

CAS CUSTOM SERVICESSM

KNOWLEDGE GRAPH-BASED APPROACHES TO DRUG REPURPOSING

Solution success story

THE CHALLENGE: A global pandemic creates a critical need for drug repurposing

In the early days of the COVID-19 pandemic, researchers worldwide raced to identify effective therapeutics for treating the disease. A great deal of effort in the pharmaceutical industry was focused on finding drugs to combat COVID-19, but initially, few treatments had received FDA authorization. To reduce development time and costs, research focused on repurposing drugs already approved for treating diseases other than COVID-19 or clinically studied small molecules. Because COVID-19 impacts multiple, interlinked physiological systems, including pulmonary hyperinflammation, severe lung injury, blood coagulopathy, renal and neurological problems, and the cellular pathways that underlie these systems, drug developers needed a fast, effective way to examine data and narrow potential candidates.

THE SOLUTION: Knowledge graphing accelerates the identification of potential drug candidates

Because of the interconnectivity of the data, an approach based on knowledge graphing added great value in identifying the links between the impacted body systems and potential therapeutics. Knowledge graphs are a database that allows users to organize and connect pieces of data based on the relationships between them. Knowledge graphs can be used to manage, explore, and navigate the interactions and connections between disparate pieces of information to gain insights and make predictions.

To support COVID-19 drug repurposing efforts, CAS built the CAS Biomedical Knowledge Graph. This knowledge graph featured data on human diseases, proteins, small-molecule inhibitors, viruses, and COVID-19-specific data, all curated from the CAS Content Collection™, linked to biomedical data from both CAS and external sources. The graph contained 6 million nodes and 18 million relationships. The goal was to identify small molecules that showed potential for repurposing as COVID-19 therapeutics.

CAS identified and ranked 1,350 small-molecule repurposing candidates from the knowledge graph. A computer algorithm-driven drug ranking method was developed to prioritize those small molecules. The top 50 molecules were analyzed according to their molecular functions. The CAS Biomedical Knowledge Graph and ranking method proved valuable - 11 of the top 50 results had been or were in clinical trials for treating COVID-19. In addition, many of the drug classes for these small molecules are well known to play important roles in combating viral infections.

Beyond their use as an information management system, knowledge graphs allow users to grasp information visually and intuitively. Users can easily zoom in on specific subsets of a large data set and then zoom back out to see how that subset fits in with the whole data. They can visually navigate the pathways connecting data to see how modules affect each other. Because knowledge graphs are both modular and flexible, data sources can be substituted in and out.

The CAS Biomedical Knowledge Graph provides researchers an opportunity to accelerate innovation and streamline the investigative process not just for COVID-19 but also for many other diseases, such as Alzheimer's, Parkinson's, cancer, and even rare or orphan diseases. Beyond life sciences, knowledge graphs can be applied in many areas of science, including diversified chemicals, materials science, food science, energy technology, environmental research, prediction and characterization of novel and emerging chem/biothreat agents, and the development of medical countermeasures for chem/bio defense.



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results were in clinical trials
for treating COVID-19

SOURCE: clinicaltrials.gov

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