EMBnet/CNB
Centro Nacional de Biotecnología, CSIC
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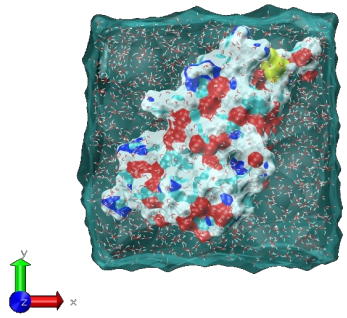
Molecular Dynamics Simulations (TINKER)



This is to certify that David Abia attended and satisfactorily completed the EMBnet (European Molecular Biology Network) course **Molecular Dynamics Simulations (TINKER)**, which took place 10th - 11th, November 2008, 9:30 to 16:30 at the *Centro Nacional de Biotecnología*, *Consejo Superior de Investigaciones Científicas*, Madrid, Spain.

This is an introductory course to Molecular Dynamics simulations for Life Scientists with an interest in understanding biological macromolecular systems. The course consists of **16 hours** of evenly split theoretical and practical sessions, and relies mainly on the use of the TINKER simulation package for the practical seesions, covering

- A general overview of the methods used in Molecular Dynamics
- Practical sessions using the TINKER molecular simulation package covering
  - installation of TINKER
  - protein simulation *in vacuo*
  - simulation of fluids using periodical boundary conditions
  - simulation of proteins in simplified solvent models
  - simulation of proteins in fully atomistic solvent models

There was considerable emphasis on developing first-hand experience through practical sessions in performing molecular mechanics, molecular dynamics, simulated annealing and other major techniques relevant to Molecular Simulations.

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