Ivan Plyushchenko

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Education

2017-22	Doctor of Philosophy (Chemistry) Lomonosov Moscow State University Moscow, Russia
2017-21	Postgraduate academic and pedagogical training (Chemistry) Lomonosov Moscow State University Moscow, Russia
2011-17	Specialist in Chemistry (equivalent to MSc), GPA: 4.67 Lomonosov Moscow State University Moscow, Russia

Key Publications

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 YA Ikhalaynen, IV Plyushchenko, IA Rodin Metabolites
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	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

Certificates

| 2019 | Data Science 201: Going Further With R: Tackling Clinical Laboratory 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 |

Grants and awards

2018-22	Russian Foundation for Basic Research Participant 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
2017	The Association for Mass Spectrometry & Advances in the Clinical Lab (MSACL) Conference EU Travel Grant Salzburg, Austria

Professional Experience

2019-22	Junior research associate	Lomonosov Moscow State University
2016-19	Lab technician	Lomonosov Moscow State University
2015-18	Analytical chemist	Analytical centre of Lomonosov Moscow State University

Skills & proficiencies

Instruments & techniques:

- MS: SCAN, SIM, MRM, DDA, DIA
- LC: RP, HILIC
- LC-MS (IT-TOF, Shimadzu; Orbitrap Exploris 120, Orbitrap Q Exactive, Thermo; QTRAP 3200, Sciex; 6470, Agilent)
- LC-DAD (1100/1200/1290 Infinity, Agilent; Ultimate 3000, Dionex; LC 20, Shimadzu; Vanquish, Thermo)
- LC-FLD (1200, Agilent; Ultimate 3000, Dionex)
- CE-UV (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, rcdk, caret, H2O, keras, ggplot2, dplyr, data.table, RMarkdown
- tool development list: URL
- full list of R packages that is used for metabolomics processing: URL
- GUI software: MetaboAnalyst, MS-DIAL, MZmine, MS-FINDER, SIRIUS+CSI:FingerID, CFM-ID, MetFrag, GNPS, Open Babel, FragPipe, DIA-NN
- Vendor Software: LabSolutions (Shimadzu); XCalibur, FreeStyle, Compound Discoverer (Thermo); OpenLab, MassHunter, ChemStation (Agilent)

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

Biomedical Chromatography	Peer Reviewer
Journal of Analytical Chemistry	Peer Reviewer
BMC Medicine	Peer Reviewer

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   YA 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, ...
Molecules

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   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   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   Monoammonium phosphate effects on glyphosate in soils: mobilization, phytotoxicity, and alteration of the microbial community   NA Kulikova, AD Zhelezova, MG Voropanov, OI Filippova, ...
Eurasian Soil Science

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

2019   Use of chemometric methods of data analysis for the identification and typification of petroleum and petroleum products   TA Bolotnik, YV Timchenko, IV Plyushchenko, VV Levkina, AV Pirogov, ...
Journal of Analytical Chemistry

2018   Identification of spillages of semi-volatile hydrocarbon fuels in soils by gas chromatography–mass spectrometry   TA Bolotnik, IV Plyushchenko, AD Smolenkov, AV Pirogov, MV Popik, ...
Journal of Analytical Chemistry

Conferences

2023   Untargeted urinary metabolomics for identification of bladder 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 on 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 task 4th International Symposium on Phytochemicals in Medicine and Food, Xi'an, China

2019   Comparison of the kinetics of dyes degradation of handwritten 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 on UPLC-MS for Preoperative Colorectal Cancer Diagnostics MSACL 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