Ivan Plyushchenko

Postdoctoral Fellow

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Education

2017-22 PhD (Chemistry) Lomonosov Moscow State University Moscow, Russia

2011-17 MSc (Chemistry), GPA: 93.4 Lomonosov Moscow State University

Moscow, Russia

[Key Publications]

2022 Deep learning for retention time prediction in reversed-phase liq-

uid chromatography ES Fedorova, DD Matyushin, IV Plyushchenko, AN

Stavrianidi, AK Buryak

Journal of Chromatography A

2022 Hopomics: Humulus lupulus Brewing Cultivars Classification

Based on LC-MS Profiling and Nested Feature Selection YA

Ikhalaynen, IV Plyushchenko, IA Rodin

Metabolites

2021 Omics Untargeted Key Script: R-Based Software Toolbox for Un-

targeted Metabolomics with Bladder Cancer Biomarkers Discovery Case Study IV Plyushchenko, ES Fedorova, NV Potoldykova, KA Polyakovskiy, ...

Journal of Proteome Research

2021 Untargeted and targeted analysis of sarin poisoning biomarkers in

rat urine by liquid chromatography and tandem mass spectrometry

MF Vokuev*, TM Baygildiev*, IV Plyushchenko*, YA Ikhalaynen, ...

Analytical and Bioanalytical Chemistry

2020 An approach for feature selection with data modelling in LC-MS

metabolomics I Plyushchenko, D Shakhmatov, T Bolotnik, T Baygildiev, PN

Nesterenko, ...

Analytical methods

Grants and Awards

2018-22	Russian Foundation f	for Basic Research	Participant
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3 grants

2017-21 Russian Science Foundation Participant

2 grants

2022 Winner of the competition of works contributing to the solution of

problems of the Development Program of Moscow State University

in the nomination 'Outstanding scientific articles'

Moscow, Russia

2022 Competition of the Russian Academy of Sciences of scientific

works of young scientists in chromatography in honor of the 150th

anniversary of the birth M.S. Tsvet

Moscow, Russia

2019 The Association for Mass Spectrometry & Advances in the Clinical

Lab (MSACL) Conference EU Travel Grant

Salzburg, Austria

2018 International Mass Spectrometry Conference Fellowship

Florence, Italy

The Association for Mass Spectrometry & Advances in the Clinical

Lab (MSACL) Conference EU Travel Grant

Salzburg, Austria

Professional Experience

2025.01- now	Postdoctoral Fellow University of Haifa, Department of Marine Biology
2022.12-	
2024.12	Graduate Researcher Technion - Israel Institute of Technology, Biology Faculty
2022.03-	
2022.11	Postdoctoral Research Fellow Lomonosov Moscow State University, Chemistry Department
2017.07-	
2022.02	Junior Research Associate Lomonosov Moscow State University, Chemistry Department
2016.05-	
2017.06	Lab Technician Lomonosov Moscow State University, Chemistry Department
2015.05-	
2018.06	Analytical Chemist Analytical centre of Lomonosov Moscow State University
	Alialy deal centre of Londonosov Proscov State Offiversity

Skills & Proficiencies

Instruments & techniques:

- MS: SCAN, SIM, MRM, DDA, DIA, PASEF, TIMS
- LC: RP, HILIC
- Nano LC: Evosep One (Evosep)
- LC-MS: IT-TOF (Shimadzu); Orbitrap Exploris 120, Orbitrap Q Exactive (Thermo); QTRAP 3200 (Sciex); 6470 (Agilent); timsTOF Pro (Bruker)
- LC-DAD: 1100, 1200, 1290 Infinity (Agilent); Ultimate 3000 (Dionex); LC 20 (Shimadzu); Vanquish (Thermo)
- LC-FLD: 1200 (Agilent); Ultimate 3000 (Dionex)
- CE-UV: G1600AX, 7100 (Agilent)
- GC-MS: GCMS-QP 2010 with SHS (Shimadzu); 7890 B (Agilent)
- GC-FID: GC-2010 (Shimadzu)

Basic lab skills:

- · Extraction from liquid & solid media
- SPE, LLE, Soxhlet extraction, centrifugation, membrane filtering
- UV/Vis analysis, pH measurement
- Preparation of calibration curves, QC/QA programs performing, daily maintenance
- · Maintenance of mammalian cell lines and bacterial cultures

Programming, Software & Bioinformatics tools:

- · R language independent user
- tidyverse, tidymass, RforMassSpectrometry families of packages
- xcms, CAMERA, IPO, MSnbase, MSstats, Biostrings, seqinr, rcdk, caret, H2O, keras, xgboost, ggplot2, dplyr, data.table, RMarkdown, plotly, Shiny
- · tool development list: URL
- full list of R packages that is used for metabolomics processing: URL
- GUI software: MetaboAnalyst, MS-DIAL, MZmine, MS-FINDER, Maven, SIR-IUS+CSI:FingerID, CFM-ID, MetFrag, GNPS, Open Babel, PathVisio, Frag-Pipe, DIA-NN, Alphapept
- Vendor Software: LabSolutions (Shimadzu); XCalibur, FreeStyle, Compound Discoverer (Thermo); OpenLab, MassHunter, ChemStation (Agilent); Compass HyStar, OtofControl (Bruker)

Certificates & Courses

2025 Introduction to Metabolomics Technion, Faculty of Medicine

• 24 hrs

2019 Data Science 201: Going Further With R: Tackling Clinical Labora-

tory Data Manipulation and Modeling

The Association for Mass Spectrometry & Advances in the Clinical

Lab (MSACL) Conference EU

• 16 hrs

2017 Metabolomics 202: Approaches, Applications and Challenges

The Association for Mass Spectrometry & Advances in the Clinical

Lab (MSACL) Conference EU

• 16 hrs

Teaching and Mentorship

2018-22 Mentoring undergraduates students of Lomonosov Moscow State University, Faculty of Chemistry, including two students' thesis supervision

2018-20 Practical and theoretical classes on analytical chemistry for students of Lomonosov Moscow State University, Faculty of Biology

2016-19 Agilent advanced training courses at the Analytical centre of Lomonosov Moscow State University in LC, LC-MS

Current Journal Roles

Metabolomics

Biomedical Chromatography Peer Reviewer Journal of Analytical Chemistry Peer Reviewer **BMC** Medicine Peer Reviewer Journal of Food Composition and Analysis Peer Reviewer Scientific Reports Peer Reviewer **PLOS Computational Biology** Peer Reviewer **BMC Infectious Diseases** Peer Reviewer PLOS One Peer Reviewer Proteome Science Peer Reviewer Journal of Proteome Research Peer Reviewer Scientific Data Peer Reviewer **BMC Bioinformatics** Peer Reviewer BMC gastroenterology Peer Reviewer Nutrition & metabolism Peer Reviewer npj Systems Biology and Applications Peer Reviewer Journal of Computational Chemistry Peer Reviewer **BMC Cancer** Peer Reviewer ACS Omega Peer Reviewer

Peer Reviewer

Publication List 2023 Glyphosate Effects on Some Characteristics of Biological Activity and Phytotoxicity of Soddy-Podzolic Soil in a Short-Term Model Experiment NV Kostina, MV Gorlenko, KA Mazurov, OI Filippova, IV Plyushchenko, ... Eurasian Soil Science 2022 Deep learning for retention time prediction in reversed-phase liquid chromatography ES Fedorova, DD Matyushin, IV Plyushchenko, AN Stavrianidi, AK Buryak Journal of Chromatography A 2022 Hopomics: Humulus lupulus Brewing Cultivars Classification Based on LC-MS Profiling and Nested Feature Selection Ikhalaynen, IV Plyushchenko, IA Rodin Metabolites 2021 Fused 1,2-Diboraoxazoles Based on closo-Decaborate Anion-Novel Members of Diboroheterocycle Class VV Voinova, NA Selivanov, IV Plyushchenko, MF Vokuev, AY Bykov, \dots Molecules 2021 Development of ELISA formats for polymyxin B monitoring in serum of critically ill patients MA Burkin, IA Galvidis, YA Surovoy, IV Plyushchenko, IA Rodin, ... Journal of Pharmaceutical and Biomedical Analysis 2021 Omics Untargeted Key Script: R-Based Software Toolbox for Untargeted Metabolomics with Bladder Cancer Biomarkers Discovery Case Study IV Plyushchenko, ES Fedorova, NV Potoldykova, KA Polyakovskiy, ... Journal of Proteome Research 2021 Algorithm of Combining Chromatography-Mass Spectrometry Untargeted Profiling and Multivariate Analysis for Identification of Marker Substances in Samples of Complex Composition Plyushchenko, DG Shakhmatov, IA Rodin **Inorganic Materials** 2021 Untargeted and targeted analysis of sarin poisoning biomarkers in rat urine by liquid chromatography and tandem mass spectrome-MF Vokuev*, TM Baygildiev*, IV Plyushchenko*, YA Ikhalaynen, ... Analytical and Bioanalytical Chemistry 2020 The degradation of glyphosate and its effect on the microbial community of agro-sod-podzolic soil under short-term model experiment conditions NA Kulikova, AD Zhelezova, OI Filippova, IV Plyushchenko, IA Rodin Moscow University Soil Science Bulletin 2020 An approach for feature selection with data modelling in LC-MS metabolomics I Plyushchenko, D Shakhmatov, T Bolotnik, T Baygildiev, PN Nesterenko, ... Analytical methods 2020 Monoammonium phosphate effects on glyphosate in soils: mobi-

lization, phytotoxicity, and alteration of the microbial community NA Kulikova, AD Zhelezova, MG Voropanov, OI Filippova, IV Plyushchenko, ...

Use of chemometric methods of data analysis for the identification and typification of petroleum and petroleum products TA Bolotnik,

Identification of spillages of semi-volatile hydrocarbon fuels in

YV Timchenko, IV Plyushchenko, VV Levkina, AV Pirogov, ...

soils by gas chromatography—mass spectrometry Plyushchenko, AD Smolenkov, AV Pirogov, MV Popik, ...

Eurasian Soil Science

Journal of Analytical Chemistry

Journal of Analytical Chemistry

2019

2018

Conferences

2023	Untargeted urinary metabolomics for identification of bladde cancer biomarkers using HPLC-MS Euroanalysis XXI, Geneva, Switzerland
2022	Application of gradient boosting machine for signal processing in LC-MS metabolomics 13th Winter Symposium on Chemometrics, Russia
2022	Untargeted metabolomics study of Humulus lupulus brewing cultivars, for genetic origin classification task 13th Winter Symposium of Chemometrics, Russia
2021	Describing metabolome diversity between Humulus lupulus genetic origin groups using UHPLC-MS/MS The 69th Annual Conference on Mass Spectrometry of MSSJ, Japan
2020	Humulus lupulus LC-MS untargeted profiling study for geographic origin classification task4th International Symposium on Phytochemicals in Medicine and Food, Xi'an, China
2019	Comparison of the kinetics of dyes degradation of handwritter strokes subjected to different types of artificial aging and studied using chromatography mass-spectrometry and statistical data processing 48th International Symposium on High-Performance Liquid Phase Separations and Related Techniques, Milan, Italy
2019	Bioassay Classification Study via LC-MS and Machine Learning in Conjunction with Dimensionality Reduction MSACL 2019 EU, Salzburg Austria
2018	Typical LC-MS metabolomics workflow for profiling urine samples of patients with colorectal cancer XXII International Mass Spectrometry Conference, Florence, Italy
2017	Simple & Robust Approach in Urinary Metabolomics Based or UPLC-MS for Preoperative Colorectal Cancer Diagnostics MSAC 2017 EU, Salzburg, Austria
2016	Complexation of sulfo-ß-cyclodextrin with fenoterol. Electrophoretic and spectroscopic study VIIIth International Symposium Design and Synthesis of Supramolecular Architectures, Kazan, Russia