# Santiago Vilar Varela

## List of Publications by Citations



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|---|---|---|---|
| 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 | 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 |
| 49 | Medicinal chemistry and bioinformatics--current trends in drugs discovery with networks topological indices. *Current Topics in Medicinal Chemistry*, **2007**, 7, 1015-29 | 3 | 216 |
| 48 | Drug-drug interaction through molecular structure similarity analysis. *Journal of the American Medical Informatics Association: JAMIA*, **2012**, 19, 1066-74 | 8.6 | 121 |
| 47 | Design, synthesis, and vasorelaxant and platelet antiaggregatory activities of coumarin-resveratrol hybrids. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 257-61 | 2.9 | 119 |
| 46 | 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 |
| 45 | Similarity-based modeling in large-scale prediction of drug-drug interactions. *Nature Protocols*, **2014**, 9, 2147-63 | 18.8 | 100 |
| 44 | High-throughput methods for combinatorial drug discovery. *Science Translational Medicine*, **2013**, 5, 205rv1 | 17.5 | 95 |
| 43 | 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 |
| 42 | 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 |
| 41 | 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 |
| 40 | Detection of drug-drug interactions by modeling interaction profile fingerprints. *PLoS ONE*, **2013**, 8, e58321 | 3.7 | 61 |
| 39 | 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 |
| 38 | 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 |
| 37 | 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 |
| 36 | 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 |
| 35 | 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 |
| 34 | Design and discovery of tyrosinase inhibitors based on a coumarin scaffold. *RSC Advances*, **2015**, 5, 94227-94235 | 3.7 | 39 |

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| 33 | 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 |
| 32 | 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 |
| 31 | 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 |
| 30 | 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 |
| 29 | 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 |
| 28 | 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 |
| 27 | Human cytidine deaminase: a biochemical characterization of its naturally occurring variants. *International Journal of Biological Macromolecules*, **2014**, 63, 64-74 | 7.9 | 23 |
| 26 | In silico screening for agonists and blockers of the (2) adrenergic receptor: implications of inactive and activated state structures. *Journal of Computational Chemistry*, **2012**, 33, 561-72 | 3.5 | 23 |
| 25 | MAO inhibitory activity of 2-arylbenzofurans versus 3-arylcoumarins: synthesis, in vitro study, and docking calculations. *ChemMedChem*, **2013**, 8, 956-66 | 3.7 | 23 |
| 24 | 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 |
| 23 | 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 |
| 22 | 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 |
| 21 | Enhancing adverse drug event detection in electronic health records using molecular structure similarity: application to pancreatitis. *PLoS ONE*, **2012**, 7, e41471 | 3.7 | 20 |
| 20 | Effect of protein backbone folding on the stability of protein-ligand complexes. *Journal of Proteome Research*, **2006**, 5, 105-11 | 5.6 | 17 |
| 19 | Similarity-based modeling applied to signal detection in pharmacovigilance. *CPT: Pharmacometrics and Systems Pharmacology*, **2014**, 3, e137 | 4.5 | 16 |
| 18 | 3D pharmacophoric similarity improves multi adverse drug event identification in pharmacovigilance. *Scientific Reports*, **2015**, 5, 8809 | 4.9 | 15 |
| 17 | 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 |
| 16 | Predicting monoamine oxidase inhibitory activity through ligand-based models. *Current Topics in Medicinal Chemistry*, **2012**, 12, 2258-74 | 3 | 14 |

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| 15 | Delineation of the molecular mechanisms of nucleoside recognition by cytidine deaminase through virtual screening. *ChemMedChem*, **2011**, 6, 1452-8 | 3.7 | 13 |
| 14 | MAO inhibitory activity of bromo-2-phenylbenzofurans: synthesis, study, and docking calculations. *MedChemComm*, **2017**, 8, 1788-1796 | 5 | 12 |
| 13 | Insight into the interactions between novel coumarin derivatives and human A3 adenosine receptors. *ChemMedChem*, **2014**, 9, 2245-53 | 3.7 | 11 |
| 12 | Monoamine oxidase (MAO) inhibitory activity: 3-phenylcoumarins versus 4-hydroxy-3-phenylcoumarins. *ChemMedChem*, **2014**, 9, 1672-6 | 3.7 | 10 |
| 11 | 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 |
| 10 | Structure-Based Optimization of Coumarin hA Adenosine Receptor Antagonists. *Journal of Medicinal Chemistry*, **2020**, 63, 2577-2587 | 8.3 | 9 |
| 9 | Application of Monte Carlo-based receptor ensemble docking to virtual screening for GPCR ligands. *Methods in Enzymology*, **2013**, 522, 263-78 | 1.7 | 8 |
| 8 | 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 |
| 7 | 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 |
| 6 | Assignment of the 1H and 13C NMR signals of some hydroxyphenylcoumarins. *Magnetic Resonance in Chemistry*, **2007**, 45, 99-101 | 2.1 | 3 |
| 5 | 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 |
| 4 | 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 |
| 3 | 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 |
| 2 | Synthesis and structural study of carbocyclic analogues of 1,2-disubstituted nucleosides. *Structural Chemistry*, **2006**, 17, 465-471 | 1.8 | 1 |
| 1 | Protein Graphs in Cancer Prediction **2010**, 125-140 | | |