CDD VAULT®
Complexity Simplified

Customer Case Study

"Having everything in the Vault means that data is easily findable, accessible, and searchable, even months later, and can be collated as required for in depth reporting."
- Koen Dechering, Ph.D., CEO, TropIQ

TROPIQ HEALTH SCIENCES

TropIQ - Digitalizing Drug Discovery for Vector-Borne Diseases

More than half of the world's population is at risk from vector-borne diseases that are transmitted by insects such as mosquitoes, flies and ticks. These diseases cause more than 1 million deaths annually, and it is primarily people in the poorest countries who are the most vulnerable.

TropIQ Health Sciences, a spin-off from Radboud University Medical Center in the Netherlands, was established in 2011 to commercialize an innovative malaria drug screening platform that was developed at the university. The high throughput platform represents the foundation of a suite of technologies that the company is leveraging commercially to enable what it sees as ground-breaking drug discovery and R&D in the field of vector-borne diseases that affect populations across the developing world.

As a critical part of its R&D infrastructure, TropIQ has implemented the CDD Vault informatics system as its primary data repository to manage the huge volumes of chemical compound, screening assay, biological and experimental data that are generated through the company's in house, partnered and contract discovery and development projects.

The breadth of TropIQ expertise is founded on a combination of parasitology, entomology and technological strengths, particularly in malaria research. The company's lab is one of the few in the world that can screen against the different life stages of the malaria parasite at scale. "There's no other lab that offers in vitro high throughput assays for all stages of the malaria parasite life cycle in both human and mosquito hosts," said Dr. Koen Dechering, co-founder and CEO of TropIQ.

The TropIQ technology labs include facilities for semi-automated cell culture, a vector lab for its insect vector experiments and associated automation and detection instrumentation. In parallel with its parasitology expertise, the company has developed a unique barcoded live insect screening technology that is being used for the discovery of novel vector control agents, such as insecticides and molecules that might block malaria transmission.

The primary focus for TropIQ remains in house/partnered malaria projects and contract research, but the firm is in addition exploiting expertise that spans discovery and R&D for multiple areas of vector-borne viral diseases, including the mosquito-borne viral infection that causes Dengue. And while the overarching aim is to progress research for global human health and tropical infectious diseases, TropIQ has more recently moved into the field of tick-borne infections, which cause huge loss of livestock across some areas of the developing world, and are a growing health concern in developed countries.

It was a combination of both the diversity of research and the breadth and volume of data that generated a significant information and data bottleneck, Dr. Dechering explained. "Managing the huge volumes of compound, screening and experimental data was a primary challenge. We had been using Excel spreadsheets but it was almost impossible to keep track of everything, remember experiments, and put in place a mechanism to combine and assess chemical and biological information in context." As Dr. Dechering pointed out, "We were struggling in house, and it wasn't feasible to retrieve all the data we needed from memory, from Excel spreadsheets and paper notebooks."

Dr. Koen Dechering, CEO of TropIQ Health Sciences

TropIQ had previously experienced the features and capabilities of CDD Vault through its partnerships and collaborations, and in 2019 made the "relatively easy" decision to acquire and roll out the technology as its primary repository for data. "Immediately we then had the functionality that allowed us to carry out structural searches on compounds, combine chemistry and biological data, and trace experiments and results."

"We have been using the Vault for registering compound sets comprising tens of thousands of compounds, together with screening data, and results generated through hit to lead, or lead optimization projects," Dr. Dechering continued. "The Vault is ideal for compound management, so we are also in the process of registering historical compound sets stored in the freezers."

TropIQ laboratory at Noviotech Campus, Nijmegen, the Netherlands

Importantly, day-to-day use of the Vault saves a considerable amount of time, and helps to prevent user errors in data transfer, Dr. Dechering noted. “When we need to write reports on projects that may have involved completing dozens of experiments, having everything in the Vault means that data is easily findable, accessible, and searchable, even months later, and can be collated as required for in depth reporting. There is also far less risk of error. Previously there was a lot of copy-pasting from Excel spreadsheets into graphics packages, and this posed a considerable error risk.”

The inherent flexibility of the CDD Vault platform means that TropIQ scientists can also program routine equipment such as plate readers to generate a Vault-compatible data output, so that data files can be deposited directly into a relevant folder in the Vault. “This allows us to ensure minimal manipulation of data between the raw data generated and the data that is entering the Vault, which again helps to reduce the risk of errors, and also frees up scientists valuable time.”

CDD Vault can be configured to manage the combination of chemical structure, biological, and experimental data generated from each project. “For example, we're currently carrying out a drug discovery project with the University, which is focusing on a novel compound series with antimalarial activity. The organic chemistry department at the University is carrying out the synthesis, and we provide the resulting assay data, so we register the compounds and combine that with biological data that we generate. The project team can then look at the data in context, to plan new syntheses.”

TropIQ is in addition engaging in an increasing number of programs focused on biologics, rather than small molecules. CDD Vault similarly offers the flexibility that will allow registration of biologics sequences directly. “All of our primer sequences, for example, are currently sitting in an Excel database, and it would be hugely beneficial to have those DNA oligonucleotides registered in the Vault, so that

we can search them as we do our chemical structures. This is something that we are working on with the CDD Vault team."

It was a chance meeting between TropIQ co-founders and old friends Dr. Koen Dechering, and Professor Robert Sauerwein that resulted in the concept of setting up a commercial entity to focus on research that has perhaps traditionally been the remit of non-profits. "With an academic background in malaria research, I had also spent a decade in pharmaceutical industry drug discovery settings. Professor Sauerwein was working on malaria vaccines at the University, and introduced me to the University's screening platform for vaccine research.

"We felt there was room for a technology platform that could bridge the divide between the excellent research that is ongoing in so many academic settings, and industrial research. We had enough confidence in our platform to establish a company, with a business model that should be sustainable, and generate revenues that could then be ploughed back in to drive the research agenda, rather than set up a foundation or non-profit."

This was, Dr. Dechering acknowledged, "something of an experiment, as we were a for-profit entity in a largely non-profit world." Nevertheless, the firm had the foresight to appreciate promising opportunities for contract research, both from the pharma world but also from non-profit organizations including the Bill and Melinda Gates Foundation or Medicines for Malaria Venture. "These are organizations with an interest in malaria R&D, but they do not have their own labs, so they outsource, and this is where we can leverage our strengths. We also have a number of small biotech customers."

Over the last 10 years since its foundation, TropIQ has grown from just three directors and a technician, to 18 people. And growth has been purely organic. The company has invited no external investment.

One of the goals for TropIQ platform development will be further miniaturization and automation of its assay technologies. "By doing this we will then be able to increase scale and throughput, and screen large libraries in 384 well format, as well as small compound sets. And this, again, is where CDD Vault comes into its own, as the repository for compounds and results from high-throughput screening assays."

Over the last decade the TropIQ has expanded its sphere of expertise, Dr. Dechering continued. "We still have a very large malaria focus working on the Plasmodium parasite, but we are also now more and more interested in mosquito vector. So, looking at how this disease is transmitted, and how we might block the spread of the disease by targeting the mosquito rather than the pathogen. And from there the business has evolved into a larger effort, where we are now working on arthropod-borne viral diseases such as dengue."

Anopheles stephensi malaria mosquitoes

The SARS-CoV-2 pandemic has resulted in a tangible reduction in investment in neglected diseases research, Dr. Dechering noted, and this at least in part, driven TropIQ to expand its own sphere of expertise and research. “For example, we have recently started a program on tick-borne diseases, which impacts both on domesticated livestock, and on human populations. We are able to use the same technologies, and effectively exploit what we are good at, which includes culturing pathogens, and working with vectors.”

About Collaborative Drug Discovery

Collaborative Drug Discovery provides a modern approach to drug discovery informatics that is trusted globally by thousands of leading researchers. Our CDD Vault is a hosted informatics platform that securely manages both private and external biological and chemical data. It provides core functionality including chemical registration, structure-activity relationship, inventory, visualization, and electronic lab notebook capabilities. For more information, visit us at www.collaborativedrug.com.