Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION
Fast Nosé-Hoover Thermostat: Molecular Dynamics in Quasi-thermodynamic Equilibrium

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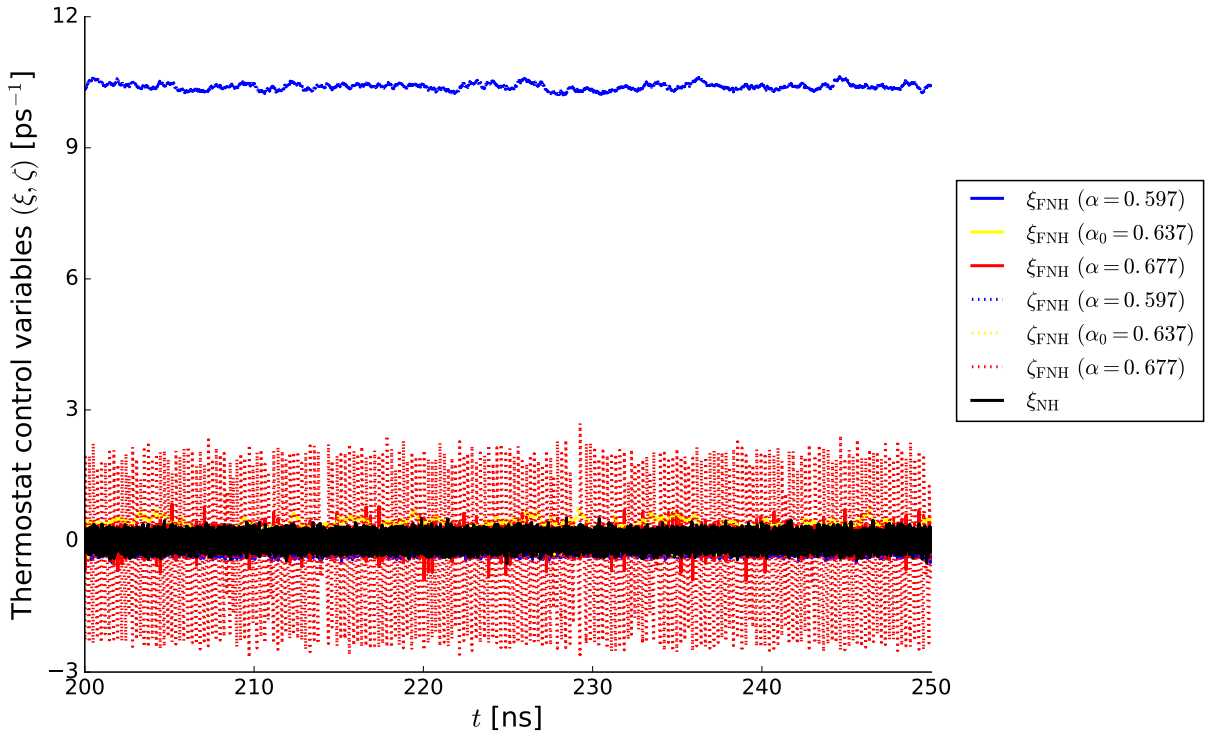

Figure S1: Time evolution of the thermostat control variables with respect to different Fast Nosé-Hoover (FNH) perturbations α for peptide 1 in methanol. On can clearly recognise that positive perturbations $\alpha = \alpha_0 + \delta\alpha$ lead to negative ζ, which are balanced by positive ξ values, and *visa versa* for negative perturbations $\alpha = \alpha_0 - \delta\alpha$. For large positive deviations $\alpha = \alpha + \Delta\alpha = 0.677$ in red, the oscillations of the thermostat variables are substantially increased involving repetitive sign changes. The Nosé-Hoover (NH) reference value for canonical equilibrium is shown in black.

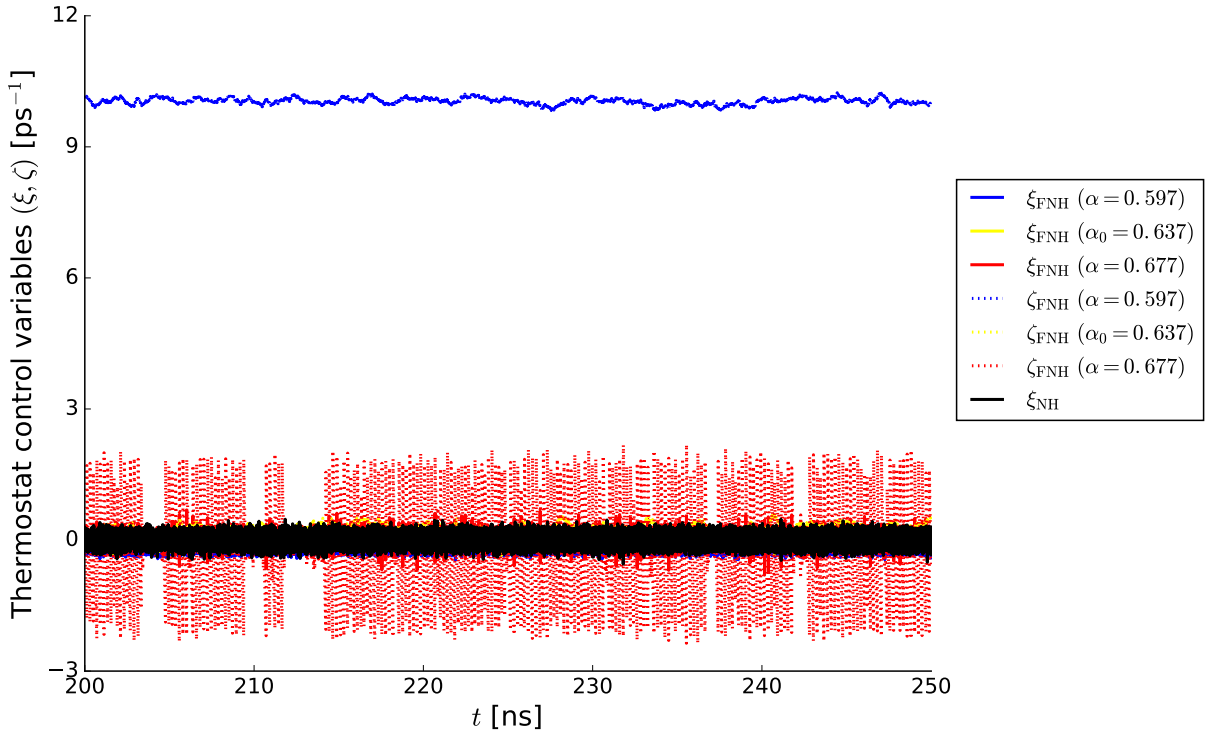

Figure S2: Time evolution of the thermostat control variables with respect to different Fast Nosé-Hoover (FNH) perturbations α for peptide 2 in methanol. On can clearly recognise that positive perturbations $\alpha = \alpha_0 + \delta\alpha$ lead to negative ζ, which are balanced by positive ξ values, and *visa versa* for negative perturbations $\alpha = \alpha_0 - \delta\alpha$. For large positive deviations $\alpha = \alpha + \Delta\alpha = 0.677$ in red, the oscillations of the thermostat variables are substantially increased also involving repetitive sign changes. However, in contrast to peptide 1 and the water test system, there exist some periods with reduced oscillatory amplitudes of ζ. The Nosé-Hoover (NH) reference value for canonical equilibrium is shown in black.