

A digital approach to chemical supply chain configuration

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Supply chain disruption during last eighteen months have increased the global understanding of the strategic vulnerabilities associated with a wide range of important chemicals, including critical medicines. In our work, we develop a semantic framework for chemical manufacturing requirements, a database of the U.S. domestic manufacturing asset inventory, and a cloud-based digital enterprise capability to index and optimize new supply patterns for chemicals important for national security.

Consider the antidote Atropine. Starting with relatively common materials, the chemistry needed to produce the active pharmaceutical ingredient (API) Atropine is relatively simple, consisting of only three chemical steps. However, to completely articulate the manufacturing requirements associated with Atropine requires more than 5,000 nodes. For more complicated pharmaceuticals, such as Remdesivir with as many as twelve chemical synthesis steps, the requirements grow exponentially. Therefore, rapid establishment of optimized, new supply patterns for a portfolio of medicines in short supply is beyond manual, human capability.

Here, we discuss a cloud-based digital enterprise that identifies manufacturing solutions for a portfolio of active pharmaceutical ingredients using automated asset allocation to chemical manufacturing requirements. This technology automates simulation and virtual scenario analysis for a wide range of supply chain challenges, including complex specialty, fine, and pharmaceutical chemicals.