

Figure 8. Experiments on 2AA test dipeptides QW (top row), HT (middle row) and GP (bottom row). Comparison of the long MD trajectory and Timewarp MCMC (Algorithm 1). (a) TICA plots. (b) Free energy comparison of the first two TICA components. (c) Autocorrelation for the TIC 0 component. (d) Time dependence of the TIC 0 component.

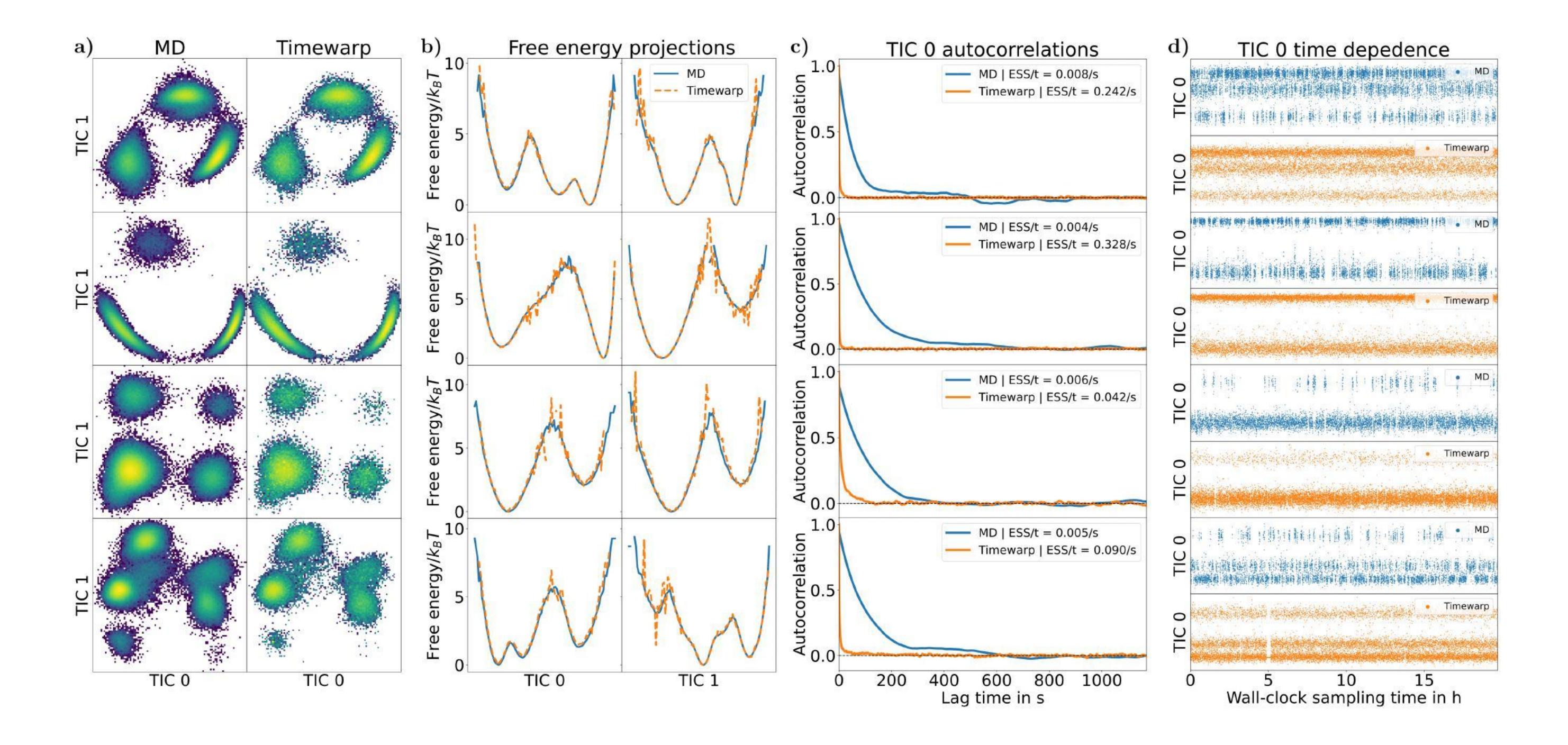


Figure 9. Experiments for the 2AA test dipeptides DH (first row), GT (second row), TK (third row), and CW (last row). Comparison of the long MD trajectory and Timewarp MCMC (Algorithm 1). (a) TICA plots. (b) Free energy comparison of the first two TICA components. (c) Autocorrelation for the TIC 0 component. (d) Time dependence of the TIC 0 component.