

Workshop
High Performance Computing for Proteomics (HPC4P)
December 12th, 2011
CINECA, via Magnanelli 6/3, I-40033 Casalecchio di Reno (BO)

09:00-09:30 Registration/welcome

09:30-10:15

Mirko Cestari/Massimiliano Culpo (CINECA HPC staff)

Introduction to biological problems addressed with HPC techniques (45 min)

10:15-11:00

Andrew Emerson (CINECA HPC staff)

High Performance Computing at CINECA:

infrastructure, architectures, HPC European framework (45 min, CINECA HPC staff)

11:00-11:15 Coffee break

11:15-12:00

Rita Casadio (UniBO, Bologna, Italy)

Introduction to protein structure (45 min)

12:00-12:25

Ivano Eberini (UniMI, Milano, Italy)

Protein structure: case study I (25 min + 5 min discussion)

12:30-13:00

Rosa Di Felice/Stefano Corni (S3, Modena, Italy)

Protein structure: case study II (25 min + 5 min discussion)

13:00-14:00 Sandwich lunch and discussion

14:00-14:45

Piercarlo Fantucci (UniMIB, Milano, Italy)

Introduction to drug design (45 min)

14:45-15:15

Giulio Rastelli (UniMORE, Modena, Italy)

Drug design: case study I (25 min + 5 min discussion)

15:15-15:45

Andrea Cavalli (IIT and UniBO, Bologna, Italy)

Drug design: case study II (25 min + 5 min discussion)

15:45-16:00 Coffee break

16:00-16:30 Wrap-up (30 min, moderated by the organizers)

16:30-16:45 Closing