

Prof. Daumantas Matulis, CV

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Short personal profile in the Biophysical Society:

<https://www.biophysics.org/profiles/daumantas-matulis> (2014)

Google Scholar profile:

<https://scholar.google.com/citations?user=4VG72SoAAAAJ&hl=lt&oi=ao>

Education

<i>Year of completion</i>	<i>Institution</i>	<i>Degree</i>
2001	University of Minnesota	Biophysics, postdoctoral associate
1998	University of Minnesota	Biochemistry and biophysics, Ph.D.
1993	Vilnius University	Biochemistry, 5-year diploma (BS/MS)
1992 Summer	University of Oslo	School of Environmental Protection

Professional experience

<i>Period</i>	<i>Institution</i>	<i>Position</i>
2005-present	Institute of Biotechnology, Life Sciences Center, Vilnius University	Head of Department
2001-2005	3-Dimensional Pharmaceuticals (acquired by Johnson&Johnson Pharmaceutical Research and Development, Inc. in 2002);	Scientist
1998-2001	University of Minnesota	Postdoctoral associate
1994-1998	University of Minnesota	Graduate student, Research/teaching Assistant
1993-1994	Institute of Biochemistry	Junior scientist
1990-1992	Ministry of Economy	Junior interpreter

Teaching experience:

1. Scientific advisor of Ph.D. student Joana Smirnovienė, who received recognition from the program “Women in Science” by L’Oreal Baltic (<https://naujienos.vu.lt/lietuves-mokslininkes-pagerbtos-prestiziniaiis-moterims-moksle-apdovanojimais/>).
2. Scientific advisor of Ph.D. student Justina Kazokaite, who has become a laureate for best Ph.D. thesis in biomedical sciences, organized by the Young Scientist Association of Lithuania, 2019.
3. 2013 - present. Member of Vilnius University studies committee.
4. “Molecular Biophysics” course for Bachelor students, Faculty of Natural Sciences, Vilnius University, 2011- present.
5. “Biophysical Chemistry of Proteins”, textbook, 1-149 pages, Vilnius University.
6. “Biothermodynamics of protein-ligand interactions” course for the Master students, 2005– present.
7. “Molecular Biophysics of proteins” course for Bachelor students, 2013–present.
8. Life Sciences Summer Undergraduate Research Program, 1999–2000, Minnesota University.
9. Biochemistry Laboratory course (academic, 130 students), 1999, Minnesota University.
10. Biochemistry Laboratory course (assistant), 1996–1997, Minnesota University.
11. Scientific supervisor or participated at defense councils (board member or an opponent) for the following Ph.D, MS, BS students:
 1. Dominyka Dapkutė. Dr. Biophysics. 2021. “Mesenchymal stem cell and cancer cell response to treatment with teranostic nanoparticles – towards cell therapy”. (Chairman of the Dissertation Defense Panel).
 2. Diana Navickaitė. Dr. Biophysics. 2021. „Influence of Calcium ions on molecular transport through plasma membrane and cell viability after electroporation and sonoporation“. (Member of the Dissertation Defense Panel).
 3. Agnė Kalnaitytė. Dr. Biophysics. 2019. „The Photostability and Phototoxicity Studies of Hydrophilic Quantum Dots in Model Biosystems“. (Chairman of the Dissertation Defense Panel).
 4. Algirdas Mikalkėnas. Dr. Biochemistry. 2019. „Application of Modified Nucleotides in Biosynthesis of Nucleic Acids“. (Chairman of the Dissertation Defense Panel).
 5. Vytautas Petkevičius. Dr. Biochemistry. 2019. „Investigation of Pyridine-ring-attacking Oxygenases“. (Member of the Dissertation Defense Panel).
 6. Ona Marija Singh. MS Biochemistry. 2019. „Recombinant production of zinc-containing metalloproteinase domain“. (scientific advisor).
 7. Evelina Zagorskaitė. PhD in biochemistry. 2018. “Recognition of Modified Cytosine by Methyl-Directed Restriction Endonucleases” (Member of the Dissertation Defense Panel).

8. Justina Kazokaitė. PhD in biochemistry. 2018. "Investigation of Human Carbonic Anhydrase VI and IX Inhibitor Efficacy and Toxicity" (scientific advisor).
9. Alexey Smirnov. PhD in chemical engineering. 2018. "Crystallographic Studies of Carbonic Anhydrase Isoforms and their Complexes with Inhibitors" (scientific advisor).
10. Paulius Toliušis. PhD in biochemistry. 2018. "Structure and Function Correlations within the Atypical ATP-Dependent Restriction Endonuclease CgII" (Chairman of the Dissertation Defense Panel).
11. Arnoldas Kaunietis. PhD in biology. 2018. "Identification, Heterologous Biosynthesis and Characterization of Novel Bacteriocins from Thermophilic Bacteria" (member of the dissertation defence panel).
12. Nanda Kumar Parvathaneni. Dr. 2017. „Targeting CAIX with small molecules: Design, Synthesis and Biological efficacy“ (member of the assessment committee). Defense was held at the Maastricht University, The Netherlands.
13. Vaida Linkuvienė. PhD in biophysics. 2017. "Observed and Intrinsic Thermodynamic and Kinetic Parameters of Sulfonamide Derivative Binding to Carbonic Anhydrases" (scientific advisor).
14. Vaida Paketurytė. BS in biochemistry. 2017. "Thermodynamic Analysis of Inhibitor–Carbonic Anhydrase Interaction and the Precision of Binding Parameters" (scientific supervisor).
15. Marija Vaitkevičienė. BS in biochemistry. 2017. "Recombinant Human Carbonic Anhydrase VII Protein: Production in E. coli and Protein Stability Analysis" (scientific supervisor).
16. Guoda Makarevičiūtė. BS in biophysics. 2017. "Determination of Recombinant Human Carbonic Anhydrase II and Acetazolamide Intrinsic Binding Heat Capacity Change Using Isothermal Titration Calorimetry" (scientific supervisor).
17. Aistė Dagtė. MS in microbiology and biotechnology. 2017. "Production of Recombinant Hsp90N from Parasitic Protozoa and Interaction with Inhibitors" (consultant).
18. Vaida Simanavičienė. Ph.D. 2017. "Molecular Diagnostics of Human Papillomavirus (HPV) and Studies on HPV Prevalence" (defense council board member).
19. Egidijus Kazlauskas. Ph.D. 2016. „Thermodynamics of Aryl-dihydroxyphenyl-thiadiazole Binding to Recombinant Human Hsp90“ (scientific supervisor).
20. Edvinas Paliulis. Bs. 2016. "Investigation of enzyme kinetics and its application in drug design" (scientific supervisor).
21. Brazdžiūnas Mikalojus. BS. 2016. "Drug Design *in silico*: Model Development for Calculation of Protein-Ligand Interaction Thermodynamics" (scientific supervisor).
22. Joana Smirnovienė. MS. 2015. "Activity, inhibition and ligand binding studies of human carbonic anhydrases" (scientific supervisor).

23. Justina Rukšnaitė. Ph.D. 2014. "Surface Plasmon Resonance and Electrochemical Imunosensores for Human Growth Hormone and Antibodies for Human Growth Hormone Detection" (defense council board member).
24. Romualdas Rudys. Ph.D. 2014. "Detection of Endogenous Porphyrins by Means of Spectroscopy and Microscopy in the Case of Rheumatoid Arthritis" (defense council board member).
25. Justina Kazokaitė. MS. 2014. "Thermodynamic Analysis of Sulfonamide Inhibitor Binding to Human Carbonic Anhydrase VI" (scientific supervisor).
26. Sandra Bakšytė. MS. 2014. "Characterization of Carbonic Anhydrase XIV Stability and Thermodynamics of Inhibitor Binding" (scientific supervisor).
27. Gediminas Skvarnavičius. BS. 2014. "Thermodynamics and of Interaction Between Polyamino Acids and Anionic Detergents" (consultant).
28. Miglė Kišonaitė. BS. 2014. "Structure and Thermodynamics Correlation of Cytosolic Carbonic Anhydrase Inhibitors" (consultant).
29. Lina Baranauskienė. Ph.D. 2013. "Analysis of Ligand Binding to Recombinant Human Carbonic Anhydrases I, II, VII, IX and XIII" (scientific supervisor).
30. Alexey Smirnov. MS. 2013. "X-ray Crystallographic Studies of Human Carbonic Anhydrase Isoforms II, XII and XIII in Complex with Inhibitors" (consultant).
31. Vaida Morkūnaitė. 2013. MS. "Inhibitors search and determination of intrinsic binding parameters to carbonic anhydrases I, II, VII, XII and XIII" (scientific supervisor).
32. Eglė Ivanauskaitė. BS. 2013. "Construction of Human Carbonic Anhydrase II Active Site Mutants and Solubility Test for Recombinant VA Protein" (consultant).
33. Joana Gylytė. BS. 2013. "Thermodynamic Analysis of Inhibitor Binding to Recombinant Human Carbonic Anhydrases" (scientific supervisor).
34. Edita Čapkauskaitė. Ph.D. 2012. "Synthesis of Carbonic Anhydrase Inhibitors and Analysis of Their Structure - Activity Relationship" (consultant).
35. Rokas Buišas. Ph.D. 2012. "The Gain of Spinal Cord Motoneurons and its Modification" (defense council board member).
36. Justė Mikučiauskaitė. BS. 2012. "Cloning and Purification of Lidless Chaperone Hsp90αN and the Measurements of Inhibitor Binding" (scientific supervisor).
37. Povilas Norvaišas. BS. 2012. "Hydrophobic Effect: Thermodynamics of Cationic and Anionic Surfactant Interaction and Laws of Additivity in the Structure-Based Drug Design" (scientific supervisor).
38. Justas Dapkūnas. Ph.D. 2011. "Computational Modeling of Cytochrome P450-Mediated Drug Metabolism" (opponent).
39. Kiril Lanevskij. Ph.D. 2011. "Absorption and Tissue Distribution of Drug-Like Compounds: Quantative Structure-Activity Relationship Analysis" (opponent).

40. Rūta Gerasimaitė. Ph.D. 2011. "A Directed Evolution Design of Target Specificity and Kinetic Analysis of Conformational Transitions in the HhaI Methyltransferase" (defense council board member).
41. Aistė Kasiliauskaitė. MS. 2011. "Cloning, Expression, Purification and Inhibition Studies of Mitochondrial Carbonic Anhydrase VB" (scientific supervisor).
42. Mantas Zakas. BS. 2011. "Production and Stability Investigation of Reptin and Hsp90C Proteins Participating in Cancer" (scientific supervisor).
43. Andrius Sazonovas. Ph.D. 2010. "Estimation of the Acute Toxicity and Prediction of the Metabolism Site for Organic Molecules Using *Galas* Methodology" (defense council board member).
44. Laura Kalinienė. Ph.D. 2010. "Investigation of Genome Sequence and Gene Expression Regulation in T4 Related Bacteriophages" (opponent).
45. Eglė Strainienė. Ph.D. 2010. "Studies of the Refolding Processes of Recombinant Growth Hormones" (defense council board member).
46. Vilma Pilipuitytė. MS. 2010. "Production of Recombinant Human Carbonic Anhydrase VII, Measurement of its Binding with Inhibitors and Characterization of its Stability" (scientific supervisor).
47. Zigmantas Toleikis. MS. 2009. "Investigations of protein-ligand binding at high pressure" (scientific supervisor).
48. Jurga Valančiūnaitė. Ph.D. 2008. "The Influence of Molecular Structure and Protein Template on the Formation of Porphyrin (TPPS_n) Aggregates: Spectroscopic Study" (opponent).
49. Renata Gasparavičiūtė. Ph.D. 2008. "Investigation of Genes Involved in Biodegradation of Pyridine and Pyridinols" (defense council board member).
50. Edita Čapkauskaitė. MS. 2008. "Synthesis of Quinoline Derivatives as Carbonic Anhydrase Inhibitors" (consultant).
51. Simona Jachimovičiūtė. MS. 2008. "The Interaction of Metal Ions with Recombinant Growth Hormones" (scientific supervisor).
52. Lina Malinauskaitė. BS. 2008. "Production of Recombinant Human Carbonic Anhydrase III and a Study of Sulfonamide Inhibitors Binding" (scientific supervisor).
53. Asta Kaušaitė. Ph.D. 2007. "Some Aspects in Development of Biofuel Cells and Biosensors" (defense council board member).
54. Pranas Japertas. Ph.D. 2007. "Application of Fragmental Descriptors and Statistical Analysis Methods in Quantitative Structure-Activity Relationships" (defense council board member).
55. Zigmantas Toleikis. BS. 2007. "Investigations of protein-ligand binding at high pressure" (scientific supervisor).

56. Milda Plečkaitytė. Ph.D. 2006. "Identification and Characterization of Hsp70 (DnaK) Chaperone System from Moderately Thermophilic Bacteria *Meiothermus Ruber*" (defense council board member).
57. Lina Mištinaitė. MS. 2006. "Thermodynamic Mechanism of Carbonic Anhydrase – Sulfonamide Inhibitor Interaction by Isothermal Titration Calorimetry" (scientific supervisor).
58. Dovilė Makarevičiūtė. BS. 2006. "Protection of Cysteine Proteases from Acid Stress by Matrix Ligands" (scientific supervisor).
59. Jovita Matukaitytė. BS. 2006. "Bromelain Isolation from Pineapple Juice Using Matrix Ligands and by Ion Exchange Chromatography" (scientific supervisor).
60. Mindaugas Zaveckas. Ph.D. 2005. "Partitioning and Refolding of Recombinant Human Granulocyte-Colony Stimulating Factor in Aqueous Two-Phase Systems Containing Chelated Metal Ions" (consultant).
61. Vida Časaitė. Ph.D. 2005. "Investigation of Glycine Betaine Catabolism in *Arthrobacter Bacteria*" (defense council board member).

Professional Societies, membership:

1. Member of the Biophysical Society (USA, 1996 – present). Chairman of the International Relations Committee (2016-18). Member of the Publications Committee (2019 – present).
2. Member of the American Chemical Society (1996 – present)
3. International Society for Biological Calorimetry (ISBC), member of the governing council.
4. International Society for Molecular Recognition (ISMR), board member.
5. Lithuanian Biochemical Society (member since 2008, President 2014 – present)
6. Lithuanian Biotechnology Association (member 2006 – present)
7. Lithuanian Biophysical Society (secretary since 2014)
8. Association "Futura Scientia" (Lithuanian scientists in the World, Chairman in 2018, member of the Board in 2019, 2011)
9. Association LGUVO "Sugrįžus" (president 2007 – 2009, member of the Board since 2009)

Public service:

- Member of the Science Prize commission of Lithuania (2019-present)
- Member of the working group on life sciences at the Ministry of Economy
- Member of the central commission at Vilnius university of employment (2018 – present)
- Member of selection committee organized by the Ministry of Science and Education for selection of Lithuanian Research Council members of FBT committee (2018)

- Member of research career program committee at the Ministry of Science and Education (2014-2017)
- Member of research output evaluation at the Ministry of Science and Education (2009-2017)
- Public consultant of the President Valdas Adamkus (2007-2009)
- President of Lithuanian Youth American Community Philadelphia section (2002-2004)

Conference organization:

1. Chairman of the organizing committee of the International Society of Biological Calorimetry conference to be held in Vilnius, June 8-10, 2022.
2. Chairman of the organizing committee of Lithuanian Biochemical Society 15-th conference, 2018.06.26-29, Dubingiai, Lithuania.
3. Member of organizing committee of the Life Sciences Baltics conferences (2016, 2018, and 2021).
4. Chairman of the organizing committee of Lithuanian Biochemical Society 14-th conference, 2016.06.27-30, Druskininkai, Lithuania.
5. Organized the meeting of COST TD0905 project in Vilnius, 2013.10.30-31.
6. Co-chaired the organizing committee of the „CEEC-TAC2 2nd Central and Eastern European Conference on Thermal Analysis and Calorimetry“, 2013.08.27-30, Vilnius.
7. Local organizer of the conference „ScanBalt Forum and ScanBalt Biomaterials Days“, 2008.09.24-26, Vilnius.

Awards:

1. Joint paper with Prof. Wen-Yih Chen has been awarded the best paper award on Jan. 6, 2022, at the annual meeting in Kaohsiung (<https://2021twiche.conf.tw>). Tai-Chih Kuo, Meng-Wei Wu, Wei-Chen Lin, Daumantas Matulis, Yuh-Shyong Yang, Si-Yu Li, Wen-Yih Chen* “Reduction of interstrand charge repulsion of DNA duplexes by salts and by neutral phosphotriesters - Contrary effects for harnessing duplex formation” *Journal of the Taiwan Institute of Chemical Engineers* (2020) <https://doi.org/10.1016/j.jtice.2020.02.023>.
2. Vilnius City Municipality St. Christophor award, 2021.
3. Justina Kazokaitė, a PhD student supervised by D. Matulis was awarded a laureate prize by the Young Lithuanian Scientist Association for the best PhD thesis in the field of biomedical sciences in Lithuania in 2019.
4. Nominated by Global Lithuanian Leaders Awards for international innovations implemented in Lithuania. 2018.
5. Joana Smirnovienė, an MS student supervised by D. Matulis was awarded a prize by the Young Lithuanian Scientist Association for the best MS thesis in the field of biomedical sciences in Lithuania in 2015.

6. Justina Kazokaitė, an MS student supervised by D. Matulis was awarded a prize by the Young Lithuanian Scientist Association for the best MS thesis in the field of biomedical sciences in Lithuania in 2014.
7. Lithuanian National Science award 2012.
8. Life Science Baltics Startup Session, Lithuania, Vilnius. 2012 (second place).
9. The Affinity 2013 “Young Investigator Award”. Co-author of the poster „20th Biennial Meeting of the International Society for Molecular Recognition“ conference. Vienna 2013.
10. The Best Poster award in the Conference “Biochemija ir biofizika Vilniaus universitete”, Lithuania, Vilnius. 2012 (third place).
11. The Best Poster award in the Conference „XVII International Society of Biological Calorimetry (ISBC) Conference“, Germany, Leipzig. 2012 (second place).
12. The Best Poster award in the Conference “ESBES+ISPPP+ISB“, Italy. 2010.
13. ScanBalt Bridge Baltic Sea Region Award, Sweden. 2009.
14. Public advisor to the President of Lithuania for the issues of emigration and repatriation, 2007-2009.
15. Selected as Lithuanian representative young scientist in the book “Portraits of Science. Scientists of Tomorrow” by European Federation of Pharmaceutical Industries and Associations, 2008.
16. Award “Direction-Home” given to Lithuanian scientist selected by an independent Swedish-Lithuanian scientific council, by “Telia Sonera” Inc., Sweden, 2007.
17. Robert Jenness Award by University of Minnesota Department of Biochemistry, Molecular Biology, and Biophysics for the best postdoctoral associate in 2000.
18. National high school Olympic competition in chemistry, third place, 1988.

Scientific Publications:

1. Baranauskiene, L., Škiudaitė, L., Michailovienė, V., Petrauskas, V., and Matulis, D. (2021). Thiazide and other Cl-benzenesulfonamide-bearing clinical drug affinities for human carbonic anhydrases. *PLOS ONE* 16, e0253608.
2. Baronas, D., Dudutienė, V., Paketurytė, V., Kairys, V., Smirnov, A., Juozapaitienė, V., Vaškevičius, A., Manakova, E., Gražulis, S., Zubrienė, A., et al. (2021). Structure and mechanism of secondary sulfonamide binding to carbonic anhydrases. *Eur Biophys J*.
3. DeLeeuw, L.W., Monsen, R.C., Petrauskas, V., Gray, R.D., Baranauskiene, L., Matulis, D., Trent, J.O., and Chaires, J.B. (2021). POT1 stability and binding measured by fluorescence thermal shift assays. *PLoS One* 16, e0245675.

4. Gulla, A., Kazlauskas, E., Liang, H., Strupas, K., Petrauskas, V., Matulis, D., and Eshleman, J.R. (2021). Heat Shock Protein 90 Inhibitor Effects on Pancreatic Cancer Cell Cultures. *Pancreas* *50*, 625–632.
5. Janonienė, A., Mazutis, L., Matulis, D., and Petrikaite, V. (2021). Inhibition of Carbonic Anhydrase IX Suppresses Breast Cancer Cell Motility at the Single-Cell Level. *Int. J. Mol. Sci.* *12*.
6. Kazlauskas, E., Petrauskas, V., Paketurytė, V., and Matulis, D. (2021). Standard operating procedure for fluorescent thermal shift assay (FTSA) for determination of protein–ligand binding and protein stability. *Eur Biophys J* *50*, 373–379.
7. Kazokaitė-Adomaitienė, J., Becker, H.M., Smirnovienė, J., Dubois, L.J., and Matulis, D. (2021). Experimental Approaches to Identify Selective Picomolar Inhibitors for Carbonic Anhydrase IX. *CMC* *28*, 3361–3384.
8. Kirchhain, A., Zubrienė, A., Kairys, V., Vivaldi, F., Bonini, A., Biagini, D., Santalucia, D., Matulis, D., and Di Francesco, F. (2021). Biphenyl substituted lysine derivatives as recognition elements for the matrix metalloproteinases MMP-2 and MMP-9. *Bioorg Chem* *115*, 105155.
9. López-Méndez, B., Baron, B., Brautigam, C.A., Jowitt, T.A., Knauer, S.H., Uebel, S., Williams, M.A., Sedivy, A., Abian, O., Abreu, C., et al. (2021). Reproducibility and accuracy of microscale thermophoresis in the NanoTemper Monolith: a multi laboratory benchmark study. *Eur Biophys J*.
10. Paketurytė, V., Petrauskas, V., Zubrienė, A., Abian, O., Bastos, M., Chen, W.-Y., Moreno, M.J., Krainer, G., Linkuvienė, V., Sedivy, A., et al. (2021). Uncertainty in protein–ligand binding constants: asymmetric confidence intervals versus standard errors. *Eur Biophys J*.
11. Skvarnavičius, G., Toleikis, Z., Michailovienė, V., Roumestand, C., Matulis, D., and Petrauskas, V. (2021). Protein–Ligand Binding Volume Determined from a Single 2D NMR Spectrum with Increasing Pressure. *J. Phys. Chem. B* *125*, 5823–5831.
12. Smirnovienė, J., Baranauskienė, L., Zubrienė, A., and Matulis, D. (2021a). A standard operating procedure for an enzymatic activity inhibition assay. *Eur Biophys J* *50*, 345–352.
13. Smirnovienė, J., Smirnov, A., Zakšauskas, A., Zubrienė, A., Petrauskas, V., Mickevičiūtė, A., Michailovienė, V., Čapkauskaitė, E., Manakova, E., Gražulis, S., et al. (2021b). Switching the Inhibitor-Enzyme Recognition Profile via Chimeric Carbonic Anhydrase XII. *ChemistryOpen* *10*, 567–580.
14. Tomašič, T., Zubrienė, A., Skok, Ž., Martini, R., Pajk, S., Sosič, I., Ilaš, J., Matulis, D., and Bryant, S.D. (2021). Selective DNA Gyrase Inhibitors: Multi-Target in Silico Profiling with 3D-Pharmacophores. *Pharmaceuticals* *14*, 789.
15. Urbelytė, L., Bagdonas, M., Grybaitė, B., Vaickelionienė, R., Mickevičiūtė, A., Michailovienė, V., Matulis, D., Mickevičius, V., and Zubrienė, A. (2021). Design and Synthesis of Hydrazone-

- Bearing Benzenesulfonamides as Carbonic Anhydrase VB Inhibitors. *ChemistrySelect* **6**, 13506–13513.
16. Zakšauskas, A., Čapkauskaitė, E., Paketurytė-Latvė, V., Smirnov, A., Leitans, J., Dvinskis, E., Stančaitis, L., Mickevičiūtė, A., Jachno, J., Jezepčikas, L., et al. (2021). Methyl 2-Halo-4-Substituted-5-Sulfamoyl-Benzoates as High Affinity and Selective Inhibitors of Carbonic Anhydrase IX. *Int. J. Mol. Sci.* **27**.
 17. Balandis, B., Ivanauskaitė, G., Smirnovienė, J., Kantminienė, K., Matulis, D., Mickevičius, V., and Zubrienė, A. (2020). Synthesis and structure–affinity relationship of chlorinated pyrrolidinone-bearing benzenesulfonamides as human carbonic anhydrase inhibitors. *Bioorganic Chemistry* **97**, 103658.
 18. Chen, W.-Y., Matulis, D., Hu, W.-P., Lai, Y.-F., and Wang, W.-H. (2020). Studies of the interactions mechanism between DNA and silica surfaces by Isothermal Titration Calorimetry. *Journal of the Taiwan Institute of Chemical Engineers*.
 19. Dudutienė, V., Zubrienė, A., Kairys, V., Smirnov, A., Smirnovienė, J., Leitans, J., Kazaks, A., Tars, K., Manakova, L., Gražulis, S., et al. (2020). Isoform-Selective Enzyme Inhibitors by Exploring Pocket Size According to the Lock-and-Key Principle. *Biophys. J.* **119**, 1513–1524.
 20. Kuo, T.-C., Wu, M.-W., Lin, W.-C., Matulis, D., Yang, Y.-S., Li, S.-Y., and Chen, W.-Y. (2020). Reduction of interstrand charge repulsion of DNA duplexes by salts and by neutral phosphotriesters – Contrary effects for harnessing duplex formation. *Journal of the Taiwan Institute of Chemical Engineers* **110**, 1–7.
 21. Matulis, D. (2020). Structural details of the enzymatic catalysis of carbonic anhydrase II via a mutation of valine to isoleucine. *IUCrJ* **7**, 953–954.
 22. Stravinskiene, D., Sliziene, A., Baranauskiene, L., Petrikaite, V., and Zvirbliene, A. (2020). Inhibitory Monoclonal Antibodies and Their Recombinant Derivatives Targeting Surface-Exposed Carbonic Anhydrase XII on Cancer Cells. *International Journal of Molecular Sciences* **21**, 9411.
 23. Zakšauskas, A., Čapkauskaitė, E., Jezepčikas, L., Linkuvienė, V., Paketurytė, V., Smirnov, A., Leitans, J., Kazaks, A., Dvinskis, E., Manakova, E., et al. (2020). Halogenated and di-substituted benzenesulfonamides as selective inhibitors of carbonic anhydrase isoforms. *European Journal of Medicinal Chemistry* **185**, 111825.
 24. Kairys, V.; Baranauskiene, L.; Kazlauskiene, M.; Matulis, D.; Kazlauskas, E. Binding Affinity in Drug Design: Experimental and Computational Techniques. *Expert Opinion on Drug Discovery* **2019**, 1–14. <https://doi.org/10.1080/17460441.2019.1623202>.
 25. Baranauskienė, L.; Matulis, D. Overview of Human Carbonic Anhydrases. In *Carbonic Anhydrase as Drug Target: Thermodynamics and Structure of Inhibitor Binding*; Matulis, D.,

- Ed.; Springer International Publishing: Cham, 2019; Chapter 1, pp 3–14. https://doi.org/10.1007/978-3-030-12780-0_1.
26. Mickevičiūtė, A.; Juozapaitienė, V.; Michailovienė, V.; Jachno, J.; Matulienė, J.; Matulis, D. Recombinant Production of 12 Catalytically Active Human CA Isoforms. In *Carbonic Anhydrase as Drug Target: Thermodynamics and Structure of Inhibitor Binding*; Matulis, D., Ed.; Springer International Publishing: Cham, 2019; Chapter 2, pp 15–37. https://doi.org/10.1007/978-3-030-12780-0_2.
 27. Baranauskienė, L.; Matulis, D. Catalytic Activity and Inhibition of Human Carbonic Anhydrases. In *Carbonic Anhydrase as Drug Target: Thermodynamics and Structure of Inhibitor Binding*; Matulis, D., Ed.; Springer International Publishing: Cham, 2019; Chapter 3, pp 39–49. https://doi.org/10.1007/978-3-030-12780-0_3.
 28. Zubrienė, A.; Matulis, D. Characterization of Carbonic Anhydrase Thermal Stability. In *Carbonic Anhydrase as Drug Target: Thermodynamics and Structure of Inhibitor Binding*; Matulis, D., Ed.; Springer International Publishing: Cham, 2019; Chapter 4, pp 51–59. https://doi.org/10.1007/978-3-030-12780-0_4.
 29. Petrauskas, V.; Zubrienė, A.; Todd, M. J.; Matulis, D. Inhibitor Binding to Carbonic Anhydrases by Fluorescent Thermal Shift Assay. In *Carbonic Anhydrase as Drug Target: Thermodynamics and Structure of Inhibitor Binding*; Matulis, D., Ed.; Springer International Publishing: Cham, 2019; Chapter 5, pp 63–78. https://doi.org/10.1007/978-3-030-12780-0_5.
 30. Paketurytė, V.; Zubrienė, A.; Chen, W.-Y.; Keller, S.; Bastos, M.; Todd, M. J.; Ladbury, J. E.; Matulis, D. Inhibitor Binding to Carbonic Anhydrases by Isothermal Titration Calorimetry. In *Carbonic Anhydrase as Drug Target: Thermodynamics and Structure of Inhibitor Binding*; Matulis, D., Ed.; Springer International Publishing: Cham, 2019; Chapter 6, pp 79–95. https://doi.org/10.1007/978-3-030-12780-0_6.
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Patents and patent applications:

Search of Patentscope database performed on 2019.01.15

1. [20180222856](#) **SELECTIVE INHIBITORS OF CARBONIC ANHYDRASE** US 09.08.2018
 C07C 311/16 15748559 VILNIUS UNIVERSITY Daumantas MATULIS

Disclosed are novel compounds—benzenesulfonamides of general formulas (I) and The compounds can be used in biomedicine as active ingredients in pharmaceutical formulations, because they

inhibit enzymes which participate in disease progression. Also disclosed are method of treatment using such compounds.

2. [3328833](#) **SELECTIVE INHIBITORS OF CARBONIC ANHYDRASE** EP 06.06.2018

C07D 215/08 15766651 VILNIUS UNIV MATULIS DAUMANTAS

Invention is related to novel compounds – benzenesulfonamides of general formulas (I) and (II). The compounds can be used in biomedicine as active ingredients in pharmaceutical formulations, because they inhibit enzymes which participate in disease progression. Acknowledgements: This research was funded by the European Social Fund under the Global Grant measure (no. VP1-3.1.-SMM-07-K-02-009).

3. [WO/2017/017505](#) **SELECTIVE INHIBITORS OF CARBONIC ANHYDRASE** WO 02.02.2017

[C07D 215/08](#) PCT/IB2015/056626 VILNIUS UNIVERSITY MATULIS, Daumantas

Invention is related to novel compounds – benzenesulfonamides of general formulas (I) and (II). The compounds can be used in biomedicine as active ingredients in pharmaceutical formulations, because they inhibit enzymes which participate in disease progression. Acknowledgements: This research was funded by the European Social Fund under the Global Grant measure (no. VP1-3.1.-SMM-07-K-02-009).

4. [20150266900](#) **Fluorinated benzenesulfonamides as inhibitors of carbonic anhydrase** US 24.09.2015

C07D 513/04 14435649 VILNIUS UNIVERSITY Daumantas Matulis

Novel fluorinated benzenesulfonamides compounds of general formula (I) can be used in biomedicine as active ingredients in pharmaceutical formulations, because they inhibit enzymes which participate in disease progression.

5. [2914583](#) **FLUORINATED BENZENESULFONAMIDES AS INHIBITORS OF CARBONIC ANHYDRASE** EP 09.09.2015

C07D 233/84 12810437 VILNIUS UNIVERSITY MATULIS DAUMANTAS

Invention is related to novel compounds - fluorinated benzenesulfonamides of general formula (I). The compounds can be used in biomedicine as active ingredients in pharmaceutical formulations, because they inhibit enzymes which participate in disease progression.

6. [WO/2014/062044](#) **FLUORINATED BENZENESULFONAMIDES AS INHIBITORS OF CARBONIC ANHYDRASE** WO 24.04.2014

[C07D 233/84](#) PCT/LT2012/000007 VILNIUS UNIVERSITY MATULIS, Daumantas

Invention is related to novel compounds - fluorinated benzenesulfonamides of general formula (I).

The compounds can be used in biomedicine as active ingredients in pharmaceutical formulations, because they inhibit enzymes which participate in disease progression.

7. [WO/2009/134110](#) **5-ARYL-4-(5-SUBSTITUTED 2,4-DIHYDROXYPHENYL)-1,2,3-THIADIAZOLES AS INHIBITORS OF HSP90 CHAPERONE AND THE INTERMEDIATES FOR PRODUCTION THEREOF** WO 05.11.2009

[C07D 285/06](#) PCT/LT2008/000003 BIOTECHNOLOGIJOS INSTITUTAS MATULIS, Daumantas

Invention is related to novel compounds - 5-aryl-4-(5-substituted 2,4-dihydroxyphenyl)-1,2,3-thiadiazoles with general formula (I). The compounds can be used in biomedicine as active ingredients in pharmaceutical formulations, because they inhibit Hsp90 chaperone which participate in cancer progression. This invention is also related to new intermediate compounds which are used for the synthesis of thiadiazoles of general formula (I).

8. [WO/2008/016288](#) **BENZIMIDAZO[1,2-C][1,2,3]THIADIAZOL-7-SULFONAMIDES AS INHIBITORS OF CARBONIC ANHYDRASE AND THE INTERMEDIATES FOR PRODUCTION THEREOF** WO 07.02.2008

[C07D 513/04](#) PCT/LT2007/000005 BIOTECHNOLOGIJOS INSTITUTAS MATULIS, Daumantas

The invention is related to novel compounds - benzimidazo[1,2-c][1,2,3]thiadiazole sulfonamides, corresponding to the general formula (I). The compounds can be used in biomedicine as active ingredients in pharmaceutical formulations, because they inhibit enzymes which participate in disease progression such as glaucoma. The compounds of formula (I) inhibits enzymes such as carbonic anhydrases and metallo proteinases. This invention is also related to new intermediate compounds which are used for the synthesis of sulfonamides of formula (I).

Patents:

1. European Patent No. 2054420. "Benzimidazo[1,2-C][1,2,3]Thiadiazol-7-Sulfonamides as Inhibitors of Carbonic Anhydrase and the Intermediates for Production Thereof". Application submitted in 2007, patent registered on 2011 06 22. Matulis, D., Dudutienė, V., Matulienė, J., Mištinaitė, L.
2. European Patent No. 2268626. "5-Aryl-4-(5-Substituted 2,4-Dihydroxyphenyl)- 1,2,3 Thiadiazoles as Inhibitors of Hsp90 Chaperone and the Intermediates for Production Thereof". Application submitted in 2008, patent registered on 2012 02 01. Čikotienė, I., Kazlauskas, E., Matulienė, J., Matulis, D.

Patent Applications:

1. Fluorinated benzenesulfonamides as inhibitors of Carbonic Anhydrase. PCT/LT2012/000007. 2012-10-30. Matulis, D., Dudutienė V., Zubrienė, A.

2. Selected inhibitors of Carbonic Anhydrase. PCT/IB2015/056626. 2015-09-01. Čapkauskaitė, E., Zakšauskas, A., Linkuvienė, V., Matulis, D.

Other important activities:

1. Together with a business partner established a startup company, a spinoff of Vilnius University, ThermoPharma Baltic, UAB, in 2014.
2. Together with a business partner established a company, ThermoPharma, Inc, in 2012.
3. Representative at the European Medicines Agency.
4. Numerous articles published on the subjects of scientific reform, the popularity of science in society, and the support for repatriating scientists.
5. Participated in several TV programs and radio shows on science popularity and administrative reforms.
6. Member of several work groups at the Ministry of Economy and the Ministry of Science and Education; discussions and preparation of legal documents in science administration.
7. Member of professional societies – American Chemical Society, Biophysical Society, an expert of the ScanBalt projects, mapping of Baltic biotechnology, discussions on international collaboration of biotechnologists. An expert to the EU FP7 “Health” program committee in Brussels.
8. Member of the ScanBalt task force for the implementation of the EU Baltic Sea strategy

Invited talks at international conferences and universities:

1. Matulis, D. “Thermodynamics-Structure Correlations of Sulfonamide Binding to Carbonic Anhydrases and the Model Systems of Molecular Interactions”. Departmental Seminar. University of Freiburg. 2019.12.10. Freiburg, Germany. Invited by Prof. Manfred Jung.
2. Matulis, D. “From Thermodynamics-Structure Correlations of Sulfonamide Binding to Carbonic Anhydrase Proteins Toward the Biology of Lead Compound Development as Anticancer”. Departmental Seminar. Skaggs School of Pharmacy. Anschutz Medical Campus, University of Colorado. 2019.03.08. Aurora, Colorado, USA. Invited by Prof. John Carpenter.
3. Matulis, D. “From Thermodynamics-Structure Correlations of Sulfonamide Binding to Carbonic Anhydrase Proteins Toward the Biology of Lead Compound Development as Anticancer”. Departmental Seminar. Purdue University. 2019.03.06. West Lafayette, Indiana, USA. Invited by Prof. Philip Low.
4. Matulis, D. “Anticancer Drug Design Targeting Carbonic Anhydrase IX and a Database of Protein-compound Binding Gibbs Energy, Enthalpy, Entropy, Heat Capacity, and Volume Correlations With the Crystal Structure”. Medicinal Chemistry Seminar Series, Department of

- Pharmacy, University of Minnesota. 2017 05 18. Minneapolis, USA. Invited by Prof. Elizabeth Ambrose.
5. Matulis, D. "Discovery and Biological Characterization of Novel Selective Inhibitors of Carbonic Anhydrase IX". European Multidisciplinary Scientific Day. 2017 04 19. Pisa, Italy. Invited by Prof. Gaetano Angelici.
 6. Matulis D. „Intrinsic thermodynamics of anticancer drug lead binding to target proteins“. Lithuanian National Physics conference. 2015 06 17-19. Vilnius, Lithuania.
 7. Matulis, D. "Intrinsic thermodynamics of fluorinated anticancer drug lead binding to target proteins". "Chemistry and Chemical Technology 2015". 2015 01 23. Vilnius, Lithuania.
 8. Matulis, D. „Intrinsic thermodynamics – structure correlations of anticancer drug lead binding to target proteins". "ARBRE meeting". 2015 01 7-10. London, Great Britain.
 9. Matulis D. "Biothermodynamics for Target Oriented Anticancer Drug Discovery". XIIIth International Conference of Lithuanian Biochemical Society, Birštonas, Lithuania. 2014 06 17-20.
 10. Matulis D. "Thermodynamics of anticancer lead binding to target carbonic anhydrases by isothermal titration calorimetry and fluorescent thermal shift assay". XVIII ISBC International Society for Biological Calorimetry Conference, Lund, Sweden. 2014 06 1-4.
 11. Matulis D. „Recombinant production of 12 human carbonic anhydrase isoforms and characterization of their stabilities and inhibitor binding“. European Biotechnology Congress 2014, Linceo, Italy. 2014 05 14-18.
 12. Matulis D. "Biophysical assays of inhibitor binding to selected CA isozymes". 2nd CA satellite meeting, Naples, Italy. 2013 10 23-25.
 13. Matulis D. "Novel inhibitors of Carbonic Anhydrase IX, an Anticancer Target". Lithuanian Trade Mission to Boston (and Washington), Boston, USA. 2013 06 16-25.
 14. Matulis D. "Intrinsic thermodynamics – structure correlations of anticancer drug lead binding to target proteins". "CEEC-TAC2", Vilnius, Lithuania. 2013 08 27-30.
 15. Matulis D. Intrinsic thermodynamics - structure correlations of anticancer drug lead binding to target proteins. „20th Biennial Meeting of the International Society for Molecular Recognition“, Vienna, Austria. 2013 06 26-29.
 16. Matulis D. Drug Design: Intrinsic Energetics – Structure Correlations, ITC, TF, Activity, X-ray. „Biophysical Society 57th Annual Meeting“, Philadelphia, USA. 2013 01 31-02 14.
 17. Matulis D. Design, synthesis, binding, crystallography, and docking of [(2-pyrimidinylthio)acetyl] benzenesulfonamides as inhibitors of human carbonic anhydrases. „COST0804“, Salerno, Italy. 2012 11 3-7.
 18. Matulis D. Overview of Lithuanian Pharmaceutical Industry. „Life Sciences Baltics Conference“. Vilnius, Lithuania. 2012 09 12-14.

19. Matulis D. Thermodynamics Of Inhibitor Binding To Recombinant Human Carbonic Anhydrases (CA) VI and XII. „Future in Chemistry and Biology for Epigenetics training school“. Poitiers, France. 2012 07 9-12
20. Matulis D. Anticancer activity of ICPD inhibitors of Hsp90 on human tumor cell lines and in murine tumor allografts. „COST0804“, Bucuresti, Romania. 2012 05 20-24.
21. Matulis D. Thiophene Sulfonamides as Carbonic Anhydrase Inhibitors by Titration Calorimetry and Thermal Shift Assay. „COST0905“, Latvia, Riga. 2012 06 26-28.
22. Matulis D. Drug Binding Energetics by Titration Calorimetry, Thermal and Pressure Shift Assay. Johns Hopkins university, Baltimore, USA. 2011 03.
23. Matulis, D. Structural biothermodynamics of inhibitor binding to human recombinant carbonic anhydrases and Hsp90. Presented at the “66th Calorimetry Conference”. Honolulu, USA. 2011 06 14.
24. Matulis D. Structural biothermodynamics of inhibitor binding to human recombinant carbonic anhydrases and Hsp90. Nordic Biacore and MicroCal User Meeting. 2011 11 17-18. Copenhagen, Denmark.
25. Matulis, D. Carbonic anhydrase inhibitors as anticancer agents. Molėtai, Lithuania. 2010 06 16.
26. Matulis, D. Structural biothermodynamics and the search for drug-like compounds. Plenary lecture given at the Institute of Theoretical Physics and Astronomy of Vilnius university, Molėtai Astronomical Observatory, Molėtai, Lithuania. 2010 07 31.
27. Matulis, D. Structural biothermodynamics and the search for drug-like compounds. Plenary lecture given at the Conference of Organic Synthesis, Kaunas University of Technology, Kaunas, Lithuania. 2009 04 22.
28. Matulis, D. Carbonic anhydrase and Hsp90 inhibitor binding measurements by TSA, ITC, and X-ray crystallography. Instruct meeting. Budapest, Hungary. 2009 03 30.
29. Matulis, D. Characterization of carbonic anhydrases and determination of inhibitor binding by thermal shift assay. Invited by Prof. Seppo Parkkila, Institute of Medical Technology / University of Tampere, Biokatu 6, 33520 Tampere, Finland. 2007 11 19.
30. Matulis, D. Characterization of carbonic anhydrases and determination of inhibitor binding by thermal shift assay. Invited by Prof. Claudiu Supuran, Universita Degli Studi Di Firenze, Dipartimento Di Chimica, Italy. 2007 11 23.
31. Matulis, D. Human Hsp90 stability and radicicol binding by thermal shift assay. Invited by Prof. Maciej Zylicz, International Institute of Molecular and Cell Biology in Warsaw, Poland. 2006 12 15.
32. Matulis, D., and Todd, M. Thermodynamics of sulfonamide inhibitor binding to carbonic anhydrase using titration calorimetry: an interesting effect of protein, ligand, and buffer protonation. Presented at the 2003 Current Trends in Microcalorimetry, Boston, USA. 2003 07.

33. Matulis, D., Rouzina, I., and Bloomfield, V. Thermodynamics of DNA binding and condensation: isothermal titration calorimetry and electrostatic mechanism. Presented at the Nucleic Acid Interest Group, University of Minnesota. 1999 11.
34. Matulis, D. Using ITC to evaluate the energetics of intermolecular interactions. Presented at the Nucleic Acid Interest Group, University of Minnesota. 1998 03.

Oral presentations given at conferences and meetings:

1. Matulis, D. "Naujų medžiagų kūrimas". Jaunųjų biochemikų mokyklos žiemos 2018 m. sesija. 2018 01 31-02 02. Vilnius, Lithuania.
2. Matulis, D. "Protein-ligand recognition in drug design". Affinity-2017. 22nd Meeting of the International Society for Molecular Recognition. 2017 06 25-29. Paris, France.
3. Matulis, D. "Design and Evaluation of Carbonic Anhydrase IX Inhibitors as Anticancer Agents - from the Thermodynamics of Binding to Biological Effects". Departmental seminar, Maastricht Clinic. 2017 06 16. Maastricht, Netherlands.
4. Linkuvienė, V., Paketurytė, V., Zubrienė, A., Petrauskas, V., Matulis, D. "Precision of Biophysical Techniques that Determine Protein – Compound Dissociation Constants, Lessons from Our Database of over 700 Ligand Kds Determined by ITC, FTSA(DSF), SPR, and SFA". Novalix Conference, Biophysics in Drug Discovery. 2017 06 06-09. Strasbourg, France.
5. Matulis, D. "What have we learned from the enthalpy database of 200 compound binding to 8 carbonic anhydrase isoforms as determined by isothermal titration calorimetry". 2nd European Microcal Symposium. 2016 09 26-27. Paris, France.
6. Matulis, D. "Expression, Purification and Characterization of Human Carbonic Anhydrase XIV for Drug Discovery". European biotechnology congress. 2016 05 05-07. Riga, Latvia.
7. Matulis, D. "Discovery and Biological characterization of Novel Selective inhibitors of Carbonic Anhydrase IX". XIVth International Conference of Lithuanian Biochemical Society, 2016 06 27-30. Druskininkai, Lithuania.
8. Matulis D. „Intrinsic thermodynamics – structure correlations of anticancer drug lead binding to target proteins“. Symposium „Aspects of Modern Drug Discovery“. 2014 10 05-08. Nottingham, Great Britain.
9. Matulis D. „ExCo meeting“. 2013 06 03-04 . Rostock, Germany.
10. Matulis D. "The Pitfalls of Drug Lead IC 50 and Binding Measurements to Target Proteins". „COST CM0804“. 2013 05 06-09. Izmir, Turkey.
11. Matulis, D., Budvytytė, R., Černiauskaitė, D. 11th ScanBalt Forum. 2012 11 20-23. Tampere, Finland.
12. Matulis, D., Budvytytė, R. „ExCo meeting“. 2012 08 28. Copenhagen, Denmark.
13. Matulis, D. Thiophene Sulfonamides as Carbonic Anhydrase Inhibitors by Titration Calorimetry and Thermal Shift Assay. COST TD 0905, Latvia, Riga. 2012 06 26-28.

14. Matulis, D. Anticancer activity of ICPD inhibitors of Hsp90 on human tumor cell lines and in murine tumor allografts. „COST0804“, Bucuresti, Romania. 2012 05 20-24.
15. Blank, W., Matulis, D., Frank, P. ScanBalt Health Region – Setting the Stage for Cross-Sectorial Innovation in Health and Life Sciences. What is in for the regions? Baltic Development Forum. 2011 10 25-27. Gdansk, Poland.
16. Matulis, D., Grinius, L., Revuckienė, J., Budvytytė, R., Černiauskaitė, D. „BSHR HealthPort“ project meeting. 10th ScanBalt Forum. 2011 09 21-24. Heringsdorf, Germany.
17. Matulis D. “Chemijos grožis ir nauda kuriant vaistus”. „LJMS vasara 2011“. 2011 07 31-08 07. Molėtai, Lietuva.
18. Matulis, D. Structural biothermodynamics of inhibitor binding to human recombinant carbonic anhydrases. “FEBS satellite CA meeting”. Montecatini, Italy. 2011 06 22-24.
19. Zubrienė, A., Kazlauskas E., Baranauskienė, L., Petrauskas, V., Matulis, D. Towards the intrinsic lead binding thermodynamics. COST TD 0905. Split, Croatia. 2011 04 28-05 01.
20. Matulis, D. Determination of the Volume Changes Induced by Ligand Binding to Hsp90 Using High Pressure Denaturation. Biophysical Society 55th Annual Meeting. Baltimore, USA. 2011 03 05-09.
21. Matulis, D. Structural biothermodynamics of inhibitor binding to human recombinant carbonic anhydrases and Hsp90. Johnson & Johnson. USA. 2011 03 10.
22. Toleikis, Z., Cimperman, P., and Matulis, D. The Volumes of Ligand Binding to Hsp90 by High Pressure Denaturation. The 6th International Conference on High Pressure Bioscience and Biotechnology (HPBB2010). Munich, Germany. 2010 08 28-09 01.
23. Zubriene, A., Matulis, D. Thermodynamics of radicicol binding to human Hsp90 alpha and beta isoforms. ESBES+ISPPP+ISB. Bologna, Italy. 2010 09 05-08.
24. Zubriene, A., Maier, E.M., Sasse, F., Kazlauskas, E., Toleikis, Z., Chaleckis, R., Michaoloviene, V., Petrikaite, V., Grinius, L., Matulienė, J., Matulis, D. Radicicol, a natural compound and an efficient inhibitor of Hsp90, as a lead for anticancer drug design. COST CM0804, “Natural Products as Drug and Leads to Drugs”. Crete, Greece. 2010 10 12-15.
25. Zubriene, A., Baranauskienė, L., Kazlauskas, E., Toleikis, Z., Chaleckis, R., Michailoviene, V., Petrikaite, V., Capkauskaitė, E., Dudutiene, V., Matulienė, J., Matulis, D. Drug Binding Energetics by Titration Calorimetry, Thermal and Pressure Shift Assay. COST Action TD09/05 Epigenetics - Bench to Bedside. Brno, Czechia. 2010 11 22-25.
26. Baranauskienė, L., Kazlauskas, E., Čikotienė, I., Matulienė, J., Zubrienė, A., Jachno, J., Torresan, J., Michailovienė, V., Cimperman, P., Gražulis, S., and Matulis D. Carbonic anhydrase and Hsp90 inhibitor binding measurements by thermal shift assay, titration calorimetry, and x-ray crystallography. INSTRUCT meeting. Budapest, Hungary. 2009 03 29-31.
27. Baranauskienė, L., Sūdžius, J., Michailovienė, V., Matulienė, J., Tumkevičius, S., Matulis, D. Carbonic anhydrase ligand binding by thermal shift assay and titration calorimetry. The 8-th International Conference on the Carbonic Anhydrases. Florence, Italy. 2009 09 16-19.

28. Cimperman, P., Zubrienė, A., Baranauskienė, L., Kazlauskas, E., Matulienė, J., and Matulis, D. Determination of protein-ligand binding thermodynamics by thermal shift assay. European Biophysics Congress Genova. Genova, Italy .2009 07 11-15.
29. Petrikaitė, V., and Matulis, D. Thermal Shift Assay and Titration Calorimetry for Protein-Ligand Interactions. COST CM0804 Conference "Chemical Biology with Natural Products. Siena, Italy. 2009 12 03-05.
30. Kazlauskas, E., Čikotienė, I., Matulienė, J., Zubrienė, A., Jachno, J., Torresan, J., Michailovienė, V., Matulis, D. Resorcinol class Hsp90 inhibitor binding thermodynamics and the effect on cancerous cells. The 4th International Conference on the Hsp90 Chaperone Machine. Bavaria, Germany. 2008 10 02-06.
31. Baranauskienė, L., Dudutienė, V., Matulis, D. Benzimidazo [1,2-c][1,2,3] thiadiazole sulfonamides as carbonic anhydrase inhibitors. 7th International Conference on Carbonic Anhydrases: CA Research in the Postgenomic Era. Whitney Laboratory of the University of Florida, St. Augustine, USA. 2006.
32. Matulis, D., and Todd, M. A. Thermodynamics of sulfonamide inhibitor binding to carbonic anhydrase using titration calorimetry: and interesting effect of protein, ligand, and buffer protonation. Presented at the 58th Calorimetry Conference, Honolulu, USA. 2003 08.
33. Matulis, D., and Bloomfield, V. Determination of hydrophobic interactions between long aliphatic hydrocarbons: aliphatic amine aggregation and protonation pKa shift. Presented at the 15th Annual Gibbs Conference on Biothermodynamics, Carbondale, USA. 2001 09.
34. Matulis, D., and Bloomfield, V. Determination of hydrophobic interactions between long aliphatic hydrocarbons: aliphatic amine aggregation and protonation pKa shift. Presented at the 56th Annual Calorimetry Conference, Colorado Springs, USA. 2001 08.
35. Matulis, D., Rouzina, I., and Bloomfield, V. Thermodynamics of cationic lipid binding to DNA by isothermal titration calorimetry. The roles of electrostatics and hydrophobicity. Presented at the 14th Annual Gibbs Conference on Biothermodynamics, Carbondale, USA. 2000 05.
36. Matulis, D., Rouzina, I., and Bloomfield, V. Thermodynamics of cationic lipid binding to DNA by isothermal titration calorimetry. The roles of electrostatics and hydrophobicity. Presented at 2000 Midwest Thermodynamics and Statistical Mechanics Conference, Minneapolis, USA. 2000 05.
37. Matulis, D., and Lovrien, R. Protection of enzymes by aromatic sulfonates from inactivation by acid. Presented at the First International Conference on Protein Stabilization, Leeds, Great Britain. 1998 07.
38. Matulis, D., and Lovrien, R. ANS anion - protein binding primarily depends on ion pair formation. Given at the 42nd Annual Meeting of the Biophysical Society, Kansas City, USA. 1998 02.

Poster Presentations at Meetings and Conferences:

1. Linkuvienė, V., Zubrienė, A., Paketurytė, V., Smirnov, A., Petrauskas, V., Matulis, D. Database of CA Protein-Ligand Binding Gibbs Energies, Enthalpies, Entropies and Crystal Structures. "ARBRE-MOBIEU ant COST Action CA 15126". Warsaw, Poland. 2018 03 19-21.
2. Linkuvienė, V., Zubrienė, A., Paketurytė, V., Smirnov, A., Petrauskas, V., Matulis, D. Database of CA Protein-Ligand Binding Gibbs Energies, Enthalpies, Entropies and Crystal Structures. "Biophysical Society 61st Annual Meeting". New Orleans, USA. 2017 02 11-19.
3. Kazokaitė, J., Aspatwar, A., Kairys, V., Parkkila, S., Matulis, D. "Fluorinated benzenesulfonamide anticancer inhibitors of carbonic anhydrase IX exhibit lower toxic effects on zebrafish embryonic development than ethoxzolamide". Vita Scientia. Vilnius. 2016 01 04. (Student presented).
4. Paketurytė, V., Paliulis, E., Matulis, D. "Enzyme survivability at acidic pH and high temperature". European Biotechnology Congress. Ryga, Latvia. 2016 05 04-07. (Student presented).
5. Smirnov, A., Manakova, E., Zubrienė, A., Čapkauskaitė, E., Dudutienė, V., Matulis, D. "Crystallography and thermodynamics of primary sulfonamide inhibitors complexed with human carbonic anhydrases I, II, XII and XIII". XIVth International Conference of Lithuanian Biochemical Society, Druskininkai, Lithuania. 2016 06 27-30. (Student presented).
6. Smirnovienė, J., Matulis, D. „Inhibition and ligand binding studies of human carbonic anhydrases". XIVth International Conference of Lithuanian Biochemical Society, Druskininkai, Lithuania. 2016 06 27-30. (Student presented).
7. Juozapaitienė, V., Bartkutė, B., Michailovienė, V., Zakšauskas, A., Baranauskienė, L., Satkūnė, S., Matulis, D. "Production and enzymatic activity detection of recombinant human carbonic anhydrase XIV". XIVth International Conference of Lithuanian Biochemical Society, Druskininkai, Lithuania. 2016 06 27-30.
8. Toleikis Z., Sirotkin, V. A., Skvarnavičius, G., Smirnovienė, J., Roumestand, C., Matulis, D., Petrauskas, V. "Protein – ligand binding volume determined by FPSA, densitometry, and NMR". XIVth International Conference of Lithuanian Biochemical Society, Druskininkai, Lithuania. 2016 06 27-30.
9. Zakšauskas, A., Čapkauskaitė, E., Linkuvienė, V., ruibys, V., Matulis, D. "Benzenesulfonamides with N-imidazolyl fragments as inhibitors of Carbonic Anhydrase VA". Balticum Organicum Syntheticum 2016, Ryga, Latvia. 2016 07 03-06.
10. Čapkauskaitė, E., Zakšauskas, A., Jezepčikas, L., Linkuvienė, V., Matulis, D. "Carbonic Anhydrase Inhibitors: 2-Halogeno-4,5-disubstituted Benzenesulfonamides". Balticum Organicum Syntheticum 2016, Ryga, Latvia. 2016 07 03-06.
11. Timm, D.D., Zubriene, A., Baranauskiene, L., Morkunaite, V., Smirnoviene, J., Matulis, D. „Binding Thermodynamics of Novel Selective Inhibitors of Carbonic Anhydrase IX". „10th European Biophysics Congress". Dresden, Germany. 2015 07 18-22.

12. Matulienė, J., Baranauskienė, L., Mickevičiūtė, A., Vegytė, A., Petrikaitė, V., Matulis, D. „Carbonic Anhydrases IX and XII as Anticancer Targets and their Inhibitors“. „41st FEBS Congress“. Berlin, Germany. 2015 07 04-10.
13. Dudutienė, V., Matulienė, J., Smirnov, A., Timm, D., Zubrienė, A., Baranauskienė, L., Morkunaitė, V., Smirnovienė, J., Michailovienė, V., Juozapaitienė, V., Mickevičiūtė, A., Kazokaitė, J., Bakšytė, S., Kasiliauskaitė, A., Jachno, J., Revuckienė, J., Kišonaitė, M., Pilipuitytė, V., Ivanauskaitė, E., Milinavičiūtė, G., Smirnovas, V., Petrikaitė, V., Kairys, V., Petrauskas, V., Norvaišas, P., Lingė, D., Gibieža, P., Čapkauskaitė, E., Zakšauskas, A., Kazlauskas, E., Manakova, E., Gražulis, S., Ladbury, J.E., Matulis, D. “Discovery and Characterization of Novel Selective Inhibitors of Carbonic Anhydrase IX”. “10th International Carbonic Anhydrase Conference”. Maastricht, Netherlands. 2015 04 19-22.
14. Matulis, D., Zubrienė, A., Baranauskienė, L., Smirnov, A., Morkunaitė, V., Smirnovienė, J., Kišonaitė, M., Norvaišas, P., Timm, D. „Intrinsic thermodynamics-structure correlation of carbonic anhydrase inhibitors“. „Biophysical Society 59th Annual Meeting“. Baltimore, USA. 2015 02 06-12.
15. Brukštus, A., Kazlauskas, E., Petrikas, H., Petrikaitė, V., Čikotienė, I., Matulis, D. „Synthesis and Biological Evaluation of 6-(5-aryl-1,2,3-thiadiazol-4-yl)-4-isopropylbenzene-1,3-dioles as Inhibitors of Hsp90 Chaperone“. „Chemistry and chemical technology. Proceedings of the international conference“. Kaunas, Lithuania. 2014 04 25.
16. Gylytė, J., Zubrienė, A., Dudutienė, V., Smirnov, A., Timm, D., Manakova, E., Gražulis, S., Matulis, D. „Intrinsic thermodynamics-structure correlations of fluorinated benzensulfonamides as inhibitors of human carbonic anhydrases“. „Biophysical Society 58th Annual Meeting“. San Francisco, USA. 2014 02 14-25.
17. Gylytė, J., Zubrienė, A., Dudutienė, V., Smirnov, A., Timm, D., Manakova, E., Gražulis, S., Matulis, D. „Intrinsic thermodynamics-structure correlations of fluorinated benzensulfonamides as inhibitors of human carbonic anhydrases“. „The Twenty-seventh Annual Gibbs Conference on Biothermodynamics“. Carbondale, USA. 2013 10 05-08.
18. Petrauskas, V., Gylytė, J., Toleikis, Z., Cimperman, P., Matulis, D. „Protein-ligand affinity correlation with the ligand binding volume“. „9th European Biophysics Congress“. Lisbon, Portugal. 2013 07 13-18.
19. Petrikaitė, V., Matulienė, J., Tauraitė, D., Villanueva, A., Berdasco, M., Huertas, A., Satein, E. F., Esteller, M., Matulis, D. „Anticancer activity of ICPD compounds in murine models and human cancer cells“. „COST TD0905“. Reykjavik, Iceland. 2013 04 29-30.
20. Kazlauskas, E., Čikotienė, I., Zubrienė, A., Matulienė, J., Mikučiauskaitė, J., Chaleckis, R., Sharp S., Workman P., Prodromou, Ch, Matulis, D. “ICPD Inhibitor Binding to Human Hsp90 alpha, beta, Full-Length, N-Terminal Domain, Lidless, and Active Site Mutant Isoforms”. „6th International Conference on the Hsp90 Chaperone Machine“. Les Diablerets, Switzerland. 2012 09 19-23.

21. Norvaišas P., Petrauskas V., Matulis D. "Thermodynamics of cationic and anionic surfactant interaction". "XVII International Society of Biological Calorimetry (ISBC) Conference". Leipzig, Germany. 2012 06 03-06.
22. Čapkauskaitė, E., Zubrienė, A., Baranauskienė, L., Manakova, E., Tamulaitienė, G., Kazokaitė, J., Kairys, V., Gražulis S., Tumkevičius, S., Matulis, D. „Design of [(2-pyrimidinylthio)acetyl]benzenesulfonamides as inhibitors of human carbonic anhydrases“. „The 9th International Conference on Carbonic Anhydrase (CA)“. Turkey, Antalya. 2012 04 11-15.
23. Petrikaitė, V., Kazlauskas, E., Matulienė, J., Matulis, D. Development of Hsp90 inhibitors as anticancer compounds. "Animal Models and Their Value in Predicting Efficacy and Toxicity". New York, USA. 2011 09 15-16.
24. Zubrienė, A., Kazlauskas, E., Michailovienė, V., Matulis D. Towards intrinsic binding thermodynamics. 8th European Biophysics Congress. Budapest, Hungary. 2011 08 23- 27.
25. Čapkauskaitė, E., Zubrienė, A., Baranauskienė, L., Tamulaitienė, G., Manakova, E., Gražulis, S., Tumkevičius, S., Matulis, D. Synthesis of pyrimidine derivatives as inhibitors of carbonic anhydrase. 23rd International Congress on Heterocyclic Chemistry (IHC-23). Glasgow, Great Britain. 2011 07 31-08 04.
26. Petrauskas, V., Matulis D. Empirical Model of Macromolecule – ligand Interaction. Ninth Triennial Congress of the world association of theoretical and computational chemist watoc 2011. Santiago de Compostela, Spain. 2011 07 16-22.
27. Petrikaitė, V., Kazlauskas, E., Matulienė, J., Matulis, D. Anticancer activity and Admet properties of resorcinol – bearing lead compounds. The 47th International Conference „Drug Discovery and Selection“. Lyon, France. 2011 07 06-08
28. Petrikaitė, V., Kazlauskas, E., Matulienė, J., Matulis, D. Rezorcinolio darinių priešvėžinis aktyvumas ir farmakokinetinių savybių tyrimas. „XV pasaulio lietuvių mokslo ir kūrybos simpoziumas“. Kaunas – Vilnius, Lithuania. 2011 07 03-05.
29. Dudutienė, V, Zubrienė, A., Kairys, V., Matulis, D. Probing of the carbonic anhydrase isozyme active center cavities with inhibitor functional groups. International Conference „Frontiers in Medicinal Chemistry“. Stocholm, Sweden. 2011 06 19-21.
30. Petrauskas, V., Zubrienė, A., Kazlauskas, E., Baranauskienė, L., Matulis, D. Intrinsic Binding Parameters as a Necessity to Correlate Energetics with Structure. 19th Biennial Meeting of the International Society for Molecular Recognition. Tavira, Portugal. 2011 06 16-19.
31. Jogaitė, V., Zubrienė, A., Gylytė, J., Michailovienė, V., Matulis, D. Inhibitors binding to Recombinant Human CAXII. „FEBS satellite CA meeting“. Montecatini, Italy. 2011 06 22-24.
32. Maksimavičiūtė, E., Petrikaitė, V., Matulis, D. Thermodynamics of Ion Pair Formations in Proteins. COST TD0905. Split, Croatia. 2011 04 29-30.
33. Čapkauskaitė, E., Zubrienė, A., Baranauskienė, L., Tumkevičius, S., Matulis, D. Pirimidino darnių, slopinančių karboanhidrazes, sintezė. Konferencija "Chemija". Kaunas, Lithuania. 2011 04 27.

34. Petrikaitė, V., Kazlauskas, E., Zubrienė, A., Michailovienė, V., Matulienė, J., Matulis, D. Anticancer activity and ADME/Tox properties of resorcinol-bearing Hsp90 inhibitors. ADMET Europe. Munchen, Germany. 2011 03 28-29.
35. Toleikis, Z., Cimperman, P., and Matulis, D. Determination of The Volume Changes Induced by Ligand Binding to Hsp90 Using High Pressure Denaturation. The 6th International Conference on High Pressure Bioscience and Biotechnology (HPBB2010). Munich, Germany. 2010 08 28-09 01.
36. Petrauskas, V., Maksimavičiūtė, E., Matulis, D. Thermodynamics of Ion Pair Formations in Proteins. ESBES+ISPPP+ISB. Bologna, Italy. 2010 09 05-08.
37. Zubrienė, A., Kazlauskas, E., Chaleckis, R., Michailovienė, V., Matulienė, J., Matulis, D. Thermodynamics of radicicol binding to human Hsp90 alpha and beta isoforms. The 5th International Conference on The Hsp90 Chaperone Machine. Les Diablerets, Switzerland. 2010 09 29-10 03.
38. Petrikaitė, V., Kazlauskas, E., Zubrienė, A., Michailovienė, V., Matulienė, J., Matulis, D. Resorcinol - Bearing Hsp90 inhibitors as anticancer agents. COST Action TD09/05 Epigenetics - Bench to Bedside. Brno, Czech. 2010 11 22-25
39. Kazlauskas, E., Čikotienė, I., Matulienė, J., Zubrienė, A., Jachno, J., Torresan, J., Michailovienė, V., Petrikaitė, V., Grinius, L., Matulis, D. Resorcinol class Hsp90 inhibitor binding thermodynamics and the effect on cancerous cells. The 4th International Conference on the Hsp90 Chaperone Machine. Bavaria, Germany. 2008 10 02-06.
40. S. Gražulis, L. Baranauskienė, E. Manakova, R. Sukackaite, D. Golovenko, G. Tamulaitienė, D. Matulis. Novel thiadiazoles inhibitors of human carbonic anhydrases. 7th ScanBalt Forum & Biomaterial Days. Vilnius, Lithuania. 2008 09 24-26.
41. S. Gražulis, L. Baranauskienė, E. Manakova, R. Sukackaite, D. Golovenko, G. Tamulaitienė, D. Matulis. Novel thiadiazoles inhibitors of human carbonic anhydrases. XXI Congress and General Assembly of the International Union of Crystallography. Osaka, Japan. 2008 08 23-31.
42. Cimperman, P., Toleikis, Z., Matulis, D. A general model to describe protein thermal stabilization and destabilization by ligands. 2nd International Symposium on Biothermodynamics, Frankfurt am Main, Germany. 2008 02 21-22.
43. Matulis, D., and Todd, M. Thermodynamics of inhibitor binding to carbonic anhydrase by titration calorimetry and ThermoFluor®. Presented at the 16th Gibbs Conference on Biothermodynamics, Carbondale, USA. 2002 09.
44. Matulis, D., and Todd, M. Thermodynamics of inhibitor binding to carbonic anhydrase by titration calorimetry and ThermoFluor®. Presented at the 57th Annual Calorimetry Conference, New Brunswick, USA. 2002 08.
45. Matulis, D., Rouzina, I., and Bloomfield, V. Determination of hydrophobic interactions between long chain aliphatic hydrocarbons by titration calorimetry. Presented at the 46th Annual Meeting of the Biophysical Society, San Francisco, USA. 2002 02.

46. Matulis, D., Rouzina, I., and Bloomfield, V. Thermodynamics cationic lipid binding to DNA by titration calorimetry: the roles of electrostatics and hydrophobicity. Presented at the 45th Annual Meeting of the Biophysical Society, Boston, USA. 2001 02.
47. Lovrien, R., Wu, C., and Matulis, D. Lectin and protease isolation from crude via coprecipitation matrix ligands. Presented at the American Chemical Society 219th National Meeting, San Francisco, USA. 2000 03.
48. Lovrien, R. and Matulis, D. Isolation of proteins from crudes: Matrix entanglement ligand basis. Presented at the American Chemical Society 219th National Meeting, San Francisco, USA. 2000 03.
49. Matulis, D., Rouzina, I., and Bloomfield, V. Thermodynamics of DNA binding and condensation: isothermal titration calorimetry and electrostatic mechanism. Presented at the 44th Annual Meeting of the Biophysical Society, New Orleans, USA. 2000 02.
50. Lovrien, R., Wu, C., and Matulis, D. Forces, energetics, topology of outer directed hydrophobicity in organic ligand-protein matrices. Presented at the 44th Annual Meeting of the Biophysical Society, New Orleans, USA. 2000 02.
51. Matulis, D., Rouzina, I., and Bloomfield, V. Thermodynamics of DNA binding and condensation: isothermal titration calorimetry and electrostatic mechanism. Presented at the Nucleic Acid Interest Group meeting. 1999 10.
52. Matulis, D., Rouzina, I., and Bloomfield, V. Thermodynamics of DNA binding and condensation: isothermal titration calorimetry and electrostatic mechanism. Presented at the 13th Annual Gibbs Conference on Biothermodynamics, Carbondale, USA. 1999 10.
53. Matulis, D., and Lovrien, R. Prediction of free energies and enthalpies of anionic aliphatic ligand binding to proteins based on experimental database and the enthalpy additivity principle. Presented at the 43rd Annual Meeting of the Biophysical Society, Baltimore, USA. 1999 02.
54. Lovrien, R., and Matulis, D. Pushing agents, pulling agents in protein isolation. Presented at the 43rd Annual Meeting of the Biophysical Society, Baltimore, USA. 1999 02.
55. Matulis, D., and Lovrien, R. Thermodynamics of the organic and inorganic anion binding to the strongest site on bovine serum albumin. Presented at the 12th Annual Gibbs Conference on Biothermodynamics, Carbondale, USA. 1998 10.
56. Matulis, D., and Lovrien, R. Protection of enzymes by aromatic sulfonates from inactivation by acid. Presented at the First International Conference on Protein Stabilization, Leeds, Great Britain. 1998 06.
57. Matulis, D., and Lovrien, R. ANS anion - protein binding primarily depends on ion pair formation. Presented at the 11th Annual Gibbs Conference on Biothermodynamics, Carbondale, USA. 1997 10.
58. Matulis, D., and Lovrien, R. Alkane sulfates (SDS) bind to proteins by forming ion pairs with the positively charged amino acids. Presented at the 3rd International Conference on Lipid-Binding Proteins, Minneapolis, USA. 1997 05.

59. Matulis, D., Wu, C., and Lovrien, R. Designing pushing, pulling, hybrid push-pull agents for protein precipitation. Presented at the 41st Annual Meeting of the Biophysical Society, New Orleans, USA. 1997 02.
60. Lovrien, R., and Matulis, D. Biophysical perspectives on protein precipitation-coprecipitation. Presented at the 40th Annual Meeting of the Biophysical Society, Baltimore, USA. 1996 02.
61. Lovrien, R. and Matulis, D. Hard and soft sulfate and sulfonate anions in protein precipitation-biorecognition. Presented at the 39th Annual Meeting of the Biophysical Society, San Francisco, USA. 1995 02.
62. Matulis, D., Meskys, R., and Rubikas, J. Removal of nickel from industrial effluents: an innovative process using the bacterial membrane transport system for nickel. Presented at the Fourth International Symposium on Biological Processing of Fossil Fuels, Alghero, Italy. 1993 09.
63. Matulis, D., Meskys, R., and Rubikas, J. Nickel uptake and efflux by bacterial cells. Presented at the International Symposium on Biological Processing of Fossil Fuel in Moscow, Russia. 1991 09.

Academic research projects:

1. Partner of the EC Horizon-2020 Marie Skłodowska-Curie project to Gaetano Angelici, acronym "ProMembrane", "Amphiphilic Peptoids as general tool for stabilization and crystallization of Membrane Proteins". (€ 4500). 2015 – 2017.
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8. Grant No. LIG-16/2010 from the Research Council of Lithuania. (€ 294 800), 2010 09 – 2011 12.

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10. Chemical Biology with natural products. COST. 2009.
11. Anticancer drug design by structural biothermodynamics“ by EEA-Norway Grants (€ 565 037), 2008 – 2010.
12. “Design of specific human carbonic anhydrase inhibitors”, by the Lithuanian Science and Studies Foundation, (€ 362 000), 2005 – 2009.
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3. Interview for TV portal LRT about virus SARS-CoV-2 <https://www.lrt.lt/naujienos/mokslas-ir-it/11/1166228/vu-biochemikas-daumantas-matulis-kuo-naujasis-koronavirusas-skiriasi-nuo-kitu>
4. Interview for the movie on Life sciences <http://www.baltic-science.org/index.php/119-life-science> (2018)
5. Greta Ališauskaitė; 50-ies tarptautinių mokslininkų formulė Lietuvai: kada baigs kepti studentus užsieniui; 2017.12.31 <https://www.tv3.lt/naujiena/940073/50-ies-tarptautiniu-mokslininku-formule-lietuvai-kada-baigs-kepti-studentus-uzsieniui>
6. Dalius Simėnas; Paruošė lengvatų paketą inovacijoms; Verslo žinios; 2017.05.04 <https://www.vz.lt/finansai-apskaita/2017/05/04/paruose-lengvatu-paketa-inovacijoms>
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16. Mokslininko užrašai. Žinių radijas. Daumantas Matulis. [2013/09/24](#)
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