Michelle M Kuttel

List of Publications by Year
in descending order

51	975	623188	454577
papers	citations	14 h-index	30 g-index

53	53	53	985
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Carbohydrate Force Fields: The Role of Small Partial Atomic Charges in Preventing Conformational Collapse. Journal of Chemical Theory and Computation, 2022, 18, 1156-1172.	2.3	8
2	Deciphering the Mechanism of Binding Selectivity of Chlorofluoroacetamide-Based Covalent Inhibitors toward L858R/T790M Resistance Mutation. Journal of Chemical Information and Modeling, 2022, , .	2.5	3
3	Comparative Molecular Modelling of Capsular Polysaccharide Conformations in Streptococcus suis Serotypes 1, 2, 1/2 and 14 Identifies Common Epitopes for Antibody Binding. Frontiers in Molecular Biosciences, 2022, 9, 830854.	1.6	1
4	Streptococcus pneumoniae serotype 15B polysaccharide conjugate elicits a cross-functional immune response against serotype 15C but not 15A. Vaccine, 2022, 40, 4872-4880.	1.7	14
5	Molecular modeling provides insights into the loading of sialic acidâ€containing antigens onto CRM197: the role of chain flexibility in conjugation efficiency and glycoconjugate architecture. Glycoconjugate Journal, 2021, 38, 411-419.	1.4	3
6	Conformational and Immunogenicity Studies of the Shigella flexneri Serogroup 6 O-Antigen: The Effect of O-Acetylation. Vaccines, 2021, 9, 432.	2.1	10
7	Cross-reactivity of Haemophilus influenzae type a and b polysaccharides: molecular modeling and conjugate immunogenicity studies. Glycoconjugate Journal, 2021, 38, 735-746.	1.4	4
8	Molecular Modeling of the Shigella flexneri Serogroup 3 and 5 O-Antigens and Conformational Relationships for a Vaccine Containing Serotypes 2a and 3a. Vaccines, 2020, 8, 643.	2.1	6
9	Mechanistic Study of Potent Fluorinated EGFR Kinase Inhibitors with a Quinazoline Scaffold against L858R/T790M/C797S Resistance Mutation: Unveiling the Fluorine Substituent Cooperativity Effect on the Inhibitory Activity. Journal of Physical Chemistry B, 2020, 124, 5813-5824.	1.2	5
10	Cryptococcus neoformans Capsular GXM Conformation and Epitope Presentation: A Molecular Modelling Study. Molecules, 2020, 25, 2651.	1.7	17
11	Effects of Glucosylation and O-Acetylation on the Conformation of Shigella flexneri Serogroup 2 O-Antigen Vaccine Targets. Journal of Physical Chemistry B, 2020, 124, 2806-2814.	1.2	9
12	Modeling the conformations of Neisseria meningitidis serogroup a CPS and a carba-analogue: Implications for vaccine development. Carbohydrate Research, 2019, 486, 107838.	1.1	7
13	A Mechanistic Study of a Potent and Selective Epidermal Growth Factor Receptor Inhibitor against the L858R/T790M Resistance Mutation. Biochemistry, 2019, 58, 4246-4259.	1.2	3
14	O-acetylation of typhoid capsular polysaccharide confers polysaccharide rigidity and immunodominance by masking additional epitopes. Vaccine, 2019, 37, 3866-3875.	1.7	24
15	Conformation and Cross-Protection in Group B Streptococcus Serotype III and Streptococcus pneumoniae Serotype 14: A Molecular Modeling Study. Pharmaceuticals, 2019, 12, 28.	1.7	12
16	A Scalable Database Model of RFI Data for the MeerKAT Radio Telescope. , 2019, , .		1
17	Conformations of Neisseria meningitidis serogroup A and X polysaccharides: The effects of chain length and O-acetylation. Carbohydrate Research, 2018, 465, 44-51.	1.1	25
18	The Role of Molecular Modeling in Predicting Carbohydrate Antigen Conformation and Understanding Vaccine Immunogenicity. ACS Symposium Series, 2018, , 139-173.	0.5	9

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19	Cross-protection in Neisseria meningitidis serogroups Y and W polysaccharides: A comparative conformational analysis. Carbohydrate Research, 2017, 446-447, 40-47.	1.1	15
20	Fluorescence and NMR spectroscopy together with molecular simulations reveal amphiphilic characteristics of a Burkholderia biofilm exopolysaccharide. Journal of Biological Chemistry, 2017, 292, 11034-11042.	1.6	11
21	Genetic and structural elucidation of capsular polysaccharides from Streptococcus pneumoniae serotype 23A and 23B, and comparison to serotype 23F. Carbohydrate Research, 2017, 450, 19-29.	1.1	18
22	Improving the usability of scientific software with participatory design. , 2017, , .		3
23	CarbBuilder: Software for building molecular models of complex oligoâ€•and polysaccharide structures. Journal of Computational Chemistry, 2016, 37, 2098-2105.	1.5	71
24	Effective Visualization of Tuberculosis Three-Drug Assays. , 2016, , .		0
25	Implementation, Validation and Profiling of a Genetic Algorithm for Molecular Conformational Optimization. , 2016, , .		1
26	An eHealth android application for mobile analysis of microplate assays. , 2016, , .		2
27	Comparison of effectiveness of two mobile application designs for encouraging children to read. , 2015, , .		0
28	Capsular polysaccharide conformations in pneumococcal serotypes 19F and 19A. Carbohydrate Research, 2015, 406, 27-33.	1.1	20
29	Scalable desktop visualisation of very large radio astronomy data cubes. New Astronomy, 2014, 30, 1-7.	0.8	11
30	Comparative simulation of pneumococcal serogroup 19 polysaccharide repeating units with two carbohydrate force fields. Carbohydrate Research, 2014, 390, 20-27.	1.1	13
31	Towards realistic and interactive sand simulation: A GPU-based framework. Powder Technology, 2013, 235, 983-1000.	2.1	38
32	Efficient compression of molecular dynamics trajectory files. Journal of Computational Chemistry, 2012, 33, 2131-2141.	1.5	7
33	Conformational properties of two exopolysaccharides produced by Inquilinus limosus, a cystic fibrosis lung pathogen. Carbohydrate Research, 2012, 350, 40-48.	1.1	16
34	CarbBuilder: An Adjustable Tool for Building 3D Molecular Structures of Carbohydrates for Molecular Simulation. , 2011, , .		12
35	The Conformational Free Energy of Carbohydrates. Mini-Reviews in Organic Chemistry, 2011, 8, 256-262.	0.6	7
36	Exhaustive computational search of ionic-charge clusters that mediate interactions between mammalian cytochrome P450 (CYP) and P450-oxidoreductase (POR) proteins. Computational Biology and Chemistry, 2010, 34, 42-52.	1.1	7

#	Article	IF	Citations
37	Panopticon. , 2010, , .		2
38	Simulation of Coarse-Grained Proteinâ"Protein Interactions with Graphics Processing Units. Journal of Chemical Theory and Computation, 2010, 6, 3588-3600.	2.3	11
39	An Electronic Health Care - Cardiac Monitoring System. , 2010, , .		9
40	Visualization of solution sets from automated docking of molecular structures. , 2010, , .		0
41	Dynamic load balancing of Lattice Boltzmann free-surface fluid animations. , 2010, , .		0
42	Visualisation of cyclic and multi-branched molecules with VMD. Journal of Molecular Graphics and Modelling, 2009, 28, 131-139.	1.3	49
43	Conformational free energy maps for globobiose (Î±-d-Galp-(1â†'4)-Î²-d-Galp) in implicit and explict aqueous solution. Carbohydrate Research, 2008, 343, 1091-1098.	1.1	11
44	Techniques for visualization of carbohydrate molecules. Journal of Molecular Graphics and Modelling, 2006, 25, 380-388.	1.3	19
45	Ramachandran free-energy surfaces for disaccharides: trehalose, a case study. Carbohydrate Research, 2005, 340, 875-879.	1.1	20
46	Free Energy Surfaces for the Î±(1 â†' 4)-Glycosidic Linkage:Â Implications for Polysaccharide Solution Structure and Dynamics. Journal of Physical Chemistry B, 2005, 109, 7468-7474.	1.2	50
47	Glycosidic Linkage Rotations Determine Amylose Stretching Mechanism. Journal of the American Chemical Society, 2005, 127, 12-13.	6.6	47
48	Carbohydrate solution simulations: Producing a force field with experimentally consistent primary alcohol rotational frequencies and populations. Journal of Computational Chemistry, 2002, 23, 1236-1243.	1.5	271
49	Water structure about the dimer and hexamer repeat units of amylose from molecular dynamics computer simulations. Journal of Computational Chemistry, 2001, 22, 445-456.	1.5	71
50	Water structure about the dimer and hexamer repeat units of amylose from molecular dynamics computer simulations. Journal of Computational Chemistry, 2001, 22, 445-456.	1.5	1
51	No expiration date. Nature Astronomy, 0, , .	4.2	1