# Oleksandr V. Savytskyi, PhD

**Citizenship:** Ukrainian ▪ **Date of birth:** 13 February 1985

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## Scientific Interests

I have completed my PhD in Molecular Biology. My interests are related to computational structural biology: structural modeling, molecular dynamics, molecular docking/virtual screening, drug discovery, grid and high-performance computing, machine learning, computer services developing, 2D/3D scientific visualization.

## Education

**10.2010 – 05.2017** **PhD in Molecular Biology**

Protein Engineering and Bioinformatics Department, Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine (IMBG of NAS of Ukraine).

***PhD Thesis:*** **"**Computational modeling and molecular dynamics simulations of *H. sapiens* tyrosyl-tRNA synthetase and its mutant forms".

***Advisor:*** Prof. Alexander I. Kornelyuk, Corresponding Member of NAS of Ukraine, Head of Protein Engineering and Bioinformatics Department in same Institute.

**09.2006 – 12.2007** **Master of Science in Biology**

Plant Protection, National University of Life and Environmental Sciences of Ukraine.

***Advisor:*** Dr. Andrii P. Gryganskyi, Assistant Professor of Plant Pathology Department.

**09.2002 – 06.2006** **Bachelor's Degree in Biology**

Plant Protection, National University of Life and Environmental Sciences of Ukraine.

***Advisor:*** Dr. Andrii P. Gryganskyi, Assistant Professor of Plant Pathology Department.

## Work Experience

**05.2022 till now** **Postdoctoral Research Fellow**, Molecular Modeling and Drug Discovery Laboratory, Department of Neuroscience, Department of Computational Biology (Div of Health Sciences), Mayo Clinic, Jacksonville, Florida, USA.

***Projects****:* various pre-clinical researches in cancer and neurological diseases (with wet labs).

**03.2019 – 10.2019** **Postdoctoral Research** in Bioinformatics and High Performance Computing Research Group, Catholic University of Murcia (UCAM, South East Spain) supported by HPC-Europa3. ***Project Title:*** The Role of Connective Peptide 1 in Human Tyrosyl-tRNA Synthetase and its Mutant Forms, Associated with Charcot-Marie-Tooth Neuropathy.

**04.2012 – 12.2016** **Subject Matter Expert** in Computational Structural Biology in collaboration with EGI.eu. ***Consulting*** IT developers based on requirements of the scientific community (MD simulations in GROMACS and NAMD software in GRID and CLOUD with GPU calculations).

**07.2008 – 05.2022** **Senior Researcher** (*Engineer* → *Junior Researcher* → *Researcher*) of Protein Engineering and Bioinformatics Department, Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine.

● Supervising the research activities in Computational and Structural Biology (pre-clinical research) ● Working on computational protocols in drug discovery process (*in silico*) ● Computer services development for the Molecular Dynamics simulations and trajectories analyses ● Control of the group's budget ● Senior Consultant

## Languages

**Ukrainian** (native) **Russian** (excellent) **English** (very good)

## Computing Qualifications and Skills

**Sequence alignments:** BLAST, FASTA, ClustalW
**Homology modeling:** Modeller, PRIME, SWISS-MODEL
**Molecular dynamics:** GROMACS, Desmond, NAMD
**Molecular docking:** Molsoft ICM Pro, GLIDE, Autodock, GOLD
**Molecular graphics:** PyMOL, VMD, Chimera, Maestro
**Data analyses:** OriginPro, Excel, gnuplot
**HPC\GRID\Cloud:** ARC, gLite, PBS Pro, Slurm, rsync, scp
**Programming lang.:** Python (basic), Bash (basic), HTML (basic)

**Other software:**
Windows, Linux (basic); 3d's Max 2013 (V-Ray, RayFire, FumeFX, RealFlow, DreamScape); Autodesk Maya 2013; Abobe Photoshop 2015, After Effects 2015, Premiere Pro 2015, Flash CC.

**Web:**
WordPress, Joomla, MySQL

## Laboratory Techniques

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| **Chemistry:** | solution preparation, titrations, extractions filtrations, separations, distillation. |
| **Microbiology:** | aseptic and sterile techniques, bacterial staining, plating methods, enumeration and identification of bacteria, use of biological safety cabinets, media and buffer preparation, food microbiology, optical microscopy, transmission electron microscope, scanning microscopy. |
| **Spectroscopy:** | UV, visible, mass spectroscopy. |
| **Molecular Biology:** | PCR, agarose gel electrophoresis, cell fractionation by centrifugation. |

## Awards and Grants *(selected)* | Full CV: http://alstudio.org/docs/Savytskyi_O.V._CV.pdf

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| **2023** | **Grant** from **International School of Crystallography** to Participation in the ***"STRUCTURAL DRUG DESIGN 2023: BIOLOGY, CHEMISTRY AND COMPUTERS"*** 2 - 10 June 2023, Erice, Sicily, Italy. |
| **2018** | **State Prize of the President of Ukraine** for young scientists, Kyiv, Ukraine. Presented by IMBG of NASU (Authors: *Oleksandr V. Savytskyi, Andrii O. Salnikov, Ievgen A. Sliusar*). |
| | **Platon Kostyuk Award 2018**, which is provided by the Shevchenko Scientific Society, Inc (New York, USA: http://shevchenko.org), 20 December 2018, Kyiv **–** New York). |
| | **Fellowship of the President of Ukraine** for young scientists (2018 – 2020). |
| | **FEBS YTF Grant and Certificate** of Participation in the FEBS Advanced Course ***"Ligand-binding theory and practice"***, 24 June - 1 July 2018, Nove Hrady, Czech Republic. |
| | **Diploma of Laureate** of Kyiv City Mayor Prize (Vitali V. Klitschko) for special achievements of youth in the development of the capital of Ukraine – Hero-City of Kyiv, 24 June 2018, Kyiv, Ukraine. |
| **2017** | **Travel Grant from iNEXT** (Horizon2020 #653706) for Participation in the Workshop on ***"Bridging Solution Methods: From NMR to Xray Scattering And Biophysics"***, 18-22 September 2017, Patras, Greece. |
| **2016** | **FEBS YTF Grant and Certificate** of Participation in the FEBS/IUBMB Advanced Lecture Course *"**Molecular basis of human diseases: 50 years anniversary of Spetses summer schools***", 27th May - 1st June, 2016, Spetses island, Greece. |
| **2015** | **Travel Grant from Cineca (IT) with PRACE (Partnership for Advanced Computing in Europe) and Certificate** of Participation in the ***"High Performance Molecular Dynamics@CINECA"***, 18-20 November 2015, CINECA – BOLOGNA, Italy. |
| **2014** | **FEBS-EMBO Travel Grant and Certificate** of Participation in the ***"FEBS-EMBO Conference 2014"***, 30 August - 4 September 2014, Paris, France. |
| **2013** | **FEBS YTF Grant and Certificate** of Participation in the FEBS/EMBO Lecture Course ***"Protein interactions, assemblies and human disease"***, 16–26 September 2013, Spetses, Greece. |
| | **Travel Grant from NAS of Ukraine and Certificate** of Participation in the ***"9th European Biophysics Congress EBSA 2013"***, 13-17 July 2013, Lisbon, Portugal. |
| | **Travel Grant from NAS of Ukraine and Certificate** of Participation in the ***"6th Theoretical Biophysics Symposium"***, 24-27 June 2013, Gothenburg, Sweden. |
| | **Travel Grant from eSSENCE and Uppsala University** for Participation in the eSSENCE International Workshop on ***"Macromolecular Structure and Dynamics"***, 3-5 June 2013, BMC, Uppsala, Sweden. |
| **2012** | **Travel Grant from NAS of Ukraine and Certificate** of Participation in the ***"NorduGrid 2012"*** Conference, 30 May - 01 June 2012, Uppsala, Sweden. |
| | **"Standard HPC Grant 2012"** on Matrix cluster (100 000 CPU hours) from CASPUR scientific research program, Roma, Italy. (collaboration with Tullio Scopigno, Taras Bryk) |
| **2011** | **FEBS YTF Grant and Certificate** of Participation in the Workshop on "***Cell Biology and Pharmacology of Mendelian Disorders***", 7-11 October 2011, Vico Equense (Naples), Italy. |
| | **Travel Grant from NAS of Ukraine and Certificate** of Participation in IEEE International Conference ***IDAACS'2011 (Intelligent Data Acquisition and Advanced Computing Systems)***, 15-17 September, Prague, Czech Republic. |
| **2010** | **FEBS YTF Grant and Certificate** of Participation in ***"Physical Chemistry of Biointerfaces"*** Workshop, 19-24 July 2010, Donostia - San Sebastian, Spain. |
| **2005** | ***Phytopharmacology Academy of Syngenta*** Awarded the **Certificate** of completion, 23 December 2005, Kyiv, Ukraine. |

## Publications *(selected)* | Full CV: http://alstudio.org/docs/Savytskyi_O.V._CV.pdf

### PAPERS IN INTERNATIONAL JOURNALS:

1. Gupta Y, **Savytskyi OV**, Coban M, Venugopal A, Pleqi V, Weber CA, Chitale R, Durvasula R, Hopkins C, Kempaiah P, Caulfield TR. (**2022**). PROTEIN STRUCTURE-BASED IN-SILICO APPROACHES TO DRUG DISCOVERY: GUIDE TO COVID-19 THERAPEUTICS. *Molecular Aspects of Medicine*. Oct 28:101151. doi: 10.1016/j.mam.2022.101151. in press (**Q1, Impact Factor: 16.4**$^{2022}$)
2. **Savytskyi O.V.**, & Kornelyuk O.I. (**2022**). COMPUTATIONAL MODELING OF THE COMPLEX BETWEEN GLYCYRRHIZIN AND SARS-CoV-2 PROTEASE 3CLpro AS A TARGET FOR THE DEVELOPMENT OF ANTIVIRAL DRUGS. Reports of the National Academy of Sciences of Ukraine, (1), 115–123. (in Ukrainian) PDF
3. Galyna P. Volynets, Larysa V. Pletnova, Vladislav M. Sapelkin, **Oleksandr V. Savytskyi**, Sergiy M. Yarmoluk (**2021**). A COMPUTATIONAL ANALYSIS OF THE BINDING FREE ENERGIES OF APOPTOSIS SIGNAL-REGULATING KINASE 1 (ASK1) INHIBITORS FROM DIFFERENT CHEMOTYPES. *Molecular Simulation,* 47:18, 1558-1568. (**Impact Factor: 1.7**$^{2021}$) PDF
4. Kravchuk, V. O., **Savytskyi, O. V.**, Odynets, K. O., Mykuliak, V. V., & Kornelyuk, A. I. (**2017**). COMPUTATIONAL MODELING AND MOLECULAR DYNAMICS SIMULATIONS OF MAMMALIAN CYTOPLASMIC TYROSYL-tRNA SYNTHETASE AND ITS COMPLEXES WITH SUBSTRATES. *J Biomol Struct Dyn*, 35(13): 2772-2788. (**Impact Factor: 2.9**$^{2016}$) PDF
5. **Savytskyi, O. V.**, & Kornelyuk, A. I. (**2015**). COMPUTATIONAL MODELING OF MOLECULAR DYNAMICS OF G41R MUTANT FORM OF HUMAN TYROSYL-tRNA SYNTHETASE, ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. *Ukr Biochem J*, 87(6), 142-153. (in Ukrainian) PDF
6. **Savytskyi, O. V.**, Yesylevskyy, S. O., & Kornelyuk, A. I. (**2013**). ASYMMETRIC STRUCTURE AND DOMAIN BINDING INTERFACES OF HUMAN TYROSYL-tRNA SYNTHETASE STUDIED BY MOLECULAR DYNAMICS SIMULATIONS. *J Mol Recognit*, 26(2), 113-120. (**Impact Factor: 3.31**$^{2013}$) PDF
7. Yesylevskyy, S. O., **Savytskyi, O. V.**, Odynets, K. A., & Kornelyuk, A. I. (**2011**). INTERDOMAIN COMPACTIZATION IN HUMAN TYROSYL-tRNA SYNTHETASE STUDIED BY THE HIERARCHICAL ROTATIONS TECHNIQUE. *Biophysical Chemistry*, 154(2-3), 90-98. (**Impact Factor: 2.276**$^{2011}$) PDF
8. Salnikov, A., Sliusar, I., Sudakov, O., **Savytskyi, O.**, & Kornelyuk, A. (**2010**). VIRTUAL LABORATORY MOLDYNGRID AS A PART OF SCIENTIFIC INFRASTRUCTURE FOR BIOMOLECULAR SIMULATIONS. *International Journal of Computing,* 9(4), 294-300. PDF
9. **Savytskyi, O. V.**, Sliusar, I. A., Yesylevskyy, S. O., Stirenko, S. G., & Kornelyuk, A. I. (**2011**). INTEGRATED TOOLS FOR MOLECULAR DYNAMICS SIMULATION DATA ANALYSIS IN THE MOLDYNGRID VIRTUAL LABORATORY. *Proceedings of the 6-th IEEE International Conference on Intelligent Data Acquisition and Advanced Computing Systems: Technology and Applications*, IDAACS 2011, 1, 209-211. (ISI Proceedings) PDF

## Oral Presentations *(selected)* | Full CV: http://alstudio.org/docs/Savytskyi_O.V._CV.pdf

1. **Oleksandr V. Savytskyi.** COMPUTATIONAL MODELING OF EML4-ALK STRUCTURES (*ALLOSTERIC INHIBITORS*), *Center of Individualized Medicine – Patient Care Technician (CIM-PCT Retreat)*. 26 August 2022, Rochester, NM, USA.
2. **O.V. Savytskyi**, V.O. Kravchuk and A.I. Kornelyuk. THE NEW ROLE OF CONNECTIVE PEPTIDE 1 IN MAMMALIAN TYROSYL-tRNA SYNTHETASE RELATED TO MUTATIONS ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. *iNEXT Workshop on "Bridging Solution Methods: From NMR to Xray Scattering And Biophysics"*, 18-22 September 2017, Patras, Greece.
3. **Oleksandr V. Savytskyi**, Semen O. Yesylevskyy and Alexander I. Kornelyuk. DOMAIN BINDING INTERFACES IN HUMAN TYROSYL-tRNA SYNTHETASE STUDIED BY THE HIEROT TECHNIQUE AND MOLECULAR DYNAMICS SIMULATIONS. *The eSSENCE International Workshop on "Macromolecular Structure and Dynamics"*, 3-5 June 2013, BMC, Uppsala, Sweden.
4. **Oleksandr Savytskyi** and Alexander Kornelyuk. MOLECULAR DYNAMICS SIMULATIONS OF TYROSYL-tRNA SYNTHETASE AND ITS MUTANTS IN MOLDYNGRID VIRTUAL LABORATORY. *The NorduGrid 2012 Conference*, 30 May – 01 June 2012, Uppsala, Sweden.
5. **O.V. Savytskyi**, I.A. Sliusar, S.O. Yesylevskyy, S.G. Stirenko, A.I. Kornelyuk. INTEGRATED TOOLS FOR MOLECULAR DYNAMICS SIMULATION DATA ANALYSIS IN THE MOLDYNGRID VIRTUAL LABORATORY**.** *The 6-th IEEE International Conference IDAACS 2011*, 15-17 September 2011, Prague, Czech Republic.

**Poster Presentations *(selected)* |** Full CV: http://alstudio.org/docs/Savytskyi_O.V._CV.pdf

1. **Oleksandr V. Savytskyi**, Alexander I. Kornelyuk, Melissa E. Murray, Thomas R. Caulfield. THE NEW ROLE OF CONNECTIVE PEPTIDE 1 (CP1) IN HUMAN TYROSYL-TRNA SYNTHETASE AND ITS MUTANT FORMS, ASSOCIATED WITH DI-CMTC NEUROPATHY STUDIED BY MOLECULAR MODELING AND MD SIMULATIONS TECHNIQUES. Proceedings of the International School of Crystallography, 58th Course: Structural Drug Design 2023: Biology, Chemistry And Computers, 2 - 10 June 2023, Erice, Sicily, Italy
2. **Oleksandr V. Savytskyi**, Tiffany N.H. Sirmans, Mathew A. Coban, Caleb A. Weber, Melissa E. Murray, Thomas R. Caulfield. (**2023**). COMPUTATIONAL MODELING AND MOLECULAR MAPPING OF SERINE PROTEASE INHIBITOR FAMILY A5 (SERPINA5) STRUCTURE, ASSOCIATED WITH TAU EXPRESSION AND ALZHEIMER'S DISEASE. *BPS Annual Meeting*, 18-22 February 2023, San Diego, CA, USA.
3. **Oleksandr V. Savytskyi**, Alexander I. Kornelyuk and Thomas R. Caulfield. THE NEW ROLE OF CONNECTIVE PEPTIDE 1 IN HUMAN TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS, ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY, STUDIED BY IN SILICO METHODS *Pacific Symposium on Biocomputing (PSB2023)*, 3-7 January 2023, Big Island of Hawaii, USA.
4. Ahmet Bilg, Imran Nasrullah, Justyna J. Gleba, Matthew Coban, **Oleksandr Savytskyi**, Thomas Caulfield, Tamas Ordog and John A. Copland III. THE DOUBLE TUDOR DOMAIN: A NOVEL THERAPEUTIC TARGET WITHIN THE HISTONE LYSINE-SPECIFIC DEMETHYLASE SUBFAMILY (KDM4) AS A MEANS TO TARGET ONCOGENIC SUPER ENHANCER FUNCTION. *Summer Undergraduate Research Fellowship (SURF) Report*, Mayo Clinic, 5 August 2022, USA.
5. **Oleksandr Savytskyi**, Andrii Salnikov, Ievgen Sliusar, Alexander Kornelyuk. MOLDYNGRID VIRTUAL LABORATORY: WEB-ORIENTED GRID-SERVICE DEDICATED TO COMPUTATIONAL STRUCTURAL BIOLOGY. *Proceedings of the 2nd European PhD and Postdoc symposium*: The Promise of Future Medicine: From Research to Therapy, 6-9th November 2018, Copenhagen, Denmark.
6. **Oleksandr V. Savytskyi** and Alexander I. Kornelyuk. MOLECULAR DYNAMICS SIMULATIONS OF TYROSYL-tRNA SYNTHETASE MUTANT FORMS ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. *FEBS/IUBMB Advanced Lecture Course "Molecular basis of human diseases: 50 years anniversary of Spetses summer schools"*, 27th May - 1st June, 2016, Spetses island, Greece.
7. **O.V. Savytskyi**, I.A. Sliusar, A.O. Salnikov and A.I. Kornelyuk. MOLDYNGRID VIRTUAL LABORATORY AS WEB-ORIENTED GRID-SERVICE FOR BIOMOLECULAR SIMULATIONS. *EGI Community Forum 2015*, 10-13 November 2015, Bari, Italy.
8. **Oleksandr V. Savytskyi**, Semen O. Yesylevskyy and Alexander I. Kornelyuk. CONFORMATIONAL FLEXIBILITY AND DOMAIN BINDING INTERFACES IN HUMAN TYROSYL-tRNA SYNTHETASE STUDIED BY MOLECULAR DYNAMICS SIMULATIONS. *FEBS-EMBO Conference 2014*, 30 August - 4 September 2014, Paris, France.
9. **O. V. Savytskyi**, A. I. Kornelyuk. LOCAL BETA-SHEET FORMATION IN 153-156delVKQV MUTANT OF HUMAN TyrRS ASSOCIATED WITH CMT DISEASE. *The 9th European Biophysics Congress (EBSA2013)*, 13-17 July 2013, Lisbon, Portugal.
10. **Oleksandr V. Savytskyi**, Semen O. Yesylevskyy and Alexander I. Kornelyuk. LOCAL β-SHEET FORMATION IN G41R MUTANT OF HUMAN TYROSYL-tRNA SYNTHETASE ASSOCIATED WITH CHARCOT-MARIE-TOOTH DISEASE. *The 6th Theoretical Biophysics Symposium*, 24-27 June 2013, Gothenburg, Sweden.

**As Research Group Leader | Networking with Students *(selected)* |**

**2022 – 2023** **Caleb Weber**, Laboratory of Drug Discovery, Design, and Optimization For Novel Therapeutics, Neuroscience Department, Clinic, Florida, USA.

***Collaboration*** in tools development (in Python) for structural analyses and drug-discovery work processes automatization. Created NN\ML protocols based on ICM-Pro by MolSoft.

***Results:*** Caleb was promoted from Graduate Research Education Program (GREP) on Special Project Associate II (SPA II) at Mayo Clinic in the same department, publication in Molecular Aspects of Medicine Journal (Impact Factor: 16.42022) and various abstracts in Proceedings Books (symposium, workshops, etc).

***Status after:*** Special Project Associate II (SPA II) at Mayo Clinic in the same department.

**2014 – 2017** **Vladyslav Kravchuk**, Department of Biotechnology, National Aviation University, Institute of High Technologies, Taras Shevchenko National University of Kyiv.

***Collaboration*** in molecular dynamics of mammalian TyrRS, High-Performance Computing.

***Results:*** Diploma for the outstanding Bachelor's thesis, paper in Journal of Biomolecular Structure and Dynamics (Awarded as the best article of the year in 2016, IMBG of NASU), oral presentations.

***Status after:*** PhD student at the Institute of Science and Technology (IST) Austria.