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, Azure, 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	NGLView, UCSF Chimera, VMD, PyMol

Positions & Education

Postdoctoral researcher in joint project for Prof. Volkamer & Prof. Chodera
Berlin & New York
Charité Universitätsmedizin (Berlin) & Memorial Sloan Kettering Cancer Center (NY)
Mar 2019 - present

- Project: Computational polypharmacology, a new paradigm for selectively promiscuous kinase inhibitors
- Funded by the Einstein Foundation and Stiftung Charité
- Developed a Python package for structure-informed machine learning in biochemistry (KinoML)
- Implemented best practices for scientific software development across the existing projects

Postdoctoral researcher in Prof. Maréchal's group
Barcelona, Spain
Autonomous University of Barcelona (UAB)
Dec 2018 - Mar 2019

- Project: Graphical interfaces for Molecular Modeling (Tangram)
- Created several extensions for UCSF Chimera, focusing on molecular dynamics, quantum mechanics, metal coordination geometry and interaction visualization

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

- Project: Optimizing computational chemistry workflows with Python
- Refactored a set of Perl scripts as a Python package for QM/MM calculations (Garleek)
- Streamlined MECP calculations with a self-contained Python script (EasyMECP)

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

- Thesis: Development and application of a computational platform for complex molecular design
- Supervised by Jean-Didier Maréchal and evaluated by Gerald Monard, Sílvia Osuna, Xavier Solans
- Funded by Government of Catalonia's FI 3-year predoctoral fellowship
- Developed and published several software projects (GaudiMM, OMMProtocol, ESIgen and others) that were applied in the fields of molecular modelling, computational chemistry, artificial metalloenzimes and drug design

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

- Project: A novel tool for computationally aided molecular design
- Supervisor: Jean-Didier Maréchal

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

Highlighted software projects

KinoML

Python 3.6+, PyTorch and more — openkinome/kinoml

- High-level library for structure-informed machine learning
- Dataset cleaner and standardizer
- Open development supported by GitHub, Netlify, and GH Actions

TeachOpenCADD

Python 3.6+, Jupyter Notebooks, rdkit and more — volkamerlab/teachopencadd

- Interactive learning materials for computer-aided drug design
- Focus on theory and code through practical examples
- Open source and easily deployable through Binder

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

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

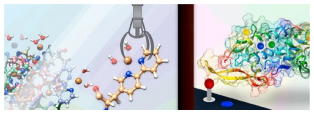
Python 2.7/3.4+; Tinker; Gaussian — insilichem/garleek

- 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

Publications

Published & In Press

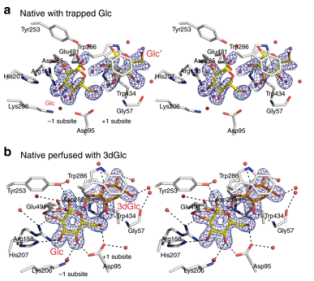
† *co-corresponding authorship*



Molecular Modeling for Artificial Metalloenzyme Design and Optimization 2020

Acc. Chem. Res. doi 10.1021/acs.accounts.0c00031

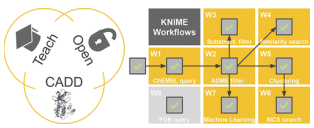
Lur Alonso-Cotchico, Jaime Rodríguez-Guerra, Agustí Lledós, Jean-Didier Maréchal



Discovery of substrate-assisted processivity by an exo-hydrolase with a pocket-shaped catalytic site 2019

Nat. Comm. 10 (1), 2222 doi 10.1021/acs.jcim.9b00662

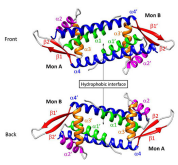
Victor Streltsov, Sukanya Luang, Alys Peisley, Joseph Varghese, James Ketudat Cairns, Sébastien Fort, Marcel Hijnen, Igor Tvaroska, Ana Ardá, Jesús Jiménez-Barbero, Mercedes Alfonso-Prieto, Carme Rovira, Fernanda Mendoza, Laura Tiessler-Sala, José-Emilio Sánchez-Aparicio, Jaime Rodríguez-Guerra, José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



TeachOpenCADD-KNIME: A Teaching Platform for Computer-Aided Drug Design Using KNIME Workflows 2019

J. Chem. Inf. Model. 59 (10) 4083-4086 doi 10.1038/s41467-019-09691-z

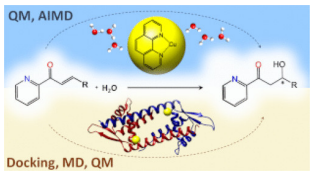
Dominique Sydow, Michele Wichmann, Jaime Rodríguez-Guerra, Daria Goldmann, Gregory Landrum, Andrea Volkamer



The effect of cofactor binding on the conformational plasticity of the biological receptors in artificial metalloenzymes: the case study of LmrR 2019

Front. Chem. 7, 211 doi 10.3389/fchem.2019.00211

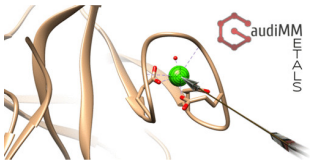
Lur Alonso-Cotchico, Jaime Rodríguez-Guerra, Agustí Lledós, Jean-Didier Maréchal



Integrated computational study of the Cu-catalyzed hydration of alkenes in water solvent and into the context of an artificial metallohydratase 2019

ACS Catal. 9 (5), 4616-4626 doi 10.1021/acscatal.8b04919

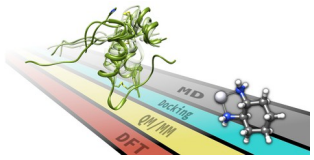
Lur Alonso-Cotchico, Giuseppe Sciortino, Jaime Rodríguez-Guerra, Ivana Drienovska, Gerard Roelfes, Agustí Lledós, Jean-Didier Maréchal



Simple coordination geometry descriptors allow to accurately predict metal binding sites in proteins 2019

ACS Omega 4 (2), 3726-3731 doi 10.1021/acsomega.8b03457

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



Computational insight on the interaction of oxaliplatin with insulin 2019

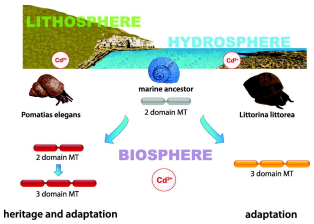
Metallomics 4 doi 10.1039/C8MT00341F

Giuseppe Sciortino, José-Emilio Sánchez-Aparicio, Jaime Rodríguez-Guerra, 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, 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, Jean-Didier Maréchal, Reinhard Dallinger

ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications 2018

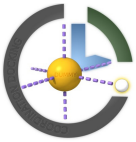
J. Chem. Inf. Model. 58 (3), 561-564 doi 10.1021/acs.jcim.7b00714 insilichem/esigen

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



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

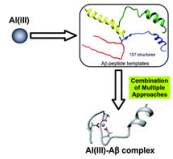
J. Comput. Chem. 39 (1), 42-51 doi 10.1002/jcc.25080

Giuseppe Sciortino, Jaime Rodríguez-Guerra, 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

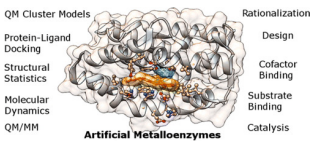
Jaime Rodríguez-Guerra,† Giuseppe Sciortino, Jordi Guasp, Martí Municoy, Jean-Didier Maréchal†



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, Xabier Lopez, Jesus M. Ugalde, Luis Rodríguez-Santiago, Mariona Sodupe, Jean-Didier Maréchal

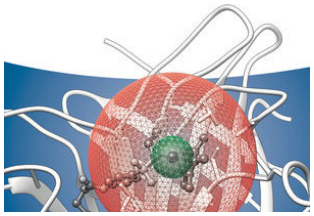


Toward the Computational Design of Artificial Metalloenzymes: From Protein–Ligand Docking to Multiscale Approaches 2015

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

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

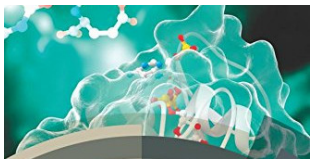
Book Chapters



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 10.1002/9783527804085.ch4

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

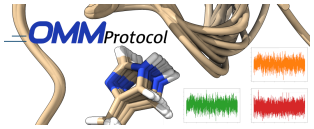


Enzyme Design 2016

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

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

Pre-prints



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

ChemRxiv 10.26434/chemrxiv.7059263 insilichem/ommprotocol

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

Presentations

15th German Conference on Cheminformatics (GCC) Mainz, Germany
Structure-based cheminformatics in the cloud: building pipelines out of free web services with Jupyter Notebooks November 3-5, 2019

RDKit User Group Meeting Hamburg, Germany
TeachOpenCADD: Open Source Teaching Platform for Computer-Aided Drug Design November 25-27, 2019

XXXV Annual Meeting of the Reference Network in Theoretical and Computational Chemistry Barcelona, Spain
Exploiting kinase pharmacology in machine learning pipelines supported by molecular modeling July 18, 2019

Molecular and Chemical Kinetics: Sampling, Design and Machine Learning Berlin, Germany
Hybrid workflows for structure-informed machine learning and free energy calculations to enable targeted kinase polypharmacology June 19-21, 2019

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, 2017
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

Computer-aided Drug Design - Methods and Application Berlin, Germany
Winter Semester Course Catalog, Free University of Berlin 2020
https://www.fu-berlin.de/vv/en/fb

Best practices for scientific software development in Python Berlin, Germany
Institute of Physiology, Charité Universitätsmedizin Berlin 2020
https://molssi.typeform.com/to/WPbljL

Computer-aided Drug Design - Methods and Application Berlin, Germany
Summer Semester Course Catalog, Free University of Berlin 2019-
https://www.fu-berlin.de/vv/en/fb

Modern Python for scientific software development — Barcelona, Spain
SGB - Servei de Genòmica i Bioinformàtica, Autonomous University of Barcelona — 2017-2018
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 — 2016-2018
http://pagines.uab.cat/chemistry-master

Introduction to Python — Barcelona, Spain
MSc Bioinformatics, Autonomous University of Barcelona — 2016-2018
http://mscbioinformatics.uab.cat

Supervised & co-supervised projects

2020	**J. Pipart, D. Köser, A. Pham, E. Kurnaz**, Structural alignment and superposition	BSc Bioinformatics, FU
2019	**B. Adas**, KNIME workflows for machine learning pipelines	MSc Bioinformatics, FU
2019	**M. Wichmann**, KNIME workflows for computer-aided drug design	BSc Bioinformatics, FU
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

JProf. Dr. Andrea Volkamer — Berlin, Germany
Assistant Professor, Institute of Physiology, Charité University of Medicine
andrea.volkamer@charite.de • http://www.volkamerlab.org

John D. Chodera, PhD — New York, USA
Assistant Member, Computational Biology Program, Memorial Sloan-Kettering Cancer Center (MSKCC)
john.chodera@choderalab.org • http://www.choderalab.org

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