

Pipelining ChemAxon

Moises Hassan, Ton van Daelen, Rob Brown, [Keith Taylor](#)

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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

- ChemAxon components

- Extend Pipeline Pilot's capabilities

- More choice in chemistry

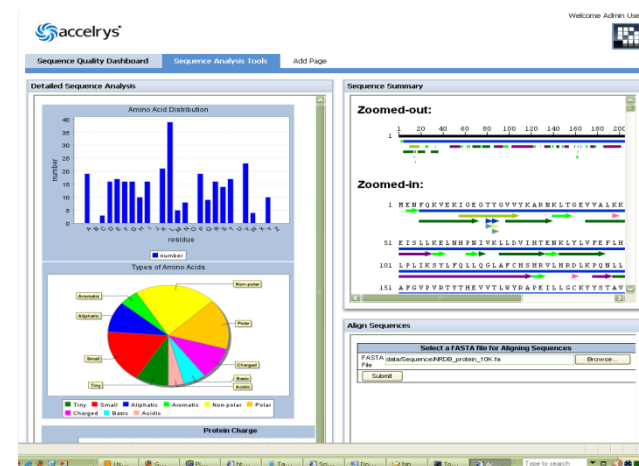
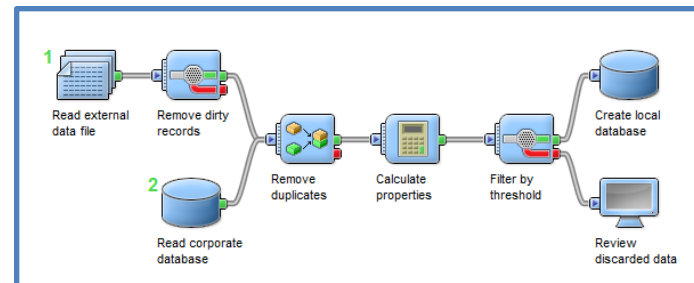
Show MDDR Activities for Sketched Molecule

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.

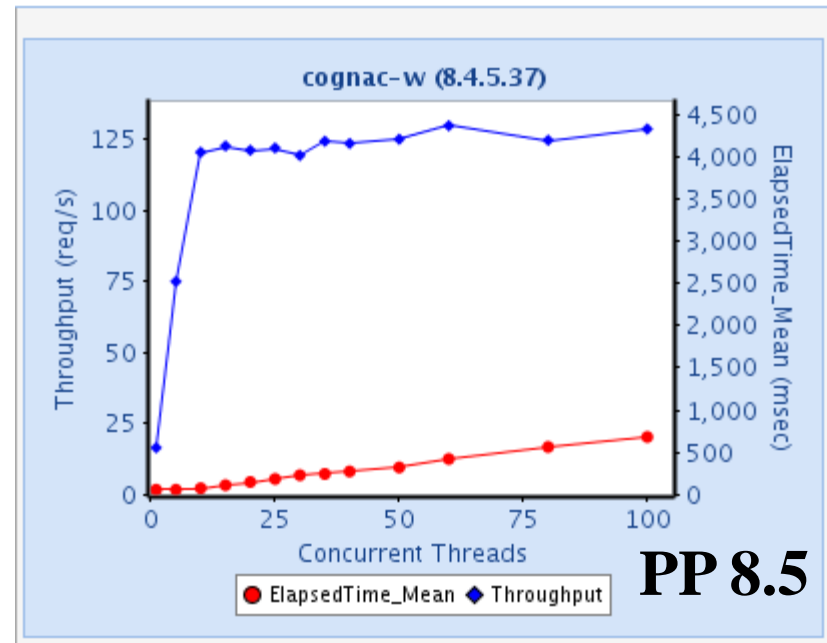
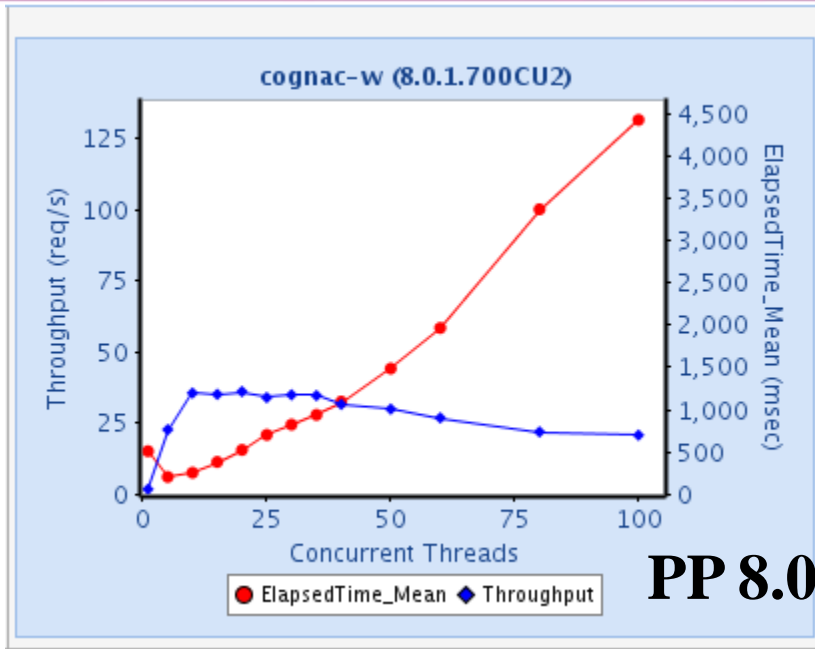
The screenshot displays the Accelrys iDraw software interface. In the center, a chemical structure is shown with a benzene ring, a carboxylic acid group, and a secondary amine. Below the structure, a table lists various MDDR activities and their predicted scores. The table has three columns: MDDR_Activity, MDDR_ActivityPredicted, and MDDR_ActivityScore. The activities listed include MDDR_ACE_inhibitor, MDDR_neutral_endonuclease_inhibitor, MDDR_Cdk2_inhibitor, MDDR_protease_inhibitor, MDDR_inhibitor_of_proteinase_activator, MDDR_Cathepsin_B_inhibitor, MDDR_inhibitor_of_endonuclease_inhibitor, MDDR_Endothelin_Formation_inhibitor, MDDR_Diacylglycerol_Agent, MDDR_Antiopsin, MDDR_Tyrosine_inhibitor, MDDR_Vasopressin_Agent, MDDR_Primidomest, MDDR_mu_Agonist, MDDR_Paraldehyde, MDDR_Paraldehyde_Agent, MDDR_Bradycinin_Antagonist, MDDR_hydroxyamino_Acetyl, MDDR_A_2_inhibitor, MDDR_Calcium_Regulator, MDDR_Thrombolytic, MDDR_antiangiogenic, MDDR_Nuclei_Promoter, and MDDR_Thapsigargin_for_Cancer. The scores range from 1 to 43,768.

MDDR_Activity	MDDR_ActivityPredicted	MDDR_ActivityScore
MDDR_ACE_inhibitor	1	139.38
MDDR_neutral_endonuclease_inhibitor	1	43,768
MDDR_Cdk2_inhibitor	1	41,622
MDDR_protease_inhibitor	1	36,332
MDDR_inhibitor_of_proteinase_activator	1	31,753
MDDR_Cathepsin_B_inhibitor	1	30,148
MDDR_inhibitor_of_endonuclease_inhibitor	1	30,056
MDDR_Endothelin_Formation_inhibitor	1	29,087
MDDR_Diacylglycerol_Agent	1	27,365
MDDR_Antiopsin	1	23,488
MDDR_Tyrosine_inhibitor	1	22,852
MDDR_Vasopressin_Agent	1	21,847
MDDR_Primidomest	1	20,094
MDDR_mu_Agonist	1	17,208
MDDR_Paraldehyde	1	16,034
MDDR_Paraldehyde_Agent	1	16,408
MDDR_Bradycinin_Antagonist	1	15,097
MDDR_hydroxyamino_Acetyl	1	13,871
MDDR_A_2_inhibitor	1	11,828
MDDR_Calcium_Regulator	1	11,332
MDDR_Thrombolytic	1	10,747
MDDR_antiangiogenic	1	10,327
MDDR_Nuclei_Promoter	1	4,9719
MDDR_Thapsigargin_for_Cancer	1	1,2023

- 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 screenshot displays the Pipeline Pilot Webport interface. The top window shows a 'Query by Form Search of Sample Drugs' with a chemical structure of Berzene, 1,2-dimethoxy-4-nitro-(BC9C) and a table of properties:

Name	Berzene, 1,2-dimethoxy-4-nitro-(BC9C)
cas_m	709-09-1
RSC	27974
Molecular_Weight	183.17
ALogP	1.69
Num_H_Acceptors	4

The bottom window shows a 3D scatter plot of molecule data with axes labeled 'Assay 1 vs. Assay 1000'. A 'Find Duplicate Molecules' dialog box is open, showing search criteria and a 'Run Protocol' button.

Acknowledgements



- ChemAxon
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 - Moises Hassan