（特別講演）

Molecular Dynamics of Proteins and Nucleic Acids

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We have used molecular dynamics simulations to study the stability and specificity of several protein-DNA/RNA complexes. In particular we have looked at the role of water molecules, which are often found in the interface regions, and which could be considered an integral part of the complexes. In addition to standard MD simulations, we have also applied free energy perturbation methods to assess the effects of mutations on the stability and specificity. Systems studied include homeodomains, DNA binding domains of nuclear hormone receptors, and RNA hairpins.