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ADVANCING DRUG DISCOVERY: FACILITATING AI-DRIVEN INITIATIVES WITH AUTOMATION IN BIOASCENT'S CENTRALISED COMPOUND MANAGEMENT

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INTRODUCTION

BioAscent Discovery Ltd., founded in 2013, is a leading provider of integrated drug discovery services based at the former Organon/MSD R&D site in Newhouse, Scotland. Our comprehensive services include de novo assay development, target analysis, bespoke screening strategies, high-throughput screening (HTS), medicinal and synthetic chemistry, computational chemistry, and compound management, with access to extensive in-house diversity and fragment libraries.

Our €20 million state-of-the-art facility in Compound Management ensuring secure storage, up-to-date inventory tracking, and rapid compound access, critical for innovative biotech. We manage over 1.5 million compounds in liquid and solid formats for more than 70 global clients across North America and Europe.

At BioAscent, our experts in medicinal chemistry, computational chemistry, data science, biology, and compound management collaborate to ensure a seamless integrated drug discovery process. From assay development to the production of preclinical and clinical candidates, we strive to achieve the highest quality and efficiency for our clients' research endeavours.

Azenta robotic -20°C liquid store

Automated cherry-picking

CENTRALISED COMPOUND MANAGEMENT

BEING PART OF INNOVATIVE PROJECTS

BioAscent's initiatives support AI-driven client drug discovery projects through automation and a centralised compound management approach. Here are a few examples:

Project A: Centralised Compound Management (CCM)

- **Automated workflow:** Robust inventory management database (Mosaic), with advanced robotics liquid handling systems » reduction in variability, cost and processing time.
- **Strategic planning through critical thinking:** Iterative approach leads to a constant influx of new data, seamless data integration back into the system for large libraries.
- **Compound Connect:** Online sample ordering interface, secure client directed sample management and request platform.

Project B: AI-driven Drug Discovery Workflow

- **Integrated Drug Discovery (IDD):** BioAscent's closely coordinated resources enable a rapid and controlled weekly workflow.
- **Optimised synthesis:** AI-driven processes streamline decision-making in the design and synthesis (~700 novel compounds, over 3 years).
- **Hit-to-Lead optimisation:** Developed five compound series, up to 23 synthetic cycles so far.
- **Budget-friendly:** Single-site IDD, rapid redirection, cost-effective screening.

Project C: Managing Large Libraries

- **Multiple large plate sets:** Production of Assay-Ready Plates (ARPs) from large libraries of small molecules or fragments (>150,000 compounds) on Echo 650 Acoustic Liquid Handler or HighRes Modular Robotic System.
- **Generation of robust datasets:** Facilitating cutting-edge High Throughput Screening (HTS) campaigns produces high-quality, comparable datasets for identifying new therapeutic targets.
- **Support for complex plate layouts and screening strategies:** From initial HTS to Active Confirmation, Potency Determination (Dose Response), and Hit-to-Lead development.

AUTOMATION & TECHNICAL CAPABILITIES
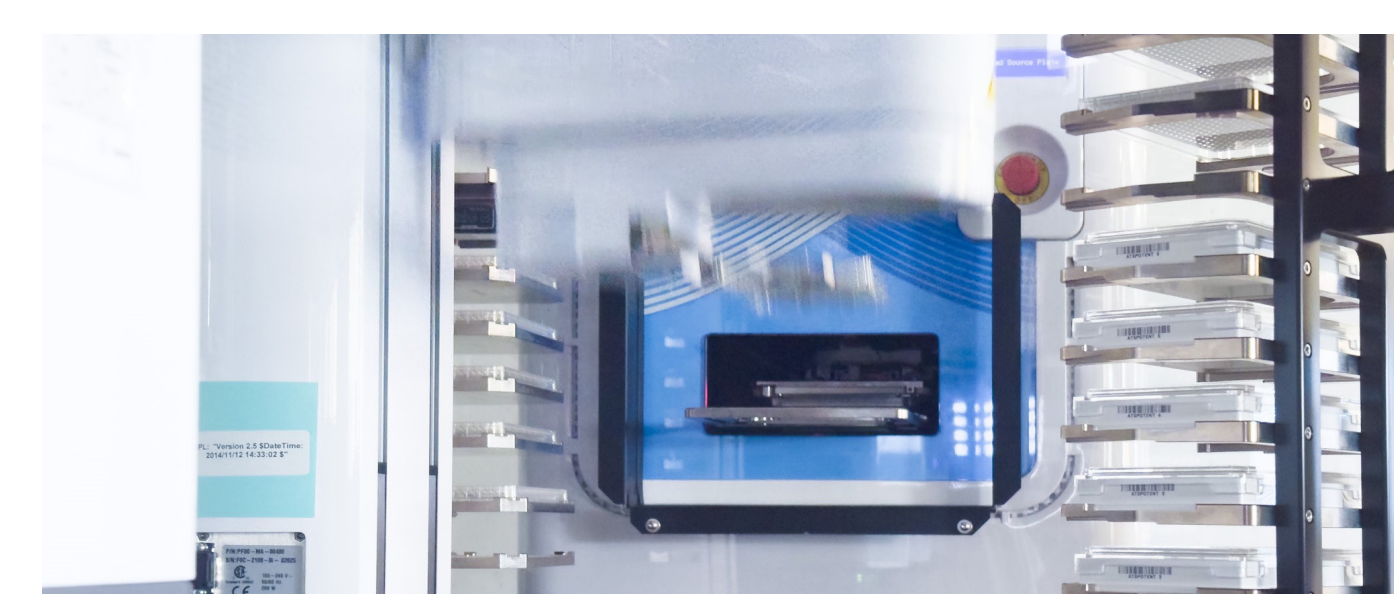

Kardex solid storage

HighRes modular robotic system

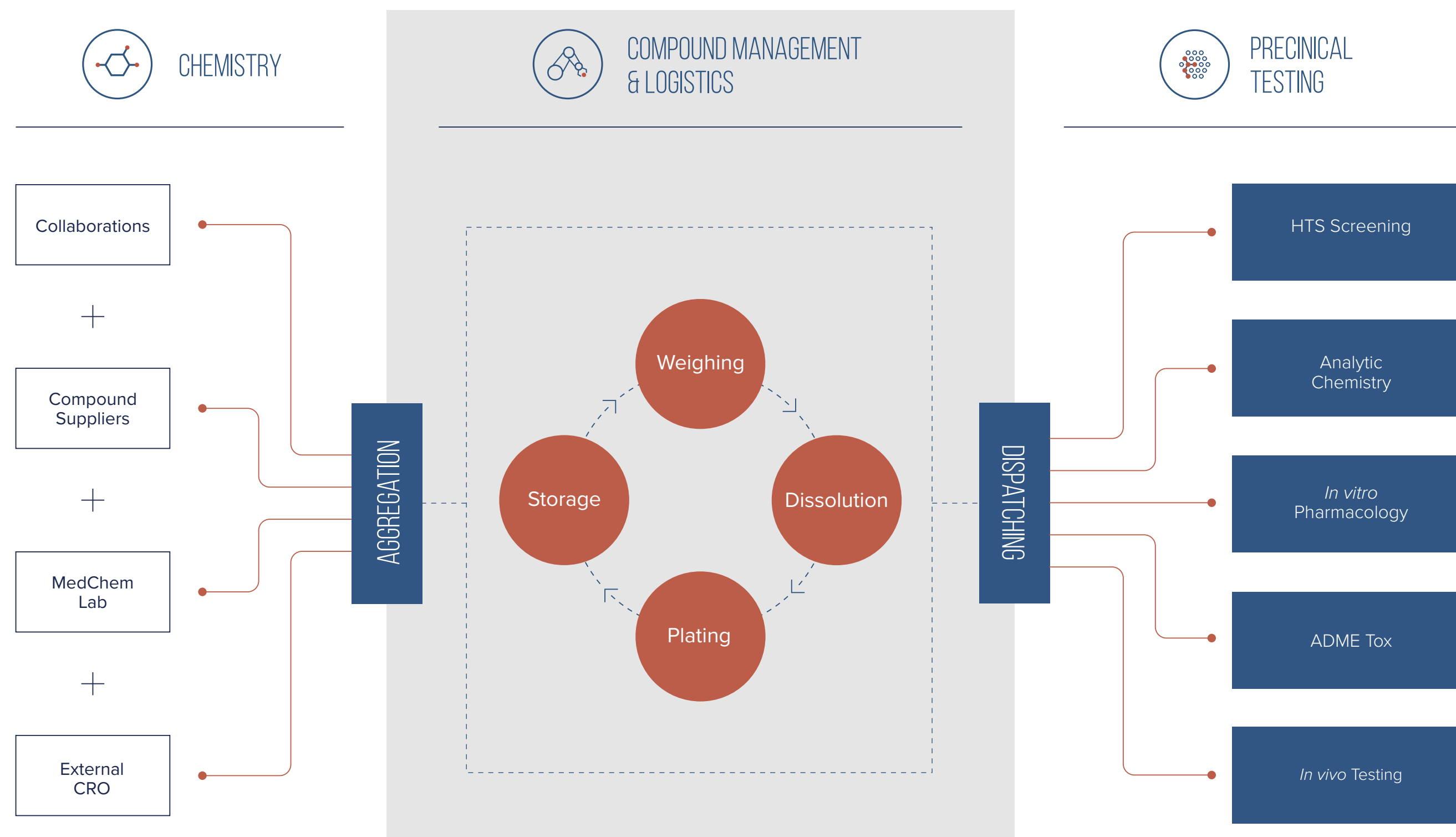
Plate Replication Platform

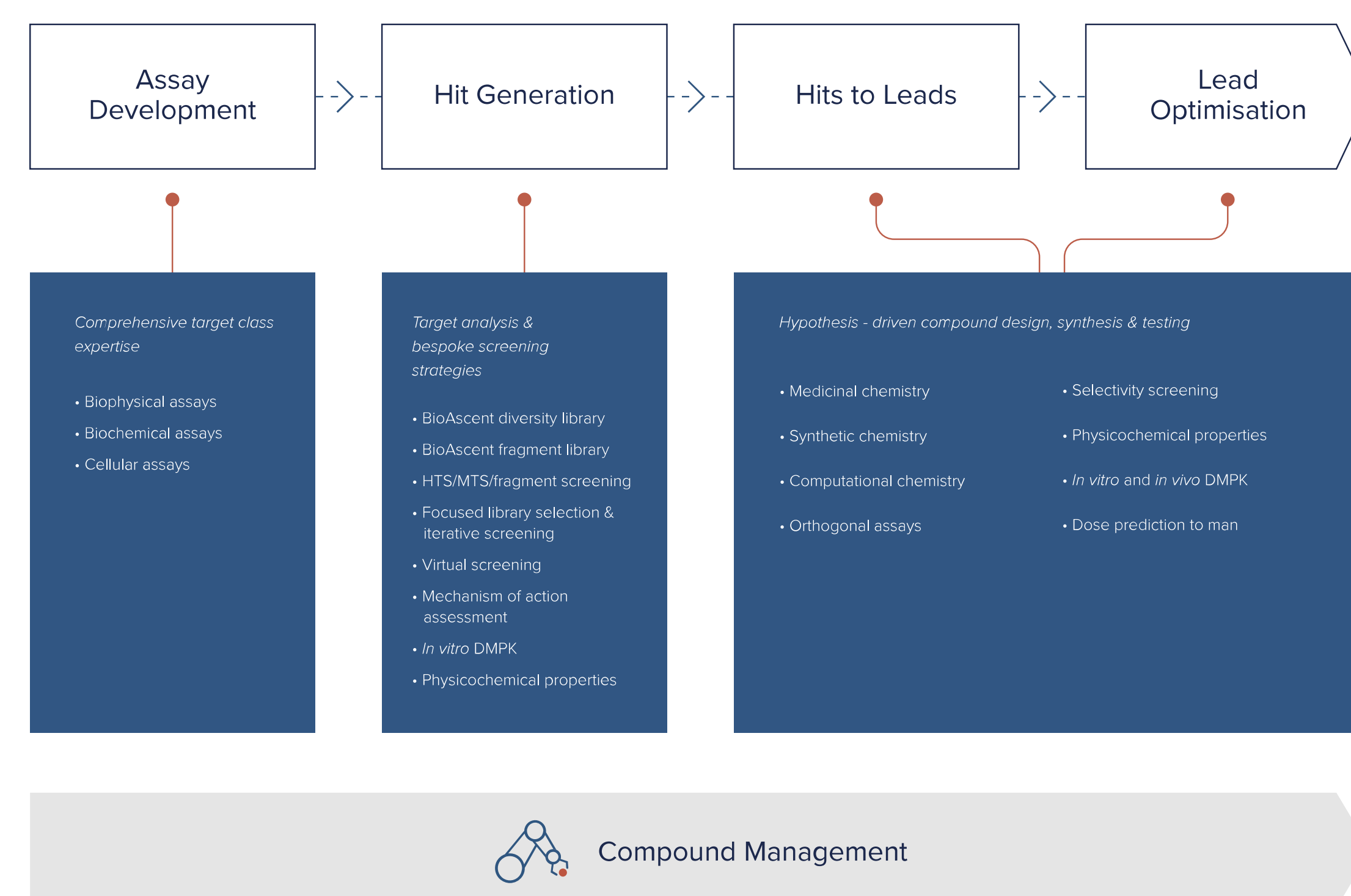Echo 650 acoustic liquid handler

INTEGRATED DRUG DISCOVERY

DISCUSSION

The intersection of artificial intelligence (AI) and automation in drug discovery represents a transformative leap for the pharmaceutical industry. BioAscent's centralised compound management system exemplifies how integrating these technologies can accelerate the discovery and development of new therapeutics.

BioAscent's centralised compound management system streamlines the process of storing, handling, and distributing chemical compounds. Automation plays a crucial role in this system, enabling precise and efficient management of compound libraries. Automated processes ensure that compounds are accurately tracked, retrieved, and dispensed, reducing the risk of human error and increasing the reliability of experimental data. AI-driven drug discovery relies heavily on large datasets to identify potential drug candidates and predict their efficacy and safety. Automation ensures that data regarding each compound's properties, and availability is consistently updated and easily accessible. We advocate for the FAIR principles; therefore, this data integrity is vital for training AI models and for performing high-throughput screening and virtual screening processes.

The synergy between AI and automation in BioAscent's centralised compound management is revolutionising drug discovery. This integrated approach not only accelerates the drug discovery timeline but also enhances the overall efficacy and cost-effectiveness of pharmaceutical research, paving the way for breakthroughs in advancing drug discovery.

FORTHCOMING DIRECTION

BioAscent is setting new trends at the intersection of AI and automation in CCM, data hungry AI demands the processing of compound screens in a timely manner to produce broad, robust high-quality datasets to feed algorithms and direct new strategies in advancing drug discovery process.

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