

Pipelining ChemAxon

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Pipeline Pilot and ChemAxon

- Pipeline Pilot
 - Not just chemistry
 - Biology, NGS, Analytical Instruments, Proteomics, Text, Imaging, Reporting
 - Enterprise solution
 - Scalable
 - Secure
 - Web deployment
 - A platform for application development
 - Accelrys Chemical, and Biological Registration
 - Market leader from a financially secure company

Show MDDR Activities for Sketched Molecule

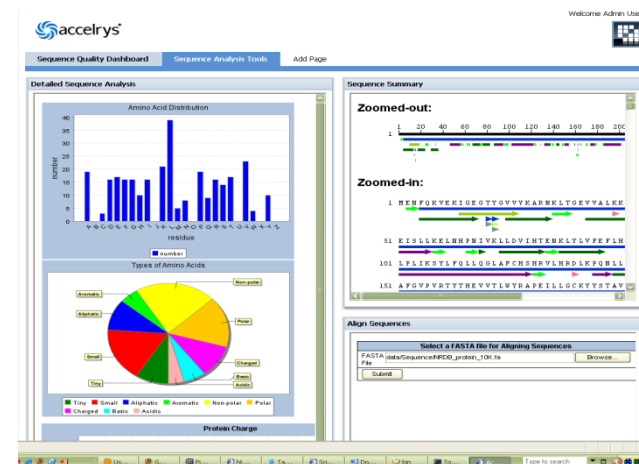
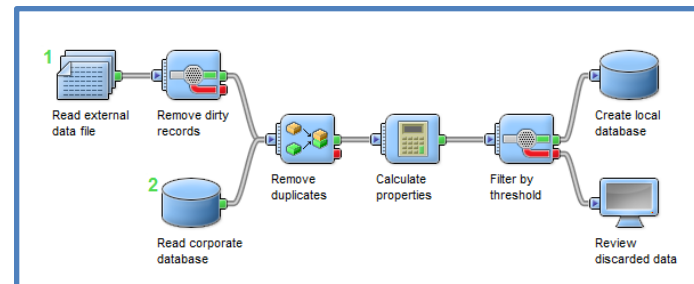
Sketch or paste a molecule in iDraw. When changes are made to the molecule, the resulting changes in MDDR activities are calculated and shown in the table.

The screenshot shows the Accelrys iDraw software interface. In the center, a chemical structure is displayed, which is a complex molecule with a benzene ring, a carboxylic acid group, and a piperidine ring. The structure is labeled 'sketchpt'. Below the structure, there is a table of MDDR activities. The table has three columns: MDDR_Activity, MDDR_ActivityPredicted, and MDDR_ActivityScore. The table lists various MDDR activities and their corresponding predicted values and scores. A 'Selected Activities' list is visible on the left, and a 'Minimum Score' field is on the right. A 'Calculate MDDR Activities' button is also present.

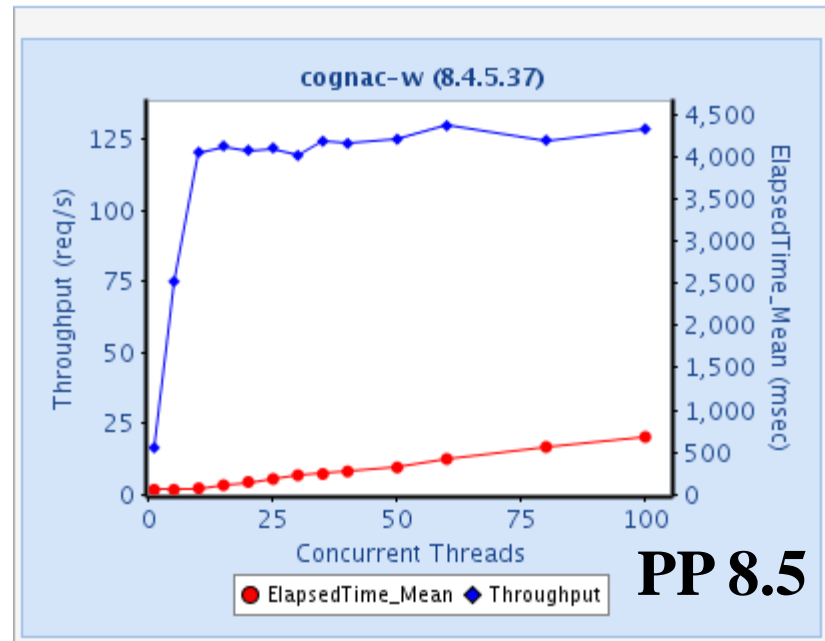
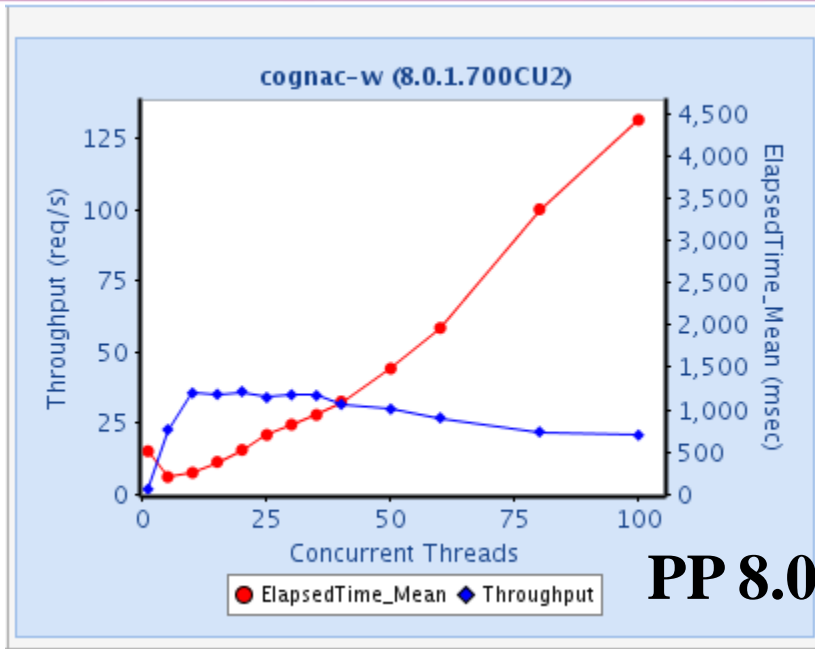
MDDR_Activity	MDDR_ActivityPredicted	MDDR_ActivityScore
MDDR_ACE_inhibitor	1	139.38
MDDR_neutral_endopeptidase_inhibitor	1	43.768
MDDR_Cathepsin_inhibitor	1	41.622
MDDR_protease_inhibitor	1	36.332
MDDR_inhibitor_of_proteinase_activator_inhibitor	1	31.753
MDDR_Cathepsin_S_inhibitor	1	30.148
MDDR_inhibitor_of_endopeptidase_inhibitor	1	30.056
MDDR_Endothelin_Formation_inhibitor	1	29.087
MDDR_Diacylglycerol_Agent	1	27.365
MDDR_Antipain	1	23.488
MDDR_Trypsin_inhibitor	1	22.852
MDDR_Vasopressin_Agent	1	21.847
MDDR_Iminostimulant	1	20.094
MDDR_mu_Agonist	1	17.208
MDDR_marijuana_Coincubant	1	16.034
MDDR_muscle_Relaxing_Agent	1	16.408
MDDR_breastkinin_Antagonist	1	15.097
MDDR_hypocretin_Receptor	1	13.871
MDDR_kd_inhibitor	1	11.828
MDDR_Calcium_Regulator	1	11.332
MDDR_Thrombolytic	1	10.747
MDDR_nongenotoxic	1	10.327
MDDR_nuclei_Promoter	1	4.9719
MDDR_inhibitor_of_cancer	1	1.2023

- ChemAxon components
 - Extend Pipeline Pilot's capabilities
 - More choice in chemistry

- Professional client
 - Research environment
 - Rapid application environment
 - Deployments: 1-500+ seats per customer
- Web Port/custom clients/SharePoint
 - End-user interface for bench scientists, managers
 - Deployment range: 10-1000+ seats per customer



Pipeline Pilot Performance and Scalability



- **Latency** and **throughput** as function of number of concurrent users
 - Latency flat up to the machine capacity and then grows linearly and slowly
 - Once machine capacity is reached, throughput remains high and constant even for large numbers of users

- Accelrys Direct Cartridge Collection
 - Manage and search
- Database Access Components
 - DiscoveryGate, PubChem, ChemSpider, ChemExper, eMolecules
- Matched Molecular Pairs protocols
- Activity models
 - Accelrys MDDR, Accelrys CMC, and Accelrys Metabolite

Conclusions

- Compatible architectures
- Pipeline Pilot good prototyping environment for ChemAxon's advanced science
- Multiple deployment options

The image displays three overlapping screenshots of the Pipeline Pilot software interface:

- Top Screenshot:** Pipeline Pilot Webport interface. It shows a "Query by Form Search of Sample Drugs" window. On the left, there are sections for "Select the database fields to display" (listing Name, CAS_m, RSC), "Select the calculated properties to search" (listing Molecular_Weight, ALogP, Num_H_Acceptors), and "Which chemical editor would you like to use?" (listing ISISDraw, ChemDraw, Bulk Form). On the right, a chemical structure of Berzene, 1,2-dimethoxy-4-nitro-(BC9C) is shown next to a table of its properties: Name, CAS_m (709-09-1), RSC (27974), Molecular_Weight (183.17), ALogP (1.69), and Num_H_Acceptors (4). Below the table, it indicates "Displaying record 1 of 578" and includes buttons for "Next", "Previous", "Jump to #", and "New Query".
- Bottom-Left Screenshot:** A 3D scatter plot window showing a large number of molecules (represented as small green and blue sticks) plotted in a 3D space. The axes are labeled with numerical values. Below the plot, there is a chemical structure and text indicating "Identifies compounds which meet 'Rule of 5'".
- Bottom-Right Screenshot:** A "Find Duplicate Molecules" dialog box. It contains fields for "Server" (http://localhost:3030), "User Name" (jcd@accelrys.com), "Password" (nc_jaswood), "New Library" (data/E_Samples/137/Brown/dependencies of), "Existing Library" (data/E_Samples/ACC/Dependencies of), "Fragment Type" (RingAssemblies), "Max Fragment Size" (10), and "Output File" (C:\testing.html). There are "Connect To Server" and "Run Protocol" buttons.

- ChemAxon
 - Szilárd Dóránt
- Accelrys
 - Moises Hassan