Stephen W Doughty

List of Publications by Year
in descending order

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	Characterization of Drug Particle Surface Energetics and Youngâ€™s Modulus by Atomic Force Microscopy and Inverse Gas Chromatography. Pharmaceutical Research, 2005, 22, 1158-1166.	3.5	70
2	Bioreductive Activation of a Series of Indolequinones by Human DT-Diaphorase:Â Structureâ^'Activity Relationships. Journal of Medicinal Chemistry, 1999, 42, 4071-4080.	6.4	64
3	Conversion of a non-selective adenosine receptor antagonist into A3-selective high affinity fluorescent probes using peptide-based linkers. Organic and Biomolecular Chemistry, 2013, 11, 5673.	2.8	47
4	Development and Validation of Decision Forest Model for Estrogen Receptor Binding Prediction of Chemicals Using Large Data Sets. Chemical Research in Toxicology, 2015, 28, 2343-2351.	3.3	47
5	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
6	Molecular Dynamics Simulations of the Adenosine A2a Receptor: Structural Stability, Sampling, and Convergence. Journal of Chemical Information and Modeling, 2013, 53, 1168-1178.	5.4	42
7	Chemical modification of the naphthoyl 3-position of JWH-015: In search of a fluorescent probe to the cannabinoid CB2 receptor. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3758-3762.	2.2	35
8	The changes in surface energetics with relative humidity of carbamazepine and paracetamol as measured by inverse gas chromatography. European Journal of Pharmaceutical Sciences, 2001, 13, 219-225.	4.0	34
9	Molecular Dynamics Simulations of the Adenosine A2a Receptor in POPC and POPE Lipid Bilayers: Effects of Membrane on Protein Behavior. Journal of Chemical Information and Modeling, 2014, 54, 573-581.	5.4	33
10	Homology modeling of the human 5-HT1A, 5-HT2A, D1, and D2 receptors: model refinement with molecular dynamics simulations and docking evaluation. Journal of Molecular Modeling, 2012, 18, 3639-3655.	1.8	26
11	Structureâ€Based Identification of Aporphines with Selective 5â€HT_{2A} Receptorâ€Binding Activity. Chemical Biology and Drug Design, 2013, 81, 250-256.	3.2	25
12	Chromatographic retention behaviour of n-alkylbenzenes and pentylbenzene structural isomers on porous graphitic carbon and octadecyl-bonded silica studied using molecular modelling and QSRR. Journal of Chromatography A, 2010, 1217, 6987-6993.	3.7	23
13	A dual-application poly (<scp>dl</scp>-lactic-co-glycolic) acid (PLGA)-chitosan composite scaffold for potential use in bone tissue engineering. Journal of Biomaterials Science, Polymer Edition, 2017, 28, 1966-1983.	3.5	23
14	The influence of l-amino acid molecular structure on the phase transition temperature of hydroxypropyl methylcellulose. Carbohydrate Polymers, 2006, 65, 22-27.	10.2	21
15	A quantitative assessment of inhaled drug particleâ€“pulmonary surfactant interaction by atomic force microscopy. Colloids and Surfaces B: Biointerfaces, 2009, 73, 97-102.	5.0	21
16	Binding of the Anticancer Prodrug CB1954 to the Activating Enzyme NQO2 Revealed by the Crystal Structure of Their Complex. Journal of Medicinal Chemistry, 2005, 48, 7714-7719.	6.4	20
17	Inhibition of cobalamin-dependent methionine synthase by substituted benzo-fused heterocycles. FEBS Journal, 2007, 274, 287-299.	4.7	19
18	Flavonoids with M1 Muscarinic Acetylcholine Receptor Binding Activity. Molecules, 2014, 19, 8933-8948.	3.8	19

#	Article	IF	Citations
19	Assessing GPCR homology models constructed from templates of various transmembrane sequence identities: Binding mode prediction and docking enrichment. Journal of Molecular Graphics and Modelling, 2018, 80, 38-47.	2.4	19
20	The application of molecular modelling to the interpretation of inverse gas chromatography data. Journal of Chromatography A, 2002, 969, 49-57.	3.7	18
21	A molecular mechanism for toxin block in N-type calcium channels. Protein Engineering, Design and Selection, 1998, 11, 95-99.	2.1	17
22	Models of ion pores in N-type voltage-gated calcium channels. Journal of Molecular Graphics, 1995, 13, 342-348.	1.1	15
23	Evaluating the performance of MM/PBSA for binding affinity prediction using class A GPCR crystal structures. Journal of Computer-Aided Molecular Design, 2019, 33, 487-496.	2.9	15
24	Toward activated homology models of the human M1 muscarinic acetylcholine receptor. Journal of Molecular Graphics and Modelling, 2014, 49, 91-98.	2.4	13
25	The influence of substituted phenols on the sol:gel transition of hydroxypropyl methylcellulose (HPMC) aqueous solutions. Carbohydrate Polymers, 2014, 101, 1198-1204.	10.2	13
26	Synthesis and evaluation of nuciferine and roemerine enantiomers as 5-HT₂ and Î±₁ receptor antagonists. MedChemComm, 2018, 9, 576-582.	3.4	12
27	In vitro functional evaluation of isolaureline, dicentrine and glaucine enantiomers at 5â€HT₂ and Î±₁ receptors. Chemical Biology and Drug Design, 2019, 93, 132-138.	3.2	12
28	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. Journal of Biomaterials Science, Polymer Edition, 2015, 26, 796-811.	3.5	9
29	A new direction in conferencing: the First Electronic Glycoscience Conference. Trends in Biochemical Sciences, 1996, 21, 31-33.	7.5	6
30	Modelling the restoration of wild-type dynamic behaviour in Î”F508-CFTR NBD1 by 8-cyclopentyl-1,3-dipropylxanthine. Journal of Molecular Graphics and Modelling, 2007, 26, 691-699.	2.4	5
31	Internet conferences in NMR spectroscopy. Progress in Nuclear Magnetic Resonance Spectroscopy, 1997, 31, 107-117.	7.5	4
32	Monitoring model drug microencapsulation in PLGA scaffolds using X-ray powder diffraction. Saudi Pharmaceutical Journal, 2016, 24, 227-231.	2.7	4
33	Effect of volume of porogens on the porosity of PLGA scaffolds in pH-controlled environment. Pharmaceutical Development and Technology, 2018, 23, 207-210.	2.4	4
34	Molecular Modelling of Human DT-Diaphorase For Enzyme-Directed Bioreductive Drug Design. Molecular Simulation, 2000, 24, 209-214.	2.0	3
35	Simulations on the activation of the bradykinin B2 receptor. Biochemical Society Transactions, 1996, 24, 259-263.	3.4	2
36	Crystallization and preliminary X-ray characterization of theBacillus amyloliquefaciensYwrO enzyme. Acta Crystallographica Section F: Structural Biology Communications, 2007, 63, 746-750.	0.7	2

#	Article	IF	Citations
37	Theoretical studies of the intramolecular mechanism for the alkoxyphosphazene to alkoxyphosphazane transformation. Journal of the Chemical Society Dalton Transactions, 1997, , 367-370.	1.1	1
38	Color plates for articles in this issue. Journal of Molecular Graphics and Modelling, 1997, 15, 101-113.	2.4	1