A Systems Biology and Ecology Framework for POPs Bioaccumulation in Marine Ecosystems

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Abstract. We propose a modelling framework for studying bioaccumulation of Persistent Organic Pollutants (POPs) and microbial bioremediation in the Adriatic food web. The integration of network estimation methods, ODE simulation and sensitivity analysis and tools from synthetic biology allows investigating multiscale effects and biological responses to POPs contamination, from the molecular level (bacteria metabolism) to the ecosystem level (food web) of a marine ecosystem.

**Keywords:** bioaccumulation modelling, PCBs, bioremediation, FBA.

When a chemical compound is released into an ecosystem, its ecological impact on living organisms and environment is hard to predict. Due to their biochemical and biophysical characteristics, *POPs* (*Persistent Organic Pollutants*) enter protein pathways at the cell surface or inside organisms, in which *bioaccumulation* occurs as the result of the uptake from contaminated environment and food. The marine ecosystem is a sink and a source of POPs that, being resistant to degradation, remain persistently into the environment and bind permanently with the fat tissue of fish. Thus, contaminants follow the same paths as biomass flows, making every species in a polluted ecosystem prone to bioaccumulation, a phenomenon that increases at higher trophic levels. What is important is not just estimating contamination levels, but also identifying which species has the largest effect on the diffusion of a pollutant through a food web (*keystones*).

On the other hand, microbial communities constitute the most prominent marine compartment in terms of abundance and diversity and, more importantly, are able to degrade POPs by using them as growth substrates in their metabolic pathways (*bioremediation*). Despite of that, the role of micro-organisms in bioaccumulation modelling has been poorly considered so far.

In this work, we investigate the systems biology of *Polychronated Biphenyls* (*PCBs*, a class of POPs) bioaccumulation in the Adriatic ecosystem, by integrating the classical food web of macro-organisms with the complex chemical pathways of the many micro-organisms involved in bioremediation. We model the microbial pool as a unique super-organism where a continuous exchange of genetic information occurs among bacteria by means of conjugative plasmids, prophages and DNA uptake [2].

Procedurally, we have estimated the food web structure in terms of trophic and contaminant flows from literature data with the *Linear Inverse Modelling (LIM)* [3] method (Fig. 1 a). Estimated rates have been used to parametrize a ODE dynamic bioaccumulation model (Fig. 1 b). Keystones have been identified with network analysis tools (trophic and topological centrality indices), and with a newly introduced index, *Sensitivity Centrality (SC)*, based on the sensitivity analysis of the ODE model. Using *Flux Balance Analysis (FBA)* we have reconstructed the metabolic pathways of PCB bioremedation, by extending a FBA model of *P. Putida* [1]. In this way, we investigate the multiscale effects of the optimization of bacterial functions and perturbations (e.g. gene knockout) in the metabolic network on the bioaccumulation dynamics in the food web.

The combination of synthetic biology and ecological analysis tools provided insights into both the key species in a contaminated network through a novel network index; and the role that the bioengineering of bacterial metabolism plays in the remediation of polluted environments.
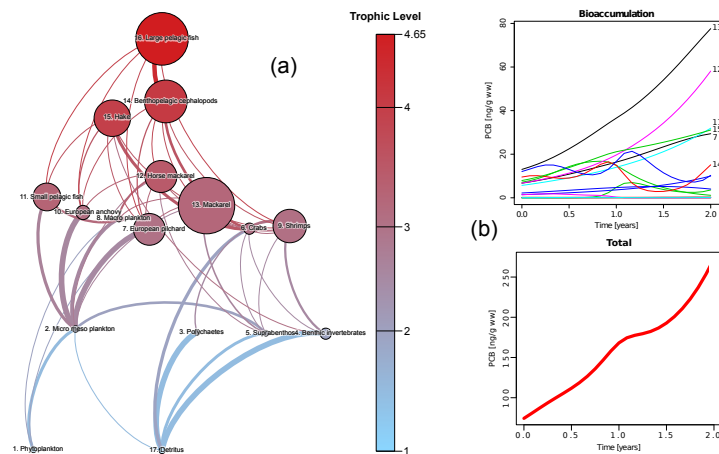
Fig. 1. PCBs bioaccumulation in Adriatic food web (a). Nodes represent species (size proportional to PCBs concentration). Edges represent feeding links. (b) Dynamic bioaccumulation model (x-axis, time; y-axis, PCB concentration).

References

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