Ivan V Grishagin PhD

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SKILLS

Informatics
- **Data Science:** R, Python, VBA, ImageJ Macro Language, MS Power Query, Neo4j, RDBMS (MySQL, Oracle, PostgreSQL), Big Data processing (10B datapoints), Cypher, SQL, data mining and organization, database design and data modeling, data harmonization.
- **Bioinformatics:** Microarray data analysis, Illumina BeadArray data processing, protein array analysis (ProtoArray), Gene Set Enrichment Analysis.
- **Software Development:** Python, Flask, Java, Play Framework, JavaScript, jQuery, Google Apps Script, Git, bash, PowerShell, Markdown, HTML5, CSS3/SASS, Materialize Framework, Java, Play Framework, Docker.

Wet Lab
- **Cell biology:** mammalian cell culture, cell viability assays, gene expression profiling (microarray, qRT-PCR), PCR, western blot, confocal and fluorescent microscopy, flow cytometry and cell sorting, luciferase reporter assay, colony formation assay, molecular cloning, protein expression and purification, low-throughput screening (20K assay points) in cell-based assays.
- **In vivo testing:** xenograft implantation into mice, IP and IV injections, euthanasia, organ harvesting, tissue handling, in vivo imaging, histology.
- **Chemistry:** organic synthesis, NMR, HPLC, LC-MS, IR, UV-Vis, dynamic/static light scattering.

General
- **Key software:** R Studio, Git, Windows Subsystem Linux, Visual Studio Code, Sublime Text 3, SQL Developer, DBeaver, MS Office 365, Excel, ImageJ, Adobe Photoshop, Adobe Lightroom.
- **Languages:** English (Fluent), Russian (Native), German (Intermediate), French (Intermediate).

EXPERIENCE

2015-present   *Various Scientific and Management Roles*
Rancho BioSciences   **Remote**

2022-present	Principal Scientist
2020-present	Team Leader
2018-2021	Senior Bioinformatics Scientist
2015-2018	Bioinformatics Scientist

- Multi-omic (microarray, protein array, sequencing, RNA-Seq), biosensor, viability assay data analysis, interpretation, formatting, and visualization.
- Data scraping, parsing, cleanup, harmonization, and alignment with ontologies.
- Preparation and evaluation of metadata models.
- R development: code refactoring, debugging, and optimization; building R packages.
- Developed a pipeline for a highly efficient analysis and transformation of a large dataset with over 500K rows and 20K columns for a consumer-grade laptop.
- Implemented complex statistical methods and visualization tools into a Protein Array Analyzer R package.

- VBA development: MS Excel/Word/Powerpoint macros and add-ins for data curation.
- Liaison, informatician, developer, and PM at NIH NCATS (see below).
- Project management:
  - project architecture and specifications
  - server organization guidelines
  - problem solving
  - liaison for the development, curation, and management teams.
- Line management: leading a team of 5 junior and senior data scientists and engineers working remotely on a wide variety of projects.
- Administrative: assisted in various aspects of the company's growth and development including
  - *de novo* design and preparation of robust and user-friendly personnel action forms for HR,
  - developing an unconventional approach to company-wide communications,
  - hiring.
- Interaction with clients, presales, proposal preparation.

2015-2022   *On-site informatician, developer, liaison, and PM*
National Center for Advancing Translational Sciences   **Remote / Rockville, MD**
- Managed, oversaw, and participated in the development of Inxight Drugs, a comprehensive portal for drug development information. Prepared the data, designed and implemented UI elements, layout of the pages, and worked out user experience aspects.
- Comprehensive annotation of 50K chemical compounds: responsible for workflow, UI/UX, and database design and specifications, management of the web UI development, annotation oversight, QC, and QnA.
- Designed and developed an R-based comprehensive pipeline for integration of key public and manually curated pathway sources, and elaborate visualization of 1,658 pathway maps for NCATS BioPlanet.
- Oversaw the development of the NCATS BioPlanet, a public resource for interactive browsing and analysis of human pathways and pathway connections. Responsible for collecting and cleaning pathway data, providing pathway visualizations, UI/UX design, and debugging.
- Designed and developed a complete web-based application for the collection of pharmacokinetic data.
- Annotation of drugs with orphan designations issued by FDA, EMA, and NIBIOHN: responsible for the data aggregation and preparation, workflow design, and project coordination.
- Performed a complete comprehensive annotation of 350 rare and novel epigenetic modifiers with over 8,000 fields. Developed workflow and R code for automated annotation, performed annotation and QC.
- Designed and developed a complete AWS-based interactive landing page, including layout, color palette, and graphics.
- Developed a web-based Flask application for 96/384/1536 plate format conversion and registration.
- Designed and co-managed the development of a curation interface for editing chemical reactions and concomitant metadata within Palantir Foundry.
- Public NCATS web resources: responsible for project management, team coordination, and support for the development of UI/UX specifications and data selection/representation.
- Responsible for coordination and management of some external collaborations.

2014-2015 *Research Fellow*
Queen's University Belfast, CCRCB **Belfast, Northern Ireland**

- Main project: repurposing FDA-approved drugs for blood cancer therapies.
- Developed a complete pipeline solution for automatic data processing of Illumina BeadArray output with R: from raw data to publication-quality figures.
- Analyzed response of leukemia to salinomycin at the transcription level using Illumina BeadArray. Processed the data, discovered 18 significantly affected genes, and confirmed by qRT-PCR.
- Used connectivity mapping with Library of Integrated Cellular Signatures (LINCS) to identify approved drugs efficacious against known drivers of leukemia.
- Designed and carried out a comprehensive screen of an FDA-approved drug library (760 compounds, 3 concentrations, 2 cell lines, 2 time points, and 2 replicates each) in two primary mouse cell lines. Analyzed the data and confirmed the hits in murine and human patient cells.
- Analyzed numerous microarray, protein array, sequencing, and viability assay data sets.

2010-2014 *Research Assistant*
University of Southern California, School of Pharmacy **Los Angeles, CA**

- Determined high in vitro and in vivo anticancer efficacy of topographical mimetics of HIF1α in disrupting hypoxia-dependent pathways.
- Investigated uptake, toxicity, and in vivo anticancer efficacy of rhomboidal Pt(II) metallacycles.
- Designed and completed a screen of 105 compounds to discover inhibitors of hypoxia-inducible signaling in breast cancer. Analyzed the data and confirmed the hits.
- Designed, developed, and published a complete, inexpensive, and robust method to count live mammalian cells automatically 10-15 times faster than the conventional approach.
- Investigated synergy of simultaneous inhibition of MAOA and hypoxia-inducible transcription in prostate cancer.
- Supervised, mentored, and taught undergraduate and junior graduate students.

2008-2010 *Research and Teaching Assistant*
University of Arizona, Department of Chemistry **Tucson, AZ**

- Optimized the synthesis of an epidithiodiketopiperazine precursor on a gram scale for a facile preparation of BC001, a designed molecule with in vivo anticancer properties, in clinically relevant quantities. BC001 was licensed to Globavir, and in 2015 exclusively licensed to Sorrento Therapeutics for $80 million in regulatory and sales milestones, in addition to multi-tiered royalty payments.
- Conducted organic chemistry labs and related lectures for undergraduate students.
- Proctored and graded the examinations in undergraduate organic chemistry classes.

EDUCATION

Tim Buchalka's Learn Programming Academy **Udemy**
Learn Python Programming Masterclass Completion Certificate, 2019

Johns Hopkins Bloomberg School of Public Health **Coursera**
R Programming Verified Certificate (with Distinction), 2014
Getting and Cleaning Data Verified Certificate (with Distinction), 2014

University of Southern California, School of Pharmacy Los Angeles, CA

PhD in Pharmaceutical Sciences (**GPA 3.91**), 2014
Dissertation: "Small Molecule Modulators of HIF1α Signaling"

University of Arizona, Department of Chemistry Tucson, AZ

Attained PhD candidacy (**GPA 4.0**), 2010
Transferred to University of Southern California

Lomonosov Moscow State University, Department of Chemistry Moscow, Russia

Diploma in Polymer Chemistry (**Summa cum Laude**, Gold Medal), 2008
Thesis: "Formation of Interpolyelectrolyte Complexes in Organic Media of Low Polarity"

PUBLICATIONS

PAPERS

- Zahoránszky-Kőhalmi, G.; Siramshetty, V.B.; Kumar, P.; Gurumurthy, M.; Grillo, B.; Mathew, B.; Metaxatos, D.; Backus, M.; Mierzwa, T.; Simon, R.; **Grishagin, I.**; Brovold, L.; Mathé, E.A.; Hall, M.D.; Michael, S.G.; Godfrey, A.G.; Mestres, J.; Jensen, L.J. and Oprea, T.I. A Workflow of Integrated Resources to Catalyze Network Pharmacology Driven COVID-19 Research. *J. Chem. Inf. Model.* **2022** DOI: 10.1021/acs.jcim.1c00431

- Siramshetty, V.B.; **Grishagin, I.**; Nguyễn, Đ.-T.; Peryea, T.; Skovpen, Y.; Stroganov, O.; Katzel, D.; Sheils, T.; Jadhav, A.; Mathé, E.A.; Southall, N.T. NCATS Inxight Drugs: a comprehensive and curated portal for translational research. *Nucleic Acids Res.* **2022**, DOI: 10.1093/nar/gkab918

- Bazdyrev, E.; Rusina, P.; Panova, M.; Novikov, F.; **Grishagin, I.**; Nebolsin, V. Lung Fibrosis after COVID-19: Treatment Prospects. *Pharmaceuticals* **2021**, 14 (8), 807, DOI: 10.3390/ph14080807

- Zhu, Q.; Nguyễn, Đ.-T.; **Grishagin, I.**; Southall, N.; Sid, E.; Pariser, A. An integrative knowledge graph for rare diseases, derived from the Genetic and Rare Diseases Information Center (GARD). *J. Biomed. Semant.* **2020**, 11(13), DOI: 10.1186/s13326-020-00232-y

- Kettyle, L.; Lebert-Ghali, C.E.; **Grishagin, I.V.**; Dickson, G.; O'Reilly, P.G.; Simpson, D.; Bijl, J.; Mills, K.; Sauvageau, G. & Thompson, A. Pathways, Processes, and Candidate Drugs Associated with *Hoxa* Cluster-Dependency Model of Leukemia *Cancers* **2019**, 11, 2036, DOI: 10.3390/cancers11122036

- Huang, R.; **Grishagin, I.**; Wang, Y.; Zhao, T.; Greene, J.; Obenauer, J.C.; Ngan, D.; Nguyen, D.-T.; Guha, R.; Jadhav, A.; Southall, N.; Simeonov, A. & Austin, C.P. The NCATS BioPlanet – An Integrated Platform for Exploring the Universe of Cellular Signaling Pathways for Toxicology, Systems Biology, and Chemical Genomics Front. *Pharmacol.* **2019**, DOI: 10.3389/fphar.2019.00445

- Matchett, K.B.; **Grishagin, I.V.**; Kettyle, L.M.; Dowling, C.; Chonghaile, T.N.; Mills, K.I.; Thompson, A. High-throughput screen identification of albendazole as a novel repurposed drug in acute myeloid leukaemia. *Blood* **2017**, 130(Supplement 1), 5062, DOI: 10.1182/blood.V130.Suppl_1.5062.5062

- Roulston, G.; Burt, C.; Kettyle, L.; Matchett, K.; Keenan, H.; Mulgrew, N.; Ramsey, J.; Dougan, C.; McKiernan, J.; **Grishagin, I.**; Mills, K.; & Thompson, A. Low-Dose Salinomycin Induces Anti-leukemic Responses in AML and MLL. *Oncotarget* **2016**, 7(45), 73448-73461, DOI: 10.18632/oncotarget.11866

- Matchett, K.B.; **Grishagin, I.**; Kettyle, L.M.; Gavory, G.; Harrison, T.; Mills, K.I.; & Thompson, A. Mebendazole: A Candidate FDA Approved Drug for Repurposing in Leukaemia. *Br. J. Haematol.* **2016**, 173(Supplement S1):5-178, 9, DOI: 10.1111/bjh.14019
- Kettyle, L.M.; Lebert-Ghali, C.; **Grishagin, I.**; Dickson, G.J.; Bijl, J.J.; McMullin, M.F.; Lappin, T.R.; Mills, K.I.; & Thompson, A. Conditional Deletion of the HOXA Cluster in MLL-AF9 is Incompatible with Leukemia Maintenance, *Hematologica* **2016**, 101(S1), 38
- Kettyle, L.M.; **Grishagin, I.**; Dickson, G.J.; Lebert-Ghali, C.; Bijl, J.J.; Mills, K.I.; & Thompson, A. Conditional Deletion of the Hoxa Cluster in MLL-AF9 is Incompatible with Leukemia Maintenance. *Br. J. Haematol.* **2016**, 173(Supplement S1):5-178, 121, DOI: 10.1111/bjh.14019
- Kettyle, L.M.; **Grishagin, I.**; Dickson, G.J.; Lebert-Ghali, C.; Bijl, J.J.; Mills, K.I.; & Thompson, A. Conditional Deletion of the Hoxa Cluster in MLL-AF9 is Incompatible with Leukemia Maintenance. *Blood* **2015**, 126(23), 3630, DOI: 10.1182/blood.V126.23.3630.3630
- **Grishagin, I.** Automatic Cell Counting with ImageJ. *Anal. Biochem.* **2015**, 473, 63-65, DOI: 10.1016/j.ab.2014.12.007
- **Grishagin, I.**; Pollock, J.B.; Kushal, S.; Cook, T.R.; Stang, P.J.; Olenyuk, B.Z. In Vivo Anticancer Activity of Rhomboidal Pt(II) Metallacycles. *PNAS* **2014**, 111, 52, 18448–18453, DOI: 10.1073/pnas.1418712111
- Lao, B.B.*; **Grishagin, I.***; Mesallati, H.; Brewer, T.; Olenyuk, B.Z.; Arora, P.S. In Vivo Modulation of Hypoxia-Inducible Signaling by Topographical Helix Mimetics. *PNAS* **2014**, 111, 21, 7531-7536, DOI: 10.1073/pnas.1402393111
  *authors contributed equally
- Dubey, R.; **Grishagin, I.**; Nagavarapu, U.; Balan, C.; Gupta, S.; Olenyuk, B.Z. Novel Selective HIF1 Alpha Inhibitor: Well Tolerated with Excellent Efficacy in Renal Cell Cancer Xenograft Studies. *Cancer Res.* **2015**, 74(19 Supplement), 1014, DOI:10.1158/1538-7445.AM2014-1014
- **Grishagin, I.**; Olenyuk, B.Z.; Bullock, B.; Arora, P.S. OOPs: Novel HIF-1α Mimics. *Cancer Res.* **2012**, 72(8 Supplement), 283, DOI:1538-7445.AM2012-283
- Burkhardt, M.; Martinez-Castro, N.; Tea, S.; Drechsler, M.; Babin, I.; **Grishagin I.**; Schweins, R.; Pergushov, D.V.; Gradzielski, M.; Zezin, A.B.; Müller, A.H.E. Polyisobutylene-block-Poly(methacrylic acid) Diblock Copolymers: Self-Assembly in Aqueous Media. *Langmuir* **2007**, 23 (26), 12864-12874, DOI: 10.1021/la701807b

PATENTS

- Arora, P.S.; Olenyuk, B.Z.; Bullock, B.; **Grishagin, I.** Control of Hypoxia-Inducible Gene Expression with Oligooxopiperazine Nonpeptidic Helix Mimetics. US Patent 9255086 B2, Feb 09, **2016**
- Arora, P.S.; Olenyuk, B.Z.; Bullock, B.; **Grishagin, I.** Control of Hypoxia-Inducible Gene Expression with Oligooxopiperazine Nonpeptidic Helix Mimetics. International Patent WO 2013123511 A1, Aug 22, **2013**

POSTERS

- BioIT World Conference & Expo, Boston, MA, April 16-18, **2019**
- BioIT World Conference & Expo, Boston, MA, May 15-17, **2018**, #54
- AACR meeting, Chicago, IL, April 1-4, **2012**, #283
- 6th International Symposium "Molecular Mobility and Order in Polymer Systems", St. Petersburg, Russia, June 2-6, **2008**
- Bayreuth Polymer Symposium, Bayreuth, Germany, September 9-11, **2007**, PI21

- 41st IUPAC World Polymer Congress, Moscow, Russia, June 27-July 1, **2005**, p.231, P9.4-23
- 5th International Symposium "Molecular Mobility and Order in Polymer Systems", St. Petersburg, Russia, June 20-24, **2005**, P-186

HONORS AND AWARDS

- Member of Phi Kappa Phi Collegiate Honor Society, US, **2014**
- Member of Rho Chi Academic Honor Society in Pharmacy, Theta Chapter, US, **2014**
- Winner of USC Norris Comprehensive Cancer Center Charles Heidelberger Predoctoral Scholarship Award in Cancer Research, Los Angeles, CA, US, **2013**
- Recipient of the Presidential Scholarship, Moscow, Russia, **2008**
- Winner of "Potanin Scholarship-2007" for the "Balance of Individualism and Leadership Qualities", Moscow, Russia, **2007**