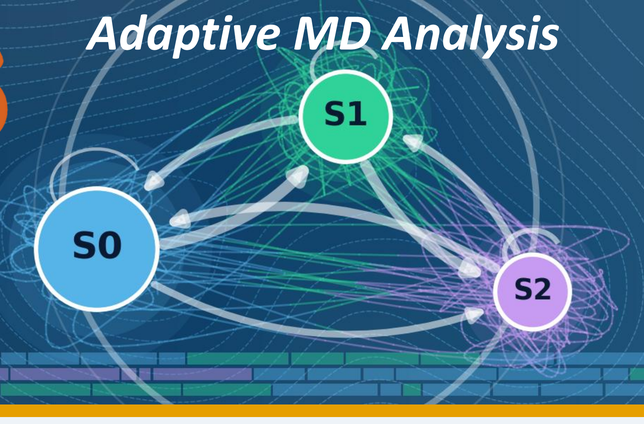
ConformaLens

Conformational states in Adaptive Molecular Dynamics

VIS2026 biovis

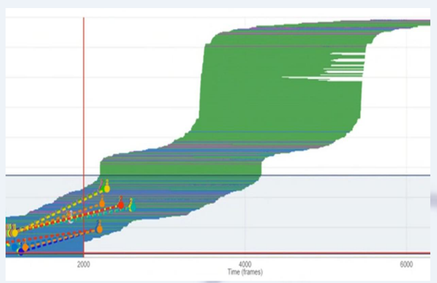


Hossein Fathollahian[1,*], Siyuan Zhao[1], Marziye Salahshour[2], Saeed Boorboor[1], G. Elisabeta Marai[1]

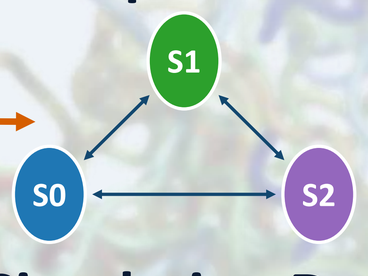
[1]University of Illinois Chicago [2]Rush University Medical Center *hfatho2@uic.edu

? How can visual analytics reveal which conformations and residue interactions drive Markov-state transitions of Aβ42, and how TMP and SPA change them, across entire adaptive-MD ensembles?

Visual Exploration of Aβ42 Dynamics



Ensemble
320 /system
16 epochs of 20 short **cluster** runs, reseeded adaptively



MSM states
2–4 states
VAMPnets cluster frames; transitions link the states



3D structure
42 residues
Atomic geometry behind each state: contacts, ligands

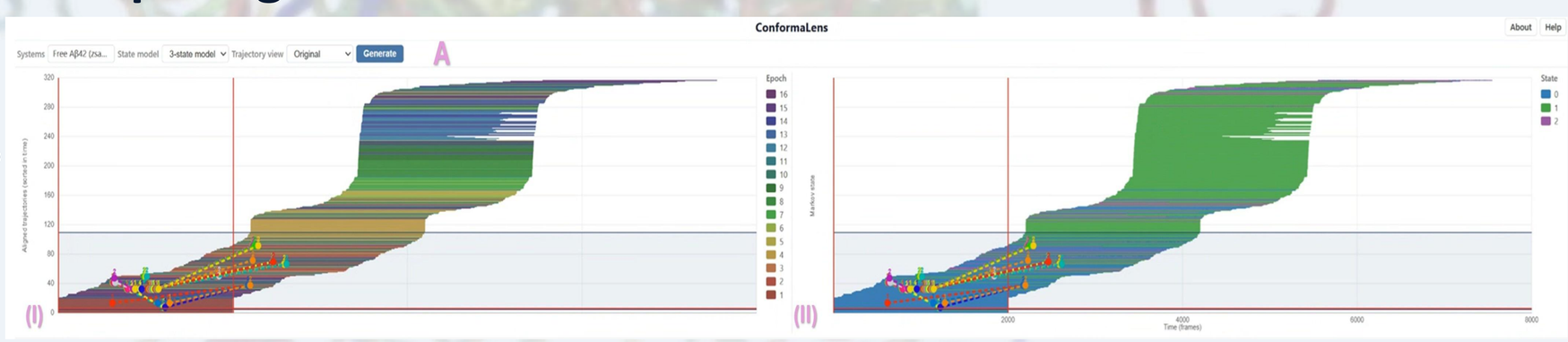
From Simulation Data to Interactive Views

INPUTS	DERIVE	LINK	COORDINATED VIEWS
Free / + TMP / + SPA	Representative frames	System	Step 1 Timelines: epochs and states overview
MSM assignments (3-state)	Structural descriptors	Trajectory	Step 2 Footprints: occupancy and transition rates
Trajectory order	Residue / atom distances	State	Step 3 StateSignature, StateDriver, 3D interactive view
Concatenated paths	Ligand-contact statistics	Frame	

Comparing Ensembles and State Transitions

Step 1 Explore ensemble coverage

View trajectories across epochs and states to identify sampling coverage and persistent states.



Brush a window → compare transition rates

Step 2 Compare state transitions

Compare footprint matrices and transition rates to examine how TMP- and SPA-bound ensembles differ from free Aβ42.



Select a state or frame → inspect residues and 3D

Step 3 Inspect structural context

Explore contact glyphs linked to interactive 3D structures to connect states with residue interactions and individual frames.

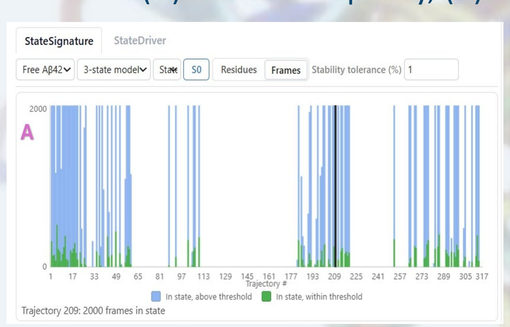


Connecting Conformational States to Residue Interactions

StateSignature

Which frames represent a state?

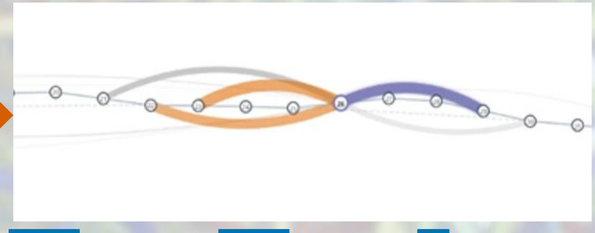
(A) frame occupancy, (B) residue-pair proximity heatmap



StateDriver

Which residues interact?

Non-local residue–residue and residue–ligand

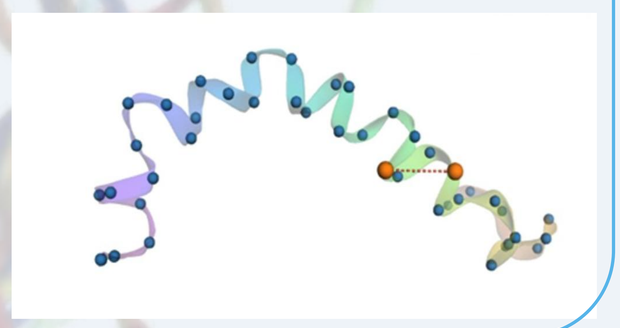


Width → frequency
Opacity → persistence
Length → proximity

3D Viewer

Where does it happen?

Ribbon with state markers and contact links



Key Insights

Linked views
Selections in timelines and matrices sync with StateSignature, StateDriver, and 3D.

Ligand effects at a glance
Gray marks behavior similar to free Aβ42; color marks deviations.

Responsive at scale
Precomputed descriptors keep large free, TMP, and SPA datasets interactive.

Evaluation

How: Task-based evaluation, rate 10 statements

Step 1: Overview
Step 2: Comparison
Step 3: Reasoning

4.0–4.8 / 5 mean rating

Who: 5 visualization researchers at EVL, UIC

Result: Coordinated views and linked interactions are valued

Limitations & Future Work

Evaluation scope
Five visualization researchers; a domain-expert study is the next step.

Offline descriptors
Structural measures are precomputed, not recomputed in the browser.

Generalization
Tested on Aβ42 with TMP and SPA; extend to other peptides and ligands.

Source code https://github.com/Hosseinfatho/BioMedVis2026

Paper

Visualization Dashboard Interface https://hosseinfatho.github.io/BioMedVis2026/

Funding: NIH NCI R01CA258827 · NIH UG3 TR004501 · NSF CNS-2320261 · UIC Institute for Health Data Science Research.

Data: Bio+MedVis Challenge 2026 (Masaryk Univ., CTU Prague; CoVAMPnet).