Biology & Medicinal Chemistry

Insights from the Industry

BIOLOGY MEDICINALCHEMISTRY

PROVENTA INTERNATIONAL

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Introduction

There are few years in living memory as disruptive and uncertain as 2020 has been. While this is true of almost every sector, the events field has seen unprecedented change in how events are held and how operations will be conducted in the future.

Proventa International was among the companies spearheading this innovation, utilising its trademark versatility to ensure that none of its important meetings were cancelled and its mission was carried out. Moving fully online, Proventa was able to facilitate connections and host expert, sector-critical discussions that would otherwise have been missed.

Despite the unforeseen challenges 2020 brought, Proventa's meetings were as successful as always, bringing together top-tier industry experts to talk through challenges and innovations with one another, make new connections and take back brand new information to their companies. Whatever challenges the rest of the year brings, those who attended the online meetings will be able to face them fully prepared and as informed as possible.

The Future of Biology and Medicinal Chemistry

While not quite as affected by the recent pandemic as some areas - for example clinical trials - manufacturing is currently entering a fascinating new era of technological growth and change. The roundtables held by Proventa this year took advantage of this, discussing among other things innovations and new methods for effective downstream viral inactivation; how to succeed in digital transformation; and how COVID-19 has changed downstreaming processing in the future.

From continuous manufacturing to CGT vectors to single-use technologies, Proventa's 2020 event looked at some of the most relevant and important changes in the field today, with leading experts offering their insights and thoughts to those who were there.

This report will look at some of the highlights of the recent Biology and MedChem events, but will also go further: it will explore what delegates are investing in right now, and look ahead to the next five years in the field: how delegates are being affected by the turbulence of Covid-19.

We hope you enjoy this report, and look forward to seeing you at our events next year,

Joshua Neil, ***Editor***
Proventa International

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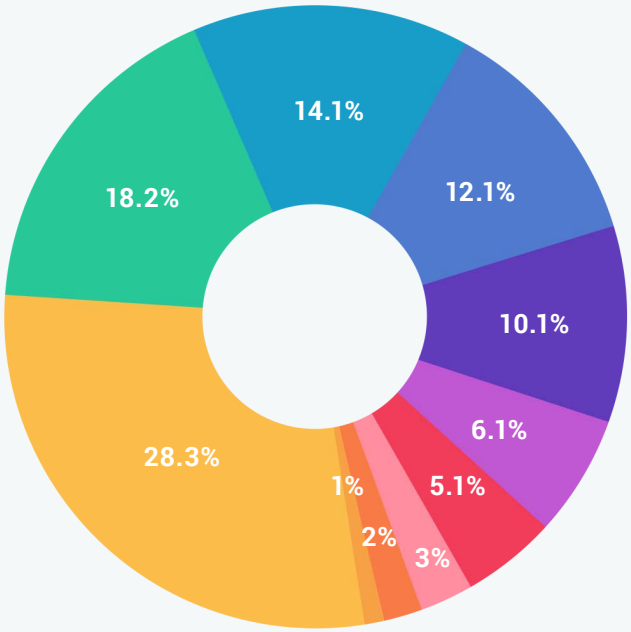


28.3% Director Level

18.2% C-Level

14.1% President / VP

12.1% Scientist

10.1% Department Head

6.1% Academia

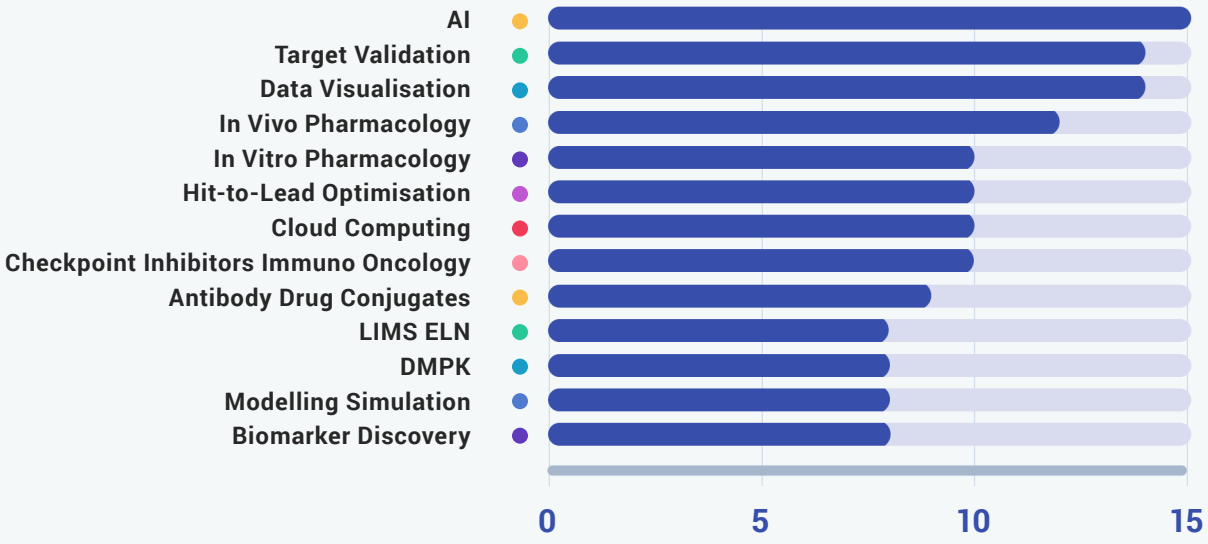
5.1% Other

3.0% Manager

2.0% Team Lead

1.0% Biology Specialist

Key Investments



2020 Delegate Breakdown

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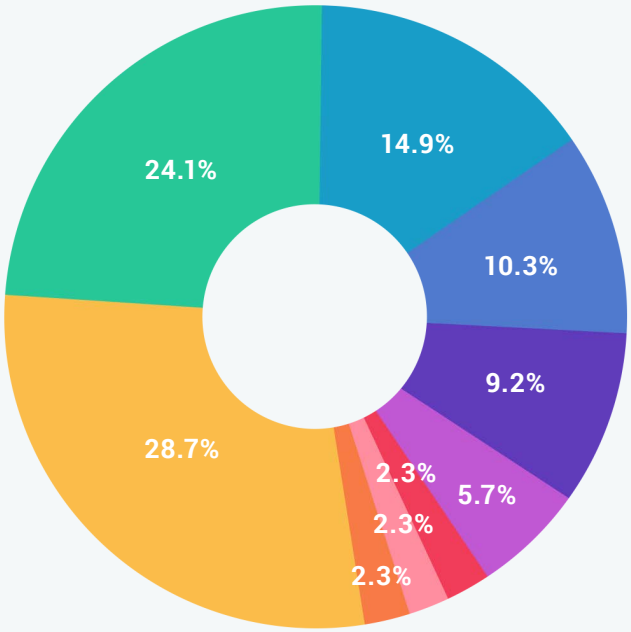
2020 Attendee Breakdown



28.7% Director Level

24.1% Scientist

14.9% Department Head

10.3% President / VP

9.2% C-Level

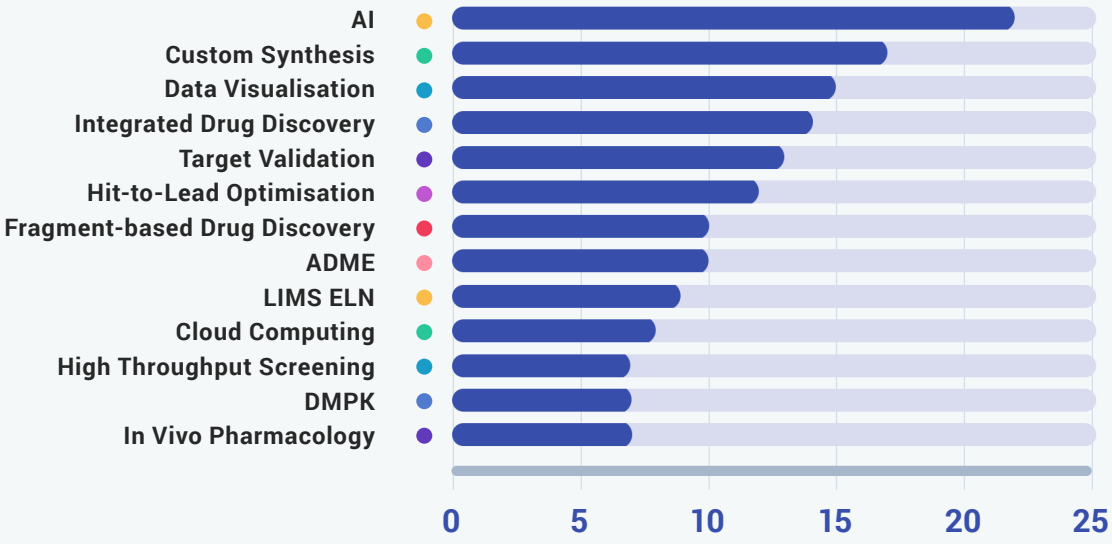
5.7% Team Lead

2.3% Other

2.3% Manager

2.3% Academia

Key Investments



2020 Event Highlights

BIOLOGY

Trends for In Vitro and In Vivo Pharmacology

One fascinating roundtable held during the Biology event was facilitated by Sonela Cavicke, VP of Discovery Services and Business Development at Sai Life Sciences. The roundtable focused on new trends for in vitro and in vivo pharmacology, and began with the question of whether pharma groups are separating teams working on in vivo and in vitro pharmacology, and whether those groups align to ensure follow-through of information and good planning in organisations.

One delegate answered this by noting that the two branches are very separate, and require animal houses, different labs and other variations. So differences, he said, were an issue. He pointed out that when his company translates they go via whole blood assays or transgenic animals, but reinforced again that the two branches are usually kept seperate. One transgression of this rule was with 3D type cellular analysis, which he noted is not used with screening currently.

Another delegate ingreed, pointing out that their key in vivo biologists with disease area expertise were all in therapeutic areas at a different site, though lab heads would often travel between the two sites. She noted both in vivo and in vitro experts were part of the biology team. Regarding assays, she noted the majority of assays used at her company were cell-based assays, and that they were using human and donor cells, patient-derived where possible - and so they would often have to backtrack to test for the preclinical model so those compounds identified in a human model worked in the preclinical species.

The conversation then moved onto new innovations in in vitro pharmacology. Delegates began by suggesting biocores for screening weak protein binders up-front. It was mentioned that non-biocore machines are coming out that will perform similar processes, not counting orthogonal screens which are vital for early-stage research. These are vital when targets have a conformational change.

The same delegate was asked if his company is moving into SPR with whole cells: he noted his company had looked at a machine that does SPR on live cells, which is fairly new and very expensive. Due to its current untested status, he said it may be too early to use.

Another delegate pointed out genomics as an exploding field, and the technologies that have grown from that including CRISPR and newer-generation base pair editing. She added anything that could streamline that process and build those models more swiftly. She also added protein degraders as an interesting new technology, to better understand what type of modality they were looking for and whether a protein degrader could be necessary to remove the protein.

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Tackling Noise and Uncertainty in Data-Driven Drug Discovery

Another excellent roundtable focused on noise and uncertainty in data-driven drug discovery, facilitated by Govinda Bhisseti, Head of Computational Chemistry at Biogen.

Govinda began by noting that good data is needed for good models, but in many companies this is not the case. He noted that over the years, it has become more important to get higher quality data, but in many spaces he still lacks sufficient data. He posed the question: which datasets were delegates working with, and what problems were they finding?

One delegate noted that while data is very important for successful model-building, she had heard opinions that some noise in data could make a model more robust. She noted there were several aspects of data quality here: the measurement itself, which always has some noise in it; and the other common aspect was the labelling of the data. She noted this was a very important aspect of pharma right now, as older pharma companies have many decades of data stored in various places, and this labelling was vital to ensure the data remained relevant. This place, she said, was something that could make all the difference.

She also pointed to FAIR data principles, which she said could be adhered to to ensure data was better identified.

Another delegate stated that his company uses semi-automatic tools to match metadata to data: he said the smaller the dataset, the more noise could make good modelling problematic. Considering much of the data in drug discovery was not big data, this was an important facet of the discussion.

This was backed up by another expert, who said that with his limited datasets keeping data quality high and paying attention to how that data was annotated was vital. He said that he has been using CDD for almost a decade, and it was helpful to ensure the dataset was properly labelled and understood.

One expert discussed his own work using structural data within the training sets for AI algorithms. He pointed out that structural data is difficult to describe, inferences from models are difficult to find. But any experimental data is difficult to work with, and AI with science is running more off the inertia it has had in other areas - quality of data in those areas is more reliable, and there's more data.

Access to large data, valid data are problems. The platforms are evolving by having data analytics / ML tied to proprietary rapid data generation process, so you're generating the data yourself and you have control over the process and you're checking the data validity constantly. There's an opportunity for someone organising this messy data.

Working with published data, noisiness or incorrect labelling is difficult. Wanted data to model transporters, and there's limited data - curate some transporter data please. We checked how they measured all this etc, it looks like a lot of data and after alignment there's actually not much data.

What are we lacking in the drug space as opposed to google etc? Experimental data produces noise into algorithm. There are some attempts to create consortia to solve this together.

Still have silos: as org gets bigger, don't know what's happening with data and algorithms. Trying to sort that in consortia: members learning from each other. Hugely important to have this collaboration. Even at discovery level, we're going into a very data-rich area.

Key Delegate Challenges - 2020 and Beyond

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Cost and Resources

The challenge most mentioned by biology experts at the event related to cost and resources: A significant number of delegates voiced concerns around the area, including issues around fund-raising, managing resources and a lack of resource availability.

Target Discovery

Target discovery and drug development were another extremely common concern mentioned by those surveyed. Among other things, delegates specified target validation, identifying 'driving' targets and novel target identification and validation as challenges to be overcome in the next few years.

COVID-19

COVID-19 was, unsurprisingly, very high up on experts' list of challenges to deal with in the near future. Delegates spoke about productivity during COVID-19, the continued impact of COVID-19 on research goals and networking during the pandemic as particular issues they were struggling to deal with.

Partnerships and Outsourcing

Working with third parties was another critical issue for biology experts. This concern covered a wide area from partnerships to outsourcing, with identifying the correct CRO, the impact of COVID-19 on CROs, and chemistry outsourcing specifically mentioned as pharma challenges.

Data and RWE

Data challenges were next highest on the list of delegate challenges, with those surveyed expressing difficulties around overall data strategy, data storage and retrieval, data integration and learning about how data science is helping drive genetics.

BIOLOGY

Translation

Translational biomarkers, translating phenotypically active drugs into genes and underlying targets and in vitro/in vivo translation were all particular challenges mentioned by delegates. While not a huge challenge to many of those present, concerns around translation were still higher than might otherwise be expected.

Staffing and Expertise

Staff recruitment, training and retention were another of the top ten concerns for delegates. Those attending the event specifically mentioned staff retention, hiring individuals with the right expertise and ensuring everyone has the same data strategy vision as problems to be overcome in the future.

New Technology and AI

Lower on the list than might have been expected, finding and implementing new technology was a key challenge of delegates surveyed. Investing in the right technologies, finding the new technologies to implement and incorporating AI and machine learning into discovery research were some of the difficulties mentioned.

Biology

Specific scientific issues related to the pharma biology field were lower down on the list of current delegate challenges, but still important to a lot of those surveyed. Specific challenges mentioned included accelerating membrane protein targets work, moving into new technologies such as single cell, and protein purification.

Clinical Trials

Finally, concerns around clinical trials were the focus of a number of delegates. Among other things, those surveyed mentioned properly designing clinical trials, clinical trial execution, and translating discoveries to the clinics as challenges for the years ahead.

Key Delegate Challenges - 2020 and Beyond

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Target Discovery/Validation

The most cited challenge faced by medicinal chemistry related to discovering and validating targets, with those surveyed mentioning in particular target validation, shortening timelines in drug discovery and picking the right discovery targets as significant issues to be overcome.

Partnerships and Outsourcing

The next most-mentioned challenge in the medicinal chemistry field related to partnerships and outsourcing. Delegates noted effective and flexible outsourcing, outsourced development, CRO selection and flexibility of CRO support as challenges to be faced in the next few years.

New Technology and AI

Making AI solutions productive in drug discovery research, investing in the right technology and using AI and machine learning to optimally speed up the drug discovery process were some of the specific concerns mentioned by delegates who pointed to implementing new technologies as a challenge in their line of work.

Data and RWE

Related to the above point, the use and management of data and Real-World Evidence were another two challenges in the medicinal chemistry sector cited by surveyed delegates at the recent Proventa event. Specific mentions included data storage and retrieval, FAIRifying inhouse data, and Big Data applications in healthcare.

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Cost and Resources

The joint challenges of funding and resources were mentioned by numerous delegates surveyed. Among other things, those attending the event mentioned the cost of data, finding funding to expand research projects, the problem of limited resources and ensuring that funding is being used effectively as difficulties they have faced in their line of work.

Covid-19

Unsurprisingly, COVID-19 was also high on the list of challenges for medicinal chemists. Those surveyed mentioned specific problems including the coronavirus' impact on the supply chain, continuity planning around COVID-19, co-ordination of CROs during the coronavirus and networking during COVID-19.

Strategic Plans

Overall strategy was another oft-cited challenge for medicinal chemists. Among other things, delegates specifically mentioned the need for clients with strategic vision, the need for better commercialisation strategies, and solid medicinal chemistry and data strategies.

Medicinal Chemistry

The day-to-day work of medicinal chemistry was a challenge discussed by several delegates, albeit one of slightly lesser importance than the above issues. Delegates pointed to fundamental insights into the biological correlates of RNA/ligand interactions, the gap between assays and chemistry, and improving prediction methods for compound properties as problems to be solved for the sector to advance.

R&D

Research and development were also a problematic factor for a number of those surveyed. Specific points raised revolved around incorporating AI and machine learning into discovery research, finding funding to expand research projects, R&D in oncology and translation research, among other things.

Staffing and Expertise

Finally, staff recruitment and training was a lower challenge for delegates. Those attending mentioned the need to find and hire subject matter experts, identifying consultants with specific expertise to address gaps, and influencing senior leadership as matters to be addressed in the future.

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