Perspective

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High Throughput Screening: Accelerating Modern Drug Discovery

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Introduction

High-throughput screening (HTS) is a cornerstone technology in modern drug discovery, enabling rapid evaluation of large chemical libraries against biological targets. By automating experimental assays and integrating robotics, HTS allows researchers to test thousands to millions of compounds efficiently, identifying potential hits for further development. This approach has revolutionized the pharmaceutical industry by accelerating lead identification, optimizing resources, and supporting the discovery of novel therapeutics for diverse diseases [1-5].

Discussion

The principle of HTS relies on miniaturized and automated assays that measure the interaction of compounds with specific targets, such as enzymes, receptors, or nucleic acids. Assays can be biochemical, detecting direct binding or enzymatic activity, or cell-based, measuring functional responses in living systems. Fluorescence, luminescence, and absorbance-based readouts are commonly used to quantify activity, while robotics and liquid handling systems ensure precision and reproducibility.

HTS offers significant advantages over traditional drug screening. Its speed and scale allow comprehensive exploration of chemical space, increasing the likelihood of identifying potent and selective hits. By integrating data analytics, cheminformatics, and structure-activity relationship (SAR) studies, HTS informs medicinal chemistry optimization and accelerates the transition from hit to lead compounds. The approach is particularly valuable for challenging targets, including protein–protein interactions, ion channels, and novel enzymes, which may not be amenable to conventional screening methods.

Recent advances in HTS technology have further expanded its capabilities. Miniaturization to microplate formats, coupled with automation and high-content imaging, enables simultaneous measurement of multiple parameters, providing rich phenotypic data. Integration with computational tools, artificial intelligence, and machine learning improves hit identification, predicts off-target effects, and enhances prioritization of promising candidates. Additionally, fragment-based and DNA-encoded library screening are being combined with HTS workflows to explore diverse chemical scaffolds efficiently.

Despite its strengths, HTS faces challenges such as assay artifacts, false positives or negatives, and the need for extensive validation of hits. Careful assay design, appropriate controls, and orthogonal screening strategies are essential to ensure data reliability and reproducibility. Moreover, translating in vitro hits to in vivo efficacy requires consideration of pharmacokinetics, bioavailability, and toxicity.

Conclusion

High-throughput screening is a transformative technology that accelerates drug discovery by enabling rapid, large-scale evaluation of chemical libraries. By combining automation, miniaturized assays, and computational analysis, HTS identifies promising lead compounds

efficiently and informs medicinal chemistry optimization. Continued innovations in assay design, data analytics, and integration with complementary screening approaches will further enhance the power of HTS, solidifying its role as a critical tool in the development of next-generation therapeutics.

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