

Antonina Dolgorukova, M.D.

Personal details

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I work at the intersection of data science and machine learning engineering, with a focus on biomedical data. I have a medical background and several years of hands-on experience in data analysis and predictive modeling using Python and R.

Applied ML experience (2022 – present)

Kaggle competitions:

[MABe Challenge - Social Action Recognition in Mice](#) (12th place of 1412 teams, Sep-Dec, 2025): Multiclass classification of mouse behaviors and temporal boundaries from pose keypoint time series under structured constraints.

[NeurIPS 2024 - Predict New Medicines with BELKA](#) (13th place of 1950 teams, Apr-Jul, 2024): Large-scale binary classification of compound-protein binding.

[Open Problems – Single-Cell Perturbations](#) (13th place of 1097 teams, Sept-Dec, 2023): Multi-output regression of gene expression responses across cell types.

[CAFA 5 Protein Function Prediction](#) (13th place of 1625 teams, Apr-Dec, 2023): Large-scale multi-label classification of protein functions.

Core Technical Contributions:

- Built a unified training and tuning pipeline supporting multiple model families for systematic comparison and ensembling.
- Developed domain-specific feature engineering.
- Implemented task-specific sampling, calibration, and postprocessing.

Key tools used: Python/R: XGBoost, LightGBM, CatBoost, PyBoost, PyTorch/Torch, TensorFlow, Chemprop (bash, docker), RDKit, pandas, NumPy, scikit-learn, scipy.

Pet projects:

CayleyPy (2024 – 2025): Developing efficient artificial intelligence-based approaches to pathfinding on extremely large graphs (spin-off [repo](#) with GPU-accelerated PyTorch implementation of machine learning-guided beam search).

[Research Project 01 Around Multimodal Single-Cell](#) (2022 – 2023): Analysis of multimodal single-cell data from the NeurIPS 2021 competition using clustering (UMAP, tSNE, PCA), gene enrichment, and feature importance analysis to uncover common regulatory signals across the transcriptome and proteome.

Education

Graduated from Pavlov First Saint Petersburg State Medical University, Saint Petersburg, Russia with a Diploma in General Medicine: Physician, M.D., 2018

Graduated from Paramedic College, Saint Petersburg, Russia with a Master's degree in emergency medical services: Paramedic, 2008

Research Experience in Experimental Neuropharmacology and Behavioral Pharmacology (2016 – 2022):

Research in animal models focusing on physiological and behavioral data collection and analysis in neuroscience and pharmacology.

Core Technical Contributions:

- Acquisition and analysis of electrophysiological and in vivo physiological measurements in rodents.
- Behavioral experiments involving operant and conditioning paradigms.
- Statistical analysis of experimental data and interpretation of biological variability.
- Reporting (publications, presentations in international conferences)

Key tools used: R, Prism, SigmaPlot, SPSS, Spike2, MED-PC.

Appointments

Biostatistician, R-Pharm (May 2022 - present) (Perform data analysis and reporting automation for clinical studies, covering data validation, statistical analysis, and reproducible report generation)

Medical translator, [Falk online mediacenter](#), Dr. Falk/Falk Foundation (June 2020 – February 2022)

Medical writer, [X7 Research](#) (February 2019 – August 2019)

Junior Researcher, Laboratory of Experimental Pharmacology and Therapy of Pain, Department of Neuropharmacology, Valdman Institute of Pharmacology, Pavlov First Saint Petersburg State Medical University, Saint Petersburg, Russia (2017 December – April 2022)

Junior Researcher, Laboratory of Behavioural Pharmacology, Department of Psychopharmacology, Valdman Institute of Pharmacology, Pavlov First Saint Petersburg State Medical University, Saint Petersburg, Russia (2016 June – 2018 January)

Professional training

Curriculum “Introduction to NGS technologies. Working with data sequencing.”, Moscow, Russia (27 January 2023 – 01 February 2023).

Online courses “Rigorous Statistics for Academics and Practitioners 2022”, “Advanced Generative Adversarial Networks”, “Neural Network Introduction”, “Natural Language Processing Introduction” by Asst. Prof. Michal Fabinger (University of Tokyo, Japan), [Acalonia school](#), (March – August 2022).

Mentee in the ECNP Mentorship programme 2020 from June 2020 to February 2022, the mentor was [Dr. Avraham Avital](#)

Online courses “Regression Analysis”, “Computer Vision”, “Neural Network Essentials”, “Probability and Statistics” by Asst. Prof. Michal Fabinger (University of Tokyo, Japan) at [Tokyo Data Science](#), February 2020 – July 2021 (weekly).

[Open Online R Streams](#) by Assoc. Prof. Wolfgang Viechtbauer (advanced R) (Maastricht University, The Netherlands), 8 October 2020 – March 2023 (weekly).

Attendee of the ECNP Workshop for Early Career Scientists in Europe, 7 - 10 March 2019, Nice, France.

ECNP Network “Preclinical Data Forum” Training Workshop for Young Scientists “How to Make Preclinical Research Robust”, Heidelberg, Germany, 3-5 July 2017 (Awarded a certificate of successful completion).

Grants and awards

- “Best student team solution” at NeurIPS 2024 - Predict New Medicines with BELKA (2024)
- “Judges” Prize at Open Problems – Single-Cell Perturbations competition (2024)
- CDE Grant at 33rd ECNP Congress, 12-15 September 2020 (Virtual)
- ALBA-FKNE-YIBRO diversity grant for participating in the FENS 2020 Virtual Forum
- Diploma of the Scientific Council of Pavlov First Saint Petersburg State Medical University for achievements in research activities, July 2018
- Awardee of the increased state academic scholarship from December 2016 to July 2018
- CDE Grant at 30th ECNP Congress, 2-5 September 2017, Paris, France.
- Russian Foundation for Basic Research (grant #16-34-01016), 2016-2018. Project: Investigation of dopaminergic mechanisms of adaptation to stress

Teaching

September – December 2019: taught a general pharmacology course for 3rd year students at Pavlov State Medical University, Saint Petersburg, Russia

Selected publications

Preprints:

1. Chervov, A., Fedoriaka, D., Konstantinova, E., Naumov, A., Kiselev, I., Sheveleva, A., Koltsov, I., Lytkin, S., Smolensky, A., ..., **Dolgorukova, A.**, Isambert, H. (2025). CayleyPy Growth: Efficient growth computations and hundreds of new conjectures on Cayley graphs (Brief version). arXiv. <https://arxiv.org/abs/2509.19162>
2. Chervov, A., Soibelman, A., Lytkin, S., Kiselev, I., Fironov, S., Lukyanenko, A., **Dolgorukova, A.**, Ogurtsov, A., ..., Khoruzhii, K., & Romanov, A. (2025). CayleyPy RL: Pathfinding and Reinforcement Learning on Cayley Graphs. arXiv. <https://arxiv.org/abs/2502.18663>

Articles:

1. **Dolgorukova, A.**, Protsenko, E., Isaeva, J., Gagloeva, V., Verbitskaya, E., Berkovich, R., & Sokolov, A. Y. (2023). Meta-analysis of the effects of anti-migraine therapeutics in the rat trigeminovascular nociception model as a tool for design optimization. *European Journal of Neuroscience*, 1– 22. <https://doi.org/10.1111/ejn.16030>
2. **Dolgorukova, A.**, Osipchuk, A. V., Murzina, A. A., Lyubashina, O. A., & Sokolov, A. Y. (2022). The implementation of transcranial Doppler ultrasonography for preclinical study of migraine. *Canadian Journal of Physiology and Pharmacology*, 100(6), 553–561. <https://doi.org/10.1139/cjpp-2021-0626>
3. **Dolgorukova, A.** & Sokolov, A. Y. (2021). Electrophysiological model of trigeminovascular nociception as a tool for experimental study of migraine pharmacotherapy. *Russian journal of pain*, 19(3), 31–38. (In Russ.). <https://doi.org/10.17116/pain20211903131>
4. Soliman, N., Haroutounian, S., Hohmann, A. G., Krane, E., Liao, J., Macleod, M., ... **Dolgorukova, A.**, ..., Rice, A. S. C. (2021). A systematic review and meta-analysis of cannabis-based medicines, cannabinoids and endocannabinoid system modulators tested for antinociceptive effects in

animal models of injury-related or pathological persistent pain. *Pain*, 162, S26-S44.

<https://doi.org/10.1097/j.pain.0000000000002269>

5. **Dolgorukova, A.**, Isaeva, J. E., Verbitskaya, E., Lyubashina, O. A., Giniatullin, R. A., & Sokolov, A. Y. (2021). Differential effects of the Piezo1 agonist Yoda1 in the trigeminovascular system: An electrophysiological and intravital microscopy study in rats. *Experimental Neurology*, 339, 113634. <https://doi.org/10.1016/j.expneurol.2021.113634>
6. **Dolgorukova, A.**, Osipchuk, A. V., Murzina, A. A., & Sokolov, A. Y. (2020). The Influence of Metoclopramide on Trigemino-vascular Nociception: Possible Anti-Migraine Mechanism of Action. *Neuroscience*, 425, 123–133. <https://doi.org/10.1016/J.NEUROSCIENCE.2019.11.026>
7. Dorotenko, A., Tur, M., **Dolgorukova, A.**, Bortnikov, N., Belozertseva, I. V., Zvartau, E. E., ... Sukhanov, I. (2020). The Action of TAAR1 Agonist RO5263397 on Executive Functions in Rats. *Cellular and Molecular Neurobiology*, 40(2), 215–228. <https://doi.org/10.1007/s10571-019-00757-6>
8. Sukhanov, I., Dorotenko, A., **Dolgorukova, A.**, Hoener, M. C., Gainetdinov, R. R., & Bernalov, A. Y. (2019). Activation of trace amine-associated receptor 1 attenuates schedule-induced polydipsia in rats. *Neuropharmacology*, 144, 184–192. <https://doi.org/10.1016/j.neuropharm.2018.10.034>
9. Sukhanov, I., Dorofeikova, M., **Dolgorukova, A.**, Dorotenko, A., & Gainetdinov, R. R. (2018). Trace Amine-Associated Receptor 1 Modulates the Locomotor and Sensitization Effects of Nicotine. *Frontiers in Pharmacology*, 9, 329. <https://doi.org/10.3389/fphar.2018.00329>
10. Mosikian, A., **Dolgorukova, A.**, & Zalevskaya, A. (2016). Possible approaches to CYP2C9-guided prescription of sulfonylureas in Russia. *Pharmacogenomics*, 17(18), 2115–2126. <https://doi.org/10.2217/pgs-2016-0121>