Laura PÃ©rez-Benito

List of Publications by Year
in descending order

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24	926	430874	610901
papers	citations	18	24
		h-index	g-index

25	25	25	1213
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Breaking the Glass Ceiling in Simulation and Modeling: Women in Pharmaceutical Discovery. Journal of Medicinal Chemistry, 2020, 63, 1929-1936.	6.4	3
2	Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152.	7.4	147
3	Accuracy and Precision of Alchemical Relative Free Energy Predictions with and without Replicaâ€Exchange. Advanced Theory and Simulations, 2020, 3, 1900195.	2.8	30
4	Modeling the Î²-secretase cleavage site and humanizing amyloid-beta precursor protein in rat and mouse to study Alzheimerâ€™s disease. Molecular Neurodegeneration, 2020, 15, 60.	10.8	37
5	GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787.	19.0	90
6	The computational modeling of allosteric modulation of metabotropic glutamate receptors. Advances in Pharmacology, 2020, 88, 1-33.	2.0	1
7	Discovery of Homobivalent Bitopic Ligands of the Cannabinoid CB₂ Receptor**. Chemistry - A European Journal, 2020, 26, 15839-15842.	3.3	20
8	Accurate Prediction of GPCR Ligand Binding Affinity with Free Energy Perturbation. Journal of Chemical Information and Modeling, 2020, 60, 5563-5579.	5.4	45
9	Monte Carlo simulations using PELE to identify a proteinâ€“protein inhibitor binding site and pose. RSC Advances, 2020, 10, 7058-7064.	3.6	7
10	Computational Drug Design Applied to the Study of Metabotropic Glutamate Receptors. Molecules, 2019, 24, 1098.	3.8	8
11	Mechanisms Underlying Allosteric Molecular Switches of Metabotropic Glutamate Receptor 5. Journal of Chemical Information and Modeling, 2019, 59, 2456-2466.	5.4	21
12	Predicting Activity Cliffs with Free-Energy Perturbation. Journal of Chemical Theory and Computation, 2019, 15, 1884-1895.	5.3	37
13	DeltaDelta neural networks for lead optimization of small molecule potency. Chemical Science, 2019, 10, 10911-10918.	7.4	48
14	Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation. Scientific Reports, 2018, 8, 4883.	3.3	43
15	Design of a True Bivalent Ligand with Picomolar Binding Affinity for a G Protein-Coupled Receptor Homodimer. Journal of Medicinal Chemistry, 2018, 61, 9335-9346.	6.4	34
16	The size matters? A computational tool to design bivalent ligands. Bioinformatics, 2018, 34, 3857-3863.	4.1	25
17	Acylguanidine Beta Secretase 1 Inhibitors: A Combined Experimental and Free Energy Perturbation Study. Journal of Chemical Theory and Computation, 2017, 13, 1439-1453.	5.3	67
18	Identification of Allosteric Modulators of Metabotropic Glutamate 7 Receptor Using Proteochemometric Modeling. Journal of Chemical Information and Modeling, 2017, 57, 2976-2985.	5.4	18

#	Article	IF	Citations
19	Molecular Switches of Allosteric Modulation of the Metabotropic Glutamate 2 Receptor. Structure, 2017, 25, 1153-1162.e4.	3.3	41
20	Molecular mechanism of positive allosteric modulation of the metabotropic glutamate receptor 2 by JNJâ€46281222. British Journal of Pharmacology, 2016, 173, 588-600.	5.4	39
21	Application of Free Energy Perturbation for the Design of BACE1 Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 1856-1871.	5.4	92
22	Discovery of 8-Trifluoromethyl-3-cyclopropylmethyl-7-[(4-(2,4-difluorophenyl)-1-piperazinyl)methyl]-1,2,4-triazolo[4,3-a]pyridine (JNJ-46356479), a Selective and Orally Bioavailable mGlu2 Receptor Positive Allosteric Modulator (PAM). Journal of Medicinal Chemistry, 2016, 59, 8495-8507.	6.4	35
23	A Versatile Approach to CF₃â€Containing 2â€Pyrrolidones by Tandem Michael Additionâ€“Cyclization: Exemplification in the Synthesis of Amidine Class BACE1 Inhibitors. Chemistry - A European Journal, 2015, 21, 11719-11726.	3.3	16
24	Gastrin-stimulated GÎ±13 Activation of Rgnef Protein (ArhGEF28) in DLD-1 Colon Carcinoma Cells. Journal of Biological Chemistry, 2015, 290, 15197-15209.	3.4	22