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Centralized Data Architecture for Multi-Site Small-Molecule Discovery with CDD Vault

Opna Bio is an early-stage biopharmaceutical enterprise headquartered in Lausanne, Switzerland, with laboratories in South San Francisco, USA. The company discovers novel oncology therapeutics targeting molecular hallmarks of cancer, spanning hit identification through lead optimization.

Following the acquisition of five preclinical oncology programs from Plexxikon, Opna expanded its pipeline to six active projects. To manage multi-site workflows and external Contract Research Organization (CRO) collaborations, Opna deployed CDD Vault (Collaborative Drug Discovery, Inc.) as its central database for chemical registration, biological profiling, and electronic laboratory notebook (ELN) entries.

Key Operational Challenges

Prior to harmonization, cross-site research generated heterogeneous datasets stored across disconnected file directories and spreadsheets.

- **Legacy Asset Integration:** Merging historical synthesis pathways, compound registries, and assay readouts from acquired Plexxikon programs into active workflows without data loss.
- **Data Dispersal:** Managing concurrent data streams from internal teams in Lausanne and California alongside external partners (including R2M Pharma).
- **Traceability Bottlenecks:** Manual file tracking created version-control risks, hindered comparative SAR evaluations, and risked redundant secondary screening.

System Architecture & Implementation

Opna established a unified database in CDD Vault to link chemical structures directly to phenotypic screening profiles and biophysical assay readouts.

Partitioned Vault Environments: Operational workflows are segregated across four distinct database instances to ensure data integrity:

1. **Chemical Registry:** Registers synthetic targets, tracks compound lineage, and records structural metadata.
2. **Biological Registry:** Tracks biological entities, including cell lines, recombinant proteins, antibodies, and assay reagents.
3. **Inventory Logistics:** Manages physical sample lots, batch numbers, storage locations, and chain-of-custody metadata linked directly to experimental readouts.
4. **Sandbox Environments:** Isolated instances used to validate protocol schemas and data templates prior to production commits.

Workflow Integration

- **Structure–Activity Relationships (SAR):** Researchers query compound libraries by registering chemical structures and automatically mapping them to primary screen readouts, values, and cellular efficacy profiles.
- **Granular Access Control:** Security rules assign write privileges strictly to local personnel, while maintaining global read-only visibility across European and US facilities. Project-level permissions grant CRO partners (such as R2M Pharma) restricted access to upload assay data without exposing broader pipeline IP.

Technical Outcomes

- **Single Source of Truth:** Consolidated historical Plexxikon records with prospective research data into an indexed, searchable architecture.
- **Eliminated Redundancy:** Direct structural search prevents re-synthesis of available analogues and avoids duplicate screening.
- **Accelerated Chemistry Cycles:** Instant correlation of structural modifications with biological activity streamlines multi-site lead optimization.

About CDD Vault

Trusted by thousands of researchers worldwide, CDD Vault is a hosted informatics platform for secure management of biological and chemical data. It combines chemical registration, SAR analysis, inventory, visualization, and ELN capabilities, all designed to make collaboration effortless without compromising security.

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