

[L3] Building compound archives for the future

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High-Throughput screening has been a valuable source for finding chemical hits against novel targets and pathways. Novel methodologies for screening can interrogate new biological modalities, and screening is an integral part of any discovery project in the pharmaceutical and agrochemical industries. There are practical limits on the number of compounds that can be stored and assayed, and this leads to strategic decisions around how to build a compound archive that is best suited for the current and future needs of screening. Chemical space is too vast to navigate purely by filters or chemical diversity. The space of the pocketome, exemplified by binding sites in proteins / DNA / RNA, is still large but more computationally tractable.

The mapping of the pocketome and link between biological and chemical universes will be discussed.