De Fabritiis, Gianni
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Experimental Sciences & Mathematics

ICREA research professor at Universitat Pompeu Fabra (UPF) and group leader of the computational biophysics laboratory and associate professor at UPF.

I have a bachelor degree in applied mathematics (1997, University of Bologna) and a PhD in computational chemistry (2002, Queen Mary University of London). I have worked at the CINECA supercomputing center (1998-1999), at University College London (2003-2006) and later I won a 5 year Ramon y Cajal tenure-track fellowship at University Pompeu Fabra and the I3 program, before becoming ICREA Professor.

I have published 80 articles in international journals (PNAS, JACS, Nat. Chem., Nat. Commun., etc). My h-index is 30 with over 3200 citations. In the last four years I gave 30 oral presentations at international conferences (18 as invited speaker) and lectures in many pharmaceutical companies. I am associate editor of “In-silico pharmacology”.

Research interests

My group research interests are centered in the application of computing as a fundamental methodology to problem solving. In particular simulations in biomedicine, machine learning of biological data and machine intelligence.

Research lines

Biomedicine. We use large distributed computational resources (GPUGRID.net) with thousands of GPUs for molecular dynamics simulations, binding prediction, binding kinetics, Markov state models, online sampling methods (ACEMD, HTMD). The approach is computational driven but we like to collaborate with experimental laboratories and pharmaceutical companies.

Machine Intelligence. In this research line we develop machine learning approaches applied to biological data. We are particularly interested in behavioral intelligence, artificial neural networks, sparse coding, deep and hierarchical learning.

Selected publications

– Martinez-Rosell G, Giorgino T & **De Fabritiis G** 2017, ‘PlayMolecule ProteinPrepare: A Web Application for Protein Preparation for Molecular Dynamics Simulations’, *Journal Of Chemical Information And Modeling*, 57, 7, 1511 – 1516.

– Martinez-Rosell G, Giorgino T, Harvey MJ & **de Fabritiis G** 2017, ‘Drug Discovery and Molecular Dynamics: Methods, Applications and Perspective Beyond the Second Timescale’, *Current Topics In Medicinal Chemistry*, 17, 23, 2617 – 2625.

– Plattner N, Doerr S, **De Fabritiis G** & Noe F 2017, ‘Complete protein-protein association kinetics in atomic detail revealed by molecular dynamics simulations and Markov modelling’, *Nature Chemistry*, 9, 10, 1005 – 1011.

– Jimenez J, Doerr S, Martinez-Rosell G, Rose A & **De Fabritiis G** 2017, ‘DeepSite: protein-binding site predictor using 3D-convolutional neural networks’, *Bioinformatics*, 33, 19, 3036 – 3042.

– Doerr S, Giorgino T, Martinez-Rosell G, Damas JM & **De Fabritiis G** 2017, ‘High-Throughput Automated Preparation and Simulation of Membrane Proteins with HTMD’, *Journal Of Chemical Theory And Computation*, 13, 9, 4003 – 4011.

– Kapoor A, Martinez-Rosell G, Provasi D, **de Fabritiis G** & Filizola M 2017, ‘Dynamic and Kinetic Elements of mu-Opioid Receptor Functional Selectivity’, *Scientific Reports*, 7, 11255.

Selected research activities

- We have obtained an EU innovation grant INUMED and one Torres Quevedo fellowship
- Member of the EU CompBioMed project with both UPF and Acellera
- Received 80K euro of private donations

- Director and chief science officier of the company Acellera ltd which I co-founded in 2006, I direct the R&D of the company and collaborate with several research organizations and pharmaceutical companies towards the goal of computerized drug discovery
- GPUGRID.net remains one of the largest worldwide distributed computing projects
- We have launched playmolecule.org