Reaxense

Diversity Compound Libraries

It is generally accepted that chemical diversity leads to diversity in bioactivity, hence majority high-throughput screening screening (HTS) efforts utilize compounds that are selected for being as unlike each other as possible. Highly diverse, optimized compound libraries improve the success of HTS by minimizing false positives and maximizing hit rates without significant increase in the library size.

We offer **diversity subsets of any size** based on Reaxense's in-stock chemical space (comprising about 300,000 compounds). The subsets can be designed on your request with various methods of choice (pairwise, clustering, shapebased, scaffold-based etc.) and finalized by applying specific physico-chemical criteria or medicinal chemistry rules.

Please contact us at <u>rxinfo@reaxense.com</u> to provide your specific needs, and our team of computational chemists and med-chem experts will be ready to help.

Currently, there are 5 pre-designed subsets (**Diversity Compound Libraries**) for immediate formatting and delivery:

Library	Number of compounds	Number of unique scaffold
1K Diversity Library	1,000	798
3K Diversity Library	3,000	2,388
6K Diversity Library	6,000	4,601
10K Diversity Library	10,000	7,456
15K Diversity Library	15,000	10,724

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REAXENSE

Features:

- 5 Diversity Compound Libraries of 1,000 15,000 drug-like compounds
- Available with various formatting options to meet any HTS needs
- No pan-assay interference (PAINS) compounds
- Compounds with reactive and toxic groups filtered out
- Highest possible diversity over each library
- Purity >90%; spectral data available

Selection Criteria:

Parameter	Value
Number of Hydrogen Bond Acceptors (HBA)	≤ 10
Number of Hydrogen Bond Donors (HBD)	≤ 5
Number of Rotatable Bonds (RB)	≤ 10
Topological Polar Surface Area (TPSA)	≤ 140
Molecular Weight (MW)	200 - 500
Octanol-water Partition Coefficient (cLogP)	≤ 5

PAINS, reactive, toxic compounds as well as compounds containing elements other than O, N, C, H, Br, Cl, F, I, S, P have been filtered out from the libraries.

Diversity analysis:



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