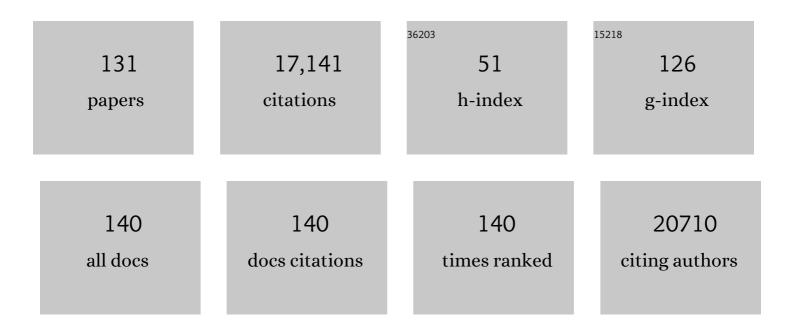
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List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	O-fucosylation stabilizes the TSR3 motif in thrombospondin-1 by interacting with nearby amino acids and protecting a disulfide bond. Journal of Biological Chemistry, 2022, 298, 102047.	1.6	3
2	PD-L1 Glycosylation and Its Impact on Binding to Clinical Antibodies. Journal of Proteome Research, 2021, 20, 485-497.	1.8	29
3	Hyper-truncated Asn355- and Asn391-glycans modulate the activity of neutrophil granule myeloperoxidase. Journal of Biological Chemistry, 2021, 296, 100144.	1.6	31
4	Heparan Sulfate Mimetics Differentially Affect Homologous Chemokines and Attenuate Cancer Development. Journal of Medicinal Chemistry, 2021, 64, 3367-3380.	2.9	11
5	Landscape and selection of vaccine epitopes in SARS-CoV-2. Genome Medicine, 2021, 13, 101.	3.6	30
6	Comparison of cellooligosaccharide conformations in complexes with proteins with energy maps for cellobiose. Carbohydrate Polymers, 2021, 264, 118004.	5.1	12
7	Discovery of rare sulfated N-unsubstituted glucosamine based heparan sulfate analogs selectively activating chemokines. Chemical Science, 2021, 12, 3674-3681.	3.7	14
8	O-glycosylation on cerebrospinal fluid and plasma apolipoprotein E differs in the lipid-binding domain. Glycobiology, 2020, 30, 74-85.	1.3	36
9	GlyGen: Computational and Informatics Resources for Glycoscience. Glycobiology, 2020, 30, 72-73.	1.3	123
10	Directed Evolution of Therapeutic Antibodies Targeting Glycosylation in Cancer. Cancers, 2020, 12, 2824.	1.7	14
11	Virus-Receptor Interactions of Glycosylated SARS-CoV-2 Spike and Human ACE2 Receptor. Cell Host and Microbe, 2020, 28, 586-601.e6.	5.1	334
12	Hierarchical Multivalent Effects Control Influenza Host Specificity. ACS Central Science, 2020, 6, 2311-2318.	5.3	20
13	Analysis of the SARS-CoV-2 spike protein glycan shield reveals implications for immune recognition. Scientific Reports, 2020, 10, 14991.	1.6	286
14	Allosteric regulation of lysosomal enzyme recognition by the cation-independent mannose 6-phosphate receptor. Communications Biology, 2020, 3, 498.	2.0	20
15	A terminal α3-galactose modification regulates an E3 ubiquitin ligase subunit in Toxoplasma gondii. Journal of Biological Chemistry, 2020, 295, 9223-9243.	1.6	6
16	Effect of hydroxylysine-O-glycosylation on the structure of type I collagen molecule: A computational study. Glycobiology, 2020, 30, 830-843.	1.3	10
17	Reconciling MA′AT and molecular dynamics models of linkage conformation in oligosaccharides. Physical Chemistry Chemical Physics, 2020, 22, 14454-14457.	1.3	12
18	Characterization of heparin and severe acute respiratory syndrome-related coronavirus 2 (SARS-CoV-2) spike glycoprotein binding interactions. Antiviral Research, 2020, 181, 104873.	1.9	233

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19	Updates to the Symbol Nomenclature for Glycans guidelines. Glycobiology, 2019, 29, 620-624.	1.3	292
20	GAG Builder: a web-tool for modeling 3D structures of glycosaminoglycans. Glycobiology, 2019, 29, 515-518.	1.3	27
21	NMR Resonance Assignment Methodology: Characterizing Large Sparsely Labeled Glycoproteins. Journal of Molecular Biology, 2019, 431, 2369-2382.	2.0	8
22	Cross-Ring Fragmentation Patterns in the Tandem Mass Spectra of Underivatized Sialylated Oligosaccharides and Their Special Suitability for Spectrum Library Searching. Journal of the American Society for Mass Spectrometry, 2019, 30, 426-438.	1.2	16
23	Fluorescent Trimeric Hemagglutinins Reveal Multivalent Receptor Binding Properties. Journal of Molecular Biology, 2019, 431, 842-856.	2.0	36
24	Use of Circular Statistics To Model αMan-(1→2)-αMan and αMan-(1→3)-α/βMan <i>O</i> -Glycosidic Linkage Conformation in ¹³ C-Labeled Disaccharides and High-Mannose Oligosaccharides. Biochemistry, 2019, 58, 546-560.	1.2	29
25	Synthesis and <i>O</i> -Glycosidic Linkage Conformational Analysis of ¹³ C-Labeled Oligosaccharide Fragments of an Antifreeze Glycolipid. Journal of Organic Chemistry, 2019, 84, 1706-1724.	1.7	15
26	A Traveling Wave Ion Mobility Spectrometry (TWIMS) Study of the Robo1-Heparan Sulfate Interaction. Journal of the American Society for Mass Spectrometry, 2018, 29, 1153-1165.	1.2	12
27	Applying Pose Clustering and MD Simulations To Eliminate False Positives in Molecular Docking. Journal of Chemical Information and Modeling, 2018, 58, 605-614.	2.5	36
28	Oligosaccharide model of the vascular endothelial glycocalyx in physiological flow. Microfluidics and Nanofluidics, 2018, 22, 21.	1.0	14
29	Structural Rearrangements Maintain the Glycan Shield of an HIV-1 Envelope Trimer After the Loss of a Glycan. Scientific Reports, 2018, 8, 15031.	1.6	17
30	Galectin binding to cells and glycoproteins with genetically modified glycosylation reveals galectin–glycan specificities in a natural context. Journal of Biological Chemistry, 2018, 293, 20249-20262.	1.6	67
31	Quantifying Weak Glycan-Protein Interactions Using a Biolayer Interferometry Competition Assay: Applications to ECL Lectin and X-31 Influenza Hemagglutinin. Advances in Experimental Medicine and Biology, 2018, 1104, 259-273.	0.8	5
32	Defining the Specificity of Carbohydrate–Protein Interactions by Quantifying Functional Group Contributions. Journal of Chemical Information and Modeling, 2018, 58, 1889-1901.	2.5	19
33	A combined computational-experimental approach to define the structural origin of antibody recognition of sialyl-Tn, a tumor-associated carbohydrate antigen. Scientific Reports, 2018, 8, 10786.	1.6	15
34	Downstream Products are Potent Inhibitors of the Heparan Sulfate 2-O-Sulfotransferase. Scientific Reports, 2018, 8, 11832.	1.6	11
35	Predicting the Structures of Glycans, Glycoproteins, and Their Complexes. Chemical Reviews, 2018, 118, 8005-8024.	23.0	130
36	Induction of Antibodies Directed Against Branched Core <i>O</i> â€Mannosyl Glycopeptides—Selectivity Complimentary to the ConA Lectin. Chemistry - A European Journal, 2017, 23, 3466-3473.	1.7	12

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37	Structural Analysis of the Glycosylated Intact HIV-1 gp120–b12 Antibody Complex Using Hydroxyl Radical Protein Footprinting. Biochemistry, 2017, 56, 957-970.	1.2	27
38	The Tetrameric Plant Lectin BanLec Neutralizes HIV through Bidentate Binding to Specific Viral Glycans. Structure, 2017, 25, 773-782.e5.	1.6	39
39	<i>O</i> -Acetyl Side-Chains in Monosaccharides: Redundant NMR Spin-Couplings and Statistical Models for Acetate Ester Conformational Analysis. Journal of Physical Chemistry B, 2017, 121, 66-77.	1.2	25
40	Synthesis of 3- <i>O</i> -Sulfated Oligosaccharides to Understand the Relationship between Structures and Functions of Heparan Sulfate. Journal of the American Chemical Society, 2017, 139, 5249-5256.	6.6	79
41	Conformational Populations of β-(1→4) <i>O</i> -Glycosidic Linkages Using Redundant NMR <i>J</i> -Couplings and Circular Statistics. Journal of Physical Chemistry B, 2017, 121, 3042-3058.	1.2	39
42	Recent H3N2 Viruses Have Evolved Specificity for Extended, Branched Human-type Receptors, Conferring Potential for Increased Avidity. Cell Host and Microbe, 2017, 21, 23-34.	5.1	163
43	Mannobiose Binding Induces Changes in Hydrogen Bonding and Protonation States of Acidic Residues in Concanavalin A As Revealed by Neutron Crystallography. Biochemistry, 2017, 56, 4747-4750.	1.2	25
44	O2 sensing–associated glycosylation exposes the F-box–combining site of the Dictyostelium Skp1 subunit in E3 ubiquitin ligases. Journal of Biological Chemistry, 2017, 292, 18897-18915.	1.6	25
45	Quantitative Protein Topography Measurements by High Resolution Hydroxyl Radical Protein Footprinting Enable Accurate Molecular Model Selection. Scientific Reports, 2017, 7, 4552.	1.6	60
46	New insights into influenza A specificity: an evolution of paradigms. Current Opinion in Structural Biology, 2017, 44, 219-231.	2.6	34
47	Gas-Phase Analysis of the Complex of Fibroblast GrowthFactor 1 with Heparan Sulfate: A Traveling Wave Ion Mobility Spectrometry (TWIMS) and Molecular Modeling Study. Journal of the American Society for Mass Spectrometry, 2017, 28, 96-109.	1.2	18
48	Three mutations switch H7N9 influenza to human-type receptor specificity. PLoS Pathogens, 2017, 13, e1006390.	2.1	83
49	NMR Spin-Couplings in Saccharides: Relationships Between Structure, Conformation and the Magnitudes of <i>J</i> HH, <i>J</i> CH and <i>J</i> CC Values. New Developments in NMR, 2017, , 20-100.	0.1	20
50	Gly-Spec: a webtool for predicting glycan specificity by integrating glycan array screening data and 3D structure. Glycobiology, 2016, 26, 1027-1028.	1.3	19
51	Extension and validation of the GLYCAM force field parameters for modeling glycosaminoglycans. Canadian Journal of Chemistry, 2016, 94, 927-935.	0.6	69
52	3D implementation of the symbol nomenclature for graphical representation of glycans. Glycobiology, 2016, 26, 786-787.	1.3	59
53	Uncovering the Relationship between Sulphation Patterns and Conformation of Iduronic Acid in Heparan Sulphate. Scientific Reports, 2016, 6, 29602.	1.6	53
54	Asn347 Glycosylation of Corticosteroid-binding Globulin Fine-tunes the Host Immune Response by Modulating Proteolysis by Pseudomonas aeruginosa and Neutrophil Elastase. Journal of Biological Chemistry, 2016, 291, 17727-17742.	1.6	27

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55	The Dependence of Carbohydrate–Aromatic Interaction Strengths on the Structure of the Carbohydrate. Journal of the American Chemical Society, 2016, 138, 7636-7648.	6.6	44
56	Vina-Carb: Improving Glycosidic Angles during Carbohydrate Docking. Journal of Chemical Theory and Computation, 2016, 12, 892-901.	2.3	94
57	Integrated Omics and Computational Glycobiology Reveal Structural Basis for Influenza A Virus Glycan Microheterogeneity and Host Interactions. Molecular and Cellular Proteomics, 2016, 15, 1895-1912.	2.5	85
58	Insights into furanose solution conformations: beyond the two-state model. Journal of Biomolecular NMR, 2016, 64, 291-305.	1.6	25
59	Combining 3D structure with glycan array data provides insight into the origin of glycan specificity. Glycobiology, 2016, 26, 772-783.	1.3	39
60	The Interaction of Heparin Tetrasaccharides with Chemokine CCL5 Is Modulated by Sulfation Pattern and pH. Journal of Biological Chemistry, 2015, 290, 15421-15436.	1.6	52
61	Specificity of Furanoside–Protein Recognition through Antibody Engineering and Molecular Modeling. Chemistry - A European Journal, 2015, 21, 1138-1148.	1.7	9
62	Analysis of site-specific <i>N</i> -glycan remodeling in the endoplasmic reticulum and the Golgi. Glycobiology, 2015, 25, 1335-1349.	1.3	60
63	Glycopeptide analogues of PSGL-1 inhibit P-selectin in vitro and in vivo. Nature Communications, 2015, 6, 6387.	5.8	69
64	Genetically Encoded Fragment-Based Discovery of Glycopeptide Ligands for Carbohydrate-Binding Proteins. Journal of the American Chemical Society, 2015, 137, 5248-5251.	6.6	67
65	Investigating changes in the gas-phase conformation of Antithrombin III upon binding of Arixtra using traveling wave ion mobility spectrometry (TWIMS). Analyst, The, 2015, 140, 6980-6989.	1.7	24
66	Impact of sulfation pattern on the conformation and dynamics of sulfated fucan oligosaccharides as revealed by NMR and MD. Glycobiology, 2015, 25, 535-547.	1.3	19
67	Calculating Binding Free Energies for Protein–Carbohydrate Complexes. Methods in Molecular Biology, 2015, 1273, 431-465.	0.4	13
68	Fucosylated Chondroitin Sulfates from the Body Wall of the Sea Cucumber Holothuria forskali. Journal of Biological Chemistry, 2014, 289, 28284-28298.	1.6	88
69	Predicting the Origins of Anti-Blood Group Antibody Specificity: A Case Study of the ABO A- and B-Antigens. Frontiers in Immunology, 2014, 5, 397.	2.2	9
70	Defining the structural origin of the substrate sequence independence of O-GlcNAcase using a combination of molecular docking and dynamics simulation. Glycobiology, 2014, 24, 85-96.	1.3	13
71	Presentation, presentation, presentation! Molecular-level insight into linker effects on glycan array screening data. Glycobiology, 2014, 24, 17-25.	1.3	80
72	Importance of ligand conformational energies in carbohydrate docking: Sorting the wheat from the chaff. Journal of Computational Chemistry, 2014, 35, 526-539.	1.5	67

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73	Recent advances in employing molecular modelling to determine the specificity of glycan-binding proteins. Current Opinion in Structural Biology, 2014, 28, 47-55.	2.6	28
74	Effect of microfibril twisting on theoretical powder diffraction patterns of cellulose Iβ. Cellulose, 2014, 21, 879-884.	2.4	62
75	BFMP: A Method for Discretizing and Visualizing Pyranose Conformations. Journal of Chemical Information and Modeling, 2014, 54, 2744-2750.	2.5	18
76	Probing the paramyxovirus fusion (F) protein-refolding event from pre- to postfusion by oxidative footprinting. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E2596-605.	3.3	44
77	Unraveling Cellulose Microfibrils: A Twisted Tale. Biopolymers, 2013, 99, 746-756.	1.2	59
78	Enzymatic Basis for N-Glycan Sialylation. Journal of Biological Chemistry, 2013, 288, 34680-34698.	1.6	116
79	Contribution of the empirical dispersion correction on the conformation of short alanine peptides obtained by gas-phase QM calculations. Canadian Journal of Chemistry, 2013, 91, 859-865.	0.6	9
80	Sugarâ€Modified Foldamers as Conformationally Defined and Biologically Distinct Glycopeptide Mimics. Angewandte Chemie, 2013, 125, 10411-10416.	1.6	9
81	Computational Screening of the Human TF-Glycome Provides a Structural Definition for the Specificity of Anti-Tumor Antibody JAA-F11. PLoS ONE, 2013, 8, e54874.	1.1	29
82	The Influence of N-Linked Glycans on the Molecular Dynamics of the HIV-1 gp120 V3 Loop. PLoS ONE, 2013, 8, e80301.	1.1	35
83	Metabolism of Vertebrate Amino Sugars with N-Glycolyl Groups. Journal of Biological Chemistry, 2012, 287, 28917-28931.	1.6	46
84	Dependence of Pyranose Ring Puckering on Anomeric Configuration: Methyl Idopyranosides. Journal of Physical Chemistry B, 2012, 116, 6380-6386.	1.2	35
85	Carbohydrate Recognition by an Architecturally Complex α-N-Acetylglucosaminidase from Clostridium perfringens. PLoS ONE, 2012, 7, e33524.	1.1	42
86	Carbohydrate force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 652-697.	6.2	87
87	Molecular Recognition of Candida albicans (1→2)-β-Mannan Oligosaccharides by a Protective Monoclonal Antibody Reveals the Immunodominance of Internal Saccharide Residues. Journal of Biological Chemistry, 2012, 287, 18078-18090.	1.6	39
88	Computational Techniques Applied to Defining Carbohydrate Antigenicity. , 2012, , 361-383.		4
89	Unusual chemical and enzymatic stability of polysialic acid containing N â€glycolylneuraminic acid. FASEB Journal, 2012, 26, 610.1.	0.2	0
90	On the Role of Water Models in Quantifying the Binding Free Energy of Highly Conserved Water Molecules in Proteins: The Case of Concanavalin A. Journal of Chemical Theory and Computation, 2011, 7, 3391-3398.	2.3	31

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91	From agonist to antagonist: Structure and dynamics of innate immune glycoprotein MD-2 upon recognition of variably acylated bacterial endotoxins. Molecular Immunology, 2011, 49, 124-133.	1.0	37
92	Structure and binding analysis of Polyporus squamosus lectin in complex with the Neu5Acα2-6Galβ1-4GlcNAc human-type influenza receptor. Glycobiology, 2011, 21, 973-984.	1.3	53
93	Computational glycoscience: characterizing the spatial and temporal properties of glycans and glycan–protein complexes. Current Opinion in Structural Biology, 2010, 20, 575-583.	2.6	74
94	Molecular simulations of carbohydrates and protein–carbohydrate interactions: motivation, issues and prospects. Drug Discovery Today, 2010, 15, 596-609.	3.2	165
95	Presentation of Membrane-Anchored Glycosphingolipids Determined from Molecular Dynamics Simulations and NMR Paramagnetic Relaxation Rate Enhancement. Journal of the American Chemical Society, 2010, 132, 1334-1338.	6.6	58
96	GLYCAM06: A generalizable biomolecular force field. Carbohydrates. Journal of Computational Chemistry, 2008, 29, 622-655.	1.5	1,778
97	Quantifying protein interface footprinting by hydroxyl radical oxidation and molecular dynamics simulation: Application to galectin-1. Journal of the American Society for Mass Spectrometry, 2008, 19, 1692-1705.	1.2	65
98	Extension of the GLYCAM06 biomolecular force field to lipids, lipid bilayers and glycolipids. Molecular Simulation, 2008, 34, 349-364.	0.9	93
99	Involvement of Water in Carbohydrateâ^ Protein Binding: Concanavalin A Revisited. Journal of the American Chemical Society, 2008, 130, 16933-16942.	6.6	89
100	On Achieving Experimental Accuracy from Molecular Dynamics Simulations of Flexible Molecules: Aqueous Glycerol. Journal of Physical Chemistry A, 2008, 112, 2634-2639.	1.1	36
101	Approach for the Simulation and Modeling of Flexible Rings:  Application to the α- <scp>d</scp> -Arabinofuranoside Ring, a Key Constituent of Polysaccharides from <i>Mycobacterium tuberculosis</i> . Journal of Chemical Theory and Computation, 2008, 4, 184-191.	2.3	24
102	The Conformational Properties of Methyl α-(2,8)-Di/Trisialosides and Their <i>N</i> -Acyl Analogues: Implications for Anti- <i>Neisseria meningitidis</i> B Vaccine Design. Biochemistry, 2008, 47, 12493-12514.	1.2	43
103	Structural glycobiology: A game of snakes and ladders. Glycobiology, 2008, 18, 426-440.	1.3	130
104	Atomic-resolution conformational analysis of the GM3 ganglioside in a lipid bilayer and its implications for ganglioside-protein recognition at membrane surfaces. Glycobiology, 2008, 19, 344-355.	1.3	62
105	The Application of Molecular Modeling Techniques to the Determination of Oligosaccharide Solution Conformations. Reviews in Computational Chemistry, 2007, , 129-165.	1.5	14
106	TIP5P-Consistent Treatment of Electrostatics for Biomolecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1721-1733.	2.3	27
107	Gaussian induced dipole polarization model. Journal of Computational Chemistry, 2007, 28, 1261-1274.	1.5	104
108	Fourier transform mass spectrometry to monitor hyaluronan-protein interactions: use of hydrogen/deuterium amide exchange. Rapid Communications in Mass Spectrometry, 2007, 21, 121-131.	0.7	14

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109	Structural Basis of the Inhibition of Golgi α-Mannosidase II by Mannostatin A and the Role of the Thiomethyl Moiety in Ligandâ^'Protein Interactions. Journal of the American Chemical Society, 2006, 128, 8310-8319.	6.6	59
110	Reconciling solvent effects on rotamer populations in carbohydrates — A joint MD and NMR analysis. Canadian Journal of Chemistry, 2006, 84, 569-579.	0.6	47
111	Predicting the Three-Dimensional Structures of AntiCarbohydrate Antibodies: Combining Comparative Modeling and MD Simulations. ACS Symposium Series, 2006, , 203-219.	0.5	7
112	Understanding the bacterial polysaccharide antigenicity of Streptococcus agalactiae versus Streptococcus pneumoniae. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 8149-8154.	3.3	41
113	Structural elucidation of type III group B Streptococcus capsular polysaccharide using molecular dynamics simulations: the role of sialic acid. Carbohydrate Research, 2005, 340, 1007-1018.	1.1	48
114	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
115	A hydration study of (1→4) and (1→6) linked α-glucans by comparative 10 ns molecular dynamics simulations and 500-MHz NMR. Journal of Computational Chemistry, 2004, 25, 573-586.	1.5	63
116	Effects of Glycosylation on Peptide Conformation:Â A Synergistic Experimental and Computational Study. Journal of the American Chemical Society, 2004, 126, 8421-8425.	6.6	124
117	Molecular dynamics simulations of galectin-1-oligosaccharide complexes reveal the molecular basis for ligand diversity. Proteins: Structure, Function and Bioinformatics, 2003, 53, 229-240.	1.5	46
118	The Xenograft Antigen Bound to Griffonia simplicifolia Lectin 1-B4. Journal of Biological Chemistry, 2002, 277, 6615-6621.	1.6	54
119	Quantum Mechanical Study of the Nonbonded Forces in Waterâ `Methanol Complexes. Journal of Physical Chemistry A, 2001, 105, 4150-4155.	1.1	101
120	Involvement of Water in Carbohydrateâ^'Protein Binding. Journal of the American Chemical Society, 2001, 123, 12238-12247.	6.6	154
121	Relative Energies of Binding for Antibodyâ^'Carbohydrate-Antigen Complexes Computed from Free-Energy Simulations. Journal of the American Chemical Society, 2000, 122, 331-338.	6.6	57
122	Computational carbohydrate chemistry: what theoretical methods can tell us. , 1998, 15, 209-216.		106
123	The high degree of internal flexibility observed for an oligomannose oligosaccharide does not alter the overall topology of the molecule. FEBS Journal, 1998, 258, 372-386.	0.2	131
124	NMR and Molecular Dynamics Studies of the Conformational Epitope of the Type III Group BStreptococcusCapsular Polysaccharide and Derivativesâ€. Biochemistry, 1997, 36, 3278-3292.	1.2	107
125	The effects of variable glycosylation on the functional activities of ribonuclease, plasminogen and tissue plasminogen activator. BBA - Proteins and Proteomics, 1995, 1248, 1-10.	2.1	97
126	Molecular Mechanical and Molecular Dynamic Simulations of Glycoproteins and Oligosaccharides. 1. GLYCAM_93 Parameter Development. The Journal of Physical Chemistry, 1995, 99, 3832-3846.	2.9	427

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127	Three-dimensional structures of oligosaccharides. Current Opinion in Structural Biology, 1995, 5, 591-598.	2.6	76
128	Molecular mechanical investigations of the properties of oxocarbenium ions. 1. Parameter development. Journal of the American Chemical Society, 1992, 114, 850-858.	6.6	27
129	Molecular mechanical investigations of the properties of oxocarbenium ions. 2. Application to glycoside hydrolysis. Journal of the American Chemical Society, 1992, 114, 859-864.	6.6	101
130	Derivation of net atomic charges from molecular electrostatic potentials. Journal of Computational Chemistry, 1990, 11, 297-310.	1.5	149
131	Combining NMR and Simulation Methods in Oligosaccharide Conformational Analysis. , 0, , 109-144.		2