GeneCDMS

Compound & Data Management System (CDMS) designed to do compound registration, batch, structural, compound storage and accompanying information into database.

Compound visualization and analysis uses Data Warriors Torx & SARVISION. Integration with Electronic Lab Notebook System, Inventory System and Analytical Ticking System.

KEY FEATURES

- Single, Batch & Legacy Compound Registration. Compound make **Auto Registration** using API.
- **Structures Drawing** Tool Integration.
- Compound property auto generation from Structure Tool.
- **Structure Search:** Exact structure, Sub-structure or Similar structure.
- Biology Assay result **data publish** & approval workflow – Manual workflow.
- Biology Assay result **data automation** using Envision and Sciex LC-MS.
- **Solid, Liquid & Solution** Compound workflow management.
- **DMSO preparation.** Compound storage, mother and daughter plate traceability.
- SAR Report with Multiple Assay and Sub Assay filtration.
- System supports Smile/SDF/MDF/Mol/Rxn & Excel File.
- TAT Report, Activity base Dashboard & Reports.
- Integration with GraphPad Prism, **Torx & SARVISION**.

BENEFITS:

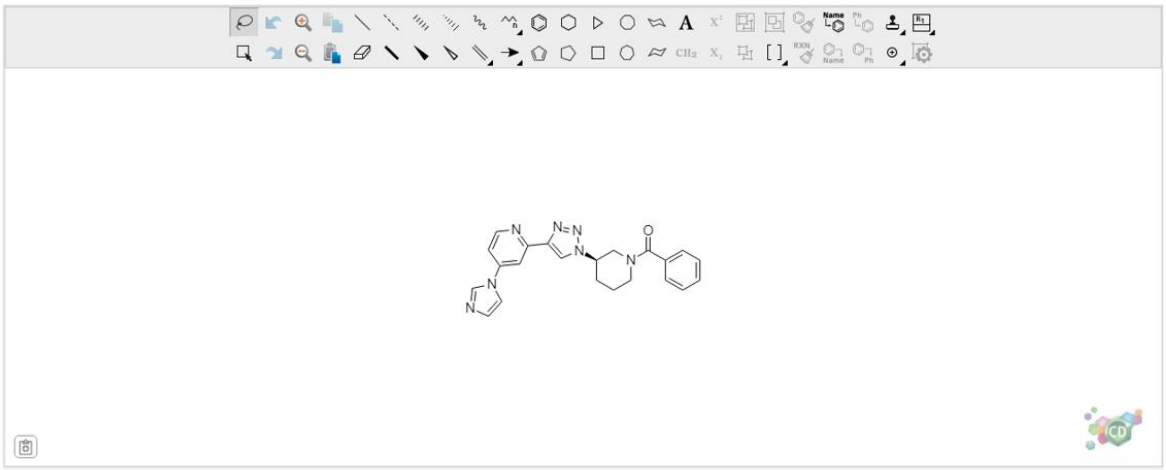
- Compound similarities can be used for multidimensional scaling methods, e.g., Kohonen nets.
- Physicochemical properties can be calculated
- Structure activity relationship tables can be created, and activity cliffs be visualized.
- Data Warrior combines dynamic graphical views and interactive row filtering with chemical intelligence.

IMAGES :

GeneCDMS

Maheshwari K
ADMIN

Home | Registration Manager | Compounds | Stores View | Scientists | Compound Issue View | Admin Panel | Enrolment Panel | Reports | Masters | Biology



PREDICTION

Confirm

Molecular Formula(Analyte)*	$C_{22}H_{21}N_7O$	Product Name*	(R)-(3-(4-(4-(1H-imidazol-1-yl)pyridin-2-yl)-1H-1,2,3-triazol-1-yl)piperidin-1-yl)(phenyl)methanone		
Molecular Weight*	399.45				
Salt Type*	01-Free base-Free base [4	cLogP		Carbon Content (%)	
No of salt counter ion*	0.00	TPSA		Hydrogen Content (%)	
Molecular Formula(Salt)*	Free base	PKa		Nitrogen Content (%)	
Formula Weight*	399.45	LogS		Oxygen Content (%)	

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