molecules

MDPI

Supplementary material

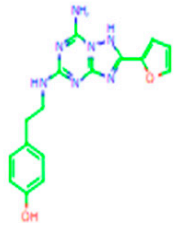
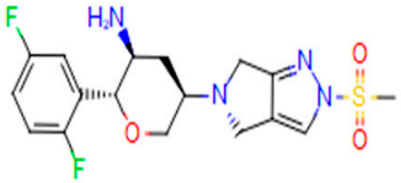
	Molecule				VIDA ID	FRED Chemgauss4 score
1	Unnamed molecule 	·	·	·	6	
2	Fragment 	·	·	·	8	-8.3346

Figure S1. Docking score of OMR (Fragment No#2) relative to the receptor ligand.

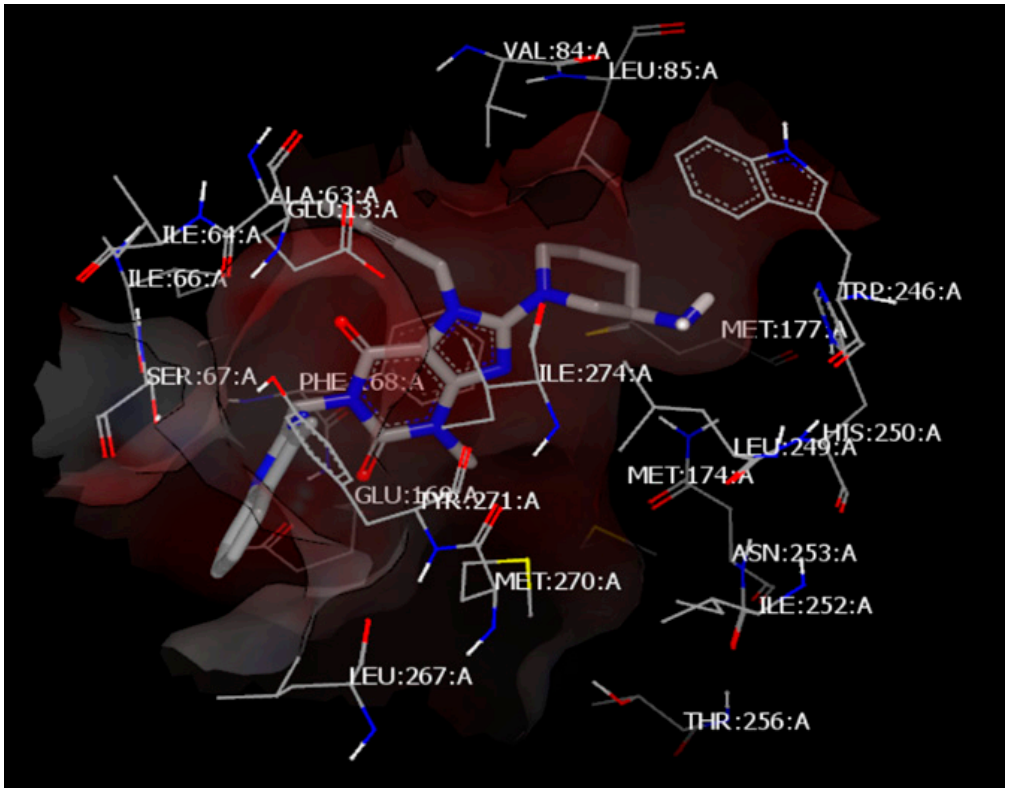


Figure S2. Predicted binding mode of alogliptin with 3PWH of A2AAR.

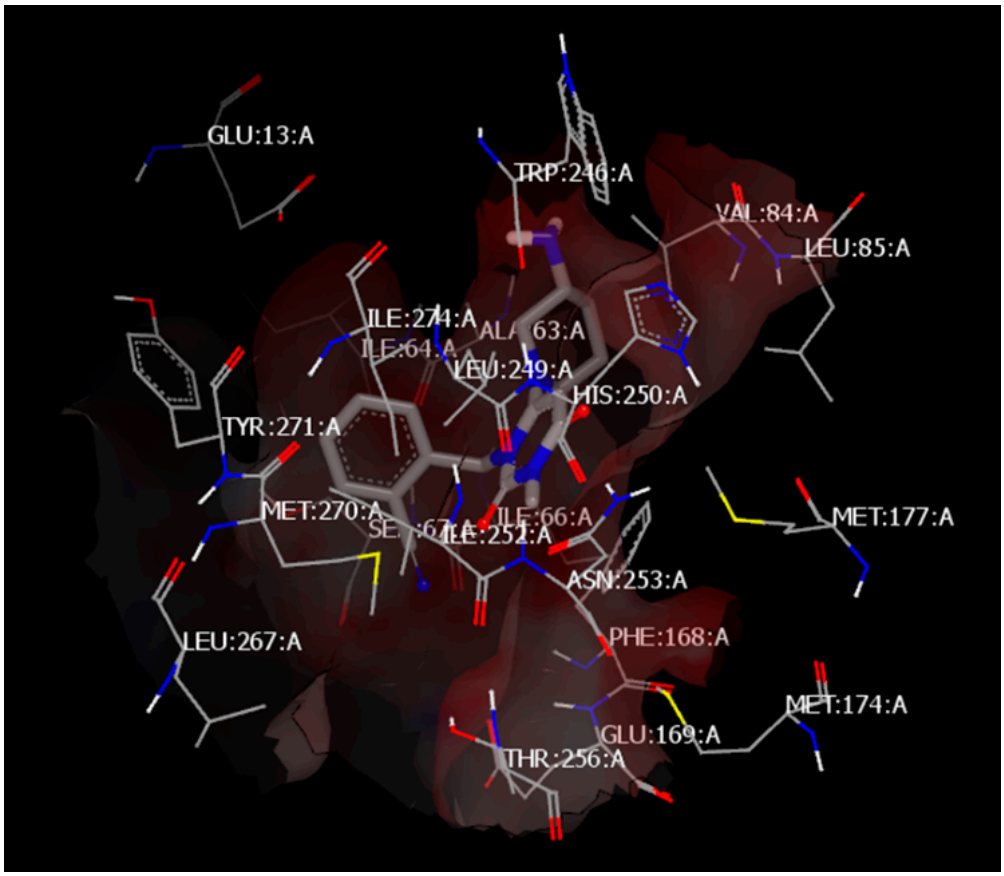


Figure S3. Predicted binding mode of linagliptin with 3PWH of A2AAR.

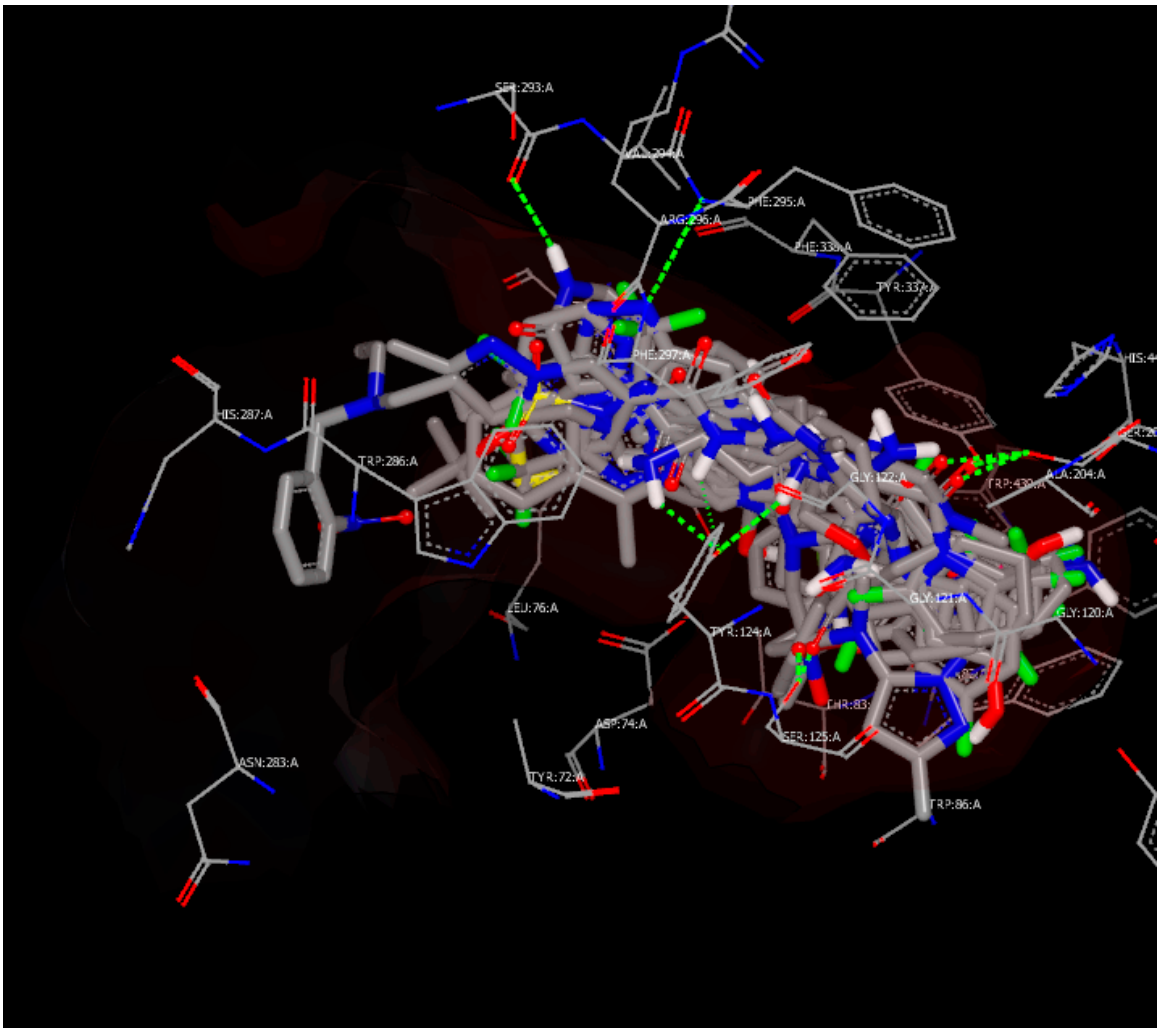


Figure S4. DPP-4 inhibitors with AChE receptor adapt different binding behaviors due to lack of structure similarity between the gliptins

Figure S5. The remarkable finding that the longer the designed structure the better to fit in the C shaped receptor pocket

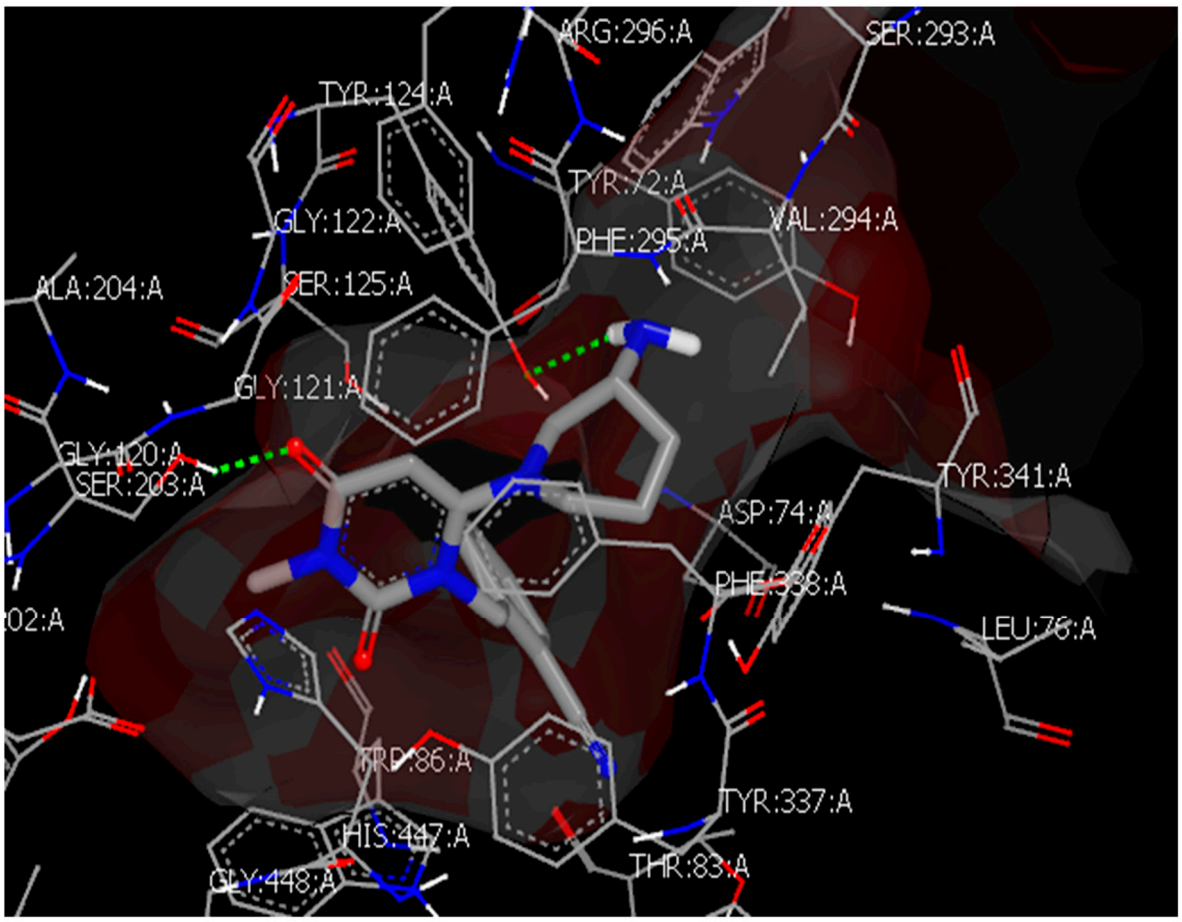


Figure S6. Alogliptin is fitted well with AChE forming two hydrogen bonds with TYR 124 and SER 203, plus the fitting within narrow bridge in receptor

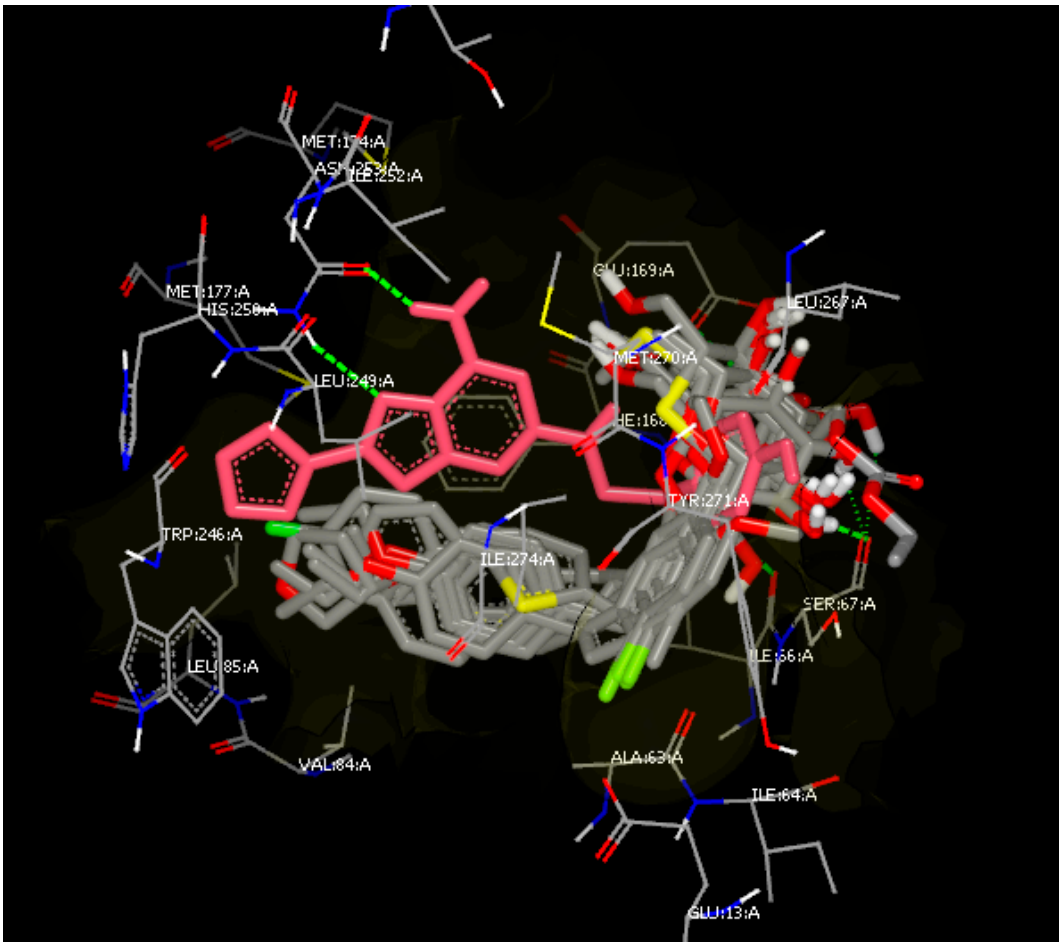


Figure S7. Different binding behavior of SGLT2 inhibitors and the cocrystlized ligand (in pink) of 6f25 in PDB.