

**University of Indiana Workshop
SBW and Modeling 8th August to 12th
2011**

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Summary of the Week's Course on Pathway Modeling

Text in **Blue** indicates Hands-on Exercises with Software

The following materials will be provided to participants of the Course:

1. e-book copies of the: "Enzyme Kinetics for Systems Biology" and an option to purchase paper copies at a considerable discount.

Visit www.analogmachine.org

Or at Amazon: <http://tinyurl.com/3gag92t>

2. A Web site containing notes and slides

Schedule:

**Morning schedule with start at 9.30 am on day 1 and go on to Noon.
Subsequent days will start at 9 am.**

There will be breaks through the morning.

The afternoon schedule will start at 1.30 pm and go on to 5 or 6pm with breaks as needed. Evening sessions can also be arranged as required. General discussion and questions are encouraged throughout the workshop.

Purpose:

The purpose of the workshop is to introduce the following:

- 1) Modeling**
- 2) Modeling Software**
- 3) Conceptual Understanding of how Cellular Networks Work**

Day 1 (Monday):

1. General Introduction (See <http://www.sys-bio.org> for downloads and other details.)
2. Cellular Networks
- 3. Installation and Introduction to the Software**
4. Basic Concepts (Chapter 1 of ebook)
 - a) Stoichiometric Amounts
 - b) Rates of Change, dx/dt
 - c) Stoichiometric Coefficients
 - d) Reaction Rates. v
 - e) Elementary Reaction Rate Laws (Mass-action)
 - f) Equilibrium Constant
 - g) Mass-Action Ratio
 - h) Disequilibrium Constant
 - i) Alternative form for Mass-action Kinetics
5. **Explore simple models**
 - a) Introduction to Jarnac, JDesigner and General Simulation Tool**
 - b) Evolution to Equilibrium**
 - c) Mass-action Ratio Experiments**
 - d) Closed, Open Systems and Boundary species**
 - e) Equilibrium, Steady State and Transient behavior**
6. Network Models, Deriving ODEs, **Stoichiometry matrix**
7. Introduction to the Various Applications in SBW
 - a) Parameter Scans
 - b) Perturbations
 - c) Collecting Data

Day 2 (Tuesday):

1. Survey of Rate Laws
 - a) Recap Mass-Action Kinetics
 - b) Michaelis-Menten
 - c) Hill Equation and Adair
 - d) Cooperativity and Allostery
 - e) Approximations and Generalized Rate Laws
 - g) Gene Regulatory Rate Laws
- 2. Investigate Rate laws using the Rate Law Explorer**
3. Introduction to Motifs
- 4. Feedforward Networks**
- 5. Positive Feedback**

Day 3 (Wednesday):

- 1. Negative Feedback**
- 2. Oscillators**
- 3. Cascades**
5. Structural Analysis – Moiety Conservation

Day 4 (Thursday):

1. Structural Analysis - Flux Conservation and FBA
2. Metabolic Control Analysis – **Simulations of Metabolism and Control**

3. Linear Pathways

- a) Signal Transfer - Effect of Irreversible and Reversible Steps
- b) Front Loading
- c) Effect of Negative Feedback

4. Branch Points

- a) Flux Amplification in a Simple Branch
- b) Flux Amplification in a Cyclic Pathway

Brief Discussion on Modeling

Day 5 (Friday):

Project

- a) Find a modeling paper online
- b) Extract the model from the paper
- c) Reproduce the results given in the paper