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**Classical synthesis characterization of an organic- inorganic
hybrid material, including *in silico* and experimental studies
of its antioxidant, antibacterial, and anti-inflammatory**

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المخلص

يتناول هذا العمل تحضير وتوصيف مركبات هجينة جديدة تعتمد على الميلمين وحمض الفوسفوريك وحمض الهيدروكلوريك، بهدف تقييم نشاطها الحيوي. شملت الدراسة تحاليل فيزيائية-كيميائية (الذوبانية، النضجار، الطيفية) وأخرى بيولوجية. أظهرت النتائج أن المركبات تمتلك خصائص مضادة للتهاب ومضادة للكسدة، خاصة عند التركيزات المنخفضة، في حين لم تسجل أي فعالية ضد البكتيريا المختبرة. دعم التحليل الجزيئي بالحاكاة (in silico) الفرضية بوجود ارتباط فعال مع مستقبلات التهاب. وتبين أن المركب 1/2 يتمتع بنشاط أعلى من 1/1 خاصة من حيث التأثير المضاد للتهاب والكسدة.

الكلمات المفتاحية: مضاد للتهابات، مضاد للكسدة, MOE software , *In vitro*, *In vivo*, *In silico*, UV-vis spectrometry, IR spectrometry .

Abstract

This work focuses on the synthesis and characterization of new hybrid compounds based on melamine, phosphoric acid, and hydrochloric acid, aiming to evaluate their biological activities. The study included physico-chemical analyses (solubility, melting point, spectral) as well as biological tests. The results showed that the compounds possess anti-inflammatory and antioxidant properties, especially at low concentrations, while no antibacterial activity was observed against the tested bacteria. Molecular modeling (in silico) supported the hypothesis of effective binding with inflammatory receptors. Compound 1/2 demonstrated higher activity than 1/1, particularly in terms of anti-inflammatory and antioxidant effects.

Keywords:

MOE software, *In vitro*, *in vivo* and *in silico* studies, UV-Vis spectrometry, IR spectrometry, Anti-inflammatory, Antioxidant.

Résumé

Ce travail porte sur la synthèse et la caractérisation de nouveaux composés hybrides à base de mélamine, d'acide phosphorique et d'acide chlorhydrique, dans le but d'évaluer leurs activités biologiques. L'étude a inclus des analyses physico-chimiques (solubilité, point de fusion, spectroscopie) ainsi que des tests biologiques. Les résultats ont montré que les composés possèdent des propriétés anti-inflammatoires et antioxydantes, notamment à faibles concentrations, tandis qu'aucune activité antibactérienne n'a été observée contre les bactéries testées. La modélisation moléculaire (in silico) a confirmé l'hypothèse d'une liaison efficace avec les récepteurs de l'inflammation. Le composé 1/2 a démontré une activité supérieure à celle du 1/1, en particulier en ce qui concerne les effets anti-inflammatoires et antioxydants.

Mots-clés :

Logiciel MOE , *Etudes in vitro*, *in vivo* et *in silico* , UV-Vis spectrometrie, IR spectrometrie , Anti-inflammatoire, Antioxydant.

LIST OF ABBREVIATIONS

ATP: Adenosine triphosphate.

BSA: Bovine Serum Albumin.

COX-1: Cyclooxygenase-1.

COX-2: Cyclooxygenase-2.

DNA: Deoxyribonucleic acid.

DMF: Dimethylformamide.

DMSO: Dimethyl sulfoxide.

DPPH: 2, 2-diphenyl-1-picrylhydrazyl.

IL-1 β : Interleukin-1 bêta.

IL6: Interleukin 6.

IUPAC: International Union of Pure and Applied Chemistry.

MBC: Minimum bactericidal concentration. **MIC:**

Minimum Inhibitory Concentration. **MOFs:**

Metal-Organic Frameworks.

M/MeOH/ HCL: (1/1)

M/MeOH/ H₃PO₄: (1/2)

M/H₂O/H₃PO₄: (1/6)

NF- κ B: Nuclear Factor kappa B.

NSAIDs: Non-steroidal anti-inflammatory drugs.

PDB: Protein Data Bank et Program Database.

PRRs: Pattern Recognition Receptors.

ROS: reactive oxygen species.

SET: Social Engineering Toolkit.

TLRs: Toll-like receptors.

TNF- α : Tumor Necrosis Factor alpha.

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Abstract

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