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Supporting Information

Modeling the Behavior of Coarse-Grained Polymer Chains in Charged Water Droplets: Implications for the Mechanism of Electrospray Ionization

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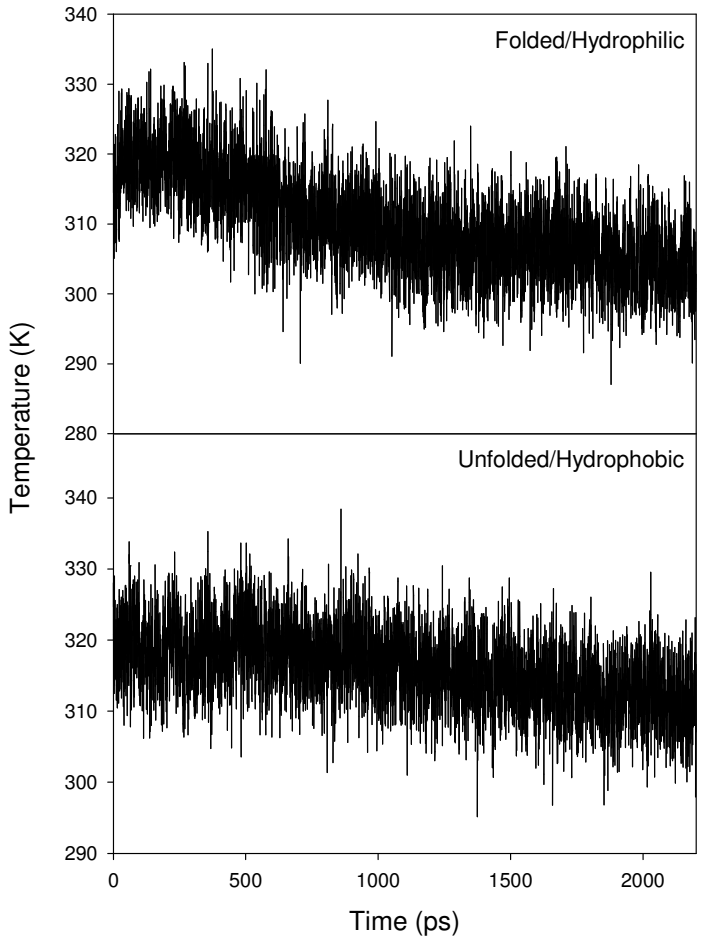

Figure S1: Temperature profiles for two different MD simulation runs. These data illustrate the occurrence of evaporative cooling during MD simulations of aqueous nanodroplets. The extent of cooling varies between different simulation runs. The top panel refers to a droplet containing a folded/hydrophilic polymer, with ejection of 28 water molecules and one ammonium ion. The bottom represents data for a droplet containing an unfolded/hydrophobic polymer, with ejection of 17 water molecules (no NH_4^+ was ejected in this particular run).