Extended Abstract | Anesthesiology and Clinical Science Research | 2021 | Vol.5 No.1

Present and future collaborative drug discovery informatics innovations

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Abstract

Collaborative Drug Discovery (CDD) provides a whole solution for today's biological and chemical data needs, differentiated by ease-of-use and superior collaborative capabilities. CDD Vault® software includes Activity & Registration, Visualization, Inventory, and ELN capabilities. Researchers can archive, mine, and securely collaborate within CDD Vault. Collaborative hypothesis generation and evaluation allow multiple perspectives for multi-parameter optimization.

Collaborative Drug Discovery (CDD) provides trailing innovation for today's chemical and biological data needs, differentiated by ease-of-use and superior collaborative data sharing workflows. Within the CDD vault software, activity and registration, visualization, inventory, and ELN capabilities all address today's markets. Secure, web-based collaborative technologies are especially applicable to the informatics needs of (and broadly used by) public-privatepartnerships (PPPs). Web-based platforms are a natural fit for collaboration due to the economic, architectural, and design benefits of a single platform that transcends any one organization's solo requirements. In contrast to the CDD vault for today's collaborations, CDD's Research Informatics Group invents bleeding edge technologies for tomorrow's needs.

For example, open source descriptors and model sharing capabilities allow for platform-independent collaborations, even for sensitive data and IP, with groups reticent to share. CDD and Pfizer have demonstrated that these open source descriptors and models were statistically like commercial models. The main idea is to democratize model building to engage experimentalists to want to use models. As a second example, the recently developed BioAssay Express (BAE) technology streamlines the conversion of human-readable assay descriptions to computer-readable information Tanimoto (Jaccard) chemical and biological sequence similarity searches. BAE uses.

CDD's unique IT architecture (true multi-tenant) allows for distinctive use cases compared to traditional (single tenant, virtualized) drug discovery informatics platforms. CDD's architectural principles and the application of modern engineering methodologies enable CDD to democratize traditionally expert informatics tools so that all scientists can benefit. CDD Vault was created from scratch to work with the cloud. As a natural consequence, CDD Vault's architecture and features accommodate those modern requirements.

Case studies will be shared from industry (Jubilant Biosys), government (NIH Neuroscience Blueprint), non-profit (Gates Foundation), and numerous leading academic collaborations. .