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A NETWORK VISUALIZATION AND FLUX ANALYSIS TOOL

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Metabolic Network Model-based Design

"All models are wrong, some are useful"

-- George Box

- "wrong" is a tautology
- Why do we need to maximize usefulness?
  - New organisms, new networks
  - Increasing accuracy and robustness
  - Expanding coverage more subsystems

Metabolic Network Models

Design networks for bioproduct production and optimization

- Understand biochemical networks
- Gene knockouts
- Gene additions
- Media optimization

- Construction and validation

Optimizing Design Process

- Increase efficiency and effectiveness
  - Maximally exploit existing knowledge
    - Organism network models
    - Metabolite/Reaction databases
  - Optimized design environment
    - Enhance human capability
    - Human--software interface
    - Manage cognitive load
- Present prototype web-based tool
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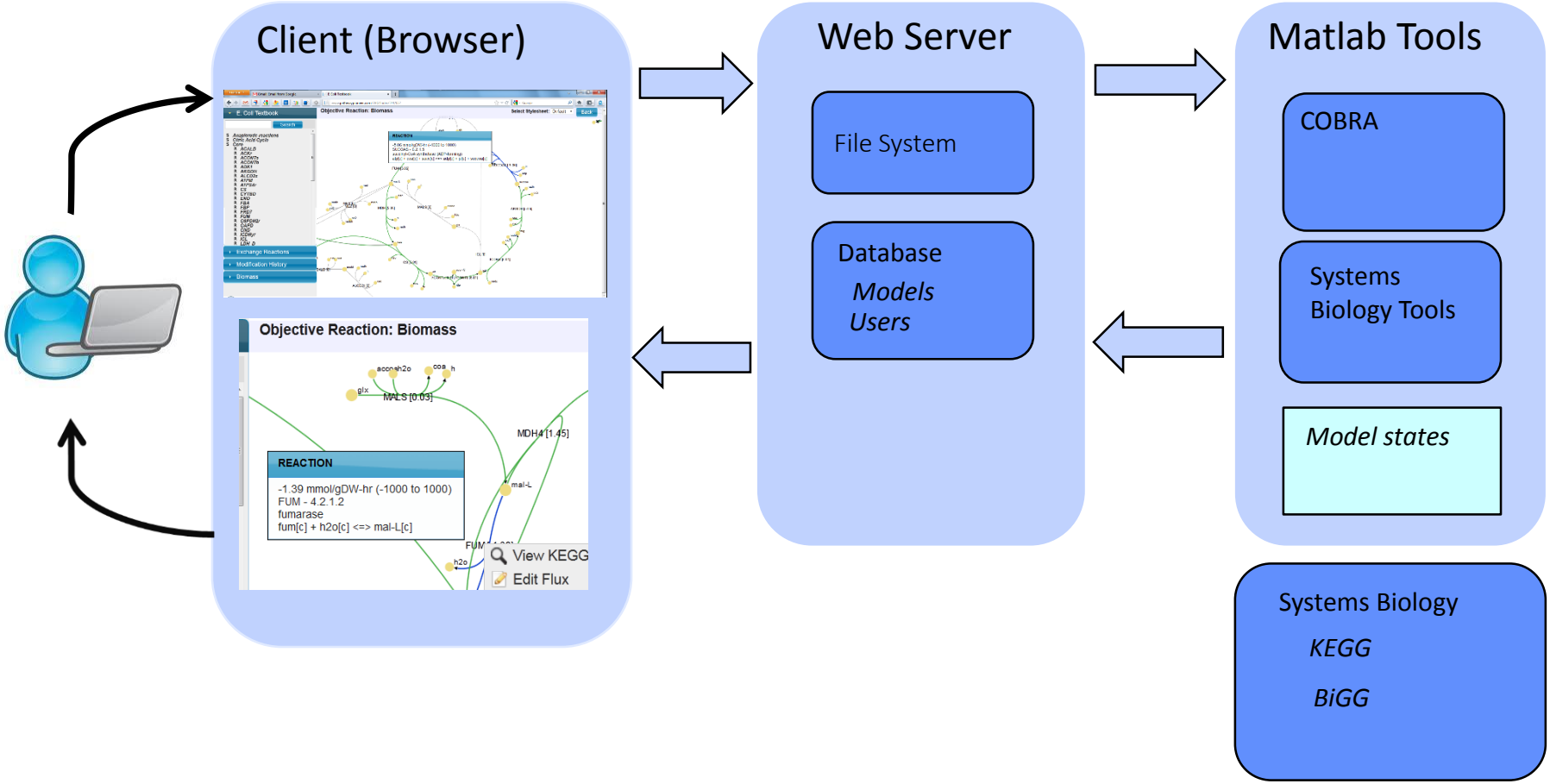
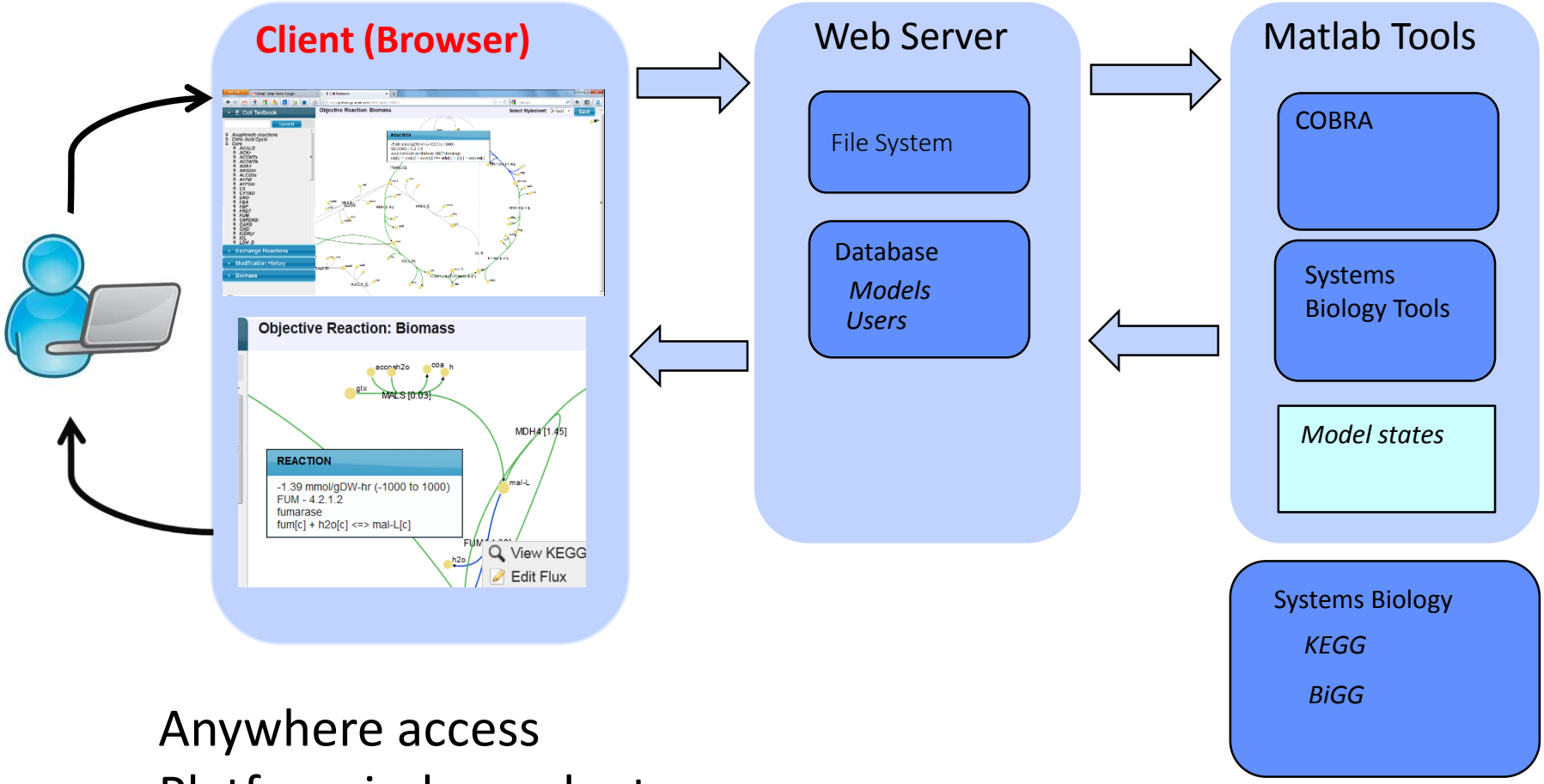
Barriers to Rapid Design

- Knowledge is dispersed
- Analysis tools are difficult to use
- State of design hard to manage
- Too slow with complex models
- Collaboration is hard

Modeling Framework

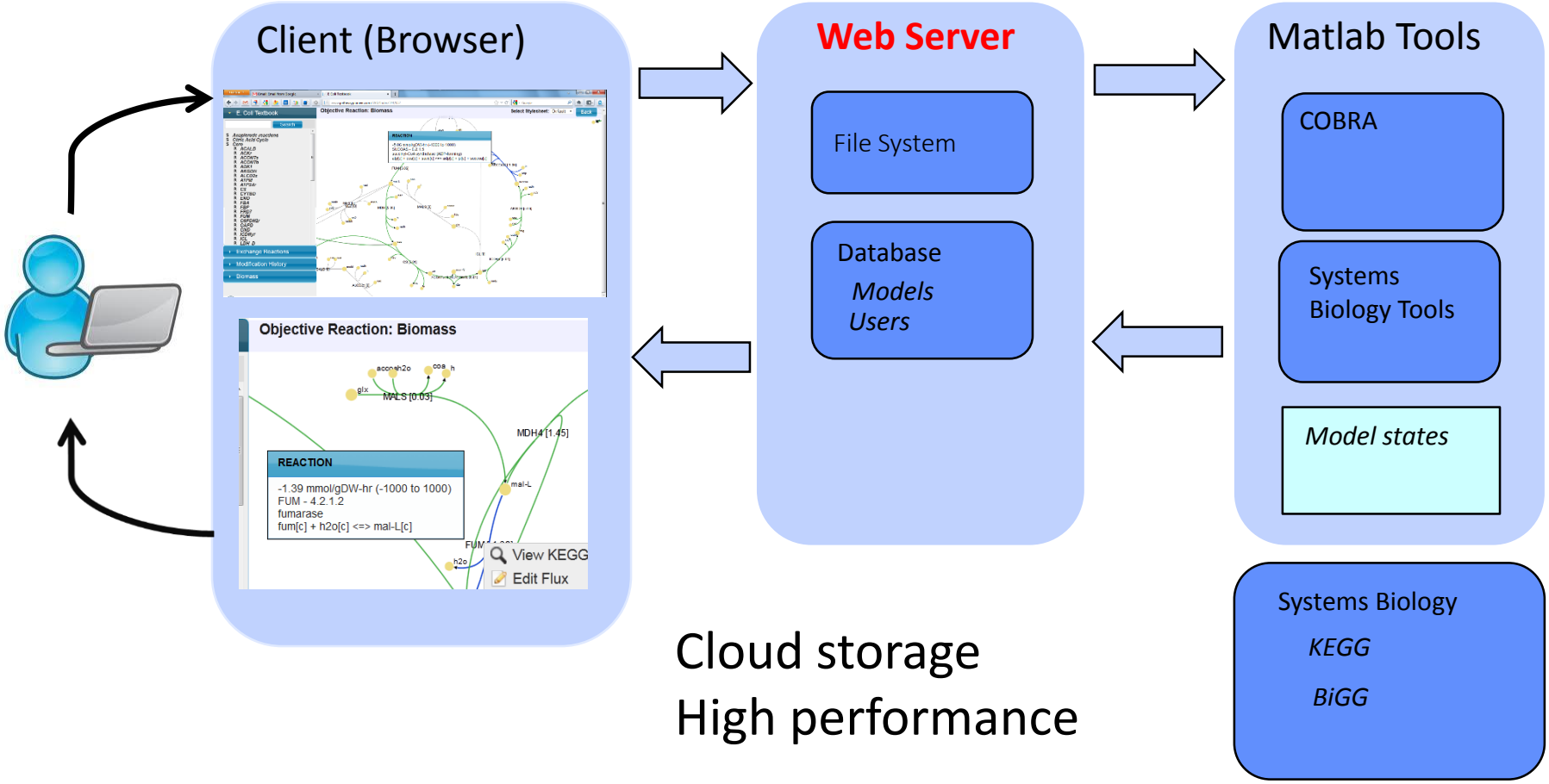


Modeling Framework



Anywhere access
Platform independent

Modeling Framework



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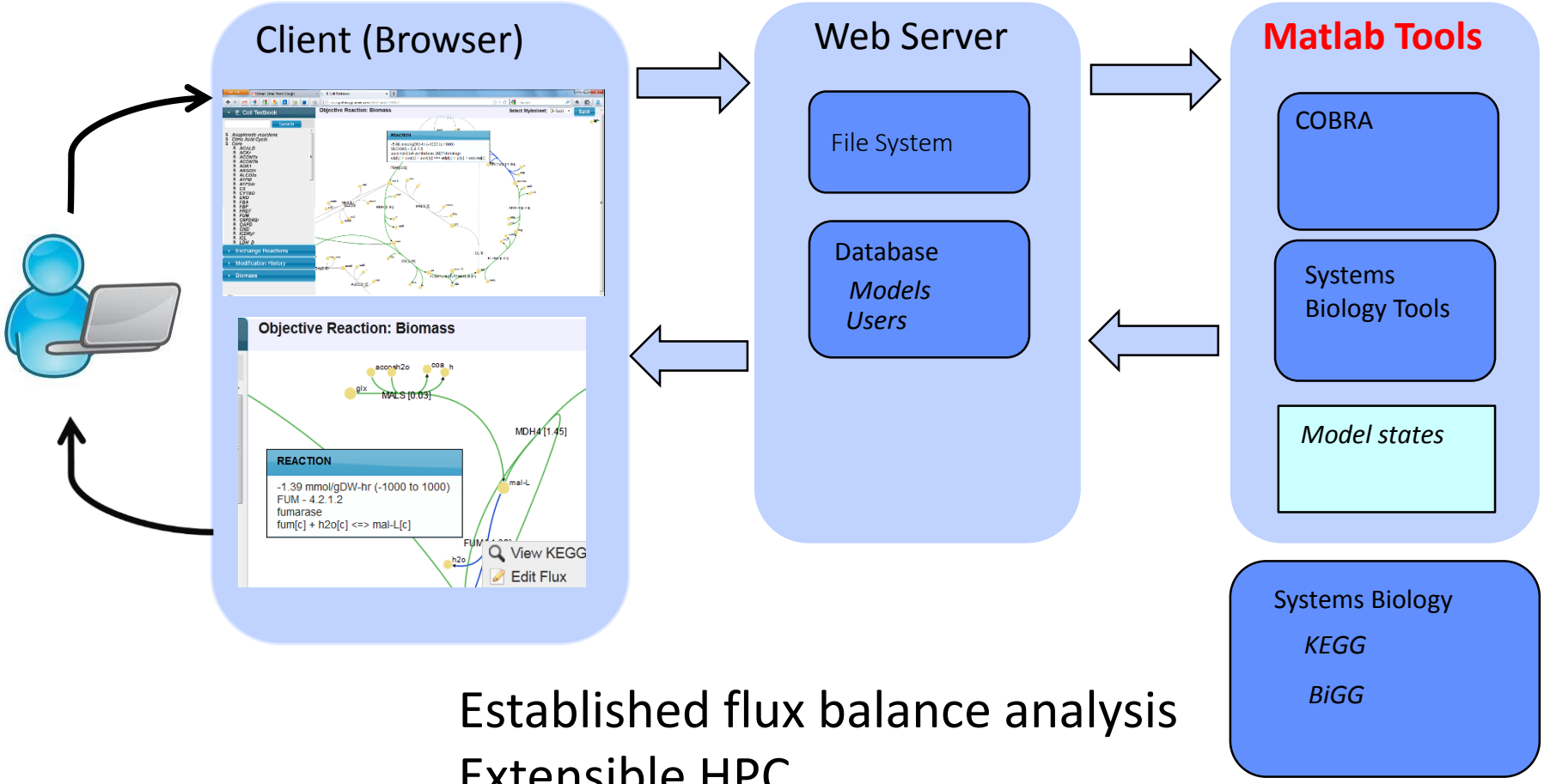

Established flux balance analysis
Extensible HPC

Demonstration

- Search
- Visualization
- Navigation
- Modification

Dynamic Solution Framework

- **Tools and knowledge together in web-based system**
- Tools run on design objects (reaction)
- Results visualized on the design (flux)
- Design state is visually organized
- Alternative model designs shared among members

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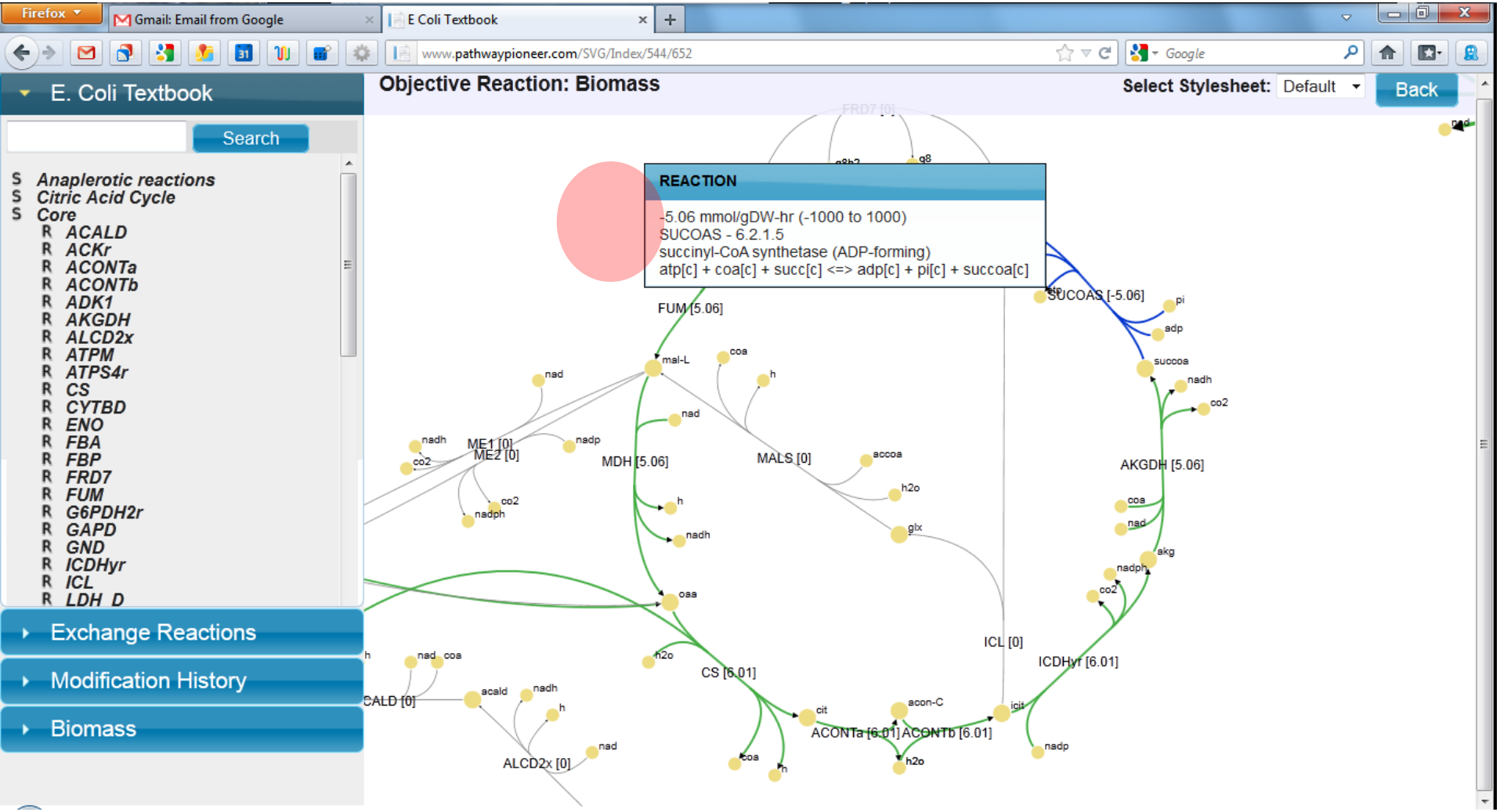

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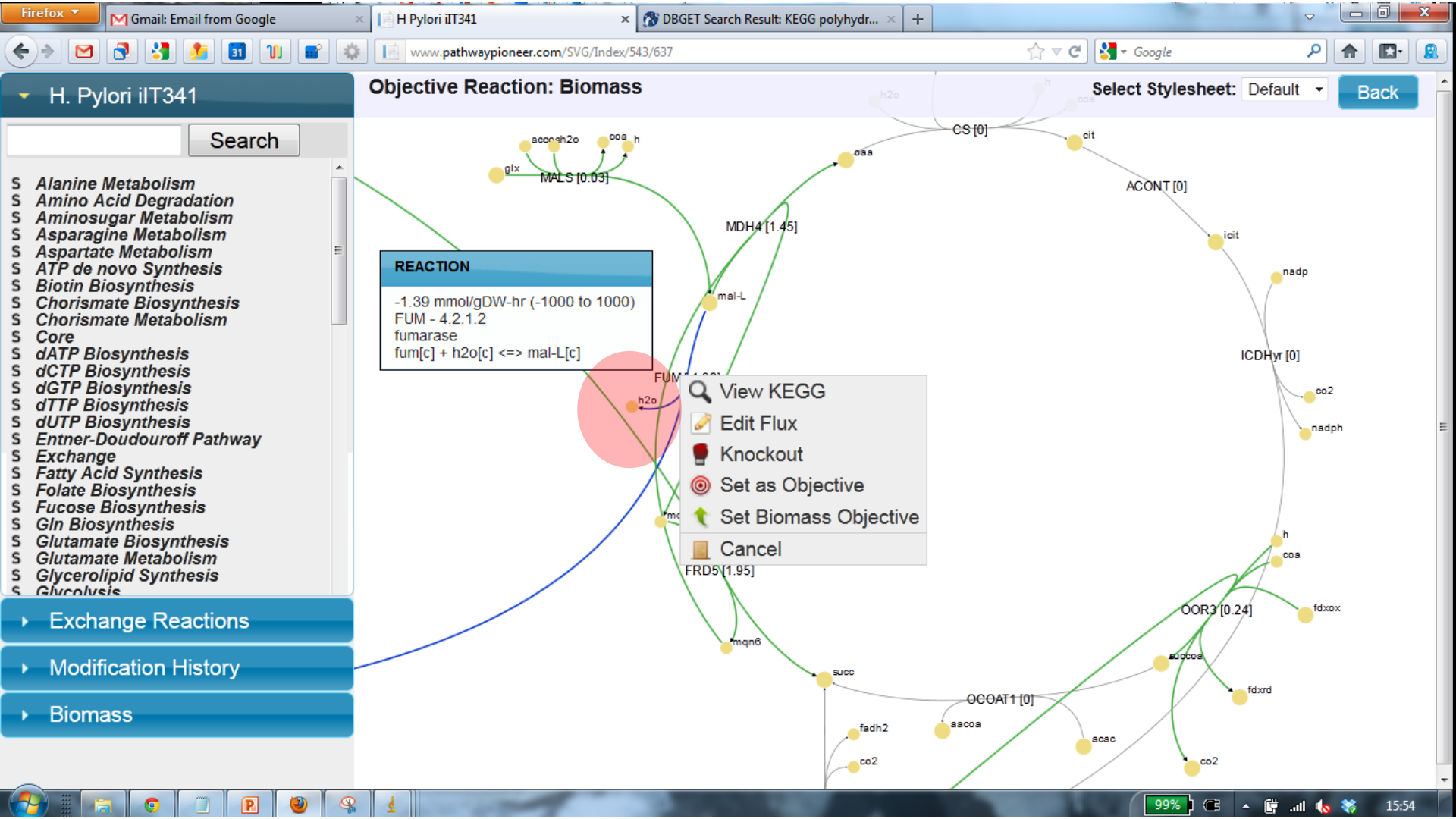

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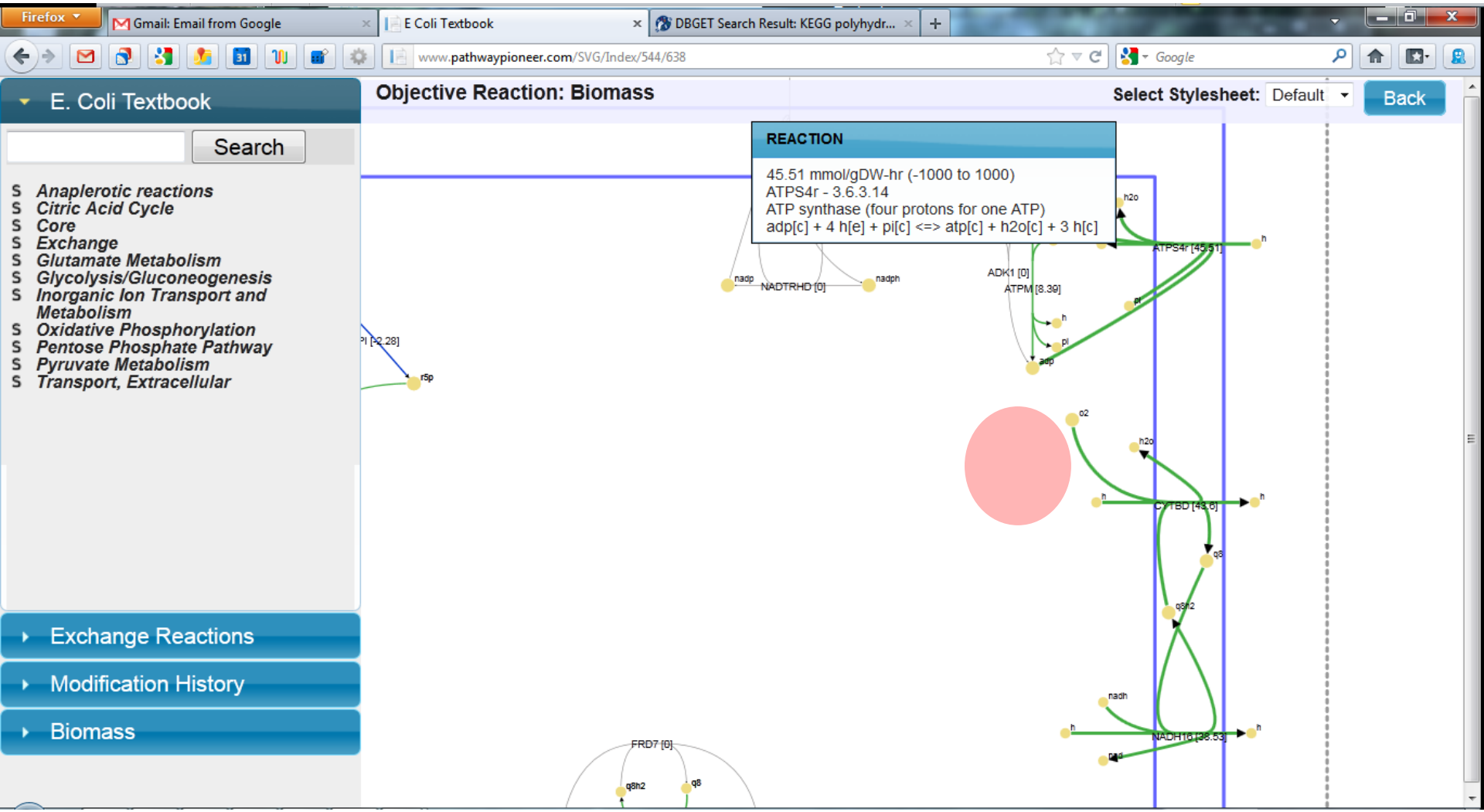
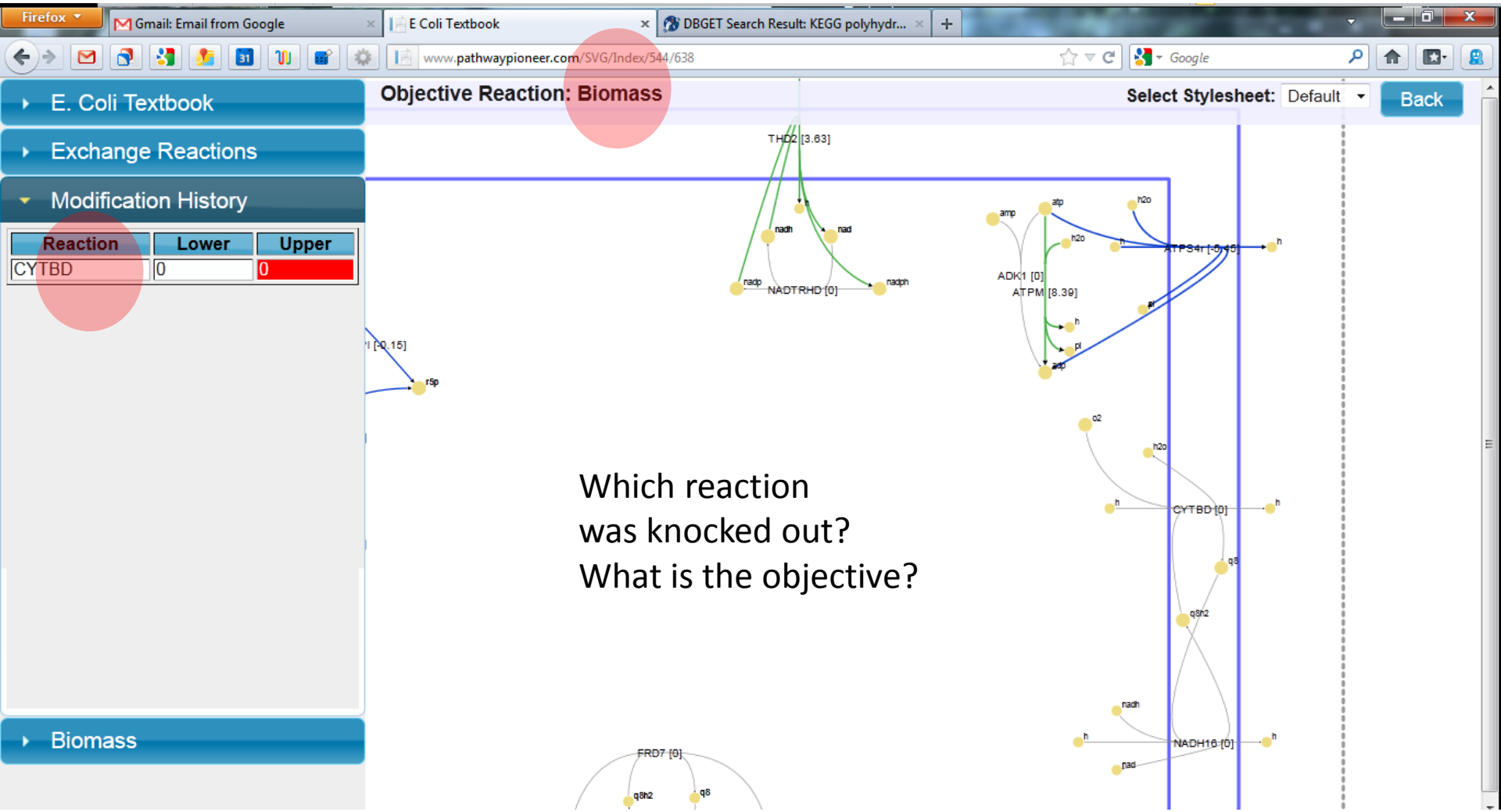


Solution Framework

- Tools and knowledge together in web-based system
- Tools run on design objects (reaction)
- Results visualized on the design (flux)
- **Design state is visually stored**
  - **No hidden state**
- Alternative model designs shared among members



Which reaction
was knocked out?
What is the objective?

Solution Framework

- Tools and knowledge together in web-based system
- Tools run on design objects (reaction)
- Results visualized on the design (flux)
- Design state is visually organized
- **Alternative model designs shared among members**

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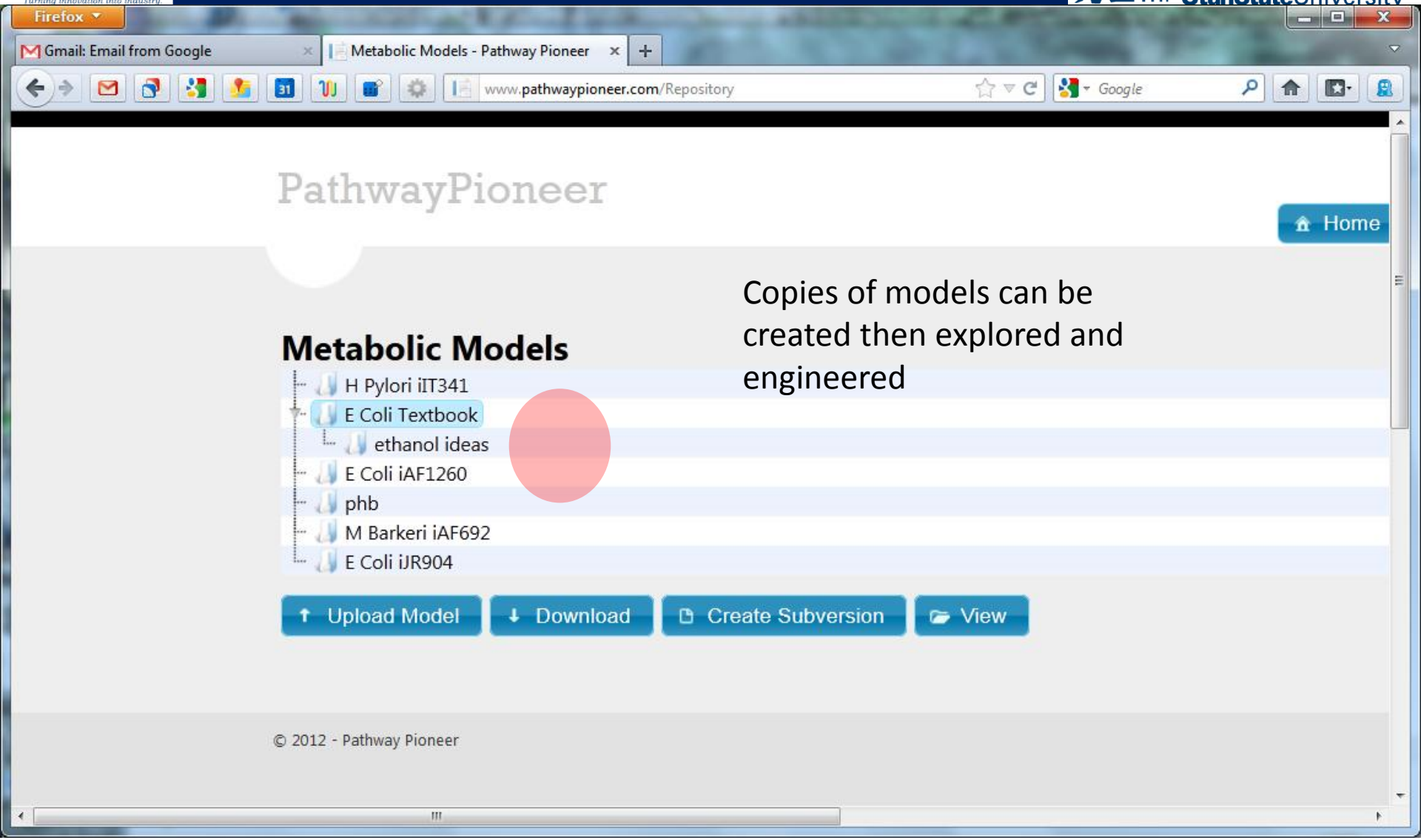

Copies of models can be created then explored and engineered

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- Applicable over multiple models
- Visually centered
- Intuitive to use
- Rapid design exploration
- Save and share designs/results
- Multiple applications within bioengineering

Future work

- Short term:
  - Expand user base
  - Apply to SBI systems
- Longer term:
  - Scale to larger more complex systems
    - Server cloud computing
    - Eukaryotic cells: SF9
    - Regulatory and Signaling
  - Model reconstruction support

Thank you
Questions?