

S4 Table. Statistical significance of VS performance between B1AR DOB-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 agonists vs. decoys (Fig 4b) and b) B1AR agonists vs. B1AR inhibitors (Fig 4c). 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 agonists vs. decoys						b) B1AR agonists vs. B1AR inhibitors			
		2Y00-A	2Y00-B	2Y01-A	2Y01-B			2Y00-A	2Y00-B	2Y01-A	2Y01-B
2Y00-A			****	****	***	2Y00-A		*	**	*	
2Y00-B				ns	ns	2Y00-B			ns	ns	
2Y01-A					ns	2Y01-A				ns	
2Y01-B						2Y01-B					