

**S5 Table. Statistical significance of VS performance between B1AR CYP-bound binding pockets.** One-way ANOVA was performed on mean NSQ\_AUC  $\pm$  S.E.M. for each of the docking experiments, followed by a Tukey multiple comparison test for a) B1AR inhibitors vs. decoys (Fig 5b) and b) B1AR inhibitors vs. B1AR agonists (Fig 5c). 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) B1AR inhibitors vs. decoys					b) B1AR inhibitors vs. B1AR agonists				
	2VT4	2YCX	2YCY	4BVN		2VT4	2YCX	2YCY	4BVN
2VT4		**	***	*	2VT4		****	***	***
2YCX			ns	ns	2YCX			ns	*
2YCY				*	2YCY				ns
4BVN					4BVN				