Ivan Plyushchenko

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Education

2017-22	PhD (Chemistry) Moscow, Russia	Lomonosov Moscow State University
2011-17	MSc (Chemistry), GPA: 93.4 Moscow, Russia	Lomonosov Moscow State University

Key Pub	lications
2022	Deep learning for retention time prediction in reversed-phase liquid chromatography ES Fedorova, DD Matyushin, <u>IV Plyushchenko</u> , 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, <u>IV Plyushchenko</u> , IA Rodin Metabolites
2021	Omics Untargeted Key Script: R-Based Software Toolbox for Untargeted Metabolomics with Bladder Cancer Biomarkers Discovery Case Study <u>IV Plyushchenko</u> , 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 <u>I Plyushchenko</u> , D Shakhmatov, T Bolotnik, T Baygildiev, PN Nesterenko, Analytical methods

2018-22	Russian Foundation for Basic Research 3 grants	Participant
2017-21	Russian Science Foundation 2 grants	Participant
2022	Winner of the competition of works contributing to the problems of the Development Program of Moscow Stain the nomination 'Outstanding scientific articles' Moscow, Russia	
2022	Competition of the Russian Academy of Sciences works of young scientists in chromatography in hono anniversary of the birth M.S. Tsvet Moscow, Russia	
2019	The Association for Mass Spectrometry & Advances Lab (MSACL) Conference EU Travel Grant Salzburg, Austria	in the Clinical
2018	International Mass Spectrometry Conference Fellow Florence, Italy	ship
2017	The Association for Mass Spectrometry & Advances Lab (MSACL) Conference EU Travel Grant Salzburg, Austria	in the Clinical

Professional Experience

Postdoctoral Fellow University of Haifa, Department of Marine Biology
Graduate Researcher Technion - Israel Institute of Technology, Biology Faculty
Postdoctoral Research Fellow Lomonosov Moscow State University, Chemistry Department
Junior Research Associate Lomonosov Moscow State University, Chemistry Department
Lab Technician Lomonosov Moscow State University, Chemistry Department
Analytical Chemist Analytical centre of Lomonosov Moscow State University

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
- · Cell culture maintenance

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
- · tool development list: URL
- full list of R packages that is used for metabolomics processing: URL
- GUI software: MetaboAnalyst, MS-DIAL, MZmine, MS-FINDER, SIR-IUS+CSI:FingerID, CFM-ID, MetFrag, GNPS, Open Babel, PathVisio, FragPipe, DIA-NN, Alphapept
- Vendor Software: LabSolutions (Shimadzu); XCalibur, FreeStyle, Compound Discoverer (Thermo); OpenLab, MassHunter, ChemStation (Agilent); Compass HyStar, OtofControl (Bruker)

Certificates & Courses

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 su-

pervision

2018-20 Practical and theoretical classes on analytical chemistry for stu-

dents 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

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

Publicati	ion 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, <u>IV Plyushchenko</u> , 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, <u>IV Plyushchenko</u> , IA Rodin Metabolites
2021	Fused 1,2-Diboraoxazoles Based on closo-Decaborate Anion—Novel Members of Diboroheterocycle Class VV Voinova, NA Selivanov, <u>IV Plyushchenko</u> , MF Vokuev, AY Bykov, 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 <u>IV Plyushchenko</u> , 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 IV 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 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 <u>I Plyushchenko</u> , D Shakhmatov, T Bolotnik, T Baygildiev, PN Nesterenko, Analytical methods
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	Monoammonium phosphate effects on glyphosate in soils: mobilization, phytotoxicity, and alteration of the microbial community

NA Kulikova, AD Zhelezova, MG Voropanov, OI Filippova, IV Plyushchenko, ...

YV Timchenko, <u>IV Plyushchenko</u>, VV Levkina, AV Pirogov, ...

Plyushchenko, AD Smolenkov, AV Pirogov, MV Popik, ...

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 soils by gas chromatography—mass spectrometry

TA Bolotnik, IV

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