

excelra

Modernization and cloud migration of legacy R&D compound registration platform

CASE STUDY





Client

Small molecule drug discovery company



Services used

- Cloud enablement
- Product design and development

The challenge

The client is a drug discovery company focused on small molecule oncology and immunology. A recurring phase of its R&D activity was the registering of compounds on a local database. The compound database was a desktop application that had been developed and primarily operated by a single user. The potential for collaboration was limited, as additional users had to download an exported and uploaded save file each time an input was required. The application was built on Microsoft Excel with unoptimized code, minimal functionality, a clunky UI, and limited security safeguards.

The sluggish legacy database was causing a bottleneck in the development pipeline, and the dependence on a single operator and single point of failure posed a significant risk to the client's operations. The limited feature set also meant that additional functions had to be executed externally, which had a knock-on effect on budgets and timelines.

The client had two core requirements. The first was to replace the legacy database with a modernized, cloud-based web application. The second was to add a suite of features to improve search capabilities, import and export functions, compound comparison, remote working, team collaboration, and user access management.

Our approach

Excelra is a leading data science company that empowers innovation across the drug development value chain. Its teams are composed of qualified scientists, cutting-edge technologists, product developers, data scientists, and data engineers. Our unique mix of competencies and specific life science expertise attracted the client, as the project required a partner that understood and respected drug development data and could recommend the most appropriate and effective technology for the requirements.

After evaluating the existing application and the functional requirements within the wider workflow, our product design team worked with the client to shape the solution to its demands and presented a comprehensive proposal.

During the initial design phase, traditional technologies like Spring BOOT and React JS were considered. These options would have provided a solid platform to develop a functional web-based application to meet the requirements. However, our architects are always looking for opportunities to exceed expectations. Given that data was held on Oracle, an alternative was proposed to build the new application in Oracle APEX—a more flexible option with low-code development functionality baked-in. Integration of the database would be seamless, and the client could employ 'citizen development' opportunities to customize the application with additional features in the future.

There was another significant benefit to this alternative proposal. The time required to deliver this setup would be up to 70% faster than the traditional approach, and iteration time would be reduced by almost 25% due to the reusability of data processing code and the out-of-the-box readiness circumventing laborious testing and QC phases.

The client was impressed by our proposal, and the project progressed to the design and development of the application's interface and functionality. An agile project delivery model was successfully executed with client approval at every stage of development to ensure security frameworks were aligned, infrastructure was effectively configured, and UI wireframes provided an efficient user experience.

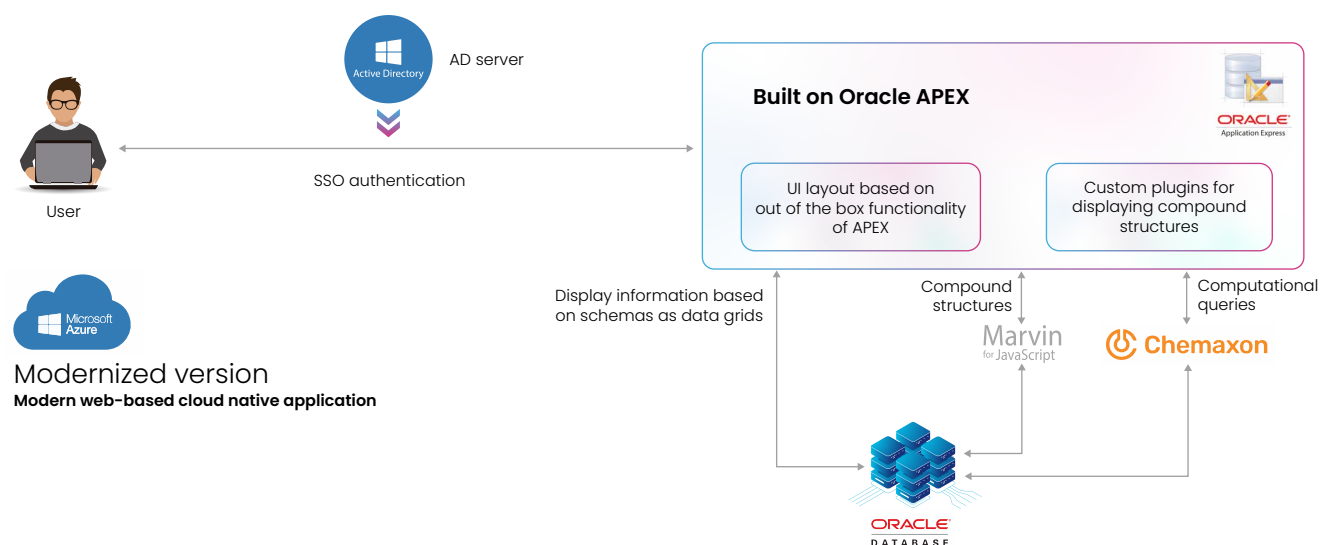
Following consultation with all end users, a feature set was developed which catered to three account variations: compound registration scientist, computational chemist, and platform admin. The compound registration user required minimal functionality, and so a clean interface with minimal graphical load was developed to streamline the addition and status editing of compounds. Likewise, the admin had a focused set of requirements, including the ability to add users, control access, review performance, search logs, and configure application settings.

The computational chemist received the broadest feature set. A powerful search functionality was developed, which allowed the user to find, save, and compare structures. An interactive viewport was developed in Marvin JS that allowed selected compounds to be viewed in multiple formats, which facilitated the identification of lead compounds to be progressed into final candidates.

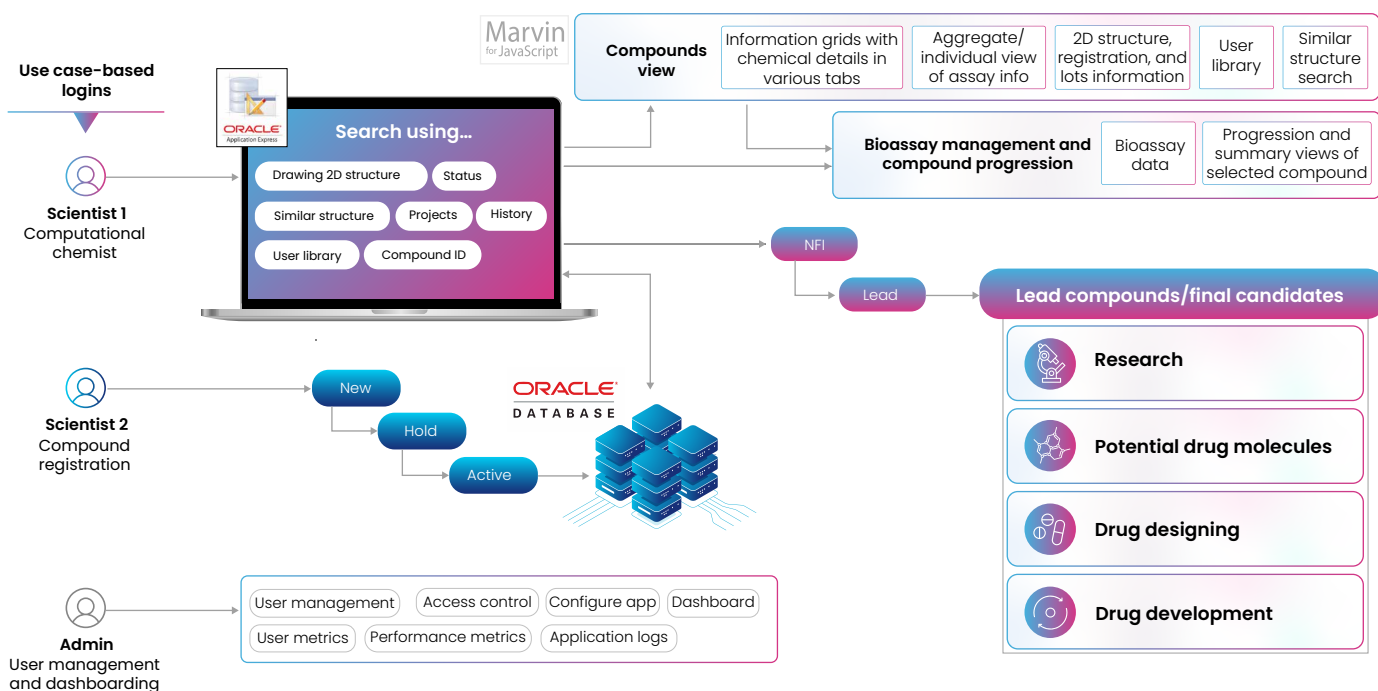
Given the deployment on Azure, all users had the ability to quickly export collections and send active links to off-premises colleagues who could instantly collaborate and contribute to the search and selection of potentially fruitful candidates.

As recommended, the deployment on Oracle APEX provided a suite of low-code plug-ins and add-ons that the client could adapt and implement on the platform. This functionality allowed the client's existing team to become citizen scientists, negating the need for an in-house programming team or external software developer.

Project overview



Platform capabilities



The results

With our help, the client was able to successfully migrate from a slow, functionally limited, single-user, legacy platform to a modern, functionally robust web application that could be used at scale across the whole enterprise. The migration was executed without any loss of service or security compromises, and the client's team was given sufficient tools and training to quickly onboard users to the responsive, intuitive platform.

The approach we proposed provided significant time and cost savings during development. It will continue to improve efficiencies and reduce expenditure thanks to the technologies utilized and the design methodology of our product development and cloud enablement teams.

Conclusion

The success of this project highlighted the efficacy of our approach. By combining domain expertise with technological innovation, we provided an exceptional solution that incorporated the flexibility required in drug discovery R&D without compromising on technical functionality.

Where science and technology meet, that's where we add value. With over 60 PhDs and 230 technologists, we help pharmas and biotechs reach their potential with data curation, bioinformatic insights, visualization services, R&D technologies, and scientific products like GOSTAR and GOBIOM.

Our service portfolio

 Data	Data curation Filter out the noise, focus your attention Clinical data Analysis-ready data for informed clinical decision-making Semantic data Refine your decisions, find your value
 Insights	Bioinformatics Illuminate the path to faster discoveries Data science Unlock the power of data Visualization Pictures paint a thousand words
 R&D technology	Product design and development Unlock your potential with data-driven design and development Cloud enablement Optimize your output on the cloud Data engineering Mitigate risks, protect your data, and rationalize your portfolio and processes.



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