

Maximizing purity and minimizing cost in oligonucleotide synthesis cycle with Snapdragon Chemistry

Sector

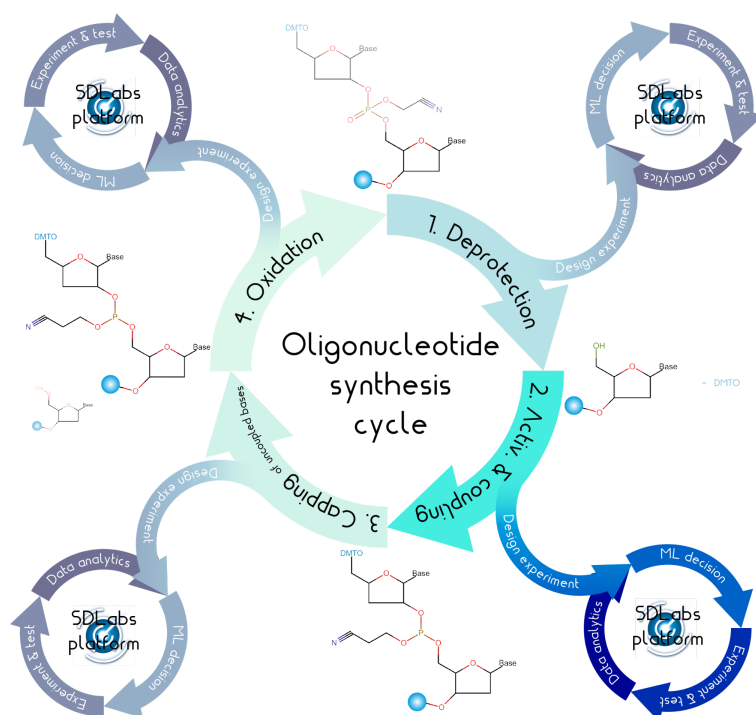
Pharma, Biotech, CDMO

Impact

Accelerated Chemical Synthesis

Overview

Oligonucleotide synthesis is the chemical process of creating short sequences of nucleotides, which are the building blocks of DNA and RNA. This synthesis typically involves a **cyclic, multistep process** where each nucleotide is added sequentially to a growing chain. The process is highly controlled and depends on several variables, such as process variables and choice of chemicals.



Schematic diagram of the cyclic and multistep process of oligonucleotide synthesis. At each step, Atinary's SDLabs platform can be applied to simultaneously optimize all variables and accelerate the identification of global optima. With the vast amount of data as input, the ML algorithms within SDLabs suggest several experimental sets of parameters that can be tested. With each new set of results, the data analytics module can identify trends and correlations without advanced analytical tools.

Challenge

One of the main challenges in oligonucleotide synthesis is the intricate **interdependence** of the various process variables. Each step in the synthesis cycle must be carefully optimized, as changes in one variable can significantly influence the outcomes of others. This complex interplay of variables makes it essential to finely tune the process altogether to achieve consistent, high-quality oligonucleotides. Currently, this optimization is typically done using a one-variable-at-a-time approach.



Use Case

The aim was to synthesize an n-mer and optimize each step of the cycle, to be repeated n times. Typical variables include the resin type, reaction time, nucleoside concentration, type of activating agent, ratio of capping agent, cleavage time and temperature, etc. The listed variables can impact the efficiency of nucleotide coupling, which in turn affects the overall yield and purity of the final product. Slight variations in these parameters will **exponentially** impact the yield and purity of the final oligonucleotide product (yieldⁿ).

Benefits

Atinary's no-code AI platform, SDLabs, allows simultaneous optimization of all variables and accelerated identification of global optima. Typically, oligonucleotide synthesis can be performed using robotic platforms, such as from Chemspeed or Unchained Labs, which can be integrated and operated seamlessly via SDLabs. During a three-month project with our customer, our AI solution led to **significant improvements, with up to an 18% increase in product yield and a 22% reduction in cost**, compared to their previously established R&D processes, demonstrating enhanced impact, efficiency, and cost-effectiveness, and paving the way for accelerated innovation and discoveries in drug development and medicine.

Resources

- [Link](#) to **Press Release**
- More about [Snapdragon Chemistry](#), a Cambrex company

