

Sanford-Burnham Medical Research Institute and Analiza, Inc. Add Large Volume of Compound Solubility Data to PubChem to Assist Future Drug Discovery Efforts

March 10, 2010 – Cleveland, OH

A collaborative project between Sanford-Burnham Medical Research Institute at Lake Nona and Analiza, Inc. has yielded aqueous solubility data for over 20,000 compounds in the NIH Molecular Library within the first 90 days of screening and characterization. The early results of the analysis are proving to be enlightening, with almost 30% of the compounds screened having low solubility – a key factor in disqualifying compounds early in the drug development process, saving later stage time and expense. The reported measurements are now part of PubChem, the largest publically available database of bioactive molecules.

In total, over 58,000 compounds from the NIH Molecular Libraries Small Molecule Repository will be analyzed during the 12 month agreement. The project is the result of Sanford-Burnham receiving a \$600,000 NIH research grant in late 2009. To date, such a large volume of solubility data, as related to chemical structure, has not been available for computational analysis. Knowing the solubility measurements of test compounds will help improve and streamline the early stages of molecular screening. Ultimately, the data will assist future drug discovery efforts by allowing an investigator to select the concentration of each compound to test within their biological studies.

“We’d like to see the more than 300,000 compounds in the NIH library analyzed for such a critical component as solubility. We are seeing upwards of 30% of the compounds having a low screening solubility measurement of less than 10 µg/mL. This is significant data for scientists who are responsible for early probe discovery and development,” said Dr. Gregory Roth, Associate Professor and Director, Medicinal Chemistry at Sanford-Burnham Medical Research Institute.

The concept of identifying properties of a compound which affect its suitability as a drug candidate early in the discovery process is not new. Until recently, the cost of analyzing such a large library of compounds for key physicochemical properties was prohibitive. “Analiza has always been focused on the automation and streamlining of the measurement process to reach a cost/value proposition that makes sense for companies” said Mark Stratton, V.P. Marketing for Analiza. Analiza uses a method that does not rely on assumptions, but rather measures the true solubility of known compounds in a biologically compatible organic solvent known as dimethyl sulfoxide that is diluted in aqueous buffers for biological analysis.

Dr. Roth stated that Sanford-Burnham Institute will continue to evaluate the results and determine how best to approach a potential second phase of measurements for the physicochemical properties of the NIH compound library. The solubility results that have been reported to date can be found at <http://pubchem.ncbi.nlm.nih.gov>. PubChem is maintained by the [National Center for Biotechnology Information](#) (NCBI), a component of the [National Library of Medicine](#), which is part of the United States [National Institutes of Health](#) (NIH). PubChem can be accessed for free through a [web user interface](#).

Analiza, Inc. is a CRO located in Cleveland with it’s emphasis on providing fast, accurate and affordable physchem services to pharmaceutical and biotech companies.

For more information:

Mark Stratton
Analiza, Inc.
216-235-2372
mstratton@analiza.com