

# Complete Publication List of Vincent ZOETE

## H-index (Clarivate analytics): 34

<sup>1</sup>: co-first author

\*: co-corresponding author

## In preparation

1. El Hage K, Daina A, Zoete V. Full analysis of the Protein DataBank reveals an overlooked role for Csp1 carbon atoms in ligand-protein binding. In preparation
2. Daina A, Zoete V. Large-scale assessment of the SwissTargetPrediction tool. In preparation
3. Krebs F, Daina A, Zoete V. Ligand-based docking. What is missing? In preparation

## Submitted

1. El Hage K, Zoete V. Strong Enrichment of Aromatic and Sulfur-Containing Residues in Ligand-Protein Binding Sites. Submitted to Sci. Rep.
2. Daina A, Michielin O, Zoete V. SwissTargetPrediction: updated data and new features for efficient prediction of protein targets of small molecules. Submitted to Nucleic Acid Research
3. Perez MAS, Bassani-Sternberg M, Michielin O, Gfeller D, Zoete V. Analysis of secondary structure biases in naturally presented HLA-I ligands. Submitted to Frontiers in Immunology.

## Published

1. Daina A, Giuliano G, Pietra C, Wang J, Chi Y, Zou Z, Li F, Yan Z, Zhou Y, Guainazzi A, Rubio SG, **Zoete V**. Rational Design, Synthesis and Pharmacological Characterization of Novel Ghrelin Receptor Inverse Agonists as Potential Treatment against Obesity-related Metabolic Diseases. *J. Med. Chem.*, in press.
2. Front S, Almeida S, **Zoete V**, Charollais-Thoenig J, Gallienne E, Marmy C, Pilloud V, Marti R, Wood T, Martin OR, Demetz S. 4-epi-Isosfagomine derivatives as pharmacological chaperones for the treatment of lysosomal diseases linked to  $\beta$ -galactosidase mutations: Improved synthesis and biological investigations. *Bioorg Med Chem.* 2018 pii: S0968-0896(18)31372-5.
3. Kapuria V, Röhrig UF, Waridel P, Lammers F, Borodkin VS, van Aalten DMF, **Zoete V**, Herr W. The conserved threonine-rich region of the HCF-1<sub>PRO</sub> repeat activates promiscuous OGT:UDP-GlcNAc glycosylation and proteolysis activities. *J Biol Chem.* 2018, in press.
4. Ansar M, Riazuddin S, Sarwar MT, Makrythanasis P, Paracha SA, Iqbal Z, Khan J, Assir MZ, Hussain M, Razaq A, Polla DL, Taj AS, Holmgren A, Batool N, Misceo D, Iwaszkiewicz J, de Brouwer APM, Guipponi M, Hanquinet S, **Zoete V**, Santoni FA, Frengen E, Ahmed J, Riazuddin S, van Bokhoven H, Antonarakis SE. Biallelic variants in LINGO1 are associated with autosomal recessive intellectual disability, microcephaly, speech and motor delay. *Genet Med.* 2018;20(7):778-784.
5. Battistello E, Katanayeva N, Dheilly E, Tavernari D, Donaldson MC, Bonsignore L, Thome M, Christie AL, Murakami MA, Michielin O, Ciriello G, **Zoete V**, Oricchio E. Pan-SRC kinase inhibition blocks B-cell receptor oncogenic signaling in non-Hodgkin lymphoma. *Blood.* 2018;131(21):2345-2356.
6. Tanyi JL, Bobisse S, Ophir E, Tuyraerts S, Roberti A, Genolet R, Baumgartner P, Stevenson BJ, Iseli C, Dangaj D, Czerniecki B, Semilietof A, Racle J, Michel A, Xenarios I, Chiang C, Monos DS, Torigian DA, Nisenbaum HL, Michielin O, June CH, Levine BL, Powell DJ Jr, Gfeller D, Mick R, Dafni U, **Zoete V**, Harari A, Coukos G, Kandalaft LE. Personalized cancer vaccine effectively mobilizes antitumor T cell immunity in ovarian cancer. *Sci Transl Med.* 2018 Apr 11;10(436).
7. Bobisse S, Genolet R, Roberti A, Tanyi JL, Racle J, Stevenson BJ, Iseli C, Michel A, Le Bitoux MA, Guillaume P, Schmidt J, Bianchi V, Dangaj D, Fenwick C, Derré L, Xenarios I, Michielin O, Romero P, Monos DS, **Zoete V**, Gfeller D, Kandalaft LE, Coukos G, Harari A. Sensitive and frequent identification of high avidity neo-epitope specific CD8<sup>+</sup> T cells in immunotherapy-naïve ovarian cancer. *Nat Commun.* 2018 Mar 15;9(1):1092
8. Makrythanasis P, Maroofian R, Stray-Pedersen A, Musaev D, Zaki MS, Mahmoud IG, Selim L, Elbadawy A, Jhangiani SN, Coban Akdemir ZH, Gambin T, Sorte HS, Heiberg A, McEvoy-Venneri J, James KN, Stanley V, Belandres D, Guipponi M, Santoni FA, Ahangari N, Tara F, Doosti M, Iwaszkiewicz J, **Zoete V**, Backe PH, Hamamy H, Gleeson JG, Lupski JR, Karimiani EG, Antonarakis SE. Biallelic variants in KIF14 cause intellectual disability with microcephaly. *Eur J Hum Genet.* 2018 Mar;26(3):330-339.
9. Daina A, Blatter MC, Gerritsen VB, **Zoete V**. Educational Tools to Introduce Computer-Aided Drug Design to Students and to the Public at Large. *Chimia (Aarau).* 2018 Feb 1;72(1):55-61.

10. Bovay A, **Zoete V**, Dolton G, Bulek AM, Cole DK, Rizkallah PJ, Fuller A, Beck K, Michielin O, Speiser DE, Sewell AK, Fuertes Marraco SA. T cell receptor alpha variable 12-2 bias in the immunodominant response to Yellow fever virus. *Eur J Immunol*. 2018 Feb;48(2):258-272.
11. Crippa S, Ancey PB, Vazquez J, Angelino P, Rougemont AL, Guettier C, **Zoete V**, Delorenzi M, Michielin O, Meylan E. Mutant CTNNB1 and histological heterogeneity define metabolic subtypes of hepatoblastoma. *EMBO Mol Med*. 2017 Nov;9(11):1589-1604.
12. Röhrig UF, **Zoete V**, Michielin O. The Binding Mode of N-Hydroxyamidines to Indoleamine 2,3-Dioxygenase 1 (IDO1). *Biochemistry*. 2017, 56(33):4323-4325.
13. Merkle PS, Irving M, Hongjian S, Ferber M, Jørgensen TJD, Scholten K, Luescher I, Coukos G, **Zoete V**, Cuendet MA, Michielin O, Rand KD. The T-Cell Receptor Can Bind to the Peptide-Bound Major Histocompatibility Complex and Uncomplexed  $\beta$ 2-Microglobulin through Distinct Binding Sites. *Biochemistry*. 2017, 56(30):3945-3961.
14. Spodzieja M, Lach S, Iwaszkiewicz J, Cesson V, Kalejta K, Olive D, Michielin O, Speiser DE, **Zoete V**, Derré L, Rodziewicz-Motowidło S. Design of short peptides to block BTLA/HVEM interactions for promoting anticancer T-cell responses. *PLoS One*. 2017, 12(6):e0179201.
15. Daina A, Michielin O, **Zoete V**. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep*. 2017, 7:42717.
16. Daina A, Blatter M-C, Baillie Gerritsen V, Palagi PM, Marek D, Xenarios I, Schwede T, Michielin O, **Zoete V**. Drug Design Workshop: A Web-Based Educational Tool To Introduce Computer-Aided Drug Design to the General Public *J. Chem. Educ.*, 2017, 94 (3), pp 335–344
17. Chaskar P, **Zoete V**, Röhrig UF. On-the-Fly QM/MM Docking with Attracting Cavities. *J Chem Inf Model*. 2017 23;57(1):73-84.
18. **Zoete V**, Daina A, Bovigny C, Michielin O. SwissSimilarity. A web tool for low to ultra high-throughput ligand-based virtual screening. *J Chem Inf Model*. 2016, 56(8):1399-404.
19. Murone M, Vaslin Chessex A, Attinger A, Ramachandra R, Shetty SJ, Dagainakatte G, Sengupta S, Marappan S, Dhodheri S, Rigotti S, Bachav Y, Brienza S, Traxler P, Lang M, Aguet M, **Zoete V**, Michielin O, Nicholas C, Johnson F, Ramachandra M and McAllister A 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, in press.
20. Röhrig UF, Majjigapu SR, Caldeleri D, Dilek N, Reichenbach P, Ascencao K, Irving M, Coukos G, Vogel P, **Zoete V**, Michielin O. 1,2,3-Triazoles as inhibitors of indoleamine 2,3-dioxygenase 2 (IDO2). *Bioorganic & Medicinal Chemistry Letters*, 2016, 26(17):4330-3.
21. Bensasson RV, Dinkova-Kostova AT, Zheng S, Saito A, Li W, **Zoete V**; Honda T. Electron affinity of tricyclic, bicyclic, and monocyclic compounds containing cyanoenones correlates with their potency as inducers of a cytoprotective enzyme. *Bioorganic & Medicinal Chemistry Letters*, 2016, 26(17):4345-9.
22. Daina, A.; **Zoete, V.**; A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem*, 2016, 11(11), 1117-1121.
23. Bonilla, X.; Parmentier, L.; King, B.; Bezrukov, F.; Kaya, G.; **Zoete, V.**; Seplyarskiy, V.B.; Sharpe, H.J.; McKee, T.; Letourneau, A.; Ribaux, P.G.; Popadin, K.; Basset-Seguín, N.; Chaabene, R.B.; Santoni, F.A.; Andrianova, M.A.; Guipponi, M.; Garieri, M.; Verdan, C.; Grosdemange, K.; Sumara, O.; Eilers, M.; Aifantis, I.; Michielin, O.; de Sauvage, F.J.; Stylli, Antonarakis S.E.; Nikolaev, S.I. Genomic analysis reveals novel drivers and progression pathways in skin basal cell carcinoma. *Nat. Gen.*, 2016, 48(4):398-406.
24. Kapuria, V.; Röhrig, U F. ; Bhuiyan, T.; Borodkin, V.S., van Aalten, D.M.F., **Zoete, V.**; Herr, W. Proteolysis of HCF-1 by glycosylation-incompetent O-GlcNAc transferase:UDP-GlcNAc complexes. *Genes and Development*, 2016, 30(8):960-72
25. **\*Zoete V**, Schuepbach T, Bovigny C, Chaskar P, Daina A, Röhrig UF, Michielin O. Attracting cavities for docking. Replacing the rough energy landscape of the protein by a smooth attracting landscape. *J Comput Chem*. 2016, 37(4):437-47.
26. Golay J, Choblet S, Iwaszkiewicz J, Cérutti P, Ozil A, Loisel S, Pugnière M, Ubiali G, **Zoete V**, Michielin O, Berthou C, Kadouche J, Mach JP, Duonor-Cérutti M. Design and Validation of a Novel Generic Platform for the Production of Tetravalent IgG1-like Bispecific Antibodies. *J Immunol*. 2016, 196(7):3199-211
27. Gfeller D, **Zoete V**. Protein Homology Reveals New Targets for Bioactive Small Molecules. *Bioinformatics*. 2015, 31(16):2721-7.
28. Röhrig UF, Majjigapu SR, Vogel P, **\*Zoete V**, Michielin O. Challenges in the Discovery of Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. *J Med Chem*. 2015, 58(24):9421-37.
29. SIB Swiss Institute of Bioinformatics Members. The SIB Swiss Institute of Bioinformatics' resources: focus on curated databases. *Nucleic Acids Res*. 2015 Nov 28. pii: gkv1310.
30. Bhuiyan T, Waridel P, Kapuria V, **Zoete V**, Herr W. Distinct OGT-Binding Sites Promote HCF-1 Cleavage. *PLoS One*. 2015 Aug 25;10(8):e0136636.
31. Daina A, Michielin O, **Zoete V**. iLOGP: A Simple, Robust, and Efficient Description of n-Octanol/Water Partition Coefficient for Drug Design Using the GB/SA Approach. *J Chem Inf Model*. 2014, 54(12):3284-301.

32. Chaskar P, **\*Zoete V**, Röhrig UF. Toward On-The-Fly Quantum Mechanical/Molecular Mechanical (QM/MM) Docking: Development and Benchmark of a Scoring Function. *J Chem Inf Model.* 2014, 54(11):3137-52.
33. Crisante G, Battista L, Iwaszkiewicz J, Nesca V, Mérrillat AM, Sergi C, **Zoete V**, Frateschi S, Hummler E. The CAP1/Prss8 catalytic triad is not involved in PAR2 activation and protease nexin-1 (PN-1) inhibition. *FASEB J.* 2014, 28(11):4792-805
34. Barras D, Chevalier N, **Zoete V**, Dempsey R, Lapouge K, Olayioye MA, Michielin O, Widmann C. A WxW Motif is required for the Anticancer Activity of TAT-RasGAP317-326. *J Biol Chem.*, 2014, 289(34):23701-11.
35. Röhrig, U.F.; Majjigapua, S.R.; Chambon, M.; Bron, S.; Pilotte, L.; Colau, D.; Van den Eynde, B.; Turcatti, G.; Vogel, P.; **\*Zoete, V.**; Michielin, O. Detailed Analysis and Follow-up Studies of a High-Throughput Screening for Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors. *Eur J Med Chem.* 2014,84:284-301.
36. Gfeller, D.; Grosdidier, A.; Wirth, M.; Daina, A.; Michielin, O.; **Zoete, V.** SwissTargetPrediction: a Web Server for Target Prediction of Bioactive Small Molecules. *Nucleic Acids Res.* 2014; 42(Web Server issue):W32-8.
37. Stockinger H, Altenhoff AM, Arnold K, Bairoch A, Bastian F, Bergmann S, Bougueleret L, Bucher P, Delorenzi M, Lane L, Mercier PL, Lisacek F, Michielin O, Palagi PM, Rougemont J, Schwede T, Mering Cv, Nimwegen Ev, Walther D, Xenarios I, Zavolan M, Zdobnov EM, **Zoete V**, Appel RD. Fifteen years SIB Swiss Institute of Bioinformatics: life science databases, tools and support. *Nucleic Acids Res.* 2014; 42(Web Server issue):W436-41.
38. Choudhary, V.; Darwiche, R.; Gfeller, D.; **Zoete, V.**; Michielin, O.; Schneiter, R. 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. *J. Lipid Res.* 2014, 55, 883–894.
39. Monaco, A.; **Zoete, V.**; Alghisi; G.C., Rüegg; C.; Michelin, O.; Prior, J.; Scapozza, L.; Seimille, Y. Synthesis and in vitro evaluation of a novel radioligand for  $\alpha\beta 3$  integrin receptor imaging: [18F]FPPA-c(RGDfK). *Bioorg Med Chem Lett.* 2013;23(22):6068-72.
40. Ding, J.; Loizides-Mangold, U.; Rando, G.; **Zoete, V.**; Michielin, O.; Reddy, J.K.; Wahli, W.; Riezman, H.; Thorens, B. The peroxisomal enzyme L-PBE is required to prevent the dietary toxicity of medium-chain fatty acids. *Cell Rep.* 2013;5(1):248-58.
41. **Zoete, V.**; Irving, M.; Ferber, M.; Cuendet, M.A.; Michielin, O. Structure-Based, Rational Design of T Cell Receptors. *Front Immunol.* 2013 Sep 12;4:268.
42. Gfeller, D.; Michielin, O.; **Zoete, V.** Shaping the interaction landscape of bioactive molecules. *Bioinformatics.* 2013;29(23):3073-9.
43. Gautschi, O.; Peters, S.; **Zoete, V.**; Aebersold-Keller, F.; Strobel, K.; Schwizer, B.; Hirschmann, A.; Michielin, O.; Diebold, J. Lung adenocarcinoma with BRAF G469L mutation refractory to vemurafenib. *Lung Cancer.* 2013;82(2):365-7.
44. Cabalzar, K.; Pelzer, C.; Wolf, A.; Lenz, G.; Iwaszkiewicz, J.; **Zoete, V.**; Hailfinger, S.; Thome, M. Monoubiquitination and activity of the paracaspase MALT1 requires glutamate 549 in the dimerization interface. *PLoS One.* 2013;8(8):e72051. doi: 10.1371/journal.pone.0072051.
45. Fagerberg, T.; **Zoete, V.**; Viatte, S.; Baumgaertner, P.; Alves, P.M.; Romero, P.; Speiser, D.E.; Michielin, O. Prediction of cross-recognition of peptide-HLA A2 by Melan-A-specific cytotoxic T lymphocytes using three-dimensional quantitative structure-activity relationships. *PLoS One.*;8(7):e65590.
46. Wirth, M.; Volkamer, A.; **Zoete, V.**; Rippmann, F.; Michielin, O.; Rarey, M.; Sauer, W.H. Protein pocket and ligand shape comparison and its application in virtual screening. *J Comput Aided Mol Des.* 2013;27(6):511-24.
47. Lapouge, K.; Perozzo, R.; Iwaszkiewicz, J.; Bertelli, C.; **Zoete, V.**; Michielin, O.; Scapozza, L.; Haas, D. RNA pentaloop structures as effective targets of regulators belonging to the RsmA/CsrA protein family. *RNA Biol.* 2013;10(6):1031-41.
48. Johansson, M.U.; **Zoete, V.**; Guex N. Recurrent structural motifs in non-homologous protein structures. *Int J Mol Sci.* 2013;14(4):7795-814.
49. Bensasson, R.V.; Sowlati-Hashjin, S.; **Zoete, V.**; Dauzonne, D.; Matta, C.F. Physicochemical properties of exogenous molecules correlated with their biological efficacy as protectors against carcinogenesis and inflammation. *Int. rev. in Phys. Chem.*, 2013;32(3),393-434.
50. Demierre, N.; **Zoete, V.**; Michielin, O.; Stauffer, E.; Zimmermann, D.R.; Betticher, D.C.; Peters, S. 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 Apr;80(1):81-4.
51. Ferber, M.; **\*Zoete, V.**; **\*Michielin, O.**; T-Cell Receptors Binding Orientation over Peptide/MHC Class I Is Driven by Long-Range Interactions. *PLoS One.* 2012;7(12):e51943.
52. Gfeller, D.; **\*Michielin, O.**; **\*Zoete, V.** SwissSidechain: a molecular and structural database of non- natural sidechains. *Nucleic Acids Res.* 2013, 41(D1):D327-32.
53. Wirth, M.; **\*Zoete, V.**; **\*Michielin, O.**; **\*Sauer, W.** SwissBioisostere: A database of molecular replacements for ligand design. *Nucleic Acids Res.* 2013, 41 (D1):D1137-43.

54. Karthikeyan, G.; Zambaldo, C.; Barluenga, S.; **Zoete, V.**; Karplus, M.; Winssinger, N. Asymmetric synthesis of pochonin E and F, revision of their proposed structure, and their conversion to potent Hsp90 inhibitors. *Chemistry* 2012, *18*, 8978–8986.
55. Irving, M.; **Zoete, V.**; Hebeisen, M.; Schmid, D.; Baumgartner, P.; Guillaume, P.; Romero, P.; Speiser, D.; Luescher, I.; Rufer, N.; Michielin, O. Interplay between T cell receptor binding kinetics and the level of cognate peptide presented by major histocompatibility complexes governs CD8+ T cell responsiveness. *J. Biol. Chem.* 2012, *287*, 23068–23078.
56. Gfeller, D.; **Zoete, V.**; Michielin, O. Expanding molecular modeling and design tools to non-natural sidechains. *J Comput Chem* 2012, *33*, 1525–1535.
57. Roehrig, U. F.; Majjigapu, S. R.; Grosdidier, A.; Bron, S.; Stroobant, V.; Pilotte, L.; Colau, D.; Vogel, P.; Van den Eynde, B. J.; **Zoete, V.**; Michielin, O.; Rational Design of 4-Aryl-1,2,3-Triazoles for Indoleamine 2,3-Dioxygenase 1 Inhibition. *J. Med. Chem.* 2012, 1–72.
58. Nikolaev, S. I.; Rimoldi, D.; Iseli, C.; Valsesia, A.; Robyr, D.; Gehrig, C.; Harshman, K.; Guipponi, M.; Bukach, O.; **Zoete, V.**; Michielin, O.; Muehlethaler, K.; Speiser, D.; Beckmann, J. S.; Xenarios, I.; Halazonetis, T. D.; Jongeneel, C. V.; Stevenson, B. J.; Antonarakis, S. E. Exome sequencing identifies recurrent somatic MAP2K1 and MAP2K2 mutations in melanoma. *Nat. Genet.* 2012, *44*, 133–139.
59. Johansson, M. U.; **Zoete, V.**; Michielin, O.; Guex, N. Defining and searching for structural motifs using DeepView/Swiss-PdbViewer. *Bmc Bioinformatics* 2012, *13*, 173.
60. Buey, R.M.; Sen, I.; Kortt, O.; Mohan, R.; Gfeller, D.; Veprintsev, D.; Kretschmar, I.; Scheuermann, J.; Neri, D.; **Zoete, V.**, Michielin, O.; de Pereda, J.M.; Akhmanova, A.; Volkmer, R., Steinmetz, M.O. Sequence determinants of a microtubule tip localization signal (MtLS). *J Biol Chem.* 2012;287(34):28227-42.
61. Sala, E.; Guasch, L.; Iwaskiewicz, J.; Mulero, M.; Salvadó, M.-J.; Blade, C.; Ceballos, M.; Valls, C.; **Zoete, V.**; Grosdidier, A.; Garcia-Vallvé, S.; Michielin, O.; Pujadas, G. 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. *Eur J Med Chem* 2011, *46*, 6098–6103.
62. Cuendet, M. A.; **Zoete, V.**; Michielin, O. How T cell receptors interact with peptide-MHCs: a multiple steered molecular dynamics study. *Proteins* 2011, *79*, 3007–3024.
63. <sup>1</sup>Bensasson, R. V.; **Zoete, V.**; Jossang, A.; Bodo, B.; Arimondo, P. B.; Land, E. J. Potency of inhibition of human DNA topoisomerase I by flavones assessed through physicochemical parameters. *Free Radic. Biol. Med.* 2011, *51*, 1406–1410.
64. **Zoete, V.**; Cuendet, M. A.; Grosdidier, A.; Michielin, O. SwissParam: a fast force field generation tool for small organic molecules. *J Comput Chem* 2011, *32*, 2359–2368.
65. Grosdidier, A.; **Zoete, V.**; Michielin, O. SwissDock, a protein-small molecule docking web service based on EADock DSS. *Nucleic Acids Res.* 2011, *39*, W270–7.
66. Grosdidier, A.; **Zoete, V.**; Michielin, O.; Fast docking using the CHARMM force field with EADock DSS. *J Comput Chem* 2011, *32*, 2149–2159.
67. Maillard, P. V.; **Zoete, V.**; Michielin, O.; Trono, D. Homology-based identification of capsid determinants that protect HIV1 from human TRIM5 $\alpha$  restriction. *J. Biol. Chem.* 2011, *286*, 8128–8140.
68. Bulliard, Y.; Narvaiza, I.; Bertero, A.; Peddi, S.; Röhrig, U. F.; Ortiz, M.; **Zoete, V.**; Castro-Díaz, N.; Turelli, P.; Telenti, A.; Michielin, O.; Weitzman, M. D.; Trono, D. Structure-function analyses point to a polynucleotide-accommodating groove essential for APOBEC3A restriction activities. *J. Virol.* 2011, *85*, 1765–1776.
69. Niel-Butschi, F.; Kantelip, B.; Iwaskiewicz, J.; **Zoete, V.**; Boimard, M.; Delpech, M.; Bourges, J.-L.; Renard, G.; D'Hermies, F.; Pisella, P.-J.; Hamel, C.; Delbosc, B.; Valleix, S. Genotype-phenotype correlations of TGFBI p.Leu509Pro, p.Leu509Arg, p.Val613Gly, and the allelic association of p.Met502Val-p.Arg555Gln mutations. *Mol. Vis.* 2011, *17*, 1192–1202.
70. Sala, E.; Guasch, L.; Iwaskiewicz, J.; Mulero, M.; Salvadó, M.-J.; Pinent, M.; **Zoete, V.**; Grosdidier, A.; Garcia-Vallvé, S.; Michielin, O.; Pujadas, G. Identification of human IKK-2 inhibitors of natural origin (part I): modeling of the IKK-2 kinase domain, virtual screening and activity assays. *PLoS ONE* 2011, *6*, e16903.
71. Leimgruber, A.; Ferber, M.; Irving, M.; Hussain-Kahn, H.; Wieckowski, S.; Derré, L.; Rufer, N.; **Zoete, V.**; Michielin, O. TCRRep 3D: an automated in silico approach to study the structural properties of TCR repertoires. *PLoS ONE* 2011, *6*, e26301.
72. Rahm, N.; Yap, M.; Snoeck, J.; **Zoete, V.**; Muñoz, M.; Radespiel, U.; Zimmermann, E.; Michielin, O.; Stoye, J.P.; Ciuffi, A.; Telenti, A. Unique spectrum of activity of prosimian TRIM5 $\alpha$  against exogenous and endogenous retroviruses. *J Virol.* 2011;85(9):4173-83.
73. **Zoete, V.**; Grosdidier, A.; Cuendet, M.; Michielin, O. Use of the FACTS solvation model for protein- ligand docking calculations. Application to EADock. *J. Mol. Recognit.* 2010, *23*, 457–461.

74. Bensasson, R. V.; **Zoete, V.**; Berthier, G.; Talalay, P.; Dinkova-Kostova, A. T. Potency ranking of triterpenoids as inducers of a cytoprotective enzyme and as inhibitors of a cellular inflammatory response via their electron affinity and their electrophilicity index. *Chem. Biol. Interact.* 2010, *186*, 118–126.
75. Schmid, D. A.; Irving, M. B.; Posevitz, V.; Hebeisen, M.; Posevitz-Fejfar, A.; Sarria, J.-C. F.; Gomez-Eerland, R.; Thome, M.; Schumacher, T. N. M.; Romero, P.; Speiser, D. E.; **Zoete, V.**; Michielin, O.; Rufer, N. Evidence for a TCR affinity threshold delimiting maximal CD8 T cell function. *J. Immunol.* 2010, *184*, 4936–4946.
76. Röhrig, U. F.; Awad, L.; Grosdidier, A.; Larrieu, P.; Stroobant, V.; Colau, D.; Cerundolo, V.; Simpson, A. J. G.; Vogel, P.; Van den Eynde, B. J.; **\*Zoete, V.**; **\*Michielin, O.**; Rational design of indoleamine 2,3-dioxygenase inhibitors. *J. Med. Chem.* 2010, *53*, 1172–1189.
77. Schüpbach, T.; **Zoete, V.**; Tsakam-Sotché, B.; Michielin, O. Fourier transform convolution integrals applied to generalized Born molecular volume. *J. Comput. Chem.* 2010, *31*, 649–659.
78. **Zoete, V.**; Irving, M. B.; Michielin, O. MM-GBSA binding free energy decomposition and T cell receptor engineering. *J. Mol. Recognit.* 2010, *23*, 142–152.
79. Hornitschek, P.; Lorrain, S.; **Zoete, V.**; Michielin, O.; Fankhauser, C. Inhibition of the shade avoidance response by formation of non-DNA binding bHLH heterodimers. *EMBO J.* 2009, *28*, 3893–3902.
80. Bulliard, Y.; Turelli, P.; Röhrig, U. F.; **Zoete, V.**; Mangeat, B.; Michielin, O.; Trono, D. Functional analysis and structural modeling of human APOBEC3G reveal the role of evolutionarily conserved elements in the inhibition of human immunodeficiency virus type 1 infection and Alu transposition. *J. Virol.* 2009, *83*, 12611–12621.
81. Röhrig, U. F.; Grosdidier, A.; **\*Zoete, V.**; **\*Michielin, O.** Docking to heme proteins. *J. Comput. Chem.* 2009, *30*, 2305–2315.
82. Grosdidier, A.; **\*Zoete, V.**; **\*Michielin, O.** Blind docking of 260 protein-ligand complexes with EADock 2.0. *J. Comput. Chem.* 2009, *30*, 2021–2030.
83. **Zoete, V.**; Grosdidier, A.; Michielin, O. Docking, virtual high throughput screening and in silico fragment-based drug design. *J. Cell. Mol. Med.* 2009, *13*, 238–248.
84. Derré, L.; Bruyninx, M.; Baumgaertner, P.; Ferber, M.; Schmid, D.; Leimgruber, A.; **Zoete, V.**; Romero, P.; Michielin, O.; Speiser, D. E.; Rufer, N. Distinct sets of alphabeta TCRs confer similar recognition of tumor antigen NY-ESO-1157-165 by interacting with its central Met/Trp residues. *PNAS* 2008, *105*, 15010–15015.
85. Rochat, B.; **Zoete, V.**; Grosdidier, A.; Grünigen, von, S.; Marull, M.; Michielin, O. In vitro biotransformation of imatinib by the tumor expressed CYP1A1 and CYP1B1. *Biopharm. Drug Dispos.* 2008, *29*, 103–118.
86. Bensasson, R. V.; **Zoete, V.** Two-step mechanism of induction of the gene expression of a prototypic cancer-protective enzyme by diphenols. *Chem. Res. Toxicol.* 2008, *21*, 805–812.
87. **\*Zoete, V.**; Grosdidier, A.; **\*Michielin, O.** Peroxisome proliferator-activated receptor structures: ligand specificity, molecular switch and interactions with regulators. *Biochim. Biophys. Acta* 2007, *1771*, 915–925.
88. Feige, J. N.; Gelman, L.; Rossi, D.; **Zoete, V.**; Métivier, R.; Tudor, C.; Anghel, S. I.; Grosdidier, A.; Lathion, C.; Engelborghs, Y.; Michielin, O.; Wahli, W.; Desvergne, B. The endocrine disruptor monoethyl-hexyl-phthalate is a selective peroxisome proliferator-activated receptor gamma modulator that promotes adipogenesis. *J. Biol. Chem.* 2007, *282*, 19152–19166.
89. **Zoete, V.**; Michielin, O. 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* 2007, *67*, 1026–1047.
90. **<sup>1</sup>Grosdidier, A.**; **<sup>1</sup>Zoete, V.**; Michielin, O. EADock: docking of small molecules into protein active sites with a multiobjective evolutionary optimization. *Proteins* 2007, *67*, 1010–1025.
91. **<sup>1</sup>Michalik, L.**; **<sup>1</sup>Zoete, V.**; Krey, G.; Grosdidier, A.; Gelman, L.; Chodanowski, P.; Feige, J. N.; Desvergne, B.; Wahli, W.; Michielin, O. Combined simulation and mutagenesis analyses reveal the involvement of key residues for peroxisome proliferator-activated receptor alpha helix 12 dynamic behavior. *J. Biol. Chem.* 2007, *282*, 9666–9677.
92. Derré, L.; Ferber, M.; Touvrey, C.; Devevre, E.; Zoete, V.; Leimgruber, A.; Romero, P.; Michielin, O.; Lévy, F.; Speiser, D. E. A novel population of human melanoma-specific CD8 T cells recognizes Melan-AMART-1 immunodominant nonapeptide but not the corresponding decapeptide. *J. Immunol.* 2007;179(11):7635–45.
93. Zhang, K.-L.; Mangeat, B.; Ortiz, M.; **Zoete, V.**; Trono, D.; Telenti, A.; Michielin, O. Model structure of human APOBEC3G. *PLoS ONE* 2007, *2*, e378.
94. **\*Zoete, V.**; **\*Meuwly, M.** Importance of individual side chains for the stability of a protein fold: computational alanine scanning of the insulin monomer. *J. Comput. Chem.* 2006, *27*, 1843–1857.
95. Koch, M.; Schmid, F. F.-F.; **Zoete, V.**; Meuwly, M. Insulin: a model system for nanomedicine? *Nanomedicine (Lond)* 2006, *1*, 373–378.

96. Yip, Y. L.; **Zoete, V.**; Scheib, H.; Michielin, O. Structural assessment of single amino acid mutations: application to TP53 function. *Hum. Mutat.* 2006, *27*, 926–937.
97. Thorsteinsdottir, H. B.; Schwede, T.; **Zoete, V.**; Meuwly, M. How inaccuracies in protein structure models affect estimates of protein-ligand interactions: Computational analysis of HIV-1 protease inhibitor binding. *Proteins* 2006, *65*, 407–423.
98. **Zoete, V.**; Meuwly, M.; Karplus, M. Study of the insulin dimerization: binding free energy calculations and per-residue free energy decomposition. *Proteins* 2005, *61*, 79–93.
99. Moulin, E.; **Zoete, V.**; Barluenga, S.; Karplus, M.; Winssinger, N. Design, synthesis, and biological evaluation of HSP90 inhibitors based on conformational analysis of radicicol and its analogues. *J. Am. Chem. Soc.* 2005, *127*, 6999–7004.
100. Ladinig, M.; Leupin, W.; Meuwly, M.; Respondek, M.; Wirz, J.; **Zoete, V.** Protonation equilibria of Hoechst 33258 in aqueous solution. *Helvetica chimica*, 2005, *88*, 53–67.
101. **Zoete, V.**; Meuwly, M.; Karplus, M. A comparison of the dynamic behavior of monomeric and dimeric insulin shows structural rearrangements in the active monomer. *J. Mol. Biol.* 2004, *342*, 913–929.
102. **Zoete, V.**; Meuwly, M. Double proton transfer in the isolated and DNA-embedded guanine- cytosine base pair. *J Chem Phys* 2004, *121*, 4377–4388.
103. **Zoete, V.**; Rougée, M.; Dinkova-Kostova, A. T.; Talalay, P.; Bensasson, R. V. Redox ranking of inducers of a cancer-protective enzyme via the energy of their highest occupied molecular orbital. *Free Radic. Biol. Med.* 2004, *36*, 1418–1423.
104. **Zoete, V.**; Meuwly, M.; Karplus, M. Investigation of glucose binding sites on insulin. *Proteins* 2004, *55*, 568–581.
105. **Zoete, V.**; Meuwly, M. On the influence of semirigid environments on proton transfer along molecular chains. *J Chem Phys* 2004, *120*, 7085–7094.
106. **Zoete, V.**; Michielin, O.; Karplus, M. Protein-ligand binding free energy estimation using molecular mechanics and continuum electrostatics. Application to HIV-1 protease inhibitors. *J. Comput. Aided Mol. Des.* 2003, *17*, 861–880.
107. Michielin, O.; **Zoete, V.**; Gierasch, T. M.; Eckstein, J.; Napper, A.; Verdine, G.; Karplus, M. Conformational analysis of a stereochemically complete set of cis-enediol peptide analogues. *J. Am. Chem. Soc.* 2002, *124*, 11131–11141.
108. **Zoete, V.**; Michielin, O.; Karplus, M. Relation between sequence and structure of HIV-1 protease inhibitor complexes: a model system for the analysis of protein flexibility. *J. Mol. Biol.* 2002, *315*, 21–52.
109. Bailly, F.; **Zoete, V.**; Vamecq, J.; Catteau, J. P.; Bernier, J. L. Antioxidant actions of ovoidiol-derived 4-mercaptoimidazoles: glutathione peroxidase activity and protection against peroxynitrite- induced damage. *FEBS Lett.* 2000, *486*, 19–22.
110. **Zoete, V.**; Maglia, F.; Rougée, M.; Bensasson, R. V. Mechanism of action in a 4,5-diarylpyrrole series of selective cyclooxygenase-2 inhibitors. *Free Radic. Biol. Med.* 2000, *28*, 1638–1641.
111. **Zoete, V.**; Bailly, F.; Vezin, H.; Teissier, E.; Duriez, P.; Fruchart, J. C.; Catteau, J. P.; Bernier, J. L. 4- Mercaptoimidazoles derived from the naturally occurring antioxidant ovoidiols 1. Antioxidant properties. *Free Radic. Res.* 2000, *32*, 515–524.
112. **Zoete, V.**; Vezin, H.; Bailly, F.; Vergoten, G.; Catteau, J. P.; Bernier, J. L. 4-Mercaptoimidazoles derived from the naturally occurring antioxidant ovoidiols 2. Computational and experimental approach of the radical scavenging mechanism. *Free Radic. Res.* 2000, *32*, 525–533.
113. **Zoete, V.**; Bailly, F.; Maglia, F.; Rougée, M.; Bensasson, R. V. Molecular orbital theory applied to the study of nonsteroidal anti-inflammatory drug efficiency. *Free Radic. Biol. Med.* 1999, *26*, 1261– 1266.
114. **Zoete, V.**; Bailly, F.; Catteau, J. P.; Bernier, J. L. Design, synthesis and antioxidant properties of ovoidiol-derived 4-mercaptoimidazoles. *Journal of the Chemical Society - Perkin Trans 1* 1998, *20*, 2983–2988.

## Patents

1. Keratan sulfate specific transporter molecules. *WO2015162287A1*.
2. C6S specific transporter molecules. *WO2015162285A1*.
3. IDO inhibitors and therapeutic uses thereof. *WO2011045341A1*
4. Electrical conductor based on proton conducting carbon nanotubes. *EP1575102A1*.
5. *Multispecific mutated antibody fab fragments*. *US20140242076A1*, *WO2013005194A2*, *WO2013005194A3*.

## Book Chapters

1. U. F. Röhrig, \* V. Zoete, \* O. Michielin, \* Inhibitors of the Kynurenine Pathway, Topics in Medicinal Chemistry, M. Waring (Ed.), Springer, Berlin, Heidelberg (2017).

2. Chapter 10: Molecular Modeling of Proteins: From Simulations to Drug Design Applications. Zoete V, Cuendet M, Röhrig UF, Grosdidier A, Michielin O. In "Bioinformatics. A Swiss Perspective". Editors Appel RD and Feytmans E, World Scientific Publishing Co., Singapore.
3. Chapter 19: Molecular Dynamics-based Free Energy Simulations. Cuendet M, Zoete V, Michielin O. In "Computational Structural Biology". Editors Schwede T and Peitsch M, World Scientific Publishing Co., Singapore.