About Bioinformatics

Anna Tramontano, I.R.B.M. Piero Angeletti, Pomezia (Roma)

The goal of Bioinformatics, in my view, is to develop and use a combination of computational approaches to learn as much as possible about proteins and the relationship between their sequence, structure and function. Molecular modelling techniques and methods for sequence and structure analysis become extremely powerful when they are combined with the results of experiments designed ad hoc and consequently all my recent projects have been carried out in collaboration with the experimental groups of IRBM. We have modelled the Hepatitis C Virus (HCV) protease, helicase, polymerase and E2 envelope glycoprotein, designed chimeric HCV proteins, analysed biochemical results in the context of the protein structures, modelled the protease domain of HCV-related viruses and, for the HCV vaccine program, we have designed a library aimed at mimicking the hypervariable region 1 of HCV and analysed the results of its selection and screening. These activities span a number of areas of Bioinfomatics and have had an impact on the development of new therapeutical agents.