

Publications List - Vincent ZOETE

¹: co-first author

*: co-corresponding author

1. **Zoete V¹***, 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.
2. 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.
3. Röhrig UF, Majjigapu SR, Caldelari D, Dilek N, Reichenbach P, Ascencao K, Irving M, Coukos G, Vogel P, **Zoete V¹***, Michielin O. 1,2,3-Triazoles as inhibitors of indoleamine 2,3-dioxygenase 2 (IDO2). *Bioorganic & Medicinal Chemistry Letters*, 2016, 26(17):4330-3.
4. Bensasson RV, Dinkova-Kostova AT, Zheng S, Saito A, Li W, **Zoete V¹***; 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.
5. Daina, A.; **Zoete, V.**; A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem*, 2016, 11(11), 1117-1121.
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9. Gfeller D, **Zoete V**. Protein Homology Reveals New Targets for Bioactive Small Molecules. *Bioinformatics*. 2015, 31(16):2721-7.
10. 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.
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Submitted Papers

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97. Daina A, Blatter MC, Baillie Gerritsen V, Palagi PM, Marek D, Xenarios I, Schwede T, Michielin O, **Zoete V.** Introducing computer-aided drug design to a wide public using a new free web-based tool. Submitted to *J. Chem. Educ.*
98. Chaskar P., **Zoete V.***, Röhrig U. On-the-fly QM/MM Docking with Attracting Cavities. Submitted to *J. Chem. Inf. Model.*
99. Daina A, Michielin O, **Zoete V.** SwissADME: a free web tool to evaluate pharmacokinetics, druglikeness and medicinal chemistry friendliness. Submitted to *Sci. Rep.*

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*.
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