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Abstract for an Invited Paper
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Conformational Dynamics of Short Peptides in Aqueous Solutions: Assessment of Molecular Dynamics Force Fields[1]

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Molecular dynamics (MD) offers deep insights into structure and dynamics of protein folding and assembly. MD predictions, however, strongly depend on the accuracy of MD force fields. In the past decade, a large number of MD force field modifications have been proposed, in particular to address the need to capture conformational dynamics of intrinsically disordered peptides and proteins. I will present our recent work elucidating three commonly used MD force fields with respect to their capacity to reproduce conformational ensembles of short unfolded cationic peptides in aqueous solutions in a way that is consistent with available spectroscopic data.

[1]MCB-1817650 DMR 1707770 OAC 1919691