Gerard Pujadas

List of Publications by Year
in descending order

60	3,737	126708	133063
papers	citations	33 h-index	59 g-index

62	62	62	5531
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular fingerprint similarity search in virtual screening. Methods, 2015, 71, 58-63.	1.9	506
2	Grape-seed procyanidins prevent low-grade inflammation by modulating cytokine expression in rats fed a high-fat diet. Journal of Nutritional Biochemistry, 2009, 20, 210-218.	1.9	260
3	Inhibition of Angiotensin-Converting Enzyme Activity by Flavonoids: Structure-Activity Relationship Studies. PLoS ONE, 2012, 7, e49493.	1.1	257
4	Grape-Seed Procyanidins Act as Antiinflammatory Agents in Endotoxin-Stimulated RAW 264.7 Macrophages by Inhibiting NFkB Signaling Pathway. Journal of Agricultural and Food Chemistry, 2007, 55, 4357-4365.	2.4	240
5	The Light and Dark Sides of Virtual Screening: What Is There to Know?. International Journal of Molecular Sciences, 2019, 20, 1375.	1.8	160
6	DecoyFinder: an easy-to-use python GUI application for building target-specific decoy sets. Bioinformatics, 2012, 28, 1661-1662.	1.8	155
7	Modulatory effect of grape-seed procyanidins on local and systemic inflammation in diet-induced obesity rats. Journal of Nutritional Biochemistry, 2011, 22, 380-387.	1.9	140
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.	1.8	123
9	Tools for in silico target fishing. Methods, 2015, 71, 98-103.	1.9	114
10	SRide: a server for identifying stabilizing residues in proteins. Nucleic Acids Research, 2005, 33, W303-W305.	6.5	107
11	Effects of a grapeseed procyanidin extract (GSPE) on insulin resistanceâ˜†. Journal of Nutritional Biochemistry, 2010, 21, 961-967.	1.9	99
12	Dietary procyanidins enhance transcriptional activity of bile acidâ€activated FXR in vitro and reduce triglyceridemia in vivo in a FXRâ€dependent manner. Molecular Nutrition and Food Research, 2009, 53, 805-814.	1.5	85
13	Oligomers of grape-seed procyanidin extract activate the insulin receptor and key targets of the insulin signaling pathway differently from insulin. Journal of Nutritional Biochemistry, 2010, 21, 476-481.	1.9	82
14	Peroxisome Proliferator-Activated Receptor Î³ (PPARÎ³) and Ligand Choreography: Newcomers Take the Stage. Journal of Medicinal Chemistry, 2015, 58, 5381-5394.	2.9	75
15	Locating the stabilizing residues in (Î±/Î²)8 barrel proteins based on hydrophobicity, long-range interactions, and sequence conservation. Proteins: Structure, Function and Bioinformatics, 2004, 55, 316-329.	1.5	73
16	Dietary procyanidins lower triglyceride levels signaling through the nuclear receptor small heterodimer partner. Molecular Nutrition and Food Research, 2008, 52, 1172-1181.	1.5	69
17	Protein-ligand Docking: A Review of Recent Advances and Future Perspectives. Current Pharmaceutical Analysis, 2008, 4, 1-19.	0.3	67
18	Grape Seed-Derived Procyanidins Decrease Dipeptidyl-peptidase 4 Activity and Expression. Journal of Agricultural and Food Chemistry, 2012, 60, 9055-9061.	2.4	66

#	Article	IF	Citations
19	Evolution of Î±-Amylases: Architectural Features and Key Residues in the Stabilization of the (Î²/Î±)8 Scaffold. Molecular Biology and Evolution, 2001, 18, 38-54.	3.5	57
20	Procyanidin Effects on Adipocyte-Related Pathologies. Critical Reviews in Food Science and Nutrition, 2006, 46, 543-550.	5.4	55
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.	1.1	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.	1.3	47
23	Procyanidin dimer B1 and trimer C1 impair inflammatory response signalling in human monocytes. Free Radical Research, 2011, 45, 611-619.	1.5	47
24	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.	5.0	46
25	Resveratrol Enhances Palmitate-Induced ER Stress and Apoptosis in Cancer Cells. PLoS ONE, 2014, 9, e113929.	1.1	45
26	Dietary catechins and procyanidins modulate zinc homeostasis in human HepG2 cells. Journal of Nutritional Biochemistry, 2011, 22, 153-163.	1.9	42
27	The good, the bad and the dubious: VHELIBS, a validation helper for ligands and binding sites. Journal of Cheminformatics, 2013, 5, 36.	2.8	42
28	Understanding the variability of the S1â€² pocket to improve matrix metalloproteinase inhibitor selectivity profiles. Drug Discovery Today, 2020, 25, 38-57.	3.2	41
29	Inhibitory Effects of Grape Seed Procyanidins on Foam Cell Formation in Vitro. Journal of Agricultural and Food Chemistry, 2009, 57, 2588-2594.	2.4	38
30	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.	1.2	36
31	BDT: an easy-to-use front-end application for automation of massive docking tasks and complex docking strategies with AutoDock. Bioinformatics, 2006, 22, 1803-1804.	1.8	35
32	Procyanidins modify insulinemia by affecting insulin production and degradation. Journal of Nutritional Biochemistry, 2012, 23, 1565-1572.	1.9	35
33	Identification of Novel Human Dipeptidyl Peptidase-IV Inhibitors of Natural Origin (Part I): Virtual Screening and Activity Assays. PLoS ONE, 2012, 7, e44971.	1.1	34
34	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.	5.0	32
35	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.	1.8	31
36	Moderate red-wine consumption partially prevents body weight gain in rats fed a hyperlipidic dietâ˜†. Journal of Nutritional Biochemistry, 2006, 17, 139-142.	1.9	30

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37	Resveratrol Potently Counteracts Quercetin Starvationâ€Induced Autophagy and Sensitizes HepG2 Cancer Cells to Apoptosis. Molecular Nutrition and Food Research, 2018, 62, 1700610.	1.5	30
38	A trimer plus a dimer-gallate reproduce the bioactivity described for an extract of grape seed procyanidins. Food Chemistry, 2009, 116, 265-270.	4.2	28
39	Evolution of Î²-amylase: Patterns of variation and conservation in subfamily sequences in relation to parsimony mechanisms. Proteins: Structure, Function and Bioinformatics, 1996, 25, 456-472.	1.5	26
40	In Vivo, in Vitro, and in Silico Studies of Cu/Zn-Superoxide Dismutase Regulation by Molecules in Grape Seed Procyanidin Extract. Journal of Agricultural and Food Chemistry, 2009, 57, 3934-3942.	2.4	25
41	Identification of PPARgamma Partial Agonists of Natural Origin (II): In Silico Prediction in Natural Extracts with Known Antidiabetic Activity. PLoS ONE, 2013, 8, e55889.	1.1	25
42	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.	1.1	23
43	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.	2.6	22
44	Identification of Novel Human Dipeptidyl Peptidase-IV Inhibitors of Natural Origin (Part II): In Silico Prediction in Antidiabetic Extracts. PLoS ONE, 2012, 7, e44972.	1.1	18
45	Ephedrine as a lead compound for the development of new DPP-IV inhibitors. Future Medicinal Chemistry, 2017, 9, 2129-2146.	1.1	17
46	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.	0.5	15
47	Development of docking-based 3D-QSAR models for PPARgamma full agonists. Journal of Molecular Graphics and Modelling, 2012, 36, 1-9.	1.3	13
48	Molecular mimicry of substrate oxygen atoms by water molecules in the Î²-amylase active site. Protein Science, 2001, 10, 1645-1657.	3.1	12
49	Grape seed procyanidins inhibit the expression of metallothione in genes in human HepG2 cells. Genes and Nutrition, 2007, 2, 105-109.	1.2	12
50	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.	0.5	11
51	Differential effects of grape-seed derived procyanidins on adipocyte differentiation markers in different in vivo situations. Genes and Nutrition, 2007, 2, 101-103.	1.2	8
52	Anti-Inflammatory and Immunomodulatory Effects of the Grifola frondosa Natural Compound o-Orsellinaldehyde on LPS-Challenged Murine Primary Glial Cells. Roles of NF-Î°Î² and MAPK. Pharmaceutics, 2021, 13, 806.	2.0	7
53	Identification of Broad-Spectrum MMP Inhibitors by Virtual Screening. Molecules, 2021, 26, 4553.	1.7	6
54	Anti-inflammatory and Proapoptotic Properties of the Natural Compound o-Orsellinaldehyde. Journal of Agricultural and Food Chemistry, 2018, 66, 10952-10963.	2.4	5

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55	Combined Ligandâ€•and Receptorâ€Based Virtual Screening Methodology to Identify Structurally Diverse Protein Tyrosine Phosphatase 1B Inhibitors. ChemMedChem, 2018, 13, 1939-1948.	1.6	5
56	Anatomy of a conformational transition of Î²â€strand 6 in soybean Pâ€amylase caused by substrate (or) Tj ETQq0 0 0 rgBT /Overlock 10	3.1	4
57	How do Detergents Work? A Qualitative Assay to Measure Amylase Activity. Journal of Biological Education, 2016, 50, 251-260.	0.8	3
58	3Dâ€QSAR Study of Pyridine Derivates as IKKâ€2 Inhibitors. QSAR and Combinatorial Science, 2009, 28, 678-695.	1.5	2
59	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.	1.1	1
60	In silico identification of red wine catechin binding sites on human and rat serotransferrins. Genes and Nutrition, 2007, 2, 99-100.	1.2	0