

## **Investment in 3CBioscreen, a High-throughput Screening Facility in Tres Cantos, Spain to Conduct Lead Identification for Texas A&M University Drug Targets.**

The identification of lead compounds which are active against a discrete molecular target-- a single protein, several associated proteins, an organelle or cell-- comprises the first step in the discovery of a drug candidate. While target evaluation and characterization is similar in both academic and pharmaceutical environments, the means of identification of tractable hits or lead compounds is accomplished differently in these two domains. In academic settings, active compounds are paired with drug targets by structure-based rational design, fragment-based screening of small compound libraries, and high-throughput screening (HTS) of compound libraries consisting of 100,000 compounds or fewer. These compound collections are generally composed of commercially-available pharmacophore sets, and represent modest chemical diversity in comparison to what may be found in the larger compound collections used in the HTS campaigns within major pharmaceutical companies. Screening by these compound-limited modalities, which after the discovery of tractable hits, require a large investment in medicinal chemistry to progress these hits to drug-candidate quality compounds. Based on the established success in lead discovery in the pharmaceutical industry, generally speaking, access to a large compound library for high-throughput screening (500,000-1,000,000 compounds) has historically provided better tractable hits as starting points for medicinal chemistry. The assembly, curation, quality-control and provision for HTS of a compound collection of 500,000 or larger requires considerable resources, rarely found in a university setting. Accordingly, having access to a large, high quality compound HTS screening collection from a pharmaceutical company could be of great benefit for those who have well-defined and validated drug targets, bio-reagents and assay materials.

Within this context GlaxoSmithKline Pharmaceuticals proposes to spin off its HTS drug discovery capabilities at Tres Cantos/Madrid in Spain and form a non-profit Research Institute (3CBioscreen) that will sit alongside but be independent of GSK's Drugs of the Developing World and Open Innovation Centre in Tres Cantos. 3CBioscreen will focus on enabling the translation of novel therapeutic hypotheses into new chemical entities for testing preclinical proof of concept. 3CBioscreen will be an independent, self-funded organisation. This new nonprofit institute will be specialized in collaborative research to advance therapeutic hypotheses into innovative medicines. Located in the largest biomedical hub in Southern Europe (Madrid, Spain), the team will build on their experience with more than 25 collaborations around the world in the last few years alone. 3CBioscreen offers an unencumbered high quality, high purity, drug-like, and chemically diverse compound collection (500K). It will also have access to the full 1.8 million screening collection from GSK under specific terms. Scientists at 3CBioscreen have an outstanding and highly innovative drug discovery track record. Only in the last 12 years they have performed more than 300 HTS's in 230 discovery programs with 90% success in identifying hits, 50% of which have yielded a chemistry effort.

3CBioscreen will provide a unique offering; (a) access to a proven drug discovery team with an outstanding track record of HTS delivery; (b) highly cost-effective access to Big Pharma drug discovery resources and HTS capabilities. The timing for the creation of 3CBioscreen will be well aligned with the proposal to create a specific fund for early drug discovery activities at Texas A&M University, will start evaluating potential collaborations in the 2<sup>nd</sup> part of 2016, with the goal to start laboratory operations and drug discovery projects by January 2017. In a full proposal, we will provide costs for access to the 3CBioscreen HTS site for screening of drug targets at Texas A&M University.