With the dawn of the twenty-first century, it appears that pharmacy's golden age has come to an end. During those years, a large number of currently used medicines were discovered, and the majority of diseases are no longer as dangerous to patients as they once were. Isn't there anything more thrilling than being a part of this brave, new world? Regrettably, there is one physiological aspect of the body that is particularly intriguing and has yet to be discovered – *aging*.

There are several theories attempting to explain it in order to identify factors responsible for its onset and progression and thus potential drug targets. The '*biological clock theory of ageing*' is perhaps the most well-known, according to which ageing is purposefully caused by evolved biological mechanisms in order to gain an evolutionary advantage. This would imply that there is no way to halt it. However, there is a ray of hope among these gloomy predictions: many scientific reports suggest that the degradation of biological structures in the cytosol and nucleus due to excessive oxidation causes functional ageing of cells (*senescence*). This lays the groundwork for the so-called '*error catastrophe theory of aging*', or more precisely, '*free radical theory of ageing'*, according to which free radicals are to blame for the accumulation of these damages, and as a result, a malfunction in cells' functioning manifested by the development of various chronic, severe, and often fatal ailments such as cancer or neurodegenerative disorders. Although cells can protect themselves from oxidants to some extent thanks to an intracellular environment made up of reducing compounds, this mechanism is becoming less and less effective in today's world, where UV radiation, smog, and air pollution are the main sources of significantly increased levels of the body's concentration of free radicals

Plants were used for therapeutic purposes in traditional Chinese medicine, Ayurveda, and shamanism, and knowledge of how to use them was passed down from generation to generation. These mythical healing powers, however, remained unknown until the chemical composition had begun to be investigated. Among the newly discovered substances, *polyphenols* piqued scientists' interest because of their activity, which is similar to that of biological antioxidants. Numerous studies have since confirmed and continue to confirm their beneficial effects.

The goal of this project is to create machine learning models to aid in the development of new drugs based on a matrix of well-known phytochemicals with enhanced antioxidant potential. The study's scope includes two types of activity: 1) direct radical scavenging and 2) inhibition of enzymes that generate them *in vivo*. Parallel to the quantitative evaluation conducted in the lab, computational chemistry studies will be carried out with the goal of understanding the molecular mechanisms underlying the observed phenomena. The obtained data will be used to create quantitative structure-activity relationship models in order to identify the structural elements modulating these activities. However, the project's ultimate goal is to turn the models into machine learning algorithms and host them on a publicly accessible server, allowing other scientists to directly influence their credibility by uploading their experimental results, which will then be processed by the server, which will adjust the parameters of the models and improve their accuracy. Another significant and anticipated benefit is the ability to use them to reduce research costs and time by discarding inactive compounds at the outset.