Vincent Zoete

List of Publications by Year
in descending order

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	SwissBioisostere 2021: updated structural, bioactivity and physicochemical data delivered by a reshaped web interface. Nucleic Acids Research, 2022, 50, D1382-D1390.	6.5	17
2	Sensitive identification of neoantigens and cognate TCRs in human solid tumors. Nature Biotechnology, 2022, 40, 656-660.	9.4	41
3	The SwissSimilarity 2021 Web Tool: Novel Chemical Libraries and Additional Methods for an Enhanced Ligand-Based Virtual Screening Experience. International Journal of Molecular Sciences, 2022, 23, 811.	1.8	53
4	A roadmap for driving CAR TÂcells toward the oncogenic immunopeptidome. Cancer Cell, 2022, 40, 20-22.	7.7	7
5	Structural Prediction of Peptideâ€“MHC Binding Modes. Methods in Molecular Biology, 2022, 2405, 245-282.	0.4	7
6	Heterozygous variants in CTR9, which encodes a major component of the PAF1 complex, are associated with a neurodevelopmental disorder. Genetics in Medicine, 2022, , .	1.1	1
7	Structure-based optimization of type III indoleamine 2,3-dioxygenase 1 (IDO1) inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1773-1811.	2.5	1
8	Actin assembly requirements of the formin Fus1 to build the fusion focus. Journal of Cell Science, 2022, 135, .	1.2	1
9	Computer-Aided Drug Design for Cancer Therapy. , 2021, , 386-401.		3
10	Durable Suppression of Acquired MEK Inhibitor Resistance in Cancer by Sequestering MEK from ERK and Promoting Antitumor T-cell Immunity. Cancer Discovery, 2021, 11, 714-735.	7.7	45
11	Azole-Based Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 2205-2227.	2.9	9
12	Dominant monoallelic variant in the PAK2 gene causes Knobloch syndrome type 2. Human Molecular Genetics, 2021, 31, 1-9.	1.4	6
13	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. Biochemistry, 2021, 60, 859-872.	1.2	3
14	Swiss-PO: a new tool to analyze the impact of mutations on protein three-dimensional structures for precision oncology. Npj Precision Oncology, 2021, 5, 19.	2.3	9
15	FGFR2Extracellular Domain In-Frame Deletions Are Therapeutically Targetable Genomic Alterations That Function as Oncogenic Drivers in Cholangiocarcinoma. Cancer Discovery, 2021, 11, 2488-2505.	7.7	46
16	VEGFR-2 redirected CAR-T cells are functionally impaired by soluble VEGF-A competition for receptor binding. , 2021, 9, e002151.		16
17	The impact of structural bioinformatics tools and resources on SARS-CoV-2 research and therapeutic strategies. Briefings in Bioinformatics, 2021, 22, 742-768.	3.2	29
18	Myeloid antigen-presenting cell niches sustain antitumor TÂcells and license PD-1 blockade via CD28 costimulation. Cancer Cell, 2021, 39, 1623-1642.e20.	7.7	64

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19	Structure and Plasticity of Indoleamine 2,3-Dioxygenase 1 (IDO1). Journal of Medicinal Chemistry, 2021, 64, 17690-17705.	2.9	17
20	T-cell repertoire analysis and metrics of diversity and clonality. Current Opinion in Biotechnology, 2020, 65, 284-295.	3.3	79
21	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. International Journal of Molecular Sciences, 2020, 21, 8021.	1.8	3
22	Deciphering the Mechanisms of Improved Immunogenicity of Hypochlorous Acid-Treated Antigens in Anti-Cancer Dendritic Cell-Based Vaccines. Vaccines, 2020, 8, 271.	2.1	13
23	Pharmacological disruption of the Notch transcription factor complex. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16292-16301.	3.3	64
24	Identification of a superagonist variant of the immunodominant Yellow fever virus epitope NS4b 214-222 by combinatorial peptide library screening. Molecular Immunology, 2020, 125, 43-50.	1.0	0
25	Disulfide-Linked Peptides for Blocking BTLA/HVEM Binding. International Journal of Molecular Sciences, 2020, 21, 636.	1.8	15
26	Cathepsin S Regulates Antigen Processing and T Cell Activity in Non-Hodgkin Lymphoma. Cancer Cell, 2020, 37, 674-689.e12.	7.7	55
27	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T f	6.8	12
28	Analysis of Secondary Structure Biases in Naturally Presented HLA-I Ligands. Frontiers in Immunology, 2019, 10, 2731.	2.2	8
29	Strong Enrichment of Aromatic and Sulfur-Containing Residues in Ligandâ€“Protein Binding Sites. Journal of Chemical Information and Modeling, 2019, 59, 4921-4928.	2.5	0
30	Inhibition Mechanisms of Indoleamine 2,3-Dioxygenase 1 (IDO1). Journal of Medicinal Chemistry, 2019, 62, 8784-8795.	2.9	59
31	Application of the SwissDrugDesign Online Resources in Virtual Screening. International Journal of Molecular Sciences, 2019, 20, 4612.	1.8	58
32	SwissTargetPrediction: updated data and new features for efficient prediction of protein targets of small molecules. Nucleic Acids Research, 2019, 47, W357-W364.	6.5	1,634
33	Bi-allelic Variants in DYNC1I2 Cause Syndromic Microcephaly with Intellectual Disability, Cerebral Malformations, and Dysmorphic Facial Features. American Journal of Human Genetics, 2019, 104, 1073-1087.	2.6	19
34	Going Beyond the Sequences: TCR Binding Patterns at the Service of Cancer Detection. Cancer Research, 2019, 79, 1299-1301.	0.4	4
35	Mutations in the palm domain disrupt modulation of acid-sensing ion channel 1a currents by neuropeptides. Scientific Reports, 2019, 9, 2599.	1.6	19
36	Herpes simplex encephalitis in adult patients with MASP-2 deficiency. PLoS Pathogens, 2019, 15, e1008168.	2.1	17

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37	Biallelic variants in FBXL3 cause intellectual disability, delayed motor development and short stature. Human Molecular Genetics, 2019, 28, 972-979.	1.4	17
38	Personalized cancer vaccine effectively mobilizes antitumor T cell immunity in ovarian cancer. Science Translational Medicine, 2018, 10, .	5.8	326
39	Biallelic variants in KIF14 cause intellectual disability with microcephaly. European Journal of Human Genetics, 2018, 26, 330-339.	1.4	52
40	Sensitive and frequent identification of high avidity neo-epitopeÂspecific CD8 + T cells in immunotherapy-naive ovarian cancer. Nature Communications, 2018, 9, 1092.	5.8	122
41	Pan-SRC kinase inhibition blocks B-cell receptor oncogenic signaling in non-Hodgkin lymphoma. Blood, 2018, 131, 2345-2356.	0.6	22
42	T cell receptor alpha variable 12â€2 bias in the immunodominant response to Yellow fever virus. European Journal of Immunology, 2018, 48, 258-272.	1.6	44
43	Biallelic variants in LINGO1 are associated with autosomal recessive intellectual disability, microcephaly, speech and motor delay. Genetics in Medicine, 2018, 20, 778-784.	1.1	21
44	4-epi-Isofagomine derivatives as pharmacological chaperones for the treatment of lysosomal diseases linked to Î²-galactosidase mutations: Improved synthesis and biological investigations. Bioorganic and Medicinal Chemistry, 2018, 26, 5462-5469.	1.4	12
45	Rational Design, Synthesis, and Pharmacological Characterization of Novel Ghrelin Receptor Inverse Agonists as Potential Treatment against Obesity-Related Metabolic Diseases. Journal of Medicinal Chemistry, 2018, 61, 11039-11060.	2.9	14
46	The conserved threonine-rich region of the HCF-1PRO repeat activates promiscuous OGT:UDP-GlcNAc glycosylation and proteolysis activities. Journal of Biological Chemistry, 2018, 293, 17754-17768.	1.6	7
47	Educational Tools to Introduce Computer-Aided Drug Design to Students and to the Public at Large. Chimia, 2018, 72, 55.	0.3	4
48	Drug Design Workshop: A Web-Based Educational Tool To Introduce Computer-Aided Drug Design to the General Public. Journal of Chemical Education, 2017, 94, 335-344.	1.1	39
49	SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Scientific Reports, 2017, 7, 42717.	1.6	7,635
50	On-the-Fly QM/MM Docking with Attracting Cavities. Journal of Chemical Information and Modeling, 2017, 57, 73-84.	2.5	42
51	Mutant <scp>CTNNB</scp> 1 and histological heterogeneity define metabolic subtypes of hepatoblastoma. EMBO Molecular Medicine, 2017, 9, 1589-1604.	3.3	38
52	The Binding Mode of N-Hydroxyamidines to Indoleamine 2,3-Dioxygenase 1 (IDO1). Biochemistry, 2017, 56, 4323-4325.	1.2	17
53	Inhibitors of the Kynurenine Pathway. Topics in Medicinal Chemistry, 2017, , 371-371.	0.4	2
54	The T-Cell Receptor Can Bind to the Peptide-Bound Major Histocompatibility Complex and Uncomplexed Î²₂-Microglobulin through Distinct Binding Sites. Biochemistry, 2017, 56, 3945-3961.	1.2	8

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55	Design of short peptides to block BTLA/HVEM interactions for promoting anticancer T-cell responses. PLoS ONE, 2017, 12, e0179201.	1.1	28
56	SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 1399-1404.	2.5	229
57	Attracting cavities for docking. Replacing the rough energy landscape of the protein by a smooth attracting landscape. Journal of Computational Chemistry, 2016, 37, 437-447.	1.5	32
58	Proteolysis of HCF-1 by Ser/Thr glycosylation-incompetent O-GlcNAc transferase:UDP-GlcNAc complexes. Genes and Development, 2016, 30, 960-972.	2.7	21
59	A BOILEDâ€Egg To Predict Gastrointestinal Absorption and Brain Penetration of Small Molecules. ChemMedChem, 2016, 11, 1117-1121.	1.6	1,249
60	1,2,3-Triazoles as inhibitors of indoleamine 2,3-dioxygenase 2 (IDO2). Bioorganic and Medicinal Chemistry Letters, 2016, 26, 4330-4333.	1.0	35
61	Electron affinity of tricyclic, bicyclic, and monocyclic compounds containing cyanoenones correlates with their potency as inducers of a cytoprotective enzyme. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 4345-4349.	1.0	2
62	Debio 0617B Inhibits Growth of STAT3-Driven Solid Tumors through Combined Inhibition of JAK, SRC, and Class III/V Receptor Tyrosine Kinases. Molecular Cancer Therapeutics, 2016, 15, 2334-2343.	1.9	7
63	Design and Validation of a Novel Generic Platform for the Production of Tetravalent IgG1-like Bispecific Antibodies. Journal of Immunology, 2016, 196, 3199-3211.	0.4	30
64	Genomic analysis identifies new drivers and progression pathways in skin basal cell carcinoma. Nature Genetics, 2016, 48, 398-406.	9.4	370
65	Distinct OGT-Binding Sites Promote HCF-1 Cleavage. PLoS ONE, 2015, 10, e0136636.	1.1	15
66	Protein homology reveals new targets for bioactive small molecules. Bioinformatics, 2015, 31, 2721-2727.	1.8	9
67	Challenges in the Discovery of Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. Journal of Medicinal Chemistry, 2015, 58, 9421-9437.	2.9	179
68	SwissTargetPrediction: a web server for target prediction of bioactive small molecules. Nucleic Acids Research, 2014, 42, W32-W38.	6.5	977
69	A WXW Motif Is Required for the Anticancer Activity of the TAT-RasGAP317â€“326 Peptide. Journal of Biological Chemistry, 2014, 289, 23701-23711.	1.6	21
70	Fifteen years SIB Swiss Institute of Bioinformatics: life science databases, tools and support. Nucleic Acids Research, 2014, 42, W436-W441.	6.5	13
71	iLOGP: A Simple, Robust, and Efficient Description of n-Octanol/Water Partition Coefficient for Drug Design Using the GB/SA Approach. Journal of Chemical Information and Modeling, 2014, 54, 3284-3301.	2.5	560
72	Toward On-The-Fly Quantum Mechanical/Molecular Mechanical (QM/MM) Docking: Development and Benchmark of a Scoring Function. Journal of Chemical Information and Modeling, 2014, 54, 3137-3152.	2.5	57

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73	The CAP1/Prss8 catalytic triad is not involved in PAR2 activation and protease nexinâ€1 (PNâ€1) inhibition. FASEB Journal, 2014, 28, 4792-4805.	0.2	13
74	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. Journal of Lipid Research, 2014, 55, 883-894.	2.0	35
75	Detailed analysis and follow-up studies of a high-throughput screening for indoleamine 2,3-dioxygenase 1 (IDO1) inhibitors. European Journal of Medicinal Chemistry, 2014, 84, 284-301.	2.6	63
76	Physicochemical properties of exogenous molecules correlated with their biological efficacy as protectors against carcinogenesis and inflammation. International Reviews in Physical Chemistry, 2013, 32, 393-434.	0.9	7
77	A dramatic lung cancer course in a patient with a rare EGFR germline mutation exon 21 V843I: Is EGFR TKI resistance predictable?. Lung Cancer, 2013, 80, 81-84.	0.9	29
78	Shaping the interaction landscape of bioactive molecules. Bioinformatics, 2013, 29, 3073-3079.	1.8	327
79	Synthesis and in vitro evaluation of a novel radioligand for Î±vÎ²3 integrin receptor imaging: [18F]FPPA-c(RGDfK). Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6068-6072.	1.0	7
80	The Peroxisomal Enzyme L-PBE Is Required to Prevent the Dietary Toxicity of Medium-Chain Fatty Acids. Cell Reports, 2013, 5, 248-258.	2.9	45
81	Lung adenocarcinoma with BRAF G469L mutation refractory to vemurafenib. Lung Cancer, 2013, 82, 365-367.	0.9	32
82	Protein pocket and ligand shape comparison and its application in virtual screening. Journal of Computer-Aided Molecular Design, 2013, 27, 511-524.	1.3	25
83	SwissBioisostere: a database of molecular replacements for ligand design. Nucleic Acids Research, 2013, 41, D1137-D1143.	6.5	101
84	Recurrent Structural Motifs in Non-Homologous Protein Structures. International Journal of Molecular Sciences, 2013, 14, 7795-7814.	1.8	5
85	RNA pentaloop structures as effective targets of regulators belonging to the RsmA/CsrA protein family. RNA Biology, 2013, 10, 1030-1041.	1.5	37
86	Prediction of Cross-Recognition of Peptide-HLA A2 by Melan-A-Specific Cytotoxic T Lymphocytes Using Three-Dimensional Quantitative Structure-Activity Relationships. PLoS ONE, 2013, 8, e65590.	1.1	3
87	Monoubiquitination and Activity of the Paracaspase MALT1 Requires Glutamate 549 in the Dimerization Interface. PLoS ONE, 2013, 8, e72051.	1.1	25
88	SwissSidechain: a molecular and structural database of non-natural sidechains. Nucleic Acids Research, 2012, 41, D327-D332.	6.5	100
89	Sequence Determinants of a Microtubule Tip Localization Signal (MtLS). Journal of Biological Chemistry, 2012, 287, 28227-28242.	1.6	44
90	Interplay between T Cell Receptor Binding Kinetics and the Level of Cognate Peptide Presented by Major Histocompatibility Complexes Governs CD8+ T Cell Responsiveness. Journal of Biological Chemistry, 2012, 287, 23068-23078.	1.6	121

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91	Rational Design of 4-Aryl-1,2,3-Triazoles for Indoleamine 2,3-Dioxygenase 1 Inhibition. Journal of Medicinal Chemistry, 2012, 55, 5270-5290.	2.9	153
92	Defining and searching for structural motifs using DeepView/Swiss-PdbViewer. BMC Bioinformatics, 2012, 13, 173.	1.2	260
93	Exome sequencing identifies recurrent somatic MAP2K1 and MAP2K2 mutations in melanoma. Nature Genetics, 2012, 44, 133-139.	9.4	369
94	T-Cell Receptors Binding Orientation over Peptide/MHC Class I Is Driven by Long-Range Interactions. PLoS ONE, 2012, 7, e51943.	1.1	8
95	Expanding molecular modeling and design tools to nonâ€natural sidechains. Journal of Computational Chemistry, 2012, 33, 1525-1535.	1.5	27
96	Asymmetric Synthesis of Pochoninâ€...E and F, Revision of Their Proposed Structure, and Their Conversion to Potent Hsp90 Inhibitors. Chemistry - A European Journal, 2012, 18, 8978-8986.	1.7	24
97	SwissDock, a protein-small molecule docking web service based on EADock DSS. Nucleic Acids Research, 2011, 39, W270-W277.	6.5	1,396
98	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. European Journal of Medicinal Chemistry, 2011, 46, 6098-6103.	2.6	22
99	Potency of inhibition of human DNA topoisomerase I by flavones assessed through physicochemical parameters. Free Radical Biology and Medicine, 2011, 51, 1406-1410.	1.3	18
100	How T cell receptors interact with peptideâ€MHCs: A multiple steered molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3007-3024.	1.5	43
101	Fast docking using the CHARMM force field with EADock DSS. Journal of Computational Chemistry, 2011, 32, 2149-2159.	1.5	384
102	SwissParam: A fast force field generation tool for small organic molecules. Journal of Computational Chemistry, 2011, 32, 2359-2368.	1.5	1,485
103	Structure-Function Analyses Point to a Polynucleotide-Accommodating Groove Essential for APOBEC3A Restriction Activities. Journal of Virology, 2011, 85, 1765-1776.	1.5	67
104	TCRep 3D: An Automated In Silico Approach to Study the Structural Properties of TCR Repertoires. PLoS ONE, 2011, 6, e26301.	1.1	24
105	Use of the FACTS solvation model for proteinâ€“ligand docking calculations. Application to EADock. Journal of Molecular Recognition, 2010, 23, 457-461.	1.1	28
106	Evidence for a TCR Affinity Threshold Delimiting Maximal CD8 T Cell Function. Journal of Immunology, 2010, 184, 4936-4946.	0.4	196
107	Rational Design of Indoleamine 2,3-Dioxygenase Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 1172-1189.	2.9	146
108	Docking, virtual high throughput screening and in silico fragmentâ€based drug design. Journal of Cellular and Molecular Medicine, 2009, 13, 238-248.	1.6	140

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109	Blind docking of 260 proteinâ€“ligand complexes with EADock 2.0. Journal of Computational Chemistry, 2009, 30, 2021-2030.	1.5	52
110	Docking to heme proteins. Journal of Computational Chemistry, 2009, 30, 2305-2315.	1.5	22
111	In vitro biotransformation of imatinib by the tumor expressed CYP1A1 and CYP1B1. Biopharmaceutics and Drug Disposition, 2008, 29, 103-118.	1.1	26
112	Distinct sets of Î±Î² TCRs confer similar recognition of tumor antigen NY-ESO-1_{157â€“165}by interacting with its central Met/Trp residues. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 15010-15015.	3.3	39
113	Combined Simulation and Mutagenesis Analyses Reveal the Involvement of Key Residues for Peroxisome Proliferator-activated ReceptorÎ± Helix 12 Dynamic Behavior. Journal of Biological Chemistry, 2007, 282, 9666-9677.	1.6	33
114	EADock: Docking of small molecules into protein active sites with a multiobjective evolutionary optimization. Proteins: Structure, Function and Bioinformatics, 2007, 67, 1010-1025.	1.5	171
115	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. Proteins: Structure, Function and Bioinformatics, 2007, 67, 1026-1047.	1.5	110