Optimizing Small Molecule Drug Discovery

How to innovate while keeping R&D costs down

Dotmatics

Contents

Small molecule drug discovery is entering a renaissance thanks to better screening technologies, improved target understanding, and novel methodologies.[1] In 2021, 62% of new drug approvals were for small molecules, including new treatments for HIV, cancer, infections, heart and kidney disease, neurological disorders, and more.[2] But as opportunity abounds, so does the need to do more with less time, money, and technical debt. To succeed, companies need to adopt processes and technologies that will help them drive innovation while controlling costs.

Rising Pressure to Do More with Less

The cost of drug discovery is higher than ever. Just look at the statistics:

>12

Years and ~1-3 billion dollars to bring a new drug to market[3,4,5,6]

$83B

Annual spend on pharmaceutical R&D in the United States in 2019[6]

12%

Increase in R&D costs in recent years[7,8]

Yet as costs soar, pressure mounts to lower drug prices and help reduce federal drug expenditures.[6] How can companies reconcile these competing demands?

Hidden Costs of Small Molecule Drug Discovery

Finding viable ways to deliver new treatments to patients requires companies to address hidden costs of small molecule drug discovery, which are driven by factors such as high failure rates, declining productivity, fragmented data, disconnected workflows, and inefficient processes. These are problems that not only impact research outcomes, but also bottom lines. Optimizing early discovery efforts to find better candidates more quickly can have a huge impact on more costly and lengthy downstream efforts in clinical testing, trials, regulatory review, and commercialization.

Teams across an organization must find ways to do more with less. Those at the forefront of discovery and innovation are no exception. Chemists, data scientists, therapeutic project leads, and CSOs must all find ways to work faster and smarter. This requires deep process scrutiny to uncover the challenges that are holding them back. Companies must then make specific changes that will ultimately help reduce the cost of downstream failures. Dotmatics has helped a lot of companies do this, and in the following sections, we highlight some of the most common challenges and opportunities for improvement.

Common Challenges

1. Unnecessary Workflow Complexity & Workarounds
2. High Failure Rate
3. Disconnected Systems
4. Compromised Data Value

1. Unnecessary Workflow Complexity & Workarounds

For years, most research teams have known that streamlining workflows is necessary, not optional. Teams have poured time and money into products promising to reduce manual processes, handle growing data volumes, and address specific workflow inefficiencies.

However, R&D productivity declined in the 2000s and stagnated in the 2010s. Why? Because point products are most often quick fixes, not long-term enterprise solutions. They may help a few users or groups with specific tasks, but they generally don't help at a larger scale when researchers need to work together and share data to move projects forward.

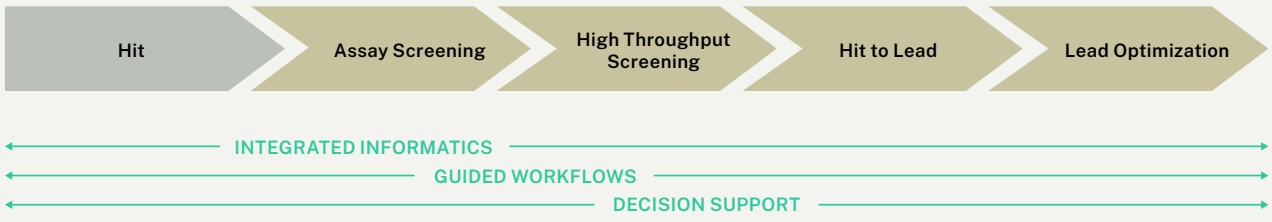
Small molecule drug discovery workflows have become increasingly complex, often demanding collaboration amongst teams who have historically worked in relative isolation, with different workflows, tools, and data types. Point solutions just can't support this. Dotmatics can.

Dotmatics provides an R&D data management platform that delivers fully integrated laboratory informatics software, guided workflows, and decision-support tools that span the entire hit-to-lead workflow. Enterprise-wide, users can leverage the same system and share data and insights seamlessly, leading to better productivity and collaboration. Dotmatics facilitates secure data exchange not only behind the scenes, but also within the user-facing tools and applications that different teams need for tasks such as library design, synthesis, sample logistics, QC analysis, screening, and SAR analysis.

With Dotmatics, teams can:

- record, search, and share experiments and results to facilitate standardization and reduce repeat experimentation,
- access their preferred tools, applications, and data from one united platform, minimizing manual data handling, and freeing time for discovery,
- securely collaborate across sites and with CROs via secure cloud data exchange,
- create reports and make decisions using a trusted master data source.

Unite Teams and Data Across Discovery



Dotmatics increases productivity and collaboration by delivering fully integrated laboratory informatics software, guided workflows, and decision-support tools that span the entire hit-to-lead workflow.

2. High Failure Rate

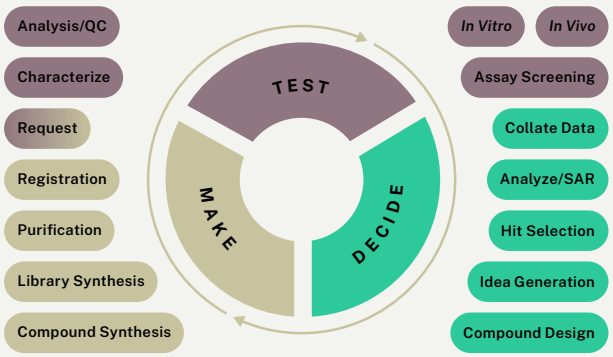
The road from hit to drug is long, winding, and expensive! The stats are staggering. Every 10,000 hits synthesized and tested generate only 250 candidates. Of those candidates, around ten make it to trials. Of those in trial, only one will make it through regulatory approval to reach market.[7]

Narrowing down candidates is an onerous process. Some companies will repeat their make-test-decide cycle up to 10,000 times, all along the way using various tests, analytics tools, and software to hone in on promising candidates and eliminate dead leads. Oftentimes, there needs to be a high rate of human touch to integrate the disparate data needed for decision-making. This is not only time-consuming, but also error-prone. It is different with Dotmatics.

Dotmatics automates data collection, integrates disparate data, and delivers the best-of-breed software that teams need throughout their make-test-decide cycle. For example, with Dotmatics:

- Chemists can make better-informed decisions with guided visualizations, preconfigured cheminformatics analytics capabilities, and easy access to all the disparate data they need to create a full picture (e.g., biochemical, structural, DMPK, patent, literature, etc.)
- Teams across locations and CRO partners can access and feed a united source of data, helping to create a complete, single source of scientific truth to drive better discovery strategies.
- Managers can merge and analyze data across multiple projects and teams, getting real-time insight into project status, results, and key department metrics.

Access Robust Capabilities From a Single Platform



Dotmatics delivers all the tools needed to efficiently capture, layer, analyze, and share data throughout the make-test-decide cycle.

Optimize Discovery to Reduce Downstream Failure Costs

FDA = FDA approval

P = Pre-Clinical Testing: feasability, iterative testing, safety data are collected, typically in vitro and in vivo (lab animals)

R= Regulatory Approval and Manufacture

Source: R&D Software Market Study: McKinsey & Co.; Jan 2022

3. Disconnected Systems

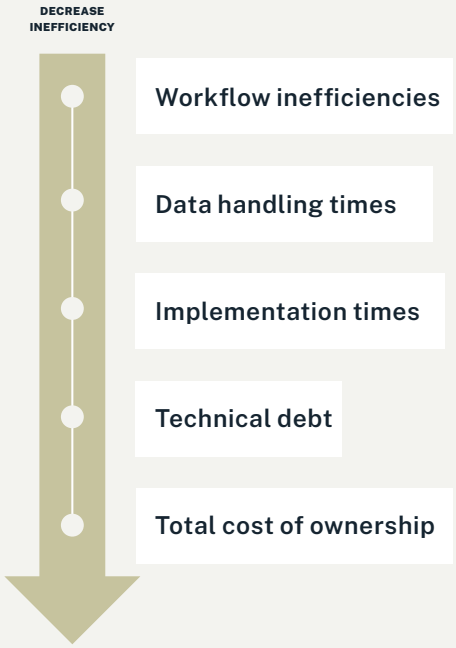
For far too long building an R&D infrastructure has meant cobbling together rigid, single-purpose lab systems, legacy software, and users' preferred research tools. Everyone suffers with approach, from IT staff implementing and supporting the solutions, to the scientists using them, to the budget managers paying for them.

Disconnected systems put IT managers under constant pressure to keep pace. They face one lengthy and costly integration project after another, and they are often left with results that are cumbersome and inflexible. Perhaps more importantly, an absence of genuine connectivity between lab solutions and a lack of truly unimpeded data flow across the research workflow impacts not just efficiency, but also insight—something that can make or break collaborative, data-driven research labs.

Break the status quo by investing in a united solution that will reduce workflow inefficiencies, implementation costs, technical debt, and total cost of ownership. By uniting all data and tools with Dotmatics, everyone benefits. For example:

- Researchers can quickly capture, find, share, and use data without the need to switch between applications and transfer data because, with Dotmatics, everything is tied back to one platform.
- IT managers can reduce the time and cost of implementing and supporting disconnected solutions and reduce technical debt by working with a single vendor whose solution spans the entire hit-to-lead research workflow.

Decrease Inefficiency With a United Platform



Dotmatics helps companies achieve higher operational efficiency by consolidating on one platform with one vendor.

4. Compromised Data Value

Beyond collecting and integrating the volumes and varieties of data being produced across early drug discovery workflows, companies need to also ensure that data are both trustworthy—to support sound decisions—and traceable, to protect IP. While many legacy informatics solutions promise to deliver process efficiency and control, most fail, leaving inefficiencies and compliance issues behind. It's different with Dotmatics.

The ways in which Dotmatics Platform handles, processes, shares, and stores data all work together to remove unnecessary risk. For example, Dotmatics Platform helps:

- Improve data integrity by eliminating error-prone manual data handling, instead automating data capture, standardization, validation, and integrity-checking.
- Standardize on a common data model by breaking away from proprietary data formats, automating QC and QA, and provisioning the model quality data need for in-depth scientific analyses.
- Optimize data acquisition from all data producers
  by supporting clean and fast data collection, whether through automated instrument data capture, database integration, or error-proof data entry via electronic laboratory notebooks (ELNs).
- Enhance compliance by recording chain-of-custody and audit-trails, supporting origin tracing, and enforcing things such as signature requirements, hazardous-product-use approvals, and standard operating procedures (SOPs).

Companies need to trust and trace their data and Dotmatics helps them do just that.

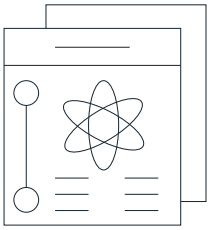
Dotmatics Small Molecule Drug Discovery Solution

For more than 15 years, we've had firsthand insight into the challenges facing small molecule drug discovery teams, as well as the solutions that help them thrive.

We've used this insight to create a Small Molecule Drug Discovery Solution that let companies:

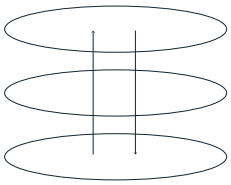
- **Support end-to-end workflows.** Adopt a single scientific R&D platform for all discovery efforts, from hit-to-lead identification, to lead optimization, to candidate selection.
- **Foster collaboration.** Let all internal teams and external CROs access the same secure platform to share data, make requests, and manage workload in areas such as:
  - Library Design
  - Compound Synthesis
  - Inventory Management
  - Sample Logistics
  - QC Analysis
  - Screening
  - Assay Data Management
  - SAR Analysis
  - Entity Registration
- **Speed up research.** Provide guided templates and focused analytics capabilities that let teams standardize experiments, record novel exploration, share results, and create a unified knowledge base.
- **Turn data into insight.** Automate data capture and provide tools to gather, clean, merge, analyze, contextualize, search, and visualize all diverse project data, including instrument data, experiments, compound data, corporate and commercial data, molecules, samples, and assays.
- **Reduce technical debt and total cost of ownership.** Replace obsolete software, fill capability gaps, and avoid the mess of working with multiple vendors whose products don't easily scale or integrate.

Some of the software and capabilities available in the Dotmatics Small Molecule Drug Discovery Solution include:



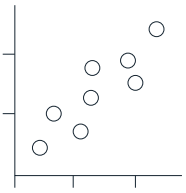
Electronic Laboratory Notebook

Capture, store and search experiments.



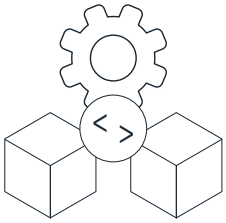
Scientific Search

Search and report across research databases.



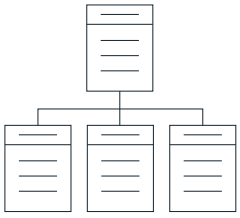
Visualization & Analytics

Analyze, graph and present your scientific work.



Assay Development

Develop new assays for screening experiments with GraphPad Prism.



Library Design

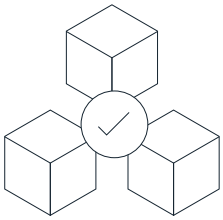
Build and execute library design workflows.

Entity Registration

Register sequence-based, chemically-modified and structureless biological entities.

Lab Data Automation Solutions

Acquire, secure, and analyze laboratory instrument and CRO data with BioBright and DarwinSync.



Assay Data Management

Capture and analyze all types of screening experiments.

Dotmatics Chemistry Solutions in Action

cerevel

Clinical stage biopharma Cerevel needed a research platform to help support their efforts to uncover novel targets to treat neuroscience diseases. They chose Dotmatics because it offers a secure, scalable research platform that supports cross-discipline workflows, while also ensuring data integrity and IP protection. Read more in the case study Unlocking Novel Targets to Treat Neuroscience Diseases at Cerevel Therapeutics.

> “We evaluated a few different vendors, but when we looked at Dotmatics we thought, ‘Wow. Everything we need is already in the Dotmatics Platform!’

HANH NHO NGUYEN
Director of Medicinal Chemistry,
Cerevel Therapeutics

See How They Did It

Dotmatics Chemistry Solutions in Action

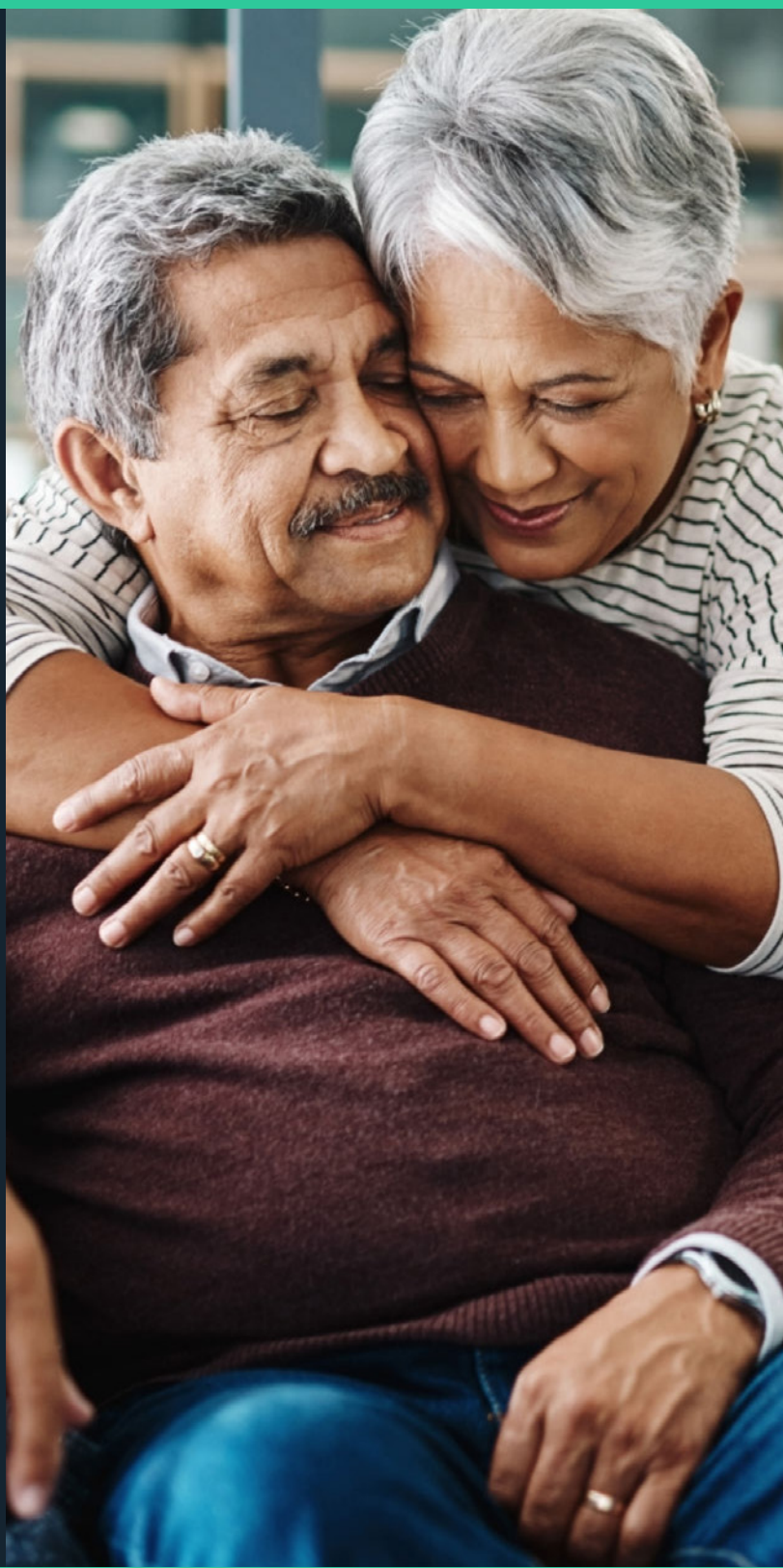
Debiopharm

Swiss biopharma leader Debiopharm uses Dotmatics solutions to support their pursuit of treatments for cancer and bacterial infections. Dotmatics solutions have helped Debiopharm streamline workflows, improve data-driven decision making, and get internal teams and CROs working better together. Read more in the case study Dotmatics as a Disruptive Technology at Debiopharm.

> “Dotmatics has truly disrupted the way the company works for the better. As soon as people saw how useful it can be to share everything in one place and how much more efficient our processes are as a result, everyone got on board with Dotmatics.”

RENÉ VAN DEN BERSSELAAR
Global Head IT and CIO, Debiopharm

See How They Did It



Make Your Small Molecule Drug Discovery Work

Request a demonstration today to explore how Dotmatics can help your small molecule drug discovery teams find better candidates, faster.

Request Demo

Dotmatics

1. **Buvalia, A. BiopharmaTrend.com**. 2022. Will Biologics Surpass Small Molecules In The Pharmaceutical Race? https://www.biopharmatrend.com/post/67-will-small-molecules-sustain-pharmaceutical-race-with-biologics/.

2. **Halford, B. Chemical and Engineering News.** 2022, 100 (2). New drug approvals held steady in 2021. https://cen.acs.org/pharmaceuticals/New-drug-approvals-held-steady/100/i2#:~:text=The%20agency%20approved%2050%20new,of%20the%20new%20drug%20pipeline.

3. **Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK.** Artificial intelligence in drug discovery and development. Drug Discov Today. 2021 Jan;26(1):80-93. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7577280/

4. **Pharmaceutical Technology.** It will take years for AI use to peak in drug discovery and development process. https://www.pharmaceutical-technology.com/comment/ai-peak-drug-discovery-development/

5. **Schlander M, Hernandez-Villafuerte K, Cheng CY, Mestre-Ferrandiz J, Baumann M.** How Much Does It Cost to Research and Develop a New Drug? A Systematic Review and Assessment. Pharmacoeconomics. 2021 Nov;39(11):1243-1269. https://pubmed.ncbi.nlm.nih.gov/34368939/

6. ***Congressional Budget Office.*** Research and Development in the Pharmaceutical Industry. 2021 April. https://www.cbo.gov/publication/57126

7. **R&D Software Market Study**; McKinsey & Co.; Jan 2022

8. **Life Science's Lab Informatics Digital Criteria to Separate Vendor Leaders From Laggards**, Gartner 2022,12,20

Dotmatics