| **Aminotransferase** | | | |
| --- | --- | --- | --- |
| in silico: Zeroshot - May 08, 2023 to May 28, 2023 | | | |
| **Acknowledgements:**  We thank Prof. Dr. U.T. Bornscheuer and M.Sc. M. J. Menke from the University of Greifswald, Dept. of Biotechnology & Enzyme Catalysis for contributing a dataset on activity data of transaminase-catalyzed conversion of bulky substrates to our Protein Engineering Tournament. | | | |
| **Citation:**  This dataset is not published (yet) in any scientific journal. Please use the citation: "Menke, M. J.; Bornscheuer, U. T. Activity data of quadruple mutants of 3FCR\_4M transaminase for bulky substrates. 2023" | | | |
| **Additional documentation and resources:**   * Transaminase engineering based on related data: „Ao, Y.-F.; Pei, S.; Xiang, C.; Menke, M. J.; Shen, L.; Sun, C.; Dӧrr, M.; Born, S.; Hӧhne, M.; Bornscheuer, U. T. Structure- and data-driven protein engineering of transaminases for improving activity and stereoselectivity. Angew. Chem. Int. Ed. 2023, 62, e20230166“. * The 3DM tool to plan the mutations: „Kuipers, R.K.P., Joosten, H.-J., Verwiel, E., Paans, S., Akerboom, J., van der Oost, J., Leferink, N.G.H., van Berkel, W.J.H., Vriend, G. and Schaap, P.J. (2009), Correlated mutation analyses on super-family alignments reveal functionally important residues. Proteins, 76: 608-616. https://doi.org/10.1002/prot.22374“ | | | |
| **Challenge Problem:**  Score how active you predict each variant is for each of the three substrates (e.g. log probabilities). The range of scoring is arbitrary. | | | |
| **Sequence Length:**  466 | **Mutation(s):**  Yes | **Classification:**  TRANSFERASE | **PDB Xtal Structure:**  3FCR |
| **Expression System:** Escherichia coli | | **Organism(s):** Ruegeria sp. TM1040 | |
| **Target Sequence:**  MLKNDQLDQWDRDNFFHPSTHLAQHARGESANRVIKTASGVFIEDRDGTKLLDAFAGLWCVNVGYGRQEIAEAIADQARELAYYHSFVGHGTEASITLAKMILDRAPKNMSKVYFGLGGSDANETNVKLIWYYNNILGRPEKKKIISRWRGFHGSGLVTGSLTGLELFHKKFDLPVEQVIHTEAPYYFRREDLNQTEEQFVAHCVAELEALIEREGADTIAAFIGEPILGAGGIVPPPAGYWEAIQTVLNKHDILLVADEVVTGFGRLGTMFGSDHYGLEPDIITIAKGLTSAYAPLSGSIVSDKVWKVLEQGTDENGPIGHGWTYSAHPIGAAAGVANLKLLDELNLVSNAGEVGAYLNATMAEALSQHANVGDVRGEGLLCAVEFVKDRDSRTFFDAADKIGPQISAKLLEQDKIIARAMPQGDILGFAPPFCLTRAEADQVVEGTLRAVKAVLGSLEHHHHHH | | | |
| **Substrates (Amino donors):**   * S-Phenylethylamine * (4-Chlorophenyl)phenylmethanamine * 1,3-Diphenyl-propane-1-amine | | | |