Robert J Woods

List of Publications by Year
in descending order

131	17,141	36203	15218
papers	citations	51 h-index	126 g-index

140	140	140	20710
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
2	GLYCAM06: A generalizable biomolecular force field. Carbohydrates. Journal of Computational Chemistry, 2008, 29, 622-655.	1.5	1,778
3	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
4	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
5	Updates to the Symbol Nomenclature for Glycans guidelines. Glycobiology, 2019, 29, 620-624.	1.3	292
6	Analysis of the SARS-CoV-2 spike protein glycan shield reveals implications for immune recognition. Scientific Reports, 2020, 10, 14991.	1.6	286
7	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
8	Molecular simulations of carbohydrates and proteinâ€“carbohydrate interactions: motivation, issues and prospects. Drug Discovery Today, 2010, 15, 596-609.	3.2	165
9	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
10	Involvement of Water in Carbohydrateâ^'Protein Binding. Journal of the American Chemical Society, 2001, 123, 12238-12247.	6.6	154
11	Derivation of net atomic charges from molecular electrostatic potentials. Journal of Computational Chemistry, 1990, 11, 297-310.	1.5	149
12	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
13	Structural glycobiology: A game of snakes and ladders. Glycobiology, 2008, 18, 426-440.	1.3	130
14	Predicting the Structures of Glycans, Glycoproteins, and Their Complexes. Chemical Reviews, 2018, 118, 8005-8024.	23.0	130
15	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
16	GlyGen: Computational and Informatics Resources for Glycoscience. Glycobiology, 2020, 30, 72-73.	1.3	123
17	Enzymatic Basis for N-Glycan Sialylation. Journal of Biological Chemistry, 2013, 288, 34680-34698.	1.6	116
18	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

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19	Computational carbohydrate chemistry: what theoretical methods can tell us. , 1998, 15, 209-216.		106
20	Gaussian induced dipole polarization model. Journal of Computational Chemistry, 2007, 28, 1261-1274.	1.5	104
21	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
22	Quantum Mechanical Study of the Nonbonded Forces in Waterâ"Methanol Complexes. Journal of Physical Chemistry A, 2001, 105, 4150-4155.	1.1	101
23	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
24	Vina-Carb: Improving Glycosidic Angles during Carbohydrate Docking. Journal of Chemical Theory and Computation, 2016, 12, 892-901.	2.3	94
25	Extension of the GLYCAM06 biomolecular force field to lipids, lipid bilayers and glycolipids. Molecular Simulation, 2008, 34, 349-364.	0.9	93
26	Involvement of Water in Carbohydrateâ"Protein Binding: Concanavalin A Revisited. Journal of the American Chemical Society, 2008, 130, 16933-16942.	6.6	89
27	Fucosylated Chondroitin Sulfates from the Body Wall of the Sea Cucumber Holothuria forskali. Journal of Biological Chemistry, 2014, 289, 28284-28298.	1.6	88
28	Carbohydrate force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 652-697.	6.2	87
29	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
30	Three mutations switch H7N9 influenza to human-type receptor specificity. PLoS Pathogens, 2017, 13, e1006390.	2.1	83
31	Presentation, presentation, presentation! Molecular-level insight into linker effects on glycan array screening data. Glycobiology, 2014, 24, 17-25.	1.3	80
32	Synthesis of 3-O-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
33	Three-dimensional structures of oligosaccharides. Current Opinion in Structural Biology, 1995, 5, 591-598.	2.6	76
34	Computational glycoscience: characterizing the spatial and temporal properties of glycans and glycanâ€"protein complexes. Current Opinion in Structural Biology, 2010, 20, 575-583.	2.6	74
35	Glycopeptide analogues of PSGL-1 inhibit P-selectin in vitro and in vivo. Nature Communications, 2015, 6, 6387.	5.8	69
36	Extension and validation of the GLYCAM force field parameters for modeling glycosaminoglycans. Canadian Journal of Chemistry, 2016, 94, 927-935.	0.6	69

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37	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
38	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
39	Galectin binding to cells and glycoproteins with genetically modified glycosylation reveals galectinâ€“glycan specificities in a natural context. Journal of Biological Chemistry, 2018, 293, 20249-20262.	1.6	67
40	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
41	A hydration study of (1â†'4) and (1â†'6) linked Î±-glucans by comparative 10 ns molecular dynamics simulations and 500-MHz NMR. Journal of Computational Chemistry, 2004, 25, 573-586.	1.5	63
42	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
43	Effect of microfibril twisting on theoretical powder diffraction patterns of cellulose Iβ. Cellulose, 2014, 21, 879-884.	2.4	62
44	Analysis of site-specificN-glycan remodeling in the endoplasmic reticulum and the Golgi. Glycobiology, 2015, 25, 1335-1349.	1.3	60
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	Structural Basis of the Inhibition of Golgi Î±-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
47	Unraveling Cellulose Microfibrils: A Twisted Tale. Biopolymers, 2013, 99, 746-756.	1.2	59
48	3D implementation of the symbol nomenclature for graphical representation of glycans. Glycobiology, 2016, 26, 786-787.	1.3	59
49	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
50	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
51	The Xenograft Antigen Bound to Griffonia simplicifolia Lectin 1-B4. Journal of Biological Chemistry, 2002, 277, 6615-6621.	1.6	54
52	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
53	Uncovering the Relationship between Sulphation Patterns and Conformation of Iduronic Acid in Heparan Sulphate. Scientific Reports, 2016, 6, 29602.	1.6	53
54	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

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55	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
56	Reconciling solvent effects on rotamer populations in carbohydrates Â— A joint MD and NMR analysis. Canadian Journal of Chemistry, 2006, 84, 569-579.	0.6	47
57	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
58	Metabolism of Vertebrate Amino Sugars with N-Glycolyl Groups. Journal of Biological Chemistry, 2012, 287, 28917-28931.	1.6	46
59	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
60	The Dependence of Carbohydrateâ€“Aromatic Interaction Strengths on the Structure of the Carbohydrate. Journal of the American Chemical Society, 2016, 138, 7636-7648.	6.6	44
61	The Conformational Properties of Methyl Î±-(2,8)-Di/Trisialosides and Their N-Acyl Analogues: Implications for Anti-Neisseria meningitidis B Vaccine Design. Biochemistry, 2008, 47, 12493-12514.	1.2	43
62	Carbohydrate Recognition by an Architecturally Complex Î±-N-Acetylglucosaminidase from Clostridium perfringens. PLoS ONE, 2012, 7, e33524.	1.1	42
63	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
64	Molecular Recognition of Candida albicans (1â†'2)-Î²-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
65	Combining 3D structure with glycan array data provides insight into the origin of glycan specificity. Glycobiology, 2016, 26, 772-783.	1.3	39
66	The Tetrameric Plant Lectin BanLec Neutralizes HIV through Bidentate Binding to Specific Viral Glycans. Structure, 2017, 25, 773-782.e5.	1.6	39
67	Conformational Populations of Î²-(1â†'4) O-Glycosidic Linkages Using Redundant NMR J-Couplings and Circular Statistics. Journal of Physical Chemistry B, 2017, 121, 3042-3058.	1.2	39
68	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
69	On Achieving Experimental Accuracy from Molecular Dynamics Simulations of Flexible Molecules:â€‰ Aqueous Glycerol. Journal of Physical Chemistry A, 2008, 112, 2634-2639.	1.1	36
70	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
71	Fluorescent Trimeric Hemagglutinins Reveal Multivalent Receptor Binding Properties. Journal of Molecular Biology, 2019, 431, 842-856.	2.0	36
72	O-glycosylation on cerebrospinal fluid and plasma apolipoprotein E differs in the lipid-binding domain. Glycobiology, 2020, 30, 74-85.	1.3	36

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73	Dependence of Pyranose Ring Puckering on Anomeric Configuration: Methyl Idopyranosides. Journal of Physical Chemistry B, 2012, 116, 6380-6386.	1.2	35
74	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
75	New insights into influenza A specificity: an evolution of paradigms. Current Opinion in Structural Biology, 2017, 44, 219-231.	2.6	34
76	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
77	Hyper-truncated Asn355- and Asn391-glycans modulate the activity of neutrophil granule myeloperoxidase. Journal of Biological Chemistry, 2021, 296, 100144.	1.6	31
78	Landscape and selection of vaccine epitopes in SARS-CoV-2. Genome Medicine, 2021, 13, 101.	3.6	30
79	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
80	Use of Circular Statistics To Model Î±Man-(1â†'2)-Î±Man and Î±Man-(1â†'3)-Î±/Î²Man O-Glycosidic Linkage Conformation in ¹³C-Labeled Disaccharides and High-Mannose Oligosaccharides. Biochemistry, 2019, 58, 546-560.	1.2	29
81	PD-L1 Glycosylation and Its Impact on Binding to Clinical Antibodies. Journal of Proteome Research, 2021, 20, 485-497.	1.8	29
82	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
83	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
84	TIP5P-Consistent Treatment of Electrostatics for Biomolecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1721-1733.	2.3	27
85	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
86	Structural Analysis of the Glycosylated Intact HIV-1 gp120â€"b12 Antibody Complex Using Hydroxyl Radical Protein Footprinting. Biochemistry, 2017, 56, 957-970.	1.2	27
87	GAG Builder: a web-tool for modeling 3D structures of glycosaminoglycans. Glycobiology, 2019, 29, 515-518.	1.3	27
88	Insights into furanose solution conformations: beyond the two-state model. Journal of Biomolecular NMR, 2016, 64, 291-305.	1.6	25
89	O-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
90	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

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91	O2 sensingâ€“associated glycosylation exposes the F-boxâ€“combining site of the Dictyostelium Skp1 subunit in E3 ubiquitin ligases. Journal of Biological Chemistry, 2017, 292, 18897-18915.	1.6	25
92	Approach for the Simulation and Modeling of Flexible Rings:â€‰ Application to the Î±-<scp>d</scp>-Arabinofuranoside Ring, a Key Constituent of Polysaccharides from Mycobacterium tuberculosis. Journal of Chemical Theory and Computation, 2008, 4, 184-191.	2.3	24
93	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
94	Hierarchical Multivalent Effects Control Influenza Host Specificity. ACS Central Science, 2020, 6, 2311-2318.	5.3	20
95	Allosteric regulation of lysosomal enzyme recognition by the cation-independent mannose 6-phosphate receptor. Communications Biology, 2020, 3, 498.	2.0	20
96	NMR Spin-Couplings in Saccharides: Relationships Between Structure, Conformation and the Magnitudes of JHH, JCH and JCC Values. New Developments in NMR, 2017, , 20-100.	0.1	20
97	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
98	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
99	Defining the Specificity of Carbohydrateâ€“Protein Interactions by Quantifying Functional Group Contributions. Journal of Chemical Information and Modeling, 2018, 58, 1889-1901.	2.5	19
100	BFMP: A Method for Discretizing and Visualizing Pyranose Conformations. Journal of Chemical Information and Modeling, 2014, 54, 2744-2750.	2.5	18
101	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
102	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
103	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
104	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
105	Synthesis and O-Glycosidic Linkage Conformational Analysis of ¹³C-Labeled Oligosaccharide Fragments of an Antifreeze Glycolipid. Journal of Organic Chemistry, 2019, 84, 1706-1724.	1.7	15
106	The Application of Molecular Modeling Techniques to the Determination of Oligosaccharide Solution Conformations. Reviews in Computational Chemistry, 2007, , 129-165.	1.5	14
107	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
108	Oligosaccharide model of the vascular endothelial glycocalyx in physiological flow. Microfluidics and Nanofluidics, 2018, 22, 21.	1.0	14

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109	Directed Evolution of Therapeutic Antibodies Targeting Glycosylation in Cancer. Cancers, 2020, 12, 2824.	1.7	14
110	Discovery of rare sulfated N-unsubstituted glucosamine based heparan sulfate analogs selectively activating chemokines. Chemical Science, 2021, 12, 3674-3681.	3.7	14
111	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
112	Calculating Binding Free Energies for Proteinâ€“Carbohydrate Complexes. Methods in Molecular Biology, 2015, 1273, 431-465.	0.4	13
113	Induction of Antibodies Directed Against Branched Core Oâ€Mannosyl Glycopeptidesâ€”Selectivity Complimentary to the ConA Lectin. Chemistry - A European Journal, 2017, 23, 3466-3473.	1.7	12
114	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
115	Reconciling MAâ€²AT and molecular dynamics models of linkage conformation in oligosaccharides. Physical Chemistry Chemical Physics, 2020, 22, 14454-14457.	1.3	12
116	Comparison of cellooligosaccharide conformations in complexes with proteins with energy maps for cellobiose. Carbohydrate Polymers, 2021, 264, 118004.	5.1	12
117	Downstream Products are Potent Inhibitors of the Heparan Sulfate 2-O-Sulfotransferase. Scientific Reports, 2018, 8, 11832.	1.6	11
118	Heparan Sulfate Mimetics Differentially Affect Homologous Chemokines and Attenuate Cancer Development. Journal of Medicinal Chemistry, 2021, 64, 3367-3380.	2.9	11
119	Effect of hydroxylysine-O-glycosylation on the structure of type I collagen molecule: A computational study. Glycobiology, 2020, 30, 830-843.	1.3	10
120	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
121	Sugarâ€Modified Foldamers as Conformationally Defined and Biologically Distinct Glycopeptide Mimics. Angewandte Chemie, 2013, 125, 10411-10416.	1.6	9
122	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
123	Specificity of Furanosideâ€“Protein Recognition through Antibody Engineering and Molecular Modeling. Chemistry - A European Journal, 2015, 21, 1138-1148.	1.7	9
124	NMR Resonance Assignment Methodology: Characterizing Large Sparsely Labeled Glycoproteins. Journal of Molecular Biology, 2019, 431, 2369-2382.	2.0	8
125	Predicting the Three-Dimensional Structures of AntiCarbohydrate Antibodies: Combining Comparative Modeling and MD Simulations. ACS Symposium Series, 2006, , 203-219.	0.5	7
126	A terminal Î±3-galactose modification regulates an E3 ubiquitin ligase subunit in Toxoplasma gondii. Journal of Biological Chemistry, 2020, 295, 9223-9243.	1.6	6

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127	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
128	Computational Techniques Applied to Defining Carbohydrate Antigenicity. , 2012, , 361-383.		4
129	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
130	Combining NMR and Simulation Methods in Oligosaccharide Conformational Analysis. , 0, , 109-144.		2
131	Unusual chemical and enzymatic stability of polysialic acid containing N â€glycolylneuraminic acid. FASEB Journal, 2012, 26, 610.1.	0.2	0