Analysis of water molecules around GTP in Hras-GTP complex and GDP in Hras-GDP complex by molecular dynamics simulations

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We investigate the structures of the Hras-GTP complex and the Hras-GDP complex 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 complex and the Hras-GDP complex in water solvents in order to study the positions and the directions of water molecules around the guanosine nucleotides in these complexes using AMBER03 and the potential parameters calculated around Mg^{2+} in these complexes.

We calculate the radial distribution functions (RDF) of water molecules with respect to the phosphorus atoms in the GTP and GDP. We define the first hydration spheres from RDF. We calculate occurrence ratio of duration time of water molecules in the first hydration sphere. For the duration time smaller than about 5.0 ps, the occurrence ratio is proportional to $t^{-1.4}$. This suggests that the network of water molecules does not break for about 5.0 ps. We also calculate the angle distribution of water molecules around PG in GTP and PB in GDP. It is shown that water molecules are distributed evenly around PG in GTP, although water molecules are distributed unevenly around PB in GDP. This suggests that the trigger of GTP hydrolysis is possibly the attack of water molecule to γ phosphate from the appropriate direction.