

De-novo geroprotector design

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Geroprotector is a therapeutics aiming at root causes of age-related diseases and as such capable of extending the life span of model animals and ultimately humans. The causes of aging are very ancient and evolutionary conservative. This means that the targets for the small molecule intervention can be identified using bio-informatics tools as the most conservative proteins in the pathways containing the largest number of genes responsible for the life span control. Together with the modern structure based drug discovery tools the approach should quickly lead to emergence of novel compounds readily testable in in-vitro models of age-related disorders and in life-span measuring experiments in multiple organisms. Once the preclinical efficacy and toxicity tests are finished the compounds can be commercialized as therapies against the specific sicknesses and as having a proven geroprotective effect. We report the specifics of the scheme and demonstrate the first de-novo design of potentially geroprotective compounds.