Weill Cornell Medicine

Affinity Map: Global Protein-Ligand Binding Affinity Profiling Using Photocatalytic Labeling

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Background & Unmet Need

- Measuring binding affinities between ligands and proteins is crucial for understanding the potency, selectivity, and specific effects of molecules in complex biological systems
- Existing methods for measuring binding affinity are typically accomplished in vitro, requiring purified proteins and prior knowledge of the interaction, limiting use in complex samples like live cells or serum
- Proximity labeling technologies can identify novel interactions in vivo (e.g., protein-protein, protein-DNA, protein-RNA) but lack quantitative binding affinity measurements
- **Unmet Need:** Robust, proteome-wide, and quantitative measurement of binding affinities in complex biological samples such as live cells, cell lysates, and organ extracts

Technology Overview

- **The Technology:** Affinity Map is a novel platform that enables robust measurement of binding affinities between ligands and proteins across the proteome using photocatalytic labeling and high-throughput mass spectrometry
- A "hot" ligand conjugated to a photocatalyst and a "cold" unmodified ligand are used to covalently label proteins, enabling competitive binding assays that yield quantitative affinity measurements
- Affinity Map is applicable to major classes of ligands: small molecules, linear and cyclic peptides, proteins
- **PoC Data:** Affinity Map measured Kd values for the protein interactions of dasatinib, a tyrosine inhibitor, and JQ1, a selective bromodomain binding compound, with high accuracy and selectivity, even identifying previously unknown interactions
- Affinity Map was used to measure Kd values for the macrocyclic cRBDfk peptide and human IgG on live cell surfaces, finding close concurrence with reported literature values

Inventors:
Jacob Geri
Charles Warren
Noah Yardeny

Patents:
PCT Application Filed

Publications:
Warren et al. *Nat Commun*. 2026.

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Technology Applications

- Global small molecule-protein, peptide-protein, or protein-protein binding affinity determination
- Can be leveraged in complex biological systems such as cell lysates, protein extracts, and live cells
- Use in early drug discovery to screen novel chemical matter or profile interactions of small molecule candidates, including binding affinity, target engagement, and proteome-wide off-target binding affinities

Technology Advantages

- Measures binding affinities across all protein classes, including membrane proteins and non-kinase targets
- Maintains a low false detection negative rate, outperforming methods like CETSA and limited proteolysis
- Provides quantitative binding affinities using competitive kinetics, offering insights beyond qualitative fold enrichment data from other platforms

Supporting Data / Figures

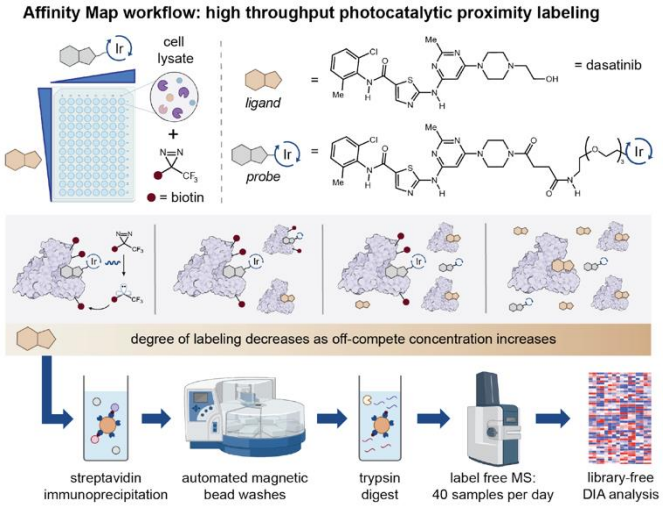

Figure 1: Affinity Map workflow for proteome-wide binding affinity measurement.

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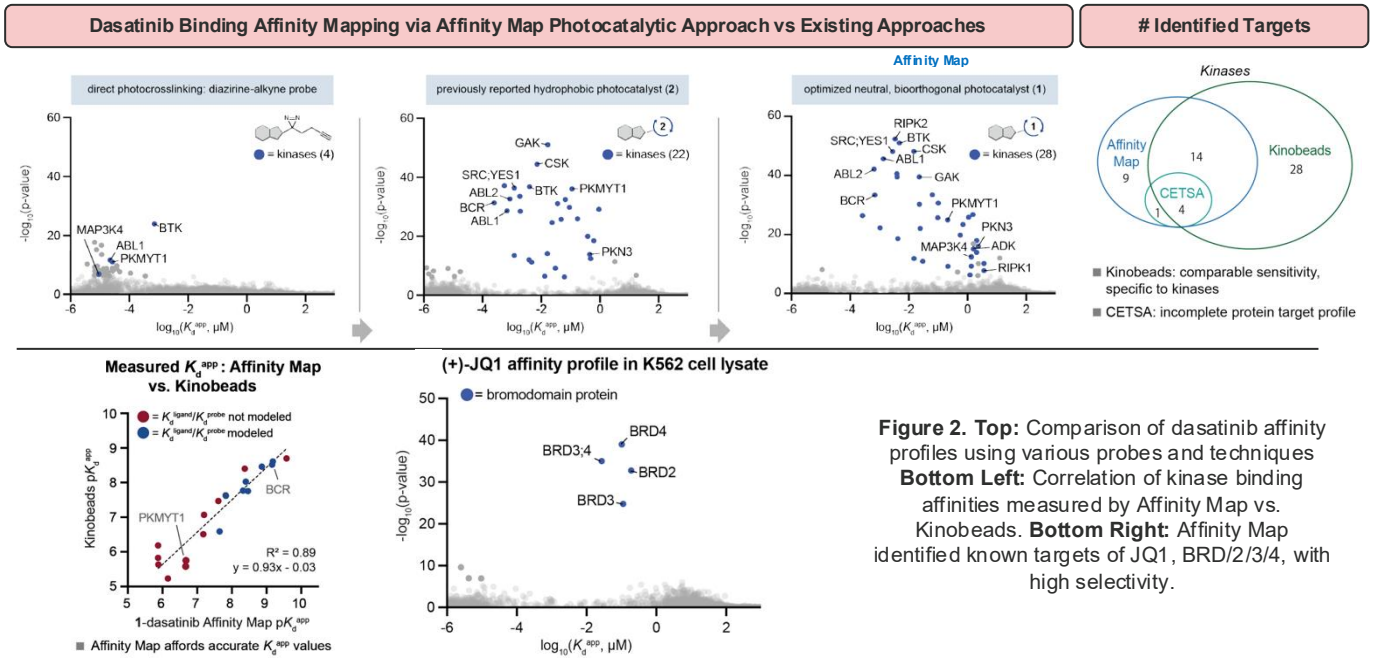

Figure 2. Top: Comparison of dasatinib affinity profiles using various probes and techniques **Bottom Left:** Correlation of kinase binding affinities measured by Affinity Map vs. Kinobeads. **Bottom Right:** Affinity Map identified known targets of JQ1, BRD/2/3/4, with high selectivity.

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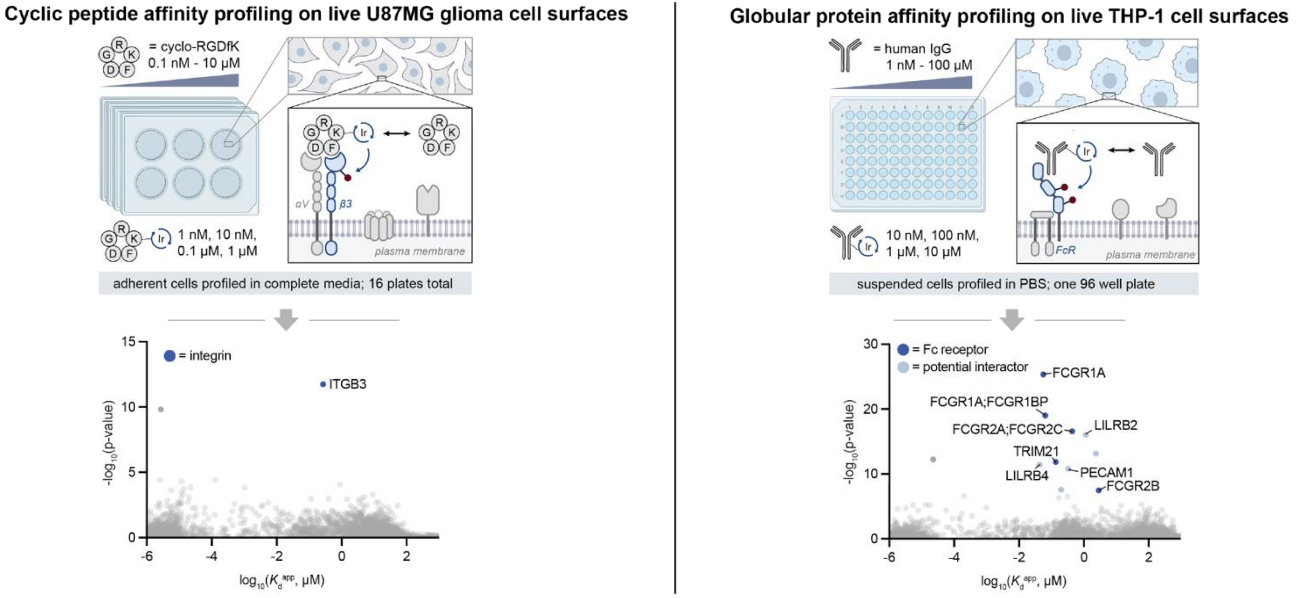

Figure 3. Left: Affinity Map measures cRGDfK binding to integrin β3 (ITGB3), consistent with known cRGDfK selectivity for the αVβ3 heterodimer **Right:** Affinity Map measures IgG affinities for several Fc-receptors.

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