

Analysis of the site-dipole fields around guanine nucleotides in the Hras-GTP and Hras-GDP complexes

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We study the behavior of water molecules around guanine nucleotides in the Hras-GTP and the Hras-GDP complexes in water solvents in order to understand the mechanism of GTP hydrolysis of GTP in the Hras-GTP complex. We performed MD simulations of the Hras-GTP and the Hras-GDP complexes and investigate the positions and the directions of water molecules around the guanine nucleotides in these complexes by the site-dipole fields using trajectories from MD simulations. We found that, in the Hras-GTP complex, there are some atoms or groups where the neighboring water molecules behave characteristically.