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Innovative Techniques Open New Avenues in Drug Discovery for Brain Diseases

The Latest from SLAS Discovery—the Journal Reporting the Latest Scientific Developments in Drug Discovery Research

Oak Brook, IL – Volume 29, Issue 2 of SLAS Discovery features two review articles, six original research articles covering phenotypic screening perspectives, medulloblastoma therapies and interventions for neurodegeneration from the SLAS2023 International Conference. Collectively, the group members' perspectives highlight various challenges, progress and proposed solutions to phenotypic screening.

Screening for molecular glues—Challenges and opportunities

This article provides an overview of molecular glues, smaller molecules that stabilize protein interactions, particularly between a target and an E3 ligase. It discusses how induced proximity can enhance activity or inhibit natural effector binding, reviews current methods for identifying molecular glues and suggests screening approaches for their discovery.

Original Research

The openOCHEM consensus model is the best-performing open-source predictive model in the First EUOS/SLAS joint compound solubility challenge

The subject of this article is the EUOS/SLAS challenge, a competition aimed at developing accurate algorithms for predicting the aqueous solubility of small molecules using experimental data from 100,000 compounds. The winning model underscores the effectiveness of Natural Language Processing methods, particularly the Transformer CNN, and suggests that incorporating information about aleatoric uncertainty could further enhance understanding and utilization of the challenge data.The subject of this article is the EUOS/SLAS challenge, a competition aimed at developing accurate algorithms for predicting the aqueous solubility of small molecules using experimental data from 100,000 compounds. The winning model underscores the effectiveness of Natural Language Processing methods, particularly the

Transformer CNN, and suggests that incorporating information about aleatoric uncertainty could further enhance understanding and utilization of the challenge data.

Development of a high-throughput screening platform to identify new therapeutic agents for Medulloblastoma Group 3

Thisarticle discusses pediatric brain tumors, emphasizing the prevalence of medulloblastoma (MB), which accounts for a significant portion of pediatric cancer deaths. The authors introduce a high-throughput screening (HTS) platform specifically tailored to identify new therapies for MB G3, showcasing promising results from a pilot HTS campaign that identified active compounds with potential clinical significance.

Screening approaches for the identification of Nrf2-Keap1 protein-protein interaction inhibitors targeting hot spot residues

Thisarticle explores the challenges of targeting protein-protein interactions in drug discovery and focuses on hot spot residues within the Kelch-like ECH-associated protein 1 (Keap1) substrate binding pocket. The study identifies small molecule compounds using(r)-1.7 (p)-0.6 (o)-4.1 (d-0.6