



Pole for Doctoral Studies
Center for Doctoral Studies Sciences, Technologies, and Medical Sciences

ANNOUNCEMENT OF DOCTORAL THESIS DEFENSE



M/. SADOQ Badr-Edine

**Will present their research work with the aim of earning a
Doctorate**

**Doctoral program: Science and Technique Engineering
Discipline: Biological Sciences**

Specialty: Nanobiotechnology, Microbiology, Bioinformatics

**On 12/05/2026 at 10H 00 at the Pr. Otman Filali Meknassi
Conference Hall, National School of Applied Sciences of Tangier,
UAE
Under the Theme**

**Evaluation of the antibacterial properties of metallic
nanoparticles, nanocomposites, and bioactive natural compounds
against pathogenic bacteria**

Front of the jury composed of :

First Name & Last Name	Establishment	Designation
Pr. BRITEL Mohammed Réda	ENSA of Tangier, UAE	President
Pr. EL RHALEB El Houssaine	FS of Rabat, UM5	Reviewer
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Pr. EL GALIOU Ouiam	FST of Tangier, UAE	Examiner
Pr. POWER Mary Deborah	CCMAR, University of Algarve, Faro, Portugal	Examiner
Pr. BOUAJAJ Adel	ENSA of Tangier, UAE	Co-Supervisor
Pr. MAURADY Amal	FST of Tangier, UAE	Supervisor

Host Research Structure: Laboratory of Innovative Technologies, National School of Applied Sciences of Tangier, Abdelmalek Essaadi University, Tetouan, Morocco

Abstract



Bacterial infections continue to pose significant challenges to public health and are causing massive alarm, prompting increased interest in alternative strategies for microbial control. Among the most promising candidates are metallic and metallic oxide nanoparticles (NPs), which exhibit diverse antibacterial mechanisms and hold considerable potential for addressing these challenges.

This thesis combines computational modelling, virtual screening, and experimental approaches to investigate the antimicrobial and antivirulence activities of metallic nanoparticles and phytochemicals targeting quorum sensing (QS) systems in *Pseudomonas aeruginosa* and other clinically relevant bacteria. The first part of this work examines metal and metal oxide nanoparticles, including AgNPs, ZnONPs and CuONPs, and their interactions with QS regulatory proteins in *P. aeruginosa*. Molecular docking and complementary bioinformatics analyses showed that these nanoparticles interact favourably with key QS enzymes and transcriptional regulators (LasI/R, RhlI/R and PqsA/R). ZnO nanoparticles displayed particularly strong binding profiles toward several targets, suggesting their capacity to interfere with signal synthesis and QS-controlled processes involved in virulence and biofilm formation.

The second part employed virtual screening to identify natural compounds with strong anti-QS activity. A curated library of 186 molecules from the *Stachys* genus was screened against the six major QS proteins of *P. aeruginosa*. Ten molecules demonstrated favourable ADMET properties and strong docking affinities, with chryso-splenetin, 5-demethoxyflavone, syringic acid, and a methoxylated flavone emerging as the most promising candidates for QS disruption. These results highlight new natural scaffolds for the development of antivirulence agents. The final part of the thesis explores the synthesis and antibacterial evaluation of graphene oxide–silver nanocomposites functionalized with PDDA. Extensive physicochemical characterization confirmed successful functionalization and improved stability.

Biological assays revealed that PDDA contributes directly to antibacterial performance, particularly against *Staphylococcus aureus*. This selective effect was further supported by molecular docking, which demonstrated stronger interaction of PDDA with the QS regulator AgrA of *S. aureus* compared to LsrR of *E. coli*. Altogether, this work provides a comprehensive evaluation of metallic nanoparticles, natural compounds and hybrid materials in the framework of bacterial communication and virulence. The combined findings from experimental and computational analyses support the exploration of alternative antimicrobial strategies and identify molecular targets that may inform future therapeutic development.

Keywords: Antibacterial nanoparticles, *Pseudomonas aeruginosa*, quorum sensing, silver nanoparticles, zinc oxide nanoparticles, graphene oxide, molecular docking, antibacterial activity, antimicrobial resistance.