Vaitea Opuu
Inselstraße 22, 04103 Leipzig, Germany
07/08/1992 (30 yo), Tahiti, French Polynesia
vopuu@mis.mpg.de & vaiteaopuu@gmail.com

Current position

Dec 2020 / Dec 2022	**From self-reproduction to evolution in the RNA world** **Max Planck Institute** for Mathematics in the Sciences, Leipzig, Germany Advisor **Matteo Smerlak** *Origin of life, RNA hypothesis, RNA designs/structure, Generative models*

Education

Oct 2017 / Oct 2020	**PhD** in **Computational Protein Design**, École Polytechnique, France Thesis title: **Computational design of proteins en enzymes** Advisor **Thomas Simonson** Defense date: **29 October 2020** *Molecular Mechanics, Molecular Dynamics, Biased Sampling, Monte Carlo Algorithms, Dynamic programming, Sequence Analysis*
Sept 2015 / Sept 2017	**Master** in **Bioinformatics**, Université Paris Saclay, France *Biostatistics, Machine learning, Sequence Analysis, Graph Theory, String Algorithms*

Publication list

2023	Vaitea Opuu and Thomas Simonson. Enzyme redesign and genetic code expansion. *Protein Engineering, Design and Selection*, page gzad017, 2023
2023	Vaitea Opuu*, Giuliano* Nigro, Christine Lazennec-Schurdevin, Yves Mechulam, Emmanuelle Schmitt, and Thomas Simonson. Redesigning methionyl-trna synthetase for β-methionine activity with adaptive landscape flattening and experiments. *Protein Science*, 32(9):e4738, 2023
2023	Kuang-Yu Chen*, Jayaprakash Karuppusamy*, Mary B. O'Neill*, Vaitea Opuu, Bahin Mathieu, Sophie Foulon, Ibanez Pnd ablo, Lluis Quintana-Murci, Tatsuhiko Ozawa, Sylvie van der Werf, Philippe Nghe, Nadia Naffakh, Andrew Griffiths, and Catherine Isel. High-throughput droplet-based analysis of influenza a virus genetic reassortment by single-virus rna sequencing. *Proceedings of the National Academy of Sciences 2023-02-07 120(6): e2211098120*, 2023
2022	Vaitea Opuu, Nono SC Merleau, Vincent Messow, and Matteo Smerlak. Rafft: Efficient prediction of rna folding pathways using the fast fourier transform. *PLoS computational biology*, 18(8):e1010448, 2022
2020	Vaitea Opuu*, Young Joo Sun*, Titus Hou, Nicolas Panel, Ernesto J. Fuentes, and Thomas Simonson. A physics-based energy function allows the computational redesign of a pdz domain. *Scientific Reports*, 10(1):11150, 2020 (* co-first authors)
2020	Vaitea Opuu, Giuliano Nigro, Thomas Gaillard, Emmanuelle Schmitt, Yves Mechulam, and Thomas Simonson. Adaptive landscape flattening allows the design of both enzyme: Substrate binding and catalytic power. *PLOS Computational Biology*, 16(1):e1007600, 2020
2020	David Mignon, Karen Druart, Eleni Michael, Vaitea Opuu, Savvas Polydorides, Francesco Villa, Thomas Gaillard, Nicolas Panel, Georgios Archontis, and Thomas Simonson. Proteus software for physics-based protein design. *The Journal of Physical Chemistry Part A*, 2021
2017	Vaitea Opuu, Martin Silvert, and Thomas Simonson. Computational design of fully overlapping coding schemes for protein pairs and triplets. *Scientific Reports*, 7(1):15873, 2017

Book chapters

2021	Vaitea Opuu, David Mignon, and Thomas Simonson. Knowledge-based unfolded state model for protein design. In *Computational Peptide Science: Methods and Protocols*. Springer, 2021
2021	Nicolas Panel, Francesco Villa, Vaitea Opuu, David Mignon, and Thomas Simonson. Computational design of pdz-peptide binding. In *PDZ Mediated Interactions*, pages 237–255. Springer, 2021

Publications submitted or in preparation

2022	Vaitea Opuu and Helene Bret. CARNAGE: trained rna structure-in-sequence compression with graph neural networks. 2022, in preparation
2022	Giuliano Nigro*, Vaitea Opuu*, Christine Lazennec, Yves Mechulam, Emmanuelle Schmitt, and Thomas Simonson. Redesigning methionyl-trna synthetase for - methionine activity using adaptive monte carlo and experiments. 2022, in preparation

Other scientific contributions

2018	Nika Abdollahi, Alexandre Albani, Eric Anthony, Agnes Baud, Mélissa Cardon, Robert Clerc, Dariusz Czernecki, Romain Conte, Laurent David, Agathe Delaune, et al. Meet-u: educating through research immersion. *PLoS computational biology*, 14(3), 2018
2018	Vaitea Opuu, Martin Silvert, and Thomas Simonson. Computational design of fully overlapping coding schemes for portein pairs and triplets. *(proceeding of) advances in systems and synthetic biology*, page 97, 2018
2018	Vaitea Opuu and Helene Bret. Investigating graph neural network for rna structural embedding. *Machine Learning for Structural Biology Workshop, NeurIPS 2022*, 2022

Oral presentations

2022	CBI seminar at ESPCI, Paris, France
2022	MASIM workshop, Paris, France
2022	ABSCICON22, Atlanta, USA (remote)
2021	MASIM workshop, Lyon, France
2019	MASIM workshop, Paris, France
2019	3rd Junior Conference on Computational Biology, Orsay, France
2019	AMMIB workshop, Gif-sur-yvette, France
2019	Seminar at Université Paris-Diderot, Paris, France
2018	17th advances in Systems and Synthetic Biology, Every, France

Computer skills

Compiled lang.	C, Java, fortran
Scripting lang.	Python, Perl, sh (bash,csh,awk...), R, Matlab, Haskell, Elisp
Markup lang.	Html, Org mode, LaTeX

Contributions to software developments

Proteus	`https://proteus.polytechnique.fr`
RAFFT	`https://github.com/strevol-mpi-mis/RAFFT`

Experimental collaborators

Project type	Collaborators	Affiliation
Enzyme designs	Emmanuelle Schmitt, Yves Mechulam	Ecole Polytechnique, France
Protein designs	Ernesto Fuentes	University of Iowa, USA
Protein designs	Gilles Travé	University of Strasbourg, France
Enzyme designs	Etienne Jourdier, Carlos Nieto	IFP Énergies nouvelles, France
RNA designs	Philippe Nghe	Ecole Superieur de Physique et Chimie Industrielle, France

References

Dr Matteo Smerlak
(PostDoc Advisor)
Group leader, Structural of evolution
Max Planck Institute for Mathematics in the Sciences, Germany
`matteo.smerlak@mis.mpg.de`

Dr Philippe Nghe
(Theoretical/experimental collaborator)
Director, Laboratory of biophysics and evolution
Ecole Superieur de Physique et Chimie Industrielle, France
`philippe.nghe@espci.psl.eu`

Pr Thomas Simonson
(PhD Advisor)
Director, Structural Biology of the Cell Laboratory
École Polytechnique, Palaiseau, France
`thomas.simonson@polytechnique.edu`

Pr Georgios Archontis
(Computational collaborator)
Associate Professor in Theoretical and Computational Biophysics
Department of physics, University of Cyprus, Cyprus
`archonti@ucy.ac.cy`

Pr Yves Mechulam
(Experimental collaborator)
Associate Professor Structural Biology of the Cell Laboratory
École Polytechnique, Palaiseau, France
`yves.mechulam@polytechnique.edu`