

Krystel El Hage

List of Publications by Year in descending order

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Version: 2024-02-01

28
papers

439
citations

687363

13
h-index

794594

19
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35
all docs

35
docs citations

35
times ranked

563
citing authors

#	ARTICLE	IF	CITATIONS
1	Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size. <i>ELife</i> , 2018, 7, .	6.0	63
2	The cooperative binding of TDP-43 to GU-rich RNA repeats antagonizes TDP-43 aggregation. <i>ELife</i> , 2021, 10, .	6.0	35
3	Molecular Mechanisms Underlying Solute Retention at Heterogeneous Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4600-4607.	4.6	26
4	Extending Halogen-based Medicinal Chemistry to Proteins. <i>Journal of Biological Chemistry</i> , 2016, 291, 27023-27041.	3.4	25
5	A Toolkit to Fit Nonbonded Parameters from and for Condensed Phase Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1479-1489.	5.4	25
6	Implications of short time scale dynamics on long time processes. <i>Structural Dynamics</i> , 2017, 4, 061507.	2.3	24
7	Impact of Quadrupolar Electrostatics on Atoms Adjacent to the Sigma-Hole in Condensed-Phase Simulations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3008-3019.	5.3	23
8	The Role of Water in the Stability of Wild-type and Mutant Insulin Dimers. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7038-7048.	2.6	23
9	Could an anisotropic molecular mechanics/dynamics potential account for sigma hole effects in the complexes of halogenated compounds?. <i>Journal of Computational Chemistry</i> , 2013, 34, 1125-1135.	3.3	21
10	Sequential Proton Coupled Electron Transfer (PCET): Dynamics Observed over 8 Orders of Magnitude in Time. <i>Journal of the American Chemical Society</i> , 2016, 138, 4401-4407.	13.7	21
11	Water Dynamics Around Proteins: T- and R-States of Hemoglobin and Melittin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6540-6554.	2.6	16
12	From in silica to in silico: retention thermodynamics at solid-liquid interfaces. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18610-18622.	2.8	15
13	Substituent-Modulated Affinities of Halobenzene Derivatives to the HIV-1 Integrase Recognition Site. Analyses of the Interaction Energies by Parallel Quantum Chemical and Polarizable Molecular Mechanics. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9772-9782.	2.5	14
14	Could the "Janus-like" properties of the halobenzene CX bond (X = Cl, Br) be leveraged to enhance molecular recognition?. <i>Journal of Computational Chemistry</i> , 2015, 36, 210-221.	3.3	14
15	Free energy simulations for protein ligand binding and stability. <i>Molecular Simulation</i> , 2018, 44, 1044-1061.	2.0	13
16	Lin28, a major translation reprogramming factor, gains access to YB-1-packaged mRNA through its cold-shock domain. <i>Communications Biology</i> , 2021, 4, 359.	4.4	13
17	Response to comment on 'Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size'. <i>ELife</i> , 2019, 8, .	6.0	13
18	YB-1 unwinds mRNA secondary structures <i>in vitro</i> and negatively regulates stress granule assembly in HeLa cells. <i>Nucleic Acids Research</i> , 2021, 49, 10061-10081.	14.5	10

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19	Polarizable molecular mechanics studies of $\langle \text{Cu(I)/Zn(II)} \rangle$ superoxide dismutase: Bimetallic binding site and structured waters. <i>Journal of Computational Chemistry</i> , 2014, 35, 2096-2106.	3.3	9
20	A Simple Isomerization of the Purine Scaffold of a Kinase Inhibitor, Roscovitine, Affords a Four- to Seven-Fold Enhancement of Its Affinity for Four CDKs. Could This Be Traced Back to Conjugation-Induced Stiffenings/Loosenings of Rotational Barriers?. <i>ACS Omega</i> , 2017, 2, 3467-3474.	3.5	8
21	Identification of a small molecule splicing inhibitor targeting UHM domains. <i>FEBS Journal</i> , 2022, 289, 682-698.	4.7	8
22	Ultrafast dynamics induced by the interaction of molecules with electromagnetic fields: Several quantum, semiclassical, and classical approaches. <i>Structural Dynamics</i> , 2017, 4, 061509.	2.3	3
23	Approaching the double-faceted nature of the CX bond in halobenzenes with a bifunctional probe. <i>Chemical Physics Letters</i> , 2015, 637, 51-57.	2.6	2
24	Effect of Single-Point Mutations on Nitric Oxide Rebinding and the Thermodynamic Stability of Myoglobin. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1961-1972.	2.6	2
25	Quantum-Chemistry Based Design of Halobenzene Derivatives With Augmented Affinities for the HIV-1 Viral G4/C16 Base-Pair. <i>Frontiers in Chemistry</i> , 2020, 8, 440.	3.6	2
26	Spectrometric and computational studies of the binding of HIV-1 integrase inhibitors to viral DNA extremities. , 0, 1, e6.		2
27	Addressing the Issues of Non-isotropy and Non-additivity in the Development of Quantum Chemistry-Grounded Polarizable Molecular Mechanics. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 1-49.	0.6	1
28	Strong Enrichment of Aromatic and Sulfur-Containing Residues in Ligand-Protein Binding Sites. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4921-4928.	5.4	0