## GOSTAR Case Study

Activity Landscape Analysis for Compound Datasets

The Purpose

Activity Landscape Analysis (ALA) methods are the emerging approaches to systematically capture structure–property/activity relationships (SPRs/SARs). SPR/SAR studies have broad applications in chemistry and related multidisciplinary areas including drug discovery. Drug discovery is one of the areas in which SPR/SAR has a large impact, wherein medicinal chemists analyze structure-pharmacokinetic relationships to optimize activity to pharmacological and toxicological systems. Such optimization not only involves the improvement of biological activity, but also decreases the toxicity while improving the overall pharmaceutical profile of the lead series.

The Excelra Approach

Excelra's Global Online Structure Activity Relationship Database (GOSTAR) provides a 360-degree view of million compounds, linking their chemical structure to biological, pharmacological and therapeutic information. GOSTAR enables medicinal chemists or cheminformaticians to quickly visualize and explore activity landscapes and evaluate SAR data. The compound datasets can be analyzed with an in-built comprehensive "Analyzer tool" within GOSTAR, to generate SAR/SPR.
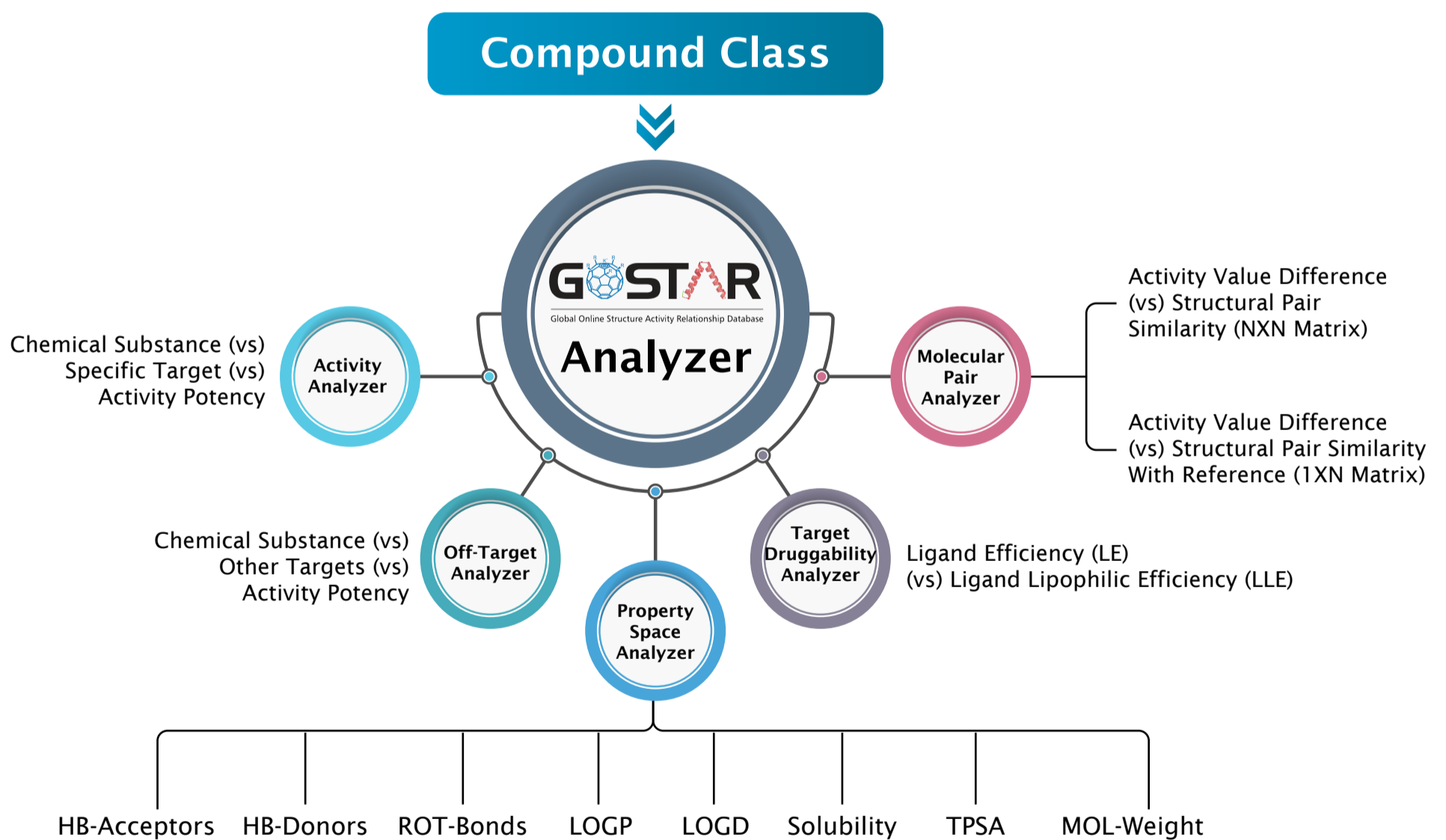
GOSTAR Utility

Excelra's GOSTAR provides tools to identify compounds' nearest neighbors or analyze activity landscapes across compound datasets.

Activity Analyzer: This analyzer provides a graphical representation of activity distribution for an end point in relation to a single target from different sources.

Off-Target Analyzer: This analyzer helps in identifying a target class of compounds potency/selectivity against other targets.

Property Space Analyzer: This analyzer is used for generating molecular encoding schemes from general chemical properties (e.g. lipophilicity, molecular weight, total charge, solubility). This helps in virtual screening of activity-enriched sets of molecules from the space of synthetically accessible structures.

Target Druggability Analyzer: This analyzer helps to identify the goodness of interaction between chemical compound vs. target protein. This provides a graphical representation of molecular properties (Ligand Efficiency (LE) vs. Ligand Lipophilic Efficiency (LLE)).

Molecular Pair Analyzer: Using this analyzer we can describe the systematic method of identifying matched molecular pairs from a set of compounds and determining the property change associated (i.e. Structural similarity vs. Activity value differences).

Our Clients

Pharmaceuticals

Biotech

Research and Academia

AI/ML Driven Drug Discovery Companies

Contract Research Organizations

Excelra's Service Portfolio

	Insights	Data
Discovery	• Data Science Driven Drug Discovery • Target Identification • Target Dossier Services	• Chemistry Curation Services • GOSTAR Structure Activity Relationship database
Translational	• Biomarker Discovery • Drug Repositioning • Life Cycle Management • Systems Biology Informatics	• Biology Curation Services • GOBIOM Biomarker intelligence database
Clinical	• Precision Oncology Informatics • Clinical Pharmacology	• Clinical Trial Outcomes Database
Value Evidence	• Outcomes Research • Epidemiology Modelling • Economic Modelling • Value Evidence Communication	• RWE & Big Data Realization • SLR & Meta-analysis
Technology Solutions	• Enterprise Data Strategy • Enterprise Cloud Ops • Enterprise Digital Transformation	

For more information, visit https://www.gostardb.com/gostar/

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About Excelra

Excelra's data and analytics solutions empower innovation in life sciences across the value chain from discovery to market. The Excelra Edge comes from a seamless amalgamation of proprietary curated data assets, deep domain expertise and data science. The company's multifaceted teams harmonize and analyse large volumes of disparate unstructured data using cutting-edge technologies. We galvanize data-driven decisions to unlock operational efficiencies to accelerate drug discovery and development. Over the past 18 years, Excelra has been the preferred data and analytics partner to over 90 global clients, including 15 of the top 20 large Pharma.

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