بيوفارم Biopharm

The 5 th Biopharm Scientific Annual Meeting
BSAM5, Alger le 28 juin 2025

BSAM5 Biopharm Scientific Annual Meeting

CRAPC

جامعة هواري بومدين للعلوم والتكنولوجيا USTHB

MOLECULAR DOCKING INVESTIGATION OF METHANOLIC EXTRACT COMPOUNDS FROM *Ricinus communis* AGAINST MICROBIAL PATHOGENS

F. AGOUILLAL[1,2,3*], D. MANCER [2*], N. NASRALLAH [1]

[1]*Laboratory of Reaction Engineering, Faculty of Mechanical and Process Engineering, University of Science and Technology Houari Boumediene (USTHB), El Alia, BP32, Bab Ezzouar, 16111, Algiers, Algeria.*
[2] *Research Unit on Physicochemical Analysis – Fluid Media and Soil, URAPC-MFS, , Algiers, Algeria.*
[3] *Scientific and Technique Research Centre on Physicochemical Analysis, CRAPC, PB. 384, RP 42004 Bou-Ismail, Tipaza, Algeria.*
[4] *Laboratory of Transfer Phenomena, Faculty of Mechanical and Process Engineering, USTHB,*

Abstract

The present study aims to isolate and identify some constituents of *R. communis* leaves, their analytical characterization, and their in-silico bioactivities against selected bacteria and fungi to establish the QSAR model of the main active compounds [1].
We have evaluated the interaction of Lupeol, Amyrin, and both Ricinine and Quercetin derivatives against twelve protein receptors of six selected pathogens (*S.aureus, E.coli, P.aeruginosa, Bacillus subtilis, S.cerevisiae* and *A.niger*); Our results shows that for *S. aureus*, ricinin is more active on the 4URM receptor and for *Saccharomyces cerivisea*, Lupeol is more active on the P47026 receptor.

Key-words: *Ricinus communis, Molecular Docking, Antimicrobial activities.*

1-INTRODUCTION

Ricinus communis is a widely studied medicinal plant as source of several active compounds displaying interesting pharmacological activities due namely to Lupeol, Amyrin, and both Ricinine and Quercetin derivatives [2].

2-MATERIELS & METHODS

Methanolic extract of *R. communis* leaves was obtained by the conventional maceration process, then, characterized by FTIR-NMR structural elucidation strategy. The identified compounds were *in-silico* tested against twelve protein receptors of six selected pathogens (*S.aureus, E.coli, P.aeruginosa, Bacillus subtilis, S.cerevisiae* and *A.niger*). The virtual docking was carried out using SwissDock software after ligand preparation using Chimera. Visualization and quantitative analysis of protein/ligand interactions were performed using Biovia Discovery Studio.

3-RESULTS & DISCUSSION

The structural elucidation allows the identification of Ricinine (R), Lupeol (L), alpha-Amyrin(A), Quercetin (Q), Quercetin-3-O- β- D-glucopyranoside (QGP) and Quercetin-3-O- β- rutinoside (QR) in the obtained extract. The binding energies ΔG (kcal/mol) of the various Ligand-Protein complexes range from -5.31 for the L-6KZV complex of *E.coli* to -11.22 for the QR-4LXJ complex of *S.cerivisea*. For *S.aureus*, ricinin is more active on the 4URM receptor (DS=-6.94), quercetin is more active on the 3FRA receptor (DS=-8.42) and finally QGP is more active on 3FRA (DS=-9.6). For *Saccharomyces cerivisea*, Lupeol is more active on the P47026 receptor (DS=-8.53), aAmyrin and Quercetin-3-O-β-rutinoside are more active on the 4LXJ receptor with a DS=-8.77 and DS=-11.22 respectively.

4-CONCLUSION

The six studied compounds are synergically more active against *Staphylococcus aureus* and *Saccharomyces cerevisiae*; the two QSAR basic models that can be deduced and written as:

QSAR R.communis-S.aureus =-6.94 [R-4URM]-8.42 [Q-3FRA]-9.6 [QGP - 3FRA].
QSAR R.communis-S.cerivisea =-8.53 [L-P47026]-8.77 [A- 4LXJ] -11.22 [QR - 4LXJ].

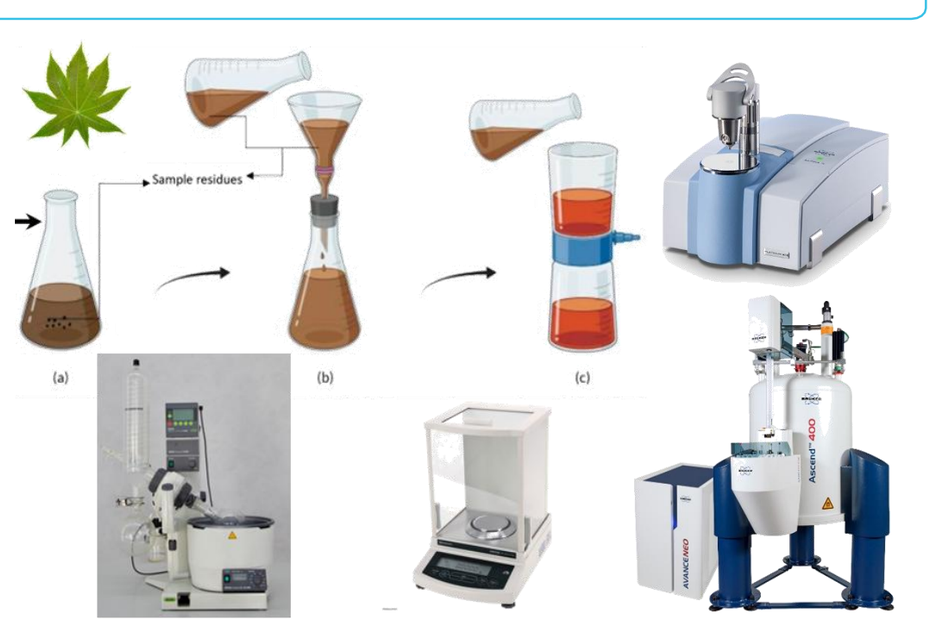

Figure 1: Steps of Methanolic extract of *R. communis* leaves & analytical charracterization

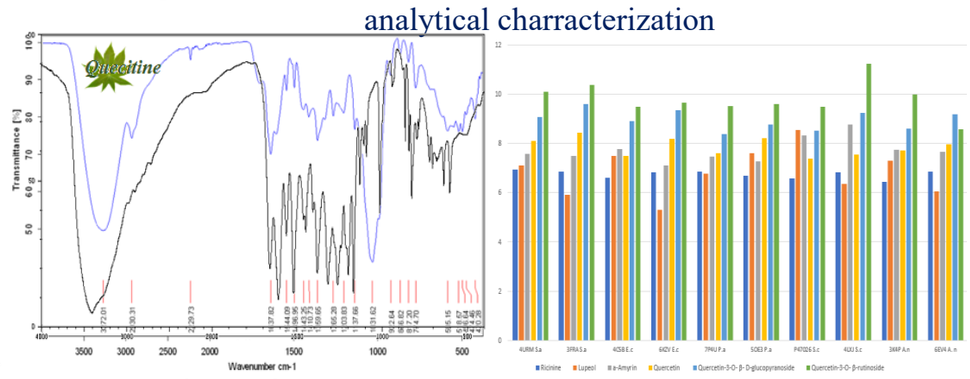

Figure 2: FTIR charracterization & *Insilico* results

Figure 3: 3 D visualisation of Ligand-Receptor complexes

References

[1] Tropsha, A., Isayev, O., Varnek, A. *et al.* Integrating QSAR modelling and deep learning in drug discovery: the emergence of deep QSAR. *Nat Rev Drug Discov* **23**, 141–155 (2024). https://doi.org/10.1038/s41573-023-00832-0

[2] Paniagua-Zambrana, N.Y., Bussmann, R.W., Kikvidze, Z. (2024). *Ricinus Communis* L. Euphorbiaceae. In: Bussmann, R.W., Paniagua-Zambrana, N.Y., Kikvidze, Z. (eds) Ethnobotany of the Mountain Regions of Eastern Europe. Ethnobotany of Mountain Regions. Springer, Cham. https://doi.org/10.1007/978-3-030-98744-2_248-1.