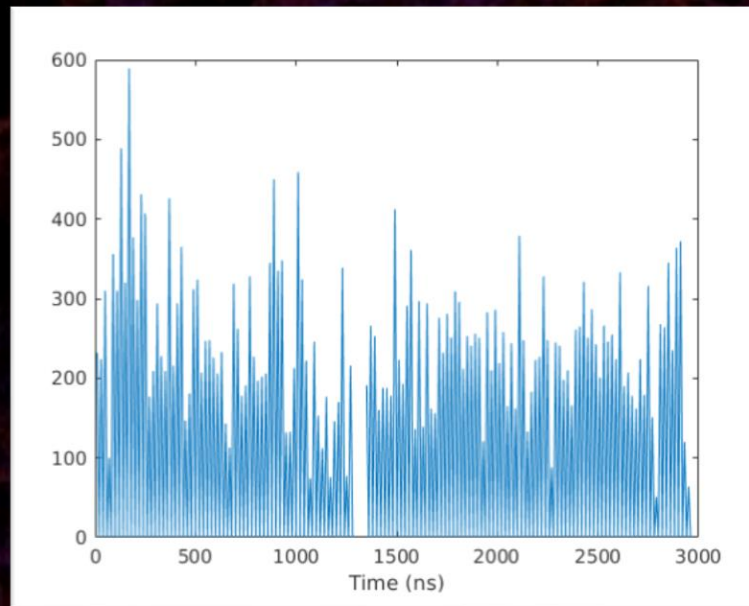
VISUALIZATION

20 microsecond long simulation



DATA ANALYSIS

EXAMPLE OF DISCOVERED POCKET



POCKET VOLUME OVER TIME



PYMOL RENDERING OF POCKET