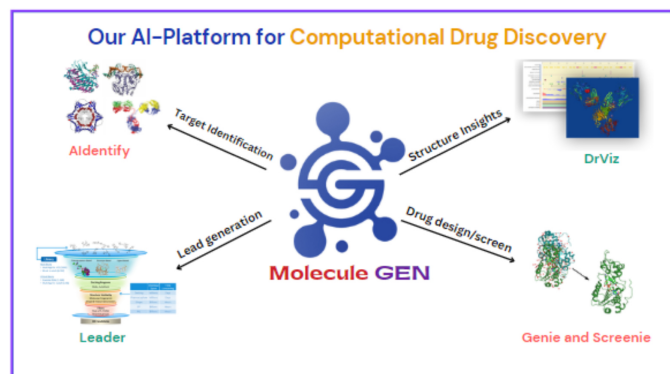# Molecule AI Harnesses AI Power to Tackle Medicine's Toughest Challenges

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Imagine experiencing sudden disorientation, confusion, agitation, and impulsivity. One day, you're clear-headedand on top of the world; the next, you're plagued by hallucinations, delusions, paranoia, and cognitive difficulties

Molecule Gen: An AI-driven platform for drug discovery

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What if there was a solution? A golden key or antidote to lift the fog and restore your mind? How far would you go to obtain it? And if it doesn't exist, how desperately would you be for someone to create it?

Imagine standing in a 100-room castle with this one Key, looking for the right lock. How much time would it take to find that lock? Half a day? What if there were a hundred such castles? What if the castles were also spread over a few thousand (or hundred thousand) square kilometres? Across a hundred countries? On multiple earths?

You still only have the one key. How many weeks or months, or years would this take?

Now, imagine that neither the lock nor the key is static. Each of them changes its shape frequently. How much time would it take then? Would you even attempt this endeavour of a few million lock & key combinations?

The researchers at Molecule AI are attempting to solve one such problem—except that they have more than a billion combinations to contend with. Led by Saurabh Singal, an IIT Delhi and Carnegie Mellon alumnus with over 20 years of experience, the AI team at Molecule AI consists of some of the sharpest minds in the country. After having developed path-breaking algorithms and models for e-commerce recommendation systems and world-beating language translation systems, they have turned their sights towards one of the most challenging problems in pharmacological research today—one with immeasurable benefits for humankind—should they succeed!

If there is any team with a fighting chance of solving such a complex problem, it is undoubtedly this one. Comprised of exceptional AI and deep learning researchers, biochemists, mathematicians, and biophysicists, their expertise is unquestioned. Interestingly, some team members are not only accomplished in their scientific pursuits but also excel in other domains. Some are also highly skilled classical musicians—routinely performing in concerts, and others start their day matching wits against chess grandmasters.

Molecule AI is an Indian-born deep tech AI startup developing cutting-edge AI algorithms and applications to further the field of Artificial Intelligence. They are one of only a handful of such organisations working on pure research in the field of AI in the country. They promise to revolutionise drug discovery by introducing Molecule GEN, their AI-powered drug discovery platform.

The research, testing and formulation of any new drug take years, if not decades. The complexity and nature of the disease-causing agents have a direct impact on how long the research will take and whether there is even foreseeable hope for success. Molecule AI has endeavoured to attack one of the most challenging known problems for clinical researchers - that of neurodegenerative diseases, such as Parkinson's and Alzheimer's. No known cures exist today. Even the deterrents available today are a shot in the dark for most patients. Over 55 Million people live with Alzheimer's induced dementia today, and over 10 Million with Parkinson's. These numbers are estimated to cross 100 Million over the next two decades.

"The challenge in finding a cure resides in the nature of the disease-causing antigens. The antigens causing neurodegenerative disorders are one of the most notorious since the proteins that make up these antigens are yet to be definitively mapped. Research so far shows us that these antigens are also shapeshifters! This makes the synthesis of any potential antibody even more laborious, especially with the current set of tools and processes available today", says Saurabh Singal.

With the use of Artificial intelligence and advanced computational models, Molecule AI hopes to be able to simulate potential antibodies and small molecules, which would have a high probability of success in combating the target antigens. However, such models do not yet exist. Even the most advanced AI models today can only work for much simpler antigens (than those causing neurodegenerative diseases) and even then, only give two-dimensional results. Therefore, the first step is to build an intelligent model that can be used to train machines that, given a set of required properties as input, can produce a small molecule, protein, or antibody and specify its 3-D structure with high accuracy.

To be able to build such a model, researchers need to perform several complex steps, such as carrying out detailed analyses of the target antigen structure and its relationship to other proteins and filtering out false positives from sets of potential drugs against these targets (whether small molecules, proteins, or antibodies) based on various parameters. While going through such steps themselves, the team at Molecule AI felt that an easy-to-use tool that could help with all the steps in this complex drug discovery and design process would be highly beneficial to the drugdiscovery field in general. With this in mind, MoleculeAI is building its drug discovery platform "Molecule Gen".

Molecule Gen incorporates various modules such as target identification, target visualization and analysis, AI-driven drug generation (both small molecule and antibody), filtration of initial hits to a few leads based on an extensive set of screening criteria, and advanced validation tools that provide high confidence that the leads generated by the computer will work in the lab. All these modules incorporate Molecule AI's proprietary algorithms with enhanced capabilities compared to current state-of-the-art tools.