



A Software for Modeling, Analysis, and Information Management of
Biochemical Pathways

... developed by  **InVetics**



SBML Workshop 2005-10-23



Fraunhofer **CHALMERS**
Research Centre
Industrial Mathematics

Mats Jirstrand, PhD
Scientific Director Systems Biology

Brief Background

-  **PATHWAY LAB** is a tool for *in silico* modeling, documentation, simulation, and computational analyses of biochemical processes
- Developed in close collaboration with end users in the Pharmaceutical industry
- Background: Software development and services for modeling and simulation of large complex engineering systems (members of Modelica design group) 

Mats Jirstrand



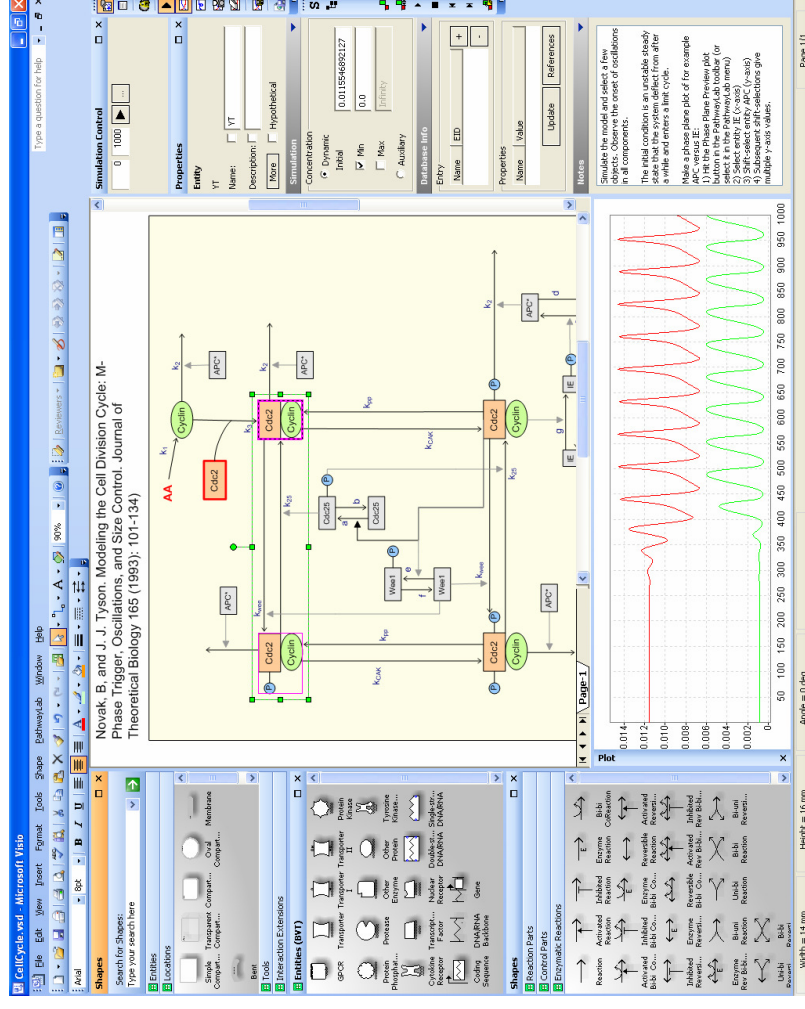
Fraunhofer
CHALMERS
Research Centre
Industrial Mathematics



List of Features

- Drag-and-drop GUI (Visio)
- User customizable graphics
- Transient simulation
- Steady-state computations
- Metabolic Control Analysis
- Parametric scanning
- Click-view visualization
- Database connectivity
- Import of data (CSV)
- Model Export
 - SBML
 - Mathematica
 - Matlab
- PathwayLab Application Package
- SB Toolbox

Mats Jirstrand

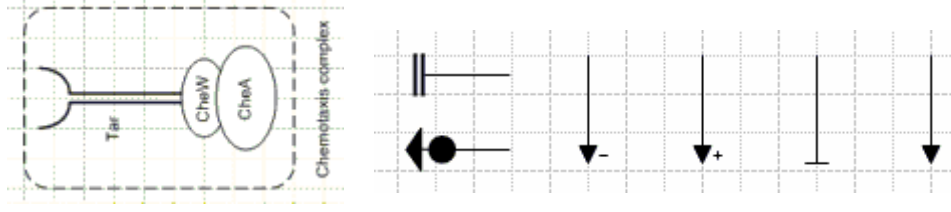
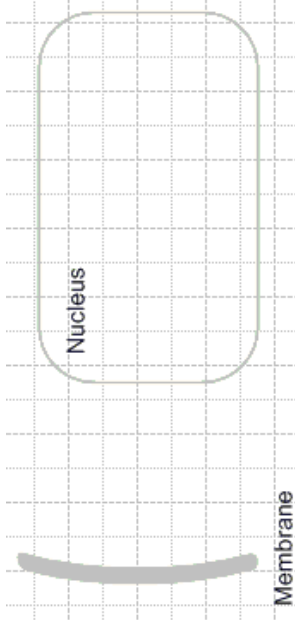
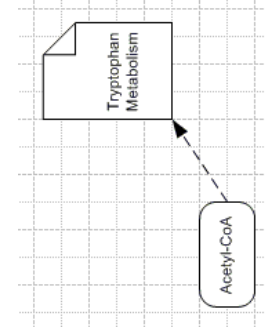
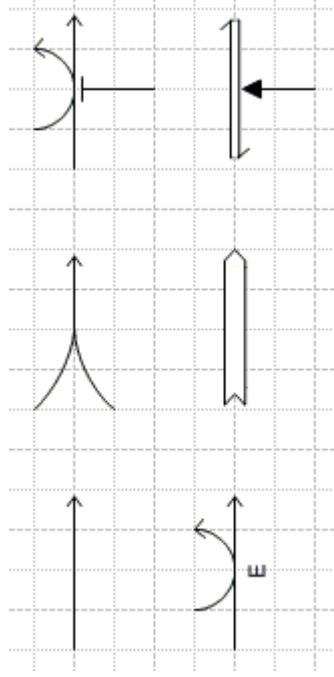
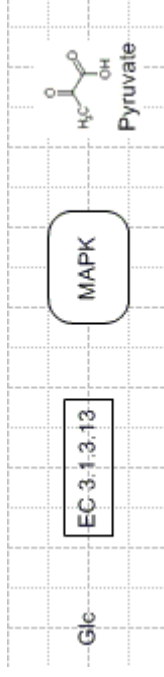


Fraunhofer
CHALMERS
 Research Centre
 Industrial Mathematics



Pathway Modeling Objects

- Entities
 - Plain
 - Complexes
- Interactions
 - Transformations
 - Controls
 - Complexes
- Locations
 - Links



Mats Jirstrand



Fraunhofer CHALMERS
Research Centre
Industrial Mathematics



Demo

Trial version
available
www.innetics.com

Mats Jirstrand



Fraunhofer
CHALMERS
Research Centre
Industrial Mathematics



LigandReceptor2.vsd - Microsoft Visio

File Edit View Insert Format Tools Shape PathwayLab Window Help

Simulation Control: Concentration 0 150

Entity Properties: Receptor Name: Receptor Description: More Hypothetical

Simulation: Concentration Dynamic Initial Rmax 0.0 Infinity

Database Info: Entry Name EID Properties Name Value Update References

Receptor Ligand Formation

Ligand

Receptor

LigandReceptorComplex

Cascade

Plot

Time	Green Line (Ligand)	Red Line (Receptor)	Blue Line (Complex)
0	5.0	0.0	0.0
10	5.0	0.0	0.0
20	5.0	0.0	0.0
30	5.0	0.0	0.0
40	5.0	0.0	0.0
45	5.0	0.0	0.0
50	4.0	1.0	1.0
60	3.0	2.0	2.0
70	2.0	3.0	3.0
80	1.0	4.0	4.0
90	1.0	4.0	4.0
100	1.0	4.0	4.0
110	1.0	4.0	4.0
120	1.0	4.0	4.0
130	1.0	4.0	4.0
140	1.0	4.0	4.0
150	1.0	4.0	4.0

Shapes: Search for Shapes: Type your search here

- Entity
- Framed Entity
- Complex

Entities: Entity

Locations

Tools

Interaction Extensions

Shapes: Reaction Parts

- Reaction Arrow 1
- Reaction Arrow 2
- Reaction Arrow 3
- Reaction Arrow 4
- Reaction Arrow 5
- Reaction Arrow 6
- Reaction Arrow 7
- Reaction Arrow 8
- Reaction Arrow 9
- Reaction Arrow 10
- Reaction Arrow 11
- Reaction Arrow 12
- Reversible Reaction
- Arc Reaction

Control Parts

Mass Action Reactions

Enzymatic Reactions

Width = 68,527 mm Height = 81,756 mm Angle = 0 deg

Page 1/2

Address: G: LigandReceptor2.vsd...

start

Simulation Control

0 150

Properties

Entity

MKKK-PP

Name: MKKK-PP

Description:

More Hypothetical

Simulation

Concentration

Dynamic Initial

0.0 0.0 Infinity

Min Max Auxiliary

Database Info

Entry

Name EID

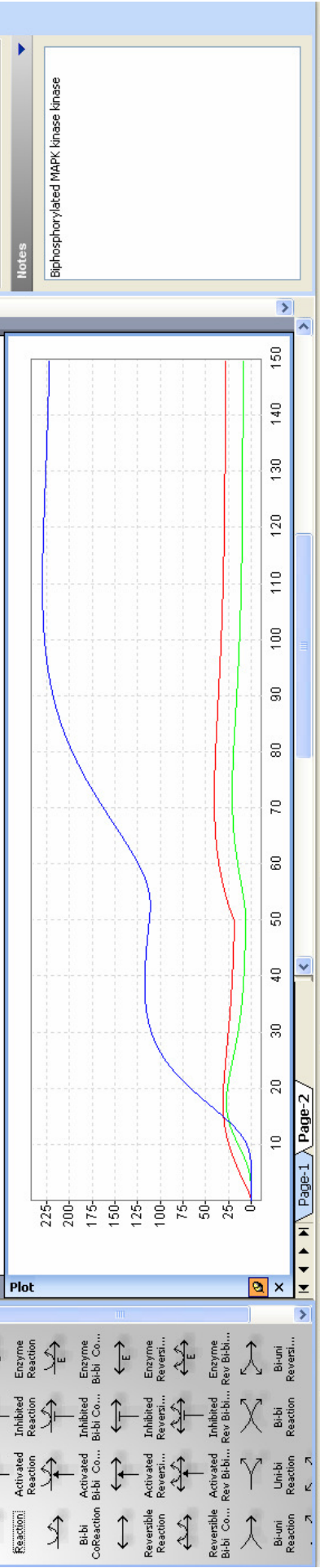
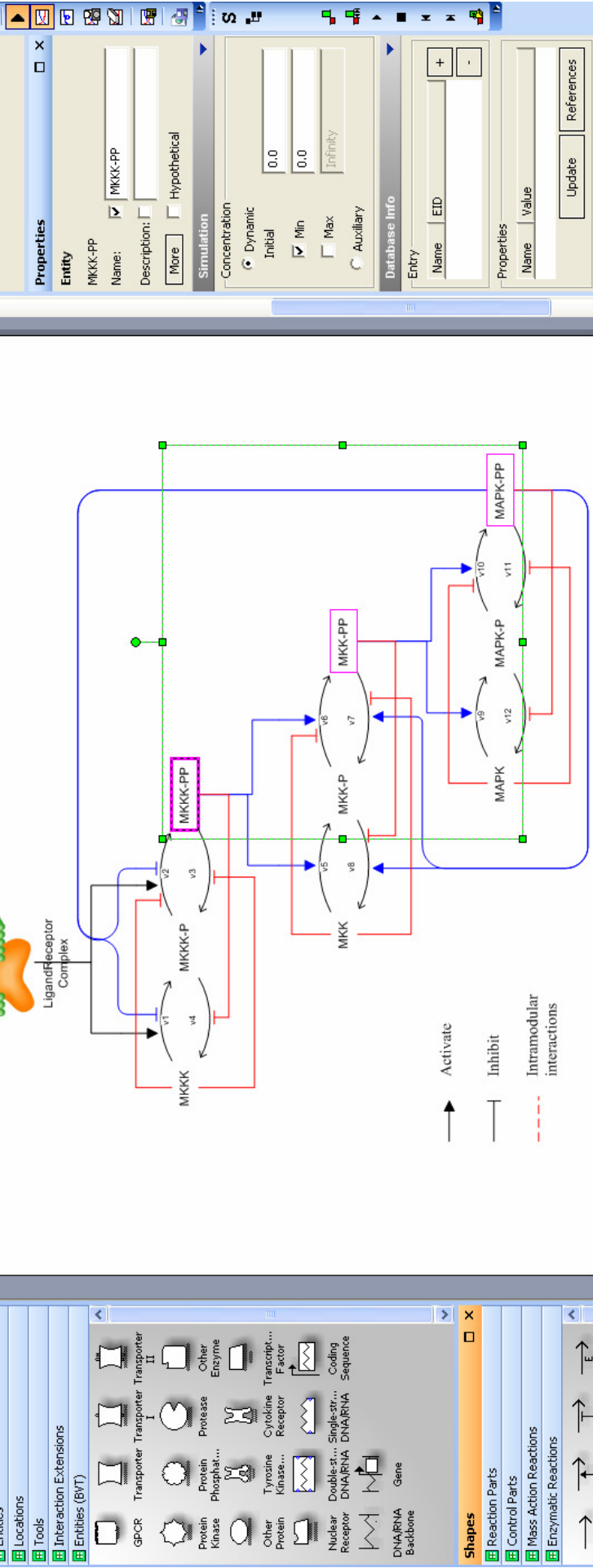
Properties

Name Value

Update References

Notes

Biphosphorylated MAPK kinase kinase



Search for Shapes:

Type your search here

Entities

Locations

Tools

Interaction Extensions

Entities (BVT)

- GPCR
- Transporter
- Transporter II
- Protein Kinase
- Protein Phosphatase
- Other Enzyme
- Protease
- Cytokine Receptor
- Tyrosine Kinase
- Other Protein
- Nuclear Receptor
- DNA/RNA
- Gene
- Backbone

Shapes

Reaction Parts

Control Parts

Mass Action Reactions

Enzymatic Reactions

- Enzyme Reaction
- Inhibited Reaction
- Activated Reaction
- Bi-bi CoReaction
- Reversible Reaction
- Reversible Activated Reaction
- Reversible Inhibited Reaction
- Bi-uni Reaction
- Uni-bi Reaction
- Bi-bi Reaction
- Reversible Bi-bi Reaction
- Reversible Activated Bi-bi Reaction
- Reversible Inhibited Bi-bi Reaction

Width = 16 mm

Height = 6 mm

Angle = 0 deg

Page-1 Page-2