Neurodegenerative diseases such as Alzheimer's disease (AD) and Parkinson's disease (PD) are one of the challenges of modern medicine. According to estimates, there are currently about 44 million AD patients worldwide, and this number is expected to triple by 2050. In contrast, the number of people with PD is estimated at 7-10 million in 2019. Both AD and PD mainly affect the elderly, and with increasing life expectancy, the problem is becoming more pronounced.

Both diseases are part of a larger group of diseases called proteinopathies. They occur when proteins in the human body form harmful aggregates. A key component of this group are amyloid fibers, which have a characteristic cross-$beta$ sheet structure. Although these fibers are very similar to each other, the proteins that form them have very different sequences, which makes it extremely difficult to design substances that will completely block aggregation. We can be aided by small-molecule compounds called amyloid modulators, which have a diverse mechanism of action and the ability to interact with amyloid at different stages of aggregation.

Many databases of amyloid proteins and peptides are now available. In addition, we have created a database of amyloid interactions (AmyloGraph; https://amylograph.com/), describing which protein interacts with another, and the nature of the interaction. Unfortunately, to date, none of these databases have included amyloid modulators. Consequently, it is impossible to train a model capable of designing new drugs that target proteinopathies.

Therefore, the main objectives of our research project are:

1. Creation of a amyloid modulators database, that will include compounds responsible for inhibition.
2. Based on the collected data, carry out training of a model capable of designing potential drugs.
3. Validate the performance of the model by conducting tests of designed molecules under laboratory conditions.