SED-ML support in JWS Online

Using SED-ML and COMBINE archives to reproduce Simulation Results

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Reproducing Simulations

About JWS Online

What’s new in JWS Online?

Summary – Achievements and Limitations
Figure 3  Model calibration with experimental data of JAK2-STAT5 signaling obtained by different experimental techniques. For all experiments, primary CFU-E cells were starved and stimulated with 5 U/ml Epo. At the indicated time points, samples were subjected to (A) quantitative immunoblotting, (B) mass spectrometry analysis or (C) qRT-PCR. Experimental data (black circles) with estimated standard errors and trajectories of the best fit (solid lines) are represented. Mass spectrometry data represent replicates of four independent experiments. (For additional experimental data used for the model calibration, see Figure 4 and Supplementary Figures S11–S23.) In total, 531 data points representing 18 different experimental conditions were used for model calibration. Source data is available for this figure at www.nature.com/msb.
Demo shows experiment database in JWS Online in action. Try it out here:

https://jjj.bio.vu.nl/models/experiments/bachmann2011/simulate
About JWS Online and the circle of reproducibility
About JWS Online and the circle of reproducibility

Scientific Review

Published Paper

Experimentation/Modeling

Feedback

???

readers
About JWS Online
a database for kinetic models

[Diagram showing the process of scientific review, technical curation, experimentation/modeling, and feedback]

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About JWS Online
and what we wanted to advance
Introducing SED-ML to JWS Online

- **Simulation Experiment Description – Markup Language**
  http://identifiers.org/combine.specifications/sed-ml.level-1.version-2

- Enabling reproducible *in silico* experiments since 2007

- Sophisticated multi-model/multi-experiment setups

- Support for experimental data and post-processing
About JWS Online and the single-click reproducibility
About JWS Online
and the single-click reproducibility
About JWS Online and COMBINE Archive support

[Diagram showing the workflow of SED-ML support in JWS Online, including steps like Technical Curation, Scientific Review, Published Paper, and Feedback, with connections to SED-ML, Web Tools, webCAT, COPASI, and Your tool supporting CAs.]
About COMBINE archives
one file to share them all

- Container format for bundling belonging to modeling or simulation experiment
- Enriched with meta information according to the OMEX standard
- Enable to bundle all necessary resources for reproduction
- http://co.mbine.org/standards/omex
• Dockerized JWS Online
  https://jws-docs.readthedocs.io/10_docker.html

• Introduced a basic set of APIs into JWS Online
  https://jws-docs.readthedocs.io/8_rest.html

• Widely extended the handling of Manuscript meta information

• Implemented **SED-ML database** into JWS Online
  https://jjj.bio.vu.nl/models/experiments/

• Enabled import and export of **COMBINE Archives**

• Introduced **Reproduction of Simulation Experiments – by a single click**
  https://jjj.bio.vu.nl/models/experiments/bachmann2011/simulate
Limitations and all the non-cool stuff

- Only Time-Course Simulations
- No Repeated-Tasks
- Excel Spreadsheets instead of NuML
- Only 2D Plots
That’s it!

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References


