

Dr. Kliment Olechnovič

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General information

Occupation Senior Researcher at Vilnius University Life Sciences Center
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Online profiles

Google Scholar https://scholar.google.lt/citations?user=uT_t5ewAAAAJ
ORCID <https://orcid.org/0000-0003-4918-9505>
GitHub <https://github.com/kliment-olechnovic>

Main research interests

- Structural bioinformatics
- Machine learning
- Computational geometry

Education

2012–2017 Ph.D. Computer Science, Vilnius University
2010–2012 M.S. Computer Science, Vilnius University (*Magna Cum Laude*)
2005–2009 B.S. Bioinformatics, Vilnius University

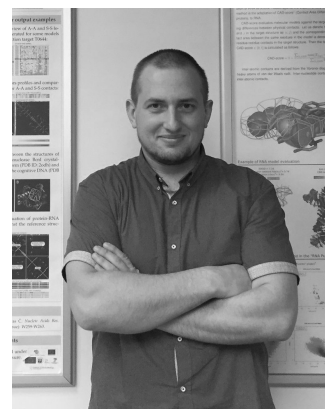
Work experience

2020–now Senior Researcher (Vilnius University / Life Sciences Center / Institute of Biotechnology)
2017–2020 Researcher (Vilnius University / Life Sciences Center / Institute of Biotechnology)
2013–2017 Junior Researcher (Vilnius University / Institute of Biotechnology)
2010–2013 Research Engineer (Vilnius University / Institute of Biotechnology)
2009–2010 Research Engineer (Institute of Biotechnology, Vilnius)
2007–2008 C++ software developer (4Team Corporation, Vilnius)

Publications

Papers in peer-reviewed journals

1. [Modeling of protein complexes in CASP14 with emphasis on the interaction interface prediction](#). Dapkūnas J, Olechnovič K, Venclovas Č. *Proteins*. 2021 Jun 27. doi:10.1002/prot.26167. PMID:34176161.
2. [VoroContacts: a tool for the analysis of interatomic contacts in macromolecular structures](#). Olechnovič K, Venclovas Č. *Bioinformatics*. 2021 Jun 16. pdf. doi:10.1093/bioinformatics/btab448. PMID:34132767.
3. [VoroCNN: Deep convolutional neural network built on 3D Voronoi tessellation of protein structures](#). Igashov I, Olechnovič K, Kadukova M, Venclovas Č, Grudinin S. *Bioinformatics*. 2021 Feb 23. doi:10.1093/bioinformatics/btab118. PMID:33620450.
4. [Template-based modeling of diverse protein interactions in CAPRI rounds 38–45](#). Dapkūnas J, Kairys V, Olechnovič K, Venclovas Č. *Proteins*. 2020 Aug;88(8):939–947. pdf. doi:10.1002/prot.25845. PMID:31697420.
5. [Blind prediction of homo- and hetero-protein complexes: The CASP13–CAPRI experiment](#). Lensink MF, Brysbaert G, Nadzirin N, Velankar S, Chaleil RAG, Gerguri T, Bates PA, Laine E, Carbone A, Grudinin S, Kong R, Liu RR, Xu XM, Shi H, Chang S, Eisenstein M, Karczynska A, Czaplewski C, Lubecka E, Lipska A, Krupa P, Mozolewska M, Golon Ł, Samsonov S, Liwo A, Crivelli S, Pagès G, Karasikov M, Kadukova M, Yan Y, Huang SY, Rosell M, Rodríguez-Lumbreras LA, Romero-Durana M, Díaz-Bueno L, Fernandez-Recio J, Christoffer C, Terashi G, Shin WH, Aderinwale T, Maddhuri Venkata Subraman SR, Kihara D, Kozakov D, Vajda S, Porter K, Padhorny D, Desta I, Beglov D, Ignatov M, Kotelnikov S, Moal IH, Ritchie DW, Chauvot de Beauchêne I, Maigret B, Devignes MD, Ruiz Echartea ME, Barradas-Bautista D, Cao Z, Cavallo L, Oliva R, Cao Y, Shen Y, Baek M, Park T, Woo H, Seok C, Braitbard M, Bitton L, Scheidman-Duhovny D, Dapkūnas J, Olechnovič K, Venclovas Č, Kundrotas PJ, Belkin S, Chakravarty D, Badal VD, Vakser IA, Vreven T, Vangaveti S, Borrmann T, Weng Z, Guest JD, Gowthaman R, Pierce BG, Xu X, Duan R, Qiu L, Hou J, Ryan Merideth B, Ma Z, Cheng J, Zou X, Koukos PI, Roel-Touris J, Ambrosetti F, Geng C, Schaarschmidt J, Trellet ME, Melquiond ASJ, Xue L, Jiménez-García B, van Noort CW, Honorato RV, Bonvin AMJJ, Wodak SJ. *Proteins*. 2019 Dec;87(12):1200–1221. doi:10.1002/prot.25838. PMID:31612567.
6. [Structural modeling of protein complexes: Current capabilities and challenges](#). Dapkūnas J, Olechnovič K, Venclovas Č. *Proteins*. 2019 Dec;87(12):1222–1232. doi:10.1002/prot.25774. PMID:31294859.
7. [Estimation of model accuracy in CASP13](#). Cheng J, Choe MH, Elofsson A, Han KS, Hou J, Maghrabi AHA, McGuffin LJ, Menéndez-Hurtado D, Olechnovič K, Schwede T, Studer G, Uziela K, Venclovas Č, Wallner B. *Proteins*. 2019 Dec;87(12):1361–1377. doi:10.1002/prot.25767. PMID:31265154.
8. [VoroMQA web server for assessing three-dimensional structures of proteins and protein complexes](#). Olechnovič K, Venclovas Č. *Nucleic Acids Res*. 2019 Jul 2;47(W1):W437–W442. doi:10.1093/nar/gkz367. PMID:31073605.
9. [Comparative analysis of methods for evaluation of protein models against native structures](#). Olechnovič K, Monastyrskyy B, Kryshatovych A, Venclovas Č. *Bioinformatics*. 2019 Mar 15;35(6):937–944. doi:10.1093/bioinformatics/bty760. PMID:30169622.
10. [Modeling of protein complexes in CAPRI Round 37 using template-based approach combined with model selection](#). Dapkūnas J, Olechnovič K, Venclovas Č. *Proteins*. 2018 Mar;86 Suppl 1:292–301. doi:10.1002/prot.25378. PMID:28905467.
11. [VoroMQA: Assessment of protein structure quality using interatomic contact areas](#). Olechnovič K, Venclovas Č. *Proteins*. 2017 Jun;85(6):1131–1145. doi:10.1002/prot.25278. PMID:28263393.
12. [The PPI3D web server for searching, analyzing and modeling protein-protein interactions in the context of 3D structures](#). Dapkūnas J, Timinskas A, Olechnovič K, Margelevičius M, Diciunas R, Venclovas Č. *Bioinformatics*. 2017 Mar 15;33(6):935–937. doi:10.1093/bioinformatics/btw756. PMID:28011769.
13. [The CAD-score web server: contact area-based comparison of structures and interfaces of proteins, nucleic acids and their complexes](#). Olechnovič K, Venclovas Č. *Nucleic Acids Res*. 2014 Jul;42(Web Server issue):W259–63. doi:10.1093/nar/gku294. PMID:24838571.
14. [The use of interatomic contact areas to quantify discrepancies between RNA 3D models and reference structures](#). Olechnovič K, Venclovas Č. *Nucleic Acids Res*. 2014 May;42(9):5407–15. doi:10.1093/nar/gku191. PMID:24623815.



15. [Voronota: A fast and reliable tool for computing the vertices of the Voronoi diagram of atomic balls](#). Olechnovič K, Venclovas Č. *J Comput Chem*. 2014 Mar 30;35(8):672-81. doi:10.1002/jcc.23538. PMID:24523197.
16. [CAD-score: a new contact area difference-based function for evaluation of protein structural models](#). Olechnovič K, Kulberkytė E, Venclovas Č. *Proteins*. 2013 Jan;81(1):149-62. doi:10.1002/prot.24172. PMID:22933340.
17. [VoroProt: an interactive tool for the analysis and visualization of complex geometric features of protein structure](#). Olechnovič K, Margelevičius M, Venclovas Č. *Bioinformatics*. 2011 Mar 1;27(5):723-4. doi:10.1093/bioinformatics/btq720. PMID:21186248.

Book chapters

- [Contact Area-Based Structural Analysis of Proteins and Their Complexes Using CAD-Score](#). Olechnovič K, Venclovas Č. In: Zoltán Gáspári (eds) *Structural Bioinformatics: Methods and Protocols, Methods in Molecular Biology, vol. 2112*. Springer. 2020.
- [In Silico Modeling of Inhibitor Binding to Carbonic Anhydrases](#). Kairys V, Olechnovič K, Raškevičius V, Matulis D. In: Matulis D. (eds) *Carbonic Anhydrase as Drug Target*. Springer, Cham. 2019.

Doctoral dissertation

- [Methods for the analysis and assessment of the three-dimensional structures of proteins and nucleic acids: development and applications](#). Olechnovič K. Doctoral dissertation, Vilnius University, 2017.
- [Baltymų ir nukleorūgščių erdvių struktūrų analizės ir vertinimo metodai: kūrimas ir taikymas](#). Olechnovič K. Doctoral dissertation summary in Lithuanian, Vilnius University, 2017.

Other publications

- [Kompiuteriai padeda pažinti sudėtingą baltymų pasaulį](#). Dapkūnas J, Olechnovič K. Popular science article in *SPECTRUM*. 2017 1(26), ISSN 1822-0147.
- [Journal cover image based on the article "VoroMQA: Assessment of protein structure quality using interatomic contact areas"](#). Olechnovič K, Venclovas Č. Cover Image for *Proteins*. 2019 Volume 85, Issue 6. doi:10.1002/prot.25129.

Presentations

Oral presentations at international conferences

- AI at CIRM, France, Marseille (2021)
- CASP14 meeting, Virtual (2020)
- COINS, Lithuania, Vilnius (2019), *keynote presentation*
- CASP13 meeting, Mexico, Riviera Maya (2018)
- VitaScientia, Lithuania, Vilnius (2018)
- CASP12 meeting, Italy, Gaeta (2016)
- CASP10 meeting, Italy, Gaeta (2012)

Poster presentations at international conferences

- AI at CIRM, France, Marseille (2021), [poster](#)
- PDB50, Virtual (2021), [poster](#)
- CASP14 meeting, Virtual (2020), [poster](#)
- ISMB, Switzerland, Basel (2019), [poster](#)
- CASP13 meeting, Mexico, Riviera Maya (2018), [poster](#)
- CASP12 meeting, Italy, Gaeta (2016), [poster](#)
- ECCB, Netherlands, Hague (2016), [poster](#)
- CASP11 meeting, Mexico, Riviera Maya (2014), [poster](#)
- ECCB, France, Strasbourg (2014), [poster](#)
- ISMB, Germany, Berlin (2013), [poster](#)
- SocBiN, Poland, Torun (2013), [poster](#)
- CASP10 meeting, Italy, Gaeta (2012), [poster](#)
- ECCB, Switzerland, Basel (2012), [poster](#)
- SAGA, Lithuania, Vilnius (2011), [poster](#)
- ISMB, Austria, Vienna (2011), [poster](#)
- ECCB, Belgium, Ghent (2010), [poster](#)
- VizBi, Germany, Heidelberg (2010), [poster](#)

Gallery of posters: www.kliment.lt/posters

Main published software

- Voronota: a standalone software package of various tools for analyzing three-dimensional structures of biological macromolecules using the Voronoi diagram of atomic balls (includes the latest versions of CAD-score and VoroMQA methods). <https://kliment-olechnovic.github.io/voronota>
- VoroMQA web server for the assessment of protein structure quality using interatomic contact areas. <https://bioinformatics.lt/wtsam/voromqa>
- VoroContacts web server for the computation and interactive querying of Voronoi tessellation-derived contacts. <https://bioinformatics.lt/wtsam/vorocontacts>
- CAD-score web server for contact area-based comparison of structures and interfaces of proteins, nucleic acids and their complexes. <https://bioinformatics.lt/cad-score/>
- VoroProt: an interactive tool for exploring some tessellation-derived features of protein structures (no longer maintained). <https://bioinformatics.lt/software/voroprot>

Achievements and awards

Achievements in CASP and CAPRI experiments

CASP (Critical Assessment of Techniques for Protein Structure Prediction) and CAPRI (Critical Assessment of PRedicted Interactions) are world-wide experiments focused on the blind testing of methods for protein structural bioinformatics.

2020

Contributed to one of the top performances (ranked 2nd) in modeling structures of protein complexes in

- CASP14 and CASP14-CAPRI experiments. Group "Venclovas", members: Olechnovič K, Dapkūnas J, Venclovas Č.
- 2019 Contributed to one of the top performances (ranked 3rd) in modeling structures of protein complexes in the CAPRI experiment rounds 38–45. Group "Venclovas", members: Dapkūnas J, Kairys V, Olechnovič K, Venclovas Č.
- 2018 Contributed to the best results (ranked 1st) in modeling structures of protein complexes in CASP13 and CASP13-CAPRI experiments. Group "Venclovas", members: Dapkūnas J, Olechnovič K, Venclovas Č.
- 2018 One of the top performances in EMA (estimation of model accuracy) in CASP13 experiment. Groups "VoroMQA-A" and "VoroMQA-B", members: Olechnovič K, Venclovas Č.
- 2016 Contributed to the best results (ranked 1st) in modeling structures of protein complexes in CASP12-CAPRI experiment. Group "Venclovas", members: Dapkūnas J, Olechnovič K, Venclovas Č.
- 2016 One of the top performances in protein structure prediction in CASP12 experiment. Group "VoroMQA-select", members: Olechnovič K, Venclovas Č.

National awards

- 2019 Lithuanian Academy of Sciences scholarship for young scientists
- 2018 Laureate of the "Best doctoral dissertation of 2017 in Lithuania" contest
- 2015 Lithuanian Academy of Sciences award for the best works by young researchers in 2014
- 2013–2014 The Research Council of Lithuania scholarship for PhD students actively conducting scientific research
- 2013 INFOBALT incentive scholarship for young scientists

Conference awards

- 2019 ISCB Art in Science Award Winner at "ISMB/ECCB 2019". Work title: ["Disassembled tessellation"](#).
- 2016 Poster selected for an oral presentation at "12th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP12 meeting)". Poster title: *VoroMQA: assessment of protein structure quality using interatomic contact areas derived from the Voronoi tessellation of atomic balls.*
- 2013 Best poster award at "Society for Bioinformatics in Northern European countries (SocBiN)". Poster title: *The use of interatomic contact areas for the assessment of RNA 3D structural models.*
- 2012 Poster selected for an oral presentation at "EMBO Conference on Critical Assessment of Protein Structure Prediction (CASP10 meeting)". Poster title: *CAD-score: a new method for the evaluation of protein structural models.*

Other achievements

- 2018 Judo champion of Lithuania, judo black belt.
- 2018 Sambo champion of Lithuania.