

Nurcan S Tuzun

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

40
papers

481
citations

12
h-index

20
g-index

43
ext. papers

534
ext. citations

3.9
avg, IF

3.88
L-index

#	Paper	IF	Citations
40	Computational Survey of Recent Experimental Developments in the Hydroxylation Mechanism of Kynurenine 3-Monooxygenase. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 9459-9477	2.8	
39	A new perspective on the beryllium sensor platform: Low symmetry phthalocyanine-based molecular design and ultra trace amount Be ²⁺ ion recognition in aqueous media. <i>Sensors and Actuators B: Chemical</i> , 2021 , 329, 129002	8.5	4
38	Non-peripherally substituted metallophthalocyanines catalyzed diastereoselective carbonyl-ylide reactions: Synthesis and DFT calculations. <i>Tetrahedron</i> , 2021 , 80, 131892	2.4	
37	Regioselectivity Patterns in Radical Cyclization of Diosphenol Derivatives with Different Ring Size: A Combined Experimental and DFT Study. <i>ChemistrySelect</i> , 2021 , 6, 1748-1755	1.8	
36	In silico methods predict new blood-brain barrier permeable structure for the inhibition of kynurenine 3-monooxygenase. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 100, 107701	2.8	0
35	Amberlyst-15-catalyzed Procedure for the Synthesis of Novel 2,4-Dihydroxybenzoyl-1,2,3-triazoles and Molecular Modelling Studies for Hsp-90 Inhibition. <i>ChemistrySelect</i> , 2019 , 4, 7278-7283	1.8	2
34	Mechanism of Kynurenine 3-Monooxygenase-Catalyzed Hydroxylation Reaction: A Quantum Cluster Approach. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 3149-3159	2.8	5
33	Superior Sensor for Be Ion Recognition via the Unprecedented Octahedral Crystal Structure of a One-Dimensional Coordination Polymer of Crown Fused Zinc Phthalocyanine. <i>Inorganic Chemistry</i> , 2019 , 58, 909-923	5.1	11
32	Computational investigation of the control of the thermodynamics and microkinetics of the reductive amination reaction by solvent coordination and a co-catalyst.. <i>RSC Advances</i> , 2018 , 8, 36662-36674	2.7	6
31	New ferrocenyl naphthoquinone fused crown ether chemosensors: Highly selective, kinetically and regio controlled colorimetric, beryllium ion recognition. <i>Journal of Organometallic Chemistry</i> , 2018 , 868, 131-143	2.3	9
30	Investigation of PDE5/PDE6 and PDE5/PDE11 selective potent tadalafil-like PDE5 inhibitors using combination of molecular modeling approaches, molecular fingerprint-based virtual screening protocols and structure-based pharmacophore development. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017 , 32, 211-222	5.6	20
29	A DFT study on the mechanism of Rh-catalyzed competitive 1,2- versus 1,3-acyloxy migration followed by [5+1] and [4+1] cycloadditions of 1,4-enynes with CO. <i>Journal of Organometallic Chemistry</i> , 2017 , 851, 97-103	2.3	7
28	Structural investigation of vesnarinone at the pore domains of open and open-inactivated states of hERG1 K channel. <i>Journal of Molecular Graphics and Modelling</i> , 2017 , 77, 399-412	2.8	3
27	Mechanism of CuAAC reaction: In acetic acid and aprotic conditions. <i>Journal of Molecular Catalysis A</i> , 2017 , 426, 150-157		6
26	In silico design of novel hERG-neutral sildenafil-like PDE5 inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 2830-2852	3.6	1
25	Ag-catalyzed azide alkyne cycloaddition: a DFT approach. <i>Dalton Transactions</i> , 2016 , 45, 5752-64	4.3	15
24	A DFT Study on the Binuclear CuAAC Reaction: Mechanism in Light of New Experiments. <i>Organometallics</i> , 2016 , 35, 2589-2599	3.8	39

23	Synthesis, reactions and DFT study of tropolone N,N-dimethylthiocarbamate. <i>Tetrahedron</i> , 2015 , 71, 5391-5398	2.4	5
22	A Quantum Mechanical Study on the Propagation Kinetics of N-methylacrylamide: Comparison With N,N-Dimethylacrylamide in Free Radical Polymerization. <i>Macromolecular Theory and Simulations</i> , 2015 , 24, 218-231	1.5	2
21	Synthesis and characterization of solution processable 6,11-dialkynyl substituted indeno[1,2-b]anthracenes. <i>Dyes and Pigments</i> , 2014 , 100, 104-117	4.6	8
20	A Theoretical Study On Rh(I) Catalyzed Enantioselective Conjugate Addition Reactions of Fluoroalkylated Olefins. <i>Organometallics</i> , 2014 , 33, 5111-5119	3.8	7
19	Stereoselective propagation in free radical polymerization of acrylamides: a DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2014 , 49, 55-67	2.8	7
18	Prediction of the 1H NMR spectra of epoxy-fused cyclopentane derivatives by calculations of chemical shifts and spin-spin coupling constants. <i>Molecular Physics</i> , 2013 , 111, 3147-3155	1.7	0
17	Reaction mechanism of ruthenium-catalyzed azide-alkyne cycloaddition reaction: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2013 , 724, 167-176	2.3	31
16	The mechanism of copper-catalyzed azide-alkyne cycloaddition reaction: a quantum mechanical investigation. <i>Journal of Molecular Graphics and Modelling</i> , 2012 , 34, 101-7	2.8	18
15	A QSPR Study on the Physical Properties of Substituted Polypyrroles and Poly(paraphenylenes). <i>Designed Monomers and Polymers</i> , 2011 , 14, 79-93	3.1	
14	Cyclopolymerization reactions of diallyl monomers: exploring electronic and steric effects using DFT reactivity indices. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 8704-11	2.8	30
13	Mechanistic Study on [3+2] Cycloaddition and Cyclopropanation Reactions of 1,3-Dioxepine Derivatives in the Presence of Copper(I) Catalyst. <i>Organometallics</i> , 2009 , 28, 4964-4973	3.8	10
12	A DFT Study on the Mechanism of Cyclopropanation via Cu(acac) ₂ -Catalyzed Diazo Ester Decomposition. <i>Organometallics</i> , 2008 , 27, 4600-4610	3.8	23
11	An experimental and quantum mechanical study on electrochemical properties of N-substituted pyrroles. <i>Computational and Theoretical Chemistry</i> , 2008 , 857, 95-104		9
10	Metal-Catalyzed Cyclization Reactions of Carbonyl Ylides: Synthesis and DFT Study of Mechanisms. <i>Organometallics</i> , 2007 , 26, 2978-2985	3.8	22
9	Modeling the cyclopolymerization of diallyl ether and methyl α -(allyloxy)methyl]acrylate. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 894-906	2.1	9
8	Modeling the effect of substitution on the Pb(OAc) ₄ mediated oxidative cleavage of steroidal 1,2-diols. <i>Journal of Organic Chemistry</i> , 2005 , 70, 7080-6	4.2	12
7	Modeling the free radical polymerization of acrylates. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 176-189	2.1	27
6	Spirodiporphyrins--as binuclear metal complexes. <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 2857-62	16.4	78

5	Cover Picture: Spirodiporphyrins As Binuclear Metal Complexes (Angew. Chem. Int. Ed. 25/2003). <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 2805-2805	16.4	
4	A theoretical study on the mechanism of the cyclopolymerization of diallyl monomers. <i>Journal of Organic Chemistry</i> , 2003 , 68, 6369-74	4.2	14
3	A Computational Study on the Substituent Effect of Diallylamine Monomers in Their Cyclopolymerization Reactions. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 8184-8190	2.8	12
2	Theoretical study of factors controlling rates of cyclization of radical intermediates from diallylamine and diallylammonium monomers in radical polymerizations. <i>Journal of Organic Chemistry</i> , 2002 , 67, 5068-75	4.2	19
1	A computational approach to the polymerizabilities of diallylamines. <i>Journal of Molecular Modeling</i> , 2001 , 7, 257-264	2	9