Supplementary Material

The simulations were performed by using the AMBER 10 package [1] with a modified version of the AMBER-99 force field, ffSB99 [2]. The modified force field has improved φ/ψ dihedral parameters that can better represent residues such as glycine and alanine [2]. The force field parameters to represent ClO_4^- anions were given by Baaden et al. [3] with the atomic charges fitted to electrostatic potentials calculated at the Hartree-Fock level using a 6-31G* basis set.

The peptide was simulated in an explicit water molecule solution and in a 0.2 M $NaClO_4$ solution. The simulations in explicit water were constructed by immersing the peptide in a cubic box containing 2317 TIP3P water molecules. Three Cl^- ions were added to counterbalance the peptide charge. The 0.2 M $NaClO_4$ solution was prepared by adding the Na^+ and ClO_4^- ions coordinates to the peptide coordinates, then three Cl^- ions were also added to counterbalance the charge and finally the water molecules in a cubic box were added. The resulting ratio of ClO_4^- ions/peptide is 9.

The energies of both systems were minimized after a total of 16000 steps. After the minimization, a 50 ps NVT equilibration run at 300 K was done with the peptide fixed, in order to equilibrate the solutions. Next, the total volume and density were adjusted with another 50 ps NPT run with the total pressure set to 1 atm. The concentration of salt after the NPT simulation was calculated resulting in 0.2 M. The production runs were carried out for both systems under NVT conditions.

We used a time step of 2 fs and trajectory data was saved every 1 ps. The simulated systems were canonical ensembles at 300 K and periodic boundary conditions were used. All bonds involving hydrogen atoms were constrained using SHAKE with a tolerance of 0.0005 Å. REMD dynamics were performed using 48 replicas at constant volume covering a range of temperatures from 270 K to 505 K. The intervals between replicas were adjusted to have a uniform acceptance ratio greater than 20%. Exchanges were attempted each 100 integration steps. Each replica was run for 10 ns, leading to a total sampling time of 480 ns.

Data collection for both cases began after 3 ns of molecular dynamics simulation in order to eliminate initial biasing.

References

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