In today's fast-paced world, technology permeates every aspect of our lives. From the way we live, work, and play, to the revolutionary advancements in various fields, one particular area that stands out is Artificial Intelligence (AI) and its close companion, Machine Learning (ML). These cutting-edge technologies have brought about significant changes and improvements across multiple industries, including the scientific community. How much do people know about these unique aforementioned developments?

AI is an interdisciplinary field that synergizes computer science with comprehensive datasets, empowering effective problem-solving. It encompasses sub-fields such as Machine Learning and Deep Learning, frequently cited in tandem with AI, which consists of algorithms aimed at developing expert systems capable of making predictions or classifications based on input data. AI has been effectively used in business to automate tasks done by humans.

ML is a part of AI based on the idea that systems can learn from data, identify patterns and make decisions with minimal human intervention. The mathematical foundations of machine learning are provided by mathematical optimization methods. With the necessary knowledge of statistics, probability, and calculus, it is possible to create a model that is best suited for the domain that is needed. Machine learning is all around us today. Banks, stores, social media, and even at home, when you watch Netflix recommendations, you too encounter the power of algorithms of this invention.

In the domain of Drug Discovery, one of the game-changing innovations is DNA-encoded library screening (DEL). This novel technology allows for the synthesis and screening of vast numbers of pharmaceutically relevant compounds cost-effectively. The integration of DEL screens with ML models enables access to an extensive chemical space in a single experiment, expediting data acquisition and significantly reducing resource requirements.

These innovations have permeated our world, and the scientific community is no exception. Chemspace has played a crucial role in this advancement by creating an ultra-large Chemical space (CS) of small molecules, comprising collections from trusted suppliers of in-stock chemicals as well as make-on-demand offer of new and unique molecules. By utilizing a DEL-ML-CS combination system, Chemspace facilitates and accelerates the drug discovery process, enabling the identification of potent hits from the first screen.
Working with large databases like the Enamine xREAL (173B) or Freedom Space (5B) requires modernized methods, because traditional approaches like

molecular docking are very computationally expesive or even impossible in traditional settings. Therefore, we introduce V-SYNTHES – a modular synthon-based approach to perform hierarchical structure-based screening. V-SYNTHES benefits from a modular and efficient algorithm, which doesn't suffer from a steep increase in computational cost as the library size grows. This scalability allows it to adapt to libraries that could reach terascale and petascale sizes. By using this approach, we can perform such screenings efficiently, which is what you need for a successful experiment. An interesting fact is that this hierarchical combinatorial method enables rapid detection of the best-scoring molecules performing molecular docking of only a small fraction (<0.1%) of the compounds.

Importantly, V-SYNTHES is not limited to a specific protein target or library. It can potentially be applied to a wide range of targets with well-defined crystal or cryo-EM structures, including orphan receptors and allosteric sites.

In essence, V-SYNTHES represents an innovative and efficient strategy for screening large compound libraries, capitalizing on computational methods to identify potential drug candidates with high affinity and potency for specific protein targets.

Our company is working every day to not only facilitate early drug discovery but also save thousands of dollars for researchers.

1. Sadybekov, A.A., Sadybekov, A.V., Liu, Y. et al. Synthon-based ligand discovery in virtual libraries of over 11 billion compounds. Nature 601, 452–459 (2022).