Over Eight Trillion Compounds and Counting!

Process Optimized Drug Discovery Efficiency Gains with eMolecules' FAIR and Integrated Unity Platform

By 20/15 Visioneers

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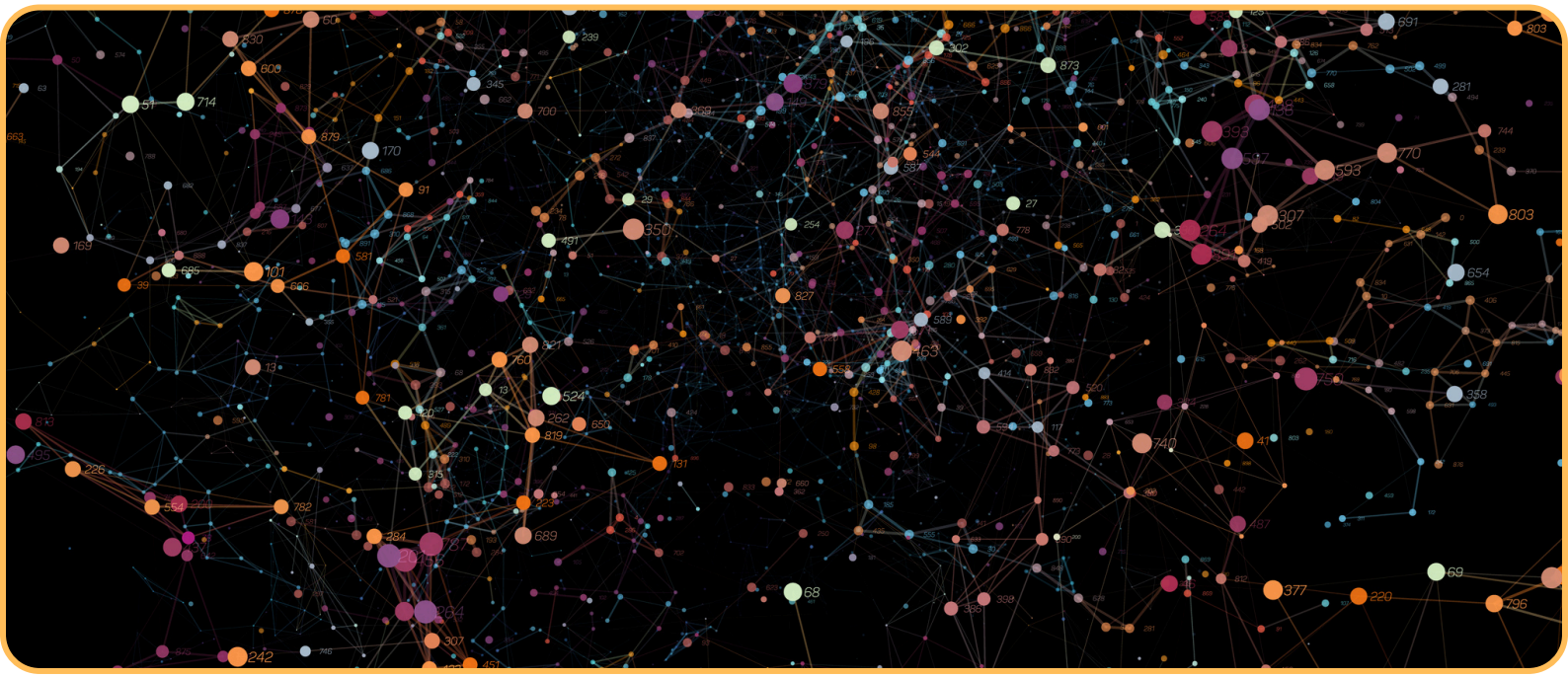

Drug hunters are accustomed to dealing with complexity, scientific and sometimes organizational. Biopharma processes follow the same pattern and anything that reduces process complexity and increases process improvement is usually a good thing. eMolecules' Unity Solution is one notable example. A platform ecosystem allows for the integration of your internal needs to its marketplace like interface, driving lead molecule discovery and optimization. The combination and integration of three (3) companies: eMolecules (eMol), Frontier Scientific Inc. (FSI), and Specs Compound Handling (Specs) now allows the seamless capability of searching, purchasing, reformatting, procuring, and managing compounds through one interface. This streamlining of previously disparate processes has resulted in a highly efficient workflow for drug hunting scientists and compound management personas. It does not end there as they just purchased Synple Chem AG, which comes with seven (7) Trillion virtual but tractable compounds and the custom synthesis group that can synthesize these virtual compounds when needed. This now gives eMolecules a total of eight (8) TRILLION tractable compounds! See Fig. 1

Figure 1- The UNITY SOLUTION

SIGNIFICANT PROCESS IMPROVEMENT

One of the biggest costs to R&D organizations is integration. Whether its data, software, hardware, services etc., integration costs run high and consume substantial amounts of time from both IT and their scientific business partners. It can also lead to costly technical debt when not done properly. To put this in perspective, it is estimated that technical debt is a 50-billion-dollar problem across all US biopharma today! [GU1] 1,2 The Unity Solution not only

reduces this integration cost to a biopharma but it is also much more efficient; 60% more efficient at one major biopharma!

Having the ability integrate and search your internal compound libraries along with the large eMolecules chemically diverse catalogs of potentially novel compounds is the beginning of the integrated and efficient journey.

One platform with multiple compound environments extends to ordering and containerization and global shipping. In addition, warehousing and storage is available to even have a just-in-time outcome saving internal space and stockroom inefficiencies, which by the way we see constantly in our assessments around the globe. If you are a biopharma in Cambridge Mass this should resonate as space is at a premium and having a “service” to manage your small molecule catalogs is probably much more a need than a nice to have.

We have experienced organizations suffering from layers of non-standard processes, antiquated software, and hardware. Having a reliable set of modern processes and thought-out automation will alleviate current bottlenecks and inefficiencies. Today’s biopharma inefficiencies are a large part of the **$314 million to $4.46 billion approved drug costs** due to delays getting to market sooner.2 These cost savings alone can be in the millions of dollars per year depending on your organizational size and current level of process automation.

WHY DIFFERENT PHARMA PERSONAS SHOULD CARE ABOUT WHAT eMOLECULES HAS BUILT

Access to this chemical space is an amazing capability to have for drug hunters (pharmacologists, biochemists/biologists, medicinal/synthetic/computational chemists), to R&D executives. Leveraging this chemical space in the IDSMTA (Ideate, Design, Simulate, Make, Test, Analyze) world does and will continue to have high value to drug discovery.

Medicinal Chemists

- **Efficiency Gain**: Improved compound screening with optimized and harmonized processes. The time that Scientists and technicians that spend synthesizing and testing compounds, adds up quickly in large organizations. Reminder that the total cost for an FTE in this domain can be on average $250,000.
- **Impact**: With access to an immense database of molecules, medicinal chemists can rapidly identify and optimize lead compounds. This accelerates the process of discovering new drug candidates, reducing the number of trial-and-error experiments in the lab. The vast chemical space also can allow for more results based on molecular properties, available descriptors, and fingerprints.

Computational Chemists

- **Efficiency Gain**: Enhanced predictive modeling and virtual screening.

- **Impact**: Computational chemists can use machine learning and AI algorithms to sift through and model this vast molecular space, predicting which compounds are likely to have favorable biological activity and ADMET (absorption, distribution, metabolism, excretion, and toxicity) profiles. In our experience *in silico* and virtual approaches have been narrowing down the list of molecules worth synthesizing, reducing costs and lab time.

Process Development Scientists

- **Efficiency Gain**: Streamlined scale-up processes.
- **Impact**: Access to a large pool of molecules may reveal novel scaffolds that are easier to synthesize and scale up, thus reducing production costs. This could make certain complex drug candidates more commercially viable by streamlining the synthesis and manufacturing processes.

Summary

Access to a vast, tractable molecular space allows for greater precision, faster iteration, and more informed decision-making across all stages of pharmaceutical development. This could significantly reduce the time, cost, and risk associated with bringing new drugs to market. The potential cost savings or ROI (Return on Investment) based on the diverse persona efficiency gains brought about by the UNITY platform is by design. With proven 60% efficiency gains, simply add up all the time how those different personas are wasting or missing opportunities not presented to them. It is millions of dollars in efficiency gains but billions in loss to missed or delayed market opportunities. eMolecules wants you to use this integrated, optimized and harmonized 8 trillion molecule universe so that you can focus on the real hard parts of science. Let the global experts at eMolecules help drive your R&D lead-molecule selection and optimization workflows with its advanced platform, and seamless procurement of over eight (8) billion tractable molecules.

Bibliography

1. https://wwa.wavestone.com/en/insight/technical_debt/

2. 20/15 Visioneer calculated 3.2% of 1.5 trillion for US Biopharma companies

3. Sertkaya A, Beleche T, Jessup A, Sommers BD. Costs of Drug Development and Research and Development Intensity in the US, 2000-2018. *JAMA Netw Open*. 2024;7(6):e2415445. doi:10.1001/jamanetworkopen.2024.15445