Andrey Smelter

Bioinformatics Ph.D. researcher and software developer

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Employment

2017-curr. **University of Kentucky**, Markey Cancer Center, Lexington, KY 40536
I am a bioinformatics researcher and software developer at Moseley Bioinformatics Lab working on developing software packages for Nuclear Magnetic Resonance (NMR) and Mass Spectrometry (MS) data analysis, analyzing and integrating data from publicly available scientific repositories, developing pipelines to facilitate deposition of metabolomics data.

Education

2013-2017 **University of Louisville**, Louisville, KY 40292
Department of Computer Engineering and Computer Science
Bioinformatics Ph.D.
My Ph.D. thesis "Algorithms for automated assignment of solution-state and solid-state protein NMR spectra"
is available through the ThinkIR: The University of Louisville's Institutional Repository: ir.library.louisville.edu/etd/2779.

2010-2013 **University of Louisville**, Louisville, KY 40292
Department of Chemistry
M.S. Chemistry

2005-2010 **Perm State University**, Perm, Russia 614990
Department of Chemistry
Specialist Degree in Physical Chemistry

Publications

2018 **Andrey Smelter**, and Hunter NB Moseley. "A Python library for FAIRer access and deposition to the Metabolomics Workbench Data Repository", Metabolomics 14.5 (2018): 64, doi:10.1007/s11306-018-1356-6
Xi Chen, **Andrey Smelter**, and Hunter N.B. Moseley. "Automatic 13 C Chemical Shift Reference Correction for Unassigned Protein NMR Spectra", Journal of Biomolecular NMR, doi:10.1007/s10858-018-0202-5

2017 **Andrey Smelter**, Eric C. Rouchka, and Hunter N.B. Moseley. "Detecting and accounting for multiple sources of positional variance in peak list registration and spin system grouping", Journal of Biomolecular NMR, doi:10.1007/s10858-017-0126-5
Andrey Smelter, Morgan Astra, and Hunter NB Moseley. "A fast and efficient python library for interfacing with the Biological Magnetic Resonance Data Bank", BMC bioinformatics 18.1 (2017): 175, doi:10.1186/s12859-017-1580-5

Presentations at Scientific and Professional Meetings

2018 "Isotopic Enumerator: a Python package to facilitate isotopically-resolved annotation and deposition of metabolomics data", **Andrey Smelter**, Hunter N.B. Moseley, Resource Center for Stable Isotope-Resolved Metabolomics Symposium, Lexington, KY

2017 "Registration and grouping algorithms in protein NMR derived peak lists and their application in protein NMR reference correction", **Andrey Smelter**, Xi Chen, Eric C.

Rouchka, Hunter N.B. Moseley, Biophysical Society Meeting, New Orleans, LA
"Registration and grouping algorithms in protein NMR derived peak lists and their application in protein NMR reference correction", **Andrey Smelter**, Xi Chen, Eric C. Rouchka, Hunter N.B. Moseley, UT-KBRIN Bioinformatics Summit, Burns, TN
"A Fast and Efficient Python Library for Interfacing with the Biological Magnetic Resonance Data Bank", **Andrey Smelter**, Morgan Astra, Hunter N.B. Moseley, UT-KBRIN Bioinformatics Summit, Burns, TN
"Application of peak list registration and spin system grouping algorithms in protein NMR derived peak lists", **Andrey Smelter**, Hunter N.B. Moseley, Commonwealth Computational Summit, Lexington, KY
"Data Quality & Consistency in Scientific Repositories", **Andrey Smelter**, Systems Biology and Omics Integration Journal Club.
"Parsing mwTab files Provided by Metabolomics Workbench NIH Metabolomics Data Repository", **Andrey Smelter**, Hunter N.B. Moseley, Metabolomics Workbench Usability Meeting.
"mwtab Python Library: facilitate reading and writing files in mwTab format", **Andrey Smelter**, Hunter N.B. Moseley, Metabolomics Workbench Usability Meeting.

2016 "Automated Assignment of Magic-Angle-Spinning Solid-State Protein NMR Spectra", **Andrey Smelter**, Eric C. Rouchka, Hunter N.B. Moseley, UT-KBRIN Bioinformatics Summit, Cadiz, KY

2015 "Automated Assignment of Magic-Angle-Spinning Solid-State Protein NMR Spectra", **Andrey Smelter**, Indraneel Reddy, Eric C. Rouchka, Hunter N.B. Moseley, UT-KBRIN Bioinformatics Summit, Buchanan, TN

Software Engineering Skills

Programming Languages: Python, working knowledge of C++, R
Python packages: NumPy, SciPy, Jupyter, Cython, bokeh, matplotlib, PyQt
Software documentation: sphinx, Doxygen, Roxygen
Software testing: pytest, unittest, testthat
Version control: Git, Github, Gitlab
Virtualization: Docker, VirtualBox, QEMU/KVM

Software

nmrstarlib

github.com/MoseleyBioinformaticsLab/nmrstarlib
I developed the nmrstarlib package – a Python library that facilitates reading and writing NMR-STAR formatted files used by the Biological Magnetic Resonance Data Bank (BMRB) for archival of Nuclear Magnetic Resonance (NMR) data and CIF formatted files used by Protein Data Bank (PDB).

mwtab

github.com/MoseleyBioinformaticsLab/mwtab
I developed the mwtab package – a Python library that facilitates reading and writing files in mwTab format used by the Metabolomics Workbench for archival of Mass Spectrometry (MS) and Nuclear Magnetic Resonance (NMR) experimental data.

jpredapi

github.com/MoseleyBioinformaticsLab/jpredapi
I developed the jpredapi package that provides a simple Python interface for submitting and retrieving jobs from JPred: A Protein Secondary Structure Prediction Server (JPred).

jpredapir

github.com/MoseleyBioinformaticsLab/jpredapir
I reimplemented jpredapi package using R programming language, the package provides R interface for submitting and retrieving jobs from JPred: A Protein Secondary Structure Prediction Server (JPred).

`chi2plookup`

github.com/MoseleyBioinformaticsLab/chi2plookup
I implemented the chi2plookup – a simple command-line interface for creating C++ header file for use in C++ projects. This header file contains pregenerated array(s) of p-values for chi-square distribution for specified degrees of freedom.

`filehandles`

github.com/MoseleyBioinformaticsLab/filehandles
I implemented the filehandles package – a Python library that facilitates processing of files by removing boilerplate code that you need to write to open files from directories, zip archives, tar archives, URL addresses of files, etc. It also automatically closes open file handle after it has been processed.

`ctfile`

github.com/MoseleyBioinformaticsLab/ctfile
I implemented the ctfile Python package (work in progress) for parsing data from files in CTfile formats, e.g. Molfiles and SDfiles widely used in chemoinformatics.

`isoenum`

github.com/MoseleyBioinformaticsLab/isoenum
I developed the isoenum Python package (work in progress) – Isotopic (iso) enumerator (enum) enumerates isotopically-resolved InChI (International Chemical Identifier) for metabolites for the purpose of unambiguous data deposition.

`ubuntu-foswiki`

github.com/andreysmelter/ubuntu-foswiki
A docker container that creates instance of running Foswiki web site - wiki document management system that facilitates collaboration.

Honors and Awards

4-year Scholarship from University of Louisville (2013-2017).
5-year Scholarship from Perm State University (2005-2010).
Outstanding student scholarship from LUKOIL energy corporation (2009-2010).

Links

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