Hugo Verli

List of Publications by Year
in descending order

99	2,604	172207	223531
papers	citations	29 h-index	46 g-index

106	106	106	4080
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	O-Glycosylated Cell Wall Proteins Are Essential in Root Hair Growth. Science, 2011, 332, 1401-1403.	6.0	287
2	GROMOS 53A6_{GLYC}, an Improved GROMOS Force Field for Hexopyranose-Based Carbohydrates. Journal of Chemical Theory and Computation, 2012, 8, 4681-4690.	2.3	132
3	Design, Synthesis, and Pharmacological Profile of Novel Fused Pyrazolo[4,3-d]pyridine and Pyrazolo[3,4-b][1,8]naphthyridine Isosteres:Â A New Class of Potent and Selective Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 2003, 46, 1144-1152.	2.9	101
4	GROMOS96 43a1 performance on the characterization of glycoprotein conformational ensembles through molecular dynamics simulations. Carbohydrate Research, 2009, 344, 491-500.	1.1	93
5	Molecular dynamics simulation of a decasaccharide fragment of heparin in aqueous solution. Carbohydrate Research, 2004, 339, 281-290.	1.1	70
6	Venomous mammals: A review. Toxicon, 2012, 59, 680-695.	0.8	58
7	Ascorbate peroxidaseâ€related (APxâ€R) is a new hemeâ€containing protein functionally associated with ascorbate peroxidase but evolutionarily divergent. New Phytologist, 2011, 191, 234-250.	3.5	57
8	Natural Plant Alkaloid (Emetine) Inhibits HIV-1 Replication by Interfering with Reverse Transcriptase Activity. Molecules, 2015, 20, 11474-11489.	1.7	56
9	Anxiolytic Effects of Erythrinian Alkaloids from Erythrina mulungu. Journal of Natural Products, 2007, 70, 48-53.	1.5	55
10	Low Accumulation of L90M in Protease from Subtype F HIVâ€1 with Resistance to Protease Inhibitors Is Caused by the L89M Polymorphism. Journal of Infectious Diseases, 2005, 191, 1961-1970.	1.9	54
11	GROMOS96 43a1 performance in predicting oligosaccharide conformational ensembles within glycoproteins. Carbohydrate Research, 2010, 345, 663-671.	1.1	50
12	Depiction of the forces participating in the 2-O-sulfo-Î±-l-iduronic acid conformational preference in heparin sequences in aqueous solutions. Carbohydrate Research, 2008, 343, 1435-1445.	1.1	49
13	Structureâ€“function studies on jaburetox, a recombinant insecticidal peptide derived from jack bean (Canavalia ensiformis) urease. Biochimica Et Biophysica Acta - General Subjects, 2014, 1840, 935-944.	1.1	48
14	Conformation of sulfated galactan and sulfated fucan in aqueous solutions: Implications to their anticoagulant activities. Journal of Molecular Graphics and Modelling, 2007, 26, 391-399.	1.3	47
15	Anticoagulant Activity of a Unique Sulfated Pyranosic (1â†’3)-Î²-l-Arabinan through Direct Interaction with Thrombin. Journal of Biological Chemistry, 2013, 288, 223-233.	1.6	46
16	A Unique 2-Sulfated Î²-Galactan from the Egg Jelly of the Sea Urchin Glyptocidaris crenularis. Journal of Biological Chemistry, 2009, 284, 18790-18800.	1.6	44
17	Structural studies of the Enterococcus faecalis SufU [Fe-S] cluster protein. BMC Biochemistry, 2009, 10, 3.	4.4	44
18	Glycyrrhizin and glycyrrhetic acid: scaffolds to promising new pharmacologically active compounds. Journal of the Brazilian Chemical Society, 2010, 21, 1595-1615.	0.6	44

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19	Extension and validation of the GROMOS 53A6_{<scp>glyc</scp>} parameter set for glycoproteins. Journal of Computational Chemistry, 2014, 35, 2087-2095.	1.5	42
20	Molecular dynamics and atomic charge calculations in the study of heparin conformation in aqueous solution. Carbohydrate Research, 2005, 340, 1499-1507.	1.1	41
21	Structural and functional behavior of biologically active monomeric melittin. Journal of Molecular Graphics and Modelling, 2007, 25, 767-772.	1.3	41
22	Psychollatine, a Glucosidic Monoterpene Indole Alkaloid from Psychotria umbellata. Journal of Natural Products, 2008, 71, 697-700.	1.5	41
23	Low Sugar Is Not Always Good: Impact of Specific O-Glycan Defects on Tip Growth in Arabidopsis. Plant Physiology, 2015, 168, 808-813.	2.3	41
24	Aromatic Rings Commonly Used in Medicinal Chemistry: Force Fields Comparison and Interactions With Water Toward the Design of New Chemical Entities. Frontiers in Pharmacology, 2018, 9, 395.	1.6	40
25	Insights into the induced fit mechanism in antithrombinâ€“heparin interaction using molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2005, 24, 203-212.	1.3	39
26	Pharmacomodulation on the 3-acetylursolic acid skeleton: Design, synthesis, and biological evaluation of novel N-{3-[4-(3-aminopropyl)piperazinyl]propyl}-3-O-acetylursolamide derivatives as antimalarial agents. Bioorganic and Medicinal Chemistry, 2008, 16, 771-782.	1.4	39
27	Ribifolin, an Orbitide from Jatropha ribifolia, and Its Potential Antimalarial Activity. Journal of Natural Products, 2015, 78, 374-380.	1.5	39
28	Thermal-induced conformational changes in the product release area drive the enzymatic activity of xylanases 10B: Crystal structure, conformational stability and functional characterization of the xylanase 10B from Thermotoga petrophila RKU-1. Biochemical and Biophysical Research Communications, 2010, 403, 214-219.	1.0	36
29	Pharmacokinetic evaluation of LASSBio-579: an N-phenylpiperazine antipsychotic prototype. Journal of Pharmacy and Pharmacology, 2010, 60, 699-707.	1.2	33
30	3-to-1: unraveling structural transitions in ureases. Die Naturwissenschaften, 2013, 100, 459-467.	0.6	32
31	Antithrombotic Effect of Chikusetsusaponin IVa Isolated fromIlex paraguariensis(MatÃ©). Journal of Medicinal Food, 2012, 15, 1073-1080.	0.8	30
32	Local intersection volume: a new 3D descriptor applied to develop a 3D-QSAR pharmacophore model for benzodiazepine receptor ligands. European Journal of Medicinal Chemistry, 2002, 37, 219-229.	2.6	27
33	New optimized piperamide analogues with potent in vivo hypotensive properties. European Journal of Pharmaceutical Sciences, 2004, 23, 363-369.	1.9	26
34	Molecular dynamics analysis of HIV-1 matrix protein: Clarifying differences between crystallographic and solution structures. Journal of Molecular Graphics and Modelling, 2007, 26, 62-68.	1.3	26
35	Characterization of JBURE-IIb isoform of Canavalia ensiformis (L.) DC urease. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1758-1768.	1.1	26
36	A cell surface arabinogalactanâ€peptide influences root hair cell fate. New Phytologist, 2020, 227, 732-743.	3.5	26

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37	Turbinatine, a Potential Key Intermediate in the Biosynthesis of Corynanthean-Type Indole Alkaloids. Journal of Natural Products, 2003, 66, 1017-1021.	1.5	25
38	Alkaloids from Hippeastrum morelianum Lem. (Amaryllidaceae). Magnetic Resonance in Chemistry, 2011, 49, 668-672.	1.1	25
39	Structural glycobiology of human Î±₁-acid glycoprotein and its implications for pharmacokinetics and inflammation. Glycobiology, 2015, 25, 1125-1133.	1.3	25
40	Current Status of Carbohydrates Information in the Protein Data Bank. Journal of Chemical Information and Modeling, 2020, 60, 684-699.	2.5	24
41	Jatrophidin I, a cyclic peptide from Brazilian Jatropha curcas L.: Isolation, characterization, conformational studies and biological activity. Phytochemistry, 2014, 107, 91-96.	1.4	23
42	Effects of glycosylation on heparin binding and antithrombin activation by heparin. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2735-2745.	1.5	22
43	Structural and thermodynamic analysis of thrombin:suramin interaction in solution and crystal phases. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 873-881.	1.1	21
44	Atomic Model and Micelle Dynamics of QS-21 Saponin. Molecules, 2014, 19, 3744-3760.	1.7	21
45	Selective PGHS-2 Inhibitors: A Rational Approach for Treatment of theInflammation. Current Medicinal Chemistry, 2002, 9, 849-867.	1.2	20
46	Insights into the N-Sulfation Mechanism: Molecular Dynamics Simulations of the N-Sulfotransferase Domain of Ndst1 and Mutants. PLoS ONE, 2013, 8, e70880.	1.1	19
47	Evidence-based docking of the urease activation complex. Journal of Biomolecular Structure and Dynamics, 2013, 31, 854-861.	2.0	15
48	The Calcium Goes Meow: Effects of Ions and Glycosylation on Fel d 1, the Major Cat Allergen. PLoS ONE, 2015, 10, e0132311.	1.1	15
49	[28]Hexaphyrin derivatives for anion recognition in organic and aqueous media. Chemical Communications, 2016, 52, 2181-2184.	2.2	15
50	Solution conformation and dynamics of exopolysaccharides from Burkholderia species. Carbohydrate Research, 2010, 345, 1922-1931.	1.1	13
51	Structural glycobiology of heparin dynamics on the exosite 2 of coagulation cascade proteases: Implications for glycosaminoglycans antithrombotic activity. Glycobiology, 2014, 24, 97-105.	1.3	13
52	In silicoInvestigation of the PglB Active Site Reveals Transient Catalytic States and Octahedral Metal Ion Coordination. Glycobiology, 2015, 25, 1183-1195.	1.3	13
53	Glycosylation is crucial for a proper catalytic site organization in human glucocerebrosidase. Glycoconjugate Journal, 2016, 33, 237-244.	1.4	13
54	Putative model for heat shock protein 70 complexation with receptor of advanced glycation end products through fluorescence proximity assays and normal mode analyses. Cell Stress and Chaperones, 2017, 22, 99-111.	1.2	13

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55	Accommodation of In-Register N-Linked Glycans on Prion Protein Amyloid Cores. ACS Chemical Neuroscience, 2020, 11, 4092-4097.	1.7	13
56	Highly diastereoselective mercury-mediated synthesis of functionalized 2-azabicyclo[3.3.0]octane derivatives. Tetrahedron Letters, 2002, 43, 1607-1611.	0.7	12
57	Characterization of the conformational ensemble from bioactive N-acylhydrazone derivatives. Journal of Molecular Graphics and Modelling, 2010, 28, 446-454.	1.3	12
58	Assessment of Glycoproteins Dynamics from Computer Simulations. Mini-Reviews in Organic Chemistry, 2011, 8, 229-238.	0.6	12
59	An Unusual Intramolecular Halogen Bond Guides Conformational Selection. Angewandte Chemie - International Edition, 2018, 57, 9970-9975.	7.2	12
60	An Unprecedented Neolignan Skeleton from Chimarrhis turbinata. Journal of Natural Products, 2011, 74, 487-491.	1.5	11
61	Unrestrained Conformational Characterization ofStenocereus erucaSaponins in Aqueous and Nonaqueous Solvents. Journal of Natural Products, 2012, 75, 1196-1200.	1.5	11
62	Homology modeling and molecular dynamics provide structural insights into tospovirus nucleoprotein. BMC Bioinformatics, 2016, 17, 489.	1.2	11
63	Molecular docking and pharmacological/toxicological assessment of a new compound designed from celecoxib and paracetamol by molecular hybridization. Inflammopharmacology, 2018, 26, 1189-1206.	1.9	11
64	Improving the Thrombin Inhibitory Activity of Glycyrrhizin, a Triterpenic Saponin, Through a Molecular Simplification of the Carbohydrate Moiety. Chemical Biology and Drug Design, 2013, 82, 756-760.	1.5	10
65	On the catalytic mechanism of polysaccharide lyases: evidence of His and Tyr involvement in heparin lysis by heparinase I and the role of Ca²⁺. Molecular BioSystems, 2014, 10, 54-64.	2.9	9
66	Pharmacological evaluation and molecular docking of new di-tert-butylphenol compound, LQFM-091, a new dual 5-LOX/COX inhibitor. European Journal of Pharmaceutical Sciences, 2017, 106, 231-243.	1.9	9
67	All-Hydrocarbon Staples and Their Effect over Peptide Conformation under Different Force Fields. Journal of Chemical Information and Modeling, 2018, 58, 2015-2023.	2.5	9
68	Molecular insight into silk fibroin based delivery vehicle for amphiphilic drugs: Synthesis, characterization and molecular dynamics studies. Journal of Molecular Liquids, 2020, 299, 112156.	2.3	9
69	Prediction, mapping and validation of tick glutathione S-transferase B-cell epitopes. Ticks and Tick-borne Diseases, 2020, 11, 101445.	1.1	9
70	Structure and Behavior of Human Î±-Thrombin upon Ligand Recognition: Thermodynamic and Molecular Dynamics Studies. PLoS ONE, 2011, 6, e24735.	1.1	8
71	Structural glycobiology of heparinase II fromPedobacter heparinus. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1092-1102.	2.0	8
72	ESIâ€MS/MS of expanded porphyrins: a look into their structure and aromaticity. Journal of Mass Spectrometry, 2016, 51, 342-349.	0.7	8

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73	Structural glycobiology of the major allergen of Artemisia vulgaris pollen, Art v 1: O-glycosylation influence on the protein dynamics and allergenicity. Glycobiology, 2012, 22, 817-825.	1.3	7
74	Dynamics on human <scp>T</scp>oll‐like receptor 4 complexation to <scp>MD</scp>‐2: The coreceptor stabilizing function. Proteins: Structure, Function and Bioinformatics, 2015, 83, 373-382.	1.5	7
75	Induction of apoptosis in Ehrlich ascites tumour cells via p53 activation by a novel small-molecule MDM2 inhibitor â€“ LQFM030. Journal of Pharmacy and Pharmacology, 2016, 68, 1143-1159.	1.2	7
76	Everyone Is a Protagonist: Residue Conformational Preferences in High-Resolution Protein Structures. Journal of Computational Biology, 2018, 25, 451-465.	0.8	7
77	Dynamics of DDB2-DDB1 complex under different naturally-occurring mutants in Xeroderma Pigmentosum disease. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 2579-2589.	1.1	7
78	Development of GROMOS-Compatible Parameter Set for Simulations of Chalcones and Flavonoids. Journal of Physical Chemistry B, 2019, 123, 994-1008.	1.2	7
79	Molecular docking and molecular dynamic studies of semi-synthetic piperidine alkaloids as acetylcholinesterase inhibitors. Journal of the Brazilian Chemical Society, 2012, 23, 163-170.	0.6	6
80	Effects of glycosylation and pH conditions in the dynamics of human arylsulfatase A. Journal of Biomolecular Structure and Dynamics, 2014, 32, 567-579.	2.0	6
81	2Â´,3Â´-Dialdehyde of ATP, ADP, and Adenosine Inhibit HIV-1 Reverse Transcriptase and HIV-1 Replication. Current HIV Research, 2014, 12, 347-358.	0.2	6
82	Um paradigma da quÃmica medicinal: a flexibilidade dos ligantes e receptores. Quimica Nova, 2005, 28, 95-102.	0.3	5
83	A knowledge-based genetic algorithm to predict three-dimensional structures of polypeptides. , 2013, , .		5
84	Conformational Characterization of Ipomotaosides and Their Recognition by COX-1 and 2. Molecules, 2014, 19, 5421-5433.	1.7	5
85	Antithrombin conformational modulation by D-myo-inositol 3,4,5,6-tetrakisphosphate (TMI), a novel scaffold for the development of antithrombotic agents. Journal of Biomolecular Structure and Dynamics, 2018, 36, 4045-4056.	2.0	5
86	Characterization of the papillomavirus Î±₁E2 peptide unfolded to folded transition upon DNA binding. FEBS Letters, 2008, 582, 3619-3624.	1.3	4
87	Dynamics of different arachidonic acid orientations bound to prostaglandin endoperoxide synthases. European Journal of Medicinal Chemistry, 2011, 46, 5212-5217.	2.6	4
88	The role of Zn2+, dimerization and N-glycosylation in the interaction of Auxin-Binding Protein 1 (ABP1) with different auxins. Glycobiology, 2017, 27, 1109-1119.	1.3	4
89	The Lazy Life of Lipid-Linked Oligosaccharides in All Life Domains. Journal of Chemical Information and Modeling, 2020, 60, 631-643.	2.5	4
90	Rotational Profiler: A Fast, Automated, and Interactive Server to Derive Torsional Dihedral Potentials for Classical Molecular Simulations. Journal of Chemical Information and Modeling, 2020, 60, 5923-5927.	2.5	4

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91	Structural Characteristics of Glycocins: Unraveling the Role of S-Linked Carbohydrates and Other Structural Elements. Journal of Chemical Information and Modeling, 2022, 62, 927-935.	2.5	4
92	A specific interdomain interaction preserves the structural and binding properties of the ModA protein from the phytopathogen Xanthomonas citri domain interaction and transport in ModA. Archives of Biochemistry and Biophysics, 2013, 539, 20-30.	1.4	3
93	Structural characterization of NETNES glycopeptide from Trypanosoma cruzi. Carbohydrate Research, 2013, 373, 28-34.	1.1	3
94	Neuropharmacological assessment in mice and molecular docking of piperazine derivative LQFM212. Behavioural Brain Research, 2020, 394, 112827.	1.2	3
95	ConfID: an analytical method for conformational characterization of small molecules using molecular dynamics trajectories. Bioinformatics, 2020, 36, 3576-3577.	1.8	3
96	Novel choline analog 2-(4-((1-phenyl-1H-pyrazol-4-yl)methyl)piperazin-1-yl)ethan-1-ol produces sympathoinhibition, hypotension, and antihypertensive effects. Naunyn-Schmiedeberg's Archives of Pharmacology, 2019, 392, 1071-1083.	1.4	2
97	Design, synthesis and pharmacological assessment of new pyrazole compounds. Inflammopharmacology, 2020, 28, 915-928.	1.9	2
98	Differential Effect of Solution Conditions on the Conformation of the Actinoporins Sticholysin II and Equinatoxin II. Anais Da Academia Brasileira De Ciencias, 2014, 86, 1949-1962.	0.3	1
99	Synthesis of Oxygenated Chalcones with Anti-Staphylococcal Activity. Letters in Drug Design and Discovery, 2013, 11, 525-530.	0.4	1