

Xavier Barril

List of Publications by Year in descending order

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94
papers

6,010
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109137

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99
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6785
citing authors

#	ARTICLE	IF	CITATIONS
1	NVP-ALU922: A Novel Heat Shock Protein 90 Inhibitor Active against Xenograft Tumor Growth, Angiogenesis, and Metastasis. <i>Cancer Research</i> , 2008, 68, 2850-2860.	0.4	433
2	rDock: A Fast, Versatile and Open Source Program for Docking Ligands to Proteins and Nucleic Acids. <i>PLoS Computational Biology</i> , 2014, 10, e1003571.	1.5	404
3	4,5-Diarylisoaxazole Hsp90 Chaperone Inhibitors: Potential Therapeutic Agents for the Treatment of Cancer. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 196-218.	2.9	386
4	Understanding and Predicting Druggability. A High-Throughput Method for Detection of Drug Binding Sites. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 5858-5867.	2.9	271
5	MDpocket: open-source cavity detection and characterization on molecular dynamics trajectories. <i>Bioinformatics</i> , 2011, 27, 3276-3285.	1.8	265
6	Structure-Activity Relationships in Purine-Based Inhibitor Binding to HSP90 Isoforms. <i>Chemistry and Biology</i> , 2004, 11, 775-785.	6.2	244
7	Novel, Potent Small-Molecule Inhibitors of the Molecular Chaperone Hsp90 Discovered through Structure-Based Design. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 4212-4215.	2.9	232
8	Unveiling the Full Potential of Flexible Receptor Docking Using Multiple Crystallographic Structures. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 4432-4443.	2.9	201
9	Binding Site Detection and Druggability Index from First Principles. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 2363-2371.	2.9	201
10	New Tacrine ⁺ Huperzine A Hybrids (Huprines): Highly Potent Tight-Binding Acetylcholinesterase Inhibitors of Interest for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 4657-4666.	2.9	185
11	Shielded Hydrogen Bonds as Structural Determinants of Binding Kinetics: Application in Drug Design. <i>Journal of the American Chemical Society</i> , 2011, 133, 18903-18910.	6.6	178
12	Combining Hit Identification Strategies: Fragment-Based and in Silico Approaches to Orally Active 2-Aminothieno[2,3- <i>d</i>]pyrimidine Inhibitors of the Hsp90 Molecular Chaperone. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 4794-4809.	2.9	157
13	Inhibition of the heat shock protein 90 molecular chaperone in vitro and in vivo by novel, synthetic, potent resorcinyl pyrazole/isoxazole amide analogues. <i>Molecular Cancer Therapeutics</i> , 2007, 6, 1198-1211.	1.9	141
14	Design and Characterization of Libraries of Molecular Fragments for Use in NMR Screening against Protein Targets. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 2157-2166.	2.8	139
15	Tacripyrines, the First Tacrine ⁺ Dihydropyridine Hybrids, as Multitarget-Directed Ligands for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 2724-2732.	2.9	134
16	3D Structure of <i>Torpedo californica</i> Acetylcholinesterase Complexed with Huprine X at 2.1 Å... Resolution: Kinetic and Molecular Dynamic Correlates. <i>Biochemistry</i> , 2002, 41, 2970-2981.	1.2	126
17	Synthesis, in Vitro Pharmacology, and Molecular Modeling of Very Potent Tacrine ⁺ Huperzine A Hybrids as Acetylcholinesterase Inhibitors of Potential Interest for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 1999, 42, 3227-3242.	2.9	101
18	Molecular Simulations with Solvent Competition Quantify Water Displaceability and Provide Accurate Interaction Maps of Protein Binding Sites. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 8530-8539.	2.9	89

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19	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 45, 428-437.	1.5	87
20	Structure-based discovery of a new class of Hsp90 inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 5187-5191.	1.0	87
21	Protein Flexibility and Ligand Recognition: Challenges for Molecular Modeling. <i>Current Topics in Medicinal Chemistry</i> , 2011, 11, 192-210.	1.0	86
22	3-(5-chloro-2,4-dihydroxyphenyl)-Pyrazole-4-carboxamides as inhibitors of the Hsp90 molecular chaperone. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 5197-5201.	1.0	83
23	Toward accurate relative energy predictions of the bioactive conformation of drugs. <i>Journal of Computational Chemistry</i> , 2009, 30, 601-610.	1.5	82
24	A fluorescence polarization assay for inhibitors of Hsp90. <i>Analytical Biochemistry</i> , 2006, 350, 202-213.	1.1	81
25	4-Amino derivatives of the Hsp90 inhibitor CCT018159. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 2543-2548.	1.0	79
26	Salt bridge interactions: Stability of the ionic and neutral complexes in the gas phase, in solution, and in proteins. , 1998, 32, 67-79.		76
27	New tacrine-dihydropyridine hybrids that inhibit acetylcholinesterase, calcium entry, and exhibit neuroprotection properties. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 7759-7769.	1.4	75
28	Adenine derived inhibitors of the molecular chaperone HSP90â€™ SAR explained through multiple X-ray structures. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 325-328.	1.0	69
29	Molecular Dynamics in Mixed Solvents Reveals Proteinâ€™Ligand Interactions, Improves Docking, and Allows Accurate Binding Free Energy Predictions. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 846-863.	2.5	68
30	Dynamic undocking and the quasi-bound state as tools for drug discovery. <i>Nature Chemistry</i> , 2017, 9, 201-206.	6.6	68
31	Ensemble Docking from Homology Models. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2547-2557.	2.3	65
32	Theoretical Methods for the Representation of Solvent. <i>Journal of Molecular Modeling</i> , 1996, 2, 1-15.	0.8	61
33	Extended connectivity interaction features: improving binding affinity prediction through chemical description. <i>Bioinformatics</i> , 2021, 37, 1376-1382.	1.8	54
34	Virtual screening: An in silico tool for interlacing the chemical universe with the proteome. <i>Methods</i> , 2015, 71, 44-57.	1.9	47
35	An investigation of structural stability in protein-ligand complexes reveals the balance between order and disorder. <i>Communications Chemistry</i> , 2019, 2, .	2.0	46
36	Synthesis, in Vitro Pharmacology, and Molecular Modeling of syn-Huprines as Acetylcholinesterase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 4733-4736.	2.9	45

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37	Fluorogenic Trp(redBODIPY) cyclopeptide targeting keratin 1 for imaging of aggressive carcinomas. <i>Chemical Science</i> , 2020, 11, 1368-1374.	3.7	42
38	Virtual Screening in Structure-Based Drug Discovery. <i>Mini-Reviews in Medicinal Chemistry</i> , 2012, 4, 779-91.	1.1	41
39	Relationship between Protein Flexibility and Binding: Lessons for Structure-Based Drug Design. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2608-2614.	2.3	41
40	Predicting Relative Binding Free Energies of Tacrine-Huperzine A Hybrids as Inhibitors of Acetylcholinesterase. <i>Journal of Medicinal Chemistry</i> , 1999, 42, 5110-5119.	2.9	36
41	A Multilevel Strategy for the Exploration of the Conformational Flexibility of Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1808-1819.	2.3	35
42	TuberQ: a Mycobacterium tuberculosis protein druggability database. <i>Database: the Journal of Biological Databases and Curation</i> , 2014, 2014, bau035-bau035.	1.4	35
43	Detecting similar binding pockets to enable systems polypharmacology. <i>PLoS Computational Biology</i> , 2017, 13, e1005522.	1.5	35
44	Fractional description of free energies of solvation. <i>Journal of Computer-Aided Molecular Design</i> , 1999, 13, 139-152.	1.3	33
45	Binding mode prediction and MD/MMPBSA-based free energy ranking for agonists of REV-ERB α /NCoR. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 755-775.	1.3	31
46	Incorporating protein flexibility into docking and structure-based drug design. <i>Expert Opinion on Drug Discovery</i> , 2006, 1, 335-349.	2.5	30
47	Druggability predictions: methods, limitations, and applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 327-338.	6.2	30
48	VAV3 mediates resistance to breast cancer endocrine therapy. <i>Breast Cancer Research</i> , 2014, 16, R53.	2.2	28
49	How accurate can molecular dynamics/linear response and Poisson-Boltzmann/solvent accessible surface calculations be for predicting relative binding affinities? Acetylcholinesterase huprine inhibitors as a test case. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 2-9.	0.5	25
50	Solvents to Fragments to Drugs: MD Applications in Drug Design. <i>Molecules</i> , 2018, 23, 3269.	1.7	25
51	Towards Improved Acetylcholinesterase Inhibitors: A Structural and Computational Approach. <i>Mini-Reviews in Medicinal Chemistry</i> , 2001, 1, 255-266.	1.1	24
52	Pharmacological chaperones for enzyme enhancement therapy in genetic diseases. <i>Pharmaceutical Patent Analyst</i> , 2013, 2, 109-124.	0.4	23
53	Rational Design of Reversible Acetylcholinesterase Inhibitors. <i>Mini-Reviews in Medicinal Chemistry</i> , 2002, 2, 27-36.	1.1	22
54	Predicting how drug molecules bind to their protein targets. <i>Current Opinion in Pharmacology</i> , 2018, 42, 34-39.	1.7	21

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55	Cosolvent-Based Protein Pharmacophore for Ligand Enrichment in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3572-3583.	2.5	21
56	Hydrophobic similarity between molecules: A MST-based hydrophobic similarity index. <i>Journal of Computational Chemistry</i> , 2002, 23, 554-563.	1.5	18
57	DUckCov: a Dynamic Undocking-Based Virtual Screening Protocol for Covalent Binders. <i>ChemMedChem</i> , 2019, 14, 1011-1021.	1.6	18
58	Extension of the MST continuum solvation model to the RM1 semiempirical hamiltonian. <i>Journal of Computational Chemistry</i> , 2008, 29, 578-587.	1.5	17
59	Molecular simulation methods in drug discovery: a prospective outlook. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 81-86.	1.3	17
60	Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1164-1172.	1.2	16
61	Computer-aided drug design: time to play with novel chemical matter. <i>Expert Opinion on Drug Discovery</i> , 2017, 12, 977-980.	2.5	14
62	Simplified descriptions of the topological distribution of hydrophilic/hydrophobic characteristics of molecules. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4897-4905.	1.3	13
63	Allosteric regulation of PKC ζ : Understanding multistep phosphorylation and priming by ligands in AGC kinases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 269-280.	1.5	12
64	Structural Stability Predicts the Binding Mode of Protein-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1644-1651.	2.5	12
65	Transferability of fragmental contributions to the octanol/water partition coefficient: An NDDO-based MST study. <i>Journal of Computational Chemistry</i> , 2003, 24, 32-45.	1.5	11
66	In Silico/In Vivo Insights into the Functional and Evolutionary Pathway of <i>Pseudomonas aeruginosa</i> Oleate-Diol Synthase. Discovery of a New Bacterial Di-Heme Cytochrome C Peroxidase Subfamily. <i>PLoS ONE</i> , 2015, 10, e0131462.	1.1	11
67	Combined Use of Oligopeptides, Fragment Libraries, and Natural Compounds: A Comprehensive Approach To Sample the Druggability of Vascular Endothelial Growth Factor. <i>ChemMedChem</i> , 2016, 11, 928-939.	1.6	10
68	Identification and Characterization of a Secondary Sodium-Binding Site and the Main Selectivity Determinants in the Human Concentrative Nucleoside Transporter 3. <i>Molecular Pharmaceutics</i> , 2017, 14, 1980-1987.	2.3	10
69	Discovery of a novel kinase hinge binder fragment by dynamic undocking. <i>RSC Medicinal Chemistry</i> , 2020, 11, 552-558.	1.7	10
70	Molecular Modelling. <i>Molecular BioSystems</i> , 2006, 2, 660.	2.9	9
71	A hydrophobic similarity analysis of solvation effects on nucleic acid bases. <i>Journal of Molecular Modeling</i> , 2007, 13, 357-365.	0.8	8
72	Discovery of an Allosteric Ligand Binding Site in SMYD3 Lysine Methyltransferase. <i>ChemBioChem</i> , 2021, 22, 1597-1608.	1.3	8

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73	Nucleic Acid Bases in Solution. Theoretical and Computational Chemistry, 1999, 8, 119-166.	0.2	7
74	Binding of calix[4]pyrroles to pyridine N-oxides probed with surface plasmon resonance. Chemical Science, 2014, 5, 4210-4215.	3.7	7
75	Inherent conformational flexibility of F ₁ -ATPase $\hat{\epsilon}$ -subunit. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1392-1402.	0.5	7
76	Testing automatic methods to predict free binding energy of host-guest complexes in SAMPL7 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 209-222.	1.3	7
77	Fragment-to-lead tailored in silico design. Drug Discovery Today: Technologies, 2021, 40, 44-57.	4.0	6
78	Discovery of Novel BRD4 Ligand Scaffolds by Automated Navigation of the Fragment Chemical Space. Journal of Medicinal Chemistry, 2021, 64, 17887-17900.	2.9	6
79	LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1741-1746.	2.5	5
80	Binding kinetics in drug discovery. Drug Discovery Today: Technologies, 2015, 17, 35-36.	4.0	4
81	Dynamic Undocking: A Novel Method for Structure-Based Drug Discovery. Methods in Molecular Biology, 2018, 1824, 195-215.	0.4	4
82	Docking points. Nature Chemistry, 2014, 6, 560-561.	6.6	3
83	Docking-undocking combination applied to the D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 805-815.	1.3	3
84	Computational Design of Inhibitors Targeting the Catalytic $\hat{\epsilon}$ Subunit of Escherichia coli FOF1-ATP Synthase. Antibiotics, 2022, 11, 557.	1.5	3
85	Cosolvent Sites-Based Discovery of Mycobacterium Tuberculosis Protein Kinase G Inhibitors. Journal of Medicinal Chemistry, 0, , .	2.9	3
86	On the transferability of fractional contributions to the hydration free energy of amino acids. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	2
87	Revealing 2-dimethylhydrazino-2-alkyl alkynyl sphingosine derivatives as sphingosine kinase 2 inhibitors: Some hints on the structural basis for selective inhibition. Bioorganic Chemistry, 2022, 121, 105668.	2.0	2
88	Chapter 4. Molecular Dynamics: a Tool to Understand Nuclear Receptors. RSC Drug Discovery Series, 2012, , 60-83.	0.2	1
89	Development of an Automatic Pipeline for Participation in the CELPP Challenge. International Journal of Molecular Sciences, 2022, 23, 4756.	1.8	1
90	Chapter 12. Expanding the Target Space: Druggability Assessments. RSC Drug Discovery Series, 2012, , 302-318.	0.2	0

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91	Hydrophobic Waters in Bromodomains. Proceedings (mdpi), 2019, 22, 80.	0.2	0
92	Targeting Novel Allosteric Sites with Confidence: Methods and Applications. Proceedings (mdpi), 2019, 22, .	0.2	0
93	Drugging the Fbw7 E3 Ligase with a Fragment-Based Approach. Proceedings (mdpi), 2019, 22, .	0.2	0
94	On the transferability of fractional contributions to the hydration free energy of amino acids. Highlights in Theoretical Chemistry, 2014, , 119-132.	0.0	0