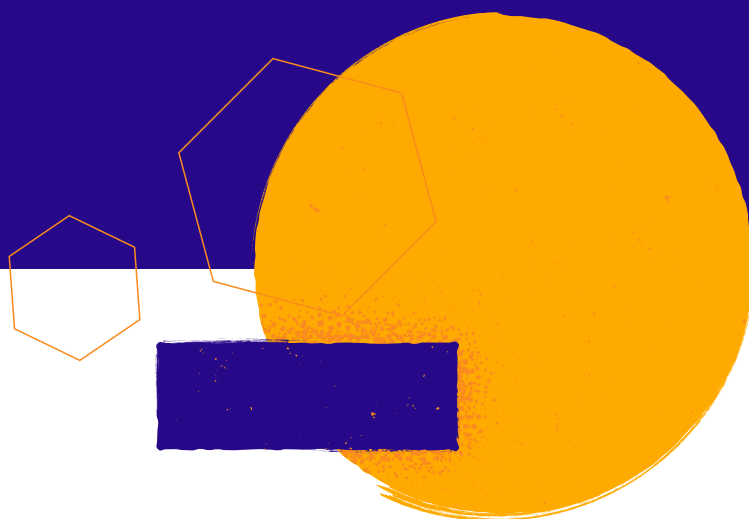




Smooth administration when collaborating with CROs



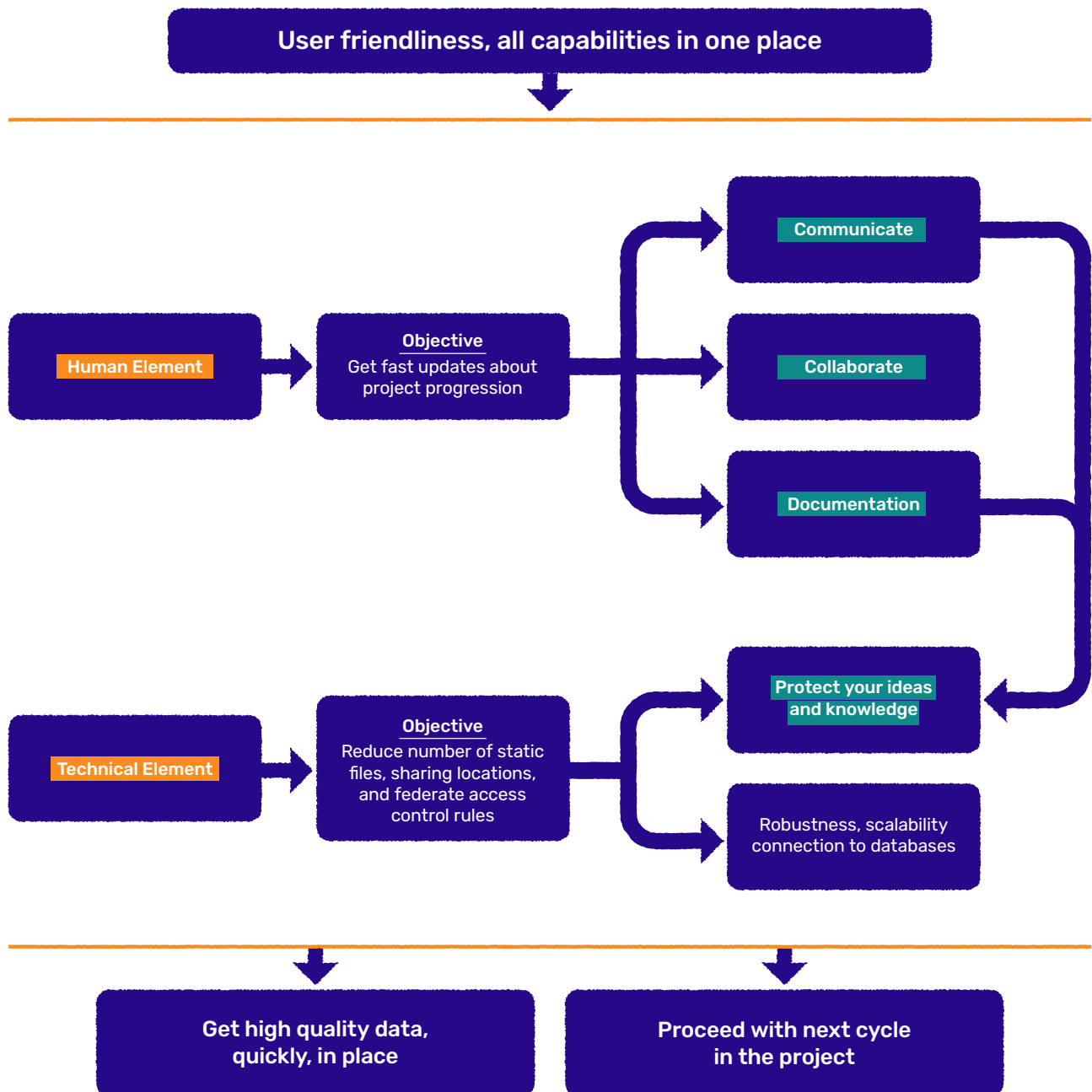


By leveraging specialized services and outsourcing to CROs, biotech and pharma companies can accelerate research, save costs, and scale resources effectively. Working with external collaborators however, brings its own challenges, in synchronizing in-house and external systems and teams, ranging from project management to documentation or technology. On the project management side, effective communication, collaboration, and documentation are essential for successful partnerships. Chemaxon's Design Hub provides a shared collaboration space to facilitate these processes without separation/segregation of design and prioritization; communication and tracking. On the technical infrastructure side, the platform also offers secure infrastructure for protecting intellectual property and sensitive data. With its innovative features and focus on data security, Design Hub enables efficient compound design, synthesis, and progression tracking, ensuring the success of drug development projects with CROs.



Introduction

Working with CROs in the biotech or pharma industry has its unique challenges, many of which fall under different aspects of the human and technical elements. The human element, people working together, includes activities like communication, aspects of collaboration, and documentation of the process. The technical element is the infrastructure supporting the project members, and includes making sure that the system is secure, robust, and efficient.





Communication



In terms of communication, one major goal for the chemistry project leader is to **decrease the time it takes to receive updates** - by this, accelerating the time to compound synthesis. Scheduled, regular meetings are often far apart, leading to delays. Ensuring that the project pace is as fast as possible requires an immediate visibility of progress, and a platform for a real-time exchange of ideas and information. Importing and exporting files while exchanging emails (or uploading them into independent file sharing systems) can result in data loss, impacting the efficiency and accuracy down the line.

Collaboration



Involving CROs in the prioritization of compounds can be another complex area. Their specialized skillset, and scalable availability enables faster processes and better results. The CRO needs to be able to access suggested synthesis routes and requirements, which are difficult to view for multiple teams with different security clearances and objectives at the same time, and require a split focus to manage from the project leader.

Documentation



Project documentation poses its own set of difficulties. **One of these is the need to increase the quality of data received from CROs.** Powerpoint files being separate from access-controlled systems make version and progression tracking near impossible in silos, resulting in inefficiency, meaning a longer time to synthesis. Exporting chemical structures in various file formats can lead to the loss of information, particularly regarding stereochemistry. Additionally, the management of static files scattered across different locations, often with version numbers, creates frustration and complexity.

Technical



From a technical standpoint, protecting intellectual property, while still providing enough information for swift collaboration can become a challenge. **There is a need to eliminate project details for CROs while safeguarding ideas, hypotheses, and knowledge.** Finding a balance between sharing essential information and hiding sensitive design hypotheses and SAR-related work is essential. In the meantime, the system needs to be scalable, as project needs vary, and further FTEs might need to be involved or phased out at any stage. Synchronization of uploaded data is another technical issue, as versions and documentation siloes across teams and collaborators can become difficult to manage.

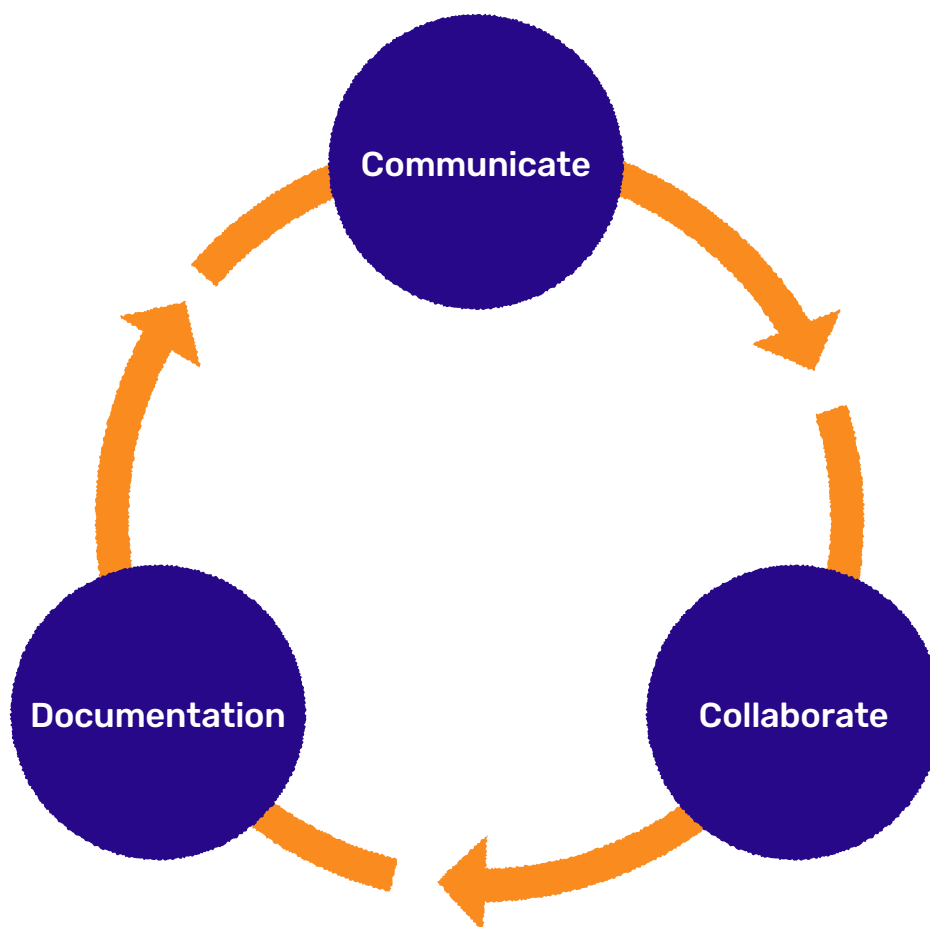


Collaboration Scenario

Imagine that, working for a pharmaceutical company, you have one system for keeping track of project progression, where you save project information such as analysis, results, your newly designed compounds that are waiting for synthesis, the hypothesis behind them, and so on.

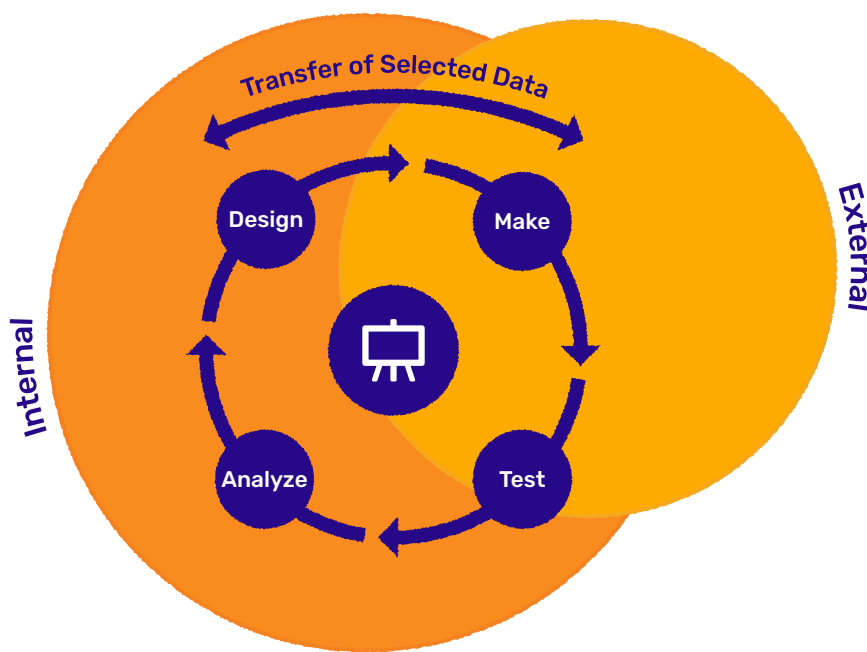
This system can also be used for internal communication of priorities for the compounds, status of synthesis with the chemistry team.

Connected to this DMTA-system, you have the database containing all compounds ever synthesized in-house and the corresponding data, such as purity, amounts, assay-results, and other data points. If these two systems are connected, your DMTA-software will immediately be updated when a new compound has been synthesized in your project, or has new assay-data - information that you can already use in your next design cycle.





Now, imagine that the project wants to perform synthesis at a CRO as well. Usually, you will not want to share any information on the protein target, the rationale behind why you make the compounds. All of this information is stored in both your DMTA system, and in your internal database. This information will be the basis for your IP, covering the drug in the market. Commonly, to avoid breaches, companies create another system, to keep track of what you should externalize. This can take the form of an email, transferring a collection of files, or an external server that is shared with the CRO.



With this, now you have your internal system, an external, clean platform, and you also need a “transit area” before uploading the compounds and meta-data from the CRO into your internal system. This means that the project leader needs a split vision to get an overview of what is going on in the project and there is an additional administrative burden. This can very quickly multiply if you have work ongoing at several CROs simultaneously.

- **Decrease the time it takes to receive updates.**
- **Involving CROs in the prioritization of compounds can be another complex area.**
- **One of these is the need to increase the quality of data received from CROs.**
- **There is a need to eliminate project details for CROs while safeguarding ideas, hypotheses, and knowledge.**



Design Hub Makes Projects Smooth

Collaboration with your Contract Research Organization partners can be made easy by inviting them into Design Hub, a shared collaboration space to collect ideas, exchange knowledge and communicate in real-time. Once a project is finished, you can simply opt your partners out of Design Hub, while still keeping the work they completed.

Example of synthesis tracking workflow

The image displays two screenshots of the Design Hub interface. The top screenshot shows a Kanban board with columns for 'Ready for review', 'For Synthesis', 'In Synthesis', 'Synthesized', and 'In shipment'. Compounds are tracked across these stages, with chemical structures and associated notes visible. The bottom screenshot shows a detailed view of a compound request, including a chemical structure, a list of comments from users like 'Jennys CRO' and 'Jenny Viklund', and a description of the request.

Keep track of all compounds in your project in one place

Get notifications when the compounds are synthesized

Select compounds for synthesis to the CRO: they will only see their assigned compounds

Write the details of your request in the "Description window"

Download the structures and meta-data into your own database (see below)

Discuss compound-related matters using the "Comments"



Our solution is to have a **shared collaboration space, with split project access**. This means that, while the internal company bears the burden of storage and administration, they can manage any number of external resources, each allocated the exact access and view they need to contribute. They will only see what you choose to share with them.

Example of CRO Workflow

The image shows two screenshots of a software interface for managing CRO workflows. The top screenshot is a Kanban board with columns: 'Ready for review', 'For Synthesis', 'In Synthesis', 'Synthesized', and 'In shipment'. Compounds are represented as cards with chemical structures and dates. The bottom screenshot is a detailed view of compound VXN0585, showing its chemical structure, a description, and a list of 'Additional fields' such as V1 Amount, V1 Barcode, V2 Amount, V2 Barcode, Purity, and Remaining solvent type. A 'Comments' section at the bottom shows a conversation between Jenny V. and Jenny Viklund.

See only the compounds and information assigned to you

Show your advancements by moving the compounds to the next level, as you are progressing with your synthesis

Write the details of your results in the customizable "Additional fields"

Discuss with the drug discovery company, ask your clarifying questions in the "Comments" window

With the integrated kanban board, you can immediately see if you need to scale the project to involve external resources. You simply assign the compounds, specify the data you need, and watch the progress in real time.

- **Shared collaboration space, with split project access.**
- **You simply assign the compounds, specify the data you need, and watch the progress in real time.**



Chemaxon offers single tenant setups, which are available using AWS infrastructure. The company and all its vendors are ISO certified, offering further peace of mind regarding secure handling of your data.

We provide a highly available system with frequent updates, built on a cloud infrastructure so you are not limited as to the capacity you need access to in an instant. The system has role and project based access, with the granularity necessary for sharing information with CROs, while keeping your IP safe.



Collaborate on original research with your medicinal and computation chemist peers. You can track compounds, identify and optimize leads while working with remote teams. Browse legacy projects and build on your internal knowledge base instantly.



Conclusion

While collaborating with CROs, there are two main areas to consider: the human element - synthesize compounds ASAP, with a need for seamless communication, efficient collaboration and exact documentation, and the technical space where the research takes place, is the need for robustness, scalability, connection to databases in a system that is designed with data protection in mind.

With its innovative features and capabilities, Chemaxon's Design Hub is engineered to make collaboration with CROs smooth and secure. It streamlines project management, makes it easy to communicate and share data, and gets you to designing and synthesizing compounds quickly while ensuring data security and intellectual property protection.

For more info contact us

