"Players like us can ease entry of Indian pharma industry into drug discovery space"

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After having developed path-breaking algorithms and models for e-commerce recommendation systems and world-beating language translation systems, researchers at New Delhi-based startup Molecule AI have turned their sights towards one of the toughest problems in pharmacological research today, one with immeasurable benefits for humankind, Drug Discovery! In conversation with Saurabh Singal, Founder, KnowDis/ Molecule AI, BioSpectrum takes you through a noble attempt on pure research in the field of AI in the country.

When did you establish KnowDis/Molecule AI, and what was the key objective?

We established KnowDis in 2018. It was a time when the Deep Learning revolution was gathering momentum, and after the huge advances in Computer Vision, Natural language processing (NLP) was making progress. We wanted to create a company that would harness the power of artificial intelligence (AI) for biomedical research and applications. As things turned out, KnowDis developed and released a series of very strong products used for e-commerce while continuing to do innovative research in the drug discovery space. Earlier this year, we launched Molecule AI, which will focus solely on computational drug discovery models and the suite of software products for that space.

Please elaborate upon the technological solutions being developed by KnowDis. How are these solutions unique in contrast to the technology already available in the market?

When discovering drugs that save lives and alleviate serious medical conditions, we prefer to talk of collaboration rather than competition. We are all trying to find solutions to complex diseases and work with, and in parallel to, multiple highly talented companies at the intersection of AI and health space. A particular Indian advantage is creating high intellectual input yet low-cost solutions that can address a vast market. Our proprietary AI platform, models and data offers one such Indian solution which will assist global teams in addressing the better treatment of severe medical conditions.

What is the current team's skill and expertise at KnowDis? Are you still expanding your team and hiring more talent?

Our team includes several PhDs, both in Chemistry and AI. We have attracted a dazzling array of very high-IQ scientists and engineers. We also have partnerships with several leading research groups globally. We are always looking to add more talented people to our team.

How can KnowDis/Molecule AI benefit the Indian pharma industry in becoming an innovation hub of drug discovery? What are the current challenges facing the Indian pharma industry with respect to developing new drugs, compared to the global counterparts?

The challenge that the Indian pharma industry faces with respect to drug discovery, and the reason it has largely remained as a producer of generic products, is the high-cost, high-rewards nature of drug discovery. Indian companies lack the financial strength to take on this risk. With rapid increase in computing power and the advent of AI, in-silico drug discovery has become a reality, with consequent significant reductions in the cost of drug discovery efforts. Therefore, Indian organisations with in-silico drug discovery capabilities, such as Molecule AI, can be key players in easing the entry of the Indian pharma industry into the drug discovery space.

In terms of KnowDis/Molecule AI helping the Indian pharma industry to become an innovation hub of drug discovery, we are happy to collaborate and partner with Indian organisations to provide access to our computational drug discovery models, platforms and team of highly skilled in-house researchers.

Your work also focuses on drug repurposing, a concept well explored during covid times. Please share more details about your tools for drug reuse.

We can broadly classify the AI-based tools we are developing into (a) screening models and (b) generative models. We will use our screening models for in-silico high-throughput screening of potential drug candidates. Therefore, these models will enable drug repurposing by using the set of known drug molecules (or any suitable subset) as the set of candidates to be screened.

What are the major plans in store for 2023 & beyond to establish your presence in the market, particularly for the pharma sector? Are you exploring new partnerships or collaborations?

Our in-house research team is strongly focused on drug discovery for neurodegenerative diseases, and we will announce significant progress within two years. Our work will identify target molecules and potential drugs, and we will conduct wet lab

testing to validate our in silico work. We will partner with pharma companies to take these drug candidates to clinical trials. We will create partnerships with research teams worldwide by making our proprietary data and platform available on a subscription basis. This will permit us to develop a pipeline of drug candidates in collaboration with world-leading researchers. We have been in discussions with leading research institutions in India and overseas to work with them on specific research projects addressing targeted diseases. We continually evaluate our ability to contribute to these initiatives and will enter into collaborations with specific objectives and milestones."

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