Molecular Dynamics Simulations of the Hras-GTP complex and the Hras-GDP comlex

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We study the structures of the Hras-GTP complex and the Hras-GDP complex in water in order to investigate the mechanism of GTP hydrolysis of the Hras-GTP comlex. We performed MD simulations of the Hras-GTP complex and the Hras-GDP complex in water in order to investigate the structures of these complexes using the modified potential parameters of AMBER03. We have shown that the structure differences between the Hras-GTP complex and Hras-GDP were found in the loop2 and loop4 mainly.