2P008 アルファとベータの二次構造を含む 40 残基の蛋白質 H-NS の folding simulation
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 究ユニット
 folding simulation of a 40-residue protein, H-NS, involving alpha and beta secondary
 sytuctures in explicit water
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Multicanonical molecular dynamics (McMD) simulations were performed for a 40-residue
 protein, the C-terminal domain of H-NS, which involves alpha and beta secondary-structure
 elements. We put the protein in explicit water, started the simulation from a disordered
 structure, and obtained the free-energy landscapes in a temperature range [280 K-700 K].
 Cooperative formation of alpha and beta structures was observed and native-topology
 structures were obtained with the smallest backbone rmsd of 3.27 Å to the NMR structure,
 although such structures were minority even when a knowledge-based force field was
 applied to the backbone dihedral potentials. Current study suggests that our McMD
 simulation could sample many different structures including the native-topology ones, and
 that the force-field issue should be critical.

2P010 分子動力学シミュレーションを用いた CARDO の酸化酵素部位の解析
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 Molecular dynamics simulation of the terminal oxygenase component of carbazole
 1,9a-dioxygenase
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CARDO (carbazole 1,9a-dioxygenase) catalyzes dihydroxylation of carbazole and
 dibenzothiophene at angular position (C1 and C9a). This reaction destroys the plane
 structure of these compounds and greatly reduces their toxicity. CARDO consists of a
 terminal oxygenase (CARDO-O), a ferredoxin (CARDO-F) and a ferredoxin reductase
 (CARDO-R). The tertiary structure of CARDO-O has been determined by X-ray
 crystallography (PDB ID: 1WW9). CARDO-O has a trimeric structure and has a Rieske
 2Fe-2S cluster and a mononuclear Fe center in each monomer. CARDO receives two
 electrons from CARDO-F with the 2Fe-2S cluster. The electrons are then transferred to the
 mononuclear Fe at the active site in the adjacent monomer and are used to reduce oxygen.
 Molecular dynamics simulation of CARDO-O will be useful to study the mechanisms of the
 electron transfer and of the substrate recognition. However, there are no parameters for the
 2Fe2S cluster and mononuclear Fe. We therefore determined their parameters by using
 quantum chemical calculations. We first optimized the geometry of the 2Fe-2S cluster
 together with two methylimidazoles and two methanethiolates that form coordinate bonds
 with Fe atoms at BP86 / 6-311+G(d) level. Then Hessian and electrostatic potential were
 calculated to obtain force constants and partial charge. The parameters of the mononuclear
 Fe center were determined similarly. Using these parameters, we are now performing
 molecular dynamics simulation of CARDO-O.

2P009 大腸菌機械受容チャネル MscL の野生型ならびに変異型モデルを用いた分子動力学シ
 ミュレーションによる開口過程の解析
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 Analysis of Opening Process of E-coli Mechanosensitive Channel MscL by Molecular
 Dynamics Simulations on Wild Type and Mutant Models
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The bacterial mechanosensitive channel of large conductance, MscL, is constituted of
 homopentamer of a subunit with two (outer and inner) transmembrane alpha-helices and
 gated by tension in the membrane. Molecular dynamics (MD) simulation studies on *E-coli*
 MscL have been proposed some models for channel opening. However, due to a lack of
 MscL-lipid interactions in previous MD studies, it remains unclear where in the structure of
 MscL senses membrane tension and how the sensed force induces channel opening. To
 address these questions, we constructed a model, in which a closed MscL was embedded in a
 lipid bilayer, and performed MD simulations with membrane tension generated in the
 membrane. The tension gave a pressure profile of the membrane with two peaks near the
 lipid headgroups. It was also found that F78 in the outer helices interacted with lipids with
 strongest tension, thus may work as a tension sensor of MscL. Upon tension F78 was
 dragged by lipids followed by tilting the rigid outer and inner helices. The inner helices cross
 and interact each other, forming the most constricted part of the pore. We calculated
 changes in the interaction energy between inner helices during pore opening and obtained a
 value consistent with experimental one. To evaluate our MD system, we modeled mutants
 that are known to open easier (G22N) or harder (F78N) than wild type. These mutant
 models successfully reproduced the experimentally observed behaviors, indicating that the
 gating profile we mentioned may depict an essence of the real MscL gating.

2P011 電子顕微鏡構造データベースウザ・EM Navigator
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 EM Navigator - Electron microscopy data browser
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 Univ; 2: Protein Data bank Japan)

EM Navigator (URL: <http://emnavi.protein.osaka-u.ac.jp/>) is our new web service for
 browsing the 3D electron microscopy (EM) structure data, based on the data from EM Data
 Bank (EMDB) and Protein Data Bank. It has been constructed so that even users who do
 not know well about 3D EM can see easily and pleasingly browse the 3D EM data.
 EM structure data have not been friendly. It is often very hard to recognize the 3D
 structures just by seeing the figures on the papers or the web pages. In case of atomic
 coordinates of proteins, we can easily get some 3D views using jV on the PDBj web site or
 opening the downloaded data using some famous software such as RasMol. On the other
 hand, it requires some skill and effort to make 3D views from 3D EM data such as 3D maps
 deposited on EMDB. The barriers are much higher to view the structure combined with the
 other data such as the atomic coordinates fitted into the EM map.
 We have been constructing movies for each the data entry in EMDB, and embedding them
 on the EM Navigator web pages. You will get easily the 3D views with the detail information
 by the web browsers without installing special software. Further movies will be added, such
 as the views with the fitted atomic models and the zoomed up views around the important
 regions. Moreover, we are making our site useful by putting the snapshots of the PDB data
 published along with the EM data, the images of the supplementary information deposited
 by authors, and so on.