Fethiye Aylin Sungur

List of Publications by Year
in descending order

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21 papers	249 citations	1039880 9 h-index	940416 16 g-index
21 all docs	21 docs citations	21 times ranked	335 citing authors

#	Article	IF	Citations
1	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
2	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
3	Modeling the deamidation of asparagine residues via succinimide intermediates. Journal of Molecular Modeling, 2001, 7, 147-160.	0.8	29
4	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
5	Conformational properties of amphotericin B amide derivatives--impact on selective toxicity. Journal of Computer-Aided Molecular Design, 2000, 14, 689-703.	1.3	25
6	A computational study on the mechanism and the kinetics of urethane formation. Computational and Theoretical Chemistry, 2011, 963, 168-175.	1.1	23
7	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
8	Solventâ€Catalyzed Ringâ€“Chainâ€“Ring Tautomerization in Axially Chiral Compounds. Chemistry - A European Journal, 2012, 18, 12725-12732.	1.7	14
9	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
10	A Theoretical Study On Rh(I) Catalyzed Enantioselective Conjugate Addition Reactions of Fluoroalkylated Olefins. Organometallics, 2014, 33, 5111-5119.	1.1	8
11	Theoretical studies on the inactivation mechanism of Î³-aminobutyric acid aminotransferase. Organic and Biomolecular Chemistry, 2011, 9, 5162.	1.5	7
12	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
13	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
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 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
16	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
17	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
18	A computational insight into cyclopropenone activated dehydration reaction of alcohols. Journal of Molecular Graphics and Modelling, 2017, 77, 106-114.	1.3	2

#	Article	IF	Citations
19	Role of then+1 amino acid residue on the deamidation of asparagine in pentapeptides. Molecular Physics, 2015, 113, 3839-3848.	0.8	1
20	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
21	Molecular Mechanism of Protein Arginine Deiminase 2: A Study Involving Multiple Microsecond Long Molecular Dynamics Simulations. Biochemistry, 0, , .	1.2	0