# CHAPTER 7

# CONCLUSION

The solvation structure of glucosamine in aqueous solution has been investigated using the Metropolis Monte Carlo scheme. Simulations have been carried out for a system containing 202 rigid particles, including one glucosamine molecule, which fixed at the center of the cube. With a volume of 201 water molecules at 298 K plus additional space occupied by the glucosamine molecule, a periodic cubic volume of side length 18.26 Å was yielded. A spherical cut-off for the site-site interaction potentials was applied at half of this length. A glucosamine-water potential has been newly developed based on DZP *ab initio* calculations, while the MCY potential was employed to describe water-water interactions. The radial distribution functions (RDFs) from O and H atoms of water molecules to the center of glucosamine molecule exhibit the weak interaction between both molecules. The first solvation shell appears at 4.6 Å from the center of glucosamine with the coordination numbers of 7 water molecules. Precise positions of these molecules have been intensively investigated and led to the conclusion that 1 water molecule lies in the ligand's plane while 2 and 4 water molecules are about 2 – 4 Å above and below the plane, respectively. Among the 7 water molecules, only W3 binding to ring oxygen atom displays linear H – bond. In addition, second solvation shell which contains 19 water molecules has been also clearly detected. However, the mobility of water molecules due to a weak glucosamine-water interaction has been also observed. This event is supported by the undefine first-minimum of RDFs, the broad distribution of the coordination numbers and the density contour plots.