S6 Table. Statistical significance of VS performance between B2AR BI-bound binding pockets. One-way ANOVA was performed on mean NSQ_AUC ± S.E.M. for each of the docking experiments, followed by a Tukey multiple comparison test for a) B2AR agonists vs. decoys (Fig 6b) and b) B2AR agonists vs. B2AR inhibitors (Fig 6c). 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 agonists vs. decoys

	3P0G	3SN6	4LDE
3P0G		***	****
3SN6			***
4LDE			

b) B2AR agonists vs. B2AR inhibitors

	3P0G	3SN6	4LDE
3P0G		ns	****
3SN6			****
4LDE			