White Paper

Planning for Quarantine/Physical Distancing: A Guidance for Scientists

As the world is confronted with the COVID-19 outbreak, leaders across industries are rapidly preparing for the possibility of significant productivity disruptions, including here at ACD/Labs. We care deeply about our customers and partners with whom we have worked over the last 26 years. While we trust that your IT has created plans to enable human-to-human interactions via modern web conferencing capabilities, the ability for scientists to leverage specialized collaboration tools is also an essential consideration. In the spirit of supporting our customers' risk mitigation, ACD/Labs felt it would be appropriate to provide a few recommendations for how a number of our tools may help in minimizing the inevitable productivity losses due to current person-to-person contact restrictions that are now in place.

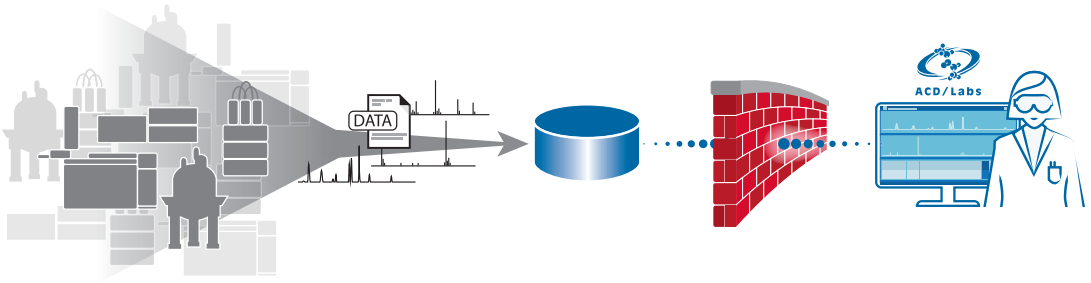
Moreover, we provide some recommendations for risk mitigation policy enhancements that are being implemented for future events that may require a remote working situation.

Remote Data Accessibility

ACD/Labs understands that many scientific experiments, particularly chemistry experiments, require a physical laboratory for work to be conducted. However, many tasks that scientists perform are directly related to experiment planning, data aggregation, analysis, and reporting—before any work is carried out in a laboratory. Given that comprehensive real-time or near real-time access to experimental data is paramount, the ability to effectively accomplish critical tasks, collaborate, and be productive from a variety of remote locations is essential for the modern scientist.

While it may be difficult to execute laboratory experiments from home, there are a variety of tools that can help provide a scientist with the capabilities necessary to support their overarching experimental lifecycle, as described above.

Presuming that a scientist can access corporate data repositories via secure network connections, ACD/Spectrus Processor, along with a variety of technique-specific workbook applications allow remote scientists to **import, process, interpret, and report analytical data and results remotely**. Moreover, using remote desktop tools to access these applications "within the firewall" reduce the degree to which specialized workstations are required. ACD/Labs also offers several browser-based web applications for even more facile access to experimental data, with little-to-no fidelity loss. The rich and broad experimental data, traditionally relegated to specialized workstations, can remotely be accessed via the browsers we all use on a daily basis.



Moreover, our variety of prediction capabilities and applications allow scientists to spend their time away from their laboratories; consider for example, new molecules to synthesize and test upon returning to the lab (or to collaborate more effectively with colleagues that have already returned to the lab).

Read on for specific application areas where ACD/Labs can help today.

Drug Development Project Decision Support

Irrespective of current face-to-face collaboration limitations, the degree to which drug development teams leverage externalized manufacturing and testing assets is only increasing. Therefore, Luminata-enabled firms can allow for the **contextually relevant organization of CMO/CRO/corporate data across the product lifecycle**, and across the internal/external development ecosystem, including:

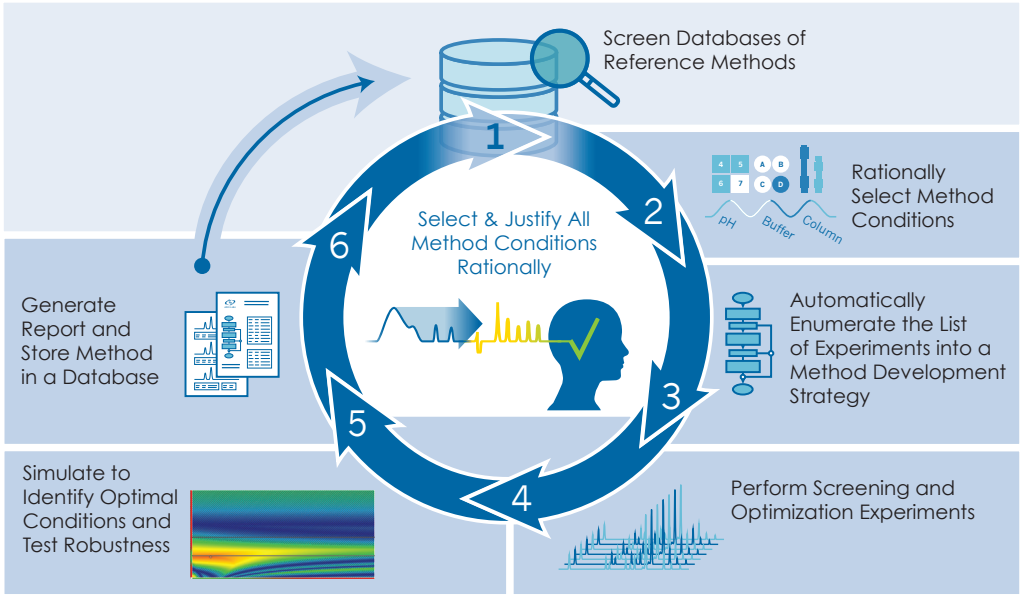
- Route and process development experimental data
- Forced degradation study data
- Process control justification data
- Fate-and-purge study data
- Formal drug substance and drug product stability study data
- And finally, Lot Release data for all development, clinical, and commercial Drug Substance and Drug Product batches—along with related raw material and intermediate characterization data—in one single interface.

Remote scientists can use the wide variety of decision-support features in Luminata to **make critical project decisions**, without the traditional encumbrance where they must access multiple systems and locations for decision-enabling data.

Moreover, Luminata offers both workstation and browser-based client user interfaces for remote scientists.

Support for Chromatographers

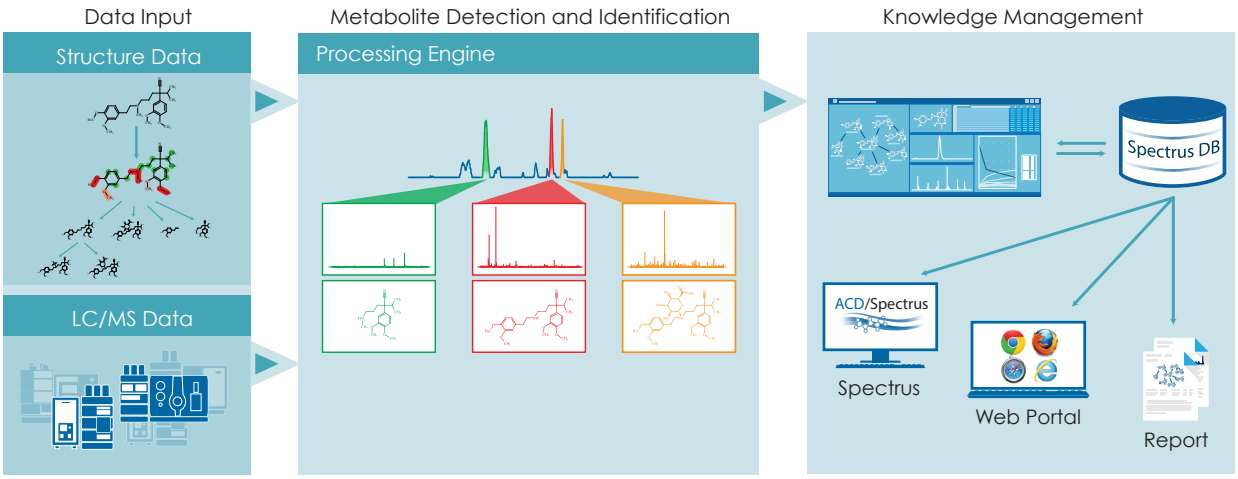
Our ACD/AutoChrom application allows for users to **design method development strategies** without ever running an experiment. Moreover, AutoChrom Online allows for direct instrument connections for seamless method parameter setting and execution. In this mode, remote colleagues can **initiate QbD-directed screening experiments, and perform automated processing and method suitability assessment, all remotely.** Finally, users can **use the results from screening experiments to build effective simulations that predict chromatographic outcomes with reasonable certainty**—hopefully arriving at developed methods that can pass validation experiments with ease.



Tools for DMPK Scientists

ACD/Labs' MetaSense product offers users a variety of tools to store and retrieve metabolic information as well as build comprehensive biotransformation maps for prospective drug candidates—across the Pharmaceutical R&D lifecycle. For remote scientists, the ability to **predict metabolic liabilities prior to investigation** (or even prior to synthesis) can allow drug discovery project teams to plan lead optimization campaigns more effectively. Additionally, for drug development candidates, MetaSense allows remote scientists to **comprehensively characterize acquired in-vitro and in-vivo incubation experimental LC/MS datasets**.

Traditionally, data processing and interpretation is limited to "instrument-specific" software interfaces; or worse, translating MS interpretation results to chemical structure-centric biotransformation maps (which ultimately serve as decision-making materials for project teams). MetaSense provides DMPK scientists with **remote processing and analysis of LC/MS data from most major instrument vendor formats** and helps to **reduce the manual effort necessary to prepare biotransformation maps**. Moreover, MetaSense allows users to **build interactive, searchable database repositories**.

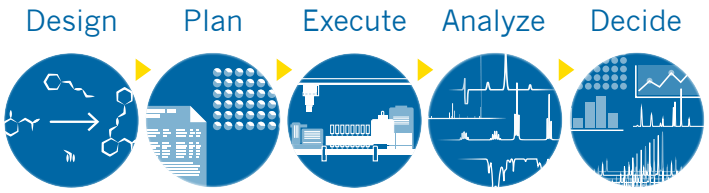


During quarantine periods, remote scientists can spend their "downtime" to construct corporate biotranformation databases, starting from only acquired LC/MSn datasets automatically. Such "future-proofing" work allows future project team efforts to perform comparative metabolic risk assessments—using structure, substructure, or structure similarity queries.

Software for Medicinal Chemists

In addition to the analytical data accessibility tools described above, the ACD/Percepta Platform can serve as a useful tool to support a variety of medicinal chemistry use cases: for the **design of new molecules during the Lead Optimization Phase of Drug Discovery**, users can **predict off-target effects**, including ADME and Toxicological Properties. More importantly, users can **predict lead series property dynamics** using Percepta's R-group substitution functionality. These two features allow remote users to **design synthesis targets** while away from their laboratories. Finally, the Percepta Platform can be deployed via desktop clients, browser-based clients, or even functionality-as-a-service, whereby prediction modules can be embedded into existing corporate web applications.

Remote Support for Automated, Parallel, and High Throughput Experimentation



As laboratories continue to introduce robotics systems to accomplish a wealth of operations, remote users need the ability to provide "machine instructions" from disparate physical locations. Katalyst D2D offers scientists the ability to **prepare their experimental design, physical experiment layouts, experiment procedures, and experiment sampling and analysis instructions**. Then, remote scientists **can submit exportable instruction lists to the appropriate automation software interfaces**. Alternatively, remote scientists can prepare human-readable instruction lists for onsite colleagues to execute preparative operations if needed. Finally, upon completion of experiments and analysis, Katalyst D2D allows remote scientists to **access all data across the high-throughput experiment lifecycle**.

Risk Mitigation for the Future

While we are hopeful that the current global efforts to mitigate the impact of the COVID-19 outbreak are effective in the coming days, weeks, and months, we recognize the importance of preparing and implementing new risk mitigation strategies. Part of this effort includes the utilization of networks to connect software interfaces, machine instructions, and robotics/automation equipment to enable continued productivity with the ability for scientists to work remotely in the event that such a situation arises again in the future.

Foundational Data Accessibility Strategies

Many of our current customers are embarking on "cloud utilization" strategies for their laboratory. The Spectrus General knowledgebase can enhance such strategies dramatically for analytical data. Silent automation and unattended instrument monitoring, data processing, and transfer-to-cloud data marshalling are all supported by various Spectrus Platform subsystems. For remote scientists, accessing live analytical data via a spectral, structure, or metadata search are all supported by our software. The ACD/Spectrus Platform has also been used to connect "externalized" data sources to corporate cloud sites. Experimental analytical data, collected by CxO laboratories, can be effectively streamed into the Spectrus Platform. Our Applications, Professional Services, and Solutions Delivery teams are ready to engage with you to determine the most effective strategy for your foundational data streaming, management, and accessibility planning efforts.

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