

Vincent Zoete

List of Publications by Year in descending order

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Version: 2024-02-01

115
papers

20,961
citations

81743

39
h-index

23472

111
g-index

118
all docs

118
docs citations

118
times ranked

24203
citing authors

#	ARTICLE	IF	CITATIONS
1	SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. <i>Scientific Reports</i> , 2017, 7, 42717.	1.6	7,635
2	SwissTargetPrediction: updated data and new features for efficient prediction of protein targets of small molecules. <i>Nucleic Acids Research</i> , 2019, 47, W357-W364.	6.5	1,634
3	SwissParam: A fast force field generation tool for small organic molecules. <i>Journal of Computational Chemistry</i> , 2011, 32, 2359-2368.	1.5	1,485
4	SwissDock, a protein-small molecule docking web service based on EADock DSS. <i>Nucleic Acids Research</i> , 2011, 39, W270-W277.	6.5	1,396
5	A BOILEDâ€Egg To Predict Gastrointestinal Absorption and Brain Penetration of Small Molecules. <i>ChemMedChem</i> , 2016, 11, 1117-1121.	1.6	1,249
6	SwissTargetPrediction: a web server for target prediction of bioactive small molecules. <i>Nucleic Acids Research</i> , 2014, 42, W32-W38.	6.5	977
7	iLOGP: A Simple, Robust, and Efficient Description of <i>n</i> -Octanol/Water Partition Coefficient for Drug Design Using the GB/SA Approach. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 3284-3301.	2.5	560
8	Fast docking using the CHARMM force field with EADock DSS. <i>Journal of Computational Chemistry</i> , 2011, 32, 2149-2159.	1.5	384
9	Genomic analysis identifies new drivers and progression pathways in skin basal cell carcinoma. <i>Nature Genetics</i> , 2016, 48, 398-406.	9.4	370
10	Exome sequencing identifies recurrent somatic MAP2K1 and MAP2K2 mutations in melanoma. <i>Nature Genetics</i> , 2012, 44, 133-139.	9.4	369
11	Shaping the interaction landscape of bioactive molecules. <i>Bioinformatics</i> , 2013, 29, 3073-3079.	1.8	327
12	Personalized cancer vaccine effectively mobilizes antitumor T cell immunity in ovarian cancer. <i>Science Translational Medicine</i> , 2018, 10, .	5.8	326
13	Defining and searching for structural motifs using DeepView/Swiss-PdbViewer. <i>BMC Bioinformatics</i> , 2012, 13, 173.	1.2	260
14	SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1399-1404.	2.5	229
15	Evidence for a TCR Affinity Threshold Delimiting Maximal CD8 T Cell Function. <i>Journal of Immunology</i> , 2010, 184, 4936-4946.	0.4	196
16	Challenges in the Discovery of Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 9421-9437.	2.9	179
17	EADock: Docking of small molecules into protein active sites with a multiobjective evolutionary optimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 1010-1025.	1.5	171
18	Rational Design of 4-Aryl-1,2,3-Triazoles for Indoleamine 2,3-Dioxygenase 1 Inhibition. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 5270-5290.	2.9	153

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19	Rational Design of Indoleamine 2,3-Dioxygenase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 1172-1189.	2.9	146
20	Docking, virtual high throughput screening and <i>in silico</i> fragment-based drug design. <i>Journal of Cellular and Molecular Medicine</i> , 2009, 13, 238-248.	1.6	140
21	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.	5.8	122
22	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, 23068-23078.	1.6	121
23	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, 1026-1047.	1.5	110
24	SwissBioisostere: a database of molecular replacements for ligand design. <i>Nucleic Acids Research</i> , 2013, 41, D1137-D1143.	6.5	101
25	SwissSidechain: a molecular and structural database of non-natural sidechains. <i>Nucleic Acids Research</i> , 2012, 41, D327-D332.	6.5	100
26	T-cell repertoire analysis and metrics of diversity and clonality. <i>Current Opinion in Biotechnology</i> , 2020, 65, 284-295.	3.3	79
27	Structure-Function Analyses Point to a Polynucleotide-Accommodating Groove Essential for APOBEC3A Restriction Activities. <i>Journal of Virology</i> , 2011, 85, 1765-1776.	1.5	67
28	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.	3.3	64
29	Myeloid antigen-presenting cell niches sustain antitumor T cells and license PD-1 blockade via CD28 costimulation. <i>Cancer Cell</i> , 2021, 39, 1623-1642.e20.	7.7	64
30	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.	2.6	63
31	Inhibition Mechanisms of Indoleamine 2,3-Dioxygenase 1 (IDO1). <i>Journal of Medicinal Chemistry</i> , 2019, 62, 8784-8795.	2.9	59
32	Application of the SwissDrugDesign Online Resources in Virtual Screening. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4612.	1.8	58
33	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, 3137-3152.	2.5	57
34	Cathepsin S Regulates Antigen Processing and T Cell Activity in Non-Hodgkin Lymphoma. <i>Cancer Cell</i> , 2020, 37, 674-689.e12.	7.7	55
35	The SwissSimilarity 2021 Web Tool: Novel Chemical Libraries and Additional Methods for an Enhanced Ligand-Based Virtual Screening Experience. <i>International Journal of Molecular Sciences</i> , 2022, 23, 811.	1.8	53
36	Blind docking of 260 protein-ligand complexes with EADock 2.0. <i>Journal of Computational Chemistry</i> , 2009, 30, 2021-2030.	1.5	52

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37	Biallelic variants in KIF14 cause intellectual disability with microcephaly. <i>European Journal of Human Genetics</i> , 2018, 26, 330-339.	1.4	52
38	<i>FGFR2</i> 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.	7.7	46
39	The Peroxisomal Enzyme L-PBE Is Required to Prevent the Dietary Toxicity of Medium-Chain Fatty Acids. <i>Cell Reports</i> , 2013, 5, 248-258.	2.9	45
40	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.	7.7	45
41	Sequence Determinants of a Microtubule Tip Localization Signal (MtLS). <i>Journal of Biological Chemistry</i> , 2012, 287, 28227-28242.	1.6	44
42	T cell receptor alpha variable 12 bias in the immunodominant response to Yellow fever virus. <i>European Journal of Immunology</i> , 2018, 48, 258-272.	1.6	44
43	How T cell receptors interact with peptide-MHCs: A multiple steered molecular dynamics study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3007-3024.	1.5	43
44	On-the-Fly QM/MM Docking with Attracting Cavities. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 73-84.	2.5	42
45	Sensitive identification of neoantigens and cognate TCRs in human solid tumors. <i>Nature Biotechnology</i> , 2022, 40, 656-660.	9.4	41
46	Distinct sets of $\hat{1}\hat{2}$ TCRs confer similar recognition of tumor antigen NY-ESO-1 ₁₅₇₋₁₆₅ 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, 15010-15015.	3.3	39
47	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.	1.1	39
48	Mutant <i>CTNNB1</i> and histological heterogeneity define metabolic subtypes of hepatoblastoma. <i>EMBO Molecular Medicine</i> , 2017, 9, 1589-1604.	3.3	38
49	RNA pentaloop structures as effective targets of regulators belonging to the RsmA/CsrA protein family. <i>RNA Biology</i> , 2013, 10, 1030-1041.	1.5	37
50	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, 883-894.	2.0	35
51	1,2,3-Triazoles as inhibitors of indoleamine 2,3-dioxygenase 2 (IDO2). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016, 26, 4330-4333.	1.0	35
52	Combined Simulation and Mutagenesis Analyses Reveal the Involvement of Key Residues for Peroxisome Proliferator-activated Receptor Helix 12 Dynamic Behavior. <i>Journal of Biological Chemistry</i> , 2007, 282, 9666-9677.	1.6	33
53	Lung adenocarcinoma with BRAF G469L mutation refractory to vemurafenib. <i>Lung Cancer</i> , 2013, 82, 365-367.	0.9	32
54	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, 437-447.	1.5	32

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55	Design and Validation of a Novel Generic Platform for the Production of Tetravalent IgG1-like Bispecific Antibodies. <i>Journal of Immunology</i> , 2016, 196, 3199-3211.	0.4	30
56	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, 81-84.	0.9	29
57	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.	3.2	29
58	Use of the FACTS solvation model for protein-ligand docking calculations. Application to EADock. <i>Journal of Molecular Recognition</i> , 2010, 23, 457-461.	1.1	28
59	Design of short peptides to block BTLA/HVEM interactions for promoting anticancer T-cell responses. <i>PLoS ONE</i> , 2017, 12, e0179201.	1.1	28
60	Expanding molecular modeling and design tools to non-natural sidechains. <i>Journal of Computational Chemistry</i> , 2012, 33, 1525-1535.	1.5	27
61	<i>In vitro</i> biotransformation of imatinib by the tumor expressed CYP1A1 and CYP1B1. <i>Biopharmaceutics and Drug Disposition</i> , 2008, 29, 103-118.	1.1	26
62	Protein pocket and ligand shape comparison and its application in virtual screening. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 511-524.	1.3	25
63	Monoubiquitination and Activity of the Paracaspase MALT1 Requires Glutamate 549 in the Dimerization Interface. <i>PLoS ONE</i> , 2013, 8, e72051.	1.1	25
64	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, 8978-8986.	1.7	24
65	TCRep 3D: An Automated In Silico Approach to Study the Structural Properties of TCR Repertoires. <i>PLoS ONE</i> , 2011, 6, e26301.	1.1	24
66	Docking to heme proteins. <i>Journal of Computational Chemistry</i> , 2009, 30, 2305-2315.	1.5	22
67	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, 6098-6103.	2.6	22
68	Pan-SRC kinase inhibition blocks B-cell receptor oncogenic signaling in non-Hodgkin lymphoma. <i>Blood</i> , 2018, 131, 2345-2356.	0.6	22
69	A WXW Motif Is Required for the Anticancer Activity of the TAT-RasGAP317-326 Peptide. <i>Journal of Biological Chemistry</i> , 2014, 289, 23701-23711.	1.6	21
70	Proteolysis of HCF-1 by Ser/Thr glycosylation-incompetent α -GlcNAc transferase:UDP-GlcNAc complexes. <i>Genes and Development</i> , 2016, 30, 960-972.	2.7	21
71	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.	1.1	21
72	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.	2.6	19

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73	Mutations in the palm domain disrupt modulation of acid-sensing ion channel 1a currents by neuropeptides. <i>Scientific Reports</i> , 2019, 9, 2599.	1.6	19
74	Potency of inhibition of human DNA topoisomerase I by flavones assessed through physicochemical parameters. <i>Free Radical Biology and Medicine</i> , 2011, 51, 1406-1410.	1.3	18
75	The Binding Mode of <i>N</i> -Hydroxyamidines to Indoleamine 2,3-Dioxygenase 1 (IDO1). <i>Biochemistry</i> , 2017, 56, 4323-4325.	1.2	17
76	Herpes simplex encephalitis in adult patients with MASP-2 deficiency. <i>PLoS Pathogens</i> , 2019, 15, e1008168.	2.1	17
77	Biallelic variants in FBXL3 cause intellectual disability, delayed motor development and short stature. <i>Human Molecular Genetics</i> , 2019, 28, 972-979.	1.4	17
78	SwissBioisostere 2021: updated structural, bioactivity and physicochemical data delivered by a reshaped web interface. <i>Nucleic Acids Research</i> , 2022, 50, D1382-D1390.	6.5	17
79	Structure and Plasticity of Indoleamine 2,3-Dioxygenase 1 (IDO1). <i>Journal of Medicinal Chemistry</i> , 2021, 64, 17690-17705.	2.9	17
80	VEGFR-2 redirected CAR-T cells are functionally impaired by soluble VEGF-A competition for receptor binding. , 2021, 9, e002151.		16
81	Distinct OGT-Binding Sites Promote HCF-1 Cleavage. <i>PLoS ONE</i> , 2015, 10, e0136636.	1.1	15
82	Disulfide-Linked Peptides for Blocking BTLA/HVEM Binding. <i>International Journal of Molecular Sciences</i> , 2020, 21, 636.	1.8	15
83	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.	2.9	14
84	Fifteen years SIB Swiss Institute of Bioinformatics: life science databases, tools and support. <i>Nucleic Acids Research</i> , 2014, 42, W436-W441.	6.5	13
85	The CAP1/Prss8 catalytic triad is not involved in PAR2 activation and protease nexin-1 (PN-1) inhibition. <i>FASEB Journal</i> , 2014, 28, 4792-4805.	0.2	13
86	Deciphering the Mechanisms of Improved Immunogenicity of Hypochlorous Acid-Treated Antigens in Anti-Cancer Dendritic Cell-Based Vaccines. <i>Vaccines</i> , 2020, 8, 271.	2.1	13
87	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.	1.4	12
88	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 142 T	0.8	12
89	Protein homology reveals new targets for bioactive small molecules. <i>Bioinformatics</i> , 2015, 31, 2721-2727.	1.8	9
90	Azole-Based Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 2205-2227.	2.9	9

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91	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.	2.3	9
92	T-Cell Receptors Binding Orientation over Peptide/MHC Class I Is Driven by Long-Range Interactions. <i>PLoS ONE</i> , 2012, 7, e51943.	1.1	8
93	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.	1.2	8
94	Analysis of Secondary Structure Biases in Naturally Presented HLA-I Ligands. <i>Frontiers in Immunology</i> , 2019, 10, 2731.	2.2	8
95	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.	0.9	7
96	Synthesis and in vitro evaluation of a novel radioligand for $\alpha_v\beta_3$ integrin receptor imaging: [18F]FPPA-c(RGDfK). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 6068-6072.	1.0	7
97	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.	1.9	7
98	The conserved threonine-rich region of the HCF-1PRO repeat activates promiscuous OGT:UDP-GlcNAc glycosylation and proteolysis activities. <i>Journal of Biological Chemistry</i> , 2018, 293, 17754-17768.	1.6	7
99	A roadmap for driving CAR T cells toward the oncogenic immunopeptidome. <i>Cancer Cell</i> , 2022, 40, 20-22.	7.7	7
100	Structural Prediction of Peptide-MHC Binding Modes. <i>Methods in Molecular Biology</i> , 2022, 2405, 245-282.	0.4	7
101	Dominant monoallelic variant in the PAK2 gene causes Knobloch syndrome type 2. <i>Human Molecular Genetics</i> , 2021, 31, 1-9.	1.4	6
102	Recurrent Structural Motifs in Non-Homologous Protein Structures. <i>International Journal of Molecular Sciences</i> , 2013, 14, 7795-7814.	1.8	5
103	Educational Tools to Introduce Computer-Aided Drug Design to Students and to the Public at Large. <i>Chimia</i> , 2018, 72, 55.	0.3	4
104	Going Beyond the Sequences: TCR Binding Patterns at the Service of Cancer Detection. <i>Cancer Research</i> , 2019, 79, 1299-1301.	0.4	4
105	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.	1.1	3
106	Trametinib Induces the Stabilization of a Dual GNAQ p.Gly48Leu- and FGFR4 p.Cys172Gly-Mutated Uveal Melanoma. The Role of Molecular Modelling in Personalized Oncology. <i>International Journal of Molecular Sciences</i> , 2020, 21, 8021.	1.8	3
107	Computer-Aided Drug Design for Cancer Therapy. , 2021, , 386-401.		3
108	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.	1.2	3

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109	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, 4345-4349.	1.0	2
110	Inhibitors of the Kynurenine Pathway. <i>Topics in Medicinal Chemistry</i> , 2017, , 371-371.	0.4	2
111	Heterozygous variants in CTR9, which encodes a major component of the PAF1 complex, are associated with a neurodevelopmental disorder. <i>Genetics in Medicine</i> , 2022, , .	1.1	1
112	Structure-based optimization of type III indoleamine 2,3-dioxygenase 1 (IDO1) inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 1773-1811.	2.5	1
113	Actin assembly requirements of the formin Fus1 to build the fusion focus. <i>Journal of Cell Science</i> , 2022, 135, .	1.2	1
114	Strong Enrichment of Aromatic and Sulfur-Containing Residues in Ligand-Protein Binding Sites. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4921-4928.	2.5	0
115	Identification of a superagonist variant of the immunodominant Yellow fever virus epitope NS4b 214-222 by combinatorial peptide library screening. <i>Molecular Immunology</i> , 2020, 125, 43-50.	1.0	0