

S8 Table. Statistical significance of VS performance between DOR NAL-bound binding pockets. An unpaired t test with Welch's correction was carried out on mean NSQ_AUC \pm S.E.M. for each of the docking experiments for a) DOR inhibitors vs. decoys (Fig 8b) and b) DOR inhibitors vs. DOR agonists (Fig 8c). 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) DOR inhibitors vs. decoys		b) DOR inhibitors vs. DOR agonists			
	4EJ4	4N6H		4EJ4	4N6H
4EJ4		**	4EJ4		**
4N6H			4N6H		