

Carol A Parish

List of Publications by Year in descending order

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60
papers

1,066
citations

394421

19
h-index

434195

31
g-index

60
all docs

60
docs citations

60
times ranked

1450
citing authors

#	ARTICLE	IF	CITATIONS
1	Halogen Bonding in DNA Base Pairs. <i>Journal of the American Chemical Society</i> , 2012, 134, 5165-5172.	13.7	108
2	Carbohydrates: A United Atom AMBER* Parameterization of Pyranoses and Simulations Yielding Anomeric Free Energies. <i>Journal of the American Chemical Society</i> , 1996, 118, 2078-2086.	13.7	97
3	Nanoaggregates of Diverse Asphaltenes by Mass Spectrometry and Molecular Dynamics. <i>Energy & Fuels</i> , 2017, 31, 9140-9151.	5.1	63
4	An extended multireference study of the electronic states of para-benzyne. <i>Journal of Chemical Physics</i> , 2008, 129, 044306.	3.0	45
5	Triphenylamine-based receptor for selective recognition of dicarboxylates. <i>Tetrahedron Letters</i> , 2010, 51, 343-347.	1.4	42
6	Mechanisms for the Reaction of Thiophene and Methylthiophene with Singlet and Triplet Molecular Oxygen. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4934-4946.	2.5	42
7	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	3.0	42
8	Cages, Baskets, Ladders, and Tubes: A Conformational Studies of Polyhedral Oligomeric Silsesquioxanes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8371-8378.	2.5	39
9	Diastereoselective synthesis and cytotoxic evaluation of new isoxazoles and pyrazoles with monoterpenic skeleton. <i>Journal of Molecular Structure</i> , 2019, 1198, 126924.	3.6	37
10	Tuning the Bergman Cyclization by Introduction of Metal Fragments at Various Positions of the Eneidyne. <i>Metalla-Bergman Cyclizations. Journal of the American Chemical Society</i> , 2007, 129, 4401-4409.	13.7	36
11	Enantioselective binding of 2,2,2-trifluoro-1-(9-anthryl)ethanol on a chiral stationary phase: a theoretical study. <i>Analytical Chemistry</i> , 1987, 59, 1731-1733.	6.5	33
12	Three-body analytical potential for interacting helium atoms. <i>Journal of Chemical Physics</i> , 1994, 101, 7618-7624.	3.0	33
13	Pairwise and many-body contributions to interaction potentials in Hen clusters. <i>Journal of Chemical Physics</i> , 1993, 98, 437-443.	3.0	32
14	A comparison of the Low Mode and Monte Carlo conformational search methods. <i>Journal of Molecular Graphics and Modelling</i> , 2002, 21, 129-150.	2.4	32
15	The Closing Mechanism of DNA Polymerase I at Atomic Resolution. <i>Structure</i> , 2015, 23, 1609-1620.	3.3	28
16	Pyrolysis Mechanisms of Thiophene and Methylthiophene in Asphaltenes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2882-2891.	2.5	27
17	Molecular Dynamics Study of the Opening Mechanism for DNA Polymerase I. <i>PLoS Computational Biology</i> , 2014, 10, e1003961.	3.2	25
18	Modeling Oil Shale Pyrolysis: High-Temperature Unimolecular Decomposition Pathways for Thiophene. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7655-7666.	2.5	25

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19	Halogen Bonding Interactions for Aromatic and Nonaromatic Explosive Detection. ACS Sensors, 2019, 4, 389-397.	7.8	23
20	Oligonucleotide Incorporation and Base Pair Stability of 9-Deaza-2- ϵ -deoxyguanosine, an Analogue of 8-Oxo-2- ϵ -deoxyguanosine. Journal of Organic Chemistry, 2010, 75, 5661-5669.	3.2	20
21	Synthesis and Conformational Analysis of Novel Trimeric Maleimide Cross-Linking Reagents. Journal of Organic Chemistry, 2007, 72, 6776-6785.	3.2	16
22	An ab Initio Exploration of the Bergman Cyclization. Journal of Physical Chemistry A, 2018, 122, 420-430.	2.5	16
23	Column design. 3. Theoretical studies of a chiral stationary phase used in column chromatography. Journal of Computational Chemistry, 1987, 8, 753-760.	3.3	15
24	A Conservative Isoleucine to Leucine Mutation Causes Major Rearrangements and Cold Sensitivity in KlenTaq1 DNA Polymerase. Biochemistry, 2015, 54, 881-889.	2.5	15
25	(<i>rac</i>)-1,1'-Binaphthyl-Based Simple Receptors Designed for Fluorometric Discrimination of Maleic and Fumaric Acids. Journal of Physical Chemistry B, 2011, 115, 8597-8608.	2.6	14
26	New 1,2,3-Triazoles from (R)-Carvone: Synthesis, DFT Mechanistic Study and In Vitro Cytotoxic Evaluation. Molecules, 2022, 27, 769.	3.8	14
27	Synthesis, Spectroscopy, and Theoretical Calculations for a Series of Push ⁺ Pull [14]-Pyridoannulenes. Journal of Organic Chemistry, 2008, 73, 474-484.	3.2	12
28	Explorations on the multidimensional potential energy surface of a chiral stationary phase. Journal of Computational Chemistry, 1988, 9, 63-66.	3.3	10
29	Comparing the Conformational Behavior of a Series of Diastereomeric Cyclic Urea HIV-1 Inhibitors Using the Low Mode:Monte Carlo Conformational Search Method. Journal of Medicinal Chemistry, 2004, 47, 4838-4850.	6.4	10
30	Evaluating Halogen-Bond Strength as a Function of Molecular Structure Using Nuclear Magnetic Resonance Spectroscopy and Computational Analysis. Journal of Physical Chemistry A, 2021, 125, 9377-9393.	2.5	10
31	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. Journal of Physical Chemistry A, 2019, 123, 2049-2057.	2.5	9
32	Dicyclobuta[de,ij]naphthalene and Dicyclopenta[cd,gh]pentalene: A Theoretical Study. Journal of Organic Chemistry, 2004, 69, 8093-8100.	3.2	8
33	Triphenylamine-Based Open and Macrocyclic Receptors: A Study Towards Selective Recognition of Aliphatic Dicarboxylates. ChemistrySelect, 2017, 2, 4794-4799.	1.5	7
34	Analysis of MEMO1 Binding Specificity for ErbB2 Using Fluorescence Polarization and Molecular Dynamics Simulations. Biochemistry, 2018, 57, 5169-5181.	2.5	7
35	A Mechanistic Study of the 2-Thienylmethyl + HO ₂ Radical Recombination Reaction. Journal of Physical Chemistry A, 2011, 115, 14546-14557.	2.5	6
36	Internal abstraction of dynemicin A: An MD approach. Journal of Molecular Graphics and Modelling, 2017, 74, 251-264.	2.4	6

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37	Design and computational support for the binding stability of a new CCR5/CXCR4 dual tropic inhibitor. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 71-79.	2.4	6
38	Title is missing!. <i>Journal of Inorganic and Organometallic Polymers</i> , 2002, 12, 31-47.	1.5	5
39	Jahn-Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4237-4243.	2.5	5
40	A Molecular Dynamics Investigation of the Thermostability of Cold-Sensitive I707L KlenTaq1 DNA Polymerase and Its Wild-Type Counterpart. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2423-2431.	5.4	5
41	Conformational Analysis of a Model for the trans-Fused FGH Ether Rings in Brevetoxin A. <i>Journal of Organic Chemistry</i> , 2010, 75, 1582-1588.	3.2	4
42	An Extended Multireference Study of the Singlet and Triplet States of the 9,10-didehydroanthracene Diradical. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3688-3696.	2.5	4
43	Isofunctional Clustering and Conformational Analysis of the Arsenate Reductase Superfamily Reveals Nine Distinct Clusters. <i>Biochemistry</i> , 2020, 59, 4262-4284.	2.5	4
44	Identification of Phenazine-Based MEMO1 Small-Molecule Inhibitors: Virtual Screening, Fluorescence Polarization Validation, and Inhibition of Breast Cancer Migration. <i>ChemMedChem</i> , 2021, 16, 1163-1171.	3.2	4
45	A comparison of the AMBER*, OPLSAA and HF potential energy surfaces for a series of diastereomeric cyclic urea HIV-1 inhibitors. <i>Computational and Theoretical Chemistry</i> , 2004, 710, 73-76.	1.5	3
46	Evidence that the kinesin light chain domain contains tetratricopeptide repeat units. <i>Journal of Structural Biology</i> , 2012, 177, 602-612.	2.8	3
47	A molecular dynamics study of the binary complexes of APP, JIP1, and the cargo binding domain of KLC. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 221-234.	2.6	3
48	Diastereoselective synthesis of new Thiazolyl-Indazole derivatives from R-carvone: A combined experimental and theoretical study. <i>Tetrahedron</i> , 2021, 78, 131830.	1.9	3
49	Understanding the Structure and Apo Dynamics of the Functionally Active JIP1 Fragment. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 324-334.	5.4	3
50	Conformational analysis of trimeric maleimide substituted 1,5,9-triazacyclododecane HIV fusion scaffolds. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 1251-1258.	3.0	2
51	A Computational Study of the Reactivity of 3,5-(Oxo/Thioxo) Derivatives of 2,7-Dimethyl-1,2,4-Triazepines. Keto-Enol Tautomerization and Potential for Hydrogen Storage. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3076-3086.	2.5	2
52	A comparison of the chemical bonding and reactivity of Si8H8O12 and Ge8H8O12: A theoretical study. <i>Journal of Chemical Physics</i> , 2021, 154, 164305.	3.0	2
53	Investigating novel thiazolyl-indazole derivatives as scaffolds for SARS-CoV-2 MPro inhibitors. <i>European Journal of Medicinal Chemistry Reports</i> , 2022, 4, 100034.	1.4	2
54	Conformational analysis of siloxane-based enzyme-mimic precursors1. <i>Macromolecular Symposia</i> , 2003, 196, 327-336.	0.7	1

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55	Energetic analyses of chair and boat conformations of maleimide substituted cyclohexane derivatives. Journal of Computational Chemistry, 2009, 30, 992-998.	3.3	1
56	A Molecular Dynamics Investigation of the Thermostability of DNA Polymerase. FASEB Journal, 2015, 29, 561.7.	0.5	0
57	A Molecular Dynamics Study of Interaction between Kinesin Light Chain and Amyloid Precursor Protein. FASEB Journal, 2015, 29, 564.9.	0.5	0
58	Molecular Dynamics Study of the Opening and Closing Mechanisms for DNA Polymerase I. FASEB Journal, 2015, 29, 561.5.	0.5	0
59	Computational Analysis of the Interaction between Kinesin Light Chain and Amyloid Precursor Protein. FASEB Journal, 2015, 29, 564.10.	0.5	0
60	Drug Design Investigation of both Traditional FDA Drugs and POSS to Serve as an Effective HIV Protease Inhibitor. FASEB Journal, 2015, 29, 894.5.	0.5	0