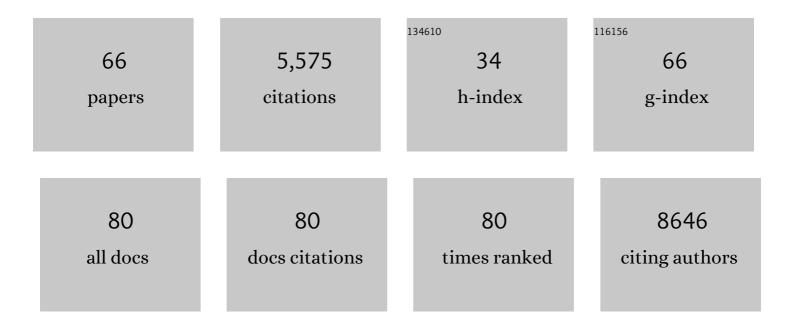
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542.	6.5	46
2	SARS-CoV-2 infects the human kidney and drives fibrosis in kidney organoids. Cell Stem Cell, 2022, 29, 217-231.e8.	5.2	146
3	Expanding the Repertoire of Lowâ€Molecularâ€Weight Pentafluorosulfanylâ€Substituted Scaffolds. ChemMedChem, 2022, 17, e202100641.	1.6	6
4	Discovery of SARS-CoV-2 main protease inhibitors using a synthesis-directed <i>de novo</i> design model. Chemical Communications, 2021, 57, 5909-5912.	2.2	30
5	Covalent flexible peptide docking in Rosetta. Chemical Science, 2021, 12, 10836-10847.	3.7	15
6	Tunable Methacrylamides for Covalent Ligand Directed Release Chemistry. Journal of the American Chemical Society, 2021, 143, 4979-4992.	6.6	41
7	Sulfopin is a covalent inhibitor of Pin1 that blocks Myc-driven tumors in vivo. Nature Chemical Biology, 2021, 17, 954-963.	3.9	73
8	Proteolysis Targeting Chimeras for BTK Efficiently Inhibit B-Cell Receptor Signaling and Can Overcome Ibrutinib Resistance in CLL Cells. Frontiers in Oncology, 2021, 11, 646971.	1.3	7
9	An automatic pipeline for the design of irreversible derivatives identifies a potent SARS-CoV-2 Mpro inhibitor. Cell Chemical Biology, 2021, 28, 1795-1806.e5.	2.5	50
10	A white-knuckle ride of open COVID drug discovery. Nature, 2021, 594, 330-332.	13.7	25
11	The rise of covalent proteolysis targeting chimeras. Current Opinion in Chemical Biology, 2021, 62, 24-33.	2.8	45
12	Electrophilic Natural Products as Drug Discovery Tools. Trends in Pharmacological Sciences, 2021, 42, 434-447.	4.0	13
13	Intracellular Protein–Drug Interactions Probed by Direct Mass Spectrometry of Cell Lysates. Angewandte Chemie - International Edition, 2021, 60, 19637-19642.	7.2	8
14	Cross-reactive antibodies against human coronaviruses and the animal coronavirome suggest diagnostics for future zoonotic spillovers. Science Immunology, 2021, 6, .	5.6	26
15	Intracellular Protein–Drug Interactions Probed by Direct Mass Spectrometry of Cell Lysates. Angewandte Chemie, 2021, 133, 19789-19794.	1.6	0
16	Targeting Pin1 renders pancreatic cancer eradicable by synergizing with immunochemotherapy. Cell, 2021, 184, 4753-4771.e27.	13.5	99
17	Covalent fragment screening. Annual Reports in Medicinal Chemistry, 2021, 56, 243-265.	0.5	2
18	Site-Specific Labeling of Endogenous Proteins Using CoLDR Chemistry. Journal of the American Chemical Society, 2021, 143, 20095-20108.	6.6	34

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19	PRosettaC: Rosetta Based Modeling of PROTAC Mediated Ternary Complexes. Journal of Chemical Information and Modeling, 2020, 60, 4894-4903.	2.5	110
20	Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease. Nature Communications, 2020, 11, 5047.	5.8	376
21	In crystallo-screening for discovery of human norovirus 3C-like protease inhibitors. Journal of Structural Biology: X, 2020, 4, 100031.	0.7	2
22	HSP40 proteins use class-specific regulation to drive HSP70 functional diversity. Nature, 2020, 587, 489-494.	13.7	140
23	Efficient Targeted Degradation via Reversible and Irreversible Covalent PROTACs. Journal of the American Chemical Society, 2020, 142, 11734-11742.	6.6	122
24	A Fast and Clean BTK Inhibitor. Journal of Medicinal Chemistry, 2020, 63, 5100-5101.	2.9	41
25	Identification of a potent and selective covalent Pin1 inhibitor. Nature Chemical Biology, 2020, 16, 979-987.	3.9	40
26	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	9.0	513
27	Hitting KRAS When It's Down. Journal of Medicinal Chemistry, 2020, 63, 6677-6678.	2.9	8
28	Crowdsourcing drug discovery for pandemics. Nature Chemistry, 2020, 12, 581-581.	6.6	88
29	Best Practices for Design and Characterization of Covalent Chemical Probes. Chemical Biology, 2020, , 69-99.	0.1	1
30	Structural basis for producing selective MAP2K7 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127546.	1.0	1
31	Overcoming insecticide resistance through computational inhibitor design. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 21012-21021.	3.3	31
32	Rapid Covalent-Probe Discovery by Electrophile-Fragment Screening. Journal of the American Chemical Society, 2019, 141, 8951-8968.	6.6	213
33	Phenotypic Screen Identifies JAK2 as a Major Regulator of FAT10 Expression. ACS Chemical Biology, 2019, 14, 2538-2545.	1.6	3
34	Covalent Docking Identifies a Potent and Selective MKK7 Inhibitor. Cell Chemical Biology, 2019, 26, 98-108.e5.	2.5	45
35	Novel K-Ras G12C Switch-II Covalent Binders Destabilize Ras and Accelerate Nucleotide Exchange. Journal of Chemical Information and Modeling, 2018, 58, 464-471.	2.5	45
36	Structural basis for chemokine recognition by a G protein–coupled receptor and implications for receptor activation. Science Signaling, 2017, 10, .	1.6	74

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37	Covalent Docking Predicts Substrates for Haloalkanoate Dehalogenase Superfamily Phosphatases. Biochemistry, 2015, 54, 528-537.	1.2	26
38	Virtual Screening for UDP-Galactopyranose Mutase Ligands Identifies a New Class of Antimycobacterial Agents. ACS Chemical Biology, 2015, 10, 2209-2218.	1.6	34
39	Covalent docking of large libraries for the discovery of chemical probes. Nature Chemical Biology, 2014, 10, 1066-1072.	3.9	225
40	Rationally designed macrocyclic peptides as synergistic agonists ofÂLPS-induced inflammatory response. Tetrahedron, 2014, 70, 7664-7668.	1.0	15
41	Prediction of Substrates for Glutathione Transferases by Covalent Docking. Journal of Chemical Information and Modeling, 2014, 54, 1687-1699.	2.5	20
42	An accurate binding interaction model in de novo computational protein design of interactions: If you build it, they will bind. Journal of Structural Biology, 2014, 185, 136-146.	1.3	12
43	Druggable protein–protein interactions – from hot spots to hot segments. Current Opinion in Chemical Biology, 2013, 17, 952-959.	2.8	199
44	Peptide docking and structure-based characterization of peptide binding: from knowledge to know-how. Current Opinion in Structural Biology, 2013, 23, 894-902.	2.6	85
45	Relacin, a Novel Antibacterial Agent Targeting the Stringent Response. PLoS Pathogens, 2012, 8, e1002925.	2.1	130
46	<i>In Silico</i> and <i>in Vitro</i> Elucidation of BH3 Binding Specificity toward Bcl-2. Biochemistry, 2012, 51, 5841-5850.	1.2	35
47	Modeling Peptide–Protein Interactions. Methods in Molecular Biology, 2011, 857, 375-398.	0.4	26
48	The Escherichia coli Extracellular Death Factor EDF Induces the Endoribonucleolytic Activities of the Toxins MazF and ChpBK. Molecular Cell, 2011, 41, 625-635.	4.5	86
49	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
50	Anchoring of bacterial effectors to host membranes through host-mediated lipidation by prenylation: a common paradigm. Trends in Microbiology, 2011, 19, 573-579.	3.5	31
51	Rosetta FlexPepDock web server—high resolution modeling of peptide–protein interactions. Nucleic Acids Research, 2011, 39, W249-W253.	6.5	351
52	Autophosphorylation Activates Dictyostelium Myosin II Heavy Chain Kinase A by Providing a Ligand for an Allosteric Binding Site in the α-Kinase Domain. Journal of Biological Chemistry, 2011, 286, 2607-2616.	1.6	22
53	Identification of a Novel Class of Farnesylation Targets by Structure-Based Modeling of Binding Specificity. PLoS Computational Biology, 2011, 7, e1002170.	1.5	58
54	Rosetta FlexPepDock ab-initio: Simultaneous Folding, Docking and Refinement of Peptides onto Their Receptors. PLoS ONE, 2011, 6, e18934.	1.1	259

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55	The Structural Basis of Peptide-Protein Binding Strategies. Structure, 2010, 18, 188-199.	1.6	370
56	On the use of structural templates for highâ€resolution docking. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1939-1949.	1.5	10
57	Sub-angstrom modeling of complexes between flexible peptides and globular proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2029-2040.	1.5	384
58	Can selfâ€inhibitory peptides be derived from the interfaces of globular protein–protein interactions?. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3140-3149.	1.5	146
59	Ubiquitination and Degradation of the Inhibitors of NF-ÂB. Cold Spring Harbor Perspectives in Biology, 2010, 2, a000166-a000166.	2.3	108
60	High-resolution Protein–Protein Docking. , 2010, , 209-235.		0
61	Allosteric Regulation of Glycogen Synthase Kinase 3β: A Theoretical Study. Biochemistry, 2010, 49, 10890-10901.	1.2	30
62	Fractured genes: a novel genomic arrangement involving new split inteins and a new homing endonuclease family. Nucleic Acids Research, 2009, 37, 2560-2573.	6.5	86
63	Funnel Hunting in a Rough Terrain: Learning and Discriminating Native Energy Funnels. Structure, 2008, 16, 269-279.	1.6	30
64	FunHunt: model selection based on energy landscape characteristics. Biochemical Society Transactions, 2008, 36, 1418-1421.	1.6	16
65	RosettaDock in CAPRI rounds 6–12. Proteins: Structure, Function and Bioinformatics, 2007, 69, 758-763.	1.5	26
66	Assessing the energy landscape of CAPRI targets by FunHunt. Proteins: Structure, Function and Bioinformatics, 2007, 69, 809-815.	1.5	15