

S3 Table. Statistical significance of VS performance between AA2AR ZM-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) AA2AR inhibitors vs. decoys (Fig 3b) and b) AA2AR inhibitors vs. AA2AR agonists (Fig 3c). Binding pocket performance is tested with P value noted as follows. *: P ≤ 0.05, **: P ≤ 0.01, ***: P ≤ 0.001, ****: P ≤ 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 inhibitors vs. decoys						b) AA2AR inhibitors vs. agonists					
	3EML	3PWH	3VG9	3VGA	4EIY		3EML	3PWH	3VG9	3VGA	4EIY
3EML		****	****	****	***	3EML		****	ns	ns	ns
3PWH			****	****	****	3PWH			****	****	****
3VG9				****	****	3VG9				ns	ns
3VGA					****	3VGA					ns
4EIY						4EIY					