Dmitry Avtonomov

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DOB: 1985-01-27

Post-Doctoral Research Fellow
University of Michigan, MI, USA
Department of Pathology
Alexey Nesvizhskii lab

Education:

Insititute for Energy Problems of Chemical Physics, Moscow, Russia — 2011
Ph.D. in Physics and Mathematics
Thesis: *Improvements to the Accurate Mass and Time (AMT) tag method and its practical use for proteome studies*

TOEFL (IBT) — 2008
Score: 111/120

Moscow Institute of Physics and Technology, Moscow, Russia — 2008
M.S. Applied Physics and Mathematics
Thesis: *Creation of Accurate Mass and Time (AMT) tags database for fast proteome screening of human body fluids*

Max Planck Institute of Biochemistry and Signal Transduction, Munich, Germany — 2006.07-10
Summer student at prof. Matthias Mann's lab (Proteomics and Signal Transduction)

Moscow Institute of Physics and Technology, Moscow, Russia — 2006
B.S. Applied Physics and Mathematics
Thesis: *Development of negative ions (Anthracene) source for ETD fragmentation of peptides in ion traps*

Research interests:

- Mass spectrometry data processing (signal processing, data visualization)
- Algorithms and software development
- Application of machine learning to bioinformatics problems
- Mass spectrometry instrumentation method development

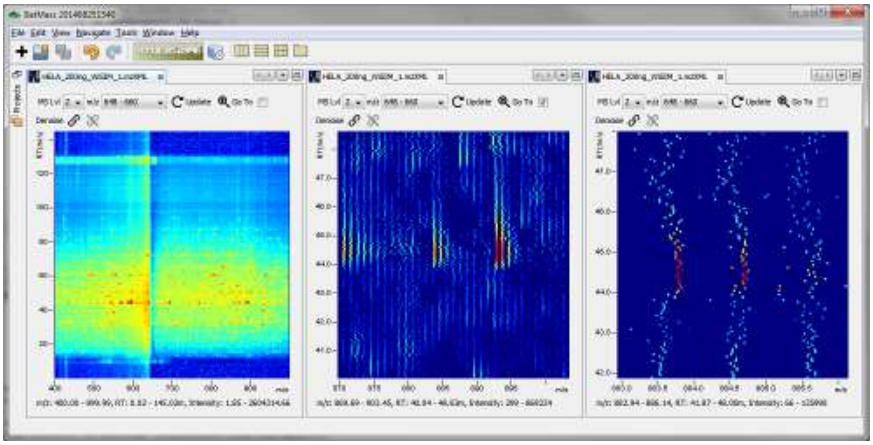
Relevant skills:

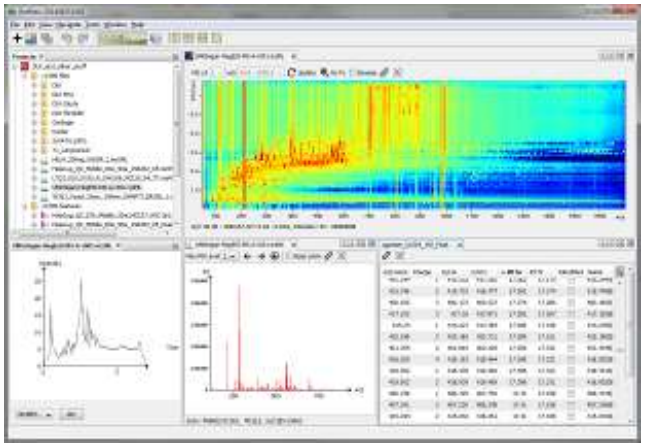
- Software development
  - Java, including desktop applications development in Java Swing and the NetBeans Platform
  - C# (including WinForms), C++, R, Python, JavaScript
  - Relational databases: MySQL, PostgreSQL, HSQLDB
- Mass spectrometry
  - MS data processing for proteomics (signal extraction, peptide and protein identification, quantitaion)
  - Raw data quality control
  - Operation and maintenance experience with Orbitrap, TOF (Bruker MicroFlex), Ion Trap (Finningan LCQ Deca XP, Thermo LTQ) and FT-ICR (Thermo LTQ-FT Ultra, Bruker Apex QE) instruments
  - HPLC systems (Agilent, Proxeon), in-house reversed phase chromatographic column packing

Research Experience:

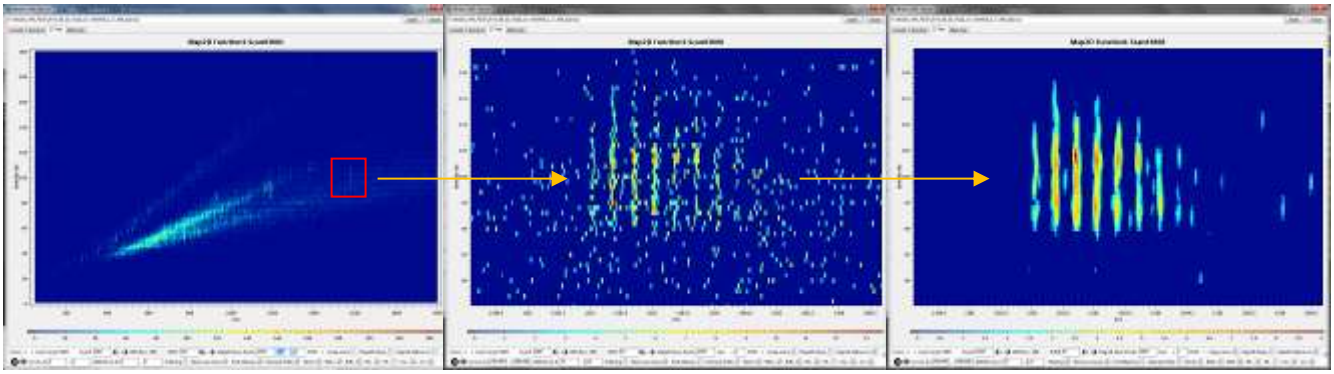
Postdoctoral Research:

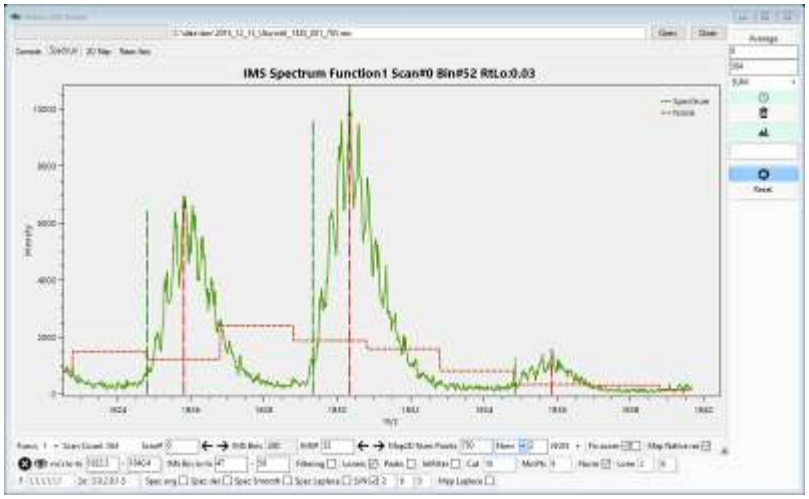
- Online instrument control software (Thermo Fusion, Exactive HF)
- Mass spectrometry (LC/MS) data visualization framework ***BatMass*** (Java, NetBeans Platform) (see http://batmass.org for an example video, more screengrabs, tutorials and downloads). Screenshots from the software:





- Data filtration and signal extraction from noisy *ion mobility* and *SONAR* spectra (Waters instruments, SynaptG2-Si, Xevo). Visualization of raw data and processing results (.NET WinForms):





- ***MSFTBX*** - high performance Java libraries for mass spectrometry data access: mzML, mzXML, pepxml, protxml, mzidentml (http://github.com/chhh/msftbx).
- ***MSDK*** – took part in development of this Java library for handling mass spectrometry data (reading/writing file formats, algorithms for alignment, feature detection, feature matching etc.) (https://github.com/msdk/msdk).
  MSDK-IO module was partially developed under our supervision during 2017 GSoC (Google Summer of Code).
- ***MSFragger*** – Ultra-fast proteomics search engine and the UI (https://github.com/chhh/MSFragger-GUI).
  The speed enables performing "open searches" (no restrictions on precursor ion mass) on a laptop computer within minutes.
- Development of processing algorithms for LC/MS (Liquid Chromatography Mass Spectrometry) DIA (Data Independent Acquisition) data. ***DIA-Umpire***: http://diaumpire.sourceforge.net.
- Isotopic fine structure calculation up to predefined total probability (http://github.com/chhh/isotree).
- Peptide retention time prediction based on confidently identified ions using supervised machine learning techniques.
- Deisotoping and deconvolution algorithms for high throughput LC-MS experiments.
- Elemental composition estimation of target molecules from ultrahigh resolution mass spectra.

Doctoral Research:

- Calculation of isotope distribution patterns for cases of non-integer atom counts. Used in optimization algorithms for mass spectra processing.
- Development of robust alignment algorithms for LC/MS data prone to outliers.
- Supercomputer modeling of ion dynamics in arbitrary geometry electrode configurations.
- Comparative study of human urinary proteomes between smokers and non-smokers (for British American Tobacco).

Undergraduate Research:

- Routine operation and maintenance of MS and LC-MS systems (including FT-ICR, Orbitrap, TOF and Ion trap instruments), optimization of LC-MS conditions to improve protein identification.
- Assembly of an AMT tag (Accurate Mass and Time) database for human urinary proteome. Development of an in-house software pipeline for storing and querying the database.
- Design, development and creation of a source of stable negative ions suitable for use in Electron Transfer Dissociation in ion trap mass-spectrometers (funded by Shimadzu corp.)

Work Experience:

University of Michigan, Department of Pathology, Ann Arbor, MI, USA — 2013-present
Post-doctoral research fellow at prof. Alexey Nesvizhskii lab

Institute for Energy Problems of Chemical Physics, Moscow, Russia — 2011-2013
Research fellow at prof. Eugene Nikolaev's laboratory of ion dynamics (INEP CP RAS).

Institute for Energy Problems of Chemical Physics, Moscow, Russia — 2007-2011
Research assistant

Other professional experience:

SoftProm (freelance work in spare time) — 2012.03-05
Development of an interactive SVG based map plugin for a web application and its integration into the existing system (ExtJS4, PostgreSQL, PHP).

LLC "New Systems" (freelance work in spare time) — 2011.09-12
Development of an online helpdesk system integrated with a hardware telephony equipment from Avaya (IPOffice).
(C/C++, Java, Play Framework, JavaScript, jQuery, Knockout.js, MySQL)

IQmen Analytics, Java programmer — 2004-2006
Development of a system for aggregating information from the internet (Java, Perl).

List of publications:

Publications

- A.T. Kong, F.V. Leprevost, D.M. Avtonomov, D. Mellacheruvu, A.I. Nesvizhskii. “MSFragger: ultrafast and comprehensive peptide identification in mass spectrometry–based proteomics”. Nature Methods, 2017, 14, pp. 513–520 (doi:10.1038/nmeth.4256)
- D.M. Avtonomov, A. Raskind, A.I. Nesvizhskii. “BatMass: a Java software platform for LC/MS data visualization in proteomics and metabolomics”. Journal of Proteome Research, Jun 16, 2016 (doi: 10.1021/acs.jproteome.6b00021)
- Chih-Chiang Tsou, Dmitry Avtonomov, Brett Larsen, Monika Tucholska, Hyungwon Choi, Anne-Claude Gingras, Alexey I Nesvizhskii. “DIA-Umpire: comprehensive computational framework for data-independent acquisition proteomics”. Nature Methods, Jan 19, 2015 (doi: 10.1038/nmeth.3255)
- Fermin D, Avtonomov D, Choi H, Nesvizhskii AI. “LuciPHOr2: Site localization of generic post-translational modifications from tandem mass spectrometry data”. Bioinformatics, Nov 25, 2014 (doi: 10.1093/bioinformatics/btu788).
- Bugrova AE , Kononikhin AS , Avtonomov DM , Popov IA , Galetskiĭ DN , Nikolaev EN , Kalamkarov GR. “Tear fluid proteome variability in healthy donors”. Rossiiskii Fiziologicheskii Zhurnal Imeni I.M. Sechenova, 2013, 99(4), pp. 527-536.
- D. M. Avtonomov, I. A. Agron, A. S. Kononikhin, I. A. Popov, E. N. Nikolaev. “A New Method for Normalization of the Peptide Retention Times in Chromatographic/Mass Spectrometric Experiments”. Bioorganic Chemistry, 2011, Vol. 37, No. 2, pp. 146–150.
- Rjumin P.A., Boldin I.A., Avtonomov D.M., Nikolaev E.N. “Capacity method in modeling of ion clouds motion in ion traps and ion transport systems having arbitrarily shaped electrodes”. Trudy MFTI, 2011, vol. 3, No.3, pp. 186-191.
- Agron I.A., Avtonomov D.M., Kononikhin A.S., Popov I.A., Melnik S.A., Moshkovskiy S.A., Nikolaev E.N. “A combination of accurate mass and time tag approach with isotopic labeling using 18O for quantitative analisys of human urinary proteome”. Trudy MFTI, 2011, Vol. 3, No. 3, pp. 3-10.
- D.M. Avtonomov, I.A. Agron, A.S. Kononikhin, I.A. Popov, E.N. Nikolaev. “Data filtration for more robust alignment of chromatograms of complex peptide mixtures.” Bioorganicheskaiakhimiia, 2010, Vol. 37, No. 2, pp. 165–170.
- A. Agron, D. M. Avtonomov, A. S. Kononikhin, I. A. Popov, S. A. Moshkovskii, E. N. Nikolaev. “Accurate Mass Tag Retention Time Database for Urine Proteome Analysis by Chromatography–Mass Spectrometry”. Biochemistry, 2010, Vol. 75, No. 5, pp. 636-641.
- Avtonomov D.M., Agron I.A., Kononikhin A.S., Nikolaev E.N. “Creation of Accurate Mass and Time tags database for quantitative and qualitative approaches in human urinary proteome research utilizing isotopic labeling”. Trudy MFTI, 2009, No.1, 18-23.

Patents

- Russian Federation Patent. Avtonomov DM, Koninokhin AS, Popov IA, Nikolaev EN, Larina IM, Pastushkova LH (start date: 2010-10-06). “A method for alignment of LC-MS chromatograms of peptide mixtures”. Application Number: 2010140839/15, Patent number: RU 2444731 C1