# Alenicheva **Alisa**

Machine Learning Researcher

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## Summary

Areas of science interests - Machine Learning in Biology&Chemistry.

## Education

**Skoltech (Skolkovo Institute of Science and Technology), GPA 4.5/5.0** — *Moscow, Russia*

M.S. in Information Science and Technology

Projects: *Sep. 2018 - Exp. Aug. 2020*

- **3D Segment Mapping using Data-Driven Descriptors**
  Labelling dataset of 3D pointclouds from KITTI dataset; extraction feature vectors from 3D pointclouds via autoencoder and classification of objects based on these vectors.
- **Thesis: Predicting the acute toxicity of organic molecules using 3D-convolutional neural networks**
  Transformation of SMILES organic molecules notation into 3D cube; reducing sparsity via convolution with specific kernels; data augmentation with molecule conformers; predict toxicity via 3D-CNN architecture: multi-label classification task (Tox21 dataset), multi-label regression task.

**MIPT (Moscow Institute of Physics and Technologies), GPA 4.9/5.0** — *Moscow, Russia*

B.S. in Applied Mathematics and Physics

Thesis: Mathematical model of light distribution inside layer of microalgae liquid *Sep. 2014 - Exp. Aug. 2018*

- Got an Abramov scholarship for academic achievements
- Graduated with Honors

## Work Experience

**JetBrains Research**

Machine Learning Applications and Deep Learning Lab — *St. Petersburg , Russia*

Machine Learning Researcher *Jul. 2020 - Present*

- Developing new neural network architectures for chemoinformatics tasks from scratch (NLP, Graph Neural Networks)
- Implementation SOTA neural network models from articles
- Participating in conferences
- Mentoring student projects
- Selected projects: Lipophilicity prediction with graph neural networks, Binding energy prediction with docking and graph neural networks, Molecule optimization with RL algorithms

**Bioinformatics Institute/Sberbank/Computer Science Center/ITMO** — *St. Petersburg , Russia*

Teaching assistant *Sep. 2020 - Now*

- Mentoring "Algorithms in Bioinformatics" course
- Teaching "Introdiction to Machine Learning" course
- Preparing lectures, seminars and homework materials

**Mobile TeleSystems (MTS)**

Artificial Intelligence Department — *Moscow, Russia*

Intern *Jun. 2019 - Sep. 2019*

- Entity Linking for the Russian language
- Collected dataset for Entity Disambiguation in the Russian language based on Wikipedia dump
- Created a prototype of software marking entities in a piece of text

**National Research Center «Kurchatov Institute»**

Biotechnology Department — *Moscow, Russia*

Research assistant *Oct. 2014 - Jun. 2019*

- Implemented software for reading and collecting data from sensors system of Bioreactor with LabView development environment
- Constructed the Arduino-based control unit of Bioreactor lighting
- Created a mathematical model of light distribution inside the Bioreactors with different geometries

## Publications

Nina Lukashina, Alisa Alenicheva, Elizaveta Vlasova, Artem Kondiukov, Aigul Khakimova, Emil Magerramov, Nikita Churikov, Aleksei Shpilman. *Lipophilicity Prediction with Multitask Learning and Molecular Substructures Representation*.

**Machine Learning for Molecules Workshop at NeurIPS'2020**, December 2020

Derek van Tilborg, Alisa Alenicheva, Francesca Grisoni. *Exposing the limitations of molecular machine learning with activity cliffs*.

**ChemRxiv**, March 2022

## Honors

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|---|---|---|
| 2019 | **1st Place, Unilever Chain Reaction Hack** - data analyst, designer | *Moscow, Russia* |
| 2019 | **1st Place, The Arctic Circle Hackathon** - data analyst, designer | *Salekhard, Russia* |
| 2020 | **2nd Place, SberCode Hackathon** - data scientist (NLP) | *Moscow, Russia* |
| 2020 | **1st Place, RaifHack** - data analyst | *Moscow, Russia* |
| 2020 | **1st Place, PandemicDataHack** - data analyst | *Moscow, Russia* |

## Skills

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|---|---|
| **Programming languages** | • Python:<br>Pytorch, Scikit-learn, Pandas, Matplotlib, Numpy, MPI4py<br>• LaTeX (Basic)<br>• SQL (Basic) |
| **Relevant Coursework (Skoltech)** | • Machine Learning<br>• Natural Language Modelling and Processing<br>• Deep Learning<br>• Bayesian Methods of Machine Learning |
| **Relevant Coursework (MIPT)** | • Biology<br>• Chemistry<br>• Quantum Physics<br>• Biochemistry |
| **Languages** | • Russian (Native)<br>• English (Upper-Intermediate) |
| **Tools** | • Linux<br>• Git<br>• ssh |