

The background of the slide is a molecular dynamics simulation of a protein's binding pocket. The protein surface is represented by a semi-transparent, wavy mesh in shades of teal and grey. A yellow, semi-transparent surface highlights a specific region within the pocket. A small molecule, likely a drug candidate, is shown in a stick representation with grey carbon atoms, red oxygen atoms, and blue nitrogen atoms, positioned within the highlighted yellow region. The title 'POCKET P.' is overlaid in a large, white, outlined font.

POCKET P.

SIMULATING MOLECULAR DYNAMICS OF POTENTIAL DRUG TARGET REGIONS

MIKE TRENFIELD

MILO LIN

JOHN YOO

UMBERTO CIRI

KEVIN NGUYEN



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



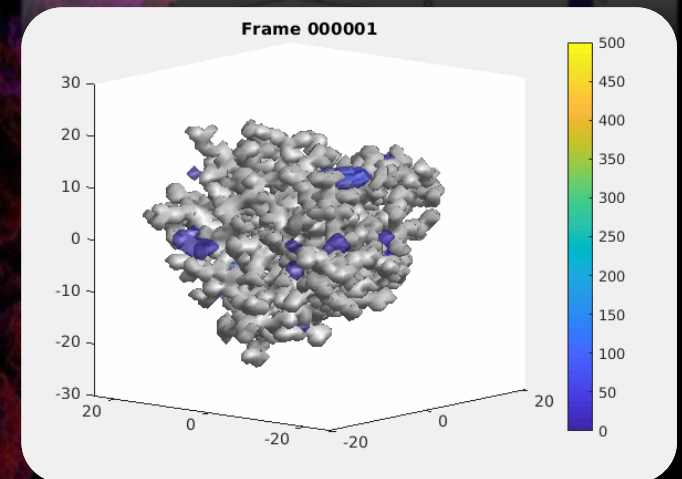
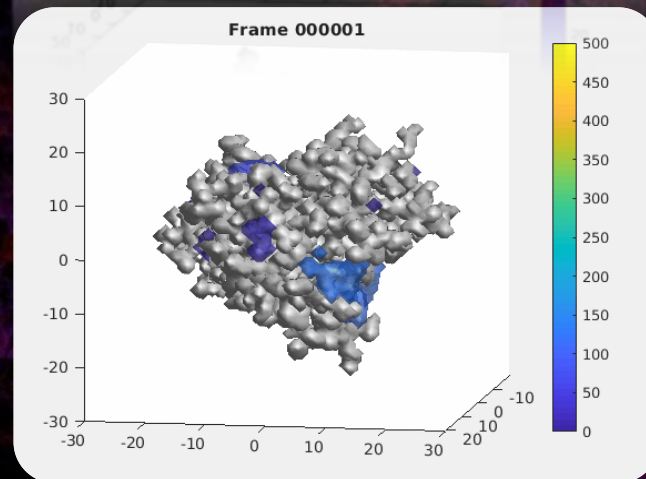
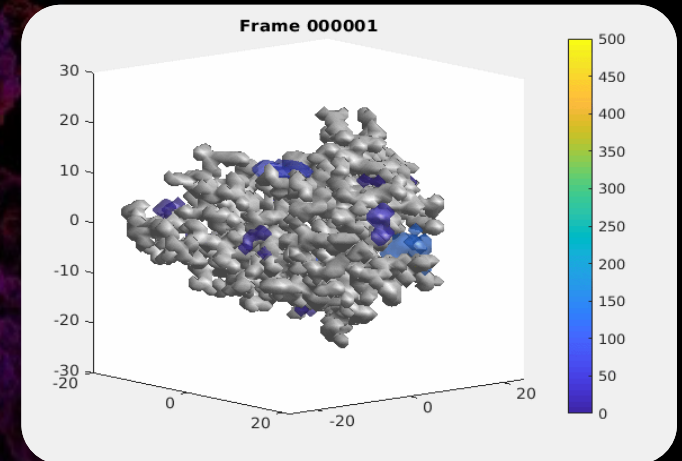
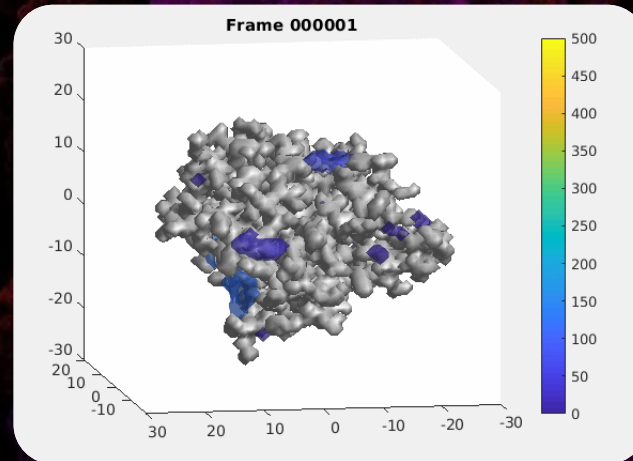
VISUALIZATION

3D IMAGE OF EACH FRAME

REAL TIME VIDEO MODULE

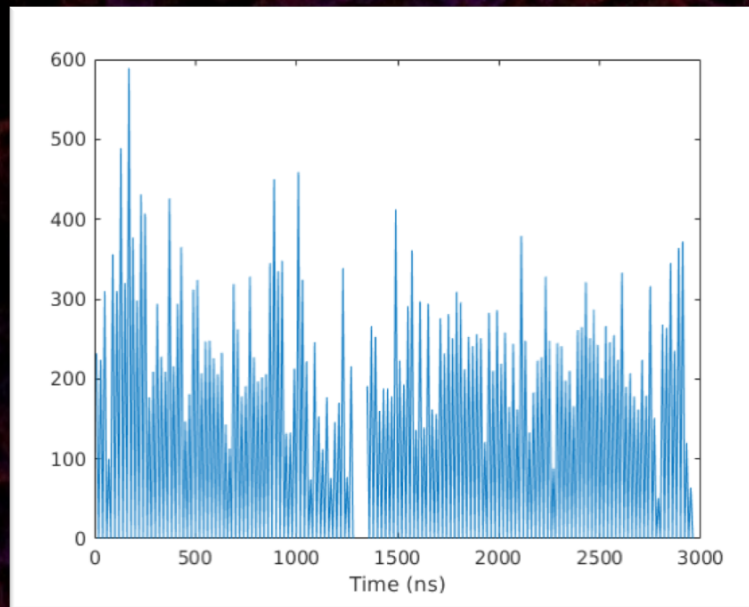
VISUALIZATION

20 microsecond long simulation



DATA ANALYSIS

EXAMPLE OF DISCOVERED POCKET



POCKET VOLUME OVER TIME



PYMOL RENDERING OF POCKET