Gugan Kothandan

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4140196/publications.pdf

Version: 2024-02-01

		1040056	839539
21	341	9	18
papers	citations	h-index	g-index

21	21	21	536
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding the dual mechanism of bioactive peptides targeting the enzymes involved in Renin Angiotensin System (RAS): An in-silico approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5044-5061.	3.5	8
2	Berberine and Emodin abrogates breast cancer growth and facilitates apoptosis through inactivation of SIK3-induced mTOR and Akt signaling pathway. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2020, 1866, 165897.	3.8	35
3	In-silico studies on Myo inositol-1-phosphate synthase of Leishmania donovani in search of anti-leishmaniasis. Journal of Biomolecular Structure and Dynamics, 2020, , 1-14.	3.5	5
4	Insights of structure-based pharmacophore studies and inhibitor design against Gal3 receptor through molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-13.	3.5	2
5	Proposing the Promiscuous Protein Structures in JNK1 and JNK3 for Virtual Screening in Pursuit of Potential Leads. ACS Omega, 2020, 5, 3969-3978.	3.5	2
6	Synthesis, X-ray crystal structure and DFT calculations of 2â€²,4â€²-dihydro-10H-spiro [anthracene-9,3â€²-benzo[b][1,4]thiazin]-10-amine and 1,3,5 -triindolyl benzene. Chemical Data Collections, 2019, 21, 100227.	2.3	3
7	Application of docking and active site analysis for enzyme linked biodegradation of textile dyes. Environmental Pollution, 2019, 248, 599-608.	7.5	77
8	Unveiling the Accuracy of Homology Modeling to Elucidate the Structure of GPCRs-HIV Co-receptor-CCR5 as a Case Study. Letters in Drug Design and Discovery, 2018, 15, 1068-1078.	0.7	1
9	Structural insights into the Aedes aegypti aquaporins and aquaglyceroporins â€“ an in silico study. Journal of Receptor and Signal Transduction Research, 2016, 36, 543-557.	2.5	2
10	In silico study of 1-(4-Phenylpiperazin-1-yl)-2-(1H-pyrazol-1-yl) ethanones derivatives as CCR1 antagonist: Homology modeling, docking and 3D-QSAR approach. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 928-933.	2.2	14
11	The nociceptin receptor (NOPR) and its interaction with clinically important agonist molecules: a membrane molecular dynamics simulation study. Molecular BioSystems, 2014, 10, 3188-3198.	2.9	9
12	Enhancement of P-gylcoprotein modulators of arylmethylamine-phenyl derivatives: an integrative modeling approach. Medicinal Chemistry Research, 2013, 22, 2511-2523.	2.4	2
13	Theoretical Characterization of Galanin Receptor Type 3 (<scp>G</scp>al₃) and Its Interaction with Agonist (<scp>GALANIN</scp>) and Antagonists (<scp>SNAP</scp> 37889 and) Tj ETQq1 1 0.784314 rgBT /Overlock 757-774.	3.2	4
14	A combined 3D QSAR and pharmacophore-based virtual screening for the identification of potent p38 MAP kinase inhibitors: an in silico approach. Medicinal Chemistry Research, 2013, 22, 1773-1787.	2.4	15
15	Large variation in electrostatic contours upon addition of steric parameters and the effect of charge calculation schemes in CoMFA on mutagenicity of MX analogues. Molecular Simulation, 2012, 38, 861-871.	2.0	30
16	Various atomic charge calculation schemes of CoMFA on HIFâ€1 inhibitors of moracin analogs. International Journal of Quantum Chemistry, 2012, 112, 995-1005.	2.0	8
17	QSAR analysis on PfPK7 inhibitors using HQSAR, CoMFA, and CoMSIA. Medicinal Chemistry Research, 2012, 21, 681-693.	2.4	9
18	Molecular modeling study of HIV-1 gp120 attachment inhibitors. Medicinal Chemistry Research, 2012, 21, 1892-1904.	2.4	6

#	Article	IF	Citations
19	Structural Insights from Binding Poses of CCR2 and CCR5 with Clinically Important Antagonists: A Combined In Silico Study. PLoS ONE, 2012, 7, e32864.	2.5	43
20	Binding Site Analysis of CCR2 Through In Silico Methodologies: Docking, CoMFA, and CoMSIA. Chemical Biology and Drug Design, 2011, 78, 161-174.	3.2	16
21	Docking and 3D-QSAR (quantitative structure activity relationship) studies of flavones, the potent inhibitors of p-glycoprotein targeting the nucleotide binding domain. European Journal of Medicinal Chemistry, 2011, 46, 4078-4088.	5.5	50