

Discovery Portal – a novel tool to increase productivity, efficiency and transparency across R&D organizations

J. Tomczak

Accelrys, Cambridge, United Kingdom

Data integration and data standardization is a major challenge and an important area of investment for most pharmaceutical companies. There are a number of commercial, in-house and even open source tools and solutions for bringing together and analyzing chemical and biological data. However, the data are usually disconnected from the processes that generate the data and internal drug discovery workflows. Furthermore, R&D scientists have to spend significant amount of time on learning and using generic tools for data extraction, mining and reporting and adapting them to their daily practices. Recognizing this bottleneck, a higher-level decision support and tracking tool can be designed on top of an existing, integrated infrastructure that fully implements internal discovery processes. The resulting Discovery Portal would be a Web-based resource where scientists and managers could not only share, mine and visualize all of their data and knowledge about drug discovery programs, but also define the programs in terms of experiments to be performed, which in turn could be requested and tracked on-line. The system developed by Accelrys combines Accelrys' products (in particular Pipeline Pilot), modern Web-based enterprise technologies and open source frameworks. The technology choice makes the system highly expandable and allows adding new capabilities to a running system. The portal demonstrates also that limitations of Web-based solutions are not as restrictive as they might seem. (Concepts will be illustrated with specific implementation examples).