

S7 Table. Statistical significance of VS performance between B2AR CAR-bound binding pockets. An unpaired t test with Welch's correction was carried out on mean NSQ_AUC \pm S.E.M. for each of the docking experiments for a) B2AR inhibitors vs. decoys (Fig 7b) and b) B2AR inhibitors vs. B2AR agonists (Fig 7c). Binding pocket performance is tested with P value noted as follows. *: $P \leq 0.05$, **: $P \leq 0.01$, ***: $P \leq 0.001$, ****: $P \leq 0.0001$, ns: not significantly different. Black asterisks signify the row structure is significantly better than the column structure, and vice-versa for red asterisks.

a) B2AR inhibitors vs. decoys		b) B2AR inhibitors vs. B2AR agonists			
	2RH1	4GBR		2RH1	4GBR
2RH1		***			**
4GBR					