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Hyderabad-based startup Excelra advances drug discovery for challenging targets

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GOSTAR provides a unique 360? view of over 8 million small molecules

A new collaboration between Hyderabad-based data science and analytics startup Excelra, and artificial intelligence pioneer X-Chem, based in the US, will accelerate preclinical drug discovery and aid scientists to find new drug candidates for currently hard-to-drug targets.

Machine learning and artificial intelligence are reshaping discovery and optimization of drug candidates. This synergistic new partnership between Excelra's GOSTAR and X-Chem's RosalindAI will enable unique and powerful tools to predict small molecules, chemical, biological, and physical properties, accelerating time and resource-intensive stages of drug discovery from hit identification to preclinical candidate selection.

GOSTAR's proprietary data set underwent rigorous analysis and large-scale ML model building to predict drug solubility in a recent joint study. X-Chem's RosalindAI delivered superior and actionable results than other similar analyses using well-known publically available datasets.

The results confirmed that RosalindAI's proprietary models are designed specifically to address challenges in chemical datasets, and when trained on the larger, more diverse GOSTAR data, yielded models twice as better than models trained on other datasets.