Chromingo Report

Specification Sheet

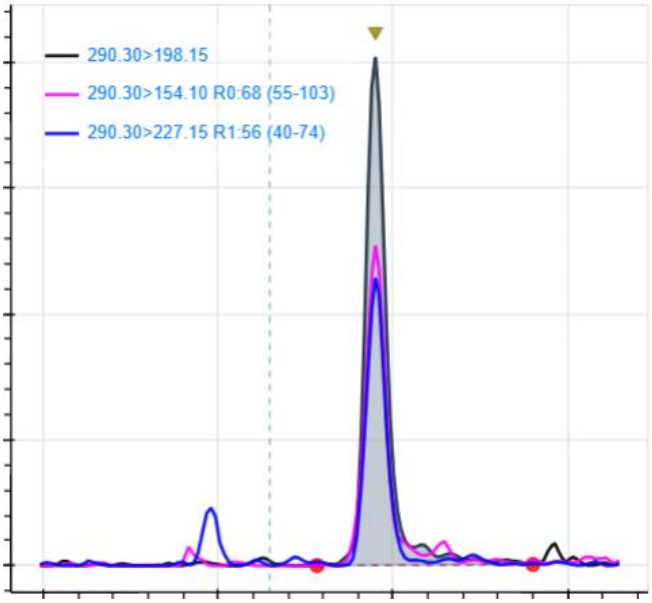
Data Upload and Processing

The system supports the upload of 2D chromatography data, including Gas Chromatography (GC), Liquid Chromatography (LC), Gas Chromatography-Mass Spectrometry (GC-MS), and Liquid Chromatography-Mass Spectrometry (LC-MS).

Data can be directly imported from the chromatographic equipment in common formats such as CDF and MzXML.

Uploaded data will be processed and analyzed, allowing visualization of the Total Ion Chromatogram (TIC) alongside associated compound chromatograms.

Intelligent algorithms will associate uploaded sample files with registered analytical methods in the system, excluding samples with irregular methods (methods differing from the dominant method of the batch). This ensures that samples can be grouped into a single batch efficiently.



Chromatogram Features and Customization

The system supports the overlay of target and reference chromatograms for the same compound, including Multiple Reaction Monitoring (MRM) and Selected Ion Monitoring (SIM) modes.

Peak annotations will display the compound name, retention time, concentration, area, and height.

The chromatogram view is interactive, allowing users to zoom, pan, and reset for detailed inspection.

Peak integration filling will be visible in the chromatogram for accurate analysis.

Chromatogram settings can be customized, including the retention time range, ion reference band range, and compound table headers (e.g., compound name, retention time, concentration, area, height).

Barcode Customization

The system allows for customization of barcode settings, supporting both Code 39 and QR codes.

For QR codes, data can be selected for embedding in the QR code format.

For standard barcodes, the Sample ID will be used as the code.

NO	Name	Unified name	m/z Ref. Ions
1	CATHINONE	CAT	150.00>105.10$_{(49.56)}$ 150.00>132.10$_{(75.34)}$
2	AMPHETAMINE	AMP	136.10>65.10$_{(22.14)}$ 136.10>119.20$_{(18.68)}$

Reference Methods

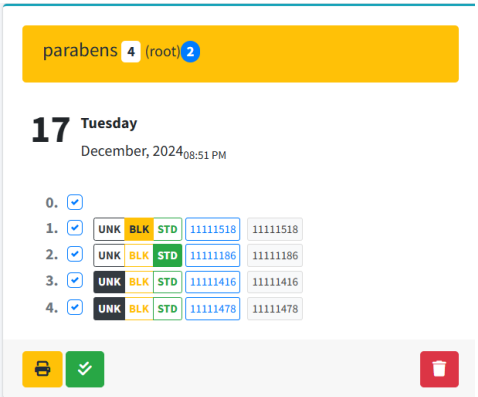
Reference methods containing compound names, fragments, and unified names can be uploaded into the system.

The unified name will be used for API integration when exporting results to a centralized platform.

Reporting Engine

Two types of reporting engines will allow users to fully customize their reports.

Users can include/exclude internal standards and combine unknown results with reference blanks and standards to align with ISO requirements.



Batch Processing and Sample Management

Batch samples can be processed and viewed, with options to add notes to each sample.

Users can delete compounds from samples if the sample is not yet approved.

Samples can be deleted if not approved yet, and sample types (UNK, STD, BLK) can be modified by users with the appropriate permissions.

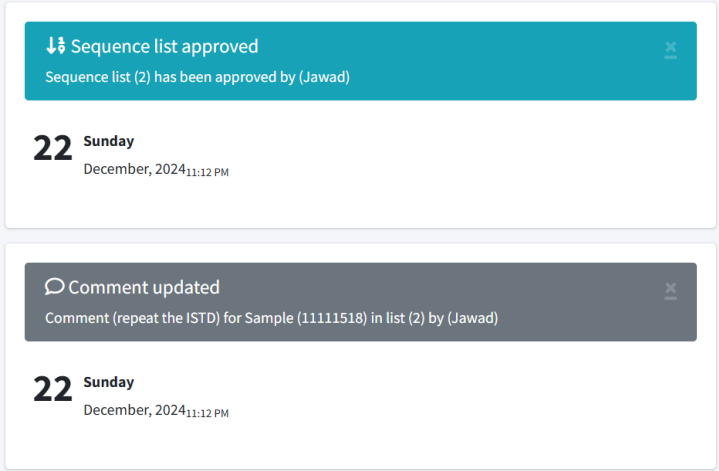
The system logs all sample actions, including upload, approval, comments, and type changes.

Sequences will be categorized as "approved" or "pending," and the process of each sequence can be monitored through logs.

Calendar and Audit Trail

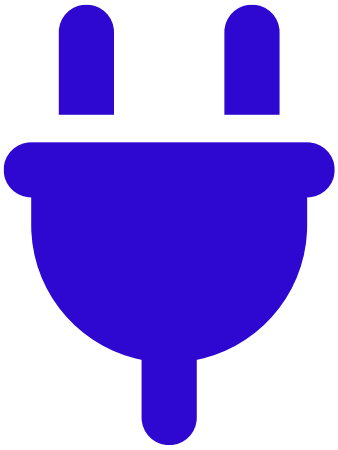
A calendar feature is available for generating analysis reports.

The system will also generate an audit trail for sequences to track all actions and modifications.



Notification System

A dual-flow notification system will notify batch uploaders when reviewers approve, modify, or delete samples. This ensures that creators of sequences are informed about any changes or actions taken on the sequences.

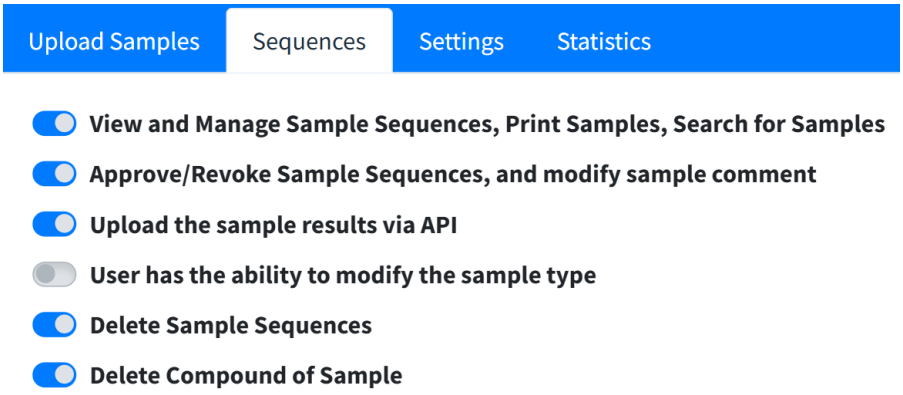


API and Metadata Customization

The system includes an API with fully customizable options for sample metadata and compound tables.

Users have the flexibility to export data either multiple times or just once.

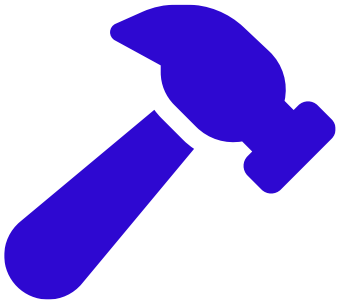
Deleted samples will be flagged and archived separately. If an exported sample is uploaded again after deletion, an automatic cross-check will be performed.



User Roles and Permissions

The system supports customizable user roles, enabling different user privileges and access levels.

IT administrators will have a server page to monitor application errors, system logs, and automated backups, as well as modify API settings and test the API.



Automated Backups

Automatic backups can be scheduled via a setup dialog, ensuring backups are made to both the primary and secondary servers.

In case of a failure in the main server, the secondary server backup can be used to restore the system.

Backups will be automatically purged after 30 days to ensure up-to-date data retention.