

Prajwal P Nandekar

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.

31 papers	397 citations	13 h-index	18 g-index
34 ext. papers	472 ext. citations	3.9 avg, IF	3.54 L-index

#	Paper	IF	Citations
31	An electron transfer competent structural ensemble of membrane-bound cytochrome P450 1A1 and cytochrome P450 oxidoreductase. <i>Communications Biology</i> , 2021 , 4, 55	6.7	10
30	The Effect of Force-Field Parameters on Cytochrome P450-Membrane Interactions: Structure and Dynamics. <i>Scientific Reports</i> , 2020 , 10, 7284	4.9	14
29	Differing Membrane Interactions of Two Highly Similar Drug-Metabolizing Cytochrome P450 Isoforms: CYP 2C9 and CYP 2C19. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	6
28	Influence of Transmembrane Helix Mutations on Cytochrome P450-Membrane Interactions and Function. <i>Biophysical Journal</i> , 2019 , 116, 419-432	2.9	13
27	A Multi-resolution Approach to the Simulation of Protein Complexes in a Membrane Bilayer 2019 , 505-514		
26	Ligand tunnels in T. brucei and human CYP51: Insights for parasite-specific drug design. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2016 , 1860, 67-78	4	18
25	An evaluation of the CYP2D6 and CYP3A4 inhibition potential of metoprolol metabolites and their contribution to drug-drug and drug-herb interaction by LC-ESI/MS/MS. <i>Biomedical Chromatography</i> , 2016 , 30, 1556-72	1.7	8
24	Synthesis and biology of ring-modified L-Histidine containing thyrotropin-releasing hormone (TRH) analogues. <i>European Journal of Medicinal Chemistry</i> , 2016 , 111, 72-83	6.8	4
23	Dynathor: Dynamics of the Complex of Cytochrome P450 and Cytochrome P450 Reductase in a Phospholipid Bilayer 2016 , 255-264		2
22	Characterization of differences in substrate specificity among CYP1A1, CYP1A2 and CYP1B1: an integrated approach employing molecular docking and molecular dynamics simulations. <i>Journal of Molecular Recognition</i> , 2016 , 29, 370-90	2.6	11
21	Structure guided design and binding analysis of EGFR inhibiting analogues of erlotinib and AEE788 using ensemble docking, molecular dynamics and MM-GBSA. <i>RSC Advances</i> , 2016 , 6, 65725-65735	3.7	27
20	Identification of leads for antiproliferative activity on MDA-MB-435 human breast cancer cells through pharmacophore and CYP1A1-mediated metabolism. <i>European Journal of Medicinal Chemistry</i> , 2016 , 115, 82-93	6.8	9
19	Discovery of a low affinity thyrotropin-releasing hormone (TRH)-like peptide that exhibits potent inhibition of scopolamine-induced memory impairment in mice. <i>RSC Advances</i> , 2015 , 5, 56872-56884	3.7	4
18	Synthesis of CNS active thyrotropin-releasing hormone (TRH)-like peptides: Biological evaluation and effect on cognitive impairment induced by cerebral ischemia in mice. <i>Bioorganic and Medicinal Chemistry</i> , 2015 , 23, 5641-53	3.4	9
17	Plasma protein binding, pharmacokinetics, tissue distribution and CYP450 biotransformation studies of fidarestat by ultra high performance liquid chromatography-high resolution mass spectrometry. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2015 , 102, 386-99	3.5	18
16	On the application of the MARTINI coarse-grained model to immersion of a protein in a phospholipid bilayer. <i>Journal of Chemical Physics</i> , 2015 , 143, 243139	3.9	15
15	Ensemble docking and molecular dynamics identify knoevenagel curcumin derivatives with potent anti-EGFR activity. <i>Gene</i> , 2014 , 539, 82-90	3.8	31

14	Characterization of forced degradation products of ketorolac tromethamine using LC/ESI/Q/TOF/MS/MS and in silico toxicity prediction. <i>Journal of Mass Spectrometry</i> , 2014 , 49, 380-91	2.2	11
13	Comparative proteomics among cytochrome p450 family 1 for differential substrate specificity. <i>Protein Journal</i> , 2014 , 33, 536-48	3.9	6
12	Design and synthesis of optically pure 3-aryl-6-methyl-2-thioxotetrahydropyrimidin-4(1H)-ones as anti-prostate cancer agents. <i>RSC Advances</i> , 2014 , 4, 37868-37877	3.7	5
11	Intestinal transport of TRH analogs through PepT1: the role of in silico and in vitro modeling. <i>Journal of Molecular Recognition</i> , 2014 , 27, 609-17	2.6	6
10	Predicting drug metabolism by CYP1A1, CYP1A2, and CYP1B1: insights from MetaSite, molecular docking and quantum chemical calculations. <i>Molecular Diversity</i> , 2014 , 18, 865-78	3.1	14
9	Pregnane X Receptor and P-glycoprotein: a connexion for Alzheimer's disease management. <i>Molecular Diversity</i> , 2014 , 18, 895-909	3.1	12
8	Human pregnane X receptor: a novel target for anticancer drug development. <i>Drug Discovery Today</i> , 2014 , 19, 63-70	8.8	4
7	Molecular dynamics simulation studies for DNA sequence recognition by reactive metabolites of anticancer compounds. <i>Journal of Molecular Recognition</i> , 2014 , 27, 138-50	2.6	6
6	Chem-bioinformatics and in vitro approaches for candidate optimization: a case study of NSC745689 as a promising antitumor agent. <i>Medicinal Chemistry Research</i> , 2013 , 22, 3728-3742	2.2	17
5	Impact of Crystal Habit on Biopharmaceutical Performance of Celecoxib. <i>Crystal Growth and Design</i> , 2013 , 13, 2824-2832	3.5	61
4	Cytochrome P450 1A1-mediated anticancer drug discovery: in silico findings. <i>Expert Opinion on Drug Discovery</i> , 2012 , 7, 771-89	6.2	20
3	An ecofriendly synthesis and DNA binding interaction study of some pyrazolo [1,5-a]pyrimidines derivatives. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012 , 22, 7566-72	2.9	20
2	Mechanistic insights into PEPT1-mediated transport of a novel antiepileptic, NP-647. <i>Molecular Pharmaceutics</i> , 2012 , 9, 2458-68	5.6	13
1	An electron transfer competent structural ensemble of membrane-bound cytochrome P450 1A1 and cytochrome P450 oxidoreductase		3