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Precision and Traceability: Advancing Protein-ligand Binding Studies Via Orthogonal Biophysical Methods

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Binding constant (Kb) is one the most important parameters describing interaction of two molecules. There are various techniques for determining Kb. These techniques have various limitations that need to be carefully considered.ITC is widely regarded as the gold standard for determining protein-ligand affinity because it can measure several parameters of a molecular interaction in a single experiment. It is limited its limited range of affinities that can be accurately determined similar to enzyme inhibition assay. TSA which can overcome these limitations, as it has an almost infinite affinity range. One limation of TSA, is complex data analysis required for Kb determination. To help with this we created a free online tool -- Thermott that assists with such analyzes.

Observed Kb is often accompanied incomplete experimental data which complicates data interpretation. This is one of the reasons we created Protein-Ligand Binding Database (PLBD), for systematically storing interaction data. It holds information not just about the affinity experiment itself but also about the molecules being used so that full data traceability could be achieved. A large, annotated dataset is crucial for enabling future machine learning driven analyses. We hope that PLBD can provide a platform for depositing carefully documented protein-ligand interaction data.