Krystel El Hage

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9497167/publications.pdf

Version: 2024-02-01

28	439	687363 13	794594 19
papers	citations	h-index	g-index

35	35	35	563
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Identification of a small molecule splicing inhibitor targeting UHM domains. FEBS Journal, 2022, 289, 682-698.	4.7	8
2	Lin28, a major translation reprogramming factor, gains access to YB-1-packaged mRNA through its cold-shock domain. Communications Biology, 2021, 4, 359.	4.4	13
3	YB-1 unwinds mRNA secondary structures in vitro and negatively regulates stress granule assembly in HeLa cells. Nucleic Acids Research, 2021, 49, 10061-10081.	14.5	10
4	The cooperative binding of TDP-43 to GU-rich RNA repeats antagonizes TDP-43 aggregation. ELife, 2021, 10, .	6.0	35
5	Quantum-Chemistry Based Design of Halobenzene Derivatives With Augmented Affinities for the HIV-1 Viral G4/C16 Base-Pair. Frontiers in Chemistry, 2020, 8, 440.	3.6	2
6	Water Dynamics Around Proteins: T- and R-States of Hemoglobin and Melittin. Journal of Physical Chemistry B, 2020, 124, 6540-6554.	2.6	16
7	Strong Enrichment of Aromatic and Sulfur-Containing Residues in Ligandâ€“Protein Binding Sites. Journal of Chemical Information and Modeling, 2019, 59, 4921-4928.	5.4	0
8	Effect of Single-Point Mutations on Nitric Oxide Rebinding and the Thermodynamic Stability of Myoglobin. Journal of Physical Chemistry B, 2019, 123, 1961-1972.	2.6	2
9	Response to comment on 'Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size'. ELife, 2019, 8, .	6.0	13
10	Free energy simulations for protein ligand binding and stability. Molecular Simulation, 2018, 44, 1044-1061.	2.0	13
11	The Role of Water in the Stability of Wild-type and Mutant Insulin Dimers. Journal of Physical Chemistry B, 2018, 122, 7038-7048.	2.6	23
12	Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size. ELife, 2018, 7, .	6.0	63
13	From in silica to in silico: retention thermodynamics at solidâ€“liquid interfaces. Physical Chemistry Chemical Physics, 2018, 20, 18610-18622.	2.8	15
14	Molecular Mechanisms Underlying Solute Retention at Heterogeneous Interfaces. Journal of Physical Chemistry Letters, 2017, 8, 4600-4607.	4.6	26
15	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?. ACS Omega, 2017, 2, 3467-3474.	3.5	8
16	Ultrafast dynamics induced by the interaction of molecules with electromagnetic fields: Several quantum, semiclassical, and classical approaches. Structural Dynamics, 2017, 4, 061509.	2.3	3
17	Implications of short time scale dynamics on long time processes. Structural Dynamics, 2017, 4, 061507.	2.3	24
18	Impact of Quadrupolar Electrostatics on Atoms Adjacent to the Sigma-Hole in Condensed-Phase Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3008-3019.	5.3	23

#	Article	IF	Citations
19	Extending Halogen-based Medicinal Chemistry to Proteins. Journal of Biological Chemistry, 2016, 291, 27023-27041.	3.4	25
20	A Toolkit to Fit Nonbonded Parameters from and for Condensed Phase Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1479-1489.	5.4	25
21	Sequential Proton Coupled Electron Transfer (PCET): Dynamics Observed over 8 Orders of Magnitude in Time. Journal of the American Chemical Society, 2016, 138, 4401-4407.	13.7	21
22	Could the â€œJanusâ€•keâ€•properties of the halobenzene CX bond (Xï£¾Cl, Br) be leveraged to enhance molecular recognition?. Journal of Computational Chemistry, 2015, 36, 210-221.	3.3	14
23	Approaching the double-faceted nature of the CX bond in halobenzenes with a bifunctional probe. Chemical Physics Letters, 2015, 637, 51-57.	2.6	2
24	Addressing the Issues of Non-isotropy and Non-additivity in the Development of Quantum Chemistry-Grounded Polarizable Molecular Mechanics. Challenges and Advances in Computational Chemistry and Physics, 2015, , 1-49.	0.6	1
25	Polarizable molecular mechanics studies of <scp>Cu(I)/Zn(II)</scp> superoxide dismutase: Bimetallic binding site and structured waters. Journal of Computational Chemistry, 2014, 35, 2096-2106.	3.3	9
26	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. Journal of Physical Chemistry A, 2014, 118, 9772-9782.	2.5	14
27	Could an anisotropic molecular mechanics/dynamics potential account for sigma hole effects in the complexes of halogenated compounds?. Journal of Computational Chemistry, 2013, 34, 1125-1135.	3.3	21
28	Spectrometric and computational studies of the binding of HIV-1 integrase inhibitors to viral DNA extremities. , 0, 1, e6.		2