Supporting information for: Spatial Heat Maps from Fast Information Matching of Fast and Slow Degrees of Freedom: Application to Molecular Dynamics Simulations

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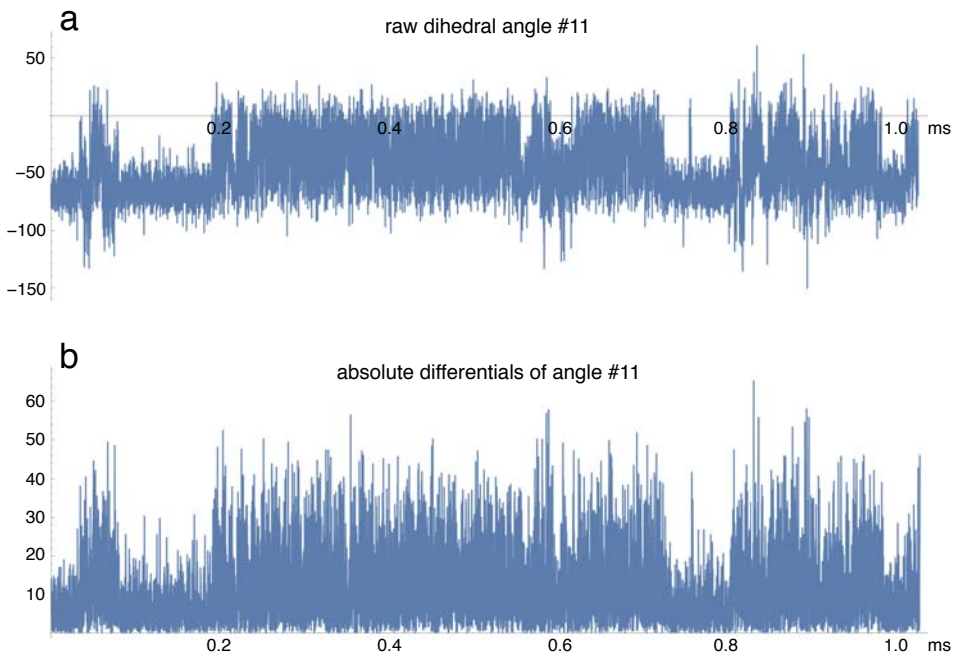

Figure S1: BPTI. **(a)** Pivot angle #11 (dihedral formed by BPTI α carbons 11,12,13,14) as a function of the simulation time in ms. **(b)** Absolute time derivative (finite difference) of the pivot angle.

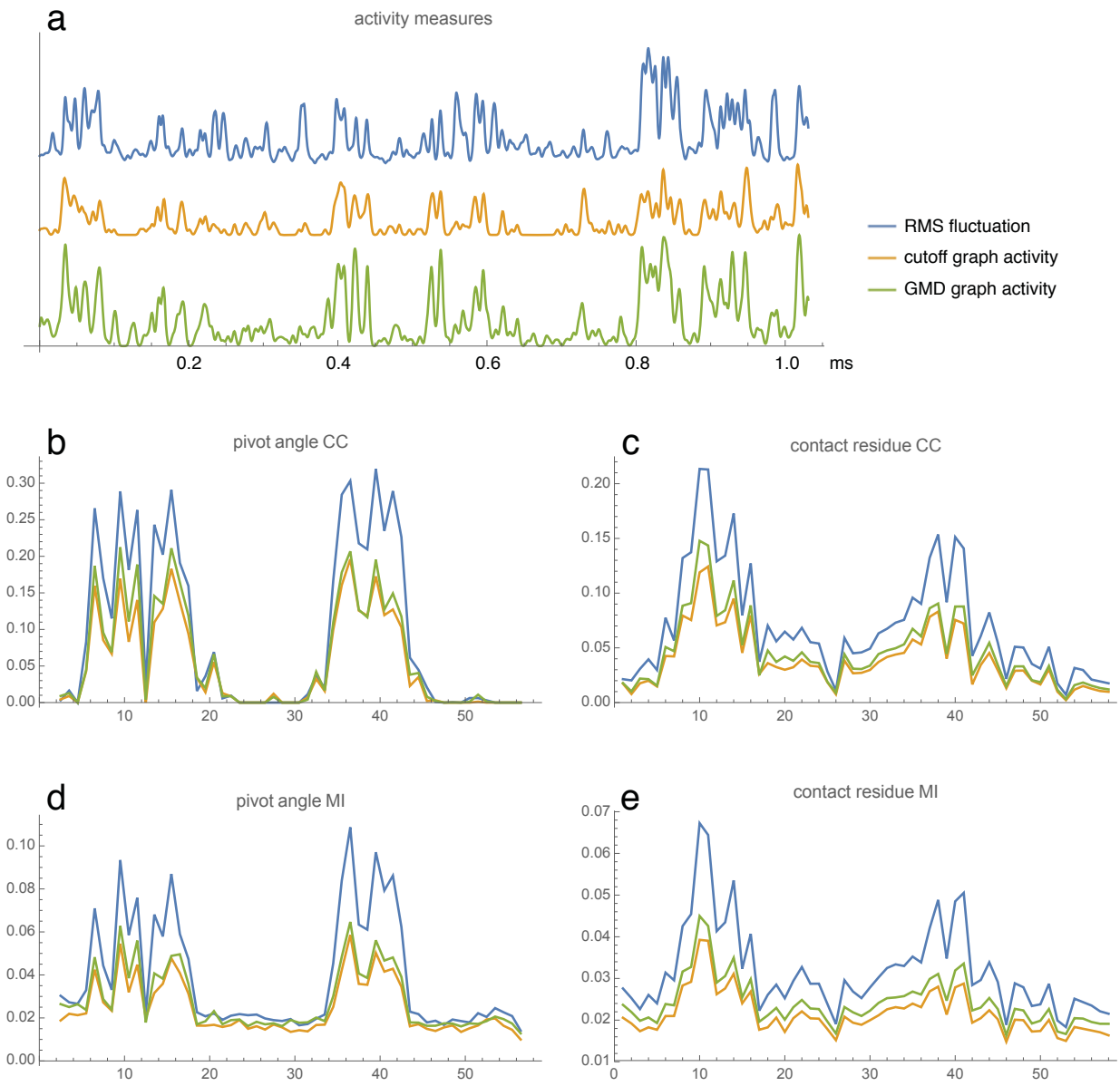

Figure S2: Complete results of the BPTI analysis shown in Figure 1 of the main text. **(a)** Three activity measures (see main text; arbitrary amplitudes and offsets) as functions of the simulation time in ms. The RMS fluctuation was computed with the *TimeScapes* `agility.py` program using a sliding window of length $\delta = 5\,\mu$s.[4] The parameters used by `terrain.py` were cut1 $= 6\,$Å, cut2 $= 7\,$Å, and $\delta = 5\,\mu$s for the cutoff graph activity, and cut1 $= 2$, cut2 $= 3$, and $\delta = 5\,\mu$s for the GMD graph activity. **(b,d)** Pivot angle CC and MI values as functions of the BPTI residue number, computed with `turning.py`, for each of the three activity measures in (a) using default parameters. **(c,e)** Contact residue CC and MI values as functions of residue number, computed with `tagging.py` with default parameters.

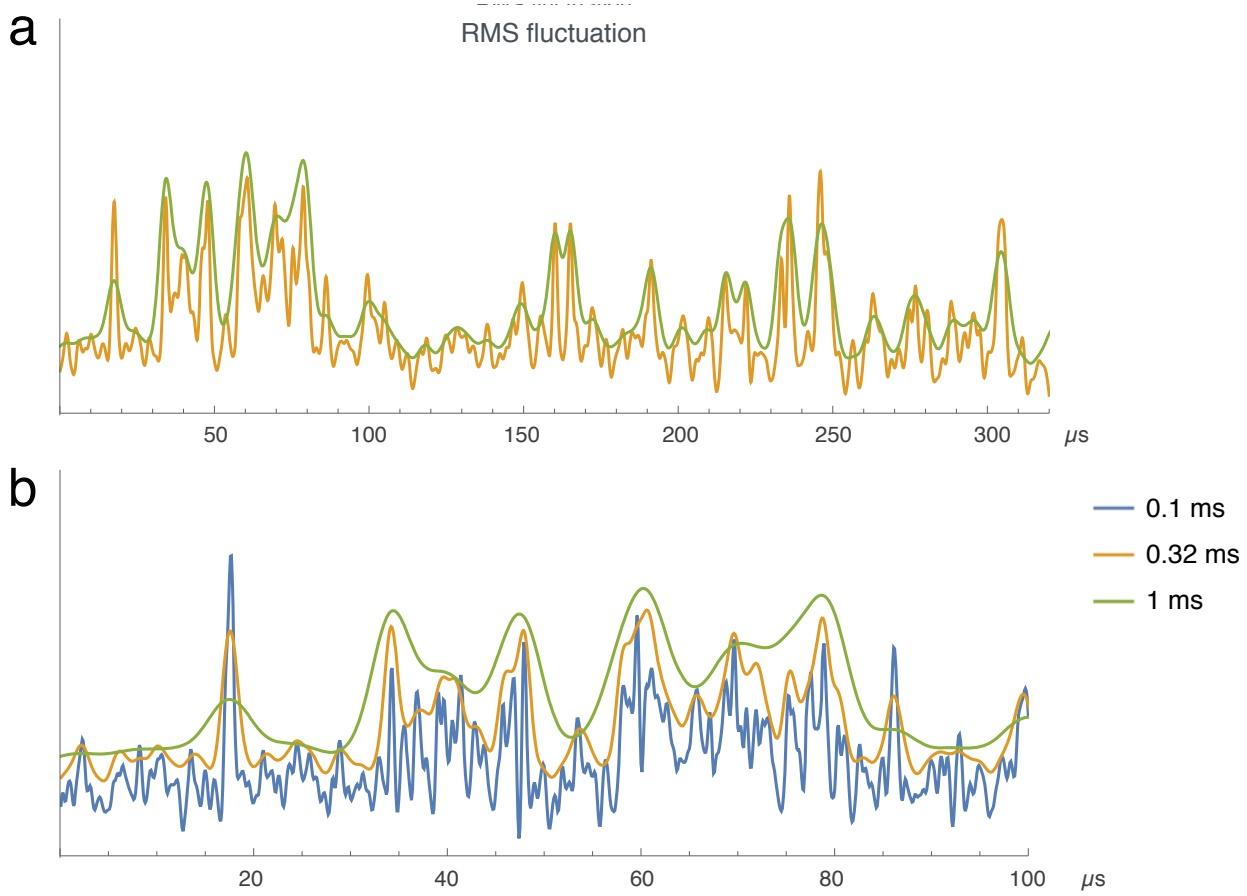

Figure S3: RMS fluctuation activity function of BPTI computed from abridged trajectories of length 0.32 ms **(a)** and 0.1 ms **(b)**. RMS fluctuation curves from longer trajectories are superimposed for comparison. The graphs are shown as functions of the simulation time in μs. The shorter trajectory subsets display higher variability due to the adjustment of the smoothing parameter δ: the 0.1 ms subset used $\delta = 500$ ns, the 0.32 ms subset used $\delta = 1.6\,\mu$s, while the full trajectory used $\delta = 5\,\mu$s.[4]

Figure S4: Heat map profiles as functions of the residue number of BPTI, for the RMS fluctuation curves shown in Figure S3: trajectories of length 0.1, 0.32, and 1 ms. **(a,b)** Pivot angle MI values, computed with `turning.py` using default parameters. **(c,d)** Contact residue MI values, computed with `tagging.py` using default parameters. The left column (unmodified MI values) shows a clear convergence of values as the subsets get longer, while the right column (matched MI values) demonstrates the robustness of the results relative to the trajectory length.

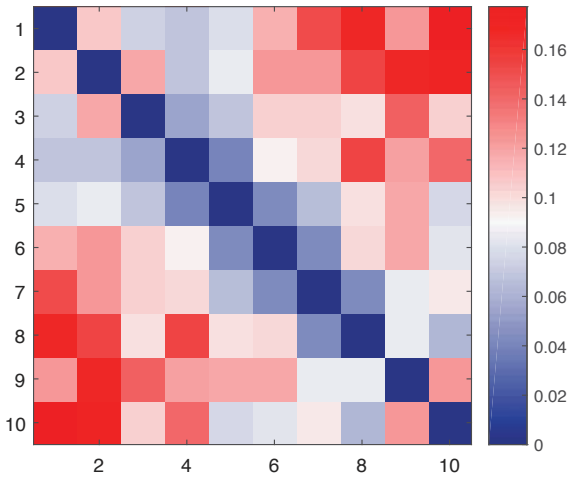

Figure S5: Chignolin. Two-dimensional pairwise residue interaction map. Colors encode the MI between the pairwise distance rate of change and the RMS fluctuation activity. Projection along rows (or columns) yields the plot in Figure 4(e) of the main text. Parameters are listed in the caption of Figure 4 of the main text. The data from this figure are also presented in the "TOC" figure of the abstract. (In that figure, the diameter or color of circles encodes the projected MI from main text Figure 4(e), whereas the height or color of the arcs encode the pairwise MI shown here.)