

Monica L. Fernández-Quintero



Personal Information

Address	Theoretical Chemistry, Faculty of Chemistry and Pharmacy, Center for Molecular Biosciences, University of Innsbruck, Innrain 82, A-6020 Innsbruck, Austria
Phone	+43 512 507 57106
Cell Phone	+43 664 / 3875663
E-mail	monica.fernandez-quintero@uibk.ac.at
Homepage	Liedllab Homepage
Google Scholar	Google Scholar Page
Nationality	Austria
Date of Birth	20.10.1993

Education

Since 2020	Post-Doctoral Researcher , Leopold-Franzens-University, Innsbruck, Austria
Since 2017	MCBO and CavX PhD Program , Medical University, Innsbruck, Austria PhD Program Chemistry , Leopold-Franzens-University, Innsbruck, Austria
2017-2020	Austria
2017	Master Program Chemistry , Leopold-Franzens-University, Innsbruck, Austria
2016	Bachelor Program Chemistry , Leopold-Franzens-University, Innsbruck, Austria

Research Experience

During my studies I had the opportunity to work on a wide range of projects. While all are related to structure prediction and drug design, I worked with antibodies, ion channels, small molecules, but also with some experimental techniques, e.g., patch clamp.

My scientific interest has been shaped by collaborating with a broad range of local and international research groups from academia and industry. Recently, I drafted a project grant for the group of Prof. Liedl, which was approved by the Austrian Science Fund (FWF) and thereby raised approximately 400000 €. So far, my research efforts have led to more than 30 publications in peer-reviewed journals and more than 10 conference presentations.

- Antibodies
- Ion Channels
- MD simulations
- Computational Drug Design

PhD Thesis

Title The Dynamic Nature of Antigen Receptors
Supervisor Univ.-Prof. DDr. Klaus R. Liedl

Master Thesis

Title Structural Ensembles of Antibody CDR-H3 Loops
Supervisor Univ.-Prof. DDr. Klaus R. Liedl

Professional and International Experience

Postdoctoral researcher, PhD student and teaching assistant coordinating the research focus on antibodies and ion channels. So far, I co-supervised eleven master and ten bachelor theses and held lectures as well as practical courses on molecular modelling and bioinformatics.

- Since 09.2020 **Post-Doctoral Researcher and Teaching Assistant**, Theoretical Chemistry, CCB Innsbruck, Innrain 82, A-6020 Innsbruck
- 09.2017-08.2020 **Research and Teaching Assistant**, Leopold-Franzens-Universität Innsbruck, Theoretical Chemistry, CCB Innsbruck, Innrain 82, A-6020 Innsbruck
- Since 09.2017 **Research and Teaching Assistant**, Medical University of Innsbruck, Physiology, Schöpfstraße 41, A-6020 Innsbruck
- 2016-2017 **Research Assistant**, Theoretical Chemistry, CCB Innsbruck, Innrain 82, A-6020 Innsbruck
- 2015-2017 **Student Co-Worker**, Theoretical Chemistry, CCB Innsbruck, Innrain 82, A-6020 Innsbruck
- 07.2015-08.2015 **Internship**, Adler-Werk Lackfabrik Johann Berghofer, Bergwerkstraße 22, 6130 Schwaz, Austria
- Since 2014 **Instructor**, Nachhilfe Institut Dr. Rampitsch, 6020 Innsbruck
- 2009-2011 **Entrepreneur's Skills Certificate**

Teaching

- Lecture** Bioinformatics of Macromolecules, University of Innsbruck
- Lecture** Structural Biology – Bioinformatics, Medical University of Innsbruck
- Lecture** Structure Prediction of Therapeutic Antibodies, University of Pavia

Extracurricular Activities

- 2019-2022 PhD representative in the student's union

Scientific Publications

- 1 Monica L. Fernández-Quintero, Katharina B. Kroell, Lukas J. Grunewald, Anna-Lena M. Fischer, Jakob R. Riccabona, Klaus R. Liedl. **CDR loop interactions determine heavy and light chain pairing preferences in bispecific antibodies.** mAbs, 2021, under review (IF: 5.5)
- 2 Johannes Kraml, Franz Waibl, Valentin J. Hoerschinger, Florian Hofer, Anna S. Kamenik, Monica L. Fernández-Quintero, Klaus R. Liedl. **A GIST for all rigid solvents.** Journal of Chemical Theory and Computation, 2021, under review (IF: 6.0)
- 3 Monica L. Fernández-Quintero, Anna Vangone, Johannes R. Loeffler, Clarissa A. Seidler, Guy Georges, Klaus R. Liedl. **Challenge Accepted – Paratope states in solution improve structure prediction and docking.** Structure, 2021, under review (IF: 4.8)
- 4 Monica L. Fernández-Quintero, Yousra El Ghaleb, Stefania Monteleone, Petronel Tuluc, Marta Campiglio, Klaus R. Liedl, Bernhard E. Flucher. **Ion-pair interactions between voltage-sensing domain IV and pore domain I regulate Cav1.1 gating.** Biophysical Journal, 2021, accepted (IF: 4.0)
- 5 Valentin J. Hoerschinger, Monica L. Fernández-Quintero, Franz Waibl, Johannes Kraml, Alexander Bujotzek, Guy Georges, Klaus R. Liedl. **OCD.py – Characterising immunoglobulin inter-domain orientations.** Bioinformatics, 2021, under review (IF: 5.9)
- 6 Monica L. Fernández-Quintero, Katharina B. Kroell, Lisa M. Bacher, Johannes R. Loeffler, Patrick K. Quoika, Guy Georges, Alexander Bujotzek, Hubert Kettenberger, Klaus R. Liedl. **Germline-dependent antibody paratope states and pairing specific V_H-V_L interface dynamics.** Frontiers in Immunology, 2021, doi: 10.3389/fimmu.2021.675655
- 7 Franz Waibl, Monica L. Fernández-Quintero, Anna S. Kamenik, Johannes Kraml, Florian Hofer, Hubert Kettenberger, Guy Georges, Klaus R. Liedl. **Conformational ensembles of antibodies determine their hydrophobicity.** Biophysical Journal, 2021, doi: 10.1016/j.bpj.2020.11.010 (IF: 4.0)
- 8 Anamika Dayal, Monica L. Fernández-Quintero, Klaus R. Liedl, Manfred Grabner. **Pore mutation N617D in the skeletal muscle DHPR blocks Ca²⁺ influx due to atypical high-affinity Ca²⁺ binding.** eLife, 2021, doi: 10.7554/eLife.63435 (IF: 6.8)

- 9 Monica L. Fernández-Quintero, Katharina B. Kroell, Jakob R. Riccabona, Klaus R. Liedl. **Mutation of framework residue 71^H results in different paratope sites in solution.** *Frontiers in Immunology*, 2021, doi: 10.3389/fimmu.2021.630034 (IF: 7.5)
- 10 Monica L. Fernández-Quintero, Guy Georges, Janos M. Varga, Klaus R. Liedl. **Ensembles in solution as a new paradigm for antibody structure prediction and design.** *mAbs*, 2021, doi: 10.1080/19420862.2021.1923122 (IF: 5.5)
- 11 Monica L. Fernández-Quintero, Clarissa A. Seidler, Patrick K. Quoika, Klaus R. Liedl. **Shark antibody variable domains rigidify upon affinity maturation – Two step conformational selection binding mechanism.** *Frontiers in Molecular Biosciences*, 2021, doi: 10.3389/fmolb.2021.639166 (IF: 5.2)
- 12 Franz Waibl, Johannes Kraml, Monica L. Fernández-Quintero, Johannes R. Loeffler, Klaus R. Liedl. **Explicit solvation thermodynamics in ionic solution – an extension of Grid Inhomogeneous Solvation Theory efficiently predicts salting-out coefficients.** *Journal of Chemical Physics*, 2021, (IF: 3.1)
- 13 Patrick K. Quoika, Monica L. Fernández-Quintero, Maren Podewitz, Florian Hofer, Klaus R. Liedl. **Implementation of the Freely Jointed Chain Model to Assess Kinetics of Thermosensitive Coil-Globule Transition by Markov States.** *Journal of Physical Chemistry B*, 2021, doi: 10.1021/acs.jpcc.1c01946 (IF: 2.9)
- 14 Alexandra Koschak, Monica L. Fernández-Quintero, Thomas Heigl, Marco Ruzza, Hartwig Seitter, Lucia Zanetti. **Cav1.4 dysfunction and congenital night blindness type 2.** *Pflügers Archiv – European Journal of Physiology*, 2021, doi: 10.1007/s00424-021-02570-x (IF: 3.2)
- 15 Johannes R. Loeffler, Monica L. Fernández-Quintero, Franz Waibl, Patrick K. Quoika, Florian Hofer, Michael Schauerl, Klaus R. Liedl. **Conformational shifts of stacked heteroaromatics: Vacuum vs. Water studied by Machine Learning.** *Frontiers in Chemistry*, 2021, doi: 10.3389/fchem.2021.641610 (IF: 5.2)
- 16 Jenna J. Guthmiller, Julianna Han, Henry A. Utset, Lei Li, Linda Yu-Ling Lan, Carole Henry, Christopher T. Stamper, Monica L. Fernández-Quintero et al. **Broadly neutralizing antibodies target a hemagglutinin anchor epitope.** *Nature*, 2021, under review (IF: 42.0)
- 17 Jenna J. Guthmiller, Linda Yu-Ling Lan, Monica L. Fernández-Quintero et al. **Polyreactive broadly neutralizing B cells are selected to**

- provide defense against pandemic threat influenza viruses.** Immunity, 2020, doi: 10.1016/j.immuni.2020.10.005 (IF: 22.6)
- 18 Yousra El Ghaleb, Pauline E. Schneeberger, Monica L. Fernández-Quintero et al. **CACNA1I gain-of function mutations differentially affect channel gating and cause neurodevelopmental disorders.** Brain, 2020, doi: 10.1093/brain/awab101 (IF: 11.3)
- 19 Monica L. Fernández-Quintero, Katharina B. Kroell, Martin C. Heiss, Johannes R. Loeffler, Patrick K. Quioka, Franz Waibl, Alexander Bujotzek, Ekkehard Moessner, Guy Georges, Klaus R. Liedl. **Surprisingly fast interface and elbow angle dynamics of antigen-binding fragments.** Frontiers in Molecular Biosciences, 2020, doi: 10.3389/fmolb.2020.609088 (IF: 4.1)
- 20 Monica L. Fernández-Quintero, Nancy D. Pomarici, Johannes R. Loeffler, Clarissa A. Seidler, Klaus R. Liedl. **T-cell receptor CDR3 loop conformations in solution shift the relative V_H-V_L domain distributions.** Frontiers in Immunology, 2020, doi: 10.3389/fimmu.2020.01440 (IF: 5.1)
- 21 Florian Hofer, Anna S. Kamenik, Monica L. Fernández-Quintero, Johannes Kraml, Klaus R. Liedl. **pH-Induced Local Unfolding of the Phl p 6 Pollen Allergen from cpH-MD.** Frontiers in Molecular Biosciences, 2020, doi: 10.3389/fmolb.2020.603644 (IF: 4.1)
- 22 Monica L. Fernández-Quintero, Nancy D. Pomarici, Barbara A. Math, Katharina B. Kroell, Franz Waibl, Alexander Bujotzek, Guy Georges, Klaus R. Liedl. **Antibodies exhibit multiple paratope states influencing V_H-V_L domain orientations.** Communications Biology, 2020, doi: 10.1038/s42003-020-01319-z (IF: 12.1)
- 23 Monica L. Fernández-Quintero, Yousra El Ghaleb, Petronel Tuluc, Marta Campiglio, Klaus R. Liedl, Bernhard E. Flucher. **Structural determinants of voltage-gating properties in calcium channels.** eLife, 2020, doi: 10.7554/eLife.64087 (IF: 6.8)
- 24 Monica L. Fernández-Quintero, Nancy D. Pomarici, Martin C. Heiss, Barbara A. Math, Klaus R. Liedl. **Antibody CDR Loops as Ensembles in Solution vs. Canonical Clusters from X-ray structures.** mAbs, 2020, doi: 10.1080/19420862.2020.1744328 (IF: 4.6)
- 25 Monica L. Fernández-Quintero, Johannes R. Loeffler, Klaus R. Liedl. **Conformational Selection of Allergen - Antibody Complexes – Surface Plasticity of Paratopes and Epitopes.** Protein Engineering, Design and Selection, 2020, doi: 10.1093/protein/gzaa014 (IF: 1.9)

- 26 Johannes R. Loeffler, Monica L. Fernández-Quintero, Michael Schauerl, Klaus R. Liedl. **STACKED – Solvation Theory of Aromatic Complexes as Key for Estimating Drug Binding.** Journal of Chemical Information and Modelling, 2020, doi: 10.1021/acs.jcim.9b01165 (IF: 4.5)
- 27 Monica L. Fernández-Quintero, Johannes R. Loeffler, Lisa M. Bacher, Clarissa A. Seidler, Franz Waibl, Klaus R. Liedl. **Local and Global Rigidification Upon Affinity Maturation.** Frontiers in Molecular Biosciences, 2020, doi: 10.3389/fmolb.2020.00182 (IF: 4.1)
- 28 Monica L. Fernández-Quintero, Clarissa A. Seidler, Klaus R. Liedl. **T-Cell Receptor Variable β Domains Rigidify During Affinity Maturation.** Scientific Reports, 2020, doi: 10.1038/s41598-020-61433-0 (IF: 3.9)
- 29 Monica L. Fernández-Quintero, Valentin J. Hoerschinger, Leonida M. Lamp, Alexander Bujotzek, Guy Georges, Klaus R. Liedl. **V_H-V_L interdomain dynamics observed by computer simulations and NMR.** Proteins, 2020, doi: 10.1002/prot.25872 (IF: 2.5)
- 30 Monica L. Fernández-Quintero, Martin C. Heiss, Klaus R. Liedl. **Antibody Humanization - The Influence of the Antibody Framework on the CDR-H3 Loop Ensemble in Solution.** Protein Engineering, Design and Selection, 2020, doi: 10.1093/protein/gzaa004 (IF: 1.9)
- 31 Leonardo H. Franca de Lima, Monica L. Fernandez-Quintéro, Rafael E. O. Rocha, Diego C. Batista Mariano, Raquel C. de Melo-Minardi, Klaus R. Liedl. **Conformational flexibility correlates with glucose tolerance for point mutations in β -glucosidases – A computational study.** Journal of Biomolecular Structure and Dynamics, 2020, doi: 10.1080/07391102.2020.1734484 (IF: 3.5)
- 32 Monica L. Fernández-Quintero, Barbara A. Math, Johannes R. Loeffler, Klaus R. Liedl. **Transitions of CDR-L3 Loop Canonical Cluster Conformations on the Micro-to-Millisecond Timescale.** Frontiers in Immunology, 2019, doi: 10.3389/fimmu.2019.02652 (IF: 5.1)
- 33 Nadja T. Hofer, Petronel Tuluc, Nadine J. Ortner, Yuliia V. Nikonishyna, Monica L. Fernández-Quintero, Klaus R. Liedl, Bernhard E. Flucher, Helen Cox, Jörg Striessnig. **Biophysical classification of a CACNA1D de novo mutation as a high-risk mutation for a severe neurodevelopmental disorder.** Molecular Autism, 2019, doi: 10.1186/s13229-019-0310-4 (IF: 5.5)
- 34 Monica L. Fernández-Quintero, Johannes Kraml, Guy Georges, Klaus R. Liedl. **CDR-H3 loop ensemble in solution–conformational**

selection upon antibody binding. mAbs, 2019, doi: 10.1080/19429862.2019.1618676 (IF: 5.5)

- 35 Monica L. Fernández-Quintero, Johannes R. Loeffler, Ursula Kahler, Johannes Kraml, Anna S. Kamenik, Klaus R. Liedl. **Characterizing the diversity of the CDR-H3 loop conformational ensembles in relationship to antibody binding properties.** Frontiers in immunology, 2019, doi: 10.3389/fimmu.2018.03065 (IF: 5.1)

Talks

- 1 **The CDR-H3 Loop as a Conformational Ensemble.** Roche, Penzberg, Germany, 2018
- 2 **Antibody Binding Properties are Reflected in Conformational Diversity.** Boehringer-Ingelheim, Biberach, DE, 2018
- 3 **Antibodies – Nano-to Millisecond-Dynamics and Design Implications.** Roche, Penzberg, Germany, 2019
- 4 **Antibodies – Nano-to Millisecond-Dynamics and Design Implications.** Computational Drug Design Conference, Boston, USA, 2019
- 5 **Structural determinants of calcium channel voltage-gating properties.** CavX Symposium, Krems, AT, 2020
- 6 **Structural determinants of calcium channel voltage-gating properties.** University of Los Angeles, LA, USA, 2020
- 7 **Antibodies exhibit multiple paratope states in solution that shift the relative V_H - V_L interdomain orientation.** Antibody Engineering and Therapeutics Europe, 2020
- 8 **Structural determinants of calcium channel voltage-gating properties.** University of Stockholm, 2021
- 9 **Ensembles in solution as a new paradigm in antibody structure prediction and design.** 13th European Biophysics Conference, Vienna, 2021
- 10 **Comparison of Antibody Interfaces – Lessons for the Design of Bispecific Antibodies.** Computational Drug Design Conference, Boston, USA, 2021
- 11 **Ensembles in solution as a new paradigm in antibody structure prediction and design.** ÖGMBT Annual Meeting, 2021

Poster Presentations

- 1 Antibodies exhibit multiple paratope states in solution that shift the relative V_H-V_L interdomain orientation.** British Society of Immunology, Virtual Meeting, 2020
- 2 Antibodies exhibit multiple paratope states in solution that shift the relative V_H-V_L interdomain orientation.** Antibody Engineering and Therapeutics Europe, Virtual Meeting, 2020
Best Poster Award
- 3 Structural determinants of calcium channel voltage-gating properties.** 64th Meeting of the Biophysical Society, San Diego, CA, USA, 2020
- 4 Transitions of CDR-L3 Loop Canonical Cluster Conformations on the Micro-to-Millisecond Timescale.** PEGS, Lisbon, Portugal, 2019
- 5 Structure Modelling of Cav1.1 reveals functional trans-domain interactions involved in voltage-sensing.** ANA Meeting, Innsbruck, Austria, 2019
- 6 Structure Modelling of Cav1.1 reveals functional trans-domain interactions involved in voltage-sensing.** PhD Life Science Meeting, Innsbruck, Austria, 2019
- 7 Structure Modelling of Cav1.1 reveals functional trans-domain interactions involved in voltage-sensing.** 63th Meeting of the Biophysical Society, Baltimore, USA, 2019
- 8 Multispecificity Reflected in Flexibility Differences of Antibodies - CDR-H3 Loop Flexibility Induces Promiscuity.** ISQBP, Barcelona, Spain, 2018
Best Poster Award
- 9 Voltage-gating of Cav1.1 based on Molecular Dynamics Simulations.** 3rd European Calcium Channel Conference, Alpbach, Austria, 2018
- 10 Voltage-gating of Cav1.1 based on Molecular Dynamics Simulations.** PhD Life Science Meeting 2018, Innsbruck, Austria
- 11 Multispecificity reflected in Flexibility Differences of Antibodies.** Gordon Research Conference on Antibody Engineering and Design, 2018, Lucca, Italy

Awards

- 1 Multispecificity Reflected in Flexibility Differences of Antibodies - CDR-H3 Loop Flexibility Induces Promiscuity.** ISQBP, Barcelona, Spain, 2018
Best Poster Award
- 2 Antibodies exhibit multiple paratope states in solution that shift the relative V_H-V_L interdomain orientation.** Antibody Engineering and Therapeutics Europe, Virtual Meeting, 2020
Best Poster Award
- 3 Antibodies Next Topmodel – Use of CDR loop ensembles *from* molecular dynamics simulations guides antibody design and docking.** Antibody Society Writing Competition, 2021
Postdoctoral Winner
- 4 The Dynamik Nature of Antigen Receptors.** Prof. Brandl Award, Prof. Brandl Foundation, 2021
Best Dissertation 2020
- 5 The Dynamik Nature of Antigen Receptors.** Prof. Sosnovsky Award, Prof. Sosnovsky Foundation, 2021
Best Dissertation 2020
- 6 The Dynamik Nature of Antigen Receptors.** Karl-Schlögl Award, Austrian Academy of Sciences, 2021
Best Dissertation 2020
- 7 The Dynamik Nature of Antigen Receptors.** Award of Excellence, National Award, 2021
Best Dissertation 2020
- 8 The Dynamik Nature of Antigen Receptors.** Wirtschaftskammerpreis, 2021
Best Dissertation 2020