

# Ivan Plyushchenko

## Postdoctoral Fellow

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University of Haifa, Department of Marine Biology

orcid.org/0000-0003-3883-4695

plyushchenko.ivan@gmail.com

plyush1993

ivan-plyushchenko-3861781a1/

## Education

2017-22	PhD (Chemistry) Moscow, Russia	Lomonosov Moscow State University
2011-17	MSc (Chemistry), GPA: 93.4 Moscow, Russia	Lomonosov Moscow State University

## Key Publications

2022	Deep learning for retention time prediction in reversed-phase liquid chromatography Stavrianidi, AK Buryak Journal of Chromatography A	ES Fedorova, DD Matyushin, IV Plyushchenko, AN
2022	Hopomics: Humulus lupulus Brewing Cultivars Classification Based on LC-MS Profiling and Nested Feature Selection Ikhlaynen, IV Plyushchenko, IA Rodin Metabolites	YA
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 Ikhlaynen, ... 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	

## Grants and Awards

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

2025.01- now	Postdoctoral Fellow University of Haifa, Department of Marine Biology
2022.12- 2024.12	Graduate Researcher Technion - Israel Institute of Technology, Biology Faculty
2022.03- 2022.11	Postdoctoral Research Fellow Lomonosov Moscow State University, Chemistry Department
2017.07- 2022.02	Junior Research Associate Lomonosov Moscow State University, Chemistry Department
2016.05- 2017.06	Lab Technician Lomonosov Moscow State University, Chemistry Department
2015.05- 2018.06	Analytical Chemist Analytical centre of Lomonosov Moscow State University

## Skills & Proficiencies

### Instruments & techniques:

- MS: SCAN, SIM, MRM, DDA, DIA, PASEF, TIMS
- LC: RP, HILIC
- 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
- Maintenance of mammalian cell lines and bacterial cultures

### 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, plotly, Shiny
- tool development list: URL
- full list of R packages that is used for metabolomics processing: URL
- GUI software: MetaboAnalyst, MS-DIAL, MZmine, MS-FINDER, Maven, SIR-IUS+CSI:FingerID, CFM-ID, MetFrag, GNPS, Open Babel, PathVisio, FragPipe, DIA-NN, Alphapept
- Vendor Software: LabSolutions (Shimadzu); XCalibur, FreeStyle, Compound Discoverer (Thermo); OpenLab, MassHunter, ChemStation (Agilent); Compass HyStar, OtofControl (Bruker)

## Certificates & Courses

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|------|--|
| 2025 | Introduction to Metabolomics<br>Technion, Faculty of Medicine <ul style="list-style-type: none"><li>• 24 hrs</li></ul>   |
| 2019 | Data Science 201: Going Further With R: Tackling Clinical Laboratory Data Manipulation and Modeling<br>The Association for Mass Spectrometry & Advances in the Clinical Lab (MSACL) Conference EU <ul style="list-style-type: none"><li>• 16 hrs</li></ul> |
| 2017 | Metabolomics 202: Approaches, Applications and Challenges<br>The Association for Mass Spectrometry & Advances in the Clinical Lab (MSACL) Conference EU <ul style="list-style-type: none"><li>• 16 hrs</li></ul>   |

## Teaching and Mentorship

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| 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
BMC Infectious Diseases	Peer Reviewer
PLOS One	Peer Reviewer
Proteome Science	Peer Reviewer
Journal of Proteome Research	Peer Reviewer
Scientific Data	Peer Reviewer
BMC Bioinformatics	Peer Reviewer
BMC gastroenterology	Peer Reviewer
Nutrition & metabolism	Peer Reviewer
npj Systems Biology and Applications	Peer Reviewer
Journal of Computational Chemistry	Peer Reviewer
BMC Cancer	Peer Reviewer
ACS Omega	Peer Reviewer
Metabolomics	Peer Reviewer
Journal of Biologically Active Products from Nature	Peer Reviewer

- 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
- 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      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 Ikhalaynen, ...  
Analytical and Bioanalytical Chemistry
- 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
- 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      Monoammonium phosphate effects on glyphosate in soils: mobilization, phytotoxicity, and alteration of the microbial community NA Kulikova, AD Zhelezova, MG Voropanov, OI Filippova, IV Plyushchenko, ...  
Eurasian Soil Science
- 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 bladder 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 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