Manuel Pastor

List of Publications by Year
in descending order

103 papers	4,203 citations	134610 34 h-index	134545 62 g-index
113 all docs	113 docs citations	113 times ranked	5163 citing authors

#	Article	IF	Citations
1	Development of In Silico Methods for Toxicity Prediction in Collaboration Between Academia and the Pharmaceutical Industry. Methods in Molecular Biology, 2022, 2425, 119-131.	0.4	0
2	New approach methods supporting read-across: Two neurotoxicity AOP-based IATA case studies. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 615-635.	0.9	9
3	Guidelines for FAIR sharing of preclinical safety and off-target pharmacology data. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 187-197.	0.9	5
4	The eTRANSAFE Project on Translational Safety Assessment through Integrative Knowledge Management: Achievements and Perspectives. Pharmaceuticals, 2021, 14, 237.	1.7	17
5	Flame: an open source framework for model development, hosting, and usage in production environments. Journal of Cheminformatics, 2021, 13, 31.	2.8	9
6	Ensemble prediction of mitochondrial toxicity using machine learning technology. Computational Toxicology, 2021, 20, 100189.	1.8	7
7	The EU-ToxRisk method documentation, data processing and chemical testing pipeline for the regulatory use of new approach methods. Archives of Toxicology, 2020, 94, 2435-2461.	1.9	30
8	Determination of benchmark concentrations and their statistical uncertainty for cytotoxicity test data and functional in vitro assays. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 155-163.	0.9	12
9	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 579-606.	0.9	48
10	Paradigm shift in safety assessment using new approach methods: The EU-ToxRisk strategy. Current Opinion in Toxicology, 2019, 15, 33-39.	2.6	7
11	Towards grouping concepts based on new approach methodologies in chemical hazard assessment: the read-across approach of the EU-ToxRisk project. Archives of Toxicology, 2019, 93, 3643-3667.	1.9	82
12	In silico assay for preclinical assessment of drug proarrhythmicity. Journal of Pharmacological and Toxicological Methods, 2019, 99, 106595.	0.3	1
13	An automated tool for obtaining QSAR-ready series of compounds using semantic web technologies. Bioinformatics, 2018, 34, 131-133.	1.8	4
14	In Silico QT and APD Prolongation Assay for Early Screening of Drug-Induced Proarrhythmic Risk. Journal of Chemical Information and Modeling, 2018, 58, 867-878.	2.5	28
15	Quantitative structureâ€“activity relationships for primary aerobic biodegradation of organic chemicals in pristine surface waters: starting points for predicting biodegradation under acclimatization. Environmental Sciences: Processes and Impacts, 2018, 20, 157-170.	1.7	21
16	Development of an Infrastructure for the Prediction of Biological Endpoints in Industrial Environments. Lessons Learned at the eTOX Project. Frontiers in Pharmacology, 2018, 9, 1147.	1.6	10
17	Hepatotoxicity Prediction by Systems Biology Modeling of Disturbed Metabolic Pathways Using Gene Expression Data. Methods in Molecular Biology, 2018, 1800, 505-518.	0.4	2
18	Generating Modeling Data From Repeat-Dose Toxicity Reports. Toxicological Sciences, 2018, 162, 287-300.	1.4	4

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19	A high-throughput approach to identify specific neurotoxicants / developmental toxicants in human neuronal cell function assays. ALTEX: Alternatives To Animal Experimentation, 2018, 35, 235-253.	0.9	46
20	Membrane cholesterol access into a G-protein-coupled receptor. Nature Communications, 2017, 8, 14505.	5.8	129
21	Combination of multiple neural crest migration assays to identify environmental toxicants from a proof-of-concept chemical library. Archives of Toxicology, 2017, 91, 3613-3632.	1.9	31
22	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
23	Hepatotoxicity prediction by systems biology modeling of disturbed metabolic pathways using gene expression data. ALTEX: Alternatives To Animal Experimentation, 2017, 34, 219-234.	0.9	13
24	Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. Scientific Reports, 2016, 6, 19839.	1.6	89
25	Toward a unifying strategy for the structure-based prediction of toxicological endpoints. Archives of Toxicology, 2016, 90, 2445-2460.	1.9	9
26	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. Molecular Informatics, 2015, 34, 477-484.	1.4	17
27	Linear Interaction Energy Based Prediction of Cytochrome P450 1A2 Binding Affinities with Reliability Estimation. PLoS ONE, 2015, 10, e0142232.	1.1	23
28	Assessing factors that affect the growth of Corylus avellana cell suspension cultures: a statistical approach. In Vitro Cellular and Developmental Biology - Plant, 2015, 51, 530-538.	0.9	15
29	eTOXlab, an open source modeling framework for implementing predictive models in production environments. Journal of Cheminformatics, 2015, 7, 8.	2.8	22
30	Detection of New Biased Agonists for the Serotonin 5-HT_{2A} Receptor: Modeling and Experimental Validation. Molecular Pharmacology, 2015, 87, 740-746.	1.0	29
31	Ensuring confidence in predictions: A scheme to assess the scientific validity of in silico models. Advanced Drug Delivery Reviews, 2015, 86, 101-111.	6.6	17
32	Multiâ€Component Protein â€“ Protein Docking Based Protocol with External Scoring for Modeling Dimers of G Proteinâ€Coupled Receptors. Molecular Informatics, 2015, 34, 246-255.	1.4	15
33	The eTOX Data-Sharing Project to Advance in Silico Drug-Induced Toxicity Prediction. International Journal of Molecular Sciences, 2014, 15, 21136-21154.	1.8	56
34	Novel insights on the structural determinants of clozapine and olanzapine multi-target binding profiles. European Journal of Medicinal Chemistry, 2014, 77, 91-95.	2.6	21
35	Applicability Domain Analysis (ADAN): A Robust Method for Assessing the Reliability of Drug Property Predictions. Journal of Chemical Information and Modeling, 2014, 54, 1500-1511.	2.5	51
36	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149

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37	A Dynamic View of Molecular Switch Behavior at Serotonin Receptors: Implications for Functional Selectivity. PLoS ONE, 2014, 9, e109312.	1.1	27
38	2D- and 3D-QSAR studies of a series of benzopyranes and benzopyrano[3,4b][1,4]-oxazines as inhibitors of the multidrug transporter P-glycoprotein. Journal of Computer-Aided Molecular Design, 2013, 27, 161-171.	1.3	17
39	Modeling Complexes of Transmembrane Proteins: Systematic Analysis of Proteinï£¿Protein Docking Tools. Molecular Informatics, 2013, 32, 717-733.	1.4	27
40	The eTOX Library of Public Resources for in Silico Toxicity Prediction. Molecular Informatics, 2013, 32, 24-35.	1.4	8
41	Rational design of the survivin/CDK4 complex by combining proteinâ€“protein docking and molecular dynamics simulations. Journal of Molecular Modeling, 2013, 19, 1507-1514.	0.8	8
42	Scientific competency questions as the basis for semantically enriched open pharmacological space development. Drug Discovery Today, 2013, 18, 843-852.	3.2	44
43	Novel Insights into Biased Agonism at G Protein-Coupled Receptors and their Potential for Drug Design. Current Pharmaceutical Design, 2013, 19, 5156-5166.	0.9	27
44	Inroads to Predict in Vivo Toxicologyâ€”An Introduction to the eTOX Project. International Journal of Molecular Sciences, 2012, 13, 3820-3846.	1.8	50
45	Tungstate activates BK channels in a Î² subunit- and Mg2+-dependent manner: relevance for arterial vasodilatation. Cardiovascular Research, 2012, 95, 29-38.	1.8	12
46	Fractal dimension as a measure of surface roughness of G protein-coupled receptors: implications for structure and function. Journal of Molecular Modeling, 2012, 18, 4465-4475.	0.8	17
47	Membrane-Sensitive Conformational States of Helix 8 in the Metabotropic Glu2 Receptor, a Class C GPCR. PLoS ONE, 2012, 7, e42023.	1.1	31
48	A Multiscale Simulation System for the Prediction of Drug-Induced Cardiotoxicity. Journal of Chemical Information and Modeling, 2011, 51, 483-492.	2.5	86
49	Progress in the structural prediction of G proteinâ€coupled receptors: D₃ receptor in complex with eticlopride. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1695-1703.	1.5	22
50	A gain-of-function SNP in TRPC4 cation channel protects against myocardial infarction. Cardiovascular Research, 2011, 91, 465-471.	1.8	31
51	Synthesis, 3Dâ€QSAR, and Structural Modeling of Benzolactam Derivatives with Binding Affinity for the D₂ and D₃ Receptors. ChemMedChem, 2010, 5, 1300-1317.	1.6	23
52	A Novel Multilevel Statistical Method for the Study of the Relationships between Multireceptorial Binding Affinity Profiles and In Vivo Endpoints. Molecular Pharmacology, 2010, 77, 149-158.	1.0	10
53	Equine Estrogens Impair Nitric Oxide Production and Endothelial Nitric Oxide Synthase Transcription in Human Endothelial Cells Compared With the Natural 17Î²-Estradiol. Hypertension, 2010, 56, 405-411.	1.3	39
54	Induced Effects of Sodium Ions on Dopaminergic G-Protein Coupled Receptors. PLoS Computational Biology, 2010, 6, e1000884.	1.5	93

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55	SHOP: A Method For Structureâ€Based Fragment and Scaffold Hopping. ChemMedChem, 2009, 4, 427-439.	1.6	15
56	Synthesis, binding affinity and SAR of new benzolactam derivatives as dopamine D3 receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1773-1778.	1.0	35
57	Suitability of GRIND-Based Principal Properties for the Description of Molecular Similarity and Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 2129-2138.	2.5	55
58	Multiâ€Receptor Binding Profile of Clozapine and Olanzapine: A Structural Study Based on the New Î²₂ Adrenergic Receptor Template. ChemMedChem, 2008, 3, 1194-1198.	1.6	51
59	Synthesis, Binding Affinity, and Molecular Docking Analysis of New Benzofuranone Derivatives as Potential Antipsychotics. Journal of Medicinal Chemistry, 2008, 51, 6085-6094.	2.9	26
60	Development and Validation of AMANDA, a New Algorithm for Selecting Highly Relevant Regions in Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2008, 48, 1813-1823.	2.5	96
61	Multistructure 3D-QSAR Studies on a Series of Conformationally Constrained Butyrophenones Docked into a New Homology Model of the 5-HT2A Receptor. Journal of Medicinal Chemistry, 2007, 50, 3242-3255.	2.9	23
62	QF2004B, a potential antipsychotic butyrophenone derivative with similar pharmacological properties to clozapine. Neuropharmacology, 2006, 51, 251-262.	2.0	26
63	Anchorâ€'GRIND:Â Filling the Gap between Standard 3D QSAR and the GRid-INdependent Descriptors. Journal of Medicinal Chemistry, 2005, 48, 2687-2694.	2.9	84
64	Novel approaches for modeling of the A1 adenosine receptor and its agonist binding site. Proteins: Structure, Function and Bioinformatics, 2004, 54, 705-715.	1.5	23
65	Comparative Analysis of Putative Agonist-Binding Modes in the Human A1 Adenosine Receptor. ChemBioChem, 2004, 5, 841-849.	1.3	10
66	Incorporating Molecular Shape into the Alignment-free GRid-INdependent Descriptors. Journal of Medicinal Chemistry, 2004, 47, 2805-2815.	2.9	78
67	Conformationally constrained butyrophenones as new pharmacological tools to study 5-HT2A and 5-HT2C receptor behaviours. European Journal of Medicinal Chemistry, 2003, 38, 433-440.	2.6	8
68	Surface Descriptors for Proteinâ€'Ligand Affinity Prediction. Journal of Medicinal Chemistry, 2003, 46, 25-33.	2.9	64
69	Suitability of Molecular Descriptors for Database Mining. A Comparative Analysis. Journal of Medicinal Chemistry, 2002, 45, 2685-2694.	2.9	52
70	GBR Compounds and Mepyramines as Cocaine Abuse Therapeutics:Â Chemometric Studies on Selectivity Using Grid Independent Descriptors (GRIND). Journal of Medicinal Chemistry, 2002, 45, 1577-1584.	2.9	17
71	Distant collaboration in drug discovery: the LINK3D project. Journal of Computer-Aided Molecular Design, 2002, 16, 809-818.	1.3	4
72	Comparison of biomolecules on the basis of Molecular Interaction Potentials. Journal of the Brazilian Chemical Society, 2002, 13, 795-799.	0.6	10

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73	Comparative Binding Energy (COMBINE) Analysis of Human Neutrophil Elastase Inhibition by Pyridone-containing Trifluoromethylketones. Combinatorial Chemistry and High Throughput Screening, 2001, 4, 627-642.	0.6	13
74	VolSurf: a new tool for the pharmacokinetic optimization of lead compounds. European Journal of Pharmaceutical Sciences, 2000, 11, S29-S39.	1.9	381
75	3D-QSAR methods on the basis of ligand-receptor complexes. Application of COMBINE and GRID/GOLPE methodologies to a series of CYP1A2 ligands. Journal of Computer-Aided Molecular Design, 2000, 14, 341-353.	1.3	59
76	Use of alignment-free molecular descriptors in diversity analysis and optimal sampling of molecular libraries. Molecular Diversity, 2000, 6, 135-147.	2.1	8
77	GRID/CPCA:Â A New Computational Tool To Design Selective Ligands. Journal of Medicinal Chemistry, 2000, 43, 3033-3044.	2.9	191
78	GRid-INdependent Descriptors (GRIND):â€‰ A Novel Class of Alignment-Independent Three-Dimensional Molecular Descriptors. Journal of Medicinal Chemistry, 2000, 43, 3233-3243.	2.9	466
79	Chemometric Detection of Binding Sites of 7TM Receptors. , 2000, , 207-212.		2
80	Comparative Binding Energy (Combine) Analysis on a Series of Glycogen Phosphorylase Inhibitors. Comparison with Grid/Golpe Models. , 2000, , 329-330.		1
81	Handling Information from 3D Grid Maps for QSAR Studies. , 2000, , 73-81.		7
82	3D QSAR on Mutagenic Heterocyclic Amines That are Substrates of Cytochrome P450 1A2. , 2000, , 321-322.		0
83	GOLPE-guided region selection. Journal of Computer - Aided Molecular Design, 1998, 12/14, 71-86.	1.0	7
84	Comparative Binding Energy Analysis of HIV-1 Protease Inhibitors:Â Incorporation of Solvent Effects and Validation as a Powerful Tool in Receptor-Based Drug Design. Journal of Medicinal Chemistry, 1998, 41, 836-852.	2.9	137
85	GOLPE-Guided Region Selection. , 1998, , 71-86.		5
86	Robust multivariate statistics and the prediction of protein secondary structure content. Protein Engineering, Design and Selection, 1997, 10, 747-749.	1.0	9
87	Azino-Fused Benzimidazolium Salts as DNA Intercalating Agents. 2.. Journal of Organic Chemistry, 1997, 62, 5476-5483.	1.7	61
88	Reliability of Comparative Molecular Field Analysis Models:â€‰ Effects of Data Scaling and Variable Selection Using a Set of Human Synovial Fluid Phospholipase A2 Inhibitors. Journal of Medicinal Chemistry, 1997, 40, 1136-1148.	2.9	62
89	Smart Region Definition:Â A New Way To Improve the Predictive Ability and Interpretability of Three-Dimensional Quantitative Structureâ^'Activity Relationships. Journal of Medicinal Chemistry, 1997, 40, 1455-1464.	2.9	137
90	GRID/GOLPE 3D Quantitative Structureâ^'Activity Relationship Study on a Set of Benzamides and Naphthamides, with Affinity for the Dopamine D3Receptor Subtype. Journal of Medicinal Chemistry, 1997, 40, 833-840.	2.9	34

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91	A Strategy for the Incorporation of Water Molecules Present in a Ligand Binding Site into a Three-Dimensional Quantitative Structureâ^'Activity Relationship Analysis. Journal of Medicinal Chemistry, 1997, 40, 4089-4102.	2.9	97
92	Simulation of alternative binding modes in a structure-based QSAR study of HIV-1 protease inhibitors. Journal of Molecular Graphics and Modelling, 1997, 15, 364-371.	1.3	20
93	N-(Pyridylmethyl)azinium Salts: Precursors of Pyridyl-stabilised Azinium N-Ylides. Tetrahedron, 1995, 51, 12425-12438.	1.0	11
94	A statistical study of the correlation between kâ€² or log kâ€² and log Pow for a group of benzene and naphthalene derivatives in micellar liquid chromatography using a C-18 column. Chromatographia, 1995, 40, 185-192.	0.7	9
95	The EDISFAR Programs. Drug Series Design in Polysubstituted Prototypes. QSAR and Combinatorial Science, 1995, 14, 24-30.	1.4	3
96	A Novel Strategy for Improving Ligand Selectivity in Receptor-Based Drug Design. Journal of Medicinal Chemistry, 1995, 38, 4637-4647.	2.9	55
97	Synthesis, Structure, and Pharmacological Evaluation of the Stereoisomers of Furnidipine. Journal of Medicinal Chemistry, 1995, 38, 2830-2841.	2.9	47
98	Hydrophobicity of Heterocycles: Determination of the ÃÂ€ Values of Substituents on N-Phenylpyrazoles. QSAR and Combinatorial Science, 1994, 13, 165-171.	1.4	0
99	New Developments of EDISFAR Programs. Experimental Design in QSAR Practice. Journal of Chemical Information and Computer Sciences, 1994, 34, 570-575.	2.8	3
100	The EDISFAR Programs. Rational Drug Series Design. QSAR and Combinatorial Science, 1991, 10, 350-358.	1.4	15
101	Development and Validation of an In Silico Rabbit Purkinje Cell Action Potential Model: A Step Towards a Drug Safety Testing Tool. , 0, , .		0
102	Region Selection in 3D-QSAR. , 0, , 379-395.		4
103	The Role of Water in Receptor-Ligand Interactions. A 3D-QSAR Approach. , 0, , 473-484.		1