excelra

Activity landscape analysis for compound datasets

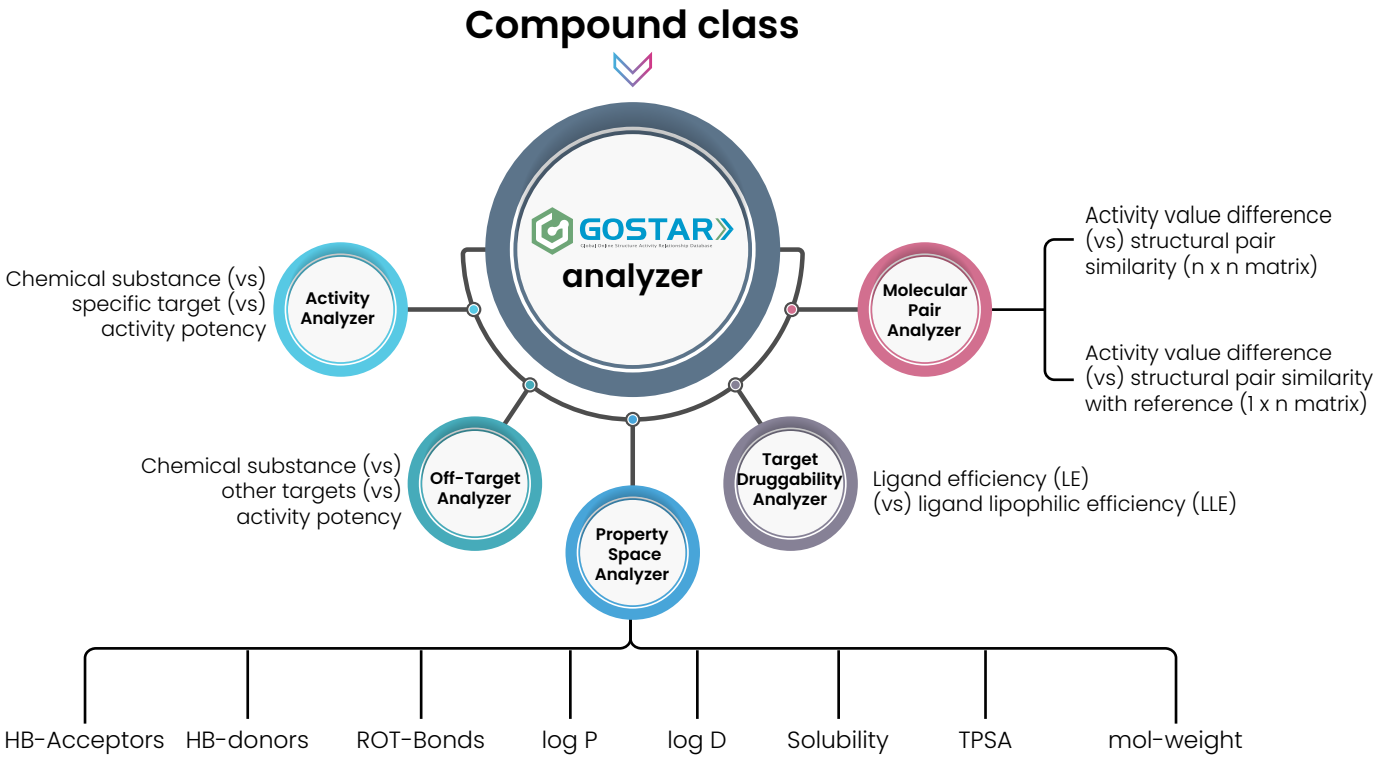
CASE STUDY

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.

Our 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

Our service portfolio

Data

Data curation
Filter out the noise, focus your attention

Clinical data
Analysis-ready data for informed clinical decision-making

Semantic data
Refine your decisions, find your value

Insights

Bioinformatics
Illuminating the path to faster discoveries

Data science
Unlock the power of data

Visualization
Pictures paint a thousand words

R&D technology

Product design and development
Unlock your potential with data-driven design and development

Cloud enablement
Optimize your output on the cloud

Data engineering
Mitigate risks, protect your data, and rationalize your portfolio and processes.

Where data means more

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