Jaime **Rodríguez-Guerra**

jaime.rogue@gmail.com • rjai.me • @jaime_rgp
jaimergp • 0000-0001-8974-1566 • imKyayEAAAAJ

Skills

Programming	Python, JavaScript, LaTeX, PHP
Web development	Flask, Hugo, React, Joomla
Code maintenance	GitHub, Readthedocs, Travis, AppVeyor
Deployment	conda, constructor, pip, npm Vultr, Heroku, Netlify, GitHub Pages

Scientific software

Molecular Dynamics	OpenMM, MDTraj, AmberTools, ParmEd
Quantum Mechanics	Gaussian, NWChem
Homology Modelling	Modeller
Docking	GOLD, AutoDock Vina
Cheminformatics	RDKit, ase, openbabel
Visualization	UCSF Chimera, VMD, PyMol, NGLView

Education & Positions

Postdoctoral researcher in Prof. Maréchal's group — Barcelona, Spain
Autonomous University of Barcelona (UAB) — Dec 2018 - present

Research assistant in Prof. Maseras' group — Tarragona, Spain
Institute of Chemical Research of Catalonia (ICIQ) — Apr - Oct 2018

PhD in Biotechnology — Barcelona, Spain
Autonomous University of Barcelona (UAB) — 2015 - 2018

- Government of Catalonia FI 3-year predoctoral fellowship
- Supervisor: Jean-Didier Maréchal
- Committee: Gerald Monard, Sílvia Osuna, Xavier Solans

MSc in Bioinformatics — Barcelona, Spain
Autonomous University of Barcelona — 2013 - 2014

BSc in Biotechnology — Salamanca, Spain
University of Salamanca — 2008 - 2013

Highlighted software projects

GaudiMM

Python 2.7, UCSF Chimera, deap and more — insilichem/gaudi

- Multi-objective genetic algorithm optimization platform for 3D molecular sketching
- Modular architecture on top of UCSF Chimera to support 3rd party libraries (OpenMM, ProDy, RDKit, NWChem, Vina, IMP)
- Open development supported by GitHub, Readthedocs, and TravisCI

OMMProtocol

Python 2.7/3.4+, OpenMM, ParmEd, MDTraj, openmoltools — insilichem/ommprotocol

- Command-line application to create MD protocols with YAML input files
- Built on top of OpenMM and enhanced with loaders, reporters and integrators found in ParmEd, MDTraj and openmoltools
- Open development and deployment supported by GitHub, Readthedocs, TravisCI, AppVeyor and conda constructor

ESIgen

Python 2.7/3.4+, cclib, Jinja, Flask; JavaScript — insilichem/esigen

- Web application to generate technical reports from computational chemistry calculations
- Exposes cclib parsers through the Jinja templating engine and serves it with Flask
- Deployed to Heroku and connected with online platforms (GitHub, FigShare, Zenodo) through JavaScript hooks

GARLEEK

Python 2.7/3.4+; Tinker; Gaussian — insilichem/garleek

- Command-line application to extend Gaussian's ONIOM engine with external MM force fields
- Modular design to accept any MM library. Tinker compatibility already available, including polarizable force fields
- Designed as a replacement for an existing collection of Bash scripts with poor maintainability

Tangram

Python 2.7, UCSF Chimera and more — insilichem/tangram

- Collection of graphical interfaces for molecular modelling in UCSF Chimera
- Setup external calculations (Gaussian, OpenMM, NCIPlot, ProDy...)
- Visualize results from external tools (PLIP, GOLD, GaudiMM, PoPMuSiC, PropKa...)

Publications

Submitted & Under Review

† *co-corresponding authorship*

On the dynamical effects of the incorporation of unnatural chemical blocks in protein backbones: the case of study of LmrR 2018

Submitted

Lur Alonso-Cotchico, Jaime Rodríguez-Guerra Pedregal, Agustí Lledós, Jean-Didier Maréchal

Molecular modelling in artificial metalloenzymes design and optimization 2018

Under review

Lur Alonso-Cotchico, Jaime Rodríguez-Guerra Pedregal, Agustí Lledós, Jean-Didier Maréchal

Simple coordination geometry descriptors allow to accurately predict metal binding sites in proteins 2018

Under review

Giuseppe Sciortino, Eugenio Garribba, Jaime Rodríguez-Guerra Pedregal,† Jean-Didier Maréchal†

Discovery of substrate-assisted processivity by an exo-hydrolase with a pocket-shaped catalytic site 2018

Under review

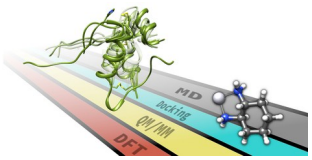
Victor Streltsov, Sukanya Luang, Alys Peisley, Joseph Varghese, James Ketudat Cairns, Sébastien Fort, Marcel Hijnen, Igor Tvaroska, Ana Ardá, Jesús Jiménez-Barbero, Mercedes Alfonso-Prieto, Carme Rovira, Fernanda Mendoza, Laura Tiessler-Sala, José-Emilio Sánchez-Aparicio, Jaime Rodríguez-Guerra Pedregal, José M. Lluch, Jean-Didier Maréchal, Laura Masgrau, Maria Hrmova

A multiscale computational study of the Cu-catalyzed hydration of alkenes in water solvent and into the context of an artificial metallohydratase 2018

Under review

Lur Alonso-Cotchico, Giuseppe Sciortino, Jaime Rodríguez-Guerra Pedregal, Ivana Drienovska, Gerard Roelfes, Agustí Lledós, Jean-Didier Maréchal

Published & In Press



Computational insight on the interaction of oxaliplatin with insulin 2019

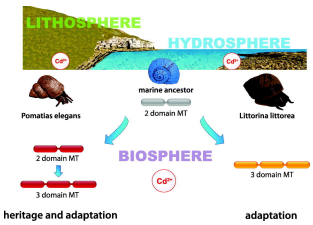
Metallomics doi 10.1039/C8MT00341F

Giuseppe Sciortino, José-Emilio Sánchez-Aparicio, Jaime Rodríguez-Guerra Pedregal, Eugenio Garribba, Jean-Didier Maréchal

GARLEEK: Adding an Extra Flavor to ONIOM 2019

J. Comput. Chem. 40, 381-386 doi 10.1002/jcc.25612 — insilichem/garleek

Jaime Rodríguez-Guerra Pedregal, Ignacio Funes-Ardoiz, Giuseppe Sciortino, José-Emilio Sánchez-Aparicio, Gregori Ujaque, Agustí Lledós, Jean-Didier Maréchal, Feliu Maseras



Differential response to Cadmium exposure by expression of a two and a three-domain metallothionein isoform in the land winkle Pomatias elegans: Valuating the marine heritage of a land snail 2018

Sci. Total. Environ. 648, 561-571 doi 10.1016/j.scitotenv.2018.07.426

Lara Schmielau, Martin Dvorak, Michael Niederwanger, Nicole Dobieszewski, Veronika Pedrini-Martha, Peter Ladurner, Jaime Rodríguez-Guerra Pedregal, Jean-Didier Maréchal, Reinhard Dallinger

ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications 2018

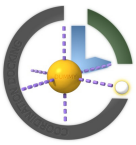
J. Chem. Inf. Model. 58 (3), 561-564 doi 10.1021/acs.jcim.7b00714 insilichem/esigen

Jaime Rodríguez-Guerra Pedregal,† Pablo Gómez-Orellana, Jean-Didier Maréchal†

PyChimera: Use UCSF Chimera modules in any Python 2.7 project 2018

Bioinf. 34 (10), 1784-1785 doi 10.1093/bioinformatics/bty021 insilichem/pychimera

Jaime Rodríguez-Guerra Pedregal,† Jean-Didier Maréchal†



Prediction of the interaction of metallic moieties with proteins: An update for protein-ligand docking techniques 2018

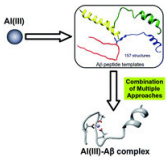
J. Comput. Chem. 39 (1), 42-51 doi 10.1002/jcc.25080

Giuseppe Sciortino, Jaime Rodríguez-Guerra Pedregal, Agustí Lledós, Eugenio Garribba, Jean-Didier Maréchal

GaudiMM: A modular multi-objective platform for molecular modeling 2017

J. Comput. Chem. 38 (24), 2118-2126 doi 10.1002/jcc.24847 insilichem/gaudi

Jaime Rodríguez-Guerra Pedregal,† Giuseppe Sciortino, Jordi Guasp, Martí Municoy, Jean-Didier Maréchal†

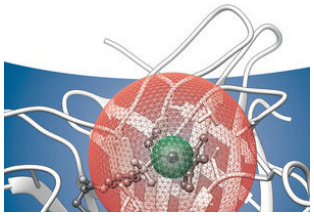


Elucidating the 3D structures of Al(III)–Aβ complexes: a template free strategy based on the pre-organization hypothesis 2017

Chem. Sci. 8, 5041-5049 doi 10.1039/C7SC01296A

Jon I. Mujika, Jaime Rodríguez-Guerra Pedregal, Xabier Lopez, Jesus M. Ugalde, Luis Rodríguez-Santiago, Mariona Sodupe, Jean-Didier Maréchal

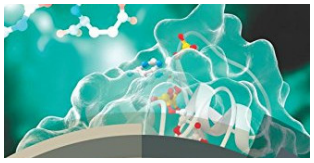
Reviews & Book Chapters



Computational Studies of Artificial Metalloenzymes: From Methods and Models to Design and Optimization 2018

Ch. 4 in "Artificial Metalloenzymes and MetalloDNAzymes in Catalysis: From Design to Applications", Wiley & Sons doi 10.1002/9783527804085.ch4

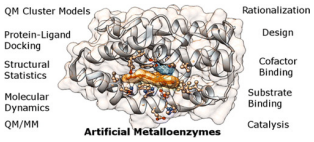
Jaime Rodríguez-Guerra Pedregal, Lur Alonso-Cotchico, Giuseppe Sciortino, Agustí Lledós, Jean-Didier Maréchal



Enzyme Design 2016

Ch. 15 in "Simulating Enzyme Reactivity", Royal Society of Chemistry doi 10.1039/9781782626831-00481

Lur Alonso-Cotchico, Jaime Rodríguez-Guerra Pedregal, Agustí Lledós and Jean-Didier Maréchal

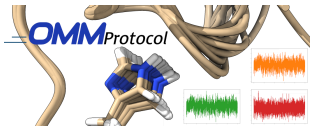


Toward the Computational Design of Artificial Metalloenzymes: From Protein–Ligand Docking to Multiscale Approaches 2015

ACS Catal. 5 (4), 2469-2480 ☒ Review doi 10.1021/acscatal.5b00010

Victor Muñoz Robles, Elisabeth Ortega-Carrasco, Lur Alonso-Cotchico, Jaime Rodriguez-Guerra Pedregal, Agustí Lledós, Jean-Didier Maréchal

Pre-prints



OMMProtocol: A Command Line Application to Launch Molecular Dynamics Simulations with OpenMM 2018

ChemRxiv doi 10.26434/chemrxiv.7059263 insilichem/ommprotocol

Jaime Rodríguez-Guerra Pedregal,† Lur Alonso-Cotchico, Lorea Velasco-Carneros, Jean-Didier Maréchal†

Presentations

XXXIV XRQTC Annual Meeting Barcelona, Spain

The InsiliChem Molecular Modelling Suite July 12, 2018

X International School on Organometallic Chemistry Marcial Moreno Mañas Ciudad Real, Spain

Multicriteria optimization of chemostructural drafts with a modular software platform July 7, 2017

XXXVI RSEQ Biennial Meeting — Sitges, Spain
A multi-objective optimization software for structural sketching of chemobiological compounds — June 28, 2018
Awarded "Best Flash Presentation"

4th COST MC Meeting "Dynamics of Biomacromolecular Machines" — Bugibba, Malta
A modular multi-objective platform for molecular modeling — March 28, 2017

IX International School on Organometallic Chemistry Marcial Moreno Mañas — San Sebastián, Spain
Solving coordination geometries for complex biometallic systems — July 7, 2016

Teaching

Modern Python for scientific software development — Barcelona, Spain
SGB - Servei de Genòmica i Bioinformàtica, Autonomous University of Barcelona — 2017-present
http://sct.uab.cat/genomica-bioinformatica/en

Practicum: Molecular Dynamics simulations in UCSF Chimera — Barcelona, Spain
MSc Industrial Chemistry and Introduction to Chemical Research, Autonomous University of Barcelona — 2016-present
http://pagines.uab.cat/chemistry-master

Introduction to Python — Barcelona, Spain
MSc Bioinformatics, Autonomous University of Barcelona — 2016-present
http://mscbioinformatics.uab.cat

Co-supervised projects

2018	**Lorea Velasco**, SAXS-driven homology modelling refinement	PhD Biomedicine & Molecular Biology, EHU
2018	**Daniel Viladrich**, Energy-corrected interpolation of molecular trajectories	BSc Physics, UAB
2018	**Mercè Alemany**, TALAIA: visual dictionary for protein residues	MSc Bioinformatics, UAB
2017	**Pablo Orenes**, Ligand-binding pathways in GaudiMM	MSc Bioinformatics, UAB
2017	**Mireia Bertrán**, Inertia tensors for protein-ligand docking	BSc Mathematics, UAB
2017	**José Emilio Sánchez**, Graph-based molecular topology generation	MSc Bioinformatics, UAB
2017	**David Teixé**, Web-based hierarchical molecular visualization	Double BSc Chemistry + Physics, UAB
2016	**Martí Municoy**, Evaluation of metal coordination geometries	Double BSc Chemistry + Physics, UAB
2016	**Daniel Soler**, Cationic Dummy Atoms Software	Double BSc Chemistry + Physics, UAB
2016	**Jordi Guasp**, Normal Modes interfacing with ProDy & UCSF Chimera	BSc Mathematics, UAB

References

Prof. Dr. Jean-Didier Maréchal — Barcelona, Spain
Associate Professor, Department of Chemistry, Autonomous University of Barcelona (UAB)
jeandidier.marechal@uab.cat • http://www.insilichem.com

Prof. Dr. Feliu Maseras — Tarragona, Spain
Group Leader, Institute of Chemical Research of Catalonia (ICIQ)
fmaseras@iciq.es • http://www.iciq.org/research/research_group/prof-feliu-maseras