Michael F Crowley

List of Publications by Year in Descending Order

117 papers	5,412 citations	46 h-index	71 g-index
120 ext. papers	6,223 ext. citations	6.6 avg, IF	5.61 L-index

#	Paper	IF	Citations
117	Towards Elucidating Structure-Spectra Relationships in Rhamnogalacturonan II: Computational Protocols for Accurate C and H Shifts for Apiose and Its Borate Esters.. *Frontiers in Molecular Biosciences*, **2021**, 8, 756219	5.6	
116	Coupling of Flavonoid Initiation Sites with Monolignols Studied by Density Functional Theory. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 1518-1528	8.3	3
115	Transition Path Sampling Study of the Feruloyl Esterase Mechanism. *Journal of Physical Chemistry B*, **2021**, 125, 2018-2030	3.4	4
114	Mechanism and Reaction Energy Landscape for Apiose Cross-Linking by Boric Acid in Rhamnogalacturonan II. *Journal of Physical Chemistry B*, **2020**, 124, 10117-10125	3.4	3
113	Reply to Cosgrove: Non-enzymatic action of expansins. *Journal of Biological Chemistry*, **2020**, 295, 6783	5.4	
112	Advances in Multiscale Modeling of Lignocellulosic Biomass. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 3512-3531	8.3	32
111	The hydrolysis mechanism of a GH45 cellulase and its potential relation to lytic transglycosylase and expansin function. *Journal of Biological Chemistry*, **2020**, 295, 4477-4487	5.4	9
110	Coupling and Reactions of Lignols and New Lignin Monomers: A Density Functional Theory Study. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 11033-11045	8.3	9
109	Molecular Lignin Solubility and Structure in Organic Solvents. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 17839-17850	8.3	16
108	Systematic parameterization of lignin for the CHARMM force field. *Green Chemistry*, **2019**, 21, 109-122	10	27
107	Glycosylation Is Vital for Industrial Performance of Hyperactive Cellulases. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 4792-4800	8.3	12
106	Message-passing neural networks for high-throughput polymer screening. *Journal of Chemical Physics*, **2019**, 150, 234111	3.9	32
105	Enabling microbial syringol conversion through structure-guided protein engineering. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 13970-13976	11.5	22
104	Nanomechanics of cellulose deformation reveal molecular defects that facilitate natural deconstruction. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 9825-9830	11.5	25
103	The dissociation mechanism of processive cellulases. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 23061-23067	11.5	21
102	Passive membrane transport of lignin-related compounds. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 23117-23123	11.5	49
101	Catalytic Mechanism of Aryl-Ether Bond Cleavage in Lignin by LigF and LigG. *Journal of Physical Chemistry B*, **2019**, 123, 10142-10151	3.4	1

100	A Quantitative Molecular Atlas for Interactions Between Lignin and Cellulose. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 19570-19583	8.3	9
99	Automated Transformation of Lignin Topologies into Atomic Structures with LigninBuilder. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 3443-3453	8.3	21
98	Engineering enhanced cellobiohydrolase activity. *Nature Communications*, **2018**, 9, 1186	17.4	47
97	Characterization and engineering of a plastic-degrading aromatic polyesterase. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E4350-E4357	11.5	369
96	Structural and molecular dynamics studies of a C1-oxidizing lytic polysaccharide monooxygenase from Heterobasidion irregulare reveal amino acids important for substrate recognition. *FEBS Journal*, **2018**, 285, 2225-2242	5.7	26
95	Iodine-Catalyzed Isomerization of Dimethyl Muconate. *ChemSusChem*, **2018**, 11, 1768-1780	8.3	11
94	Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. *Wiley Interdisciplinary Reviews: Energy and Environment*, **2018**, 7, e297	4.7	23
93	The impact of -glycan chemistry on the stability of intrinsically disordered proteins. *Chemical Science*, **2018**, 9, 3710-3715	9.4	12
92	Different Behaviors of a Substrate in P450 Decarboxylase and Hydroxylase Reveal Reactivity-Enabling Actors. *Scientific Reports*, **2018**, 8, 12826	4.9	7
91	Prediction of reaction knockouts to maximize succinate production by Actinobacillus succinogenes. *PLoS ONE*, **2018**, 13, e0189144	3.7	8
90	Membrane Permeability of Terpenoids Explored with Molecular Simulation. *Journal of Physical Chemistry B*, **2018**, 122, 10349-10361	3.4	14
89	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. *Nature Communications*, **2018**, 9, 2487	17.4	77
88	Estimation of the Maximum Theoretical Productivity of Fed-Batch Bioreactors. *IFAC-PapersOnLine*, **2017**, 50, 9883-9888	0.7	
87	Membrane Permeability of Fatty Acyl Compounds Studied via Molecular Simulation. *Journal of Physical Chemistry B*, **2017**, 121, 11311-11324	3.4	15
86	Structural, mutagenic and in silico studies of xyloglucan fucosylation in Arabidopsis thaliana suggest a water-mediated mechanism. *Plant Journal*, **2017**, 91, 931-949	6.9	36
85	Distinct roles of N- and O-glycans in cellulase activity and stability. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 13667-13672	11.5	52
84	Efficient estimation of the maximum metabolic productivity of batch systems. *Biotechnology for Biofuels*, **2017**, 10, 28	7.8	8
83	Density Functional Theory Study of Spirodienone Stereoisomers in Lignin. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 7188-7194	8.3	12

82	Diffraction pattern simulation of cellulose fibrils using distributed and quantized pair distances. *Journal of Applied Crystallography*, **2016**, 49, 2244-2248	3.8	7
81	Who's on base? Revealing the catalytic mechanism of inverting family 6 glycoside hydrolases. *Chemical Science*, **2016**, 7, 5955-5968	9.4	20
80	Coupling and Reactions of 5-Hydroxyconiferyl Alcohol in Lignin Formation. *Journal of Agricultural and Food Chemistry*, **2016**, 64, 4742-50	5.7	10
79	Comparison of the simulations of cellulosic crystals with three carbohydrate force fields. *Carbohydrate Research*, **2016**, 422, 17-23	2.9	9
78	Simulations of cellulose translocation in the bacterial cellulose synthase suggest a regulatory mechanism for the dimeric structure of cellulose. *Chemical Science*, **2016**, 7, 3108-3116	9.4	11
77	Comparing Residue Clusters from Thermophilic and Mesophilic Enzymes Reveals Adaptive Mechanisms. *PLoS ONE*, **2016**, 11, e0145848	3.7	17
76	Strategies to reduce end-product inhibition in family 48 glycoside hydrolases. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 295-304	4.2	8
75	Radical Nature of C-Lignin. *ACS Sustainable Chemistry and Engineering*, **2016**, 4, 5327-5335	8.3	34
74	Effects of lytic polysaccharide monooxygenase oxidation on cellulose structure and binding of oxidized cellulose oligomers to cellulases. *Journal of Physical Chemistry B*, **2015**, 119, 6129-43	3.4	72
73	The molecular origins of twist in cellulose I-beta. *Carbohydrate Polymers*, **2015**, 125, 146-52	10.3	34
72	Electronic coupling through natural amino acids. *Journal of Chemical Physics*, **2015**, 143, 225102	3.9	12
71	New perspective on glycoside hydrolase binding to lignin from pretreated corn stover. *Biotechnology for Biofuels*, **2015**, 8, 214	7.8	57
70	O-glycosylation effects on family 1 carbohydrate-binding module solution structures. *FEBS Journal*, **2015**, 282, 4341-56	5.7	15
69	Biomass Particle Models with Realistic Morphology and Resolved Microstructure for Simulations of Intraparticle Transport Phenomena. *Energy & Fuels*, **2015**, 29, 242-254	4.1	51
68	Experimental and modeling studies of an unusual water-filled pore structure with possible mechanistic implications in family 48 cellulases. *Journal of Physical Chemistry B*, **2014**, 118, 2306-15	3.4	6
67	The mechanism of cellulose hydrolysis by a two-step, retaining cellobiohydrolase elucidated by structural and transition path sampling studies. *Journal of the American Chemical Society*, **2014**, 136, 321-9	16.4	134
66	Predicting enzyme adsorption to lignin films by calculating enzyme surface hydrophobicity. *Journal of Biological Chemistry*, **2014**, 289, 20960-9	5.4	91
65	Simulation analysis of the cellulase Cel7A carbohydrate binding module on the surface of the cellulose I *Cellulose*, **2014**, 21, 951-971	5.5	17

64	Response to Comment on "Revealing nature's cellulase diversity: the digestion mechanism of Caldicellulosiruptor bescii CelA". *Science*, **2014**, 344, 578	33.3	1
63	Carbohydrate-protein interactions that drive processive polysaccharide translocation in enzymes revealed from a computational study of cellobiohydrolase processivity. *Journal of the American Chemical Society*, **2014**, 136, 8810-9	16.4	79
62	The structure of the catalytic domain of a plant cellulose synthase and its assembly into dimers. *Plant Cell*, **2014**, 26, 2996-3009	11.6	46
61	New faster CHARMM molecular dynamics engine. *Journal of Computational Chemistry*, **2014**, 35, 406-13	3.5	84
60	Towards a molecular-level theory of carbohydrate processivity in glycoside hydrolases. *Current Opinion in Biotechnology*, **2014**, 27, 96-106	11.4	73
59	Endoglucanase peripheral loops facilitate complexation of glucan chains on cellulose via adaptive coupling to the emergent substrate structures. *Journal of Physical Chemistry B*, **2013**, 117, 10750-8	3.4	14
58	3D electron tomography of pretreated biomass informs atomic modeling of cellulose microfibrils. *ACS Nano*, **2013**, 7, 8011-9	16.7	60
57	Crystal structure and computational characterization of the lytic polysaccharide monooxygenase GH61D from the Basidiomycota fungus Phanerochaete chrysosporium. *Journal of Biological Chemistry*, **2013**, 288, 12828-39	5.4	131
56	Revealing nature's cellulase diversity: the digestion mechanism of Caldicellulosiruptor bescii CelA. *Science*, **2013**, 342, 1513-6	33.3	221
55	Initial recognition of a cellodextrin chain in the cellulose-binding tunnel may affect cellobiohydrolase directional specificity. *Biophysical Journal*, **2013**, 104, 904-12	2.9	29
54	Binding site dynamics and aromatic-carbohydrate interactions in processive and non-processive family 7 glycoside hydrolases. *Journal of Physical Chemistry B*, **2013**, 117, 4924-33	3.4	48
53	Glycoside hydrolase processivity is directly related to oligosaccharide binding free energy. *Journal of the American Chemical Society*, **2013**, 135, 18831-9	16.4	71
52	Loop motions important to product expulsion in the Thermobifida fusca glycoside hydrolase family 6 cellobiohydrolase from structural and computational studies. *Journal of Biological Chemistry*, **2013**, 288, 33107-17	5.4	23
51	Computational investigation of the pH dependence of loop flexibility and catalytic function in glycoside hydrolases. *Journal of Biological Chemistry*, **2013**, 288, 12175-86	5.4	27
50	Glycosylated linkers in multimodular lignocellulose-degrading enzymes dynamically bind to cellulose. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 14646-51	11.5	131
49	Conversion of cellulose I to I via a high temperature intermediate (I-HT) and other cellulose phase transformations. *Cellulose*, **2012**, 19, 297-306	5.5	27
48	Binding preferences, surface attachment, diffusivity, and orientation of a family 1 carbohydrate-binding module on cellulose. *Journal of Biological Chemistry*, **2012**, 287, 20603-12	5.4	67
47	Comparison of Cellulose I Simulations with Three Carbohydrate Force Fields. *Journal of Chemical Theory and Computation*, **2012**, 8, 735-48	6.4	101

46	Computational investigation of glycosylation effects on a family 1 carbohydrate-binding module. *Journal of Biological Chemistry*, **2012**, 287, 3147-55	5.4	52
45	Product binding varies dramatically between processive and nonprocessive cellulase enzymes. *Journal of Biological Chemistry*, **2012**, 287, 24807-13	5.4	49
44	Cellulase linkers are optimized based on domain type and function: insights from sequence analysis, biophysical measurements, and molecular simulation. *PLoS ONE*, **2012**, 7, e48615	3.7	76
43	Examination of the α-chitin structure and decrystallization thermodynamics at the nanoscale. *Journal of Physical Chemistry B*, **2011**, 115, 4516-22	3.4	61
42	Decrystallization of Oligosaccharides from the Cellulose Iβ Surface with Molecular Simulation. *Journal of Physical Chemistry Letters*, **2011**, 2, 1546-1550	6.4	50
41	Protein allostery at the solid-liquid interface: endoglucanase attachment to cellulose affects glucan clenching in the binding cleft. *Journal of the American Chemical Society*, **2011**, 133, 16617-24	16.4	22
40	Molecular-level origins of biomass recalcitrance: decrystallization free energies for four common cellulose polymorphs. *Journal of Physical Chemistry B*, **2011**, 115, 4118-27	3.4	161
39	Coarse-Grain Model for Glucose, Cellobiose, and Cellotetraose in Water. *Journal of Chemical Theory and Computation*, **2011**, 7, 2137-50	6.4	26
38	High-temperature behavior of cellulose I. *Journal of Physical Chemistry B*, **2011**, 115, 2155-66	3.4	110
37	Sugar-binding sites on the surface of the carbohydrate-binding module of CBH I from Trichoderma reesei. *Carbohydrate Research*, **2011**, 346, 839-46	2.9	24
36	Applications of computational science for understanding enzymatic deconstruction of cellulose. *Current Opinion in Biotechnology*, **2011**, 22, 231-8	11.4	111
35	Modeling the self-assembly of the cellulosome enzyme complex. *Journal of Biological Chemistry*, **2011**, 286, 5614-23	5.4	37
34	Probing carbohydrate product expulsion from a processive cellulase with multiple absolute binding free energy methods. *Journal of Biological Chemistry*, **2011**, 286, 18161-9	5.4	64
33	Multiple functions of aromatic-carbohydrate interactions in a processive cellulase examined with molecular simulation. *Journal of Biological Chemistry*, **2011**, 286, 41028-35	5.4	88
32	Atomistic Simulation of Lignocellulosic Biomass and Associated Cellulosomal Protein Complexes. *ACS Symposium Series*, **2010**, 55-73	0.4	4
31	The O-glycosylated linker from the Trichoderma reesei Family 7 cellulase is a flexible, disordered protein. *Biophysical Journal*, **2010**, 99, 3773-81	2.9	89
30	Identification of amino acids responsible for processivity in a Family 1 carbohydrate-binding module from a fungal cellulase. *Journal of Physical Chemistry B*, **2010**, 114, 1447-53	3.4	102
29	Modeling the Cellulosome Using Multiscale Methods. *ACS Symposium Series*, **2010**, 75-98	0.4	

28	CHAMBER: Comprehensive support for CHARMM force fields within the AMBER software. *International Journal of Quantum Chemistry*, **2009**, 109, 3767-3772	2.1	64
27	Building a foundation for structure-based cellulosome design for cellulosic ethanol: Insight into cohesin-dockerin complexation from computer simulation. *Protein Science*, **2009**, 18, 949-59	6.3	17
26	Computational simulations of the Trichoderma reesei cellobiohydrolase I acting on microcrystalline cellulose Ibeta: the enzyme-substrate complex. *Carbohydrate Research*, **2009**, 344, 1984-92	2.9	46
25	The energy landscape for the interaction of the family 1 carbohydrate-binding module and the cellulose surface is altered by hydrolyzed glycosidic bonds. *Journal of Physical Chemistry B*, **2009**, 113, 10994-1002	3.4	69
24	Developing improved MD codes for understanding processive cellulases. *Journal of Physics: Conference Series*, **2008**, 125, 012049	0.3	2
23	Interactions of the complete cellobiohydrolase I from Trichodera reesei with microcrystalline cellulose I. *Cellulose*, **2008**, 15, 261-273	5.5	43
22	The implementation of a fast and accurate QM/MM potential method in Amber. *Journal of Computational Chemistry*, **2008**, 29, 1019-31	3.5	289
21	A biophysical perspective on the cellulosome: new opportunities for biomass conversion. *Current Opinion in Biotechnology*, **2008**, 19, 218-27	11.4	79
20	Molecular modeling suggests induced fit of Family I carbohydrate-binding modules with a broken-chain cellulose surface. *Protein Engineering, Design and Selection*, **2007**, 20, 179-87	1.9	72
19	Study of a highly accurate and fast protein–ligand docking method based on molecular dynamics. *Concurrency Computation Practice and Experience*, **2005**, 17, 1627-1641	1.4	22
18	Studying protein folding on the Grid: experiences using CHARMM on NPACI resources under Legion. *Concurrency Computation Practice and Experience*, **2004**, 16, 385-397	1.4	6
17	Modeling of the metallo-beta-lactamase from B. fragilis: structural and dynamic effects of inhibitor binding. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 448-59	4.2	41
16	A molecular level picture of the stabilization of A-DNA in mixed ethanol-water solutions. *Proceedings of the National Academy of Sciences of the United States of America*, **1997**, 94, 9626-30	11.5	99
15	Molecular dynamics simulation study of DNA dodecamer d(CGCGAATTCGCG) in solution: conformation and hydration. *Journal of Molecular Biology*, **1997**, 272, 553-72	6.5	98
14	Adventures in Improving the Scaling and Accuracy of a Parallel Molecular Dynamics Program. *Journal of Supercomputing*, **1997**, 11, 255-278	2.5	79
13	Stabilizing steady and periodic behavior in propagating flame fronts. *Physica D: Nonlinear Phenomena*, **1995**, 84, 12-22	3.3	1
12	AN ADAPTIVE CONTROL ALGORITHM FOR TRACKING UNSTABLE PERIODIC ORBITS. *International Journal of Bifurcation and Chaos in Applied Sciences and Engineering*, **1994**, 04, 1311-1317	2	15
11	Controlling spatiotemporal dynamics of flame fronts. *Journal of Chemical Physics*, **1994**, 101, 6606-6614	3.9	7

10	Tracking unstable periodic orbits in the Belousov-Zhabotinsky reaction. *Physical Review Letters*, **1994**, 72, 2955-2958	7.4	54
9	Molecular dynamics investigation of the MBE growth of Si on Si{110}. *Surface Science*, **1993**, 284, 91-102	1.8	12
8	Experimental and theoretical studies of a coupled chemical oscillator: phase death, multistability and in-phase and out-of-phase entrainment. *The Journal of Physical Chemistry*, **1989**, 93, 2496-2502		196
7	Electrically coupled Belousov-Zhabotinskii oscillators. 1. Experiments and simulations. *The Journal of Physical Chemistry*, **1986**, 90, 1907-1915		90
6	Electrically Coupled Belousov-Zhabotinskii Oscillators: Experimental Observation of Chaos in a Chemical System and Identification of its Source in the Field-Noyes Equations. *Lecture Notes in Biomathematics*, **1986**, 68-97		3
5	Observation of a peculiar phenomenon in the cerium-ion-catalyzed Belousov-Zhabotinskii oscillator with acetylacetone in CSTR mode. *Reaction Kinetics and Catalysis Letters*, **1985**, 28, 233-238		
4	Asymptotic solutions of a reduced Oregonator model of the Belousov-Zhabotinsky reaction. *The Journal of Physical Chemistry*, **1984**, 88, 762-766		5
3	Electrically Coupled Belousov-Zhabotinsky Oscillators: A Potential Chaos Generator. *Springer Series in Synergetics*, **1981**, 147-153	0.4	6
2	Studying protein folding on the grid: experiences using CHARMM on NPACI resources under Legion		16
1	Computational Approaches to Study Cellulose Hydrolysis306-330		2