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Nanotechnology Platform for Identification of Ligand Binding Sites on a Protein

The ability to identify target ligand binding sites on a protein surface is of great importance to drug design, discovery and screening, as well as general and bionanotechnology research. Protein-ligand interactions allow for a complex network of molecular interactions. While it is possible to experimentally screen large amounts of binders, computational prediction methods for binding sites are still not at the level that would allow one to in silico off-load the binding site design. Currently available machine learning methods can annotate likely binding sites, but often contain many false positives.

Researchers at the Biodesign Institute of Arizona State University have developed a new platform that combines molecular modeling and experimental measurements with DNA nanotechnology structures to identify unknown binding sites of a ligand (peptide, small molecule, aptamer) on a target protein. This platform enables researchers to weed out false positives from a candidate list of possible binding sites.

Identification of ligand binding site on a target protein is of major importance for drug design pipelines and diagnostics, thus, this platform could be incredibly useful in pharmaceutical and biotechnology industries.

Potential Applications

- Drug screening/discovery/design
- Diagnostics
- Research
- Bionanotechnology

Benefits and Advantages

- Can weed out false positives from a candidate list of binding sites
- Complements existing computational and experimental approaches to identify binding sites
- Can cover all possible combinations of predicted binding sites, which are then measured for affinity to weed out the non-binders (and the incorrectly predicted binding sites)
- The DNA nanostructures can be designed so that the positions of the ligands have well defined angles and distances
- Makes it possible to sample different regions that can be reached with a bivalent nanostructure

For more information about the inventor(s) and their research, please see

[Dr. Sulc's laboratory webpage](#)

[Dr. Stephanopoulos' laboratory webpage](#)