

S2 Table. Statistical significance of VS performance between AA2AR CGS-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) AA2AR agonists vs. decoys (Fig 1b) and b) AA2AR agonists vs. AA2AR inhibitors (Fig 1c). 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) AA2AR agonists vs. decoys		4UG2-A	4UG2-B	4UHR
4UG2-A			ns	***
4UG2-B				**
4UHR				

b) AA2AR agonists vs. AA2AR inhibitors		4UG2-A	4UG2-B	4UHR
4UG2-A			*	***
4UG2-B				**
4UHR				