Curriculum Vitae of 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

2019- Principal Investigator at the Laboratory of Molecular Modeling, Department of Theoretical Chemistry, Faculty of Chemistry, University of Gdańsk.

2018 Title of dr. habil. at the University of Tours. *Cum laude*.

2017-2019 Principal Investigator at the Laboratory of Molecular Modeling, Department of Theoretical Chemistry, Faculty of Chemistry, University of Gdańsk in Polonez Grant Project: *'Computational approaches to study protein-glycosaminoglycan interactions'.*

2016-2017 Postdoctoral researcher at BIOTEC TU Dresden in Structural Bioinformatics group led by Dr. M. Teresa Pisabarro, topic 'Protein-DNA interactions in target-specific recombination'.

2009-2016 Postdoctoral researcher at BIOTEC TU Dresden in Structural Bioinformatics group led by Dr. M. Teresa Pisabarro in German Research Council Project TRR67 'Molecular Modeling and Simulation of Glycosaminoglycans-Protein Interactions'.

2006-2010 PhD in Biophysics and Biochemistry, Saint-Petersburg State University, Russia, supervised by Prof. L. Puchkova. PhD Thesis: 'Expression of mammalian CTR1 in different type of copper metabolism and in silico analysis of its protein product'.

2006-2009 PhD in Structural Bioinformatics at BIOTEC TU Dresden, Germany, supervised by Dr. Maria Teresa Pisabarro. PhD Thesis 'Protein-protein interactions: impact of solvent and effects of fluorination'. *Summa cum laude.*

2006 Master Degree (*with honors*) in Biophysics, Department of Biophysics, Faculty of Physics and Mechanics, State Polytechnical University of Saint-Petersburg, Russia. Master Thesis: 'Mammalian CTR1 gene expression and *in silico* analysis of its product'.

2004 Bachelor Degree (*with honors*) in Physics, Department of Biophysics, Faculty of Physics and Mechanics, State Polytechnical University of Saint-Petersburg, Russia. Bachelor's Thesis: 'Structural analysis of putative gene Ctr1 protein product and study of its expression in mammals'.

1990-2000 High school, Saint-Petersburg, Russia

RESEARCH INTERESTS

Protein-glycosaminoglycans interactions, glycosaminoglycans conformational analysis, protein-DNA interactions, solvent in protein interfaces, non-natural amino acids, molecular dynamics, molecular docking, QM, ONIOM, QM/MM, force field parameters development, coarse-grained modeling.

COMPUTER PROGRAMS/SKILLS

– AMBER, GAUSSIAN03/09, R.E.D. III, GAMESS, Autodock, eHiTs, Glide, FlexX, GRID, Discovery Studio, MOE, VMD, Chimera UCSF, Cambridge Structural Database, ProHit, R statistical package, bash/awk/sed scripting, Python, Gnuplot, high performance computing.

GRANTS AND AWARDS

– **2020**: University of Gdańsk Rector Award for the scientific achievement of the Lab in the year 2019.

– **2019**: BEETHOVEN CLASSIC 3 Grant from National Science Center (Poland). It is a joint grant with the Prof. Huster group (University of Leipzig) supported by the German Research Council from the German side. Project: '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). Project: '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. Project: 'Modeling of interactions between glycosaminoglycans and the anticancer agent ellipticine'. 860 Euro.

– **2017**: German Research Council Grant for Temporary Positions for Principal Investigators. Project: 'Computational approaches for analyzing protein-glycosaminoglycan interactions'. 264 950 Euro. Duration: 3 years.

– **2016**: POLONEZ 2 Grant from National Science Center (Poland). Project: '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.

– **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 (from 2017)
– Expert member of NAWA (Polish National Agency for Academic Exchange)
– Marie Curie Alumni Association

LIST OF PUBLICATIONS IN PEER-REVIEWED JOURNALS

*Corresponding author; +Co-first co-author

1. Kogut M.M., Marcisz M., **Samsonov S.A.** Modeling glycosaminoglycan-protein complexes. *Current Opinion in Structural Biology*. 2022. In press.

2. 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.
doi: 10.3390/molecules26216565.

3. 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.

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

5. 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.

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

7. 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.

8. 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.

9. 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.

10. 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.

11. 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. doi: 10.1515/hsz-2021-0119

12. 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 binding and processivity of mannuronan C-5 epimerase AlgE4. *Glycobiology*. 2021. doi: 10.1093/glycob/cwab025/

13. 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. doi: 10.1093/glycob/cwab016

14. **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.

15. 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.

16. 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.

17. 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.

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

19. 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.

20. 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. doi: 10.1016/j.carbpol.2020.117261

21. 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.

22. 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.

23. 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.

24. 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.

25. 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. doi: 10.1002/prot.25860.

26. 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.

27. 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.

28. Lensink M.F., Brysbaert G., Nadzirin N., Velankar S., Chaleil R.A.G., Gerguri T., Bates P.A., Laine E., Carbone A., Grudinin S., Kong R., Liu R.R., Xu X.M., Shi H., Chang S., Eisenstein M., Karczynska A., Czaplewski C., Lubecka E., Lipska A., Krupa P., Mozolewska M., Golon Ł., **Samsonov S.**, Liwo A., Crivelli S., Pagès G., Karasikov M., Kadukova M., Yan Y., Huang S.Y., Rosell M., Rodríguez-Lumbreras L.A., Romero-Durana M., Díaz-Bueno L., Fernandez-Recio J., Christoffer C., Terashi G., Shin W.H., Aderinwale T., Maddhuri Venkata Subraman S.R., Kihara D., Kozakov D., Vajda S., Porter K., Padhorny D., Desta I., Beglov D., Ignatov M., Kotelnikov S., Moal I.H., Ritchie D.W., Chauvot de Beauchêne I., Maigret B., Devignes M.D., Ruiz Echartea M.E., Barradas-Bautista D., Cao Z., Cavallo L., Oliva R., Cao Y., Shen Y., Baek M., Park T., Woo H., Seok C., Braitbard M., Bitton L., Scheidman-Duhovny D., Dapkūnas J., Olechnovič K., Venclovas Č., Kundrotas P.J., Belkin S., Chakravarty D., Badal V.D., Vakser I.A., Vreven T., Vangaveti S., Borrman T., Weng Z., Guest J.D., Gowthaman R., Pierce B.G., Xu X., Duan R., Qiu L., Hou J., Ryan Merideth B., Ma Z., Cheng J., Zou X., Koukos P.I., Roel-Touris J., Ambrosetti F., Geng C., Schaarschmidt J., Trellet M.E., Melquiond A.S.J., Xue L., Jiménez-García B., van Noort C.W., Honorato R.V., Bonvin A.M.J.J., Wodak S.J. Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins*. 2019, Vol. 87:1200-1221.

29. 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.

30. 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.

31. 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.

32. 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.

33. 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.

34. **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.

35. 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.

36. 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.

37. 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.

38. **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.

39. **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.

40. 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.

41. 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.

42. 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.

43. 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.

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

45. 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.

46. **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.

47. 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.

48. 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.

49. 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.

50. Anders G., Hasseipen U., Theisgen S., Heymann S., Muller L., Panigada T., Huster D., **Samsonov S.A.**[*] The Intrinsic Pepsin Resistance of Interleukin-8 Can be Explained from a Combined Bioinformatical and Experimental Approach. *IEEE/ACM Trans Comp Biol Bioinf*. 2016. Vol. 15, No. 1, 300–308.

51. Rother S., **Samsonov S.A.**, Hempel U., Vogel S., Moeller S., Blaszkiewicz J., Köhling S.,

Schnabelrauch M., Rademann J., Pisabarro M.T., Hintze V., Scharnweber D. Sulfated hyaluronan alters the interaction profile of TIMP-3 with the endocytic receptor LRP-1 cluster II and IV and increases the extracellular TIMP-3 level of human bone marrow stromal cells. *Biomacromolecules*. Vol. 17, No. 10, 2016, 3252-3261.

52. Rother S., **Samsonov S.A.**, Hofmann T., Blaszkiewicz J., Köhling S., Schnabelrauch M., Möller S., Rademann J., Kalkhof S., von Bergen M., Pisabarro M.T., Scharnweber D., Hintze V. Structural and functional insights into the interaction of sulfated glycosaminoglycans with tissue inhibitor of metalloproteinase-3 - a possible regulatory role on extracellular matrix homeostasis. *Acta Biomaterialia*. 2016, Vol 45, 143-154.

53. Panitz N., Theisgen S., **Samsonov S.A.**, Gehrcke J.-P., Baumann L., Pisabarro M.T., Bellmann-Sickert K., Rademann J., Huster D., Beck-Sickinger A. The Structural Investigation of Glycosaminoglycan Binding to CXCL12 Displays Distinct Interaction Sites. *Glycobiology,* 2016, Vol. 26, No. 11, 1209-1221.

54. **Samsonov S.A.**[*], Pisabarro M.T[*]. Computational analysis of interactions in structurally available protein-glycosaminoglycan complexes. *Glycobiology* 2016, Vol. 26, No. 8, 850-861.

55. Scharnweber D., Hübner L., Rother S., Hempel U., Anderegg U., **Samsonov S.A.**, Pisabarro M.T., Hofbauer L., Schnabelrauch M., Franz S., Simon J., Hintze V. Glycosaminoglycan derivatives - promising candidates for the design of functional biomaterials. *JMSM*, 2015, Vol. 26, No. 9, 232.

56. Salbach-Hirsch J., **Samsonov S.A.**, Hintze V., Hofbauer C., Picke A.-K., Rauner M., Gehrcke J.-P., Moeller S., Schnabelrauch M., Scharnweber D., Pisabarro M.T., Hofbauer L.C. Structural and functional insights into sclerostin-glycosaminoglycan interactions in bone. *Biomaterials*, 2015, Vol. 67, 335-345.

57. Andrault P.-M., **Samsonov S.A.**, Weber G., Coquet L., Nazmi K., Bolscher J., Lalmanach A.-C., Jouenne T., Bromme D., Pisabarro M.T., Lalmanach G., Lecaille F. The antimicrobial peptide LL-37 is both a substrate of cathepsins S and K and a selective inhibitor of cathepsin L. *Biochemistry*, 2015, Vol. 54 No. 17, 2785-2798.

58. 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.

59. Abi-Ghanem J., **Samsonov S.A.**, Pisabarro M.T. Insights into the preferential order of strand exchange in the Cre/loxP recombinase system: impact of the DNA spacer flanking sequence and flexibility. *J Comput Aided Mol Des*, 2015, Vol. 29 No. 3, 271-282.

60. **Samsonov S.**[*], Bichmann L., Pisabarro M.T. Coarse-grained model of glycosaminglycans. *J Chem Inf Mod*, 2015, Vol. 55 No. 2, 114-124.

61. Hintze V.[+], **Samsonov S.**[+], Anselmi M., Moeller S., Becher J., Schnabelrauch M., Scharnweber D., Pisabarro M.T. Sulfated glycosaminoglycans exploit the conformational plasticity of bone morphogenetic protein-2 (BMP-2) and alter the interaction profile with its receptor. *Biomacromolecules*, 2014, Vol. 15, No. 8, 3083-3092.

62. **Samsonov S.**[+], Gehrcke J.-P.[+], Pisabarro M.T. Flexibility and explicit solvent in molecular dynamics-based docking of protein-glycosaminoglycan systems. *J Chem Inf Mod*, 2014, Vol. 54 No. 2, 582-592.

63. **Samsonov S.A.**[*,+], Theisgen S.[+]**,** Riemer T., Huster D., Pisabarro M.T. Glycosaminoglycan monosaccharide blocks analysis by quantum mechanics, molecular dynamics and nuclear magnetic resonance. *BioMed Res Int, Special Issue "Glycosaminoglycans and Derivatives for the Regulation of Healing Processes: From Synthesis to Biomaterial Application"*, 2014:808071.

64. Atkovska K., **Samsonov S.A.**[*,+], Paszkowski-Rogacz M., Pisabarro M.T[*]. Multipose binding in molecular docking. *Int J Mol Sci, Special Issue "Proteins and Protein-Ligand Interactions"*, 2014, Vol. 15, No. 2, 2622-2645.

65. **Samsonov S.A.**[*], Pisabarro M.T.[*] Importance of IdoA and IdoA(2S) ring conformations in computational studies of glycosaminoglycan-protein interactions. *Carb Res*, No. 381, 2013. p. 133–137.

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Formation of a Heterodimeric Coiled Coil. *Chem Eur J,* 2009, Vol. 15, No. 31, 7628-7636.

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79. 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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81. **Sergey A. Samsonov**, Andrey V. Vasin, Natalia A. Platonova, Alexey N. Skvortsov, Nadezhda V. Tsymbalenko, Ludmila V. Puchkova. Tissue-specific *Ctr1* Gene Expression and *in silico* Analysis of Its Putative Protein Product // *AIP Conference Proceedings (peer-reviewed)*, 2006, Vol. 851, 185-191.

82. **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.

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LIST OF ABSTRACTS AND PROCEEDINGS OF THE MEETINGS

Oral presentations

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

2. 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.

3. 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.

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

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

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

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

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

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

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

11. 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.

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

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

14. 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.

15. 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.

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

17. 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.

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

19. 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.

20. 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.

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

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

23. 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.

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

25. 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.

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

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

28. 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.

29. 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.

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

31. 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.

32. 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.

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

34. 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.

35. 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.

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

37. 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.

38. 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.

39. 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.

40. 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.

– Regular peer-reviews (~15 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.

STUDENTS SUPERVISION

2014-2015 (15 months) Supervision of the Erasmus Student Project 'Molecular docking and MD study of FGF heparin interactions' of Sándor Babik with the continuation of the supervision of his Master Thesis (together with Budapest Pázmány Péter Catholic University)

2014-2015 (6 months) Supervision of the Lab Rotation Project 'Exploring conformational space of GAGs using computational methods' of Leon Bichmann

2014 (6 months) Supervision of the Master Thesis 'Computational analysis of glycosaminoglycan-specific glycosidases' of Josue Manik Nava Sedeno (Grade 1.3, good)

2012 (6 months) Supervision of the Master Thesis 'Computational study for characterization of multipose binding' of Kalina Atkovska (Grade 1.0, excellent)

TEACHING EXPERIENCE

2016 (one summer term) Lectures and seminars in the course 'Introduction to Molecular Cellular Biology' in the International Master Program 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 Programs Molecular Bioengineering and Nanobiophysics at BIOTEC TU Dresden. 9 lectures, audience ~60 students.

Since 2009 Giving practicals for PhD students at Dresden International PhD Programme.

Since 2009 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
– 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

LANGUAGES

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

HOBBIES

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