Dr. Saulius Gražulis

Chief Researcher
Vilnius University Institute of Biotechnology

1968-08-19, Kaunas, Lietuva (Lithuania)
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Education

1994 – 2000 Ph.D.; Munich Technical University (Technische Universität München), Munich, Germany.
Thesis title: *Structure and function of the restriction endonucleases Bse634I and MunI*

1986 – 1994 MSc, engineer-researcher physicist; Moscow Institute of Physics and Technology (Московский Физико-Технический Институт), Moscow, Russia.
Thesis title: *Isolation and biochemical characterisation of the laminarinase from hyperthermophilic eubacteria* Thermotoga neapolitana

1975 – 1986 Secondary education; Jonas Jablonskis Secondary School, Kaunas, Lithuania.

Employment

Primary employment

2013 – . . . Chief Researcher, VU Institute of Biotechnology, Life Science Centre.
2003 – 2013 Senior Researcher, VU Institute of Biotechnology.
2000 – 2003 Research Associate, Institute of Biotechnology.
1994 – 2000 Junior Researcher, Institute of Biotechnology.

Secondary employment

2014 – . . . Full Professor, VU Faculty of Mathematics and Informatics.
2010 – 2014 Associate Professor, VU Faculty of Mathematics and Informatics.
2008 – 2010 Lecturer, VU Faculty of Mathematics and Informatics.
2009 – 2014 Associate Professor, VU Faculty of Chemistry, Faculty of Natural Sciences.
2007 – 2009 Lecturer, VU Faculty of Chemistry, Faculty of Natural Sciences.

Research interests

Crystallography; crystallographic databases; structural biology – structure-function relations of biological macromolecules; computer science – programming and data description languages, computer architecture; scientific databases; data management; ontologies; philosophy of science – epistemology.

Language Proficiency

According to levels approved by EC:

Gimtoji kalba/mother tongue:			Lietuvių (Lithuanian)		
Kitos kalbos Other languages	Supratimas Understanding		Kalbėjimas Speaking		Rašymas Writing
	Klausymas Listening	Skaitymas Reading	Pokalbis Spoken Interaction	Monologas Spoken Production	
Rusų (Russian)	C2	C2	C2	C2	C2
Anglų (English)	C1	C2	C2	C2	C1
Vokiečių (German)	B2	B2	B1	B1	A2
Lenkų (Polish)	B1	B2	A2	A2	A1
Esperanto	A1	A2	A1	A1	A1
Japonų (Japanese)	A1	A1	A1	A1	A1
French (Prancūzų)	A1	A1	A1	A1	A1

Life-long learning

- 2011 — 3 days BIOTEFA-A courses on the Virtual learning environment, Vilnius, Lithuania.
- 2011 — 1 week Crystallographic Computing School, Mieres/Oviedo, Spain.
- 2008 — 1 week Crystallographic Computing School, Kyoto, Japan.
- 2009 — 2 months The University of York, York Structural Biology Laboratory, (visit to Dr. G. Murshudov), York, UK.
- 2005 — 1 week M2M courses, EMBL, DESY, Hambug, Germany.
- 1994 — 2000 — 6 years Max-Planck Institute of Biochemistry, Dept. of Structural Research (dept. leader Dr. FRS R. Huber), Martinsried (by Munich), Germany

Teaching activities

Courses offered

- Computer Architecture, II year Bioinformatics and Computer Science students, (fall term), in English and in Lithuanian, 66 hours/semester, 5 ECTS credits.
- Programming methodology for bioinformatics, III year bioinformatics students, 64 hours/semester.
- Bioinformatics III – analysis of biological macromolecule 3-d structures, III year bioinformatics students, 48 hours/semester.
- Macromolecular X-ray crystallography.
- Physical analysis methods – introduction into crystallography (part of the course), IV year biochemistry students, 20 hours/semester.
- GNU/Linux operating systems, I year master students, Systems Biology programme, 5 ECTS credits.

Doctoral students

- 2016 – . . . — Antanas Vaitkus
- 2017 – . . . — Algirdas Grybauskas

Teaching activities (continued)

2013 – 2017 Andrius Merkys, thesis defended in 2018.

2004 – 2012 Dmitrij Golovenko, thesis defended in 2012.

2004 – 2009 Rasa Sukackaitė, thesis defended in 2009.

2002 – 2007 Giedrė Tamulaitienė, thesis defended in 2007.

Undergraduate students

2000 – 2014 Supervised Andrius Merkys, Antanas Vaitkus, Erikas Raginis, Alina Belova, Saulė Girdzijauskaitė, Aleksandras Konovalovas, Rolandas Porėjus, Adriana Daškevič BSc and/or MSc thesis.

Research grants

2016 – 2020 S. Gražulis, A. Merkys, A. Vaitkus, A. Grybauskas (the VU group) participated in the H2020 project 689868 — SOLSA "Sonic Drilling coupled with Automated Mineralogy and chemistry On-Line-On-Mine-Real-Time" (call H2020 — H2020-SC5-2015-one-stage). Project coordinator: ERAMET (France); leader of the Vilnius University group: S. Gražulis; funds allocated for the project are 9 775 488 €; the part allocated to the Vilnius University is 602 000 €.

2013 – 2015 S. Gražulis, A. Smirnov, A. Merkys, V. Kairys, M. Okulič-Kazarinas have been participating in the project MIP-025/2013 "Expansion of the Crystallography Open Database (COD) and statistical analysis of crystal structures", funded by the Lithuanian Research Council (LRC). S. Gražulis was the project leader. funding received: 317 400 Lt.

2014 – 2015 S. Gražulis, V. Siksnys et al. together with partners from Latvia and Estonia, participated in the BioStruct-X BAG project to receive access to synchrotron beamlines. Principal Investigator – S. Gražulis. 75 MX time shifts for protein crystallography and 27 SAXS shifts for small-angle scattering experiments were received (1 shift is 8 measurement hours).

2011 – 2015 Dr. S. Gražulis took part in the RCL Global grant project "Structural and molecular mechanisms of bacteria defence systems", contract No. R100, the leader - prof. V. Šikšnys. Estimated value: 1 599 781 Lt (EUR 463 398). The objects of the project were type III restriction endonucleases and I-E and Type II CRISPR systems.

2009 – 2013 Dr. S. Gražulis participated in the EU-funded project, FP7-REGPOT-2009-1 call. The project contract was No. 245721, project title was "Strengthening and Sustaining the European Perspectives of Molecular Biotechnology in Lithuania (MoBiLi)". Estimated value – 1 603 788 €.

2010 – 2011 Research Council of Lithuanian grant No. MIP-124/2010 "Open access crystallographic database COD", project leader S.Gražulis, 190 thous. Lt.

2008 – 2010 EEA contract No. 2004-LT0019-IP-1EEE "Anti-cancer drug design using methods of structural thermodynamics", project leader Dr. D. Matulis, total financing (for the whole project) 565 thous. EUR, S. Gražulis was responsible for the crystallographic part of the investigations.

2007 – 2010 LVMSF project grant No. N-0711 "Search of compounds specifically inhibiting human carbonic anhydrases using methods of biotechnology" , project leader Dr. D. Matulis, 350 thous. Lt, S. Gražulis was responsible the crystallographic investigations.

2008 – 2010 Lithuanian high priority research programme, contract No. C-01/2008 "Investigations of structure and function of the phage T4 replisome", project leader V.Šikšnys, 220 thous. Lt, S. Gražulis was responsible the crystallographic investigations.

Conferences

- 2012 ECM27, The 27th European Crystallographic Meeting, invited talk "Use of the Crystallography Open Database as a source of prior knowledge for molecular modelling" at the microsymposium "Advances in Refinement and Validation", Bergen, Norway;
- 2011 IUCr Crystallographic Computing School, invited talk and 2 tutorial sessions „Crystallography Open Database: plans, wishes, perspectives", Oviedo, Spain;
- 2008 21st Congress of IUcr pre-congress workshop „On New Routes to Crystallographic Data Publication", invited talk „A Tale of COD (selection, curation and maintenance of the Crystallography Open Database)", Osaka, Japan;
- IUCr Crystallographic Computing School, invited talk „A Tale of COD (selection, curation and maintenance of the Crystallography Open Database)", Kyoto, Japan.

Participation in professional organisations

- 2007 – . . . Member of the Crystallography Open Database (COD) Advisory Board
- 2018 – . . . Member of the Raman Open Database (ROD) Advisory Board

Organisation of international workshops and conferences

- 2022 Participation in organising an international CECAM Flagship Workshop "Open Databases Integration for Materials Design"
- 2021 Member of the scientific advisory board and participant of the international "Workshop on Ontologies for Materials-Databases Interoperability", Linköping University, Sweden.
- 2019–2021 Participation in organising an international CECAM workshops "Open Databases Integration for Materials Design"

Publication output

- papers $>$ 50 papers in the peer reviewed press;
- books 3 book chapters based on the research results;
- citations 4318 citations; $h-$index $= 30$ (Google Scholar, 2021-12-20)

List of Research Publications

Books and Chapters

1. Gražulis, S., Merkys, A., Vaitkus, A., Chateigner, D., Lutterotti, L., Moeck, P., Quiros, M., Downs, R. T., Kaminsky, W. & Le Bail, A. (2019). *Crystallography open database: History, development, and perspectives* (O. Isayev, A. Tropsha & S. Curtarolo, Eds.). Wiley. https://doi.org/10.1002/9783527802265.ch1
2. Smirnov, A., Manakova, E., Gražulis, S., McKenna, R. & Matulis, D. (2019). *Structures of carbonic anhydrases and their complexes with inhibitors* (D. Matulis, Ed.). Springer. https://tinyurl.com/y5hqomv8
3. Gražulis, S., Merkys, A. & Vaitkus, A. (2018). *Crystallography Open Database (COD)* (W. Andreoni & S. Yip, Eds.). Springer International Publishing. https://doi.org/10.1007/978-3-319-42913-7_66-1

Journal Articles

1. Petrauskas, K., Merkys, A., Vaitkus, A., Laibinis, L. & Gražulis, S. (2022). Proving the correctness of the algorithm for building a crystallographic space group. *Journal of Applied Crystallography*, *55*(3), 515–525. https://doi.org/10.1107/s1600576722003107

2. Andersen, C. W., Armiento, R., Blokhin, E., Conduit, G. J., Dwaraknath, S., Evans, M. L., Fekete, Á., Gopakumar, A., Gražulis, S., Merkys, A., Mohamed, F., Oses, C., Pizzi, G., Rignanese, G.-M., Scheidgen, M., Talirz, L., Toher, C., Winston, D., Aversa, R., ... Yang, X. (2021). OPTIMADE, an API for exchanging materials data. *Scientific Data*, *8*(1). https://doi.org/10.1038/s41597-021-00974-z

3. Smirnovienė, J., Smirnov, A., Zakšauskas, A., Zubrienė, A., Petrauskas, V., Mickevičiūtė, A., Michailovienė, V., Čapkauskaitė, E., Manakova, E., Gražulis, S., Baranauskienė, L., Chen, W.-Y., Ladbury, J. E. & Matulis, D. (2021). Switching the inhibitor-enzyme recognition profile via chimeric Carbonic anhydrase XII. *ChemistryOpen*, *10*(5), 567–580. https://doi.org/10.1002/open.202100042

4. Vaitkus, A., Merkys, A. & Gražulis, S. (2021). Validation of the crystallography open database using the crystallographic information framework. *Journal of Applied Crystallography*, *54*(2), 661–672. https://doi.org/10.1107/s1600576720016532

5. Mendili, Y. E., Vaitkus, A., Merkys, A., Gražulis, S., Chateigner, D., Mathevet, F., Gascoin, S., Petit, S., Bardeau, J.-F., Zanatta, M., Secchi, M., Mariotto, G., Kumar, A., Cassetta, M., Lutterotti, L., Borovin, E., Orberger, B., Simon, P., Hehlen, B. & Guen, M. L. (2019). Raman Open Database: First interconnected Raman–X-ray diffraction open-access resource for material identification. *Journal of Applied Crystallography*, *52*(3), 618–625. https://doi.org/10.1107/s1600576719004229

6. Tamulaitienė, G., Manakova, E., Jovaišaitė, V., Tamulaitis, G., Gražulis, S., Bochtler, M. & Šikšnys, V. (2018). Unique mechanism of target recognition by PfoI restriction endonuclease of the CCGG-family. *Nucleic Acids Research*, 997–1010. https://doi.org/10.1093/nar/gky1137

7. Smirnov, A., Zubrienė, A., Manakova, E., Gražulis, S. & Matulis, D. (2018). Crystal structure correlations with the intrinsic thermodynamics of human carbonic anhydrase inhibitor binding. *PeerJ*, *6*, e4412. https://doi.org/10.7717/peerj.4412

8. Quirós, M., Gražulis, S., Girdzijauskaitė, S., Merkys, A. & Vaitkus, A. (2018). Using smiles strings for the description of chemical connectivity in the crystallography open database. *Journal of Cheminformatics*. https://doi.org/10.1186/s13321-018-0279-6

9. Merkys, A., Mounet, N., Cepellotti, A., Marzari, N., Gražulis, S. & Pizzi, G. (2017). A posteriori metadata from automated provenance tracking: Integration of AiiDA and TCOD. *Journal of Cheminformatics*, *9*(1), 56. https://doi.org/10.1186/s13321-017-0242-y

10. Mickevičiūtė, A., Timm, D. D., Gedgaudas, M., Linkuvienė, V., Chen, Z., Waheed, A., Michailovienė, V., Zubrienė, A., Smirnov, A., Čapkauskaitė, E., Baranauskienė, L., Jachno, J., Revuckienė, J., Manakova, E., Gražulis, S., Matulienė, J., Cera, E. D., Sly, W. S. & Matulis, D. (2017). Intrinsic thermodynamics of high affinity inhibitor binding to recombinant human carbonic anhydrase IV. *European Biophysics Journal*, *47*(3), 271–290. https://doi.org/10.1007/s00249-017-1256-0

11. Bruno, I., Gražulis, S., Helliwell, J. R., Kabekkodu, S. N., McMahon, B. & Westbrook, J. (2017). Crystallography and databases. *Data Science Journal*, *16*, 38. https://doi.org/10.5334/dsj-2017-038

12. Fuentes-Cobas, L. E., Chateigner, D., Fuentes-Montero, M. E., Pepponi, G. & Grazulis, S. (2017). The representation of coupling interactions in the Material Properties Open Database (MPOD). *Advances in Applied Ceramics*, *116*(8), 428–433. https://doi.org/10.1080/17436753.2017.1343782

13 Long, F., Nicholls, R. A., Emsley, P., Gražulis, S., Merkys, A., Vaitkus, A. & Murshudov, G. N. (2017a). ACEDRG: A stereo-chemical description generator for ligands. *Acta Crystallographica Section D*, *73*(2), 112–122. https://doi.org/10.1107/S2059798317000067

14 Long, F., Nicholls, R. A., Emsley, P., Gražulis, S., Merkys, A., Vaitkus, A. & Murshudov, G. N. (2017b). Validation and extraction of stereochemical information from small molecular databases. *Acta Crystallographica Section D*, *73*(2), 103–111. https://doi.org/10.1107/S2059798317000079

15 Tamulaitienė, G., Jovaišaitė, V., Tamulaitis, G., Songailiene, I., Manakova, E., Zaremba, M., Gražulis, S., Xu, S.-y. & Šikšnys, V. (2016). Restriction endonuclease AgeI is a monomer which dimerizes to cleave DNA. *Nucleic Acids Research*, 3547–3558. https://doi.org/10.1093/nar/gkw1310

16 Bernstein, H. J., Bollinger, J. C., Brown, I. D., Gražulis, S., Hester, J. R., McMahon, B., Spadaccini, N., Westbrook, J. D. & Westrip, S. P. (2016). Specification of the Crystallographic Information File format, version 2.0. *Journal of Applied Crystallography*, *49*(1), 277–284. https://doi.org/10.1107/s1600576715021871

17 Merkys, A., Vaitkus, A., Butkus, J., Okulič-Kazarinas, M., Kairys, V. & Gražulis, S. (2016). *COD::CIF::Parser*: an error-correcting CIF parser for the Perl language. *Journal of Applied Crystallography*, *49*(1), 292–301. https://doi.org/10.1107/S1600576715022396

18 Gražulis, S., Sarjeant, A. A., Moeck, P., Stone-Sundberg, J., Snyder, T. J., Kaminsky, W., Oliver, A. G., Stern, C. L., Dawe, L. N., Rychkov, D. A., Losev, E. A., Boldyreva, E. V., Tanski, J. M., Bernstein, J., Rabeh, W. M. & Kantardjieff, K. A. (2015). Crystallographic education in the 21st century. *Journal of Applied Crystallography*, *48*(6), 1964–1975. https://doi.org/10.1107/S1600576715016830

19 Tamulaitis, G., Rutkauskas, M., Zaremba, M., Gražulis, S., Tamulaitienė, G. & Šikšnys, V. (2015). Functional significance of protein assemblies predicted by the crystal structure of the restriction endonuclease BsaWI. *Nucleic Acids Research*, *43*(16), 8100–8110. https://doi.org/10.1093/nar/gkv768

20 Dudutienė, V., Zubrienė, A., Smirnov, A., Timm, D. D., Smirnovienė, J., Kazokaitė, J., Michailovienė, V., Zakšauskas, A., Manakova, E., Gražulis, S. & Matulis, D. (2015). Functionalization of fluorinated benzenesulfonamides and their inhibitory properties toward carbonic anhydrases. *Chemmedchem*, *10*(4), 662–687. https://doi.org/10.1002/cmdc.201402490

21 Gražulis, S., Merkys, A., Vaitkus, A. & Okulič-Kazarinas, M. (2015). Computing stoichiometric molecular composition from crystal structures. *Journal of Applied Crystallography*, *48*, 85–91. https://doi.org/10.1107/S1600576714025904

22 Zubrienė, A., Smirnovienė, J., Smirnov, A., Morkūnaitė, V., Michailovienė, V., Jachno, J., Juozapaitienė, V., Norvaišas, P., Manakova, E., Gražulis, S. & Matulis, D. (2015). Intrinsic thermodynamics of 4-substituted-2,3,5,6-tetrafluorobenzenesulfonamide binding to carbonic anhydrases by isothermal titration calorimetry. *Biophysical Chemistry*, *205*, 51–65. https://doi.org/10.1016/j.bpc.2015.05.009

23 Dudutienė, V., Matulienė, J., Smirnov, A., Timm, D. D., Zubrienė, A., Baranauskienė, L., Morkūnaitė, V., Smirnovienė, J., Michailovienė, V., Juozapaitienė, V., Mickevičiūte, A., Kazokaitė, J., Bakšytė, S., Kasiliauskaitė, A., Jachno, J., Revuckiene, J., Kišonaitė, M., Pilipuitytė, V., Ivanauskaitė, E., ... Matulis, D. (2014). Discovery and characterization of novel selective inhibitors of carbonic anhydrase IX. *Journal of Medicinal Chemistry*, *57*(22), 9435–9446. https://doi.org/10.1021/jm501003k

24 Golovenko, D., Manakova, E., Zakrys, L., Zaremba, M., Sasnauskas, G., Gražulis, S. & Šikšnys, V. (2014). Structural insight into the specificity of the B3 DNA-binding domains provided by the co-crystal structure of the C-terminal fragment of BfiI restriction enzyme. *Nucleic Acids Research*, *42*(6), 4113–4122. https://doi.org/10.1093/nar/gkt1368

25 Kišonaitė, M., Zubrienė, A., Čapkauskaitė, E., Smirnov, A., Smirnovienė, J., Kairys, V., Michailovienė, V., Manakova, E., Gražulis, S. & Matulis, D. (2014). Intrinsic thermodynamics and structure correlation of

benzenesulfonamides with a pyrimidine moiety binding to carbonic anhydrases I, II, VII, XII, and XIII. *Plos One*, *9*(12), e114106. https://doi.org/10.1371/journal.pone.0114106

26 Rutkauskas, K., Zubrienė, A., Tumošiene, I., Kantminienė, K., Kazemekaitė, M., Smirnov, A., Kazokaitė, J., Morkūnaitė, V., Čapkauskaitė, E., Manakova, E., Gražulis, S., Beresnevičius, Z. J. & Matulis, D. (2014). 4-amino-substituted benzenesulfonamides as inhibitors of human carbonic anhydrases. *Molecules*, *19*(11), 17356–17380. https://doi.org/10.3390/molecules191117356

27 Tamulaitienė, G., Šilanskas, A., Gražulis, S., Zaremba, M. & Šikšnys, V. (2014). Crystal structure of the R-protein of the multisubunit ATP-dependent restriction endonuclease NgoAVII. *Nucleic Acids Research*, *42*(22), 14022–14030. https://doi.org/10.1093/nar/gku1237

28 Čapkauskaitė, E., Zubrienė, A., Smirnov, A., Torresan, J., Kišonaitė, M., Kazokaitė, J., Gylytė, J., Michailovienė, V., Jogaite, V., Manakova, E., Gražulis, S., Tumkevicius, S. & Matulis, D. (2013). Benzenesulfonamides with pyrimidine moiety as inhibitors of human carbonic anhydrases I, II, VI, VII, XII, and XIII. *Bioorganic & Medicinal Chemistry*, *21*(22), 6937–6947. https://doi.org/10.1016/j.bmc.2013.09.029

29 Dudutienė, V., Zubrienė, A., Smirnov, A., Gylytė, J., Timm, D., Manakova, E., Gražulis, S. & Matulis, D. (2013). 4-substituted-2,3,5,6-tetrafluorobenzenesulfonamides as inhibitors of carbonic anhydrases I, II, VII, XII, and XIII. *Bioorganic & Medicinal Chemistry*, *21*(7), 2093–2106. https://doi.org/10.1016/j.bmc.2013.01.008

30 Matulis, D., Čapkauskaitė, E., Zubrienė, A., Baranauskienė, L., Tamulaitienė, G., Manakova, E., Kairys, V., Gražulis, S. & Tumkevicius, S. (2013). Design, synthesis, binding, crystallography, and docking of [(2-pyrimidinylthio) acetyl] benzenesulfonamides as inhibitors of human carbonic anhydrases. *Biophysical Journal*, *104*(2), 558A–559A. https://doi.org/10.1016/j.bpj.2012.11.3095

31 Čapkauskaitė, E., Zubrienė, A., Baranauskienė, L., Tamulaitienė, G., Manakova, E., Kairys, V., Gražulis, S., Tumkevicius, S. & Matulis, D. (2012). Design of [(2-pyrimidinylthio)acetyl]benzenesulfonamides as inhibitors of human carbonic anhydrases. *European Journal of Medicinal Chemistry*, *51*, 259–270. https://doi.org/10.1016/j.ejmech.2012.02.050

32 Gražulis, S., Daškevič, A., Merkys, A., Chateigner, D., Lutterotti, L., Quirós, M., Serebryanaya, N. R., Moeck, P., Downs, R. T. & Le Bail, A. (2012). Crystallography Open Database (COD): An open-access collection of crystal structures and platform for world-wide collaboration. *Nucleic Acids Research*, *40*(D1), http://nar.oxfordjournals.org/content/40/D1/D420.full.pdf+html, D420–D427. https://doi.org/10.1093/nar/gkr900

33 Manakova, E., Gražulis, S., Zaremba, M., Tamulaitienė, G., Golovenko, D. & Šikšnys, V. (2012). Structural mechanisms of the degenerate sequence recognition by Bse634I restriction endonuclease. *Nucleic Acids Research*, *40*(14), 6741–6751. https://doi.org/10.1093/nar/gks300

34 Pepponi, G., Gražulis, S. & Chateigner, D. (2012). MPOD: A material property open database linked to structural information [E-MRS 2011 Spring Meeting, Symposium M: X-ray techniques for materials research-from laboratory sources to free electron lasers]. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, *284*(0), 10–14. https://doi.org/10.1016/j.nimb.2011.08.070

35 Sukackaitė, R., Gražulis, S., Tamulaitis, G. & Šikšnys, V. (2012). The recognition domain of the methyl-specific endonuclease McrBC flips out 5-methylcytosine. *Nucleic Acids Research*, *40*(15), 7552–7562. https://doi.org/10.1093/nar/gks332

36 Čapkauskaitė, E., Baranauskienė, L., Golovenko, D., Manakova, E., Gražulis, S., Tumkevičius, S. & Matulis, D. (2010). Indapamide-like benzenesulfonamides as inhibitors of carbonic anhydrases I, II, VII, and XIII. *Bioorg Med Chem*, *18*(21), 7357–7364. https://doi.org/10.1016/j.bmc.2010.09.016

37 Sūdžius, J., Baranauskienė, L., Golovenko, D., Matulienė, J., Michailovienė, V., Torresan, J., Jachno, J., Sukackaitė, R., Manakova, E., Gražulis, S., Tumkevičius, S. & Matulis, D. (2010). 4-[n-(substituted

4-pyrimidinyl)amino]benzenesulfonamides as inhibitors of carbonic anhydrase isozymes I, II, VII, and XIII. *Bioorg Med Chem*, *18*(21), 7413–7421. https://doi.org/10.1016/j.bmc.2010.09.011

38 Gražulis, S., Butkus, J., Downs, R., Olozábal, M. Q. & Le Bail, A. (2010). Software for maintaining and expanding the Crystallography Open Database. *Acta Crystallogr. A*, *66*(a1), s313. https://doi.org/10.1107/S0108767310092810

39 Baranauskienė, L., Hilvo, M., Matulienė, J., Golovenko, D., Manakova, E., Dudutienė, V., Michailovienė, V., Torresan, J., Jachno, J., Parkkila, S., Maresca, A., Supuran, C., Gražulis, S. & Matulis, D. (2010). Inhibition and binding studies of carbonic anhydrase isozymes I, II and IX with benzimidazo[1,2-c][1,2,3]thiadiazole-7-sulphonamides. *Enzyme Inhib. Med. Chem.*, *25*(6), 863–870. https://doi.org/10.3109/14756360903571685

40 Golovenko, D., Manakova, E., Tamulaitienė, G., Gražulis, S. & Šikšnys, V. (2009). Structural mechanisms for the 5'-CCWGG sequence recognition by the N- and C-terminal domains of EcoRII. *Nucleic Acids Res*, *37*(19), 6613–6624. https://doi.org/10.1093/nar/gkp699

41 Gražulis, S., Chateigner, D., Downs, R. T., Yokochi, A. F. T., Quirós, M., Lutterotti, L., Manakova, E., Butkus, J., Moeck, P. & Le Bail, A. (2009). Crystallography open database – an open-access collection of crystal structures. *Journal of Applied Crystallography*, *42*(4), 726–729. https://doi.org/10.1107/S0021889809016690

42 Sukackaitė, R., Gražulis, S., Bochtler, M. & Šikšnys, V. (2008). The recognition domain of the BpuJI restriction endonuclease in complex with cognate DNA at 1.3 Å resolution. *J Mol Biol*, *378*(5), 1084–1093. https://doi.org/10.1016/j.jmb.2008.03.041

43 Bartolucci, C., Lamba, D., Gražulis, S., Manakova, E. & Heumann, H. (2008). Crystal structure of wild-type chaperonin GroEL (vol 354, pg 940, 2005). *Journal of Molecular Biology*, *380*(4), 775. https://doi.org/10.1016/j.jmb.2005.09.101

44 Tamulaitienė, G., Jakubauskas, A., Urbanke, C., Huber, R., Gražulis, S. & Šikšnys, V. (2006). The crystal structure of the rare-cutting restriction enzyme SdaI reveals unexpected domain architecture. *Structure*, *14*(9), 1389–1400. https://doi.org/10.1016/j.str.2006.07.002

45 Bochtler, M., Szczepanowski, R. H., Tamulaitis, G., Gražulis, S., Czapinska, H., Manakova, E. & Šikšnys, V. (2006). Nucleotide flips determine the specificity of the Ecl18kI restriction endonuclease. *EMBO J*, *25*(10), 2219–2229. https://doi.org/10.1038/sj.emboj.7601096

46 Bartolucci, C., Lamba, D., Gražulis, S., Manakova, E. & Heumann, H. (2005). Crystal structure of wild-type chaperonin GroEL. *J Mol Biol*, *354*(4), 940–951. https://doi.org/10.1016/j.jmb.2005.09.096

47 Gražulis, S., Manakova, E., Roessle, M., Bochtler, M., Tamulaitienė, G., Huber, R. & Šikšnys, V. (2005). Structure of the metal-independent restriction enzyme BfiI reveals fusion of a specific DNA-binding domain with a nonspecific nuclease. *Proc Natl Acad Sci U S A*, *102*(44), 15797–15802. https://doi.org/10.1073/pnas.0507949102

48 Neely, R. K., Daujotytė, D., Gražulis, S., Magennis, S. W., Dryden, D. T. F., Klimašauskas, S. & Jones, A. C. (2005). Time-resolved fluorescence of 2-aminopurine as a probe of base flipping in m.hhai-dna complexes. *Nucleic Acids Res*, *33*(22), 6953–6960. https://doi.org/10.1093/nar/gki995

49 Tamulaitienė, G., Gražulis, S., Janulaitis, A., Janowski, R., Bujacz, G. & Jaskolski, M. (2004). Crystallization and preliminary crystallographic studies of a bifunctional restriction endonuclease Eco57I. *Biochim Biophys Acta*, *1698*(2), 251–254. https://doi.org/10.1016/j.bbapap.2003.12.006

50 Gražulis, S., Deibert, M., Rimseliene, R., Skirgaila, R., Sasnauskas, G., Lagunavicius, A., Repin, V., Urbanke, C., Huber, R. & Šikšnys, V. (2002). Crystal structure of the Bse634I restriction endonuclease: Comparison of two enzymes recognizing the same DNA sequence. *Nucleic Acids Res*, *30*(4), 876–885. https://doi.org/10.1093/nar/30.4.876

51 Deibert, M., Gražulis, S., Sasnauskas, G., Šikšnys, V. & Huber, R. (2000). Structure of the tetrameric restriction endonuclease NgoMIV in complex with cleaved DNA. *Nat Struct Biol*, *7*(9), 792–799. https://doi.org/10.1038/79032

52 Deibert, M., Gražulis, S., Janulaitis, A., Šikšnys, V. & Huber, R. (1999). Crystal structure of MunI restriction endonuclease in complex with cognate DNA at 1.7 Å resolution. *EMBO J*, *18*(21), 5805–5816. https://doi.org/10.1093/emboj/18.21.5805

53 Šikšnys, V., Skirgaila, R., Sasnauskas, G., Urbanke, C., Cherny, D., Gražulis, S. & Huber, R. (1999). The Cfr10I restriction enzyme is functional as a tetramer. *J Mol Biol*, *291*(5), 1105–1118. https://doi.org/10.1006/jmbi.1999.2977

54 Skirgaila, R., Gražulis, S., Bozic, D., Huber, R. & Šikšnys, V. (1998). Structure-based redesign of the catalytic/metal binding site of Cfr10I restriction endonuclease reveals importance of spatial rather than sequence conservation of active centre residues. *J Mol Biol*, *279*(2), 473–481. https://doi.org/10.1006/jmbi.1998.1803

55 Lagunavicius, A., Gražulis, S., Balčiūnaitė, E., Vainius, D. & Šikšnys, V. (1997). DNA binding specificity of MunI restriction endonuclease is controlled by pH and calcium ions: Involvement of active site carboxylate residues. *Biochemistry*, *36*(37), 11093–11099. https://doi.org/10.1021/bi963126a

56 Bozic, D., Gražulis, S., Šikšnys, V. & Huber, R. (1996). Crystal structure of *Citrobacter freundii* restriction endonuclease *Cfr*10I at 2.15 Å resolution. *J Mol Biol*, *255*(1), 176–186. https://doi.org/10.1006/jmbi.1996.0015

Conference Proceedings

1 Matulis, D., Gylytė, J., Zubrienė, A., Dudutienė, V., Smirnov, A., Manakova, L. & Gražulis, S. (2014). Structure-thermodynamics correlations of fluorinated benzensulfonamides as inhibitors of human carbonic anhydrases. https://doi.org/10.1016/j.bpj.2013.11.1543

2 Timm, D., Zubrienė, A., Gylytė, J., Dudutienė, V., Smirnov, A., Manakova, E., Gražulis, S. & Matulis, D. (2013). Thermodynamics of inhibitor binding to several recombinant carbonic anhydrases isoforms. https://doi.org/10.1111/febs.12340

3 Zubrienė, A., Dudutienė, V., Smirnov, A., Timm, D., Gylytė, J., Manakova, E., Gražulis, S. & Matulis, D. (2013). Thermodynamics of 4-substituted-2,3,5,6-tetrafluorobenzenesulfonamides binding to carbonic anhydrase isozymes. https://link.springer.com/journal/249/42/1/suppl

4 Manakova, E., Golovenko, D., Gražulis, S., Zaremba, M. & Šikšnys, V. (2012). Structural mechanism of cognate DNA recognition by the BfiI restriction enzyme. https://doi.org/10.1111/j.1742-4658.2010.08705.x