



For Immediate Release

New ThemePair™ Libraries bridge gap between fragments and hits

Intermediates allow wide exploration without the need for specialised techniques

Chesterford Research Park, UK, 12 September 2005... With the launch of the first ThemePair™ Library, BioFocus has created a unique opportunity for drug researchers to find ligands that bind to proteins without having to invest in specialised structural biology assay techniques.

ThemePair™ libraries of low molecular weight compounds bridge the gap between screening very small molecular weight ligands ("fragments"), which requires structure-based assays to show any affinity at millimolar concentrations, and the screening of higher molecular weight compounds which often require very large numbers of such compounds to be screened at low micromolar concentrations to find hits. In contrast, low molecular weight compounds created using the new paired monomer approach (ThemePair™) can be readily screened for activity using standard bio-assays at high concentrations due to a particular focus on the solubility of the novel, low molecular weight ThemePair™ compounds.

In developing its latest library, BioFocus has used knowledge gained from its design of the pioneering SoftFocus® libraries, coupled to more than seven years of successful drug discovery. Each of the 10 different scaffolds in the 500 member ThemePair™ library has been extensively elaborated in one position with either an amine or aryl group. These substituents have been chosen specifically to enable the exploration of a wide range of characteristics, including: steric; electronic factors and the ability to form H-bonds. However, the substituents have been chosen to generate only low molecular weight products (mostly less than 300 daltons) which assists in producing compounds with good solubility and thus having a better chance of being screened at high concentrations. During library validation, a subset of the library has indeed been proven to have excellent measured solubility. Furthermore, as they are highly novel, active compounds possess excellent potential for elaboration into more potent candidate compounds.

According to Phil Dudfield, Director of Discovery Products, at BioFocus, "We have developed this approach to ligand discovery in order to allow drug researchers to strike a balance between fragments, which typically need X-ray crystallography or NMR-based screening, and conventional libraries, which comprise a large number of compounds to screen. This unique concept, which is founded on our proven drug discovery capabilities, creates a genuine new entry point into ligand binding studies."

About BioFocus

BioFocus offers a full range of pre-clinical expertise for discovery biology, medicinal chemistry and molecular informatics to pharmaceutical and biotechnology companies. Founded in 1997, BioFocus is now a recognised expert in three key areas of drug discovery – kinases, GPCRs and ion channels, and provides SoftFocus libraries targeted at all these gene families.

Renowned for generating the highest rate of tractable hit series for onward development into pre-clinical candidates, BioFocus has provided its services and/or products to 17 out of the top 20 pharmaceutical companies worldwide.

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