Sergey A Samsonov

List of Publications by Year
in descending order

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	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
2	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
3	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
4	Docking glycosaminoglycans to proteins: analysis of solvent inclusion. Journal of Computer-Aided Molecular Design, 2011, 25, 477-489.	1.3	69
5	Binding of Chondroitin 4-Sulfate to Cathepsin S Regulates Its Enzymatic Activity. Biochemistry, 2013, 52, 6487-6498.	1.2	63
6	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
7	Computational analysis of interactions in structurally available proteinâ€“glycosaminoglycan complexes. Glycobiology, 2016, 26, 850-861.	1.3	58
8	Glycosaminoglycan derivatives: promising candidates for the design of functional biomaterials. Journal of Materials Science: Materials in Medicine, 2015, 26, 232.	1.7	53
9	Multipose Binding in Molecular Docking. International Journal of Molecular Sciences, 2014, 15, 2622-2645.	1.8	51
10	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
11	Coarse-Grained Model of Glycosaminoglycans. Journal of Chemical Information and Modeling, 2015, 55, 114-124.	2.5	43
12	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
13	Structural and functional insights into sclerostin-glycosaminoglycan interactions in bone. Biomaterials, 2015, 67, 335-345.	5.7	39
14	Insights into the structure and dynamics of lysyl oxidase propeptide, a flexible protein with numerous partners. Scientific Reports, 2018, 8, 11768.	1.6	39
15	The influence of glycosaminoglycans on IL-8-mediated functions of neutrophils. Carbohydrate Research, 2012, 356, 196-203.	1.1	37
16	Cm³⁺/Eu³⁺induced structural, mechanistic and functional implications for calmodulin. Physical Chemistry Chemical Physics, 2019, 21, 21213-21222.	1.3	34
17	The promotion of osteoclastogenesis by sulfated hyaluronan through interference with osteoprotegerin and receptor activator of NF-Î²B ligand/osteoprotegerin complex formation. Biomaterials, 2013, 34, 7653-7661.	5.7	32
18	Importance of IdoA and IdoA(2S) ring conformations in computational studies of glycosaminoglycanâ€“protein interactions. Carbohydrate Research, 2013, 381, 133-137.	1.1	31

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19	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
20	Docking software performance in protein-glycosaminoglycan systems. Journal of Molecular Graphics and Modelling, 2019, 90, 42-50.	1.3	31
21	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
22	Sulfated Hyaluronan Derivatives Modulate TGF-Î²1:Receptor Complex Formation: Possible Consequences for TGF-Î²1 Signaling. Scientific Reports, 2017, 7, 1210.	1.6	30
23	Molecular dynamics insights into proteinâ€glycosaminoglycan systems from microsecondâ€scale simulations. Biopolymers, 2019, 110, e23252.	1.2	30
24	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. Biomolecules, 2021, 11, 1347.	1.8	29
25	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
26	NMR and molecular modeling reveal specificity of the interactions between CXCL14 and glycosaminoglycans. Glycobiology, 2019, 29, 715-725.	1.3	28
27	The structural investigation of glycosaminoglycan binding to CXCL12 displays distinct interaction sites. Glycobiology, 2016, 26, 1209-1221.	1.3	27
28	Computational drill down on FGF1-heparin interactions through methodological evaluation. Glycoconjugate Journal, 2017, 34, 427-440.	1.4	27
29	Residue 75 of Interleukinâ€8 is Crucial for its Interactions with Glycosaminoglycans. ChemBioChem, 2012, 13, 2558-2566.	1.3	26
30	Molecular dynamics-based model of VEGF-A and its heparin interactions. Journal of Molecular Graphics and Modelling, 2018, 82, 157-166.	1.3	24
31	Structural analysis of the interleukin-8/glycosaminoglycan interactions by amide hydrogen/deuterium exchange mass spectrometry. Methods, 2015, 89, 45-53.	1.9	21
32	The effect of interleukinâ€8 truncations on its interactions with glycosaminoglycans. Biopolymers, 2018, 109, e23103.	1.2	19
33	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
34	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
35	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
36	Modeling glycosaminoglycanâ€“protein complexes. Current Opinion in Structural Biology, 2022, 73, 102332.	2.6	16

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37	Modeling large proteinâ€“glycosaminoglycan complexes using a fragmentâ€based approach. Journal of Computational Chemistry, 2019, 40, 1429-1439.	1.5	15
38	Modeling Proteinâ€“Glycosaminoglycan Complexes: Does the Size Matter?. Journal of Chemical Information and Modeling, 2021, 61, 4475-4485.	2.5	14
39	Glycosaminoglycan Monosaccharide Blocks Analysis by Quantum Mechanics, Molecular Dynamics, and Nuclear Magnetic Resonance. BioMed Research International, 2014, 2014, 1-11.	0.9	13
40	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
41	Computational insights into the role of calcium ions in proteinâ€“glycosaminoglycan systems. Physical Chemistry Chemical Physics, 2021, 23, 3519-3530.	1.3	13
42	Coarseâ€grained and atomic resolution biomolecular docking with the ATTRACT approach. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1018-1028.	1.5	12
43	Proteinâ€“Ligand Interaction Energy-Based Entropy Calculations: Fundamental Challenges For Flexible Systems. Journal of Physical Chemistry B, 2018, 122, 7821-7827.	1.2	11
44	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
45	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
46	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
47	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
48	Rat cathepsin K: Enzymatic specificity and regulation of its collagenolytic activity. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2020, 1868, 140318.	1.1	9
49	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
50	Further analyses of APRIL/APRIL-receptor/glycosaminoglycan interactions by biochemical assays linked to computational studies. Glycobiology, 2021, 31, 772-786.	1.3	9
51	Synthesis and in silico characterization of artificially phosphorylated glycosaminoglycans. Journal of Molecular Structure, 2019, 1197, 401-416.	1.8	8
52	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
53	Evaluation of replica exchange with repulsive scaling approach for docking glycosaminoglycans. Journal of Computational Chemistry, 2021, 42, 1040-1053.	1.5	8
54	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

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55	Molecular interactions of the anticancer agent ellipticine with glycosaminoglycans by in silico analysis. Carbohydrate Research, 2018, 462, 28-33.	1.1	7
56	Local and long range potentials for heparinâ€protein systems for coarseâ€grained simulations. Biopolymers, 2019, 110, e23269.	1.2	7
57	Effect of Tetraphenylborate on Physicochemical Properties of Bovine Serum Albumin. Molecules, 2021, 26, 6565.	1.7	7
58	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
59	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
60	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
61	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
62	Advanced Molecular Dynamics Approaches to Model a Tertiary Complex APRIL/TACI with Long Glycosaminoglycans. Biomolecules, 2021, 11, 1349.	1.8	6
63	Role of Oligosaccharide Chain Polarity in Proteinâ€“Glycosaminoglycan Interactions. Journal of Chemical Information and Modeling, 2021, 61, 455-466.	2.5	6
64	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
65	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
66	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
67	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
68	Computational Analysis of Solvent Inclusion in Docking Studies of Proteinâ€“Glycosaminoglycan Systems. Methods in Molecular Biology, 2018, 1762, 445-454.	0.4	3
69	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
70	Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins. Journal of Molecular Modeling, 2022, 28, .	0.8	3
71	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
72	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

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73	The potential role of glycosaminoglycans in serum amyloid A fibril formation by in silico approaches. Matrix Biology Plus, 2021, 12, 100080.	1.9	2
74	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
75	Molecular Dynamics Approaches Dissect Molecular Mechanisms Underlying Methylene Blueâ€“Glycosaminoglycan Interactions. Molecules, 2022, 27, 2654.	1.7	2
76	Probing the Proton-Loading Site of Cytochrome C Oxidase Using Time-Resolved Fourier Transform Infrared Spectroscopy. Molecules, 2020, 25, 3393.	1.7	1
77	Physics-Based Coarse-Grained Modeling in Bio- and Nanochemistry. , 2022, , 31-69.		1
78	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
79	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