Bioactive Compound Collections: From Design to Target Identification

The discovery of bioactive compounds underpins many areas of basic biomedical research and constitutes a large part of medicinal chemistry and chemical biology. Synthetic chemistry is now able to provide almost any drug-like molecule imaginable. Therefore, attention has turned to increasing the biological relevance of the compounds to be used in chemical biology and medicinal chemistry research, as well as maximizing their diversity within this large area of chemical space. In this review, we outline key concepts for the design of biologically relevant compound collections by taking inspiration from nature and natural products. We highlight efficient ways to screen the resulting libraries in order to maximize hit rates and the chance of discovering new modes of action. Finally, we discuss state-of-the-art techniques for the identification of molecular targets of hits identified through phenotypic screening approaches.

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