**Figure 1 – Model Summary**

**a.** Overview of model inputs to *inSilicoCellModel* and output as pictures of cellular distributions colored according to where cells are in the cycle.

**b.** Adaptation from Drasdo-Hohme of how the model works.

**c.** Hierarchy of the model and what can be replaced.

**Figure 2 – Growth Parameters**

**a.** Multiple growth rates in boundary and no boundary (show every curve)

**b.** Show density over time in both bounded and unbounded

**Figure 3 – Fitting Data with Drug Simulation**

Real Data from experiment plotted with points, simulation fits plotted with lines. PBS fitted from all simulations without drug effect, then initial density and cycle length are fixed and all drug simulations are fit with some drug effect. Fit done by minimizing L2.

**Figure 4 – Gene Expression Simulation and Comparison to Data**

**a.** Cartoon overview of how we simulate gene expression.

**b.** Illustrating how the scaling varies between 0 to 1 for each pathway.

**c.** Pick one dosage (10 um/mL) from **Figure 3** and plot each of the effective pathways vs time for that selection. Y-axis is % of pathway activity and all pathways can be plotted together. Show difference in pathways for drug effect.

**d.** Comparison to real gene expression data along each pathway.

**Figure 5 – Multiple Cell Types**

two cell types, low enough density so one can overtake, not so low (equivalent to no boundary) so that overtaking always happens

**a** heatmap for 2 cell types w/ boundary

**b.** Varying mean (normal) of drug effect w/o boundary in a simulation where you would typically observe a balance in the cellular populations.

**c.** Varying SD (normal) of drug effect w/o boundary where you would typically observe a balance in the cellular populations.

**d.** gene expression

**Figure 6**

fig 4 but with single cell rna-seq