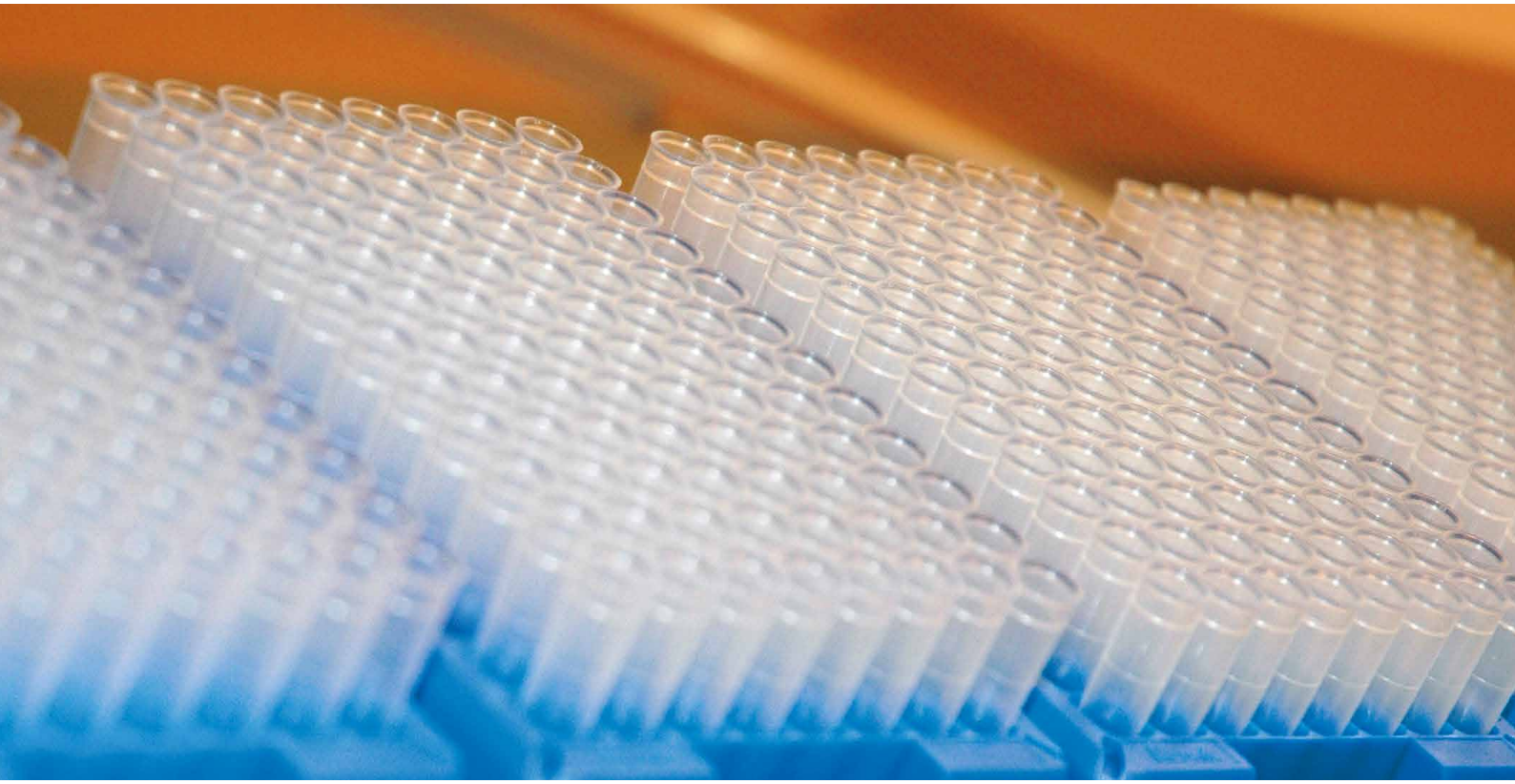
Fragment library



Fragment-based drug discovery has developed into one of the sound pillars for providing small molecule lead compounds. Specs offers a fragment-based library of 4,532 compounds of low molecular molecules as an off-the-shelf, pre-plated screening set.

Fragment-based drug design has emerged as an effective alternative to high throughput screening for the identification of lead compounds in drug discovery in the past twenty years. Fragment based screening and optimization methods have achieved credible success in many drug discovery projects with one approved drug and many more compounds in clinical trials.

Fragments

The fragment-based drug design starts with the identification of fragments or low molecular weight compounds that generally bind with weak affinity to the target of interest. These small molecules tend to be more polar and more soluble than larger drug-like molecules and are therefore thought to translate into compounds with favorable physicochemical properties.

Lipinski's Rule of Five, later enhanced by Verber and co-workers, provided the original framework for the development of orally bioavailable drug candidates. More recently, Congreve and co-workers have found that, after analysis of a diverse set of fragment hits against a range of targets, small molecules seem to obey a 'Rule of Three', in which molecular weight is <300, the number of hydrogen bond donors is ≤3, the number of hydrogen bond acceptors is ≤3 and ClogP is ≤3. In addition, the results suggested NROT (≤3) and PSA (≤60) might also be useful criteria for fragment selection.

Plate specification

Applying these and other filters to our own compound repository, we have selected 4,532 compounds which are offered as a complete, off-the shelf, general purpose pre-plated fragment-based screening library. The plates are available in Beckman 96 deep well plates containing 80 compounds per plate as 200µl 10mM DMSO solution or as dry film.

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