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	New 1,2,3-Triazoles from (R)-Carvone: Synthesis, DFT Mechanistic Study and In Vitro Cytotoxic Evaluation. Molecules, 2022, 27, 769.	3.8	14
2	Investigating novel thiazolyl-indazole derivatives as scaffolds for SARS-CoV-2 MPro inhibitors. European Journal of Medicinal Chemistry Reports, 2022, 4, 100034.	1.4	2
3	Identification of Phenazineâ€Based MEMO1 Smallâ€Molecule Inhibitors: Virtual Screening, Fluorescence Polarization Validation, and Inhibition of Breast Cancer Migration. ChemMedChem, 2021, 16, 1163-1171.	3.2	4
4	Diastereoselective synthesis of new Thiazolyl-Indazole derivatives from R-carvone: A combined experimental and theoretical study. Tetrahedron, 2021, 78, 131830.	1.9	3
5	A comparison of the chemical bonding and reactivity of Si8H8O12 and Ge8H8O12: A theoretical study. Journal of Chemical Physics, 2021, 154, 164305.	3.0	2
6	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
7	Understanding the Structure and Apo Dynamics of the Functionally Active JIP1 Fragment. Journal of Chemical Information and Modeling, 2021, 61, 324-334.	5.4	3
8	Isofunctional Clustering and Conformational Analysis of the Arsenate Reductase Superfamily Reveals Nine Distinct Clusters. Biochemistry, 2020, 59, 4262-4284.	2.5	4
9	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
10	Diastereoselective synthesis and cytotoxic evaluation of new isoxazoles and pyrazoles with monoterpenic skeleton. Journal of Molecular Structure, 2019, 1198, 126924.	3.6	37
11	Halogen Bonding Interactions for Aromatic and Nonaromatic Explosive Detection. ACS Sensors, 2019, 4, 389-397.	7.8	23
12	A Molecular Dynamics Investigation of the Thermostability of Cold-Sensitive I707L KlenTaq1 DNA Polymerase and Its Wild-Type Counterpart. Journal of Chemical Information and Modeling, 2019, 59, 2423-2431.	5.4	5
13	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. Journal of Physical Chemistry A, 2019, 123, 2049-2057.	2.5	9
14	A Computational Study of the Reactivity of 3,5-(Oxo/Thioxo) Derivatives of 2,7-Dimethyl-1,2,4-Triazepines. Ketoâ€“Enol Tautomerization and Potential for Hydrogen Storage. Journal of Physical Chemistry A, 2018, 122, 3076-3086.	2.5	2
15	An Extended Multireference Study of the Singlet and Triplet States of the 9,10-didehydroanthracene Diradical. Journal of Physical Chemistry A, 2018, 122, 3688-3696.	2.5	4
16	An ab Initio Exploration of the Bergman Cyclization. Journal of Physical Chemistry A, 2018, 122, 420-430.	2.5	16
17	Analysis of MEMO1 Binding Specificity for ErbB2 Using Fluorescence Polarization and Molecular Dynamics Simulations. Biochemistry, 2018, 57, 5169-5181.	2.5	7
18	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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19	Triphenylamineâ€Based Open and Macrocyclic Receptors: A Study Towards Selectivite Recognition of Aliphatic Dicarboxylates. ChemistrySelect, 2017, 2, 4794-4799.	1.5	7
20	Design and computational support for the binding stability of a new CCR5/CXCR4 dual tropic inhibitor. Journal of Molecular Graphics and Modelling, 2017, 75, 71-79.	2.4	6
21	Modeling Oil Shale Pyrolysis: High-Temperature Unimolecular Decomposition Pathways for Thiophene. Journal of Physical Chemistry A, 2017, 121, 7655-7666.	2.5	25
22	Nanoaggregates of Diverse Asphaltenes by Mass Spectrometry and Molecular Dynamics. Energy & Fuels, 2017, 31, 9140-9151.	5.1	63
23	A molecular dynamics study of the binary complexes of APP, JIP1, and the cargo binding domain of KLC. Proteins: Structure, Function and Bioinformatics, 2017, 85, 221-234.	2.6	3
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	The Closing Mechanism of DNA Polymerase I at Atomic Resolution. Structure, 2015, 23, 1609-1620.	3.3	28
26	Jahnâ€“Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations. Journal of Physical Chemistry A, 2015, 119, 4237-4243.	2.5	5
27	A Molecular Dynamics Investigation of the Thermostability of DNA Polymerase. FASEB Journal, 2015, 29, 561.7.	0.5	0
28	A Molecular Dynamics Study of Interaction between Kinesin Light Chain and Amyloid Precursor Protein. FASEB Journal, 2015, 29, 564.9.	0.5	0
29	Molecular Dynamics Study of the Opening and Closing Mechanisms for DNA Polymerase I. FASEB Journal, 2015, 29, 561.5.	0.5	0
30	Computational Analysis of the Interaction between Kinesin Light Chain and Amyloid Precursor Protein. FASEB Journal, 2015, 29, 564.10.	0.5	0
31	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
32	Molecular Dynamics Study of the Opening Mechanism for DNA Polymerase I. PLoS Computational Biology, 2014, 10, e1003961.	3.2	25
33	Evidence that the kinesin light chain domain contains tetratricopeptide repeat units. Journal of Structural Biology, 2012, 177, 602-612.	2.8	3
34	Mechanisms for the Reaction of Thiophene and Methylthiophene with Singlet and Triplet Molecular Oxygen. Journal of Physical Chemistry A, 2012, 116, 4934-4946.	2.5	42
35	Halogen Bonding in DNA Base Pairs. Journal of the American Chemical Society, 2012, 134, 5165-5172.	13.7	108
36	(rac)-1,1â€²-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

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37	Pyrolysis Mechanisms of Thiophene and Methylthiophene in Asphaltenes. Journal of Physical Chemistry A, 2011, 115, 2882-2891.	2.5	27
38	A Mechanistic Study of the 2-Thienylmethyl + HO2Radical Recombination Reaction. Journal of Physical Chemistry A, 2011, 115, 14546-14557.	2.5	6
39	Triphenylamine-based receptor for selective recognition of dicarboxylates. Tetrahedron Letters, 2010, 51, 343-347.	1.4	42
40	Conformational Analysis of a Model for the trans-Fused FGH Ether Rings in Brevetoxin A. Journal of Organic Chemistry, 2010, 75, 1582-1588.	3.2	4
41	Oligonucleotide Incorporation and Base Pair Stability of 9-Deaza-2â€²-deoxyguanosine, an Analogue of 8-Oxo-2â€²-deoxyguanosine. Journal of Organic Chemistry, 2010, 75, 5661-5669.	3.2	20
42	Energetic analyses of chair and boat conformations of maleimide substituted cyclohexane derivatives. Journal of Computational Chemistry, 2009, 30, 992-998.	3.3	1
43	Conformational analysis of trimeric maleimide substituted 1,5,9-triazacyclododecane HIV fusion scaffolds. Bioorganic and Medicinal Chemistry, 2009, 17, 1251-1258.	3.0	2
44	An extended multireference study of the electronic states of para-benzyne. Journal of Chemical Physics, 2008, 129, 044306.	3.0	45
45	Synthesis, Spectroscopy, and Theoretical Calculations for a Series of Pushâ€'Pull [14]-Pyridoannulenes. Journal of Organic Chemistry, 2008, 73, 474-484.	3.2	12
46	Synthesis and Conformational Analysis of Novel Trimeric Maleimide Cross-Linking Reagents. Journal of Organic Chemistry, 2007, 72, 6776-6785.	3.2	16
47	Tuning the Bergman Cyclization by Introduction of Metal Fragments at Various Positions of the Enediyne. Metalla-Bergman Cyclizations. Journal of the American Chemical Society, 2007, 129, 4401-4409.	13.7	36
48	Cages, Baskets, Ladders, and Tubes:â€‰Conformational Studies of Polyhedral Oligomeric Silsesquioxanes. Journal of Physical Chemistry A, 2005, 109, 8371-8378.	2.5	39
49	A comparison of the AMBER*, OPLSAA and HF potential energy surfaces for a series of diastereomeric cyclic urea HIV-1 inhibitors. Computational and Theoretical Chemistry, 2004, 710, 73-76.	1.5	3
50	Dicyclobuta[de,ij]naphthalene and Dicyclopenta[cd,gh]pentalene:Â A Theoretical Study. Journal of Organic Chemistry, 2004, 69, 8093-8100.	3.2	8
51	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
52	Conformational analysis of siloxane-based enzyme-mimic precursors1. Macromolecular Symposia, 2003, 196, 327-336.	0.7	1
53	A comparison of the Low Mode and Monte Carlo conformational search methods. Journal of Molecular Graphics and Modelling, 2002, 21, 129-150.	2.4	32
54	Title is missing!. Journal of Inorganic and Organometallic Polymers, 2002, 12, 31-47.	1.5	5

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55	Carbohydrates:Â United Atom AMBER* Parameterization of Pyranoses and Simulations Yielding Anomeric Free Energies. Journal of the American Chemical Society, 1996, 118, 2078-2086.	13.7	97
56	Threeâ€body analytical potential for interacting helium atoms. Journal of Chemical Physics, 1994, 101, 7618-7624.	3.0	33
57	Pairwise and manyâ€body contributions to interaction potentials in Hen clusters. Journal of Chemical Physics, 1993, 98, 437-443.	3.0	32
58	Explorations on the multidimensional potential energy surface of a chiral stationary phase. Journal of Computational Chemistry, 1988, 9, 63-66.	3.3	10
59	Enantioselective binding of 2,2,2-trifluoro-1-(9-anthryl)ethanol on a chiral stationary phase: a theoretical study. Analytical Chemistry, 1987, 59, 1731-1733.	6.5	33
60	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