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Monte Carlo Simulations with reference interaction site model theory for simulating peptide molecules in aqueous solution AYORI MITSUTAKE, Keio Univ., YUTAKA MARUYAMA, IMS, TAKASHI IMAI, Ritsumei Univ., MASAHIRO KINOSHITA, Kyoto Univ., YUKO OKAMOTO, Nagoya Univ., FUMIO HIRATA, IMS — We have developed Monte Carlo simulations with reference interaction site model theory for simulating proteins in aqueous solution. The reference interaction site model theory based on the liquid theory of statistical mechanics can treat solvent effect with solvent molecular shape and estimate solvation free energy around proteins. We have developed simulation algorithms which combine with generalized-ensemble algorithms and reference interaction site model theory. We showed results of a simulated annealing Monte Carlo simulation, a multicanonical Monte Carlo simulation, and a replica-exchange Monte Carlo simulation with one dimensional reference interaction site model theory for Met-Enkephalin, a penta-peptide [1,2,3]. Recently we have performed a Monte Carlo simulation with three-dimensional reference interaction site model theory for simulating C-peptide in aqueous solution. We will describe these attempts and discuss results of these simulations. [1] M. Kinoshita, Y. Okamoto, and F. Hirata, *J. Am. Chem. Soc.* **120**, 1855 (1998) [2] A. Mitsutake, M. Kinoshita, Y. Okamoto, and F. Hirata, *Chem. Phys. Lett.* **329**, 295 (2000) [3] A. Mitsutake, M. Kinoshita, Y. Okamoto, and F. Hirata, *J. Phys. Chem. B* **108**, 19002 (2004)

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