Case study 1: *Natural example: Bacillus subtilis*

Protein: protein interaction network:

1 – Select both Organism 1 and Organism 2 as '*Bacillus subtilis'*

2 – select the desired node shape and layout (e.g. database and nicely) and click on Submit

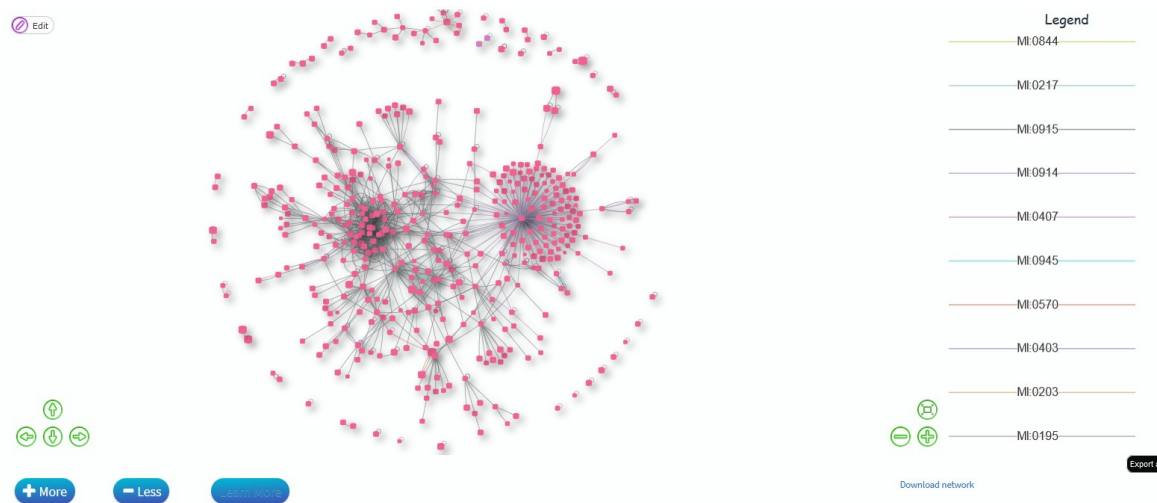The first 100 interactions will be shown. For more interaction, click on the button +More (Figure 1).

	From_A	To_B	Interaction_Type	Gene_A	Gene_B	Taxonomy_A	Taxonomy_B	Organism_A	Organism_B
1	P33112	P33113	MI:0844	spaR	spaK	1423	1423	Bacillus subtilis	Bacillus subtilis
2	P33113	P33113	MI:0217	spaK	spaK	1423	1423	Bacillus subtilis	Bacillus subtilis
3	P20429	O31602	MI:0915	rpoA	spx	224308	224308	Bacillus subtilis (strain 168)	Bacillus subtilis (strain 168)
4	P37871	O31602	MI:0915	rpoC	spx	224308	224308	Bacillus subtilis (strain 168)	Bacillus subtilis (strain 168)
5	P25144	O31662	MI:0914	ccpA	mtnA	224308	224308	Bacillus subtilis (strain 168)	Bacillus subtilis (strain 168)

Figure 1: View of 850 experimentally validated protein-protein interactions of B. subtilis

Dynamical modelling:

1 – download the test data from the GIT (https://github.com/salihoglu/PRO-Simat) (testJimena.txt) and enter the JIMENA module in the PRO-Simat page

2 – On the left side, choose 'upload your data' and click the Convert Graphml button, then Run Jimena.

3 – Look at the table at the bottom to analyse the network. The analysis results for each node can be displayed by clicking on each time point (green button).

4 – to change the activation, click on the Add perturbation and select the Spo0A with a start point 0, endpoint 1000 and the value 1. This will lead to the activation of the biofilm production almost immediately after the activation (from time point 1, figure 2). To delay the activation of the biofilm production, postpone the activation of Spo0A protein (delay the time point), and observe the delayed production of the biofilm production and its effect on other proteins.

5 – To activate the cannibalism process, decrease the activity of DeS protein (value 0) and activate the DegS, group of Miner proteins, SDK and SDP proteins (value above 0.5), and run the Jimena analysis. The cannibalism process will be activated at a particular time point (Figure 3). Observe also the activity of other proteins and processes (not shown).
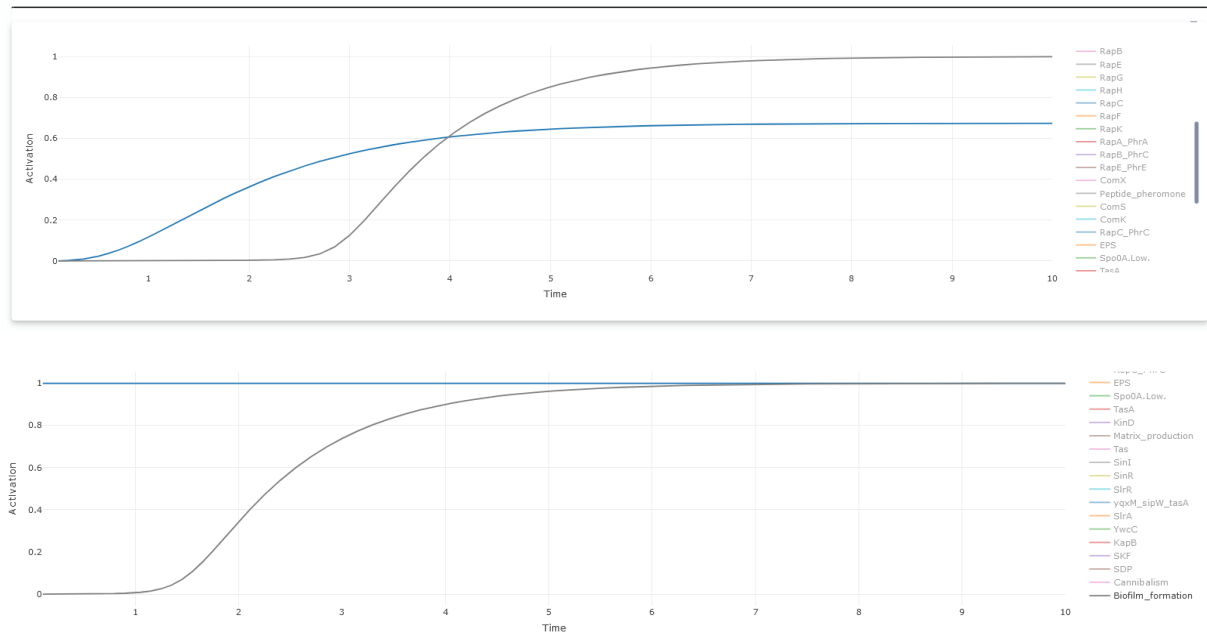

Figure 2: Dynamic modelling of biofilm production. Upper graph: native conditions, below: modified accelerated Spo0A
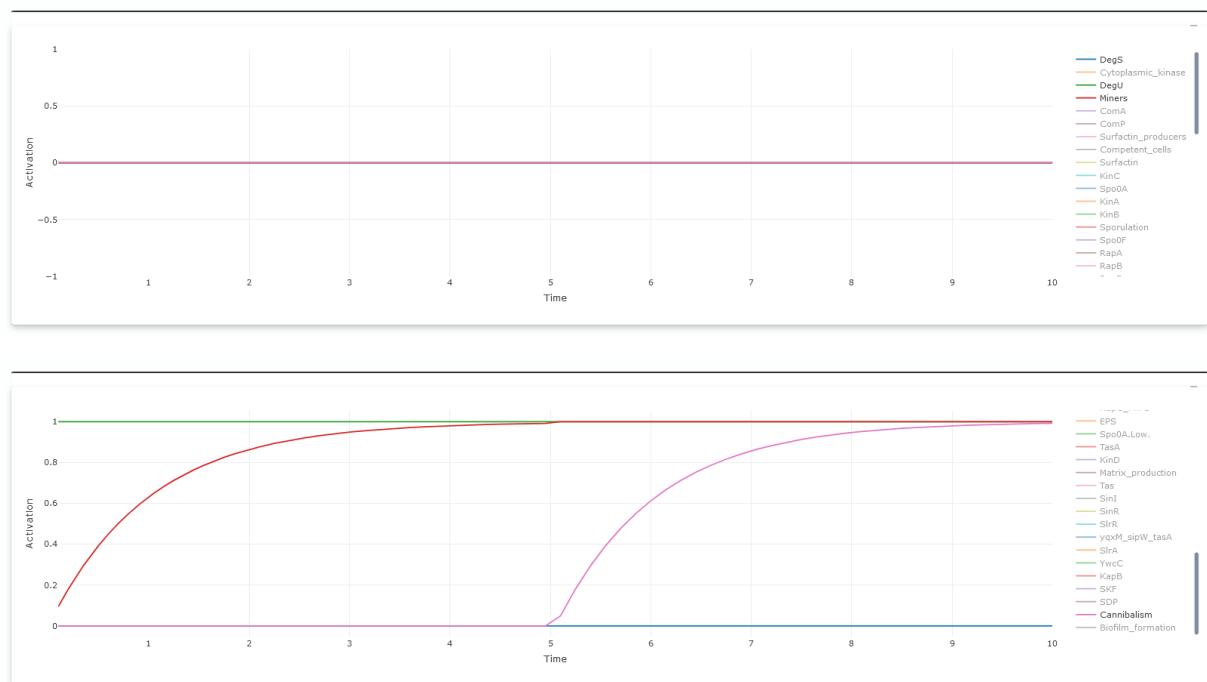

Figure 3: Dynamic modelling of cannibalism. Only differently activated proteins are shown. Upper graph: native conditions, proteins are not activated. Below: modified conditions as listed in point 5.