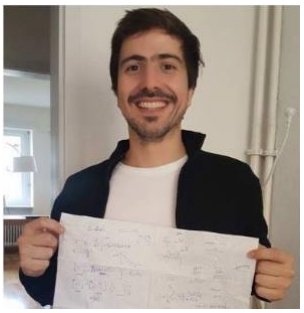
Z. Faidon Brotzakis
Doctor of Philosophy



Institute of Bioinovation (IBI)
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Place of birth: Athens, Greece
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PROFLE

My field of expertise is computational biophysics by utilizing principles of statistical physics and machine learning. In biology, the function or misfunction of the cell attributed to disease is greatly manifested as (de)regulation of molecular reactions occurring at the level of biomolecules such as DNA, RNA and proteins. To be able to understand and control such a molecular microverse against disease, I develop and use state of the art computational chemistry/biology methods based on statistical physics, machine learning and structural biology falling under the specific scientific disciplines:

- **Protein dynamics**: By development and use of Enhanced Sampling-based Molecular Dynamics (Transition Path Sampling, Metadynamics)
- **Integrative Structural Biology** by integrating experimental data (Cryo-EM, NMR and transition rate constants) or AlphaFold predictions into enhanced sampling (bio)molecular simulations that enable the swift determination of atomistic protein dynamics.
- **Computer Aided Drug Discovery** against disease, by using Molecular Simulations and Machine Learning.
- **Computational Protein Design** for targeted protein functions against disease, by combining Deep Learning and Molecular Simulations.

#computational biophysics, #statistical physics, #integrative structural biology, #machine learning, #molecular simulations, #enhanced sampling molecular dynamics #computational protein design, #computational chemistry, #computational biology, #physical chemistry, #chemical physics, #rare events, #host pathogen interactions, #misfolding disease, #antibodies, #fibrils, #protein plasticity, #protein-protein interactions, #drug discovery

WORK EXPERIENCE

Nov. 2023-Now	**Senior post-doctoral researcher**: Development of in-silico physics & machine learning based tools to design therapeutic and diagnostic protein binders. Host Institute: BSRC Fleming (Project member of the Boost4Bio EraChair consortium. Project ID: Grant Agreement No. 101087471, PI: G. Skretas)
Nov. 2023-Now	**Senior post-doctoral researcher** Visitor: University of Cambridge (PI: M. Vensruscolo)
Sept 2022- Oct 2023	**Bodossaki individual post-doc fellow**: Development of therapeutic and Diagnostic strategies against COVID-19 by combining cryo-electron microscopy with artificial intelligence. Host institute: University of Cambridge (PI: M. Vendruscolo) Collaborating institute: BSRC Al. Fleming (PI: G. Skretas).
May 2019- Aug. 2022	**FEBS individual post-doc fellow**: Novel therapeutic strategies based on

	the determination of the structure and dynamics of misfolded proteins using molecular simulations and CryoEM data. Host institute: University of Cambridge. Host PI: Prof. M. Vendruscolo.
March 2017-December 2018	**Post-doc**: Development of enhanced sampling molecular simulation rare-event methods for drug-discovery and protein folding. PI: Prof. Dr. M. Parrinello. ETH Zurich and Universita della Svizzera Italiana.

EDUCATION

Sept 2012 – Sept 2016	**PhD**: Computational Chemistry of Biomolecules. PhD title: Hydration layer dynamics and association mechanisms of food and antifreeze proteins. A Molecular Dynamics and Transition Path Sampling study. PI: Prof. Dr. P.G. Bolhuis. University of Amsterdam. (Project member of NanoNextNL consortium, PI: P. G. Bolhuis)
Sept 2006 – June 2012	**Majors degree** in Chemical Engineering, National Technical University of Athens (NTUA).
Sept 2011 – June 2012	**Diploma Thesis** in the Department of Materials Science of NTUA. Thesis title: *"Computational investigation of the significance of inherent structures in the dynamical behavior of glassy materials."* Scientific supervisor: Prof. dr. D.N Theodorou, National Technical University of Athens and Lecturer (470/80) Dr G.C Boulougouris, University of West Macedonia **. Grade 10/10.**
Sept 2009 - June 2011	**Academic studies** in chemical engineering at the NTUA in the direction of material science and engineering (equivalent to master).
Sept 2006 - June 2009	**Academic studies** in NTUA, Greece (university entering grade 17.7/20).

LIST OF PUBLICATIONS

38. Murtada Mhd. H., Brotzakis Z. F. , Vendruscolo M. (2024). Language Models for Molecular Dynamics. bioRxiv https://doi.org/10.1101/2024.11.25.625337 (under revision in Nature Machine Intelligence with reference number: NATMACHINTELL-A24123996)

37. Santabrogio A., Horne R. I., Metrick M., Brotzakis Z. F. et. al.(2024). Design of Potent Tau Aggregation Inhibitors Using Iterative Machine Learning and a Polymorph-Specific Brain-Seeded Fibril Amplification Assay. (under revision in Nature Computational Science with reference number: NATCOMPUTSCI-24-2775)

36. Tribello G.A.,Bonomi M. Bussi G., Caimloni C. et. al. (2024) PLUMED Tutorials: a collaborative, community-driven learning ecosystem, arXiv arXiv:2412.03595 (under revision in Journal of Chemical Physics)

35. Horne R.I., Andrzejewska, E.A., Alam P., Brotzakis Z.F. et. al. (2024). Discovery of potent inhibitors of α-Synuclein aggregation using structure-based iterative learning. Nature Chemical Biology, **20**, 634–645

34. Vendruscolo, M. Berzinova, M. Brotzakis, Z.F. et. al. (2024). Identification of high-affinity secondary nucleation inhibitors of Aβ42 aggregation from an ultra-large chemical library using Deep Docking. Researchsquare ,10.21203/rs.3.rs-4512167/v1 (under revision in Nature Machine Intelligence, reference number: NATMACHINTELL-A24051579A)

33. P. Karatzas, Z.F. Brotzakis, H. Sarimveis. (2024), Small molecules targeting the structural dynamics of AR-V7 partially disordered protein using deep learning and physics based models. bioRxiv https://doi.org/10.1101/2024.02.23.581804 (Under revision in JCTC)
32. D. Papadopoulou, et al. (2024), Discovery of the First-in-Class Inhibitors of Hypoxia Up-Regulated Protein 1 (HYOU1) Suppressing Pathogenic Fibroblast Activation. Angew Chem Int Ed, e202319157
31. Horne R. Wilson-Godber J., González Díaz A., Brotzakis Z.F.,Seal S., Gregory R., Possenti A., Chia S., Vendruscolo M. (2024) Using generative modelling to endow with potency initially inert compounds with good bioavailability and low toxicity. J. Chem. Inf. Model. 64, 590–596
30. Milanesi+, M. Brotzakis+, Z.F. Vendruscolo, M. (2024) Transient interactions between the fuzzy coat and the cross-β core of brain-derived Aβ42 filaments. bioRxiv https://doi.org/10.1101/2024.01.08.574772. *Accepted in Science Advances*
29. Horne R., Metrick M.A., Man W., Rinauro D.J., Brotzakis Z.F., Chia S., Meisl G. & Vendruscolo, M (2023). Secondary Processes Dominate the Quiescent, Spontaneous Aggregation of α-Synuclein at Physiological pH with Sodium Salts. *ACS Chem. Neurosci.* 14 (17), 3125-3131
28. Staats,R., Brotzakis Z.F., Chia S., Horne R.I. & Vendruscolo M. (2023). Optimization of a small molecule inhibitor of secondary nucleation in α-synuclein aggregation. *Front. Mol. Biosci.* 10, 1155753
27. Bolhuis P.G., Brotzakis Z.F., Keller B. (2023). Optimizing molecular potential models by imposing kinetic constraints with path reweighting *J. Chem. Phys.*159, 074102
26. Horne, R.I, Murtada, H.M. Donghui, H, Brotzakis, Z.F., Gregory, R.C. et al. (2023). Exploration and Exploitation Approaches Based on Generative Machine Learning to Identify Potent Small Molecule Inhibitors of α-Synuclein Secondary Nucleation. *J. Chem. Theory. Comput.* doi: 10.1021/acs.jctc.2c01303
25. Bhardwaj T, Gadhave K, Kapuganti S.K., Kumar P., Brotzakis Z.F. et al (2023). Amyloidogenic proteins in the SARS-CoV and SARS-CoV-2 proteomes. *Nat Communications* **14**, 945
24. Brotzakis Z. F., Zhang S. Murtada Mhd H., Vendruscolo M. (2023) AlphaFold Prediction of Structural Ensembles of Disordered Proteins. https://doi.org/10.1101/2024.11.09.622758. *Accepted in Nature Communications*
23. Sandler S.E., Horne R.I., Rocchetti S, Novak R., Hsu N-S, Cruz M.C., Brotzakis Z.F., Chia S., Bernardes G.J.L., Keyser U.F. & Vendruscolo M.(2023). Multiplexed Digital characterisation of Misfolded Protein Oligomers via Solid-State Nanopores. *J. Am. Chem. Soc.* 2023, 145, 47, 25776–25788
22. Brotzakis Z. F*. (2023) Guide for determination of protein structural ensembles by combining Cryo-EM data with metadynamics. *FEBS Open Bio* 13 (7), 1193-1203
21. Brotzakis Z. F., Löhr T. Truong S. Hoff S.E., Bonomi M & Vendruscolo M. (2023) Determination of the structure and dynamics of the fuzzy coat of an amyloid fibril of IAPP using cryo-electron microscopy. *Biochemistry*, 62, 16, 2407–2416
20. Mikolajek+ H, Weckener+M, Brotzakis+ Z.F., Huo J et. al. (2022) Correlation between binding affinity and the conformational entropy of nanobodies targeting the SARS-CoV-2 spike protein. *Proc Nat. Acad. Sci. USA*, 119 (31):e2205412119
19. Chia, S., Brotzakis, Z.F. Possenti, A.,Mannini, B., Cataldi, R.,Nowinska, M., Staats, R.,Linse, S., Knowles,T., Habchi, J. & Vendruscolo, MV. (2022). Structure-based discovery of small molecule inhibitors of the autocatalytic proliferation of α-synuclein aggregates. *Mol. Pharmaceutics*, 20, 1, 183–193
18. Brotzakis, Z.F., Lohr, T. & Vendruscolo, M.(2021), Determination of intermediate state structures in the opening pathway of SARS-CoV-2 spike using cryo-electron microscopy. *Chem Sci*, 12, 9168-9175.
17. Brotzakis Z.F., Lisdstedt P., Taylor R., Rinauro D. J., Gallagher N., Bernardes G. & Vendruscolo M. (2021) A structural ensemble of a tau-microtubule complex reveals regulatory tau phosphorylation and acetylation mechanisms. *ACS Central Sci*. 7 (12) 1986-1995
16. Brotzakis Z.F., Vendruscolo M. & Bolhuis P.G. (2021) A method of incorporating rate constants as kinetic constraints in molecular dynamics simulations, *Proc. Nat. Acad. Sci*. USA 118 (2) e2012423118
15. Bolhuis P.G., Brotzakis Z.F. & Vendruscolo M. (2021) A maximum caliber approach for continuous path ensembles, *European Phys. J.* B 94 (9),1-21
14. Brotzakis Z.F. & Bolhuis P.G. (2019) Approximating Committor and Free Energy Landscapes in standard Transition Path Sampling using Virtual Interface Exchange, *J. Chem. Phys.* 151 (17), 174111
13. Brotzakis Z.F. & Bolhuis P.G. (2019) Unbiased Atomistic Insight in the Mechanisms and Solvent Role for Globular Protein Dimer Dissociation *J. Phys. Chem. B* 123 (9), 1883-1895
12. Brotzakis Z.F., Mendels D. & Parrinello M. (2019) Augmented Harmonic Linear Discriminant Analysis, *arXiv* preprint arXiv:1902.08854
11. Brotzakis Z.F. & Parrinello M. (2019) Enhanced Sampling of Protein Conformational Transitions via Dynamically Optimized Collective Variables. *J. Chem. Theory Comput*. 15(2),1393-1398

10. Brotzakis Z.F., Limongelli V. & Parrinello M. (2019) Accelerating the Calculation of Protein-Ligand Binding Free Energy and Residence Times using Dynamically Optimized Collective Variables. *J. Chem. Theory Comput*. 15(1) 743-750
9. Mendels D., Piccini G.M., Brotzakis Z.F., Yang Y. & Parrinello M. (2018) Folding a Small Protein Using Harmonic Linear Discriminant Analysis. *J. Chem. Phys*. 149(19), 194113
8. Dutta R., Brotzakis Z.F. & Mira A. (2018) Bayesian Calibration of Force-fields from Experimental Data: TIP4P Water. J. Chem. Phys. 149: 154110
7. Brotzakis Z.F., Voets IK & Bolhuis PG (2018) Water Structure and Dynamics in the Hydration Layer of a Type III Anti-Freeze Protein. *Phys. Chem. Chem. Phys* 20: 6996-7006
6. Jagannath V., Brotzakis Z.F., Parrinello M., Walitza S. & Grunblatt E. (2017) Controversial Effects of D-Amino Acid Oxidase Activator (DAOA)/G72 on D-Amino Acid Oxidase (DAO) Activity in Human Neuronal, Astrocyte, and Kidney Cell Lines: The N-methyl D-Aspartate (NMDA) Receptor Hypofunction Point of View. *Front. Mol. Neurosci*. 10: 342
5. Brotzakis Z.F., Gehre M., Voets I.K. & Bolhuis P.G. (2017) Stability and Growth Mechanism of Self-Assembling Putative Antifreeze Cyclic Peptides. *Phys. Chem. Chem. Phys*. 19: 19032-19042
4. Brotzakis Z.F. & Bolhuis P.G. (2016) A One-Way Shooting Algorithm for Transition Path Sampling of Systems with Asymmetric Barriers. *J. Chem. Phys*. 145: 164112-12
3. Brotzakis Z.F., Groot C.C.M, Brandeburgo W.H., Bakker H.J. & Bolhuis P.G. (2016) Dynamics of Hydration Water around Native and Misfolded α-Lactalbumin. *J. Phys. Chem. B*. 120: 4756-4766

BOOK CHAPTERS AND CONFERENCE PROCEEDINGS

2. Book chapter: Z. F. Brotzakis*. (2024), Cryo-electron Microscopy and Molecular Modeling Methods to Characterize the Dynamics of Tau Bound to Microtubules. Methods in Molecular Biology, Springer 77–90
1. Conference proceedings: Hirakis S.,Venkatakrishnan V.,Brotzakis, Z. F. et.al. (2024). Where cryo-electron and computational microscopy converge: The story of the elusive flipback conformation of protein kinase A and its critical role in phosphodiesterase cyclic AMP channeling *Biophys. J.*123,3

TEACHING EXPERIENCE

2023-2024 Teaching: "In-silico Protein Design" lectures of the "*Protein and enzyme biotechnology*" course of the NKUA *Biotechnology masters* of the Biology department (winter semester)
2024-now Co-supervision of the master thesis of Kyriakos Lemonis in the context of the "*Biotechnology*" masters at the department of Biology of the NKUA, entitled "Computational design of inhibitors against the misfolding and problematic aggregation of the TDP-43 protein, involved in Amyotrophic Lateral Sclerosis disease."
2024-now Co-supervision of the master thesis of Eva Kladou in the context of the "*Biotechnology*" masters at the department of Biology of the NKUA, entitled "Computational design of inhibitors against the misfolding and problematic aggregation of the Huntingtin protein, involved in Huntington's disease."
2024-now Co-supervision of the master thesis of Iliana Ziori in the context of the "*Biotechnology*" masters at the department of Biology of the NKUA, entitled "Computational design of selective antibody binder inhibitors targeting distinct Tumor Necrosis Factor Receptors."
2022 Co-supervision of the master thesis of Michaela Brezinova at the Chemistry Department of the University of Cambridge, entitled "*Deep Docking: Pipeline optimization and case study on Aβ amyloid peptide*". Grade: 74%, leading to a submission in Nature Machine Intelligence.
2016 Co-supervision of the master thesis of Mascha Gehre at the HIMS of University of Amsterdam, entitled "Stability and self-assembly process of an anti-freezing nanotue", leading to a publication in the Journal of Physical Chemistry Chemical Physics, entitled "*Stability and Growth Mechanism of Self-Assembling Putative Antifreeze Cyclic Peptide*". Grade: 8.5/10
2016 Lab assistant, *"Molecular Simulations workshop (MolSim)",* University of Amsterdam.
2015 Lab assistant, *"Molecular Simulations workshop (MolSim)",* University of Amsterdam.
2015 Teaching assistant, *"Biomolecular Simulations"*, spring semester, University of Amsterdam.
2014 Lab assistant, *"Molecular Simulations workshop (MolSim)",* lab assistant, University of Amsterdam.
2014 Teaching assistant, *"Introduction to Thermodynamics"*, winter semester,University of Amsterdam.

GRANTS-AWARDS-HONOURS

Award	**Academy of Athens prize in Chemistry** (2023): "*G. Foteinos award for pioneering research published in distinguished journal in the field of Chemistry*". 1500 euro
Grant	**FEBS Excellence** (2023): Co-Principal Investigator with P. Santucci (PI @ CNRS Marseille) project "Molecular investigation of pyrazinamide action and resistance against tuberculous and environmental mycobacteria (MoNPyRATE)". 100 keuro
Fellowship	**Bodossaki individual post-doc fellowship** (2022-2023): "Development of therapeutic and diagnostic strategies against COVID-19 by combining cryo-electron microscopy with artificial intelligence". Department of Chemistry, University of Cambridge UK (host) & BSRC Fleming, GR (collaborating). 37.5 keuro
Award	**Poster Award**: "*Hellenic polymer society international conference"*, Athens, Greece 2021.
Fellowship	**FEBS individual post-doc fellowship** (2019-2022): *"Simultaneous Determination of the Structure and Dynamics of a Tau-Microtubule Complex"*, Department of Chemistry, University of Cambridge UK. 100 keuro
Travel grant	**Travel Grant**: *"Advanced Simulations for Biomolecular Research*" BioExcel 2nd SIG Meeting, Athens, Greece, 2018.
Fellowship	**HPC Europa-3 individual short visiting fellowship** (1/1/2019 - 31/3/2019) at BRFAA
Award	**Poster Award**: "*Nanocity 2015, the national event on nanotechnology*" conference, Amersfoort, Netherlands, 2015.
Distinction	**Article in the cover of the JCP special edition** "*Machine Learning Hits Molecular Simulations*": Bolhuis P.G., Brotzakis Z.F., Keller B. (2023). Optimizing molecular potential models by imposing kinetic constraints with path reweighting *J. Chem. Phys.*159, 074102
Distinction	**CASP16 challenge.** AlphaFold Metainference [https://doi.org/10.1101/2024.11.09.622758] was ranked 5th out of 35 participant teams in the CASP16 **"**Integrative modelling **"**challenge. (group ID:084)
Participation	Project member of Boost4Bio EraChair project ID: Grant Agreement No. 101087471 supporting my PostDoc funding.(PI: G. Skretas)
Participation	Project member of NanonextNL (2012-2016) supporting my PhD funding. (PI: P. G. Bolhuis)

COMPUTATIONAL GRANTS

Grant	**Amazon AWS resources, GRNET call** (2024): ID: **ResQPMDs,** equivalent budget of $45k.
Grant	**Amazon AWS resources, GRNET call** (2024): ID: **Cryo-EM Modellin**, equivalent budget of $347k.
Grant	**PRACE-ICEI 8th call computer-resource-time** (2022): grant project icp017 of 124000 nodehours equivalent budget of 20k euro.
Grant	**Preparatory project** for PRACE-ICEI 8th call computer-resource-time (2022).
Grant	**Preparatory project** n2010PA5371 for PRACE 8th call computer-resource-time (2020).

DISSEMINATION & OPENS SCIENCE

Workshop co-organizer	"Twin4Promis training workshop: Folding and misfolding of soluble and integral membrane proteins" 12-14 June 2024, NHRF, Athens, Greece
Summer school co-organizer	"Bioinnovation and bioentrepreneurship summer school", 7-11 June 2024, BSRC Fleming, Vari, Greece.
Open science	Method developed code and analysis scripts are publicly available in Github **.**
Open data	Data from publications are made publicly available in Zenobo and PlumedNest.
Dissemination	Personal website, with updated newsfeed on the new scientific publications, methods, conferences, workshops.
Dissemination	FEBS news interview **.**
Dissemination	Interview at Athens Macedonian News Agency https://www.amna.gr/home/article/785838/Kainotoma-protasi-beltionei-ti-gnosi-mas-gia-tis-spanies-domes-proteinon-me-efarmoges-stis-neuroekfulistikes-astheneies-kai-brabeuetai-apo-tin-Akadimia-Athinon
Dissemination	Interview at Dnews agency. https://www.dnews.gr/eidhseis/science/469571/i-sokaristiki-voitheia-tis-texnitis-noimosynis-stin-anakalypsi-farmakon-gia-to-parkinson

PDB databank submissions PDBID: 9A8E, 9A8E, 7PQC, 7PQP

Professional activity

2022-today **Reviewer** for ACS Journal of Chemical Theory and Computation, Journal Chemical Physics Letters.
2022-today **Reviewer** for Journal of Molecular Liquids.
2018-2021 **Member** of the Biochemical Society.
2022-today **Member** of the Hellenic Society of Biochemistry and Molecular Biology.

Scientific achievements

- 36 publications
- 1 book chapter
- 1 conference proceeding
- H-index: 16 (google scholar)
- i10-index: 23 (google scholar)
- 12 invited speaker presentations in conference
- 12 poster presentations in conferences
- 3 international post-doc fellowships
- 1 research grant as co-PI
- 5 computational grants
- 1 travel grant
- 17 courses/workshops
- 3 awards
- 2 distinction
- 2 participations in grants as consortium member.

CONFERENCES

2024 5th International Conference on Materials Science-Nanotechnology, Athens, GR ***invited speaker***
2024 7th Conference of Young Scientists Hellenic Pasteur Institute, ***speaker***
2024 Twin4Promis training workshop, NHRF, Athens, Greece, **invited speaker**
2024 Twin2Pipsa & Twin4Promis Twinned Training Schools, U. Cambridge, UK, **invited speaker**
2023 Annual Hellenic Society of Biochemistry and Molecular Biology conference, Athens GR, **invited speaker**
2023 Hbio. 3rd Hellenic Biocluster Forum**. poster presentation**
2022 Annual Hellenic Society of Biochemistry and Molecular Biology conference, Patras GR, **invited speaker**.
2022 "20 years of Metadynamics" CECAM meeting, Lausanne, Switzerland**, invited speaker.**
2022 "The Biochemistry Global Summit", Lisbon, Portugal. **poster presentation.**
2022 **"**5th FEBS fellows meeting", Vimeiro, Portugal**, invited speaker.**
2021 "ECR webinar series, Biochemistry focus, Computational biology and bioinformatics", Biochemical society **, invited speaker**.
2021 "*Computer Simulation and Theory of Macromolecules*" 2021, Hunfeld, Germany, **invited speaker**.
2021 "*18th Hellenic Symposium on Medicinal Chemistry*" 2021, **Invited speaker**.
2021 "*7th Annual meeting of the Centre of Misfolding Diseases*", CMD, Cambridge UK**, invited speaker**.
2021 "*Hellenic polymer society international conference"*, Athens, Greece 2021, **poster presentation**.
2019 "*Showcase week Theory symposium*", Department of Chemistry, University Cambridge, Cambridge UK, **chair.**
2019 "*6th Annual meeting of the Centre of Misfolding Diseases*", CMD, Cambridge UK**, invited speaker**.
2019 "5th Molecular and Chemical Kinetics workshop (MolKin2019)" Berlin, Germany, **poster presentation**.

2018 *"Advanced Simulations for Biomolecular Research"*, BioExcel 2nd SIG Meeting,Athens, Greece, **poster presentation**.
2018 "Multiscale simulations of allosteric regulatory mechanisms in cancer-associated proteins and signaling protein networks" CECAM workshop, Lugano, Switzerland, **poster presentation**.
2017 *"Structure Based Drug Discovery",* Lausanne, Switzerland, **poster presentation**.
2016 *"Nanocity 2016, the national event on nanotechnology",* Amsterdam, Netherlands **poster presentation**.
2016 *"Computer Simulations",* Gordon Conference, Girona, Spain **poster presentation**.
2016 "Dutch Molecular Dynamics day", Groningen, Netherlands, **co-organizer**.
2015 "*CHAINS, the Dutch chemistry conference*", Veldhoven, Netherlands, **invited speaker**.
2015 *"Nanocity 2015, the national event on nanotechnology",* Amersfoort, Netherlands **poster presentation**.
2015 *"Dutch Biophysics conference",* Veldhoven, Netherlands**, poster presentation**.
2014 *Physics@FOM, physics conference",* Veldhoven, Netherlands, **poster presentation**.

COURSES/WORKSHOPS

2024 Boost4bio summer school "Bioinnovation and entrepreneurship", BSRC Fleming, Vari, Greece.
2022 "Lost in Integration - Probing Biomolecules with Electrons, Photons, Neutrons and Magnetic Spins", Spetses, Greece.
2021 Centre of Misfolding Disease annual meeting, Cambridge, United Kingdom.
2021 *"Accelerating the Understanding of Rare Events"*, Leiden, Netherlands.
2021 *"Advances and challenges in biomolecular simulations", EMBO Virtual Workshop*
2020 *"Machine learning how to coarse grain", CECAM workshop, Mainz, Germany.*
2019 "Extended Software Development Workshop:Topics in Classical MD", Lyon, France.
2018 *"Colloid Assembly Engineering",* Riva del Garda, Italy.
2015 *"From trajectories to reaction coordinates: making sense of molecular simulation data"*, Vienna, Austria.
2015 *"Writing Scientific Proposals and Survival Guide for Peer Review workshop"*, Leiden, Netherlands
2014 *"Computer simulation and theory of macromolecules workshop"*, Hunfeld, Germany.
2013 *"Risk analysis and technology assessment"* course, NanonextNL course, Netherlands.
2013 *"Computational structural biology"* course, Amsterdam, Netherlands.
2013 *"Biomolecular Simulations"* course, Amsterdam, Netherlands.
2013 *"Molecular Simulations workshop (MolSim)",* poster presentation, Amsterdam, Netherlands.
2013 *"Methods in molecular simulations (CCP5) summer* school", poster presentation, Manchester,UK.
2012 *"Scientific programing in python"* course, Amsterdam, Netherlands.

RELEVANT SKILLS

Molecular simulations and modelling.

- PLUMED:
  Free energy enhanced sampling methods: Metadynamics, Umbrella Sampling, Hamiltonian Replica Exchange Molecular Dynamics, Reaction Coordinate optimization algorithms (VAC-MetaD, HLDA, Deep-LDA, Committor based, Path-Metadynamics).
- GROMACS:
  Free energy enhanced sampling methods: Free Energy Perturbation, Replica Exchange Molecular Dynamics, λ-dynamics.
  Coarse grained molecular dynamics: Martini, Vodka.
- Open Path Sampling:
  Path based enhanced sampling methods for kinetics: Transition Path Sampling, Transition Interface Sampling, spring-shooting TPS (developer), VIE-TPS (developer)
- Language Models for Molecular dynamics:
  GPT-based molecular dynamics

AI-based structure prediction and sequence design: AlphaFold, ESM, Inverse Folding, proteinMPNN
Homology modelling: Modeller, Swiss-Model.

Integrative structural biology methods.

- PLUMED:
  AlphaFold data: AlphaFold Metainference (developer)
  Cryo-EM data: Metadynamics Electron Microscopy MetaInference (MEMMI) (developer)

NMR data: Metadynamics Metainference

- Python-based:
  Rate constants-time dependent data: CoPE-MaxCal (developer)

Computational Protein Design. Inverse folding. Inverse folding molecular dynamics (developer)
Drug discovery methods.

- Binding site identification: Fpocket,SiteMap
- Virtual screening/molecular docking: Deep Docking (developer), Deep Ensemble Docking (developer) FRED, Autodock Vina, Glide, ensemble dockinng
- Toxicity estimation: Marvin Suite
- Deep Neural Networks: Python, tensorflow, pytorch, keras, matplotlib, scikitlearn, RDKIT
- Shallow learning: Gaussian process regression: Python, tensorflow, keras
- Clustering in chemical space: Butina, UMAP
- Lead optimization: FEP, λ-dynamics (PLUMED, GROMACS)
- Small molecule classical force field parametrisation: Gaussian, Antechamber

Other tools. Chimera, Modeller, VMD, Pymol, Coot, RosettaFold, MDTraj, Matlab, Gnuplot
Programming experience. Python,Fortran-90, C/C++, bash scripting, Matlab, Perl,tcl
Operating system. Microsoft operating systems, UNIX, MacOS
Office automation. Microsoft Office, Latex, Mendeley
Fluent in English. Certificate of Proficiency in English, 2010
Native speaker of Greek