3P116 The coarse grained GBSA method for simulations of biomolecular system

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The Generalized Born with solvent accessible surface area (GBSA) method has been widely used as a quick and reasonably accurate implicit solvation free energy model in all-atom (AA) molecular dynamics (MD) simulations of biomolecules. However, it has never been used in coarse grained (CG) MD simulations. Here, using a one-bead-per-residue CG representation, we provide the protocols to apply GBSA method in CGMD simulations. The CG GB term is fitted against AA Poisson-Boltzmann solvation energy. The CG SA is fitted against AA SA. Together, the CG GBSA method will give better accuracy for electrostatic and hydrophobic interactions than traditional CG force fields.

3P117 DNA 結合蛋白質はどのようにして障害物を回避するか。分子シミュレーションによるアプローチ

How DNA-binding proteins can bypass obstacles? Molecular simulation approaches

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Recent researches suggest that DNA-binding proteins(DBPs) search target sites by 1D-sliding, hopping and 3D-diffusion because the theoretical search time with only 3D-diffusion is much longer than the time from experimental results. But it is unclear how DBPs bypass the obstacles consisted of other DBPs and nucleosome on DNA.

This research aims to reveal how DBPs bypass the obstacles by using coarse-grained molecular dynamics simulation software, CafeMol.

3P118 転写因子 p53 の特異的結合部位探索・認識機構：マルチスケールシミュレーション研究

Specific DNA sequence search and recognition mechanism of transcription factor p53: multi-scale simulation study

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A transcription factor p53 is composed of five domains, of which three are intrinsically disordered regions, which prevent to elucidate the functional mechanism based on static structural analyses. In order to elucidate the role of functional cross-talks among these domains from a dynamic structural analysis, we constructed coarse-grained model for p53 based on the result of all-atom simulation. The result of multi-scale MD simulation using the constructed model revealed the specific DNA sequence search and recognition mechanism of p53 and the effect of post-translational modification on it, suggesting efficacy of multi-scale approach to elucidation of functional mechanism of the highly flexible proteins.

3P119 DNA 塩基対の安定性に及ぼすコリンイオンの効果の分子動力学計算による解析

Analysis for the effect of choline ions on the stability of DNA base pairs using molecular dynamics simulation

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In physiological-condition, G-C base pairs are more stable than A-T base pairs. However, A-T base pairs are stabilized in the solution containing choline ion while G-C base pairs are destabilized. In this study, we clarified unique binding style of choline ion with DNA atoms using molecular dynamics simulation. The binding style of sodium ion to DNA is tight but fragile; in contrast, the style of choline ion is relatively loose but stable through multiple-hydrogen-bond network. Choline ions prevent the formation of hydrogen bonds between G-C base pairs by binding to atoms between base pairs, while choline ions stabilize by fitting their narrow minor groove. We will discuss about the effects of choline ions on the stability of DNA base pairs in the presentation.

3P120 粗視化分子動力学シミュレーションによる一本鎖 DNA 領域形成機構の駆動力の解明

DNA unwinding mechanisms in *E. coli*, *oriC* region studied by coarse grained molecular dynamics simulations

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In the initiation of DNA replication of *E.coli*, unwinding DNA duplex at *oriC* region is a critical step. When DnaA proteins bind DNA to form DnaA-*oriC* complex, *oriC* region is bent to be positive supercoil structure and then DNA duplex is unwound. But, mechanisms of how this region is unwound are poorly understood. We assumed that *oriC* is a characteristic region which is easy to be ssDNA by a kind of driving force. In this study we first addressed thermodynamic stability of duplex in the *oriC* region, especially in AT-rich region, using coarse grained molecular dynamics simulation. We then investigated what kind of force play crucial role for DNA unwinding by reproducing the DnaA-*oriC* complex forming.

3P121 粗視化シミュレーションによる多ヌクレオソーム系の構造ダイナミクス

Poly-nucleosome structural dynamics by coarse-grained simulations

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Nucleosome is a basic unit of chromatin structure in which DNA duplex wraps about 1 and 3/4 times around a histone octamer. Poly-nucleosome takes higher order chromatin structure to store the very long genome into a compact form. Density fluctuation of chromatin structure may be essential for the searching mechanism of transcription factors to achieve the target sites on DNA duplex. Previously, we simulated mono-nucleosome dynamics by using coarse-grained DNA-protein model, in which one amino acid is represented by one bead and one nucleotide is represented by three beads corresponding to phosphate, sugar, and base. In this study, we try to reproduce poly-nucleosome conformations at various densities of nucleosomes.