"Attempts are being made to establish a standard form of what a model should be like, how it should be described and documented...This is intended in part to facilitate communication of information about models, which may be difficult owing to their complexity. In building a model one has to keep track of why one made the decisions one did, what mistakes were made, what was learned along the way, etc. It may be desirable in describing a model to also include its unsuccessful predecessors, and the reasons for their failure to fit the data or other inadequacies."

-D. Garfinkel. FEBS Letters 2:S9-S13, 1969.

### BISEN: Biochemical Simulation Environment

#### Caveats:

#1. We get paid to do science, not software.

not an excuse or an apology ©

#2. Our unique tools are driven by our unique needs.

sub-caveat: I am hoping to convince you that it is worth thinking about some of things we do.

## Chemical versus Biochemical Reactions

A "biochemical" reaction:

$$ATP = ADP + Pi$$

A "chemical" reaction:

$$ATP^{4-} + H_2O = ADP^{3-} + HPO_4^{2-} + H^+$$

# Another Example

A "biochemical" reaction:

acetyl-CoA + OAA = CoA + citrate

A "chemical" reaction:

 $acetyl-CoA^{0} + OAA^{2-} + H_{2}O = CoA-S^{1-} + citrate^{3-} + 2 H^{+}$ 

### Reactome:

 $acetyl-CoA + OAA + H_2O = CoA + citrate$ 

### **BIOCYK:**

 $acetyl-CoA + OAA + H_2O = CoA + citrate + H^+$ 

## BISEN: Biochemical Simulation Environment

