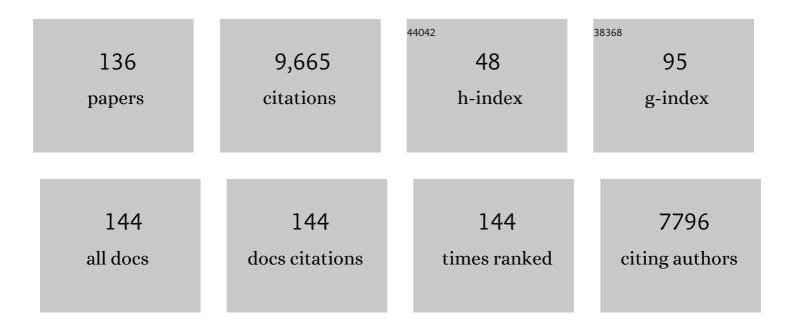
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Idealized powder diffraction patterns for cellulose polymorphs. Cellulose, 2014, 21, 885-896.	2.4	2,081
2	Cellulose polymorphy, crystallite size, and the Segal Crystallinity Index. Cellulose, 2013, 20, 583-588.	2.4	663
3	Segal crystallinity index revisited by the simulation of X-ray diffraction patterns of cotton cellulose IÎ <sup>2</sup> and cellulose II. Carbohydrate Polymers, 2016, 135, 1-9.	5.1	417
4	Effects of ball milling on the structure of cotton cellulose. Cellulose, 2019, 26, 305-328.	2.4	253
5	About the structure of cellulose: debating the Lindman hypothesis. Cellulose, 2012, 19, 589-598.	2.4	232
6	Neutron Crystallography, Molecular Dynamics, and Quantum Mechanics Studies of the Nature of Hydrogen Bonding in Cellulose I <sub>1²</sub> . Biomacromolecules, 2008, 9, 3133-3140.	2.6	215
7	Increment in evolution of cellulose crystallinity analysis. Cellulose, 2020, 27, 5445-5448.	2.4	214
8	Glucose, not cellobiose, is the repeating unit of cellulose and why that is important. Cellulose, 2017, 24, 4605-4609.	2.4	196
9	Comparative properties of cellulose nano-crystals from native and mercerized cotton fibers. Cellulose, 2012, 19, 1173-1187.	2.4	192
10	Relative stability of alternative chair forms and hydroxymethyl conformations of β-d-glucopyranose. Carbohydrate Research, 1995, 276, 219-251.	1.1	184
11	Evaluation of Density Functionals and Basis Sets for Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 679-692.	2.3	183
12	Characterization of cellulose II nanoparticles regenerated from 1-butyl-3-methylimidazolium chloride. Carbohydrate Polymers, 2013, 94, 773-781.	5.1	154
13	A comparison and chemometric analysis of several molecular mechanics force fields and parameter sets applied to carbohydrates. Carbohydrate Research, 1998, 314, 141-155.	1.1	150
14	Modeling of aldopyranosyl ring puckering with MM3 (92). Carbohydrate Research, 1994, 264, 1-19.	1.1	148
15	Factors controlling relative stability of anomers and hydroxymethyl conformers of glucopyranose. Journal of Computational Chemistry, 1998, 19, 1111-1129.	1.5	122
16	Conformational analysis of the anomeric forms of sophorose, laminarabiose, and cellobiose using MM3. Carbohydrate Research, 1992, 233, 15-34.	1.1	121
17	Characterization of cellulose I/II hybrid fibers isolated from energycane bagasse during the delignification process: Morphology, crystallinity and percentage estimation. Carbohydrate Polymers, 2015, 133, 438-447.	5.1	117
18	Cellulose nanofibers reinforced sodium alginate-polyvinyl alcohol hydrogels: Core-shell structure formation and property characterization. Carbohydrate Polymers, 2016, 147, 155-164.	5.1	116

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19	Conformational analysis of the anomeric forms of kojibiose, nigerose, and maltose using MM3. Carbohydrate Research, 1992, 230, 223-244.	1.1	105
20	Exploration of disaccharide conformations by molecular mechanics. Computational and Theoretical Chemistry, 1993, 286, 183-201.	1.5	104
21	Conformational Flexibility of Soluble Cellulose Oligomers: Chain Length and Temperature Dependence. Journal of the American Chemical Society, 2009, 131, 14786-14794.	6.6	102
22	Exo-anomeric effects on energies and geometries of different conformations of glucose and related systems in the gas phase and aqueous solution. Carbohydrate Research, 1997, 298, 1-14.	1.1	94
23	The effects of changes in ring geometry on computer models of amylose. Carbohydrate Research, 1973, 27, 391-406.	1.1	87
24	Comparison of different force fields for the study of disaccharides. Carbohydrate Research, 2009, 344, 2217-2228.	1.1	87
25	Linkage position in oligosaccharides by fast atom bombardment ionization, collision-activated dissociation, tandem mass spectrometry and molecular modeling. L-Fucosylp-(.alpha.1.fwdarw.X)-D-N-acetyl-D-glucosaminylp-(.beta.1.fwdarw.3)-D-galactosylp-(.beta.1-O-methyl) where X = 3. 4. or 6. Journal of the American Chemical Society, 1988, 110, 6931-6939.	6.6	86
26	Conformational analysis of trehalose disaccharides and analogues using MM3. Journal of Computational Chemistry, 1992, 13, 102-114.	1.5	86
27	Diffraction from nonperiodic models of cellulose crystals. Cellulose, 2012, 19, 319-336.	2.4	86
28	Miniature crystal models of cellulose polymorphs and other carbohydrates. International Journal of Biological Macromolecules, 1993, 15, 30-36.	3.6	83
29	HF/6-31G* energy surfaces for disaccharide analogs. Journal of Computational Chemistry, 2001, 22, 65-78.	1.5	78
30	Structural variations of cotton cellulose nanocrystals from deep eutectic solvent treatment: micro and nano scale. Cellulose, 2019, 26, 861-876.	2.4	73
31	pH-Responsive Water-Based Drilling Fluids Containing Bentonite and Chitin Nanocrystals. ACS Sustainable Chemistry and Engineering, 2018, 6, 3783-3795.	3.2	69
32	Constructing and evaluating energy surfaces of crystalline disaccharides. Journal of Molecular Graphics and Modelling, 2000, 18, 95-107.	1.3	63
33	Conformational Analyses of Native and Permethylated Disaccharides. Journal of Physical Chemistry A, 2002, 106, 4115-4124.	1.1	63
34	Cellulose and the twofold screw axis: modeling and experimental arguments. Cellulose, 2009, 16, 959-973.	2.4	62
35	Nanocellulose-Based Biosensors: Design, Preparation, and Activity of Peptide-Linked Cotton Cellulose Nanocrystals Having Fluorimetric and Colorimetric Elastase Detection Sensitivity. Engineering, 2013, 05, 20-28.	0.4	62
36	Effect of microfibril twisting on theoretical powder diffraction patterns of cellulose Iβ. Cellulose, 2014, 21, 879-884.	2.4	62

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#	Article	IF	CITATIONS
37	Immobilization of lysozyme-cellulose amide-linked conjugates on cellulose I and II cotton nanocrystalline preparations. Cellulose, 2012, 19, 495-506.	2.4	61
38	Relaxed-residue conformational mapping of the three linkage bonds of isomaltose and gentiobiose with MM3(92). Biopolymers, 1994, 34, 625-638.	1.2	60
39	What crystals of small analogs are trying to tell us about cellulose structure. Cellulose, 2004, 11, 5-22.	2.4	60
40	Quantum mechanics studies of cellobiose conformations. Canadian Journal of Chemistry, 2006, 84, 603-612.	0.6	59
41	Unraveling Cellulose Microfibrils: A Twisted Tale. Biopolymers, 2013, 99, 746-756.	1.2	59
42	Comparisons of rigid and relaxed conformational maps for cellobiose and maltose. Carbohydrate Research, 1989, 188, 206-211.	1.1	56
43	Chromophores in lignin-free cellulosic materials belong to three compound classes. Chromophores in cellulosics, XII. Cellulose, 2015, 22, 1053-1062.	2.4	56
44	The crystal structure of the α-cellobiose·2 Nal·2 H2O complex in the context of related structures and conformational analysis. Carbohydrate Research, 2002, 337, 851-861.	1.1	55
45	Conformational analysis of cellobiose by electronic structure theories. Carbohydrate Research, 2012, 350, 68-76.	1.1	55
46	Rigid- and relaxed-residue conformational analyses of cellobiose using the computer program mm2. Biopolymers, 1988, 27, 1519-1525.	1.2	54
47	van der Waals versus Hydrogen-Bonding Forces in a Crystalline Analog of Cellotetraose: Cyclohexyl 4′- <i>O</i> -Cyclohexyl l²- <scp>d</scp> -Cellobioside Cyclohexane Solvate. Journal of the American Chemical Society, 2008, 130, 16678-16690.	6.6	53
48	Young's modulus calculations for cellulose lβ by MM3 and quantum mechanics. Cellulose, 2011, 18, 505-516.	2.4	53
49	Chromophores in cellulosics, VI. First isolation and identification of residual chromophores from aged cotton linters. Cellulose, 2011, 18, 1623-1633.	2.4	50
50	A QM/MM analysis of the conformations of crystalline sucrose moieties. Carbohydrate Research, 2000, 326, 305-322.	1.1	48
51	Chemical and Physical Properties of Fructans. Journal of Plant Physiology, 1989, 134, 125-136.	1.6	45
52	Atomic resolution of cotton cellulose structure enabled by dynamic nuclear polarization solid-state NMR. Cellulose, 2019, 26, 329-339.	2.4	44
53	Modeling of Glucopyranose. ACS Symposium Series, 1990, , 120-140.	0.5	42
54	Molecular modeling methodology of β-cyclodextrin inclusion complexes. Computational and Theoretical Chemistry, 1996, 366, 113-117.	1.5	42

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55	Nanocellulose as a colorimetric biosensor for effective and facile detection of human neutrophil elastase. Carbohydrate Polymers, 2019, 216, 360-368.	5.1	42
56	Advanced conformational energy surfaces for cellobiose**. Cellulose, 2004, 11, 449-462.	2.4	41
57	Quantum Mechanics Studies of the Intrinsic Conformation of Trehalose. Journal of Physical Chemistry A, 2002, 106, 4988-4997.	1.1	39
58	The quintessential sustainable resource: cellulose, and the journal named for it. Cellulose, 2019, 26, 1-3.	2.4	39
59	Computer Modeling of Carbohydrates. ACS Symposium Series, 1990, , 1-19.	0.5	37
60	Linkage and pyranosyl ring twisting in cyclodextrins. Carbohydrate Research, 2007, 342, 1223-1237.	1.1	37
61	Molecular Mechanics Modeling of α-(1→2)-, α-(1→3)-, and α-(1→6)-Linked Mannosyl Disaccharides with MM3(92) <sup>1</sup> . Journal of Carbohydrate Chemistry, 1995, 14, 589-600.	0.4	36
62	Covalent attachment of lysozyme to cotton/cellulose materials: protein verses solid support activation. Cellulose, 2011, 18, 1239-1249.	2.4	36
63	Kinetic and structural analysis of fluorescent peptides on cotton cellulose nanocrystals as elastase sensors. Carbohydrate Polymers, 2015, 116, 278-285.	5.1	35
64	Electron (charge) density studies of cellulose models. Cellulose, 2014, 21, 1051-1063.	2.4	33
65	Preliminary potential energy calculations of cellulose i $\hat{l}\pm$ crystal structure. Macromolecular Theory and Simulations, 1994, 3, 185-191.	0.6	32
66	Analysis of the ring-form tautomers of psicose with MM3 (92). Journal of Computational Chemistry, 1994, 15, 561-570.	1.5	32
67	Accessible conformations of the β-d-(2→1)- and -(2→6)-linked d-fructans inulin and levan. Carbohydrate Research, 1988, 176, 17-29.	1.1	31
68	Conformational Analysis of a Disaccharide (Cellobiose) with the Molecular Mechanics Program (MM2). ACS Symposium Series, 1990, , 191-212.	0.5	31
69	Incremented alkyl derivatives enhance collision induced glycosidic bond cleavage in mass spectrometry of disaccharides. Journal of the American Society for Mass Spectrometry, 2003, 14, 63-78.	1.2	31
70	Comparative physical and chemical analyses of cotton fibers from two near isogenic upland lines differing in fiber wall thickness. Cellulose, 2017, 24, 2385-2401.	2.4	31
71	Cellulose nanofibers from rapidly microwave-delignified energy cane bagasse and their application in drilling fluids as rheology and filtration modifiers. Industrial Crops and Products, 2020, 150, 112378.	2.5	31
72	The external-anomeric torsional effect. Carbohydrate Research, 2005, 340, 853-862.	1.1	29

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73	Human neutrophil elastase detection with fluorescent peptide sensors conjugated to cellulosic and nanocellulosic materials: part II, structure/function analysis. Cellulose, 2016, 23, 1297-1309.	2.4	29
74	Disaccharide conformational maps: adiabaticity in analogues with variable ring shapes. Molecular Simulation, 2008, 34, 373-389.	0.9	28
75	Combining Computational Chemistry and Crystallography for a Better Understanding of the Structure of Cellulose. Advances in Carbohydrate Chemistry and Biochemistry, 2012, 67, 19-93.	0.4	28
76	Conformational analysis of 1-kestose by molecular mechanics and by n.m.r. spectroscopy. Carbohydrate Research, 1991, 217, 29-42.	1.1	27
77	Comparison and validation of Fourier transform infrared spectroscopic methods for monitoring secondary cell wall cellulose from cotton fibers. Cellulose, 2018, 25, 49-64.	2.4	27
78	Surface wetting behavior of nanocellulose-based composite films. Cellulose, 2018, 25, 5071-5087.	2.4	27
79	Overlapping anomeric effects in a sucrose analogue. Carbohydrate Research, 1993, 239, 51-60.	1.1	26
80	Computer modeling of the tetrasaccharide nystose. Carbohydrate Research, 1993, 247, 51-62.	1.1	26
81	Conformational analysis of inulobiose by molecular mechanics. Carbohydrate Research, 1990, 207, 221-235.	1.1	25
82	Chromophores in cellulosics, XI: isolation and identification of residual chromophores from bacterial cellulose. Cellulose, 2014, 21, 2271-2283.	2.4	25
83	Studies of crystalline native celluloses using potential energy calculations. Cellulose, 1994, 1, 161-168.	2.4	24
84	Determining the crystal structure of cellulose IIII by modeling. Carbohydrate Research, 2005, 340, 827-833.	1.1	24
85	QM/MM distortion energies in di- and oligosaccharides complexed with proteins. International Journal of Quantum Chemistry, 2001, 84, 416-425.	1.0	23
86	MM3(96) CONFORMATIONAL ANALYSIS OF d-GLUCARAMIDE AND X-RAY CRYSTAL STRUCTURES OF THREE d-GLUCARIC ACID DERIVATIVES—MODELS FOR SYNTHETIC POLY(ALKYLENE d-GLUCARAMIDES). Journal of Carbohydrate Chemistry, 2002, 21, 27-51.	0.4	23
87	1H and 13C solid-state NMR of Gossypium barbadense (Pima) cotton. Journal of Molecular Structure, 2008, 878, 177-184.	1.8	23
88	Twisting of glycosidic bonds by hydrolases. Carbohydrate Research, 2009, 344, 2157-2166.	1.1	23
89	Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. Tetrahedron: Asymmetry, 2005, 16, 577-586.	1.8	21
90	Structure/Function Analysis of Cotton-Based Peptide-Cellulose Conjugates: Spatiotemporal/Kinetic Assessment of Protease Aerogels Compared to Nanocrystalline and Paper Cellulose. International Journal of Molecular Sciences, 2018, 19, 840.	1.8	21

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91	Ab Initio-MIA and Molecular Mechanics Studies of the Distorted Sucrose Linkage of Raffinose. Journal of the American Chemical Society, 1994, 116, 9590-9595.	6.6	20
92	When anomeric effects collide. Journal of Computational Chemistry, 2001, 22, 1194-1204.	1.5	20
93	Chemistry of 2,5-dihydroxy-[1,4]-benzoquinone, a Key Chromophore in Aged Cellulosics. Mini-Reviews in Organic Chemistry, 2013, 10, 309-315.	0.6	20
94	Hydroxyl orientations in cellobiose and other polyhydroxyl compounds: modeling versus experiment. Cellulose, 2011, 18, 897-909.	2.4	18
95	Modeling of deoxy- and dideoxyaldohexopyranosyl ring puckering with MM3(92). Carbohydrate Research, 2001, 335, 261-273.	1.1	16
96	Contributions of Dexter French (1918–1981) to cycloamylose/cyclodextrin and starch science. Carbohydrate Polymers, 2021, 257, 117620.	5.1	16
97	Stepwise allomorphic transformations by alkaline and ethylenediamine treatments on bamboo crystalline cellulose for enhanced enzymatic digestibility. Industrial Crops and Products, 2022, 177, 114450.	2.5	16
98	An NMR, X-ray crystal structure, and molecular mechanics study of di-(3-deoxy-d-glycero-pentulose) 1,2′:2,1′ dianhydride. Carbohydrate Research, 1994, 260, 1-15.	1.1	15
99	MM3 MODELING OF ALDOPENTOSE PYRANOSE RINGS. Journal of Carbohydrate Chemistry, 2002, 21, 11-25.	0.4	14
100	Conformational analysis of xylobiose by DFT quantum mechanics. Cellulose, 2020, 27, 1207-1224.	2.4	14
101	N-Methylmorpholine-N-oxide (NMMO): hazards in practice and pitfalls in theory. Cellulose, 2021, 28, 5985-5990.	2.4	14
102	Conformational differences and steric energies for compounds containing α-d-glucopyranose chairs having a range of 0–4-0–1 distances. Carbohydrate Research, 1980, 87, 1-10.	1.1	13
103	Crystal structure of penta-O-acetyl-β-d-galactopyranose with modeling of the conformation of the acetate groups. Carbohydrate Research, 2002, 337, 2301-2310.	1.1	13
104	Octa-O-propanoyl-β-maltose: crystal structure, acyl stacking, related structures, and conformational analysis. Carbohydrate Research, 2007, 342, 1210-1222.	1.1	13
105	Experimental and theoretical electron density distribution of α,α-trehalose dihydrate. Carbohydrate Research, 2010, 345, 1469-1481.	1.1	13
106	Comparison of cellooligosaccharide conformations in complexes with proteins with energy maps for cellobiose. Carbohydrate Polymers, 2021, 264, 118004.	5.1	12
107	Chemistry of 5,8-dihydroxy-[1,4]-naphthoquinone, a Key Chromophore in Aged Cellulosics. Mini-Reviews in Organic Chemistry, 2013, 10, 302-308.	0.6	12
108	Molecular Modeling of Two Disaccharides Containing Fructopyranose Linked to Glucopyranose. Journal of Carbohydrate Chemistry, 1993, 12, 449-457.	0.4	11

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109	Synthesis and characterization of TEMPO-oxidized peptide-cellulose conjugate biosensors for detecting human neutrophil elastase. Cellulose, 2022, 29, 1293-1305.	2.4	11
110	Cotton Fiber Properties and Moisture: Water of Imbibition. Textile Reseach Journal, 2005, 75, 177-180.	1.1	10
111	2,4′:2′,4 Dianhydride of 3-keto-glucoside, a precursor to chromophores of aged, yellow cellulose, and its weak interactions. Cellulose, 2017, 24, 1227-1234.	2.4	10
112	Quantum mechanics models of the methanol dimer: O Hâ∢O hydrogen bonds of β- d -glucose moieties from crystallographic data. Carbohydrate Research, 2017, 443-444, 87-94.	1.1	10
113	Cotton Fiber Structure. , 2018, , 13-39.		9
114	Availability and disposition of hydroxyl groups on surfaces of crystalline cellulose II. Journal of Polymer Science: Polymer Chemistry Edition, 1974, 12, 445-454.	0.8	8
115	A Dehydration Method for Immature or Wet Cotton Fibers for Light and Electron Microscopy. Textile Reseach Journal, 2006, 76, 514-518.	1.1	8
116	In defense of adiabatic Ï•/l̈́ mapping for cellobiose and other disaccharides. Cellulose, 2011, 18, 889-896.	2.4	8
117	Computerized Molecular Modeling of Carbohydrates. Methods in Molecular Biology, 2011, 715, 21-42.	0.4	8
118	Detection of Human Neutrophil Elastase by Fluorescent Peptide Sensors Conjugated to TEMPO-Oxidized Nanofibrillated Cellulose. International Journal of Molecular Sciences, 2022, 23, 3101.	1.8	8
119	Cellulose Shapes. , 2007, , 257-284.		5
120	Energy Maps for Glycosidic Linkage Conformations. Methods in Molecular Biology, 2015, 1273, 333-358.	0.4	5
121	Modelling the Effect of Solvents on Carbohydrates. Mini-Reviews in Organic Chemistry, 2011, 8, 249-255.	0.6	5
122	Digital comparison of x-ray diffraction data from cotton textiles. Journal of Applied Polymer Science, 1980, 25, 1469-1478.	1.3	4
123	An Assessment of Surface Properties and Moisture Uptake of Nonwoven Fabrics from Ginning By-products. , 0, , .		4
124	100Âyears of cellulose fiber diffraction and the emergence of complementary techniques. Cellulose, 2014, 21, 1087-1089.	2.4	3
125	Structure/Function Analysis of Truncated Amino-Terminal ACE2 Peptide Analogs That Bind to SARS-CoV-2 Spike Glycoprotein. Molecules, 2022, 27, 2070.	1.7	3
126	Comments on the paper †The behavior of cellulose molecules in aqueous environments' by Tanaka and Fukui. Cellulose, 2004, 11, 39-42.	2.4	2

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127	Computerized Models of Carbohydrates. , 2014, , 1-38.		2
128	Synthesis and Molecular Structure of the 5-Methoxycarbonylpentyl α-Glycoside of the Upstream, Terminal Moiety of the O-Specific Polysaccharide of Vibrio cholerae O1, Serotype Inaba. Molecules, 2015, 20, 2892-2902.	1.7	2
129	The molecular structure and conformation of cellulose II (Fortisan) using accurate X-ray diffraction intensities. Journal of Macromolecular Science - Physics, 1985, 24, 229-245.	0.4	1
130	Thermally Induced Structural Transitions in Cotton Fiber Revealed by a Finite Mixture Model of Tenacity Distribution. ACS Sustainable Chemistry and Engineering, 2018, 6, 7420-7431.	3.2	1
131	When anomeric effects collide. Journal of Computational Chemistry, 2001, 22, 1194-1204.	1.5	1
132	Computerized Molecular Modeling of Carbohydrates. Methods in Molecular Biology, 2020, 2149, 513-539.	0.4	1
133	Combining Computational Chemistry and Crystallography for a Better Understanding of the Structure of Cellulose. Advances in Carbohydrate Chemistry and Biochemistry, 2021, 80, 15-93.	0.4	1
134	Comments on the proposed helical structure of cellulose I. Journal of Applied Polymer Science, 1972, 16, 1579-1579.	1.3	0
135	Paradigm for Improving the Catalytic Ability of Industrial Enzymes: Linkage Distortions of Carbohydrates in Complexes with Crystalline Proteins. ACS Symposium Series, 2007, , 207-219.	0.5	0

136 Computerized Models of Carbohydrates. , 2015, , 1397-1440.