The CDD SAR Data Platform – Features At a Glance

1. Introduction
   CDD is an on-line data management platform designed to organize and mine scientific data, particularly chemical structures and biological results. The CDD relational database allows quick access from any computer to structure-activity data (SAR) stored in private databases (“CDD Vault”), collaborative shared data (“CDD Collaborate”), and published SAR (“CDD Public”). CDD’s interface and tools are simple enough for novice database users, and sophisticated enough for seasoned chem and bioinformatics professionals. Key features are outlined below, but please contact us for an in-depth demonstration.

2. Database Configuration
   CDD’s flexible database organization permits many different types of experimental results to be stored. Flexible user access controls allow to fine-tune data permissions and sharing.
   ✓ User-specified database configuration.
   ✓ Flexible molecule and protocol definition with customizable database fields.
   ✓ Data access and security control with user roles.
   ✓ Data sharing control with private databases (CDD Vault), private data sharing between Vaults (CDD Collaborate), public repository of SAR data (CDD Public).

3. Compound registration
   CDD provides simplified compound registration with many of the powerful tools of costlier traditional packages (ActivityBase, ISIS/Base), plus additional unique features.
   ✓ Structure drawing capability integrated into the website, eliminating the need to purchase a separate application.
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- Support for SMILES, MOL, IUPAC structure representation.
- Individual compound registration, or upload from SDF and CSV files.
- Salt stripping and registration of batches and lots.
- Structure validation with a detailed QC report when new molecules are registered.
- User-defined molecule and batch fields.
- Automatic calculation of chemical properties based on structure, such as the Lipinski rule of 5, and physicochemical properties.

4. **Chemical intelligence**
   CDD has partnered with ChemAxon to provide our users with industry standard chem-informatics tools:
   - Substructure, Tanimoto similarity, and R-group searching capability.
   - Searchable custom molecule and batch fields.
   - Searchable chemical properties, such as Lipinski Rule of 5, logP and pKa.

5. **Biological Data Management**
   Biological data is organized intuitively into “Protocols” and experimental “Runs”, just like it is in the lab. Flexibility of the system allows biological data to be accumulated for each compound throughout the drug discovery life cycle, from HTS to in-vivo.
   - Easy organization of screening data, enzymatic assays (IC50), Cell/Animal Data, ADME-TOX data.
   - IC50 calculation and Dose Response plot generation.
   - Streamlined routine data uploads with an intuitive 4-step import wizard, and data mapping templates.
   - Plate control assignment, with Z/Z'-factor and z-score calculations.

6. **Visualization and Analysis**
   CDD’s search tools and visualizations help draw knowledge and information from the data. These tools will allow chemists, biologists and managers to make research and business critical decisions.
   - Simple display of compound structures with associated biological results (SAR) with configurable viewing options, including dose response plots.
   - Intuitive and powerful protocol and molecule search tools for quick identification of hits, or data quality control with multi-level Boolean queries.
   - Heat-maps for visual data inspection.
   - Scatterplot visualization of chemical properties and biological results.
   - Export options, including export to excel with structure images and dose response plots, and to SD and csv file formats.