# Sergey A Samsonov

List of Publications by Year
in descending order



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|---|---|---|---|
| 79 papers | 1,736 citations | 236612 25 h-index | 329751 37 g-index |
| 79 all docs | 79 docs citations | 79 times ranked | 1557 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Physics-Based Coarse-Grained Modeling in Bio- and Nanochemistry. , 2022, , 31-69. | | 1 |
| 2 | Modulation of the expression and activity of cathepsin S in reconstructed human skin by neohesperidin dihydrochalcone. Matrix Biology, 2022, 107, 97-112. | 1.5 | 2 |
| 3 | Modeling glycosaminoglycanâ€“protein complexes. Current Opinion in Structural Biology, 2022, 73, 102332. | 2.6 | 16 |
| 4 | Biglycan Interacts with Type I Insulin-like Receptor (IGF-IR) Signaling Pathway to Regulate Osteosarcoma Cell Growth and Response to Chemotherapy. Cancers, 2022, 14, 1196. | 1.7 | 7 |
| 5 | In silico and in vitro mapping of specificity patterns of glycosaminoglycans towards cysteine cathepsins B, L, K, S and V. Journal of Molecular Graphics and Modelling, 2022, 113, 108153. | 1.3 | 8 |
| 6 | Molecular Dynamics Approaches Dissect Molecular Mechanisms Underlying Methylene Blueâ€“Glycosaminoglycan Interactions. Molecules, 2022, 27, 2654. | 1.7 | 2 |
| 7 | Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins. Journal of Molecular Modeling, 2022, 28, . | 0.8 | 3 |
| 8 | Molecular dynamics-based descriptors of 3-O-Sulfated Heparan sulfate as contributors of protein binding specificity. Computational Biology and Chemistry, 2022, 99, 107716. | 1.1 | 3 |
| 9 | Binding of heparan sulfate to human cystatin C modulates inhibition of cathepsin L: Putative consequences in mucopolysaccharidosis. Carbohydrate Polymers, 2022, 293, 119734. | 5.1 | 3 |
| 10 | Explicit solvent repulsive scaling replica exchange molecular dynamics (<scp>RSâ€REMD</scp>) in molecular modeling of proteinâ€glycosaminoglycan complexes. Journal of Computational Chemistry, 2022, 43, 1633-1640. | 1.5 | 6 |
| 11 | Impact of calcium ions on the structural and dynamic properties of heparin oligosaccharides by computational analysis. Computational Biology and Chemistry, 2022, 99, 107727. | 1.1 | 1 |
| 12 | The abnormal accumulation of heparan sulfate in patients with mucopolysaccharidosis prevents the elastolytic activity of cathepsin V. Carbohydrate Polymers, 2021, 253, 117261. | 5.1 | 13 |
| 13 | Computational insights into the role of calcium ions in proteinâ€“glycosaminoglycan systems. Physical Chemistry Chemical Physics, 2021, 23, 3519-3530. | 1.3 | 13 |
| 14 | Evaluation of replica exchange with repulsive scaling approach for docking glycosaminoglycans. Journal of Computational Chemistry, 2021, 42, 1040-1053. | 1.5 | 8 |
| 15 | Further analyses of APRIL/APRIL-receptor/glycosaminoglycan interactions by biochemical assays linked to computational studies. Glycobiology, 2021, 31, 772-786. | 1.3 | 9 |
| 16 | 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. | 1.3 | 6 |
| 17 | Investigation of the structure of regulatory proteins interacting with glycosaminoglycans by combining NMR spectroscopy and molecular modelingÂâ€“ the beginning of a wonderful friendship. Biological Chemistry, 2021, 402, 1337-1355. | 1.2 | 16 |
| 18 | Acute phase Î±1-acid glycoprotein as a siderophore-capturing component of the human plasma: A molecular modeling study. Journal of Molecular Graphics and Modelling, 2021, 105, 107861. | 1.3 | 3 |

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|---|---|---|---|
| 19 | The potential role of glycosaminoglycans in serum amyloid A fibril formation by in silico approaches. Matrix Biology Plus, 2021, 12, 100080. | 1.9 | 2 |
| 20 | Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. Biomolecules, 2021, 11, 1347. | 1.8 | 29 |
| 21 | Computational insights into heparin-small molecule interactions: Evaluation of the balance between stacking and non-stacking binding modes. Carbohydrate Research, 2021, 507, 108390. | 1.1 | 5 |
| 22 | Modeling Proteinâ€“Glycosaminoglycan Complexes: Does the Size Matter?. Journal of Chemical Information and Modeling, 2021, 61, 4475-4485. | 2.5 | 14 |
| 23 | Advanced Molecular Dynamics Approaches to Model a Tertiary Complex APRIL/TACI with Long Glycosaminoglycans. Biomolecules, 2021, 11, 1349. | 1.8 | 6 |
| 24 | Physicochemical nature of sodium dodecyl sulfate interactions with bovine serum albumin revealed by interdisciplinary approaches. Journal of Molecular Liquids, 2021, 340, 117185. | 2.3 | 10 |
| 25 | Modeling protein structures with the coarse-grained UNRES force field in the CASP14 experiment. Journal of Molecular Graphics and Modelling, 2021, 108, 108008. | 1.3 | 17 |
| 26 | Role of Oligosaccharide Chain Polarity in Proteinâ€“Glycosaminoglycan Interactions. Journal of Chemical Information and Modeling, 2021, 61, 455-466. | 2.5 | 6 |
| 27 | Effect of Tetraphenylborate on Physicochemical Properties of Bovine Serum Albumin. Molecules, 2021, 26, 6565. | 1.7 | 7 |
| 28 | Rat cathepsin K: Enzymatic specificity and regulation of its collagenolytic activity. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2020, 1868, 140318. | 1.1 | 9 |
| 29 | Probing the Proton-Loading Site of Cytochrome C Oxidase Using Time-Resolved Fourier Transform Infrared Spectroscopy. Molecules, 2020, 25, 3393. | 1.7 | 1 |
| 30 | Mind Your Dye: The Amyloid Sensor Thioflavin T Interacts with Sulfated Glycosaminoglycans Used To Induce Cross-Î²-Sheet Motifs. Journal of Physical Chemistry B, 2020, 124, 11625-11633. | 1.2 | 8 |
| 31 | Truncation of Huia versabilis Bowman-Birk inhibitor increases its selectivity, matriptase-1 inhibitory activity and proteolytic stability. Biochimie, 2020, 171-172, 178-186. | 1.3 | 5 |
| 32 | Role of Glycosaminoglycans in Procathepsin B Maturation: Molecular Mechanism Elucidated by a Computational Study. Journal of Chemical Information and Modeling, 2020, 60, 2247-2256. | 2.5 | 9 |
| 33 | Improved Consensus-Fragment Selection in Template-Assisted Prediction of Protein Structures with the UNRES Force Field in CASP13. Journal of Chemical Information and Modeling, 2020, 60, 1844-1864. | 2.5 | 11 |
| 34 | Coarseâ€grained and atomic resolution biomolecular docking with the ATTRACT approach. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1018-1028. | 1.5 | 12 |
| 35 | Case of Early-Onset Parkinsonâ€™s Disease in a Heterozygous Mutation Carrier of the ATP7B Gene. Journal of Personalized Medicine, 2019, 9, 41. | 1.1 | 6 |
| 36 | Cm<sup>3+</sup>/Eu<sup>3+</sup>induced structural, mechanistic and functional implications for calmodulin. Physical Chemistry Chemical Physics, 2019, 21, 21213-21222. | 1.3 | 34 |

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| 37 | In silico analysis of heparin and chondroitin sulfate binding mechanisms of the antiprotozoal drug berenil and pentamidine. Carbohydrate Research, 2019, 482, 107742. | 1.1 | 4 |
| 38 | Synthesis and in silico characterization of artificially phosphorylated glycosaminoglycans. Journal of Molecular Structure, 2019, 1197, 401-416. | 1.8 | 8 |
| 39 | NMR and molecular modeling reveal specificity of the interactions between CXCL14 and glycosaminoglycans. Glycobiology, 2019, 29, 715-725. | 1.3 | 28 |
| 40 | Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221. | 1.5 | 99 |
| 41 | Analysis of Procollagen C-Proteinase Enhancer-1/Glycosaminoglycan Binding Sites and of the Potential Role of Calcium Ions in the Interaction. International Journal of Molecular Sciences, 2019, 20, 5021. | 1.8 | 11 |
| 42 | Evaluation of the scale-consistent UNRES force field in template-free prediction of protein structures in the CASP13 experiment. Journal of Molecular Graphics and Modelling, 2019, 92, 154-166. | 1.3 | 19 |
| 43 | Molecular dynamics insights into proteinâ€glycosaminoglycan systems from microsecondâ€scale simulations. Biopolymers, 2019, 110, e23252. | 1.2 | 30 |
| 44 | The molecular mechanism of structural changes in the antimicrobial peptide CM15 upon complex formation with drug molecule suramin: a computational analysis. Physical Chemistry Chemical Physics, 2019, 21, 10644-10659. | 1.3 | 11 |
| 45 | Local and long range potentials for heparinâ€protein systems for coarseâ€grained simulations. Biopolymers, 2019, 110, e23269. | 1.2 | 7 |
| 46 | Docking software performance in protein-glycosaminoglycan systems. Journal of Molecular Graphics and Modelling, 2019, 90, 42-50. | 1.3 | 31 |
| 47 | Modeling large proteinâ€“glycosaminoglycan complexes using a fragmentâ€based approach. Journal of Computational Chemistry, 2019, 40, 1429-1439. | 1.5 | 15 |
| 48 | Meglumine acridone acetate, the ionic salt of CMA and N-methylglucamine, induces apoptosis in human PBMCs via the mitochondrial pathway. Scientific Reports, 2019, 9, 18240. | 1.6 | 6 |
| 49 | Computational Analysis of Solvent Inclusion in Docking Studies of Proteinâ€“Glycosaminoglycan Systems. Methods in Molecular Biology, 2018, 1762, 445-454. | 0.4 | 3 |
| 50 | Molecular interactions of the anticancer agent ellipticine with glycosaminoglycans by in silico analysis. Carbohydrate Research, 2018, 462, 28-33. | 1.1 | 7 |
| 51 | The effect of interleukinâ€8 truncations on its interactions with glycosaminoglycans. Biopolymers, 2018, 109, e23103. | 1.2 | 19 |
| 52 | Molecular dynamics-based model of VEGF-A and its heparin interactions. Journal of Molecular Graphics and Modelling, 2018, 82, 157-166. | 1.3 | 24 |
| 53 | The Intrinsic Pepsin Resistance of Interleukin-8 Can Be Explained from a Combined Bioinformatical and Experimental Approach. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2018, 15, 300-308. | 1.9 | 0 |
| 54 | Proteinâ€“Ligand Interaction Energy-Based Entropy Calculations: Fundamental Challenges For Flexible Systems. Journal of Physical Chemistry B, 2018, 122, 7821-7827. | 1.2 | 11 |

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| 55 | Insights into the structure and dynamics of lysyl oxidase propeptide, a flexible protein with numerous partners. Scientific Reports, 2018, 8, 11768. | 1.6 | 39 |
| 56 | Computational drill down on FGF1-heparin interactions through methodological evaluation. Glycoconjugate Journal, 2017, 34, 427-440. | 1.4 | 27 |
| 57 | Sulfated Hyaluronan Derivatives Modulate TGF-Î²1:Receptor Complex Formation: Possible Consequences for TGF-Î²1 Signaling. Scientific Reports, 2017, 7, 1210. | 1.6 | 30 |
| 58 | Structural and functional insights into the interaction of sulfated glycosaminoglycans with tissue inhibitor of metalloproteinase-3 â€“ A possible regulatory role on extracellular matrix homeostasis. Acta Biomaterialia, 2016, 45, 143-154. | 4.1 | 31 |
| 59 | The structural investigation of glycosaminoglycan binding to CXCL12 displays distinct interaction sites. Glycobiology, 2016, 26, 1209-1221. | 1.3 | 27 |
| 60 | Computational analysis of interactions in structurally available proteinâ€“glycosaminoglycan complexes. Glycobiology, 2016, 26, 850-861. | 1.3 | 58 |
| 61 | Structural analysis of the interleukin-8/glycosaminoglycan interactions by amide hydrogen/deuterium exchange mass spectrometry. Methods, 2015, 89, 45-53. | 1.9 | 21 |
| 62 | Coarse-Grained Model of Glycosaminoglycans. Journal of Chemical Information and Modeling, 2015, 55, 114-124. | 2.5 | 43 |
| 63 | Structural and functional insights into sclerostin-glycosaminoglycan interactions in bone. Biomaterials, 2015, 67, 335-345. | 5.7 | 39 |
| 64 | Glycosaminoglycan derivatives: promising candidates for the design of functional biomaterials. Journal of Materials Science: Materials in Medicine, 2015, 26, 232. | 1.7 | 53 |
| 65 | Multipose Binding in Molecular Docking. International Journal of Molecular Sciences, 2014, 15, 2622-2645. | 1.8 | 51 |
| 66 | Glycosaminoglycan Monosaccharide Blocks Analysis by Quantum Mechanics, Molecular Dynamics, and Nuclear Magnetic Resonance. BioMed Research International, 2014, 2014, 1-11. | 0.9 | 13 |
| 67 | Sulfated Glycosaminoglycans Exploit the Conformational Plasticity of Bone Morphogenetic Protein-2 (BMP-2) and Alter the Interaction Profile with Its Receptor. Biomacromolecules, 2014, 15, 3083-3092. | 2.6 | 76 |
| 68 | Flexibility and Explicit Solvent in Molecular-Dynamics-Based Docking of Proteinâ€“Glycosaminoglycan Systems. Journal of Chemical Information and Modeling, 2014, 54, 582-592. | 2.5 | 59 |
| 69 | Importance of IdoA and IdoA(2S) ring conformations in computational studies of glycosaminoglycanâ€“protein interactions. Carbohydrate Research, 2013, 381, 133-137. | 1.1 | 31 |
| 70 | Binding of Chondroitin 4-Sulfate to Cathepsin S Regulates Its Enzymatic Activity. Biochemistry, 2013, 52, 6487-6498. | 1.2 | 63 |
| 71 | The promotion of osteoclastogenesis by sulfated hyaluronan through interference with osteoprotegerin and receptor activator of NF-ÎºB ligand/osteoprotegerin complex formation. Biomaterials, 2013, 34, 7653-7661. | 5.7 | 32 |
| 72 | Artificial extracellular matrix composed of collagen I and highly sulfated hyaluronan interferes with TGFÎ²1 signaling and prevents TGFÎ²1-induced myofibroblast differentiation. Acta Biomaterialia, 2013, 9, 7775-7786. | 4.1 | 49 |

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| 73 | Investigation of lysine side chain interactions of interleukin-8 with heparin and other glycosaminoglycans studied by a methylation-NMR approach. Glycobiology, 2013, 23, 1260-1269. | 1.3 | 40 |
| 74 | Residue 75 of Interleukinâ€8 is Crucial for its Interactions with Glycosaminoglycans. ChemBioChem, 2012, 13, 2558-2566. | 1.3 | 26 |
| 75 | Characterization of the interaction of interleukin-8 with hyaluronan, chondroitin sulfate, dermatan sulfate and their sulfated derivatives by spectroscopy and molecular modeling. Glycobiology, 2012, 22, 134-145. | 1.3 | 120 |
| 76 | The influence of glycosaminoglycans on IL-8-mediated functions of neutrophils. Carbohydrate Research, 2012, 356, 196-203. | 1.1 | 37 |
| 77 | Docking glycosaminoglycans to proteins: analysis of solvent inclusion. Journal of Computer-Aided Molecular Design, 2011, 25, 477-489. | 1.3 | 69 |
| 78 | SCOWLP update: 3D classification of protein-protein, -peptide, -saccharide and -nucleic acid interactions, and structure-based binding inferences across folds. BMC Bioinformatics, 2011, 12, 398. | 1.2 | 28 |
| 79 | A molecular dynamics approach to study the importance of solvent in protein interactions. Proteins: Structure, Function and Bioinformatics, 2008, 73, 515-525. | 1.5 | 30 |