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“We're exploring AI, ML techniques for molecular design & various predictions of drug candidates"

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Aurigene is a clinical stage biotech company committed to bringing novel therapeutics for the treatment of cancer and inflammation. Based in Bangalore and Kuala Lumpur, it has fully integrated Drug Discovery & Development infrastructure from Hit Generation to Clinical Development. In over 15 years of working with Pharma, Biotech and Academic partners, in a variety of Therapeutic Areas, Biologies and Chemistries and over 80 integrated Drug Discovery projects, Aurigene has contributed to delivering over 15 small molecule and peptide drug candidates to its biotech and pharmaceutical partners. Aurigene has out-licensed several first-in-class and best-in-class compounds to pharma and biotech companies for global clinical development, while undertaking clinical POC studies in a few programmes in India.

Dr Murali Ramachandra, CEO, Aurigene Discovery Technologies Ltd shares his views with BioSpectrum, about the role of new age technology in drug discovery. Edited excerpts;

New-age technology-based interventions are playing a major role in transforming pharmaceutical processes and operations. The same applies to drug discovery too. How according to you has tech applications been a major advantage in drug discovery?

New-age technological development has revolutionised the drug discovery process like all other fields. I would like to divide the impact into three major buckets as follows:

Informatics

1. ***Information flow management:*** With availability of various software tools, management of information became very easy and error free, helping save enormous time in the drug discovery process. For example, various search engines like PubMed, Thomson Reuters, Scifinder, Reaxys, MARPAT, STN etc. to name a few, help in gathering accurate and up-to-date information that would have been taking very long otherwise. Almost all the research journals have made available online with searchable annotation and keyword enabled notification systems that help researchers keep themselves updated almost real-time. Many specialised bio and chemo informatics databases have been made available over the last few years that help in identifying high quality drug discovery projects (biological target). These tools also help in designing right experiments supported by knowledge bases accessible on the fingertip. In addition to the above explained global informatics systems researchers also create their own local informatics by using tools like electronic lab notebooks, data management systems and various inventory systems. These local tools gather historical data over the years to cater future researchers with precious knowledge that is organisational experience which was missing before these information technology tools were made available. All the tools and technologies explained above help in improving the quality of drug candidates and shortening drug discovery timeline significantly.
2. **Project management:** Drug Discovery is an expensive and time-consuming process. Using various project management tools tracking of the project progress and project budget has become more streamlined. Important project milestones could be tracked down effectively using various IT tools.

Data Analytics: Usage of computer software to calculate results from complex experiments helped in improving data accuracy. Now statistical analysis of these data with high accuracy gathered over time generates power to predict. Various data analysis tools using global publicly available large data sets or locally available small data sets enable predictability reducing time and cost of innovation.

Innovation support: In the highly complex domain of drug discovery various computational algorithms developed over the last few years that are helping in predicting certain aspects of drug design. AI and machine learning are being used more and more in recent times powering computer aided drug design (CADD), however, one needs to wait before assessing the effectiveness of these tools.

How has your company exploited technologies in drug discovery? Does it have a significant impact on timelines and cost of the processes in drug discovery?

We have deployed almost all the above-described tools and technologies in our drug discovery process and operation. We have subscribed to many of the global databases assisting our projects. We have developed electronic lab notebooks, compound and data management systems and chemical inventory management systems etc. inhouse saving a significant amount of money and time. We utilise computer aided drug design technology for assisting novel drug design in many of our drug discovery projects. All standard data analysis tools and informatics databases are being used at Aurigene routinely to help reduce the overall timeline for each project. Lately, we are exploring AI and machine learning techniques for molecular design and various predictions like efficacy and toxicity of the drug candidates.

Providing data-driven, personalised cure to patients and most importantly cost-effective cure is the need of the hour. What is your take on the use of technology to deliver personalised medicine, in an Indian scenario?

Personalised medicine is an emerging concept in the field of drug discovery, especially in oncology. Due to extremely high heterogeneity cancer of the same organ (lineage) for two different patients could have very distinct characteristics. This heterogeneity could be in such a high degree that the cancer of the same lineage of two different patients should rather be called different diseases requiring completely different treatment regimens. Under these circumstances it is essential to analyse and understand the character of the disease for each person separately and decide upon the treatment which is known as personalised treatment. To my understanding, use of various technologies (e.g. next generation sequencing, cell signal pathway analyser) and informatics database tools enabled personalised medicine to some extent. More than money, significant improvement in long term survival of patients with many cancer types could be achieved due to personalised or

precision oncology therapy. However, constant development in fundamental research in biology is needed to make significant progress in this front both globally and locally for India.

Has the pandemic had any influence on adopting technologies for drug discovery?

COVID-19 has taught all sectors how to work remotely in a very effective manner. In drug discovery also usage of various Virtual Reality (VR) tools has become popular that helped in effective team activity otherwise was not feasible without sitting across the table. One such example is usage of VR software for simultaneous viewing of crystal structures and molecular design from remote by various team members.

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