a computational model for understanding and predicting the chemical and physical properties of protein-solid surface systems.
As a test example, adsorption of the BLIP (beta-lactamase inhibitor protein) protein fused with different homotripeptides to the gold surface is explored. The computational algorithm is based on Brownian dynamics simulations of a protein in the presence of a metal surface with interactions described by electrostatic, Lennard-Jones (LJ), and desolvation energy terms. The interatomic LJ potential describes both the van der Waals and the chemical interaction between amino acids and the gold surface with parameters derived from ab initio calculations and experimental data. The desolvation term includes protein desolvation as well as surface water desorption effects. The results of the computer simulations are compared with the experimentally observed binding characteristics of the systems under consideration.
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Gold clusters as Spatial Probes of Residue Position on Protein in Small Angle X-ray Scattering
Hyun Chul Lee[1], Bruce A. Craig[1], Chris Bailey-Kellogg[2], Alan M. Friedman[1].
[1]Purdue University, West Lafayette, IN, USA, [2]Dartmouth College, Hanover, NH, USA.
We are developing a new method for using proteins labeled with one or two gold clusters in small angle X-ray scattering. Gold cluster labeling provides strong cluster-cluster (for double-label) and cluster-protein (for single and double-labels) interference. Analysis of the former provides the distance between gold clusters, while the analysis of the latter provides the distance and relative orientation between gold cluster and protein.
Here, we have investigated what structural information can be extracted from labeled protein. Simulated scattering curves of single or double-cluster labeled hypothetical template structures (PDB models modified with monomaleimido undecagold) were generated by the Debye formula using effective-atomic-scattering factors in solution. The template scattering curve is compared to the simulated scattering curves of trial structures generated by exhaustive rigid body searches for a fixed protein with rotated and translated gold cluster(s). For both single and double-labeled rigid body modeling (RBM), inter-body distance information was predicted within 1-2 Å error. However, the prediction of gold cluster position(s) was inaccurate (20-40 Å error for double-label, 5-50 Å error for single-label) presumably because inter-body distance information dominates over the relative orientation of gold cluster and protein. To predict accurate gold cluster position(s), we corrected inter-body distance(s) of trial structure by moving gold cluster(s) along the vector from protein to cluster during RBM. Gold cluster position(s) were improved significantly by correcting to the simulated template distance (2-7 Å for double-label, 2-5 Å for single-label), although the accuracy was reduced when using distance(s) determined by RBM (5-70 Å double-label, 2-12 Å single-label). Combining single and double-labeled data is being pursued.
This technique is being developed for two main applications: (1) discrimination of threading structures, (2) protein-protein docking model prediction.

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Molecular Dynamics Study of Carbon Nanotubes Interacting with Humic Acid - Towards a Mechanistic Understanding of Nanomaterial Transport in the Environment
Praveen Nedumpully Govindan[1], Jukka Määttä[1], Tatsiana Ratnikova[2], Sijie Lin[2], Pu-Chun Ke[2], Emppu Salonen[1].
[1]Helsinki University of Technology, Espoo, Helsinki, Finland, [2]Clemson University, Clemson, SC, USA.
A general concern with nanomaterials used in contemporary nanotechnology applications and consumer products is their potential discharge into the nature [1,2]. At present, there is still very little knowledge about the environmental and biological effects of nanomaterials, and the factors contributing to their transport, uptake and transformation in biological organisms. As one of the most important class of nanomaterials, carbon nanotubes (CNTs) pose a specifically important topic of study. Being essentially hydrophobic needle-like molecules, CNTs are not inherently water-soluble. Yet, it is known that CNTs can be solubilized by various types of amphiphilic molecules. In the case of CNTs discharged into the environment, such molecules capable of inducing solubilization are abundant in the ubiquitous natural organic matter (NOM) within soil and natural water sources. We have used molecular dynamics simulations to study the binding of humic acid (HA) - a major constituent of NOM - with a single-walled carbon nanotube (SWNT). As a representative structure for HA we have used an oligomer consisting of 12 monomers of the so-called Temple-Northeastern-Birmingham (TNB) HA model [3]. We describe in detail the factors affecting the binding of the HA oligomer to the SWNT, and its subsequent solubilization. In addition, aggregation processes of solubilized SWNTs, leading to their eventual precipitation with HA in experiments, are elucidated. The computational modeling is complemented by spectroscopic measurements of the HA-SWNT modes of binding.
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Analysis Of Side-chain Dynamics Of PhoB Dna Binding/transactivation Domain Using Molecular Dynamics Simulations
Tsutomu Yamane[1], Hideyasu Okamura[2], Yoshifumi Nishimura[1], Akinori Kidera[1,3], Mitsunori Ikeguchi[1].
[1]Yokohama City University, Yokohama, Japan, [2]Nathonal Institute of Agrobiological Sciences, Tsukuba, Japan, [3]Research Program for Computational Science, RIKEN, Wako, Japan.
PhoB is a transcription activator protein involved in the regulation of 39 genes constituting the *pho* regulon of bacteria. The DNA-binding/transactivation domain is a C-terminal functional domain of the PhoB for binding of the *pho* box, which is situated upstream of the pho regulon. The NMR structure of the DNA binding form of the PhoB DNA-binding/transactivation domain was solved by our group (PDB: 2z33) (1). In addition, backbone and side-chain dynamics of PhoB-DNA binding/transactivation domain were analyzed using the NMR relaxation spectroscopy (2).
In the present study, molecular dynamics (MD) simulations of the free-form and DNA- binding form of PhoB-DNA binding/transactivation domain were carried out, and resulting backbone and side-chain dynamics were compared with those of NMR relaxation experiments. The model-free order parameters for the backbone N-H bond (S^2_{NH}) and the methyl-averaging axis (S^2_{axis}) obtained from the MD simulations were in agreement with experimental values. It was found that S^2_{NH} and S^2_{axis} correlate well with the root-mean-square fluctuation (RMSF) of the backbone nitrogen atoms and the methyl carbon atoms obtained from the MD simulations, respectively, in contrast to weak correlations between the order parameters and crystal temperature factors. The S^2_{axis} - RMSF plot showed the clear dependence of S^2_{axis} on amino-acid species and the positions of the methyl groups in the side-chains, suggesting that dynamics of the methyl group in side chains are strongly affected by geometry of side chains in amino-acid species.
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Conformational Change of F_1-ATPase ϵ Subunit upon ATP Binding Studied by Molecular Dynamics Simulations and Small-angle X-ray Scattering
Tomotaka Oroguchi[1], Yasuyuki Kato-Yamada[2], Hiroshi Hashimoto[1], Satoru Unzai[1], Mamoru Sato[1], Mitsunori Ikeguchi[1].
[1]International Graduate School of Arts and Sciences, Yokohama City University, Yokohama, Japan, [2]Department of Life Science, Rikkyo University, Tokyo, Japan.
The ϵ subunit of F_1-ATPase acts as an endogenous inhibitor of the ATPase activity in F_1-ATPase. Biochemical and structural studies have shown that the ϵ subunit from the thermophilic Bacillus strain PS3 (TF1) binds ATP specifically, and the ATP binding induces the conformational change of the C-terminal domain of the ϵ subunit from the extended form to the folded form that allows ATP hydrolysis in F_1 motor. The mechanism of how ATP binding induces the conformational change of the ϵ subunit remains unclear, because the atomic detail of the conformational ensemble of the ATP-free form is still not known.
In this study, to address the above question, we used molecular dynamics (MD) simulations and small-angle X-ray scattering (SAXS) experiments. Analysis of the SAXS data measured at SPring-8 has shown that the overall structural characteristics of the ATP-bound form in solution are consistent with the crystal structure, while the molecular shape determined for the ATP-free form shows a more expanded conformation. We performed MD simulations for both the ATP-bound and ATP-free forms to obtain conformational ensemble of these forms, and the validity of the calculated ensembles was checked by a comparison of simulation-derived SAXS profiles with the experimentally observed profiles.