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q-REM: NOVEL METHOD OF CONFORMATIONAL SEARCH FOR PROTEIN FOLDING DYNAMICS

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There have been considerable recent progresses regarding the fast conformational sampling of proteins. Various strategies to circumvent quasi-ergodic problem by introducing non-Boltzmann weight factors have been proposed. The replica exchange method (REM) is considered to be one of the most promising sampling methods. We have applied REM to the folding simulations of small peptides in explicit water environments.

We have developed a new scheme for fast conformational searches by combining the REM with MD simulations using the generalized effective potential. Unlike theconventional REM, the new scheme (termed as 'q-REM') uses 'q' values in Tsallis transformation as a coupling parameter. It is found that the new method requires much smaller number of replicas than the conventional REM for effective conformational sampling of complex systems. The advantage of the present method has been demonstrated with *ab initio* folding simulations of small peptides and proteins.

Here, we report q-REM study of a 20-residue mini-protein tc5b (Trp-Cage molecule, PDB-code 1L2Y), which is a representative molecule in protein folding study for its stable helix structure. Six replicas were employed for q-REM simulation in this work. Set of q values, with the same , were taken to maintain overall exchange rate around 30 %. Exchange occurred only between neighboring two replicas, and was tried every 80 step. Information on the canonical ensemble for given temperature was extracted from the $q1$ ($q1$=1.000000) replica.