Supplementary Information for:

Extracting Markov models of peptide conformational dynamics from simulation data

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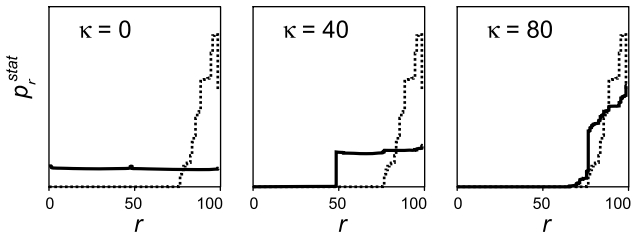

Figure 1: Solid lines: Stationary distributions $\mathbf{p}_{stat}$ for $\kappa \in \{0, 40, 80\}$ and $x_t = 0.66$ as in Fig. 4 of the manuscript. At $\kappa = 0$ the peaked initial distribution (dashed lines) converges to the uniform distribution, at $\kappa \in \{40, 80\}$ it becomes more and more localized near the intermediate metastable states of the linear dynamics (cf. Fig. 4 of our article) in the right half of the 100-dimensional state space.

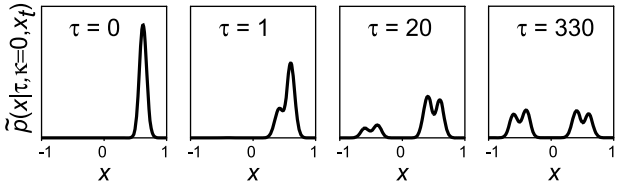

Figure 2: Temporal evolution of the virtual density $\tilde{p}(\mathbf{x}|\tau, \kappa = 0, x_t)$ for a linear dynamics (cf. Fig. 4 of the manuscript). As dictated by the starting value $x_t = 0.66$ the density is initially ($\tau = 0$) concentrated near the right maximum $x_4 = 0.6$ of the data distribution (cf. Fig. 2 of our article) and immediately starts spreading towards the mixture model (2) of the invariant density $p_{inv}(\mathbf{x})$.

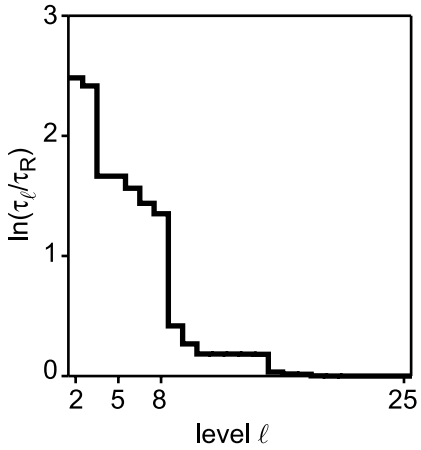

Figure 3: Logarithmic plot of the fastest relaxation time scales τ_ℓ measured in units of τ_R at the 24 steps of the recursive coarse-graining procedure applied to the transfer operator of the tripeptide. The figure is analogous to Fig. 9 of our article, which pertains to the one-dimensional model trajectory. In the transition from hierarchy level $\ell = 9$ to $\ell = 8$ a large increase of the fastest relaxation time scale is observed, which indicates that an eight-state model should describe the key features of the conformational dynamics in the peptide.