Santiago Vilar Varela

List of Publications by Year in Descending Order

50 papers	2,342 citations	23 h-index	48 g-index
52 ext. papers	2,734 ext. citations	4.8 avg, IF	4.82 L-index

#	Paper	IF	Citations
50	Structure-Based Optimization of Coumarin hA Adenosine Receptor Antagonists. *Journal of Medicinal Chemistry*, **2020**, 63, 2577-2587	8.3	9
49	MAO inhibitory activity of bromo-2-phenylbenzofurans: synthesis, study, and docking calculations. *MedChemComm*, **2017**, 8, 1788-1796	5	12
48	Progress in the development of small molecules as new human A3 adenosine receptor ligands based on the 3-thiophenylcoumarin core. *MedChemComm*, **2016**, 7, 845-852	5	2
47	Potent and selective MAO-B inhibitory activity: amino- versus nitro-3-arylcoumarin derivatives. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 642-8	2.9	21
46	3D pharmacophoric similarity improves multi adverse drug event identification in pharmacovigilance. *Scientific Reports*, **2015**, 5, 8809	4.9	15
45	Design and discovery of tyrosinase inhibitors based on a coumarin scaffold. *RSC Advances*, **2015**, 5, 94227-94235	3.7	39
44	Insight into the functional and structural properties of 3-arylcoumarin as an interesting scaffold in monoamine oxidase B inhibition. *ChemMedChem*, **2014**, 9, 1488-500	3.7	29
43	Monoamine oxidase (MAO) inhibitory activity: 3-phenylcoumarins versus 4-hydroxy-3-phenylcoumarins. *ChemMedChem*, **2014**, 9, 1672-6	3.7	10
42	Similarity-based modeling in large-scale prediction of drug-drug interactions. *Nature Protocols*, **2014**, 9, 2147-63	18.8	100
41	Synthesis, pharmacological study and docking calculations of new benzo[f]coumarin derivatives as dual inhibitors of enzymatic systems involved in neurodegenerative diseases. *Future Medicinal Chemistry*, **2014**, 6, 371-83	4.1	23
40	A method for controlling complex confounding effects in the detection of adverse drug reactions using electronic health records. *Journal of the American Medical Informatics Association: JAMIA*, **2014**, 21, 308-14	8.6	30
39	Human cytidine deaminase: a biochemical characterization of its naturally occurring variants. *International Journal of Biological Macromolecules*, **2014**, 63, 64-74	7.9	23
38	Similarity-based modeling applied to signal detection in pharmacovigilance. *CPT: Pharmacometrics and Systems Pharmacology*, **2014**, 3, e137	4.5	16
37	Insight into the interactions between novel coumarin derivatives and human A3 adenosine receptors. *ChemMedChem*, **2014**, 9, 2245-53	3.7	11
36	Recent structural advances of 1 and 2 adrenoceptors yield keys for ligand recognition and drug design. *Journal of Medicinal Chemistry*, **2013**, 56, 8207-23	8.3	22
35	Application of Monte Carlo-based receptor ensemble docking to virtual screening for GPCR ligands. *Methods in Enzymology*, **2013**, 522, 263-78	1.7	8
34	Comparative study of the 3-phenylcoumarin scaffold: Synthesis, X-ray structural analysis and semiempirical calculations of a selected series of compounds. *Journal of Molecular Structure*, **2013**, 1050, 185-191	3.4	2

33	MAO inhibitory activity of 2-arylbenzofurans versus 3-arylcoumarins: synthesis, in vitro study, and docking calculations. *ChemMedChem*, **2013**, 8, 956-66	3.7	23
32	Novel (coumarin-3-yl)carbamates as selective MAO-B inhibitors: synthesis, in vitro and in vivo assays, theoretical evaluation of ADME properties and docking study. *European Journal of Medicinal Chemistry*, **2013**, 63, 151-61	6.8	37
31	Synthesis, NMR characterization, X-ray structural analysis and theoretical calculations of amide and ester derivatives of the coumarin scaffold. *Journal of Molecular Structure*, **2013**, 1041, 144-150	3.4	3
30	Combing signals from spontaneous reports and electronic health records for detection of adverse drug reactions. *Journal of the American Medical Informatics Association: JAMIA*, **2013**, 20, 413-9	8.6	117
29	High-throughput methods for combinatorial drug discovery. *Science Translational Medicine*, **2013**, 5, 205rv1	17.5	95
28	Detection of drug-drug interactions by modeling interaction profile fingerprints. *PLoS ONE*, **2013**, 8, e58321	3.7	61
27	In silico screening for agonists and blockers of the β(2) adrenergic receptor: implications of inactive and activated state structures. *Journal of Computational Chemistry*, **2012**, 33, 561-72	3.5	23
26	Enhancing adverse drug event detection in electronic health records using molecular structure similarity: application to pancreatitis. *PLoS ONE*, **2012**, 7, e41471	3.7	20
25	Drug-drug interaction through molecular structure similarity analysis. *Journal of the American Medical Informatics Association: JAMIA*, **2012**, 19, 1066-74	8.6	121
24	Predicting monoamine oxidase inhibitory activity through ligand-based models. *Current Topics in Medicinal Chemistry*, **2012**, 12, 2258-74	3	14
23	Delineation of the molecular mechanisms of nucleoside recognition by cytidine deaminase through virtual screening. *ChemMedChem*, **2011**, 6, 1452-8	3.7	13
22	Docking-based virtual screening for ligands of G protein-coupled receptors: not only crystal structures but also in silico models. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 614-23	2.8	58
21	In silico analysis of the binding of agonists and blockers to the β2-adrenergic receptor. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 809-17	2.8	43
20	Facilitating adverse drug event detection in pharmacovigilance databases using molecular structure similarity: application to rhabdomyolysis. *Journal of the American Medical Informatics Association: JAMIA*, **2011**, 18 Suppl 1, i73-80	8.6	47
19	Ligand and structure-based models for the prediction of ligand-receptor affinities and virtual screenings: Development and application to the beta(2)-adrenergic receptor. *Journal of Computational Chemistry*, **2010**, 31, 707-20	3.5	36
18	Prediction of passive blood-brain partitioning: straightforward and effective classification models based on in silico derived physicochemical descriptors. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 899-903	2.8	80
17	Protein Graphs in Cancer Prediction **2010**, 125-140		
16	A network-QSAR model for prediction of genetic-component biomarkers in human colorectal cancer. *Journal of Theoretical Biology*, **2009**, 261, 449-58	2.3	62

15	Structural basis of the selectivity of the beta(2)-adrenergic receptor for fluorinated catecholamines. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 7987-92	3.4	15
14	Medicinal chemistry and the molecular operating environment (MOE): application of QSAR and molecular docking to drug discovery. *Current Topics in Medicinal Chemistry*, **2008**, 8, 1555-72	3	510
13	QSAR model for alignment-free prediction of human breast cancer biomarkers based on electrostatic potentials of protein pseudofolding HP-lattice networks. *Journal of Computational Chemistry*, **2008**, 29, 2613-22	3.5	45
12	Inhibitor docking screened by the modified SAFE_p scoring function: application to cyclic urea HIV-1 PR inhibitors. *Journal of Computational Chemistry*, **2007**, 28, 2216-25	3.5	1
11	Assignment of the 1H and 13C NMR signals of some hydroxyphenylcoumarins. *Magnetic Resonance in Chemistry*, **2007**, 45, 99-101	2.1	3
10	On the applicability of QSAR for recognition of miRNA bioorganic structures at early stages of organism and cell development: embryo and stem cells. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 2544-50	3.4	23
9	Quantitative Structure Vasodilatory Activity Relationship Synthesis and In Silico and In Vitro Evaluation of Resveratrol-Coumarin Hybrids. *QSAR and Combinatorial Science*, **2007**, 26, 317-332		9
8	Medicinal chemistry and bioinformatics--current trends in drugs discovery with networks topological indices. *Current Topics in Medicinal Chemistry*, **2007**, 7, 1015-29	3	216
7	Probabilistic neural network model for the in silico evaluation of anti-HIV activity and mechanism of action. *Journal of Medicinal Chemistry*, **2006**, 49, 1118-24	8.3	72
6	Effect of protein backbone folding on the stability of protein-ligand complexes. *Journal of Proteome Research*, **2006**, 5, 105-11	5.6	17
5	Design, synthesis, and vasorelaxant and platelet antiaggregatory activities of coumarin-resveratrol hybrids. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 257-61	2.9	119
4	Synthesis and structural study of carbocyclic analogues of 1,2-disubstituted nucleosides. *Structural Chemistry*, **2006**, 17, 465-471	1.8	1
3	3D comparative structural study of 6-hydroxy-4-methyl-5,7-dinitrocoumarin using experimental and theoretical approaches. *Structural Chemistry*, **2006**, 17, 459-464	1.8	6
2	In silico studies toward the discovery of new anti-HIV nucleoside compounds through the use of TOPS-MODE and 2D/3D connectivity indices. 2. Purine derivatives. *Journal of Chemical Information and Modeling*, **2005**, 45, 502-14	6.1	34
1	In silico studies toward the discovery of new anti-HIV nucleoside compounds with the use of TOPS-MODE and 2D/3D connectivity indices. 1. Pyrimidyl derivatives. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 1194-203		46