北尾彰朗（きたおあきお）

【研究課題名】原子解像度で探る巨大分子・分子集合体の柔らかさと機能の関係

東京大学分子細胞生物学研究所　准教授

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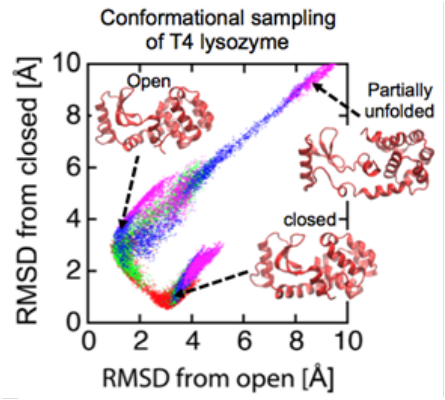
【専　門】理論化学、生物物理学、情報生物学

【キーワード】分子シミュレーション、巨大分子、複合体形成、分子機能

柔らかさの特徴を織り込んだ理論開発と柔らかさと機能の関係解明を進めます。また理論と実験の比較に基づく理論計算の改良と柔らかさの統合的な理解を目指した研究を行います。更に柔らかさを考慮した立体構造・分子機能の予測と設計を目指します。

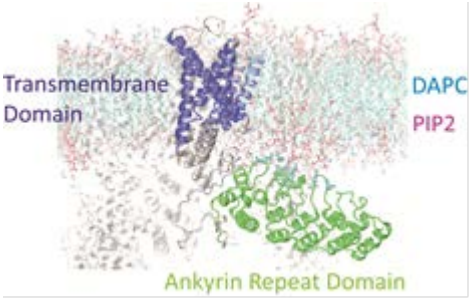
〈研究グループアクティビティー〉

柔らかさの特徴を織り込んだ理論開発



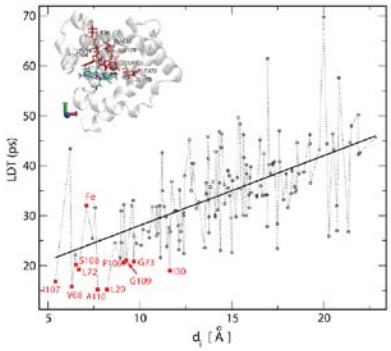
nt-PaCS-MD による柔らかな構造変化の探索

巨大分子・分子集合体の柔らかさと機能の関係



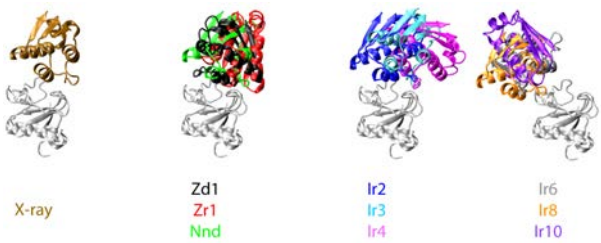
脂質との相互作用による TRPV1 の柔らかな構造変化

理論と実験の比較に基づく柔らかさの統合的な理解



線型応答理論によるタンパク質の応答

柔らかさを考慮した立体構造・分子機能の予測と設計



タンパク質ータンパク質複合体の立体構造予測

Akio KITAO

【Research Subject】Softness-function relationship in large molecules and molecular assemblies investigated at atomic resolution

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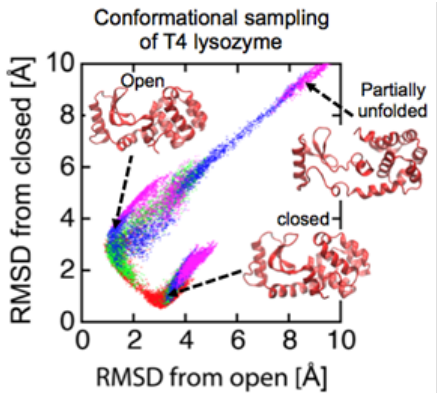
【Specialty】Theoretical Chemistry, Biophysics, Computational Biology

【Keywords】Molecular Simulation, Large Molecule, Complex Formation, Molecular Function

We will consider softness of complex molecular systems in the development of simulation methods and apply them to investigate softness-function relationship. Integrated approaches to elucidate the softness will be conducted by comparison between computation and experiment. Considering the softness, molecular design and prediction will be also addressed.

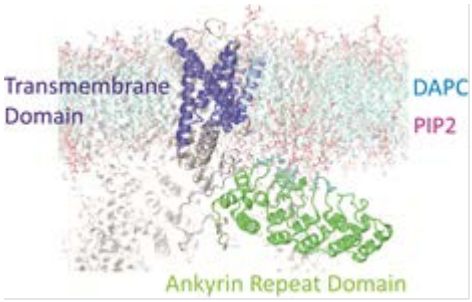
Research Group Activity

Consideration of the softness in the development of simulation



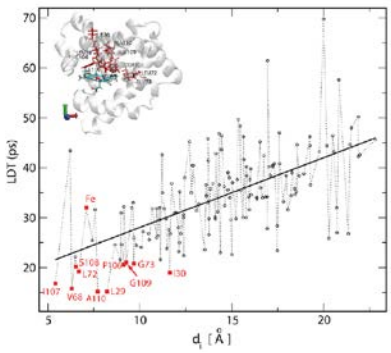
Searching soft conformational change by nt-PaCS-MD

Softness-function relationships



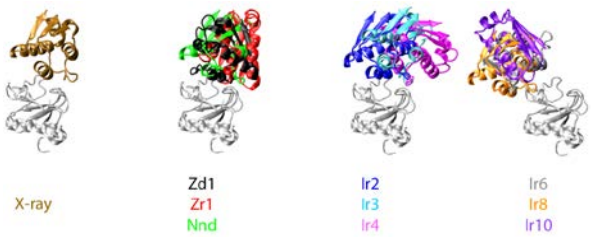
Soft conformational change of TRPV1 induced by interaction with lipids

Integrated understanding of softness from theory and experiment



Protein response from linear response theory

Consideration of the softness in prediction and design



Protein-protein complex structure prediction