Jordi Mestres

List of Publications by Year
in descending order

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138 papers	6,367 citations	61945 43 h-index	79644 73 g-index
147 all docs	147 docs citations	147 times ranked	8702 citing authors

#	Article	IF	Citations
1	A Workflow of Integrated Resources to Catalyze Network Pharmacology Driven COVID-19 Research. Journal of Chemical Information and Modeling, 2022, 62, 718-729.	2.5	2
2	Rare Variation in Drug Metabolism and Long QT Genes and the Genetic Susceptibility to Acquired Long QT Syndrome. Circulation Genomic and Precision Medicine, 2022, 15, CIRCGEN121003391.	1.6	7
3	Environmental levels of carbaryl impair zebrafish larvae behaviour: The potential role of ADRA2B and HTR2B. Journal of Hazardous Materials, 2022, 431, 128563.	6.5	14
4	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	1.8	5
5	Extended connectivity interaction features: improving binding affinity prediction through chemical description. Bioinformatics, 2021, 37, 1376-1382.	1.8	54
6	Identification of the Core Chemical Structure in SureChEMBL Patents. Journal of Chemical Information and Modeling, 2021, 61, 2241-2247.	2.5	12
7	Androgenic activation, impairment of the monoaminergic system and altered behavior in zebrafish larvae exposed to environmental concentrations of fenitrothion. Science of the Total Environment, 2021, 775, 145671.	3.9	48
8	Congenericity of Claimed Compounds in Patent Applications. Molecules, 2021, 26, 5253.	1.7	6
9	In silico approaches in carcinogenicity hazard assessment: Current status and future needs. Computational Toxicology, 2021, 20, 100191.	1.8	19
10	PRIMAGE project: predictive in silico multiscale analytics to support childhood cancer personalised evaluation empowered by imaging biomarkers. European Radiology Experimental, 2020, 4, 22.	1.7	41
11	Skin sensitization in silico protocol. Regulatory Toxicology and Pharmacology, 2020, 116, 104688.	1.3	27
12	Comparison of Zebrafish Larvae and hiPSC Cardiomyocytes for Predicting Drug-Induced Cardiotoxicity in Humans. Toxicological Sciences, 2019, 171, 283-295.	1.4	23
13	Closing the Gap Between Therapeutic Use and Mode of Action in Remedial Herbs. Frontiers in Pharmacology, 2019, 10, 1132.	1.6	1
14	The human endogenous metabolome as a pharmacology baseline for drug discovery. Drug Discovery Today, 2019, 24, 1806-1820.	3.2	9
15	Information Loss in Network Pharmacology. Molecular Informatics, 2019, 38, 1900032.	1.4	6
16	EU-OPENSCREEN: A Novel Collaborative Approach to Facilitate Chemical Biology. SLAS Discovery, 2019, 24, 398-413.	1.4	12
17	Identification of a Tool Compound to Study the Mechanisms of Functional Selectivity between D₂ and D₃ Dopamine Receptors. ACS Omega, 2018, 3, 17368-17375.	1.6	1
18	Dual Inhibitors of PARPs and ROCKs. ACS Omega, 2018, 3, 12707-12712.	1.6	5

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19	Mechanisms of the Development of Allergy (MeDALL): Introducing novel concepts in allergy phenotypes. Journal of Allergy and Clinical Immunology, 2017, 139, 388-399.	1.5	145
20	Design, Synthesis and Biological Evaluation of Potent Antioxidant 1â€(2,5â€Dimethoxybenzyl)â€4â€arylpiperazines and Nâ€Azolyl Substituted 2â€(4â€Arylpiperazinâ€1â€yl) ChemistrySelect, 2017, 2, 3854-3859.	0.7	4
21	Synthesis, pharmacological evaluation and molecular docking of pyranopyrazole-linked 1,4-dihydropyridines as potent positive inotropes. Molecular Diversity, 2017, 21, 533-546.	2.1	9
22	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
23	Polypharmacology in Precision Oncology: Current Applications and Future Prospects. Current Pharmaceutical Design, 2017, 22, 6935-6945.	0.9	65
24	Biological substantiation of antipsychotic-associated pneumonia: Systematic literature review and computational analyses. PLoS ONE, 2017, 12, e0187034.	1.1	20
25	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. PLoS Pathogens, 2016, 12, e1005763.	2.1	244
26	Paving the way of systems biology and precision medicine in allergic diseases: the Me <scp>DALL</scp> success story. Allergy: European Journal of Allergy and Clinical Immunology, 2016, 71, 1513-1525.	2.7	77
27	The In Vitro Pharmacological Profile of Drugs as a Proxy Indicator of Potential In Vivo Organ Toxicities. Chemical Research in Toxicology, 2016, 29, 637-648.	1.7	9
28	Distant Polypharmacology among MLP Chemical Probes. ACS Chemical Biology, 2015, 10, 395-400.	1.6	28
29	In Silico Prescription of Anticancer Drugs to Cohorts of 28 Tumor Types Reveals Targeting Opportunities. Cancer Cell, 2015, 27, 382-396.	7.7	290
30	Large-Scale Predictive Drug Safety: From Structural Alerts to Biological Mechanisms. Chemical Research in Toxicology, 2015, 28, 1875-1887.	1.7	49
31	Insights from Fragment Hit Binding Assays by Molecular Simulations. Journal of Chemical Information and Modeling, 2015, 55, 2200-2205.	2.5	25
32	Effects of BDE-209 contaminated sediments on zebrafish development and potential implications to human health. Environment International, 2014, 63, 216-223.	4.8	47
33	Design of a Generalâ€Purpose European Compound Screening Library for EUâ€OPENSCREEN. ChemMedChem, 2014, 9, 2309-2326.	1.6	29
34	Identification of host interactions for phenotypic antimalarial hits. Journal of Cheminformatics, 2014, 6, O12.	2.8	0
35	Linking off-target kinase pharmacology to the differential cellular effects observed among PARP inhibitors. Oncotarget, 2014, 5, 3023-3028.	0.8	49
36	On the origins of drug polypharmacology. MedChemComm, 2013, 4, 80-87.	3.5	124

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37	Chemoisosterism in the Proteome. Journal of Chemical Information and Modeling, 2013, 53, 279-292.	2.5	20
38	Exploring the effect of PARP-1 flexibility in docking studies. Journal of Molecular Graphics and Modelling, 2013, 45, 192-201.	1.3	16
39	Scientific competency questions as the basis for semantically enriched open pharmacological space development. Drug Discovery Today, 2013, 18, 843-852.	3.2	44
40	Prediction of the P. falciparum Target Space Relevant to Malaria Drug Discovery. PLoS Computational Biology, 2013, 9, e1003257.	1.5	47
41	Identification of Similar Binding Sites to Detect Distant Polypharmacology. Molecular Informatics, 2013, 32, 976-990.	1.4	50
42	The EUâ€ADR Web Platform: delivering advanced pharmacovigilance tools. Pharmacoepidemiology and Drug Safety, 2013, 22, 459-467.	0.9	36
43	Drug-Induced Acute Myocardial Infarction: Identifying â€˜Prime Suspectsâ€™ from Electronic Healthcare Records-Based Surveillance System. PLoS ONE, 2013, 8, e72148.	1.1	41
44	Gathering and Exploring Scientific Knowledge in Pharmacovigilance. PLoS ONE, 2013, 8, e83016.	1.1	15
45	Automatic Filtering and Substantiation of Drug Safety Signals. PLoS Computational Biology, 2012, 8, e1002457.	1.5	34
46	Combination of Biological Screening in a Cellular Model of Viral Latency and Virtual Screening Identifies Novel Compounds That Reactivate HIV-1. Journal of Virology, 2012, 86, 3795-3808.	1.5	28
47	Identification of Pim Kinases as Novel Targets for PJ34 with Confounding Effects in PARP Biology. ACS Chemical Biology, 2012, 7, 1962-1967.	1.6	65
48	Drug Repurposing: Far Beyond New Targets for Old Drugs. AAPS Journal, 2012, 14, 759-763.	2.2	212
49	PharmaTrek: A Semantic Web Explorer for Open Innovation in Multitarget Drug Discovery. Molecular Informatics, 2012, 31, 537-541.	1.4	17
50	Myxobacteria: natural pharmaceutical factories. Microbial Cell Factories, 2012, 11, 52.	1.9	32
51	Identification of Small Molecule Inhibitors of Amyloid Î²-Induced Neuronal Apoptosis Acting through the Imidazoline I₂ Receptor. Journal of Medicinal Chemistry, 2012, 55, 9838-9846.	2.9	14
52	New chromene scaffolds for adenosine A2A receptors: Synthesis, pharmacology and structureâ€“activity relationships. European Journal of Medicinal Chemistry, 2012, 54, 303-310.	2.6	33
53	A Chemocentric Approach to the Identification of Cancer Targets. PLoS ONE, 2012, 7, e35582.	1.1	19
54	Response to the comment by Wolf Ihlenfeldt on the paper â€œIndexing molecules with chemical graph identifiersâ€• Journal of Computational Chemistry, 2012, 33, 238-238.	1.5	0

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55	Linking Pharmacology to Clinical Reports: Cyclobenzaprine and Its Possible Association With Serotonin Syndrome. Clinical Pharmacology and Therapeutics, 2011, 90, 662-665.	2.3	46
56	MeDALL (Mechanisms of the Development of ALLergy): an integrated approach from phenotypes to systems medicine. Allergy: European Journal of Allergy and Clinical Immunology, 2011, 66, 596-604.	2.7	146
57	Multiâ€targeted activity of maslinic acid as an antimalarial natural compound. FEBS Journal, 2011, 278, 2951-2961.	2.2	53
58	Chemical probes for biological systems. Drug Discovery Today, 2011, 16, 99-106.	3.2	25
59	Ligand-Based Approaches to In Silico Pharmacology. Methods in Molecular Biology, 2011, 672, 489-502.	0.4	73
60	In Silico Target Profiling of One Billion Molecules. Molecular Informatics, 2011, 30, 405-409.	1.4	13
61	Indexing molecules with chemical graph identifiers. Journal of Computational Chemistry, 2011, 32, 2638-2646.	1.5	12
62	Fragment-based discovery of 6-substituted isoquinolin-1-amine based ROCK-I inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 97-101.	1.0	27
63	Cross-Pharmacology Analysis of G Protein-Coupled Receptors. Current Topics in Medicinal Chemistry, 2011, 11, 1956-1963.	1.0	33
64	Shaping the future of safer innovative drugs in Europe. Nature Biotechnology, 2011, 29, 789-790.	9.4	3
65	A canonical cationâ€“Ï€ interaction stabilizes the agonist conformation of estrogen-like nuclear receptors. European Biophysics Journal, 2010, 39, 1471-1475.	1.2	5
66	Drugâ€Target Networks. Molecular Informatics, 2010, 29, 10-14.	1.4	73
67	In Silico Receptorome Screening of Antipsychotic Drugs. Molecular Informatics, 2010, 29, 543-551.	1.4	66
68	In silico directed chemical probing of the adenosine receptor family. Bioorganic and Medicinal Chemistry, 2010, 18, 3043-3052.	1.4	28
69	iPHACE: integrative navigation in pharmacological space. Bioinformatics, 2010, 26, 985-986.	1.8	24
70	Anticipating drug side effects by comparative pharmacology. Expert Opinion on Drug Metabolism and Toxicology, 2010, 6, 1253-1263.	1.5	47
71	A chemogenomic approach to drug discovery: focus on cardiovascular diseases. Drug Discovery Today, 2009, 14, 479-485.	3.2	57
72	The topology of drugâ€“target interaction networks: implicit dependence on drug properties and target families. Molecular BioSystems, 2009, 5, 1051.	2.9	196

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73	Conciliating binding efficiency and polypharmacology. Trends in Pharmacological Sciences, 2009, 30, 470-474.	4.0	59
74	Coverage and bias in chemical library design. Current Opinion in Chemical Biology, 2008, 12, 359-365.	2.8	33
75	Data completenessâ€"the Achilles heel of drug-target networks. Nature Biotechnology, 2008, 26, 983-984.	9.4	290
76	A Ligand-Based Approach to Mining the Chemogenomic Space of Drugs. Combinatorial Chemistry and High Throughput Screening, 2008, 11, 669-676.	0.6	104
77	Connecting Small Molecules to Nuclear Receptor Pathways. Current Topics in Medicinal Chemistry, 2007, 7, 1530-1536.	1.0	8
78	In silico pharmacology for drug discovery: methods for virtual ligand screening and profiling. British Journal of Pharmacology, 2007, 152, 9-20.	2.7	522
79	In silico pharmacology for drug discovery: applications to targets and beyond. British Journal of Pharmacology, 2007, 152, 21-37.	2.7	269
80	SHED:Â Shannon Entropy Descriptors from Topological Feature Distributions. Journal of Chemical Information and Modeling, 2006, 46, 1615-1622.	2.5	104
81	Ligand-Based Approach to In Silico Pharmacology:â€‰ Nuclear Receptor Profiling. Journal of Chemical Information and Modeling, 2006, 46, 2725-2736.	2.5	100
82	Mapping the Chemogenomic Space. , 2006, , 39-57.		1
83	Putting molecular similarity into context: asymmetric indices for field-based similarity measures. Journal of Mathematical Chemistry, 2006, 39, 107-118.	0.7	11
84	FCP: functional coverage of the proteome by structures. Bioinformatics, 2006, 22, 1792-1793.	1.8	15
85	Representativity of target families in the Protein Data Bank: impact for family-directed structure-based drug discovery. Drug Discovery Today, 2005, 10, 1629-1637.	3.2	34
86	Chemical and Biological Profiling of an Annotated Compound Library Directed to the Nuclear Receptor Family. Current Topics in Medicinal Chemistry, 2005, 5, 763-772.	1.0	45
87	Mutual induced fit in cyclodextrinâ€"rocuronium complexes. Organic and Biomolecular Chemistry, 2005, 3, 1863.	1.5	28
88	Unsupervised guided docking of covalently bound ligands. Journal of Computer-Aided Molecular Design, 2004, 18, 635-650.	1.3	18
89	Structure conservation in cytochromes P450. Proteins: Structure, Function and Bioinformatics, 2004, 58, 596-609.	1.5	70
90	Guided Docking Approaches to Structure-Based Design and Screening. Current Topics in Medicinal Chemistry, 2004, 4, 687-700.	1.0	62

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91	Computational chemogenomics approaches to systematic knowledge-based drug discovery. Current Opinion in Drug Discovery & Development, 2004, 7, 304-13.	1.9	22
92	Identification of â€œLatent Hitsâ€•in Compound Screening Collections. Journal of Medicinal Chemistry, 2003, 46, 3441-3444.	2.9	37
93	Exploring the active site of human factor Xa protein by NMR screening of small molecule probes. Organic and Biomolecular Chemistry, 2003, 1, 4235.	1.5	17
94	Virtual screening: a real screening complement to high-throughput screening. Biochemical Society Transactions, 2002, 30, 797-799.	1.6	41
95	A General Analysis of Field-Based Molecular Similarity Indices. Journal of Mathematical Chemistry, 2002, 31, 251-270.	0.7	26
96	Mechanism of the Addition Reaction of Alkyl Azides to [60]Fullerene and the Subsequent N2Extrusion to Form Monoimino-[60]fullerenes. Journal of Organic Chemistry, 2001, 66, 433-442.	1.7	91
97	Comparing protein structures: A Gaussian-based approach to the three-dimensional structural similarity of proteins. Journal of Molecular Graphics and Modelling, 2001, 19, 168-178.	1.3	16
98	Atomic transferability within the exchange-correlation density. Journal of Computational Chemistry, 2000, 21, 1361-1374.	1.5	11
99	Similarity-driven flexible ligand docking. Proteins: Structure, Function and Bioinformatics, 2000, 40, 623-636.	1.5	87
100	A molecular-field-based similarity study of non-nucleoside HIV-1 reverse transcriptase inhibitors. 2. The relationship between alignment solutions obtained from conformationally rigid and flexible matching. Journal of Computer-Aided Molecular Design, 2000, 14, 39-51.	1.3	20
101	Similarity versus docking in 3D virtual screening. , 2000, 20, 191-207.		26
102	Gaussian-based Alignment of Protein Structures: Deriving a Consensus Superposition when Alternative Solutions Exist. Journal of Molecular Modeling, 2000, 6, 539-549.	0.8	4
103	The mapping of the local contributions of Fermi and Coulomb correlation into intracule and extracule density distributions. Journal of Chemical Physics, 2000, 113, 2530-2543.	1.2	9
104	Interpretation of Molecular Intracule and Extracule Density Distributions in Terms of Valence Bond Structures:â€‰ Two-Electron Systems and Processes. Journal of Physical Chemistry A, 2000, 104, 8445-8454.	1.1	11
105	Comparative electronic analysis between hydrogen transfers in the CH₄/CH₃⁺, CH₄/CH₃^{Â•}, and CH₄/CH₃⁻ systems: on the electronic nature of the hydrogen (H⁻, H^{Â•}, H⁺) being transferred. II. Analysis of electron-pair interactions from intracule and extracule densities. Canadian Journal of Chemistry, 2000, 78, 328-337.	0.6	5
106	Similarity versus docking in 3D virtual screening. , 2000, , 191-207.		6
107	Gaussian-Based Approaches to Protein-Structure Similarity. , 2000, , 83-88.		1
108	Comparative electronic analysis between hydrogen transfers in the CH₄/CH₃⁺, CH₄/CH₃^{â€¢}, and CH₄/CH₃⁻ systems: on the electronic nature of the hydrogen (H⁻, H^{â€¢}, H⁺) being transferred. II. Analysis of electron-pair interactions from intracule and eÂ—tracule densities. Canadian Journal of Chemistry, 2000, 78, 328-337.	0.6	7

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109	A molecular-field-based similarity study of non-nucleoside HIV-1 reverse transcriptase inhibitors. Journal of Computer-Aided Molecular Design, 1999, 13, 79-93.	1.3	33
110	Comparison of quantum similarity measures derived from one-electron, intracule, and extracule densities. Advances in Molecular Similarity, 1999, , 215-243.	0.5	1
111	Exploring the possibility of a bimolecular reaction channel for the F2SS/FSSF rearrangement process. Computational and Theoretical Chemistry, 1998, 455, 123-129.	1.5	5
112	The use of ab initio quantum molecular self-similarity measures to analyze electronic charge density distributions. International Journal of Quantum Chemistry, 1998, 58, 361-372.	1.0	31
113	Second-order quantum similarity measures from intracule and extracule densities. Theoretical Chemistry Accounts, 1998, 99, 44-52.	0.5	11
114	Dielsâ^'Alder Cycloadditions of 1,3-Butadiene to Polycyclic Aromatic Hydrocarbons (PAH). Quantifying the Reactivity Likeness of Bowl-Shaped PAHs to C60. Journal of Organic Chemistry, 1998, 63, 7556-7558.	1.7	24
115	The relevance of the Laplacian of intracule and extracule density distributions for analyzing electronâ€"electron interactions in molecules. Journal of Chemical Physics, 1997, 107, 3576-3583.	1.2	28
116	Preparation and characterization of pyridinium-n-carboxylate trioxochromate (VI) (n=3, 4) and pyridinium-4-carboxylic pyridine-4 carboxylate trioxochromate (VI) hemihydrate. Inorganica Chimica Acta, 1997, 258, 53-63.	1.2	10
117	A molecular field-based similarity approach to pharmacophoric pattern recognition. Journal of Molecular Graphics and Modelling, 1997, 15, 114-121.	1.3	36
118	MIMIC: A molecular-field matching program. Exploiting applicability of molecular similarity approaches. Journal of Computational Chemistry, 1997, 18, 934-954.	1.5	104
119	Theoretical Study of the Regioselectivity of Successive 1,3-Butadiene Dielsâ^'Alder Cycloadditions to C60. Journal of the American Chemical Society, 1996, 118, 8920-8924.	6.6	37
120	A comparative analysis by means of quantum molecular similarity measures of density distributions derived from conventional ab initio and density functional methods. Journal of Chemical Physics, 1996, 104, 636-647.	1.2	54
121	Comparative electronic analysis between hydrogen transfers in the CH4/CH3+, CH4/CH3â€¢, and CH4/CH3â^' systems: on the electronic nature of the hydrogen (Hâ^', Hâ€¢, and H+) being transferred. Canadian Journal of Chemistry, 1996, 74, 1253-1262.	0.6	3
122	Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. Computational and Theoretical Chemistry, 1996, 371, 171-183.	1.5	26
123	Characterization of the Transition State for the Hydride Transfer in a Model of the Flavoprotein Reductase Class of Enzymes. Bioorganic Chemistry, 1996, 24, 69-80.	2.0	15
124	Effect of Solvation on the Charge Distribution of a Series of Anionic, Neutral, and Cationic Species. A Quantum Molecular Similarity Study. The Journal of Physical Chemistry, 1996, 100, 606-610.	2.9	27
125	Theoretical Study of Dielsâ^'Alder Cycloadditions of Butadiene to C70. An Insight into the Chemical Reactivity of C70as Compared to C60. The Journal of Physical Chemistry, 1996, 100, 7449-7454.	2.9	64
126	The use of ab initio quantum molecular selfâ€similarity measures to analyze electronic charge density distributions. International Journal of Quantum Chemistry, 1996, 58, 361-372.	1.0	25

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127	Conformational analysis from the viewpoint of molecular similarity. Advances in Molecular Similarity, 1996, , 135-165.	0.5	6
128	Genetic algorithms: A robust scheme for geometry optimizations and global minimum structure problems. Journal of Computational Chemistry, 1995, 16, 729-742.	1.5	54
129	Is there a hydride transfer between N2OH+ and saturated hydrocarbons?. Chemical Physics, 1995, 192, 99-110.	0.9	3
130	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10752-10758.	2.9	50
131	Foundations and recent developments on molecular quantum similarity. Topics in Current Chemistry, 1995, , 31-62.	4.0	72
132	Ab initio electronic analysis of the hydride transfer in the [CH3-H-CH3]+ system. Theoretica Chimica Acta, 1994, 88, 325-338.	0.9	16
133	An AM1 study of the reactivity of buckminsterfullerene (C60) in a Diels-Alder model reaction. Chemical Physics Letters, 1994, 231, 325-330.	1.2	49
134	On the calculation ofab initioquantum molecular similarities for large systems: Fitting the electron density. Journal of Computational Chemistry, 1994, 15, 1113-1120.	1.5	46
135	Use of ab Initio Quantum Molecular Similarities as an Interpretative Tool for the Study of Chemical Reactions. Journal of the American Chemical Society, 1994, 116, 5909-5915.	6.6	54
136	Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M) Tj ETQq0 0 0 rgBT /Overlock 10 T 1047-1053.	2.8	25
137	Intrinsic reaction coordinate of perturbed potential energy surfaces: Construction of perturbed energy profiles. International Journal of Quantum Chemistry, 1993, 47, 307-317.	1.0	1
138	Ab initio theoretical study on geometries, chemical bonding, and infrared and electronic spectra of the M2O72- (M = chromium, molybdenum, tungsten) anions. Inorganic Chemistry, 1993, 32, 4708-4713.	1.9	23