

IRB BARCELONA 2011 ANNUAL REPORT

Research Programmes

STRUCTURAL AND COMPUTATIONAL BIOLOGY

Modesto Orozco: Molecular Modelling and Bioinformatics



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Highlights

- We have determined the conformational nature of a prototypical molten-globule moonlighting protein and advanced in the description of the unfolded state of proteins.
- We have gained ground in the description of chromatin structure using both experimental and theoretical approaches.
- We have progressed in describing the connection between changes in DNA sequence and structure and genetic pathologies such as cancer.

Publications

- Kowalczyk L, Ratera M, Paladino A, Bartoccioni P, Errasti-Murugarren E, Valencia E, Portella G, Bial S, Zorzano A, Fita I, Orozco M, Carpena X, Vázquez-Ibar JL and Palacín M.
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- Luque FJ, Dehez F, Chipot C and Orozco M
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- Orozco M, Orellana L, Hospital A, Naganathan AN, Emperador A, Carrillo O and Gelpí JL.
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The protein folding transition-state ensemble from a G?-like model
Phys Chem Chem Phys, **13**, 15166-74 (2011)
- Naganathan AN and Orozco M.
The native ensemble and folding of a protein molten-globule: functional consequence of downhill folding
J Am Chem Soc, **133**, 12154-61 (2011)

- Flores O and Orozco M.
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- Stein A, Rueda M, Panjkovich A, Orozco M and Aloy P.
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Whole-genome sequencing identifies recurrent mutations in chronic lymphocytic leukaemia
Nature, **475**, 101-5 (2011)
- D'Abramo M, Orozco M and Amadei A.
Effects of local electric fields on the redox free energy of single stranded DNA
Chem Commun, **47**, 2646-8 (2011)
- Ayuso-Tejedor S, García-Fandiño R, Orozco M, Sancho J and Bernadó P.
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Research projects

- Desarrollo de nuevas etiquetas peptídicas (EpiTag). INNPACTO (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
- 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". (RDo7/0067/0009). 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
- Palau Pharma 2011-2012 Modesto Orozco

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Collaborations

- *Definition of new generation simulation methods*, Department of Physical Chemistry. Pharmacy School, University of Barcelona (Barcelona, Spain)
- *Essential deformation patterns in protein recognition*, University of California (San Diego, United States)
- *Genotyping of chronic lymphocytic leukemia*, University of Oviedo (Oviedo, Spain)
- *Representation of DNA conductivity*, Department of Chemistry, University La Sapienza of Rome (Rome, Italy)
- *Representation of partially folded proteins*. Department of Chemistry, University of Zaragoza (Zaragoza, Spain)



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