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AgPlenus takes fungicide discovery beyond chemistry

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AgPlenus CEO Dr. Dan J. Gelvan on using AI, novel targets and predictive biology to reduce the time, cost and risk of developing next-generation fungicides



Fungicide discovery is confronting a difficult equation: resistance is accelerating, while finding genuinely new modes of action remains costly, slow and inherently high-risk. In this exclusive **AgroSpectrum interview, Dr. Dan J. Gelvan, CEO of AgPlenus**, explains how artificial intelligence could alter that equation by improving the odds of identifying viable molecules before they enter the laboratory. AgPlenusâ?? Antifungal Potency Predictor (APP) is built to reduce the experimental burden of conventional discovery, but Gelvan argues that chemistry is only the beginning. The bigger prize is predictive biologyâ??anticipating field performance, toxicology, phytotoxicity and environmental behaviour before costly development decisions are made. AgPlenus therefore sees AI not as a faster screening tool, but as a way to progressively de-risk the entire fungicide pipeline. Its target-based strategy deliberately focuses on novel modes of action, with Septoria, Botrytis and Fusarium among the pathogen areas under consideration. As resistance reshapes crop protection, the interview explores whether AI can make first-in-class fungicide discovery not just faster, but economically viable.

The fungicide industry has struggled with resistance for decades despite continuous innovation. How fundamentally does the Antifungal Potency Predictor change the economics and success rates of fungicide discovery compared with conventional R&D approaches?

The Antifungal Potency Predictor (APP) should be assessed alongside our broader developmental approach, which includes discovering novel fungicide targets to establish new modes of action. Resistance is typically tied to a fungicideâ??s target and mode of action, so introducing novel targets into the discovery pipeline creates an opportunity to develop truly novel fungicides that can help address resistance.

The challenge is that discovering entirely new chemical entities against novel targets is, by definition, a high-risk, time-consuming and expensive process. Conventional approaches require significant experimental work to identify and validate promising molecules. The APP is designed to improve the odds of success within that inherently risky process by helping us

identify molecules with greater potential before we invest heavily in synthesis and downstream testing. In doing so, it can reduce unnecessary experimentation, saving both time and money while improving the efficiency of the discovery process.

AI models are only as robust as the data they are trained on. Without revealing proprietary information, what distinguishes AgPlenus' datasets and machine learning architecture from those used by competitors developing AI-driven crop protection solutions?

We have invested significant resources in building a proprietary dataset specifically for this purpose. It combines both external data and internal data generated specifically for the project, giving us a foundation that is tailored to the questions we are trying to answer in antifungal discovery.

The quality and curation of the dataset are particularly important. We collected and curated the data using state-of-the-art AI tools, with the objective of understanding not only which molecular features are associated with activity, but also which features are associated with a lack of activity. Having sufficient and well-chosen negative examples is essential for effective machine learning because the model needs to distinguish between molecules that are likely to work and those that are not. This allows the APP to learn a more meaningful representation of the relationship between molecular structure and antifungal activity, rather than simply identifying patterns among successful compounds.

ChemPass AI for Ag now predicts target affinity and antifungal potency before synthesis. What remains the biggest scientific bottleneck in bringing an AI-discovered molecule from computational prediction to commercial fungicide registration?

Fungicides go through a long development process that is focused not only on efficacy, but also on environmental safety and the overall suitability of a molecule for practical use. The main sources of failure tend to be field performance, toxicological profile and off-target phytotoxicity. A molecule can perform well at an early discovery stage and still fail when it encounters the much more complex conditions of development and field use.

We see this as an opportunity as much as a threat. Every time a molecule advances through the development funnel, it risks failing at the next step. Rather than viewing AI simply as a tool for identifying molecules, our goal is to build a string of predictive algorithms, with each algorithm targeting a different stage of the process. Together, these models could progressively de-risk the entire discovery and development pipeline. The objective is therefore to extend predictive capability beyond chemistry and potency to the biological, safety and performance questions that ultimately determine whether a fungicide can become a successful commercial product.

The crop protection industry is increasingly shifting from discovering 'better molecules' to discovering entirely new modes of action. How confident are you that AI can consistently identify first-in-class fungicides rather than incremental improvements to existing chemistry?

AgPlenus works exclusively on new modes of action. Our mission is to help overcome the rising resistance of crops to pesticides by developing fundamentally new approaches to crop protection. Our process starts with an AI-based workstream that we call Target Selector, which identifies new essential targets in the target organism. Our molecular discovery process is then target-based: we look for molecules that bind to a specific protein target in order to elicit the desired biological effect. The choice of target is therefore central to the discovery process.

By choosing new targets, we are, by definition, choosing new modes of action for our lead candidates. This is different from taking an existing mode of action and attempting to optimise the chemistry around it. Our focus is on identifying biological vulnerabilities that can provide the foundation for an entirely new class of fungicides.

Your pipeline currently includes targets against Septoria Wheat Blotch, with plans to expand into Botrytis and Fusarium. What criteria determine which pathogens become priorities, and where do you see the greatest unmet commercial opportunity over the next decade?

We closely monitor resistance pressures as they emerge in the field and combine that information with commercial analysis to determine which fungi and crops should be prioritised. Resistance is an important part of the equation, but it is not the only consideration. We also need to understand the commercial relevance of the crop and pathogen and whether our target-based discovery approach can address the biological problem effectively.

Because our discovery approach is target-based, a compound that inhibits a particular protein will not necessarily be active against fungi in which that target is absent or is not essential. That biological constraint is an important part of how we think about the pipeline.

We therefore favour targets that are expressed across multiple fungi where possible, but we are not pursuing the conventional path of trying to build one broad-spectrum fungicide that works indiscriminately across pathogens. Instead, the potential scope of the fungi we can address is defined by the target itself. This target-driven approach allows us to focus our resources on pathogens where there is both a meaningful need and a compelling biological rationale.

Large agrochemical companies are investing heavily in AI-driven discovery, while biotech startups are pursuing similar ambitions. Beyond speed, what competitive advantage will ultimately determine leadership in AI-enabled crop protectionâ??data ownership, algorithms, biological validation, or strategic partnerships?

AI has largely levelled the playing field for startups. The old paradigm relied heavily on massive parallel synthesis and high- or ultra-high-throughput screening, which required significant capital investment and large experimental infrastructures. AI-based discovery changes that equation by reducing the need for synthesis by orders of magnitude and, consequently, shrinking the experimental burden.

However, speed alone will not determine success. Biological validation, and predictive biology more broadly, will remain the biggest challenge in this field. Chemistry matters, but a pesticide ultimately has to perform under real field conditions, where biological systems are considerably more complex than the controlled environments used during early discovery.

That means the real competitive advantage will come from our ability to predict the biology, not simply the chemistry. The APP is an example of this approach: it is designed to predict antifungal potency before synthesis. We see the same principle extending across the development pipeline, with predictive tools helping us understand which candidates are most likely to succeed as they move from computational discovery into increasingly complex biological and field environments.

With regulatory expectations and sustainability demands becoming increasingly stringent worldwide, how do you anticipate AI-driven molecule discovery influencing the environmental profile, development timelines, and regulatory approval process for future fungicides?

Environmental profiling and regulatory approval are among the hardest things to predict, which is precisely where we believe AI needs to be applied. The value of AI is not limited to solving relatively easy optimisation problems. It should also be applied to the difficult questions that determine whether a molecule can ultimately become a viable pesticide.

As we develop predictive capabilities across the discovery and development process, environmental and regulatory characteristics are important areas where those capabilities can potentially create value. If we can identify potential issues earlier, we can make better-informed decisions about which molecules to advance and which ones to deprioritise.

It is tempting to use AI to solve easy problems, such as finding the fastest route home, but the real value comes from putting it to work on hard problems. That is exactly what we are doing at AgPlenus: applying AI to difficult biological and development questions where better prediction could have a meaningful impact on the efficiency and risk profile of pesticide discovery.

Looking ahead five to ten years, do you envision AgPlenus evolving primarily as an AI-powered discovery engine partnering with global crop protection companies, or as a developer advancing proprietary fungicide assets further toward commercialization? What strategic milestones should the industry watch for?

We are building a pipeline of partnered products. Whether we initiate a given project ourselves or collaborate with a partner that initiated it is less important than our core business model: building a unique pipeline of novel mode-of-action pesticides.

Our objective is to create value through that pipeline and through the ability to discover and develop products based on new biological targets. Partnerships are an important part of that model because they provide a route to combining our discovery capabilities with the development and commercial capabilities required to bring products to market.

From our perspective, therefore, any progress in the pipeline is strategic. The key milestones are not limited to the evolution of the AI platform itself; they include progress in identifying and validating novel targets, discovering active molecules, advancing candidates through development and ultimately building a portfolio of partnered products based on genuinely new modes of action.

-- Suchetana Choudhury (suchetana.choudhuri@agrospectrumindia.com)