

# Ivan Plyushchenko

January 2023



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## Education

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

## 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, 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

### Programming, Software & Bioinformatics tools:

- R language independent user
- tidyverse family of packages
- xcms, CAMERA, IPO, MSnbase, caret, H2O, keras, ggplot2
- 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, rcdk
- 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

- 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 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 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  
**Industrial laboratory. Diagnostics of materials**
- 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

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