

## Current position

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| Dec 2020 /<br>Dec 2022 | <b>From self-reproduction to evolution in the RNA world</b><br><b>Max Planck Institute</b> for Mathematics in the Sciences, Leipzig, Germany<br>Advisor <b>Matteo Smerlak</b><br><i>Origin of life, RNA hypothesis, RNA designs/structure, Generative models</i> |
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## Education

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

## Publication list

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|------|--|
| 2023 | Kuang-Yu Chen*, Jayaprakash Karuppusamy*, Mary B. O'Neill*, <u>Vaitea Opuu</u> , Bahin Mathieu, Sophie Foulon, Ibanez Pnd ablo, Lluís 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. <i>Proceedings of the National Academy of Sciences</i> 2023-02-07 120(6): e2211098120, 2023 |
| 2022 | <u>Vaitea Opuu</u> , Nono SC Merleau, Vincent Messow, and Matteo Smerlak. Rafft: Efficient prediction of rna folding pathways using the fast fourier transform. <i>PLoS computational biology</i> , 18(8):e1010448, 2022   |
| 2020 | <u>Vaitea Opuu</u> *, 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. <i>Scientific Reports</i> , 10(1):11150, 2020<br>(* co-first authors)  |
| 2020 | <u>Vaitea Opuu</u> , 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. <i>PLOS Computational Biology</i> , 16(1):e1007600, 2020  |
| 2020 | David Mignon, Karen Druart, Eleni Michael, <u>Vaitea Opuu</u> , Savvas Polydorides, Francesco Villa, Thomas Gaillard, Nicolas Panel, Georgios Archontis, and Thomas Simonson. Proteus software for physics-based protein design. <i>The Journal of Physical Chemistry Part A</i> , 2021  |
| 2017 | <u>Vaitea Opuu</u> , Martin Silvert, and Thomas Simonson. Computational design of fully overlapping coding schemes for protein pairs and triplets. <i>Scientific Reports</i> , 7(1):15873, 2017  |

## Book chapters

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

## Publications submitted or in preparation

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| 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

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| 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. <i>PLoS computational biology</i> , 14(3), 2018 |
| 2018 | Vaitea Opuu, Martin Silvert, and Thomas Simonson. Computational design of fully overlapping coding schemes for portein pairs and triplets. ( <i>proceeding of</i> ) <i>advances in systems and synthetic biology</i> , page 97, 2018                           |
| 2018 | Vaitea Opuu and Helene Bret. Investigating graph neural network for rna structural embedding. <i>Machine Learning for Structural Biology Workshop, NeurIPS 2022</i> , 2022   |

## Oral presentations

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|------|---|
| 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 | 3 <sup>rd</sup> Junior Conference on Computational Biology, Orsay, France |
| 2019 | AMMIB workshop, Gif-sur-yvette, France                                    |
| 2019 | Seminar at Université Paris-Diderot, Paris, France                        |
| 2018 | 17 <sup>th</sup> advances in Systems and Synthetic Biology, Every, France |

## Computer skills

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|-----------------|---|
| Compiled lang.  | C, Java, fortran  |
| Scripting lang. | Python, Perl, sh (bash,csh,awk...), R, Matlab, Haskell, Elisp |
| Markup lang.    | Html, Org mode, L <sup>A</sup> T <sub>E</sub> X               |

## Contributions to software developments

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| Proteus | <a href="https://proteus.polytechnique.fr">https://proteus.polytechnique.fr</a>                 |
| RAFFT   | <a href="https://github.com/strevol-mpi-mis/RAFFT">https://github.com/strevol-mpi-mis/RAFFT</a> |

## 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 Supérieur 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 Supérieur 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

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