

# Sergey A Samsonov

## List of Publications by Year in descending order

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79  
papers

1,736  
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236925

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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.	3.6	2
3	Modeling glycosaminoglycan-protein complexes. Current Opinion in Structural Biology, 2022, 73, 102332.	5.7	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.	3.7	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.	2.4	8
6	Molecular Dynamics Approaches Dissect Molecular Mechanisms Underlying Methylene Blue-Glycosaminoglycan Interactions. Molecules, 2022, 27, 2654.	3.8	2
7	Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins. Journal of Molecular Modeling, 2022, 28, .	1.8	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.	2.3	3
9	Binding of heparan sulfate to human cystatin C modulates inhibition of cathepsin L: Putative consequences in mucopolysaccharidosis. Carbohydrate Polymers, 2022, 293, 119734.	10.2	3
10	Explicit solvent repulsive scaling replica exchange molecular dynamics (<scp>REMD</scp>) in molecular modeling of protein-glycosaminoglycan complexes. Journal of Computational Chemistry, 2022, 43, 1633-1640.	3.3	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.	2.3	1
12	The abnormal accumulation of heparan sulfate in patients with mucopolysaccharidosis prevents the elastolytic activity of cathepsin V. Carbohydrate Polymers, 2021, 253, 117261.	10.2	13
13	Computational insights into the role of calcium ions in protein-glycosaminoglycan systems. Physical Chemistry Chemical Physics, 2021, 23, 3519-3530.	2.8	13
14	Evaluation of replica exchange with repulsive scaling approach for docking glycosaminoglycans. Journal of Computational Chemistry, 2021, 42, 1040-1053.	3.3	8
15	Further analyses of APRIL/APRIL-receptor/glycosaminoglycan interactions by biochemical assays linked to computational studies. Glycobiology, 2021, 31, 772-786.	2.5	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.	2.5	6
17	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.	2.5	16
18	Acute phase $\beta$ -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.	2.4	3

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19	The potential role of glycosaminoglycans in serum amyloid A fibril formation by in silico approaches. <i>Matrix Biology Plus</i> , 2021, 12, 100080.	3.5	2
20	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. <i>Biomolecules</i> , 2021, 11, 1347.	4.0	29
21	Computational insights into heparin-small molecule interactions: Evaluation of the balance between stacking and non-stacking binding modes. <i>Carbohydrate Research</i> , 2021, 507, 108390.	2.3	5
22	Modeling Protein-Glycosaminoglycan Complexes: Does the Size Matter?. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4475-4485.	5.4	14
23	Advanced Molecular Dynamics Approaches to Model a Tertiary Complex APRIL/TACI with Long Glycosaminoglycans. <i>Biomolecules</i> , 2021, 11, 1349.	4.0	6
24	Physicochemical nature of sodium dodecyl sulfate interactions with bovine serum albumin revealed by interdisciplinary approaches. <i>Journal of Molecular Liquids</i> , 2021, 340, 117185.	4.9	10
25	Modeling protein structures with the coarse-grained UNRES force field in the CASP14 experiment. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 108008.	2.4	17
26	Role of Oligosaccharide Chain Polarity in Protein-Glycosaminoglycan Interactions. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 455-466.	5.4	6
27	Effect of Tetraphenylborate on Physicochemical Properties of Bovine Serum Albumin. <i>Molecules</i> , 2021, 26, 6565.	3.8	7
28	Rat cathepsin K: Enzymatic specificity and regulation of its collagenolytic activity. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2020, 1868, 140318.	2.3	9
29	Probing the Proton-Loading Site of Cytochrome C Oxidase Using Time-Resolved Fourier Transform Infrared Spectroscopy. <i>Molecules</i> , 2020, 25, 3393.	3.8	1
30	Mind Your Dye: The Amyloid Sensor Thioflavin T Interacts with Sulfated Glycosaminoglycans Used To Induce Cross- $\beta$ -Sheet Motifs. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11625-11633.	2.6	8
31	Truncation of <i>Huia versabilis</i> Bowman-Birk inhibitor increases its selectivity, matriptase-1 inhibitory activity and proteolytic stability. <i>Biochimie</i> , 2020, 171-172, 178-186.	2.6	5
32	Role of Glycosaminoglycans in Procathepsin B Maturation: Molecular Mechanism Elucidated by a Computational Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2247-2256.	5.4	9
33	Improved Consensus-Fragment Selection in Template-Assisted Prediction of Protein Structures with the UNRES Force Field in CASP13. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1844-1864.	5.4	11
34	Coarse-grained and atomic resolution biomolecular docking with the ATTRACT approach. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 1018-1028.	2.6	12
35	Case of Early-Onset Parkinson's Disease in a Heterozygous Mutation Carrier of the ATP7B Gene. <i>Journal of Personalized Medicine</i> , 2019, 9, 41.	2.5	6
36	Cm <sup>3+</sup> /Eu <sup>3+</sup> induced structural, mechanistic and functional implications for calmodulin. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21213-21222.	2.8	34

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37	In silico analysis of heparin and chondroitin sulfate binding mechanisms of the antiprotozoal drug berenil and pentamidine. <i>Carbohydrate Research</i> , 2019, 482, 107742.	2.3	4
38	Synthesis and in silico characterization of artificially phosphorylated glycosaminoglycans. <i>Journal of Molecular Structure</i> , 2019, 1197, 401-416.	3.6	8
39	NMR and molecular modeling reveal specificity of the interactions between CXCL14 and glycosaminoglycans. <i>Glycobiology</i> , 2019, 29, 715-725.	2.5	28
40	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 1200-1221.	2.6	99
41	Analysis of Procollagen C-Proteinase Enhancer-1/Glycosaminoglycan Binding Sites and of the Potential Role of Calcium Ions in the Interaction. <i>International Journal of Molecular Sciences</i> , 2019, 20, 5021.	4.1	11
42	Evaluation of the scale-consistent UNRES force field in template-free prediction of protein structures in the CASP13 experiment. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 154-166.	2.4	19
43	Molecular dynamics insights into protein-glycosaminoglycan systems from microsecond-scale simulations. <i>Biopolymers</i> , 2019, 110, e23252.	2.4	30
44	The molecular mechanism of structural changes in the antimicrobial peptide CM15 upon complex formation with drug molecule suramin: a computational analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10644-10659.	2.8	11
45	Local and long range potentials for heparin-protein systems for coarse-grained simulations. <i>Biopolymers</i> , 2019, 110, e23269.	2.4	7
46	Docking software performance in protein-glycosaminoglycan systems. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 42-50.	2.4	31
47	Modeling large protein-glycosaminoglycan complexes using a fragment-based approach. <i>Journal of Computational Chemistry</i> , 2019, 40, 1429-1439.	3.3	15
48	Meglumine acridone acetate, the ionic salt of CMA and N-methylglucamine, induces apoptosis in human PBMCs via the mitochondrial pathway. <i>Scientific Reports</i> , 2019, 9, 18240.	3.3	6
49	Computational Analysis of Solvent Inclusion in Docking Studies of Protein-Glycosaminoglycan Systems. <i>Methods in Molecular Biology</i> , 2018, 1762, 445-454.	0.9	3
50	Molecular interactions of the anticancer agent ellipticine with glycosaminoglycans by in silico analysis. <i>Carbohydrate Research</i> , 2018, 462, 28-33.	2.3	7
51	The effect of interleukin-8 truncations on its interactions with glycosaminoglycans. <i>Biopolymers</i> , 2018, 109, e23103.	2.4	19
52	Molecular dynamics-based model of VEGF-A and its heparin interactions. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 82, 157-166.	2.4	24
53	The Intrinsic Pepsin Resistance of Interleukin-8 Can Be Explained from a Combined Bioinformatical and Experimental Approach. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2018, 15, 300-308.	3.0	0
54	Protein-Ligand Interaction Energy-Based Entropy Calculations: Fundamental Challenges For Flexible Systems. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7821-7827.	2.6	11

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55	Insights into the structure and dynamics of lysyl oxidase propeptide, a flexible protein with numerous partners. <i>Scientific Reports</i> , 2018, 8, 11768.	3.3	39
56	Computational drill down on FGF1-heparin interactions through methodological evaluation. <i>Glycoconjugate Journal</i> , 2017, 34, 427-440.	2.7	27
57	Sulfated Hyaluronan Derivatives Modulate TGF- $\beta$ 1:Receptor Complex Formation: Possible Consequences for TGF- $\beta$ 21 Signaling. <i>Scientific Reports</i> , 2017, 7, 1210.	3.3	30
58	Structural and functional insights into the interaction of sulfated glycosaminoglycans with tissue inhibitor of metalloproteinase-3 – A possible regulatory role on extracellular matrix homeostasis. <i>Acta Biomaterialia</i> , 2016, 45, 143-154.	8.3	31
59	The structural investigation of glycosaminoglycan binding to CXCL12 displays distinct interaction sites. <i>Glycobiology</i> , 2016, 26, 1209-1221.	2.5	27
60	Computational analysis of interactions in structurally available protein-glycosaminoglycan complexes. <i>Glycobiology</i> , 2016, 26, 850-861.	2.5	58
61	Structural analysis of the interleukin-8/glycosaminoglycan interactions by amide hydrogen/deuterium exchange mass spectrometry. <i>Methods</i> , 2015, 89, 45-53.	3.8	21
62	Coarse-Grained Model of Glycosaminoglycans. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 114-124.	5.4	43
63	Structural and functional insights into sclerostin-glycosaminoglycan interactions in bone. <i>Biomaterials</i> , 2015, 67, 335-345.	11.4	39
64	Glycosaminoglycan derivatives: promising candidates for the design of functional biomaterials. <i>Journal of Materials Science: Materials in Medicine</i> , 2015, 26, 232.	3.6	53
65	Multipose Binding in Molecular Docking. <i>International Journal of Molecular Sciences</i> , 2014, 15, 2622-2645.	4.1	51
66	Glycosaminoglycan Monosaccharide Blocks Analysis by Quantum Mechanics, Molecular Dynamics, and Nuclear Magnetic Resonance. <i>BioMed Research International</i> , 2014, 2014, 1-11.	1.9	13
67	Sulfated Glycosaminoglycans Exploit the Conformational Plasticity of Bone Morphogenetic Protein-2 (BMP-2) and Alter the Interaction Profile with Its Receptor. <i>Biomacromolecules</i> , 2014, 15, 3083-3092.	5.4	76
68	Flexibility and Explicit Solvent in Molecular-Dynamics-Based Docking of Protein-Glycosaminoglycan Systems. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 582-592.	5.4	59
69	Importance of IdoA and IdoA(2S) ring conformations in computational studies of glycosaminoglycan-protein interactions. <i>Carbohydrate Research</i> , 2013, 381, 133-137.	2.3	31
70	Binding of Chondroitin 4-Sulfate to Cathepsin S Regulates Its Enzymatic Activity. <i>Biochemistry</i> , 2013, 52, 6487-6498.	2.5	63
71	The promotion of osteoclastogenesis by sulfated hyaluronan through interference with osteoprotegerin and receptor activator of NF- $\kappa$ B ligand/osteoprotegerin complex formation. <i>Biomaterials</i> , 2013, 34, 7653-7661.	11.4	32
72	Artificial extracellular matrix composed of collagen I and highly sulfated hyaluronan interferes with TGF $\beta$ 21 signaling and prevents TGF $\beta$ 21-induced myofibroblast differentiation. <i>Acta Biomaterialia</i> , 2013, 9, 7775-7786.	8.3	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. <i>Glycobiology</i> , 2013, 23, 1260-1269.	2.5	40
74	Residue 75 of Interleukin-8 is Crucial for its Interactions with Glycosaminoglycans. <i>ChemBioChem</i> , 2012, 13, 2558-2566.	2.6	26
75	Characterization of the interaction of interleukin-8 with hyaluronan, chondroitin sulfate, dermatan sulfate and their sulfated derivatives by spectroscopy and molecular modeling. <i>Glycobiology</i> , 2012, 22, 134-145.	2.5	120
76	The influence of glycosaminoglycans on IL-8-mediated functions of neutrophils. <i>Carbohydrate Research</i> , 2012, 356, 196-203.	2.3	37
77	Docking glycosaminoglycans to proteins: analysis of solvent inclusion. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 477-489.	2.9	69
78	SCOWLP update: 3D classification of protein-protein, -peptide, -saccharide and -nucleic acid interactions, and structure-based binding inferences across folds. <i>BMC Bioinformatics</i> , 2011, 12, 398.	2.6	28
79	A molecular dynamics approach to study the importance of solvent in protein interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 515-525.	2.6	30