Juan Eiros Zamora

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Education

Imperial College London **London**

PhD, Computational Chemistry *2015–2018*

I study the structure and dynamics of proteins using molecular dynamics simulations. I use machine learning techniques such as dimensionality reduction, clustering and Markov State Models to build interpretable models from large simulation datasets.

Imperial College London **London**

MRes, GPA: 79.9/100 (Distinction) *2014–2015*

Chemical Biology: Multidisciplinary Scientists for Next Generation Biological, Biomedical and Pharmaceutical Research Development

Institut Químic de Sarrià – Universitat Ramon Llull **Barcelona**

BSc, GPA: 84/100 *2010–2014*

Degree in Chemistry

Work Experience

BASF Spain **Barcelona**

Operational Excellence Summer Intern *Jul 2017–Sep 2017*

I developed an Excel based tool for the analysis and visualization of relevant Key Performance Indicators from Asset Effectiveness data. The aim was to monitor the improvement actions and to synchronise the historical production data in SAP with the real capacity of an asset.

Biomedical Research Foundation of the Academy of Athens **Athens**

PRACE Summer of HPC Participant *Jul 2016–Sep 2016*

I developed a re-ranking algorithm to post process compounds arising from virtual screening to enhance protein selectivity. The algorithm has been added to the ChemBioServer for general use. Additional activities of the programme involved writing blog posts in the Summer of HPC website as well as the preparation of a final manuscript and presentation.

Volunteer and Teaching Experience

Imperial College London **London**

Graduate Teaching Assistant *Oct 2016 – Current*

Courses taught: Molecular Driving Forces, Data Visualization and Analysis, Introduction to Programming, Molecular Reaction Dynamics, Measurement Science II

Software Carpentry Foundation **London**

Certified Instructor *Jan 2018–Current*

The Software Carpentry Foundation is an open source project that aims to to teach researchers the computing skills they need to get more done in less time and with less pain. I have become a volunteer certified instructor, and teach Python programming and data analysis in the workshops run at Imperial College London.

TuringLab **London**

Coding Instructor *2016–2017*

The aim of Turinglab is to introduce coding and computational thinking to young children. We use JavaScript and Scratch to program simple videogames.

Exscitec **London**

Reaching Further Instructor *2014–2016*

I developed an outreach activity to engage potential STEM careers students into multidisciplinary teams such as Structural Biology and Computational Chemistry.

Scholarships and Awards

Hackathon Innovation Price

British Petrol & Imperial College London *Jun 2017*

Our team won the Innovation Price for developing an autopilot system integrating Computer Vision and Voice Assisted technologies enabling an AI agent to detect a driver's identity and fatigue. The agent reduces the risk of accidents by engaging with the driver through a set of different voice-activated activities, such as finding the closest gas station, texting a friend, calling emergencies or playing music.

Research Grant **PhD**

Engineering and Physical Sciences Research Council *2016-2018*

I've been funded by the EPSRC during the last two years of my PhD.

Sir Alan Fersht Certificate of Excellence **MRes**

Institute of Chemical Biology – Imperial College London *2015*

Prize awarded for an outstanding Chemical Biology MRes Research Project.

Grant for Postgraduate Studies in Europe **MRes**

Obra Social La Caixa *2014–2016*

Full economic grant for the first two years of postgraduate studies. Around a hundred of these scholarships are awarded yearly to the best performing students (of any discipline) in Spain.

Grant for Academic Excellence **BSc**

Fundació Francesc Castelló *2010–2014*

Economic scholarship for the undergraduate studies in Chemistry. Awarded and maintained each year to the best performing students in the cohort.

Languages

Spanish, Catalan: Native speaker

English: Proficient User *C2*

French: Independent User *B1*

Computer skills

Languages

Proficient: Python, R, Bash scripting **Intermediate**: C, C++, CUDA, Javascript, VBA

Technologies

Git, GNU/Linux, HPC environments, Microsoft Office, LATEX, Apache, HTML5, CSS, Biomolecular modelling software, SAP

Articles

Zamora, Juan Eiros, Maria Papadaki, et al. (2016). "Troponin structure: its modulation by Ca2+ and phosphorylation studied by molecular dynamics simulations". In: *Phys. Chem. Chem. Phys.* 18 (30), pp. 20691–20707. DOI: 10.1039/C6CP02610A. URL: http://dx.doi.org/10.1039/C6CP02610A.

Conference and Oral Communications

Zamora, Juan Eiros, Gil Hoben, et al. (2017). "EGCG and Silybin as treatment for inherited cardiomyopathies: Binding simulations to cardiac troponin". In: ed. by American Chemical Society. San Francisco, CA. DOI: 10.13140/RG.2.2.25103.38563.

Zamora, Juan Eiros, Alice Sheehan, et al. (2016). "Troponin Structure and Effects of Phosphorylation and Mutations Studied by Molecular Dynamics Simulations". In: ed. by Biophysical Journal. Vol. 110. 3. Los Angeles, CA, 208a. DOI: 10.1016/j.bpj.2015.11.1157.

Zamora, Juan Eiros et al. (2017). "Markov State Models of cardiac Troponin dynamics". In: ed. by MGMS Young Modellers' Forum. London, UK. URL: http://www.mgms.org/YMF2017.