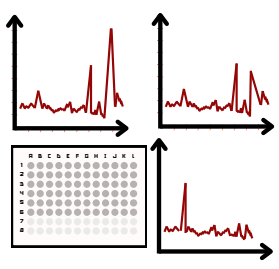
Mestrelab Research

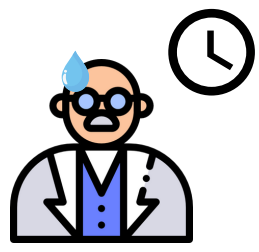
Affinity Screen:
Screening libraries within minutes made possible

Affinity Selection Mass Spectrometry (AS-MS) has emerged as a powerful technique for elucidating protein-ligand interactions, providing valuable insights into complex biological systems and playing a pivotal role in advancing the development of novel therapeutics and diagnostics. To enhance the efficiency of AS-MS, ligand multiplexing is often employed, enabling researchers to simultaneously screen up to 200 ligands within a single well and thus screen more extensive compound libraries.
However, analyzing high-throughput AS-MS data can be a challenging and time-consuming endeavor, requiring specialized tools and expertise. That's where our software, Affinity Screen, comes in. It automates data analysis, making it easier for researchers to extract meaningful insights from their experiments, accelerating the understanding of protein-ligand interactions and expediting the discovery process.

High throughput screenings causes data bottlenecks



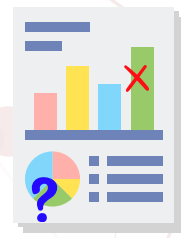
Scientists spend plenty of time on LC-MS data analysis



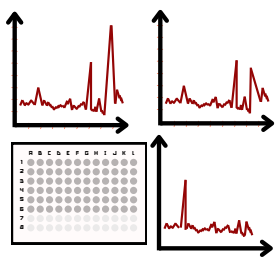
Manual work implies data quality issues that bleeds into reports

SAMPLE	LIGAND	M+H	RESULT
SAMPLE 1	N01	470.055	Hit
SAMPLE 1	N02	453.261	Hit
SAMPLE 1	N03	411.097	Not hit
SAMPLE 2	N04	411.127	Not hit
SAMPLE 2	N05	375.084	Hit

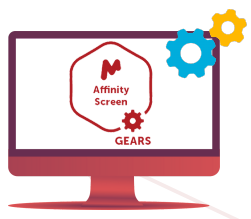
Inconclusive experiments cannot always be re-run due to limited sample sizes



Affinity Screen has been developed with real customer challenges in mind to simplify and accelerate mass spectrometry analysis process, offering a comprehensive suite of features that ensure precision and efficiency.



Batch data analysis and automated mapping of LC-MS data to sample information

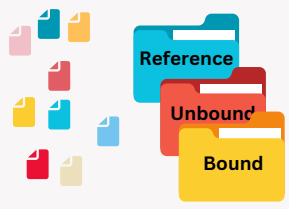


Automation of data extraction, processing, analysis, and reporting

End-to-end data workflow which eliminates error-prone manual steps and increases accuracy and reproducibility

Possibility to review data and re-analyze ambiguous results without the need to re-run a whole experiment !

Data Detection & Sorting

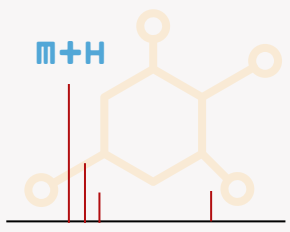


Easily finds and categorizes input data files, distinguishing between bound, unbound, and reference ligands for each sample

Peak Assignment

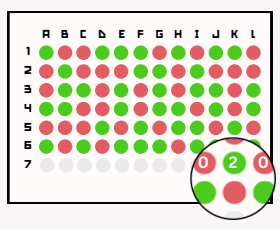
Assigns MS peaks utilizing: Molecular Formula, SMILES, or MW data provided in a CSV file, then generates analytical EICs for each compound

Compound Mass Matching



Applies the desired method for compound mass matching, whether by assigning the largest peak of the EIC or using mol match scoring, or a combination of both

Binding Assessment

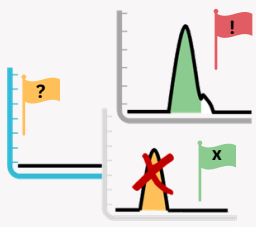


Calculates a score to determine whether a molecule effectively binds to a target or not, and classifies hits by score

Interactive Dashboards

Allows review-by-exception, and provides the ability to override results when necessary

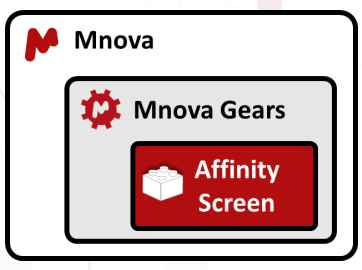
Alerts and Warnings



Displays flags and warnings when encountering MS overlaps, peak assignment failures, or missing peaks

Real-time Updates

Automatically updates all analysis outputs when changes are introduced by the scientist, maintaining consistency and accuracy throughout the research process

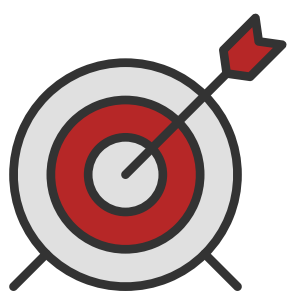


Unmatched flexibility to adapt to your needs

Affinity Screen operates within Mnova, our vendor neutral software suite which can handle most LCMS data formats, and Mnova Gears, our low code automation engine which seamlessly integrates with your lab and informatics systems. Affinity Screen boasts a comprehensive array of customizable features, offering the freedom to incorporate custom scripts, thereby enabling a heightened degree of personalization to effortlessly meet your distinct workflow needs.

Transform raw data to actionable results

Eliminate the burdensome overhead associated with extensive LC-MS analyses; benefit from faster and more rigorous data workflows to streamline decision making. Our interactive dashboards simplify data exploration and comprehension eliminating the need to sift through irrelevant data and allow better control over result quality. Identify interesting hits within minutes and expedite your transition to hit validation and optimization.



Learn more by visiting our website

Contact us

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