Troy W Whitfield

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Characterizing Protein–Ligand Binding Using Atomistic Simulation and Machine Learning: Application to Drug Resistance in HIV-1 Protease. Journal of Chemical Theory and Computation, 2020, 16, 1284-1299.	2.3	19
2	Molecular Determinants of Epistasis in HIV-1 Protease: Elucidating the Interdependence of L89V and L90M Mutations in Resistance. Biochemistry, 2019, 58, 3711-3726.	1.2	15
3	Constrained Mutational Sampling of Amino Acids in HIV-1 Protease Evolution. Molecular Biology and Evolution, 2019, 36, 798-810.	3.5	10
4	Synonymous Mutations at the Beginning of the Influenza A Virus Hemagglutinin Gene Impact Experimental Fitness. Journal of Molecular Biology, 2018, 430, 1098-1115.	2.0	16
5	Chromatin dynamics regulate mesenchymal stem cell lineage specification and differentiation to osteogenesis. Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms, 2017, 1860, 438-449.	0.9	55
6	Demethylated HSATII DNA and HSATII RNA Foci Sequester PRC1 and MeCP2 into Cancer-Specific Nuclear Bodies. Cell Reports, 2017, 18, 2943-2956.	2.9	76
7	Elucidating the Interdependence of Drug Resistance from Combinations of Mutations. Journal of Chemical Theory and Computation, 2017, 13, 5671-5682.	2.3	27
8	Structural Basis of the Disorder in the Tandem Zinc Finger Domain of the RNA-Binding Protein Tristetraprolin. Journal of Chemical Theory and Computation, 2016, 12, 4717-4725.	2.3	2
9	Genome-Wide Studies Reveal that H3K4me3 Modification in Bivalent Genes Is Dynamically Regulated during the Pluripotent Cell Cycle and Stabilized upon Differentiation. Molecular and Cellular Biology, 2016, 36, 615-627.	1.1	53
10	Genome-wide co-occupancy of AML1-ETO and N-CoR defines the t(8;21) AML signature in leukemic cells. BMC Genomics, 2015, 16, 309.	1.2	30
11	The bone-specific Runx2-P1 promoter displays conserved three-dimensional chromatin structure with the syntenic Supt3h promoter. Nucleic Acids Research, 2014, 42, 10360-10372.	6.5	28
12	Genomic occupancy of Runx2 with global expression profiling identifies a novel dimension to control of osteoblastogenesis. Genome Biology, 2014, 15, R52.	13.9	122
13	Epigenetic landscape during osteoblastogenesis defines a differentiation-dependent Runx2 promoter region. Gene, 2014, 550, 1-9.	1.0	28
14	Quantum Drude oscillator model of atoms and molecules: Many-body polarization and dispersion interactions for atomistic simulation. Physical Review B, 2013, 87, .	1.1	65
15	Sequence features and chromatin structure around the genomic regions bound by 119 human transcription factors. Genome Research, 2012, 22, 1798-1812.	2.4	762
16	Functional analysis of transcription factor binding sites in human promoters. Genome Biology, 2012, 13, R50.	13.9	136
17	An integrated encyclopedia of DNA elements in the human genome. Nature, 2012, 489, 57-74.	13.7	15,516
18	A machine learning approach for the prediction of protein surface loop flexibility. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2467-2474.	1.5	8

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19	A Combined Experimental and Theoretical Study of Ion Solvation in Liquid <i>N</i> -Methylacetamide. Journal of the American Chemical Society, 2010, 132, 10847-10856.	6.6	35
20	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	2.3	401
21	Identification of functional modules that correlate with phenotypic difference: the influence of network topology. Genome Biology, 2010, 11, R23.	13.9	67
22	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	1.2	122
23	Low variance energy estimators for systems of quantum Drude oscillators: Treating harmonic path integrals with large separations of time scales. Journal of Chemical Physics, 2007, 126, 074104.	1.2	17
24	Theoretical Study of Aqueous Solvation of K ⁺ Comparing ab Initio, Polarizable, and Fixed-Charge Models. Journal of Chemical Theory and Computation, 2007, 3, 2068-2082.	2.3	87
25	A unified formalism for many-body polarization and dispersion: The quantum Drude model applied to fluid xenon. Chemical Physics Letters, 2006, 424, 409-413.	1.2	29
26	Liquid NMA: A surprisingly realistic model for hydrogen bonding motifs in proteins. Chemical Physics Letters, 2005, 414, 210-214.	1.2	36
27	Gravitational smoothing as a global optimization strategy. Journal of Computational Chemistry, 2002, 23, 1100-1103.	1.5	4
28	Generalized parallel sampling. Physica A: Statistical Mechanics and Its Applications, 2002, 305, 157-171.	1.2	49
29	Uncertainty of path integral averages at low temperature. Journal of Chemical Physics, 2001, 115, 6834-6840.	1.2	4