



CONCEPT LIFE SCIENCES
a spectris company



FRAGMENT-BASED DRUG DESIGN

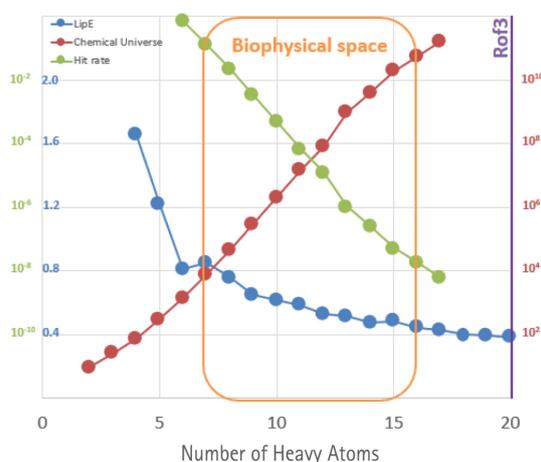
Over the last twenty years fragment-based drug design (FBDD) has emerged as one of the most prominent strategies used to identify innovative drug discovery Hits. FBDD presumes drug molecules are made of a combination of small fragments, each contributing to the affinity of the drug for its biological target. Unlike HTS, which aims to identify moderate to high affinity Hits the size of a typical drug molecule, fragment screening scouts for small molecule Hits with weaker but leaner affinity to their biological target. The FBDD strategy had led to many drug discovery successes including 4 approved drugs and another 40 under clinical investigation. At Concept Life Sciences, our FBDD service is designed to enhance success rate and speed of delivery.



THE BIOPHYSICAL SWEET SPOT

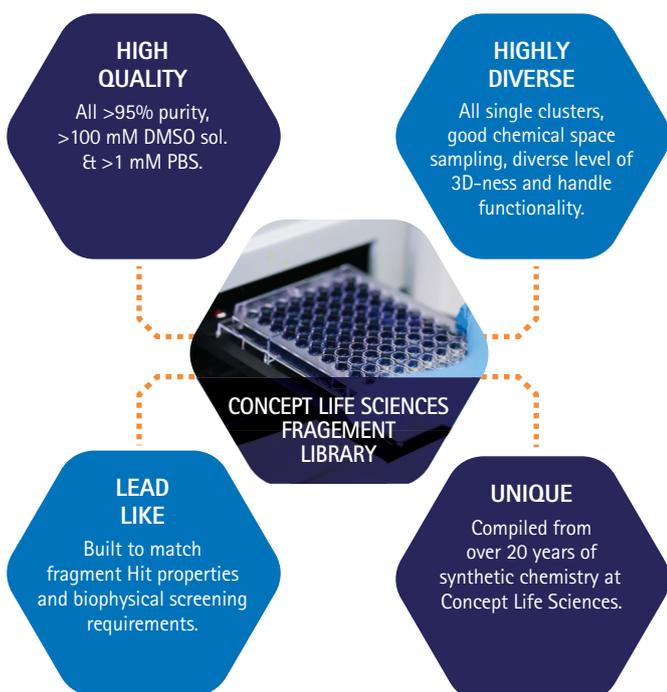
The efficient sampling of the chemical universe is one of the key benefits of FBDD and is correlated with the size of the molecules in a compound collection. It is underexploited in most fragment collections as they are populated with many large fragments (20-25 heavy atoms). Many biophysical screening technologies have emerged in recent years, providing tools to detect weak but lean binding events associated with molecules (typically 8-16 heavy atoms). Scientists at Concept Life Sciences have pushed the boundaries of fragment screening by designing a compound collection that samples this biophysically accessible space. Our Biophysical Fragments exploit the power of biophysical screening to identify lean and tractable start points for drug discovery campaigns.

The probability of hitting the target ("Hit rate") and leanness of the hit ("LipE") is inversely correlated with the size of the compounds ("Number of Heavy Atoms") screened".



OUR BIOPHYSICAL FRAGMENT COLLECTION

Our team of computational and medicinal chemists have selected compounds from the > 55,000 internal collection to build a bespoke Biophysical Fragment collection. Our collection contains 1133 highly diverse (Tanimoto = 0.7) and functionalized fragments typically containing between 8 and 16 heavy atoms, ideal for biophysical screening. Unlike the many other fragment collections, the physicochemical properties associated with our fragment collection are in perfect accordance with those of reported fragment Hits. This, combined with our thorough quality control (solubility > 1 mM in PBS pH 7.4, > 100 mM in DMSO and purity > 95%), provides us with a unique and high-quality compound collection for FDBB campaigns.



SCREENING BIOPHYSICAL FRAGMENTS

Our team of biologists have access and expertise in state of the art instrumentation for biophysical screening including Surface Plasmon Resonance (SPR), Thermal Shift Assay (TSA), MicroScale Thermophoresis (MST) and Isothermal Titration Calorimetry (ITC), and we collaborate with experts in X-ray crystallography to obtain and exploit structural information to drive project progression. Fragment Hits are rapidly progressed through the drug discovery process by our team of chemistry, biology and ADMET experts.

SUPPORTING YOUR FBDD PROJECTS

Identifying the right Hits is a critical step for any drug discovery pipeline management. Concept Life Sciences offers an integrated FBDD service which combines our exclusive Biophysical fragment collection with our expertise in Biophysical screening. This provides our team of drug hunters with excellent starting points for taking your programme all the way to the clinic. Our team of experienced scientists, with depth and breadth of knowledge and expertise, share your passion for delivering science.

AS YOUR DEDICATED PARTNER AND COLLEAGUE, WE ARE HERE TO HELP YOU ACHIEVE YOUR GOALS

