

Dandamudi Usharani

List of Publications by Year in descending order

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44
papers

1,494
citations

471509

17
h-index

315739

38
g-index

48
all docs

48
docs citations

48
times ranked

1704
citing authors

#	ARTICLE	IF	CITATIONS
1	Dichotomous Hydrogen Atom Transfer vs Proton-Coupled Electron Transfer During Activation of X-H Bonds (X = C, N, O) by Nonheme Iron-Oxo Complexes of Variable Basicity. <i>Journal of the American Chemical Society</i> , 2013, 135, 17090-17104.	13.7	216
2	A Theory for Bioinorganic Chemical Reactivity of Oxometal Complexes and Analogous Oxidants: The Exchange and Orbital-Selection Rules. <i>Accounts of Chemical Research</i> , 2013, 46, 471-482.	15.6	154
3	Nonheme Iron Oxidant Formed in the Presence of H ₂ O ₂ and Acetic Acid Is the Cyclic Ferric Peracetate Complex, Not a Ferryl-oxo Complex. <i>ACS Catalysis</i> , 2013, 3, 1334-1341.	11.2	96
4	Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations [XYO ₂] ⁺ (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer. <i>Journal of the American Chemical Society</i> , 2016, 138, 7973-7981.	13.7	90
5	How Does Tunneling Contribute to Counterintuitive H-Abstraction Reactivity of Nonheme Fe(IV)O Oxidants with Alkanes?. <i>Journal of the American Chemical Society</i> , 2015, 137, 722-733.	13.7	89
6	Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions. <i>Journal of the American Chemical Society</i> , 2016, 138, 11368-11377.	13.7	85
7	Targeting COVID-19 (SARS-CoV-2) main protease through active phytochemicals of ayurvedic medicinal plants - Emblica officinalis (Amla), Phyllanthus niruri Linn. (Bhumi Amla) and Tinospora cordifolia (Giloy) - A molecular docking and simulation study. <i>Computers in Biology and Medicine</i> , 2021, 136, 104683.	7.0	77
8	Modeling C-H Abstraction Reactivity of Nonheme Fe(IV)O Oxidants with Alkanes: What Role Do Counter Ions Play?. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2610-2617.	4.6	66
9	Does the TauD Enzyme Always Hydroxylate Alkanes, While an Analogous Synthetic Non-Heme Reagent Always Desaturates Them?. <i>Journal of the American Chemical Society</i> , 2011, 133, 176-179.	13.7	64
10	Theory Uncovers an Unusual Mechanism of DNA Repair of a Lesioned Adenine by AlkB Enzymes. <i>Journal of the American Chemical Society</i> , 2014, 136, 13895-13901.	13.7	64
11	A tutorial for understanding chemical reactivity through the valence bond approach. <i>Chemical Society Reviews</i> , 2014, 43, 4968-4988.	38.1	58
12	Trends in Aromatic Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes: A Valence Bond Modeling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 327-339.	5.3	53
13	Subtype Selectivity in Phosphodiesterase 4 (PDE4): A Bottleneck in Rational Drug Design. <i>Current Pharmaceutical Design</i> , 2008, 14, 3854-3872.	1.9	51
14	The Origins of Dramatic Axial Ligand Effects: Closed-Shell Mn ^V O Complexes Use Exchange-Enhanced Open-Shell States to Mediate Efficient H-Abstraction Reactions. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 4421-4425.	13.8	40
15	Design, Synthesis, and DNA Binding Properties of Photoisomerizable Azobenzene-Distamycin Conjugates: An Experimental and Computational Study. <i>Bioconjugate Chemistry</i> , 2008, 19, 2332-2345.	3.6	32
16	A Single-Site Mutation (F429H) Converts the Enzyme CYP 2B4 into a Heme Oxygenase: A QM/MM Study. <i>Journal of the American Chemical Society</i> , 2012, 134, 4053-4056.	13.7	31
17	Brain Chemistry: How Does P450 Catalyze the O-Demethylation Reaction of 5-Methoxytryptamine to Yield Serotonin?. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7078-7089.	2.6	28
18	Sesaminol diglucoside, a water-soluble lignan from sesame seeds induces brown fat thermogenesis in mice. <i>Biochemical and Biophysical Research Communications</i> , 2018, 507, 155-160.	2.1	17

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19	Intramolecular Gas-Phase Reactions of Synthetic Nonheme Oxoiron(IV) Ions: Proximity and Spin-State Reactivity Rules. <i>Chemistry - A European Journal</i> , 2012, 18, 11747-11760.	3.3	15
20	Structural and Functional Characterization of a Cytochrome P450 2B4 F429H Mutant with an Axial Thiolate-Histidine Hydrogen Bond. <i>Biochemistry</i> , 2014, 53, 5080-5091.	2.5	14
21	Redox-Associated Variation of Hückel Aromaticity from Lactam-Embedded Smallest Antiaromatic trans-Doubly N-Confused Porphyrins: Synthesis and Characterization. <i>Journal of Organic Chemistry</i> , 2020, 85, 2059-2067.	3.2	14
22	Photophysical and Duplex-DNA-Binding Properties of Distamycin Dimers Based on 4,4'- and 2,2'-Dialkoxyazobenzenes as the Core. <i>Chemistry - an Asian Journal</i> , 2008, 3, 1949-1961.	3.3	13
23	Salt bridges are pivotal for the kinetic stability of GH26 endo-mannanase (ManB-1601). <i>International Journal of Biological Macromolecules</i> , 2019, 133, 1236-1241.	7.5	13
24	Electronic structure and bonding studies on triple-decker sandwich complexes with a P6 middle ring. <i>Journal of Computational Chemistry</i> , 2007, 28, 310-319.	3.3	11
25	<i>meso</i> -Aryl substituted stable unorthodox 5,10-porphodimethenes with $\hat{1}^{\pm}, \hat{1}^2$ and $\hat{1}^2, \hat{1}^2$ - <i>N</i> -methyl pyrrole connectivities: synthesis and spectroscopic, solid state and theoretical characterization. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6131-6135.	2.8	8
26	Perimeter Coordinated Diastereomeric Rh(I) Complex of Helically Twisted Weakly Aromatic Hybrid Singly N-Confused $\hat{1}^2$ - $\hat{1}^2$ Fused Ferrocenoporphyrinoids. <i>Journal of Organic Chemistry</i> , 2021, 86, 8015-8026.	3.2	8
27	Targeted synthesis of <i>meso</i> -aryl substituted aromatic trans-doubly N-confused dithia/diselena [18] porphyrins (1.1.1.1) with NIR absorption: spectroscopic and theoretical characterization. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 6058-6062.	2.8	8
28	Electronic Structure and Bonding in Neutral and Dianionic Boradiphospholes: $R^2BC_2P_2R_2$ ($R=H, t\text{-}Bu, R^2=H, Ph$). <i>Chemistry - A European Journal</i> , 2009, 15, 8429-8442.	3.3	7
29	Conformationally Rigid Ethynylene-Cumulene Conjugated Aromatic [30] Heteroannulenes with NIR Absorption: Synthesis, Spectroscopic and Theoretical Characterization. <i>Journal of Organic Chemistry</i> , 2019, 84, 5203-5212.	3.2	7
30	A Rationally Designed Multifunctional Antibiotic for the Treatment of Drug-Resistant Acne. <i>Journal of Investigative Dermatology</i> , 2018, 138, 1400-1408.	0.7	6
31	Mono-nuclear copper complexes mimicking the intermediates for the binuclear copper center of the subunit II of cytochrome oxidase: a peptide based approach. <i>Dalton Transactions</i> , 2016, 45, 17624-17632.	3.3	5
32	A bioactive polypeptide from sugarcane selectively inhibits intestinal sucrase. <i>International Journal of Biological Macromolecules</i> , 2020, 156, 938-948.	7.5	4
33	Structural isolation of NIR absorbing ferrocenyl bridged N-confused fused expanded phlorin, N-confused porphodimethene and the $\hat{1}^2$ -extended corrorin isomer: synthesis and characterization. <i>Dalton Transactions</i> , 2021, 50, 14421-14431.	3.3	4
34	Zn ²⁺ stapling of N and C-terminal maintains stability and substrate affinity in GH26 endo-mannanase. <i>Enzyme and Microbial Technology</i> , 2020, 135, 109497.	3.2	3
35	Molecular insights into the mechanism of substrate binding and catalysis of bifunctional FAD synthetase from <i>Staphylococcus aureus</i> . <i>Biochimie</i> , 2021, 182, 217-227.	2.6	3
36	Ni(II) and Cu(III) organometallic complexes of trans doubly N-confused porphodimethenes: Synthesis, spectroscopic and theoretical characterization. <i>Journal of Porphyrins and Phthalocyanines</i> , 2021, 25, 966-974.	0.8	3

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37	Chemical transformation of doubly N-confused porphodimethenes to variants of (anti)aromatic doubly N-confused porphyrinoids and If-aromatic doubly N-confused isophlorinoids. Organic Chemistry Frontiers, 0, , .	4.5	3
38	pH Dependence of a 310-Helix versus a Turn in the M-Loop Region of PDE4: Observations on PDB Entries and an Electronic Structure Study. Journal of Chemical Theory and Computation, 2008, 4, 974-984.	5.3	2
39	Structure and Bonding in Stannadiphospholes and their Dianions SnC ₂ P ₂ R ₂ ^m (R=H, t-Bu, m=0, 2): A Comparative Study with C ₅ H ₅ ⁺ and C ₅ H ₅ ⁺ Analogues. Chemistry - A European Journal, 2011, 17, 9142-9152.	3.3	1
40	Tropylium cation-fused aromatic [26]dicarbaporphyrinoids with NIR absorptions: Synthesis, spectroscopic and theoretical characterization. Journal of Porphyrins and Phthalocyanines, 2020, 24, 161-170.	0.8	1
41	Metalloincorporated Hybrid Singly N-Methyl N-Confused Calixphyrins: Synthesis, Characterization, Protonation and Deprotonation Studies. Chemistry - an Asian Journal, 2022, 17, .	3.3	1
42	Insights into the role of F26 residue in the FMN: ATP adenylyltransferase activity of Staphylococcus aureus FAD synthetase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2022, 1870, 140781.	2.3	1
43	Fluoride ion promoted NH deprotonation of dioxaPhlorin with NIR absorption vs. acid induced facile conversion to aromatic dioxaSapphyrin: Synthesis, spectroscopic and theoretical characterization. Journal of Porphyrins and Phthalocyanines, 2021, 25, 436-446.	0.8	0
44	Prevailing charge transfer in the reaction of protonated and neutral nitric oxide: A theoretical and experimental study. International Journal of Mass Spectrometry, 2022, 471, 116724.	1.5	0