ILIA IGASHOV
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EDUCATION

PhD in Computational Biology, École Polytechnique Fédérale de Lausanne, expected 2025
M.Sc. in Applied Mathematics, Université Grenoble Alpes, 2021
M.Sc. in Computer Science, Moscow Institute of Physics and Technology, 2021
B.Sc. in Applied Mathematics and Physics, Moscow Institute of Physics and Technology, 2019

CURRENT AND PREVIOUS SCIENTIFIC ACTIVITIES

11/2022 – 01/2023	Research Intern Monte Rosa Therapeutics, Basel, Switzerland Supervised by Pablo Gainza Development of machine learning algorithms for design of molecular glues
10/2021 – 10/2025 (ongoing)	PhD Student École Polytechnique Fédérale de Lausanne, Switzerland Supervised by Bruno Correia and Michael Bronstein Development of machine learning methods for drug discovery
02/2021 – 07/2021	Research Intern Laboratoire Jean Kuntzmann, Grenoble, France Supervised by Sergei Grudinin Development of group-equivariant neural networks for molecular data
11/2019 – 05/2020	Research Intern Inria, Grenoble, France Supervised by Sergei Grudinin Development of graph neural networks from protein model quality assessment

SCHOLARSHIPS AND AWARDS

2025	Spotlight Paper Award, ICLR 2025
2024	Spotlight Paper Award, ICLR 2024
2023	Community Grant, HuggingFace
2022	Travel Award: Keystone Symposia on Computational Design and Modeling of Biomolecules
2021 – 2025	EPFLglobaLeaders Doctoral Fellowship part of the EU Horizon 2020 research and innovation program, co-funded by the Marie Skłodowska-Curie Actions
2019	Inria Scholarship
2015 – 2019	Russian Government Scholarship for Undergraduate Students

PROFESSIONAL EXPERIENCE

05/2020 – 08/2021	Data Science Team Leader, PeakData (remote) Management of the data science team in the healthcare start-up aimed to gather and process information on medical topics

09/2018 – 10/2019 Software Engineer, Yandex, Moscow, Russia
Development of the music recommender system

03/2018 – 08/2018 Software Engineer, S7 Airlines, Moscow, Russia
Development of the frequent flyer loyalty platform

07/2017 – 08/2017 Summer Intern, Intel, Nizhny Novgorod, Russia
Implementation of machine learning algorithms in
Intel Data Analytics Acceleration Library

OTHER SCIENTIFIC ACTIVITIES

Co-organizer of Learning on Graphs Conference (LoG) local meetup in Lausanne, 2023
Co-organizer of Learning on Graphs Conference (LoG), 2022 and 2023
Co-organizer of AI & the Molecular World Track @ AMLD EPFL, 2022 and 2024

PUBLICATIONS

Schneuing, A.*, Igashov, I.*, Dobbelstein, A., Castiglione, T., Bronstein, M., & Correia, B. (2024). Multi-domain Distribution Learning for De Novo Drug Design. ICLR 2025. https://openreview.net/forum?id=g3VCIM94ke

Cretu, M., Harris, C., Igashov, I., Schneuing, A., Segler, M., Correia, B., Roy, J., Bengio, E., & Liò, P. (2024). SynFlowNet: Design of Diverse and Novel Molecules with Synthesis Constraints. ICLR 2025 Spotlight. https://openreview.net/forum?id=uvHmnahyp1

Schneuing, A.*, Igashov, I.*, Castiglione, T., Bronstein, M., & Correia, B. (2024) Towards Structure-based Drug Design with Protein Flexibility. In ICLR 2024 Workshop on Generative and Experimental Perspectives for Biomolecular Design.

Igashov I.*, Schneuing A.*, Segler M., Bronstein M., & Correia B. (2024). RetroBridge: Modeling Retrosynthesis with Markov Bridges. ICLR 2024 Spotlight. arXiv:2308.16212.

Igashov I., Stärk H., Vignac C., Satorras V. G., Frossard P., Welling M., Bronstein M., & Correia B. (2024). Equivariant 3D-conditional diffusion models for molecular linker design. Nature Machine Intelligence. https://doi.org/10.1038/s42256-024-00815-9

Khakzad H.*, Igashov I.*, Schneuing A.*, Goverde C., Bronstein M., & Correia B. (2023). A new age in protein design empowered by deep learning. Cell Systems, 14(11), 925-939.

Schneuing A., Du Y., Harris C., Jamasb A., Igashov I., Du W., Blundell T, Lió P., Gomes C., Welling M., Bronstein M., & Correia B. (2022). Structure-based drug design with equivariant diffusion models. Nature Computational Science. https://doi.org/10.1038/s43588-024-00737-x

Igashov, I., Jamasb, A. R., Sadek, A., Sverrisson, F., Schneuing, A., Lio, P., Blundell, T., Bronstein, M., & Correia, B. (2022). Decoding surface fingerprints for protein-ligand interactions. In ICLR2022 Machine Learning for Drug Discovery Workshop. bioRxiv (2022): 2022-04.

Zhemchuzhnikov D., Igashov I., & Grudinin S. (2022). 6DCNN with roto-translational convolution filters for volumetric data processing. In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 36, No. 4, pp. 4707-4715).

Igashov I., Olechnovič K., Kadukova M., Venclovas Č., & Grudinin S. (2021). VoroCNN: deep convolutional neural network built on 3D Voronoi tessellation of protein structures. Bioinformatics, 37(16), 2332-2339.

Igashov I., Pavlichenko N., & Grudinin S. (2021). Spherical convolutions on molecular graphs for protein model quality assessment. Machine Learning: Science and Technology, 2(4), 045005.

INVITED TALKS

- Generative drug design: the next paradigm shift in therapeutic development? IBS Grenoble (2025).
- Design of functional biomolecules using deep generative models, AlgoSB 2024, Cargèse (2024).
- RetroBridge: Modeling Retrosynthesis with Markov Bridges, Cambridge AI Group Talks (2023).
- Fragment-Based Drug Discovery Using Protein Surface Fingerprints, Symposium: Biochemical Machine Learning, IOCB Prague (2023).
- Equivariant 3D-Conditional Diffusion Models for Molecular Linker Design, Interplay between AI and mathematical modelling in the post-structural genomics era, CIRM, Marseille (2023).
- Equivariant 3D-Conditional Diffusion Models for Molecular Linker Design, M2D2 Seminar Series (2023).
- Fragment-Based Drug Discovery Using Protein Surface Fingerprints, Keystone Symposia on Computational Design and Modeling of Biomolecules, Banff (2023).
- Fragment-Based Drug Discovery Using Protein Surface Fingerprints, CIS SV Retreat 2022 “AI in life sciences: challenges and opportunities”, Lausanne (2022).

TEACHING ACTIVITIES

2023 – 2024 Analysis I and II, Teaching Assistant
École Polytechnique Fédérale de Lausanne

2022 – 2023 Numerical Analysis, Teaching Assistant
École Polytechnique Fédérale de Lausanne

2021 Graph as models in life sciences: Machine learning and integrative approaches, Lecturer
Université Paris Saclay Thematic School 2021, Paris

2021 Machine Learning Course, Lecturer
Moscow Institute of Physics and Technology & Yandex School of Data Analysis, Moscow

2019 Machine Learning Course, Lecturer
Sberbank, Moscow

PATENTS

"Decoding surface fingerprints for protein-ligand interactions". Bruno Correia, Ilia Igashov. US patent application - 63/455,819