Curriculum Vitae of Prof. dr. hab. Sergey A. Samsonov

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PERSONAL INFORMATION

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

RESEARCH EXPERIENCE AND ACADEMIC DEGREES

2024 The academic title of Professor was granted by the President of the Republic of Poland
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 computational 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

– **2024:** SMART LOIRE VALLEY (SLV) Programme LE STUDIUM VISITING RESEARCHER Award at the Laboratory of The Research Center for Respiratory Diseases, Team 2: Proteolytic Mechanisms in Inflammation (Host: Prof. Lecaille), University of Tours, project "**C**omputational **A**pproache**s** for ca**t**heps**in**-**g**lycosaminoglycan systems (CASTING)". July-October 2024.
– **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

– 2024: University of Gdańsk Rector Individual Award for the scientific achievement in the year 2023.
– 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

– Research Center for Future Medicine at Samsung Medical Center: Advisory Board Member
– 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: **31** (SCOPUS, 24.03.2025)

1. Kapica M., Grabowska O., Dębowski D., Marszałek M., Tesmar A., Kamysz E., Wyrzykowski D., **Samsonov S.A.** Physicochemical Insights into the Interaction of Cationic Peptides (KR12 and TAT47-57) with Decavanadate: An Integrated ITC and Molecular Dynamics Study. *PCCP*. 2026. In press.

2. Grzywacz D., Nutti F., Żamojć K., **Samsonov S.A.**, Malinowska M., Paduszyńska M., Papini A.M., Makowska J. Influence of N- and O-glycosylation on metal binding and structural properties of a C-terminal LL-37 fragment. *Carbohydr Res*. 2026. Vol. 563, 109872.

3. Le Fournis C., Maszota-Zeleniak M., Kulesza A., Chopra P., Boons G.-J., Aubrey N., Liesecke F., **Samsonov S.A.**, Weber G. Structural determinants of glycosaminoglycan oligosaccharides as LL-37-inhibitors in breast cancer. *Glycobiology*. 2026. Vol. 36, cwag010.

4. Kapica M., Grabowska O., Kamysz E., Kamysz J., **Samsonov S.A.**, Wyrzykowski D. Cyclodextrin and KR12-Lipopeptide Interactions: A Thermodynamic View of Binding Mechanisms and Impact on the Structure of α-Helical Peptides. *J Phys Chem B*. 2026. Vol. 130, 1167–1174.

5. Clark J., Zykwinska A., Colliec-Jouault S., **Samsonov S.A.** Modeling highly sulfated Infernan. *Carbohydr Res*. 2025. Vol. 558, 109759.

6. Tsushima S., Seal A., Samsonov S.A., Fahmy K., Takao K. Macrocyclic and Hydroxamate Ligands for ^{225}Ac Radiopharmaceuticals: Evaluating SSTR2-Targeting Potential. *Inorganic Chemistry*. 2025. https://doi.org/10.1021/acs.inorgchem.5c04349

7. Pavan N., Grabowska O., Wyrzykowski D. **Samsonov S.A.** Heparin Inclusion in Cyclodextrins: A Combined MD and ITC Study. *TASK Quaterly*. 2024. Vol. 28.

8. David A., Domain R., Surback F., Vibert A., Buisson P., Maszota-Zieleniak M., Landemarre L., Schuler M., Lalmanach G., **Samsonov S.A.**, Lopin-Bon C., Lecaille F. Deciphering minimal size of chondroitin 4-sulfate oligomers to develop innovative inhibitors of cathepsin S. *Polysaccharides*. 2025. Vol. 6, 99.

9. **Samsonov S.A.**, Frączyk T., Ufnalska I., Bal W. Molecular dynamics study of the impact of glycosylation on conformational properties of trimeric N-terminal domain of human copper transporter 1. *Carbohydr Res*. 2025. Vol. 558, 109708.

10. **Samsonov S.A.**, Ricard-Blum S. Molecular Dynamics Insights into Glycosaminoglycan Effects on the Extracellular Domains of Syndecan 2 and 4 Dimers. *Carbohydr Res*. 2025. Vol. 558, 109690.

11. Clark J.A., **Samsonov S.A.**, Clark J. Modeling and simulation of protein-carbohydrate interaction. *Comprehensive Biophysics*, 2nd Ed. Editor: Zacharias. Elsevier. 2025.

12. Grabowska O., Żamojć K., Kloska A., Niedziałkowski P., **Samsonov S.A.**, Wyrzykowski D. An interdisciplinary study of lysozyme interactions with hexacyanoferrate(III)/(II) ions. *International Journal of Molecular Sciences*. 2025. Vol. 26, 8511.

13. David A., Rigoux B., Maszota-Zieleniak M., Sinquin C., Neau C., Zykwinksa A., Saidi A.,

Lalmanach G., **Samsonov S.A.**, Colliec-Jouault S., Lecaille F. Selective inhibition of cathepsin S elastolytic activity by exopolysaccharides from deep-sea hydrothermalbacteria. *Carbohydrate Polymers*. 2025. Vol. 367, 123968.

14. Babuty A., Zykwinska A., **Samsonov S.A.**, Candia N., Veinstein C., Pugniere M., Ngo T. H. G., Sinquin C., Munoz-Garcia J., Colliec-Jouault S., Heymann D. Anticoagulant Potential of Modified Sulfated Exopolysaccharides from Deep-Sea Bacteria: Toward Non-Animal Heparin Alternatives. *Polysaccharides*. 2025. Vol. 6, 54.

15. Grabowska O., Kogut-Günthel M., **Samsonov S.A.**, Wyrzykowski D., Makowska J. β-CD saves lysozyme from the clutches of 1-alkylsulfonates. *Journal of Molecular Liquids*. 2025. Vol. 428. 127543.

16. Kapica M., Kamysz E., Grabowska O., Tesmar A., Pająk M., Chmur K., Brzeski J., **Samsonov S.A.**, Wyrzykowski D. Interactions of Laurylated and Myristoylated KR12 Fragment of the LL37 peptide with Polyoxidovanadates. *Molecules*. 2025. Vol. 30. 1589.

17. **Samsonov S.A.**, Marcisz M. Decrypting Glycosaminoglycan "sulfation code" with Computational Approaches. *Handbook of Experimental Pharmacology - Complex Carbohydrates*. Editors: Tauber, Pfengle, Pagel. Springer. 2025. 1-23.

18. Pągielska M., **Samsonov S.A.** The Amazing World of Glycosaminoglycans through the Eyes of a Theoretician. *Glycoforum*. 2024. Vol. 27, A25 (in English and Japanese).

19. Danielsson A., **Samsonov S.A.**, Sieradzan A.K. Implementation of the UNRES/SUGRES-1P Coarse-Grained Model of Heparin for Simulating Protein/Heparin Interactions. *J Chem Theor Comp*. 2024. Vol: 20: 10703-10715.

20. Uciechowska-Kaczmarzyk U., Frank M., **Samsonov S.A.**, Maszota-Zieleniak M. Structural insights into the endostatin-heparan sulfate interactions by modeling approaches. *Molecules*. 2024. Vol. 29: 4040.

21. Mańkowska M., Krzymiński K., Wyrzykowski D., Zadykowicz B., **Samsonov S.A.** Why do ionic surfactants significantly alter the chemiluminogenic properties of acridinium salt? *Molecules*. 2024. Vol. 29: 3736.

22. Santini B.L., Gaardløs M., Wyrzykowski D., Rothemund S., Penk A., Zacharias M., **Samsonov S.A.** Rational Design of Glycosaminoglycan Binding Cyclic Peptides using cPEPmatch. *Computational and Structural Biotechnology Journal*. 2024. Vol. 23: 2985–2994.

23. Bojarski K.K., David A., Lecaille F., **Samsonov S.A.** *In silico* approaches for better understanding cysteine cathepsin-glycosaminoglycan interactions. *Carbohydrate Research*. 2024. Vol. 543: 109201.

24. Bertozo L., Tadeu H.S., Sebastian A., Maszota-Zieleniak M., **Samsonov S.A.**, Ximenes V. A Role for Carboxylic Acid Moiety in NSAIDs: Favoring the Binding at Site II of Bovine Serum Albumin. *Molecular Pharmaceutics*. 2024. Vol. 21: 2501–2511.

25. Grabowska O., **Samsonov S.A.**, Kogut-Günthel M., Żamojć K., Wyrzykowski D. Elucidation of binding mechanisms of bovine serum albumin and 1-alkylsulfonates with different hydrophobic chain lengths. *International Journal of Biological Macromolecules*. 2024. Vol. 266: 131134.

26. Anila S., **Samsonov S.A.** Benchmarking Water Models in Molecular Dynamics of Protein-Glycosaminoglycan Complexes. *J Chem Inf Mod.* 2024. Vol. 64: 1691–1703.

27. 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.

28. 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.

29. 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.

30. 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.

31. 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.

32. 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.

33. 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.

34. 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.

35. 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.

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

37. 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.

38. 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.

39. 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.

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

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

42. 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.

43. 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.

44. 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.

45. 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.

46. 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.

47. 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.

48. 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.

49. 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.

50. 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.

51. 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.

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

53. 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.

54. 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.

55. 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.

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

57. 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.

58. 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.

59. 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.

60. 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.

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

62. 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.

63. 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.

64. 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.

65. 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.

66. 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.

67. 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.

68. 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.

69. **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.

70. 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.

71. 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.

72. 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.

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

74. 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.

75. 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.

76. 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.

77. 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.

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PRESENTATIONS

Oral presentations and invitated talks (~50)

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, A1 level
– Korean, Beginner

HOBBIES

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