

## **Project 4.15. Aggregation and gellation of the intrinsically disordered proteins (theoretical)**

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### **Background:**

In recent years, there has been a tremendous interest in the properties of the intrinsically disordered proteins, primarily in the context of the neurodegenerative diseases. Oftentimes the solutions of these proteins undergo liquid-liquid phase transitions that result in the formations of the proteinaceous droplets. The droplets act as membrane-less organelles that provide a more concentrated environment to perform various biological functions. The idea of the project is to involve such droplets in the fish aquaculture to capture toxins that plague breeding of salmon and other species.

### **Aim:**

Ultimately, the aim of the project is to design novel ways to control diseases of fish in aquaculture. The idea is to use selected affibodies connected to some intrinsically disordered proteins to bind with toxins. Due to the presence of the disordered segments, such objects would first form droplets and then transform into gels. The gels will be removed from the aquaculture. Such a capture of toxins is expected to replace the current widespread application of antibiotics.

This topic involves collaboration with two laboratories in Spain, one in Italy, one in France, one in Ireland, and IFPAN. The IFPAN group is the only unit in the consortium that is supposed to provide theoretical modelling. The modelling will be based both on all-atom and coarse-grained simulations. The latter will be based on the available in-house programs.

### **Requirements:**

The project will involve a lot of numerical simulations and programming so the background in such tasks is required.

- an M.Sc. degree in physics, chemistry or information science is welcome.
- knowledge of biology, biophysics, or biochemistry would certainly help.
- a sufficient proficiency in English is necessary.

### **Funding:**

Standard Polish PhD scholarship, with the possibility of additional work in the European H2020-FETOPEN-2018-2020 project PathoGelTrap.