Pierre Tuffery

List of Publications by Citations

75 papers	4,570 citations	27 h-index	67 g-index
81 ext. papers	5,479 ext. citations	9.7 avg, IF	5.64 L-index

#	Paper	IF	Citations
75	Fpocket: an open source platform for ligand pocket detection. *BMC Bioinformatics*, **2009**, 10, 168	3.6	680
74	PEP-FOLD: an updated de novo structure prediction server for both linear and disulfide bonded cyclic peptides. *Nucleic Acids Research*, **2012**, 40, W288-93	20.1	400
73	PEP-FOLD3: faster de novo structure prediction for linear peptides in solution and in complex. *Nucleic Acids Research*, **2016**, 44, W449-54	20.1	399
72	Improved PEP-FOLD Approach for Peptide and Miniprotein Structure Prediction. *Journal of Chemical Theory and Computation*, **2014**, 10, 4745-58	6.4	373
71	PEP-FOLD: an online resource for de novo peptide structure prediction. *Nucleic Acids Research*, **2009**, 37, W498-503	20.1	279
70	Mobyle: a new full web bioinformatics framework. *Bioinformatics*, **2009**, 25, 3005-11	7.2	238
69	A model for the photosystem II reaction center core including the structure of the primary donor P680. *Biochemistry*, **1996**, 35, 14486-502	3.2	201
68	fpocket: online tools for protein ensemble pocket detection and tracking. *Nucleic Acids Research*, **2010**, 38, W582-9	20.1	170
67	Frog2: Efficient 3D conformation ensemble generator for small compounds. *Nucleic Acids Research*, **2010**, 38, W622-7	20.1	161
66	A fast method for large-scale de novo peptide and miniprotein structure prediction. *Journal of Computational Chemistry*, **2010**, 31, 726-38	3.5	140
65	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. *Chemical Society Reviews*, **2014**, 43, 4871-93	58.5	118
64	MTiOpenScreen: a web server for structure-based virtual screening. *Nucleic Acids Research*, **2015**, 43, W448-54	20.1	101
63	FAF-Drugs: free ADME/tox filtering of compound collections. *Nucleic Acids Research*, **2006**, 34, W738-44	20.1	96
62	Isotype modulates epitope specificity, affinity, and antiviral activities of anti-HIV-1 human broadly neutralizing 2F5 antibody. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 12680-5	11.5	90
61	The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. *Bioinformatics*, **2011**, 27, 2018-20	7.2	70
60	Interfering peptides targeting protein-protein interactions: the next generation of drugs?. *Drug Discovery Today*, **2018**, 23, 272-285	8.8	69
59	Missense mutations in SLC26A8, encoding a sperm-specific activator of CFTR, are associated with human asthenozoospermia. *American Journal of Human Genetics*, **2013**, 92, 760-6	11	68

58	SABBAC: online Structural Alphabet-based protein BackBone reconstruction from Alpha-Carbon trace. *Nucleic Acids Research*, **2006**, 34, W147-51	20.1	67
57	Flexibility and binding affinity in protein-ligand, protein-protein and multi-component protein interactions: limitations of current computational approaches. *Journal of the Royal Society Interface* , **2012**, 9, 20-33	4.1	64
56	PEP-SiteFinder: a tool for the blind identification of peptide binding sites on protein surfaces. *Nucleic Acids Research*, **2014**, 42, W221-6	20.1	62
55	The pepATTRACT web server for blind, large-scale peptide-protein docking. *Nucleic Acids Research*, **2017**, 45, W361-W364	20.1	59
54	InterEvDock: a docking server to predict the structure of protein-protein interactions using evolutionary information. *Nucleic Acids Research*, **2016**, 44, W542-9	20.1	52
53	Protease profiling of liver fibrosis reveals the ADAM metallopeptidase with thrombospondin type 1 motif, 1 as a central activator of transforming growth factor beta. *Hepatology*, **2011**, 54, 2173-84	11.2	51
52	PCE: web tools to compute protein continuum electrostatics. *Nucleic Acids Research*, **2005**, 33, W372-5	20.1	49
51	SA-Search: a web tool for protein structure mining based on a Structural Alphabet. *Nucleic Acids Research*, **2004**, 32, W545-8	20.1	39
50	A triple-mutated allele of granzyme B incapable of inducing apoptosis. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 2562-7	11.5	36
49	Enhanced protein fold recognition using a structural alphabet. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 129-37	4.2	32
48	InterEvDock2: an expanded server for protein docking using evolutionary and biological information from homology models and multimeric inputs. *Nucleic Acids Research*, **2018**, 46, W408-W416	20.1	27
47	Improved greedy algorithm for protein structure reconstruction. *Journal of Computational Chemistry*, **2005**, 26, 506-13	3.5	27
46	DaReUS-Loop: accurate loop modeling using fragments from remote or unrelated proteins. *Scientific Reports*, **2018**, 8, 13673	4.9	21
45	Dependency between consecutive local conformations helps assemble protein structures from secondary structures using Go potential and greedy algorithm. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 732-40	4.2	20
44	wwLigCSRre: a 3D ligand-based server for hit identification and optimization. *Nucleic Acids Research* , **2009**, 37, W504-9	20.1	19
43	Fast protein fragment similarity scoring using a Binet-Cauchy kernel. *Bioinformatics*, **2014**, 30, 784-91	7.2	17
42	Ligand scaffold hopping combining 3D maximal substructure search and molecular similarity. *BMC Bioinformatics*, **2009**, 10, 245	3.6	17
41	Lys53 of ribosomal protein L36AL and the CCA end of a tRNA at the P/E hybrid site are in close proximity on the human ribosome. *ChemBioChem*, **2012**, 13, 1791-7	3.8	16

40	Progress with peptide scanning to study structure-activity relationships: the implications for drug discovery. *Expert Opinion on Drug Discovery*, **2016**, 11, 771-84	6.2	16
39	DaReUS-Loop: a web server to model multiple loops in homology models. *Nucleic Acids Research*, **2019**, 47, W423-W428	20.1	15
38	Packing and recognition of protein structural elements: a new approach applied to the 4-helix bundle of myohemerythrin. *Proteins: Structure, Function and Bioinformatics*, **1993**, 15, 413-25	4.2	15
37	Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets. *Oncotarget*, **2018**, 9, 32346-32361	3.3	15
36	Probing the quality control mechanism of the twin-arginine translocase with folding variants of a -designed heme protein. *Journal of Biological Chemistry*, **2018**, 293, 6672-6681	5.4	14
35	BactPepDB: a database of predicted peptides from a exhaustive survey of complete prokaryote genomes. *Database: the Journal of Biological Databases and Curation*, **2014**, 2014,	5	13
34	Detecting protein candidate fragments using a structural alphabet profile comparison approach. *PLoS ONE*, **2013**, 8, e80493	3.7	12
33	The CCA-end of P-tRNA Contacts Both the Human RPL36AL and the A-site Bound Translation Termination Factor eRF1 at the Peptidyl Transferase Center of the Human 80S Ribosome. *The Open Biochemistry Journal*, **2014**, 8, 52-67	0.9	11
32	A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	10
31	Accessing external innovation in drug discovery and development. *Expert Opinion on Drug Discovery* , **2015**, 10, 579-89	6.2	10
30	aes, the gene encoding the esterase B in Escherichia coli, is a powerful phylogenetic marker of the species. *BMC Microbiology*, **2009**, 9, 273	4.5	9
29	Cloning and modeling of CD8 beta in the amphibian ambystoma Mexicanum. Evolutionary conserved structures for interactions with major histocompatibility complex (MHC) class I molecules. *Gene*, **2002**, 288, 95-102	3.8	9
28	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo Community). *F1000Research*, **2020**, 9,	3.6	9
27	A critical assessment of hidden markov model sub-optimal sampling strategies applied to the generation of peptide 3D models. *Journal of Computational Chemistry*, **2016**, 37, 2006-16	3.5	8
26	In silico characterization of the interaction between LSKL peptide, a LAP-TGF-beta derived peptide, and ADAMTS1. *Computational Biology and Chemistry*, **2016**, 61, 155-61	3.6	7
25	HHalign-Kbest: exploring sub-optimal alignments for remote homology comparative modeling. *Bioinformatics*, **2015**, 31, 3850-2	7.2	7
24	Coarse-grained and atomic resolution biomolecular docking with the ATTRACT approach. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 1018-1028	4.2	6
23	In silico structural characterization of protein targets for drug development against Trypanosoma cruzi. *Journal of Molecular Modeling*, **2016**, 22, 244	2	6

22	PMG: online generation of high-quality molecular pictures and storyboarded animations. *Nucleic Acids Research*, **2007**, 35, W483-8	20.1	5
21	De novo peptide structure prediction: an overview. *Methods in Molecular Biology*, **2015**, 1268, 1-13	1.4	5
20	InterEvDock3: a combined template-based and free docking server with increased performance through explicit modeling of complex homologs and integration of covariation-based contact maps. *Nucleic Acids Research*, **2021**, 49, W277-W284	20.1	5
19	BCSearch: fast structural fragment mining over large collections of protein structures. *Nucleic Acids Research*, **2015**, 43, W378-82	20.1	4
18	PPG: online generation of protein pictures and animations. *Nucleic Acids Research*, **2005**, 33, W320-3	20.1	4
17	Bioinformatics Applications Discovery and Composition with the Mobyle Suite and MobyleNet. *Lecture Notes in Computer Science*, **2012**, 11-22	0.9	4
16	PatchSearch: a web server for off-target protein identification. *Nucleic Acids Research*, **2019**, 47, W365-W372	20.1	3
15	Probing Protein Interaction Networks by Combining MS-Based Proteomics and Structural Data Integration. *Journal of Proteome Research*, **2020**, 19, 2807-2820	5.6	3
14	A Computational Methodology to Overcome the Challenges Associated With the Search for Specific Enzyme Targets to Develop Drugs Against. *Bioinformatics and Biology Insights*, **2017**, 11, 1177932217712471	5.3	3
13	A Functional Role for the Monomethylated Gln-51 and Lys-53 Residues of the 49GGQTK53 Motif of eL42 from Human 80S Ribosomes. *The Open Biochemistry Journal*, **2017**, 11, 8-26	0.9	3
12	Bi-Functional Peptides as a New Therapeutic Tool for Hepatocellular Carcinoma. *Pharmaceutics*, **2021**, 13,	6.4	3
11	Identification of peptides interfering with the LRRK2/PP1 interaction. *PLoS ONE*, **2020**, 15, e0237110	3.7	3
10	Proteo3Dnet: a web server for the integration of structural information with interactomics data. *Nucleic Acids Research*, **2021**, 49, W567-W572	20.1	2
9	The CH1 domain of mucosal gp41 IgA contributes to antibody specificity and antiviral functions in HIV-1 highly exposed Sero-Negative individuals. *PLoS Pathogens*, **2020**, 16, e1009103	7.6	1
8	Semantic Map for Structural Bioinformatics: Enhanced Service Discovery Based on High Level Concept Ontology. *Lecture Notes in Computer Science*, **2012**, 57-70	0.9	1
7	Evolutionary conserved protein motifs drive attachment of the plant nucleoskeleton at nuclear pores		1
6	Isolation of Primary Hepatocytes for Testing Tumor Penetrating Peptides. *Methods in Molecular Biology*, **2022**, 2383, 413-427	1.4	0
5	Modelling of transmembrane helix bundles. *Molecular Engineering*, **1995**, 5, 1-9		

4	Modelling of Transmembrane Helix Bundles. *Jerusalem Symposia on Quantum Chemistry and Biochemistry*, **1995**, 1-9	
3	Peptide Suboptimal Conformation Sampling for the Prediction of Protein-Peptide Interactions. *Methods in Molecular Biology*, **2017**, 1561, 21-34	1.4
2	The search of sequence variants using a constrained protein evolution simulation approach. *Computational and Structural Biotechnology Journal*, **2020**, 18, 1790-1799	6.8
1	Dynamics of Amyloid Formation from Simplified Representation to Atomistic Simulations.. *Methods in Molecular Biology*, **2022**, 2405, 95-113	1.4