accelrys®

Discovery Studio®

Product Brief

Configurable science at its best—from target identification to lead optimization

Discovery Studio offers unparalleled capabilities for customizing the research solutions to best suit your needs.

- Choose from a wealth of validated Discovery Studio computational chemistry and biology tools.
- Leverage an open and scalable platform to automate processes, create custom workflows, and integrate data types, databases, and third-party or in-house tools.
- Boost both individual and team productivity with flexible deployment options, workflow sharing functionality, and reporting tools.

With a research solution customized to your needs, the possibilities are endless. Study your systems more completely and thoroughly. Work with your team more efficiently. Make your decisions more confidently. Drive your research further.

Trusted Science

By offering a wealth of tools within a graphical interface (Table 1), Discovery Studio makes it easier than ever to examine the properties of large and small molecules, study systems, identify leads, and optimize candidates. Moreover, you can have confidence knowing that Discovery Studio tools are built on validated, published scientific algorithms. The science at Discovery Studio's core has undergone years of continuous innovation based on the input of customers, internal scientists, and renowned scientific advisors. With citations in over hundreds of research publications, Discovery Studio is a trusted resource for many of the industry's top research teams.

Trusted Science within Discovery Studio (Table 1)

- 2D and 3D visualization
- 2D and 3D molecular descriptors
- Quantum mechanics/molecular mechanics
- SAR analysis, 2D and 3D QSAR
- Bayesian statistics, neural networks, recursive partitioning, GFA, etc.
- Library analysis
- Library design
- Predictive ADME and toxicology (TOPKAT®)
- Conformation generation and analysis
- Structure-based and structure-guided design, docking, scoring
- Virtual screening and compound ranking/scoring
- Receptor-ligand interactions analysis
- Fragment-based design
- *de novo* design (LUDI)
- Pharmacophore generation (Catalyst®)
- Scaffold hopping
- 3D database screening
- Simulations, molecular mechanics/dynamics (CHARMm®)
- Explicit/implicit solvation models
- Transmembrane protein modeling
- Homology modeling
- Antibody modeling
- Electrostatics calculations, protein ionization and pK prediction
- Protein modeling (MODELER®) and analysis, protein engineering
- Protein-protein docking and refinement
- Sequence analysis, sequence alignment, phylogenetic analysis
- X-Ray (CNX), structure refinement and analysis

Powerful Platform

Discovery Studio is part of the open and scalable Accelrys Scientific Informatics Platform. The features of this powerful platform (Figure 1, Table 2) will impact your research on every level, allowing you to:

- make better decisions by integrating, processing, and simultaneously considering diverse data types, from protein sequences and structures to molecular properties and experimental data
- streamline your work environment and optimize resource utilization by integrating all the tools you need into the platform, from in-house code, to third-party software, to public or internal databases
- process data efficiently by automating tasks and leveraging parallel computing
- ensure best practices are enforced with algorithm customization and workflow sharing (See below)

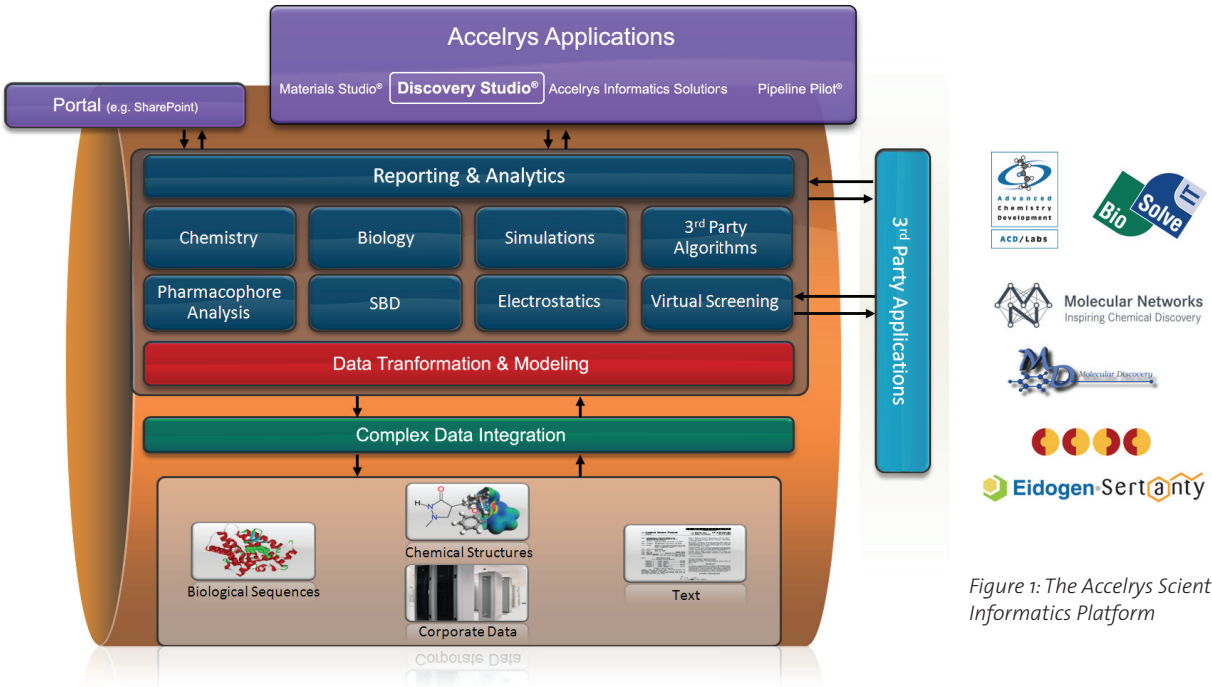

Figure 1: The Accelrys Scientific Informatics Platform

Benefits of the Accelrys Scientific Informatics Platform (Table 2)

- Algorithm and protocol customization
- Automation of tasks (via Perl scripting)
- Data integration (protein sequence, structures, molecular properties, experimental data, etc.)
- Data model manipulation (via Perl scripting)
- Database access (e.g., corporate cheminformatics databases with chemical and biological data for modeling)
- In-house/proprietary code integration
- Parallel computing (grid and cluster-computing and multi-core technology for quickly processing large tasks)
- Third-party software integration
- Web-resource integration (e.g., PDB, PubChem)
- Workflow creation and sharing (via componentized science and simple graphical, drag-and-drop programming)

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Customization and Collaboration

Differences in user proficiencies and work styles often derail projects, prevent goals from being reached or inhibit resources from being utilized. Discovery Studio's customization and collaboration features (Table 3) not only improve the individual user experience, they also enhance communication and teamwork. Because Discovery Studio utilizes the Pipeline Pilot® Enterprise Server, your team members can more easily share their expertise, collaborate on results, and work towards a common goal by developing common-purpose workflows (figure 2).

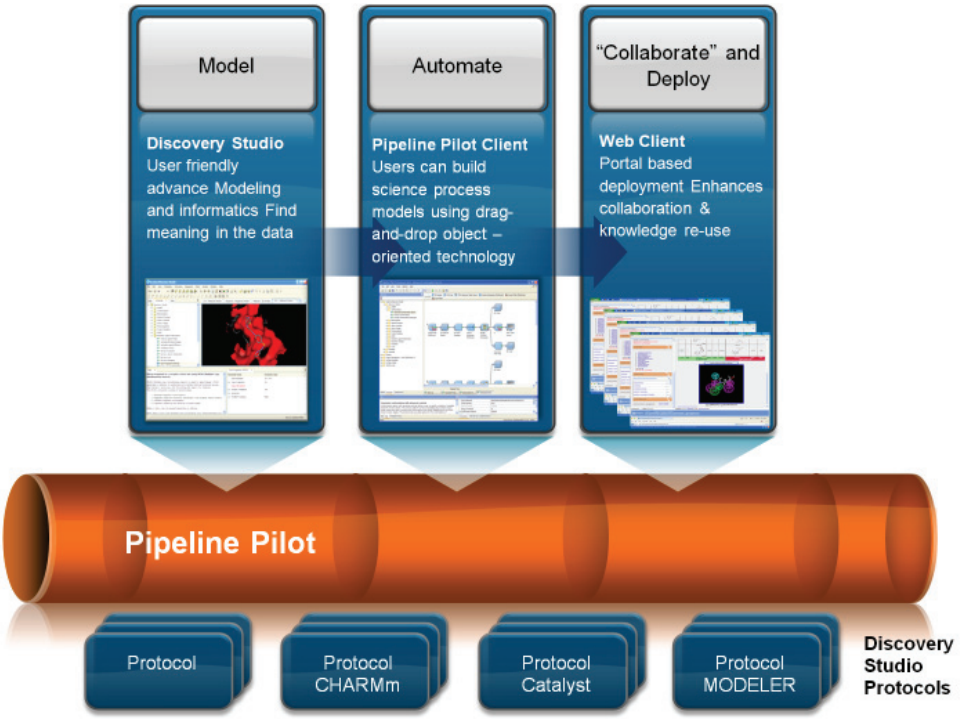

Figure 2: Discovery Studio utilizes the Pipeline Pilot Enterprise Server, making it easy for users within various roles to model, automate, decide, and collaborate.

Customization and Collaboration Features of Discovery Studio (Table 3)

- Access/interface options (via graphical Discovery Studio client, scripting and protocol sharing environment, command-line)
- Data viewing/customization options (view 3D data simultaneously with data tables and scripting/protocol controls)
- Deployment options (standalone solution for individuals or part of enterprise-level, client-server installation)
- Reporting and result-sharing tools
- Task-based workflow sharing (walk other users through complex, task-based procedures)
- User-community (online collaboration and script/protocol sharing, user group meetings)
- Workflow creation (via componentized science and simple graphical, drag-and-drop programming)
- Workflow sharing (via internal web pages, Microsoft® SharePoint®)

No matter what your role on the team, you'll see the benefits of Discovery Studio (Table 4, next page). For example, computational experts can combine data and scientific algorithms to create meaningful models and visualizations, which can then be shared with the experimentalists, who will use the information to design meaningful experiments that move projects toward their goals.

User-Specific Benefits of Discovery Studio (Table 4)	
Biologists	• Illustrate relationships between sequence and structural data • Communicate advanced biological data with colleagues in different disciplines
Computational chemists	• Apply the validated Accelrys science you've trusted for years, and augment with new algorithms or workflows • Publish your results and methods to a broad base of users • Create customized workflows to enable access to common procedures (Figure 3)
Medicinal chemists	• Visualize the impact of structural information on your projects • Easily organize comprehensive small molecule libraries using a synchronized 2D/3D working environment (Figure 4, next page) • Understand complex relationships between biological and chemical experimental data
IT members	• Reduce the time needed to manage the installation, licensing, and update requirements of different vendors by using a consolidated platform • Simplify user training with straightforward, customizable interfaces
Project / program managers	• Save time by implementing consistent workflows and procedures • Give team members the 'big picture' and project status updates more easily • Gain consensus on projects through more 'seeing is believing' and less 'faith-based' methods

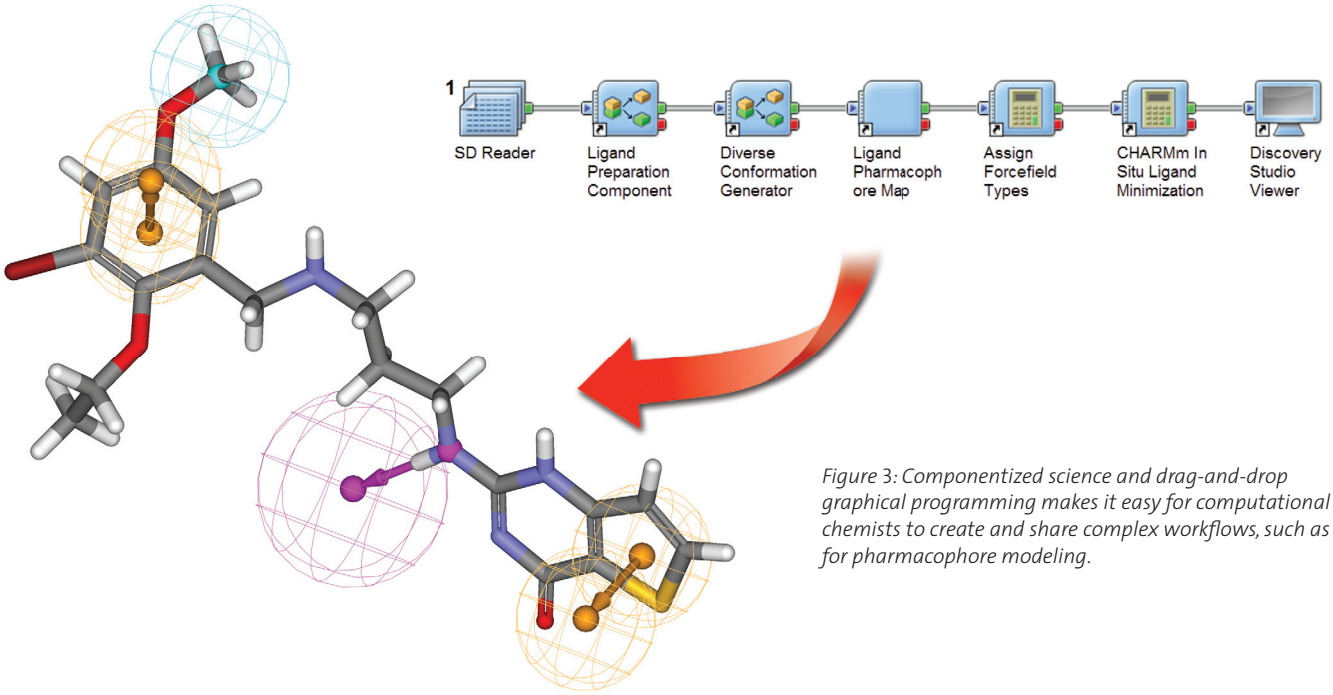

Figure 3: Componentized science and drag-and-drop graphical programming makes it easy for computational chemists to create and share complex workflows, such as for pharmacophore modeling.

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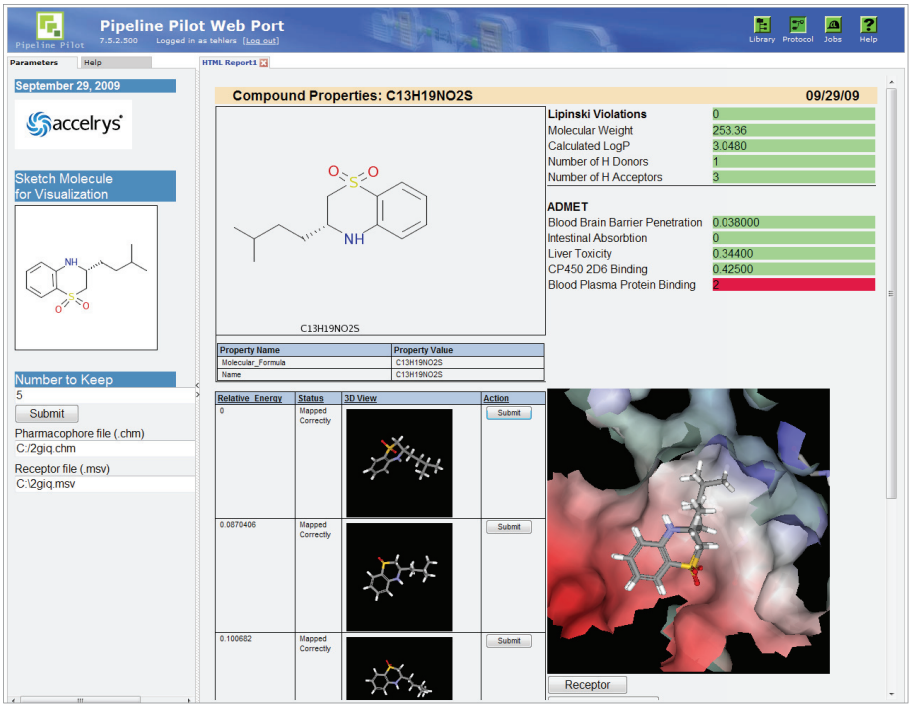

Figure 4: Access to complex science from a user-friendly, web-based interface makes it easy for medicinal chemists to visualize and explore the complex relationship between biological and chemical experimental data using both 2D and 3D data.

More than Software

At Accelrys, we know that you may need more than a one-size-fits-all solution to succeed. In addition to the benefits offered by Discovery Studio and the Accelrys Scientific Informatics Platform, we'll also help you succeed with:

- Outstanding customer support – Accelrys customers report a 98% satisfaction rate with the Accelrys support team.
- Commitment to innovation – With over 100 PhDs in the field, working daily with researchers in industry and academia, Accelrys is committed to delivering cutting-edge technology.
- Scientific consulting – Accelrys has dozens of PhDs who have expertise in implementing scientific solutions for drug design and are available for short-term engagements to help you in whatever way you may require, whether it be performing modeling experiments or creating a tailored solution.

Learn More

Fill out our online contact form to have an Accelrys representative contact you to discuss how Discovery Studio and the Accelrys Scientific Informatics Platform can help boost your research.

http://accelrys.com/company/contact/

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