

Stephen W Doughty

List of Publications by Year in descending order

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38
papers

791
citations

430874

18
h-index

526287

27
g-index

41
all docs

41
docs citations

41
times ranked

1296
citing authors

#	ARTICLE	IF	CITATIONS
1	Evaluating the performance of MM/PBSA for binding affinity prediction using class A GPCR crystal structures. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 487-496.	2.9	15
2	In vitro functional evaluation of isolaureline, dicentrine and glaucine enantiomers at 5-HT ₂ and 1 ₁ receptors. <i>Chemical Biology and Drug Design</i> , 2019, 93, 132-138.	3.2	12
3	Synthesis and evaluation of nuciferine and roemerine enantiomers as 5-HT ₂ and 1 ₁ receptor antagonists. <i>MedChemComm</i> , 2018, 9, 576-582.	3.4	12
4	Assessing GPCR homology models constructed from templates of various transmembrane sequence identities: Binding mode prediction and docking enrichment. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 80, 38-47.	2.4	19
5	Effect of volume of porogens on the porosity of PLGA scaffolds in pH-controlled environment. <i>Pharmaceutical Development and Technology</i> , 2018, 23, 207-210.	2.4	4
6	A dual-application poly (DL-lactic-co-glycolic) acid (PLGA)-chitosan composite scaffold for potential use in bone tissue engineering. <i>Journal of Biomaterials Science, Polymer Edition</i> , 2017, 28, 1966-1983.	3.5	23
7	Monitoring model drug microencapsulation in PLGA scaffolds using X-ray powder diffraction. <i>Saudi Pharmaceutical Journal</i> , 2016, 24, 227-231.	2.7	4
8	Development and Validation of Decision Forest Model for Estrogen Receptor Binding Prediction of Chemicals Using Large Data Sets. <i>Chemical Research in Toxicology</i> , 2015, 28, 2343-2351.	3.3	47
9	Physicomechanical properties of sintered scaffolds formed from porous and protein-loaded poly(DL-lactic-co-glycolic acid) microspheres for potential use in bone tissue engineering. <i>Journal of Biomaterials Science, Polymer Edition</i> , 2015, 26, 796-811.	3.5	9
10	Flavonoids with M1 Muscarinic Acetylcholine Receptor Binding Activity. <i>Molecules</i> , 2014, 19, 8933-8948.	3.8	19
11	Toward activated homology models of the human M1 muscarinic acetylcholine receptor. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 49, 91-98.	2.4	13
12	The influence of substituted phenols on the sol:gel transition of hydroxypropyl methylcellulose (HPMC) aqueous solutions. <i>Carbohydrate Polymers</i> , 2014, 101, 1198-1204.	10.2	13
13	Molecular Dynamics Simulations of the Adenosine A2a Receptor in POPC and POPE Lipid Bilayers: Effects of Membrane on Protein Behavior. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 573-581.	5.4	33
14	Conversion of a non-selective adenosine receptor antagonist into A3-selective high affinity fluorescent probes using peptide-based linkers. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 5673.	2.8	47
15	Structure-Based Identification of Aporphines with Selective 5-HT _{2A} Receptor Binding Activity. <i>Chemical Biology and Drug Design</i> , 2013, 81, 250-256.	3.2	25
16	Molecular Dynamics Simulations of the Adenosine A2a Receptor: Structural Stability, Sampling, and Convergence. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1168-1178.	5.4	42
17	Homology modeling of the human 5-HT1A, 5-HT2A, D1, and D2 receptors: model refinement with molecular dynamics simulations and docking evaluation. <i>Journal of Molecular Modeling</i> , 2012, 18, 3639-3655.	1.8	26
18	Chromatographic retention behaviour of n-alkylbenzenes and pentylbenzene structural isomers on porous graphitic carbon and octadecyl-bonded silica studied using molecular modelling and QSRR. <i>Journal of Chromatography A</i> , 2010, 1217, 6987-6993.	3.7	23

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19	A quantitative assessment of inhaled drug particle-pulmonary surfactant interaction by atomic force microscopy. <i>Colloids and Surfaces B: Biointerfaces</i> , 2009, 73, 97-102.	5.0	21
20	Crystallization and preliminary X-ray characterization of the <i>Bacillus amyloliquefaciens</i> enzyme. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 746-750.	0.7	2
21	Inhibition of cobalamin-dependent methionine synthase by substituted benzo-fused heterocycles. <i>FEBS Journal</i> , 2007, 274, 287-299.	4.7	19
22	Modelling the restoration of wild-type dynamic behaviour in Δ F508-CFTR NBD1 by 8-cyclopentyl-1,3-dipropylxanthine. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 691-699.	2.4	5
23	The influence of l-amino acid molecular structure on the phase transition temperature of hydroxypropyl methylcellulose. <i>Carbohydrate Polymers</i> , 2006, 65, 22-27.	10.2	21
24	Chemical modification of the naphthoyl 3-position of JWH-015: In search of a fluorescent probe to the cannabinoid CB2 receptor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 3758-3762.	2.2	35
25	Characterization of Drug Particle Surface Energetics and Young's Modulus by Atomic Force Microscopy and Inverse Gas Chromatography. <i>Pharmaceutical Research</i> , 2005, 22, 1158-1166.	3.5	70
26	Binding of the Anticancer Prodrug CB1954 to the Activating Enzyme NQO2 Revealed by the Crystal Structure of Their Complex. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7714-7719.	6.4	20
27	The application of molecular modelling to the interpretation of inverse gas chromatography data. <i>Journal of Chromatography A</i> , 2002, 969, 49-57.	3.7	18
28	The changes in surface energetics with relative humidity of carbamazepine and paracetamol as measured by inverse gas chromatography. <i>European Journal of Pharmaceutical Sciences</i> , 2001, 13, 219-225.	4.0	34
29	Molecular Modelling of Human DT-Diaphorase For Enzyme-Directed Bioreductive Drug Design. <i>Molecular Simulation</i> , 2000, 24, 209-214.	2.0	3
30	Bioreductive Activation of a Series of Indolequinones by Human DT-Diaphorase: Structure-Activity Relationships. <i>Journal of Medicinal Chemistry</i> , 1999, 42, 4071-4080.	6.4	64
31	A molecular mechanism for toxin block in N-type calcium channels. <i>Protein Engineering, Design and Selection</i> , 1998, 11, 95-99.	2.1	17
32	Theoretical studies of the intramolecular mechanism for the alkoxyphosphazene to alkoxyphosphazane transformation. <i>Journal of the Chemical Society Dalton Transactions</i> , 1997, , 367-370.	1.1	1
33	Color plates for articles in this issue. <i>Journal of Molecular Graphics and Modelling</i> , 1997, 15, 101-113.	2.4	1
34	Internet conferences in NMR spectroscopy. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1997, 31, 107-117.	7.5	4
35	Simulations on the activation of the bradykinin B2 receptor. <i>Biochemical Society Transactions</i> , 1996, 24, 259-263.	3.4	2
36	A new direction in conferencing: the First Electronic Glycoscience Conference. <i>Trends in Biochemical Sciences</i> , 1996, 21, 31-33.	7.5	6

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37	Prediction of the three-dimensional structure of human interleukin-7 by homology modeling. Protein Engineering, Design and Selection, 1996, 9, 493-498.	2.1	44
38	Models of ion pores in N-type voltage-gated calcium channels. Journal of Molecular Graphics, 1995, 13, 342-348.	1.1	15