Xavier Barril

List of Publications by Year
in descending order

94 papers	6,010 citations	109137 35 h-index	74018 75 g-index
99 all docs	99 docs citations	99 times ranked	6785 citing authors

#	Article	IF	Citations
1	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
2	Computational Design of Inhibitors Targeting the Catalytic Î² Subunit of Escherichia coli FOF1-ATP Synthase. Antibiotics, 2022, 11, 557.	1.5	3
3	Development of an Automatic Pipeline for Participation in the CELPP Challenge. International Journal of Molecular Sciences, 2022, 23, 4756.	1.8	1
4	Extended connectivity interaction features: improving binding affinity prediction through chemical description. Bioinformatics, 2021, 37, 1376-1382.	1.8	54
5	Discovery of an Allosteric Ligand Binding Site in SMYD3 Lysine Methyltransferase. ChemBioChem, 2021, 22, 1597-1608.	1.3	8
6	Fragment-to-lead tailored in silico design. Drug Discovery Today: Technologies, 2021, 40, 44-57.	4.0	6
7	Testing automatic methods to predict free binding energy of hostâ€“guest complexes in SAMPL7 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 209-222.	1.3	7
8	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
9	Fluorogenic Trp(redBODIPY) cyclopeptide targeting keratin 1 for imaging of aggressive carcinomas. Chemical Science, 2020, 11, 1368-1374.	3.7	42
10	Discovery of a novel kinase hinge binder fragment by dynamic undocking. RSC Medicinal Chemistry, 2020, 11, 552-558.	1.7	10
11	Structural Stability Predicts the Binding Mode of Proteinâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2020, 60, 1644-1651.	2.5	12
12	Cosolvent-Based Protein Pharmacophore for Ligand Enrichment in Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 3572-3583.	2.5	21
13	Hydrophobic Waters in Bromodomains. Proceedings (mdpi), 2019, 22, 80.	0.2	0
14	Targeting Novel Allosteric Sites with Confidence: Methods and Applications. Proceedings (mdpi), 2019, 22, .	0.2	0
15	An investigation of structural stability in protein-ligand complexes reveals the balance between order and disorder. Communications Chemistry, 2019, 2, .	2.0	46
16	DUckCov: a Dynamic Undockingâ€Based Virtual Screening Protocol for Covalent Binders. ChemMedChem, 2019, 14, 1011-1021.	1.6	18
17	Drugging the Fbw7 E3 Ligase with a Fragment-Based Approach. Proceedings (mdpi), 2019, 22, .	0.2	0
18	Solvents to Fragments to Drugs: MD Applications in Drug Design. Molecules, 2018, 23, 3269.	1.7	25

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19	Dynamic Undocking: A Novel Method for Structure-Based Drug Discovery. Methods in Molecular Biology, 2018, 1824, 195-215.	0.4	4
20	Predicting how drug molecules bind to their protein targets. Current Opinion in Pharmacology, 2018, 42, 34-39.	1.7	21
21	Identification and Characterization of a Secondary Sodium-Binding Site and the Main Selectivity Determinants in the Human Concentrative Nucleoside Transporter 3. Molecular Pharmaceutics, 2017, 14, 1980-1987.	2.3	10
22	Molecular Dynamics in Mixed Solvents Reveals Proteinâ€“Ligand Interactions, Improves Docking, and Allows Accurate Binding Free Energy Predictions. Journal of Chemical Information and Modeling, 2017, 57, 846-863.	2.5	68
23	Binding mode prediction and MD/MMPBSA-based free energy ranking for agonists of REV-ERBÎ±/NCoR. Journal of Computer-Aided Molecular Design, 2017, 31, 755-775.	1.3	31
24	Computer-aided drug design: time to play with novel chemical matter. Expert Opinion on Drug Discovery, 2017, 12, 977-980.	2.5	14
25	LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1741-1746.	2.5	5
26	Dynamic undocking and the quasi-bound state as tools for drug discovery. Nature Chemistry, 2017, 9, 201-206.	6.6	68
27	Detecting similar binding pockets to enable systems polypharmacology. PLoS Computational Biology, 2017, 13, e1005522.	1.5	35
28	Docking-undocking combination applied to the D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 805-815.	1.3	3
29	Combined Use of Oligopeptides, Fragment Libraries, and Natural Compounds: A Comprehensive Approach To Sample the Druggability of Vascular Endothelial Growth Factor. ChemMedChem, 2016, 11, 928-939.	1.6	10
30	Inherent conformational flexibility of F 1 -ATPase Î±-subunit. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1392-1402.	0.5	7
31	In Silico/In Vivo Insights into the Functional and Evolutionary Pathway of Pseudomonas aeruginosa Oleate-Diol Synthase. Discovery of a New Bacterial Di-Heme Cytochrome C Peroxidase Subfamily. PLoS ONE, 2015, 10, e0131462.	1.1	11
32	Binding kinetics in drug discovery. Drug Discovery Today: Technologies, 2015, 17, 35-36.	4.0	4
33	Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands. Journal of Physical Chemistry B, 2015, 119, 1164-1172.	1.2	16
34	Virtual screening: An in silico tool for interlacing the chemical universe with the proteome. Methods, 2015, 71, 44-57.	1.9	47
35	rDock: A Fast, Versatile and Open Source Program for Docking Ligands to Proteins and Nucleic Acids. PLoS Computational Biology, 2014, 10, e1003571.	1.5	404
36	Molecular Simulations with Solvent Competition Quantify Water Displaceability and Provide Accurate Interaction Maps of Protein Binding Sites. Journal of Medicinal Chemistry, 2014, 57, 8530-8539.	2.9	89

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37	TuberQ: a Mycobacterium tuberculosis protein druggability database. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau035-bau035.	1.4	35
38	VAV3 mediates resistance to breast cancer endocrine therapy. Breast Cancer Research, 2014, 16, R53.	2.2	28
39	Binding of calix[4]pyrroles to pyridine N-oxides probed with surface plasmon resonance. Chemical Science, 2014, 5, 4210-4215.	3.7	7
40	Docking points. Nature Chemistry, 2014, 6, 560-561.	6.6	3
41	Relationship between Protein Flexibility and Binding: Lessons for Structure-Based Drug Design. Journal of Chemical Theory and Computation, 2014, 10, 2608-2614.	2.3	41
42	On the transferability of fractional contributions to the hydration free energy of amino acids. Highlights in Theoretical Chemistry, 2014, , 119-132.	0.0	0
43	On the transferability of fractional contributions to the hydration free energy of amino acids. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	2
44	Pharmacological chaperones for enzyme enhancement therapy in genetic diseases. Pharmaceutical Patent Analyst, 2013, 2, 109-124.	0.4	23
45	Druggability predictions: methods, limitations, and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 327-338.	6.2	30
46	Virtual Screening in Structure-Based Drug Discovery. Mini-Reviews in Medicinal Chemistry, 2012, 4, 779-91.	1.1	41
47	Chapter 4. Molecular Dynamics: a Tool to Understand Nuclear Receptors. RSC Drug Discovery Series, 2012, , 60-83.	0.2	1
48	A Multilevel Strategy for the Exploration of the Conformational Flexibility of Small Molecules. Journal of Chemical Theory and Computation, 2012, 8, 1808-1819.	2.3	35
49	Allosteric regulation of PKCÎ¸: Understanding multistep phosphorylation and priming by ligands in AGC kinases. Proteins: Structure, Function and Bioinformatics, 2012, 80, 269-280.	1.5	12
50	Chapter 12. Expanding the Target Space: Druggability Assessments. RSC Drug Discovery Series, 2012, , 302-318.	0.2	0
51	Molecular simulation methods in drug discovery: a prospective outlook. Journal of Computer-Aided Molecular Design, 2012, 26, 81-86.	1.3	17
52	Shielded Hydrogen Bonds as Structural Determinants of Binding Kinetics: Application in Drug Design. Journal of the American Chemical Society, 2011, 133, 18903-18910.	6.6	178
53	Protein Flexibility and Ligand Recognition: Challenges for Molecular Modeling. Current Topics in Medicinal Chemistry, 2011, 11, 192-210.	1.0	86
54	MDpocket: open-source cavity detection and characterization on molecular dynamics trajectories. Bioinformatics, 2011, 27, 3276-3285.	1.8	265

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55	Understanding and Predicting Druggability. A High-Throughput Method for Detection of Drug Binding Sites. Journal of Medicinal Chemistry, 2010, 53, 5858-5867.	2.9	271
56	Ensemble Docking from Homology Models. Journal of Chemical Theory and Computation, 2010, 6, 2547-2557.	2.3	65
57	Toward accurate relative energy predictions of the bioactive conformation of drugs. Journal of Computational Chemistry, 2009, 30, 601-610.	1.5	82
58	Combining Hit Identification Strategies: Fragment-Based and in Silico Approaches to Orally Active 2-Aminothieno[2,3-d]pyrimidine Inhibitors of the Hsp90 Molecular Chaperone. Journal of Medicinal Chemistry, 2009, 52, 4794-4809.	2.9	157
59	Binding Site Detection and Druggability Index from First Principles. Journal of Medicinal Chemistry, 2009, 52, 2363-2371.	2.9	201
60	Tacripyrines, the First Tacrineâˆ'Dihydropyridine Hybrids, as Multitarget-Directed Ligands for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2009, 52, 2724-2732.	2.9	134
61	Extension of the MST continuum solvation model to the RM1 semiempirical hamiltonian. Journal of Computational Chemistry, 2008, 29, 578-587.	1.5	17
62	New tacrine-dihydropyridine hybrids that inhibit acetylcholinesterase, calcium entry, and exhibit neuroprotection properties. Bioorganic and Medicinal Chemistry, 2008, 16, 7759-7769.	1.4	75
63	4,5-Diarylisoxazole Hsp90 Chaperone Inhibitors: Potential Therapeutic Agents for the Treatment of Cancer. Journal of Medicinal Chemistry, 2008, 51, 196-218.	2.9	386
64	NVP-AUY922: A Novel Heat Shock Protein 90 Inhibitor Active against Xenograft Tumor Growth, Angiogenesis, and Metastasis. Cancer Research, 2008, 68, 2850-2860.	0.4	433
65	Inhibition of the heat shock protein 90 molecular chaperone in vitro and in vivo by novel, synthetic, potent resorcinylic pyrazole/isoxazole amide analogues. Molecular Cancer Therapeutics, 2007, 6, 1198-1211.	1.9	141
66	A hydrophobic similarity analysis of solvation effects on nucleic acid bases. Journal of Molecular Modeling, 2007, 13, 357-365.	0.8	8
67	4-Amino derivatives of the Hsp90 inhibitor CCT018159. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2543-2548.	1.0	79
68	A fluorescence polarization assay for inhibitors of Hsp90. Analytical Biochemistry, 2006, 350, 202-213.	1.1	81
69	Molecular Modelling. Molecular BioSystems, 2006, 2, 660.	2.9	9
70	Incorporating protein flexibility into docking and structure-based drug design. Expert Opinion on Drug Discovery, 2006, 1, 335-349.	2.5	30
71	Structure-based discovery of a new class of Hsp90 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5187-5191.	1.0	87
72	3-(5-chloro-2,4-dihydroxyphenyl)-Pyrazole-4-carboxamides as inhibitors of the Hsp90 molecular chaperone. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5197-5201.	1.0	83

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73	Unveiling the Full Potential of Flexible Receptor Docking Using Multiple Crystallographic Structures. Journal of Medicinal Chemistry, 2005, 48, 4432-4443.	2.9	201
74	Novel, Potent Small-Molecule Inhibitors of the Molecular Chaperone Hsp90 Discovered through Structure-Based Design. Journal of Medicinal Chemistry, 2005, 48, 4212-4215.	2.9	232
75	Adenine derived inhibitors of the molecular chaperone HSP90â€"SAR explained through multiple X-ray structures. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 325-328.	1.0	69
76	Structure-Activity Relationships in Purine-Based Inhibitor Binding to HSP90 Isoforms. Chemistry and Biology, 2004, 11, 775-785.	6.2	244
77	Design and Characterization of Libraries of Molecular Fragments for Use in NMR Screening against Protein Targets. Journal of Chemical Information and Computer Sciences, 2004, 44, 2157-2166.	2.8	139
78	Transferability of fragmental contributions to the octanol/water partition coefficient: An NDDO-based MST study. Journal of Computational Chemistry, 2003, 24, 32-45.	1.5	11
79	Rational Design of Reversible Acetylcholinesterase Inhibitors. Mini-Reviews in Medicinal Chemistry, 2002, 2, 27-36.	1.1	22
80	3D Structure of Torpedo californica Acetylcholinesterase Complexed with Huprine X at 2.1 Ã... Resolution:â€‰ Kinetic and Molecular Dynamic Correlates,. Biochemistry, 2002, 41, 2970-2981.	1.2	126
81	Hydrophobic similarity between molecules: A MST-based hydrophobic similarity index. Journal of Computational Chemistry, 2002, 23, 554-563.	1.5	18
82	Synthesis, in Vitro Pharmacology, and Molecular Modeling ofsyn-Huprines as Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 4733-4736.	2.9	45
83	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. Theoretical Chemistry Accounts, 2001, 106, 2-9.	0.5	25
84	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2001, 45, 428-437.	1.5	87
85	Towards Improved Acetylcholinesterase Inhibitors: A Structural and Computational Approach. Mini-Reviews in Medicinal Chemistry, 2001, 1, 255-266.	1.1	24
86	New Tacrineâ^'Huperzine A Hybrids (Huprines):â€‰ Highly Potent Tight-Binding Acetylcholinesterase Inhibitors of Interest for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 2000, 43, 4657-4666.	2.9	185
87	Simplified descriptions of the topological distribution of hydrophilic/hydrophobic characteristics of molecules. Physical Chemistry Chemical Physics, 2000, 2, 4897-4905.	1.3	13
88	Nucleic Acid Bases in Solution. Theoretical and Computational Chemistry, 1999, 8, 119-166.	0.2	7
89	Fractional description of free energies of solvation. Journal of Computer-Aided Molecular Design, 1999, 13, 139-152.	1.3	33
90	Predicting Relative Binding Free Energies of Tacrineâ^'Huperzine A Hybrids as Inhibitors of AcetylcholinesteraseÂ§. Journal of Medicinal Chemistry, 1999, 42, 5110-5119.	2.9	36

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91	Synthesis, in Vitro Pharmacology, and Molecular Modeling of Very Potent Tacrineâ˜Huperzine A Hybrids as Acetylcholinesterase Inhibitors of Potential Interest for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 1999, 42, 3227-3242.	2.9	101
92	Salt bridge interactions: Stability of the ionic and neutral complexes in the gas phase, in solution, and in proteins. , 1998, 32, 67-79.		76
93	Theoretical Methods for the Representation of Solvent. Journal of Molecular Modeling, 1996, 2, 1-15.	0.8	61
94	Cosolvent Sites-Based Discovery of Mycobacterium Tuberculosis Protein Kinase G Inhibitors. Journal of Medicinal Chemistry, 0, , .	2.9	3