

Oleksandr V. Savytskyi, PhD

Citizenship: Ukrainian • Date of birth: 13 February 1985

Address: Mayo Clinic, Jacksonville, Florida, USA, 32224

Contacts

tel: +38 068 321-39-75 sms: +38 068 321-39-75

web: https://alstudio.org/savytskyi/ email: savytskyi@moldyngrid.org

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, 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.

01.2017 – 05.2021 Co-lecturer in course "Computational modeling of biopolymers and grid technologies" for PhD students in Department of Biology at IMBG of NAS of Ukraine, Q1, Ukraine. – 3 ECTS

(90 hours per year).

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).

04.2018 - 05.2022 Senior Researcher, Protein Engineering and Bioinformatics Department, Institute of

Molecular Biology and Genetics, National Academy of Sciences of Ukraine.

10.2016 - 04.2018 Researcher, Protein Engineering and Bioinformatics Department, Institute of Molecular

Biology and Genetics, National Academy of Sciences of Ukraine.

03.2011 - 10.2016 Junior Researcher, Protein Engineering and Bioinformatics Department, Institute of

Molecular Biology and Genetics, National Academy of Sciences of Ukraine.

07.2008 - 03.2011 Engineer, 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

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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

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 Gra	nts
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
2019	Travel Grant from HPC-Europa3 (H2020) for Postdoctoral Research in Catholic University of Murcia (UCAM), South East Spain. Collaboration with Prof. Horacio Pérez Sánchez. Supported by HPC Grant (200k CPU hours) in Barcelona Supercomputing Center, Spain.
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).
	Travel Grant from Biotechnology Business Institute and Certificate of Participation in the "The 2nd European PhD and Postdoc symposium: The Promise of Future Medicine: From Research to Therapy", 6th to the 9th of November 2018, Copenhagen, Denmark.
	Fellowship of the President of Ukraine for young scientists (2018-2020).
	Travel Grant from the Association of Guangdong Science and Technology Enterprise Cooperation for Participation in the Scientific Forums "Tour Of Foreign Experts In Guangdong province", 10-20 September 2018, Guangzhou, Republic of China.
	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 Biotechnology Business Institute to Participation in the ENABLE "1st European PhD and Postdoc symposium", 15-17 November 2017, Barcelona, Spain.
	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	Diploma of the Best Poster Presentation and Certificate of Participation in the XI International Conference "Factors in Experimental Evolution of Organisms", 12-16 September 2016, Odessa, Ukraine.
	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.
2016 - 2018	Fellowship of the National Academy of Sciences of Ukraine for young scientists.
2015	CINECA HPC Grant 2015 for GPU Cluster (nVidia Tesla k40) in Bologna, Italy.
	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.

	Travel Grant from EGI-Engage (The EU Framework Programme HORIZON 2020) and Certificate of Participation in the "EGI Community Forum 2015", 10-13 November 2015, Bari, Italy.
	Diploma of the Best Poster Presentation and Certificate of Participation in the "VI Meeting of Ukrainian Biophysical Society", 28-30 May 2015, Luts'k-Svityaz, Ukraine.
2014	Travel Grant from COMBIOM (7 th EU Framework Program) and Certificate of Participation in the Workshop on "Practical Training on IPR, Project Management and Equipment", 22-26 September 2014, Warsaw, Poland.
	FEBS-EMBO Travel Grant and Certificate of Participation in the "FEBS-EMBO Conference 2014", 30 August - 4 September 2014, Paris, France.
2014	FEBS-EMBO Travel Grant and Certificate of Participation in the "Young Scientific Forum 2014", 27-30 August 2014, Paris, France.
	The 2st prize award from the Scientific Council of the IMBG of NAS of Ukraine for the best 3nd year PhD thesis report on the "VIII Young Scientist Conference", 20-21 May 2014, Kyiv, Ukraine.
2013	Travel Grant from COMBIOM (7th EU Framework Program) for Participation in the "Opening of the Academic Year 2013/2014 at Biocentrum Ochota", 25 October 2013, Warsaw, Poland.
	FEBS YTF Grant and Certificate of Participation in the FEBS/EMBO Lecture Course " <i>Protein interactions, assemblies and human disease</i> ", 16–26 September 2013, Spetses, Greece.
2013	Travel Grant from NAS of Ukraine and Certificate of Participation in the Satellite Meeting of the EBSA2013 "Molecular Biology in Portugal and EMBL (and EMBL Alumni)", 18 July 2013, Lisbon, Portugal.
	Travel Grant from NAS of Ukraine and Certificate of Participation in the "9 th European Biophysics Congress EBSA 2013", 13-17 July 2013, Lisbon, Portugal.
	Travel Grant from NAS of Ukraine (additionally EBSA) and Certificate of Participation in the Satellite Meeting of the EBSA2013 " <i>Bionanotechnology – Recent Advances</i> ", 10-13 July 2013, Sesimbra, Portugal.
	Travel Grant from NAS of Ukraine and Certificate of Participation in the "6 th Theoretical Biophysics Symposium", 24-27 June 2013, Gothenburg, Sweden.
	Travel Grant from eSSENCE and Uppsala University for Participation in the eSSENCE International Workshop on " <i>Macromolecular Structure and Dynamics</i> ", 3-5 June 2013, BMC, Uppsala, Sweden.
	The 1st prize award from the Scientific Council of the IMBG of NAS of Ukraine for the best 3nd year PhD thesis report on the "VII Young Scientist Conference", 28-29 May 2013, Kyiv, Ukraine.
2012	Travel Grant from COMBIOM (7th EU Framework Program) and Certificate of Participation in the Workshop on "Scientific Communication", 1-5 October 2012, Warsaw, Poland.
2012 - 2014	Fellowship of the National Academy of Sciences of Ukraine for Young Scientists.
	Travel Grant from NAS of Ukraine and Certificate of Participation in the "NorduGrid 2012" Conference, 30 May - 01 June 2012, Uppsala, Sweden.
	The 2nd prize award from the Scientific Council of the IMBG of NAS of Ukraine for the best 2nd year PhD thesis report on the "VI Young Scientist Conference", 24-25 May 2012, Kyiv, Ukraine.
	"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.
	Certificate of Participation in the 4th International IMBG Conference for Young Scientists "Molecular Biology: Advances And Perspectives", 14-17 September 2011, Kyiv, Ukraine.

	Travel Grant from NAS of Ukraine and Certificate of Participation in the "V Meeting of Ukrainian Biophysical Society", 22-25 June 2011, Luts'k, Ukraine.
	Certificate from WIPO (World Intellectual Property Organization), certify successfully completed the distance learning " <i>DL-101 General Course on Intellectual Property</i> " from 2 April to 20 May 2011.
2010	Certificate of Participation in "Autodesk Forum in Kyiv", 1 October 2010, Kyiv, Ukraine.
	FEBS YTF Grant and Certificate of Participation in " <i>Physical Chemistry of Biointerfaces</i> " Workshop, 19-24 July 2010, Donostia - San Sebastian, Spain.
2009	Travel Grant from NAS of Ukraine and Certificate of Participation in IEEE Workshop <i>IDAACS'2009</i> (<i>Intelligent Data Acquisition and Advanced Computing Systems</i>), 21-23 September, Rende (Cosenza), Italy.
	NAS of Ukraine Grant "Virtual Laboratory MolDynGrid Development as a Part of the Ukrainian Academic Grid infrastructure". Head of Project: Prof. A.I. Kornelyuk (IMBG of NAS of Ukraine).
2008	Certificate of Participation in <i>UCG-December</i> , 2D/3D Visualization Workshop, 3 December 2008, Kyiv, Ukraine.
	Certificate of Participation in the 21st International CODATA (Committee on Data for Science and Technology) Conference, 5 - 8 October 2008, Kyiv, Ukraine.
	The 2nd prize award of the Scientific Center of agricultural education of Ukraine competition for the best Master's Thesis in the field of plant protection, Kyiv, Ukraine.
2005	Phytopharmacology Academy of Syngenta Awarded the Certificate of completion, 23 December 2005, Kyiv, Ukraine.

2017	XII International Summer School "Molecular Microbiology and Biotechnology" 4-20 June 2017, Odessa, Ukraine.
	"Useful cases in molecular modeling of biopolymers and their structural complexes"
	"High-Performance Computing and molecular dynamics simulations of proteins"
	"Grid computing and infrastructures for biomolecular research"
	"Virtual Laboratory MolDynGrid as efficient infrastructure for automation of molecular dynamics simulations (moldyngrid.org)"
	molecular dynamics simulations (moldyngrid.org)" 2 nd Conference for Young Scientists (CYS-2017), 6-9 June 2017, Kyiv, Uk "Computational molecular modeling and visualization of biopolymers"

International Collaboration		
2019	HPC-Europa3 Transnational Access programme. Collaboration with Bioinformatics and High Performance Computing Research Group (Prof. Horacio Pérez Sánchez), 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.	
2015 till now	EGI Federated Cloud (JRA2.4) Accelerated Computing. laaS-type cloud, made of academic private clouds and virtualized resources and built around open standards. Its development is driven by requirements of the scientific community. (EGI-Engage, Horizon 2020 EU, grant №654142)	
2015 till now	EGI-Engage:WP4 (JRA2.4) Accelerated Computing. Technologies for using GPUs in grid and cloud. Analysis of requirements from user communities. (EGI-Engage, Horizon 2020 EU, grant №654142)	
2012 – 2013	VT GPGPU (the Virtual Team project aims to collect detailed requirements from existing and new EGI user communities and their support teams about using GPGPU services in the European Grid Infrastructure).	
2010 – 2011	NVIDIA's Tesla Bio Workbench. Recently the GPU Test Drive system was installed in Ukraine within the scope of NVIDIA's Tesla Bio Workbench Project. This project aims at evaluation of performance of molecular dynamics simulations and trajectory analysis computations employing GPU accelerator support in specialized software including GROMACS 4.5, AMBER 11 and NAMD 2.7.	

Local projects	
2017 – 2018	NAS of Ukraine Grant "Distributed Database development for molecular dynamics trajectories and NMR data in the virtual laboratory MolDynGrid". (collaboration with KNU)
2014 – 2016	NAS of Ukraine Grant "Cloud-technologies development and introduction in GRID services for the virtual laboratory MolDynGrid". (collaboration with KNU)
2013 – 2017	NAS of Ukraine Grant "Local conformational changes and formation of metastable structural elements in eukaryotic tyrosyl-tRNA synthetase".
2013 – 2014	NAS of Ukraine Grant "Software Development and adaptation on clusters SCIT-4 super computer for solving tasks in structural biology", Kyiv, Ukraine. (collaboration with KNU, IOP, ICYB, ISMA)
2011 – 2012	NAS of Ukraine Grant "Software package development, adaptation and implementation in Ukrainian National Grid infrastructure for trajectories analysis of molecular dynamics of proteins", Kyiv, Ukraine. (collaboration with KNU, IOP of NASU, ISS of NASU)
2010 – 2013	NAS of Ukraine Grant "Software package development, adaptation and implementation in Ukrainian National Grid infrastructure for trajectories analysis of molecular dynamics of proteins", Kyiv, Ukraine. (collaboration with KNU, IOP of NASU, ISS of NASU)
2008 – 2012	NAS of Ukraine Grant "Dynamic aspects of eukaryotic tyrosyl-tRNA synthetase and study the effect of mutations on tRNA aminoacylation process and the emergence of neurodegenerative diseases".

Professional Affiliations	
2022 – now	Co-Collection Editor in peer-reviewed journal (Biomolecules , IF:6.06, ISSN 2218-273X). Topical Collection "Biomolecules In Silico: Contemporary Advances in Computational Approaches to Investigating the Molecular Dynamics of Biological Systems".
	International Society for Computational Biology (ISCB). Certificate from October 2022.
	Member of the Biophysical Society. Certificate from October 2022.
2018 till now	Expert Committee Member in peer-reviewed journal (Computational Biology and Chemistry, Impact Factor: 3.5).
2013 till now	Expert Committee Member (Peer Reviewer) of annual scientific conferences HPC-UA are devoted to development of high-performance computing systems and their applications to physics, biology and astronomy.
	Member of the EBSA (European Biophysical Societies' Association). Certificate from the Ukrainian Biophysical Society, since 2 April 2013.

2013 till now	Member of GGUS in EGI project (the Global Grid User Support officer in the European Grid Infrastructure/National Grid Initiatives).
2010 till now	Member of the FEBS (Federation of European Biochemical Societies). Certificate from Ukrainian Biochemical Society, since 22 February 2010.
	Member of the VO: enmr.eu (WeNMR - e-Infrastructure-based global virtual research community for structural biology in the life sciences).
2009 till now	Member and Administrator of the Virtual Laboratory MolDynGrid (VO: moldyngrid).
	Member of the UNG (Ukrainian National Grid) and EGI (X509v3 certificate).

Publications

PAPERS IN INTERNATIONAL JOURNALS:

- 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: 16.4²⁰²²)
- 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
- 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: 1.7²⁰²¹) PDF
- 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: 2.9²⁰¹⁶) 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: 3.31²⁰¹³) PDF
- 7. Vislovukh, A. A., Shalak, V. F., **Savytskyi, O. V.**, Kovalenko, N. I., Gralievska, N. L., Negrutskii, B. S., & El'skaya, A. V. (2012). PTI-1: NOVEL WAY TO ONCOGENICITY. *Biopolym. Cell.*, 28(5), 404-410. PDF
- 8. 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
- 9. 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
- 10. Salnikov, A., Sudakov, O., **Savytskyi, O.**, Sliusar, I., & Kornelyuk, A. (**2010**). THE INTEGRATED ENVIRONMENT OF VIRTUAL LABORATORY MOLDYNGRID FOR CALCULATION OF MOLECULAR DYNAMICS OF BIOPOLYMERS. *Medical Informatics and Engineering*, 1, 24-32. (in Ukrainian) PDF

PROCEEDINGS BOOKS:

- 11. 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
- 12. Salnikov, A. O., Sliusar, I. A., Sudakov, O. O., **Savytskyi, O. V.**, & Kornelyuk, A. I. (**2009**). MOLDYNGRID VIRTUAL LABORATORY AS A PART OF UKRAINIAN ACADEMIC GRID INFRASTRUCTURE. *Proceedings of the 5th IEEE International Workshop on Intelligent Data Acquisition and Advanced Computing Systems: Technology and Applications*, IDAACS 2009, 1, 237-240. (ISI Proceedings) PDF
- 13. A. Gryganskyi, N. Goncharenko, **O. Savytskyi**, O. Tereshchenko, O. Pererva (**2007**). DISEASE AND ITS CONTROL ON MUSHROOMS GROWING FARMS IN UKRAINE. *Proceedings Book of Scientific student's conference of NAU*, October 2007, Kyiv, Ukraine, 1, 33-36. (in Ukrainian)

CONFERENCE, MEETING, SYMPOSIA ABSTRACTS:

- 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, p. #
- 2. Tiffany Sirmans, Oleksandr Savytskyi, Matt Coban, Kelly Hinkle, Caleb Weber, Evette Radisky, Thomas Caulfield, Melissa Murray. STRUCTURAL MODELING OF NOVEL TAU INTERACTION PARTNER, SERPINA5, REVEALS METASTABLE CONFORMATION OF DISEASE RELEVANT N-TERMINUS. Proceedings of the AD/P D™ 2023 Advances in Science; Therapy (International Conference on Alzheimer's and Parkinson's Diseases and related neurological disorders). 28 March 1 April 2023, Gothenburg, Sweden. OD095 / #1630
- 3. 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. Biophysical Journal 122 (3), 471a.
- 4. 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. Proceedings of the Pacific Symposium on Biocomputing (PSB2023), 3-7 January 2023, Big Island of Hawaii, USA, p. 32.
- Oleksandr V. Savytskyi. THE ROLE OF CONNECTIVE PEPTIDE 1 IN HUMAN TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS ASSOCIATED WITH DI-CMTC NEUROPATHY STUDIED BY MOLECULAR DYNAMICS SIMULATIONS. Proceedings of the 2nd Transnational Access Meeting (TAM), 22-23 October 2020, Barcelona, Spain, p.22.
- 6. **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*, 6-9 November 2018, Copenhagen, Denmark, p. 209.
- 7. **Oleksandr Savytskyi.** HIGH PERFORMANCE COMPUTING IN BIOMEDICAL RESEARCH. *Scientific Forums "Tour of Foreign Experts in Guangdong Province"*, 10-20 September 2018, Guangzhou, Republic of China, p. 91-104.
- 8. **O. Savytskyi**, A. Kornelyuk. THE NEW ROLE OF CONNECTIVE PEPTIDE 1 IN HUMAN TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS, ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. *Proceedings of the Advanced practical and laboratory course "Ligand-binding theory and practice"*, 24 June 1 July 2018, Nove Hrady, Czech Republic., p. 26.
- 9. Oleksandr V. Savytskyi and Alexander I. Kornelyuk. THE NEW ROLE OF CONNECTIVE PEPTIDE 1 IN HUMAN TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS ASSOCIATED WITH DI-CMTC NEUROPATHY STUDIED BY MOLECULAR DYNAMICS SIMULATIONS. Proceedings of the 1st European PhD and Postdoc symposium", 15-17 November 2017, Barcelona, Spain, p.106.
- 10. 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, p. 32.
- 11. Petrychenko V.O, **Savytskyi O.V.**, Kornelyuk A.I.. COMPUTATIONAL MODELLING AND MOLECULAR DYNAMICS SIMULATIONS OF *Bos taurus* TYROSYL-tRNA SYNTHETASE IN COMPLEX WITH tRNA Tyr. *Proceedings of the "Shevchenkivska Vesna: bioscience advances 2017"*, 18-21 April 2017, Kyiv, Ukraine, p. 23.
- 12. V.O. Kravchuk, **O.V. Savytskyi**, K.O. Odynets, V.V. Mykuliak, A.I. Kornelyuk. *IN SILICO* STUDY OF THE COMPLEXES OF *B. TAURUS* TYROSYL-tRNA SYNTHETASE WITH SUBSTRATES. *Biopolymers & Cell*, 32 (5), p. 399.
- 13. Oleksandr V. Savytskyi and Alexander I. Kornelyuk. MOLECULAR DYNAMICS SIMULATIONS OF TYROSYL-tRNA SYNTHETASE MUTANT FORMS ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. Proceedings of 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, p. 41.
- 14. Grom M.Yu., **Savytskyi O.V.** BIOINFORMATICS ANALYSIS OF IMMUNOGENICITY OF TYROSYL-tRNA SYNTHETASE AND ITS SEPARATED DOMAINS. *Proceedings of the 10th International Young Scientists' Biology Conference "From A Molecule Up To The Biosphere"*, 2-4 December 2015, Kharkiv, Ukraine, p. 119-120.

- 15. **O.V. Savytskyi**, I.A. Sliusar, A.O. Salnikov and A.I. Kornelyuk. MOLDYNGRID VIRTUAL LABORATORY AS WEB-ORIENTED GRID-SERVICE FOR BIOMOLECULAR SIMULATIONS. *Proceedings of the "EGI Community Forum 2015"*, 10-13 November 2015, Bari, Italy, p. 107.
- 16. **O.V. Savytskyi**, A.I. Kornelyuk. CONFORMATIONAL CHANGES IN MUTANT FORMS G41R OF TYROSYLtRNA SYNTHETASE AND G526R OF GLYCYL-tRNA SYNTHETASE ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. *Proceedings of the "VI Meeting of Ukrainian Biophysical Society"*, 28-30 May 2015, Luts'k-Svityaz, Ukraine, p. 46. (in Ukrainian)
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Oral Presentations

- 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. Oleksandr V. Savytskyi. THE ROLE OF CONNECTIVE PEPTIDE 1 IN HUMAN TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS, ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. The 2nd Transnational Access Meeting (TAM) of the HPC Europa-3 program. 22-23 October 2020, Barcelona, Spain.
- 3. **Oleksandr V. Savytskyi.** COPMUTATIONAL STRUCTURAL BIOLOGY: METHODS AND APPLIED TASKS. *Odessa I.I.Mechnikov National University*, 14 18 September 2020, Odesa, Ukraine.

- 4. **Oleksandr Savytskyi.** HIGH PERFORMANCE COMPUTING IN BIOMEDICAL RESEARCH. *Scientific Forums "Tour of Foreign Experts in Guangdong Province"*, 10-20 September 2018, Guangzhou, Republic of China.
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- 6. **Oleksandr Savytskyi**. MOLECULAR DYNAMICS SIMULATIONS OF TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS, ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. *Biomolecular Modelling Course by Politecnico di Milano*, May 10-16, 2018, Kyiv, Ukraine.
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- 9. **Oleksandr Savytskyi**. COMPUTATIONAL MODELING OF TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS ASSOSIETED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. Workshop in the Institute for Condensed Matter Physics of NAS of Ukraine, 24 December 2015, Lviv, Ukraine.
- 10. Oleksandr Savytskyi. USE CASES FROM "EGI COMMUNITY FORUM 2015". *Grid Reports 2015*, Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, 8 December 2015, Kyiv, Ukraine.
- 11. Marco Verlato, **Oleksandr Savytskyi**, Andrii Salnikov. GPU ACCELERATION FOR MOLECULAR DYNAMICS SIMULATIONS IN GRID: FIRST RESULTS AND PERSPECTIVES. USE CASES FROM OTHER COMMUNITIES. *The EGI Conference 2015*, 18-22 May 2015, Lisbon, Portugal.
- 12. Oleksandr V. Savytskyi. CLOUD-TECHNOLOGIES DEVELOPMENT AND INTRODUCTION IN GRID SERVICES FOR THE VIRTUAL LABORATORY MOLDYNGRID. *Grid Reports 2014*, Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, 16 December 2014, Kyiv, Ukraine. (in Ukrainian)
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Poster Presentations

- 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.
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- 7. Oleksandr V. Savytskyi and Alexander I. Kornelyuk. THE NEW ROLE OF CONNECTIVE PEPTIDE 1 IN HUMAN TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS ASSOCIATED WITH DI-CMTC NEUROPATHY STUDIED BY MOLECULAR DYNAMICS SIMULATIONS. Proceedings of the 1st European PhD and Postdoc symposium, 15-17 November 2017, Barcelona, Spain
- 8. 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.
- 9. **Oleksandr V. Savytskyi** and Alexander I. Kornelyuk. COMPUTATIONAL MODELING OF MOLECULAR DYNAMICS SIMULATIONS OF TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. *XI International Conference "Factors in Experimental Evolution of Organisms"*, 12-16 September 2016, Odessa, Ukraine.
- 10. **Oleksandr V. Savytskyi** and Alexander I. Kornelyuk. MOLECULAR DYNAMICS SIMULATIONS OF TYROSYLtRNA 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.
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- 22. **O. Savytskyi,** R. Nikolaenko, A. Kornelyuk. MOLECULAR DYNAMICS SIMULATION OF MUTANT TYROSYL-tRNA SYNTHETASE ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY REVEALS THE STABILIZATION OF ENZYME DIMER INTERFACE. *Physical Chemistry of Biointerfaces Workshop*, CIC biomaGUNE, 19-24 July 2010, Donostia San Sebastian, Spain.
- 23. A.P. Gryganskyi, A. Litvintseva, S.C. Lee, M.E. Smith, G. Bonito, T.M. Porter, I.M. Anishchenko, O. Savytskyi, W. Colquhoun, J. Heitman, R. Vilgalys. STRUCTURE, FUNCTION, AND PHYLOGENY OF THE SEX LOCUS IN THE RHIZOPUS ORYZAE COMPLEX. Joint Meeting of the Mycological Society of America and The International Symposium on Fungal Endophytes of Grasses, June 28-July 1, 2010, University of Kentucky, Lexington, Kentucky, USA.
- 24. R. Nikolaenko, F. Tereschenko, O. Savytskyi, A. Kornelyuk. MOLECULAR DYNAMICS SIMULATION OF HUMAN TYROSYL-tRNA SYNTHETASE AND ITS MUTANT FORMS ASSOCIATED WITH CHARCOT-MARIE-TOOTH NEUROPATHY. Polish – Ukrainian research collaboration meeting, International Institute of Molecular and Cell Biology, 14 May 2009, Warsaw, Poland.

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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.

2014 - 2017

Valentyn Petrychenko, ESC "Institute of Biology and Medicine", Taras Shevchenko National University of Kyiv.

Collaboration in molecular dynamics of mammalian TyrRS in complex with tRNA, High-Performance Computing.

Results: Diploma for the outstanding Bachelor's thesis, Diploma for the best oral presentation on the *Shevchenkivska Vesna: bioscience advances 2017*, 18-21 April 2017, Kyiv, Ukraine.

Status after: M.Sc. Molecular biology at the Georg-August-Universität Göttingen, Germany.

2009 - 2010

Anastasiia Kamenska, Taras Shevchenko National University of Kyiv

Collaboration in aggregation analysis *in silico* of *H. sapiens* TyrRS's mutant forms, associated with Charcot-Marie-Tooth neuropathy.

Results: Bachelor thesis, abstracts, poster presentations in EU.

Status after: PhD student at the University of Cambridge, United Kingdom.

2008 - 2010

Roman Nikolaienko, NTUU "Igor Sikorsky Igor Sikorsky Kyiv Polytechnic Institute".

Collaboration in molecular dynamics of *H. sapiens* TyrRS's mutant forms, associated with Charcot-Marie-Tooth neuropathy. HPC and GRID computing.

Results: Master thesis, abstracts, poster presentations.

Status after: PhD student at the University of Missouri - Kansas City.

Participation in Meetings and Courses without Presented Materials (selected)

- 1. The EGI Community Forum 2014, 19-23 May, Helsinki, Finland. (via Web).
- 2. HPC Day 2013, 10-11 October 2013, Kyiv, Ukraine.
- 3. HPC-UA: International Conferences on High Performance Computing, 7-9 October 2013, Kyiv, Ukraine.
- 4. Satellite Meeting of the EBSA2013 "Molecular Biology in Portugal and EMBL (and EMBL Alumni)", 18 July 2013, Lisbon, Portugal.
- 5. Satellite Meeting of the EBSA2013 "Bionanotechnology Recent Advances", 10-13 July 2013, Sesimbra, Portugal.
- 6. EGI Community Forum 2013, Manchester, United Kingdom, 8-12 April 2013. (via Web)
- 7. Erik Lindahl, and Devang Sachdev. GROMACS and Kepler GPUs. GPU Technology Conference, 4 April 2013. (via Web).

Activities and Interests

Traveling, cooking, photo and filming short films, reading (popular-science, science fiction), swimming.