



AVIS DE SOUTENANCE DE THESE

Le Doyen de la Faculté des Sciences Dhar El Mahraz –Fès – annonce que

Mr **ALLOUI Mourad**

Soutiendra : **le Jeudi 29/10/2026 à 10H00**

Lieu : **FSDM – Centre Visioconférence**

Une thèse intitulée :

Conception in silico de nouveaux agents anticancéreux par intégration des approches 2D/3D-QSAR, docking moléculaire, dynamique moléculaire et étude de leurs propriétés ADMET

En vue d'obtenir le **Doctorat**

FD : Ressources Naturelles, Environnement et Développement Durable

Spécialité : Chimie-physique appliquée

Devant le jury composé comme suit :

Nom et prénom	Etablissement	Grade	Qualité
Pr. OUAMMOU Abdelkrim	Faculté des Sciences Dhar El Mahraz, Fès	PES	Président
Pr. CHALLIOUI Allal	Faculté des Sciences, Oujda	PES	Rapporteur
Pr. BOUAMMALI Boufelja	Faculté des Sciences, Oujda	PES	Rapporteur
Pr. TOUIMI BENJELLOUN Adil	Faculté des Sciences Dhar El Mahraz, Fès	PES	Rapporteur
Pr. SFAIRA Mouhcine	Faculté des Sciences Dhar El Mahraz, Fès	PES	Examineur
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2D/3D-QSAR, cancer, conception de nouveaux composés, docking moléculaire, dynamique moléculaire, propriétés ADMET.

In silico design of new anticancer agents through the integration of 2D/3D-QSAR, molecular docking, and molecular dynamics approaches, and investigation of their ADMET properties

Abstract :

Cancer remains one of the leading causes of mortality worldwide, as it can affect multiple organs and body systems, thus representing a major global public health challenge. Nevertheless, recent scientific advances have provided deeper insights into the molecular and cellular mechanisms underlying this disease, paving the way for more selective treatments, the development of personalized therapies, as well as novel strategies for prevention and early detection. These achievements have significantly contributed to reducing both the incidence and mortality rates associated with cancer.

In this context, Computer-Aided Drug Design (CADD) has emerged as a powerful theoretical tool that enables the identification of novel drug candidates in a faster, more rational, and cost-effective manner. The present thesis is situated within this framework, aiming to exploit *in silico* approaches for the rational design of potential anticancer agents with high therapeutic value.

The adopted methodology was carried out in several steps:

- Statistical analysis of molecular descriptors and molecular interaction fields (2D/3D-QSAR) to investigate structure–activity relationships in three different series of candidate molecules.
- Application of molecular docking to elucidate protein–ligand interaction modes and identify the most relevant binding sites.
- Implementation of molecular dynamics simulations to assess the stability of the protein–ligand complexes obtained from docking studies, thereby ensuring the reliability of the models.

The three applications provided reliable and predictive models that allowed the design of new biologically active compounds. The most promising molecules were subsequently subjected to drug-likeness filters and evaluated for their ADMET properties. The results of these analyses led to the identification of compounds with high affinity toward the selected enzymes and protein targets, highlighting their potential as future therapeutic agents.

Key Words :

2D/3D-QSAR, cancer, design of novel compounds, molecular docking, molecular dynamics, ADMET properties.