

Jaime Rodríguez-Guerra

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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

AUTONOMOUS UNIVERSITY OF BARCELONA (UAB)

Barcelona, Spain

Dec 2018 - present

Research assistant in Prof. Maseras' group

INSTITUTE OF CHEMICAL RESEARCH OF CATALONIA (ICIQ)

Tarragona, Spain

Apr - Oct 2018

PhD in Biotechnology

AUTONOMOUS UNIVERSITY OF BARCELONA (UAB)

Barcelona, Spain

2015 - 2018

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

MSc in Bioinformatics

AUTONOMOUS UNIVERSITY OF BARCELONA

Barcelona, Spain

2013 - 2014

BSc in Biotechnology

UNIVERSITY OF SALAMANCA

Salamanca, Spain

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, Gerard Roelfes, Jean-Didier Maréchal

Molecular modelling in artificial metalloenzymes design and optimization

2018

SUBMITTED

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

SUBMITTED

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

SUBMITTED

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

SUBMITTED

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

Computational insight on the interaction of oxaliplatin with insulin

2018

SUBMITTED

Giuseppe Sciortino, José-Emilio Sánchez-Aparicio, [Jaime Rodríguez-Guerra Pedregal](#), Eugenio Garribba, Jean-Didier Maréchal

Pillar[5]arene glyco(mimetic)rotaxanes for the functional interrogation of multivalency responsive glycosidases

2018

SUBMITTED

Iwona Nierengarten, Manuel González-Cuesta, [Jaime Rodríguez-Guerra Pedregal](#), Uwe Hahn, Sonia Romero-Téllez, Jean-Didier Maréchal, Laura Masgrau, José Manuel García Fernández, Jean-François Nierengarten, Carmen Ortiz Mellet

PUBLISHED & IN PRESS



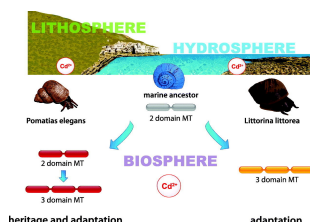
GARLEEK: Adding an Extra Flavor to ONIOM

2019

J. Comput. Chem. 40, 381-386  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  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[†]



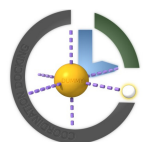
PyChimera: Use UCSF Chimera modules in any Python 2.7 project

2018

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

insilichem/pychimera

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

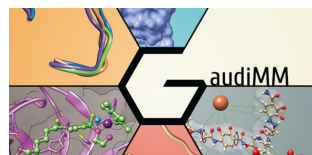


Prediction of the interaction of metallic moieties with proteins: An update for protein-ligand docking techniques

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



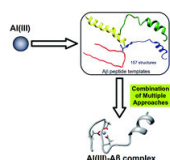
GaudiMM: A modular multi-objective platform for molecular modeling

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[†]



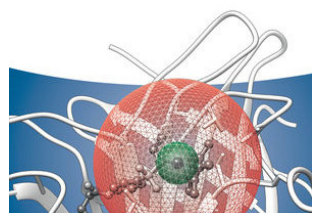
Elucidating the 3D structures of Al(III)-Aβ complexes: a template free strategy based on the pre-organization hypothesis

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

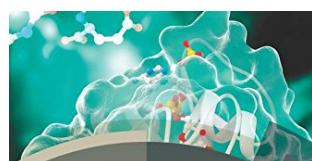


Computational Studies of Artificial Metalloenzymes: From Methods and Models to Design and Optimization

2018

Ch. 4 in "Artificial Metalloenzymes and MetalloDNAs 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

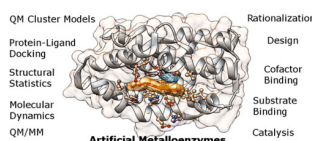


Enzyme Design

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



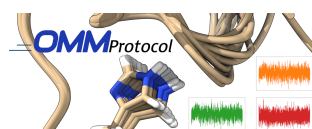
Toward the Computational Design of Artificial Metalloenzymes: From Protein-Ligand Docking to Multiscale Approaches

2015

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

Victor Muñoz Robles, Elisabeth Ortega-Carrasco, Lur Alonso-Cotchico, Jaime Rodríguez-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

THE INSILICHEM MOLECULAR MODELLING SUITE

Barcelona, Spain

July 12, 2018

X International School on Organometallic Chemistry Marcial Moreno Mañas

MULTICRITERIA OPTIMIZATION OF CHEMOSTRUCTURAL DRAFTS WITH A MODULAR SOFTWARE PLATFORM

Ciudad Real, Spain

July 7, 2017

XXXVI RSEQ Biennial Meeting

A MULTI-OBJECTIVE OPTIMIZATION SOFTWARE FOR STRUCTURAL SKETCHING OF CHEMOBIOLOGICAL COMPOUNDS

🏆 Awarded “Best Flash Presentation”

Sitges, Spain

June 28, 2018

4th COST MC Meeting “Dynamics of Biomacromolecular Machines”

A MODULAR MULTI-OBJECTIVE PLATFORM FOR MOLECULAR MODELING

Bugibba, Malta

March 28, 2017

IX International School on Organometallic Chemistry Marcial Moreno Mañas

SOLVING COORDINATION GEOMETRIES FOR COMPLEX BIOMETALLIC SYSTEMS

San Sebastián, Spain

July 7, 2016

Teaching

Modern Python for scientific software development

SGB - SERVEI DE GENÒMICA I BIOINFORMÀTICA, AUTONOMOUS UNIVERSITY OF BARCELONA

🌐 <http://sct.uab.cat/genomica-bioinformatica/en>

Barcelona, Spain

2017-present

Practicum: Molecular Dynamics simulations in UCSF Chimera

MSC INDUSTRIAL CHEMISTRY AND INTRODUCTION TO CHEMICAL RESEARCH, AUTONOMOUS UNIVERSITY OF BARCELONA

🌐 <http://pagines.uab.cat/chemistry-master>

Barcelona, Spain

2016-present

Introduction to Python

MSC BIOINFORMATICS, AUTONOMOUS UNIVERSITY OF BARCELONA

🌐 <http://mscbioinformatics.uab.cat>

Barcelona, Spain

2016-present

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

ASSOCIATE PROFESSOR, DEPARTMENT OF CHEMISTRY, AUTONOMOUS UNIVERSITY OF BARCELONA (UAB)

✉ jeandidier.marechal@uab.cat • 🌐 <http://www.insilichem.com>

Barcelona, Spain

Prof. Dr. Feliu Maseras

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