Ivan Plyushchenko

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plyush1993

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, Russia
Key Ρι	ublications
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 <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

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

2017

	tory Data Manipulation and Modeling	The Association for Mass
	Spectrometry & Advances in the Clinical Lab (MSACI 16 hrs	L) Conference EU
2017	Metabolomics 202: Approaches, Applications and Challenges Association for Mass Spectrometry & Advances in the Clinical Lab (MSACL) C ference EU 16 hrs	

Data Science 201: Going Further With R: Tackling Clinical Labora-

Grants and awards

2018-22	Russian Foundation for Basic Research 3 grants	Participant
2017-21	Russian Science Foundation 2 grants	Participant
2022	Competition of the Russian Academy of Sciences of works of young scientists in chromatography in honor of anniversary of the birth M.S. Tsvet Mos	
2019	The Association for Mass Spectrometry & Advances in the Lab (MSACL) Conference EU Travel Grant Salzb	ne Clinical ourg, Austria
2018	International Mass Spectrometry Conference Fellowship Italy	Florence,

Lab (MSACL) Conference EU Travel Grant

The Association for Mass Spectrometry & Advances in the Clinical

Salzburg, Austria

Professional Experience

Junior research associate

2016-19 Lab technician Lomonosov Moscow State University

Lomonosov Moscow State University

2015-18 Analytical chemist Analytical centre of Lomonosov Moscow State University

Skills & proficiencies

Instruments:

2019-22

- 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)

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
- 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

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 on LC, LC-MS

Current journal roles

Biomedical Chromatography

Peer Reviewer

Russian Journal of Analytical Chemistry

Peer Reviewer

Publication list

2022	Deep learning for retention time prediction in reversed-phase liq- uid 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	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	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

Connerci	ices,
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