

ChemCart Registration

...a full-featured registration system built on the ChemCart web interface

The **ChemCart Registration** module provides functionality needed to implement a corporate registration system. Integration of business rules, structure checking, and registrar capabilities ensures the validity of molecules and reactions registered to the corporate database.

The screenshot displays the 'ChemCart - CHEMCART_REGISTRATION' web interface. It features a 'Structure' field with a chemical structure of a tertiary amine, a 'Compound Registration' title, and a 'New Compound' / 'New Batch' button. Below this are two tables: one for compound details (Corp ID, Reg. No., Batch ID, Mol Formula, Batch Formula, Mol Weight, MW with Salt, Exact Mass, Reg Date, Reg By, Alias) and another for project and physical properties (Project, Therapeutic Target, Solvate, Solubility, Purity, Purification Method, Melting Point, Boiling Point, Library, External Source, External Reg. #). A 'Salt Form' dropdown is set to 'No Salt'. Other fields include 'Notebook Ref', 'Amount Submitted', 'Submitter', 'Stereocenter', 'Appearance', 'Reference', 'Chemical Name', and 'Comments'.

Basic ChemCart features that support registration

- Insert, update, or delete structures and data using customizable forms
- Query, view, report on structures and data through the same form interface
- Extensive list handling capability
- Support for role-based security and Oracle Fine Grained Access Control
- Integrated API for extending functionality
- Supports several popular chemistry formats, such as Accelrys, CambridgeSoft, ChemAxon, Daylight, Symyx

ChemCart Registration provides enhanced 'registration specific' functionality

- Duplicate checking for structures, MF, and text
- Register new compounds or create batches of existing ones
- Batch load data (structures, text, and images) from a variety of file types using a powerful field mapper; check for duplicates against any database field
- Save and re-use registration templates
- Full Registrar functionality including accept/reject flagged registrations and option to bypass business rules
- Integrate structure validation and standardization tools
- Configure for use as a component-based registration system
- Use the Business Rule Engine to implement corporate registration policies

The 'Issue Dialog' window shows a list of issues. The first issue, 'Structure was modified for standardization.', has a green checkmark and an 'Address' button. The second issue, 'Potential duplicate structures found in database.', has a red 'X' and a 'Resolve Duplicates' button. At the bottom are buttons for 'Clear', 'Clear All', 'Flag Registrar', 'Resubmit', and 'Hide'.

The Issue Dialog provides a resolution mechanism during registration.

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