

Signature Libraries

Addressing challenging targets

Areas of unmet medical need are often linked to novel “challenging” targets which are poorly addressed by current early drug discovery efforts. Most screening collections consist of compounds from previous projects; these compounds are “Rule-of-Five compliant” but lack the diversity and the proper configuration to address “challenging” targets.

At ASINEX, we focus on targets of high unmet need due to the lack of appropriate chemical probes; examples of these research areas are

- protein-protein interactions,
- protein-nucleic acid interactions
- protein-carbohydrate interactions

Many important signaling pathways are governed by these interactions. Aberrations of these pathways correlate with the onset of disease, maintenance of the disease state, and chemoresistance.

Our solution to the problem

ASINEX has addressed “cutting edge” chemistry in early drug discovery, developed its own direction, and combined this new direction with *in silico* and *in vitro* screening validation. Favorable results are packaged in an easy to use, one plate, 80 compound format which is our “Signature”.

Our technology is based on the creation of permeable small molecules and macrocycles with natural product-like features able to probe biologically relevant chemical space.

Nature often utilizes conservative protein-structural domains (i.e. PDZ, SH2, BH3 etc.) to govern protein interactions; therefore, many macromolecules can be grouped into related “superfamilies” based upon similar 3D architectures. We create small molecules and macrocycles that can recognize nature’s privileged set of architectures.

Initial design is validated through target-based and/or phenotypic screening approaches. This allows us to minimize the time for initial hit identification and also supports quick progress during the lead optimization stage. The value of this approach has been demonstrated through several successful projects in multiple target and therapeutic areas

Our recent research has focused on several underexplored clusters of chemical space that are particularly interesting in screening against challenging targets: α -helix mimetics, macrocycles, glycomimetics, and natural product-like compounds