

Michelle M Kuttel

List of Publications by Year in descending order

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Version: 2024-02-01

51
papers

975
citations

623188

14
h-index

454577

30
g-index

53
all docs

53
docs citations

53
times ranked

985
citing authors

#	ARTICLE	IF	CITATIONS
1	Carbohydrate solution simulations: Producing a force field with experimentally consistent primary alcohol rotational frequencies and populations. <i>Journal of Computational Chemistry</i> , 2002, 23, 1236-1243.	1.5	271
2	Water structure about the dimer and hexamer repeat units of amylose from molecular dynamics computer simulations. <i>Journal of Computational Chemistry</i> , 2001, 22, 445-456.	1.5	71
3	CarbBuilder: Software for building molecular models of complex oligo- and polysaccharide structures. <i>Journal of Computational Chemistry</i> , 2016, 37, 2098-2105.	1.5	71
4	Free Energy Surfaces for the $\alpha(1 \rightarrow 4)$ -Glycosidic Linkage: Implications for Polysaccharide Solution Structure and Dynamics. <i>Journal of Physical Chemistry B</i> , 2005, 109, 7468-7474.	1.2	50
5	Visualisation of cyclic and multi-branched molecules with VMD. <i>Journal of Molecular Graphics and Modelling</i> , 2009, 28, 131-139.	1.3	49
6	Glycosidic Linkage Rotations Determine Amylose Stretching Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 12-13.	6.6	47
7	Towards realistic and interactive sand simulation: A GPU-based framework. <i>Powder Technology</i> , 2013, 235, 983-1000.	2.1	38
8	Conformations of <i>Neisseria meningitidis</i> serogroup A and X polysaccharides: The effects of chain length and O-acetylation. <i>Carbohydrate Research</i> , 2018, 465, 44-51.	1.1	25
9	O-acetylation of typhoid capsular polysaccharide confers polysaccharide rigidity and immunodominance by masking additional epitopes. <i>Vaccine</i> , 2019, 37, 3866-3875.	1.7	24
10	Ramachandran free-energy surfaces for disaccharides: trehalose, a case study. <i>Carbohydrate Research</i> , 2005, 340, 875-879.	1.1	20
11	Capsular polysaccharide conformations in pneumococcal serotypes 19F and 19A. <i>Carbohydrate Research</i> , 2015, 406, 27-33.	1.1	20
12	Techniques for visualization of carbohydrate molecules. <i>Journal of Molecular Graphics and Modelling</i> , 2006, 25, 380-388.	1.3	19
13	Genetic and structural elucidation of capsular polysaccharides from <i>Streptococcus pneumoniae</i> serotype 23A and 23B, and comparison to serotype 23F. <i>Carbohydrate Research</i> , 2017, 450, 19-29.	1.1	18
14	<i>Cryptococcus neoformans</i> Capsular GXM Conformation and Epitope Presentation: A Molecular Modelling Study. <i>Molecules</i> , 2020, 25, 2651.	1.7	17
15	Conformational properties of two exopolysaccharides produced by <i>Inquilinus limosus</i> , a cystic fibrosis lung pathogen. <i>Carbohydrate Research</i> , 2012, 350, 40-48.	1.1	16
16	Cross-protection in <i>Neisseria meningitidis</i> serogroups Y and W polysaccharides: A comparative conformational analysis. <i>Carbohydrate Research</i> , 2017, 446-447, 40-47.	1.1	15
17	<i>Streptococcus pneumoniae</i> serotype 15B polysaccharide conjugate elicits a cross-functional immune response against serotype 15C but not 15A. <i>Vaccine</i> , 2022, 40, 4872-4880.	1.7	14
18	Comparative simulation of pneumococcal serogroup 19 polysaccharide repeating units with two carbohydrate force fields. <i>Carbohydrate Research</i> , 2014, 390, 20-27.	1.1	13

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19	CarbBuilder: An Adjustable Tool for Building 3D Molecular Structures of Carbohydrates for Molecular Simulation. , 2011, , .		12
20	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
21	Conformational free energy maps for globobiose (β -d-Galp-(1 \rightarrow 4)- β -d-Galp) in implicit and explicit aqueous solution. Carbohydrate Research, 2008, 343, 1091-1098.	1.1	11
22	Simulation of Coarse-Grained Protein-Protein Interactions with Graphics Processing Units. Journal of Chemical Theory and Computation, 2010, 6, 3588-3600.	2.3	11
23	Scalable desktop visualisation of very large radio astronomy data cubes. New Astronomy, 2014, 30, 1-7.	0.8	11
24	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
25	Conformational and Immunogenicity Studies of the Shigella flexneri Serogroup 6 O-Antigen: The Effect of O-Acetylation. Vaccines, 2021, 9, 432.	2.1	10
26	An Electronic Health Care - Cardiac Monitoring System. , 2010, , .		9
27	The Role of Molecular Modeling in Predicting Carbohydrate Antigen Conformation and Understanding Vaccine Immunogenicity. ACS Symposium Series, 2018, , 139-173.	0.5	9
28	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
29	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
30	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
31	The Conformational Free Energy of Carbohydrates. Mini-Reviews in Organic Chemistry, 2011, 8, 256-262.	0.6	7
32	Efficient compression of molecular dynamics trajectory files. Journal of Computational Chemistry, 2012, 33, 2131-2141.	1.5	7
33	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
34	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
35	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
36	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

#	ARTICLE	IF	CITATIONS
37	Improving the usability of scientific software with participatory design. , 2017, , .		3
38	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
39	Molecular modeling provides insights into the loading of sialic acid-containing antigens onto CRM197: the role of chain flexibility in conjugation efficiency and glycoconjugate architecture. Glycoconjugate Journal, 2021, 38, 411-419.	1.4	3
40	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
41	Panopticon. , 2010, , .		2
42	An eHealth android application for mobile analysis of microplate assays. , 2016, , .		2
43	Implementation, Validation and Profiling of a Genetic Algorithm for Molecular Conformational Optimization. , 2016, , .		1
44	No expiration date. Nature Astronomy, 0, , .	4.2	1
45	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
46	A Scalable Database Model of RFI Data for the MeerKAT Radio Telescope. , 2019, , .		1
47	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
48	Comparison of effectiveness of two mobile application designs for encouraging children to read. , 2015, , .		0
49	Effective Visualization of Tuberculosis Three-Drug Assays. , 2016, , .		0
50	Visualization of solution sets from automated docking of molecular structures. , 2010, , .		0
51	Dynamic load balancing of Lattice Boltzmann free-surface fluid animations. , 2010, , .		0