

Making Data Science Accessible for Domain Experts and Creating Real Business Value

Wave Life Sciences is a drug discovery company that makes oligonucleotide therapeutics for the treatment of life threatening diseases. In an industry that moves quickly and has costly development cycles, being able to make timely decisions is essential. KNIME plays a significant role in efficiently managing resources, building quick prototypes, and easily evaluating the results.

A Modern Platform that Covers the Entire Data Science Process

An important question in this setting is how to quickly and reliably develop, test, and deploy software that uses modern data science tools and answers key business questions. The answer lies in finding a platform that provides tools for the entire data science process: from data access and transformation, to visualization and predictive analytics, through to reporting and feedback. For Wave, the solution was KNIME Analytics Platform, later followed by KNIME Server and KNIME WebPortal. KNIME provides access not only to robust data science tools, but also a means for productionizing data science solutions for broad use and delivering these to domain experts via the browser. Wave was able to apply this in different life science domains including cheminformatics and bioinformatics - as seen in the following examples.

Mix and Match Technologies for Creating a KNIME WebPortal GUI that Analyzes qPCR Data

A qPCR workflow for mRNA measurements is a Guided Analytics application for scientists that analyzes 384-well bioassay data. Guided Analytics enables scientists to interact with and explore the data through interactive web pages where a KNIME workflow is running under the hood. "This is one of the nicest features of KNIME WebPortal. Users get to interact as they move with the data and move through the workflow" says Kenneth Longo, Vice President - Discovery Data Science, Wave Life Sciences. "Scientists get a sense of what is going on in their experiment. It's very easy to interact with users at this point to check things that might have gone wrong - which is often a make or break moment" he continues. This close collaboration with scientists can save a lot of time and resources as problems can be detected early on and appropriate decisions can be made.

The workflow is triggered through interactions on the web pages and contains "ready-made" features of KNIME including components with interactive JavaScript graphs, context properties extraction, and controlled metadata through flow variables. In addition, due to the open nature of KNIME, Wave combines this with advanced statistical features and custom visualizations in R, as well as connections to various databases, data sources, and data APIs - some in AWS and some local. And all of this in one platform. The workflow has allowed Wave to process over 200,000 observations in a period of 24 months.

Company

Wave Life Sciences is a biotechnology company focused on delivering transformational therapies for patients with serious, genetically-defined diseases.

Solution highlights

Saving significant amount of time and empowering domain experts.

Biotechnology

Guided Analytics

Research & Development

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Kenneth Longo, Vice President - Discovery Data Science, Wave Life Sciences

Using KNIME as a Data Science and Chemistry Collaboration Framework

Wave develops oligonucleotide therapeutics. The precise design and optimization of those oligonucleotides enables the development of molecules with greater efficacy and safety. With KNIME and its dedicated chemistry extensions, Wave can explore chemical features of these large molecules, do substructure searches, and select and categorize molecules of interest. KNIME has become an integral tool for interactions and collaborations between functional groups at Wave. Through KNIME's strength in cheminformatics, combined with the ability to easily create web applications, it serves as a powerful collaborative framework for data science and chemistry groups.

Creating a Bioinformatics Gene-Species Alignment Network

Evaluating the homology between DNA or RNA sequences is a common task in bioinformatics. Detecting the presence of homologous relationships between relatively short oligonucleotide sequences and the genomes or transcriptomes of different animal species can be a useful predictor of intended (or unintended) gene targets. Command-line tools such as bowtie are commonly used to perform computationally efficient sequence alignments against large genomes. With KNIME it's possible to integrate these command-line tools and enhance the analysis with KNIME components in one reproducible workflow. This built-in functionality includes dedicated nodes for interactive network analysis and visualization, made available on the KNIME WebPortal. For example, users can interactively select clinically-relevant species of interest and investigate the resulting gene-species network of sequence alignments.

Giving Domain Experts Access to Data and Saving Significant Amounts of Time

Since using KNIME Software, Wave has been able to give domain experts the ability to access, view, process, and interact with data. It's empowered them in their research to get a better feeling and understanding of their data – thereby allowing them to find errors early on. Significant amounts of time have been saved because data scientists are no longer spending time hand-processing the data, and ideas can be evaluated quickly. Lastly, human error has been considerably reduced through the workflow-based automation of these processes.

Why KNIME?

KNIME Software is the perfect end-to-end data software development tool – enabling the connection of multiple data sources and domains, the ability to build workflows with a simple, visual drag and drop method, and do automated reporting. One of the strongest benefits of KNIME is the flexibility it offers to mix and match different technologies and features. Being able to augment KNIME workflows by integrating R or Python code is a huge plus. Deployment of KNIME in the AWS cloud enables a powerful and flexible resource architecture.

Getting started with KNIME is easy for new users and has a short learning curve. This is due to the intuitive nature of the KNIME visual interface and the fact that zero coding is required (but possible if needed). KNIME hastens prototype development; the journey from idea to proof-of-concept is short, which is essential in the dynamic and fast-moving biopharma landscape. Lastly, because KNIME works well within a modern software environment, there is less work and risk for IT to integrate it into pre-existing software stacks.