ELODIE LAINE

MAITRESSE DE CONFÉRENCES

elodie.laine@sorbonne-universite.fr | http://www.lcqb.upmc.fr/laine/ | +33 (0)6 71 22 69 41

ORIGINAL ARTICLES IN INTERNATIONAL PEER-REVIEW JOURNALS

46 published or accepted research articles, 13 as first author, 15 as co-corresponding last or next-to-last author (supervised students or post-docs are underlined, the stars indicate corresponding authors).

46. Abakarova M., C. Marquet, M. Rera, B. Rost, and **E. Laine*** (**2023**). Alignment-based protein mutational landscape prediction: doing more with less. Gen Biol Evol *(accepted).* **doi:** 10.1101/2022.12.13.520259

45. Szatkownik A., Zea DJ., H. Richard* and **E. Laine*** (**2023**). Building alternative splicing and evolution-aware sequence-structure maps for protein repeats. *J. Struct. Biol.* 215:107997 **doi:** 10.1016/j.jsb.2023.107997

44. Nashed S., H. El Barbry, M. Benchouaia, A. Dijoux-Marechal, N. Ruiz Gutierrez, L. Gaulier, G. Chevreux, S. Le Crom, B. Palancade, F. Devaux, **E. Laine**, M. Garcia (**2023**). Functional mapping of N-terminal residues in the yeast proteome uncovers novel determinants for mitochondrial protein import. *PLOS Genetics* 19:e1010848 **doi:** 10.1101/2022.08.19.504527

43. Tsuboyama K., J. Dauparas, J. Chen, **E. Laine**, Y. Mohseni Behbahani, J. Weinstein *et al.* (**2023**). Mega-scale experimental analysis of protein folding stability in biology and protein design. *Nature* 1:11 **doi**: 10.1101/2022.12.06.519132

42. Mohseni Behbahani Y., P. Saighi, F. Corsi, **E. Laine*** and A. Carbone* (**2023**). LEVELNET to visualize, explore, and compare protein–protein interaction networks. *Proteomics* 2200159 **doi:** 10.1101/2021.07.31.453756

41. Mohseni Behbahani Y., **E. Laine*** and A. Carbone* (**2023**). Deep Local Analysis deconstructs protein-protein interfaces and accurately estimates binding affinity changes upon mutation. *Bioinformatics* 39:i544–i552 **doi:** 10.1101/2022.12.04.519031

40. Mohseni Behbahani Y., S. Crouzet, **E. Laine*** and A. Carbone* (**2022**). Deep Local Analysis evaluates protein docking conformations with locally oriented cubes. *Bioinformatics* 38:4505–4512 **doi:** 10.1101/2021.07.31.453756

39. Vicedomini R., J-P. Bouly, **E. Laine**, A. Falciatore and A. Carbone (**2022**) Multiple probabilistic models extract features from protein sequence data and resolve functional diversity of very different protein families. *Mol Biol Evol.* 39:msac070 **doi:** 10.1101/717249

38. Zea DJ., H. Richard* and **E. Laine***. (**2022**) ASES: Visualising evolutionary conservation of alternative splicing in proteins. *Bioinformatics* 38:2615-2616

37. Dequeker C., Y. M. Behbahani, L. David, **E. Laine***, and A. Carbone* (**2022**). From complete cross-docking to partners identification and binding sites predictions. *PLoS Comput Biol* 18: e1009825

36. Kryshtafovych A. *et al.* (**2021**) Modeling severe acute respiratory syndrome—coronavirus-2 proteins in the Critical Assessment of Structure Prediction-commons experiment. *Proteins* 89: 1987–1996

35. Zea DJ., S. Laskina, A. Baudin, H. Richard* and **E. Laine***. (**2021**) Assessing conservation of alternative splicing with evolutionary splicing graphs. *Genome Research* 31:1462-1473

34. Danko D. *et al.* (**2021**) A global metagenomic map of urban microbiomes and antimicrobial resistance. *Cell* 184:3376-3393.e17

33. Laine E.* and S. Grudinin* (**2021**). HOPMA: Boosting protein functional dynamics with colored contact maps. *J. Phys. Chem. B.* 125:2577–2588

32. Karami Y.*, P. Saighi, R. Vanderhaegen, S. Longhi, D. Gerlier, **E. Laine*** and A. Carbone* (**2020**) Predicting substitutions to modulate disorder and stability in coiled-coils. *BMC Bioinformatics* 21:1-20

31. Grudinin S.[+], **E. Laine**[+] and A. Hoffmann (**2020**) Predicting protein functional motions: an old recipe with a new twist. *Biophys. J.* 118:2513-2525 (+equal contributions)

30. Ait-hamlat A., DJ. Zea, A. Labeeuw, L. Polit, H. Richard* and **E. Laine***. (**2020**) Transcripts' evolutionary history and structural dynamics give mechanistic insights into the functional diversity of the JNK family. *J Mol Biol* 432:2121-2140.

29. Corsi F., R. Lavery, **E. Laine*** and A Carbone*. (**2019**) Multiple protein-DNA interfaces unravelled by evolutionary information, physico-chemical and geometrical properties. *PLoS Comput Biol* 16:e1007624

28. Lensink MF., G. Brysbaert, N. Nadzirin, S. Velankar, RAG. Chaleil, T. Gerguri *et al.* (**2019**) The CASP13-CAPRI experiment. *Proteins: Structure, Function, and Bioinformatics* 87: 1200-1221.

27. **Laine E.***, Y. Karami and A. Carbone*. (**2019**) GEMME: a simple and fast global epistatic model predicting mutational effects. *Mol Biol Evol.* 36:2604–2619

26. Dequeker C., **E. Laine*** and A. Carbone*. (**2019**) Decrypting protein surfaces by combining evolution, geometry, and molecular docking. *Proteins*. 87:952-965

25. Karami Y., T. Bitard-Feildel, **E. Laine*** and A. Carbone*. (**2018**) "Infostery" analysis of short molecular dynamics simulations identifies highly sensitive residues and predicts deleterious mutations*, Scientific Reports.* 8 :16126

24. Raucci R., **E. Laine**, A. Carbone. (**2018**) Local Interaction Signal Analysis Predicts Protein-Protein Binding Affinity. *Structure*. 26:905-915

23. Dequeker C., **E. Laine*** and A. Carbone*. (**2017**) INTerface Builder: A Fast Protein-Protein Interface Reconstruction Tool. *J Chem Inf Model.*, 57:2613-2617

22. **Laine E.** and A. Carbone. (**2017**) Protein social behaviour gives a stronger signal for protein partner identification than geometrical docking, *Proteins*, 85:137-154

21. Ripoche H.[+], **E. Laine**[+], N. Ceres and A. Carbone. (**2017**) JET2 Viewer: a database of predicted multiple, possibly overlapping, protein-protein interaction sites for PDB structures, *Nucl. Acids Res. (database issue)*, 45:D236-D242 (+equal contributions)

20. T. Delaveau, D. Davoine, A. Jolly, A. Vallot, J.O. Rouviere, A. Gerber, S. Brochet, M. Plessis, R. Roquigny, J. Merhej, T. Leger, C. Garcia, G. Lelandais, **E. Laine**, B. Palancade, F. Devaux and M. Garcia. (**2016**) Tma108, a putative M1 aminopeptidase, is a specific nascent-chain associated protein in *Saccharomyces cerevisiae*. *Nucl. Acids Res.*, 44:8826-8841

19. Champeimont R., **E. Laine**, S.-W. Hu, F. Penin and A. Carbone. (**2015**) Coevolution analysis of Hepatitis C virus genotypes to identify the structural and functional dependency network of viral proteins, *Sci. Reports*, 6:26401

18. **Laine E.*** and A. Carbone*. (**2015**) Local geometry and evolutionary conservation of protein surfaces reveal the multiple recognition patches in protein-protein interactions. *PLoS Comput Biol*, **11**: e1004580

17. Karami Y., **E. Laine*** and A. Carbone*. (**2015**) Dissecting protein architecture with communication blocks and communicating segment pairs. *BMC Bioinformatics*, 17:13

16. Couve S., C. Ladroue, **E. Laine**, K. Mahtouk, J. Guégan, S. Gad, H. Lejeune, M. Le Gentil, G. Nuel *et al.*. (**2014**) Genetic evidence of a precisely tuned dysregulation in the hypoxia signaling pathway during oncogenesis. *Cancer Research* 74:6554-64

15. Chauvot de Beauchêne I., A. Allain, N. Panel, **E. Laine**, A. Trouve, P. Dubreuil and L. Tchertanov. (**2014**) Hotspot mutations in KIT receptor differentially modulate its allosterically coupled conformational dynamics: impact on activation and drug sensitivity. *PLoS Comput Biol* 10:e1003749

14. Da Silva Figueiredo Celestino Gomes P., N. Panel, **E. Laine**, P.G. Pascutti, E. Solary and L. Tchertanov. (**2014**) Differential effects of CSF-1R D802V and KIT D816V homologous mutations on receptor tertiary structure and allosteric communication. *PLoS ONE* 9:e97519

13. Allain A., I. C. de Beauchêne, F. Langenfeld, Y. Guarracino, **E. Laine**, L. Tchertanov (**2014**) Allosteric pathway identification through network analysis: from molecular dynamics simulations to interactive 2D and 3D graphs. *Faraday discussions* 169:303-321

12. Lopes A., S. Sacquin-Mora, V. Dimitrova, **E. Laine**, Y. Ponty and A. Carbone. (**2013**) Protein-protein interactions in a crowded environment: an analysis via cross-docking simulations and evolutionary information. *PLoS Comput Biol.* 9:e1003369

11. Arora R., I.C. de Beauchene, J. Polanski, **E. Laine** and L. Tchertanov. (**2013**) Raltegravir flexibility and its impact on recognition by the HIV-1 IN targets. *J Mol Recognit.* 26:383-401

10. **Laine E.**, C. Auclair and L. Tchertanov. (**2012**) Allosteric Communication across the Native and Mutated KIT Receptor Tyrosine Kinase. *PLoS Comput Biol.* 8:e1002661

9. Ni X.[+], S. Abdel-Azeim[+], **E. Laine**[+], R. Arora, O. Osemwota, AG. Marcelin, V. Calvez, JF. Mouscadet and L. Tchertanov. (**2012**) *In silico* and *in vitro* Comparison of HIV-1 Subtypes B and CRF02_AG Integrases Susceptibility to Integrase Strand Transfer Inhibitors. *Adv Virol.* 2012:548657 ([+]equal contributions)

8. Selwa E., **E. Laine** and TE. Malliavin. (**2011**) Differential role of Calmodulin and Calcium ions in the stabilization of the catalytic domain of adenyl cyclase CyaA from *Bordetella pertussis*. *Proteins.* 80:1028-40

7. Serafin K., P. Mazur, A. Bak, **E. Laine**, L. Tchertanov, JF. Mouscadet, J. Polanski. (**2011**) Ethyl malonate amides: A diketo acid offspring fragment for HIV integrase inhibition. *Bioorg Med Chem.* 19:5000-5

6. **Laine E.***, I. Chauvot de Beauchêne, D. Perahia, C. Auclair, L. Tchertanov*. (**2011**) Mutation D816V alters the internal structure and dynamics of KIT cytoplasmic region: implications for dimerization and activation mechanisms. *PLoS Comput Biol.* 7:e1002068

5. **Laine E.**, L. Martínez, A. Blondel and TE. Malliavin. (**2010**) Activation of the edema factor of *Bacillus anthracis* by calmodulin: evidence of an interplay between the EF-calmodulin interaction and calcium binding. *Biophys J.* 99:2264-72

4. **Laine E.**, C. Goncalves, J. Karst, A. Lesnard, S. Rault, W.-J. Tang, TE. Malliavin, D. Ladant and A. Blondel. (**2010**) Use of allostery to identify inhibitors of calmodulin-induced activation of *Bacillus anthracis* edema factor. *Proc. Natl. Acad. Sci. U.S.A.* 107:11277-82

3. Martínez L., **E. Laine**, TE. Malliavin, M. Nilges and A. Blondel. (**2009**) ATP conformations and ion binding modes in the active site of anthrax edema factor: A computational analysis. *Proteins.* 77:971-83

2. **Laine E.**, A. Blondel and TE. Malliavin. (**2009**) Dynamics and energetics: a consensus analysis of the impact of calcium on EF-CaM protein complex.*Biophys. J.* 96:1249-63

1. **Laine E.**, JD. Yoneda, A. Blondel and TE. Malliavin. (**2008**) The conformational plasticity of calmodulin upon calcium complexation gives a model of its interaction with the oedema factor of *Bacillus anthracis*. *Proteins.* 71:1813-29

REVIEW ARTICLES IN INTERNATIONAL PEER-REVIEW JOURNALS

Laine E.[+], S. Eismann[+], A. Elofsson[+], S. Grudinin[+]. (**2021**) Protein sequence-to-structure learning: Is this the end (-to-end revolution)? *Proteins* 89:1770-1786 ([+]equal contributions)

Colas C., **E. Laine.** (**2020**) Targeting Solute Carrier Transporters through Functional Mapping. *Trends Pharmacol Sci.* 21:S0165-6147(20)30255-8.

Laine E., L. Martínez, D. Ladant, TE. Malliavin and A. Blondel. (**2012**) Functional Molecular Motions in Edema Factor of Anthrax Toxin: a Structural and Energetic Interplay to Target for Drug Design (review). *Toxins* 4:580-604

EDUCATION ARTICLE IN INTERNATIONAL PEER-REVIEW JOURNALS

N. Abdollahi, A. Albani, E. Anthony, A. Baud, M. Cardon, …., **E. Laine*** and A. Lopes*. (**2018**) Meet-U: Educating through research immersion. *PLoS Comput Biol.* 14:e1005992

BOOK CHAPTER

Laine E. (**2017**) Decrypting how protein move and change their shape. *published in Mathematical Biology And Biological Physics, edited by Rubem P. Mondaini.*

PATENTS

Tchertanov L., **E. Laine**, A. Allain and I. Chauvot de Beauchêne (**2013**) MOdular NETwork Analysis (MONETA) version 2.0. *IDDN.FR.001.020012.000.S.P.2014.000.31235*

Malliavin T.E., **E. Laine**, A. Blondel, D. Ladant, J. Karst, S. Rault and A. Lesnard (**2011**) Methods of identifying compounds that inhibit the activation of a biomolecule and methods of treatment using the compounds*. US Patent Application* n° 20110065782

LIST OF SELECTED TOOLS, WEB SERVERS AND DATABASES

I systematically make my developments available to the scientific community: http://www.lcqb.upmc.fr/laine/software.html. https://github.com/PhyloSofS-Team, http://www.lcqb.upmc.fr/AnalGenom/software.html.

Tools: **ASPRING** (**2023**), an efficient and versatile method for charting the alternative usage of protein repeats in evolution; **DLA-Ranker** (**2022**), an efficient geometric deep learning-based method for evaluating protein complex candidate conformations; **ThorAxe** (**2021**), an efficient and robust method for assessing alternative splicing evolutionary conservation; **PhyloSofS** (**2020**), a tool to infer plausible evolutionary scenarios for transcripts and model proteoform 3D structures; **HOPMA** (**2020**), an unsupervised method for boosting protein conformational dynamics; **INTerface Builder** (**2017**), a fast easy- to-use software to screen millions of protein complex structures and detect their interfaces; **JET2DNA** (**2020**), **dynJET2** (**2019**), and **JET2** (**2015**), a suite of methods to predict protein- and DNA-binding sites on protein surfaces and learn about their functions; **COMmunication MApping** (v2 in **2018**, v1 in **2015**), a method to dissect proteins dynamical architectures and identify sensitive residues; **MONETA** (**2012**), an original method to decipher allosteric communication across protein structures.

Web servers: **LEVELNET (2022)**, a user-friendly interactive tool to explore protein-protein interaction networks; **ASES** (**2022**), a versatile and interactive tool for assessing and visualising evolutionary conservation of alternative splicing in proteins; **GEMME** (**2019**), a fast, scalable, and interpretable method to predict mutational landscapes from natural sequences.

Database: **ThorAxe KB** (**2021**), a knowledge base of alternative transcripts and their differential expressions across species and tissues; **JET2 Viewer** (**2017**), a very large knowledge base of protein binding sites.

ARTICLES SELECTED IN INTERNATIONAL PEER-REVIEW CONFERENCES

Mohseni Behbahani Y., **E. Laine*** and A. Carbone* (**2023**). Deep Local Analysis deconstructs protein-protein interfaces and accurately estimates binding affinity changes upon mutation. *The 31st Annual Intelligent Systems For Molecular Biology and the 22nd Annual European Conference on Computational Biology, published in Bioinformatics 39:i544–i552.*

Mohseni Behbahani Y., **E. Laine*** and A. Carbone* (**2022**). Deep Local Analysis estimates effects of mutations on protein-protein interactions *Machine Learning in Structural Biology workshop at the thirty-sixth Conference on Neural Information Processing Systems Meeting (NeurIPS), New Orleans, USA*

Mohseni Behbahani Y., **E. Laine*** and A. Carbone* (**2021**). DLA-Ranker: Evaluating protein docking conformations with many locally oriented cubes. *Machine Learning in Structural Biology workshop at the thirty-sixth Conference on Neural Information Processing Systems Meeting (NeurIPS), online.*

ORAL COMMUNICATIONS WITH PROCEEDINGS

Laine E., H. Ripoche and A. Carbone. (**2016**) Local geometry and evolutionary conservation of protein surfaces reveal the multiple recognition patches in protein-protein interactions *60th Annual Meeting of the Biophysical-Society, Los Angeles, CA, USA, published in Biophys J.* 110:S347A-348A

Laine E. and A. Carbone. (**2013**) Identification of protein interaction partners from shape complementarity molecular cross-docking. *New Trends in Image Analysis and Processing - ICIAP 2013, Naples, IT, published in LNCS* 8158:318-325

Laine E., I. Chauvot de Beauchêne, C. Auclair and L. Tchertanov. (**2011**) Propagation of D816V/H mutation effects across KIT receptor. *8th European Biophysics Congress*, August 23-27 2011, Budapest, HN, *published in Eur. Biophys. J. Biophys. Lett.* 40:S109

Laine E., JD. Yoneda, A. Blondel & TE. Malliavin. (**2009**) The Residue Network Architecture of a Protein-Protein Complex Reveals the Linkage between Dynamics and Energetics. *Biophysical Society 53rd Annual Meeting*, Feb. 28. - March 4 2009, Boston, MA, USA, *published in Biophys. J.* 96:S585a

Laine E., J. Huguenin & TE. Malliavin. (**2007**) Analysis of the calcium-dependent activation of the anthrax oedema factor by calmodulin. *6th European Biophysical Congress*, July 14-19, London, UK, *published in Eur. Biophys. J.* 36:S107

INVITED SEMINARS IN CONFERENCES, WORKSHOPS, AND SCHOOLS

13 in total, 7 in international events.

- Deciphering the multiplicity of protein surface usage (**2022**) *Nobel Symposium NS #184*, Stockholm, S
- Deciphering protein sequence variations' functional outcomes (**2021**) *Artificial Intelligence and Structural Biology Workshop*, CIRM, Marseille, FR
- Lessons from Protein Evolution: from Sequences through Structures to Functions, and back (**2021**) *Plenary Annual Meeting of the GDR Molecular Bioinformatics*, Lyon, FR
- Machine learning in the post CASP14 era : from protein structure to protein interactions (**2021**) *algoSB Winter School*, CIRM, Marseille, FR (seminar + hands-on)
- Mutational scanning predictions (**2021**) *INDEPTH Training School on Protein-Protein Interactions,* Warsaw (online), PL (seminar + hands-on)
- Protein sequence-structure-dynamics-function relationships: efficient tools for mining experimental and simulated data (**2020**) *PDCLifeS workshop of EURO-PAR 2020*, online
- Prediction d'effets de mutations à partir de l'histoire évolutive des protéines (**2019**) *Evolution à Paris monthly meeting*, Paris, FR
- Learning about protein-molecules interactions (**2017**) *MASIM kick-off meeting*, Paris, FR
- Modeling protein-protein interactions at large scale (**2017**), *Première journée de Biologie Structurale à l'UPMC*, Paris, FR
- Protein infostery : a new way to look into protein motions to predict deleterious mutations (**2016**), *16th International Symposium on Mathematical and Computational Biology*, Chern Institute of Mathematics, Nankai University, Tianjin, CN
- Protein evolution and structural dynamics (**2014**) *Journée MESU*, invited by P. Frey, ICS, Paris, FR
- Etude des mécanismes d'activation de cibles thérapeutiques & recherche d'inhibiteurs (**2011**) *Congrès GGMM 2011*, **as the recipient of the GGMM award**, La Rochelle, FR
- Use of allostery to identify inhibitors of calmodulin-induced activation of *Bacillus anthracis* Edema Factor (**2010**) *EMBO Practical Course on Biomolecular Simulation*, Institut Pasteur, Paris, FR (seminar)

ORGANISATION OF SCIENTIFIC MEETINGS

11 in total, 5 at the international level.

- **LEGO First Research Day, Machine Learning for Genomics (2023),** kickoff meeting of a French national working group (90 participants), Paris, FR. Session Chairperson, Scientific Committee Member, Fund Raiser, and Local Chairperson
- **Interplay between AI and mathematical modelling in the post-structural genomics era (2023)**, international workshop (70 participants), CIRM, Marseille, FR. Session Chairperson, Scientific Committee Member, Fund Raiser, and Local Chairperson
- **UPMC Young Researchers' Meeting: Modeling Complex Biological Systems, 2nd edition (2023)**, meeting day for student and post-doc at Sorbonne Université (30 participants), Paris, FR. Session Chairperson, Scientific Committee Member, Fund Raiser, and Local Chairperson
- **New directions of AI in structural biology** (**2021**), international workshop (35 participants), FR. Session Chairperson, Scientific Committee Member, and Local Chairperson
- **Integrative structural modeling in the era of big data and artificial intelligence** **(2021)**, mini-symposium at the *French Society for Bioinformatics* annual meeting (80 participants), online. Session Chairperson and Scientific Committee Member
- **Meet-4EU+ Symposium** (**2021**), international symposium mixing education and research (100 participants), online. General Chairperson

- **Noncanonical amino acids (ncAAs): tools for biological and biophysical investigations** (**2019**), international symposium (100 participants), Paris, FR. Session Chairperson and Scientific Committee Member
- **Meet-U Symposium** (**2018**), symposium mixing education and research (120 participants), Paris, FR. Session Chairperson, Scientific Committee Member, Fund Raiser, and Local Chairperson
- **UPMC Young Researchers' Meeting: Modeling Complex Biological Systems, 1st edition** (**2017**), meeting day for student and post-doc at Sorbonne Université (60 participants), Paris, FR. Session Chairperson, Scientific Committee Member, Fund Raiser, and Local Chairperson
- **Formal methods in the eyes of biological data (2017)**, symposium at the *French Society for Applied Mathematics* meeting, (35 participants), Ronce-les-Bains, FR. Session Chairperson, Scientific Committee Member, and Fund Raiser
- **Evolution of alternative splicing (2015)**, international symposium at the *Society for Molecular Biology and Evolution* annual congress, (70 participants), Vienna, AU. Session Chairperson and Scientific Committee Member

ORGANISATION OF SUMMER SCHOOLS

- **AI for biologists** (**2022**) *i-Bio* initiative for interfaces between biology and other disciplines, July 25-29 **2022**, Banyuls-sur-Mer, FR. Executive chair, fund raiser, and teacher
- **Scientific Trends at the Interfaces – Bioinformatics and Visualization** (**2017**), *Institut des Sciences du Calcul et des Données*, Roscoff, FR. Program Committee Member and teacher
- **Scientific Trends at the Interfaces – Bioinformatics and Visualization** (**2014**), *Institut du Calcul et de la Simulation*, Roscoff, FR. Program Committee Member and teacher

ORAL PRESENTATIONS (SELECTED)

16 total, 10 in international events.

- Evolutionary splicing graphs for matching non-globular protein sequences nd describing protein repeats alternative usage in evolution (**2023**), **Best talk award,** *1st meeting of the ML4NGP COST Action*, Bratislava, SK
- Evolutionary decomposition and structural characterization of functionally distinct protein isoforms (**2019**) *MASIM colloquium @BIM meeting days,* Paris, FR
- Meet-U: education through research immersion (**2019**) *ISMB-ECCB 2019*, Basel, CH
- Towards a large-scale prediction of protein partners (**2017**) *MAPPING conference – Understanding protein interactions: from molecules to organisms*, Lyon, FR
- The impact of alternative splicing evolution on protein structure and conformational dynamics (**2017**) *1st qBio mini-Workshop*, Milan, IT
- Accurately predicting and dissecting protein-protein interfaces with Joint Evolutionary Trees (**2014**) *Bringing Maths to Life Meeting*, Naples, IT
- A Modular Network Analysis (MONETA) of Protein Structures for Exploring and Predicting Allosteric Communication (**2012**) *JOBIM 2012*, Rennes, FR
- Propagation de perturbation à travers les structures protéiques : le récepteur tyrosine kinase KIT (**2011**) *Atelier Modélisation Gros Grains des Système Biologiques*, Paris, FR
- Role of Mutation D816V in the deregulation of KIT receptor: hypotheses & perspectives (**2011**) *Modeling and Beyond, 2nd ENSC-Schrödinger Meeting/Workshop*, Cachan, FR
- Mutation D816V alters the internal structure and dynamics of KIT cytoplasmic region (**2011**) *CECAM Dynamics and Thermodynamics of Biomolecular Recognition*, Palaiseau, FR
- Effect of the D816V mutation on c-Kit kinase domain: implications for the receptor molecular recognition (**2010**) *1st Aegean International Conference on Molecular Recognition*, Heraklion, GR
- Structural mobility of the anthrax toxin and search for inhibitors (**2009**) *MGMS Annual Molecular Modelling Workshop*, Erlangen, DE
- Mobilité Structurale de la Toxine de l'Anthrax et Recherche d'Inhibiteurs (**2009**) *16ème Congrès Annuel du GGMM*, Mittelwihr, FR

- Modeling the effect of Ca^{2+} through the residue network of the complex between EF and calmodulin (**2008**) *Computer Simulation and Theory of Macromolecules*, Hünfeld, DE
- The conformational plasticity of CaM upon Ca^{2+} complexation gives a model of its interaction with EF (**2008**) *CCPB Annual Conference: frontiers of biomolecular simulation*, Bristol, UK
- Analyse de l'activation de facteur oedémateux de Bacillus anthracis par dynamique moléculaire (**2007**) *Atelier Modélisation Gros-Grains pour la Biologie et la Matière Molle*, Evry, FR

POSTER PRESENTATIONS IN INTERNATIONAL CONFERENCES (SELECTED)

- Deep Local Analysis deciphers protein-protein interfaces (**2022**) *Critical Assessment of Protein Structure Prediction (CASP 15 meeting)*, Antalya, TR
- DLA-Ranker: Evaluating protein docking conformations with many locally oriented cubes (**2021**) *Machine Learning for Structural Biology Workshop at the Thirty Fifth Conference on Neural Information Processing Systems (NeurIPS)*, online
- Assessing conservation of alternative splicing with evolutionary splicing graphs (**2021**) *CSHL Virtual Meeting: Eukaryotic mRNA Processing*, online
- GEMME: a simple and fast global epistatic model predicting mutational effects (**2019**) *ISMB-ECCB 2019*, Basel, CH
- Decrypting protein surfaces using evolutionary information, geometry and docking (**2019**) *7th CAPRI evaluation meeting*, Cambridge, UK
- Local geometry and evolutionary conservation of protein surfaces reveal the multiple recognition patches in protein-protein interactions (**2016**) *6th CAPRI evaluation meeting,* Tel-Aviv, IL
- Accurate prediction of protein-protein contacts: from patches to sites (**2013**) *ISMB/ECCB Conference,* Berlin, DE
- Propagation of point mutation effect throughout tyrosine kinase c-Kit structure, probed by MD (**2010**) *2nd NaBi Workshop, CNRS-Weizmann*, Annecy, FR
- Propagation of point mutation effect throughout tyrosine kinase c-Kit structure, probed by MD (**2010**) *TAGp 2010*, Annecy-le-Vieux, FR
- Analysis of the activation of the edema factor of *Bacillus anthracis*, probed by molecular dynamics (**2006**), *20th Pasteur Weizmann Symposium: Structural Biology*, Paris, FR

INVITED SEMINARS

- Assessing the impact of sequence variations on protein functioning (**2023**), *IBENS seminar*, *Ecole Normale Supérieure*, invited by A. Lambert, Paris, FR
- Assessing the impact of sequence variations on protein functioning (**2023**), *LAAS seminar*, invited by J. Cortes, Toulouse, FR
- Assessing the impact of sequence variations on protein functioning (**2023**), *Biology Department seminar*, *University of Copenhagen*, invited by K. Lindorff-Larsen, Copenhagen, DK
- Deep local analysis for decrypting protein-protein complexes (**2023**), *bioinformatics seminar, University Paris Saclay,* invited by F. Jay, Saclay, FR
- High-throughput computational assessment of the functional impact of protein sequence variations (**2022**) *CaSToRC HPC National Competence Center Seminar Series,* The Cyprus Institute, invited by S. Erotokritou, online, CY
- Deep local analysis for assessing protein complexes and the effects of mutations at their interfaces (**2022**) *SAD-ABI seminar*, National Museum of Natural History, invited by M. Carpentier, Paris, FR
- Assessing conservation of alternative splicing with evolutionary splicing graphs (**2022**) *CRISTAL team seminar*, invited by J.-S. Varré, Lille, FR
- Functional protein sites deciphered by evolution and conformational dynamics (**2020**) *Genopole seminar*, invited by C. Maroun, Evry, FR
- Functional protein sites deciphered by evolution and conformational dynamics (**2020**) *Structural Biology Institute seminar*, invited by S. Grudinin, Grenoble, FR

- Functional protein sites deciphered by evolution and conformational dynamics (**2019**) *Guest lecture at University of Vienna/MolTag Doctoral Program*, invited by C. Colas, Vienna, AU
- Modeling protein-protein interactions at large scale (**2018**) *Séminaire CMLA*, invited by L. Tchertanov, CMLA, Cachan, FR
- Protein evolution and structural dynamics (**2015**) *Séminaire EMC2*, invited par Y. Maday, April 24, LIP6, Paris, FR
- Méthodes de modélisation moléculaire pour extraire des réseaux fonctionnels de résidus dans les protéines (**2013**) *Séminaire Math-Bio*, invited by V. Milisik LAGA, Paris 13, FR
- Mécanismes d'activation des récepteurs tyrosine kinases par des mutations oncogènes (**2011**) *Séminaire LERMIT*, invited by R. Fischmeister, UMR-S 769, Châtenay-Malabry, FR
- Modeling the regulatory impact of cancer mutation on c-Kit kinase structure, dynamics and stability (**2010**) *Séminaire LBT*, invited by S. Sacquin-Mora, LBT, IBPC, Paris, FR
- Interview at D.E. Shaw Research (**2010**) invited by Y. Shan, New York, NY, USA
- Mobilité structurale de la toxine de l'anthrax et recherche d'inhibiteurs (**2008**) *Séminaire 3Bio*, invited by M. Marchi, CEA de Saclay, FR

INTERNAL OR WORK GROUP SEMINARS

- All letters are not equal, *IBPS Day*, Dec 6, **2018**, Paris, FR
- Protein social behaviour makes a stronger signal for partner identification than surface geometry, *6th MAPPING Meeting*, Jan. 25 **2016**, Lyon, FR
- Wait and see: JET2 false positives are true positives, *5th MAPPING Meeting*, July 3 **2015**, Paris, FR
- The geometry of protein-protein interfaces reveals the multiple origins of recognition patches, *Séminaire Institut de Biologie Paris-Seine*, March 27 **2015**, IBPS, Paris, FR
- Accurately predicting and dissecting protein-protein interfaces with Joint Evolutionary Trees, *4th MAPPING Meeting*, Dec 3 **2014**, Lyon, FR
- Accurate prediction of protein-protein contacts with JET: from patches to sites, *3rd MAPPING Meeting*, May 6 **2014**, Paris, FR
- Identification of protein interaction partners from shape complementarity molecular docking, *2nd MAPPING Meeting*, Sept. 16 **2013**, Lyon, FR
- Predicting protein binding patches by combining evolutionary signals, physico-chemical and structural properties, *Kickoff Meeting of the MAPPING Project*, Jan. 23 **2013**, Paris, FR
- Mobilité structurale de la toxine de l'anthrax et recherche d'inhibiteurs, *Journées Dép. de Biologie Structurale et Chimie*, Institut Pasteur, Dec. 13-14 **2007**, Paris, FR

REVIEWING ACTIVITIES

- Member of the hiring committees for 2 Associate Professor positions (**2023, 2017**) France.
- PhD jury member in 17 committees, 8 as reviewer and 7 as examiner (**since 2019**), Europe.

Javier Gonzales-Delgado, Oct. 12 **2023**, Université Paul Sabatier, FR, ***reviewer***
Matteo Cagiada, Oct. 3 **2023**, University of Copenhagen, ***reviewer (opponent)***
Salomé Nashed, July 17 2023, Sorbonne University, FR, ***invited***
Adam Abellaïche, April 21 **2023**, University Paris Cité, FR, ***examiner***
Antoine Villié, March 31 **2023**, University Claude Bernard Lyon 1, FR, ***reviewer***
Ilyes Hamitouche, March 29 **2023**, Sorbonne University, FR, ***examiner***
Hélène Bret, March 27 **2023**, University Paris-Saclay, FR, ***reviewer***
Luc Blassel, Dec. 2 **2022**, Sorbonne University, FR, ***examiner***
Cyril Malbranke, Nov. 30 **2022**, Ecole Normale Supérieure, FR, ***reviewer***
Paul de Boissier, Oct. 24 **2022**, University of Aix Marseille, FR, ***reviewer***
Zineb Belkacemi, July 6 **2022**, Ecole des Ponts, FR, ***examiner***
Nicolas Guillaudeux, Dec. 16 **2021**, University of Rennes, FR, ***reviewer***
Dina El Adhab, Oct. 18 **2021**, Sorbonne University and University Saint-Joseph of Beyrouth, FR, ***examiner***
Nicolas Scalzitti, Sept. 29 **2021**, University of Strasbourg, FR, ***reviewer***
Irène Pitard, Oct. 23 **2020**, Sorbonne University, ***invited***
Guillaume Pagès, Sept. 12 **2019**, University of Grenoble Alpes, FR, ***examiner***
Akhila Melarkode Vattekatte, March 25 **2019**, University of Reunion Island, FR, ***examiner***

- Program Committee Member to 6 international conferences (**since 2019**): Intelligent Systems for Molecular Biology ISMB (2019-2023), WABI (2021-2023), ACM-BCB 2019.
- Reviewer for 6 grant applications to French and European agencies (**since 2018**): French National Research Agency (France), the Austrian Science Fund (Austria), the Biotechnology and Biological Sciences Research Council (BBSRC, United Kingdom), the Medical Research Council (MRC, United Kingdom), the Israel Science Foundation (ISF, Israel) and Partnership for Advanced Computing in Europe (PRACE, Europe).
- Reviewer for top international journals in biochemistry and molecular biology (**since 2015**): *Nucleic Acids Research*, *Molecular Biology and Evolution*, and in bioinformatics and computational biology: *Bioinformatics* and *PLOS Computational Biology*, among others.

DIFFUSION OF SCIENTIFIC CULTURE

- **Participation to articles for the general public** in La Recherche (07/2021, 08/2022), Sciences et Vie Junior (11/2021), Sciences et Avenir (01/2022, 04/2021), Sciences et Vie (08/2021), and in the Data Analytics Post (01/2021)
- **Sharing of experience with young women,** Sorbonne Université and Rêv'Elles, 11 Feb. 2021, online
- **Participation to the design of a** video for the general public**,** realized by La Bande Destinée (2019)
- **Sharing of experience with high school students,** Institut Henri Poincaré, 17 Dec. 2015, Paris, FR

PARTICIPATION IN PHD COMMITTEES

Nagi Debbah (Oct. 2023, Oct. 2022), Alexandre Detruit (July 2022), Lilian Marchand (July 2022), Barthélémy Meynard (Jan. 2023, Oct. 2021), Adam Bellaïche (Oct. 2022 and July 2021), Blandine Baudon (June 2022 and May 2021), Martin Romei (Oct. 2020 and Sept. 17 2019), Kai Shimagaki (Jan. 2021 and Nov. 2019), Chloé Quignot (July 2019).