Nicolas PANEL

PhD

Education

2022 **CNU qualification for senior lecturer position** - Sections 31 and 64

2014–2017 **PhD in Computational biology** - École Polytechnique, Palaiseau, France

2012–2014 **Master of Bioinformatic** - Université Paris-Diderot, Paris, France (ranking 4/21)

2009–2012 **Bachelor of Biology – Bioinformatic** - UVSQ, Versailles, France (ranking 2/104)

Professional experience

Research

march. 2022 - now **Researcher at Toulouse Biotechnology Institute, INSA Toulouse, Toulouse, France** - Molecular modelling and design of enzymes for industrial processes (Dr Isabelle André)
- Computational protein design for enzyme stability and activity

feb. 2018 - feb. 2022 **Researcher at Uppsala University, Dept. of Cell and Molecular Biology, Uppsala, Sweden** - Development and applications of methods for structure-based drug discovery applied to G protein-coupled receptors (Pr Jens Carlsson)
- Virtual screening for discovery of GPCRs modulators
- Ligand pharmacology prediction

nov. 2017 - jan. 2018 **Postdoctoral research at École Polytechnique, Laboratoire de Biochimie, Palaiseau, France** - Computational study of the Tiam1 PDZ domain using computational protein design approach and free energy models (Pr Thomas Simonson)

oct. 2014 - sept. 2017 **Doctoral research at École Polytechnique, Laboratoire de Biochimie, Palaiseau, France** - Computational study of the Tiam1 PDZ domain using computational protein design approach and free energy models (Pr Thomas Simonson)
- Parameters optimisation for computational protein design
- Molecular modelling and simulations of protein:peptide complexes
- Free energy calculations (LIE, MMPBSA, alchemical simulations)

jan. 2014 - june 2014 **Master internship (2nd year) at ENS Cachan, LPBA, Cachan, France** - Characterization of mutation effects on allosteric pathways in KIT receptor (Dr Luba Tchertanov and Dr Priscila Da Silva Figueiredo Celestino Gomes)
- Exploring effects of point mutations on the dynamic of the KIT receptor
- Affinity prediction of tyrosine kinase inhibitors with MMPBSA model

march 2013 - june 2013 **Master internship (1st year) at École Polytechnique, Laboratoire de Biochimie, Palaiseau, France** - Protein side chain conformation predictions using a computational protein design approach (Dr Thomas Gaillard)
- Performance comparison between two softwares for sidechain conformation predictions

Teaching

2019-2022 **Teaching assistant at Uppsala University, Uppsala, Sweden**
R programming, structural biology for Master degree

2015-2017 **Teaching assistant at Université Paris-Diderot, Paris, France**
Biostatistics and sequence analysis for Master degree (128h)

Mentored Students

2024 **Assia Djilali (4th year Student-engineer)** - Production and *in vitro* characterization of novel enzymes for plastic oligomers degradation.

2021 **Adam Hallberg (2nd year Master)** - Adam synthesized compounds indentified by virtual screening against the Neurotensin receptor 1 to study structure activity relationship.

Qingtian Gong, Molly Ångström, Tova Rane (1st year Master) - Lead optimization of SARS-CoV-2 Mpro inhibitors using molecular docking approaches.

2020 **Nour Kahlous (2nd year Master)** - Nour optimized and applied a free energy calculation pipeline to predict ligand efficacy at the β_2 adrenergic receptor.

Yupei Li (2nd year Master) - Yupei generated homology models of the active state of the dopamine D_2 receptor in order to perform high throughput screening.

Technical skills

Theory Molecular mechanics, molecular modelling, free energy calculation, docking, computational protein design, machine learning, sequence analysis

Softwares **Molecular dynamics packages:** NAMD, Q, GROMACS, CHARMM, XPLOR, AMBER

Molecular docking: DOCK3.7, AutoDock

Computational Chemistry RDKit, ChemAxon

Computational Protein Design: Proteus, Rosetta, SCWRL

Homology modelling: Modeller

Molecular visualization: PyMOL, VMD, Chimera

Languages Python, shell script (bash,grep,sed Awk,...), R, Perl, C, LaTeX

Language

French Native

English Fluent

Swedish Occasional

Publications and communications

Publications

Panel N., Vo D.D., Huebner H., Pach S., Hilge M., Plückthun A., Gmeiner P., and Carlsson J. **Structure-based discovery of small-molecule agonists of the Neurotensin receptor 1.** *In preparation*.

Nguyen A.T.N.*, Panel N.*, Vo D.D., Thai B.S, Chia L.Y., Tran Q.L, Hellyer S., Langiu M., Gregory K.J., Kihlberg J., White P.J., Scammells P., Christopoulos A., Carlsson J., and May1 L.T. **Structure-based discovery of positive allosteric modulators of the A_1 adenosine receptor**. *Submitted*. *co-first authors.

Panel N., Vo D.D., Aldin Kahlous N., Hübner H., Tiedt S., Matricon P., Pacalon J., Fleetwood O., Kampen S., Luttens A., Delemotte L., Kihlberg J., Gmeiner P., and Carlsson J. **Design of Drug Efficacy Guided by Free Energy Simulations of the β_2-Adrenoceptor**. *Angewandte Chemie International Edition*, 2023.

Draper-Joyce C.J., Bhola R., Wang J., Bhattarai A., Anh T.N., Nguyen A.T.N., Cowie-Kent I., O'Sullivan K., Yeong Chia L.Y., Venugopal H., Valant C., Thal D.M., Wootten D., Panel N., Carlsson J., Macdonald J.C., White P.J., Scammells P, May L.T., Sexton P.M., Danev R., Yinglong Miao Y., Glukhova A., Imlach W., and A. Christopoulos. **Positive allosteric mechanisms of adenosine A1 receptor-mediated analgesia**. *Nature*, 2021.

Kampen S., Vo D.D., Zhang X., Panel N., Yang Y., Jaiteh M., Matricon P., Svenningsson P., Brea J., Loza M.I., Kihlberg J., and Carlsson J. **Structure-guided Design of G Protein-coupled Receptor Polypharmacology**. *Angewandte Chemie*, 2021.

Matricon P., Suresh R.R., Gao Z.G., Panel N., Jacobson K.A., and Carlsson J. **Ligand design by targeting a binding site water**. *Chemical Science*, 2020.

Mignon D., Druart K., Michael E., Opuu V., Polydorides S., Villa F., Gaillard T., Panel N., Archontis G., and Simonson T. **Physics-Based Computational Protein Design: An Update**. *Journal of physical chemistry A*, 2020.

Opuu V., Sun Y.J., Hou T., Panel N., Fuentes E.J., and Simonson T. **A physics-based energy function allows the computational redesign of a PDZ domain**. *Scientific Reports*, 2020.

Villa F., Panel N., Chen X., and Simonson T. **Adaptive landscape flattening in amino acid sequence space for the computational design of protein:peptide binding**. *Journal of Chemical Physics*, 149, 2018.

Panel N.*, Villa F.*, Fuentes E.J., and Simonson T. **Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations**. *Biophysical Journal*, 114, 2018. *co-first authors.

Panel N., Sun Y.J., Fuentes E.J., and Simonson T. **A simple PB/LIE free energy function accurately predicts the peptide binding specificity of the Tiam1 PDZ domain**. *Frontiers in Molecular Biosciences*, 4, 2017.

Mignon D.*, Panel N.*, Chen X., Fuentes E.J., and Simonson T. **Computational Design of the Tiam1 PDZ Domain and Its Ligand Binding**. *Journal of Chemical Theory and Computation*, 13(5):2271–2289, 2017. *co-first authors.

Gaillard T., Panel N., and Simonson T. **Protein side chain conformation predictions with an MMGBSA energy function**. *Proteins: Structure, Function, and Bioinformatics*, 84(6):803–819, 2016.

P. Da Silva Figueiredo Celestino Gomes, I. Chauvot De Beauchêne, Panel, N., S. Lopez, P. De Sepulveda, P. Geraldo Pascutti, E Solary, and L. Tchertanov. **Insight on Mutation-Induced Resistance from Molecular Dynamics Simulations of the Native and Mutated CSF-1R and KIT**. *PLOS ONE*, 11:1–25, 2016.

Chauvot de Beauchêne I., Allain A., Panel N., Laine E., Dubreuil P., and Tchertanov L. **Hotspot mutations in KIT receptor differentially modulate its allosterically coupled conformational dynamics: impact on activation and drug sensitivity**. *PLOS Computational Biology*, 2014.

Da Silva Figueiredo Celestino Gomes P., Panel N., Laine E., Pascutti P.G., Solary E., and Tchertanov L. **Differential effects of CSF-1R D802V and KIT D816V homologous mutations on receptor tertiary structure and allosteric communication**. *PLOS ONE*, 2014.

Vita M., Tisserand J.C., Chauvot de Beauchêne I., Panel N., Tchertanov L., Agopian J., Mescam-Mancini L., Fouet B., Fournier B., Dubreuil P., Bertucci F., and De Sepulveda P. **Characterization of S628N, a novel KIT mutation found in a metastatic melanoma**. *JAMA Dermatology*, 2014.

Book chapters

Panel N., Villa F., Opuu V., Mignon D., and Simonson T. **Computational Design of PDZ-Peptide Binding**, PDZ Mediated Interactions: Methods and Protocols, pages 237–255. Springer US, New York, NY, 2021.

Patents

Canu N., El Bachiri M., Nigro C., Panel N., Raghunathan G., Sharma R., Remaud-Siméon M., Bozonnet S., and André I. **Optimisation d'une polykétide synthase de type III pour la production de phloroglucinol**. *In preparation*.

Canu N., El Bachiri M., Nigro C., Panel N., Raghunathan G., Sharma R., Remaud-Siméon M., Bozonnet S., and André I. **Utilisation de polykétide synthases de type III de champignons Ascomycètes comme phloroglucinol synthases (FR2302961)**. Filed on april 2023 by Compagnie générale des établissements Michelin.

Canu N., El Bachiri M., Nigro C., Panel N., Raghunathan G., Sharma R., Remaud-Siméon M., Bozonnet S., and André I. **Utilisation de polykétide synthases de type III de cyanobactéries comme phloroglucinol synthases (FR2302963)**. Filed on april 2023 by Compagnie générale des établissements Michelin.

Oral Communications

Panel N., Cabeza de Vaca I., Ballante F., Aldin Kahlous N., Vasile S., and Carlsson J. Accurate modeling of gpcr-peptide complexes by combining homology modeling, machine learning, and molecular dynamics simulations. *7th iHuman Forum*, April 2022, ShanghaiTech University, Shanghai, China, Virtual Meeting, *invited speaker*.

Panel N., Vo D.D., Huebner H., Pacalon J., Matricon P., Gmeiner P., and Carlsson J. Design of GPCR agonists using free energy calculations. *ACS Fall 2020 National Meeting Exposition*, August 2020, Virtual Meeting.

Panel N. Computation protein design of the Tiam1 PDZ domain. *Seminar at Uppsala Biomedicinska Centrum - Jens Carlsson's group meeting*, November 2017, Uppsala, Sweden.

Panel N. Computational protein design of protein:peptide recognition. *5th workshop AMMIB - Atelier de Modélisation des Molécules d'Intérêt Biologique*, April 2017, Orsay, France.

Panel N. and Simonson T. Computation protein design of the Tiam1 PDZ domain. *Seminar at Pasteur Institute*, June 2016, Paris, France.

Panel N. and Simonson T. Peptide-PDZ recognition: designing peptide ligands to inhibit the tiam1 pdz domain. *4th workshop AMMIB - Atelier de Modélisation des Molécules d'Intérêt Biologique*, April 2016, Châtenay-Malabry, France.

Posters

Panel N., Aldin Kahlous N., Vo D.D., Hübner H., Stefanie K., Andreas L., Jan K., Pierre M., Pacalon J., Gmeiner P., and Carlsson J. Design of GPCR agonists by free energy calculations. *GGMM conference*, october 2021, Lille, France. **Best Poster Award**.

Panel N., Matricon P., Pacalon J., Zeifman A., and Carlsson J. Design of GPCR agonists using molecular docking and simulations. *ERNEST, COST CA19133, GPCR Pharmacology: Activation, Signalling and Drug Design*, october 2019, Belfast, Northern Ireland, UK.

Panel N., Mignon D., Chen X., Young J.S., Fuentes E.J., and Simonson T. Computational protein design of the Tiam1 PDZ domain. *GGMM conference*, may 2017, Reims, France.

Panel N. and Simonson T. Designing peptide ligands to inhibit the Tiam1 PDZ domain. *ISQBP President's Meeting*, june 2016, Bergen, Norway. **Best Poster Award**.

Guarracino Y.*, Langenfeld F., Panel N.*, and Tchertanov L. Extension of moneta to analysis of allosteric communication in protein-protein and protein-dna complexes. *Faraday Discussion 169*, may 2014, Nottingham, UK. **Best Poster Award**. *presenting authors.

Scholarships and grants

2020 Wenner-Gren foundations, travel grant

2014 IDEX - IDI 2014, Paris-Saclay, PhD scholarship

References

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