Simulated Western Blots: Visualizations of Computational Systems Biology Model Predictions

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Keywords: computational biology, computer visualization, mechanistic mathematical modeling, systems biology, computational toxicology

Computational and experimental toxicology have historically been conducted in parallel and often with less-than-ideal levels of interaction and cross-fertilization. Differences in training between quantitatively oriented computational modelers and the often more qualitatively oriented experimenters are one reason for this situation. To facilitate communication between modelers and experimenters and enable essential correlative studies, we are developing special visualization and analysis tools to compare computational systems biology model predictions of protein concentrations with western blot data. To simulate western blots, a physics-based mathematical model of gel electrophoresis was developed to determine the migration rate and spatial distribution of proteins based on their molecular weight and concentration. A computer visualization program was created to display the simulated western blot images from the computational biology model–predicted protein concentrations. Using a graphical user interface, the display parameters can be interactively adjusted to improve the correspondence between the simulated and experimental western blot images. The visualization of simulated western blots will enable more effective interactions between modelers and experimenters, allow experimenters to identify possible matching data, and enable modelers to qualitatively compare model predictions with literature data typically published as western blot images.

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