

Sergey A Samsonov

List of Publications by Year in descending order

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79
papers

1,736
citations

236925

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330143

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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. <i>Glycobiology</i> , 2012, 22, 134-145.	2.5	120
2	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
3	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
4	Docking glycosaminoglycans to proteins: analysis of solvent inclusion. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 477-489.	2.9	69
5	Binding of Chondroitin 4-Sulfate to Cathepsin S Regulates Its Enzymatic Activity. <i>Biochemistry</i> , 2013, 52, 6487-6498.	2.5	63
6	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
7	Computational analysis of interactions in structurally available protein-glycosaminoglycan complexes. <i>Glycobiology</i> , 2016, 26, 850-861.	2.5	58
8	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
9	Multipose Binding in Molecular Docking. <i>International Journal of Molecular Sciences</i> , 2014, 15, 2622-2645.	4.1	51
10	Artificial extracellular matrix composed of collagen I and highly sulfated hyaluronan interferes with TGF β 1 signaling and prevents TGF β 1-induced myofibroblast differentiation. <i>Acta Biomaterialia</i> , 2013, 9, 7775-7786.	8.3	49
11	Coarse-Grained Model of Glycosaminoglycans. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 114-124.	5.4	43
12	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
13	Structural and functional insights into sclerostin-glycosaminoglycan interactions in bone. <i>Biomaterials</i> , 2015, 67, 335-345.	11.4	39
14	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
15	The influence of glycosaminoglycans on IL-8-mediated functions of neutrophils. <i>Carbohydrate Research</i> , 2012, 356, 196-203.	2.3	37
16	Cm ³⁺ /Eu ³⁺ induced structural, mechanistic and functional implications for calmodulin. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21213-21222.	2.8	34
17	The promotion of osteoclastogenesis by sulfated hyaluronan through interference with osteoprotegerin and receptor activator of NF- κ B ligand/osteoprotegerin complex formation. <i>Biomaterials</i> , 2013, 34, 7653-7661.	11.4	32
18	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

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19	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
20	Docking software performance in protein-glycosaminoglycan systems. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 42-50.	2.4	31
21	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
22	Sulfated Hyaluronan Derivatives Modulate TGF- β 1:Receptor Complex Formation: Possible Consequences for TGF- β 1 Signaling. <i>Scientific Reports</i> , 2017, 7, 1210.	3.3	30
23	Molecular dynamics insights into protein-glycosaminoglycan systems from microsecond-scale simulations. <i>Biopolymers</i> , 2019, 110, e23252.	2.4	30
24	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. <i>Biomolecules</i> , 2021, 11, 1347.	4.0	29
25	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
26	NMR and molecular modeling reveal specificity of the interactions between CXCL14 and glycosaminoglycans. <i>Glycobiology</i> , 2019, 29, 715-725.	2.5	28
27	The structural investigation of glycosaminoglycan binding to CXCL12 displays distinct interaction sites. <i>Glycobiology</i> , 2016, 26, 1209-1221.	2.5	27
28	Computational drill down on FGF1-heparin interactions through methodological evaluation. <i>Glycoconjugate Journal</i> , 2017, 34, 427-440.	2.7	27
29	Residue 75 of Interleukin-8 is Crucial for its Interactions with Glycosaminoglycans. <i>ChemBioChem</i> , 2012, 13, 2558-2566.	2.6	26
30	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
31	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
32	The effect of interleukin-8 truncations on its interactions with glycosaminoglycans. <i>Biopolymers</i> , 2018, 109, e23103.	2.4	19
33	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
34	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
35	Investigation of the structure of regulatory proteins interacting with glycosaminoglycans by combining NMR spectroscopy and molecular modeling " the beginning of a wonderful friendship. <i>Biological Chemistry</i> , 2021, 402, 1337-1355.	2.5	16
36	Modeling glycosaminoglycan-protein complexes. <i>Current Opinion in Structural Biology</i> , 2022, 73, 102332.	5.7	16

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37	Modeling large protein-glycosaminoglycan complexes using a fragment-based approach. <i>Journal of Computational Chemistry</i> , 2019, 40, 1429-1439.	3.3	15
38	Modeling Protein-Glycosaminoglycan Complexes: Does the Size Matter?. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4475-4485.	5.4	14
39	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
40	The abnormal accumulation of heparan sulfate in patients with mucopolysaccharidosis prevents the elastolytic activity of cathepsin V. <i>Carbohydrate Polymers</i> , 2021, 253, 117261.	10.2	13
41	Computational insights into the role of calcium ions in protein-glycosaminoglycan systems. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3519-3530.	2.8	13
42	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
43	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
44	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
45	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
46	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
47	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
48	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
49	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
50	Further analyses of APRIL/APRIL-receptor/glycosaminoglycan interactions by biochemical assays linked to computational studies. <i>Glycobiology</i> , 2021, 31, 772-786.	2.5	9
51	Synthesis and in silico characterization of artificially phosphorylated glycosaminoglycans. <i>Journal of Molecular Structure</i> , 2019, 1197, 401-416.	3.6	8
52	Mind Your Dye: The Amyloid Sensor Thioflavin T Interacts with Sulfated Glycosaminoglycans Used To Induce Cross- β -Sheet Motifs. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11625-11633.	2.6	8
53	Evaluation of replica exchange with repulsive scaling approach for docking glycosaminoglycans. <i>Journal of Computational Chemistry</i> , 2021, 42, 1040-1053.	3.3	8
54	In silico and in vitro mapping of specificity patterns of glycosaminoglycans towards cysteine cathepsins B, L, K, S and V. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 113, 108153.	2.4	8

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55	Molecular interactions of the anticancer agent ellipticine with glycosaminoglycans by in silico analysis. <i>Carbohydrate Research</i> , 2018, 462, 28-33.	2.3	7
56	Local and long range potentials for heparin-protein systems for coarse-grained simulations. <i>Biopolymers</i> , 2019, 110, e23269.	2.4	7
57	Effect of Tetraphenylborate on Physicochemical Properties of Bovine Serum Albumin. <i>Molecules</i> , 2021, 26, 6565.	3.8	7
58	Biglycan Interacts with Type I Insulin-like Receptor (IGF-IR) Signaling Pathway to Regulate Osteosarcoma Cell Growth and Response to Chemotherapy. <i>Cancers</i> , 2022, 14, 1196.	3.7	7
59	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
60	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
61	Insights into the roles of charged residues in substrate binding and mode of action of mannuronan C-5 epimerase AlgE4. <i>Glycobiology</i> , 2021, 31, 1616-1635.	2.5	6
62	Advanced Molecular Dynamics Approaches to Model a Tertiary Complex APRIL/TACI with Long Glycosaminoglycans. <i>Biomolecules</i> , 2021, 11, 1349.	4.0	6
63	Role of Oligosaccharide Chain Polarity in Protein-Glycosaminoglycan Interactions. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 455-466.	5.4	6
64	Explicit solvent repulsive scaling replica exchange molecular dynamics (scpr-REMD) in molecular modeling of protein-glycosaminoglycan complexes. <i>Journal of Computational Chemistry</i> , 2022, 43, 1633-1640.	3.3	6
65	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
66	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
67	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
68	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
69	Acute phase α 1-acid glycoprotein as a siderophore-capturing component of the human plasma: A molecular modeling study. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107861.	2.4	3
70	Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins. <i>Journal of Molecular Modeling</i> , 2022, 28, .	1.8	3
71	Molecular dynamics-based descriptors of 3-O-Sulfated Heparan sulfate as contributors of protein binding specificity. <i>Computational Biology and Chemistry</i> , 2022, 99, 107716.	2.3	3
72	Binding of heparan sulfate to human cystatin C modulates inhibition of cathepsin L: Putative consequences in mucopolysaccharidosis. <i>Carbohydrate Polymers</i> , 2022, 293, 119734.	10.2	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.	3.5	2
74	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
75	Molecular Dynamics Approaches Dissect Molecular Mechanisms Underlying Methylene Blueâ€™Glycosaminoglycan Interactions. Molecules, 2022, 27, 2654.	3.8	2
76	Probing the Proton-Loading Site of Cytochrome C Oxidase Using Time-Resolved Fourier Transform Infrared Spectroscopy. Molecules, 2020, 25, 3393.	3.8	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.	2.3	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.	3.0	0