

Ivan Plyushchenko

April 2023



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Education

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| 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

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| 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, <u>IV Plyushchenko</u> , 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 | |

Certificates

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| 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

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| 2018-22 | Russian Foundation for Basic Research | Participant |
| | 3 grants | |
| 2017-21 | Russian Science Foundation | Participant |
| | 2 grants | |

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| 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

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| 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, tidyproteomics, 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, SIR-IUS+CSI:FingerID, CFM-ID, MetFrag, GNPS, Open Babel
- 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

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| Biomedical Chromatography | Peer Reviewer |
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| Journal of Analytical Chemistry | Peer Reviewer |
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| BMC Medicine | Peer Reviewer |
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- 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 Ikhlaynen, 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 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 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 Ikhlaynen, ...
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 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 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
- 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

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| 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- β -cyclodextrin with fenoterol. Electrophoretic and spectroscopic study | VIIIth International Symposium Design and Synthesis of Supramolecular Architectures, Kazan, Russia |