2019—current Senior Scientist in Computational Structural Biology, Merck KGaA, Global Analytical-Pharmaceutical Science and Innovation, Rome (Italy).

Activity

! Computational structural biology in pharmaceutical product development;

! Protein characterization via Molecular Dynamics simulations of the role of glycosylation and major post translational modifications;

! Machine learning methods development for the prediction of protein structural PTMs;

! Computational investigation of protein formulation via protein-excipient modeling and Molecular Dynamics simulations; ! PhD supervision

2014—2019 Senior Research Scientist, Bioinformatics Institute (BII, A*STAR) Singapore, Dr Igor N. Berezovsky.

2019—current Affiliated

Activity

! Structure-based molecular modeling development of allosteric communication in proteins;

! Perturbation based Free energy calculations from ligand binding and mutations;

! Server and Database development for fast calculation of allosteric properties of proteins;

! Machine learning method development for data driven Chromatin 3D structure reconstruction; !

2010—2013 Postdoctoral Research Fellow**,** Courant Institute of Mathematical Sciences (CIMS) - New York University, New York US, Prof. E. Vanden-Eijnden

Activity

! Molecular Dynamics simulations and Markov State Modeling to characterize protein functional dynamics

! Free energy barrier estimation from non-equilibrium simulations

! PhD supervision

2008—2009 Postdoctoral Scientist, Department of Bioengineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland, group of Prof. F. Naef

Activity

! Development of tools for the analysis of high-throughput sequencing data for the characterization of Protein-DNA interactions

! Multidimensional Markov modeling of gene expression time series data for characterizing cell cycle

2002–-2008 PhD student

2009–-2010 Postdoctoral Scientist, Department of Biochemistry, University of Zurich, Zurich Switzerland, Prof. A. Caflisch

Activity

! Several projects to investigate protein folding and aggregation via Molecular Dynamics simulations;

! Focus on biophysics of “primordial” proteins with low complexity amino acid sequences;

! Markov State Modeling to extrapolate long time dynamics of folding and aggregation;

! Complex Network modeling of protein free energy landscapes;