Curriculum-Vitae

Balasubramanian Chandramouli,
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Research/Education

Post Doctoral Fellow, Scuola Normale Superiore, Pisa , Italy	2012-present
Doctorate Student, University of Rome, Tor Vergata, Italy	2008-2012
Project Associate, Institute of Genomics & Integrative Biology, India	2005-2008
Masters in Biophysics, University of Madras, India	2004
Bachelors in Physics, Bharathidasan University, India	2002

Research methodologies

Classical MD Simulations (Experience with protein, nucleic acids and lipid membranes)

QM calculations (Optimization and forcefield parameterization)

Enhanced sampling methods (Adaptive biasing technique, steered MD and Umbrella sampling)

Computational biology (Bioinformatics and modeling techniques)

Data analytics: Development of in-house analysis codes and statistical computing.

Research Expertise

- Hydration effects on nucleic acid structures and small molecule interaction
- Unusual DNA and RNA structural biology
- Protein structural-function relationship
- Membrane structure and dynamics

Tutoring contributions

- Masters course on “Application of MD simulations to study membrane proteins”. SNS (2013,2014).
- Python Data analystics and visualization. SNS, 2016.

Recent publications

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(1) Flex, E.; Niceta, M.; Cecchetti, S.; Thiffault, I.; Au, M. G.; Capuano, A.; Piermarini, E.; Ivanova, A. A.; Francis, J. W.; Chillemi, G.; **Chandramouli, B**. et al., Biallelic Mutations in TBCD, Encoding the Tubulin Folding Cofactor D, Perturb Microtubule Dynamics and Cause Early-Onset Encephalopathy. *Am. J. Hum. Genet*. 2016, 99 (4), 962–973.

(2) Grubišić, S.; **Chandramouli, B**.; Barone, V.; Brancato, G. Chain Length, Temperature and Solvent Effects on the Structural Properties of α-Aminoisobutyric Acid Homooligopeptides. *Phys. Chem. Chem. Phys*. 2016, 18 (30), 20389–20398.

(3) **Chandramouli, B**.; Silvestri, V.; Scarno, M.; Ottini, L.; Chillemi, G. Smyd3 Open & Closed Lock Mechanism for Substrate Recruitment: The Hinge Motion of C-Terminal Domain Inferred from μ-Second Molecular Dynamics Simulations. *Biochim. Biophys. Acta* 2016, 1860 (7), 1466–1474.

(4) Di Maio, D.; **Chandramouli, B**.; Yan, R.; Brancato, G.; Pastore, A. Understanding the Role of Dynamics in the Iron Sulfur Cluster Molecular Machine. *Biochim. Biophys. Acta* 2016.

(5) Mancini, G.; Brancato, G.; **Chandramouli, B**.; Barone, V. Organic Solvent Simulations under Non-Periodic Boundary Conditions: A Library of Effective Potentials for the GLOB Model. *Chem. Phys. Lett.* 2015.

(6) **Chandramouli, B**.; Di Maio, D.; Mancini, G.; Barone, V.; Brancato, G. Breaking the Hydrophobicity of the MscL Pore: Insights into a Charge-Induced Gating Mechanism. *PLoS One* 2015, 10 (3), e0120196.

(7) Di Maio, D.; **Chandramouli, B**.; Brancato, G. Pathways and Barriers for Ion Translocation through the 5-HT3A Receptor Channel. *PLoS One* 2015, 10 (10), e0140258.

(8) Bhartiya, D.; **Chandramouli, B**.; Kumar, N. Co-Evolutionary Analysis Implies Auxiliary Functions of HSP110 in Plasmodium Falciparum. *Proteins* 2015, 83 (8), 1513–1525.

(9) **Chandramouli, B**.; Zazza, C.; Mancini, G.; Brancato, G. Boundary Condition Effects on the Dynamic and Electric Properties of Hydration Layers. *J. Phys. Chem. A* 2015, 119 (21).

(10) **Chandramouli, B**.; Di Maio, D.; Mancini, G.; Brancato, G. Introducing an Artificial Photo-Switch into a Biological Pore: A Model Study of an Engineered α-Hemolysin. *Biochim. Biophys. Acta* - Biomembr. 2015.