

# Ivan Plyushchenko

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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, <a href="#">IV Plyushchenko</a> , 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, <a href="#">IV Plyushchenko</a> , IA Rodin                                   |
|      | Metabolites   |   |
| 2021 | Omics Untargeted Key Script: R-Based Software Toolbox for Untargeted Metabolomics with Bladder Cancer Biomarkers Discovery Case Study | <a href="#">IV Plyushchenko</a> , 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, <a href="#">IV Plyushchenko</a> , YA Ikhalaynen, ...              |
|      | Analytical and Bioanalytical Chemistry  |   |
| 2020 | An approach for feature selection with data modelling in LC-MS metabolomics   | <a href="#">I Plyushchenko</a> , 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, 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 family of packages
- xcms, CAMERA, IPO, MSnbase, RforMassSpectrometry, TidyMass, tidyproteomics, Biostrings, bioseq, seqinr, rcdk, caret, H2O, keras, ggplot2, dplyr, data.table
- 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

Biomedical Chromatography      Peer Reviewer

Journal of Analytical Chemistry      Peer Reviewer

BMC Medicine      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 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

|      |   |  |
|------|---|--|
| 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             |