

Vincent Zoete

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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 | A roadmap for driving CAR T cells toward the oncogenic immunopeptidome.. <i>Cancer Cell</i> , 2022 , 40, 20-22 | 4.3 | 0 |
| 109 | Structural Prediction of Peptide-MHC Binding Modes.. <i>Methods in Molecular Biology</i> , 2022 , 2405, 245-282 | 1.4 | 1 |
| 108 | SwissBioisostere 2021: updated structural, bioactivity and physicochemical data delivered by a reshaped web interface. <i>Nucleic Acids Research</i> , 2021 , | 20.1 | 2 |
| 107 | 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 |
| 106 | Sensitive identification of neoantigens and cognate TCRs in human solid tumors. <i>Nature Biotechnology</i> , 2021 , | 44.5 | 9 |
| 105 | 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 |
| 104 | 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 |
| 103 | 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 |
| 102 | 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 |
| 101 | Computer-Aided Drug Design for Cancer Therapy 2021 , 386-401 | | 2 |
| 100 | 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 |
| 99 | Azole-Based Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 2205-2227 | 8.3 | 4 |
| 98 | VEGFR-2 redirected CAR-T cells are functionally impaired by soluble VEGF-A competition for receptor binding 2021 , 9, | | 4 |
| 97 | Structure and Plasticity of Indoleamine 2,3-Dioxygenase 1 (IDO1).. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 17690-17705 | 8.3 | 0 |
| 96 | 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 |
| 95 | 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 |
| 94 | 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 |

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| 93 | Identification of a superagonist variant of the immunodominant Yellow fever virus epitope NS4b by combinatorial peptide library screening. <i>Molecular Immunology</i> , 2020 , 125, 43-50 | 4.3 | |
| 92 | Disulfide-Linked Peptides for Blocking BTLA/HVEM Binding. <i>International Journal of Molecular Sciences</i> , 2020 , 21, | 6.3 | 10 |
| 91 | 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 |
| 90 | A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo Community). <i>F1000Research</i> , 2020 , 9, | 3.6 | 9 |
| 89 | T-cell repertoire analysis and metrics of diversity and clonality. <i>Current Opinion in Biotechnology</i> , 2020 , 65, 284-295 | 11.4 | 11 |
| 88 | Inhibition Mechanisms of Indoleamine 2,3-Dioxygenase 1 (IDO1). <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 8784-8795 | 8.3 | 33 |
| 87 | Application of the SwissDrugDesign Online Resources in Virtual Screening. <i>International Journal of Molecular Sciences</i> , 2019 , 20, | 6.3 | 25 |
| 86 | 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 |
| 85 | 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 |
| 84 | Going Beyond the Sequences: TCR Binding Patterns at the Service of Cancer Detection. <i>Cancer Research</i> , 2019 , 79, 1299-1301 | 10.1 | 4 |
| 83 | Analysis of Secondary Structure Biases in Naturally Presented HLA-I Ligands. <i>Frontiers in Immunology</i> , 2019 , 10, 2731 | 8.4 | 4 |
| 82 | 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 | 6.1 | |
| 81 | 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 |
| 80 | Herpes simplex encephalitis in adult patients with MASP-2 deficiency. <i>PLoS Pathogens</i> , 2019 , 15, e1008168 | 6.8 | 14 |
| 79 | 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 |
| 78 | Personalized cancer vaccine effectively mobilizes antitumor T cell immunity in ovarian cancer. <i>Science Translational Medicine</i> , 2018 , 10, | 17.5 | 205 |
| 77 | Biallelic variants in KIF14 cause intellectual disability with microcephaly. <i>European Journal of Human Genetics</i> , 2018 , 26, 330-339 | 5.3 | 37 |
| 76 | 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 |

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|----|---|-----|------|
| 75 | Pan-SRC kinase inhibition blocks B-cell receptor oncogenic signaling in non-Hodgkin lymphoma. <i>Blood</i> , 2018 , 131, 2345-2356 | 2.2 | 15 |
| 74 | 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 |
| 73 | 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 |
| 72 | 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 |
| 71 | 4-epi-Isosagomine 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 |
| 70 | 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 |
| 69 | 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 |
| 68 | 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 |
| 67 | 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 |
| 66 | On-the-Fly QM/MM Docking with Attracting Cavities. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 73-84 | 6.1 | 33 |
| 65 | 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 |
| 64 | Mutant and histological heterogeneity define metabolic subtypes of hepatoblastoma. <i>EMBO Molecular Medicine</i> , 2017 , 9, 1589-1604 | 12 | 28 |
| 63 | The Binding Mode of N-Hydroxyamidines to Indoleamine 2,3-Dioxygenase 1 (IDO1). <i>Biochemistry</i> , 2017 , 56, 4323-4325 | 3.2 | 14 |
| 62 | Inhibitors of the Kynurenine Pathway. <i>Topics in Medicinal Chemistry</i> , 2017 , 371-371 | 0.4 | 1 |
| 61 | The T-Cell Receptor Can Bind to the Peptide-Bound Major Histocompatibility Complex and Uncomplexed β Microglobulin through Distinct Binding Sites. <i>Biochemistry</i> , 2017 , 56, 3945-3961 | 3.2 | 6 |
| 60 | 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 |
| 59 | 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 |
| 58 | 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 |

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| 57 | 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 |
| 56 | Genomic analysis identifies new drivers and progression pathways in skin basal cell carcinoma. <i>Nature Genetics</i> , 2016 , 48, 398-406 | 36.3 | 242 |
| 55 | 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 |
| 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, 437-47 | 3.5 | 27 |
| 53 | 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 |
| 52 | A BOILED-Egg To Predict Gastrointestinal Absorption and Brain Penetration of Small Molecules. <i>ChemMedChem</i> , 2016 , 11, 1117-21 | 3.7 | 591 |
| 51 | Protein homology reveals new targets for bioactive small molecules. <i>Bioinformatics</i> , 2015 , 31, 2721-7 | 7.2 | 8 |
| 50 | 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 |
| 49 | Distinct OGT-Binding Sites Promote HCF-1 Cleavage. <i>PLoS ONE</i> , 2015 , 10, e0136636 | 3.7 | 13 |
| 48 | 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 |
| 47 | 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 |
| 46 | SwissTargetPrediction: a web server for target prediction of bioactive small molecules. <i>Nucleic Acids Research</i> , 2014 , 42, W32-8 | 20.1 | 557 |
| 45 | 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 |
| 44 | 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 |
| 43 | 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 |
| 42 | 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 |
| 41 | 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 |
| 40 | 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 |

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| 39 | 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 |
| 38 | Shaping the interaction landscape of bioactive molecules. <i>Bioinformatics</i> , 2013 , 29, 3073-9 | 7.2 | 185 |
| 37 | Synthesis and in vitro evaluation of a novel radioligand for $\alpha\beta$ integrin receptor imaging: [18F]FPPA-c(RGDfK). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013 , 23, 6068-72 | 2.9 | 7 |
| 36 | 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 |
| 35 | Lung adenocarcinoma with BRAF G469L mutation refractory to vemurafenib. <i>Lung Cancer</i> , 2013 , 82, 365-79 | 5.9 | 25 |
| 34 | 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 |
| 33 | SwissBioisostere: a database of molecular replacements for ligand design. <i>Nucleic Acids Research</i> , 2013 , 41, D1137-43 | 20.1 | 75 |
| 32 | Recurrent structural motifs in non-homologous protein structures. <i>International Journal of Molecular Sciences</i> , 2013 , 14, 7795-814 | 6.3 | 3 |
| 31 | 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 |
| 30 | 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 |
| 29 | Monoubiquitination and activity of the paracaspase MALT1 requires glutamate 549 in the dimerization interface. <i>PLoS ONE</i> , 2013 , 8, e72051 | 3.7 | 21 |
| 28 | SwissSidechain: a molecular and structural database of non-natural sidechains. <i>Nucleic Acids Research</i> , 2013 , 41, D327-32 | 20.1 | 74 |
| 27 | 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 |
| 26 | Defining and searching for structural motifs using DeepView/Swiss-PdbViewer. <i>BMC Bioinformatics</i> , 2012 , 13, 173 | 3.6 | 185 |
| 25 | 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 |
| 24 | Expanding molecular modeling and design tools to non-natural sidechains. <i>Journal of Computational Chemistry</i> , 2012 , 33, 1525-35 | 3.5 | 21 |
| 23 | 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 |
| 22 | Sequence determinants of a microtubule tip localization signal (MtLS). <i>Journal of Biological Chemistry</i> , 2012 , 287, 28227-42 | 5.4 | 36 |

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| 21 | 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 |
| 20 | Exome sequencing identifies recurrent somatic MAP2K1 and MAP2K2 mutations in melanoma. <i>Nature Genetics</i> , 2011 , 44, 133-9 | 36.3 | 313 |
| 19 | 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 |
| 18 | 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 |
| 17 | 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 |
| 16 | Fast docking using the CHARMM force field with EADock DSS. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2149-59 | 3.5 | 269 |
| 15 | SwissParam: a fast force field generation tool for small organic molecules. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2359-68 | 3.5 | 1025 |
| 14 | SwissDock, a protein-small molecule docking web service based on EADock DSS. <i>Nucleic Acids Research</i> , 2011 , 39, W270-7 | 20.1 | 984 |
| 13 | 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 |
| 12 | 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 |
| 11 | Evidence for a TCR affinity threshold delimiting maximal CD8 T cell function. <i>Journal of Immunology</i> , 2010 , 184, 4936-46 | 5.3 | 148 |
| 10 | Rational design of indoleamine 2,3-dioxygenase inhibitors. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 1172-39 | 2.9 | 126 |
| 9 | 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 |
| 8 | 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 |
| 7 | Blind docking of 260 protein-ligand complexes with EADock 2.0. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2021-30 | 3.5 | 46 |
| 6 | Docking to heme proteins. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2305-15 | 3.5 | 14 |
| 5 | 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 |
| 4 | 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 |

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|---|--|-----|-----|
| 3 | 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 |
| 2 | 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 |
| 1 | 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 |