

Excelra licenses drug discovery database to Canadian firm

21 October 2020 | News

GOSTAR ultimately equips researchers with insights to generate novel ideas in drug design in the early as well as optimization stages of drug discovery.

Excelra, a global data & analytics organization based in Hyderabad, has announced that it has licensed its Global Online Structure Activity Relationship Database (GOSTAR) to Toronto based Cyclica Inc., a leading biotechnology company whose Al-augmented integrated platform enables multi-objective, polypharmacology-informed design of drug molecules.

<u>GOSTAR</u> is the largest online structure activity relationship database comprising of over 5.5 million small molecules and their associated chemical, biological and pharmacological properties. The database is manually curated by our scientific team who excerpt and enrich datasets from functional assays, in vitro and in vivo studies. A variety of small molecule activities encompassing SAR, physicochemical, metabolic, ADME and toxicological profiles are captured and structured into a relational database. GOSTAR ultimately equips researchers with insights to generate novel ideas in drug design in the early as well as optimization stages of drug discovery.

Dr. Raveendra Dayam, Director, Chemistry Services, Excelra said: "GOSTAR provides access to more than 28 million experimentally determined quantitative interactions between small molecules and the vast druggable target space. Insights derived from these interactions complement Cyclica's polypharmacology approach in novel compound drug discovery. GOSTAR is a rich qualitative and quantitative dataset that is applied by many AI/ML companies and we are excited that the data will support Cyclica with its predictive analytics."

The breadth of data provided by GOSTAR will broaden the domain of applicability of Cyclica's models, as Dr.Stephen MacKinnon, VP of R&D at Cyclica indicates: "The collaboration with GOSTAR strengthens Cyclica's training data for our platform models by allowing Cyclica to annotate our proteome screening data, thus enhancing our predicted interaction capabilities. This will have a direct impact on the development of more precise and efficacious medicines for patients in need."