APPLICATION

datavisyn

Discover visynChem

The Intelligent Chemical Workbench

You Want to Transform High-Dimensional Chemical Data into Laboratory-Ready Roadmaps?

Experience visynChem

A specialized cheminformatics application providing a native chemical data model with first-class support for SMILES identifiers.

Integrated Evidence

Merges interactive structural rendering with asynchronous machine learning to assess experiment libraries and compound success.

Seamless Orchestration

Within the visynPlatform, visynChem bridges the gap between chemical and CMC raw quantitative test data and actionable, reproducible lead insights.

Discovery Workflows

- **Lead Triage:** Ranking compounds by predicted efficacy and synthetic feasibility
- **Reaction Optimization:** Identify high-yield clusters based on catalysts and solvents.
- **Scaffold Exploration:** Visualizing chemical space via UMAP projections
- **Model Validation:** Verify structural drivers behind AI-generated success scores.

Part of Ordino & Aevidence

www.datavisyn.io

Strategic Capabilities

Advanced Visual Analytics

visynChem moves beyond standard tables

Move beyond standard tables with Hierarchical Facet Plots (HFP) to instantly surface high-yield clusters. Use UMAP Projection Plots to explore chemical space with fully synchronized data selection.

Explainable AI (XAI)

Validate model logic before moving to laboratory

Validate model logic using SHAP visualizations to demystify ranking drivers. Identify whether structural features or secondary variables drive predicted success to ensure transparent triage decisions.

Scalable Lead Discovery

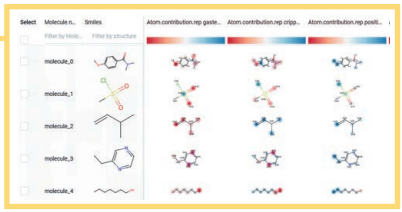
Targeted screening for high-throughput analysis

Identify top-performing conditions and apply a learning-to-rank approach to predict the success of all remaining rows in a dataset, ensuring every laboratory cycle is statistically robust and reproducible.

Precision Reporting Modules

Interactive Structural Tables

Scan hundreds of reaction sets with real-time rendering. Rows integrate chemical structures via SMILES with quantitative data for a high-level view of your experiment library.



Chemistry Toolbox

Compute RDKit descriptors and Morgan Fingerprints directly within the workbench. Run clustering algorithms to identify which chemical families perform best as a group.

Predictive Model Integrations

Rank compounds by efficacy using live recommender models or custom-trained predictive tools, while filtering out candidates that are difficult or expensive to synthesize.

Request a Demo

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