Orlando Acevedo

List of Publications by Year
in descending order

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		218677	161849
62	2,973	26	54
papers	citations	h-index	g-index

63	63	63	3168
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Development of OPLS-AA Force Field Parameters for 68 Unique Ionic Liquids. Journal of Chemical Theory and Computation, 2009, 5, 1038-1050.	5.3	435
2	Revisiting OPLS Force Field Parameters for Ionic Liquid Simulations. Journal of Chemical Theory and Computation, 2017, 13, 6131-6145.	5.3	296
3	Advances in Quantum and Molecular Mechanical (QM/MM) Simulations for Organic and Enzymatic Reactions. Accounts of Chemical Research, 2010, 43, 142-151.	15.6	221
4	Discovery of a Potent, Selective, and Efficacious Class of Reversible Î±-Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase Effective as Analgesicsâ‡. Journal of Medicinal Chemistry, 2005, 48, 1849-1856.	6.4	201
5	OPLS Force Field for Choline Chloride-Based Deep Eutectic Solvents. Journal of Physical Chemistry B, 2018, 122, 9982-9993.	2.6	132
6	Solvent Effects and Mechanism for a Nucleophilic Aromatic Substitution from QM/MM Simulations. Organic Letters, 2004, 6, 2881-2884.	4.6	97
7	Claisen Rearrangements: Insight into Solvent Effects and â€œon Waterâ€•Reactivity from QM/MM Simulations. Journal of the American Chemical Society, 2010, 132, 1966-1975.	13.7	91
8	Elucidation of Hydrolysis Mechanisms for Fatty Acid Amide Hydrolase and Its Lys142Ala Variant via QM/MM Simulations. Journal of the American Chemical Society, 2006, 128, 16904-16913.	13.7	82
9	Understanding Rate Accelerations for Dielsâ^'Alder Reactions in Solution Using Enhanced QM/MM Methodology. Journal of Chemical Theory and Computation, 2007, 3, 1412-1419.	5.3	78
10	Elucidation of Rate Variations for a Dielsâ^'Alder Reaction in Ionic Liquids from QM/MM Simulations. Journal of Chemical Theory and Computation, 2007, 3, 132-138.	5.3	77
11	Kobophenol A Inhibits Binding of Host ACE2 Receptor with Spike RBD Domain of SARS-CoV-2, a Lead Compound for Blocking COVID-19. Journal of Physical Chemistry Letters, 2021, 12, 1793-1802.	4.6	77
12	Mechanism of Photolytic Decomposition of N-Halamine Antimicrobial Siloxane Coatings. ACS Applied Materials & Interfaces, 2010, 2, 2456-2464.	8.0	76
13	Cope Elimination:Â Elucidation of Solvent Effects from QM/MM Simulations. Journal of the American Chemical Society, 2006, 128, 6141-6146.	13.7	74
14	Influence of Inter- and Intramolecular Hydrogen Bonding on Kemp Decarboxylations from QM/MM Simulations. Journal of the American Chemical Society, 2005, 127, 8829-8834.	13.7	57
15	Multidimensional Exploration of Valleyâ^'Ridge Inflection Points on Potential-Energy Surfaces. Journal of the American Chemical Society, 2009, 131, 2530-2540.	13.7	56
16	Exploring Solvent Effects upon the Menshutkin Reaction Using a Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 8425-8430.	2.6	53
17	Virtual Site OPLS Force Field for Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2018, 122, 2962-2974.	2.6	46
18	Characterization and Mechanism for the Protection of Photolytic Decomposition of N-Halamine Siloxane Coatings by Titanium Dioxide. ACS Applied Materials & Interfaces, 2016, 8, 3516-3523.	8.0	42

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19	Quantum and molecular mechanical Monte Carlo techniques for modeling condensedâ€phase reactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 422-435.	14.6	37
20	Medium Effects on the Decarboxylation of a Biotin Model in Pure and Mixed Solvents from QM/MM Simulations. Journal of Organic Chemistry, 2006, 71, 4896-4902.	3.2	35
21	Pairwise Alternatives to Ewald Summation for Calculating Long-Range Electrostatics in Ionic Liquids. Journal of Chemical Theory and Computation, 2013, 9, 944-950.	5.3	35
22	Computation of Accurate Activation Barriers for Methyl-Transfer Reactions of Sulfonium and Ammonium Salts in Aqueous Solution. Journal of Chemical Theory and Computation, 2007, 3, 1028-1035.	5.3	33
23	An Ionic Liquid Dependent Mechanism for Base Catalyzed Î²-Elimination Reactions from QM/MM Simulations. Journal of the American Chemical Society, 2013, 135, 1065-1072.	13.7	33
24	Simulating Chemical Reactions in Ionic Liquids Using QM/MM Methodology. Journal of Physical Chemistry A, 2014, 118, 11653-11666.	2.5	32
25	A New Solvent-Dependent Mechanism for a Triazolinedione Ene Reaction. Journal of Organic Chemistry, 2008, 73, 912-922.	3.2	30
26	Density Functional Theory Determination of an Axial Gateway To Explain the Rate and Endo Selectivity Enhancement of Dielsâ€'Alder Reactions by Bis(oxazoline)-Cu(II). Journal of the American Chemical Society, 2004, 126, 6043-6047.	13.7	26
27	c-Phycocyanin primed silver nano conjugates: Studies on red blood cell stress resilience mechanism. Colloids and Surfaces B: Biointerfaces, 2020, 194, 111211.	5.0	26
28	Benchmarking Continuum Solvent Models for Ketoâ€“Enol Tautomerizations. Journal of Physical Chemistry A, 2015, 119, 8724-8733.	2.5	25
29	Curcumin-based pyrazoline analogues as selective inhibitors of human monoamine oxidase A. MedChemComm, 2018, 9, 1164-1171.	3.4	25
30	Effect of Phenyl Derivatization on the Stabilities of AntimicrobialN-Chlorohydantoin Derivatives. Industrial & Engineering Chemistry Research, 2010, 49, 11188-11194.	3.7	24
31	A Remodeled Protein Arginine Methyltransferase 1 (PRMT1) Generates Symmetric Dimethylarginine. Journal of Biological Chemistry, 2014, 289, 9320-9327.	3.4	24
32	Ionic Liquid Effects on Nucleophilic Aromatic Substitution Reactions from QM/MM Simulations. Journal of Physical Chemistry B, 2015, 119, 743-752.	2.6	24
33	Enhanced sampling by multiple molecular dynamics trajectories: carbonmonoxy myoglobin 10 Î¼s A0 â†' A1â€"3 transition from ten 400 picosecond simulations. Journal of Molecular Graphics and Modelling, 2004, 22, 369-376.	2.4	23
34	Using Electronic Theory To Identify Metabolites Present in 17Î±-Ethinylestradiol Biotransformation Pathways. Environmental Science & Technology, 2012, 46, 760-768.	10.0	23
35	Determination of local effects for chloroaluminate ionic liquids on Dielsâ€"Alder reactions. Journal of Molecular Graphics and Modelling, 2009, 28, 95-101.	2.4	22
36	Exploring the Aldol Reaction using Catalytic Antibodies and â€œOnÂWaterâ€•Organocatalysts from QM/MM Calculations. Journal of the American Chemical Society, 2014, 136, 147-156.	13.7	22

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37	Simulation of deep eutectic solvents: Progress to promises. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1598.	14.6	22
38	Phe71 in Type III Trypanosomal Protein Arginine Methyltransferase 7 (TbPRMT7) Restricts the Enzyme to Monomethylation. Biochemistry, 2018, 57, 1349-1359.	2.5	21
39	Identification of HIV Inhibitors Guided by Free Energy Perturbation Calculations. Current Pharmaceutical Design, 2012, 18, 1199-1216.	1.9	20
40	The Effect of Solvent on a Lewis Acid Catalyzed Dielsâ^'Alder Reaction, Using Computed and Experimental Kinetic Isotope Effects. Organic Letters, 2003, 5, 649-652.	4.6	18
41	Computational Insight into Small Molecule Inhibition of Cyclophilins. Journal of Chemical Information and Modeling, 2011, 51, 475-482.	5.4	16
42	Optimal scaling factors for CM1 and CM3 atomic charges in RM1â€based aqueous simulations. Journal of Computational Chemistry, 2011, 32, 2836-2842.	3.3	16
43	Role of Water in the Multifaceted Catalytic Antibody 4B2 for Allylic Isomerization and Kemp Elimination Reactions. Journal of Physical Chemistry B, 2009, 113, 15372-15381.	2.6	15
44	Substrate-Dependent Mobile Loop Conformational Changes in Alkanesulfonate Monooxygenase from Accelerated Molecular Dynamics. Biochemistry, 2020, 59, 3582-3593.	2.5	14
45	Accurate Diels-Alder Energies and Endo Selectivity in Ionic Liquids Using the OPLS-VSIL Force Field. International Journal of Molecular Sciences, 2020, 21, 1190.	4.1	13
46	Design, development and evaluation of novel dual PPARÎ´/PPARÎ³ agonists. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 873-879.	2.2	12
47	Partial Charges Optimized by Genetic Algorithms for Deep Eutectic Solvent Simulations. Journal of Chemical Theory and Computation, 2021, 17, 3078-3087.	5.3	12
48	Non-carboxylic acid inhibitors of aldose reductase based on N-substituted thiazolidinedione derivatives. European Journal of Medicinal Chemistry, 2021, 223, 113630.	5.5	12
49	Understanding protein arginine methyltransferase 1 (PRMT1) product specificity from molecular dynamics. Bioorganic and Medicinal Chemistry, 2016, 24, 4949-4960.	3.0	11
50	Examining Ionic Liquid Effects on Mononuclear Rearrangement of Heterocycles Using QM/MM Simulations. Journal of Physical Chemistry B, 2016, 120, 10786-10796.	2.6	10
51	Examining Product Specificity in Protein Arginine Methyltransferase 7 (PRMT7) Using Quantum and Molecular Mechanical Simulations. Journal of Chemical Information and Modeling, 2019, 59, 2913-2923.	5.4	10
52	Naturally occurring cancer-associated mutations disrupt oligomerization and activity of protein arginine methyltransferase 1 (PRMT1). Journal of Biological Chemistry, 2021, 297, 101336.	3.4	9
53	Mechanism of 5,5-Dimethylhydantoin Chlorination:â€‰ Monochlorination through a Dichloro Intermediate. Journal of Chemical Theory and Computation, 2007, 3, 2282-2289.	5.3	8
54	Comparison between Ab Initio Molecular Dynamics and OPLS-Based Force Fields for Ionic Liquid Solvent Organization. Journal of Physical Chemistry B, 2022, 126, 3908-3919.	2.6	8

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55	Primer for Designing Main Protease (M^{pro}) Inhibitors of SARS-CoV-2. Journal of Physical Chemistry Letters, 2022, 13, 5776-5786.	4.6	8
56	Computing Free-Energy Profiles Using Multidimensional Potentials of Mean Force and Polynomial Quadrature Methods. Annual Reports in Computational Chemistry, 2010, 6, 37-49.	1.7	5
57	Inter- and Intramolecular Mechanisms for Chlorine Rearrangements in Trimethyl-Substituted N-Chlorohydantoins. Journal of Physical Chemistry A, 2012, 116, 7245-7252.	2.5	5
58	Exploring the Catalytic Mechanism of Alkanesulfonate Monooxygenase Using Molecular Dynamics. Biochemistry, 2014, 53, 3308-3317.	2.5	5
59	Hydration of divalent lanthanides, Sm ²⁺ and Eu ²⁺ : A molecular dynamics study with polarizable <scp>AMOEBA</scp> force field. Journal of Computational Chemistry, 0, , .	3.3	4
60	Brain permeable curcumin-based pyrazoline analogs: MAO inhibitory and antioxidant activity. Journal of Molecular Structure, 2022, 1268, 133681.	3.6	3
61	Transition Structure Models of Organic Reactions in Chloroaluminate Ionic Liquids. ACS Symposium Series, 2003, , 174-190.	0.5	2
62	Discovery of 3-chlorobenzyl-linked 1,9-diazaspiro[5.5]undecane derivatives, a lead for dengue virus type 2 infection. New Journal of Chemistry, 2022, 46, 1087-1098.	2.8	2