Ivan Plyushchenko

March 2024

orcid.org/0000-0003-3883-4695

plyushchenko.ivan@gmail.com

plyush1993

Education

Haifa, Israel
Doctor of Philosophy (Chemistry) Lomonosov Moscow State University Moscow, Russia
Postgraduate academic and pedagogical training (Chemistry) Lomonosov Moscow State University Moscow, Russia
Specialist in Chemistry (equivalent to MSc), GPA: 4.67 Lomonosov Moscow State University Moscow, Russia

2017

	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 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	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			
Grants and awards				
2018-22	Russian Foundation for Basic Research Participant 3 grants			
2017-21	Russian Science Foundation Participant			

	3 grants	·
2017-21	Russian Science Foundation 2 grants	Participant
2022	Winner of the competition of works contributing to the so problems of the Development Program of Moscow State U in the nomination 'Outstanding scientific articles' Mosc	
2022	Competition of the Russian Academy of Sciences of works of young scientists in chromatography in honor of the anniversary of the birth M.S. Tsvet Mosc	
2019	The Association for Mass Spectrometry & Advances in the Lab (MSACL) Conference EU Travel Grant Salzbu	e Clinical urg, 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

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 & techniques:

• MS: SCAN, SIM, MRM, DDA, DIA, PASEF, TIMS

Junior research associate

· LC: RP, HILIC

2019-22

- Nano LC: Evosep One (Evosep)
- LC-MS: IT-TOF (Shimadzu); Orbitrap Exploris 120, Orbitrap Q Exactive (Thermo); QTRAP 3200 (Sciex); 6470 (Agilent); timsTOF Pro (Bruker)
- LC-DAD: 1100, 1200, 1290 Infinity (Agilent); Ultimate 3000 (Dionex); LC 20 (Shimadzu); Vanquish (Thermo)
- LC-FLD: 1200 (Agilent); Ultimate 3000 (Dionex)
- CE-UV: G1600AX, 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, seqinr, rcdk, caret, H2O, keras, xgboost, 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, FragPipe, DIA-NN, Alphapept
- Vendor Software: LabSolutions (Shimadzu); XCalibur, FreeStyle, Compound Discoverer (Thermo); OpenLab, MassHunter, ChemStation (Agilent); Compass HyStar, OtofControl (Bruker)

Certificates

2019 Data Science 201: Going Further With R: Tackling Clinical Labora-

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) Con-

ference EU 16 hrs

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

Journal of Food Composition and Analysis Peer Reviewer

Scientific Reports Peer Reviewer

PLOS Computational Biology Peer Reviewer

Publication list 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

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

ES Fedorova, DD Matyushin, IV Plyushchenko, AN

Hopomics: Humulus lupulus Brewing Cultivars Classification
Based on LC-MS Profiling and Nested Feature Selection
YA
Ikhalaynen, IV Plyushchenko, IA Rodin
Metabolites

uid chromatography

Journal of Chromatography A

Stavrianidi, AK Buryak

- 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
- 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
- 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 An approach for feature selection with data modelling in LC-MS metabolomics I Plyushchenko, D Shakhmatov, T Bolotnik, T Baygildiev, PN Nesterenko. ...

Analytical methods

2022

- 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

- 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 bladde 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 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