RESEARCH ARTICLE
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Bioinformatic and Experimental Evaluation of Compounds Targeting *Acinetobacter baumannii*

ABSTRACT

Background: This study combined cheminformatics and in vitro approaches to identify novel antimicrobial compounds against *Acinetobacter baumannii*, a major multidrug-resistant ESKAPE pathogen.

Methods: Initially, 350 000 compounds with three-dimensional structures and specific physicochemical properties were selected from the ZINC20 database. These were further filtered using DataWarrior software based on logP, logD, polar surface area, globularity, rotatable bonds, and ionizable nitrogen groups. Molecular docking analyses targeted *A. baumannii* methionyl-tRNA synthetase (MetRS). One of the available molecules with the highest predicted binding affinity from the in silico analyses was evaluated for antimicrobial activity.

Results: Data curation according to the specific physicochemical properties yielded a library of 530 compounds. Docking analyses validated critical binding residues (Tyr12, Leu10, and Trp251) within the crystal structure (PDB: 5URB). Ten candidate compounds exhibited binding energies between −7.1 and −6.2 kcal/mol—approximately twice as strong as methionine. Due to stock and logistical constraints, the fourth-ranked compound (ZINC000037626221) was purchased instead of the top three. In vitro antimicrobial susceptibility testing showed minimum inhibitory concentrations of 62.5 µg/mL for *A. baumannii*, 125 µg/mL for *Pseudomonas aeruginosa*, and ≥500 µg/mL for *Escherichia coli* and *Staphylococcus aureus*.

Conclusion: The results indicate that the selected compound displayed relatively specific activity against *A. baumannii* compared with the other bacteria tested. Overall, the findings confirm that combining computational screening with experimental validation can effectively narrow down large chemical libraries to a manageable set of promising candidates. This integrative approach highlights the potential of MetRS as a therapeutic target and provides a framework for discovering new antimicrobial agents against multidrug-resistant Gram-negative pathogens.

Keywords: *Acinetobacter baumannii,* antimicrobial, bioinformatics, cheminformatics, compound screening

What is already known on this topic?

- *Acinetobacter baumannii* is recognized as a multidrug-resistant ESKAPE pathogen and a critical global health threat due to its ability to cause severe hospital-acquired infections.
- Aminoacyl-tRNA synthetases, including methionyl-tRNA synthetase (MetRS), are essential enzymes in protein synthesis and have been proposed as promising antibacterial targets.
- Previous virtual screening studies against *A. baumannii* proteins have demonstrated that computational approaches can identify candidate compounds with strong predicted binding affinities.

What this study adds on this topic?

- This study applied a 2-step cheminformatics filtering strategy combined with molecular docking to generate a focused library of 530 compounds targeting *A. baumannii* MetRS.
- It experimentally validated one of the top-ranked candidates, demonstrating moderate but selective activity against *A. baumannii* compared with other bacteria.
- The findings highlight the potential of integrating in-silico screening with in vitro testing to accelerate the discovery of new antimicrobial agents targeting multidrug-resistant Gram-negative pathogens.

INTRODUCTION

Integrating computer-based approaches has become a highly effective strategy for identifying new antimicrobial drug candidates.[1] Contemporary computational approaches are transforming the drug discovery process by facilitating the straightforward identification of drug targets and drug candidates.[2,3] Today, antimicrobial drug discovery efforts against resistant pathogens are incorporating omics-based approaches—such as metabolic pathway analysis and structural bioinformatics on extensive protein and chemical libraries—as complementary strategies to conventional methods in the fight against antimicrobial resistance.[4]

Within this scope, it is possible to access large datasets and highly effective web- or operating system-based computational software and algorithms within the bioinformatics field.[5] The evaluation of new drug targets and candidates is of critical importance in the fight against bacteria with high drug-resistance potential. The combination of bioinformatics-derived data with in vitro analyses offers the potential to provide effective solutions for diversifying new and potential antimicrobial agents.

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Acinetobacter baumannii stands out as a global public health threat as one of the multidrug-resistant ESKAPE pathogens (including *Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa,* and *Enterobacter* spp.). This attention is largely due to its ability to cause hospital-acquired infections and to develop multiple mechanisms of antibiotic resistance.[6] *Acinetobacter baumannii* plays a role in a range of nosocomial infections—including pneumonia, bacteremia, urinary tract infections, meningitis, and wound infections—and is strongly associated with high morbidity and mortality rates, especially in intensive care units, often following prolonged hospital stays.[7] In this context, the World Health Organization has included *A. baumannii* on its list of antibiotic-resistant priority pathogens and classified it as "critical" according to the urgency of the need for new antibiotics.[8]

Aminoacyl-tRNA synthetases (aaRS) play a crucial role in protein synthesis by correctly matching with their corresponding amino acids. In most prokaryotes, tRNA aminoacylation is carried out by 20 different aminoacyl-tRNA synthetases, one for each amino acid. Targeting these enzymes has the potential to inhibit protein synthesis in pathogens.[9,10] This study aimed to use cheminformatics to screen novel compounds targeting methionine-tRNA synthetase (MetRS) in silico and to evaluate the antimicrobial activity of selected compounds against *A. baumannii* in vitro.

MATERIALS AND METHODS

In Silico Analyses

Database Curation: From among the millions of compounds available in the chemical database, those possessing three-dimensional structures and specific physicochemical properties were selected. These properties were evaluated to determine the compounds' potential as drug candidates. Lipinski's Rule of Five and similar physicochemical criteria—widely applied in mammalian drug design—served as initial guidelines. However, the unique cell wall architecture of bacteria can restrict chemical uptake, necessitating consideration of physicochemical features beyond classical rules.

In this context, the limited number of studies available—particularly on *Escherichia coli* and other Gram-negative bacteria—has indicated that certain physicochemical and structural characteristics improve the ability of compounds to penetrate Gram-negative cell walls. Based on these studies, recommended properties included: molecular weight ≤400, high polarity (logD ≤ 1), hydrophilicity (logP < 0), neutral or slightly positive charge (0 or +1), low three-dimensionality (globularity ≤ 0.25), high structural rigidity (≤5 rotatable bonds), low polar surface area (PSA < 90), and the presence of ionizable nitrogen groups (primary, secondary, or tertiary amines).

The chemical database was generated using a 2-step filtering strategy. In the first step, compounds from the ZINC20 database (https://zinc20.docking.org/) with three-dimensional structures, molecular weights between 200 and 400, near-neutral charges (0 or +1), and confirmed in-stock availability were selected. Compounds meeting these criteria were downloaded from the ZINC20 platform, and the second filtering step was performed using DataWarrior v5.5 software.

In this second step, the downloaded .sdf files were merged and saved in DataWarrior format. The software was used to calculate key parameters, including molecular weight, SMILES formulas, cLogP, cLogS, hydrogen-bond acceptor and donor counts, rotatable bond counts, and PSA. Compounds that fit the predefined physicochemical reference values were subsequently filtered and selected. Furthermore, chemicals with potentially toxic properties for mammalian cells (e.g., mutagenic, carcinogenic, or irritant) were excluded, whereas compounds containing $-NH_2$ or $-NH_3$ functional groups were preferentially retained.

This 2-step filtering process resulted in the establishment of a curated chemical database for subsequent bioinformatic analyses.

Molecular Docking Analysis

The crystal structure of *A. baumannii* methionine-tRNA synthetase was retrieved from the Protein Data Bank (RCSB PDB; https://www.rcsb.org/). Among the 4 structures resolved with amino acid ligands (6BQZ, 5URB, 5E3I, and 8G98), the 5URB structure (1.90 Å; Armstrong) was selected for further analysis because it showed the highest PDB validation score. For molecular docking, the selected protein structure was prepared using AutoDockTools v1.5.7[11] by removing water molecules, adding missing atoms, and assigning appropriate charges. Grid coordinates were defined for the protein's active site, and docking simulations were performed using AutoDock Vina and the free version of PyRx (https://pyrx.sourceforge.io/), which implements the same algorithms. Since the crystal structure of the MetRS protein (PDB: 5URB) contains the methionine binding site, this region was taken as the center for docking. The grid box coordinates were defined as follows:

center_x = −2.02440

center_y = 12.32793

center_z = −29.71518

size_x = 12.91765

size_y = 8.795413

size_z = 9.042616

Each ligand was docked in 10 independent runs and ranked according to its binding energy. Binding poses of

compounds exhibiting higher affinities than methionine were subsequently visualized and validated using PyMOL (https://pymol.org/2/).

In Vitro Analyses

Antimicrobial Susceptibility Testing: One of the available molecules with the highest predicted binding affinity from the in silico analyses was purchased and evaluated for antimicrobial activity against the reference *A. baumannii* strain (ATCC 19606), *E. coli* (ATCC 25922), *P. aeruginosa* (ATCC 27853), *and S. aureus* (ATCC 29213). The minimum inhibitory concentration (MIC) was determined by the microdilution method according to the Clinical and Laboratory Standards Institute (CLSI) M27-A standard.[12] The stock solution of the candidate compound was prepared at 1 mg/mL in DMSO, and the bacterial suspension density was adjusted to the McFarland 0.5 standard in sterile PBS. Using 96-well plates, the compound was serially 2-fold diluted in Mueller–Hinton broth (Sigma-Aldrich, St. Louis, MO) and inoculated with 10 µL of the bacterial suspension. Each plate included positive and negative bacterial controls as well as antibiotic controls (ampicillin and ciprofloxacin). The MIC values were determined both visually and spectrophotometrically at 450 nm after 18 hours of incubation at 37°C.

RESULTS

In Silico Analysis

A 2-step filtering process was applied using the ZINC20 database to create a chemical library with the desired physicochemical and structural characteristics. In the first step, compounds with three-dimensional structures, molecular weights between 200 and 400, near-neutral charges (0 or +1), and confirmed in-stock availability were selected; a total of 350 000 compounds meeting these criteria were downloaded from ZINC20. In the second step, more specific physicochemical and structural filtering was performed using the DataWarrior software. This filtering prioritized compounds with high polarity (logD ≤ 1), hydrophilicity (logP < 0), neutral or slightly positive charge (0 or +1), low three-dimensionality (globularity ≤ 0.25), high structural rigidity (≤5 rotatable bonds), low PSA (PSA < 90), and the presence of ionizable nitrogen groups. As a result of this 2-step filtering process, a final database of 530 chemical compounds was obtained. Among these chemicals, the top 10 compounds showing the strongest binding to MetRS protein were identified as ZINC000409427210, ZINC000952975349, ZINC000037626221, ZINC000095095731, ZINC000044699326, ZINC000096024198, ZINC000222406432, ZINC000095095729, and ZINC000095095731. The binding energies of these molecules ranged from −7.1 to −6.2 kcal/mol (Table 1). In contrast, the natural substrate of the target protein, methionine, exhibited a maximum binding energy of −3.8 kcal/mol. Accordingly, the selected compounds demonstrated approximately twice the binding affinity compared to methionine. Molecular docking studies revealed that among these, the compound coded as ZINC000409424224 exhibited the strongest binding to the target protein, with a binding energy of −7.1 kcal/mol (Figure 1). Analysis of the crystal structure of the target protein with methionine (PDB: 5URB) revealed that the strongest binding positions were Tyr12, Leu10, and Trp251. In addition, the $-NH_2$ group of methionine was observed to form hydrogen bonds with Leu10 and Asp49. Molecular docking analyses produced results highly consistent with the crystal structure (5URB), confirming Tyr12, Leu10, and Trp251 as the strongest binding positions and showing that the $-NH_2$ group of methionine formed a hydrogen bond between Leu10 and Asp49. These findings supported the accuracy of the analyses. Among the top compounds, ZINC000409424224, ZINC000409427210, and ZINC000037626221 showed their strongest interactions at the Leu10 amino acid position, while additional interactions involved Trp251, Ile295, Ala9, Tyr12, and Asp49 (Figure 2). Compared with the binding positions of methionine, these compounds exhibited strong interactions with critical residues such as Tyr12, Leu10, and Trp251, indicating their potential to inhibit the binding of methionine (the natural substrate) to the target protein (Figure 3).

Table 1. ZINC Codes, SMILES Formulas, and Binding Energies (kcal/mol) of the Top-Ranked Molecules Binding to the Target Protein Based on Molecular Docking Analyses

ZINC codes	SMILES	Affinity (kcal/mol)	Ki
ZINC000409424224	CC(=O)N1CCC[C@@H](n2cc(CN)nn2)C1	−7.1	6.16
ZINC000409427210	CC(=O)N1CCC[C@@H]1Cn1cc(CN)nn1	−6.8	10.23
ZINC000952975349	Cc1nnnn1-c1cccc(NC(=O)[C@@H](N)[C@@H](C)O)c1	−6.8	10.23
ZINC000037626221*	**C[C@H](NC(=O)[C@H](N)CC(N)=O)c1cccnc1**	**−6.4**	**20.12**
ZINC000095095731	NCc1nc(CC(=O)N2CCOCC2)no1	−6.4	20.12
ZINC000044699326	N[C@@H]1[C@H](O)[C@@H](O)[C@H](CO)O[C@H]1OCc1ccccc1	−6.3	23.82
ZINC000096024198	NCCn1nc(-n2cncn2)ccc1=O	−6.3	23.82
ZINC000222406432	N[C@@H](CO)C(=O)NCc1cccc(-c2nnn[nH]2)c1	−6.3	23.82
ZINC000095095729	NCc1nc(CC(=O)N2CCCC2)no1	−6.2	28.20
ZINC000095095731	NCc1nc(CC(=O)N2CCOCC2)no1	−6.2	28.20

*The molecule procured and tested in vitro.

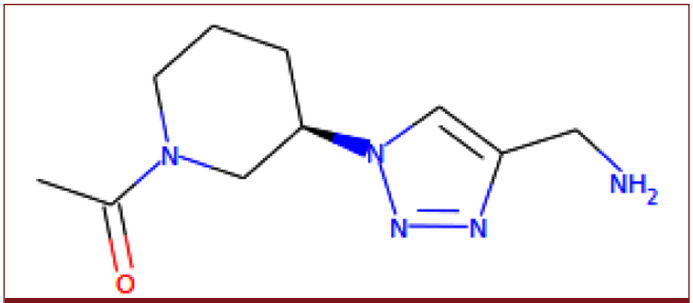

Figure 1. The structure of the compound coded as ZINC000409424224.

In Vitro Analysis

In the context of antimicrobial susceptibility testing, procurement issues arose for the top 3 molecules with the strongest predicted interactions—ZINC000409424224, ZINC000409427210, and ZINC000952975349—due to stock shortages or additional customs fees associated with international suppliers. Therefore, the fourth-ranked compound, ZINC000037626221 (Figure 4), was procured instead from Enamine (https://new.enaminestore.com/; Catalog No: Z594252176). The minimum inhibitory concentration (MIC) values of the compound were recorded as 62.5 µg/mL for *A. baumannii* (ATCC 19606), 125 µg/mL for *P. aeruginosa* (ATCC 27853), and ≥500 µg/mL for *E. coli* (ATCC 25922) and *S. aureus* (ATCC 29213). Although the inhibitory activity of the compound against the primary target organism *A. baumannii* was moderate, it was observed to exhibit relatively more specific activity toward *A. baumannii* compared to the other tested bacteria. Considering that this compound represented the fourth-strongest interaction in the in silico analyses, it is likely that the top 3 ranked compounds (ZINC000409424224, ZINC000409427210, and ZINC000952975349) may display similar or even higher inhibitory activity against *A. baumannii*.

DISCUSSION

In this study, both in silico and in vitro approaches were combined to identify compounds with stronger binding affinity to the target protein than its natural substrate, methionine. A 2-step filtering process was applied starting from the ZINC20 database: first, a broad selection based on molecular weight, charge, and stock availability, followed by a more selective screening using DataWarrior software according to parameters such as logP, logD, PSA, globularity, rotatable bonds, and ionizable nitrogen groups. This strategy yielded a library of 530 compounds characterized by high polarity and structural rigidity, well suited to fit the binding pocket of the *A. baumannii* MetRS protein (PDB : 5URB). The analysis

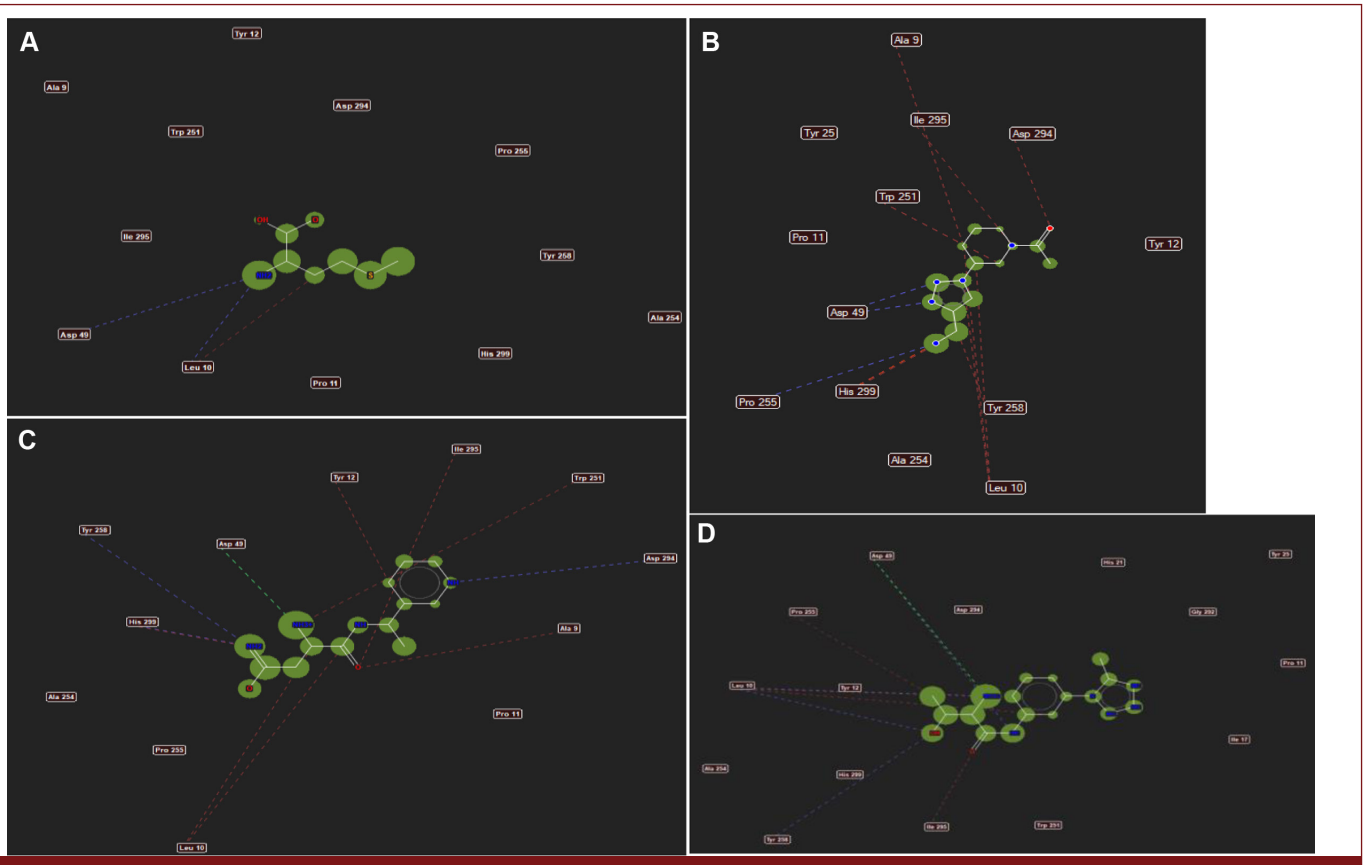

Figure 2. Interactions of (A) methionine, (B) ZINC000409424224, (C) ZINC000409427210, and (D) ZINC000037626221 with the *A. baumannii* MetRS protein (5URB).

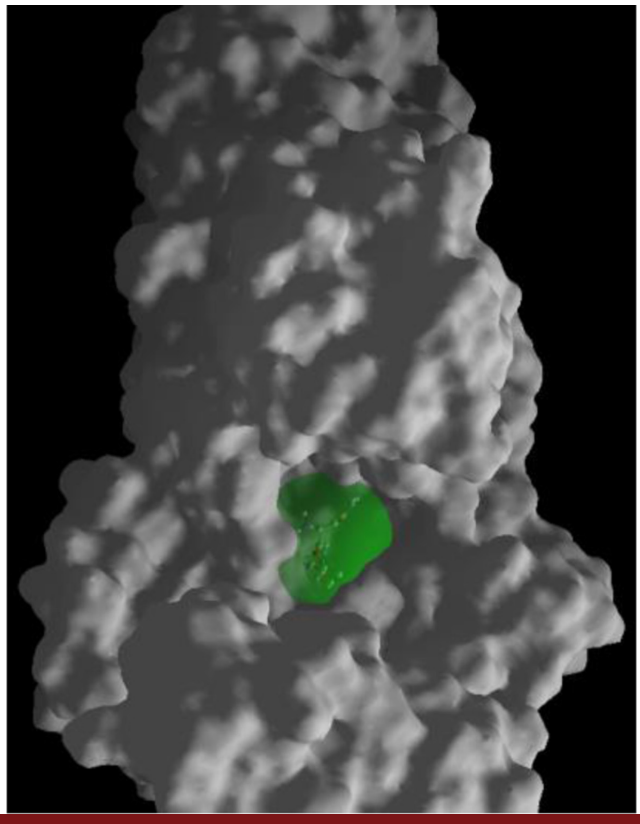

Figure 3. Appearance of docked compound ZINC000037626221 in the cavity of *A. baumannii* MetRS protein (PDB: 5URB).

showed strong interaction with the crystal structure with key binding residues of Tyr12, Leu10, and Trp251. In particular, the compound ZINC000409424224 exhibited the strongest interaction with a binding energy of −7.1 kcal/mol. Due to stock and logistical limitations, the top 3 predicted compounds could not be procured for in vitro testing, necessitating the evaluation of the fourth-ranked compound, ZINC000037626221. This compound showed moderate inhibition against *A. baumannii* with an MIC of 62.5 μg/mL and activity against *P. aeruginosa* at 125 μg/mL. These results suggest a selective activity profile of the compound against Gram-negative bacteria, particularly *A. baumannii*. Compared with methionine's binding energy of

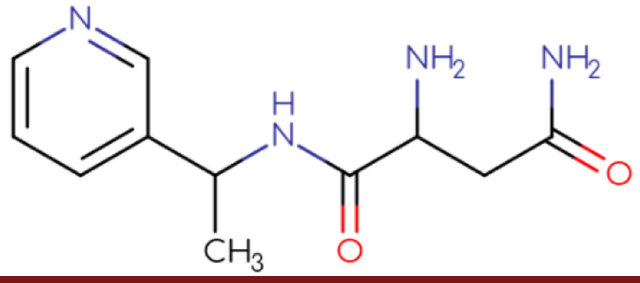

Figure 4. The structure of the procured compound ZINC000037626221 (Enamine: Z594252176) was tested for antimicrobial activity.

−3.8 kcal/mol, the selected compounds exhibited approximately twice the binding strength, indicating their potential to modulate the target protein's function.

The MetRS target has long been investigated in the literature using substrate mimetics and tRNA-competitive scaffolds (e.g., methionyl-adenylate analogues and diaryldiamine derivatives).[13-15] For instance, REP8839 was developed as a MetRS inhibitor for Gram-positive bacteria, and Met-AMP analogues mimic the activated intermediate of MetRS, thereby exerting inhibitory effects.[16,17] These compound classes provide valuable starting points for structure-based re-targeting and virtual screening of *A. baumannii* MetRS.[18] Consequently, the structural similarity between the docking-filtered compounds and known MetRS inhibitor chemotypes in the literature offers a strong rationale for future lead optimization efforts.

Comparable approaches have also been reported for other Gram-negative pathogens (e.g., *P. aeruginosa*, *K. pneumoniae*), where thousands of compounds have been screened and validated in vitro against essential targets such as aaRS enzymes and lipid A biosynthesis pathways.[19] This body of work underscores the importance of chemoinformatics filtering in selecting viable candidates despite the outer membrane barrier and efflux pumps characteristic of Gram-negative bacteria.

Other virtual screening studies have been assessed for different *A. baumannii* targets in the literature. For example, Swain et al[20] found scores ranging from −8.7 to −9.8 kcal/mol for the SecA protein, while Bhati et al[21] screened thousands of compounds against the DHPS enzyme and validated their results using MM/PBSA analyses. Likewise, Zoghlami et al[22] identified LpxC inhibitors through structure-based virtual screening and subsequently confirmed their activity in vitro. Collectively, these studies indicate that virtual screening scores in *A. baumannii* typically fall within the −6 to −10 kcal/mol range and that some selected candidates display measurable in vitro activity.

Nevertheless, it should be recognized that docking scores do not directly translate to biological activity; factors such as membrane permeability, metabolic stability, and efflux mechanisms can strongly influence in vivo efficacy.[23] Therefore, subsequent ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiling, molecular dynamics simulations, and MIC validation using different clinical isolates are recommended, as these represent the main limitations of this study.

CONCLUSION

In conclusion, the study used chemoinformatics tools to distill millions of database entries into a unique set, whose inhibitory potential was assessed both in silico and in vitro. These findings underscore the power of integrating computational and experimental approaches to discover new

drug candidates, and further in vitro testing will be highly valuable.

Data Availability Statement: The data that support the findings of this study are available on request from the corresponding author.

Ethics Statement: Ethical approval and patient consensus were not necessary

Peer-review: Externally peer-reviewed.

Author Contributions: Concept – E.M., E.Y.D.; Design – E.M., E.Y.D.; Supervision – E.M., E.Y.D.; Resources – E.M., E.Y.D.; Materials – E.M., E.Y.D.; Data Collection and/or Processing – E.M., E.Y.D.; Analysis and/or Interpretation – E.M., E.Y.D.; Literature Search – E.M., E.Y.D.; Writing – E.M., E.Y.D.; Critical Review – E.M., E.Y.D.

Declaration of Interests: The authors have no conflicts of interest to declare.

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