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	Molecular fingerprint similarity search in virtual screening. Methods, 2015, 71, 58-63.	3.8	506
2	OPTIMIZER: a web server for optimizing the codon usage of DNA sequences. Nucleic Acids Research, 2007, 35, W126-W131.	14.5	467
3	CAIcal: A combined set of tools to assess codon usage adaptation. Biology Direct, 2008, 3, 38.	4.6	447
4	Horizontal Gene Transfer in Bacterial and Archaeal Complete Genomes. Genome Research, 2000, 10, 1719-1725.	5.5	329
5	Inhibition of Angiotensin-Converting Enzyme Activity by Flavonoids: Structure-Activity Relationship Studies. PLoS ONE, 2012, 7, e49493.	2.5	257
6	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
7	HGT-DB: a database of putative horizontally transferred genes in prokaryotic complete genomes. Nucleic Acids Research, 2003, 31, 187-189.	14.5	207
8	Horizontal Gene Transfer of Glycosyl Hydrolases of the Rumen Fungi. Molecular Biology and Evolution, 2000, 17, 352-361.	8.9	191
9	The Light and Dark Sides of Virtual Screening: What Is There to Know?. International Journal of Molecular Sciences, 2019, 20, 1375.	4.1	160
10	DecoyFinder: an easy-to-use python GUI application for building target-specific decoy sets. Bioinformatics, 2012, 28, 1661-1662.	4.1	155
11	E-CAI: a novel server to estimate an expected value of Codon Adaptation Index (eCAI). BMC Bioinformatics, 2008, 9, 65.	2.6	142
12	Papillomaviruses: different genes have different histories. Trends in Microbiology, 2005, 13, 514-521.	7.7	133
13	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
14	TOPD/FMTS: a new software to compare phylogenetic trees. Bioinformatics, 2007, 23, 1556-1558.	4.1	120
15	Tools for in silico target fishing. Methods, 2015, 71, 98-103.	3.8	114
16	Peroxisome Proliferator-Activated Receptor Î³ (PPARÎ³) and Ligand Choreography: Newcomers Take the Stage. Journal of Medicinal Chemistry, 2015, 58, 5381-5394.	6.4	75
17	RCDI/eRCDI: a web-server to estimate codon usage deoptimization. BMC Research Notes, 2010, 3, 87.	1.4	71
18	Grape Seed-Derived Procyanidins Decrease Dipeptidyl-peptidase 4 Activity and Expression. Journal of Agricultural and Food Chemistry, 2012, 60, 9055-9061.	5.2	66

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	Haste makes waste: A critical review of dockingâ€based virtual screening in drug repurposing for SARSâ€CoVâ€2 main protease (Mâ€pro) inhibition. Medicinal Research Reviews, 2022, 42, 744-769.	10.5	46
24	Resveratrol Enhances Palmitate-Induced ER Stress and Apoptosis in Cancer Cells. PLoS ONE, 2014, 9, e113929.	2.5	45
25	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
26	Understanding the variability of the S1â€² pocket to improve matrix metalloproteinase inhibitor selectivity profiles. Drug Discovery Today, 2020, 25, 38-57.	6.4	41
27	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
28	Procyanidins modify insulinemia by affecting insulin production and degradation. Journal of Nutritional Biochemistry, 2012, 23, 1565-1572.	4.2	35
29	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
30	Gaining and losing the thermophilic adaptation in prokaryotes. Trends in Genetics, 2008, 24, 10-14.	6.7	33
31	Activity and selectivity cliffs for DPPâ€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
32	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
33	Resveratrol Potently Counteracts Quercetin Starvationâ€Induced Autophagy and Sensitizes HepG2 Cancer Cells to Apoptosis. Molecular Nutrition and Food Research, 2018, 62, 1700610.	3.3	30
34	Prokaryotic origin of cytidylyltransferases and Î±-ketoacid synthases. Trends in Microbiology, 2004, 12, 120-128.	7.7	28
35	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
36	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

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37	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
38	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
39	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
40	Genetic variation between Helicobacter pylori strains: gene acquisition or loss?. Trends in Microbiology, 2002, 10, 445-447.	7.7	18
41	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
42	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
43	Ephedrine as a lead compound for the development of new DPP-IV inhibitors. Future Medicinal Chemistry, 2017, 9, 2129-2146.	2.3	17
44	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
45	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
46	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
47	Development of docking-based 3D-QSAR models for PPARgamma full agonists. Journal of Molecular Graphics and Modelling, 2012, 36, 1-9.	2.4	13
48	Completely sequenced genomes of pathogenic bacteria: A review. Enfermedades Infecciosas Y MicrobiologÃa ClÃnica, 2008, 26, 88-98.	0.5	11
49	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
50	PairWise Neighbours database: overlaps and spacers among prokaryote genomes. BMC Genomics, 2009, 10, 281.	2.8	9
51	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
52	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
53	Anti-Inflammatory and Immunomodulatory Effects of the Grifola frondosa Natural Compound o-Orsellinaldehyde on LPS-Challenged Murine Primary Glial Cells. Roles of NF-Î¹Î²2 and MAPK. Pharmaceutics, 2021, 13, 806.	4.5	7
54	Identification of Broad-Spectrum MMP Inhibitors by Virtual Screening. Molecules, 2021, 26, 4553.	3.8	6

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55	Anti-inflammatory and Proapoptotic Properties of the Natural Compound o-Orsellinaldehyde. Journal of Agricultural and Food Chemistry, 2018, 66, 10952-10963.	5.2	5
56	Combined Ligandâ€•and Receptorâ€Based Virtual Screening Methodology to Identify Structurally Diverse Protein Tyrosine Phosphatase 1B Inhibitors. ChemMedChem, 2018, 13, 1939-1948.	3.2	5
57	Circular permutants in Î²-glucosidases (family 3) within a predicted double-domain topology that includes a (Î²/Î±)8-barrel. , 1998, 31, 214-223.		4
58	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
59	Annapurna expedition game: applying molecular biology tools to learn genetics. Journal of Biological Education, 2019, 53, 516-523.	1.5	4
60	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
61	How do Detergents Work? A Qualitative Assay to Measure Amylase Activity. Journal of Biological Education, 2016, 50, 251-260.	1.5	3
62	Towards reconstructing a metabolic tree of life. Bioinformation, 2007, 2, 135-144.	0.5	3
63	Frameshift mutation events in Î²-glucosidases. Gene, 2003, 314, 191-199.	2.2	2
64	3Dâ€QSAR Study of Pyridine Derivates as IKKâ€2 Inhibitors. QSAR and Combinatorial Science, 2009, 28, 678-695.	1.4	2
65	An Unsupervised Algorithm for Host Identification in Flaviviruses. Life, 2021, 11, 442.	2.4	2
66	Discovery of Natural Products that Modulate the Activity of PPARgamma: A Source for New Antidiabetics. , 2014, , 151-176.		1
67	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