Santiago Garcia-Vallve

List of Publications by Year
in descending order

67 papers	**4,803** citations	159585 **30** h-index	106344 **65** g-index
69 all docs	**69** docs citations	**69** times ranked	**7716** citing authors

#	Article	IF	Citations
1	Haste makes waste: A critical review of docking‐based virtual screening in drug repurposing for SARS‐CoV‐2 main protease (M‐pro) inhibition. Medicinal Research Reviews, 2022, 42, 744-769.	10.5	46
2	Functional and genomic comparative study of the bitter taste receptor family TAS2R: Insight into the role of human TAS2R5. FASEB Journal, 2022, 36, e22175.	0.5	4
3	A Review of the Current Landscape of SARS-CoV-2 Main Protease Inhibitors: Have We Hit the Bullseye Yet?. International Journal of Molecular Sciences, 2022, 23, 259.	4.1	31
4	Anti-Inflammatory and Immunomodulatory Effects of the Grifola frondosa Natural Compound o-Orsellinaldehyde on LPS-Challenged Murine Primary Glial Cells. Roles of NF-κβ and MAPK. Pharmaceutics, 2021, 13, 806.	4.5	7
5	An Unsupervised Algorithm for Host Identification in Flaviviruses. Life, 2021, 11, 442.	2.4	2
6	Identification of Broad-Spectrum MMP Inhibitors by Virtual Screening. Molecules, 2021, 26, 4553.	3.8	6
7	Understanding the variability of the S1′ pocket to improve matrix metalloproteinase inhibitor selectivity profiles. Drug Discovery Today, 2020, 25, 38-57.	6.4	41
8	Prediction of Novel Inhibitors of the Main Protease (M-pro) of SARS-CoV-2 through Consensus Docking and Drug Reposition. International Journal of Molecular Sciences, 2020, 21, 3793.	4.1	123
9	Annapurna expedition game: applying molecular biology tools to learn genetics. Journal of Biological Education, 2019, 53, 516-523.	1.5	4
10	Mining large databases to find new leads with low similarity to known actives: application to find new DPP-IV inhibitors. Future Medicinal Chemistry, 2019, 11, 1387-1401.	2.3	1
11	The Light and Dark Sides of Virtual Screening: What Is There to Know?. International Journal of Molecular Sciences, 2019, 20, 1375.	4.1	160
12	Activity and selectivity cliffs for DPP‐IV inhibitors: Lessons we can learn from SAR studies and their application to virtual screening. Medicinal Research Reviews, 2018, 38, 1874-1915.	10.5	32
13	Resveratrol Potently Counteracts Quercetin Starvation‐Induced Autophagy and Sensitizes HepG2 Cancer Cells to Apoptosis. Molecular Nutrition and Food Research, 2018, 62, 1700610.	3.3	30
14	Anti-inflammatory and Proapoptotic Properties of the Natural Compound o-Orsellinaldehyde. Journal of Agricultural and Food Chemistry, 2018, 66, 10952-10963.	5.2	5
15	Combined Ligand‐and Receptor‐Based Virtual Screening Methodology to Identify Structurally Diverse Protein Tyrosine Phosphatase 1B Inhibitors. ChemMedChem, 2018, 13, 1939-1948.	3.2	5
16	Ephedrine as a lead compound for the development of new DPP-IV inhibitors. Future Medicinal Chemistry, 2017, 9, 2129-2146.	2.3	17
17	How do Detergents Work? A Qualitative Assay to Measure Amylase Activity. Journal of Biological Education, 2016, 50, 251-260.	1.5	3
18	Peroxisome Proliferator-Activated Receptor γ (PPARγ) and Ligand Choreography: Newcomers Take the Stage. Journal of Medicinal Chemistry, 2015, 58, 5381-5394.	6.4	75

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19	Molecular fingerprint similarity search in virtual screening. Methods, 2015, 71, 58-63.	3.8	506
20	Tools for in silico target fishing. Methods, 2015, 71, 98-103.	3.8	114
21	Resveratrol Enhances Palmitate-Induced ER Stress and Apoptosis in Cancer Cells. PLoS ONE, 2014, 9, e113929.	2.5	45
22	Discovery of Natural Products that Modulate the Activity of PPARgamma: A Source for New Antidiabetics. , 2014, , 151-176.		1
23	The good, the bad and the dubious: VHELIBS, a validation helper for ligands and binding sites. Journal of Cheminformatics, 2013, 5, 36.	6.1	42
24	Grape seed procyanidin extract reduces the endotoxic effects induced by lipopolysaccharide in rats. Free Radical Biology and Medicine, 2013, 60, 107-114.	2.9	56
25	Identification of PPARgamma Partial Agonists of Natural Origin (II): In Silico Prediction in Natural Extracts with Known Antidiabetic Activity. PLoS ONE, 2013, 8, e55889.	2.5	25
26	The lipid-lowering effect of dietary proanthocyanidins in rats involves both chylomicron-rich and VLDL-rich fractions. British Journal of Nutrition, 2012, 108, 208-217.	2.3	36
27	Identification of Novel Human Dipeptidyl Peptidase-IV Inhibitors of Natural Origin (Part II): In Silico Prediction in Antidiabetic Extracts. PLoS ONE, 2012, 7, e44972.	2.5	18
28	Procyanidins modify insulinemia by affecting insulin production and degradation. Journal of Nutritional Biochemistry, 2012, 23, 1565-1572.	4.2	35
29	Grape Seed-Derived Procyanidins Decrease Dipeptidyl-peptidase 4 Activity and Expression. Journal of Agricultural and Food Chemistry, 2012, 60, 9055-9061.	5.2	66
30	Identification of Novel Human Dipeptidyl Peptidase-IV Inhibitors of Natural Origin (Part I): Virtual Screening and Activity Assays. PLoS ONE, 2012, 7, e44971.	2.5	34
31	Inhibition of Angiotensin-Converting Enzyme Activity by Flavonoids: Structure-Activity Relationship Studies. PLoS ONE, 2012, 7, e49493.	2.5	257
32	Identification of PPARgamma Partial Agonists of Natural Origin (I): Development of a Virtual Screening Procedure and In Vitro Validation. PLoS ONE, 2012, 7, e50816.	2.5	48
33	Characterization of the activity and stability of amylase from saliva and detergent: Laboratory practicals for studying the activity and stability of amylase from saliva and various commercial detergents. Biochemistry and Molecular Biology Education, 2012, 40, 254-265.	1.2	15
34	DecoyFinder: an easy-to-use python GUI application for building target-specific decoy sets. Bioinformatics, 2012, 28, 1661-1662.	4.1	155
35	Development of docking-based 3D-QSAR models for PPARgamma full agonists. Journal of Molecular Graphics and Modelling, 2012, 36, 1-9.	2.4	13
36	Identification of human IKK-2 inhibitors of natural origin (Part II): In Silico prediction of IKK-2 inhibitors in natural extracts with known anti-inflammatory activity. European Journal of Medicinal Chemistry, 2011, 46, 6098-6103.	5.5	22

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37	Structural insights for the design of new PPARgamma partial agonists with high binding affinity and low transactivation activity. Journal of Computer-Aided Molecular Design, 2011, 25, 717-728.	2.9	47
38	Characterization of the protease activity of detergents laboratory practicals for studying the protease profile and activity of various commercial detergents. Biochemistry and Molecular Biology Education, 2011, 39, 280-290.	1.2	11
39	Identification of Human IKK-2 Inhibitors of Natural Origin (Part I): Modeling of the IKK-2 Kinase Domain, Virtual Screening and Activity Assays. PLoS ONE, 2011, 6, e16903.	2.5	23
40	RCDI/eRCDI: a web-server to estimate codon usage deoptimization. BMC Research Notes, 2010, 3, 87.	1.4	71
41	PairWise Neighbours database: overlaps and spacers among prokaryote genomes. BMC Genomics, 2009, 10, 281.	2.8	9
42	Adaptation of the short intergenic spacers between co-directional genes to the Shine-Dalgarno motif among prokaryote genomes. BMC Genomics, 2009, 10, 537.	2.8	8
43	3Dâ€QSAR Study of Pyridine Derivates as IKKâ€2 Inhibitors. QSAR and Combinatorial Science, 2009, 28, 678-695.	1.4	2
44	E-CAI: a novel server to estimate an expected value of Codon Adaptation Index (eCAI). BMC Bioinformatics, 2008, 9, 65.	2.6	142
45	Gaining and losing the thermophilic adaptation in prokaryotes. Trends in Genetics, 2008, 24, 10-14.	6.7	33
46	Completely sequenced genomes of pathogenic bacteria: A review. Enfermedades Infecciosas Y MicrobiologÃa ClÃnica, 2008, 26, 88-98.	0.5	11
47	CAIcal: A combined set of tools to assess codon usage adaptation. Biology Direct, 2008, 3, 38.	4.6	447
48	In SilicoPrediction of the Origin of Replication among Bacteria: A Case Study ofBacteroides thetaiotaomicron. OMICS A Journal of Integrative Biology, 2008, 12, 201-210.	2.0	4
49	HEG-DB: a database of predicted highly expressed genes in prokaryotic complete genomes under translational selection. Nucleic Acids Research, 2007, 36, D524-D527.	14.5	64
50	OPTIMIZER: a web server for optimizing the codon usage of DNA sequences. Nucleic Acids Research, 2007, 35, W126-W131.	14.5	467
51	TOPD/FMTS: a new software to compare phylogenetic trees. Bioinformatics, 2007, 23, 1556-1558.	4.1	120
52	Towards reconstructing a metabolic tree of life. Bioinformation, 2007, 2, 135-144.	0.5	3
53	Use of a multi-way method to analyze the amino acid composition of a conserved group of orthologous proteins in prokaryotes. BMC Bioinformatics, 2006, 7, 257.	2.6	26
54	Different papillomaviruses have different repertoires of transcription factor binding sites: convergence and divergence in the upstream regulatory region. BMC Evolutionary Biology, 2006, 6, 20.	3.2	28

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55	Papillomaviruses: different genes have different histories. Trends in Microbiology, 2005, 13, 514-521.	7.7	133
56	Contribution of each complex of the mitochondrial respiratory chain in the generation of the proton-motive force. Biochemistry and Molecular Biology Education, 2004, 32, 17-19.	1.2	7
57	Prokaryotic origin of cytidylyltransferases and α-ketoacid synthases. Trends in Microbiology, 2004, 12, 120-128.	7.7	28
58	HGT-DB: a database of putative horizontally transferred genes in prokaryotic complete genomes. Nucleic Acids Research, 2003, 31, 187-189.	14.5	207
59	Frameshift mutation events in β-glucosidases. Gene, 2003, 314, 191-199.	2.2	2
60	Analysis of highly phosphorylated inositols in avian and crocodilian erythrocytes. Comparative Biochemistry and Physiology - B Biochemistry and Molecular Biology, 2003, 135, 169-175.	1.6	14
61	Genetic variation between Helicobacter pylori strains: gene acquisition or loss?. Trends in Microbiology, 2002, 10, 445-447.	7.7	18
62	Simultaneous Horizontal Gene Transfer of a Gene Coding for Ribosomal Protein L27 and Operational Genes in Arthrobacter Sp.. Journal of Molecular Evolution, 2002, 55, 632-637.	1.8	18
63	Horizontal Gene Transfer of Glycosyl Hydrolases of the Rumen Fungi. Molecular Biology and Evolution, 2000, 17, 352-361.	8.9	191
64	Horizontal Gene Transfer in Bacterial and Archaeal Complete Genomes. Genome Research, 2000, 10, 1719-1725.	5.5	329
65	Horizontal gene transfer in glycosyl hydrolases inferred from codon usage in Escherichia coli and Bacillus subtilis. Molecular Biology and Evolution, 1999, 16, 1125-1134.	8.9	240
66	Circular permutants in β-glucosidases (family 3) within a predicted double-domain topology that includes a (β/α)8-barrel. , 1998, 31, 214-223.		4
67	Nuclear receptors, nuclear-receptor factors, and nuclear-receptor-like orphans form a large paralog cluster in Homo sapiens. Molecular Biology and Evolution, 1998, 15, 665-682.	8.9	16