**Molecular dynamics simulation for understanding in dynamic water structures of aqueous solution of biomolecules**

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It has been pointed out that the water structure in the body is important for understanding in the molecular mechanism of structures and functions of biomolecules. The role of water has, however, not been fully understood on the molecular level. It is necessary to consider interactions among constituent molecules, in order to understand dynamic structures and functions of biomolecules. Therefor, interactions of water molecules surrounding biomolecules through hydrogen bonds are necessarily considered. In the present work, dynamic behaviors and relaxation phenomena of biomolecules and surrounding water molecules were analyzed by Discovery Studio 2017 R2 and CHARMm(General Information Center, Tokai University). The MD simulation was carried out with conditions; number of molecules: 282, temperature: 300K, ensemble: TNP. The dielectric relaxation curve obtained from the MD simulation for water is shown in Fig.1. The composition with experimental results indicate that the difference in the relaxation time and the numerical error in higher frequency region. It should be considered if the reduce temperature / time is required or not from evaluations of the correlation function approach and numerical calculation.

Fig.1.Dielecrric relaxation curves at 25℃ for water from literature (green and light-green ) and red and blue plots are obtained from the Cole’s theory with MD simulation for water at 300K



References: [1] S. Yagihara, N. Shinyashiki, R. Kita, Dynamics of in vivo water structure and broadband dielectric spectroscopy, 2007 [2] Robert. H. Cole, Evaluation of Dielectric Behavior by Time Domain Spectroscopy, 1945