Vaitea Opuu
6 rue Jean Calvin 75005, Paris, France
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Research positions

now / Dec 2022	**Machine learning applied to RNA** **UMR CNRS-ESPCI 8231 Chimie, Biologie Innovation**, Paris, France Advisor **Philippe Nghe** *Origin of life, RNA designs/structure, Generative models*
Dec 2022 / Dec 2020	**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: 8 articles, 6 first author, 1 corresponding

2023	**V. Opuu** and T. Simonson. Enzyme redesign and genetic code expansion. *Protein Engineering, Design and Selection*, 2023
2023	**V. Opuu***, G. Nigro*, C. Lazennec-Schurdevin, Y. Mechulam, E. Schmitt, and T. Simonson. Redesigning methionyl-trna synthetase for β-methionine activity with adaptive landscape flattening and experiments. *Protein Science*, 32(9):e4738, 2023
2023	K.-Y. Chen*, J. Karuppusamy*, M. B. O'Neill*, **V. Opuu**, B. Mathieu, S. Foulon, I. P. ablo, L. Quintana-Murci, T. Ozawa, S. van der Werf, P. Nghe, N. Naffakh, A. Griffiths, and C. 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	**V. Opuu**‡, N. S. Merleau, V. Messow, and M. Smerlak. Rafft: Efficient prediction of rna folding pathways using the fast fourier transform. *PLoS computational biology*, 18(8):e1010448, 2022
2020	**V. Opuu***, Y. J. Sun*, T. Hou, N. Panel, E. J. Fuentes, and T. Simonson. A physics-based energy function allows the computational redesign of a pdz domain. *Scientific Reports*, 10(1):11150, 2020
2020	**V. Opuu**, G. Nigro*, T. Gaillard, E. Schmitt, Y. Mechulam, and T. Simonson. Adaptive landscape flattening allows the design of both enzyme: Substrate binding and catalytic power. *PLOS Computational Biology*, 16(1):e1007600, 2020
2020	D. Mignon, K. Druart, E. Michael, **V. Opuu**, S. Polydorides, F. Villa, T. Gaillard, N. Panel, G. Archontis, and T. Simonson. Proteus software for physics-based protein design. *The Journal of Physical Chemistry Part A*, 2021
2017	**V. Opuu**, M. Silvert, and T. Simonson. Computational design of fully overlapping coding schemes for protein pairs and triplets. *Scientific Reports*, 7(1):15873, 2017

Book chapters

2021	**V. Opuu**, D. Mignon, and T. Simonson. Knowledge-based unfolded state model for protein design. In *Computational Peptide Science: Methods and Protocols*. Springer, 2021
2021	N. Panel, F. Villa, **V. Opuu**, D. Mignon, and T. Simonson. Computational design of pdz-peptide binding. In *PDZ Mediated Interactions*, pages 237–255. Springer, 2021

Publications submitted or in preparation

2023	M. Deyell*, **V. Opuu***, A. D. Griffiths, S. J. Tans, and P. Nghe. Global regulators facilitate adaptation to a phenotypic trade-off
2023	S. Wang, A. Alluzen, P. Nghe, and **V. Opuu**‡. One parameter-genotype model design for genotype-fitness maps

Other scientific contributions

2018	N. Abdollahi, A. Albani, E. Anthony, A. Baud, M. Cardon, R. Clerc, D. Czernecki, R. Conte, L. David, A. Delaune, et al. Meet-u: educating through research immersion. *PLoS computational biology*, 14(3), 2018
2018	**V. Opuu**, M. Silvert, and T. 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	**V. Opuu**‡ and H. Bret. Investigating graph neural network for rna structural embedding. *Machine Learning for Structural Biology Workshop, NeurIPS 2022*, 2022

Co-supervision of PhD students

Paul Dupuyds	advisor Philippe Nghe, starting date 2024
Shuhui Wang	advisor Philippe Nghe, starting date 2023

Teaching

Master	Master of Bioinformatics at **Sorbonne University** in Structural Biology (4 hours) and Meet-UE (7×2 hours)

Oral presentations

2023	Biological sequence variation school, Corsica, France
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 Philippe Nghe
(Postdoc advisor)
Principal investigator, 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 Alexandre Allauzen
(AI collaborator)
Professor, LAMSADE
ESPCI and Université Paris Dauphine, Paris, France
alexandre.allauzen@espci.psl.eu