Martin McCullagh

List of Publications by Year
in descending order

40	849	567281 15	501196 28
papers	citations	h-index	g-index

49	49	49	1169
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conserved motifs in the flavivirus <scp>NS3 RNA</scp> helicase enzyme. Wiley Interdisciplinary Reviews RNA, 2022, 13, e1688.	6.4	12
2	Size-and-Shape Space Gaussian Mixture Models for Structural Clustering of Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2022, 18, 3218-3230.	5.3	18
3	Implicit Solvation Using the Superposition Approximation (IS-SPA): Extension to Peptides in a Polar Solvent. Journal of Chemical Theory and Computation, 2021, 17, 703-713.	5.3	3
4	Role of ATP in the RNA Translocation Mechanism of SARS-CoV-2 NSP13 Helicase. Journal of Physical Chemistry B, 2021, 125, 8787-8796.	2.6	8
5	Using molecular simulations to investigate how intermolecular interactions dictate liquid structure. , 2021, , 71-91.		1
6	Motif V regulates energy transduction between the flavivirus NS3 ATPase and RNA-binding cleft. Journal of Biological Chemistry, 2020, 295, 1551-1564.	3.4	18
7	Deterring Effect of Resins on the Aggregation of Asphaltenes in n-Heptane. Energy & Fuels, 2020, 34, 16081-16088.	5.1	15
8	A Hyperactive Kunjin Virus NS3 Helicase Mutant Demonstrates Increased Dissemination and Mortality in Mosquitoes. Journal of Virology, 2020, 94, .	3.4	2
9	The Role of Hydrophobicity in the Stability and pH-Switchability of (RXDX)₄ and Coumarinâ€“(RXDX)₄ Conjugate Î²-Sheets. Journal of Physical Chemistry B, 2020, 124, 1723-1732.	2.6	3
10	RNA-Dependent Structures of the RNA-Binding Loop in the Flavivirus NS3 Helicase. Journal of Physical Chemistry B, 2020, 124, 2371-2381.	2.6	3
11	Residue-Level Allostery Propagates through the Effective Coarse-Grained Hessian. Journal of Chemical Theory and Computation, 2020, 16, 3385-3395.	5.3	21
12	Molecular Analysis of Dengue NS3 Helicase Function. Biophysical Journal, 2019, 116, 489a-490a.	0.5	0
13	LÎ²3Î²4 Conformations of the Flaviviridae NS3h Protein. Biophysical Journal, 2019, 116, 434a.	0.5	0
14	Molecular Dynamics Simulations of 2-Aminopurine-Labeled Dinucleoside Monophosphates Reveal Multiscale Stacking Kinetics. Journal of Physical Chemistry B, 2019, 123, 2291-2304.	2.6	4
15	Characterization of the Search Complex and Recognition Mechanism of the AlkDâ€“DNA Glycosylase. Journal of Physical Chemistry B, 2019, 123, 95-105.	2.6	5
16	Elucidating Structural Evolution of Perylene Diimide Aggregates Using Vibrational Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 4891-4900.	2.6	10
17	Molecular Analysis of Dengue NS3 Helicase Function. Biophysical Journal, 2018, 114, 233a.	0.5	0
18	Initial Aggregation and Ordering Mechanism of Diphenylalanine from Microsecond All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 12331-12341.	2.6	7

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19	Allostery in the dengue virus NS3 helicase: Insights into the NTPase cycle from molecular simulations. PLoS Computational Biology, 2018, 14, e1006103.	3.2	38
20	Selfâ€Assembly of Perylenediimideâ€“Singleâ€Strandâ€DNA Conjugates: Employing Hydrophobic Interactions and DNA Baseâ€Pairing To Create a Diverse Structural Space. Chemistry - A European Journal, 2017, 23, 10328-10337.	3.3	12
21	Molecular Allostery in Dengue NS3 Helicase along the ATP Hydrolysis Cycle. Biophysical Journal, 2017, 112, 497a.	0.5	0
22	Implicit Solvation Using the Superposition Approximation (IS-SPA): An Implicit Treatment of the Nonpolar Component to Solvation for Simulating Molecular Aggregation. Journal of Chemical Theory and Computation, 2017, 13, 5911-5924.	5.3	6
23	Deriving Coarse-Grained Charges from All-Atom Systems: An Analytic Solution. Journal of Chemical Theory and Computation, 2016, 12, 4390-4399.	5.3	5
24	Electrostatic Interactions between the Bni1p Formin FH2 Domain and Actin Influence Actin Filament Nucleation. Structure, 2015, 23, 68-79.	3.3	24
25	Ground and excited state electronic spectra of perylenediimide dimers with flexible and rigid geometries in DNA conjugates. Chemical Science, 2014, 5, 973-981.	7.4	19
26	Thymine photodimer formation in DNA hairpins. Unusual conformations favor (6 â˜’ 4) vs. (2 + 2) adducts. Photochemical and Photobiological Sciences, 2014, 13, 266-271.	2.9	10
27	Unraveling the Mystery of ATP Hydrolysis in Actin Filaments. Journal of the American Chemical Society, 2014, 136, 13053-13058.	13.7	74
28	The Theory of Ultra-Coarse-Graining. 1. General Principles. Journal of Chemical Theory and Computation, 2013, 9, 2466-2480.	5.3	149
29	Unraveling the Role of the Protein Environment for [FeFe]-Hydrogenase: A New Application of Coarse-Graining. Journal of Physical Chemistry B, 2013, 117, 4062-4071.	2.6	37
30	Electronic Interactions in Helical Stacked Arrays of the Modified DNA Base Pyrrolocytosine. Journal of Physical Chemistry B, 2012, 116, 5199-5204.	2.6	6
31	Defects in DNA: Lessons from Molecular Motor Design. Journal of Physical Chemistry Letters, 2012, 3, 689-693.	4.6	11
32	Conformational Control of Thymine Photodimerization in Purine-Containing Trinucleotides. Journal of Physical Chemistry Letters, 2011, 2, 1432-1438.	4.6	26
33	Electron Donorâ€“Acceptor Interactions with Flanking Purines Influence the Efficiency of Thymine Photodimerization. Journal of the American Chemical Society, 2011, 133, 20793-20798.	13.7	47
34	DNA-Based Optomechanical Molecular Motor. Journal of the American Chemical Society, 2011, 133, 3452-3459.	13.7	56
35	Theoretical Studies of Thymineâ€“Thymine Photodimerization: Using Ground State Dynamics to Model Photoreaction. , 2011, , 385-413.		1
36	Conformational Control of Thymine Photodimerization in Single-Strand and Duplex DNA Containing Locked Nucleic Acid TT Steps. Journal of the American Chemical Society, 2010, 132, 12856-12858.	13.7	28

#	Article	IF	Citations
37	Conformational Control of TT Dimerization in DNA Conjugates. A Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 5215-5221.	2.6	62
38	Modeling Self-Assembly Processes Driven by Nonbonded Interactions in Soft Materials. Journal of Physical Chemistry B, 2008, 112, 10388-10398.	2.6	78
39	Effect of Loop Distortion on the Stability and Structural Dynamics of DNA Hairpin and Dumbbell Conjugates. Journal of Physical Chemistry B, 2008, 112, 11415-11421.	2.6	17
40	Modeling Catalysis in Allosteric Enzymes: Capturing Conformational Consequences. Topics in Catalysis, 0, , 1.	2.8	3