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Author Erik Marklund		
Title (English) Proteins under electrospray conditions: a simulation study		
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Abstract <p>The final stages of electrospray ionization (ESI) of four different proteins were simulated with molecular dynamics and the resulting trajectories analyzed with respect to structure preservation, evaporation and the protecting effect of hydrating water layers. For all proteins except insulin the structure was well preserved in the presence of a hydrating water layer. The results provide new insight in the mechanistic details of ESI and are promising for future single particle imaging experiments with X-ray free electron lasers (XFEL).</p>		
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