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SEE-Tx® Platform

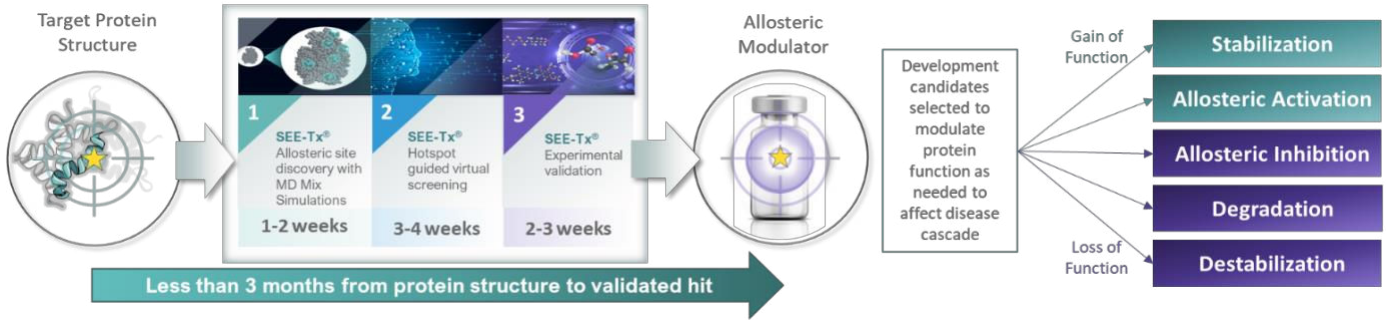
Fast – SEE-Tx® transforms drug discovery by enabling the identification of novel protein binding sites and hit compounds for experimental testing in 4-6 weeks.

Versatile – SEE-Tx® can be applied in any therapeutic area and generates small molecule hits that can elicit either a gain of function or a loss of function of the target protein through the full range of possible compound-protein interactions, including stabilization, activation, inhibition, degradation or destabilization.

Powerful – SEE-Tx® expands the target universe to the 90% of protein targets that have so far been undruggable and generates a more than 100-fold greater output of chemically diverse hit compounds compared to traditional high-throughput screening.

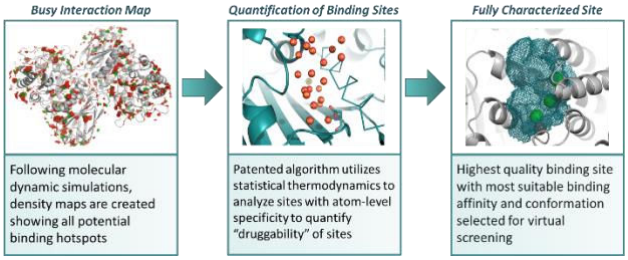
How it works

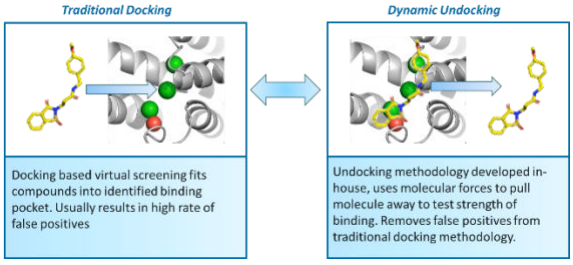
Gain's computational drug discovery platform SEE-Tx® was developed to exploit the untapped opportunities of allosteric binding sites and allosteric modulators. Using AI-supported structural biology and our supercomputer-powered physics-based methods, SEE-Tx® utilizes 3-dimensional protein structures and molecular dynamic modeling pioneered by our CTO Dr. Xavier Barrill to simulate physiologically relevant protein conformations. Organic solvents are added as probes to mimic a drug-like molecule and map the protein surface. A proprietary algorithm is applied to generate quantitative data of the "druggability" to enable the selection of the allosteric binding sites best suited for binding a small molecule. Virtual screening of millions of chemical structures, guided by binding hotspots discovered during the site identification stage, leads to the discovery of small molecule hits. A chemically diverse set of approx. 100 hit compounds is selected for experimental validation in primary screens established in Gain's lab facilities. Our success rate of about 15% of experimentally confirmed hit compounds represents a >100-fold increase compared to the hit rate in traditional high-throughput screening.



Platform Differentiation and Competitive Edge

SEE-Tx® provides several key advantages over other methods available in the field. Different from AI-based platforms that require big data inputs, SEE-Tx® applies a physics-based approach that only requires a 3-D protein structure, which can be generated from predictive models like Google/DeepMind's Alphafold. Gain's patented algorithm[1] integrated into the screening workflow provides atom-level specificity and quantification of binding interactions, which enables the selection of binding sites most suitable for targeting by small molecules.





The SEE-Tx® platform integrates hotspot-guided virtual screening of small molecule structures, including unique methods for analyzing the binding properties of hit molecules. Gain's Dynamic Undocking Protocol[2] incorporated into the virtual screening workflow provides quantitative information to remove more than 80% of molecules that appear be promising hits based on initial docking data alone.

Gain's extensive product pipeline was generated with SEE-Tx® - a testament to the capability of our discovery and chemistry team to select suitable allosteric sites and hit compounds based on computational predictions. This expertise in combination with the differentiated SEE-Tx® modeling technology tailored for drug discovery in the allostery space represents an invaluable competitive edge compared to subscription-based computational tools that are intended for general research or mass market use.

[1]Patented methodology and algorithm (WO/2013/092922); [2]Dynamic undocking and the quasi-bound state as tools for drug discovery. Nat Chem. 2017 Mar;9(3):201-206. PMID: 28221352.