

# Design of pharmaceuticals of potential application in conformational diseases

Computer-Aided Strategies in  
Medicinal Chemistry

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Dipartimento di Scienza e Tecnologia del Farmaco



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## The Project

A large and diverse number of diseases are now recognized as 'conformational diseases'. Adoption of non native conformations by some proteins involved in a given cellular mechanism could lead to protein misfolding, i.e. cascade of reactions giving rise to aberrant protein polymerization. Among brain diseases due to misfolding and subsequent aggregation of proteins, AD is one of the most important also for its social implications.

In AD two types of deposit are to be found: intracellular neurofibrillary tangles containing paired helical filaments of Tau (PHF-Tau), and extracellular neuritic plaques consisting of fibrillar deposits of amyloid- $\beta$  peptide. Moreover also deposits of lithostathine have also been recently observed in the brain of patients with AD.

Given this scenario, there is nowadays a huge and increasing interest in the search for pharmaceuticals that can interfere with the protein aggregation pathway and thus prevent AD from occurring. A successful drug should a) interact with the defective protein and hence inhibiting its aggregation by blocking key proteinprotein contact, b) be specific for the undesirable protein associated with AD and c) cross the blood-brain barrier (BBB) to reach the brain.

The ultimate scope of this project is to design molecular structures of potential application in the AD therapy. To reach this aim a medicinal chemistry approach is used through the application of commercial and in-house computational tools.

## More details

The project will take place in the CASMedChem laboratory and in the Centro per l'Ottimizzazione di Molecole Bioattive at the Center of innovation of the University of Torino ([www.centro-innovazione.it](http://www.centro-innovazione.it))

Deadline admission exam subscription: about august-september 2009

The admission exam will take place in Torino

## Information

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