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# Narek **Abelyan**

Yerevan, Armenia

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## PROFESSIONAL EXPERIENCE

### CO-FOUNDER OF BIOCENTRIC.AI

*Drug design and discovery startup*
*2022 – 2024* *Yerevan, Armenia*

### COMPUTATIONAL BIOLOGY EXPERT

*DeNovo Sciences*
*FAST (Foundation for Armenian Science and Technology)*
*2020 – 2022* *Yerevan, Armenia*

### SCIENTIFIC RESEARCHER

*Research group "Solving antibiotic resistance problem by molecular modeling methods"*
*Russian-Armenian University*
*2019 – 2023* *Yerevan, Armenia*

### RESEARCHER

*Critical Technologies Research Center*
*Russian-Armenian University*
*2019 – 2021* *Yerevan, Armenia*

### JUNIOR SCIENTIFIC RESEARCHER

*Laboratory of MS-Analytics*
*Russian-Armenian University*
*2018 – 2019* *Yerevan, Armenia*

### JUNIOR SCIENTIFIC RESEARCHER

*Research group "Molecular modeling of the biological systems"*
*Russian-Armenian University*
*2016 – 2019* *Yerevan, Armenia*

## EDUCATION

**BIOINFORMATICS**
**PHD**
*Institute of Biomedicine and Pharmacy, Russian-Armenian University*
*2019 – 2022*

BIOINFORMATICS AND BIOENGINEERING
**MASTERS DEGREE**
*Institute of Mathematics and High Technologies, Russian-Armenian University*
*Graduated (Diploma with Honours)*
*2014 – 2019*

*School N3, Sisian Syunik, Armenia*
***Graduated (Red Certificate)***

*Jewish school "Geula", Pyatigorsk, Stavropol Krai, Russia*

*School N5, Sisian Syunik, Armenia*

## LANGUAGES

**Armenian(native)**
**Russian(fluent)**
**English(good)**

## CITIZENSHIP

**Armenian**

## AWARDS

PRESIDENTIAL EDUCATIONAL AWARD

*Best student, Annual Educational Award of the President of the Republic of Armenia 2018*

THE BEST REPORT OF THE "BIOINFORMATICS" section at the Lomonosov International Scientific Conference 2019

THE BEST ORAL REPORT at the IV International Conference of the YSU SSS 2017

CERTIFICATE FOR THE HIGH SCIENTIFIC LEVEL of the presented report at the annual scientific conference of the Russian-Armenian University 2019

WINNER OF THE PHD SUPPORT PROGRAM implemented by Enterprise Incubator Foundation (EIF) with support of Philip Morris International (PMI) Science, Yerevan, Armenia, 2019, 2021

WINNER OF FACULTY RESEARCH FUNDING PROGRAM Implemented by Enterprise Incubator Foundation (EIF) with support of Philip Morris International (PMI) Science, Yerevan, Armenia, 2020

DIPLOMA: ACTIVE PARTICIPATION in the second all-Russian scientific and practical conference on the advancement and implementation of scientific developments in 2017

2017, 2018-2019 RECEIVED A STATE ACADEMIC SCHOLARSHIP for excellent studies and scientific work

FIRST-DEGREE DIPLOMA. Best Graduation work 2019 (*Russian-Armenian University*)

CERTIFICATE OF "SCIENCE CHAMPIONS" by Philip Morris International and EIF. 2020, Yerevan, Armenia

ANSEF-2021, Research Grant molbio-2521 from The Armenian National Science and Education Fund

INNOVATION MATCHING GRANT - member of the DeNovo Sciences team that won the Innovation Matching Grant

NATIONAL FINALIST OF EWC ARMENIA

Member of the DeNovo Sciences team that won National Champion prize during the Entrepreneurship World Cup - Armenia's National Finals (2021)

"NERUZH 3.0" grant WINNER

Co-Founder at BioCentric.AI that was awarded 1st place

## RESEARCH INTERESTS

- **Computational Biology**
- **Molecular biology**
- **Bioinformatics**
- **Structural biology**
- **Chemoinformatics**
- **Computer Science**

## KEY SKILLS

- **Computer Aided Drug Design**
- **Molecular docking**
- **Large scale virtual screening**
- **Pharmacophore modelling**
- **Drug target identification and validation**
- **Hit identification**
- **Lead optimization**
- **QSAR, QSPR ADMET, DMPK.**
- **Molecular Modeling**
- **Molecular dynamics simulations**
- **De novo and homology modelling**

## PROGRAMMING LANGUAGES & SOFTWARE

| | |
|---|---|
| ✓ **Python** | ✓ **Bash** |
| ✓ **R** | ✓ **ICM** |
| ✓ **GROMACS** | ✓ **AMBER** |
| ✓ **LigandSC** | ✓ **Vina & AD4** |
| ✓ **Rosetta** | ✓ **OpenEye** |
| ✓ **RDKit** | ✓ **OBabel** |
| ✓ **UGENE** | ✓ **. and other** |

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## PUBLICATION LIST

- **Nanomedicine,** 2024; Tannin–albumin particles as stable carriers of medicines; N.Ohanyan, N.Abelyan et al. **2024**
  DOI : https://doi.org/10.2217/nnm-2023-0275
- **Antiviral Research**, 2023; Advanced virtual screening enables the discovery of a host-targeting and broad-spectrum antiviral agent; G. Chilingaryan, R. Izmailyan, N.Abelyan et al. **2023**
  DOI: https://doi.org/10.1016/j.antiviral.2023.105681
- **Journal of Biomolecular Structure & Dynamics,** 2023; Design of new chemical entities targeting both native and H275Y mutant influenza a virus by deep reinforcement learning; Matevosyan M., Abelyan N. et al. **2023**
  DOI: https://doi.org/10.1080/07391102.2022.2158936
- **PLOS ONE**, 2022; T. 17. – №. 9. – C. e0272065; Combination of ligand and structure based virtual screening approaches for the discovery of potential PARP1 inhibitors; Al-Sanea M. M., Abelyan N. et al. (Impact Factor = 3.2, Q1) **2022**
  DOI: https://doi.org/10.1371/journal.pone.0272065
- **ACS Omega,** 2022; Network Pharmacology Analysis of Cytotoxic Triterpenes Isolated from Euphorbia abyssinica Latex Supported by Drug-likeness and ADMET Studies; Ahmed S. R., Abelyan N. et al. (Impact Factor = 3.5, Q1) **2022**
  DOI: https://doi.org/10.1021/acsomega.2c00750
- **ACS Omega,** 2022; Cancer Chemopreventive Potential and Chemical Profiling of Euphorbia abyssinica Endowed with Docking Studies; Ahmed, S. R., Abelyan, N., Al-Sanea, M. M. et al. (Impact Factor = 3.5, Q1) **2022**
  DOI:https://pubs.acs.org/doi/10.1021/acsomega.1c06148
- **Nature Scientific Report,** 11(1), 11417; Combination of consensus and ensemble docking strategies for the discovery of human dihydroorotate dehydrogenase inhibitors; G. Chilingaryan, N.Abelyan, A. Sargsyan, K. Nazaryan, A. Serobian, H. Zakaryan. (Impact Factor = 4.4, Q1) **2021**
  DOI: https://doi.org/10.1038/s41598-021-91069-7
- **MDPI Antibiotics,** 2021; 10(7):824; Strawberry and Ginger Silver Nanoparticles as Potential Inhibitors for SARS-CoV-2 Assisted by In Silico Modeling and Metabolic Profiling. Al-Sanea MM, Abelyan N. et al. **2021**
  (Impact Factor = 4.6, Q1)
  DOI: https://doi.org/10.3390/antibiotics10070824
- **Nature Scientific Report,** 11(1), 15516; Identification of non-classical hCA XII inhibitors using combination of computational approaches for drug design and discovery; Mm. Al-Sanea, G. Chilingaryan, N. Abelyan et al. **2021**
  (Impact Factor = 4.4, Q1)
  DOI: https://doi.org/10.1038/s41598-021-94809-x
- **Journal of Applied Microbiology,** 2021; SoyBean-Associated Endophytic Fungi as Potential Source for Anti-COVID-19 Metabolites supported by docking analysis; El-hawary S. S., Mohammed R., Bahr, H. S., Attia E. Z. El-Katatny, Abelyan N.N. et al. (Impact Factor = 3.7, Q1) **2021**
  DOI: 10.1111/jam.15031

- **MDPI Life,** 2021; 11(10):1070; Identification of Novel Potential VEGFR-2 Inhibitors Using a Combination of Computational Methods for Drug Discovery. Al-Sanea MM, Chilingaryan G, Abelyan N, et al. (Impact Factor = 3.8, Q2) DOI: https://doi.org/10.3390/life11101070 **2021**

- **Journal of Biomolecular Structure & Dynamics;** Multitarget in silico studies of Ocimum menthiifolium, family Lamiaceae against SARS-CoV-2 supported by molecular dynamics simulation; Amgad Albohy, Eman Maher Zahran, MM. Al-Sanea, Narek Abelyan, Mohamed Salah Kamel et al. (Impact Factor = 3.5, Q2) DOI: 10.1080/07391102.2020.1852964 **2020**

- **Molecular Biology;** 54(1), 134- 143, (2020); In silico Screening of Flavones and its Derivatives as Potential Inhibitors of Quorum-Sensing Regulator LasR of Pseudomonas aeruginosa; Abelyan, N., Grabski, H., & Tiratsuyan, S. DOI: 10.1134/S0026893320010021 **2020**

- **Молекулярная биология,** 2019, 54, 153-163, In silico скрининг флавонов и их производных как потенциальных ингибиторов кворум-сенсинг регулятора LasR Pseudomonas aeruginosa; Abelyan N.N., Grabski O.V., Tiratsuyan S.G. DOI: 10.31857/S0026898420010024 **2020**

- **PLOS ONE,** T. 14. – №. 8. – C. e0221532; In silico study of colchicine resistance molecular mechanisms caused by tubulin structural polymorphism; Sahakyan, H., Abelyan, N., Arakelov, V., Arakelov, G., & Nazaryan, K.; (Impact Factor = 3.2, Q1) DOI: https://doi.org/10.1371/journal.pone.0221532 **2019**

- Vestnik of RAU No. 1 physical-mathematical and natural sciences; Modeling the interaction of taxifolin with human telomeric hybrid G-quadruplex DNA using the molecular dynamics method; G.V. Chilingaryan, N.N. Abelyan; 02/26/2019, p. 141-149 **2019**

- Vestnik of RAU No. 1 physical-mathematical and natural sciences; Virtual screening of flavones and its derivatives for inhibition of transcriptional regulator LasR of Pseudomonas aeruginosa . N.N. Abelyan; 02/26/2019, p. 110-120 **2019**

- Materials of the VI international scientific Internet - conference: "Physico-Chemical Biology"; The music of the evolution of the insulin gene; N.N. Abelyan, S.G. Tiratsuyan, G.R. Vardapetyan; pp. 15-20, 2018 **2018**

- Materials of the IV international scientific-practical conference "Biotechnology: a look into the future"; Virtual screening of potential quorum sensing inhibitors of an antibiotic-resistant opportunistic pathogen (Pseudomonas aeruginosa); Abelyan N.N., Grabsky O.V., Tiratsuyan S.G.; p. 6-9, 2018 **2018**

- The second practical conference on the implementation of scientific developments (Collection of reports); Virtual screening of flavones and their derivatives to inhibit the LasR transcriptional regulator Pseudomonas aeruginosa; N.N. Abelyan, O. V Grabsky., L.S. Hunanyan, S. G. Tiratsuyan, G.R. Vardapetyan; October 25-26, 2017, p. 43 - 44; **2017**

- Vestnik of RAU No. 2 physical, mathematical and natural sciences; In silico screening of low molecular weight ligands that stabilize telomeric G-quadruplex DNA; G.V. Chilingaryan, N.N. Abelyan, S.G. Tiratsyan, L.S. Hunanyan, G.R. Vardapetyan; October 18, 2017, pp. 112-121 **2017**

- **FEBS OPEN BIO**, silico screening of flavones and its derivatives as potential inhibitors of quorum-sensing regulator LasR of Pseudomonas aeruginosa. Abelyan, N., Grabski, H., Tiratsuyan, S. (2021). 11, p. 101, DOI: 10.1002/2211-5463.13205 **2021**

- Abelyan N., Chilingaryan G., Farsiyan L., Hovhannisyan A., Tiratsuyan S. Computational Modeling of Potential Inhibitors of the QS System of Antibiotic-Resistant Bacteria P. aeruginosa, **V International Conference of Biotechnology and Health.** Book of Abstracts. Yerevan, Armenia October 29–31, p. 15-16. ISBN 978-9939-67-254-0 **2020**

- Абелян Н.Н., Тирацуян С.Г. (2020). Молекулярное моделирование взаимодействия потенциальных ингибиторов регулятора кворум-сенсинга LasR бактерии Pseudomonas aeruginosa. Материалы Международного молодежного научного форума **«ЛОМОНОСОВ-2020».** ISBN 978-5-317-06417-4 **2020**

- Абелян Н., Тирацуян С. (2019). In silico скрининг низкомолекулярных ингибиторов кворум-сенсинга антибиотико-резистентной бактерии Pseudomonas aeruginosa, активирующих иммунный ответ хозяина. XXVI Международная конференция студентов, аспирантов и молодых учёных **«Ломоносов» 2019**. ISBN 978-5-317-06100-5 **2019**

- Ghrejyan E., Ohanyan S., Abelyan N., Hovhannisyan A. (2020). Assessment of Sensitivity of AgNPs-Resistant E. coli to Antibiotics and Antibiotic-Nanoparticle Complexes, V International Conference of Biotechnology and Health. Book of Abstracts. Yerevan,Armenia October 29–31, p. 59-60, ISBN 978-9939-67-254-0 **2020**

- Абелян Н., Тирацуян С. (2019). In silico скрининг низкомолекулярных ингибиторов кворумсенсинга антибиотикорезистентной бактерии Pseudomonas aeruginosa, активирующих иммунный ответ хозяина. Сборник докладов конференции Летней школы по биоинформатике. Москва 2019, 29 июля – 3 августа, стр. 4 **2019**

## SPEECH AT THE CONFERENCES

INTERNATIONAL YOUTH SCIENTIFIC FORUM "LOMONOSOV-2019", Moscow, Lomonosov Moscow State University; In silico screening of low molecular weight quorum sensing inhibitors of the antibiotic-resistant bacterium Pseudomonas aeruginosa, activating the host's immune response; Abelyan N.N., Ph.D., Associate Professor Tiratsuyan S.G.; 2019

INTERNATIONAL YOUTH SCIENTIFIC FORUM "LOMONOSOV-2020", Moscow, Lomonosov Moscow State University; Молекулярное моделирование взаимодействия потенциальных ингибиторов регулятора кворум-сенсинга LasR бактерии Pseudomonas aeruginosa; Abelyan N.N., Tiratsuyan S.G.; 2020

YSU SSS 4TH INTERNATIONAL CONFERENCE DEDICATED TO THE 70TH ANNIVERSARY OF YSU SSS; Virtual screening of flavones and its derivatives for inhibition of transcriptional regulator LasR of Pseudomonas Aeruginosa; Narek Abelyan; 2017

SECOND ALL-RUSSIAN SCIENTIFIC AND PRACTICAL CONFERENCE ON THE IMPLEMENTATION OF SCIENTIFIC DEVELOPMENTS October 25-26, 2017; Virtual screening of flavones and their derivatives to inhibit the transcriptional regulator LasR Pseudomonas aeruginosa; N.N. Abelyan

INTERNATIONAL YOUTH SCIENTIFIC FORUM "LOMONOSOV-2018", Moscow, Lomonosov Moscow State University; Virtual screening of potential quorum sensing inhibitors of antibiotic-resistant Pseudomonas aeruginosa; Abelyan N.N., Ph.D., Associate Professor Tiratsuyan S.G.; 2018

INTERNATIONAL CONFERENCE FEBS: CURRENT ADVANCES IN PATHOGEN RESEARCH; 25–30 March 2019 Molecular modeling of artemisinin and flavones with transcriptional regulator LasR of pseudomonas aeruginosa; Narek A., Siranush G., Hovakim G., Susanna T.

TWELFTH ANNUAL SCIENTIFIC CONFERENCE Dedicated to the 20th anniversary of the founding of the Russian-Armenian University on December 4–8, 2017; Virtual screening of flavones and their derivatives to inhibit the transcriptional regulator LasR - Pseudomonas aeruginosa; N.N. Abelyan, O.V. Grabsky, Doctor of Biological Sciences, Ph.D. L.S. Hunanyan, Ph.D., Assoc. S.G. Tiratsuyan, prof. G.R. Vardapetyan.

STUDENT'S ANNUAL SCIENTIFIC CONFERENCE Dedicated to the 20th anniversary of the founding of the Russian-Armenian University on April 18–20, 2017; Study of subsequent nucleotides of the same gene in different organisms; Abelyan N.N., Doctor of Biological Sciences, prof. Vardapetyan G.R., Ph.D., Associate Professor Tiratsuyan S.G.

THIRTEENTH ANNUAL SCIENTIFIC CONFERENCE OF RAU; Study of the molecular mechanisms of the functioning of horseradish peroxidase (HRP); Ph.D., Assoc. A.A. Hovhannisyan, student N.N. Abelyan

THIRTEENTH ANNUAL SCIENTIFIC CONFERENCE OF RAU; In silico screening for potential quorum sensing inhibitors that make the antibiotic resistant Pseudomonas aeruginosa vulnerable for human immune system; Ph.D., Assoc. S.G. Tiratsuyan, graduate student O.V. Grabsky, student N.N. Abelyan

THIRTEENTH ANNUAL SCIENTIFIC CONFERENCE OF RAU; Colchicine resistance molecular mechanisms caused by tubulin structural polymorphism; Prof., D.Sc. K. Nazaryan, PhD student H. Sahakyan, student N. Abelyan

RAU STUDENT ANNUAL SCIENTIFIC CONFERENCE April 26-30, 2019; (First plenary meeting, opening of the conference); In silico screening for low molecular weight quorum sensing inhibitors of the antibiotic resistance bacterium Pseudomonas aeruginosa that activate the host's immune response; Abelyan N.N., Ph.D., Assoc. Tiratsuyan S.G.

IV INTERNATIONAL SCIENTIFIC AND PRACTICAL CONFERENCE "BIOTECHNOLOGY: LOOKING FORWARD" 2018; Virtual screening of potential quorum-sensing inhibitors of an antibiotic-resistant opportunistic pathogen Pseudomonas aeruginosa; Abelyan N.N., Grabsky O.V., Tiratsuyan S.G.

VI INTERNATIONAL SCIENTIFIC CONFERENCE "NEW FUNCTIONAL MATERIALS AND HIGH TECHNOLOGIES": MUSIC OF EVOLUTION OF THE GENE INSULIN; N.N. Abelyan, S.G. Tiratsuyan, G.R. Vardapetyan

CONFERENCE OF THE SUMMER SCHOOL ON BIOINFORMATICS 2019; In silico screening for low molecular weight quorum sensing inhibitors of the antibiotic resistance bacterium Pseudomonas aeruginosa that activate the host's immune response; Abelyan N.N., Ph.D., Assoc. Tiratsuyan S.G.

INVITATION TO THE 20TH FEBS YOUNG SCIENTISTS' FORUM TO BE HELD IN LOVRAN, CROATIA, 1-4 July 2020, which has moved to 30th June- 3rd July 2021

INVITATION TO THE 45TH FEBS CONGRESS TO BE HELD IN LJUBLJANA, SLOVENIA, 4-9 July 2020, which has moved to 3-8 July 2021 due to pandemic