

# Unlocking Novel Targets to Treat Neuroscience Diseases at Cerevel Therapeutics

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## Cerevel Therapeutics

- *Founded in 2018 in partnership with Pfizer and Bain Capital*
- *A clinical-stage biopharmaceutical company unraveling the mysteries of the brain to treat neuroscience diseases*
- *Leverage both in-house expertise and external partners including in vitro pharmacology, chemistry, DMPK, in vivo pharmacology, and safety assessments to support a broad and diverse pipeline of neuroscience drug candidates*
- *Select Dotmatics platform, biology/chemistry ELN, and across-the-board solutions for data searching and data analytics, workflow creation, assay management, one-way CRO data upload for chemical and biological result registrations, inventory management, sample and asset management, highly secured cloud-based hosting with version controls, and more*

Cerevel Therapeutics was founded in 2018 with the vision of unraveling the mysteries of the brain to treat neuroscience diseases. The company is tackling diseases with a targeted approach to neuroscience that combines expertise in neurocircuitry with a focus on receptor selectivity. Cerevel has a diversified pipeline with the potential to treat a range of neuroscience diseases, including Parkinson's, epilepsy, schizophrenia, and dementia-related apathy.

Cerevel has a diverse team of experts in biology and chemistry who work both internally and at CRO partner locations across the globe.

As a company with a bold vision, Cerevel knew they needed to find a software provider whose solutions would support their complex research workflows and help meet their ambitious goals. Due diligence early on would pay off in the long term. That being, Cerevel put together a cross-functional team to evaluate a number of vendors in hopes of finding a provider whose solutions would:

1. A single software for data warehouse and analytics with cloud-based hosting
2. Facilitate cross-functional research
3. Ensure strong security and safeguard IP
4. Scale as they grow both externally and internally

Very quickly, the Cerevel team conclusively determined that Dotmatics offered the best overall solutions for their needs.

In this case study, Cerevel's Director of Medicinal Chemistry, Hanh Nho Nguyen, explains why Dotmatics is such a great fit for Cerevel and he presents some specific examples of how his team has put Dotmatics solutions to work across their research workflow.

*"We evaluated a few different vendors, but when we looked at Dotmatics we thought, 'Wow. Everything we need is already in the Dotmatics Platform!' But on top of that, it was easy to see that the Dotmatics team would be flexible and easy to work with. This was a very critical factor for us in choosing a software partner. We wanted to pick someone who would be a partner for the long haul and we found that with Dotmatics."*



*Hanh Nho Nguyen,*

*Director of Medicinal Chemistry,  
Cerevel Therapeutics*



## Why Cerevel Therapeutics Chose Dotmatics

Of course, a big reason Cerevel chose Dotmatics solutions was because they met the team's three key needs surrounding research, which includes enablement, security, and scalability. But there was more to it. Dotmatics, as a company, also stood out. Dr. Nguyen mentioned, *"We evaluated a few different vendors, but when we looked at Dotmatics we thought, 'Wow. Everything we need is already in the Dotmatics Platform!' But on top of that, it was easy to see that the Dotmatics team would be flexible and easy to work with. This was a very critical factor for us in choosing a software partner. We wanted to pick someone who would be a partner for the long haul and we found that with Dotmatics."*

Dr. Nguyen walked us through the three key reasons his team chose Dotmatics, explaining which features stood out during the evaluation and giving us a sneak peek at how his team has put the solutions in action.

### Key Reason #1: Dotmatics Facilitates Cross-Functional Research

The Cerevel team wanted a solution that would support their entire research workflow—from design and synthesis, to registration, to testing and data analyses. They needed to not just capture research data from their lab environment, but also easily search and view that data in real time. They wanted a solution that would unite their data and equip all scientific team members with the specific capabilities they needed. They didn't want to deal with burdensome technology integrations and data transfers. So, the team decided to pursue a platform solution instead of standalone pieces, and they found the perfect solution in Dotmatics.

#### Key features of the Dotmatics Platform that stood out to the Cerevel team were its:

- Unifying access to all corporate data (legacy, preclinical, HTS, virtual compounds, etc.)
  - Powerful data browsing, querying, viewing, and analyzing capabilities for guiding compound designs
  - Fully integrated lab informatics and analytical tools to help with profiling the compounds, such as prediction of physical properties and efficiency indices
  - Cross-functional capabilities to unite chemistry and biology teams and facilitate cross-functional collaboration
- Integrated chemical and biological registrations
  - Real-time inventory functionality (e.g., both solid and DMSO stock solution)
  - Compound re-testing expiry and re-testing alerts to ensure batch quality is up-to-date
  - Assay registration and assay-data handing (including from non-GLP *in vitro/in vivo* studies)

### Informatics Requirements at Cerevel

- Integrated mining and analysis of all corporate data
- Web-based ELN for all scientists
- Test and task management and tracking
- Assay management and analysis
- Scientific data visualization and analyses
- Sample and asset management
- Chemical registration and reagent management
- Peptide and protein registration



## Solution at Work: Cross-Functional Research

The Cerevel teams leverage the Dotmatics ELN across all departments. This has greatly streamlined the team's workflows by allowing them to:

- Use the same web-based ELN for all disciplines, including chemistry, biology, analytical chemistry, DMPK, and safety assessments
- Record experiments with all necessary details, such as date stamps, experiment numbers, ownership, reaction drawings, reagent and solvent data, experimental conditions, procedures, etc.
- Handling thousands of high throughput screening compounds
- Capture diverse data, including text, images, files, assay results, high throughput screening results, kinetics, calculated dose-response values, documents, and encrypted PDFs
- Potentially upload data from lab instruments with Dotmatics BioBright (e.g., QC data files and reports)
- Use integrated chemical and biological registrations
- Let CROs upload data into an approval queue that internal scientists can review, approve, publish, and share
- See real-time compound inventory and know instantly what needs to be scaled up
- Feel confident using a system that ensures data is fully archived, secure, auditable, and searchable

The team has found that one of the great things about Dotmatics ELN is not just how easy it is to get data in, but also how easy it is to then query and analyze that data.

Dr. Nguyen explains, "A lot of ELNs are good at getting data in, but not so great at getting data out. That's not the case with Dotmatics. You can easily query your data with Dotmatics Browser. You can even set up your ELN to automatically push data into Dotmatics Browser, where you can create tabs to cleanly organize project data. You can then push data to Dotmatics Vortex for automatic merging and detailed analysis."



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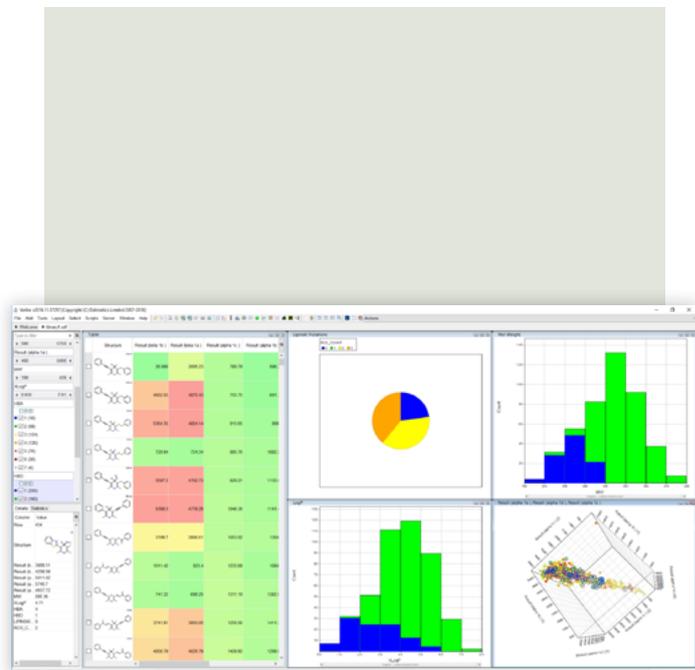
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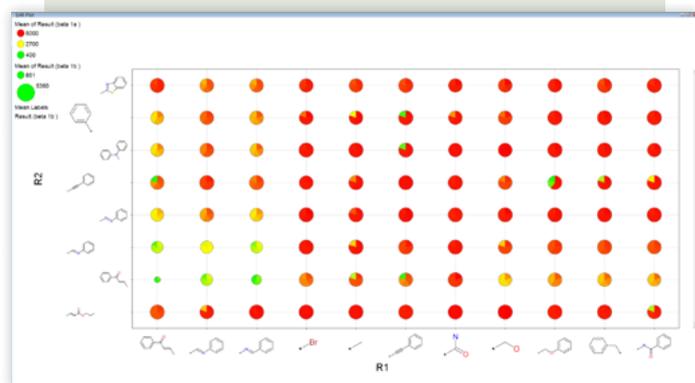
Streamlining the early parts of their research workflow has freed a ton of time for the team to focus on data analysis. This is where Dotmatics Vortex comes into play. Dotmatics Vortex is a powerful data visualization and analysis program that Cerevel uses to garner insight from their data and guide their research decisions.

#### Some of the key Vortex features the teams appreciate are:

- Calculation and analysis capabilities:
  - physical properties
  - customized formulas (e.g., LE, LipE)
  - selectivity ratio
  - K-mean clustering
  - match-pair analysis
  - R-group analysis
- Ability to export to PowerPoint for presentation and sharing
- Merging and combining multiple spreadsheets using compound code as the key
- Graph features:
  - Different graph types:
    - scatter
    - pie
    - bar
  - Manipulation tools:
    - size by value
    - color/shape by series
    - trendlines
    - structure and compound code viewing



Dotmatics Vortex Dashboard



Dotmatics Vortex Dashboard

Dr. Nguyen comments, “Dotmatics Vortex is a really powerful tool for data mining and analysis. One of the features we like most is how easy it is to merge files like SDF files and Excel files. With just one click, your data is merged. No deleting columns, no manual editing. It really frees a ton of time to focus on analysis. It’s a breeze!”

## Key Reason #2: Dotmatics Solutions Are Secure and Safeguard IP

During vendor evaluation, Cerevel's IT and legal teams were onboard to ensure that any solutions chosen would meet their strict security standards.

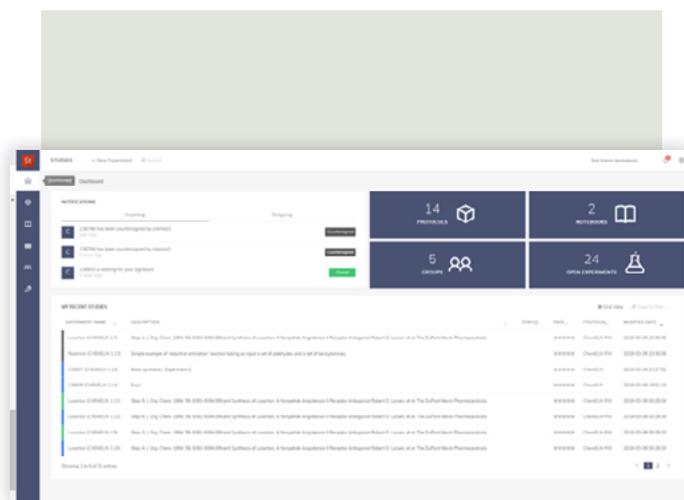
A few data security features stood out, including the Dotmatics Platform's:

- Regular distributed data backups
- Secure data transfer with encryption and valid web-app certification
- Trusted cloud security (e.g., AWS security and encryption)
- Full compliance with applicable rules and regulations (e.g., electronic records and signature, ISO)
- Reliable data transfer and flow
- Secure version control

The Cerevel team also felt that using the Dotmatics Platform, in particular the ELN, would help protect their IP because it would keep electronic records of work done in all areas of research, including medicinal chemistry, chemistry, formulation, in vitro and in vivo pharmacology, DMPK, and safety assessment.

However, it wasn't just behind-the-scenes security that impressed the Cerevel team, it was also the Dotmatics Platform's user-level security features. With the Dotmatics Platform, the Cerevel team can easily:

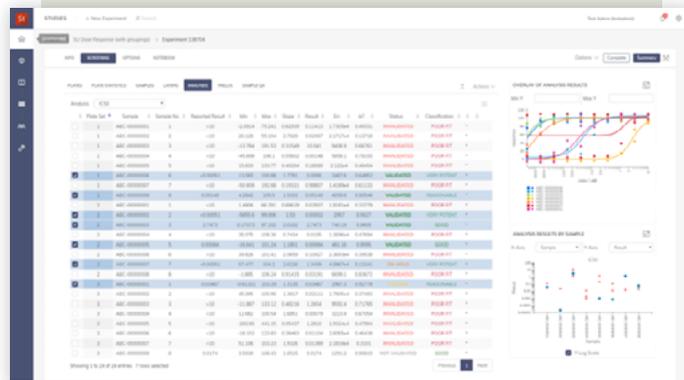
- Define which users have access to specific Dotmatics functionality
- Restrict admin access
- Limit users to data deposition and block data retrieval
- Prohibit enterprise-wide querying for specific users
- Assign internal codes and aliases for compounds (if desired)
- Encrypt PDF reports



Dotmatics ELN Dashboard



Dotmatics Bioregister for registering sequence-based, chemically-modified and structure-less biological, including uniqueness checking



Assay data management with Dotmatics

## Solution at Work: Secure CRO Collaboration and Compound Registration

The Cerevel team has used Dotmatics Register to create a secure process for registering their small molecules and proteins with unique IDs that have eliminated the registration of duplicated compounds. Because Dotmatics permission levels are easy to fine-tune, both CRO and Cerevel scientists can securely work together on the same Dotmatics Platform.

CRO partners are given restricted access to the Cerevel database with:

- One-way data upload only (including batch uploading for time savings)
- No direct registration capabilities (but rather entry into a review queue)
- No access to viewing other data or making edits or deletions
- Aliased/coded compound, assay, and project names

Cerevel chemists and biologists are given additional functionality, such as:

- Sketching and stoichiometric calculation capabilities
- Compound and assay registration (with unique Cerevel IDs)
- Access to audit trails and countersigning capabilities
- Ability to create customizable PDF reports with optional encryption

To streamline collaboration, the Cerevel team has created multiple-field templates for their CRO partners to record compounds and associated details (e.g., who made it, what purity it is, etc.). The CROs enter all the data themselves and then do a single batch upload to the Cerevel database. Cerevel scientists then review and publish the data after it has been reviewed.

The Cerevel team loves that Dotmatics solutions make it easier to collaborate with their CROs. Dr. Nguyen explains, *“The option of secure, one-way data upload for our CROs has saved a ton of time for us internally. We can let the Dotmatics system acts as an intermediary and don’t have to take on this task ourselves. The process has been really fail-proof. In fact, since implementing Dotmatics, we haven’t had any duplicate compounds!”*



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### Key Reason #3: Dotmatics Scales with Growth

The Cerevel team needed to position themselves for growth. They felt a cloud-based solution would let them seamlessly scale as their projects increased and their internal and external teams grew.

### Solution at Work: Virtual Machine for HTS

Building their research platform using scalable, cloud-based computational resources has already benefited the Cerevel team. One example Dr. Nguyen cites is managing HTS compounds and screening results. He explains that when he has a project that requires more computing power, he simply asks his IT team to spin up a virtual machine. With Dotmatics and the power of the cloud, his team can register thousands of compounds with no issues at all, something he believes wouldn't be feasible with Excel sheets or even other free software. He concludes, *“Having this option of linking out to a virtual machine is really key for us, especially in the area of HTS, where we're dealing with structural features and trying to register thousands of compounds.”*



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## Starting Up for Success

By partnering with Dotmatics early on, the Cerevel team has positioned themselves for success. They believe that without Dotmatics' suite of solutions, they would have faced great challenges in not just organizing all their research data, but perhaps more importantly, leveraging that data to gain insight and guide efforts. The team summarized their thoughts by providing a quick list of the benefits they've seen since adopting Dotmatics.

### Benefits Since Dotmatics Adoption

- Compound searching with codes and aliases
- Up-to-date inventory
- Compound re-testing dates
- One ELN for all functions
- Secure CRO collaboration
- Biology assay results registration
- Results can be viewed and analyzed in Vortex to elucidate structure-activity relationships and trends that allow the medicinal chemists to design better compounds
- No more duplicated compounds
- Time savings across all processes
- More insight from easier analysis
- Power to manage thousands upon thousands of compounds

The Cerevel team plans to continue working with Dotmatics to add additional functionality for computational chemistry and predictive modeling. Dr. Nguyen concludes, *"We here at Cerevel consider Dotmatics a partner. They continue to support us and they truly want us to succeed. We look forward to working with them more in the future."*



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