Curriculum Vitae of dr hab. Sergey A. Samsonov, prof. UG

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PERSONAL INFORMATION

Date of birth: 28.02.1983
Birth place: Leningrad, USSR
Citizenship: Russian

RESEARCH EXPERIENCE AND ACADEMIC DEGREES

2022-now Associate Professor at the University of Gdańsk, Poland
2018 Title of dr. habil. (HDR) at the University of Tours, France. *Cum laude*.
2017-now Principal Investigator at Faculty of Chemistry, University of Gdańsk, Poland
2009-2017 Postdoctoral researcher at BIOTEC TU Dresden, Germany
2006-2010 PhD in Biophysics and Biochemistry, Saint-Petersburg State University, Russia
2006-2009 PhD in Structural Bioinformatics at BIOTEC TU Dresden, Germany. *Suma cum laude*.
2006 Master Degree (*with honors*) in Biophysics, Department of Biophysics, Faculty of Physics and Mechanics, State Polytechnical University of Saint-Petersburg, Russia
2004 Bachelor Degree (*with honors*) in Physics, Department of Biophysics, Faculty of Physics and Mechanics, State Polytechnical University of Saint-Petersburg, Russia.
1990-2000 High school, Saint-Petersburg, Russia

RESEARCH INTERESTS

Modeling glycosaminoglycan molecular systems, protein-glycosaminoglycans interactions, glycosaminoglycans conformational analysis, development of novel compuatational approaches for gycosaminoglycan containing systems, solvent in molecular interfaces, non-natural amino acids, molecular dynamics, molecular docking, force field parameters development, coarse-grained modeling.

COMPUTER PROGRAMS/SKILLS

– AMBER, GAUSSIAN, Autodock, eHiTs, Glide, FlexX, GRID, Discovery Studio, MOE, VMD, Chimera UCSF, Cambridge Structural Database, R statistical package, bash/awk/sed scripting, Python, Gnuplot, high performance computing.

GRANTS

– **2023:** OPUS 25 Grant from National Science Center (Poland) “Decrypting the "sulfation code" of glycosaminoglycans for understanding their function in the extracellular matrix” 2 128 604 zł (~490 000 Euro). Duration 4 years.
– **2022**: a joint PHC Polonium mobility grant from French Republic and NAWA (the Polish National Agency for Academic Exchange) with the title “Characterization of protein-glycosaminoglycan interactions” together with the group of prof. Ricard-Blum at the University of Lyon (France) (~5000 Euro).

– **2021**: a joint mobility grant from DAAD (The German Academic Exchange Service) and NAWA (the Polish National Agency for Academic Exchange) with the title "Advanced and innovative computational approaches to study protein-glycosaminoglycan systems" together with the group of prof. Zacharias at the Technical University of Munich (~5000 Euro) .

– **2019**: BEETHOVEN CLASSIC 3 Grant from National Science Center (Poland) "Mechanistic insights into the specificity of glycosaminoglycan interactions with regulatory proteins" 976 500 zł (~232 500 Euro). Duration: 3 years.

– **2019**: SONATA BIS 8 Grant from National Science Center (Poland) "Modeling of glycosaminoglycan-induced formation of protein structure and enhancement of biologically relevant protein-ligand interactions" 2 477 304 zł (579 000 Euro). Duration: 5 years.

– **2018**: Faculty of Chemistry, University of Gdansk "Research of Young Scientists" grant "Modeling of interactions between glycosaminoglycans and the anticancer agent ellipticine". 860 Euro.

– **2017**: German Research Council Grant for Temporary Positions for Principal Investigators "Computational approaches for analyzing protein-glycosaminoglycan interactions". 264 950 Euro. Duration: 3 years. The grant was not accepted by the grantee.

– **2016**: POLONEZ 2 Grant from National Science Center (Poland) "Computational approaches to study protein-glycosaminoglycan interactions". 944 874 zł (217 970 Euro). This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 665778. Duration: 2 years.

AWARDS

– 2022: University of Gdańsk Rector Award for the scientific achievement of the Lab in the year 2021.
– 2020: University of Gdańsk Rector Award for the scientific achievement of the Lab in the year 2019.
– **2018**: HDR Thesis. *Cum laude*.
– 2014: Award for the contributed talk at the conference 'From Computational Biophysics to Systems Biology'. Gdańsk, Poland.
– **2009**: PhD Thesis. *Summa cum laude*.
– **2006**: Master Thesis was awarded with the first prize of Russian Academy of Science as the best Thesis in Biology.
– **2006**: Student's Fellowship awarded by FEBS for participation in FEBS Young Scientists Forum. Istanbul, Turkey.
– **2005**: First prize award for the talk at International Scientific-Practical Conference of Young Scientists. Odessa, Ukraine.
– **2005**: First prize award for the talk at the 33rd Week of Science at the State Polytechnical University. Saint-Petersburg, Russia.
– **2005**: Travel grant awarded by Center for International Mobility (CIMO) for participation in Scientific Winter School in Bioinformatics.
– **2004**: Bachelor Thesis was awarded with the diploma at the Russian Competition for Student Thesis.

MEMBERSHIPS

– International Society of Matrix Biology
– INNOGLY COST Action
– Marie Curie Alumni Association
– Expert member of NAWA (Polish National Agency for Academic Exchange)

LIST OF PUBLICATIONS IN PEER-REVIEWED JOURNALS

H-index: **27** (SCOPUS, 13.09.2023)

1. Marcicz M., Anila S., Gaardløs M., Zacharias M., **Samsonov S.A.** Studying specificity in protein-glycosaminoglycan recognition with umbrella sampling. *Beilstein Journal of Organic Chemistry*. 2023. Vol. 19: 1933–1946.

2. Penk A., Danielsson A., Gaardløs M., Montag C., Schöler A., Huster D., **Samsonov S.A.**, Künze G. Detecting protein-ligand interactions with nitroxide based paramagnetic cosolutes. *Chemistry - A European Journal*. 2023. e202303570. doi: 10.1002/chem.202303570

3. Brzeski J., Nowicka P., **Samsonov S.A.** The effect of Pd(II) and Pt(II) coordination on the affinity of avibactam to OXA-48 β-lactamase. *Eur J Med Chem Rep*. 2023. Vol. 9: 100118.

4. Lensink M., ... **Samsonov S.**, … Wodak S.J. Impact of AlphaFold on Structure Prediction of Protein Complexes: The CASP15-CAPRI Experiment. *Proteins*. 2023. Vol. 91: 1658–1683.

5. Schulze C., Danielsson A., Liwo A., Huster D., **Samsonov S.A.**, Penk A. Ligand Binding of Interleukin-8: A Comparison of Glycosaminoglycans and Acidic Peptides. *Phys Chem Chem Phys*. 2023. Vol. 25: 24930–24947.

6. Maszota-Zieleniak M., **Samsonov S.A.** Molecular dynamics simulation-based prediction of glycosaminoglycan interactions with drug molecules. *Computational Drug Discovery and Design (2nd Ed.). Methods in Molecular Biology Series. Springer.* 2023. 143–154.

7. Maszota-Zieleniak M., Liwo A., Ricard-Blum S., **Samsonov S.A.** Interplay of heparan sulfate chains with the core proteins of syndecans 2 and 4. *Proteoglycan Research*. 2023. Vol. 1: e10.

8. Danielsson A., **Samsonov S.A.**, Liwo A., Sieradzan A.K. Extension of the SUGRES-1P Coarse-Grained Model of Polysaccharides to Heparin. *J Chem Theor Comp*. 2023. Vol. 17: 6023–6036.

9. Kowalska D., Dołżonek J., Żamojć K., **Samsonov S.A.**, Maszota-Zieleniak M., Makowska J., Stepnowski P., Białk-Bielińska A., Wyrzykowski D. Insights into the interaction of Human Serum Albumin with Ionic Liquids – Thermodynamic, spectroscopic and molecular modelling studies. *International Journal of Biological Macromolecules*. 2023. Vol. 249: 125883.

10. Marcisz M., **Samsonov S.A.** Solvent models benchmark for molecular dynamics of glycosaminoglycans. *J Chem Inf Mod.* 2023. Vol 63: 2147–2157.1

11. Gaardløs M., Lervik A., **Samsonov S.A.** Computational modeling of the molecular basis for the calcium-dependence of the mannuronan C-5 epimerase AvAlgE6 from Azotobacter vinelandii. *Computational and Structural Biotechnology Journal*. 2023. Vol. 21: 2188–2196.

12. Gitlin-Domagalska A., Dębowki D., Maciejewska A., **Samsonov S.A.**, Maszota-Zieleniak M., Ptaszyńska N., Łęgowska A., Rolka K. Cyclic peptidic furin inhibitors developed by combinatorial chemistry. *ACS Medicinal Chemistry Letters*. 2023. Vol. 14: 458–465.

13. Grabowska O., **Samsonov S.A.**, Chmurzyński L., Wyrzykowski D., Żamojć K. Investigation of hexacyanoferrate(II)/(III) charge-dependent interactions with bovine and human serum albumins. *Spectrochimica Acta Part A*. 2023. Vol. 293: 122505.

14. Pągielska M., **Samsonov S.A.** Molecular dynamics-based comparative analysis of chondroitin and dermatan sulfates. *Biomolecules*. 2023. Vol. 13: 247.

15. Bojarski K.K., **Samsonov S.A.** In silico insights into procathepsin S maturation mediated by glycosaminoglycans. *J Mol Graph Mod.* 2023. Vol. 120: 108406.

16. Marcisz M., Maszota-Zieleniak M., **Samsonov S.A.** Repulsive Scaling Replica Exchange

Molecular Dynamics in Modeling Protein-Glycosaminoglycan Complexes. *Nikos K. Karamanos (ed.), Proteoglycans: Methods and Protocols, Methods in Molecular Biology Series. Springer.* 2023. Vol. 2619.

17. Perez S., Makshakova O., Angulo J., Bedini E., Bisio A., de Paz J.L., Fadda E., Guerrini M., Hricovini M., Hricovini M., Lisacek F., Nieto P.M., Pagel K., Pairardi G., Richter R., **Samsonov S.A.**, Vives R., Nikitovic D., Ricard-Blum S. Glycosaminoglycans: What remains to be deciphered? *JACS Au*. 2023. Vol. 323: C1740-C1756.

18. Giatagana E-M., Berdiaki A., Gaardløs M., Tsatsakis A., **Samsonov S.A.**, Nikitovic D. Rapamycin-induced autophagy in osteosarcoma cells is mediated via the biglycan/Wnt/β-catenin signaling axis. *American Journal of Physiology-Cell Physiology*. 2022. Vol. 323: C1740-C1756.

19. Kogut M.M., Grabowska O., Wyrzykowski D., **Samsonov S.A.** Affinity and putative entrance mechanisms of alkyl sulfates into the β-CD cavity. *Journal of Molecular Liquids*. 2022. Vol. 364: 119978.

20. Kogut M.M., Danielsson A., Ricard-Blum S., **Samsonov S.A.** Impact of calcium ions on the structural and dynamic properties of heparin oligosaccharides by computational analysis. *Computational Biology and Chemistry*. 2022. Vol. 99: 107727.

21. Marcisz M., Gaardløs M., Bojarski K.K., Siebenmorgen T., Zacharias M., **Samsonov S.A**. Explicit Solvent Repulsive Scaling Replica Exchange Molecular Dynamics (RS-REMD) in Molecular Modeling of Protein-Glycosaminoglycan Complexes. *J Comp Chem*. 2022. Vol. 43: 1633–1640.

22. Danielsson A., Kogut M.M., Maszota-Zieleniak M., Chopra P., Boons G.J., **Samsonov S.A**. Molecular Dynamics-based descriptors of 3-O-Sulfated Heparan Sulfate as Contributors of Protein Binding Specificity. *Computational Biology and Chemistry*. 2022. Vol. 99: 107716.

23. Denamur S., Chazeirat T., Maszota-Zieleniak M., Vives R., Saidi A., Zhang F., Linhardt R.J., Labarthe F., **Samsonov S.A.**, Lalmanach G., Lecaille F. Binding of heparan sulfate to human cystatin C modulates inhibition of cathepsin L:consequences in mucopolysaccharidosis. *Carbohydrate Polymers*. 2022. Vol. 293: 119734.

24. Bertozo L., Kogut M., Maszota-Zieleniak A., **Samsonov S.A.**, Ximenez V.F. Induced Circular Dichroism as a Tool to Monitor the Displacement of Ligands Between Albumins. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy.* 2022, Vol. 278: 121374.

25. Lipska A.G., Anoniak A. M., Wesolowski P., Warszawski A., **Samsonov S.A.**, Sieradzan A.K. Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins. *Journal of Molecular Modeling*. 2022.

26. Maszota-Zieleniak M., Zsila F., **Samsonov S.A.** Molecular Dynamics Approaches Dissect Molecular Mechanisms Underlying Methylene Blue–Glycosaminoglycan Interactions. *Molecules.* 2022, Vol. 27: 2654.

27. Giatagana E-M., Berdiaki A., Gaardløs M., **Samsonov S.A.**, Tzanakakis G.N., Nikitovic D. Biglycan interacts with type I insulin-like receptor (IGF-IR) signaling pathway to regulate osteosarcoma progression and response to chemotherapy. *Cancers*. 2022. Vol 14: 1196.

28. Bojarski K.K., Sage J., Lalmanach G., Lecaille F., **Samsonov S.A.** *In silico* and *in vitro* mapping of specificity patterns of glycosaminoglycans towards cysteine cathepsins B, L, K, S and V. *J Mol Graph Mod.* 2022. Vol. 113: 108153.

29. Sage J., Renault J., Domain R., Bojarski K.K., Chazeirat T., Saidi A., Leblanc E., Nizard C., **Samsonov S.A.**, Kurfurst R., Lalmanach G., Lecaille F. Modulation of the expression and activity of cathepsin S in reconstructed human skin by neohesperidin dihydrochalcone. *Matrix Biology*. 2022. Vol. 107: 97–112.

30. Kogut M.M., Marcisz M., **Samsonov S.A.** Modeling glycosaminoglycan-protein complexes. *Current Opinion in Structural Biology*. 2022. Vol. 73: 102332.

31. Liwo A., Sieradzan A.K., Karczyńska A.S., Lubecka E.A., **Samsonov S.A.**, Czaplewski C., Krupa P., Mozolewska M. Practical Aspects of Computational Chemistry V. Physics-Based Coarse-Grained Modeling in Bio- and Nanochemistry. *Springer Nature Switzerland AG*. 2022.

32. Grabowska O., Kogut M.M., Żamojć K., **Samsonov S.A.**, Makowska J., Tesmar A., Chmur K., Wyrzykowski D., Chmurzyński L. Effect of Tetraphenylborate on Physicochemical Properties of Bovine Serum Albumin. *Molecules*. 2021. Vol. 26: 6565.

33. Marcisz M., Maszota-Zieleniak M., Huard B., **Samsonov S.A.** Advanced Molecular Dynamics Approaches to Model a Tertiary Complex APRIL/TACI with Long Glycosaminoglycans. *Biomolecules*. 2021. Vol. 11: 1349.

34. Liwo A., Czaplewski C., Sieradzan A.K., Lipska A.G., **Samsonov S.A.**, Murarka R.K. Theory and practice of coarse-grained molecular dynamics of biologically important systems. *Biomolecules*. 2021. Vol. 11: 1347.

35. Marcisz M., Zacharias M., **Samsonov S.A.** Modeling protein-glycosaminoglycan complexes: does the size matter? *J Chem Inf Mod.* 2021. Vol. 61: 4475–4485.

36. Antoniak A., Biskupek I., Bojarski K.K., Czaplewski C., Giełdoń A., Kogut M., Kogut M.M., Krupa P., Lipska A.G., Liwo A., Lubecka E.A., Marcisz M., Maszota-Zieleniak M., **Samsonov S.A.**, Sieradzan A.K., Ślusarz M.J., Ślusarz R., Wesołowski P.A., Zięba K. Modeling protein structures with the coarse-grained UNRES force field in the CASP14 experiment. *J Mol Graph Mod.* 2021.108:108008.

37. Tesmar A., Kogut M.M., Żamojć K., Grabowska O., Chmur K., **Samsonov S.A.**, Makowska J., Wyrzykowski D., Chmurzyński L. Physicochemical nature of sodium dodecyl sulfate interactions with bovine serum albumin revealed by interdisciplinary approaches. *Journal of Molecular Liquids*. 2021. Vol. 340: 117185.

38. Maszota-Zieleniak M., Danielsson A., **Samsonov S.A.** The potential role of glycosaminoglycans in serum amyloid A fibril formation by in silico approaches. *Matrix Biology Plus*. 2021. Vol. 12: 1000080.

39. Maszota-Zieleniak M., Zsila F., **Samsonov S.A.** Computational insights into heparin-small molecule interactions: evaluation of the balance between stacking and non-stacking binding modes. *Carbohydrate Research*. 2021. Vol. 507: 108390.

40. Künze G., Huster D., **Samsonov S.A**. Investigation of the Structure of Regulatory Proteins Interacting with Glycosaminoglycans by Combining NMR Spectroscopy and Molecular Modeling – The Beginning of a Wonderful Friendship. *Biological Chemistry*. 2021. 402: 1337–1355.

41. Gaardløs M., **Samsonov S.A.**, Sletmoen M., Sætrom G.I., Hjørnevik M., Sletta H., Tøndervik A., Aachmann F.L. Insights into the roles of charged residues in substrate binding and mode of action of mannuronan C-5 epimerase AlgE4. *Glycobiology*. 2021. 31: 1616–1635.

42. Marcisz M., Huard B., Lipska A.G., **Samsonov S.A.** Further analyses of APRIL/APRIL-Receptor/Glycosaminoglycan interactions by biochemical assays linked to computational studies. *Glycobiology*. 2021. 31: 772–786.

43. **Samsonov S.A.**, Zsila F., Maszota-Zieleniak M. Acute phase α1-acid glycoprotein as a siderophore-capturing component of the human plasma: a molecular modeling study. *J Mol Graph Mod.* 2021. 105:107861.

44. Maszota-Zieleniak M., Marcisz M., Kogut M.M., Siebenmorgen T., Zacharias M., **Samsonov S.A**.

Evaluation of Replica Exchange with Repulsive Scaling Approach for Docking Glycosaminoglycans. *J Comp Chem*. 2021. Vol. 42: 1040–1053.

45. Bertozo L. C., Maszota-Zieleniak M., Bolean M., Ciancaglini P., **Samsonov S.A.**, Ximenes V.F. Binding of fluorescent dansyl amino acids in albumin: when the access to the protein cavity is more important than the strength of binding. *Dyes and Pigments*. 2021. Vol. 188: 109195.

46. Kogut M.M., Maszota-Zieleniak M., Marcisz M., **Samsonov S.A**. Computational insights into the calcium ions role in protein-glycosaminoglycan systems. *Phys Chem Chem Phys*. 2021. Vol. 23: 3519–3530.

47. Bojarski K.K., **Samsonov S.A.** Role of oligosaccharide chain polarity in protein-glycosaminoglycan interactions. *J Chem Inf Mod.* 2021. Vol. 61: 455–466.

48. Zsila F., **Samsonov S.A.**, Maszota-Zieleniak M. Mind your dye: the amyloid sensor thioflavin T interacts with sulfated glycosaminoglycans used to induce cross-β-sheet motifs. *J Phys Chem B*. 2020. Vol. 124: 11625–11633.

49. Chazeirat T., Denamur S., Bojarski K.K., Andrault P.-M., Sizaret D., Zhang F., Saidi A., Tardieu M., Linhardt R.J., Labarthe F., Brömme D., **Samsonov S.A.**, Lalmanach G., Lecaille F. The abnormal accumulation of heparan sulfate in patients with mucopolysaccharidosis prevents the elastolytic activity of cathepsin V. *Carbohydrate Polymers*. 2020. Vol. 253. 117261.

50. Gorbikova E., **Samsonov S.A.**, Kalendar R. Probing proton-loading site of cytochrome c oxidase by time-resolved Fourier transform infrared spectroscopy. *Molecules*. 2020. Vol. 25: 3393.

51. Bojarski K.K., Karczyńska A.S., **Samsonov S.A.** The role of glycosaminoglycans in procathepsin B maturation – molecular mechanism elucidated by a computational study. *J Chem Inf Mod.* 2020. Vol. 60:2247-2256.

52. Gitlin-Domagalska A., Dębowski D., Gucwa K., Starego D., Ptaszyńska N., Sieradzan A., Karczyńska A., **Samsonov S.A.**, Mangold M., Gütschow M., Łęgowska A., Rolka K. Truncation of Huia versabilis Bowman-Birk inhibitor increases its selectivity, matriptase-1 inhibitory activity and proteolytic stability. *Biochemie*. Vol. 171-172:178-186.

53. Karczyńska A., Zięba K., Uciechowska U., Mozolewska, M., Krupa P., Lubecka E., Lipska A., Sikorska C., **Samsonov S.**, Sieradzan A., Gieldon A., Liwo A., Ślusarz R., Ślusarz M., Lee, J., Joo K., Czaplewski C. Improved consensus-fragment selection in template-assisted prediction of protein structures with the UNRES force field in CASP13. *J Chem Inf Mod.* 2020. 60:1844-1864.

54. Glashagen G., de Vries S., Uciechowska-Kaczmarzyk U., **Samsonov S.A.**, Murail S., Tuffery P., Zacharias M. Coarse-grained and atomic resolution biomolecular docking with the ATTRACT approach. *Proteins*. 2019. Vol. 88:1018-1028.

55. Lecaille F., Chazeirat T., Bojarski K.K., Renault J., Saidi A., Prasad V.G.N.V, **Samsonov S.A.**, Lalmanach G. Rat cathepsin K: enzymatic specificity and regulation of its collagenolytic activity. *BBA – Proteins and Proteomics*. 2019, Vol. 1868:140318.

56. Plotnikova M.A., Klotchenko S.A., Kiselev A.A., Gorshkov A.N., Shurygina A.S., Vasilyev K.A., Uciechowska-Kaczmarzyk U., **Samsonov S.A.**, Kovalenko A.L., Vasin A.V. Meglumine acridone acetate, the ionic salt of CMA and N-methylglucamine, induces apoptosis in human PBMCs via the mitochondrial pathway. *Sci Rep*. 2019, Vol. 9:18240.

57. Lensink M.F., ... **Samsonov S.**, … Wodak S.J. Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins*. 2019, Vol. 87:1200-1221.

58. Potthoff J., Bojarski K.K., Kohut G., Lipska A.G., Liwo A., Kessler E., Ricard-Blum S., **Samsonov S.A.** Analysis of procollagen C-proteinase enhancer-1/glycosaminoglycan binding sites and of the

potential role of calcium ions in the interaction. *Int J Mol Sci, Special Issue: "Recent Developments on Protein–Ligand Interactions: From Structure, Function to Applications"*. 2019, Vol. 20:5021.

59. Ilyechova E., Miliukhina I., Karpenko M., Orlov I., Puchkova L., **Samsonov S.A.** A case of Parkinson's disease with early onset in a heterozygous carrier of mutation in Atp7b gene. *J Pers Med*. 2019, Vol. 9:41.

60. Drobot B., Schmidt M., Mochizuki Y., Abe T., Okuwaki K., Brulfert F., Falke S., **Samsonov S.A.**, Komeiji Y., Betzel C., Stumpf T., Raff J., Tsushima S. Cm^{3+}/Eu^{3+} induced structural, mechanistic and functional implications for calmodulin. *Phys Chem Chem Phys*. 2019, Vol. 21: 21213-21222.

61. Lubecka E.A., Karczynska A.S., Lipska A.G., Sieradzan A.K., Zieba K., Sikorska C., Uciechowska U., **Samsonov S.A.**, Krupa P., Mozolewska M.A., Golon L., Gieldon A., Czaplewski C., Slusarz R., Slusarz M., Crivelli S.N., Liwo A. Evaluation of the scale-consistent UNRES force field in template-free prediction of protein structures in the CASP13 experiment. *J Mol Graph Mod.* 2019, Vol. 92:154-166.

62. Bojarski K.K., Becher J., Riemer T., Lemmnitzer K., Möller S., Schiller J., Schnabelrauch M., **Samsonov S.A.** Synthesis and *in silico* characterization of artificially phosphorylated glycosaminoglycans. *J Mol Struct*. 2019, Vol. 1197:401-416.

63. **Samsonov S.A.**, Freza S., Zsila F. *In silico* analysis of heparin and chondroitin sulfate binding mechanisms of the antiprotozoal drug berenil and pentamidine. *Carb Res*. 2019, 482:107742.

64. Penk A., Baumann L., Huster D., **Samsonov S.A.** NMR and Molecular Modeling Reveal Specificity of the Interactions between CXCL14 and Glycosaminoglycans. *Glycobiology*. 2019, Vol. 29: 715-725.

65. Kohut G., Sieradzan A., Zsila F., Tunde J., Bosze S., Liwo A., **Samsonov S.A.**, Beke-Somfai T. The Molecular Mechanism of Structural Changes in the Antimicrobial Peptide CM15 Upon Complex Formation with Drug Molecule Suramin: a Computational Analysis. *Phys Chem Chem Phys*. 2019, Vol. 21: 10644-10659.

66. Uciechowska-Kaczmarzyk U., Chauvot de Beauchene I., **Samsonov S.A.** Docking software performance in protein-glycosaminoglycan systems. *J Mol Graph Mod.* 2019, Vol. 90:42-50.

67. **Samsonov S.A.**, Lubecka E. A., Bojarski K. K., Ganzynkowicz R., Liwo A. Local and Long Range Potentials for Heparin-Protein Systems for Coarse-Grained Simulations. *Biopolymers*. 2019, Vol. 110:e23269.

68. **Samsonov S.A.**, Zacharias M., Chauvot de Beauchene I. Modeling large protein-glycosaminoglycan complexes using a fragment-based approach. *J Comp Chem*. 2019, Vol. 40:1429-1439.

69. Bojarski K.K., Sieradzan A.K., **Samsonov S.A.** Molecular Dynamics Insights into Protein-Glycosaminoglycan Systems from Microsecond-Scale Simulations. *Biopolymers*. 2019, Vol. 110:e23252.

70. Kohut G., Liwo A., Bosze S., Beke-Somfai T., **Samsonov S.A.** Protein-Ligand Interaction Energy-Based Entropy Calculations: Fundamental Challenges for Flexible Systems. *J Phys Chem B*. 2018, Vol. 122, No. 32: 7821-7827.

71. Vallet S.D., Miele A.E., Uciechowska-Kaczmarzyk U., Liwo A., Duclos B., **Samsonov S.A.**, Ricard-Blum S. Insights into the structure and dynamics of lysyl oxidase propeptide, a flexible protein with numerous partners. *Sci Rep*. 2018. Vol. 8:11768.

72. Uciechowska-Kaczmarzyk U., Babik S., Zsila F., Bojarski K.K., Beke-Somfai T., **Samsonov S.A.** Molecular Dynamics-Based Model of VEGF-A and Its Heparin Interactions. *J Mol Graph Mod.* 2018.

Vol. 82, 157-166.

73. Zsila F., **Samsonov S.A.** Molecular interactions of the anticancer agent ellipticine with glycosaminoglycans by in silico analysis. *Carb Res*. 2018. 462:28–33.

74. Nordsieck K., Baumann L., Hintze V., Pisabarro M.T., Schnabelrauch M., Beck-Sickenger A.G., **Samsonov S.A.** The effect of interleukin-8 truncations on its interactions with glycosaminoglycans. *Biopolymers*. 2018. 109(10):e23103.

75. **Samsonov S.A.** Computational analysis of solvent inclusion in docking studies of protein-glycosaminoglycan systems. *Computational Drug Discovery and Design. Methods in Molecular Biology Series. Springer.* 2018. 1762: 445-454.

76. Babik S., **Samsonov S.A.**, Pisabarro M.T. Computational drill down on FGF1-heparin interactions through methodological evaluation. *Glycoconj J*, *Special Issue on Glycosaminoglycans*, 2017, Vol. 34, No. 3, 1-14.

77. Koehler L., **Samsonov S.A.**, Rother S., Vogel S., Köhling S., Moeller S., Schnabelrauch S., Rademann J., Hempel U., Pisabarro M.T., Scharnweber D., Hintze V. Sulfated Hyaluronan Derivatives Modulate TGF-β1:Receptor Complex Formation: Possible Consequences for TGF-β1 Signaling. *Scientific Reports*, 2017, Vol. 7, No. 1: 1210.

78. Rother S., **Samsonov S.A.**, Moeller S., Schnabelrauch M., Rademann J., Blaszkiewicz J., Köhling S., Waltenberger J., Pisabarro M.T., Scharnweber D., Hintze V. Sulfated Hyaluronan Alters Endothelial Cell Activation in Vitro by Controlling the Biological Activity of the Angiogenic Factors Vascular Endothelial Growth Factor-A and Tissue Inhibitor of Metalloproteinase-3. *ACS Appl Mater Interface*s, Vol. 9, No. 11, 2017, 9539-9550.

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87. Hofmann T., **Samsonov S.A.**, Pichert A., Lemmnitzer K., Schiller J., Huster D., Pisabarro M.T., von Bergen M., Kalkhof S. Structural analysis of the Interleukin-8/Glycosaminoglycan interactions by amide hydrogen/deuterium exchange mass spectrometry. *Methods*, 2015, Vol. 89, 45-55.

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myofibroblastdifferentiation. *Acta Biomaterialia*, 2013, Vol. 9, No. 8, 7775-7786.

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108. Vagt T., Jäckel C., **Samsonov S.**, Pisabarro M.T., Koksch B. Selection of a buried salt bridge by phage display. *Bioorg Med Chem Lett*, 2009, Vol. 19, No. 14, 3924-3927.

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110. **Samsonov S.A.**, Vasin A.V., Platonova N.A., Skvortsov A.N., Tsymbalenko N.V., Puchkova L.V. Tissue-specific *Ctr1* Gene Expression and *in silico* Analysis of Its Putative Protein Product // *AIP Conference Proceedings*, 2006, Vol. 851, 185-191.

111. **Samsonov S. A.**, Platonova N. A., Skvortsov A. N., Tsymbalenko N. V., Vasin A. V., Puchkova L. V. Relations between *CTR1* gene activity and copper status in different rat organs // *Molecular Biology (Moscow, Russia)*, 2006, Vol. 40, No. 2, 1-13.

112. Vasin A. V., Platonova N. A., Povalikhin R. G., Klotchenko S. A., **Samsonov S. A.**, Tsymbalenko N. V., Puchkova L. V. Mitochondrial ceruloplamin of mammals // *Mol Biol (Moscow, Russia)*, 2005 Vol. 39, No. 1, 42-52.

LIST OF ABSTRACTS AND PROCEEDINGS OF THE MEETINGS

Oral presentations

1. Computational approaches to understand protein-glycosaminoglycan recognition. Invited talk at HS-Seq, Berlin Symposium. Berlin, Germany. 14-15 December 2023.

2. The dynamic dance: exploring protein-carbohydrate recognition with molecular dynamics. Invited talk at the University of Leipzig, Germany. 8 December 2023.

3. Dynamic Dance of Sugars and Proteins: Unveiling the Secrets of Protein-Carbohydrate Complex Structures with Molecular Dynamics. Invited talk at the 8th Polish-Korean Conference on Protein Folding. 24-27.09.2023. Jastrzębia Góra, Poland.

4. Modeling glycosaminoglycan containing biologically relevant systems. Invited talk at the Chair for Theoretical Biophysics at Technical University of München, Germany, 3 April 2023.

5. Theoretical chemistry approaches to biologically relevant problems in the molecular systems containing glycosaminoglycans. Chemistry Towards Biology (CTB10). 11-14.09.2022. Bratislava, Slovakia.

6. Modeling Biologically Relevant Interactions of Glycosaminoglycans. Invited talk at Innogly Annual Meeting. 4-6.05.2022. Lugano, Switzerland.

7. Modeling protein-glycosaminoglycan interactions in biologically relevant systems. Invited talk at Intercollegiate Faculty of Biotechnology of University of Gdańsk/Medical University of Gdańsk. 8 April 2022.

8. Modeling molecular interactions of glycosaminoglycans. Invited talk at the Lab of Theory of Biopolymers, Faculty of Chemistry, Warsaw University. 19 January 2022.

9. Computational approaches to study glycosaminoglycan interactions. Invited talk at the University of Leipzig, Germany. 14 December 2021.

10. Recent advances in computational approaches to model biologically relevant interactions of glycosaminoglycans. Invited talk at the 6th Polish-Korean Conference on Protein Folding. 17-21.10.2021. Jastrzębia Góra, Poland.

11. Challenges and advances in molecular docking of glycosaminoglycans. Invited talk at Hybrid Symposium “GlycosAminoGlycans: What remains to be solved?”. 27-29.09.2021. Heraklion, Greece.

12. Modeling glycosaminoglycans in biologically relevant molecular systems. Online seminar at VCU edical Chemistry Department. Virginia Commonwealth University, USA, 24 September 2021.

13. Modeling molecular interactions of glycosaminoglycans. Invited talk at the Chair for Theoretical Biophysics at Technical University of München, Germany, 14 July 2021.

14. Computational insights into modeling protein-glycosaminoglycan interactions. Online Joint Warren and Beilstein Symposium on Glycosciences. 25 June 2021.

15. Glycosaminoglycan binding: specific or not? Invited talk at the Chair for Theoretical Biophysics at Technical University of München, Germany, 11 November 2019.

16. Modeling insights into glycosaminoglycan biologically relevant functions. Invited talk at the 5th Korean-Polish Conference on Protein Folding. 16-18.09.2019. Seoul, Korea.

17. Modeling insights into molecular mechanisms underlying the role of glycosaminoglycans in cell signaling processes. Oral presentation. EuroCarb XX, Leiden (the Netherlands). 4 July 2019.

18. Modeling glycosaminoglycans – key molecules for tissue regeneration. International Conference "Sakharov Readings 2019: enviromental problems of the XXI century" Minsk (Belarus). 23 May 2019.

19. Protein-ligand Interaction Energy-based Entropy Calculations: Fundamental Challenges For

Flexible Systems. Webinar for Institute of Physics (Polish Academy of Sciences) and Thai Nguyen University (Vietnam). Together with Gergely Kohut from Hyngarian Academy of Sciences. 29 March 2019.

20. Invited talk at the Institute of Physics of Kazimierz Wielki University, (in Polish), Bydgoszcz, Poland. 29 January 2019.

21. Computational approaches to study glycosaminoglycan mediation of biologically relevant protein-ligand interactions. Invited talk at the University of Reims, France. 7 December 2018.

22. Modeling of glycosaminoglycan-induced formation of protein structure and enhancement of biologically relevant protein-ligand interactions. Invited talk at Institute for Medical Physics and Biophysics, Leipzig University, Germany. 25 September 2018.

23. Computational insights into the glycosaminoglycan-mediated molecular mechanisms underlying cell signaling. Invited talk at the 4th Polish-Korean Conference on Protein Folding. 9-13.09.2018. Iława, Poland.

24. Modeling protein-glycosaminoglycan interactions. Invited talk at Research Institute of Influenza (in Russian), Saint-Petersburg, Russia. 16 July 2018.

25. Computational approaches to study interactions in protein-glycosaminoglycan molecular systems. Invited talk at Institute for Molecular and Supramolecular Chemistry and Biochemistry, University of Lyon, France. 15 October 2017.

26. Computational analysis of protein-GAG interactions. Invited talk at Department of Biochemistry, University of Tours, France. 5 October 2017.

27. Interactions in protein-glycosaminoglycan systems: computational approaches. Invited talk at Institute of Materials and Environmental Chemistry, Hungarian Academy of Science, Budapest, Hungary. 22 September 2017.

28. Evaluation of computational approaches for the analysis of FGF1-heparin interactions. 5th Beilstein Symposium on Glyco-Bioinformatics: 'Discovering the Subtleties of Sugars', 13-15 June 2017, Berlin, Germany. p. 23.

29. Molecular docking in protein-glycosaminoglycan systems. Invited talk at Institute for Medical Physics and Biophysics, Leipzig University, Germany, 10 March 2017.

30. Computational approaches to study protein-glycosaminoglycan interactions. Invited Talk at Department of Chemistry, University of Gdańsk, Poland, 9 December 2016.

31. Combining computational and experimental approaches to characterize IL-8/glycosaminoglycan interactions. Invited Talk at Department of Theoretical Chemistry, University of Lund, Sweden, 3 October 2016.

32. Computational approaches to study protein-glycosaminoglycan interactions. Talk at Leibniz Institute for Polymer Research, Dresden, 8 September 2016.

33. Combining computational and experimental approaches to characterize IL-8/glycosaminoglycan interactions. Invited talk at the Chair for Theoretical Biophysics at Technical University of München, Germany, 18 July 2016.

34. Computational approaches to study protein-glycosaminoglycan interactions. JungChemikerForum, Chemistry Department, TU Dresden, 14 January 2016.

35. Computational insights into protein-GAG interactions: BMP-2 system. Transregio 67 Afternoon. CRTD Dresden, 26 October 2015.

36. IL-8 interactions with glycosaminoglycans: merging computational and experimental approaches.

Invited talk at the Chair of Biophysics, Pavol Jozef Šafárik University in Košice, Slovakia, 2 October 2015.

37. Elucidation of molecular mechanisms behind the interaction of sulfated hyaluronan with TGF-β1 by *in silico* and experimental approaches. 4th Beilstein Symposium on Glyco-Bioinformatics: 'Discovering the Subtleties of Sugars', 22-25 June 2015, Potsdam, Germany. p. 18.

38. IL-8 interactions with glycosaminoglycans: merging computational and experimental approaches. Postdoc Seminar, CRTD Dresden, 17 April 2015.

39. Computational analysis of the interactions of sulfated glycosaminglycans and bone morphogenetic protein-2 (BMP-2). 13th Bratislava Symposium on Saccharides „Recent Advances in Glycomics". Smolenice Castle, Slovakia, 22-26 June 2014. p. 61.

40. Dynamic Molecular Docking (DMD): a new approach to treat flexibility and explicit solvent in docking of protein-glycosaminoglycan systems. From Computational Biophysics to Systems Biology. Gdańsk (Poland), 25-27 May 2014.

41. Interleukin-8 interactions with glycosaminoglycans: merging computational and experimental approaches. 17th European Carbohydrate Symposium. Tel Aviv (Israel), 7-12 July 2013.

42. Computational analysis of Interleukin-8 interactions with hyaluronan and chondroitin-sulfate derivatives. Conformational Analysis of Carbohydrates & Protein/Carbohydrate Interactions (CAC-PCI, Naples (Italy), 2nd July 2011). Abstracts, p48. 16th European Carbohydrate Symposium. Sorrento (Italy), 3-7 July 2011.

43. Theoretical analysis of fluorinated amino acids in protein enviroments. International workshop in memoriam of Angel Ramirez Ortiz "Structural Bioinformatics and Beyond", 26-28 January 2009, Madrid, Spain. Book of abstracts, p. 29.

44. High performance computing in molecular dynamics approaches for studying protein-protein interactions. High-performance Computing Workshop. Dresden (Germany), 6-7 December 2010.

45. Organ-specific mammalian *Ctr1* gene expression and *in silico* analysis of its putative protein product // FEBS Young Scientists Forum (Istanbul, Turkey). Abstracts. 2006. p.18.

46. Organ-specific rat *CTR1* expression and its relations to copper status in ontogenesis // Biology-Science of XXI Century, the 9th International Pushchino School-Conference of Young Scientists. Abstracts. Pushchino, Russia. 2006. p. 45.

47. Rat *CTR1* gene expression and *in silico* analysis of its putative protein product // Scientists of the Future. International Scientific-Practical Conference of Young Scientists. Abstracts. State Medical University, Odessa, Ukraine. 2005. p.55-56.

48. Computer analysis of structural and functional domains in putative Ctr1 gene protein product // 33rd Scientific Week at the State Polytechnical University. Abstracts. Part IV. Saint-Petersburg, Russia. 2005. p.156-157.

Poster presentations (~30)

PARTICIPATION IN SCIENTIFIC SCHOOLS/WORKSHOPS

– Workshop Series (Self Effectiveness, Working with Others, Management, Intellectual Property, Communication: 10 days/80 hours in total) for POLONEZ Fellows by VITAE - The Career Development Organisation (*www.vitae.ac.uk*) within Horizon 2020 Programme, **2018-2019 ,** Warsaw (Poland):

– SCIGRESS Workshop, 8.11, **2017**, Gdańsk (Poland).

– Gaussian Workshop, 11-15.07, **2011**, Santiago de Compostella (Spain).

– MOE Applications training and basic SVL training at European User Group Meeting, 29.09-2.10, **2009**, Basel (Switzerland).

– Modeling of Biomolecular Systems Summer School, 30.05-1.06, 2005, Helsinki (Finland).

– Center for International Mobility (CIMO) Scientific Winter School in Bioinformatics. 17-23.01, **2005**, Tvärminne (Finland).

OTHER RESEARCH-RELATED ACTIVITIES:

– Research Grant review for The National Fund for Scientific and Technological Development (Chile) in 2018; ERC Advanced Grant in 2021; The Agence Nationale de la Recherche Grant in 2021; Swiss National Science Foundation in 2023.

– Regular peer-reviews (~20 papers per year) for journals including Glycobiology, BMC Bioinformatics, Journal of Physical Chemistry B, Journal of Bioorganic Chemistry, Journal of Chemical Information and Modeling, Journal of Computational Biology and Chemistry, Journal of Computer-Aided Molecular Design, Acta Biomaterialia, Computational and Structural Biotechnology Journal, Frontiers and MDPI Journals.

SUPERVISION

– 3 Postdoctoral Researchers (2 at the moment)

– 4 PhD students (1 at the moment, 3 successfully defended)

– 6 Undergraduate Students (2 at the moment, 4 successfully defended or submitted reports)

TEACHING EXPERIENCE

2016 (one summer term) Lectures and seminars in the course 'Introduction to Molecular Cellular Biology' in the International Master's Programme of Nanobiophysics at BIOTEC TU Dresden. 28 lectures, audience ~20 students.

2011-2017 (every winter term) Lectures and seminars in the course 'Computational and Structural Biology' in the International Master's Programmes Molecular Bioengineering and Nanobiophysics at BIOTEC TU Dresden. 9 lectures, audience ~60 students.

2009-2016 Giving practicals for PhD students at Dresden International PhD Programme.

2009-2016 Giving lectures in the PhD course of 'Bioanalysis' within TR67 'Functional Biomaterials for Controlling Healing Processes in Bone and Skin - From Material Science to Clinical Application'.

2007-2009 Giving several open lectures on 'Computational approaches to study protein-protein interactions' at the Department of Biophysics at State Polytechnical University of Saint-Petersburg.

COLLABORATIONS

– Adam Liwo, University of Gdańsk, Poland
– Dariusz Wyrzykowski, University of Gdańsk, Poland
– Daniel Huster, University of Leipzig, Germany
– Martin Zacharias, Technical University of Munich, Germany
– Sylvie Ricard-Blum, Claude Bernard University Lyon 1, France
– Fabien Lecaille, François Rabelais University, Tours, France

– Bertrand Huard, University of Grenoble Alps, France
– Tamás Beke-Somfai and Ferenc Zsila, Hungarian Academy of Sciences, Budapest, Hungary
– Finn Lillelund Aachmann and Marit Sletmoen, University of Trondheim, Norway
– Satoru Tsushima, University of Tokyo, Japan/Helmholtz-Zentrum Dresden-Rossendorf, Germany
– Ludmila Puchkova, Peter the Great St. Petersburg Polytechnic University, Russia
– Aliaksei Sysa, Belarusian State University, Minsk, Belarus
– Valdecir Farias Ximenes, University of the State of Sao Paulo, Brasil
– Dragana Nikitovic, University of Crete, Greece
– Gerardus Boons, University of Georgia Athens, USA

LANGUAGES

– Russian, native
– English, fluent
– Polish, fluent
– German, fluent
– Norwegian (bokmål), fluent
– Italian, B1/B2 level
– French, B1 level
– Finnish, A2 level

HOBBIES

Cross-country skiing, running, football, reading, learning languages, traveling