

Vincent Zoete

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110
papers

11,536
citations

33
h-index

107
g-index

118
ext. papers

15,784
ext. citations

8.2
avg, IF

7.12
L-index

#	Paper	IF	Citations
110	SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. <i>Scientific Reports</i> , 2017 , 7, 42717	4.9	3362
109	SwissParam: a fast force field generation tool for small organic molecules. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2359-68	3.5	1025
108	SwissDock, a protein-small molecule docking web service based on EADock DSS. <i>Nucleic Acids Research</i> , 2011 , 39, W270-7	20.1	984
107	SwissTargetPrediction: updated data and new features for efficient prediction of protein targets of small molecules. <i>Nucleic Acids Research</i> , 2019 , 47, W357-W364	20.1	631
106	A BOILED-Egg To Predict Gastrointestinal Absorption and Brain Penetration of Small Molecules. <i>ChemMedChem</i> , 2016 , 11, 1117-21	3.7	591
105	SwissTargetPrediction: a web server for target prediction of bioactive small molecules. <i>Nucleic Acids Research</i> , 2014 , 42, W32-8	20.1	557
104	Exome sequencing identifies recurrent somatic MAP2K1 and MAP2K2 mutations in melanoma. <i>Nature Genetics</i> , 2011 , 44, 133-9	36.3	313
103	iLOGP: a simple, robust, and efficient description of n-octanol/water partition coefficient for drug design using the GB/SA approach. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 3284-301	6.1	294
102	Fast docking using the CHARMM force field with EADock DSS. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2149-59	3.5	269
101	Genomic analysis identifies new drivers and progression pathways in skin basal cell carcinoma. <i>Nature Genetics</i> , 2016 , 48, 398-406	36.3	242
100	Personalized cancer vaccine effectively mobilizes antitumor T cell immunity in ovarian cancer. <i>Science Translational Medicine</i> , 2018 , 10,	17.5	205
99	Shaping the interaction landscape of bioactive molecules. <i>Bioinformatics</i> , 2013 , 29, 3073-9	7.2	185
98	Defining and searching for structural motifs using DeepView/Swiss-PdbViewer. <i>BMC Bioinformatics</i> , 2012 , 13, 173	3.6	185
97	Challenges in the Discovery of Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2015 , 58, 9421-37	8.3	161
96	Evidence for a TCR affinity threshold delimiting maximal CD8 T cell function. <i>Journal of Immunology</i> , 2010 , 184, 4936-46	5.3	148
95	EADock: docking of small molecules into protein active sites with a multiobjective evolutionary optimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 67, 1010-25	4.2	131
94	Rational design of 4-aryl-1,2,3-triazoles for indoleamine 2,3-dioxygenase 1 inhibition. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 5270-90	8.3	129

93	SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1399-404	6.1	129
92	Rational design of indoleamine 2,3-dioxygenase inhibitors. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 1172-89	5.8	126
91	Docking, virtual high throughput screening and in silico fragment-based drug design. <i>Journal of Cellular and Molecular Medicine</i> , 2009 , 13, 238-48	5.6	103
90	Comparison between computational alanine scanning and per-residue binding free energy decomposition for protein-protein association using MM-GBSA: application to the TCR-p-MHC complex. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 67, 1026-47	4.2	98
89	Interplay between T cell receptor binding kinetics and the level of cognate peptide presented by major histocompatibility complexes governs CD8+ T cell responsiveness. <i>Journal of Biological Chemistry</i> , 2012 , 287, 23068-78	5.4	86
88	Sensitive and frequent identification of high avidity neo-epitope-specific CD8 T cells in immunotherapy-naïve ovarian cancer. <i>Nature Communications</i> , 2018 , 9, 1092	17.4	82
87	SwissBioisostere: a database of molecular replacements for ligand design. <i>Nucleic Acids Research</i> , 2013 , 41, D1137-43	20.1	75
86	SwissSidechain: a molecular and structural database of non-natural sidechains. <i>Nucleic Acids Research</i> , 2013 , 41, D327-32	20.1	74
85	Structure-function analyses point to a polynucleotide-accommodating groove essential for APOBEC3A restriction activities. <i>Journal of Virology</i> , 2011 , 85, 1765-76	6.6	63
84	Detailed analysis and follow-up studies of a high-throughput screening for indoleamine 2,3-dioxygenase 1 (IDO1) inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2014 , 84, 284-301	6.8	56
83	Toward on-the-fly quantum mechanical/molecular mechanical (QM/MM) docking: development and benchmark of a scoring function. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 3137-52	6.1	51
82	Blind docking of 260 protein-ligand complexes with EADock 2.0. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2021-30	3.5	46
81	Biallelic variants in KIF14 cause intellectual disability with microcephaly. <i>European Journal of Human Genetics</i> , 2018 , 26, 330-339	5.3	37
80	How T cell receptors interact with peptide-MHCs: a multiple steered molecular dynamics study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 3007-24	4.2	36
79	Sequence determinants of a microtubule tip localization signal (MtLS). <i>Journal of Biological Chemistry</i> , 2012 , 287, 28227-42	5.4	36
78	On-the-Fly QM/MM Docking with Attracting Cavities. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 73-84	6.1	33
77	Inhibition Mechanisms of Indoleamine 2,3-Dioxygenase 1 (IDO1). <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 8784-8795	8.3	33
76	Distinct sets of alphabeta TCRs confer similar recognition of tumor antigen NY-ESO-1157-165 by interacting with its central Met/Trp residues. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 15010-5	11.5	33

75	The peroxisomal enzyme L-PBE is required to prevent the dietary toxicity of medium-chain fatty acids. <i>Cell Reports</i> , 2013 , 5, 248-58	10.6	32
74	RNA pentaloop structures as effective targets of regulators belonging to the RsmA/CsrA protein family. <i>RNA Biology</i> , 2013 , 10, 1031-41	4.8	32
73	Combined simulation and mutagenesis analyses reveal the involvement of key residues for peroxisome proliferator-activated receptor alpha helix 12 dynamic behavior. <i>Journal of Biological Chemistry</i> , 2007 , 282, 9666-9677	5.4	31
72	Drug Design Workshop: A Web-Based Educational Tool To Introduce Computer-Aided Drug Design to the General Public. <i>Journal of Chemical Education</i> , 2017 , 94, 335-344	2.4	30
71	Mutant and histological heterogeneity define metabolic subtypes of hepatoblastoma. <i>EMBO Molecular Medicine</i> , 2017 , 9, 1589-1604	12	28
70	Attracting cavities for docking. Replacing the rough energy landscape of the protein by a smooth attracting landscape. <i>Journal of Computational Chemistry</i> , 2016 , 37, 437-47	3.5	27
69	Application of the SwissDrugDesign Online Resources in Virtual Screening. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	25
68	Lung adenocarcinoma with BRAF G469L mutation refractory to vemurafenib. <i>Lung Cancer</i> , 2013 , 82, 365-79	5.9	25
67	Use of the FACTS solvation model for protein-ligand docking calculations. Application to EADock. <i>Journal of Molecular Recognition</i> , 2010 , 23, 457-61	2.6	25
66	Cathepsin S Regulates Antigen Processing and T Cell Activity in Non-Hodgkin Lymphoma. <i>Cancer Cell</i> , 2020 , 37, 674-689.e12	24.3	23
65	1,2,3-Triazoles as inhibitors of indoleamine 2,3-dioxygenase 2 (IDO2). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016 , 26, 4330-3	2.9	23
64	The caveolin-binding motif of the pathogen-related yeast protein Pry1, a member of the CAP protein superfamily, is required for in vivo export of cholesteryl acetate. <i>Journal of Lipid Research</i> , 2014 , 55, 883-94	6.3	23
63	A dramatic lung cancer course in a patient with a rare EGFR germline mutation exon 21 V843I: Is EGFR TKI resistance predictable?. <i>Lung Cancer</i> , 2013 , 80, 81-4	5.9	23
62	In vitro biotransformation of imatinib by the tumor expressed CYP1A1 and CYP1B1. <i>Biopharmaceutics and Drug Disposition</i> , 2008 , 29, 103-18	1.7	22
61	Pharmacological disruption of the Notch transcription factor complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 16292-16301	11.5	21
60	Design of short peptides to block BTLA/HVEM interactions for promoting anticancer T-cell responses. <i>PLoS ONE</i> , 2017 , 12, e0179201	3.7	21
59	T cell receptor alpha variable 12-2 bias in the immunodominant response to Yellow fever virus. <i>European Journal of Immunology</i> , 2018 , 48, 258-272	6.1	21
58	Expanding molecular modeling and design tools to non-natural sidechains. <i>Journal of Computational Chemistry</i> , 2012 , 33, 1525-35	3.5	21

57	Monoubiquitination and activity of the paracaspase MALT1 requires glutamate 549 in the dimerization interface. <i>PLoS ONE</i> , 2013 , 8, e72051	3.7	21
56	Asymmetric synthesis of pochonin E and F, revision of their proposed structure, and their conversion to potent Hsp90 inhibitors. <i>Chemistry - A European Journal</i> , 2012 , 18, 8978-86	4.8	20
55	Protein pocket and ligand shape comparison and its application in virtual screening. <i>Journal of Computer-Aided Molecular Design</i> , 2013 , 27, 511-24	4.2	20
54	Biallelic variants in LINGO1 are associated with autosomal recessive intellectual disability, microcephaly, speech and motor delay. <i>Genetics in Medicine</i> , 2018 , 20, 778-784	8.1	16
53	Identification of human IKK-2 inhibitors of natural origin (Part II): in Silico prediction of IKK-2 inhibitors in natural extracts with known anti-inflammatory activity. <i>European Journal of Medicinal Chemistry</i> , 2011 , 46, 6098-103	6.8	16
52	Potency of inhibition of human DNA topoisomerase I by flavones assessed through physicochemical parameters. <i>Free Radical Biology and Medicine</i> , 2011 , 51, 1406-10	7.8	16
51	The impact of structural bioinformatics tools and resources on SARS-CoV-2 research and therapeutic strategies. <i>Briefings in Bioinformatics</i> , 2021 , 22, 742-768	13.4	16
50	Pan-SRC kinase inhibition blocks B-cell receptor oncogenic signaling in non-Hodgkin lymphoma. <i>Blood</i> , 2018 , 131, 2345-2356	2.2	15
49	Design and Validation of a Novel Generic Platform for the Production of Tetravalent IgG1-like Bispecific Antibodies. <i>Journal of Immunology</i> , 2016 , 196, 3199-211	5.3	15
48	A WXW motif is required for the anticancer activity of the TAT-RasGAP317-326 peptide. <i>Journal of Biological Chemistry</i> , 2014 , 289, 23701-11	5.4	15
47	TCRep 3D: an automated in silico approach to study the structural properties of TCR repertoires. <i>PLoS ONE</i> , 2011 , 6, e26301	3.7	15
46	The Binding Mode of N-Hydroxyamidines to Indoleamine 2,3-Dioxygenase 1 (IDO1). <i>Biochemistry</i> , 2017 , 56, 4323-4325	3.2	14
45	Docking to heme proteins. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2305-15	3.5	14
44	Herpes simplex encephalitis in adult patients with MASP-2 deficiency. <i>PLoS Pathogens</i> , 2019 , 15, e1008168	6.8	14
43	Distinct OGT-Binding Sites Promote HCF-1 Cleavage. <i>PLoS ONE</i> , 2015 , 10, e0136636	3.7	13
42	Proteolysis of HCF-1 by Ser/Thr glycosylation-incompetent O-GlcNAc transferase:UDP-GlcNAc complexes. <i>Genes and Development</i> , 2016 , 30, 960-72	12.6	13
41	Fifteen years SIB Swiss Institute of Bioinformatics: life science databases, tools and support. <i>Nucleic Acids Research</i> , 2014 , 42, W436-41	20.1	12
40	Rational Design, Synthesis, and Pharmacological Characterization of Novel Ghrelin Receptor Inverse Agonists as Potential Treatment against Obesity-Related Metabolic Diseases. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 11039-11060	8.3	12

39	T-cell repertoire analysis and metrics of diversity and clonality. <i>Current Opinion in Biotechnology</i> , 2020 , 65, 284-295	11.4	11
38	Extracellular Domain In-Frame Deletions Are Therapeutically Targetable Genomic Alterations That Function as Oncogenic Drivers in Cholangiocarcinoma. <i>Cancer Discovery</i> , 2021 , 11, 2488-2505	24.4	11
37	Durable Suppression of Acquired MEK Inhibitor Resistance in Cancer by Sequestering MEK from ERK and Promoting Antitumor T-cell Immunity. <i>Cancer Discovery</i> , 2021 , 11, 714-735	24.4	11
36	Disulfide-Linked Peptides for Blocking BTLA/HVEM Binding. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	10
35	The CAP1/Prss8 catalytic triad is not involved in PAR2 activation and protease nexin-1 (PN-1) inhibition. <i>FASEB Journal</i> , 2014 , 28, 4792-805	0.9	10
34	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo Community). <i>F1000Research</i> , 2020 , 9,	3.6	9
33	Sensitive identification of neoantigens and cognate TCRs in human solid tumors. <i>Nature Biotechnology</i> , 2021 ,	44.5	9
32	Biallelic variants in FBXL3 cause intellectual disability, delayed motor development and short stature. <i>Human Molecular Genetics</i> , 2019 , 28, 972-979	5.6	9
31	Bi-allelic Variants in DYNC112 Cause Syndromic Microcephaly with Intellectual Disability, Cerebral Malformations, and Dysmorphic Facial Features. <i>American Journal of Human Genetics</i> , 2019 , 104, 1073-1087	11.1	8
30	Protein homology reveals new targets for bioactive small molecules. <i>Bioinformatics</i> , 2015 , 31, 2721-7	7.2	8
29	T-cell receptors binding orientation over peptide/MHC class I is driven by long-range interactions. <i>PLoS ONE</i> , 2012 , 7, e51943	3.7	8
28	Mutations in the palm domain disrupt modulation of acid-sensing ion channel 1a currents by neuropeptides. <i>Scientific Reports</i> , 2019 , 9, 2599	4.9	8
27	4-epi-Isogomine derivatives as pharmacological chaperones for the treatment of lysosomal diseases linked to β -galactosidase mutations: Improved synthesis and biological investigations. <i>Bioorganic and Medicinal Chemistry</i> , 2018 , 26, 5462-5469	3.4	8
26	Debio 0617B Inhibits Growth of STAT3-Driven Solid Tumors through Combined Inhibition of JAK, SRC, and Class III/V Receptor Tyrosine Kinases. <i>Molecular Cancer Therapeutics</i> , 2016 , 15, 2334-2343	6.1	7
25	Synthesis and in vitro evaluation of a novel radioligand for α _v β 3 integrin receptor imaging: [18F]FPPA-c(RGDfK). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013 , 23, 6068-72	2.9	7
24	Deciphering the Mechanisms of Improved Immunogenicity of Hypochlorous Acid-Treated Antigens in Anti-Cancer Dendritic Cell-Based Vaccines. <i>Vaccines</i> , 2020 , 8,	5.3	6
23	The T-Cell Receptor Can Bind to the Peptide-Bound Major Histocompatibility Complex and Uncomplexed β 2-Microglobulin through Distinct Binding Sites. <i>Biochemistry</i> , 2017 , 56, 3945-3961	3.2	6
22	Physicochemical properties of exogenous molecules correlated with their biological efficacy as protectors against carcinogenesis and inflammation. <i>International Reviews in Physical Chemistry</i> , 2013 , 32, 393-434	7	5

21	Going Beyond the Sequences: TCR Binding Patterns at the Service of Cancer Detection. <i>Cancer Research</i> , 2019 , 79, 1299-1301	10.1	4
20	Analysis of Secondary Structure Biases in Naturally Presented HLA-I Ligands. <i>Frontiers in Immunology</i> , 2019 , 10, 2731	8.4	4
19	Swiss-PO: a new tool to analyze the impact of mutations on protein three-dimensional structures for precision oncology. <i>Npj Precision Oncology</i> , 2021 , 5, 19	9.8	4
18	Azole-Based Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 2205-2227	8.3	4
17	VEGFR-2 redirected CAR-T cells are functionally impaired by soluble VEGF-A competition for receptor binding 2021 , 9,		4
16	Educational Tools to Introduce Computer-Aided Drug Design to Students and to the Public at Large. <i>Chimia</i> , 2018 , 72, 55-61	1.3	3
15	Recurrent structural motifs in non-homologous protein structures. <i>International Journal of Molecular Sciences</i> , 2013 , 14, 7795-814	6.3	3
14	Prediction of cross-recognition of peptide-HLA A2 by Melan-A-specific cytotoxic T lymphocytes using three-dimensional quantitative structure-activity relationships. <i>PLoS ONE</i> , 2013 , 8, e65590	3.7	3
13	Myeloid antigen-presenting cell niches sustain antitumor T cells and license PD-1 blockade via CD28 costimulation. <i>Cancer Cell</i> , 2021 ,	24.3	3
12	Electron affinity of tricyclic, bicyclic, and monocyclic compounds containing cyanoenones correlates with their potency as inducers of a cytoprotective enzyme. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016 , 26, 4345-9	2.9	2
11	SwissBioisostere 2021: updated structural, bioactivity and physicochemical data delivered by a reshaped web interface. <i>Nucleic Acids Research</i> , 2021 ,	20.1	2
10	Computer-Aided Drug Design for Cancer Therapy 2021 , 386-401		2
9	The conserved threonine-rich region of the HCF-1 repeat activates promiscuous OGT:UDP-GlcNAc glycosylation and proteolysis activities. <i>Journal of Biological Chemistry</i> , 2018 , 293, 17754-17768	5.4	2
8	Inhibitors of the Kynurenine Pathway. <i>Topics in Medicinal Chemistry</i> , 2017 , 371-371	0.4	1
7	Probing the Conformational Dynamics of Affinity-Enhanced T Cell Receptor Variants upon Binding the Peptide-Bound Major Histocompatibility Complex by Hydrogen/Deuterium Exchange Mass Spectrometry. <i>Biochemistry</i> , 2021 , 60, 859-872	3.2	1
6	Structural Prediction of Peptide-MHC Binding Modes.. <i>Methods in Molecular Biology</i> , 2022 , 2405, 245-282	1.4	1
5	Trametinib Induces the Stabilization of a Dual p.Gly48Leu- and p.Cys172Gly-Mutated Uveal Melanoma. The Role of Molecular Modelling in Personalized Oncology. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	0
4	A roadmap for driving CAR T cells toward the oncogenic immunopeptidome.. <i>Cancer Cell</i> , 2022 , 40, 20-22	24.3	0

- 3 Structure and Plasticity of Indoleamine 2,3-Dioxygenase 1 (IDO1).. *Journal of Medicinal Chemistry*, **2021**, 64, 17690-17705 8.3 o
- 2 Identification of a superagonist variant of the immunodominant Yellow fever virus epitope NS4b by combinatorial peptide library screening. *Molecular Immunology*, **2020**, 125, 43-50 4.3
- 1 Strong Enrichment of Aromatic and Sulfur-Containing Residues in Ligand-Protein Binding Sites. *Journal of Chemical Information and Modeling*, **2019**, 59, 4921-4928 6.1