

Dr. Kliment Olechnovič

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General information

Occupation MSCA Postdoctoral Fellow at CNRS Laboratoire Jean Kuntzmann, Grenoble, France (from 2023-09-01 to 2025-08-31)
on sabbatical leave as Senior Researcher at Vilnius University Life Sciences Center until 2025-09-01

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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

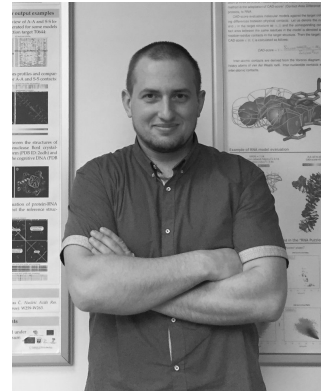
Work experience

2023–now MSCA Postdoctoral Fellow (CNRS Laboratoire Jean Kuntzmann, Grenoble, France)
2020–2023 Senior Researcher (Vilnius University / Life Sciences Center / Institute of Biotechnology)
2021–2023 Visiting researcher, for 28 weeks in total (CNRS Laboratoire Jean Kuntzmann, Grenoble, France)
2017–2020 Researcher (Vilnius University / Life Sciences Center / Institute of Biotechnology)
2019–2020 Visiting researcher, for 9 weeks (Inria, Grenoble, France)
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

Research papers

1. **FTDMP: A Framework for Protein-Protein, Protein-DNA, and Protein-RNA Docking and Scoring.** Olechnovič K, Banciul R, Dapkūnas J, Venclovas Č. *Proteins*. 2025 Jan 2. doi:10.1002/prot.26792. PMID:39748638.
2. (preprint) **Voronota-LT: efficient, flexible and solvent-aware tessellation-based analysis of atomic interactions.** Olechnovič K, Grudin S. Preprint in bioRxiv. 2024. doi:10.1101/2024.02.05.577169.
3. **PPI3D: a web server for searching, analyzing and modeling protein-protein, protein-peptide and protein-nucleic acid interactions.** Dapkūnas J, Timinskas A, Olechnovič K, Tomkuvienė M, Venclovas Č. *Nucleic Acids Res*. 2024 Apr. doi:10.1093/nar/gkae278. PMID:38619046.
4. **TemStaPro: protein thermostability prediction using sequence representations from protein language models.** Pudžiuvėlytė I, Olechnovič K, Godliauskaitė E, Sermokas K, Urbaitis T, Gasiunas G, Kazlauskas D. *Bioinformatics*. 2024 Apr 4. doi:10.1093/bioinformatics/btae157. PMID:38507682.
5. **VoroIF-GNN: Voronoi tessellation-derived protein-protein interface assessment using a graph neural network.** Olechnovič K, Venclovas Č. *Proteins*. 2023 Jul 21. doi:10.1002/prot.26554. PMID:37482904.
6. **Prediction of protein assemblies by structure sampling followed by interface-focused scoring.** Olechnovič K, Valančauskas L, Dapkūnas J, Venclovas Č. *Proteins*. 2023 Aug 14. doi:10.1002/prot.26569. PMID:37578163.
7. **Impact of AlphaFold on Structure Prediction of Protein Complexes: The CASP15-CAPRI Experiment.** Lensink M, Brysbaert G, Raouraoua N, Bates P, Giuliani M, Vargas Honorato R, van Noort C, Teixeira J, MJJ Bonvin A, Kong R, Shi H, Lu X, Chang S, Liu J, Guo Z, Chen X, Morehead A, Roy R, Wu T, Giri N, Quadri F, Chen C, Cheng J, Del Carpio C, Ichiishi E, Fernández-Recio J, Harmalkar A, Chu L, Canner S, Smanta R, Gray J, Li H, Lin P, He J, Tao H, Huang S, Roel J, Jimenez-Garcia B, Christoffer C, Jain A, Kagaya Y, Kannan H, Nakamura T, Terashi G, Verburg J, Zhang Y, Zhang Z, Fujuta H, Sekijima M, Kihara D, Khan O, Kotelnikov S, Ghani U, Padhorny D, Beglov D, Vajda S, Kozakov D, Negi S, Ricciardelli T, Barradas-Bautista D, Cao Z, Chawla M, Cavallo L, Oliva R, Yin R, Cheung M, Guest J, Lee J, Pierce B, Shor B, Cohen T, Halfon M, Schneidman-Duhovny D, Zhu S, Yin R, Sun Y, Shen Y, Maszota-Zieleniak M, Bojarski K, Lubecka E, Marcisz M, Danielsson A, Dziadek L, Gaardlos M, Giełdoń A, Liwo J, Samsonov S, Slusarz R, Zieba K, Sieradzian A, Czaplewski C, Kobayashi S, Miyakawa Y, Kiyota Y, Takeda-Shitaka M, Olechnovič K, Valančauskas L, Dapkūnas J, Venclovas C, Wallner B, Yang L, Hou C, He X, Guo S, Jiang S, Ma X, Duan R, Qiu L, Xu X, Zou X, Velankar S, Wodak S. *Proteins*. 2023 Oct 31. doi:10.1002/prot.26609. PMID:37905971.
8. **Discriminating Physiological from Non-Physiological Interfaces in Structures of Protein Complexes: A Community-Wide Study.** Schweke H, Xu Q, Tauriello G, Pantolini L, Schwede T, Cazals F, Lhéritier A, Fernandez-Recio J, Rodríguez-Lumbreras LA, Schueler-Furman O, Varga JK, Jiménez-García B, Réau MF, Bonvin A, Savojardo C, Martelli P-L, Casadio R, Tubiana J, Wolfson H, Oliva R, Barradas-Bautista D, Ricciardelli T, Cavallo L, Venclovas Č, Olechnovič K, Guerois R, Andreani J, Martin J, Wang X, Kihara D, Marchand A, Correia B, Zou X, Dey S, Dunbrack R, Levy E, Wodak S. *Proteomics*. 2023 Jun 27. doi:10.1002/pmic.202200323. PMID:37365936.
9. **Modeling SARS-CoV2 proteins in the CASP-commons experiment.** Kryshchak A, Moulton A, Billings WM, Della Corte D, Fidelis K, Kwon S, Olechnovič K, Seok C, Venclovas Č, Won J, et al. *Proteins*. 2021 Aug 30. doi:10.1002/prot.26231. PMID:34462960.
10. **Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment.** Lensink MF, Brysbaert G, Mauri T, Nadzirin N, Velankar S, Chaleil RAG, Clarence T, Bates PA, Kong R, Liu B, Yang G, Liu M, Shi H, Lu X, Chang S, Roy RS, Quadri F, Liu J, Cheng J, Antoniak A, Czaplewski C, Giełdoń A, Kogut M, Lipska AG, Liwo A, Lubecka EA, Maszota-Zieleniak M, Sieradzian AK, Slusarz R, Wesolowski PA, Zięba K, Del Carpio Muñoz CA, Ichiishi E, Harmalkar A, Gray JJ, Bonvin AMJJ, Ambrosetti F, Honorato RV, Jandova Z, Jiménez-García B, Koukous PI, Van Keulen S, Van Noort CW, Réau M, Roel-Touris J, Kotelnikov S, Padhorny D, Porter KA, Alekseenko A, Ignatov M, Desta I, Ashizawa R, Sun Z, Ghani U, Hashemi N, Vajda S, Kozakov D, Rosell



- M, Rodríguez-Lumbreras LA, Fernandez-Recio J, Karczynska A, Grudinin S, Yan Y, Li H, Lin P, Huang SY, Christoffer C, Terashi G, Verburgt J, Sarkar D, Aderinwale T, Wang X, Kihara D, Nakamura T, Hanazono Y, Gowthaman R, Guest JD, Yin R, Taherzadeh G, Pierce BG, Barradas-Bautista D, Cao Z, Cavallo L, Oliva R, Sun Y, Zhu S, Shen Y, Park T, Woo H, Yang J, Kwon S, Won J, Seok C, Kiyota Y, Kobayashi S, Harada Y, Takeda-Shitaka M, Kundrotas PJ, Singh A, Vakser IA, Dapkūnas J, **Olechnovič K**, Venclovas Č, Duan R, Qiu L, Zhang S, Zou X, Wodak SJ. *Proteins*. 2021 Aug 28. doi:10.1002/prot.26222. PMID:34453465.
11. [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.
 12. [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.
 13. [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.
 14. [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.
 15. [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 E, 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 Echarte 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.
 16. [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.
 17. [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.
 18. [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.
 19. [Comparative analysis of methods for evaluation of protein models against native structures](#). **Olechnovič K**, Monastyrskyy B, Kryshchak A, Venclovas Č. *Bioinformatics*. 2019 Mar 15;35(6):937-944. doi:10.1093/bioinformatics/bty760. PMID:30169622.
 20. [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.
 21. [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.
 22. [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.
 23. [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.
 24. [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.
 25. [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.
 26. [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.
 27. [Voroport: 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 analizė 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 and posters

Oral presentations at international conferences

- 2nd ML4NGP Meeting on Machine Learning and Non-globular proteins, Thessaloniki, Greece (2024)
- Joint ICB Workshop and 8th CAPRI Assessment Meeting, France, Grenoble (2024)
- CASP15 meeting, Turkey, Antalya (2022)
- 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

- CASP16 meeting, Punta Cana, Dominican Republic (2024), [poster](#)
- NCSB meeting, Nancy, France (2024), [poster](#)
- CASP15 meeting, Antalya, Turkey (2022), [poster](#)
- 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>
- Voronota-JS: an expansion of the core Voronota software. Voronota-JS provides a way to write JavaScript scripts for the comprehensive analysis of macromolecular structures, including the Voronoi tessellation-based analysis. https://kliment-olechnovic.github.io/voronota/expansion_js/
- Voronota-LT: an expansion of the core Voronota software. Voronota-LT (pronounced ‘voronota lite’) is an alternative, significantly faster version of Voronota for constructing tessellation-derived atomic contact areas and volumes. https://kliment-olechnovic.github.io/voronota/expansion_lt/
- Voronota-GL: a visual tool for the comprehensive interactive analysis of macromolecular structures, including the Voronoi tessellation-based analysis. https://kliment-olechnovic.github.io/voronota/expansion_gl/
- FTDMP: a software system for running docking experiments and scoring/ranking multimeric models (includes VoroIF-jury and VoroIF-GNN methods). <https://kliment-olechnovic.github.io/ftdmp/>
- 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.

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|-------------|---|
| 2022 | Contributed to one of the top performances in modeling structures of protein complexes in CASP15 and CASP15-CAPRI experiments (ranked 2nd in CASP, ranked 1st in CAPRI). Group “Venclovas”, members: Olechnovič K, Valančauskas L, Dapkūnas J, Venclovas Č. |
| 2022 | One of the top performances in EMA (estimation of model accuracy) in CASP15 experiment (and ranked 1st in CASP15-CAPRI scoring experiment). Groups “Venclovas” and “VoroIF”. |
| 2020 | Contributed to one of the top performances in modeling structures of protein complexes in CASP14 and CASP14-CAPRI experiments (ranked 2nd in CASP, ranked 1st in CAPRI jointly with two other groups). 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 (ranked 1st in prediction of unreliable regions). Groups “VoroMQA-A” and “VoroMQA-B”.
- 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”.

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.