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	In silico pharmacology for drug discovery: methods for virtual ligand screening and profiling. British Journal of Pharmacology, 2007, 152, 9-20.	2.7	522
2	Data completenessâ€"the Achilles heel of drug-target networks. Nature Biotechnology, 2008, 26, 983-984.	9.4	290
3	In Silico Prescription of Anticancer Drugs to Cohorts of 28 Tumor Types Reveals Targeting Opportunities. Cancer Cell, 2015, 27, 382-396.	7.7	290
4	In silico pharmacology for drug discovery: applications to targets and beyond. British Journal of Pharmacology, 2007, 152, 21-37.	2.7	269
5	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. PLoS Pathogens, 2016, 12, e1005763.	2.1	244
6	Drug Repurposing: Far Beyond New Targets for Old Drugs. AAPS Journal, 2012, 14, 759-763.	2.2	212
7	The topology of drugâ€"target interaction networks: implicit dependence on drug properties and target families. Molecular BioSystems, 2009, 5, 1051.	2.9	196
8	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
9	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
10	On the origins of drug polypharmacology. MedChemComm, 2013, 4, 80-87.	3.5	124
11	MIMIC: A molecular-field matching program. Exploiting applicability of molecular similarity approaches. Journal of Computational Chemistry, 1997, 18, 934-954.	1.5	104
12	SHED:Â Shannon Entropy Descriptors from Topological Feature Distributions. Journal of Chemical Information and Modeling, 2006, 46, 1615-1622.	2.5	104
13	A Ligand-Based Approach to Mining the Chemogenomic Space of Drugs. Combinatorial Chemistry and High Throughput Screening, 2008, 11, 669-676.	0.6	104
14	Ligand-Based Approach to In Silico Pharmacology:â€‰ Nuclear Receptor Profiling. Journal of Chemical Information and Modeling, 2006, 46, 2725-2736.	2.5	100
15	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
16	Similarity-driven flexible ligand docking. Proteins: Structure, Function and Bioinformatics, 2000, 40, 623-636.	1.5	87
17	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
18	Drugâ€Target Networks. Molecular Informatics, 2010, 29, 10-14.	1.4	73

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19	Ligand-Based Approaches to In Silico Pharmacology. Methods in Molecular Biology, 2011, 672, 489-502.	0.4	73
20	Foundations and recent developments on molecular quantum similarity. Topics in Current Chemistry, 1995, , 31-62.	4.0	72
21	Structure conservation in cytochromes P450. Proteins: Structure, Function and Bioinformatics, 2004, 58, 596-609.	1.5	70
22	In Silico Receptorome Screening of Antipsychotic Drugs. Molecular Informatics, 2010, 29, 543-551.	1.4	66
23	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
24	Polypharmacology in Precision Oncology: Current Applications and Future Prospects. Current Pharmaceutical Design, 2017, 22, 6935-6945.	0.9	65
25	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
26	Guided Docking Approaches to Structure-Based Design and Screening. Current Topics in Medicinal Chemistry, 2004, 4, 687-700.	1.0	62
27	Conciliating binding efficiency and polypharmacology. Trends in Pharmacological Sciences, 2009, 30, 470-474.	4.0	59
28	A chemogenomic approach to drug discovery: focus on cardiovascular diseases. Drug Discovery Today, 2009, 14, 479-485.	3.2	57
29	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
30	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
31	Genetic algorithms: A robust scheme for geometry optimizations and global minimum structure problems. Journal of Computational Chemistry, 1995, 16, 729-742.	1.5	54
32	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
33	Extended connectivity interaction features: improving binding affinity prediction through chemical description. Bioinformatics, 2021, 37, 1376-1382.	1.8	54
34	Multiâ€targeted activity of maslinic acid as an antimalarial natural compound. FEBS Journal, 2011, 278, 2951-2961.	2.2	53
35	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10752-10758.	2.9	50
36	Identification of Similar Binding Sites to Detect Distant Polypharmacology. Molecular Informatics, 2013, 32, 976-990.	1.4	50

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37	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
38	Large-Scale Predictive Drug Safety: From Structural Alerts to Biological Mechanisms. Chemical Research in Toxicology, 2015, 28, 1875-1887.	1.7	49
39	Linking off-target kinase pharmacology to the differential cellular effects observed among PARP inhibitors. Oncotarget, 2014, 5, 3023-3028.	0.8	49
40	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
41	Anticipating drug side effects by comparative pharmacology. Expert Opinion on Drug Metabolism and Toxicology, 2010, 6, 1253-1263.	1.5	47
42	Prediction of the P. falciparum Target Space Relevant to Malaria Drug Discovery. PLoS Computational Biology, 2013, 9, e1003257.	1.5	47
43	Effects of BDE-209 contaminated sediments on zebrafish development and potential implications to human health. Environment International, 2014, 63, 216-223.	4.8	47
44	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
45	Linking Pharmacology to Clinical Reports: Cyclobenzaprine and Its Possible Association With Serotonin Syndrome. Clinical Pharmacology and Therapeutics, 2011, 90, 662-665.	2.3	46
46	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
47	Scientific competency questions as the basis for semantically enriched open pharmacological space development. Drug Discovery Today, 2013, 18, 843-852.	3.2	44
48	Virtual screening: a real screening complement to high-throughput screening. Biochemical Society Transactions, 2002, 30, 797-799.	1.6	41
49	Drug-Induced Acute Myocardial Infarction: Identifying â€˜Prime Suspectsâ€™ from Electronic Healthcare Records-Based Surveillance System. PLoS ONE, 2013, 8, e72148.	1.1	41
50	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
51	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
52	Identification of â€œLatent Hitsâ€•in Compound Screening Collections. Journal of Medicinal Chemistry, 2003, 46, 3441-3444.	2.9	37
53	A molecular field-based similarity approach to pharmacophoric pattern recognition. Journal of Molecular Graphics and Modelling, 1997, 15, 114-121.	1.3	36
54	The EUâ€ADR Web Platform: delivering advanced pharmacovigilance tools. Pharmacoepidemiology and Drug Safety, 2013, 22, 459-467.	0.9	36

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55	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
56	Automatic Filtering and Substantiation of Drug Safety Signals. PLoS Computational Biology, 2012, 8, e1002457.	1.5	34
57	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
58	Coverage and bias in chemical library design. Current Opinion in Chemical Biology, 2008, 12, 359-365.	2.8	33
59	Cross-Pharmacology Analysis of G Protein-Coupled Receptors. Current Topics in Medicinal Chemistry, 2011, 11, 1956-1963.	1.0	33
60	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
61	Myxobacteria: natural pharmaceutical factories. Microbial Cell Factories, 2012, 11, 52.	1.9	32
62	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
63	Design of a Generalâ€Purpose European Compound Screening Library for EUâ€OPENSCREEN. ChemMedChem, 2014, 9, 2309-2326.	1.6	29
64	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
65	Mutual induced fit in cyclodextrinâ€“rocuronium complexes. Organic and Biomolecular Chemistry, 2005, 3, 1863.	1.5	28
66	In silico directed chemical probing of the adenosine receptor family. Bioorganic and Medicinal Chemistry, 2010, 18, 3043-3052.	1.4	28
67	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
68	Distant Polypharmacology among MLP Chemical Probes. ACS Chemical Biology, 2015, 10, 395-400.	1.6	28
69	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
70	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
71	Skin sensitization in silico protocol. Regulatory Toxicology and Pharmacology, 2020, 116, 104688.	1.3	27
72	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

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73	Similarity versus docking in 3D virtual screening. , 2000, 20, 191-207.		26
74	A General Analysis of Field-Based Molecular Similarity Indices. Journal of Mathematical Chemistry, 2002, 31, 251-270.	0.7	26
75	Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M) Tj ETQq1 1 0.784314 rgBT /Over 1047-1053.	2.8	25
76	Chemical probes for biological systems. Drug Discovery Today, 2011, 16, 99-106.	3.2	25
77	Insights from Fragment Hit Binding Assays by Molecular Simulations. Journal of Chemical Information and Modeling, 2015, 55, 2200-2205.	2.5	25
78	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
79	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
80	iPHACE: integrative navigation in pharmacological space. Bioinformatics, 2010, 26, 985-986.	1.8	24
81	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
82	Comparison of Zebrafish Larvae and hiPSC Cardiomyocytes for Predicting Drug-Induced Cardiotoxicity in Humans. Toxicological Sciences, 2019, 171, 283-295.	1.4	23
83	Computational chemogenomics approaches to systematic knowledge-based drug discovery. Current Opinion in Drug Discovery & Development, 2004, 7, 304-13.	1.9	22
84	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
85	Chemoisosterism in the Proteome. Journal of Chemical Information and Modeling, 2013, 53, 279-292.	2.5	20
86	Biological substantiation of antipsychotic-associated pneumonia: Systematic literature review and computational analyses. PLoS ONE, 2017, 12, e0187034.	1.1	20
87	A Chemocentric Approach to the Identification of Cancer Targets. PLoS ONE, 2012, 7, e35582.	1.1	19
88	In silico approaches in carcinogenicity hazard assessment: Current status and future needs. Computational Toxicology, 2021, 20, 100191.	1.8	19
89	Unsupervised guided docking of covalently bound ligands. Journal of Computer-Aided Molecular Design, 2004, 18, 635-650.	1.3	18
90	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

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91	PharmaTrek: A Semantic Web Explorer for Open Innovation in Multitarget Drug Discovery. Molecular Informatics, 2012, 31, 537-541.	1.4	17
92	Ab initio electronic analysis of the hydride transfer in the [CH3-H-CH3]+ system. Theoretica Chimica Acta, 1994, 88, 325-338.	0.9	16
93	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
94	Exploring the effect of PARP-1 flexibility in docking studies. Journal of Molecular Graphics and Modelling, 2013, 45, 192-201.	1.3	16
95	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
96	FCP: functional coverage of the proteome by structures. Bioinformatics, 2006, 22, 1792-1793.	1.8	15
97	Gathering and Exploring Scientific Knowledge in Pharmacovigilance. PLoS ONE, 2013, 8, e83016.	1.1	15
98	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
99	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
100	In Silico Target Profiling of One Billion Molecules. Molecular Informatics, 2011, 30, 405-409.	1.4	13
101	Indexing molecules with chemical graph identifiers. Journal of Computational Chemistry, 2011, 32, 2638-2646.	1.5	12
102	EU-OPENSCREEN: A Novel Collaborative Approach to Facilitate Chemical Biology. SLAS Discovery, 2019, 24, 398-413.	1.4	12
103	Identification of the Core Chemical Structure in SureChEMBL Patents. Journal of Chemical Information and Modeling, 2021, 61, 2241-2247.	2.5	12
104	Second-order quantum similarity measures from intracule and extracule densities. Theoretical Chemistry Accounts, 1998, 99, 44-52.	0.5	11
105	Atomic transferability within the exchange-correlation density. Journal of Computational Chemistry, 2000, 21, 1361-1374.	1.5	11
106	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
107	Putting molecular similarity into context: asymmetric indices for field-based similarity measures. Journal of Mathematical Chemistry, 2006, 39, 107-118.	0.7	11
108	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

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109	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
110	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
111	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
112	The human endogenous metabolome as a pharmacology baseline for drug discovery. Drug Discovery Today, 2019, 24, 1806-1820.	3.2	9
113	Connecting Small Molecules to Nuclear Receptor Pathways. Current Topics in Medicinal Chemistry, 2007, 7, 1530-1536.	1.0	8
114	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
115	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
116	Similarity versus docking in 3D virtual screening. , 2000, , 191-207.		6
117	Information Loss in Network Pharmacology. Molecular Informatics, 2019, 38, 1900032.	1.4	6
118	Congenericity of Claimed Compounds in Patent Applications. Molecules, 2021, 26, 5253.	1.7	6
119	Conformational analysis from the viewpoint of molecular similarity. Advances in Molecular Similarity, 1996, , 135-165.	0.5	6
120	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
121	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
122	A canonical cationâ€“Ï€ interaction stabilizes the agonist conformation of estrogen-like nuclear receptors. European Biophysics Journal, 2010, 39, 1471-1475.	1.2	5
123	Dual Inhibitors of PARPs and ROCKs. ACS Omega, 2018, 3, 12707-12712.	1.6	5
124	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	1.8	5
125	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
126	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

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127	Is there a hydride transfer between N2OH+ and saturated hydrocarbons?. Chemical Physics, 1995, 192, 99-110.	0.9	3
128	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
129	Shaping the future of safer innovative drugs in Europe. Nature Biotechnology, 2011, 29, 789-790.	9.4	3
130	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
131	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
132	Mapping the Chemogenomic Space. , 2006, , 39-57.		1
133	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
134	Closing the Gap Between Therapeutic Use and Mode of Action in Remedial Herbs. Frontiers in Pharmacology, 2019, 10, 1132.	1.6	1
135	Gaussian-Based Approaches to Protein-Structure Similarity. , 2000, , 83-88.		1
136	Comparison of quantum similarity measures derived from one-electron, intracule, and extracule densities. Advances in Molecular Similarity, 1999, , 215-243.	0.5	1
137	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
138	Identification of host interactions for phenotypic antimalarial hits. Journal of Cheminformatics, 2014, 6, O12.	2.8	0