



# POGORELOV LAB: MOLECULAR INFORMATION TRANSFER IN THE CELL

Department of Chemistry, Center of Biophysics and Quantitative Biology, School of Chemical Sciences,  
Beckman Institute for Advanced Science and Technology, National Center for Supercomputing  
Applications, University of Illinois at Urbana-Champaign, URL: pogorelov.scs.illinois.edu E-mail: pogorelo@illinois.edu



TARAS  
POGORELOV  
Research Assistant  
Professor



VADIM  
MUSTAEV  
Research  
Programmer



KEVIN  
CHENG  
PhD student Biophysics  
Research Interests:  
Developing workflows to  
characterize protein-lipid  
interactions



SHASHANK  
SHASTRY  
PhD student  
Biophysics



SEPEHR  
ALAEEN  
PhD student  
Biophysics,  
co-advised with  
Martin Gruebele



AINGARAN  
BALA RAMAN  
PhD student Chemical  
and Biomolecular  
Engineering,  
co-advised with  
Baron Peters



MELANIE  
BRUNET  
Chemical and Biomolecular  
Engineering, co-advised  
with Mary Kraft  
Fellow, NIH



IMMANUEL (MANI)  
SCHMIDT  
Biophysics, co-advised  
with Martin Gruebele



JUAN DAVID  
CAMPOLARGO  
Engineering  
Class of 2024



ANIKA  
HONG  
Bioengineering  
Class 2026

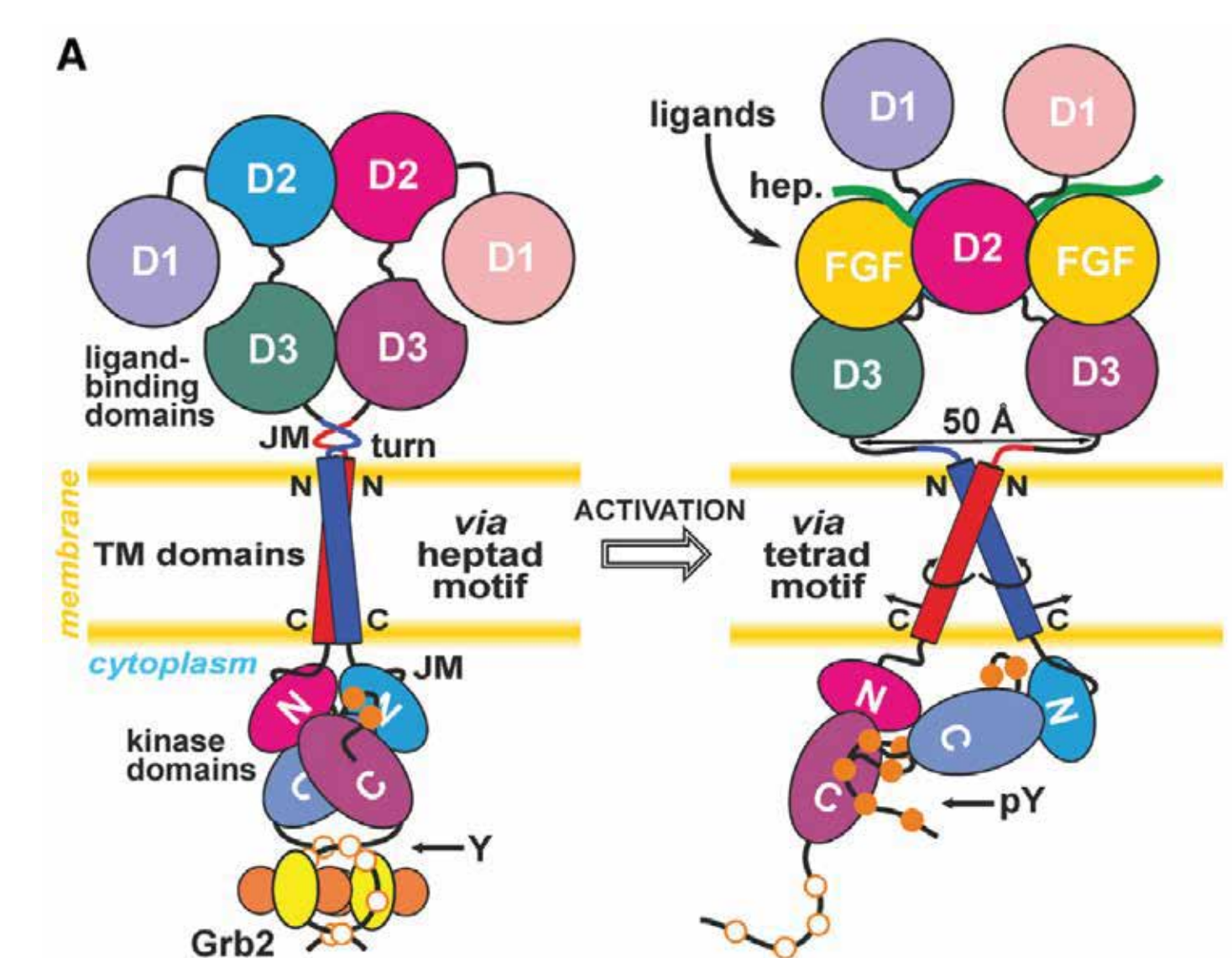


HAJUN  
LEE  
Bioengineering  
Class 2026

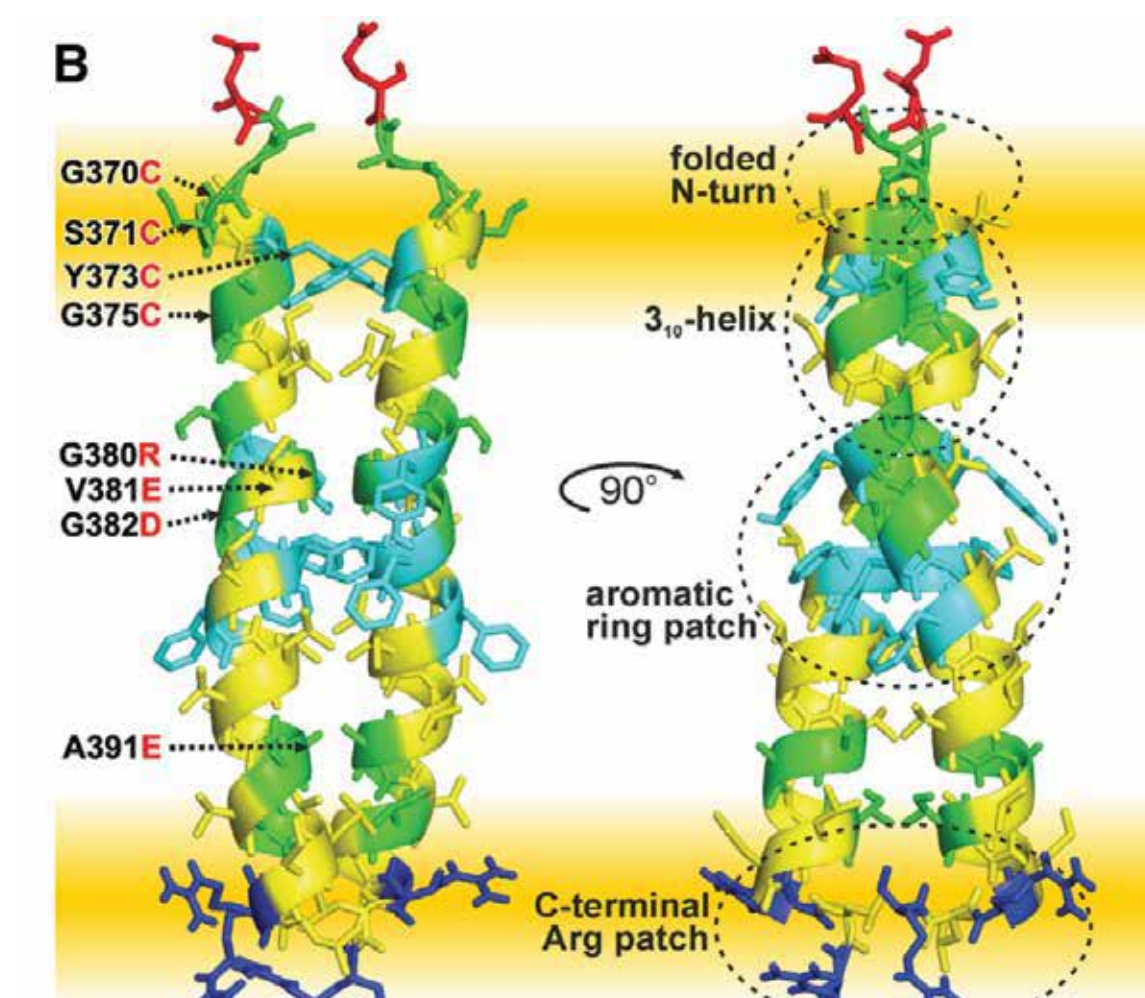
Collaborators: Kalina Hristova (JHU), Kai Zhang, Chad Rienstra (U Wisconsin-Madison)

## Signaling through cell membranes

Receptor tyrosine kinases: dimer structures and pathological mutations



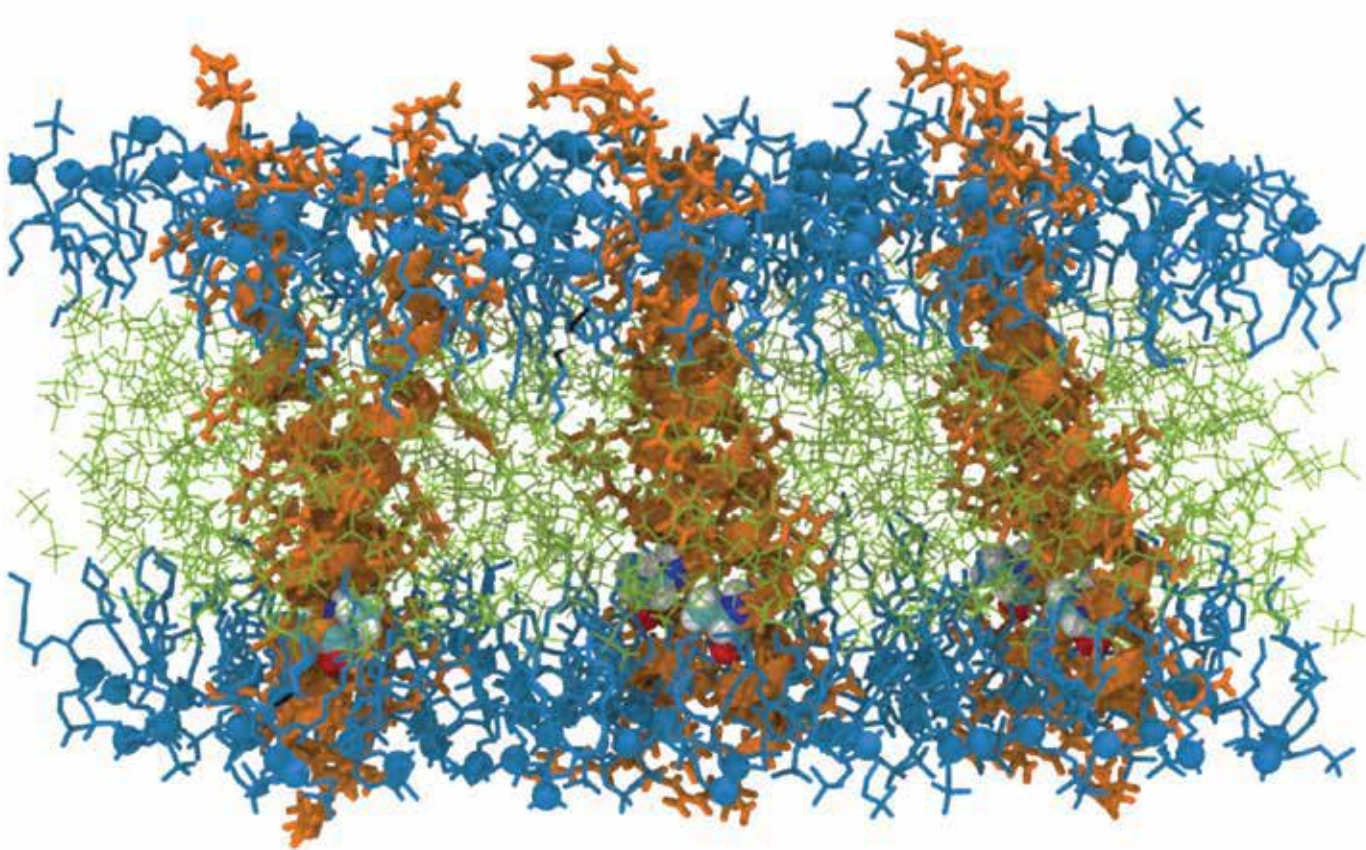
Fibroblast growth factor receptor FGFR3-TM  
– human receptor tyrosine kinase  
– dimer (33/43 res) PDB ID 2LZL (micelle)  
– extended heptad motif: YA<sub>37</sub>X<sub>1</sub>L<sub>1-377</sub>X<sub>2</sub>G<sub>380</sub>X<sub>2</sub>FF<sub>384</sub>X<sub>2</sub>IL<sub>386</sub>X<sub>2</sub>A<sub>391</sub>



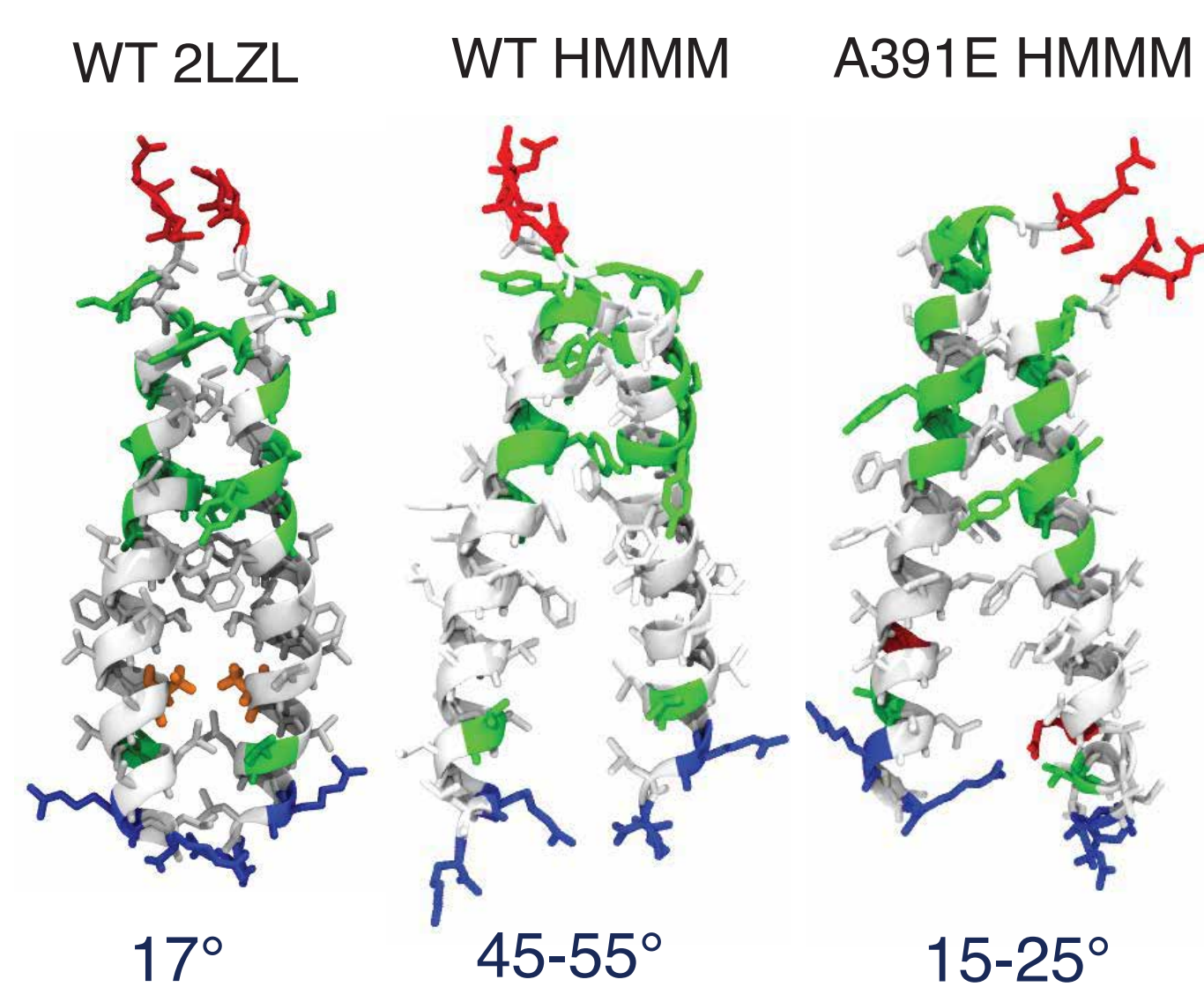
Bocharov, E.V., et al., Structure 21, 2087–2093, 2013

FGFR3-TM A391E mutant  
– development disorders and cancer  
– increases dimerization and activation

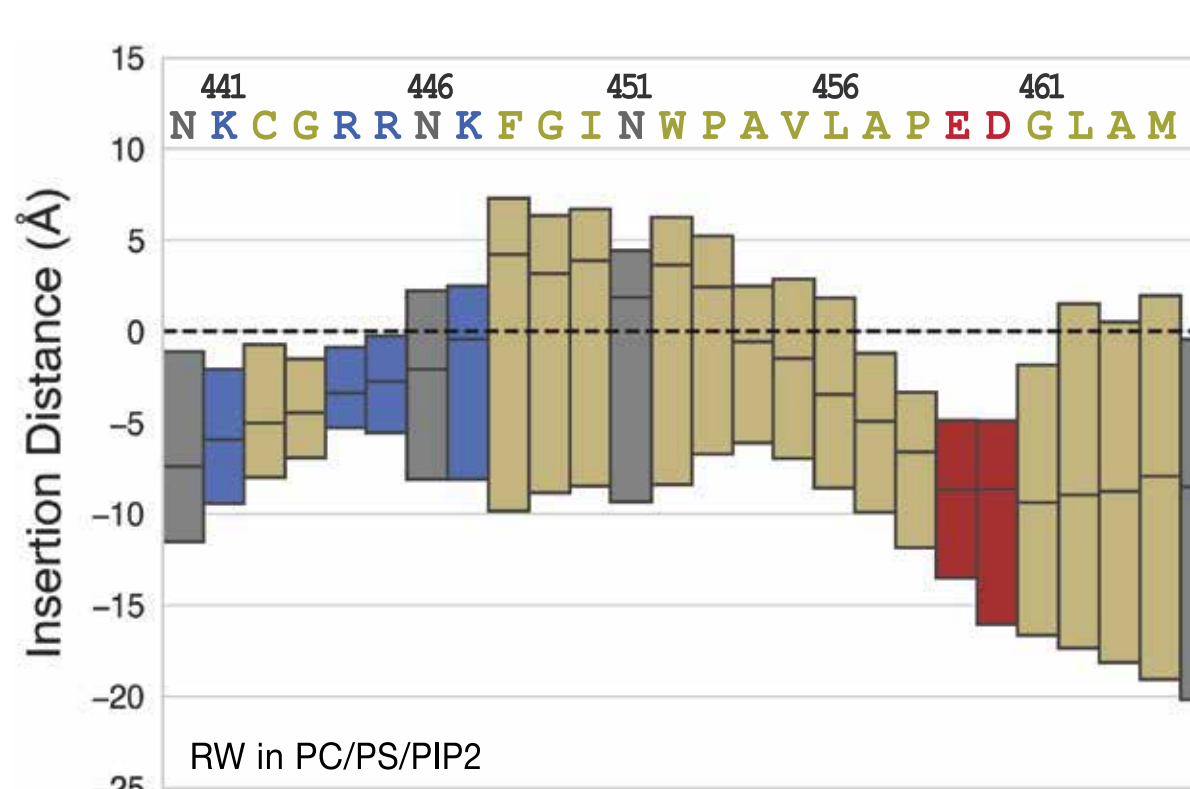
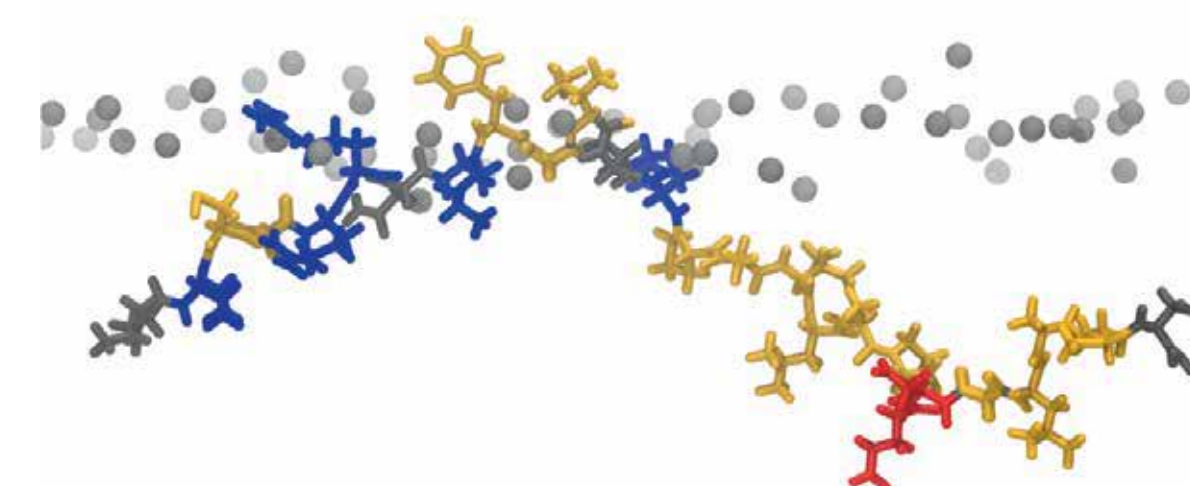
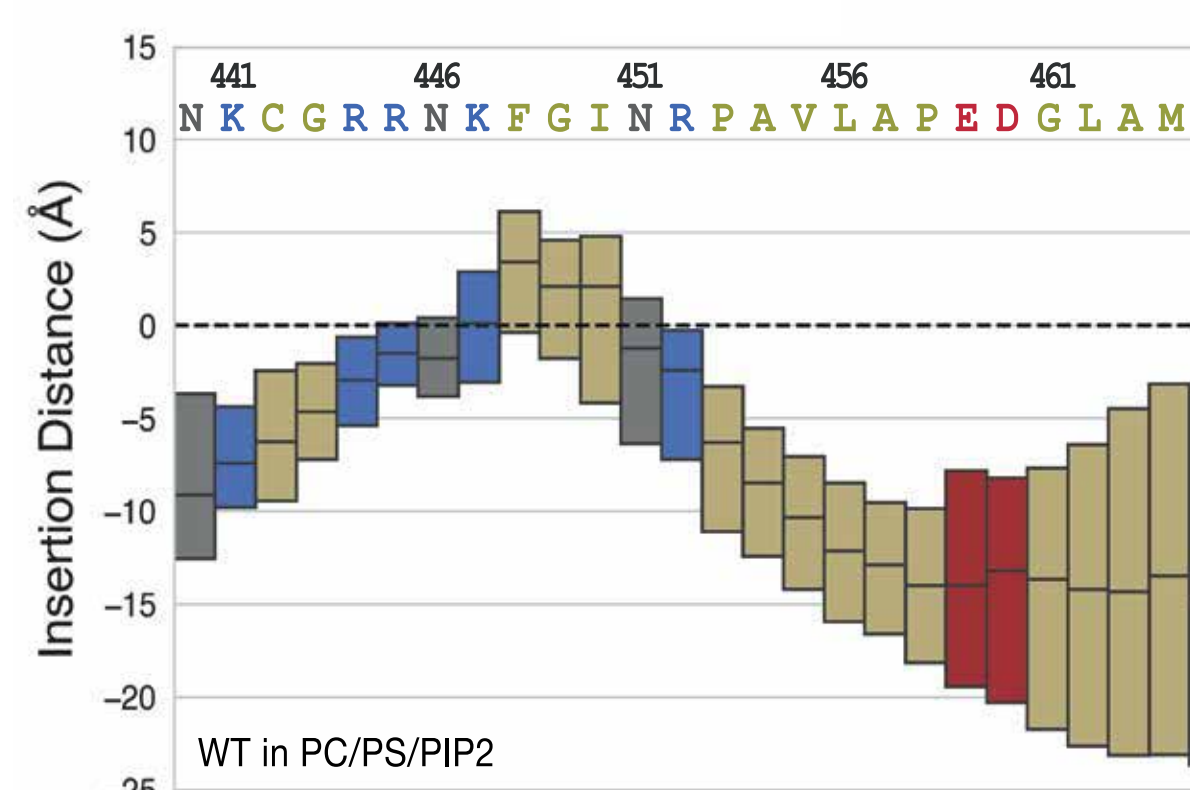
Spontaneous TM dimer formation:  
MD with HMMM



TM domain structure influenced by  
pathological mutations



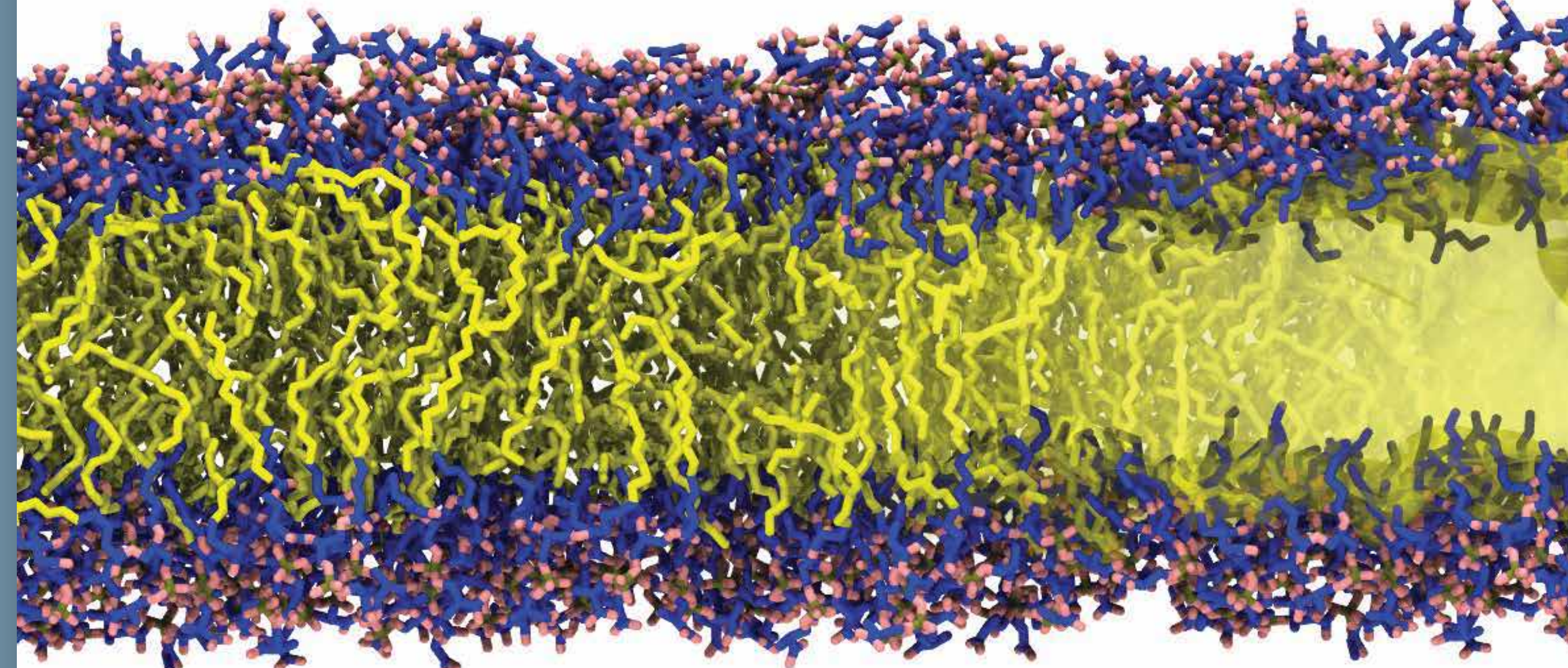
Disordered TrkA juxtamembrane  
domain insertion into membrane



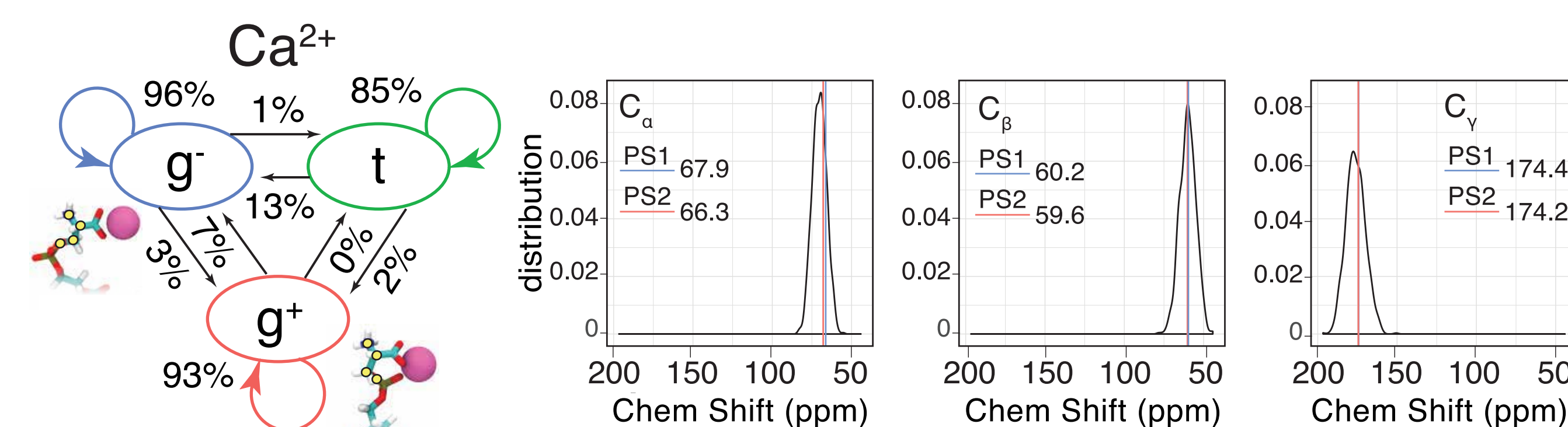
Collaborators: Chad Rienstra, Marty Burke, Jim Morrissey, Emad Tajkhorshid

## Membrane-associated phenomena

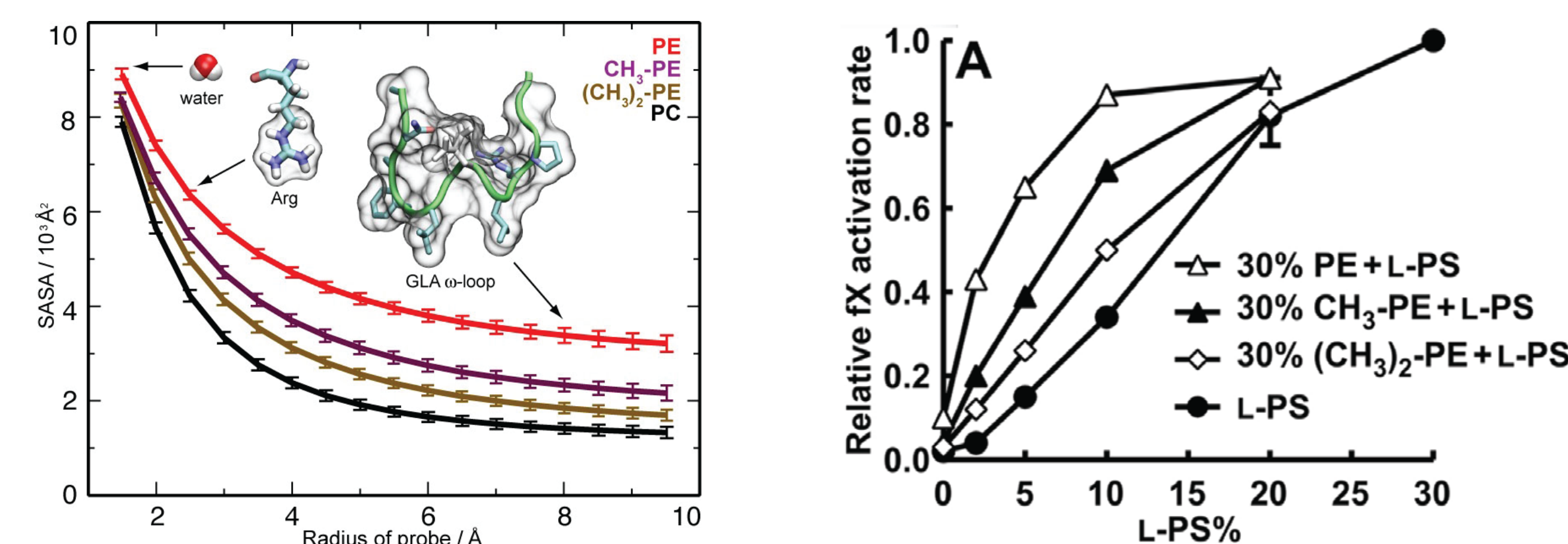
HMMM: Highly Mobile Membrane Mimetic Model



Membrane sculpting by charges: phosphatidylserine and calcium

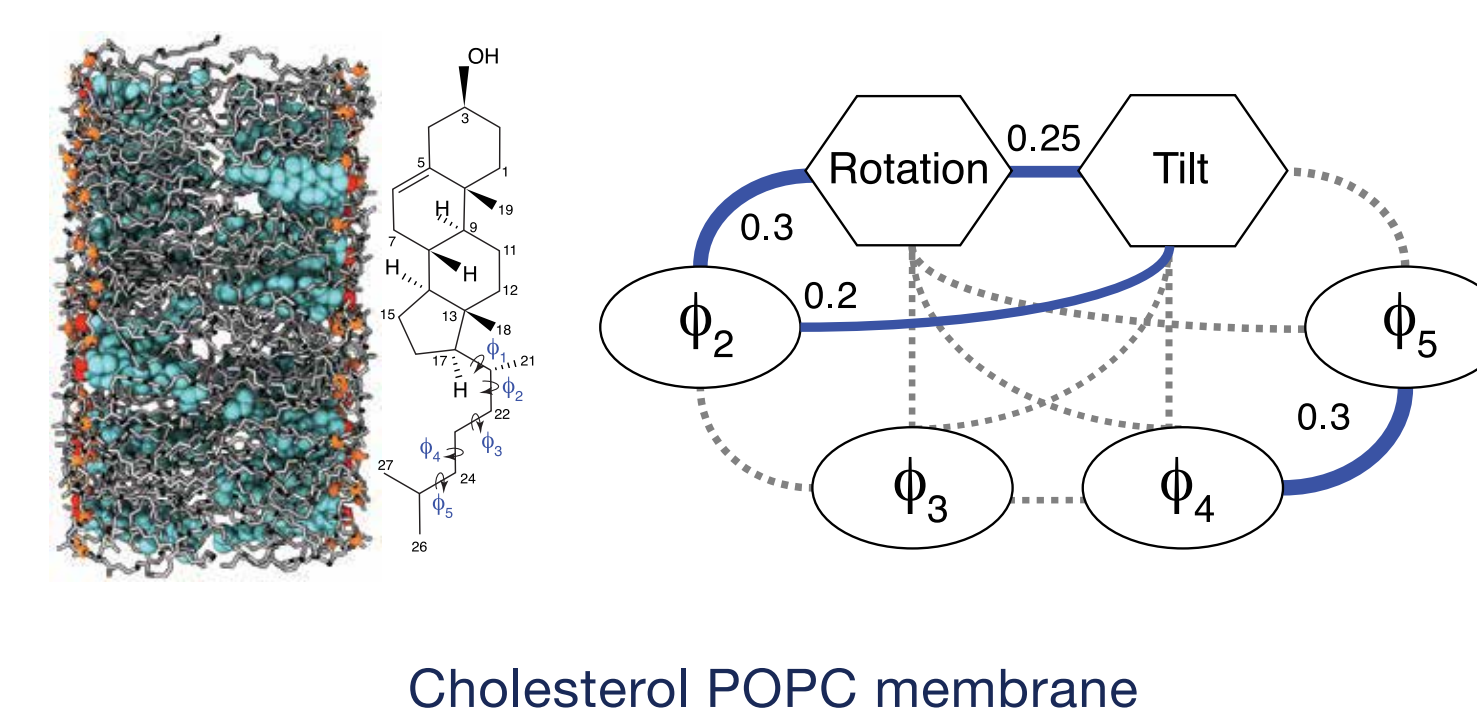


Membrane as platform for protein activation: blood coagulation cascade

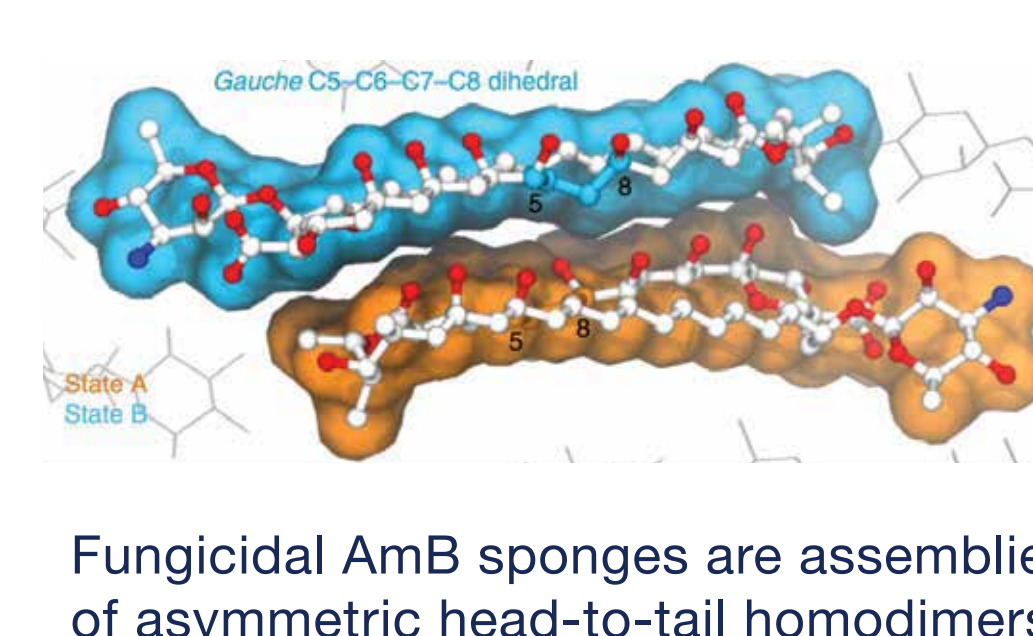


Membrane active agents and sterols

Cholesterol dynamics in membrane is coupled



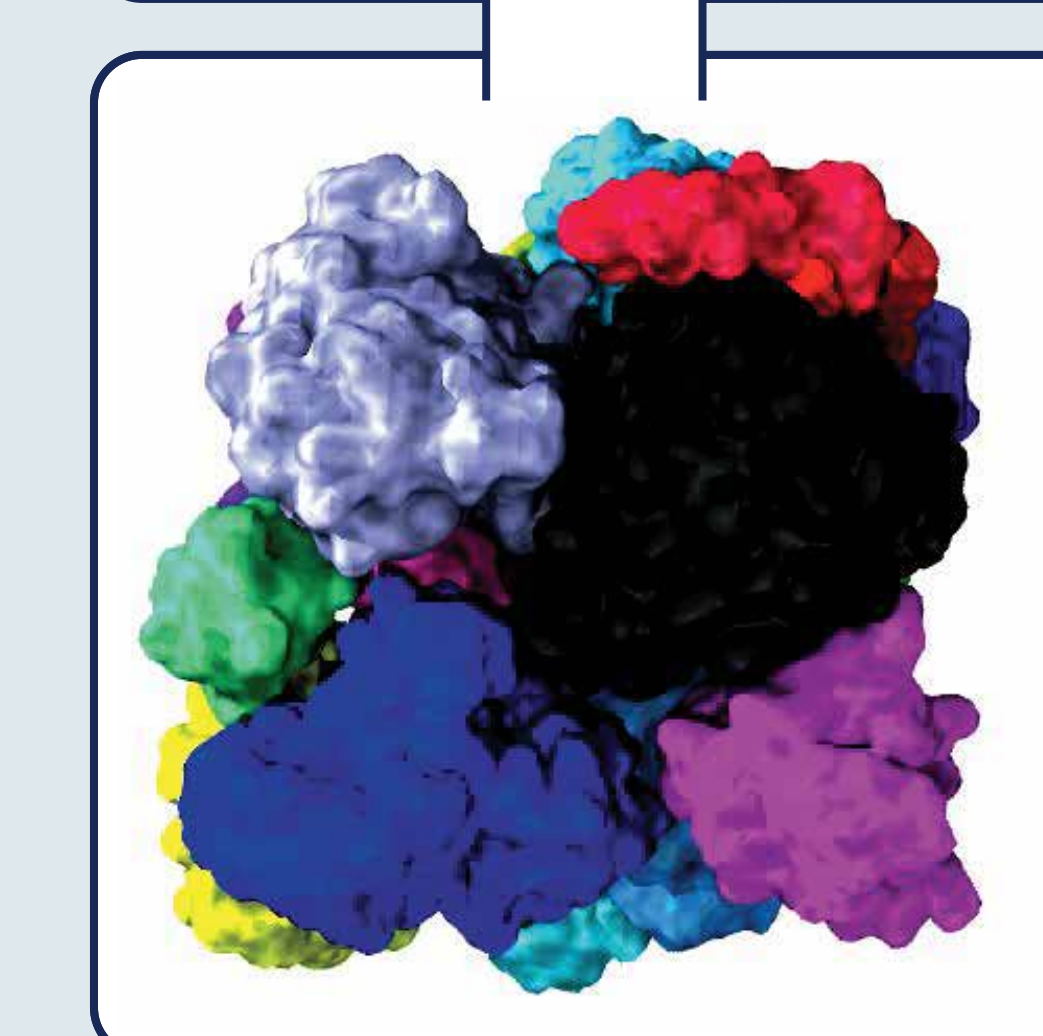
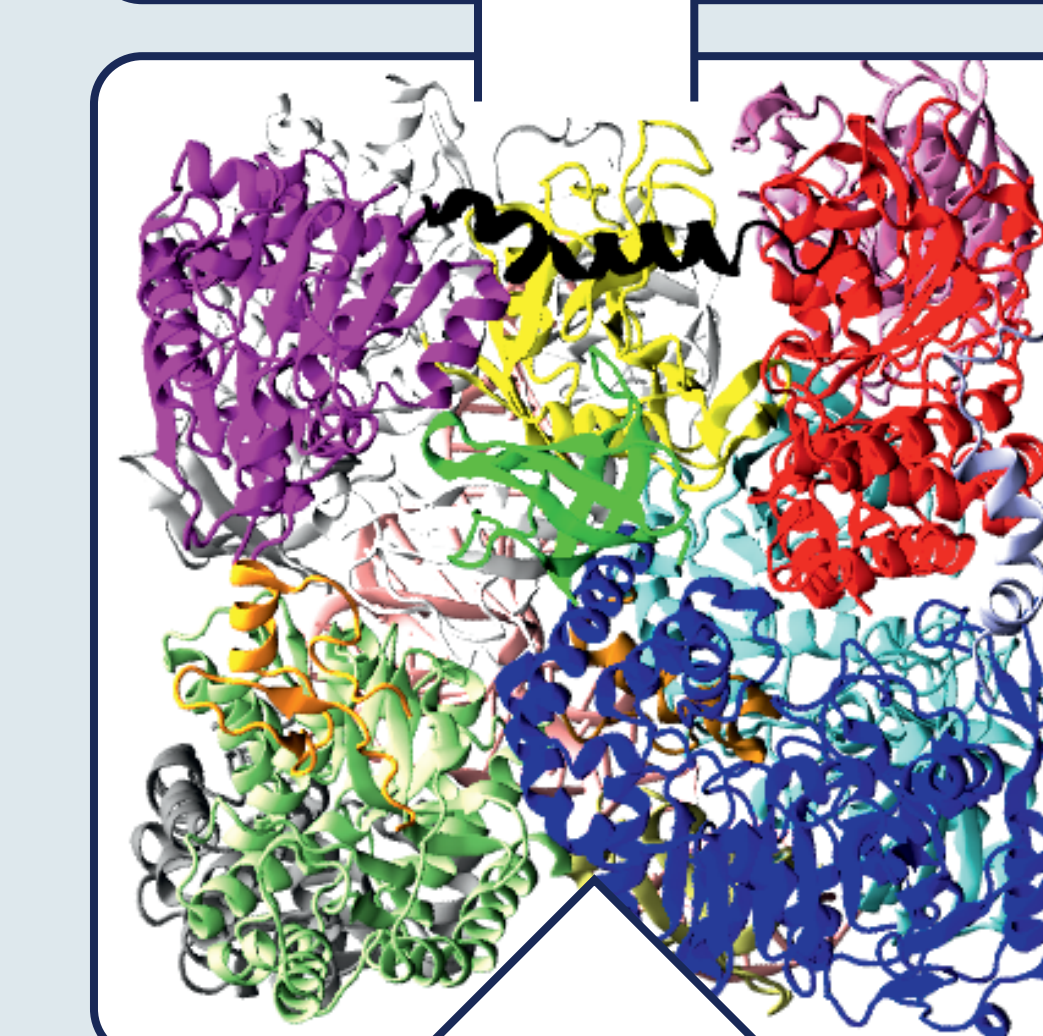
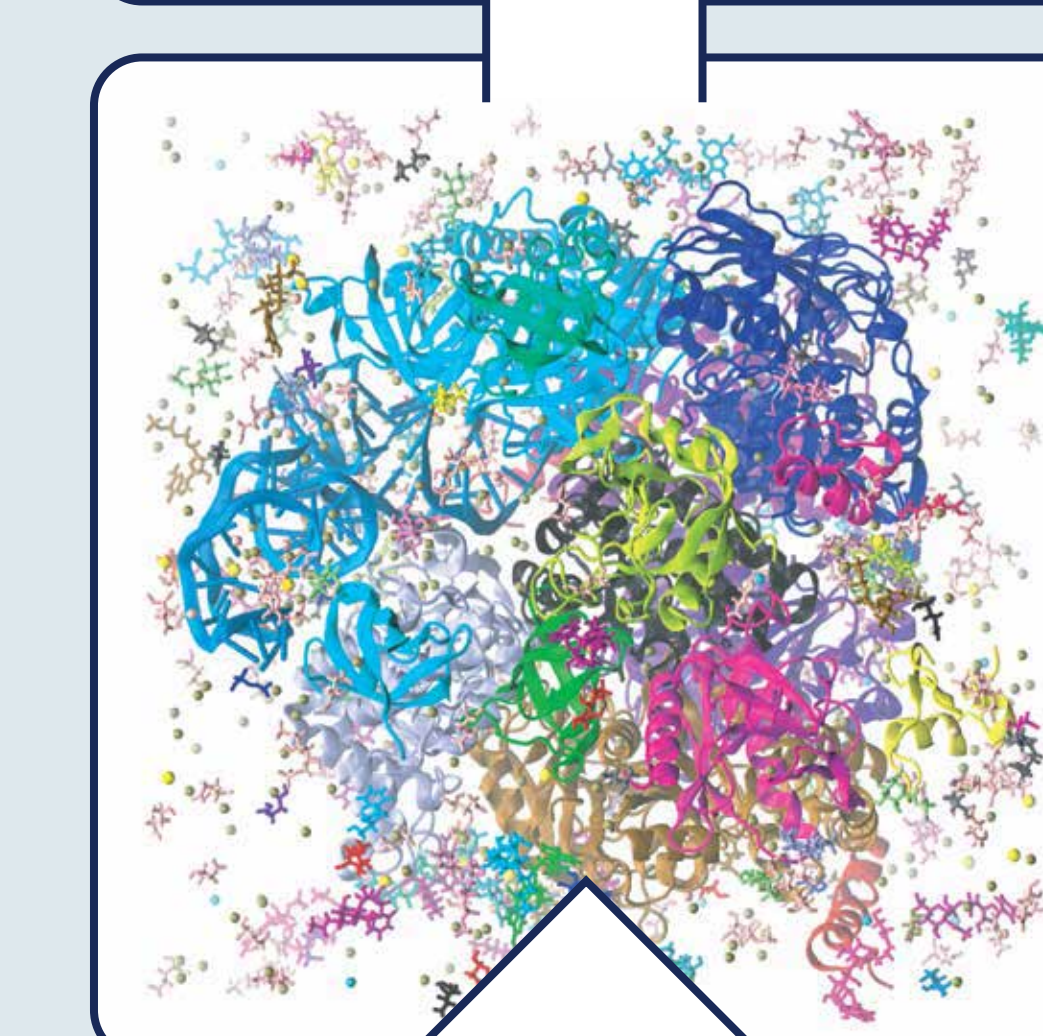
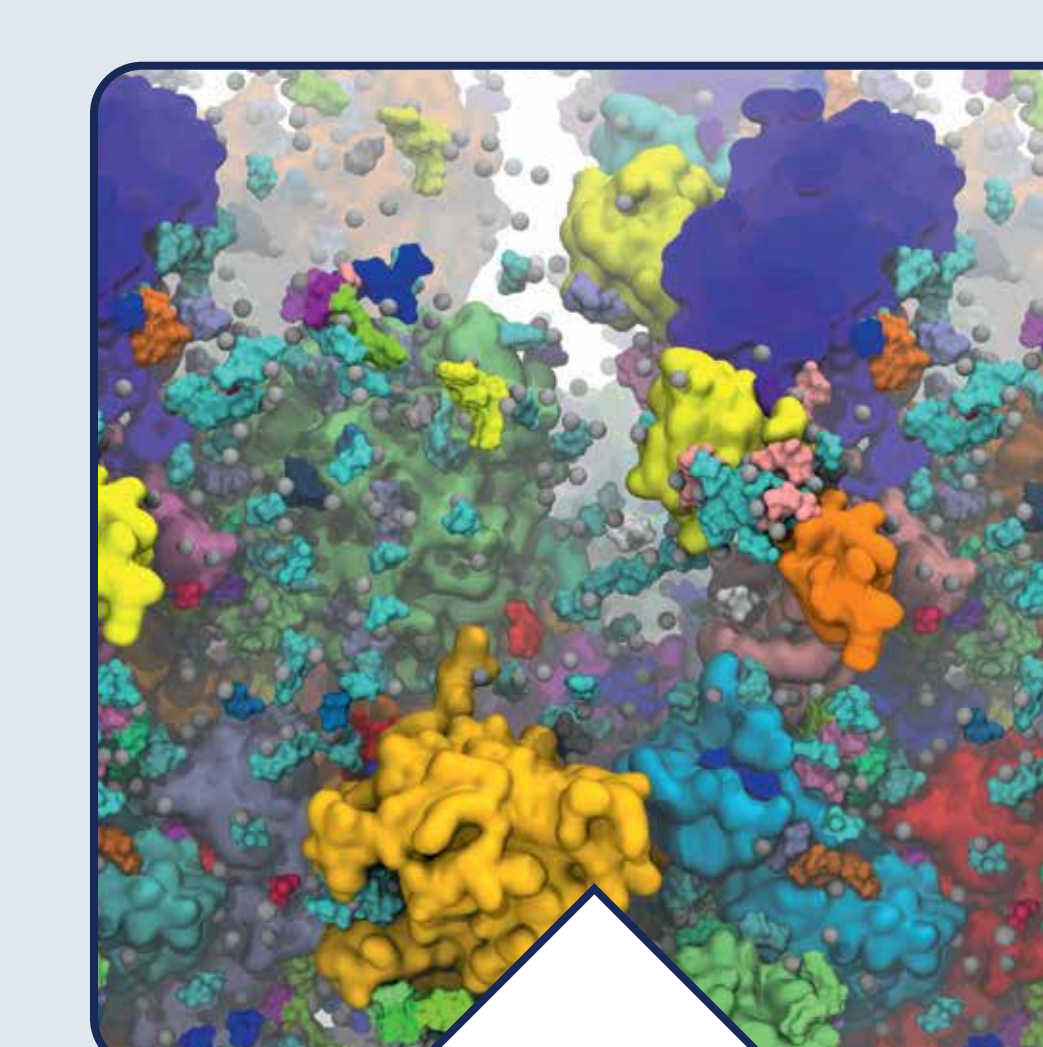
Antifungal drugs:  
Amphotericin B (AmB)



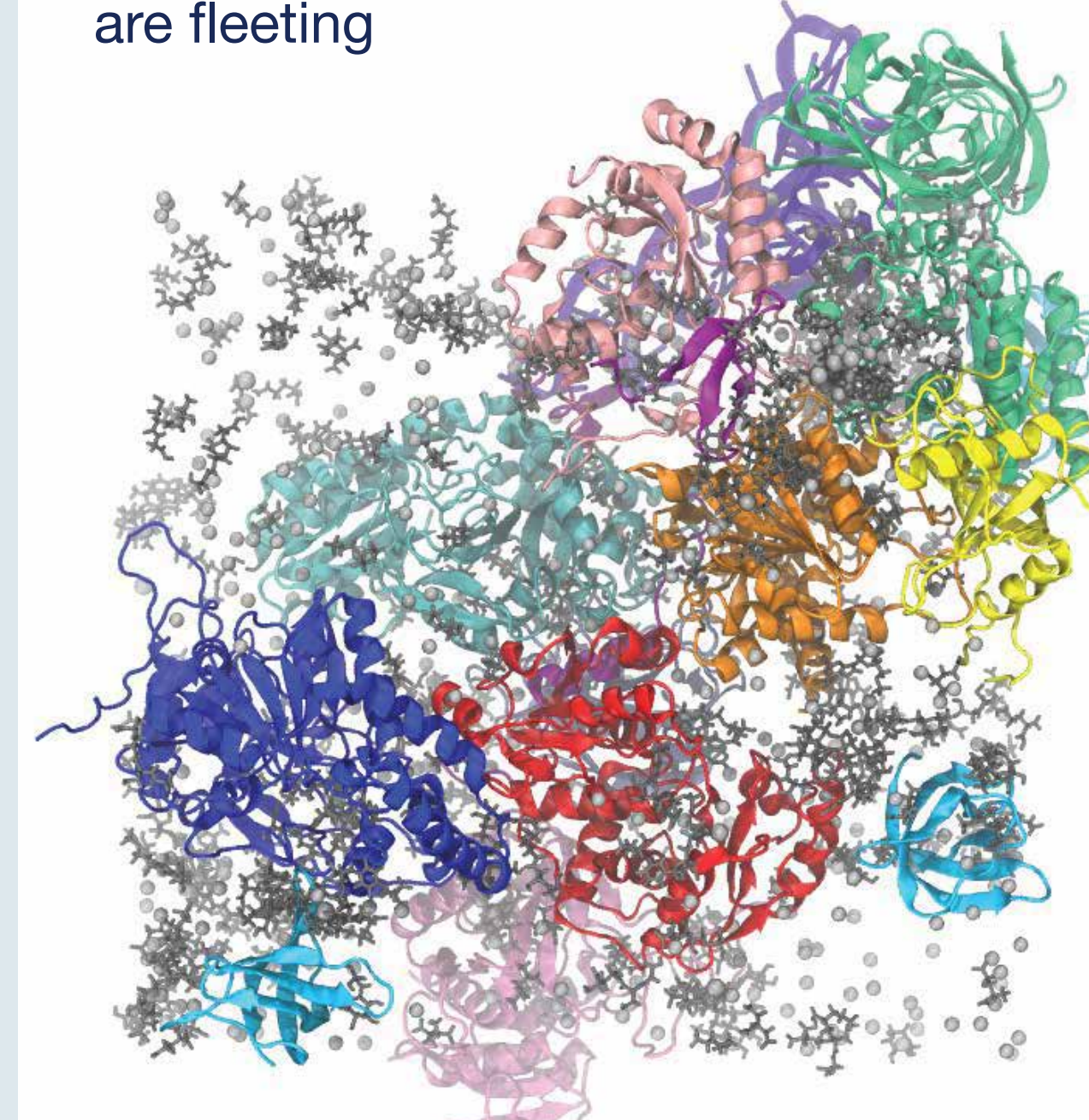
Collaborators: Martin Gruebele, Matthias Heyden (ASU)

## In silico cell: protein dynamics

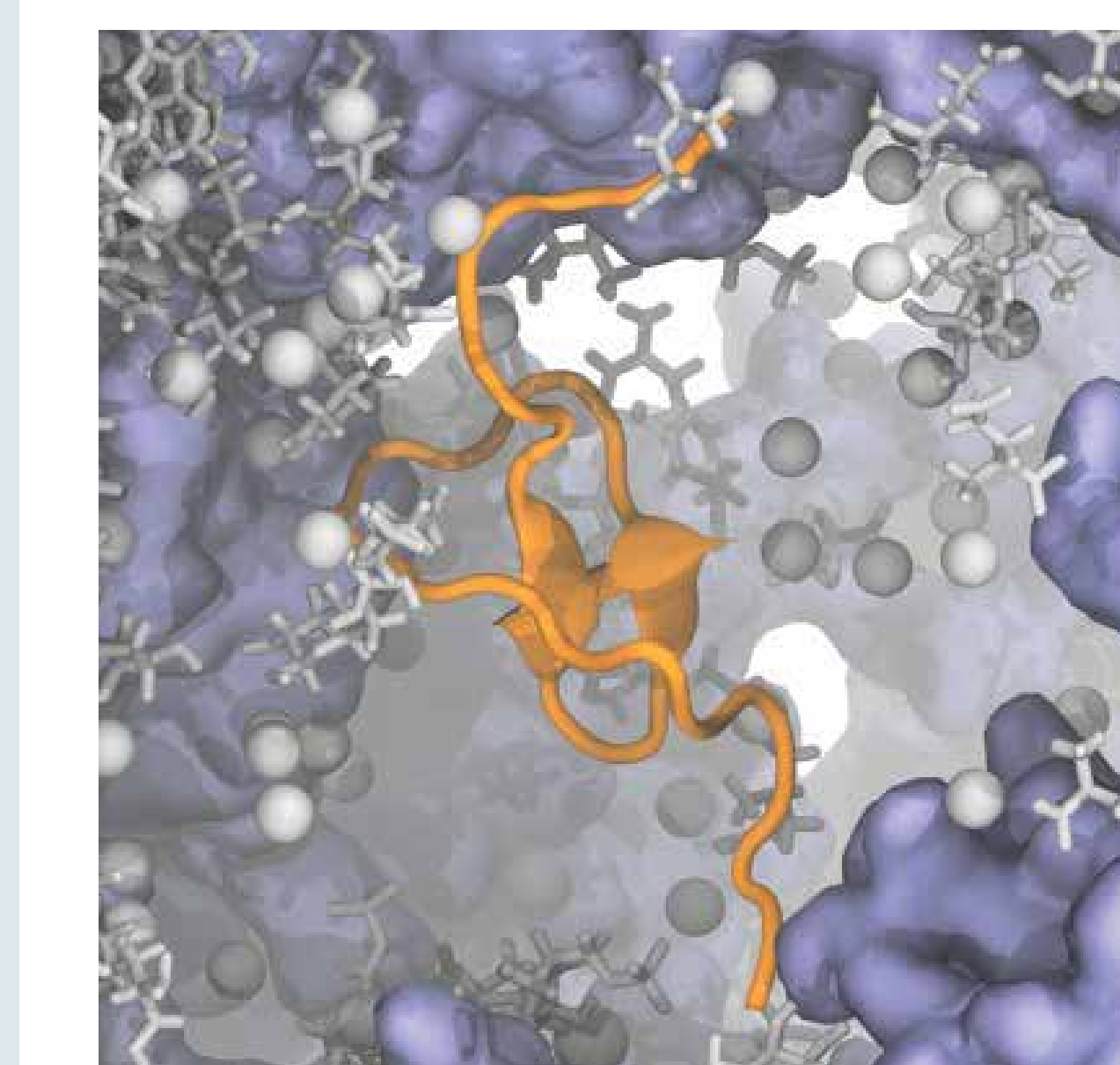
Building cytoplasm models: *E. coli*



Transient protein-protein interactions  
are fleeting



WW domain folding: secondary &  
“chimeric” structures



ATP dynamics is impacted

