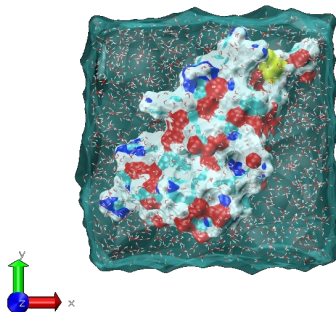


## Molecular Dynamics Simulations (TINKER)

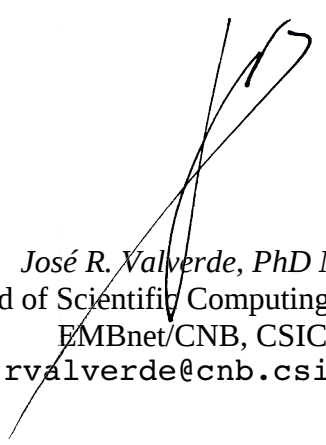


This is to certify that Herminia Loza Tavera attended and satisfactorily completed the EMBnet (European Molecular Biology Network) course **Molecular Dynamics Simulations (TINKER)**, which took place 10<sup>th</sup> - 11<sup>th</sup>, November 2008, 9:30 to 16:30 at the *Centro Nacional de Biotecnología, 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 sessions, 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.

  
José R. Valverde, PhD MD  
Head of Scientific Computing Services  
EMBnet/CNB, CSIC.  
jrvalverde@cnb.csic.es