Workflow Customization with the DS Developer Client

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July 24th, 2008
• June 12, 2008 - Advances in Protein Modeling and Protein-Protein Interactions in Discovery Studio
• June 19, 2008 - Physics-Based Protein Ionization and pK Estimation
• June 26, 2008 - Towards Increased Accuracy in Computational Drug Discovery with QM/MM
• July 10, 2008 - Pharmacophore Guided Fragment-Based Drug Design
• July 17, 2008 - Advances in Pharmacophore Modeling and Parallel Screening
• July 24, 2008 - Workflow Customization with DS Developer Client
• July 31, 2008 - Tips and Tricks in using Discovery Studio

• Recordings Available:
  • http://accelrys.com/events/webinars/discovery-studio-21/recordings.html
• BUSINESS ISSUE → How can we address common hurdles researchers face everyday?
  – Automating repetitive tasks
  – Integration with corporate data repositories or 3rd party applications
  – Develop complete workflow solutions to meet the demands of your research endeavors

• SOLUTION → Discovery Studio (DS) Developer Client allows you to easily customize an existing protocol or to create a new protocol and publish it within the Discovery Studio interface for interactive modeling

Customizing and Automating Discovery Studio Workflows

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What is the DS Developer Client?

• The DS Developer Client will give you an unprecedented ability to customize and automate

• The DS Developer Client consists of:
  – Scaled-down version of the Pipeline Pilot Professional Client with the necessary technology (component collections) to facilitate such customization of Discovery Studio science

• DS Developer Client is offered as a 1-year promotion of a limited version of Pipeline Pilot Professional Client to all Discovery Studio 2.1 customers at no additional charge
  – The promotion expires on April 30, 2009 (or the maintenance end date, whichever comes first)

• What happens at the end of the one year DS Developer Client promotion period?
  – At the end of the year
    • We have several deployment strategies we are investigating for the future
    • You will not lose the functionality that you have in this promotion
• Architecture of Discovery Studio 2.1

• Protocols, Pipelines, and Components

• Customization of Protocols for Discovery Studio

• Integration

• Demonstration

• Getting Started
Customizing and Automating Discovery Studio Workflows

Discovery Studio 2.1 is built on

- Pipeline Pilot 6.1.6
- Scitegic Enterprise Server (SES) 7.0.1

Protocol
- CHARMM
- MODELER
- BLAST
- LigandFit
- Ludi
User Clients

Web Port (web access)
DS Dev Client
ISV Client (e.g., Spotfire)
PP Pro Client
Discovery Studio Client
Accord Clients

Client Integration Layer

Pipeline Pilot Platform

Tool Integration Layer

Chemistry
Biology
Materials
Accord

Data Access Layer

Accord
IDBS
Oracle
ISIS

Isentris

Tools

Reporting
Statistics
ISV

Databases
Accelrys Discovery Studio Application

Create and modify protocols and components

DS Dev Client

ISV Client (e.g., Spotfire)

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Databases

Use DS protocols in PP

Use new protocols and components in DS

Create and modify protocols and components
• Discovery Studio offers a high-end 3D modeling environment to Pipeline Pilot protocols

• This client supports tables, 3D views, scripting, etc.

• To support submission to a protocol of
  – Proteins
  – Nucleic Acids
  – Small Molecules
  – Pharmacophores
  – Sequences Alignments
  – Other “datatypes”

• DS client can also display HTML report
• Components
  – Are the building blocks used to create workflows
  – Each component performs a task like reading, writing or manipulating data
  – Can have one input and up to two output ports
  – Organized in folders by application area (sequence alignment, simulations, etc)
• **Pipelines**

  - A series of components connected through pipes through which data flows
  
  - Each component acts on the data and passes it on to subsequent components
• **Protocols**

- Consist of one or multiple pipelines that are run sequentially
- Are executed left to right, top to bottom
- Pipeline 2 will not start processing data until pipeline 1 has completely finished processing all the records
Solutions Powered by 3D Modeling Components

- Structure Based Drug Design
- Pharmacophore Modeling
- Virtual Screening
- Protein Modeling
- Sequence Analysis
- Simulations
- QSAR
- Library Design
- Antibody Modeling
- ADME/Tox

3D Modeling Components in PP

- Readers
- Writers
- Manipulators
- Analysis Components
- 3D Model Generators

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Additional Collections in the DS Developer Client

- The Generic, Chemistry, and Integration Collections are available through the DS Developer Client

- Other collections are “embedded” in the Discovery Studio server
  - Sequence Analysis
  - Data Modeling
  - Advanced Data Modeling
  - Reporting

  - Additional licensing required for access in your DS Developer Client
Special DS Parameter Types: DS Readers

- Specific readers are provided with DS collection

- Source parameter are of type “URL” when used in DS Dev Client (PP Client) Web Port

- When used in DS client they provide advanced interface for selection

- Tip: View the HELP for each reader (click F1)
Pharmacophore Modeling Workflow Example

- Generate a hypothesis from structure and activity data
- Search database for compounds that match
- Design new molecules to fit your hypothesis
- Synthesize and assay the most promising candidates

Add new molecules. As you increase the range of activities and diversity of structures, new information is gained
• DS protocols are identical to any other PP protocol

• Promoting Parameters
  – “Grant” access to user-defined parameters
  • only promoted parameters will be accessible through DS client

• Documentation
  – Help section of protocol and parameters are displayed in DS client
• Standard results of Pipeline Pilot protocols are:
  – Text files
  – HTML reports
  – Molecular files in various format
  – Sequence and alignment files

• Simply write these files in \$(RunDirectory) to make them accessible to users
Integration of a 3rd Party Application

- DS has published and validated science, but DS Dev Client allows you to integrate alternative methods into Discovery Studio
  - Prepare a PP protocol to call the 3rd party program
  - Use PP components to assist in input, output, and analysis
  - Apply DS specific components to the new protocol
  - Use the new protocol in the DS client
  - Example: integrate CORINA command line into a DS-ready protocol
PERL scripting API

Develop client-side scripts

Embed in Pipeline Pilot protocols through Integration comp collection available in DS Dev Client

```perl
#!/usr/bin/perl
#
# HelloMolecule.pl - shows how to open icrn from a URL and report molecular information
use strict;
use MdmDiscoveryScript;

my $document = DiscoveryScript::OpenFromUrl("http://www.rcsb.org/pdb/files/icrn.pdb");

my $firstMolecule = $document->Molecules->[0];
my $atomCount = $firstMolecule->AtomCount;
my $moleculeName = $firstMolecule->Label;

print "There are $atomCount atoms in $moleculeName";
```
• Create Simple Protocol, Promote Parameters, Run in DS Client

• Appending a Final Minimization Stage to the Standard Dynamics Cascade Protocol

• Integration of a 3rd Party Application into Discovery Studio

• Calculate 3D Properties From Low Energy Conformers in a 3D database

• Recharge Ligand (QM/MM) Component Followed by Docking

• Building Homology Models and Optimization Loops

• Processing Ligand Data with Pharmacophore Filtering and Minimization
How Do I Get Started?

• DS Developer Client is available by sending an email to support@accelrys.com

• Installation Overview
  – DS Developer Client is available only on Windows
    • Discovery Studio 2.1 (Server Components) can be on Linux
  – Instructions will guide you through the simple steps to install the DS Developer Client

• Is there a good way to jump start using the DS Developer Client?
  – Online Tutorials (coming very soon!)
  – Discovery Studio and Pipeline Pilot Training → http://accelrys.com/services/training/
  – Review “Examples” in the DS Developer Client
  – Contact Customer Support
    • Our expert scientists can quickly turnaround customized protocols or scripts for you
    • Enterprise-level customization available through Professional Services
  – Download this Recording
  – Last by certainly not least..
• Customized Workflows and Protocols available now

• Accelrys Community Site ➔ www.accelrys.org

• Nearly 100 customized DS solutions for your unique research needs
• Customize (i.e. promote or de-promote) parameters of existing DS protocols/components

• Add or remove available components from existing DS protocols/components

• Create a new component and add to an existing DS protocol

• Increase automation of DS Protocols
  – automate DS protocol to run over all files in a specific folder

• Easily connect to an external relational database (ORACLE, mySQL, etc)

• Integrate third-party algorithms (e.g., CORINA, proprietary codes for descriptor calculations, etc.)
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• Accelrys Customer Support → support@accelrys.com

• Accelrys Contact Form → http://accelrys.com/company/contact/

• Please visit us at an upcoming events (http://accelrys.com/events/conferences/)
  – Drug Discovery Technologies (DDT), Boston MA, Aug 4-7, Booth 512
  – National Meeting of the American Chemical Society (ACS), Philadelphia PA, Aug 17-21, Booth 211
  – EFMC -ISMC 2008 International Symposium on Medicinal Chemistry, Vienna Austria, Aug 31-Sep 4, Booth 29

• Next Webinar in the “New Science and Customized Workflows for Drug Discovery Research” Series
  – Tips and Tricks in Using Discovery Studio
    – Al Maynard, Manager, R/D, Simulations and Structure Based Design
    – Next Thursday, July 31st, 2008
    – Register online → http://accelrys.com/events/webinars/discovery-studio-21/