



**Supplementary information, Fig. S6| The two dihedrals of the F<sup>45.52</sup> sidechain plotted against each for the  $\beta_1$ AR and  $\beta_2$ AR.**

The data is shown for the crystal structures and simulations of epinephrine bound to  $\beta_1$ AR and  $\beta_2$ AR. The means of the dihedral values of the two simulation conditions are shown as big dots. The respective values from the crystal structures are shown as stars. The difference of F<sup>45.52</sup> rotamers present in the crystal structures is not observed in simulations.