

[ActiProbe-10K](#) is a selection of distinctly drug-like molecules that probe broad pharmacore space. Compounds with activity potential were gathered from ActiGlobe-50K through Jarvis-Patrick clustering. ActiProbe Series is the result of refined medicinal chemistry compound selection from global sources of over 2,000,000 compounds.

ActiProbe-10K, 10,000 compounds, is available in several formatting options to choose from, in dry form or dissolved in DMSO. Custom formatting is always available.

Please contact us for attractive quotations.

Each order is accompanied with electronic files, including our easy-to-use and search ChemBD soft format.

Compound Selection

The Collection is a screening set of 10,000 compounds that has been assembled from the ActiProbe-25 library through Jarvis-Patrick clustering. In its turn ActiProbe-25 originated from ActiGlobe-50K. Jarvis-Patrick clustering permits sampling of large library pools through selection of molecules that are representative of a group (cluster) within this library. 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.

Purity of compounds in this, and all our collections, is generally at least 95% as determined by high-field ¹H-NMR and/or MS.

ActiProbe 10K purchasing information.

ActiProbe-10K, [10,000 compounds](#) , is available in several formatting options to choose from in dry form or DMSO:

- 0.5 micromol in 50 microliter of DMSO
- 1 micromol in 100 microliters of DMSO
- 2 micromol in 200 microliters of DMSO
- 1mg of each compound in dry form

Prices start from \$12,500.00

[ActiProbe-25K, 25,000 compounds](#) , is also available for larger screening projects!

If custom formatting is required, please inquire a quotation.

Prices do not include shipping. (Shipping is free until January 1st 2007)

We have flexible payment options for Academic institutions.

Each order is accompanied with electronic files, including our easy-to-use and search [Chem BD chemical format](#)

[Contact TimTec](#) for for orders and more information:

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