

# Approximations of binding affinity of CellTalkDB sequences with AutoDock Vina

Pete Rigas

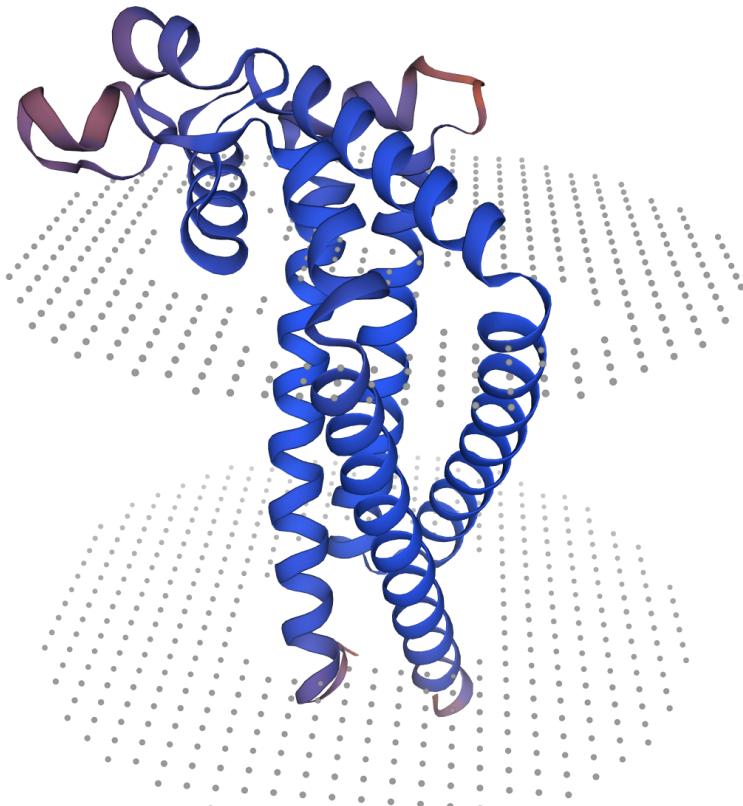


Figure 1: Receptor CD63

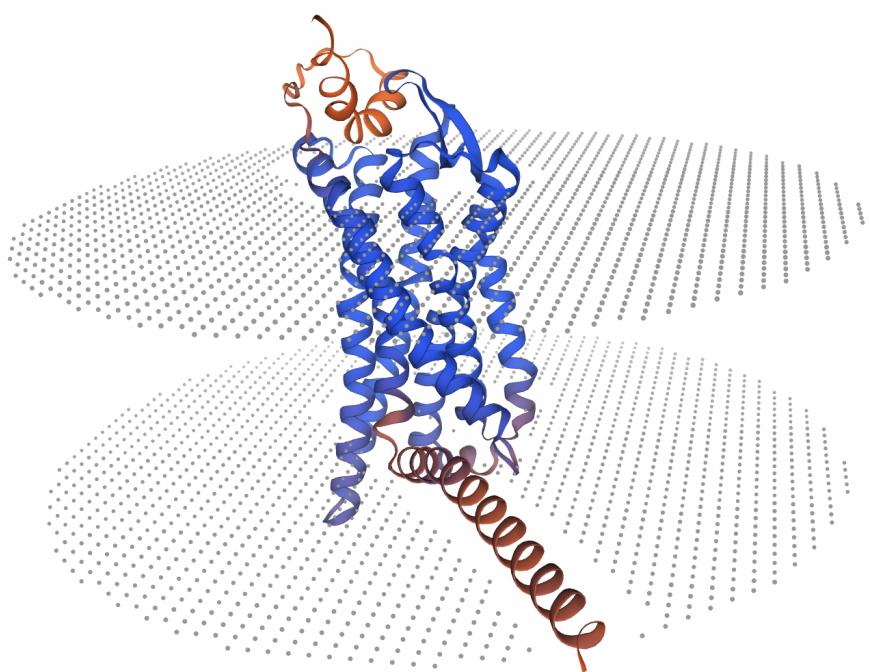


Figure 2: Receptor AGTR2

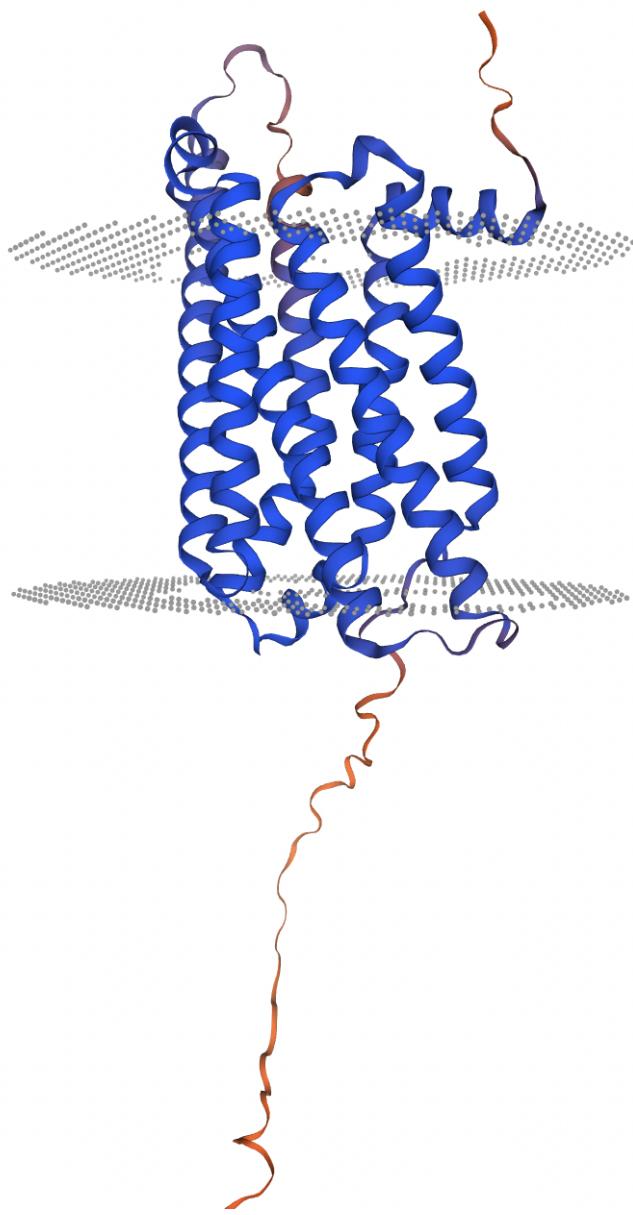


Figure 3: Receptor MC3R

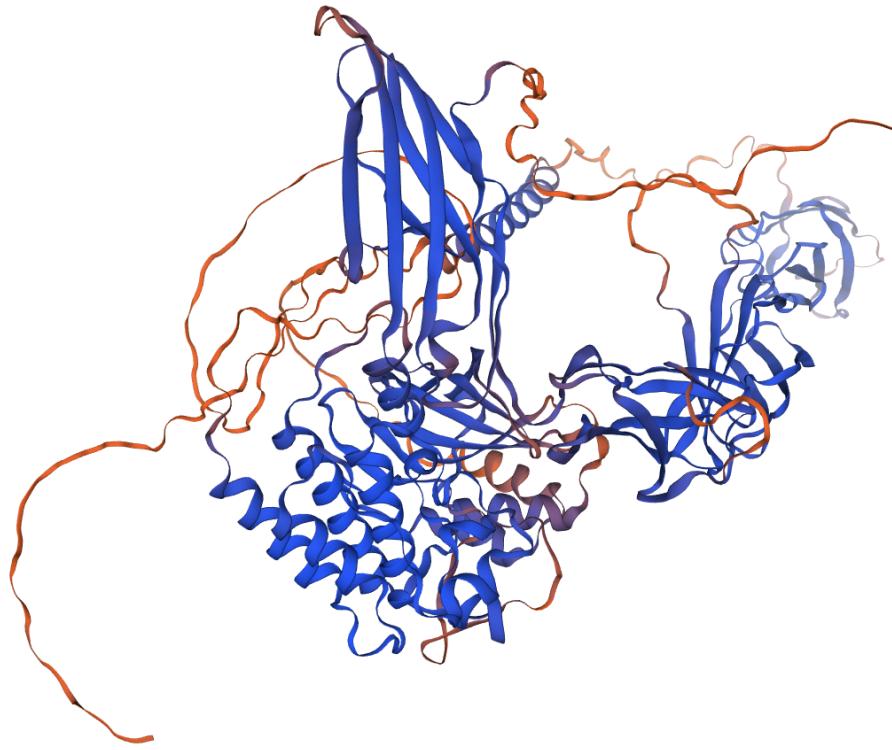


Figure 4: Receptor APCD1

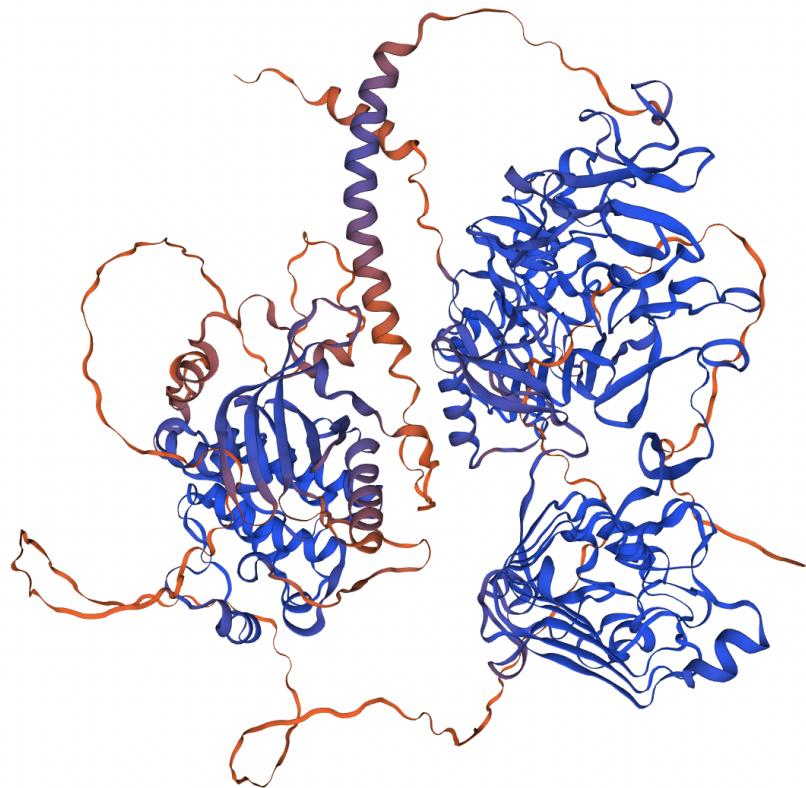


Figure 5: Receptor EGFR

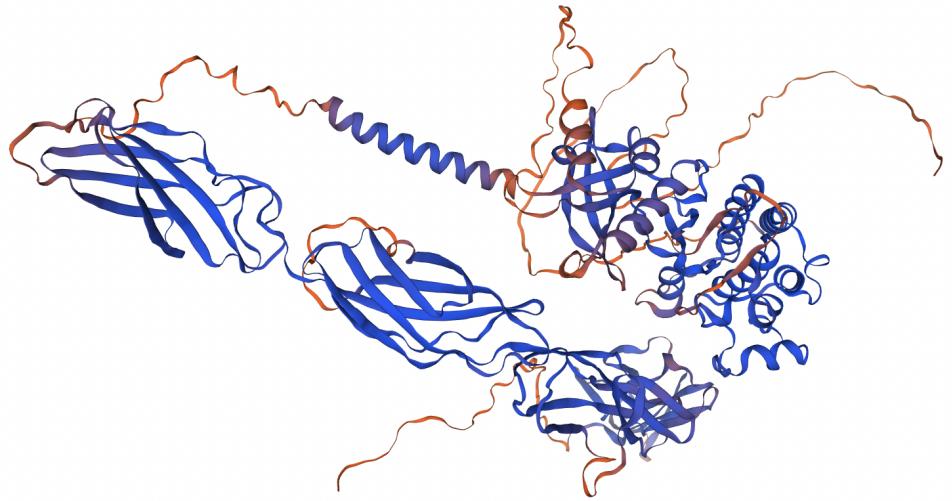


Figure 6: Receptor UFO

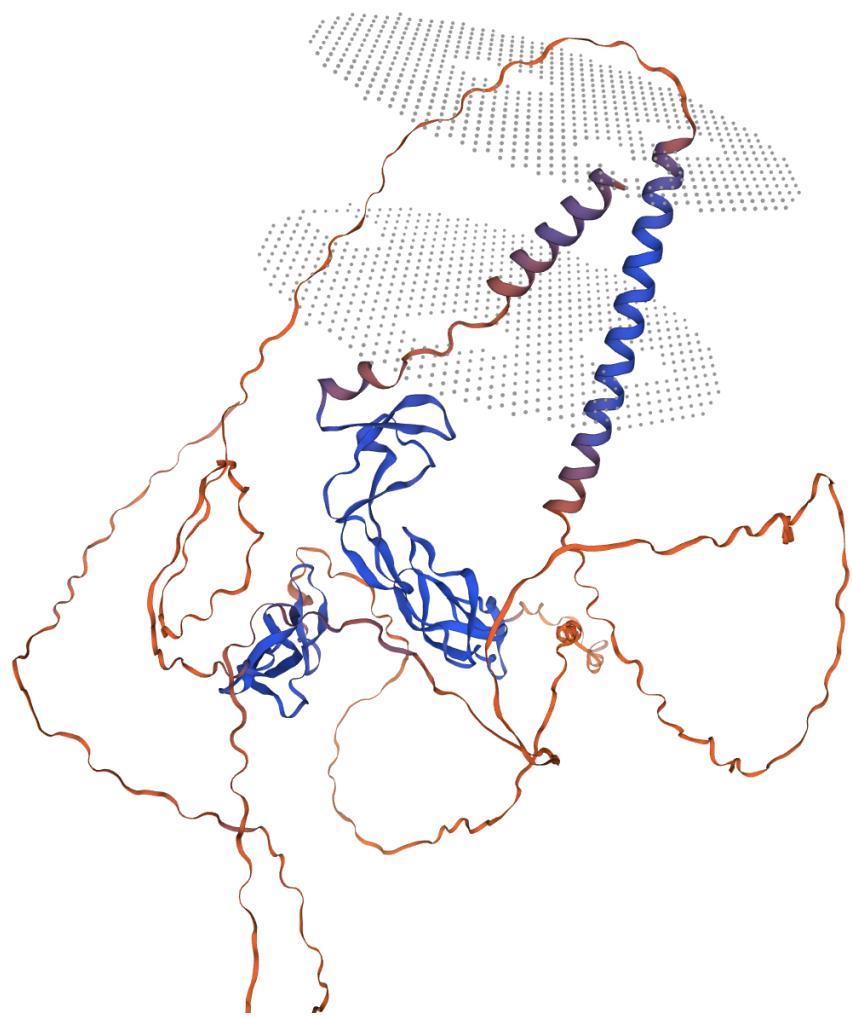


Figure 7: Receptor TNR8

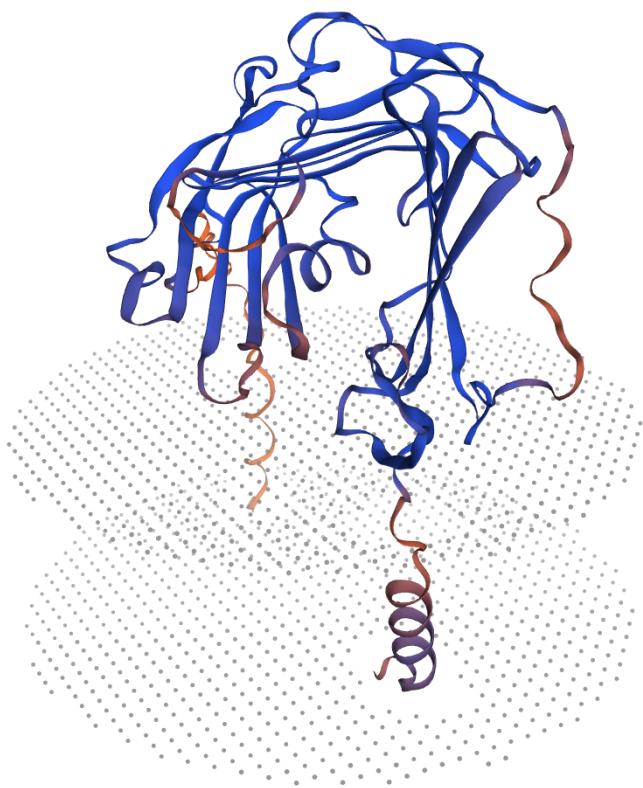


Figure 8: Receptor UPAR

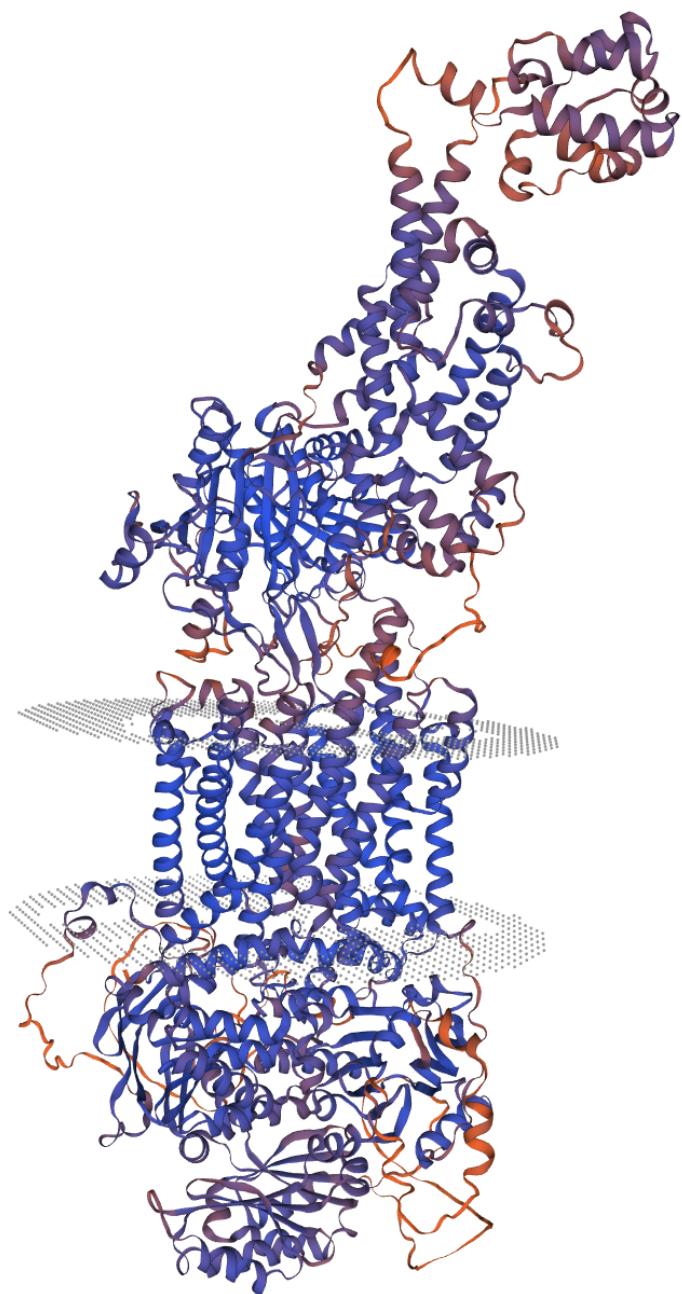


Figure 9: Receptor ABCA1

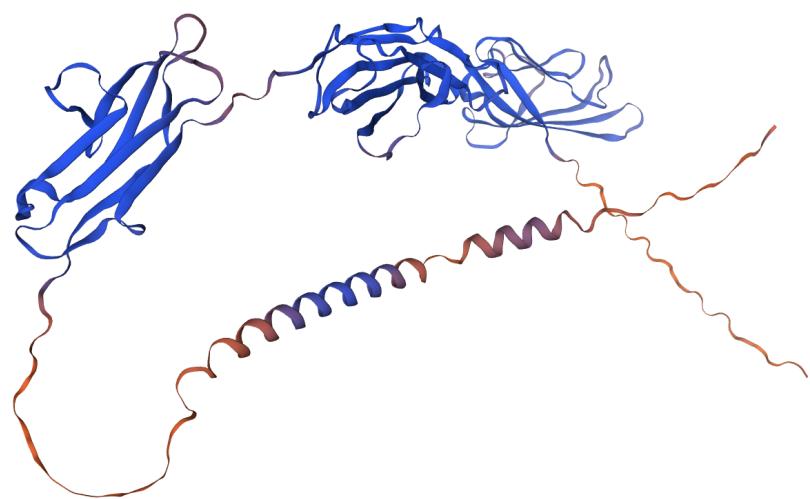


Figure 10: Receptor RAGE

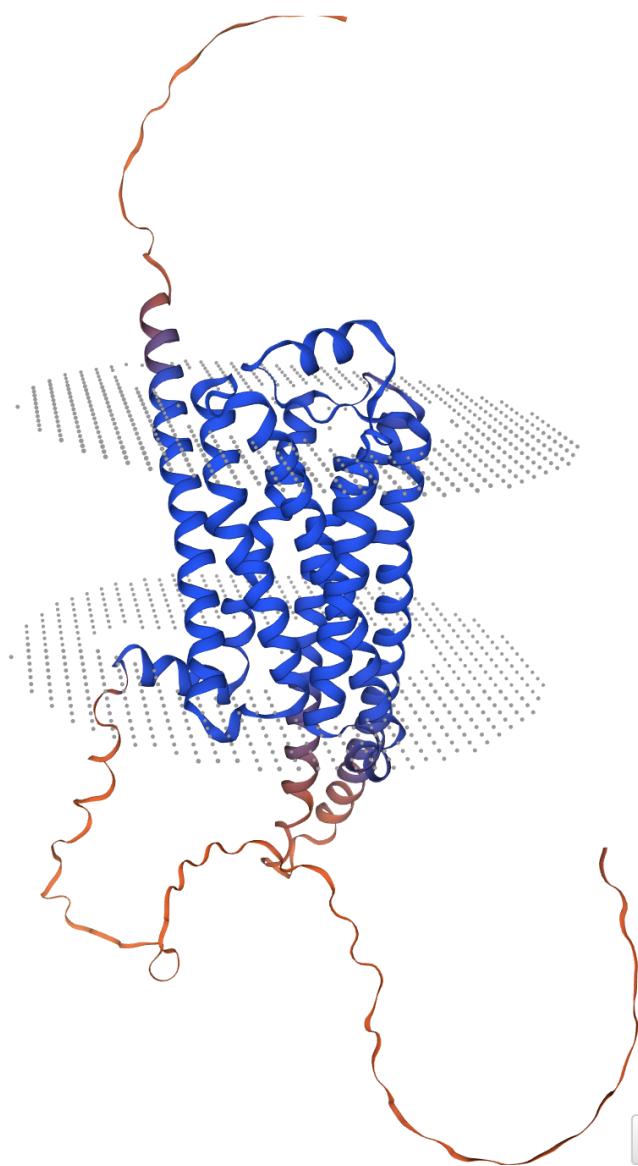


Figure 11: Receptor ADRB2

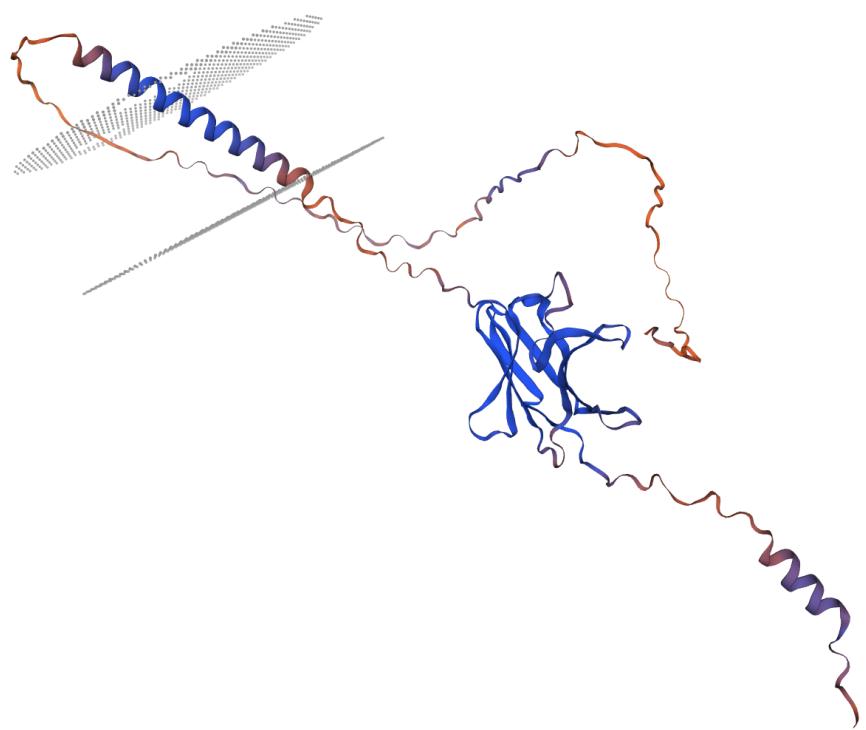


Figure 12: Receptor PDCD1

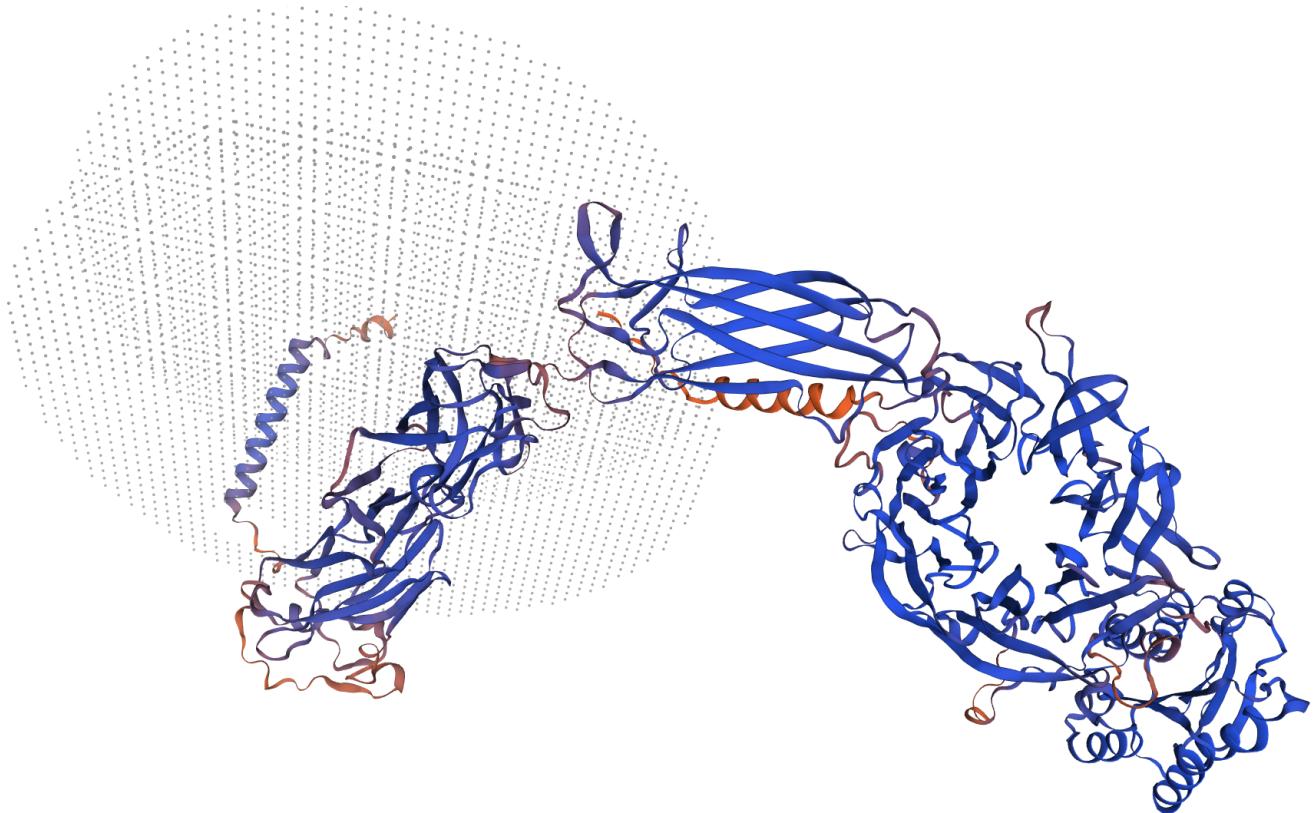


Figure 13: Receptor ITA1

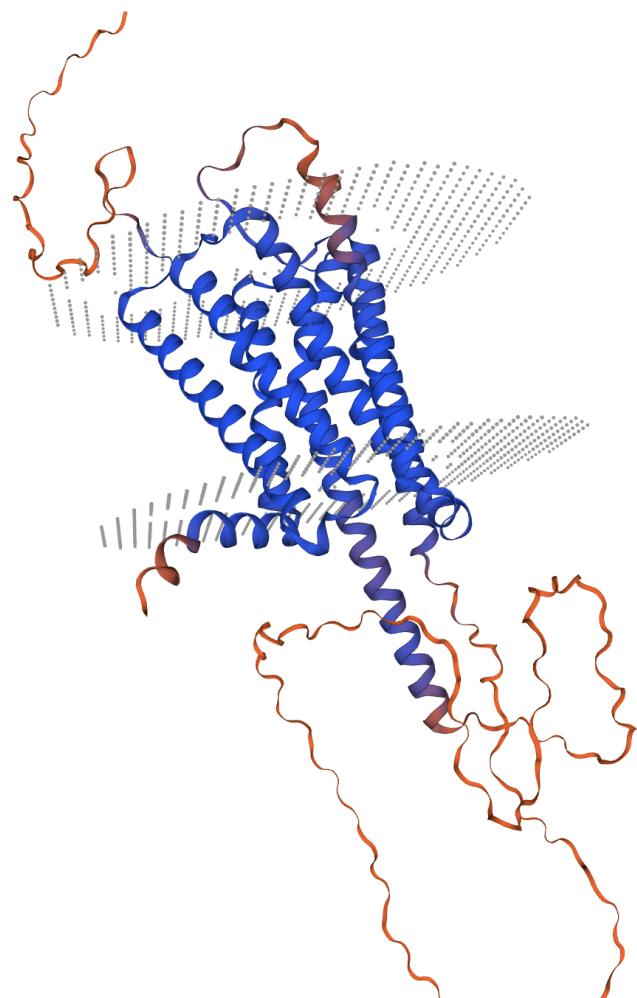


Figure 14: Receptor ADA2A

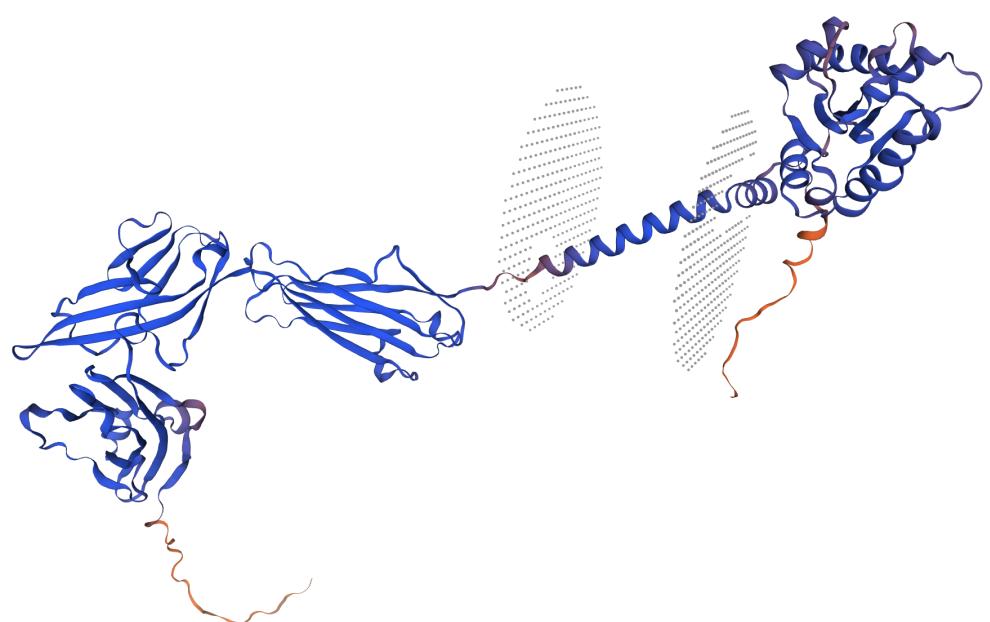


Figure 15: Receptor IL1AP

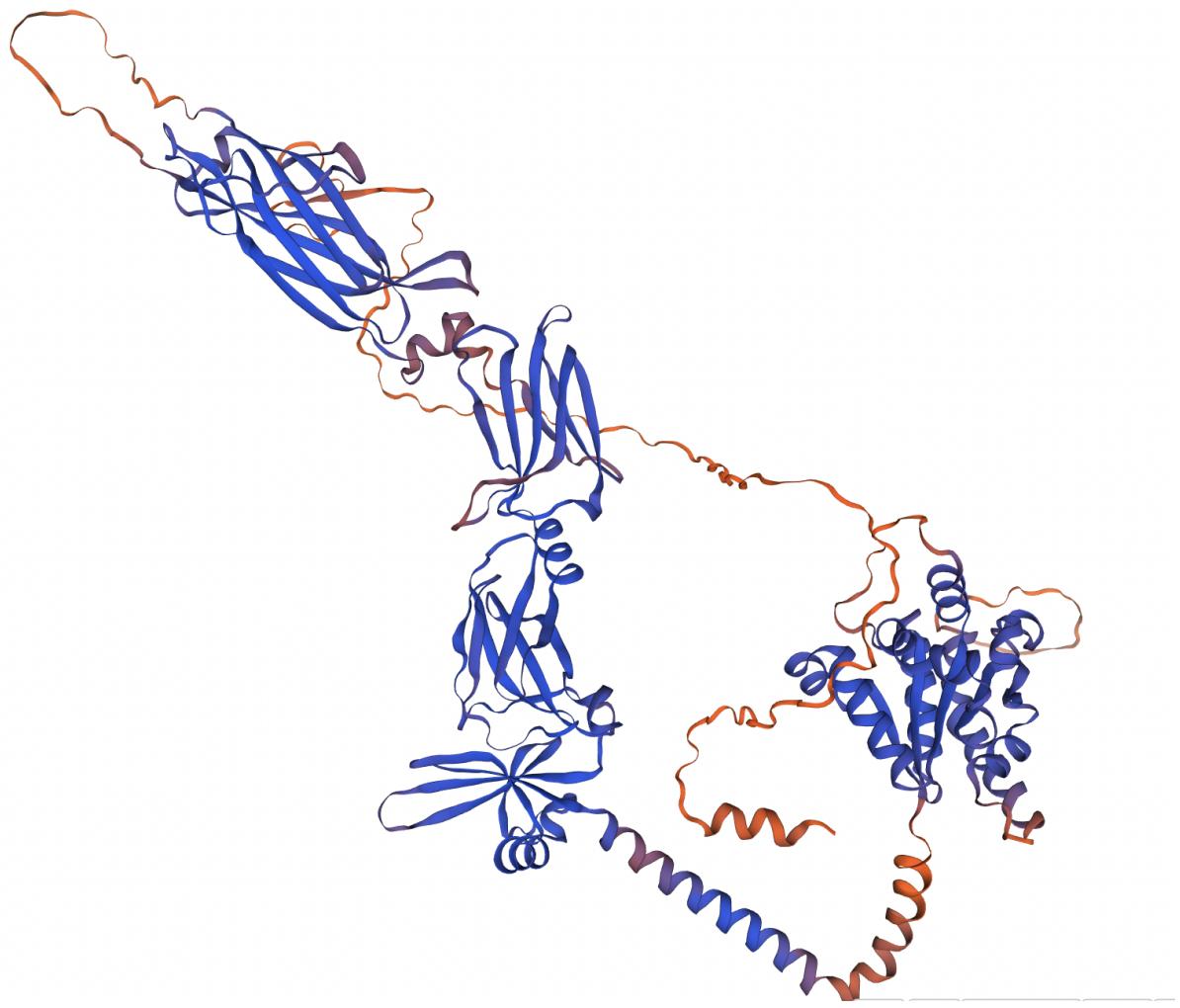


Figure 16: Receptor L17RC



Figure 17: Receptor INLR1

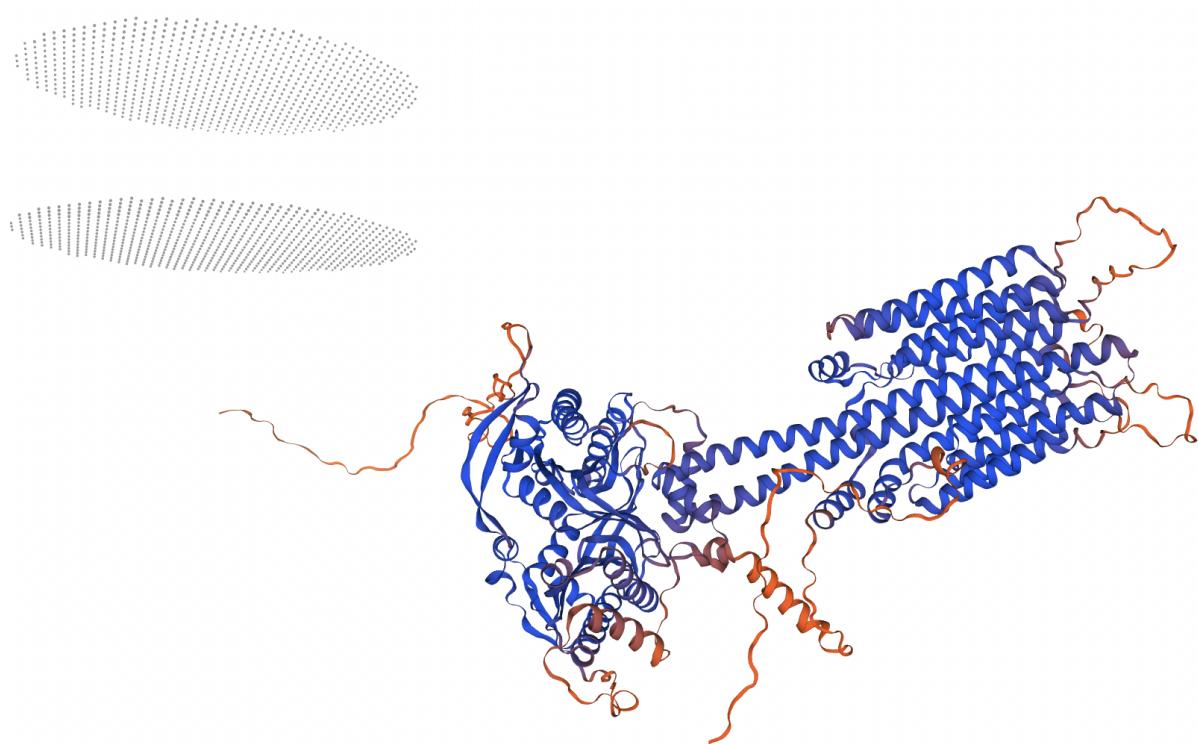


Figure 18: Receptor ADCY1

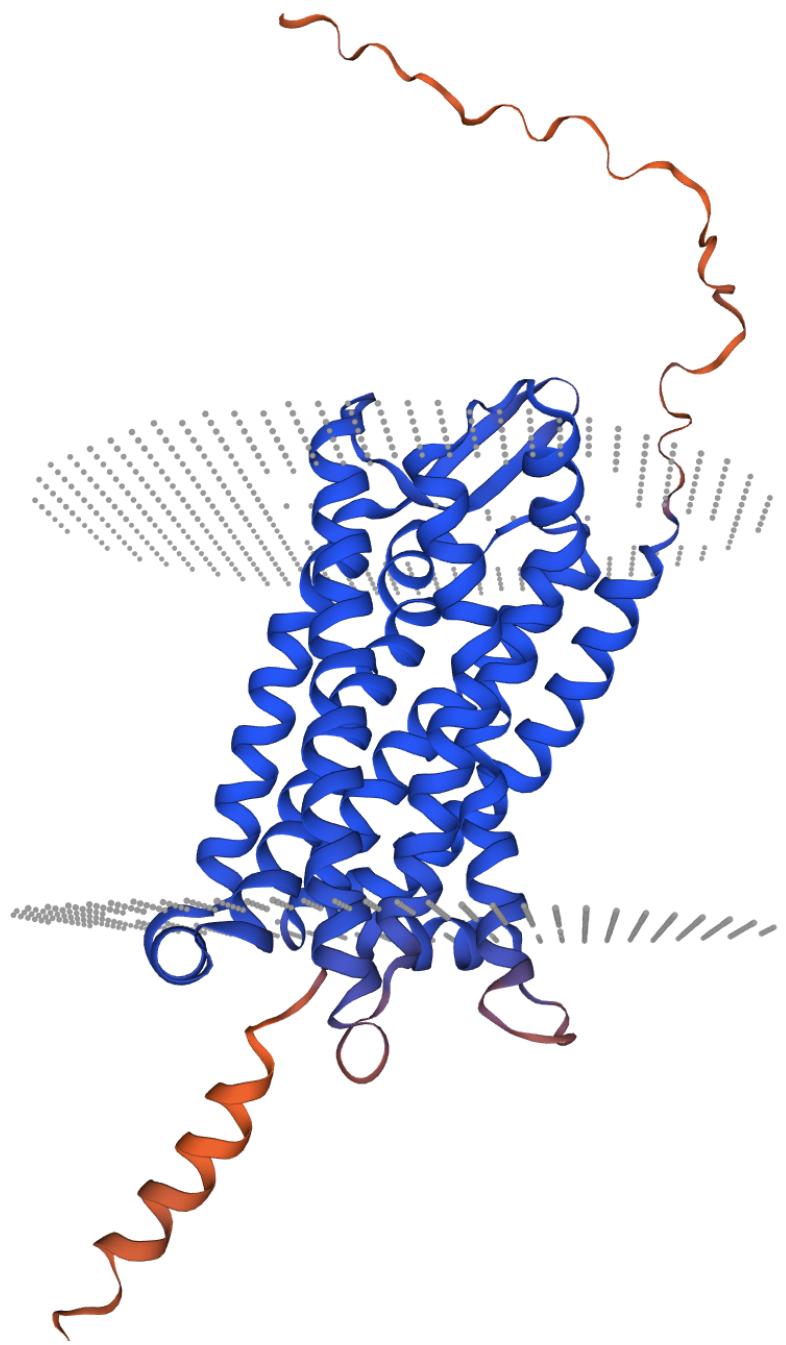


Figure 19: Receptor C5AR1

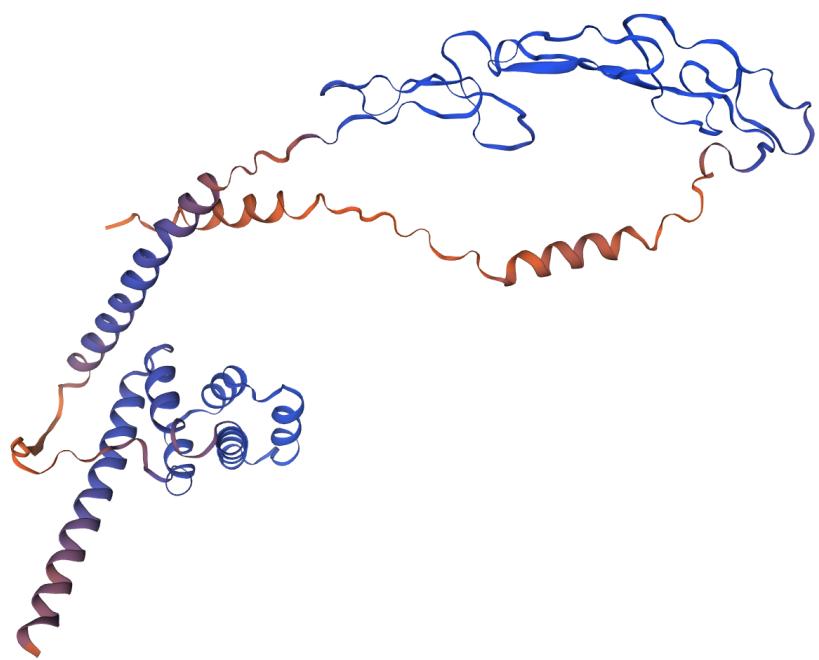


Figure 20: Receptor TNR6

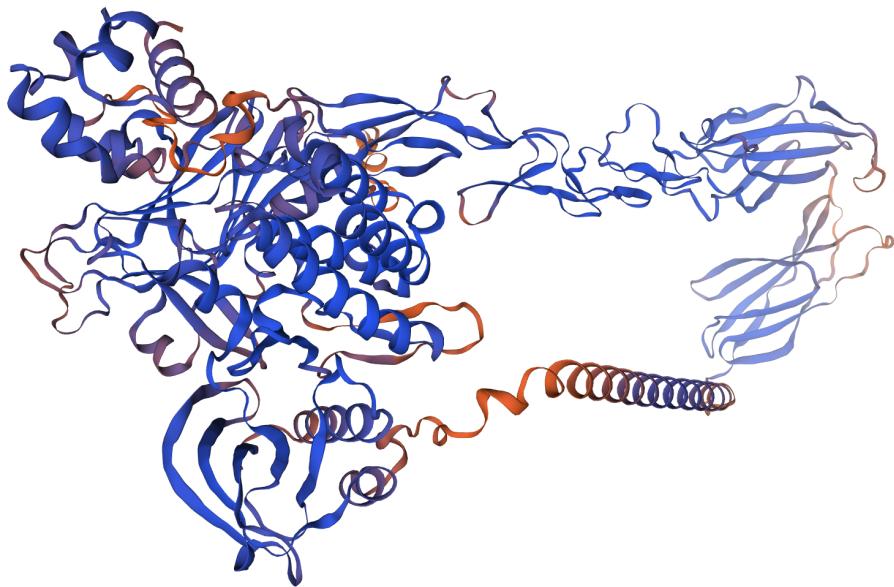


Figure 21: Receptor EPHA1

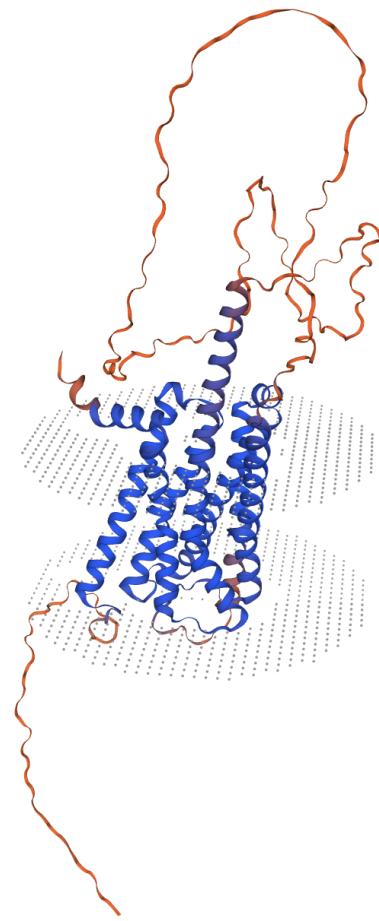


Figure 22: Receptor ADA2A

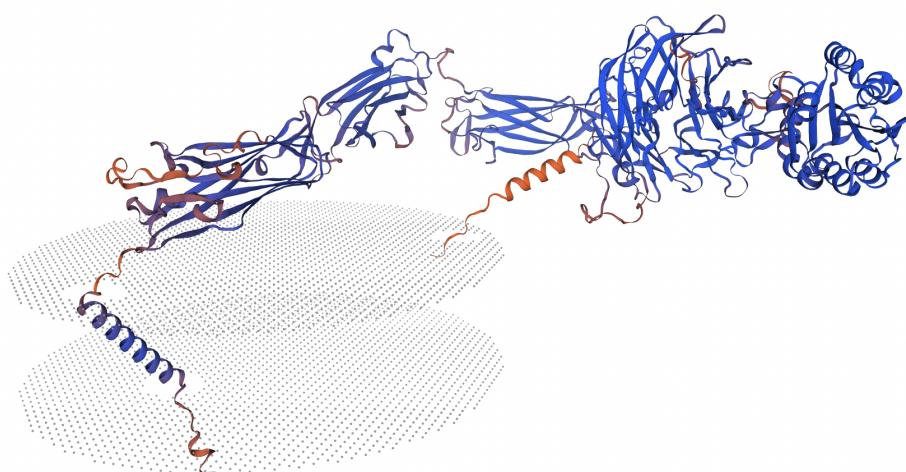


Figure 23: Receptor ITA1

# 1 References

- [1] Bienert, S., Waterhouse, A., de Beer, T.A.P., Tauriello, G., Studer, G., Bordoli, L., Schwede, T. The SWISS-MODEL Repository - new features and functionality. *Nucleic Acids Res.* **45**, D313-D319 (2017).
- [2] Benkert, P., Biasini, M., Schwede, T. Toward the estimation of the absolute quality of individual protein structure models. *Bioinformatics* **27**, 343-350 (2011).
- [3] Bertoni, M., Kiefer, F., Biasini, M., Bordoli, L., Schwede, T. Modeling protein quaternary structure of homo- and hetero-oligomers beyond binary interactions by homology. *Scientific Reports* **7** (2017).
- [4] Guex, N., Peitsch, M.C., Schwede, T. Automated comparative protein structure modeling with SWISS-MODEL and Swiss-PdbViewer: A historical perspective. *Electrophoresis* **30**, S162-S173 (2009).
- [5] Karplus, M., McCammon, J.A. Molecular dynamics simulations of biomolecules. *Nature Structural Biology* **9**: 646-652 (2002).
- [6] Karplus, M., Kuriyan, J. Molecular dynamics and protein function. *PNAS* **102** (19): 6679-6685 (2005).
- [7] Phillips, J.C. et al. Scalable molecular dynamics with NAMD. *Journal of Computational Chemistry* **26**(16): 1781-1802 (2005).
- [8] Mariani, V., Biasini, M., Barbato, A., Schwede, T. lDDT: a local superposition-free score for comparing protein structures and models using distance difference tests. *Bioinformatics* **29**, 2722-2728 (2013).
- [9] Sutmann, G. Classical Molecular Dynamics. *NIC Series* **10**: 211-254 (2002).
- [10] Shao X, Liao J, Li C, Lu X, Cheng J, Fan X. CellTalkDB: a manually curated database of ligand-receptor interactions in humans and mice. *Brief Bioinform.* 2021 Jul 20;22(4):bbaa269. doi: 10.1093/bib/bbaa269. PMID: 33147626.
- [11] Studer, G., Biasini, M., Schwede, T. Assessing the local structural quality of transmembrane protein models using statistical potentials (QMEANBrane), *Bioinformatics* **30**, i505–i511 (2014).
- [12] Studer, G., Tauriello, G., Bienert, S., Biasini, M., Johner, N., Schwede, T. ProMod3 - A versatile homology modelling toolbox. *PLOS Comp. Biol.* **17**(1), e1008667 (2021).
- [13] Studer, G., Rempfer, C., Waterhouse, A.M., Gumienny, R., Haas, J., Schwede, T. QMEANDisCo - distance constraints applied on model quality estimation. *Bioinformatics* **36**, 1765-1771 (2020).
- [14] Toukan, K., Rahman, A. Molecular-dynamics study of atomic motions in water. *Physical Review B* **31**:5 (1985).
- [15] Vlachakis, D., Bencurova, E., Papangelopoulos, N., Kossida, S. Chapter Seven- Current State-of-the-Art Molecular Dynamics Methods and Applications. *Science Direct* **94** : 269-313 (2014).
- [16] Volter, A.F. A method for accelerating the molecular dynamics simulation of infrequent events. *The Journal of Chemical Physics* **106**: 4665-4677 (1997).
- [17] van Gunsteren, W.F., Berendsen, H.J.C. Computer Simulation of Molecular Dynamics: Methodology, Applications, and Perspectives in Chemistry. *Angewandte Chemie International* **29**(9): 992-1023 (1990).
- [18] Waterhouse, A., Bertoni, M., Bienert, S., Studer, G., Tauriello, G., Gumienny, R., Heer, F.T., de Beer, T.A.P., Rempfer, C., Bordoli, L., Lepore, R., Schwede, T. SWISS-MODEL: homology modelling of protein structures and complexes. *Nucleic Acids Res.* **46**, W296-W303 (2018).