

# Gugan Kothandan

## List of Publications by Year in descending order

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Version: 2024-02-01

21  
papers

341  
citations

1040056

9  
h-index

839539

18  
g-index

21  
all docs

21  
docs citations

21  
times ranked

536  
citing authors

#	ARTICLE	IF	CITATIONS
1	Application of docking and active site analysis for enzyme linked biodegradation of textile dyes. Environmental Pollution, 2019, 248, 599-608.	7.5	77
2	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
3	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
4	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
5	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
6	Binding Site Analysis of CCR2 Through <i>In Silico</i> Methodologies: Docking, CoMFA, and CoMSIA. Chemical Biology and Drug Design, 2011, 78, 161-174.	3.2	16
7	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
8	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
9	QSAR analysis on Pfk7 inhibitors using HQSAR, CoMFA, and CoMSIA. Medicinal Chemistry Research, 2012, 21, 681-693.	2.4	9
10	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
11	Various atomic charge calculation schemes of CoMFA on HIF-1 inhibitors of moracin analogs. International Journal of Quantum Chemistry, 2012, 112, 995-1005.	2.0	8
12	Understanding the dual mechanism of bioactive peptides targeting the enzymes involved in Renin Angiotensin System (RAS): An <i>in-silico</i> approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5044-5061.	3.5	8
13	Molecular modeling study of HIV-1 gp120 attachment inhibitors. Medicinal Chemistry Research, 2012, 21, 1892-1904.	2.4	6
14	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
15	Theoretical Characterization of Galanin Receptor Type 3 ( $G_{\alpha 3}$ ) and Its Interaction with Agonist (GALANIN) and Antagonists (SNAP 37889 and) Tj ETQq1 1 0.784314 rgBT 4/Overl... 757-774.	3.2	4
16	Synthesis, X-ray crystal structure and DFT calculations of 2,4-dihydro-10H-spiro [anthracene-9,3-benzo[b][1,4]thiazin]-10-amine and 1,3,5-triindolyl benzene. Chemical Data Collections, 2019, 21, 100227.	2.3	3
17	Enhancement of P-glycoprotein modulators of arylmethylamine-phenyl derivatives: an integrative modeling approach. Medicinal Chemistry Research, 2013, 22, 2511-2523.	2.4	2
18	Structural insights into the <i>Aedes aegypti</i> aquaporins and aquaglyceroporins – an <i>in silico</i> study. Journal of Receptor and Signal Transduction Research, 2016, 36, 543-557.	2.5	2

#	ARTICLE	IF	CITATIONS
19	Insights of structure-based pharmacophore studies and inhibitor design against Gal3 receptor through molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 39, 1-13.	3.5	2
20	Proposing the Promiscuous Protein Structures in JNK1 and JNK3 for Virtual Screening in Pursuit of Potential Leads. <i>ACS Omega</i> , 2020, 5, 3969-3978.	3.5	2
21	Unveiling the Accuracy of Homology Modeling to Elucidate the Structure of GPCRs-HIV Co-receptor-CCR5 as a Case Study. <i>Letters in Drug Design and Discovery</i> , 2018, 15, 1068-1078.	0.7	1