Barry Bunin, Med Chem 2014, 4:12
http://dx.doi.org/10.4172/2161-0444.S1.013

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
December 08-10, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA

10 Years securely hosting collaborative drug discovery CDD vault in a single, privately managed "cloud"

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Drug Discovery Collaborations have been securely hosted in the CDD Vault since before "The Cloud" was part of our everyday vocabulary. A decade of experience provides unique insights to make individual drug discovery collaborations, and complex collaborations economically scale. Layering unique collaborative capabilities upon sophisticated drug discovery informatics functionality unlocks and amplifies synergy between biologists and chemists. In addition to intuitive registration, structure activity relationship tools, and secure collaboration tools, CDD has given back to the community public data sets (in CDD Public and Pubchem), Open Source Descriptors and Models (in GitHub and CDK toolkits), and via free mobile applications (TB Mobile). Researchers need to have tools that balance individual needs for robust, intuitive registration and bioactivity analyses while at the same time facilitating collaborations with secure data partitioning, communication, and group engagement. Collaborative technologies have crossed the chasm from academic, neglected disease to mainstream commercial drug discovery applications. Since collaborative technology is "therapeutic area agnostic", it has generally been proven equally applicable for commercial applications. Representative commercial case studies include broad consortia such as the NIH Neuroscience Blueprint collaboration between drug discovery companies, CROs, together with seven leading academic biology laboratories as part of a 5-year government contract to advance new CNS drugs into the clinic. As well as more focused examples following the lean venture funded model such as the collaboration between Acetyton Pharmaceuticals with Harvard and a Chinese CRO to bring a selective HDAC inhibitor into the clinic. Collaborative innovation allows well-integrated specialization required for drug discovery both within and between laboratories. Particularly for collaborations between large and small companies or between industry and academia - superior collaborative tools are fundamentally important to catalyze faster progress. In summary, by spanning the continuum of private, collaborative and public modes, researchers globally can now seamlessly collaborate across the pre-competitive and competitive landscape.

Biography

Barry A Bunin, PhD, is the CEO of Collaborative Drug Discovery. Prior to CDD, he was an Entrepreneur in Residence with Eli Lilly & Co. He is on a patent for Kyprolis™ (carfilzomib) for Injection, a proteasome inhibitor that received accelerated FDA approval for the treatment of patients with multiple myeloma. He was the founding CEO, President, & CSO of Libraria (now Eidogen-Sertanty). At Libraria, he led a team that integrated exhaustive reaction capture (synthetic chemistry) with gene-family wide SAR capture (medicinal chemistry). On the scientific side, he co-authored "*Chemoinformatics: Theory, Practice, and Products"* (Springer-Verlag), a text that overviews modern chemoinformatics technologies, and *"The Combinatorial Index"* (Academic Press), a widely used text on high-throughput chemical synthesis. In the lab, he did medicinal synthetic chemistry developing patented new chemotypes for protease inhibition at Axys Pharmaceuticals (now Celera) and RGD mimics to inhibit GP-IIbIIIa at Genentech. He received his BA from Columbia University and his PhD from UC Berkeley, where he synthesized and tested the initial 1, 4-benzodiazepine libraries with Professor Jonathan Ellman.

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