

IRB BARCELONA 2010 ANNUAL REPORT

SCIENCE AT IRB BARCELONA

Research Programmes

Structural and Computational Biology

Modesto Orozco: Molecular modelling and bioinformatics



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Highlights

- We have determined for the first time the mechanistic pathways in DNA chemothermal unfolding.
- We have defined at the microscopic level the atomistic pathways of the folding of small DNA hairpins.
- We have completed the largest atlas of protein dynamics in the world, creating a series of tools for the mining of the approx 20 Tb of data collected. We have found interesting correlations between the dynamic properties and biological function of proteins.

Publications

- Aviñó A, Cubero E, Gargallo R, González C, Orozco M and Eritja R. Structural properties of g,t-parallel duplexes. *J Nucleic Acids*, 2010, 1-11 (2010)
- Banás, P.; Hollas, D, Zgarbová Jurecka P, Orozco M, Cheatham TE, Sponer J and Otyepka M. Performance of molecular mechanics force-fields for RNA simulations. Stability of UUCG and GNRA hairpins. *J Chem Theory Comput*, 6, 3836-3849 (2010)
- Emperador A, Meyer T and Orozco M. Protein flexibility from discrete molecular dynamics simulations using quasi-physical potentials. *Proteins*, 78 (1), 83-94 (2010)
- Novoa EM, Ribas de Pouplana L, Barril X and Orozco M. Ensemble docking from homology models. *J Chem Theory Comput*, 6 (8), 2547-2557 (2010)
- Faustino I, Pérez A and Orozco M. Toward a consensus view of duplex RNA flexibility. *Biophys J*, 99 (6), 1876-85 (2010)
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- Meyer T, D'Abramo M, Hospital A, Rueda M, Ferrer-Costa C, Pérez A, Carrillo O, Camps J, Fenollosa C, Repchevsky D, Gelpí JL and Orozco M. MoDEL (Molecular Dynamics Extended Library): a database of atomistic molecular dynamics trajectories. *Structure*, 18 (11), 1399-409 (2010)
- Novoa EM, Castro de Moura M, Orozco M and Ribas de Pouplana L. A genomics method to identify pathogenicity-related proteins. Application to aminoacyl-tRNA synthetase-like proteins. *FEBS Lett*, 584 (2), 460-6 (2010)
- Orellana L, Rueda M, Ferrer-Costa C, López-Blanco JR, Chacón P and Orozco M. Approaching elastic network models to atomistic molecular dynamics. *J Chem Theory Comput*, 6, 2910-2923 (2010)
- Perez A and Orozco M. Real-time atomistic description of DNA unfolding. *Angew Chem Int Edit*, 49 (28), 4805-8 (2010)
- Pettifer, S. and the EMBRACE and INB-consortia including Orozco, M. The EMBRACE web service collection. *Nucleic Acids Res*, 38, W683-W688 (2010)
- Pons C, D'Abramo M, Svergun DI, Orozco M, Bernadó P and Fernández-Recio J. Structural characterization of protein-protein complexes by integrating computational docking with small-angle scattering data. *J Mol Biol*, 403 (2), 217-30 (2010)
- Pons C, Tlavera D, de la Cruz X, Orozco M and Fernández-Recio J. Scoring by intermolecular pairwise propensities of exposed residus (SIPPER): A new efficient potential for protein-protein docking. *J Chem Inf Model*, In Press (2010)

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- Portella G and Orozco M. Multiple routes to characterize the folding of a small DNA hairpin *Angew Chem Int Edit*, 49 (42), 7673-6 (2010)
- Raimondi F, Orozco M and Fanelli F. Deciphering the deformation modes associated with function retention and specialization in members of the Ras superfamily. *Structure*, 18 (3), 402-14 (2010)
- Soteras I, Orozco M and Luque FJ. Performance of the IEF-MST solvation continuum model in the SAMPL2 blind test prediction of hydration and tautomerization free energies. *J Comput Aid Mol Des*, 24 (4), 281-91 (2010)
- Watts JK, Martín-Pintado N, Gómez-Pinto I, Schwartzentruber J, Portella G, Orozco M, González C and Damha MJ. Differential stability of 2'F-ANA*RNA and ANA*RNA hybrid duplexes: roles of structure, pseudohydrogen bonding, hydration, ion uptake and flexibility. *Nucleic Acids Res*, 38 (7), 2498-511 (2010)

Collaborations

- A genomics method to identify pathogenicity-related proteins. Application to aminoacyl-tRNA synthetase-like proteins. ICREA (Barcelona, Spain)
- Deciphering the deformation modes associated with function retention and specialization in members of the Ras superfamily. Dulbecco Telethon Institute and Department of Chemistry (Modena, Italy)
- Performance of molecular mechanics force fields for RNA simulations: Stability of UUCG and GNRA Hairpins. University of Utah (Salt Lake City, United States)
- Structural properties of G,T-parallel duplexes. Department of Spectroscopy and Molecular Structure (Madrid, Spain)

Research projects

- Desarrollo de nuevas etiquetas peptídicas (EpiTag). INNFACTO (IPT-010000-2010-19). Spanish Ministry of Science and Innovation (MICINN). 2010-2012. Principal investigator: Modesto Orozco
- European life-science infrastructure for biological information, European Commission (214227), 2007-2011. Principal investigator: Modesto Orozco
- Exascale challenges in computational biology. ARCS 2010. Agency for Administration of University and Research Grants (AGAUR). Principal investigator: Modesto Orozco
- Modelització molecular i bioinformàtica, Grups de Recerca reconeguts per la Generalitat de Catalunya 2009-2013 (2009 SGR 1348). Agency for Administration of University and Research Grants (AGAUR). 2009-2013. Principal investigator: Modesto Orozco
- Molecular recognition, Fundación Marcelino Botín, (2007-2010). Principal investigator: Modesto Orozco
- Red temática de investigación cooperativa en biomedicina computacional "COMBIOMED". Carlos III Health Institute (ISCIII). 2008-2012. Principal investigator: Modesto Orozco
- Scalable Software Services for Life Science (ScalaLife), European Commission (261523). 2010-2013. Principal investigator: Modesto Orozco
- Simulaciones de formas inusuales o tensionadas de los ácidos nucleicos de potencial interés biotecnológico o biomédico. Proyectos de investigación fundamental (BIO2009-10964). Spanish Ministry of Science and Innovation (MICINN). 2010-2012. Principal investigator: Modesto Orozco
- Supercomputación y e-ciencia. Consolider Ingenio-2010 (CSD2007-00050). Spanish Ministry of Science and Innovation (MICINN). 2007-2012. Principal investigator: Modesto Orozco.
- Plataforma en Red de Bioinformática (INB-ISCIII). Carlos III Health Institute (ISCIII). 2004-2011. Principal investigator: Modesto Orozco
- Spanish Ministry of Science and Innovation (MICINN). 2010. Principal investigator: Modesto Orozco
- Pfizer Research and Technology Center. 2010. Principal investigator: Modesto Orozco



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