



LUND UNIVERSITY



UNIVERSITÀ DEGLI STUDI DI TORINO

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Faculty of Pharmacy  
Master Degree in Medicinal Chemistry

*“Discovery of new human DHODH inhibitors using a Structure-Based and a Ligand-Based Pharmacophore approaches.”*

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The Dihydroorate Dehydrogenase (DHODH) is an enzyme involved in the *de novo* biosynthesis of pyrimidine, i.e. DNA/RNA's building blocks. This biosynthetic pathway is particularly important in rapid proliferating cells such T cells and metastatic cells, involved in inflammation processes and cancer respectively. In this sense DHODH is an ideal target for developing new drugs. To block the activity of this enzyme is an important strategy for threatening disorders such Rheumatoid Arthritis and cancer, which still diseases without a definitive and efficient drug therapy. The aim of this Master Thesis project is to develop a model that will be used “to sieve” huge library of compounds, in order to discover new possible active molecules. The work will be achieved using new computational technologies and the resulting molecules will be bought in order to be tested using *in vitro* assays.