

Mining structure information using NAMD(Amber) and VMD

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Protein Structures

- Increase wealth information on the molecular foundation of living cells as new primary sequences and atomic resolution structures are deposited in the data base.
- The structures of crucial proteins which were essentially unknown 10 years ago are being resolved at a rapid pace.
- Structure yield static information
- Mining dynamic information from static structures
- Dynamic information leads to understanding function and mechanism of proteins, intellectual guideposts for medical research
- How to access mined dynamic information from structures

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Research tools

- Software tools: NAMD (Amber) and sister software VMD, and Excel.
- Mathematics tools: Optimization, Langevin equation, Numerical Methods and basic statistics.
- Chemistry tools
- Biology tools
- NAMD and VMD[**PB**].

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Frontier in Integrative Biological Research (FIBR)

The research

- tackles major questions in the Biological Sciences
- identifies major under-studied or unanswered questions in biology
- uses research tools across disciplines: Biology, Chemistry and Math
- biological significance is understanding molecular information of living cells.
- train young scientists in an interdisciplinary environment using.

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RIHC structure using pdb file

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Short dynamics of RIHC in the water

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(RIHC-wild-force-tube.mpg)



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