ETNA: Equilibrium transitions network and Arrhenius equation for extracting folding kinetics from REMD simulations SUPPLEMENTARY MATERIAL

S. Muff* and A. Caflisch*

Department of Biochemistry, University of Zurich,

Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

(Dated: December 1, 2008)

Keywords:

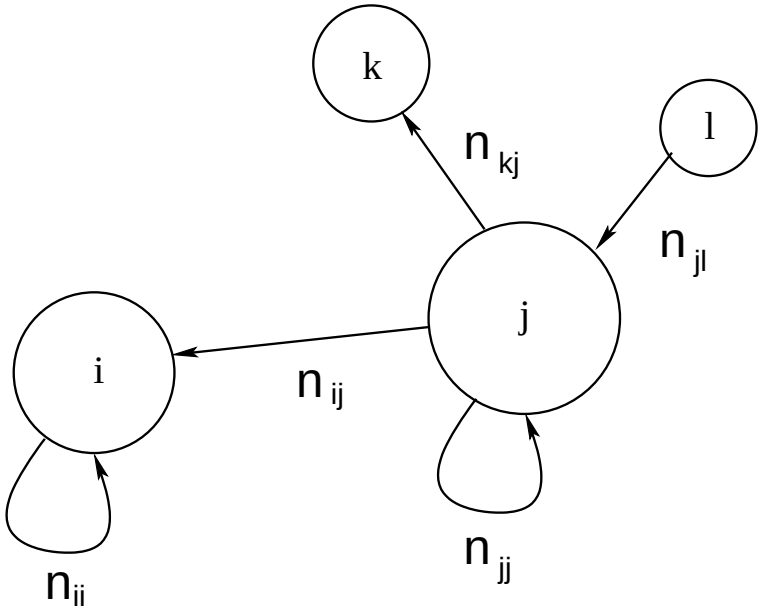

FIG. S1: Schematic representation of the transition matrix The absolute number of transitions from node j to node i is n_{ij}. The transition probability from node j to node i is calculated by $p_{ij} = \frac{n_{ij}}{\sum_k n_{kj}}$.

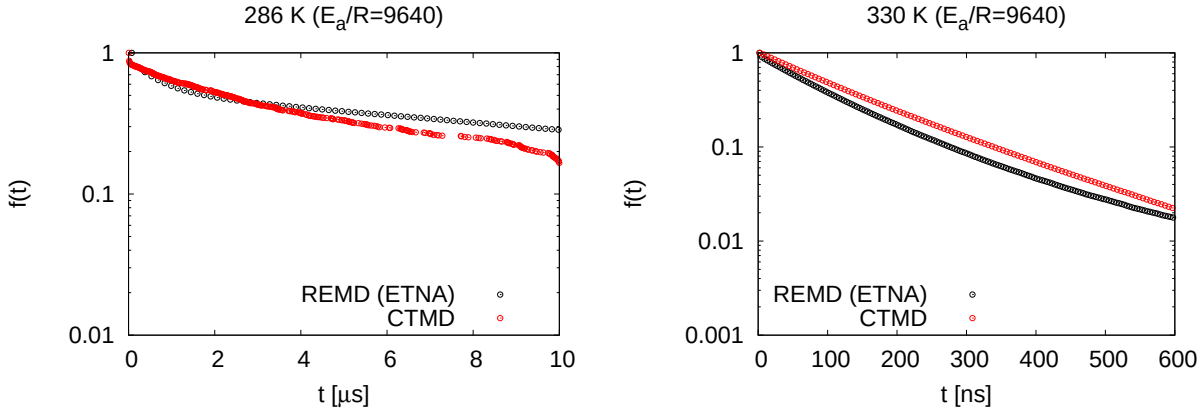

FIG. S2: Cumulative folding time distributions at 286 K (left) and 330 K (right) with ETNA using the Arrhenius parameter $E_a/R = 9640$ K, as calculated from the fit of unfolding rates on the ETNs of REMD.

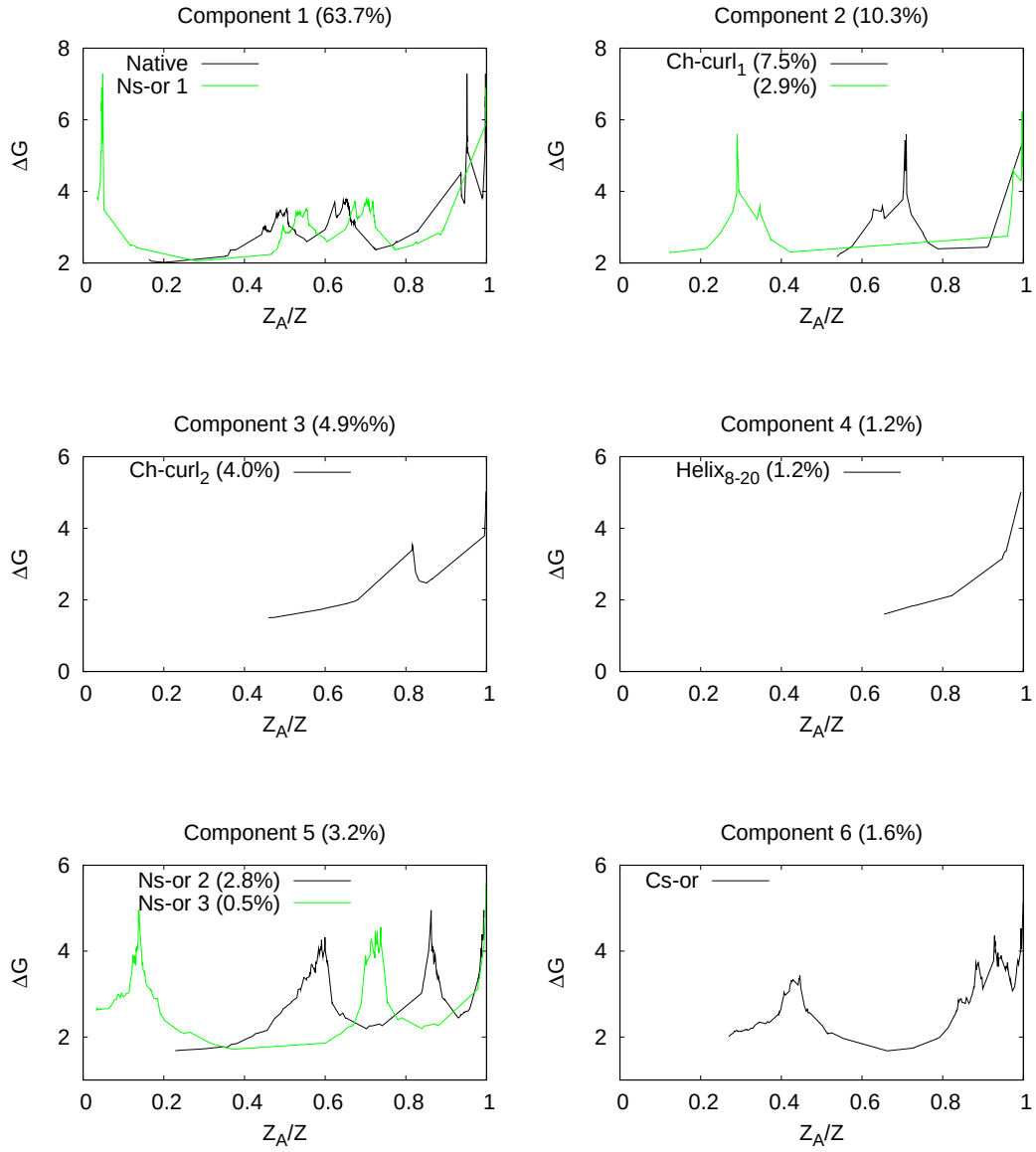

FIG. S3: cFEPs from the six most populated REMD components at 286 K. Component 1 is the NC.

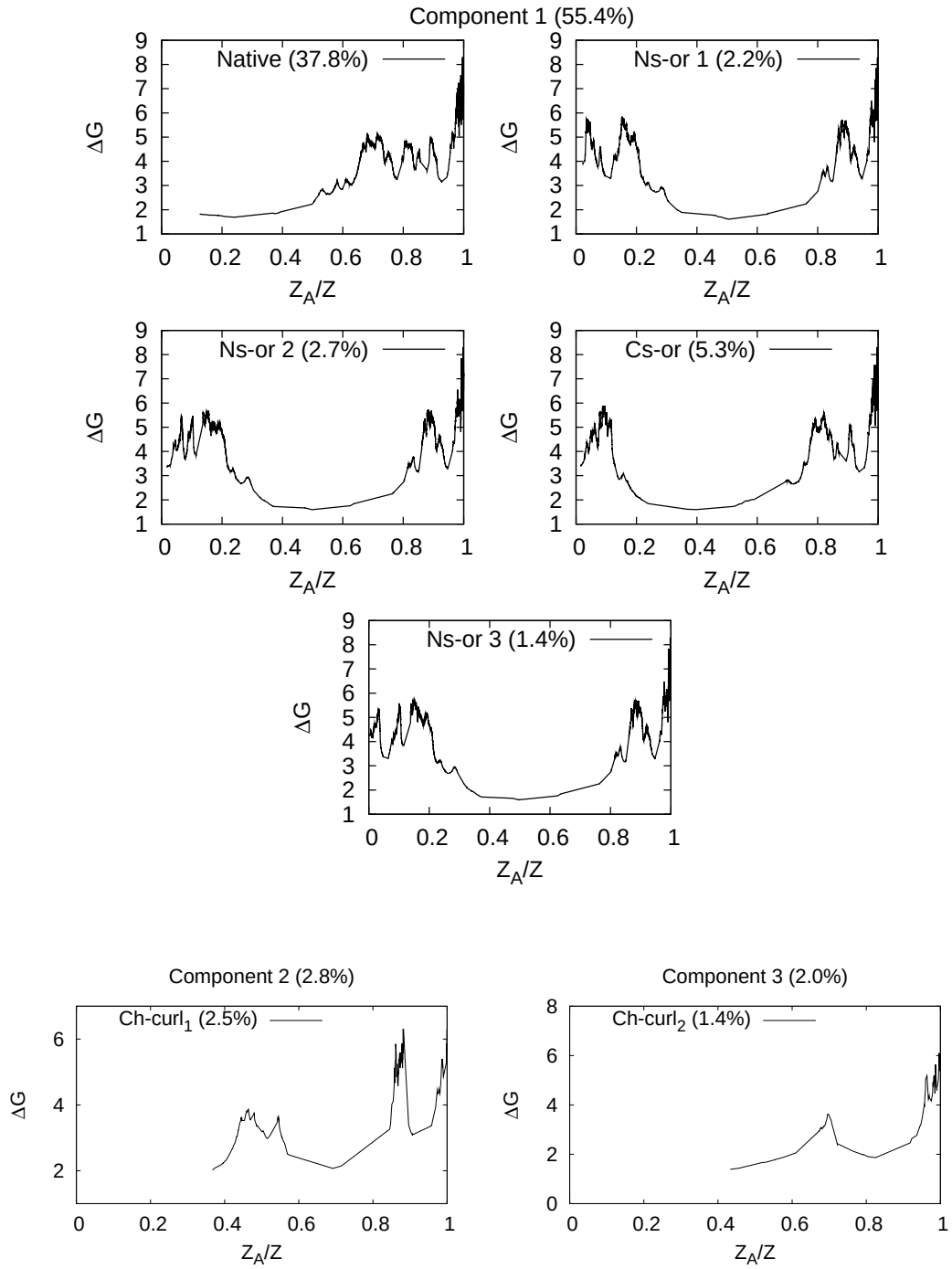

FIG. S4: cFEPs from the three most populated REMD components at 330 K. Component 1 is the NC.

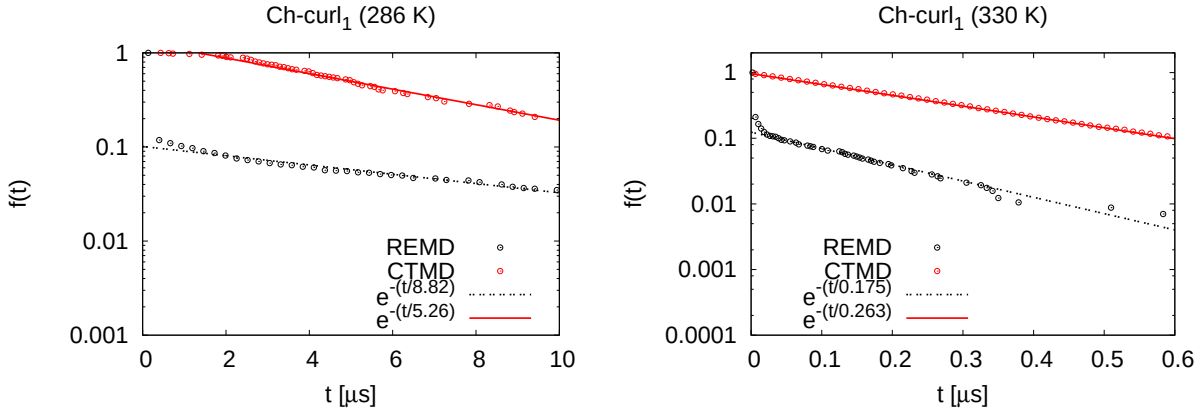

FIG. S5: Example fits to the cumulative folding time distributions from CTMD folding runs (red) and from ETNA scaling (black).

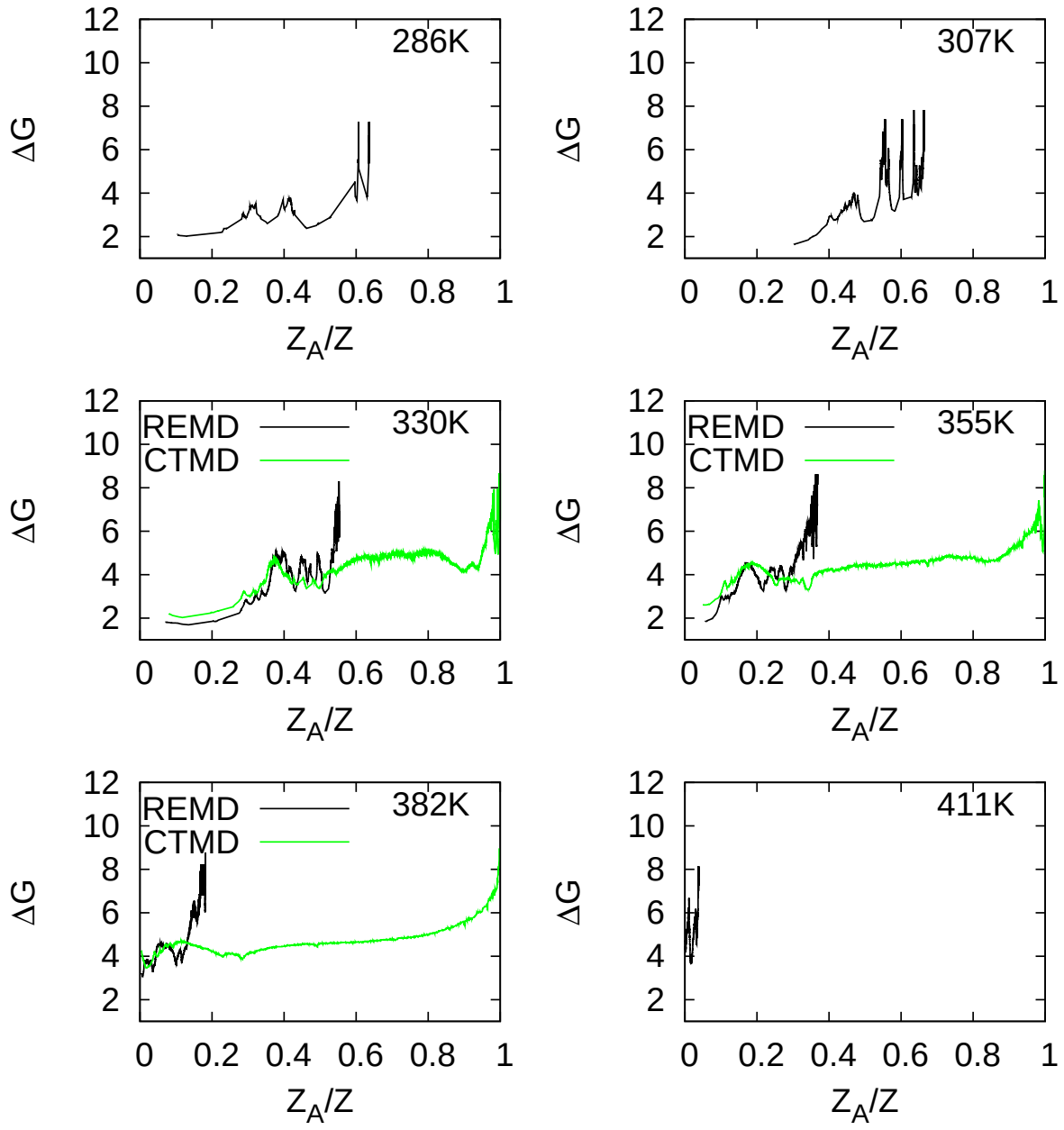

FIG. S6: cFEPs calculated from the REMD (black) and CTMD (green) simulation data. The REMD-cFEPs show only the NC, whose relative size is the Z_A/Z value of the rightmost black data point. At very low temperature (top) the ETN from REMD is disconnected because of high free-energy barriers. At high temperature (bottom), large entropic contributions have the same effect. All ΔG values are in kcal/mol.

* tel: +41 44 635 55 21 e-mail:caflisch@bioc.uzh.ch,smuff@bioc.uzh.ch