



# The Computerworld Honors Program

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## Final Copy of Case Study

**LOCATION:**  
*San Ramon, CA, US*

**ORGANIZATION:**  
Accelrys, Inc.

**YEAR:**  
*2011*

**ORGANIZATION URL:**  
<http://www.accelrys.com>

**STATUS:**  
*Laureate*

**PROJECT NAME:**  
Informatics for Neglected Diseases Collaborations

**CATEGORY:**  
*Innovation*

### PROJECT OVERVIEW

Tropical infectious diseases affect millions of individuals, predominantly in the developing world. The low financial viability for the sale of new pharmaceutical products in these poor countries does not offer an incentive to enable the high and risk-associated investments in R&D required for the discovery of new treatments for these diseases. Consequently, while these 'neglected diseases' affect many individuals, the research effort has been minimal for the past several decades. Drugs currently used to treat these diseases are of limited availability and efficacy, are costly, and in many cases are based on old molecules, some of which have severe toxic effects. Furthermore, resistance to these drugs has emerged in several of these neglected diseases. To address the need for better treatment of neglected diseases, several not-for-profit organizations have emerged in the past decade. These organizations are known as public-private partnerships (PPPs), as they share a common model that combines investment and expertise from the public sector and industry. Examples of such PPPs include the Drugs for Neglected Diseases initiative (DNDi) and the Medicines for Malaria Ventures (MMV). The breadth and complexity of these collaborations require informatics solutions that facilitate and support a virtual, global R&D organization and are able to overcome these challenges:

- Data integration from multiple scientific disciplines and contributors.
- The immediate and secure exchange of scientific information among the members of the network.
- An institutional memory that records the collaborative efforts in a central database, thus avoiding unnecessary duplication of effort.
- Scientists involved in the collaborations require access to bioinformatics and cheminformatics software, both of which are traditionally used to perform data analysis and to help design future experiments in silico.
- To permit secure remote access by any member of the partnership and to manage the diversity of environments, the software must be offered via a web-based front end and must be able to operate with all data captured by the network.

Several vendors collaborated to solve this problem:

- SCYNEXIS Inc. provides a SaaS platform for drug discovery -- the Hit Explorer Operating System (HEOS). HEOS has hosted data for several major PPPs, including



the DNDi and the MMV. • Accelrys Inc. provides free licenses to its scientific informatics platform, Pipeline Pilot and Accord Cheminformatics Software. The workflow technology embodied in Pipeline Pilot lends itself to the facile execution of several cheminformatics tasks, including, but not limited to, substructure searching, clustering, construction of Bayesian models, combinatorial library enumeration and the numerical characterization of compounds for further statistical analyses. • Tibco Software Inc.'s Spotfire Analytics provides a platform for visual analysis that allows an end-user to interact with data in real-time. This is particularly useful for interpreting relationships in multidimensional data. Interactive filters further aid the data analysis workflow; end-users can quickly identify compounds of particular interest within a data set. Pipeline Pilot and Spotfire are integrated within HEOS, affording end-users access to state-of-the-art data analysis, visualization and mining tools.

## **SOCIETAL BENEFITS**

Allows scientists worldwide to collaborate in development of new medicines for underfunded but important global diseases (Appendix 2); creates economic opportunities for underdeveloped economies to have their scientific IP made known through a global collaboration. • Creates momentum for solving an important problem at a faster pace, lower cost.

## **PREVIOUS PROJECT UPDATED/EXPANDED?**

The Program was greatly enhanced in 2008 with the addition of Accelrys Accord Chemical Registration and Pipeline Pilot workflow. The newer state-of-the-art implementation has shown a dramatic increase in Data (2007 – 200K biological results, 2010 - 1.3 Million biological results) and Users (2007 – 50 users, 2010 – 450 users). The new enhancements have promoted more use and more groups willing to use the software.

## **PROJECT IMPLEMENTATION COMPLETE? Yes**

## **PROJECT BENEFIT EXAMPLE**

The Drugs for Neglected Diseases initiative (DNDi) human African trypanosomiasis (HAT) program has also benefitted from the project. Also known as sleeping sickness, HAT is one of the most devastating diseases in sub-Saharan Africa. Initiated in 2006, this program involved a high-throughput screen of approximately 110,000 compounds for their ability to kill *Trypanosoma brucei*, the causative parasite of HAT, and has progressed through hit-to-lead and lead optimization phases. A preclinical candidate, SCYX-7158 (Anacor Pharmaceuticals Inc/Drugs for Neglected Diseases initiative/Pace University/SCYNEXIS Inc.) has now been selected. As this project evolved, geographically distributed partners from industry, government and academia have been engaged to contribute experimental capabilities and expertise. <http://www.dndi.org/> "HEOS® is a fully secured, easily accessible, user-friendly and robust solution for the management of screening data generated through DNDi activities. We are entirely satisfied by this web-based tool along with the top quality support that has been provided by SCYNEXIS." - Jean-Robert Loset, DNDi The Medicines for Malaria Venture (MMV) is a PPP focused on the discovery, development and delivery of new small molecule antimalarials for the world's poor. MMV began to use HEOS® in 2009. It has subsequently become a database comprising over 40,000 antimalarial actives (and >400,000 inactives from screening campaigns) from global projects and the literature. This database, along with the built-in features, has proved invaluable for teams to store, share and securely communicate data. Furthermore, the protocols have enabled MMV to implement analyses and studies that would otherwise be inaccessible. MMV has over 25 projects in Discovery research with a portfolio that is

progressing and maturing – and this software technology platform is contributing to this success. <http://www.mmv.org/> “The last two years have seen a hundred-fold increase in the amount of data on active antimalarial compounds. This is a tremendous opportunity, but also a tremendous challenge and working with HEOS has enabled us to simplify our management of this data and provide more clarity for our partners.” Tim Wells, CSO MMV.

## **IS THIS PROJECT AN INNOVATION, BEST PRACTICE?** Yes

### **ADDITIONAL PROJECT INFORMATION**

The PPPs have effectively raised money from different funding sources, including governments and charitable organizations such as The Bill and Melinda Gates Foundation and the Wellcome Trust. PPPs use these funds to conduct virtual drug discovery and development programs for various neglected diseases and have established a global network of multidisciplinary partners, including large pharmaceutical companies, biotechnology companies, not-for-profit organizations, CROs and academic institutions. As well as repositioning goals, such as expanding the applications of existing drugs, the PPPs have now evolved to address the entire cycle of drug discovery and development in order to sustain the delivery of innovative technologies. The PPPs coordinate multiple projects at every stage, managing a portfolio in a similar manner to large pharmaceutical and biotechnology companies. Examples of such portfolios, managed by the DNDi and MMV respectively, are available at <http://www.dndi.org/index.php/portfolio.html?ids=2> and <http://www.mmv.org/research-development/science-portfolio>. The visibility of the PPPs has improved the level of interest from biotechnology and large pharmaceutical companies in the area of neglected diseases by increasing awareness of both social responsibility within corporations and the strong need for the expertise of these companies in drug discovery and development. By coupling the historical involvement of academic groups in research for neglected diseases with industry partners, it is now common for each PPP to manage collaborations with 30-40 different organizations worldwide. In fact, one of the PPPs is working with over 140 organizations and around 70-80 partners. Conclusion Neglected diseases collaborations consist of many different organizations working together to find cures for the diseases of the world's underprivileged. The ability of these collaborations to combine public and private expertise and investment has contributed to several success stories. Because of the geographical distribution and virtual nature of these collaborations, the support of customized informatics solutions can have a significant impact. The potential of these solutions has led to the early adoption and evolution of the SaaS drug-discovery and development web-based platforms by this community. Because of these platforms, several major PPPs now control data management for various collaborations. As these platforms grow and are further interfaced with powerful data-analysis tools, scientists will have a greater ability to convert data into knowledge. These SaaS platforms have evolved to provide solutions similar to the ones developed and used within the firewall of large pharmaceutical and biotechnology companies. The combination of secure and scientific services offered by the SaaS platform for experimental data management, data analysis, remote collaborations and advanced communication can significantly aid virtual team members in the building and leveraging of knowledge shared among the organizations, and thus increase the chances of finding new treatments against diseases affecting the most neglected.



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