Fragments.Rainer Mutsch's abstract installation, 2006.

Molecular fragment as a part of something yet invisible and more functional structural whole defines Fragment-Based Drug Discovery (FBDD) being used more and more on its own and along with HTS campaigns. FBDD is well established by now with the first fragment-based screening drug being approved, Zelboraf (vemurafenib).

FBDD is credited with covering greater chemical diversity space multiplying optimization options. It is also an economical precursor to HTS as active moieties are identified early on and SAR data can be generated faster.

Fragment screening economy also means smaller library size. Active hits can be identified among just about 500 fragments or less. TimTec Fragment-Based Library, FBL , gathers the pool of 3,200 small and diverse fragments ready for customized subsets selection. Some screening techniques, especially the ones involving fragment mixtures, would make entire FBL-3,200 approachable. FBL design criteria stay mid-way accommodating greater structural diversity and versatility including and going beyond, for example, Ro3 restrictions and playing around “half-molecules”, larger fragments with up to three rings.

We are pleased to report recently published favorable screening results:

Meiby E, Knapp S, et.al. Fragment screening of cyclin G-associated kinase by weak affinity chromatography. Anal Bioanal Chem. 2012 Nov;404(8):2417-25. doi: 10.1007/s00216-012-6335-6

Fragment screening methods vary and can accomodate challenging targets. There is one notable screening method that just has been announced: weak affinity LC/MS. The method

allows screening fragments under high-throughput conditions corresponding to >3,500 fragments per day.

Duong-Thi M-D, Bergstrom M, et al. High-Throughput Fragment Screening by Affinity LC-MS. J Biomol Screen. Pub online: Sept 13, 2012. doi:1087057112459271

Extended information about FBL-3,200 design and the screening results

Please e-mail support@timtec.net your inquiries or call us.