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Aurigene Pharmaceutical Services introduces AI and machine learning assisted drug discovery platform

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Aurigene Pharmaceutical Services, a contract research, development, and manufacturing services organisation and a Dr. Reddy’s Laboratories company, has introduced Aurigene.AI, an artificial intelligence (AI) and machine learning (ML)-assisted platform for accelerating drug discovery projects from hit identification to candidate nomination.

Aurigene.AI combines advanced physics-based simulation, generative and predictive AI models, and CADD (Computer-Aided Drug Design) in one platform, allowing users to pick the appropriate algorithms for a given application. The modular platform also consists of a meticulously curated database of 180 million compounds and 1.6 million validated bioassay data points. This database is ever-expanding and serves as training data for the platform.

Aurigene.AI is hosted on Google Cloud, which offers a scalable infrastructure for handling large datasets and efficient computation while safeguarding client data confidentiality.

Integrating AI and ML-based solutions with Aurigene's core capabilities in chemical design, synthesis, and assessment in bioassays will facilitate faster development of novel therapeutics. Discovery scientists at Aurigene have validated the platform using a case study and demonstrated that the application of Aurigene.AI reduced the cycle time from chemical design to synthesis and testing by 35%.