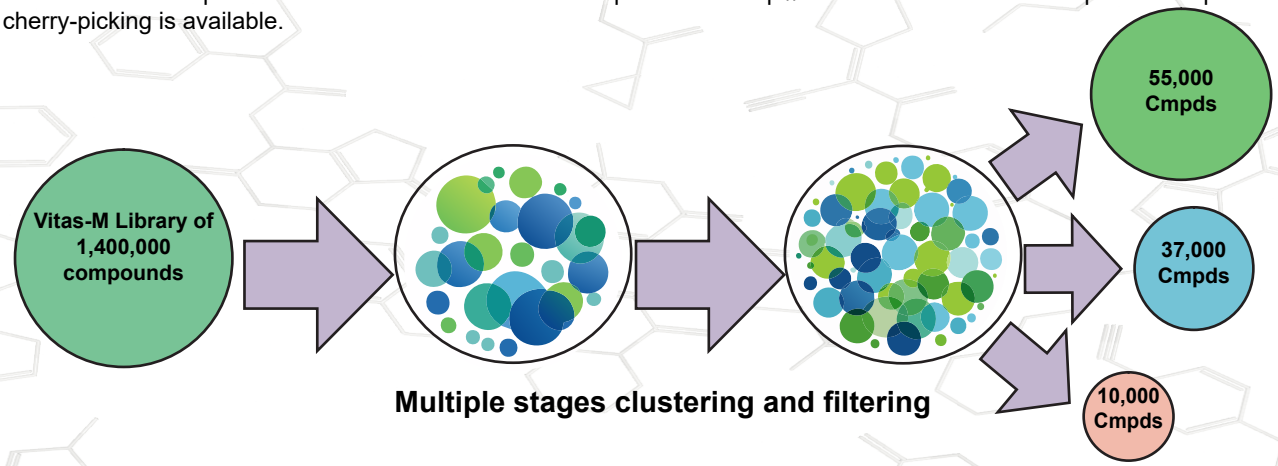
Diversity_Vitas-55000
55k Compounds Diversity Library

Chemical diversity of screening set enhances the chances of finding compounds with unique mechanisms of action, particularly against complex or underexplored targets. Our Diversity Libraries can act as way to expand your ongoing project or as a starting point to overcome significant challenges, including drug resistance, unmet medical needs, and the high failure rates of clinical candidates.

These libraries represent broad range of 3D and 2D chemical diversity with focus on maximizing variety of pharmacophores and structural features so maximum amount of possible interactions would be covered. We have designed diversity libraries based off our collection of more than 1,400,000 compounds using a combination of K-means/K-Medoids, graph-based (Jarvis-Patrick), hiearchical and density-based clustering methods with similarity coefficients in the 0.85-0.95 range. In order to better suit your project's specific needs, three libraries of different sizes were created: 10k, 37k and 55k compounds, that cover different ranges of potential chemical interactions and structural varieties. Majority of compounds presented are drug-like and follow rule-of-5; in order to maximize structrural diversity and to not miss potential unique interactions, compounds outside this rule are also present. Libraries without those compounds can be provided upon your request. You can download samples of databases as well as our other products at http://www.vitasmlab.biz. Partial purchase option and cherry-picking is available.



Vitas-M Diversity Libraries

Diversity_Vitas-55000 is designed to be used either as a stand-alone or as a supplementary to smaller diversity libraries to maximize potential interactions. It includes additional compounds, including "wildcard" ones, that did not make it to smaller libraries, but represent broader range of characteristics and further expand structural diversity.

Distribution of Parameters