

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 <i>Molecular Mechanics, Molecular Dynamics, Biased Sampling, Monte Carlo Algorithms, Dynamic programming, Sequence Analysis</i>
Sept 2015 / Sept 2017	Master in Bioinformatics , Université Paris Saclay, France <i>Biostatistics, Machine learning, Sequence Analysis, Graph Theory, String Algorithms</i>

Publication list

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. <i>Scientific Reports</i> , 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. <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, accepted
2020	Nicolas Panel, <u>Vaitea Opuu</u> , Francesco Villa, David Mignon, and Thomas Simonson. in <i>Methods in Molecular Biology: PDZ domains</i> . JP Borg. Springer Verlag, New York, 2020 (book chapter)
2017	Vaitea Opuu, 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

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. <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

Oral presentations

2019	MASIM workshop, Paris, France
2019	3 rd Junior Conference on Computational Biology, Orsay, France
2019	AMMIB workshop, Gif-sur-yvette, France
2019	Seminar at Université Paris-Diderot, Paris, France
2018	17 th 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, L ^A T _E X

Contributions to software developments

Proteus	https://proteus.polytechnique.fr
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References

Pr Thomas Simonson

(PhD Advisor)

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Pr Georgios Archontis

(Computational collaborator)

Associate Professor in Theoretical and Computational Biophysics

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Pr Yves Mechulam

(Experimental collaborator)

Associate Professor Structural Biology of the Cell Laboratory

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