Fethiye Aylin Sungur

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8734489/publications.pdf

Version: 2024-02-01

21 papers	249 citations	1039406 9 h-index	940134 16 g-index
21 all docs	21 docs citations	21 times ranked	335 citing authors

#	Article	IF	Citations
1	Repurposing of <scp>FDA</scp>â€approved drugs against active site and potential allosteric drugâ€binding sites of <scp>COVID</scp>â€19 main protease. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1425-1441.	1.5	30
2	Monte Carlo and Molecular Dynamics Simulations suggest controlled release of corticosteroids from mesoporous host MIL-101 (Cr). Molecular Simulation, 2021, 47, 1530-1539.	0.9	1
3	Bismuth nitrate-promoted disproportionative condensation of indoles with cyclohexanone: a new-type azafulvenium reactivity of indole. New Journal of Chemistry, 2017, 41, 9674-9687.	1.4	7
4	A computational insight into cyclopropenone activated dehydration reaction of alcohols. Journal of Molecular Graphics and Modelling, 2017, 77, 106-114.	1.3	2
5	Molecular dynamics simulations of apo, holo, and inactivator bound GABAâ€at reveal the role of active site residues in PLP dependent enzymes. Proteins: Structure, Function and Bioinformatics, 2016, 84, 875-891.	1.5	4
6	Role of then+1 amino acid residue on the deamidation of asparagine in pentapeptides. Molecular Physics, 2015, 113, 3839-3848.	0.8	1
7	A Theoretical Study On Rh(I) Catalyzed Enantioselective Conjugate Addition Reactions of Fluoroalkylated Olefins. Organometallics, 2014, 33, 5111-5119.	1.1	8
8	Stereoelectronic explanations for the mechanistic details of transimination and HF elimination reactions. Journal of Molecular Graphics and Modelling, 2014, 51, 173-183.	1.3	2
9	Theoretical Study on HF Elimination and Aromatization Mechanisms: A Case of Pyridoxal 5â€² Phosphate-Dependent Enzyme. Journal of Organic Chemistry, 2012, 77, 5533-5543.	1.7	5
10	Solventâ€Catalyzed Ringâ€“Chainâ€“Ring Tautomerization in Axially Chiral Compounds. Chemistry - A European Journal, 2012, 18, 12725-12732.	1.7	14
11	Theoretical studies on the inactivation mechanism of Î³-aminobutyric acid aminotransferase. Organic and Biomolecular Chemistry, 2011, 9, 5162.	1.5	7
12	A computational study on the mechanism and the kinetics of urethane formation. Computational and Theoretical Chemistry, 2011, 963, 168-175.	1.1	23
13	Mechanistic Study on [3+2] Cycloaddition and Cyclopropanation Reactions of 1,3-Dioxepine Derivatives in the Presence of Copper(I) Catalyst. Organometallics, 2009, 28, 4964-4973.	1.1	10
14	Coupling of structural fluctuations to deamidation reaction in triosephosphate isomerase by Gaussian network model. Proteins: Structure, Function and Bioinformatics, 2005, 62, 715-727.	1.5	5
15	Theoretical Approach to the Wear and Tear Mechanism in Triosephoshate Isomerase:Â A QM/MM Study. Journal of Physical Chemistry B, 2004, 108, 3925-3934.	1.2	5
16	Barriers to internal rotation around the Câ€“N bond in 3-(o-aryl)-5-methyl-rhodanines using NMR spectroscopy and computational studies. Electron density topological analysis of the transition states. Organic and Biomolecular Chemistry, 2004, 2, 2426-2436.	1.5	14
17	Modelling the hydrolysis of succinimide: formation of aspartate and reversible isomerization of aspartic acid via succinimide. Organic and Biomolecular Chemistry, 2003, 1, 2290.	1.5	30
18	Theoretical Study on the Alkaline and Neutral Hydrolysis of Succinimide Derivatives in Deamidation Reactions. Journal of Physical Chemistry A, 2002, 106, 11205-11214.	1.1	27

#	Article	IF	Citations
19	Modeling the deamidation of asparagine residues via succinimide intermediates. Journal of Molecular Modeling, 2001, 7, 147-160.	0.8	29
20	Conformational properties of amphotericin B amide derivatives--impact on selective toxicity. Journal of Computer-Aided Molecular Design, 2000, 14, 689-703.	1.3	25
21	Molecular Mechanism of Protein Arginine Deiminase 2: A Study Involving Multiple Microsecond Long Molecular Dynamics Simulations. Biochemistry, 0, , .	1.2	0