MD simulations of wild-type, phosphorylated and mutant versions of E2 enzymes belonging to family 3 involved in the ubiquitin-conjugating system, for which phosphorylations, which affect its activity, have been experimentally investigated. The simulations and their experimental validation by mutagenesis provide a molecular model in which relevant conformational changes promoted by the post-translational modifications are responsible of effects on E2 activity.

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[P-S.34]

Effects of glucose and inoculum concentrations on production of bioactive molecules by *Paenibacillus polymyxa* RNC-D: A statistical experimental design

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Keywords: Bioactive molecules; *Paenibacillus polymyxa* RNC-D; Process variables; Statistical design

The composition of culture media and the microbial cell mass influence on secondary metabolites production in fermentative procedures. The effect of two process variables, namely glucose and inoculum concentrations on biomass formation, bioactivity and surface tension of extract obtained during the cultivation of endophytic *Paenibacillus polymyxa* RNC-D was evaluated. Assays were performed using glucose and inoculum concentrations varying from 5.0 to 40.0 g.l⁻¹ and from 2.5% to 5.0% (v/v), respectively, according to a 2² full factorial design. The microorganism was cultivated in orbital shaker (30 °C, 180 rpm) for 96 h. Cell growth was estimated by optical density (600 nm) vs dry weight calibration curve. Bioassays were performed using two-fold serially diluted extract displayed in 96-well plates. *Escherichia coli* ATCC 25923 and *Staphylococcus aureus* ATCC 25922 were used as indicator strains. The minimal inhibitory concentration (MIC) was expressed in µg.ml⁻¹. Surface tension (mN.m⁻¹) of extracts was measured using a tensiometer.

A significant (p<0.01) and positive effect of glucose and inoculum concentrations was observed on biomass formation. Bioactivity results were also affected by the two studied variables (p<0.01). The lowest MIC value of *E. coli* was obtained when the highest glucose and inoculum concentrations were used. Otherwise, MIC of *S. aureus* was increased when the maximum glucose was applied. Surface tension was affected by the two evaluated variables and also by their interaction (all of negative signal, p<0.1). The highest biomass formation (4.11 g.l⁻¹) and the lowest MIC of *E. coli* (15.6 µg.ml⁻¹) were attained under the highest concentrations of glucose and inoculum, while the surface tension reduction reached the maximum (20.0 mN.m⁻¹) when using the lowest glucose and the highest inoculum concentrations. Such results can still be improved by performing additional assays for the establishment of the quadratic models, as suggested by analysis of the experimental design.

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[P-S.35]

Behavioral dynamic modelling of fast responses: the *Escherichia coli* SOS system as a case study

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Keywords: Modelling; Gene expression; Stress; Fast response

The mathematical description of gene expression time profiles is generally a very hard task, given the overwhelming complexity of the underlying molecular components and their interaction network. In this paper we approach this problem from a different perspective: in the presence of very stringent requirements (time, energy consumption,...) the behaviour of a biological entity may be forced to follow a stereotyped pattern amenable, as such, of formal mathematical description. For example, the crowd behavior induced by panic is well described by mathematical models able to accurately simulate group decisions. Here, we discuss the peculiar features of a generic “fast” response at the mRNA level and translate them in a straightforward mathematical model characterized by tunable parameters each having a precise biological meaning. The example of the SOS system in *Escherichia coli* will be considered together with experimental data provided by our laboratory.

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[P-S.36]

Towards a yeast cell cycle hybrid model: network analysis for model building of the coordination between cell growth and division

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Keywords: Cell Cycle; Systems Biology; Dynamic modeling; *Saccharomyces cerevisiae*

Proliferating eukaryotic cells are continuously increasing in mass throughout the cell cycle. As pointed out as early as 1971 by Mitchinson, the “continuous events of the growth cycle” (i.e., increase in cell mass) and the “discontinuous events of the DNA division cycle” (i.e., DNA replication, mitosis, and cell division) need to be tightly coordinated in order to maintain cell size homeostasis.

We present here a network analysis of gene products involved in cell growth and cell cycle regulation. Gene products belonging to the network have been chosen based on available literature data. They include products of genes identified through genome wide screening for size mutants, products of genes whose expression is correlated with the growth rate, gene products involved in the core cell cycle machinery, gene products involved in ribosome biogenesis and function and selected gene products involved in metabolism.

In the budding yeast *Saccharomyces cerevisiae*, two quantitative parameters characterize each exponentially growing population: the rate of growth (l, min⁻¹) and the critical cell size at