
Education

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|--------------------------|---|
| 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

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| 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. <i>in 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

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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 |

Oral presentations

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| 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

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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 ^A T _E X |

Contributions to software developments

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| 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
Department of physics, University of Cyprus, Cyprus
archonti@ucy.ac.cy

Pr Yves Mechulam

(Experimental collaborator)

Associate Professor Structural Biology of the Cell Laboratory
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