Violeta I PÃ©rez-Nueno

List of Publications by Year
in descending order

26 papers	712 citations	471509 17 h-index	580821 25 g-index
29 all docs	29 docs citations	29 times ranked	1063 citing authors

#	Article	IF	Citations
1	Comprehensive Comparison of Ligand-Based Virtual Screening Tools Against the DUD Data set Reveals Limitations of Current 3D Methods. Journal of Chemical Information and Modeling, 2010, 50, 2079-2093.	5.4	121
2	APIF: A New Interaction Fingerprint Based on Atom Pairs and Its Application to Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 1245-1260.	5.4	102
3	Comparison of Ligand-Based and Receptor-Based Virtual Screening of HIV Entry Inhibitors for the CXCR4 and CCR5 Receptors Using 3D Ligand Shape Matching and Ligandâ^'Receptor Docking. Journal of Chemical Information and Modeling, 2008, 48, 509-533.	5.4	67
4	Discovery of Novel HIV Entry Inhibitors for the CXCR4 Receptor by Prospective Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 810-823.	5.4	39
5	Using Consensus-Shape Clustering To Identify Promiscuous Ligands and Protein Targets and To Choose the Right Query for Shape-Based Virtual Screening. Journal of Chemical Information and Modeling, 2011, 51, 1233-1248.	5.4	39
6	Clustering and Classifying Diverse HIV Entry Inhibitors Using a Novel Consensus Shape-Based Virtual Screening Approach: Further Evidence for Multiple Binding Sites within the CCR5 Extracellular Pocket. Journal of Chemical Information and Modeling, 2008, 48, 2146-2165.	5.4	34
7	Detecting Drug Promiscuity Using Gaussian Ensemble Screening. Journal of Chemical Information and Modeling, 2012, 52, 1948-1961.	5.4	28
8	Recent Trends and Future Prospects in Computational GPCR Drug Discovery: From Virtual Screening to Polypharmacology. Current Topics in Medicinal Chemistry, 2013, 13, 1069-1097.	2.1	27
9	GESSE: Predicting Drug Side Effects from Drugâ€“Target Relationships. Journal of Chemical Information and Modeling, 2015, 55, 1804-1823.	5.4	23
10	Improving VEGFR-2 Docking-Based Screening by Pharmacophore Postfiltering and Similarity Search Postprocessing. Journal of Chemical Information and Modeling, 2011, 51, 777-787.	5.4	22
11	Computational proteomics pitfalls and challenges: HavanaBioinfo 2012 Workshop report. Journal of Proteomics, 2013, 87, 134-138.	2.4	19
12	Impact of the CXCR4 structure on docking-based virtual screening of HIV entry inhibitors. Journal of Molecular Graphics and Modelling, 2012, 38, 123-136.	2.4	18
13	GES Polypharmacology Fingerprints: A Novel Approach for Drug Repositioning. Journal of Chemical Information and Modeling, 2014, 54, 720-734.	5.4	18
14	Using quantitative systems pharmacology for novel drug discovery. Expert Opinion on Drug Discovery, 2015, 10, 1315-1331.	5.0	18
15	Discovery of Novel Nonâ€Cyclam Polynitrogenated CXCR4 Coreceptor Inhibitors. ChemMedChem, 2008, 3, 1549-1557.	3.2	17
16	Biological Profiling of Antiâ€HIV Agents and Insight into CCR5 Antagonist Binding Using inâ€...silico Techniques. ChemMedChem, 2009, 4, 1153-1163.	3.2	17
17	Novel Monocyclam Derivatives as HIV Entry Inhibitors: Design, Synthesis, Antiâ€HIV Evaluation, and Their Interaction with the CXCR4 Coâ€receptor. ChemMedChem, 2010, 5, 1272-1281.	3.2	17
18	Recent Trends and Applications in 3D Virtual Screening. Combinatorial Chemistry and High Throughput Screening, 2012, 15, 749-769.	1.1	16

#	ARTICLE	IF	CITATIONS
19	Studying the binding interactions of allosteric agonists and antagonists of the CXCR4 receptor. Journal of Molecular Graphics and Modelling, 2015, 60, 1-14.	2.4	16
20	Highly Specific and Sensitive Pharmacophore Model for Identifying CXCR4 Antagonists. Comparison with Docking and Shape-Matching Virtual Screening Performance. Journal of Chemical Information and Modeling, 2013, 53, 1043-1056.	5.4	15
21	Identifying and characterizing promiscuous targets: Implications for virtual screening. Expert Opinion on Drug Discovery, 2012, 7, 1-17.	5.0	14
22	Using Spherical Harmonic Surface Property Representations for Ligandâ€Based Virtual Screening. Molecular Informatics, 2011, 30, 151-159.	2.5	10
23	Predicting Drug Promiscuity Using Spherical Harmonic Surface Shape-Based Similarity Comparisons. The Open Conference Proceedings Journal, 2011, 2, 113-129.	0.6	7
24	Predicting drug polypharmacology using a novel surface property similarity-based approach. Journal of Cheminformatics, 2011, 3, .	6.1	4
25	Applying in silico tools to the discovery of novel CXCR4 inhibitors. Drug Development Research, 2011, 72, 95-111.	2.9	4
26	Polypharmacology within CXCR4: Multiple binding sites and allosteric behavior. , 2014, , .		0