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Drug discovery informatics for collaborative teams: Innovations available today and planned for tomorrow

ollaborative 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. Here the main idea is to allow researchers to easily search and combine similar bioassay protocols, even though those similarity searches are much more difficult than semantic standards to markup bioprotocols, which unleashes the full power of informatics technology on data that could previously only be organized by crude text searching (https://peerj.com/articles/cs-61/). These two newer web-technologies may be used not only with the CDD Vault, but also with other commercial, academic, or government built software tools. All open source components are in GitHub.

Speaker Biography

Luke's background brings twenty years of experience in scientific informatics solutions. Managing Pre-Sales, Post-Sales and working in Account Management has expanded his domain knowledge of scientific informatics and provided him the ability to maintain a successful track record. Luke serves leading pharmaceutical, biotech, agricultural, chemicals, academic and government labs. Luke has experience in scientific software solutions from the smaller scale deployment of point solutions like molecular modeling packages to the larger enterprise scale of ELNs, scientific workflow technologies, data content, analysis and visualization. His background also includes managing the support complexity of software integration strategies based on numerous mergers and acquisitions.

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