With ActiProbe Series of screening collections you get access to some most diverse chemotypes among distinctly drug-like molecules available from TimTec extended stock.

All collections share the same design approach. Each smaller collection is assembled from a larger one in the Series through Jarvis-Patrick clustering that permits sampling of large library pools through selection of molecules that are representative of a group (cluster) within this library.

ActiProbe includes a different number of compounds to suit your assays. Start with one ActiProbe collection and add others as your research progresses.

ActiProbe's largest collection is **ActiGlobe-50K** , which includes 50,000 compounds. Other stand-alone collections are part of ActiGlobe:

ActiProbe-2K (2,000 molecules)
ActiProbe-5K (5,000 molecules)
ActiProbe-10K (10,000 molecules)
ActiProbe-15K (15,000 molecules)
ActiProbe-25K (25,000 molecules)

You are welcome to customize an ActiProbe collection with your choice of molecules to match your assay capacity and budget.

Smaller subsets are perfect “screen-boosters” being comprehensive in size and dense in chemical diversity within strictly defined drug-like parameters. Larger subsets allow building on initial screening results from smaller ones and are suitable for larger screenings.

The grand diversity collection of 50,000 compounds, ActiMol-50K, has been assembled from worldwide sources numbering over 2,000,000 compounds-candidates. The collection has

molecules representing the chemical diversity of screening samples produced by labs and research centers throughout the world. In addition to adherence to Lipinski parameters, dozens of advanced filters have eliminated undesirable atoms, functionalities and fragments creating a library that provides exceptionally good chemical starting points for hit and ADMET optimization.

Jarvis-Patrick Clustering

Here, molecular characterization is based on 2D fragment descriptors consisting of a central atom and neighboring atoms connected to it within a predefined sphere size -- bonds between central and edge atoms. Groups of molecules are based on the structural similarity of fingerprints (bit strings of these fragments), and the centroid has the highest degree of similarity to other members of a cluster. Chemically unique compounds (singletons) with low similarity to other members of the collection are also identified. Sampling libraries are created from centroid and singleton selection along with augmentation with other members from the largest groups.

Structural data and pricing information is available on request. We look forward to hearing from you