Carlos J Camacho

List of Publications by Year
in descending order

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74 papers	5,505 citations	159585 30 h-index	82547 72 g-index
84 all docs	84 docs citations	84 times ranked	7443 citing authors

#	Article	IF	Citations
1	ClusPro: an automated docking and discrimination method for the prediction of protein complexes. Bioinformatics, 2004, 20, 45-50.	4.1	809
2	ClusPro: a fully automated algorithm for protein-protein docking. Nucleic Acids Research, 2004, 32, W96-W99.	14.5	717
3	Lessons Learned in Empirical Scoring with smina from the CSAR 2011 Benchmarking Exercise. Journal of Chemical Information and Modeling, 2013, 53, 1893-1904.	5.4	675
4	Anchor residues in protein-protein interactions. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 11287-11292.	7.1	327
5	ZINCPharmer: pharmacophore search of the ZINC database. Nucleic Acids Research, 2012, 40, W409-W414.	14.5	311
6	Free Energy Landscapes of Encounter Complexes in Protein-Protein Association. Biophysical Journal, 1999, 76, 1166-1178.	0.5	181
7	Kinetics of Desolvation-Mediated Proteinâ€“Protein Binding. Biophysical Journal, 2000, 78, 1094-1105.	0.5	141
8	Pharmer: Efficient and Exact Pharmacophore Search. Journal of Chemical Information and Modeling, 2011, 51, 1307-1314.	5.4	134
9	Scoring docked conformations generated by rigid-body protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2000, 40, 525-537.	2.6	112
10	FastContact: rapid estimate of contact and binding free energies. Bioinformatics, 2005, 21, 2534-2536.	4.1	111
11	Proteinâ€“protein association kinetics and protein docking. Current Opinion in Structural Biology, 2002, 12, 36-40.	5.7	107
12	ANCHOR: a web server and database for analysis of protein-protein interaction binding pockets for drug discovery. Nucleic Acids Research, 2010, 38, W407-W411.	14.5	102
13	Toward a quantitative theory of intrinsically disordered proteins and their function. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 19819-19823.	7.1	92
14	Enabling Large-Scale Design, Synthesis and Validation of Small Molecule Protein-Protein Antagonists. PLoS ONE, 2012, 7, e32839.	2.5	90
15	Dynamical View of the Positions of Key Side Chains in Protein-Protein Recognition. Biophysical Journal, 2001, 80, 635-642.	0.5	88
16	SUMOylation of nuclear actin. Journal of Cell Biology, 2009, 186, 193-200.	5.2	85
17	De novo emergence of adaptive membrane proteins from thymine-rich genomic sequences. Nature Communications, 2020, 11, 781.	12.8	84
18	Species-specific immune responses generated by histidyl-tRNA synthetase immunization are associated with muscle and lung inflammation. Journal of Autoimmunity, 2007, 29, 174-186.	6.5	83

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19	PocketQuery: protein-protein interaction inhibitor starting points from protein-protein interaction structure. Nucleic Acids Research, 2012, 40, W387-W392.	14.5	79
20	Small-molecule inhibitor starting points learned from proteinâ€“protein interaction inhibitor structure. Bioinformatics, 2012, 28, 784-791.	4.1	59
21	Tenascin cytotactin epidermal growth factor-like repeat binds epidermal growth factor receptor with low affinity. Journal of Cellular Physiology, 2007, 211, 748-758.	4.1	58
22	Successful discrimination of protein interactions. Proteins: Structure, Function and Bioinformatics, 2003, 52, 92-97.	2.6	56
23	Restricted Protein Phosphatase 2A Targeting by Merkel Cell Polyomavirus Small T Antigen. Journal of Virology, 2015, 89, 4191-4200.	3.4	54
24	Predicting protein targets for drug-like compounds using transcriptomics. PLoS Computational Biology, 2018, 14, e1006651.	3.2	51
25	Predicting oligomeric assemblies: N-mers a primer. Journal of Structural Biology, 2005, 150, 233-244.	2.8	46
26	Ensemble Modeling of Substrate Binding to Cytochromes P450:Â Analysis of Catalytic Differences between CYP1A Orthologsâ€,â€¡. Biochemistry, 2007, 46, 2640-2654.	2.5	45
27	Structural and Thermodynamic Approach to Peptide Immunogenicity. PLoS Computational Biology, 2008, 4, e1000231.	3.2	39
28	Modeling side-chains using molecular dynamics improve recognition of binding region in CAPRI targets. Proteins: Structure, Function and Bioinformatics, 2005, 60, 245-251.	2.6	38
29	FastContact: a free energy scoring tool for protein-protein complex structures. Nucleic Acids Research, 2007, 35, W556-W560.	14.5	35
30	Extensive Citrullination Promotes Immunogenicity of HSP90 through Protein Unfolding and Exposure of Cryptic Epitopes. Journal of Immunology, 2016, 197, 1926-1936.	0.8	32
31	Improving small molecule virtual screening strategies for the next generation of therapeutics. Current Opinion in Chemical Biology, 2018, 44, 87-92.	6.1	32
32	Crossâ€docking benchmark for automated pose and ranking prediction of ligand binding. Protein Science, 2020, 29, 298-305.	7.6	31
33	Performance of the first protein docking server ClusPro in CAPRI rounds 3-5. Proteins: Structure, Function and Bioinformatics, 2005, 60, 239-244.	2.6	30
34	Peroxidase activation of cytoglobin by anionic phospholipids: Mechanisms and consequences. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2016, 1861, 391-401.	2.4	30
35	Rational design and synthesis of 1,5-disubstituted tetrazoles as potent inhibitors of the MDM2-p53 interaction. European Journal of Medicinal Chemistry, 2017, 126, 384-407.	5.5	30
36	<scp>A</scp>nchor<scp>Q</scp>uery: <scp>R</scp>apid online virtual screening for smallâ€molecule proteinâ€“protein interaction inhibitors. Protein Science, 2018, 27, 229-232.	7.6	29

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37	A network-centric approach to drugging TNF-induced NF-Î¹B signaling. Nature Communications, 2019, 10, 860.	12.8	26
38	Tandem phosphorylation within an intrinsically disordered region regulates ACTN4 function. Science Signaling, 2015, 8, ra51.	3.6	25
39	Modeling the Assembly of the Multiple Domains of Î±-actinin-4 and Its Role in Actin Cross-linking. Biophysical Journal, 2013, 104, 705-715.	0.5	22
40	Discovery of a Potent Allosteric Kinase Modulator by Combining Computational and Synthetic Methods. Angewandte Chemie - International Edition, 2015, 54, 13933-13936.	13.8	22
41	Scoring a diverse set of high-quality docked conformations: A metascore based on electrostatic and desolvation interactions. Proteins: Structure, Function and Bioinformatics, 2006, 63, 868-877.	2.6	21
42	Optimal strategies for virtual screening of induced-fit and flexible target in the 2015 D3R Grand Challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 695-706.	2.9	20
43	Probing protein flexibility reveals a mechanism for selective promiscuity. ELife, 2017, 6, .	6.0	20
44	Choosing the Optimal Rigid Receptor for Docking and Scoring in the CSAR 2013/2014 Experiment. Journal of Chemical Information and Modeling, 2016, 56, 1004-1012.	5.4	19
45	Novel FOXM1 inhibitor identified via gene network analysis induces autophagic FOXM1 degradation to overcome chemoresistance of human cancer cells. Cell Death and Disease, 2021, 12, 704.	6.3	19
46	A resource of high-quality and versatile nanobodies for drug delivery. IScience, 2021, 24, 103014.	4.1	19
47	Experimentally based contact energies decode interactions responsible for proteinâ€“DNA affinity and the role of molecular waters at the binding interface. Nucleic Acids Research, 2009, 37, 4076-4088.	14.5	18
48	Continuum electrostatic analysis of preferred solvation sites around proteins in solution. , 2000, 38, 176-188.		17
49	Symmetry breaking during homodimeric assembly activates an E3 ubiquitin ligase. Scientific Reports, 2017, 7, 1789.	3.3	17
50	Tripeptide IRW Upregulates NAMPT Protein Levels in Cells and Obese C57BL/6J Mice. Journal of Agricultural and Food Chemistry, 2021, 69, 1555-1566.	5.2	16
51	The carboxyl tail of alpha-actinin-4 regulates its susceptibility to m-calpain and thus functions in cell migration and spreading. International Journal of Biochemistry and Cell Biology, 2013, 45, 1051-1063.	2.8	15
52	A Teach-Discover-Treat Application of ZincPharmer: An Online Interactive Pharmacophore Modeling and Virtual Screening Tool. PLoS ONE, 2015, 10, e0134697.	2.5	15
53	A specific inhibitor of ALDH1A3 regulates retinoic acid biosynthesis in glioma stem cells. Communications Biology, 2021, 4, 1420.	4.4	15
54	Optimal affinity ranking for automated virtual screening validated in prospective D3R grand challenges. Journal of Computer-Aided Molecular Design, 2018, 32, 287-297.	2.9	14

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55	SIMPLE estimate of the free energy change due to aliphatic mutations: Superior predictions based on first principles. Proteins: Structure, Function and Bioinformatics, 2007, 68, 850-862.	2.6	12
56	Consensus alignment server for reliable comparative modeling with distant templates. Nucleic Acids Research, 2004, 32, W50-W54.	14.5	10
57	Fluorescence Polarization Screening Assays for Small Molecule Allosteric Modulators of ABL Kinase Function. PLoS ONE, 2015, 10, e0133590.	2.5	10
58	A Discovery Strategy for Selective Inhibitors of câ€Src in Complex with the Focal Adhesion Kinase SH3/SH2â€binding Region. Chemical Biology and Drug Design, 2015, 86, 144-155.	3.2	10
59	Electrostatic hot spot on DNA-binding domains mediates phosphate desolvation and the pre-organization of specificity determinant side chains. Nucleic Acids Research, 2010, 38, 2134-2144.	14.5	9
60	Focal segmental glomerulosclerosis ACTN4 mutants binding to actin: regulation by phosphomimetic mutations. Scientific Reports, 2019, 9, 15517.	3.3	9
61	A heterotypic assembly mechanism regulates <scp>CHIP E3</scp> ligase activity. EMBO Journal, 2022, 41, .	7.8	9
62	Defining the Kv2.1â€“syntaxin molecular interaction identifies a first-in-class small molecule neuroprotectant. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 15696-15705.	7.1	8
63	Acidic groups docked to well defined wetted pockets at the core of the binding interface: A tale of scoring and missing protein interactions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2007, 69, 786-792.	2.6	7
64	Discovery of Non-peptide Small Molecule Allosteric Modulators of the Src-family Kinase, Hck. Frontiers in Chemistry, 2019, 7, 822.	3.6	6
65	Novel modulation factor quantifies the role of water molecules in protein interactions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3226-3234.	2.6	5
66	Indexing volumetric shapes with matching and packing. Knowledge and Information Systems, 2015, 43, 157-180.	3.2	5
67	A combined computational and experimental approach reveals the structure of a C/EBPÎ²â€“Spi1 interaction required for IL1B gene transcription. Journal of Biological Chemistry, 2018, 293, 19942-19956.	3.4	5
68	Focusing on shared subpockets â€“ new developments in fragment-based drug discovery. Expert Opinion on Drug Discovery, 2015, 10, 1179-1187.	5.0	4
69	Case series: Pyramidal cataracts, intact irides and nystagmus from three novel PAX6 mutations. American Journal of Ophthalmology Case Reports, 2018, 10, 172-179.	0.7	4
70	Transcription with a laser: Radiation-damage-free diffraction of RNA Polymerase II crystals. Methods, 2019, 159-160, 23-28.	3.8	4
71	Fragment oriented molecular shapes. Journal of Molecular Graphics and Modelling, 2016, 66, 143-154.	2.4	3
72	Quantitative Modeling of Currents from a Voltage Gated Ion Channel Undergoing Fast Inactivation. PLoS ONE, 2008, 3, e3342.	2.5	2

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73	OTME-20. Chitinase-3-like-1(CHI3L1) Protein Complexes Regulate the immunosuppressive Microenvironment in Glioblastoma. Neuro-Oncology Advances, 2021, 3, ii17-ii18.	0.7	0
74	On Modulating the Regulatory Role of Intrinsically Disordered Proteins Using Small Molecules. FASEB Journal, 2015, 29, 491.3.	0.5	0