and SwissProt. The basic information in the database is provided by expert bench researchers, edited by Reactome staff and, following peer review, is

published online. Knowledge from experts in the field, cast into this unambiguous but impressive data model by human curators (as opposed to computational text processing), makes Reactome data suitable for a variety of computational modelling approaches.

# NIH chemical genomics network takes off

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The National Institutes of Health (NIH; http://www.nih.gov/) announced that it has established the first in a series of chemical genomics screening centres that will allow academic and government scientists in the USA a currently unprecedented access to large libraries of organic chemical compounds.

### Ten pilot centres

The NIH Chemical Genomics Center will be based at the National Human Genome Research Institute (NHGRI; http://www.genome.gov/) with the plan of funding ten pilot centres across the USA within the 2005 fiscal year. To support the network, NIH will establish a repository to acquire, maintain and distribute a collection of up to one million chemical compounds.

The compounds in question, referred to as 'small molecules' because their size is less than that of proteins, can be used to modulate gene function and so improve understanding of the biological pathways involved in human health and disease. Most marketed drugs are small molecules and, as a result, have been the focus of intense screening efforts by the pharmaceutical industry for many years. In contrast, researchers within academia, government and non-profit research institutions have previously not been able to access large libraries of these molecules.

## Redressing the balance

Director of the NHGRI, Francis S. Collins, hopes that the centres will help



to redress the balance without impinging on the pharmaceutical industry; 'It should not be viewed as an effort to turn public sector researchers into drug developers. What we are doing is simply giving academic and government researchers a chance to contribute in a much more vigorous way to the earliest stages of the drug development pipeline.'

The network of chemical genomics centres will explore the vast majority of the human genome for which no smallmolecule chemical probes have been identified. Pharmaceutical research tends to concentrate on small molecules that act upon molecular targets with known relevance to human disease, which constitutes a relatively narrow group. To date, of the hundreds of thousands of proteins thought to be encoded by the 25,000 genes within the human genome, less than 500 have been discovered to possess a chemical compound with which they interact. The NIH Chemical Genomics Center plans to substantially build upon this number by screening more than

100,000 small molecules within its first year of operation.

#### Ultra-high throughput screening

To help achieve its goals, the centre has selected a suite of ultra-high throughput target and pathway screening technologies from Kalypsys of San Diego (http://www.kalypsys.com/). The agreement, potentially worth up to US\$30 million over the four-year contract, will deliver a series of technologies, materials and services including an automated robotic system capable of screening in excess of a million compounds per day in a variety of biochemical and cellular assays.

It is hoped that the information generated by the chemical genomics network will identify new targets for therapy and the tools to study them and, as a result, enable these targets to move more rapidly through the drug development pipeline.

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