Title: **In silico study of the structure-activity relationship in a family of antitumor platinum(II) complexes.**

Student: Laia Casanova Farràs

Date: June 2014

Supervisor: Dr. Ángel Montaña Pedrero
Departament of Organic

There are many factors that force the scientists to keep working on the development of new platinum compounds as anticancer drugs, despite the success of cisplatin and also of the following generations of platinum complexes.

In this project, a chemical library of nine platinum(II) complexes having different organic functions in their ligands were selected in order to evaluate their structure-activity relationship.

Different parameters (like logP, logS, Connoly surfaces and volumes, etc, as well as topological parameters like ovality, electronic properties like electron densities, among other parameters) were calculated by using different software. Determination of structural parameters allows the evaluation of the drug likeness of a molecule and facilitates the rational design.

Finally, various comparisons among calculated parameters of complexes and their cytotoxic activity were carried out to withdraw some conclusions about structure-activity relationship. Some evidences about their structure were drawn but, we can not forget that they are approximations, it is therefore advisable to complement computational results with experimental data in order to ensure representative conclusions.

Keywords: Computer calculations, structural parameters, rational design, structure-activity relationship.