

# **Supporting Information**

**Order Through Disorder :  
Hyper-mobile C-terminal Residues  
Stabilize the Folded State of a Helical Peptide.  
A Molecular Dynamics Study.**

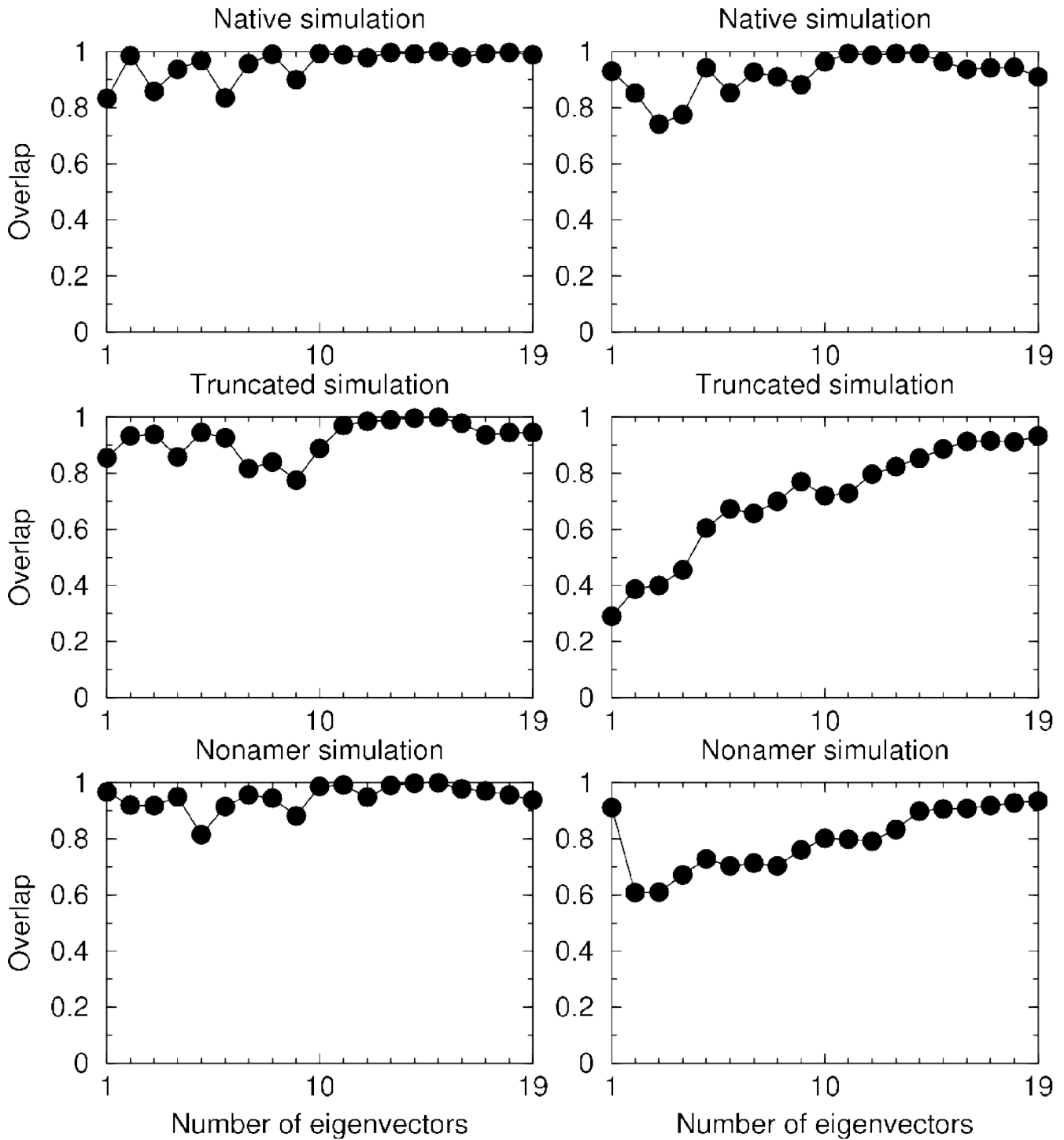
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# Sufficient sampling

Cartesian PCA

Dihedral PCA



**Sufficient sampling:** Eigenspace overlap as a function of the number of eigenvectors for all three simulations and using both Cartesian (left column) and dihedral (right column) PCA.

# Determination of rmsd cutoff for folded structures

## Truncated simulation

Distribution of RMSDs from helical structure (only 1–7)



**Determination of rmsd cutoff for folded structures:** Histogram of the distribution of the RMSDs of the truncated peptide's simulation from the representative  $\alpha$ -helical structure. The folded (helical) structures correspond to the first peak from the left. The minimum of the histogram separating the folded helical structures from the next peak is at 0.78Å (indicated by an arrow head in the figure above).