Curriculum Vitae

(01/2025)

Miguel Ângelo dos Santos Machuqueiro

1. PERSONAL DATA

Name:	Miguel Ângelo dos Santos Machuqueiro
Place & Birth Date:	Palmela, 27-12-1974
Nationality:	Portuguese
Address:	BioISI - Biosystems & Integrative Sciences Institute
	Departamento de Química e Bioquímica
	Faculdade de Ciências, Universidade de Lisboa
	Campo Grande, Edifício C8 (sala 8.5.52), 1749-016 Lisboa, Portugal
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Group Webpage:	http://mms.rd.ciencias.ulisboa.pt
ORCID ID:	http://orcid.org/0000-0001-6923-8744
SCOPUS:	https://www.scopus.com/authid/detail.uri?authorId=57221975472
R-ID:	https://publons.com/researcher/C-8012-2011
Google Scholar:	https://scholar.google.com/citations?hl=en-US&user=vMBlK7AAAAAJ

2. LANGUAGES

Portuguese	–	all levels;
English	–	all levels;
French	–	reading and conversation;
Spanish/Castilian	–	reading and conversation;
Italian	–	reading and conversation;
German	–	reading;

3. INFORMATICS

System Administrator of the BioISI scientific computer cluster (~2500 CPUs, ~40 GPUs, ~200 TB). Advanced user of Linux and Windows.

Advanced user of many scientific tools for MD, QM, Continuum Electrostatics, Monte Carlo techniques, Molecular Docking, Molecular Visualization, etc.

Very good skills in a variety of programming (Python, C, etc…) and scripting (AWK, SED, BASH, etc) languages.

4. ACADEMIC

2024- Assistant Professor at the Chemistry and Biochemistry Department, Faculty of Sciences, University of Lisbon and member of the BioISI – Biosystems & Integrative Sciences Institute.

2019-2024 Assistant Researcher (CEECIND/02300/2017) at the BioISI – Biosystems & Integrative Sciences Institute and at the Chemistry and Biochemistry Department, Faculty of Sciences, University of Lisbon.

2015-2018 Invited Assistant Professor at the Chemistry and Biochemistry Department, Faculty of Sciences, University of Lisbon.

2009-2014 Assistant Researcher (Investigador Auxiliar do Programa Ciência2008) at the Chemistry and Biochemistry Center, Faculty of Sciences, University of Lisbon.

2006-2009 Pos-doctoral fellow at the Molecular Simulation and Protein Modelling Groups under the supervision of Dr. António M. Baptista and Prof. Cláudio M. Soares, at Instituto de Tecnologia Química e Biológica, Oeiras, Portugal. The project was entitled "Membrane-induced structural changes in proteins: a computer simulation study".

2003-2006 Pos-doctoral fellow at the Molecular Simulation Group under the supervision of Dr. António M. Baptista, Instituto de Tecnologia Química e Biológica, Oeiras, Portugal. The project was entitled "pH and redox effects in structure and dynamics of biomolecules: Studies in molecular modelling".

1999-2003 Ph.D. from the University of Bern, Switzerland (Doctor of Philosophy; Ph.D.; Dr. phil.-nat.), with a thesis entitled "Chemical Models of Zinc-dependent Enzymes: Methyltransferases and Class II Aldolases", supervised by Prof. Tamis Darbre and Prof. Jean-Louis Reymond.

1992-1998 Diploma in Biochemistry, at the Faculty of Sciences University of Lisbon, with a thesis entitled "Simulação do Ciclo de Oxidação e Redução das Ubiquinonas num Modelo de Transporte Electrónico - Aplicação ao Peroxissoma".

5. SPECIALIZATION DOMAINS

- Chemistry and Biochemistry
- Theoretical Chemistry and Biochemistry:
    - Computational (Bio)chemistry
    - Molecular Mechanics
    - Quantum Mechanics
    - Force Field Development
    - Molecular Dynamics
    - Continuum Electrostatics
    - Molecular Docking
    - Biological Membrane Biophysics
    - Artificial Intelligence

6. SCIENTIFIC INTERESTS

- (Bio)chemistry: Theoretical (Bio)chemistry
- Computational methods for biomolecular simulations
- The influence of pH and reduction potential in biomolecules
- Protein/peptide structure, folding, and stabilization
- Protein misfolding and disease
- The role of the biological membrane in protein/peptide structure and function

- The protonation/conformation coupling in lipids and its influence on the structure of biological membranes

7. TEACHING (14 items)

2018- Theoretical and practical course in *Biochemistry Simulation* for Biochemistry undergrads at the Faculty of Sciences, University of Lisbon. I was responsible for the "Molecular Dynamics" block, including its evaluation.

2018- *Molecular Modeling and Simulation of Biomolecules* module in UC: "Projecto Experimental I" given to the master's degree in Biochemistry at the Faculty of Sciences, University of Lisbon. I was responsible for this module, including its evaluation.

2013- Introductory course on *Structural Databases in (Bio)Chemistry*, given to the master's degree in Chemistry at the Faculty of Sciences, University of Lisbon.

2013-17 Introductory course on *Computational Modeling of Biomembranes*, given to the master's degree in Biochemistry at the Faculty of Sciences, University of Lisbon.

2011-17 Introductory course on *Drug Design*. Given to the Biochemistry undergrads at the Faculty of Sciences, University of Lisbon.

2010-14 Practical course in *Computational Biochemistry* to Biochemistry undergrads at the Faculty of Sciences, University of Lisbon.

2012-14 Practical course in *Chemical Systems and Reactivity* to Chemistry Master at the Faculty of Sciences, University of Lisbon.

2009-13 Theoretical and practical course in *Biochemistry Simulation* for Biochemistry undergrads at the Faculty of Sciences, University of Lisbon. I was responsible for the "Molecular Docking and Molecular Dynamics" block, including its evaluation.

2011-13 Theoretical and practical course in *Molecular Modeling and Simulation* to Inorganic and Biomedical Chemistry master at Faculty of Sciences, University of Lisbon.

2007-08 Practical course in Molecular Docking, a part of the Ph.D. program in Computational Biology of Instituto Gulbenkian da Ciência, Oeiras, Portugal.

2005-09 Practical course in Continuum Electrostatics, a part of the Ph.D. program in Computational Biology of Instituto Gulbenkian da Ciência, Oeiras, Portugal.

2004-09 Practical course on molecular visualization, a part of the Ph.D. program at Instituto de Tecnologia Química e Biológica, Oeiras, Portugal.

2002-03 Practical course "Chemie im alltag" (transl: everyday chemistry), for students in Educational Chemistry, University of Bern, Switzerland.

1999-02 Practical course of Organic Chemistry for students in Pharmaceutical Chemistry, University of Bern, Switzerland. This was a part of my Ph.D. program.

8. TEACHING MATERIAL (5 items)

2024- Tutorial on "Visualização molecular com o PyMOL e previsão de estrutura de proteínas com IA": Online Access

2023- Tutorial on Molecular Visualization, 3D Structure Prediction, and Molecular Docking of the S100B Protein and its Single Domain Antibody: Online Access

2023- Tutorial on the Study of the S100B/Antibody interactions using Molecular Dynamics: Online Access

2020- Online tutorials on Molecular Modelling: http://insilicotutorials.rd.ciencias.ulisboa.pt. These tutorials were converted from a basic to an intermediate level and published on ACS Synth. Biol. [10.1021/acssynbio.1c00368].

2019- Tutorial on Molecular Dynamics using GROMACS software package: Online Access

9. SUPERVISING

- *PosDoc (5 items):*

2019-20 **Pedro Lopes** (contract from the project: PTDC/MED-QUI/29036/2017)

2018-18 **Pedro Rafael Magalhães** (grant from the project: PTDC/QEQ-COM/5904/2014)

2017-18 **Diogo Vila Viçosa** (grant from the project: PTDC/QEQ-COM/5904/2014)

2016-17 **Bruno Lourenço da Silva Victor** (grant from the project: PTDC/QEQ-COM/5904/2014)

2011-15 **Vitor Hugo Oliveira Teixeira** (grant from the project: PTDC/QUI-BIQ/113721/2009)

- *Ph.D. (14 items):*

2023- **Inês Pires** with the project "*In silico study of the electrochemical gradient role in Cytochrome c Oxidase proton gating mechanism"* (2023.01155.BD) at FCUL, co-supervision of Dr. António Baptista, ITQB-NOVA.

2023- **Marta Baptista** (co-supervisor) with the project "*Unclothing the dichotomic pH regulation in aquaporin-7 and aquaporin-10"* (2023.03251.BD) at FCUL, supervision of Dr. Bruno Victor, FCUL.

2022- **João Vitorino** with the project "*Coupling CpHMD with MMPBSA to Study the Dopaminergic GPCRs Binding Interactions*" (2022.11124.BD) at FCUL, in co-supervision with Prof. Irina Moreira (CNC, Universidade de Coimbra, PT).

2022- **João Sequeira** with the project "*A new AMBER CpHMD implementation to study the acid-sensing ion channels inhibition*" (2022.10517.BD) at FCUL, in co-supervision with Prof. Adrian Roitberg (Univ. Florida, USA).

2022- **Ana Beatriz Caniceiro** (co-supervisor) with the project "*Pluridimensional signaling of GPCR - understanding mutagenesis effect on the receptorsome*" (2022.12479.BD) at Universidade de Coimbra, supervised by Prof. Irina Moreira (CNC, Universidade de Coimbra, PT).

2022- **Sara Ferreira** with the project "*In silico insights on the role of protein knots in mechanical stability and self-association*" (UI/BD/153055/2022) at FCUL, in co-supervision with Prof. Patrícia Faísca (BioISI, FCUL, PT).

2021- **Nuno Oliveira** with the project "*Development of computational methods to study and help revert tumor MDR*" (2021.06409.BD) at FCUL.

2021- **Filipe Rodrigues** with the project "*In silico study of peptidic dendrimers as transfection agents in DNA/RNA vaccines*" (2021.05909.BD) at FCUL, in co-supervision with Dr. Tamis Darbre (Univ. Bern, CH).

2021- **Mohannad Yousef** with the project entitled "*pH effects for improved computer-aided drug design*" at FCUL.

2019-24 **Carlos Barreto** (co-supervision) with the project "*A computational approach to the structural and dynamical characterization of the ghrelin receptor function and mechanism.*" (SFRH/BD/145457/2019) at the University of Coimbra, supervised by Prof. Irina Moreira (CNC, Universidade de Coimbra, PT).

2018-23 **Pedro Reis** with the project "*Melhoramento da eficiência das simulações de dinâmica molecular a pH constante em sistemas biológicos complexos*" (SFRH/BD/136226/2018) in co-supervision with Dr. Diogo Vila Viçosa (FCUL) and Dr. Walter Rocchia (Instituto Italiano di Tecnologia, Genova, IT). Grade: **Aprovação com Distinção e Louvor**

2018-23 **Tomás Fernandes Silva** with the project "*Desenvolvimento e aplicação de técnicas de amostragem aumentada dependente do pH na optimização da tecnologia pHLIP como marcador tumoral*" (SFRH/BD/140886/2018) in co-supervision with Dr. Diogo Vila Viçosa (FCUL). Grade: **Aprovação com Distinção e Louvor**

2012-16 **Luís Carlos Santos Filipe** (co-supervision) with the project "*Studying the structural features of peptide dendrimers using a combined computational and experimental approach*" (SFRH/BD/76085/2011) at ITQB, supervised by Dr. António M. Baptista (ITQB-UNL, PT) and co-supervised by Dr. Tamis Darbre (Univ. Bern, CH).

2012-15 **Diogo Vila Viçosa** with the project "*Modelação e simulação do efeito do pH em membranas lipídicas*" (SFRH/BD/81017/2011) in co-supervision with Prof. Maria José Calhorda (FCUL, PT). Grade: **Aprovação com Distinção e Louvor**

- *Master Degree (19 items):*

2024- **Gonçalo Cunha** (Engenharia Biomédica, FCT, NOVA) with the project "*Deteção de traços moleculares de triclosano em meios líquidos complexos*".

2024- **Ana Figueiredo** (Biochemistry, FCUL) with the project "*Computational Model of Phosphatidylinositol Protonation: Insights into Membrane and Protein Interactions*".

2024- **Francisco Duarte** (Chemistry, FCUL) with the project "*An In Silico Protocol to Evaluate and Optimize Cyclodextrins for Drug Delivery*", in co-supervision with Dr. Paulo Costa (FCUL, PT).

2022-24 **Rita Guerra** (Bioinformatics, FCUL) with the project "*A computational study on the impact of adding anionic groups to tyrosine kinase inhibitors*" in co-supervision with Dr. Bruno Victor (FCUL, PT).

2022-24 **André Gomes** (Medicinal and Biopharmaceutical Chemistry, FFUL) with the project "*What drives the membrane permeability of drugs? A study on untackled effects*" in co-supervision with Dr. Paulo Costa (FCUL, PT) and Prof. Maria José Umbelino Ferreira (FFUL). Grade: **19/20**

2021-23 **Inês Pires** (Biochemistry, FCUL) with the project "*New antitumor Ru-based compound derivatives optimized using in silico methods*". Grade: **20/20**

2020-22 **João Sequeira** (Bioinformatics, FCUL) with the project "*High-throughput virtual screening to identify non-covalent inhibitors of CRM1 with anti-tumoral potential*". Grade: **19/20**

2020-22 **Pedro Suzano** (Biochemistry, FCUL) with the project "*Developing a computational method to calculate pH-dependent membrane permeabilities for anti-tumor drugs*". Grade: **19/20**

2020-22 **João Vitorino** (Biochemistry, FCUL) with the project "*PyBindE: Development of a Simple Python MM-PBSA Implementation for Estimating Protein-Protein and Protein-Ligand Binding Energies*". Grade: **20/20**

2019-20 **Nuno Oliveira** (Biochemistry, FCUL) with the project "*The role of electrostatics in the mechanism of ATP/ADP carrier function: an in silico study*". Grade: **20/20**

2019-20 **Filipe Rodrigues** (Biochemistry, FCUL) with the project "*Study of the interaction between the amyloid β peptide and the S100B protein using computational techniques*". Grade: **19/20**

2016-17 **Bárbara Rodrigues** (FCT-UNL) with the project "*Encapsulamento da Catequina EGCG no Lipossoma: Múltiplas Abordagens*" in co-supervision with Prof. Maria de Fátima Raposo (FCT-UNL, PT). Grade: **19/20**

2016-17 **Tomás Fernandes Silva** (Biochemistry, FCUL) with the project "*Computational study of pH-dependent membrane insertion mechanism of pHLIP peptides*" in co-supervision with Dr. Diogo Vila Viçosa (FCUL, PT). Grade: **20/20**

2016-17 **Pedro Reis** (Biochemistry, FCUL) with the project "*Improving pKa calculations of membrane inserting amino acids using replica exchange CpHMD simulations.*" in co-supervision with Dr. Diogo Vila Viçosa (FCUL, PT). Grade: **20/20**

2013-15 **Rafael de Santana Nunes** (Chemistry, FCUL) with the project "*Synthesis of new antibiotic glycosides and computational studies on their interaction with model lipid bilayers*" in co-supervision with Prof. Amélia Pilar Rauter (FCUL, PT). Grade: **20/20**

2013-14 **Bruno Calçada** (Chemistry, FCUL) with the project "*Cyclodextrins as anti-asthmatic drug carriers*" in co-supervision with Prof. Helena Marques (FFUL, PT). Grade: **19/20**

2012-13 **Hugo Alexandre Feiteira dos Santos** (Biochemistry, FCUL) with the project "*Constant-pH MD simulations of higher complexity lipid bilayer models: PA/PC binary mixtures*". Grade: **20/20**

2011-12 **Ana Sofia Capacho** (Inorganic and Biomedicinal Chemistry, FCUL) with the project "*Avaliação in silico da tioredoxina redutase como alvo para a terapia anti-tumoral*". Grade: **19/20**

2009-10 **João Manuel Almeida Henriques** (Biochemistry, FCUL) with the project "*Application of QM and MM methodologies to cytochrome c_3: Charge parametrization of the heme group for classic force fields*". Grade: **19/20**

2009-10 **Diogo Vila Viçosa** (Biochemistry, FCUL) with the project "*Reversibility of Prion Misfolding by Constant-pH Molecular Dynamics Simulations*" in co-supervision with Dr. António M. Baptista. Grade: **19/20**

- *Undergrad Project (10 items):*

2024- **Maria João Pintassilgo** (Chemistry, FCUL) with the project "*Principles in Computational Chemistry*".

2023-24 **Ana Figueiredo** (Biochemistry, FCUL) with the project "*Introduction to Molecular Dynamics Simulations*".

2022-24 **Francisco Duarte** (Chemistry, FCUL) with the project "*Avaliação computacional de novos derivados da isoniazida com ação antitubercular*".

2019-20 **João Vitorino** (Biochemistry, FCUL) with the project "*Estudo computacional da protonação dos fosfatidilinositóis em diferentes ambientes com relevo biológico*".

2018-19 **Inês Pires** (Biochemistry, FCUL) with the project "*Estudo in silico da permeabilidade da proteína membranar bacteriana OmpG e da sua regulação através do pH do meio*".

2018-19 **Nuno Oliveira** (Biochemistry, FCUL) with the project "*Estudo computacional do efeito do pH no mecanismo de acção do transportador mitocondrial de ATP/ADP*".

2015-18 **José Ricardo Dias** (Biochemistry, FCUL) with the project "Development of a new GROMOS *54A7 based force-field for lipids*".

2016 **Ricardo Rosa** (Biochemistry, FCT-UNL) with a diploma project entitled "*Interacções proteína:ligando via ligações de halogéneo: uma nova abordagem com vista a aplicações em design de fármacos*" in co-supervision with Dr. Paulo J. Costa.

2014-16 **Pedro Reis** (Biochemistry, FCUL) with the project "*Protonation behavior of Ala pentapeptides interacting with lipid bilayers*".

2015 **Ana Grosso** (Biochemistry, FCT-UNL) with a diploma project entitled "*In silico study of the protonation state of pHLIP peptide inserted in a lipid bilayer*".

10. PROJECTS

- *Coordinator (PI) (5 items):*

2024-25 "Optimizing MDR-Evading Drugs: Unveiling P-gp Transport Dynamics" (2023.10710.CPCA.A2; DOI: 10.54499/2023.10710.CPCA.A2). 256k CPU core.hours/250GB storage. Funding: **€ 6.3k**

2023-24 "In silico study of peptidic dendrimers as transfection agents in RNA vaccines" (2022.15878.CPCA; DOI: 10.54499/2022.15878.CPCA.A2). 768k CPU core.hours/750GB storage. Funding: **€ 9.5k**

2021-23 "A fast deep learning approach to improve protein pK_a predictions" (2021.09635.CPCA; DOI: 10.54499/2021.09635.CPCA). 841k CPU core.hours/4.5k GPU core.hours/4TB storage. Funding: **€ 11.4k**

2015-19 "CpHMD-L simulations of pHLIP peptides: design of new tumor-targeted drug delivery systems" (PTDC/QEQ-COM/5904/2014). Funding: **€ 185k**

2010-14 "Adding realism to the molecular modeling of lipidic membranes: inclusion of pH effects" (PTDC/QUI-BIQ/113721/2009). Funding: **€ 150k**

- *Co-PI (3 items):*

2018-22 "Physical Basis of Disease: The case of Dialysis Related Amyloidosis" (PTDC/FIS-OUT/28210/2017) (Coordination: Patrícia Faísca, FCUL). Funding: **€ 195k**

2018-22 "Targeting multi-resistant tuberculosis with new potent isoniazid derivatives: an integrated medicinal chemistry approach" (PTDC/MED-QUI/29036/2017) (Coordination: Filomena Leitão, FCUL) Funding: **€ 226k**

2018-22 "Deal with PAINS: strategies to identify membrane modulators" (PTDC/BIA-BFS/28419/2017) (Coordination: Bruno L. Victor, FCUL) Funding: **€ 235k**

- *Team member (16 items):*

2022- "TWIN2PIPSA: Twinning for Excellence in Biophysics of Protein Interactions and Self-Assembly" (HORIZON-WIDERA-2021-ACCESS-03). Funding: **€ ~30k**

2022- "COZYME: Establishing a Pan-European Network on Computational Redesign of Enzymes" (COST Action CA21162: **Management Committee**). Funding: **€ ~7.5k**

2022- "EURESTOP: European Network for diagnosis and treatment of antibiotic-resistant bacterial infections" (COST Action CA21145). Funding: **€ ~1.5k**

2021-24 "Ruthenium-peptide conjugates: arrows for selectively targeting breast cancer" (PTDC/QUI-QIN/0146/2020) (Coordination: Tânia Morais, FCUL). Funding: **€ 250k**

2018-22 "EuroMicropH: Understanding and exploiting the impacts of low pH on micro-organisms" (COST Action CA18113). Funding (FCUL): **€ ~1.5k**

2018-22 "STRATAGEM: New diagnostic and therapeutic tools against multidrug-resistant tumors" (COST Action CA17104). Funding (FCUL): **€ ~7.5k**

2018-22 "EUTOPIA: EUropean TOPology Interdisciplinary Action" (COST Action CA17139). Funding (FCUL): **€ ~1.5k**

2018-22 "Uncovering blind spots in halogen bonding applications" (PTDC/QUI-QFI/28455/2017) (Coordination: Paulo J. Costa, FCUL). Funding: **€ 239k**

2012-15 "Multivalent Glycosystems for Nanoscience - MultiGlycoNano" (CMST COST Action CM1102: **Management Committee**). Funding (FCUL): **€ ~7.5k**

2013-15 "Aumentando o realismo da modelação de membranas em métodos de dinâmica molecular a pH constante: inclusão de gradientes electroquímicos e titulação de lípidos" (PTDC/QEQ-COM/1623/2012) (Coordination: António M. Baptista, ITQB). Funding (FCUL): **€ ~5k**

2011-12 "Complexos de metais de transição usados como intercaladores de DNA: investigação teórica." (Programa Bilateral PESSOA: Strasbourg, France) (Coordination: Maria José Calhorda, FCUL)

2010-11 "Síntese, estudos computacionais e propriedades biológicas de compostos de ouro" (Bilateral FCT-CSIC: Zaragoza, Spain) (Coordination: Maria José Calhorda, FCUL)

2008-13 "Understanding structure-activity relationships in peptide dendrimers using a molecular modelling approach" (PTDC/QUI-QUI/100416/2008) (Coordination: António M. Baptista, ITQB)

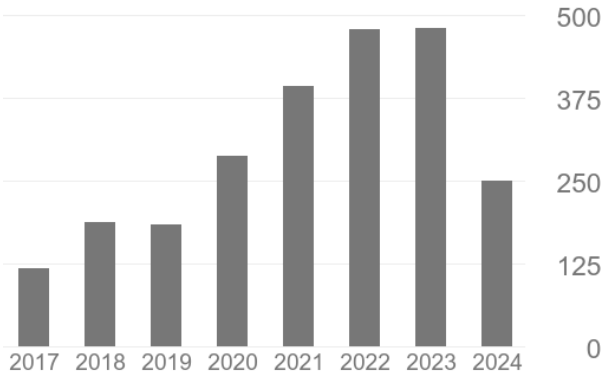
2008-13 “Study of pH-dependent protein misfolding using state-of-the-art molecular modeling methods” (PTDC/QUI-BIQ/105238/2008) (Coordination: António M. Baptista, ITQB)

2008-13 “Including protonation effects in the simulation of peptides and proteins in membrane environments” (PTDC/BIA-PRO/104378/2008) (Coordination: António M. Baptista, ITQB)

2002-06 “Increasing realism in protein modelling: including pH and redox effects into molecular dynamics simulations” (POCTI/BME/45810/2002) (Coordination: António M. Baptista, ITQB)

11. PUBLICATIONS STATS (Google Scholar)

	Todos	Desde 2019
Citações	3274	2086
Índice h	32	23
Índice i10	66	54



(data retrieved on 29/06/2024 from Google Scholar)

12. PUBLICATIONS IN PEER-REVIEWED JOURNALS/BOOKS (100 items/39 as Corresp. Auth.)

(Corresponding Authors are marked with ✉ symbol)

101. Oliveira, N. F. B., Ladokhin, A. S.✉, Machuqueiro, M.✉ (**2024**) "Constant-pH MD Simulations of the Protonation-Triggered Conformational Switching in Diphtheria Toxin Translocation Domain", *Biophys. J.,* 123, 24, 4266-4273.
https://doi.org/10.1016/j.bpj.2024.08.023
Impact Factor: ***3.4*** *Citations: N/A*

100. Barreto, C.A.V., Vitorino, J.N.M., Reis, P. B. P. S., Machuqueiro, M.✉, Moreira, I.S.✉ (**2024**) "pK_a Calculations of GPCRs: Understanding Protonation States in Receptor Activation", *J. Chem. Inf. Model.,* 64, 17, 6850-6856.
https://doi.org/10.1021/acs.jcim.4c01125
Impact Factor: ***6.2*** *Citations: N/A*

99. Salaroglio, I.C., Stefanova, D., Teixeira, R.G., Oliveira, N.F.B., Ahmed, A., Fusi, F., Tzankova, V., Yordanov, Y., Machuqueiro, M., Saponara, S., Valente, A.✉, Riganti, C.✉ (**2024**) "A novel combinatory treatment against a CDDP-resistant non-small cell lung cancer based on a Ruthenium(II) cyclopentadienyl compound", *Pharmacol. Res.,* 208, 107353.
https://doi.org/10.1016/j.phrs.2024.107353

Impact Factor: ***9.1*** *Citations: N/A*

98. Ferreira, S. G. F., Sriramoju, M. K., Hsu, S.-T. D., Faísca, P. F. N., Machuqueiro, M. (**2024**) "Is there a functional role for the knotted topology in protein UCH-L1?", *J. Chem. Inf. Model.,* 64, 17, 6827-6837.

https://doi.org/10.1021/acs.jcim.4c00880

Impact Factor: ***6.2*** *Citations: N/A*

97. Reis, P. B. P. S., Clevert, D.-A., Machuqueiro, M. (**2024**) "PypKa Server: online pKa predictions and biomolecular structure preparation with precomputed data from PDB and AlphaFold DB", *Nucleic Acids Res.,* 52, W294-W298.

https://doi.org/10.1093/nar/gkae255

Impact Factor: ***14.9*** *Citations: N/A*

96. Rodrigues, F. E. P., Darbre, T., Machuqueiro, M. (**2024**) "High Charge Density in Peptide Dendrimers is Required to Destabilize Membranes: Insights into Endosome Evasion", *J. Chem. Inf. Model.,* 64, 3430.

https://doi.org/10.1021/acs.jcim.4c00018

Impact Factor: ***6.2*** *Citations: N/A*

95. Machado, J., Sá, M., Pires, I. D. S.; Silva, M. T., Marques, F., Coelho, J. A. S.; Mendes, F., Minas da Piedade, M.; Machuqueiro, M., Jiménez, M. A., Garcia, M.H., Correia, J.D.G., Morais, T.S. (**2024**) "Dual FGFR-targeting and pH-activable Ruthenium-Peptide Conjugates for targeted therapy of Breast Cancer", *Dalton Trans.,* 53, 7682. **See also the Journal Cover:**

https://doi.org/10.1039/D4DT00497C

Impact Factor: ***4.4*** *Citations: N/A*

94. Fortuna, A., Suzano, P. M. S., Machuqueiro, M., Costa, P. J. (**2024**) "Influence of Iodine Merz-Singh-Kollman Radius on the Calculated Charges and Hydration Free Energies of Iodinated Molecule", *J. Comput. Biophys. Chem.,* 23, 481.

https://doi.org/10.1142/S2737416523500722

Impact Factor: ***2.4*** *Citations:* ***1***

93. Bueschbell, B., Magalhães, P. R., Barreto, C. A. V., Melo, R., Schiedel, A. C., Machuqueiro, M., Moreira, I. S. (**2023**) "The world of GPCR dimers - mapping dopamine receptor D2 homodimers in different activation states and configuration arrangements", *Comput. Struct. Biotechnol. J.*, 21, P4336.

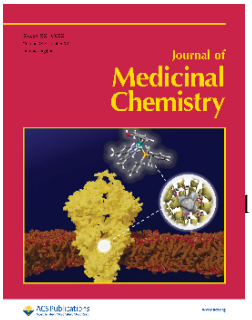
https://doi.org/10.1016/j.csbj.2023.08.032

Impact Factor: ***6.2*** *Citations: N/A*

92. Gomes, A. M. M., Costa, P. J., Machuqueiro, M. (**2023**) "Recent Advances on Molecular Dynamics-Based Techniques to Address Drug Membrane Permeability with Atomistic Detail", *BBA Advances*, 4, 100099.

https://doi.org/10.1016/j.bbadva.2023.100099

Impact Factor: ***-.-*** *Citations:* ***5***



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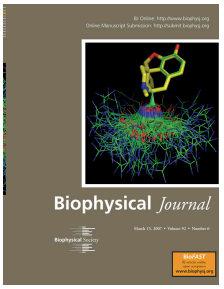

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13. ABSTRACTS IN CONFERENCE PROCEEDINGS (9 items)

2015 D. Vila-Viçosa, V. H. Teixeira, **M. Machuqueiro**. "Computational study of the pH-dependent insertion of pHLIP peptide into lipid bilayers". 10th EBSA European Biophysics Congress. Eur. Biophys. J. (2015) 44 (Suppl 1):S175. http://dx.doi.org/10.1007/s00249-015-1045-6

2013 **Machuqueiro, M.** (2013) "pH effects on lipid bilayer structures: A computational study", Abstracts of Papers of the American Chemical Society, Vol. 246, Meeting Abstract: 168-PHYS.

2013 Estácio, S. G., Krobath, H., Vila-Viçosa, D., **Machuqueiro, M.**, Shakhnovich, E.I., Faísca, P.F.N. (2013) "An intermediate state for folding and aggregation provides new insights into the amyloidogenic behavior of β2-microglobulin", Prot. Sci.: The 27th Annual Symposium of The Protein Society 22(Suppl. 1), i–ii, 1–258.

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14. SELECTED ORAL PRESENTATIONS AT INTERNATIONAL VENUES (35 items)

2024 **Machuqueiro, M**, "In silico methods to capture the pH effects in drug binding to proteins and membranes", Online Seminar at the Ciclo de Seminários do Programa de Pós-Graduação em Ciências Biomoleculares e Farmacológicas (PPG-CBF), IBILCE/IBB/UNESP, (BR), May. 2024.

2024 Silva, T.F.D., Oliveira, N.F.B., Vitorino, J.N.M., Lorena, C, Borges, P.T., Martins, L.O., and **Machuqueiro, M**, "Constant-pH MD simulations as a tool to unveil the effects of pH on proteins: the case of DyP-type peroxidases", Cozyme COST Action MC and WG meeting, Zagreb (HR), Apr. 2024.

2024 **Machuqueiro, M**, "In silico methods to capture the pH effects in drug binding to proteins and membranes", BioISI Seminar, FCUL (PT), Apr. 2024.

2024 **Machuqueiro, M**, "Increasing the realism of MD simulations by adding pH effects", Online Seminar at the Theoretical and Computational Biophysics group, Beckman Institute, University of Illinois (USA), Feb. 2024.

2023 **Machuqueiro, M**, "Increasing the realism of MD simulations of proteins, drugs, and lipid bilayers by adding pH effects", TWIN2PIPSA Scientific Exchange to the Yusuf Hamied Department of Chemistry, University of Cambridge (UK), Oct. 2023.

2023 **Machuqueiro, M**, "Using computational methods to evaluate the role of tumor microenvironment acidity in multi-drug resistance", Protein Electrostatics 2023 meeting, Genoa, IT. June 2023.

2023 **Machuqueiro, M**, "The pH-dependent multidrug resistance mechanism in tumors" Post-graduated Course: Cancer therapy - from basic research to clinic (remote). Organized by CBMA, Univ. Minho. April 28, 2023.

2023 **Machuqueiro, M**, "pH effects in molecular dynamics simulations at the water/membrane interface" Post-graduated Course: Computational modelling - in silico screening for drug design (remote). Organized by Sapienza University, Rome, IT. March 15, 2023.

2022 Reis, PBPS and **Machuqueiro, M**, "Can deep learning models help accelerate electrostatics-driven protein pK_a predictions?" EGI Webinar Programme 2022 (remote). November 23, 2022.

2022 Sequeira, JGN, Rodrigues, FEP, Reis, PBPS and **Machuqueiro, M**, "CpHMD battle: GROMOS54A7 vs CHARMM36m", Protein Electrostatics 2022 (remote) meeting, Telluride, CO, USA. June 2022.

2022 **Machuqueiro, M**, "The pH-dependent membrane crossing mechanism of Lewis-base anti-cancer drugs" Post-graduated Course: Cancer therapy - from basic research to clinic (remote). Organized by CBMA, Univ. Minho. April 29, 2022.

2021 **Machuqueiro, M** "How to deal with pH effects in GROMACS: from simple peptides to membrane proteins", GROMACS Workshop: a collaboration between BIOEXCEL and national EuroHPC competence center - Portugal (https://www.biodata.pt/node/330), September 9, 2021.

2021 Silva, TFD, **Machuqueiro, M** "The pH-dependent membrane crossing mechanism of Lewis bases antitumor drugs", Protein Electrostatics Webinar Series, Genova, Italy, February 3, 2021.

2020 Silva, TFD, **Machuqueiro, M** "The pH-dependent mechanism underlying membrane crossing of Lewis base drugs", CBIOS Meeting, Universidade Lusófona, Lisboa, December 2020.

2020 **Machuqueiro, M**, Silva, TFD, Assaraf, Y.G "The pH-dependent membrane crossing mechanism of Lewis bases antitumor drugs", Stratagem, COST Action CA17104, Belgrade, Serbia, February 2020.

2020 **Machuqueiro, M**, Silva, TFD, Vila-Vicosa, D, Reshetnyak, YK, Andreev, OA, "Computational methods to study pH at the molecular level", EuroMicropH, COST Action CA18113, Lisbon, PT, February 2020.

2019 Silva, TFD, Vila-Vicosa, D, Reshetnyak, YK, Andreev, OA, **Machuqueiro, M**, "In silico studies of pHLIPs: the pH-sensitive peptides that target the acidity of tumor cell surfaces", 4th Meeting of the College of Chemistry of ULisboa (4ECQUL), Lisbon, Portugal, July 2019.

2019 **Machuqueiro, M**, Vila-Vicosa, D, Silva, TFD, Slaybaugh, G, Reshetnyak, YK, Andreev, OA, "Modeling pH effects at the water/membrane interface: application to the pHLIP peptide", Invited Lecture to Rhode island University, RI, USA, July 2019.

2019 **Machuqueiro, M**, Silva, TFD, Vila-Vicosa, D, Reshetnyak, YK, Andreev, OA, "Modeling pH effects of pHLIP peptide with a pH gradient", Protein Electrostatics 2019 meeting, Telluride, CO, USA. June 2019.

2019 **Machuqueiro, M**, "Computational Molecular Modelling of Cell Membranes", Invited Lecture to CNC, University of Coimbra, Portugal, March 2019.

2019 **Machuqueiro, M**, Vila-Vicosa, D, Silva, TFD, Slaybaugh, G, Reshetnyak, YK, Andreev, OA, "In silico studies of pHLIPs: the pH-sensitive peptides that target the acidity of tumor cell surfaces", COST Action CA17104, Torino, Italy, January 2019.

2018 D. Vila-Viçosa, P. B. P. S. Reis, T. Silva, **M. Machuqueiro**. "Coupling enhanced sampling and biased MD simulations with CpHMD" Protein Electrostatics, Belgrade, Serbia, June 2018.

2017 P. Reis, T. Silva, B.Victor, D. Vila-Viçosa, and **M. Machuqueiro**, "Molecular modeling pH effects in proteins: including membrane interactions and drug binding", Invited talk at the Department of Biochemistry and Molecular Biology, University of Kansas Medical Center, Kansas City, KS, USA, June 2017.

2017 D. Vila-Viçosa, P. Reis, T. Silva, B. Victor, and **M. Machuqueiro**, "Sampling issues in protonation equilibria: advanced methods vs. complex problems", Protein Electrostatics, Telluride 2017, CO, USA, June 2017.

2017 P. Reis, T. Silva, B. Victor, D. Vila-Viçosa and **M. Machuqueiro**, "pK_a shifts in protein and membrane binding", Free Energy Calculations from Molecular Simulation Workshop, London, UK, May 2017.

2016 **M. Machuqueiro**, "Computational methods to calculate pK_a values at the water/membrane interface", Protein Electrostatics Berlin, Germany, July 2016.

2016 **M. Machuqueiro**, "Computational methods to calculate pK_a values at the water/membrane interface", 5th International Iberian Biophysics Congress, Porto, Portugal, June 2016.

2014 **M. Machuqueiro**, "New *in silico* methods to model biological membranes with increased realism", Protein Electrostatics, Lisboa, Portugal, July 2014.

2014 **M. Machuqueiro**, "Interaction of antibacterial sugar-based surfactants with lipid bilayers: a computational approach", COST-CM1102, Siena, Italy, June 2014.

2013 **M. Machuqueiro**, D. Vila-Viçosa, H. A. F. Santos, V. H. Teixeira, "pH effects on lipid bilayer structures: a computational study" ACS Meeting, Indianapolis, USA, September 2013.

2013 **M. Machuqueiro**, D. Vila-Viçosa, "pH-dependent conformational study of a synthetic receptor for molecular recognition of carbohydrates", COST-CM1102, Prague, Czech Republic, April 2013.

2012 **M. Machuqueiro**, "pH effects on lipid bilayer structures: a computational study", Invited lecture at the Institut de Chimie, Université de Strasbourg, Strasbourg, France, November 2012.

2012 **M. Machuqueiro**, D. Vila-Viçosa, V. H. Teixeira, "pH effects on lipid bilayer structures: a computational study", X Girona Seminar on Theoretical and Computational Chemistry for the Modeling of Biochemical Systems: From Theory to Applications, Girona, Spain, July 2012.

2012 **M. Machuqueiro**, "Structure-function relationship in biomolecular systems: Insights from molecular simulations", COST-CM1102, Bern, Switzerland, February 2012.

2011 **M. Machuqueiro**, "Is the prediction of pK_a values by constant-pH molecular dynamics being hindered by inherited problems?", THEOBio, 5th Theoretical Biophysics International Symposium, Funchal, Portugal, June 2011.

2010 **M. Machuqueiro**, "Constant-pH MD of Lipid Bilayers", Proton Transfer in Biology, Telluride, Colorado, USA, August 2010.

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15. AWARDS AND ACHIEVEMENTS (11 items)

2023 Ciencias ULisboa Merit Award in Chemical Sciences and Technologies for work and productivity in 2022, Ciências@ULisboa.

2016 Conference grant awarded by the *German Research Foundation (DFG)* for participation in the *Protein Electrostatics Berlin* in Berlin, Germany (400 €).

2015 36-month grant for postdoctoral studies awarded by the Portuguese Foundation for Science and Technology in a highly competitive call.

2013 Conference grant awarded by *Fundação Luso-Americana para o Desenvolvimento* for participation in the *246th ACS Meeting* in Indianapolis, USA (900 €).

2010 Conference grant awarded by *Fundação Luso-Americana para o Desenvolvimento* for participation in the *Proton Transfer Electrostatics* in Telluride, CO, USA (1200 €).

2009 5-year contract under the Ciência2008 program by the Portuguese Foundation for Science and Technology in a highly competitive call.

2010 Conference grant awarded by *Fundação Calouste Gulbenkian* for participation in the *Quantum Pharmacology - 30 years on* meeting in Oxford, England (1500 €).

2006 36-month grant for postdoctoral studies awarded by the Portuguese Foundation for Science and Technology in a highly competitive call.

2003 36-month grant for postdoctoral studies awarded by the Portuguese Foundation for Science and Technology in a highly competitive call.

1999 48-month grant for doctoral studies awarded by the Swiss National Science Foundation.

1997 Prize awarded by the Portuguese office of the Ministry of Education under the program PRODEP for excellence in the completion of undergraduate studies.

16. TEAM AWARDS (11 items)

2024 Pedro Reis: FCiências.ID award (€750) for PhD thesis in the research field of Chemical Sciences and Technologies

2024 Inês Pires: Student and Early Carrer Research Poster Award (shortlisted) – 21st IUPAB Congress 2024, Kyoto, JP.

2024 João Vitorino: Student and Early Carrer Research Poster Award (shortlisted) – 21st IUPAB Congress 2024, Kyoto, JP.

2024 João Sequeira: Student and Early Carrer Research Poster Award (shortlisted) – 21st IUPAB Congress 2024, Kyoto, JP.

2024 EBSA pos-doc work visit grant (€800) attributed to Rózsa Zsófia Borbála (University of Miskolc, HU) to visit the Machuqueiro Lab for 3 weeks.

2024 Nuno Oliveira: SPBf Bursary (€350) and EBSA Grant (€300) for attending the ESAB 2024 conference, San Sebastian, ES.

2024 Marta Batista: SPBf Bursary (€350) and EBSA Grant (€300) for attending the ESAB 2024 conference, San Sebastian, ES.

2024 João Sequeira: SPBf Bursary (€350) and EBSA Grant (€300) for attending the ESAB 2024 conference, San Sebastian, ES.

2023 Sara Ferreira: Best Poster Award (€250) – Protein Electrostatics 2023, Genoa, IT.

2018 Tomás Silva: Best Scientific Poster in Protein Electrostatics Conference at Belgrade, RS.

2018 Pedro Reis: Best Oral Communication @ EJIBCE, Porto, Portugal

17. MANAGEMENT (4 items)

2022- **Data Management Plan Manager** of the European twinning project **TWIN2PIPSA** (https://twin2pipsa.campus.ciencias.ulisboa.pt/consortium.html).

2020- **Coordinator** of the **Computational Biology** thematic line in **BioISI** - Biosystems & Integrative Sciences Institute, Faculty of Sciences, University of Lisbon.

2019- **Coordinator** and **System Administrator** of the **BioISI** scientific **Computational Infrastructure** (~2500 CPUs, ~40 GPUs, ~200 TB).

2018-19 Member of the management **Coordination** of the **Chemistry and Biochemistry Center** at the Faculty of Sciences, University of Lisbon.

18. Ph.D., MASTER, AND DIPLOMA JURYS (24 items)
(excluding jury presences as (co-)supervisor or president)

2024 *Lucie da Rocha*: **Ph.D. degree**, Instituto de Tecnologia Química e Biológica António Xavier | Universidade Nova de Lisboa, entitled "*Unravelling the molecular determinants underlying pH effects on BLG using molecular simulation"*.

2024 *Carlota José Fernandes da Conceição*: **Ph.D. degree**, NOVA School of Science and Technology, NOVA University Lisbon, entitled "*PARP1 inhibitors for cancer combination therapy: merging liposome encapsulation and UVC irradiation"*.

2024 *Ana Carolina Borges Araújo*: **Master's degree**, Instituto de Tecnologia Química e Biológica António Xavier, NOVA University Lisbon, entitled: "*Poking holes in membranes with coarse-grained simulations*".

2023 *Ana Filipa Santana Fernandes*: **Master's degree**, Instituto Superior Técnico, Universidade de Lisboa, entitled: "*In silico evaluation of HER2-virus-like particles for treating breast cancer in the era of precision medicine*".

2023 *António José de Jesus Matos Figueira*: **2nd year Ph.D. Evaluation**, Faculdade de Ciências da Universidade de Lisboa, entitled "*Brain S100 proteins as a toolbox of novel chaperones to prevent amyloid aggregation and toxicity in neurodegeneration*".

2023 Benedict Braunsfeld, **1st year Ph.D. Thesis Committee**, University of Vienna, Austria.

2023 *Ana Catarina Marques Pereira*: **2nd year Ph.D. Evaluation**, Faculdade de Ciências da Universidade de Coimbra, entitled "*Cutting-Edge Virus-Host Interactome Discovery: A Multi-Omics AI-Driven Approach*".

2023 *Marianna Bufano*: **External Reviewer of a Ph.D. thesis**, Sapienza University of Roma, entitled "*Application of Computer Aided Drug Design techniques for the identification of bioactive compounds"*.

2023 *Cátia Alexandra Marques Bonito Ferreira*: **Ph.D. degree**, Faculdade de Ciências da University of Porto, entitled "*Overcoming Multidrug Resistance: search for human P-glycoprotein modulators and insights on drug efflux mechanism"*.

2023 *António José de Jesus Matos Figueira*: **1st year Ph.D. Evaluation**, Faculdade de Ciências da Universidade de Lisboa, entitled "*Brain S100 proteins as a toolbox of novel chaperones to prevent amyloid aggregation and toxicity in neurodegeneration*".

2022 *Gonçalo Miguel Fonseca Monteiro*: **Masters' degree**, Escola Superior de Tecnologia do Barreiro, do Instituto Politécnico de Setúbal, entitled: "*Analysis of residue interaction networks in molecular dynamics simulations*".

2021 *Manuel Maria Moura Neves Moreira Pires*: **Master's degree**, Faculdade de Ciências da Universidade do Porto, entitled: "*SARS-CoV-2 membrane protein: from genomic data to structural new insights*".

2021 *Bárbara Sofia Valente Almeida*: **Diploma degree**, University of Lisbon, entitled "*Identificação de novos inibidores do complexo p53-MDM2 como potenciais novas terapias anticancerígenas"*.

2021 *Carla Sílvia Silva Teixeira*: **Ph.D. degree**, University of Porto, entitled "*Computational studies addressed to multifunctional enzyme complexes"*.

2020 *Raquel Pina Gouveia*: **Master's degree**, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, entitled: "*The Structural and Functional Role of CACNG2 Mutations in Psychiatric Disorders*".

2019 *Rui João de Sousa Loureiro*: **Ph.D. degree**, University of Lisbon, entitled "*Disclosing the aggregation mechanism of β2-microglobulin in amyloid disease"*.

2018 *Lucie da Rocha*: **Masters' degree**, ITQB-NOVA, entitled: "*Molecular modeling study of ß-lactoglobulin dimerization: a first step to hypoallergen design for immunotherapy*".

2017 *Ricardo José Diogo Grácio Ferreira*: **Ph.D. degree**, University of Lisbon, entitled "*Reversing multidrug resistance (MDR) in cancer cells by targeting P-glycoprotein (Pgp)— Insights into the mechanism of MDR reversal from in silico Pgp modeling"*.

2016 *Jorge Miguel Penela de Deus Antunes*: **Master's degree**, University of Lisbon, entitled "*Modelação molecular/Bioinformática estrutural da hemaglutinina do virus influenza"*.

2015-17 *Rui João de Sousa Loureiro*: **1st, 2nd, and 3rd year Ph.D. Evaluations**, University of Lisbon, entitled "*The aggregation mechanism of β2-microglobulin in amyloid disease investigated through molecular simulations*".

2013 *Rita Leonor Veiga da Silva e Veiga Ferro*: **Ph.D. degree**, University of Lisbon, entitled "*Theoretical investigation of the energy of olefin- and sila-olefin insertion/β-H elimination reactions of two late transition metals – DFT MO calculations"*.

2013 *Marta Andreia Silva Perez Gomes*: **Ph.D. degree**, University of Porto, entitled "*Estudos de Inibição Enzimática"*.

2012 *Maria Margarida Pires dos Santos Mateus*: **Ph.D. degree**, University of Lisbon, entitled "*Propriedades Electrónicas de Espécies Hidrofóbicas Micro-solvatadas e em Solução"*.

2011 *Igor de Oliveira Marques*: **Master's degree**, University of Aveiro, entitled "*Molecular Modelling of transmembranar transporters for Chloride"*.

19. INTERNATIONAL EVALUATIONS (3 items)

2023 Grant evaluation for the Grantová Agentura České Republiky (Standard Projects 2024)

2023 Evaluation of computational production projects for the Swiss National Supercomputing Centre (CSCS), Switzerland.

2016 Evaluation of FCT's PESSOA program: "Cooperação Bilateral Portugal-França 2016"

20. GRANTS AND CONTRACTS EVALUATION JURYS (6 items)

2021-23 Member of the Evaluation Panel for the annual evaluation of the DL-57 type contracts within the BioISI research unit. 15 researchers have been evaluated by this 5-member evaluation board (the coordinators of 5 BioISI Thematic Lines).

2022 Member of the Evaluation Committee of BioISI Projects 2022. 9 research projects were evaluated and 5 were selected for funding. This was a 5-member evaluation board (the coordinators of 5 BioISI Thematic Lines).

2022 Member of the Evaluation Panel for the BioISI Junior Program (Second Edition). This call awarded 8 Research Fellowships for R&D Initiation (BII) in Systems Biology and 24 applications were evaluated.

2022 Member of the Evaluation Panel for the BioISI "Verão com Ciência" Special Initiative from FCT. This call awarded 9 Research Fellowships for R&D Initiation (BII) and 26 applications were evaluated.

2021 Member of the Evaluation Panel for the BioSYS2 Ph.D. program. This is the second call of the BioISI Ph.D. program where 15 applications were evaluated and 8 Ph.D. grants have been attributed.

2021 Member of the Evaluation Panel for the BioISI Junior Program. This call awarded 8 Research Fellowships for R&D Initiation (BII) in Systems Biology and 17 applications were evaluated.

21. ACADEMIC EDITOR OR EDITORIAL BOARD IN INTERNATIONAL JOURNALS (3 items)

- PlosOne
- Journal of Computational Biophysics and Chemistry
- The Journal of Membrane Biology

22. REFEREEING IN INTERNATIONAL JOURNALS (23 selected items)

- Journal of the American Chemical Society
- Journal of Chemical Theory and Computation
- Journal of Chemical Information and Modeling
- The Journal of Physical Chemistry Letters

- The Journal of Physical Chemistry B
- ACS Omega
- Nature Scientific Reports
- Nucleic Acids Research
- Journal of Computational Chemistry
- Biochemistry
- Langmuir
- PROTEINS: Structure, Function, and Bioinformatics
- FEBS Open Bio
- RSC Advances
- PlosOne
- PeerJ
- Physical Chemistry Chemical Physics
- The European Physical Journal B
- Journal of Molecular Modeling
- Journal of Biophysics
- Frontiers in Molecular Biosciences
- BioMed Research International
- Journal of Drug Delivery Science and Technology

23. CONFERENCE ORGANIZING (4 items)

- Organizer of the 3D-BioInfo-PT Advanced Workshop held on April 12th, 2024 at FCUL (https://3d-bioinfo-pt.github.io/events)
- Organizer of the EJIBCE 2019 (Encontro de Jovens Investigadores de Biologia Computacional Estrutural). The meeting is held on 20th of December 2019 at FCUL. (http://ejibce.github.io/images/abstracts_2019.pdf)
- Organizer of the "Protein Electrostatics" – satellite meeting of EBEC 2014. The meeting was held on 08-11 of July 2014 at FCUL. (https://proteinelectrostatics.org/past-editions-archive/lisbon-2014/home.html)
- Organizer of the EJIBCE 2014 (Encontro de Jovens Investigadores de Biologia Computacional Estrutural). The meeting was held on 18-19 of December 2014 at FCUL. (http://ejibce.github.io/images/abstracts_2014.pdf)

24. NATIONAL AND INTERNATIONAL COLLABORATIONS (only ongoing/22 items)

- Walter Rocchia (Genova, IT), for the DelPHI and PypKa development project
- Chris Oostenbrink (Vienna, AT), for the enhanced sampling CpHMD projects
- Djork-Arné Clevert (Berlin, DE), for the AI-based projects
- Adrian Roitberg (Univ. Florida, USA) for the Amber ff CpHMD project

- Profs. Oleg Andreev and Yana Reshetnyak (Rhode Island, US), and Donald Engelman (Yale, US) for the pHLIP project
- Yehuda Assaraf (Haifa, IL), for the Lewis drugs project
- Alexey Ladokhin (Kansas, US), for the DTT project
- Wolfgang Link (Univ. Madrid, ES) for the CRM1 project
- Tamis Darbre (Univ. Bern, CH) for the peptide dendrimers project
- P. Drączkowski and K. Jóźwiak (Univ. Lublin, PL) for the AChE project
- Ross Anderson (Univ. Bristol, UK) for the C(pH,*E*)MD development project
- Adrian Mulholland (Univ. Bristol, UK) for the heme parameterization projects
- Irina Moreira (Univ. Coimbra, PT) for the GPCR projects
- Lígia Martins (ITQB-NOVA, PT) for the DyP-type Peroxidase projects
- Filomena Martins (FCUL, PT) for the antitubercular isoniazid derivatives project
- Patrícia Faísca (FCUL, PT) for the β2M and the protein knots projects
- Cláudio Gomes (FCUL, PT) for the S100 projects
- Andreia Valente (FCUL, PT) for the P-gp inhibition project
- Tânia Morais (FCUL, PT) for the Ru-drug membrane interactions project
- Andreia Figueiredo (FCUL, PT) for the vineyard defense subtilases project
- Bruno Victor (FCUL, PT) for the PAINS project
- Paulo J. Costa (FCUL, PT) for the X-bonds in CpHMD project

25. SOFTWARE DEVELOPMENT (7 items)

- PypKa - A protein pK_a calculation tool and server (https://pypka.org) where users can submit online their pK_a calculations.
- PypKa-MD - A Python wrapper for the stochastic titration CpHMD method used in our group (https://pypi.org/project/pypkamd).
- pKPDB - A protein pK_a database encompassing almost the complete PDB Databank (https://pypka.org/pKPDB).
- pKAI - An AI tool developed to speed up the protein pK_a calculations (https://github.com/bayer-science-for-a-better-life/pKAI).
- MembIT - A Python-based tool to calculate several membrane properties (drug/protein insertion or drug/protein-induced deformations) from MD trajectories (https://github.com/mms-fcul/MembIT).
- pKa_Profiler - A Python-based tool to calculate pK_a values along a membrane-insertion coordinate (https://github.com/mms-fcul/pKaProfiler).
- PyBindE - A Python wrapper to calculate binding free energies (MM/PBSA) for protein/drug and protein/protein complexes (https://github.com/mms-fcul/PyBindE).

For more details check out our website: https://mms.rd.ciencias.ulisboa.pt/software.html

26. OUTREACH (6 items)

2022- **European Researcher's Night** initiative with an outreach activity entitled *From structure to function - Three-dimensional visualization of the molecules of life*. With this activity, we reached out to the community and showed how small modifications (mutations) in proteins can trigger diseases.

2021- **Speed Dating with Scientists** outreach activity in the *"Ciências Research Day"*. With this initiative, we help young students choose their future at FCUL.

2020 Participation in the "90 segundos de ciência" Antena 1 radio podcast about science. https://www.90segundosdeciencia.pt/episodes/ep-931-miguel-machuqueiro

2019- Several **High School** presentations entitled "Será que posso vir a ser Cientista?" aimed at attracting young students to FCUL, in particular to Chemistry and Biochemistry. The venues include: Escola Secundária (ES) do Restelo; ES Lumiar; ES Seomara da Costa Primo (Amadora); ES Cacilhas-Tejo; ES Externato de S. José (Lisboa); ES Torres Vedras; ES Baixa Banheira.

2016-17 **FCUL Open Day 2016** initiative with an outreach activity entitled *Bioquímica e Bioquímica Computacional na FCUL*. With this informative activity, we reached out to young students and helped them choose their future at FCUL.

2015 **Noite dos Investigadores 2015** initiative with an outreach activity entitled *Simulação Computacional em Química e Bioquímica*. With this activity, we reached out to the community and shared our most recent findings in the design of new anti-tuberculosis drugs.

27. COMPLETE LIST OF ORAL AND PANEL COMMUNICATIONS IN BOTH NATIONAL AND INTERNATIONAL CONFERENCES (234 items)

https://docs.google.com/document/d/18peiR34AjQkTGH5KMnU67nAkOUSgNeB_HwBG5YM5VSY/edit?usp=sharing