

Jaime Rodríguez-Guerra

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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

CHARITÉ UNIVERSITÄTSMEDIZIN (BERLIN) & MEMORIAL SLOAN KETTERING CANCER CENTER (NY)

Berlin & New York

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

AUTONOMOUS UNIVERSITY OF BARCELONA (UAB)

Barcelona, Spain

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

INSTITUTE OF CHEMICAL RESEARCH OF CATALONIA (ICIQ)

Tarragona, Spain

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

AUTONOMOUS UNIVERSITY OF BARCELONA (UAB)

Barcelona, Spain

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 metalloenzymes and drug design

MSc in Bioinformatics

AUTONOMOUS UNIVERSITY OF BARCELONA

Barcelona, Spain

2013 - 2014

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

BSc in Biotechnology

UNIVERSITY OF SALAMANCA

Salamanca, Spain

2008 - 2013

Highlighted software projects

KinoML

Python 3.6+, PyTorch and more

 [openkinome/kinoml](https://github.com/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](https://github.com/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](https://github.com/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

ESlgen

Python 2.7/3.4+, cclib, Jinja, Flask; JavaScript

 [insilichem/esigen](https://github.com/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

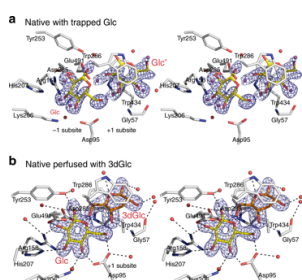
 [insilichem/garleek](https://github.com/insilichem/garleek)

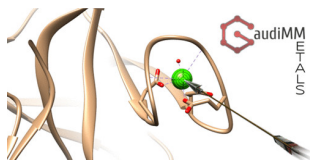
- Command-line application to extend Gaussian's ONIOM engine with external MM force fields
- Modular design to accept any MM library. Tinker compatibility already available, including polarizable force fields
- Designed as a replacement for an existing collection of Bash scripts with poor maintainability

Publications

PUBLISHED & IN PRESS

† co-corresponding authorship



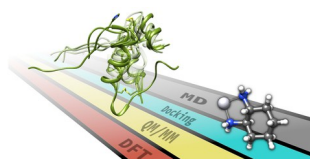


Simple coordination geometry descriptors allow to accurately predict metal binding sites in proteins

2019

ACS Omega 4 (2), 3726-3731 [doi 10.1021/acsomega.8b03457](https://doi.org/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](https://doi.org/10.1039/C8MT00341F)

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



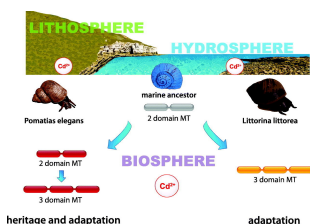
GARLEEK: Adding an Extra Flavor to ONIOM

2019

J. Comput. Chem. 40, 381-386 [doi 10.1002/jcc.25612](https://doi.org/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 snail 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](https://doi.org/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](https://doi.org/10.1021/acs.jcim.7b00714)

[insilichem/esigen](#)

[Jaime Rodríguez-Guerra](#),[†] Pablo Gómez-Orellana, Jean-Didier Maréchal[†]



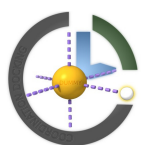
PyChimera: Use UCSF Chimera modules in any Python 2.7 project

2018

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

[insilichem/pychimera](#)

[Jaime Rodríguez-Guerra](#),[†] Jean-Didier Maréchal[†]

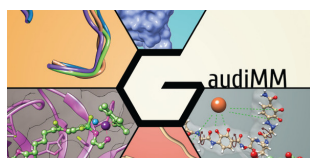


Prediction of the interaction of metallic moieties with proteins: An update for protein-ligand docking techniques

2018

J. Comput. Chem. 39 (1), 42-51 [doi 10.1002/jcc.25080](https://doi.org/10.1002/jcc.25080)

Giuseppe Sciortino, [Jaime Rodríguez-Guerra](#), Agustí Lledós, Eugenio Garribba, Jean-Didier Maréchal



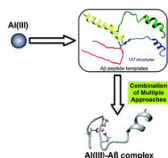
GaudiMM: A modular multi-objective platform for molecular modeling

2017

J. Comput. Chem. 38 (24), 2118-2126 [doi 10.1002/jcc.24847](https://doi.org/10.1002/jcc.24847)

[insilichem/gaudi](#)

[Jaime Rodríguez-Guerra](#),[†] Giuseppe Sciortino, Jordi Guasp, Martí Municoy, Jean-Didier Maréchal[†]

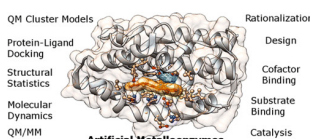


Elucidating the 3D structures of Al(III)-Aβ complexes: a template free strategy based on the pre-organization hypothesis

2017

Chem. Sci. 8, 5041-5049 [doi 10.1039/C7SC01296A](https://doi.org/10.1039/C7SC01296A)

Jon I. Mujika, [Jaime Rodríguez-Guerra](#), Xabier Lopez, Jesus M. Ugalde, Luis Rodríguez-Santiago, Mariona Sodupe, Jean-Didier Maréchal



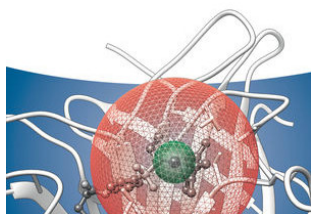
Toward the Computational Design of Artificial Metalloenzymes: From Protein-Ligand Docking to Multiscale Approaches

2015

ACS Catal. 5 (4), 2469-2480 [doi 10.1021/acscatal.5b00010](https://doi.org/10.1021/acscatal.5b00010)

Victor Muñoz Robles, Elisabeth Ortega-Carrasco, Lur Alonso-Cotichico, [Jaime Rodríguez-Guerra](#), Agustí Lledós, Jean-Didier Maréchal

BOOK CHAPTERS

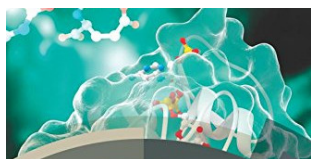


Computational Studies of Artificial Metalloenzymes: From Methods and Models to Design and Optimization

2018

Ch. 4 in "Artificial Metalloenzymes and MetalloDNAs in Catalysis: From Design to Applications", Wiley & Sons [doi 10.1002/9783527804085.ch4](https://doi.org/10.1002/9783527804085.ch4)

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



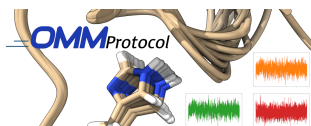
Enzyme Design

2016

Ch. 15 in "Simulating Enzyme Reactivity", Royal Society of Chemistry [doi 10.1039/9781782626831-00481](https://doi.org/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 [doi 10.26434/chemrxiv.7059263](https://doi.org/10.26434/chemrxiv.7059263)

[insilichem/ommprotocol](https://insilichem.github.io/ommprotocol)

[Jaime Rodríguez-Guerra](#),[†] Lur Alonso-Cotchico, Lorea Velasco-Carneros, Jean-Didier Maréchal[†]

Presentations

15th German Conference on Cheminformatics (GCC)

STRUCTURE-BASED CHEMINFORMATICS IN THE CLOUD: BUILDING PIPELINES OUT OF FREE WEB SERVICES WITH JUPYTER NOTEBOOKS

Mainz, Germany
November 3-5, 2019

RDKit User Group Meeting

TEACHOPENCADD: OPEN SOURCE TEACHING PLATFORM FOR COMPUTER-AIDED DRUG DESIGN

Hamburg, Germany
November 25-27, 2019

XXXV Annual Meeting of the Reference Network in Theoretical and Computational Chemistry

EXPLOITING KINASE PHARMACOLOGY IN MACHINE LEARNING PIPELINES SUPPORTED BY MOLECULAR MODELING

Barcelona, Spain
July 18, 2019

Molecular and Chemical Kinetics: Sampling, Design and Machine Learning

HYBRID WORKFLOWS FOR STRUCTURE-INFORMED MACHINE LEARNING AND FREE ENERGY CALCULATIONS TO ENABLE TARGETED KINASE POLYPHARMACOLOGY

Berlin, Germany
June 19-21, 2019

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, 2017

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

Computer-aided Drug Design - Methods and Application

WINTER SEMESTER COURSE CATALOG, FREE UNIVERSITY OF BERLIN
<https://www.fu-berlin.de/vv/en/fb>

Berlin, Germany
2020

Best practices for scientific software development in Python

INSTITUTE OF PHYSIOLOGY, CHARITÉ UNIVERSITÄTSMEDIZIN BERLIN
<https://molssi.typeform.com/to/WPbljL>

Berlin, Germany
2020

Computer-aided Drug Design - Methods and Application

SUMMER SEMESTER COURSE CATALOG, FREE UNIVERSITY OF BERLIN
<https://www.fu-berlin.de/vv/en/fb>

Berlin, Germany
2019-

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

2017-2018

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

2016-2018

Introduction to Python

MSc BIOINFORMATICS, AUTONOMOUS UNIVERSITY OF BARCELONA

✉ <http://mscbioinformatics.uab.cat>

Barcelona, Spain

2016-2018

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

ASSISTANT PROFESSOR, INSTITUTE OF PHYSIOLOGY, CHARITÉ UNIVERSITY OF MEDICINE

✉ andrea.volkamer@charite.de • <http://www.volkamerlab.org>

Berlin, Germany

John D. Chodera, PhD

ASSISTANT MEMBER, COMPUTATIONAL BIOLOGY PROGRAM, MEMORIAL SLOAN-KETTERING CANCER CENTER (MSKCC)

✉ john.chodera@choderalab.org • <http://www.choderalab.org>

New York, USA

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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