



Achieve Business Goals with Integrated Informatics

Introduction

Agrochemical R & D is dominated, in both spend and discovery, by half a dozen large global corporations that use three primary approaches to identify new active ingredient classes: high-throughput screening, targeted synthesis, and rational design.

UK-based Redag Crop Protection is a company dedicated to the discovery of novel agrochemicals. Its niche is in pursuing original manufacturer patents to find comparable actives and innovative molecule designs. Founded in 2014 as a spin-off from RedX Pharma, Redag was in the enviable position of “starting from scratch” to equip its new facilities at the Alderley Park life sciences complex with state-of-the-art technologies.

Fit-for-business Informatics

To support its best-in-class discovery capabilities, gain the strongest return on its investment, and be able to both compete against and partner with industry leaders, Redag was determined to build a solid foundation around fit-for-business informatics system. The start-up’s management and science leaders knew they

wanted to implement an electronic laboratory notebook (ELN), as well as analytic solutions, to drive productivity in their labs and accelerate time-to-value for their scientists.

“We had the opportunity to assess all the informatics solutions that were available on the market and look at what was fit-for-purpose for our business,” said Victoria Jackson, chemistry team leader at Redag. As a small business with fewer than 20 employees, the goal was to select a “bedrock” solution that:

- Could justify its total cost of ownership
- Free scientists to focus on more productive work, not paperwork
- Required minimal IT intervention, both to deploy and maintain
- Leveraged shared learning and experience of other users

The solution needed to serve both management and end-users, from being modern, nimble, and efficient, to producing and tracking high quality data, registering and uniquely coding new chemical entities, and visualizing chemical and biological data for analysis.

From a user perspective, the ELN and analytics platform had to be an intuitive and easy to use with capabilities for easily entering, finding, and reusing data. Redag wanted all experimental data and notes stored in a single location, accessible to everyone in the organization. In addition, they wanted systems for risk assessment and regulatory compliance.

For inventory control, Redag wanted to minimize the number and amount of chemicals stored, minimize waste generation and control waste disposal costs, and, importantly, enhance safety by having immediate access to information on chemicals in use and their locations.

For registration, they wanted a solution that would register compounds straight from an experiment, enable multiple users to register simultaneously without confusion or duplication, and link all experiment information and data back to the ELN.

Additionally, they wanted an integrated solution that required little to no customization, supported several scientific domains/functions, and enhanced collaboration – both within the organization and with external partners.

In short, they wanted an informatics platform that would enable them to partner with larger organization, while meeting needs for flexibility, efficiency, and performance.

Platform Selection

Redag's evaluation process which was led by Victoria Jackson, included three vendors. The company reviewed each solution against the stated criteria and user feedback.

Redag selected PerkinElmer's platform, which included the E-Notebook lab notebook with Inventory and Registration enterprise modules, ChemDraw for chemical drawing, and TIBCO Spotfire® for data analysis and visualization.

"PerkinElmer's platform was simpler to use, it was more efficient, it produced high quality results, and there wasn't that much customization required for us to get started," Victoria said. "It was just the overall quality of the solution that really stood out for us."

The integrated solutions approach allows Redag's chemists and biologists manage their experiments and data, while business leaders can track progress with dashboard visualizations.

Victoria estimated they initially used approximately 40% of E-Notebook and TIBCO Spotfire's® functionality and this has steadily risen to over 60% as they further explored and tested the platform's capabilities. Areas for additional growth include exporting and visualizing more data and entering more biological data.

As PerkinElmer has developed cloud-based software-as-a-service versions of its leading informatics solutions, Redag will leverage these capabilities in the future to increase collaboration and data-sharing.

Measuring Success

Victoria said that, in addition to user feedback, the informatics platform is proving its value in three important ways:

- Number of compounds registered
- Number of patents filed
- Number of partners secured

"One sign of high-quality data is if the business is prepared to patent it," Victoria said. "The fact that we filed multiple patents in the last few months of 2016 really shows that we want to protect that high-quality data. We finished filing half a dozen patents, and for a small business of 18 employees to be able to do that as well as carrying on your day-to-day work, is important."

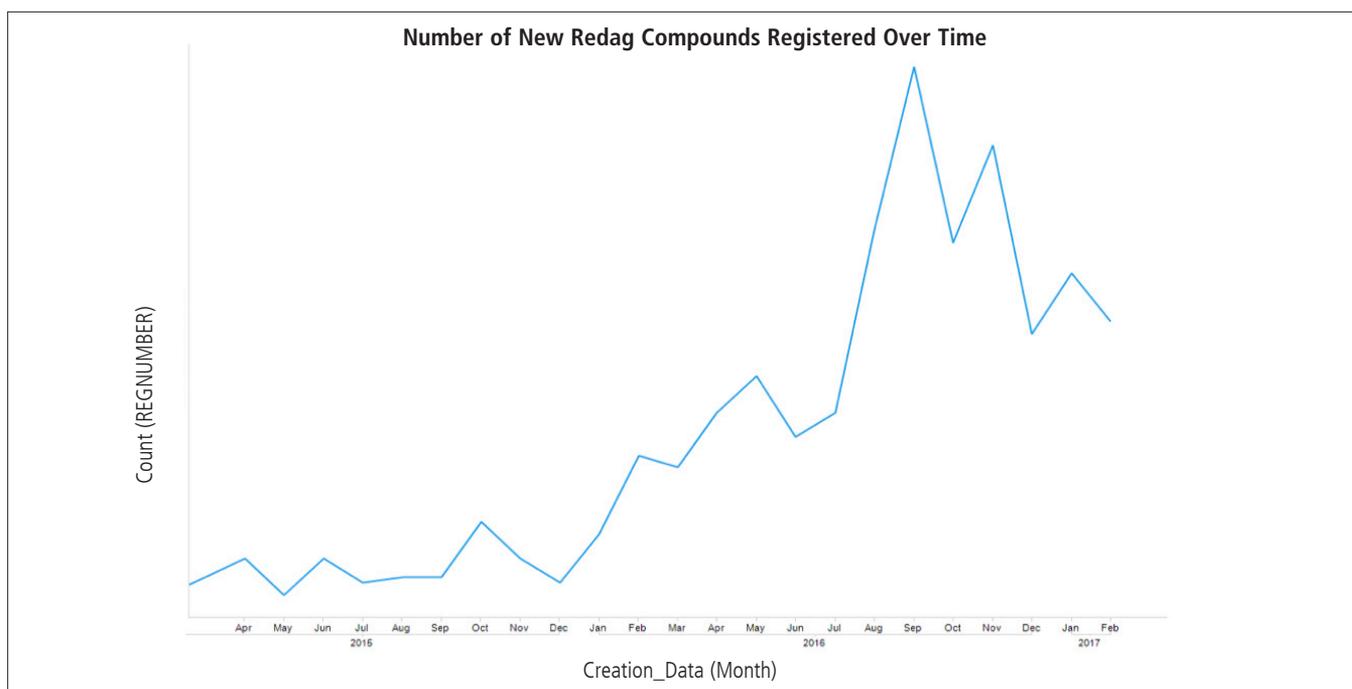


Figure 1. E-Notebook usage has led to increased productivity as shown here in acceleration of the number of compounds registered.

Redag registered more than four times the number of novel compounds in 2016 compared to 2015, which Victoria said increases opportunities for collaboration and licensing to partners. Its portfolio in 2017 demonstrates Redag’s opportunities and capabilities – they had herbicide, fungicide, insecticide, and nematocidal targets identified, plus five projects in lead exploration in primary screening phase with their activity under evaluation, and another four being optimized with the dosage rate defined and work is ongoing to progress one of these projects to field trials in the second half of 2017. (See Table below.)

Advice On Selecting Informatics

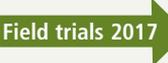
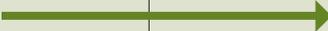
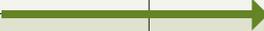
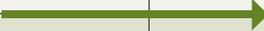
For an informatics platform to add value, particularly to small organizations for which this is a significant investment, Victoria recommends businesses “aim high and demand the best.”

“Be prepared to challenge your company to be the best they can and to have access to the right informatics solutions,” she said. “Think of what you want, especially for the future. If you start off having those solutions in place it makes achieving your goals a lot easier, and your data management a lot easier as well.”

Building a business case helps senior managers and investors in a start-up to understand the value of high-quality data to the organization, and the risk of lesser quality data. The system must be able to grow with the business, and the vendor must be as responsive to the needs of small businesses and start-ups as to its larger enterprise customers.

“We want to be a professional, innovative agrochemical business that’s respected in our industry for the the high-quality data we produce,” Victoria said. “PerkinElmer’s platform is the bedrock for our scientists to make their discoveries.”

Table 1. RedAg Crop Protection's Portfolio.

Research Stage	Lead Generation	Lead Exploration	Optimization	Candidate Selection
Activity	Target identified, synthesis underway	Primary screen, activity under evaluation	Dose rate definition, optimization underway	Field Evaluation and Regulatory assessment
Herbicide	R17 - Monocot.  R35 – Total herbicide R37 – Monocot & Dicot. R46 – Monocot & Dicot. Burn down	R36 – Monocot. & Dicot.	Rx02 – Burn down, BLW	
Fungicide	R39 – Cereal/F&V R44 – Cereal/Soy 	R35 – Fruit and Veg R33 – Downy Mildew/Blight	R10 – Downy Mildew/Blight R21 – Cereal and veg	 Field trials 2017
Insecticide	R18 – Broad spectrum R38/R39 – Aphids and public health 		R34 Leps	
Nematocidal	R35 – M. incognita 	Rx01– M. Incognita 		
Plant Stress	R45 Growth Promoter 	R30 – Drought and gaseous exchange		