Supplementary material for

Markov state models from hierarchical density based assignment

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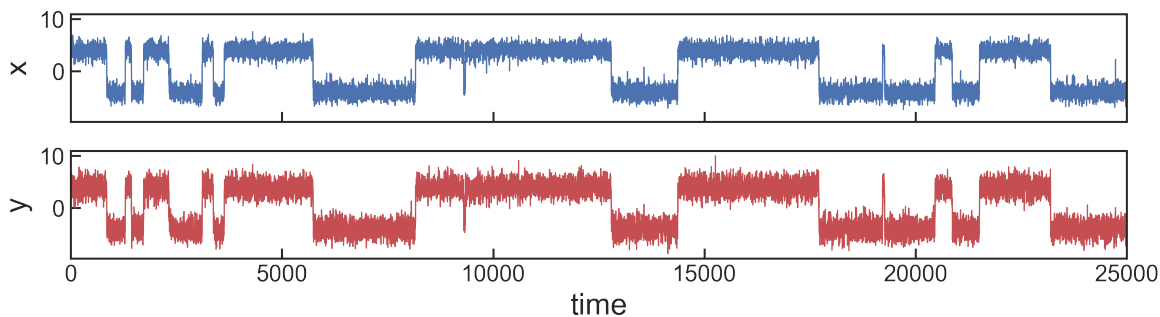[a]Electronic mail: david.desancho@ehu.eus

FIG. S1: Time series data corresponding to the brownian dynamics trajectory on a two-dimensional potential.
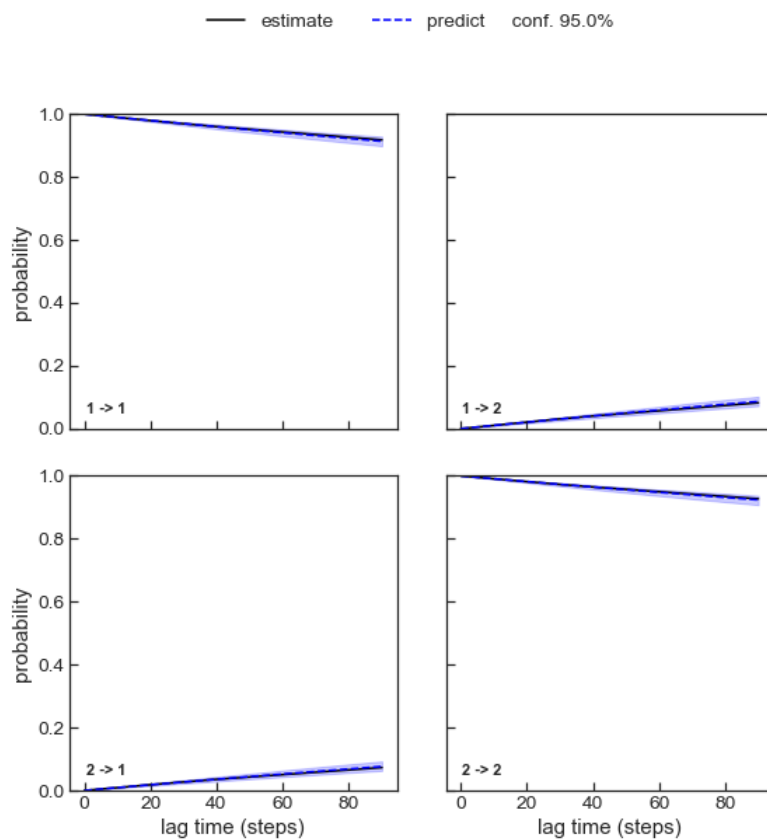

FIG. S2: Chapman-Kolmogorov tests corresponding to the two-dimensional potential from PCCA+.
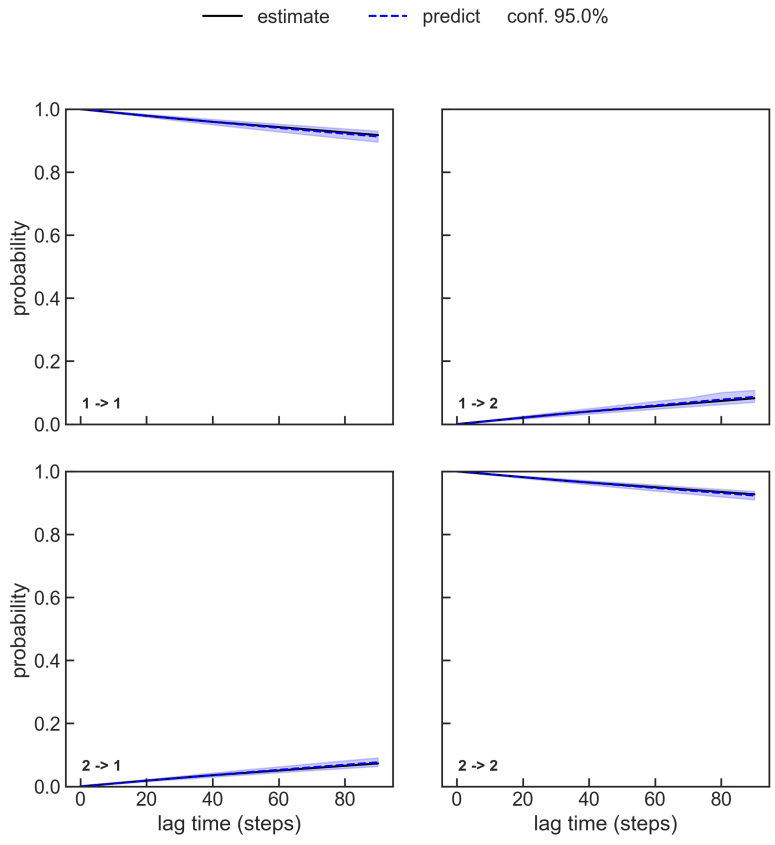
FIG. S3: Chapman-Kolmogorov tests corresponding to the two-dimensional potential for the hdbMSM.
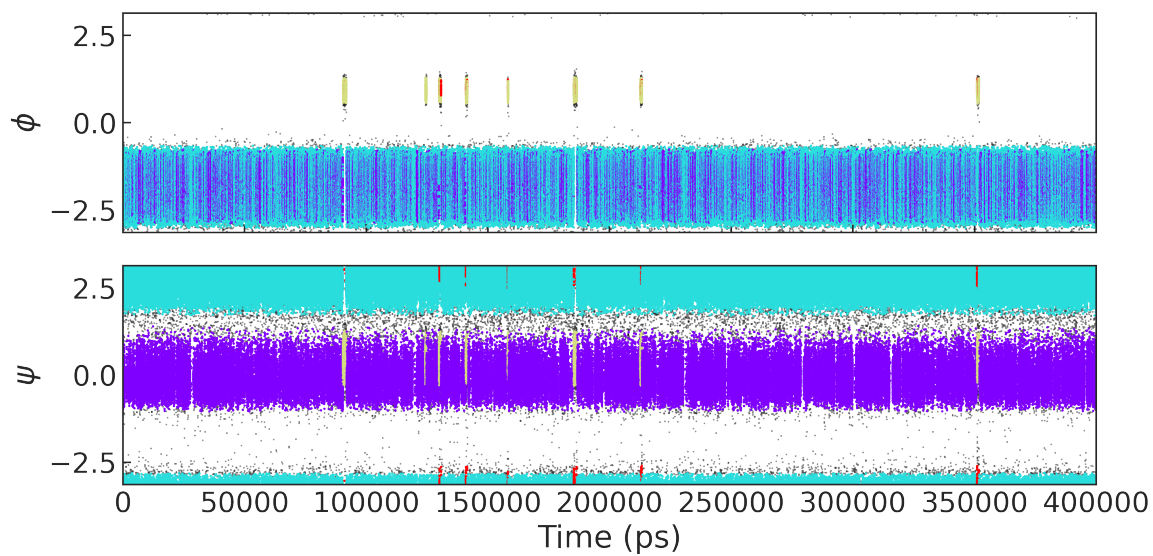
FIG. S4: Backbone torsion angles with different colours for each HDBSCAN cluster along simulation trajectory of alanine dipeptide.
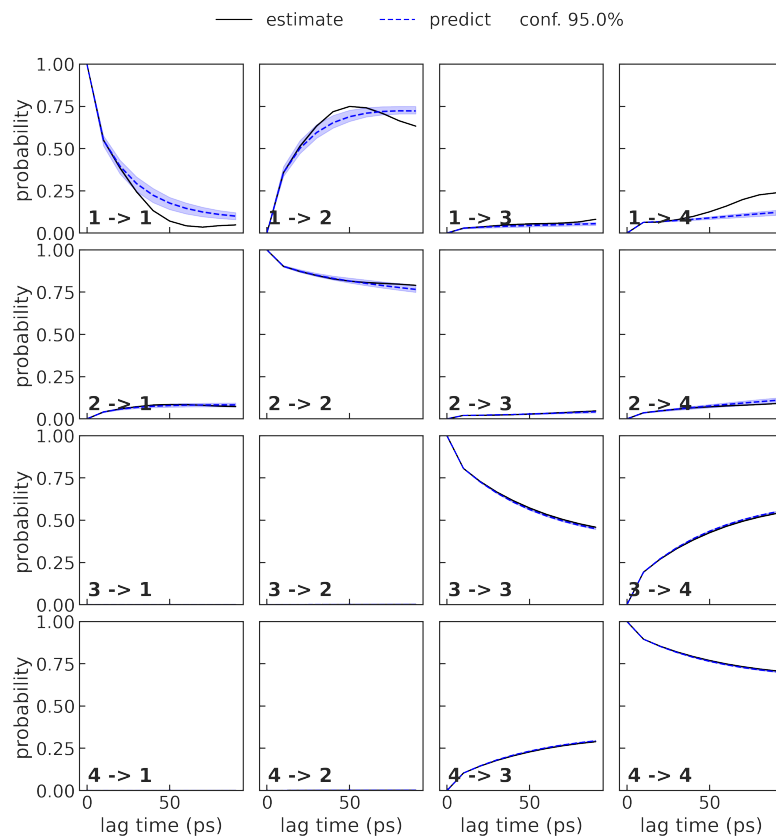
FIG. S5: Chapman-Kolmogorov tests corresponding to alanine dipeptide. for the PCCA+ coarse-grained MSM.
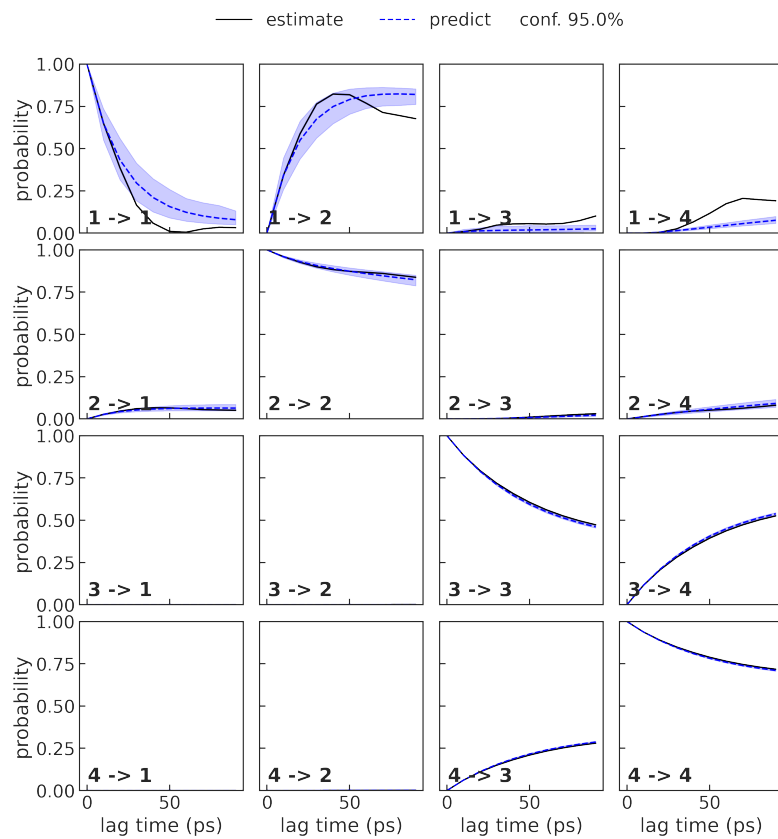
FIG. S6: Chapman-Kolmogorov tests corresponding to the hdbMSM for the alanine dipeptide
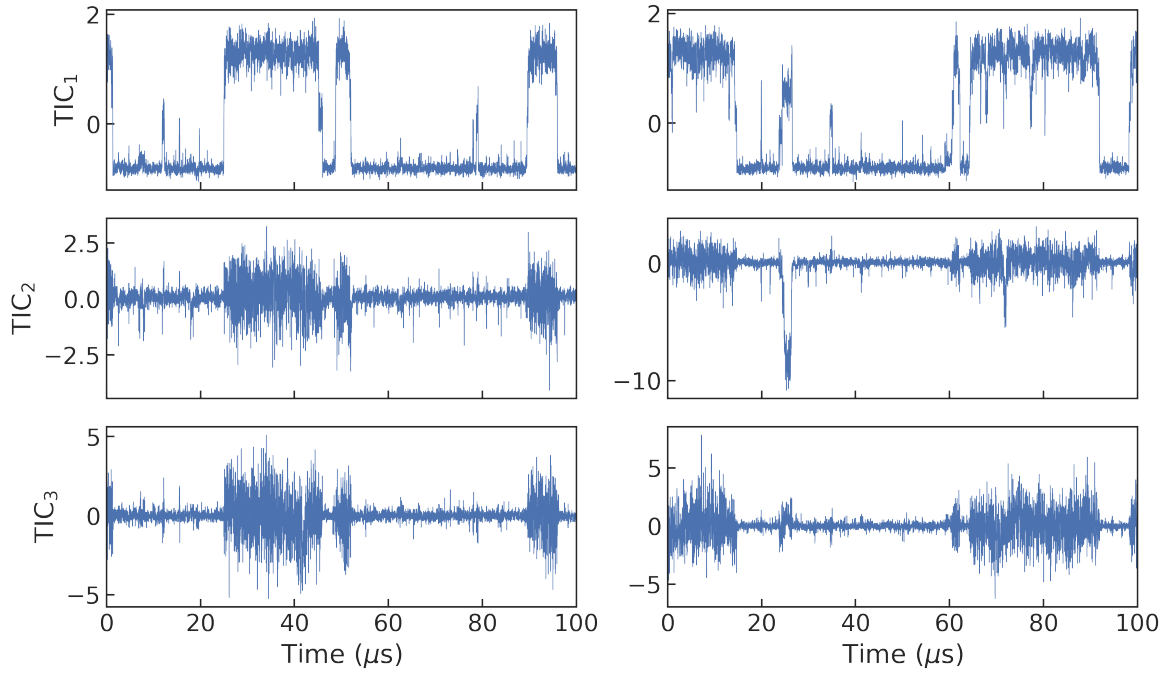
FIG. S7: Time series data for the projection on the first three TICA coordinates for the two long equilibrium trajectories of the FiP35 Pin WW domain.
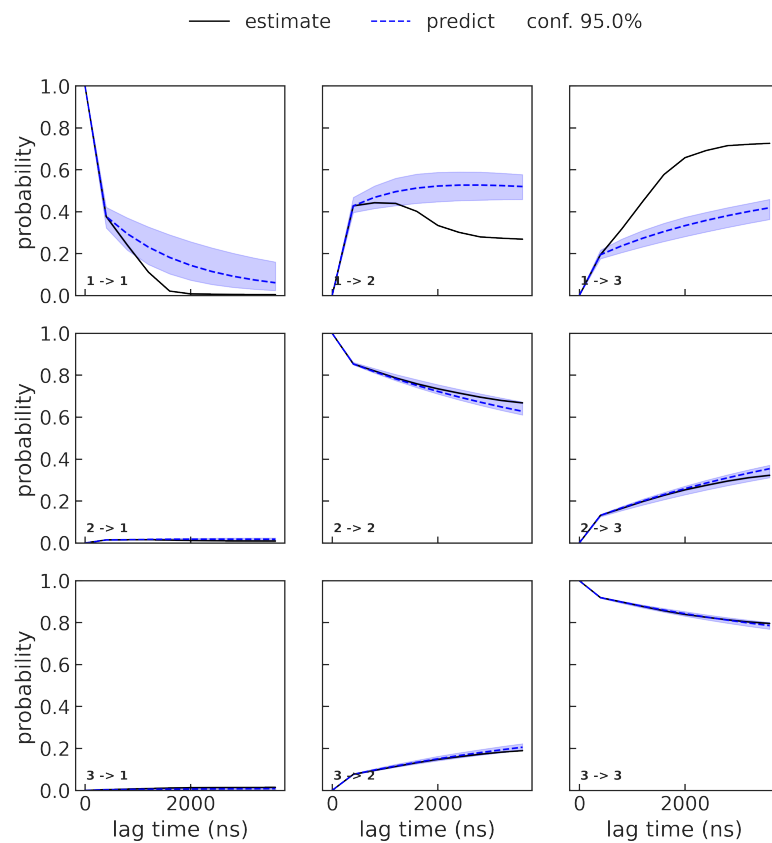
FIG. S8: Chapman-Kolmogorov tests corresponding to the FiP35 WW domain from the MSM coarse-grained using PCCA+.
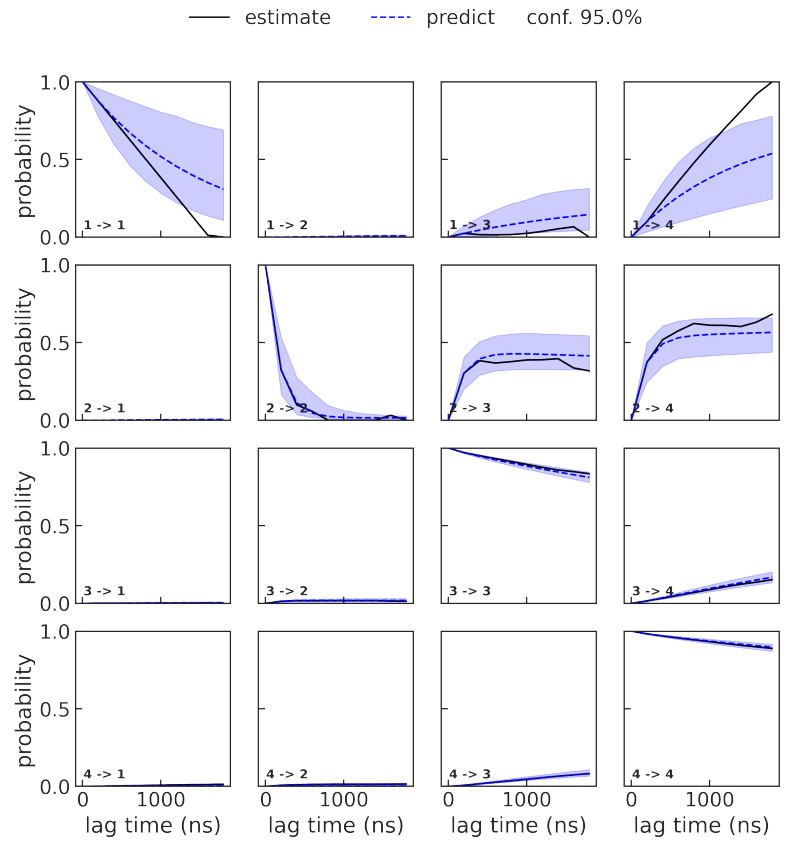
FIG. S9: Chapman-Kolmogorov tests corresponding to the hdbMSM for the FiP35 WW domain.
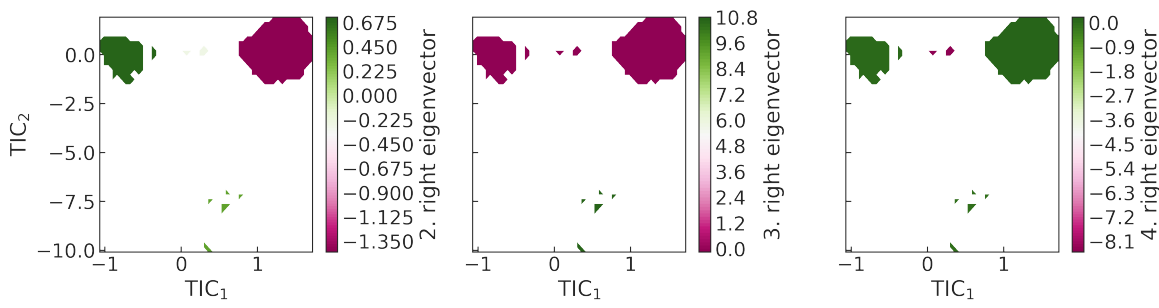

FIG. S10: Right eigenvectors corresponding to the three slowest modes of the hdbMSM for the Fip35 WW domain.