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摘要: Sub-terahertz (THz) vibrational modes of the protein thioredoxin in a water environment were simulated using molecular dynamics (MD) in order to find the conditions needed for simulation convergence, improve the correlation between experimental and simulated absorption frequencies, and ultimately enhance the predictive capabilities of computational modeling. Thioredoxin from E. coli was used as a model molecule for protocol development and to optimize the simulation parameters. The empirically parameterized software packages Amber 8 and 10 were used in this work. Using atomic trajectories from the constant energy and volume MD simulations, thioredoxin's sub-THz vibrational spectra and absorption coefficients were calculated in a quasi-harmonic approximation. An optimal production run length similar to 100 ps was found, in agreement with experimental data on thioredoxin relaxation dynamics. At the same time, a new procedure was developed for averaging correlation matrices of atomic coordinates in MD simulations. In particular, the open source package ptraj was edited to improve a matrix-analyzing function. Averaging only six matrices gave much more consistent results, with absorption peak intensities exceeding those from the individual spectra and a rather good correlation between simulated vibrational frequencies and experimental data.
作者关键词: THz absorption; Vibrational modes; Thioredoxin; Convergence; Molecular dynamics
KeyWords Plus: PARTICLE MESH EWALD; PROTEIN DYNAMICS; CONFIGURATIONAL ENTROPY; TERAHERTZ SPECTROSCOPY; POTENTIAL FUNCTIONS; ESCHERICHIA-COLI; NUCLEIC-ACIDS; LIQUID WATER; FORCE-FIELD; SIMULATIONS
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