GENERAL MEDICINE
ISSN:1311-1817

ISSN: 1311-1817
Volume 28, Issue 06, June, 2026

Chemical Extraction for the Sodium 4-amino-2-(2,3-dioxido-2H-thiopyran-5-yl)-4H-hiochromene-3,5,7-tris(olate) and isolated from Allium sativum against multidrug-resistant Acinetobacter baumannii

Fatima Waleed Abdul-ameer[1], Mohammed Abdul-Imam Almazini[2], H. N. K. AL-Salman[3*]

Biology Department, College of Science, University of Basrah, Iraq[1,2]
Pharmaceutical Chemistry Department, College of Pharmacy, University of Basrah, Iraq[3]

Corresponding Author: 3*

ABSTRACT— The compound 4-amino-2-(2,3-dioxido-2H-thiopyran-5-yl)-4H-thiochromine-3,5,7-tris(oleate)sodium was isolated from garlic (Allium sativum) for its resistance to multidrug-resistant Acinetobacter baumannii. The garlic-derived compound was characterized using analytical physics techniques, specifically carbon-13 NMR and 1H-NMR spectroscopy, as well as GC-mass spectroscopy and FTIR to validate its structure. The bactericidal activity of various bacterial cells can be enhanced using pharmaceutical preparations that achieve physiological homeostasis by eliminating both pathogens and bacterial cells. However, studies investigating this type of reaction using 4-amino-2-(2,3-dioxido-2H-thiopyran-5-yl)-4H-thiochromine-3,5,7-tris(oleate)sodium as a novel derivative are rare. Therefore, in this study, the evaluate the effects of this novel compound on colony-forming unit (CFU) cells involved in bacterial activity. An increase in the bactericidal activity of Acinetobacter baumannii was observed, as evidenced by the significant elimination of this bacterium. A statistically significant increase ($p<0.0001$) in bacterial cell killing was recorded. Further analyses revealed that sodium 4-amino-2-(2,3-deoxydo-2H-thiopran-5-yl)-4H-thiochromine-3,5,7-tris(oleate), extracted from garlic (Allium sativum), (This will be addressed in future studies), significantly modulates the levels of inflammatory cytokines such as tumor necrosis factor-alpha (TNF-α), interleukin-2 (IL-2), interleukin-1 beta (IL-1β), and interleukin-17 (IL-17) in the supernatant of RAW macrophage cell cultures. (In future studies) 264.7. Based on the above, sodium may enhance the 4-amino-2-(2,3-deoxydo-2H-thiopyran-5-yl)-4H-thiochromine-3,5,7-tris(olate) complex, which promotes the cytotoxic activity of Acinetobacter baumannii bacteria by increasing reactive oxygen species (ROS) and cell size.

KEYWORDS: Allium sativum, multidrug-resistant, Acinetobacter baumannii

DOI:
06.10562/GM.30.06.2026.01

Introduction

Medicinal plants (MPs) are plants that contain biologically active substances of therapeutic value or serve as raw materials for the synthesis of pharmaceutical drugs. These substances may be found in different parts of the plant, including leaves, roots, seeds, or flowers. The therapeutic effects of medicinal plants are mainly due to their secondary metabolites, such as alkaloids, flavonoids, tannins, and phenolic compounds, which possess antimicrobial, antioxidant, and anti-inflammatory activities [16], [2].

In addition, compounds produced from plants have shown significant potential for inhibiting microbial growth and combating drug-resistant infections. Many plants are used as food additives, condiments, and aromatic or cosmetic compounds [7], [4].

for example, Pharmacological Properties of Garlic (Allium sativum L.) It is a bulbous herb that has been utilized as a natural treatment for a number of illnesses since ancient times. It is commonly used as a spice, food additive, and medicinal plant and is a member of the Alliaceae family [38]. Garlic's medicinal properties are mainly attributed to bioactive sulfur compounds such as allicin, diallyl trisulfide, diallyl disulfide, vinyldithiins, and S-allylcysteine [19].

Recent studies indicate that these sulfur compounds contribute to the numerous health benefits of garlic, including its antibacterial, antifungal, and anticancer properties, as well as its ability to lower blood pressure, protect the heart, prevent atherosclerosis, lower cholesterol, and prevent diabetes and rheumatism. The many therapeutic applications of garlic products, whether they are fresh or processed (extracts, powder, or oil), emphasize the importance of garlic as a natural agent with broad efficacy and low toxicity. [34].

For a very long period, it was difficult to define what bioactive chemicals were. The term "bioactive" is described in only few instances. It is made up of two words: active and bio-. In terms of etymology, the word "active" comes from the Latin word "activus," which means dynamic and full of energy, while bio- comes from the Greek word "bios," which means life. [21].

Secondary metabolites that are abundant in plants are called bioactive substances. Isolated polysaccharides, phenols, terpenes, and alkaloids found in these therapeutic plants exhibit a range of properties, such as anti-inflammatory, antioxidant, stress-resistant, healing, and even the capacity to alter immunological pathways [18]. They have even demonstrated resistance to a number of chronic conditions, including diabetes, cardiovascular disease, neurological diseases, and even shown promise in the treatment of cancer. The majority of the substances have demonstrated anti-oxidative qualities, which aid in improved cell repair, relatively reduced cell damage, and heightened resistance to oxidative stress. [35].
Bioactive substances are essentially secondary metabolic products derived from plants that have either toxicological or therapeutic effects on humans and animals based on their structure and function. [35].

About 2000 physiologically active substances can be found in garlic, such as volatile, water-soluble, and oil-soluble organosulfur compounds (such as Diallyl sulfide (DAS), Diallyl disulfide, DADS, and Diallyl trisulfide (DATS)), essential oils, dietary fiber, sugars (32%), flavonoids, and pectin. [13]. The authors acknowledge the assistance of the College of Pharmacy, University of Basrah, for offering them laboratory facilities. We would like to acknowledge the Microbiology Laboratory staff at Basrah Teaching Hospital for their help in providing as well as characterizing the clinical isolates used in this study. The writers have no conflicting interests.

Furthermore, as illustrated in Figure 1, recent research has established the antibacterial, antioxidant, and other biological activities of garlic essential oil as well as its effects on human health, including its anticancer, hypoglycemic, and anti-inflammatory qualities. [23].

GENERAL MEDICINE
ISSN:1311-1817
ISSN: 1311-1817
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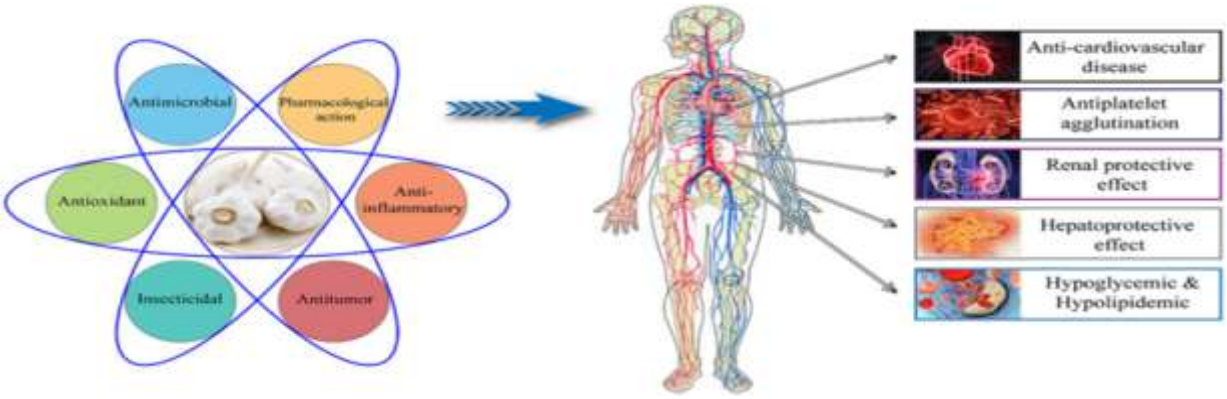
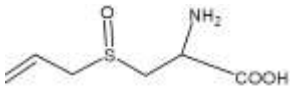
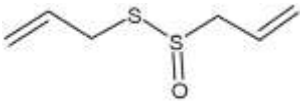
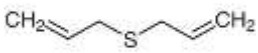
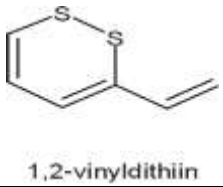
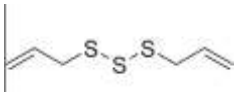


Figure 1: Garlic essential oil's biological function and impact on human health. In 2023, [23].

Table 1. Garlic's biological active chemicals' chemical makeup and biological roles.

Biological active compound	Chemical structure	Biological functions	References
Alliin	 S-allylcysteine sul foxi de (Al liin)	Antioxidant Antimicrobial Anticancer	[14], [43]
Allicin	 Dia llylthi osulfi nate(Al Lic in)	Anticancer Anti-inflammatory Antimicrobial Antioxidant Cardioprotective Imunomodulatory	[12]
diallyl sulfide (DAS)		Anticancer Antimicrobials Antioxidant Antithrombotic	[17], Suman & Shukla, 2016)
DADS	 Diallyl disulfide (DADS)	Anti-inflammatory, Antioxidant, Anticancer, Regulation of Metabolism, Detoxifying effects, Antimicrobial Activity, Antifungal Activity,	[30], [37]

		Antiviral Activity, Cardiovascular protection, Neuroprotection	
1,2-vinyldithiin	 1,2-vinyldithiin	Antimicrobials, Antioxidants, Antithrombotic	[39]
Diallyl trisulfide (DATS)		Antioxidant, Anticancer, Cardiovascular protection	[33]

Result and Discussion

Physical Properties of the extracted compound

Table 1 shows the recorded physical properties of the extracted compound, which include molecular formula, molecular weight, melting point, appearance, and percentage yield

Table 1: Physical Properties of the extracted compound

Compd.	Molecular formula	Molecular weight(g/mol)	Melting point (°C)	Appearance	Yield (%)
Thiochromene	$C_{14}HNS_2O_5(Na)_5$	426	349.5-350°C	Yellow powder	100

FT-IR of extracted compound thiochromene

There is no generally defined frequency value for the C–S bond in the infrared (IR) spectrum because it lies in the fingerprint region between 1400–400 cm^{-1}, which is highly specific to each compound. Therefore, absorption bands in this region are typically weak but unique, making them difficult to identify conclusively compared to other functional groups. Additionally, the aromatic C–N bond exhibits stretching vibrations in the range of approximately 1200 to 1350 cm^{-1}. Furthermore, the N–H bond frequency of compound Sodium 4-amino-2-(2,3-dioxido-2H-thiopyran-5-yl)-4H-hiochromene-3,5,7-tris(olate) lies in the range of 3200 to 3500 cm^{-1}. The C–O bond stretching vibration frequency in the infrared spectrum lies in the region of 1210–1320 cm^{-1}. Moreover, the sp^2 hybridized C–H stretching bonds of alkenes show absorption in the range of 3000–3100 cm^{-1}. The C–C bond stretching vibration frequency appears as a weak band in the fingerprint region, i.e., between 1200 and 800 cm^{-1}, and often overlaps and is difficult to determine precisely due to its weakness. Finally, the C=C bond stretching vibration frequency in aromatic compounds typically lies in the range of approximately 1600–1585 cm^{-1}, with another range appearing between 1500–1400 cm^{-1} as a result of intra-ring C–C stretches. The values of the characteristic bands observed in each spectrum are presented in Figures 1.

GENERAL MEDICINE
ISSN:1311-1817
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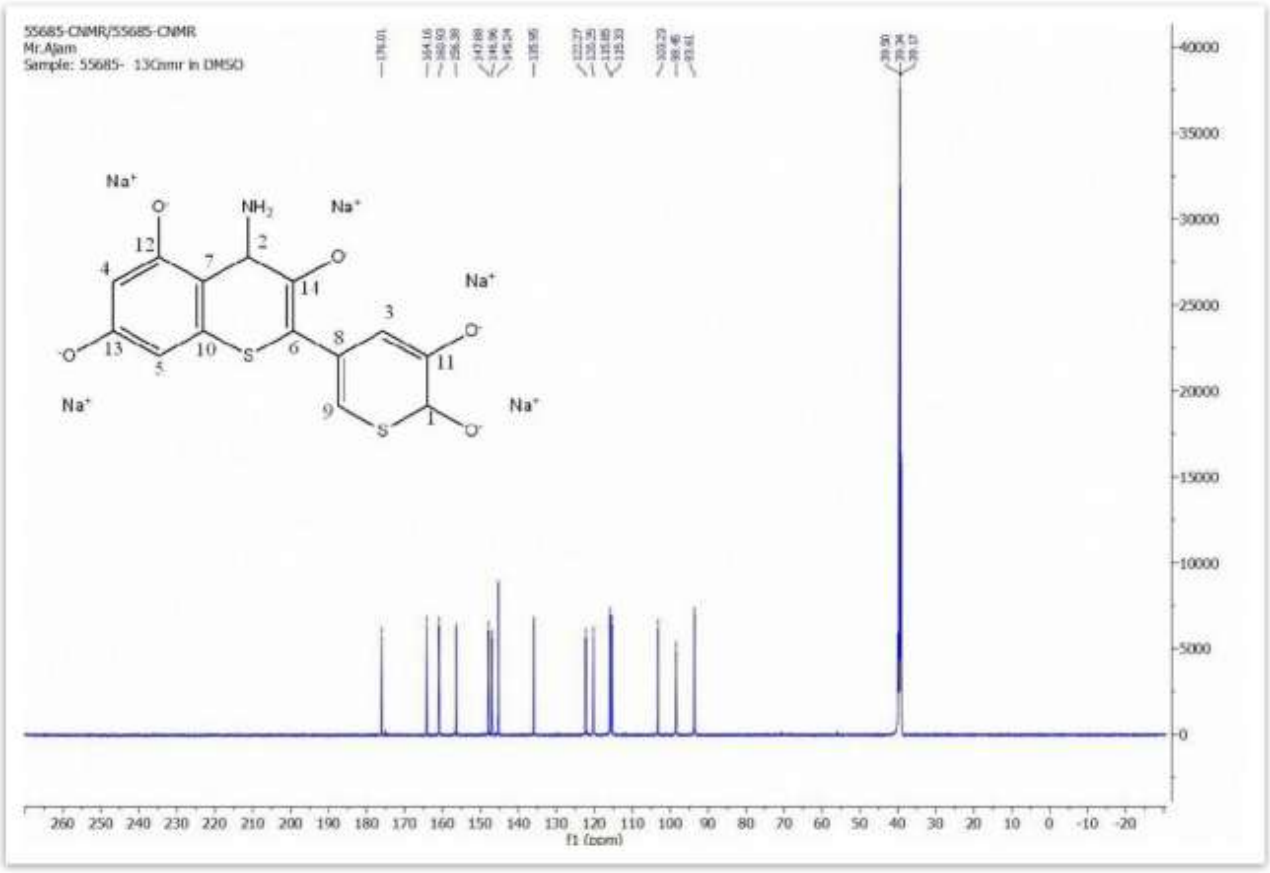

Figure 1: FT-IR spectrum of thiochromene

NMR ^{13}C-NMR spectra of extracted compound thiochromene

In the (^{13}C-NMR) Spectrum of thiochromene Figure 3 illustrates the carbon-13 nuclear magnetic resonance (^{13}C-NMR) spectrum of thiochromene. The spectrum is characterized by the appearance of the signals as shown in Table 2: In ddition, Carbon atoms 6 and 7 have similar environments; therefore, they are expected to show a single signal.

Table 2: ^{13}C-NMR data of thiochromene

Comp.	Chemical shift ppm												
	C 1	2	3	C 4	C 5	C 6	C 7	C 8	C 9	C 10	C 11	12	C 13
thiochromene	9 3.61	8.45	15.85	1 20.25	1 22.27	1 35.95	45.24	1 46.96	1 47.88	1 56.38	1 60.93	64.16	1 76.01

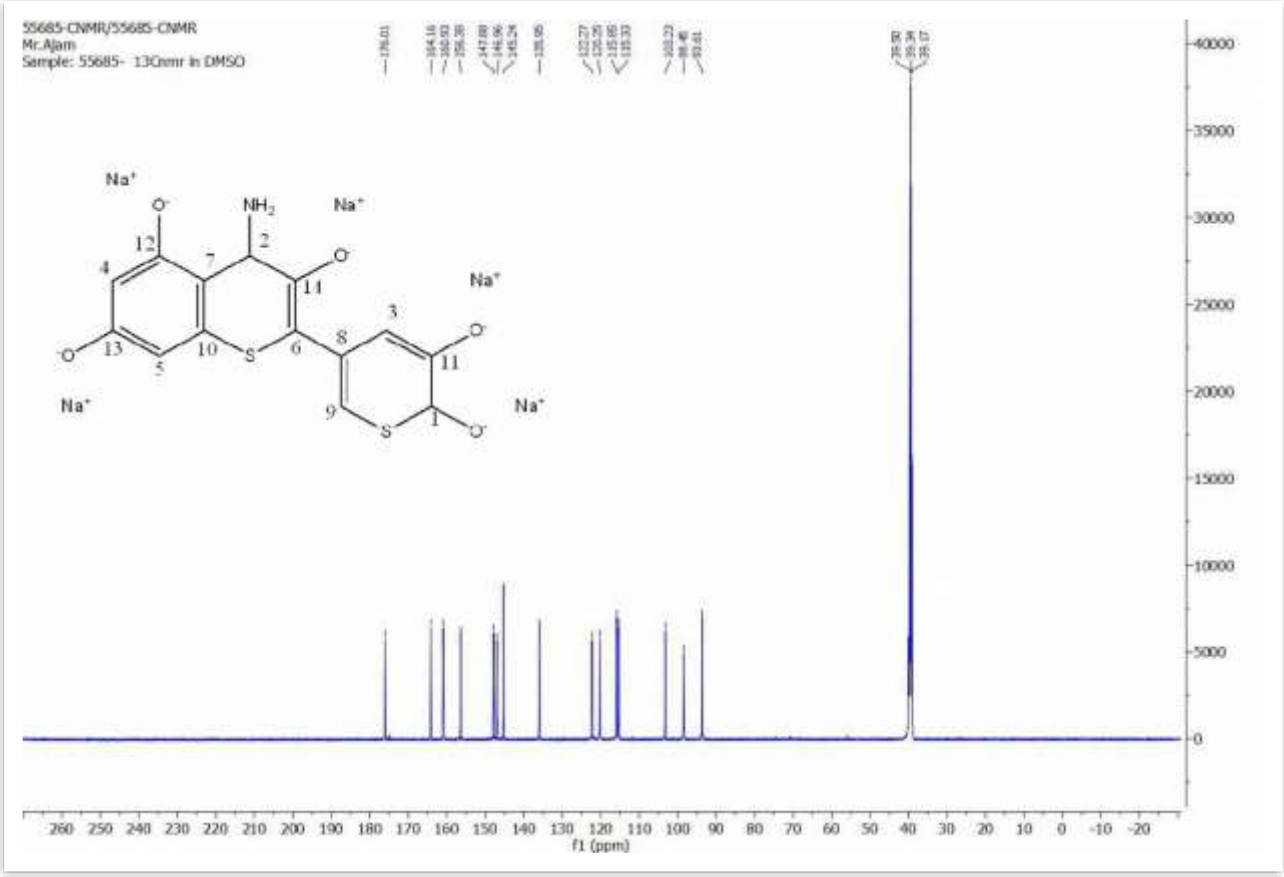

Figure 2: The (^{13}C-NMR) Spectrum of thiochromene

NMR ^{1}H-NMR spectra of extracted compound thiochromene

The (^{1}H-NMR) Spectrum of thiochromene Figure 4.3 illustrates the proton nuclear magnetic resonance (^{1}H-NMR) spectrum of thiochromene. The spectrum is characterized by the appearance of the following signals, as shown in Table 3.

Table3: ^{1}H-NMR data of thiochromene

compound	Chemical shift ppm						
	NH_2	H2	H3	H4	H5	H6	H7
thiochromene	3.8	5.08	6.18	6.40	6.89	7.54	7.70

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ISSN:1311-1817
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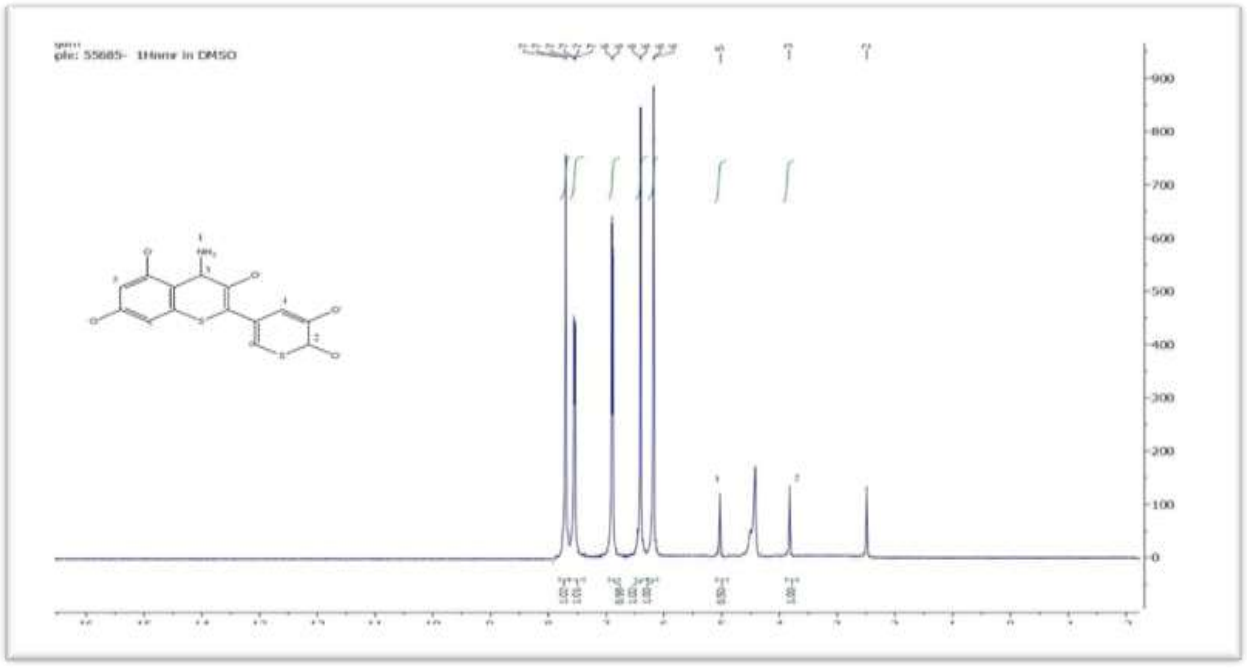

Figure 3: The (^{1}H-NMR) Spectrum of thiochromene

Mass Spectra of extracted compound thiochromene

The observed molecular weight of the synthesized compounds is identical to the calculated molecular weight. That indicates the compounds are correctly prepared, as in Table (4) and Figure (4).

Table 4: Mass spectra of thiochromene

M/Z	**53**	**69**	**108**	**137**	**222**	**254**	**300**	**333**
A	$C_3H_3O^+$	$C_4H_5O^+$	$C_6H_4O_2^+$	$C_7H_5O_3^+$	$C_{12}H_6O_3S^+$	$C_{12}H_6O_4S_2^+$	$C_{13}H_8O_6S_2^{\bullet+}$	$C_{14}H_8NO_5S_2$

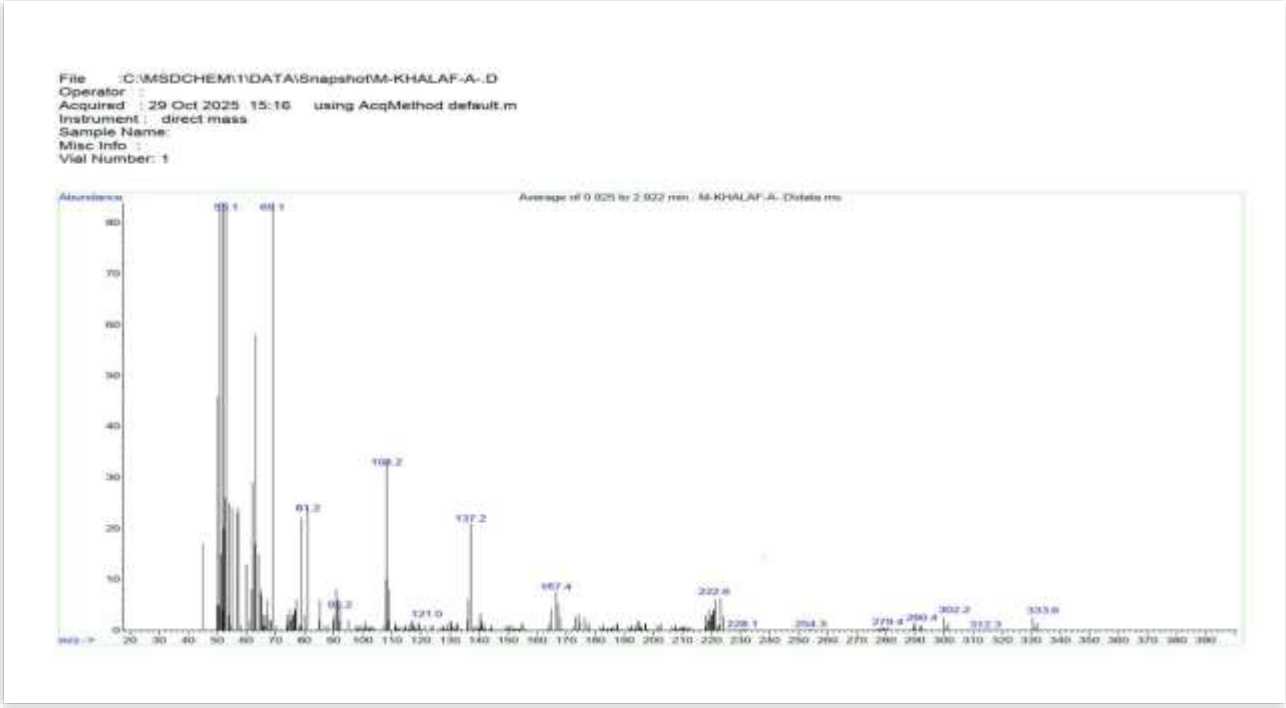

Figure 4: The Mass spectra of thiochromene

Antibacterial Activity of compound against *Acinetobacter baumannii*

The results showed the ability of thiochromene sample to inhibits *Acinetobacter baumannii*. The results was concentration dependent manner as indicated in Figure 5.

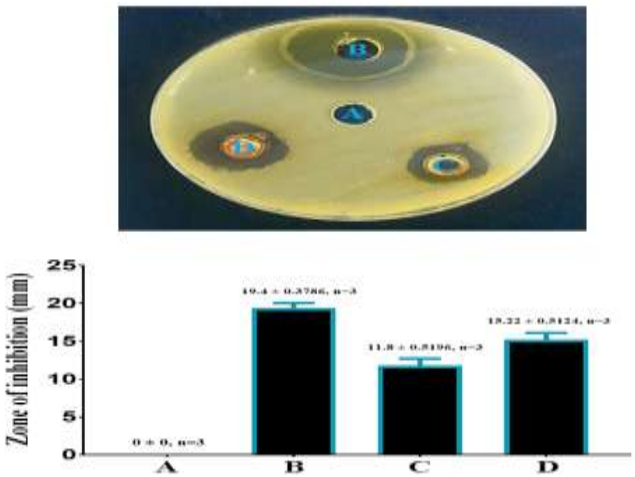

Figure 5: Antibacterial activity of (x sample) against *Acinetobacter baumannii*. A, Negative Control. B, Positive control. C, x sample at concentration 250 µg/mL. D, x sample at concentration 500 µg/mL.

Drug likeness and ADMET predictions

The physicochemical properties, toxicity, absorption characteristics, and metabolism of compound (Thiochromene)and its derivatives have been analyzed in this study. The data given give a detailed account of the possible uses of these compounds in future medicines. Toxicity (LD50) and Graphical Analysis: The acute toxicity (LD50) value of compound Thiochromene was plotted against DrugBank data. Its LD50 value was also compared with those of other compounds in this database [9], [25].

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The compound is noted to fall with moderate LD50 which indicates neither too toxic nor non-toxic. This suggests that the compound can be useful for therapeutic applications requiring controlled doses or conditions which need low toxicity. According to the data in table 5, Thiochromene has 449.30 daltons as molecular weight and -16.91 as logP value. The compound has a low tendency to dissolve in non-aqueous solvents but is likely to be soluble in aqueous ones. The significant hydrogen bond acceptor (8) and donor (1) values suggest that this compound may have an enhanced ability to interact with biological molecules, thus enhancing its biological activity in cells and tissues. Based on the findings of [5] shown in Table 6, the Thiochromene compound has good intestinal absorption (0.92) and good oral bioavailability (0.87) of the compound. As a proof that the compound is absorbed efficiently through the gut and reaches systemic circulation by way of oral dosing.

The aqueous solubility of -0.64 indicates that there is a good capacity to move within aqueous biological environments that favour distribution. Moreover, the cell permeability values indicate the capacity of a compound to cross cellular membranes and further enhances their potential biological efficacy. Table 7 shows that thiochromene interacts with cytochromes such as CYP1A2, CYP2C9, and CYP3A4. These enzymes are important for drug metabolism.

This compound has a moderate effect on these enzymes and therefore needs further evaluation to assess any actions with other drugs. Interactions like this may reduce the drug's effectiveness when used in combination with other drugs. According to the Radar Plot, the pharmacological properties of (thiochromene) such as Blood Brain Barrier Penetrability, Cardiac Toxicity (hERG), Oral Bioavailability, Aqueous Solubility and Toxicity are as shown in Figure 7. The radar model suggests that the compound has high attributes of aqueous solubility and bioavailability, although has relatively less toxicity which indicates a good PK profile. This image suggests that the compound exhibits properties similar to those of a drug, indicating that it could be an ideal candidate to be developed [24].

Table 5: Drug-likeness descriptors: Physicochemical properties of Thiochromene

Property	Value	Drug Bank Percentile	Units
Molecular Weight	449.30	75.03%	Dalton
LogP	-16.91	0.27%	log-ratio
Hydrogen Bond Acceptors	8.00	82.36%	#
Hydrogen Bond Donors	1.00	36.68%	#
Lipinski Rule of 5	4.00	63.80%	# of 4
Quantitative Estimate of Drug Likeness (QED)	0.42	35.98%	
Stereo Centers	2.00	68.86%	
Topological Polar Surface Area (TPSA)	120	83.09%	Å^2

Table 6: ADMET Absorption parameters for Thiochromene Derivatives

Property	Value	Drug Bank Percentile	Units
Human Intestinal Absorption	0.92	27.57%	-
Oral Bioavailability	0.87	64.29%	-
Aqueous Solubility	-0.64	87.63%	Log (mol/L)
Lipophilicity	0.93	40.95%	log-ratio
Hydration Free Energy	-7.70	69.17%	kcal/mol
Cell Effective Permeability	-5.34	29.66%	Log (10^-6 cm/s)
PAMPA Permeability	0.37	28.23%	Log (10^-6 cm/s)
P-glycoprotein Inhibition	0.25	64.02%	-

Table 7. ADMET Metabolism parameters for Thiochromene derivatives

Property	Value	Drug Bank Percentile
CYP1A2 Inhibition	0.19	69.25%
CYP2C19 Inhibition	0.26	69.17%
CYP2C9 Inhibition	0.36	85.15%
CYP2D6 Inhibition	0.03	44.75%
CYP3A4 Inhibition	0.35	74.33%
CYP2C9 Substrate	0.29	77.01%
CYP2D6 Substrate	0.17	62.66%
CYP3A4 Substrate	0.41	43.00%

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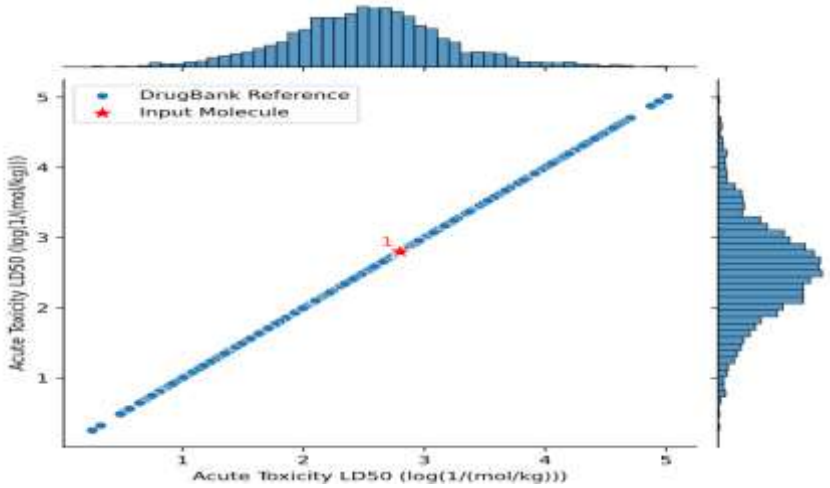

Figure 6: Relationship between Acute Toxicity (LD50) of the Input Thiochromene and Drug Bank Reference: Distribution of LD50 for a Set of Compounds.

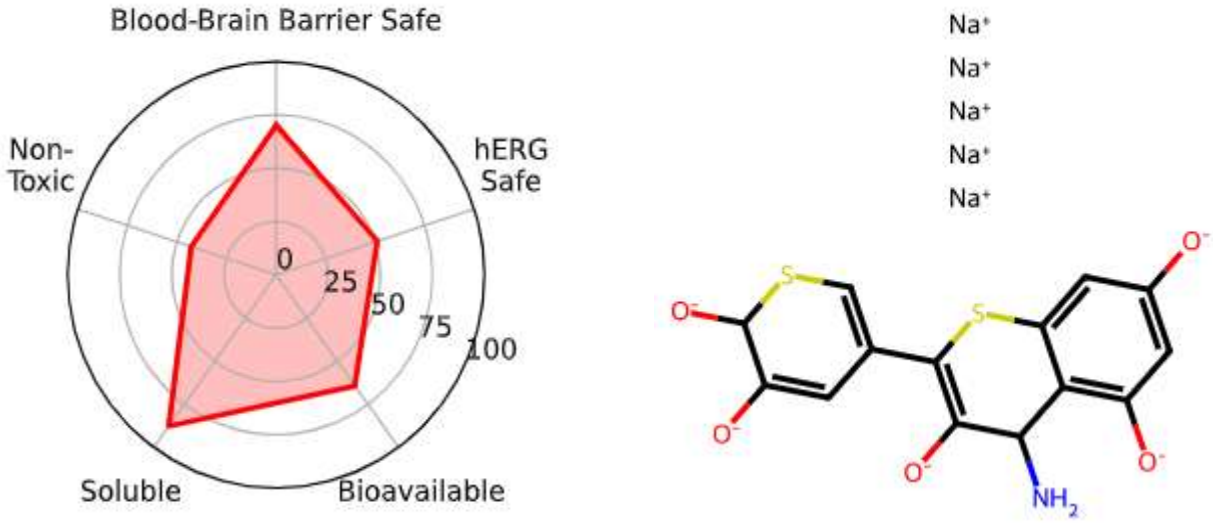

Figure 7: Radar model of the predicted Thiochromene derivatives

Molecular Docking for Antibacterial

As observed from Table 8 and Figures 8, 8DK1 and 8SCA Receptor (Thiochromene) (PDB ID: 8DK1) of (PDB ID: 8IOM) docking results [6]. The Noval Thiochromene Ligand Molecular Docking Results Interacting with the Receptors of A. Pseudomonas, Acinetobacter, and Stenotrophomonas Mutants show great potential. The ligand binding scores are evident, with A at -7.1312 kcal/mol. The binding energies of A. baumannii, P aeruginosa and S. are −7.0802 kcal/mol, −7.0613 kcal/mol, and −6.9463 kcal/mol, respectively. The mutants showed strong binding to the active sites of these pathogens. The RMSD values, which reflect the proximity of the docked conformation to the reference structure, range from 1.7121 Å for A. The distance is 1.6310 A for P. aeruginosa and 1.5510 A for S. Deviants The binding mode of the ligand at the receptor active site appears to be stable and reasonable as all the above RMSD values are below 2 Å, which is generally considered acceptable. The ligand is making important interactions with LYS, PHE etc in all three bacterial receptors [42].

The distance between them has been found to be in the range of 2.89 Å to 4.03 Å suitable for H-bonding. Most of the interactions involve H-bonds (H-donor and H-acceptor), which stabilize the ligand-receptor

complex. The total binding energy value of A is -34.5465 kcal/mol The binding energy for haumannii was -36.5330 kcal/mol, -33.0160 kcal/mol for P. aeruginosa, S with -30.1215 kcal/mol. mutants These values show a strong binding but S. The total binding energy of the mutants are slightly lower, this may imply ligand interaction with S. Mutants exhibit lower potency than the other two bacteria. The structural differences in the active sites may be one reason or the presence of some mechanism reducing binding indicates the cause of this.

A. thiochromene looks to be a promising antimicrobial agent. The activity of S was substantially less than Bauman and P aeruginosa. Mutants may need more optimization. However, it is necessary to conduct in vivo and experimental investigations to verify the computational predictions and the compound's potential in clinical applications [5].

Table 8: Molecular Docking Results of (Thiochromene) Ligand with the (*A. baumannii*, *P. aeruginosa*, and *S. mutants*) Receptor.

Bonds between (Thiochromene) with Active Site Residues									
Compd. NO	**Score (kcal/mol)**	**RMSD (Å)**	**Compd. Atoms**	**Receptor Atoms**	**Receptor Residues**	**Interaction**	**d (Å)**	**E (kcal/ mol)**	**Total E (kcal/mol)**
A. baumannii	-7.1312	1.7121	S 10	O	VAL 545 (A)	H-donor	3.77	-1.5	-34.5465
			O 13	O	PHE 541 (A)	H-donor	3.24	-0.5	
			O 19	NZ	LYS 533 (A)	H-acceptor	2.89	-6.2	
			O 21	CE	LYS 544 (A)	H-acceptor	3.35	-1.4	
P. aeruginosa	-7.0802	1.6310	S 10	O	VAL 545 (A)	H-donor	3.70	-2.0	-33.0160
			O 19	NZ	LYS 533 (A)	H-acceptor	2.85	-7.0	
			O 19	CE	LYS 544 (A)	H-acceptor	4.03	-0.5	
			O 21	CA	ILE 546 (A)	H-acceptor	3.62	-0.7	
S. mutants	-7.0613	1.5510	O 13	O	PHE 541 (A)	H-donor	3.07	-0.6	-30.1215
			O 19	NZ	LYS 533 (A)	H-acceptor	2.82	-4.5	
			O 21	CE	LYS 544 (A)	H-acceptor	3.37	-1.4	

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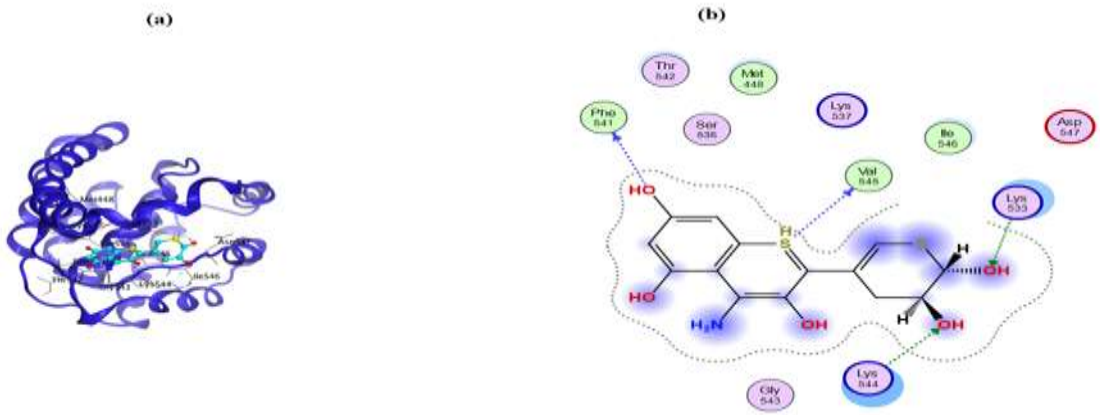

Figure 8: Representations of Molecular Docking (a) The binding site of the top-ranked conformer from the docking simulation between the A. baumannii receptor and thiochromene (PDB Code: 8IOM). (b) A three-dimensional illustration of how the amino acids surround and interact with the most stable conformer.

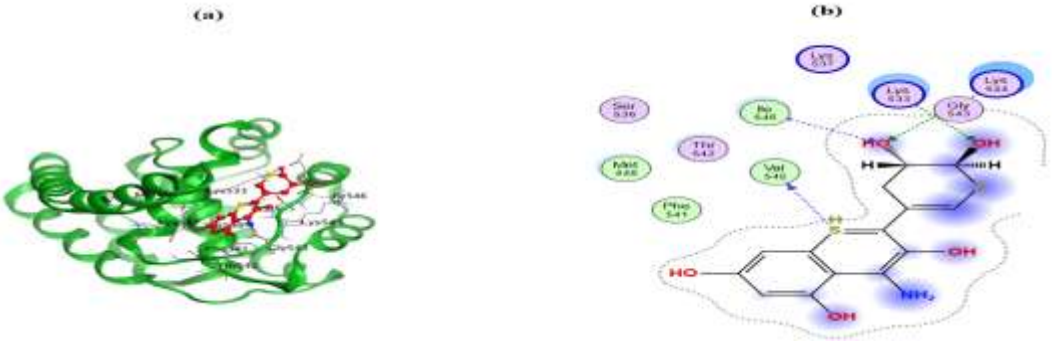

Figure 9: Representations of Molecular Docking (a) The binding site from the top-ranked conformer from the docking simulation between the A. baumannii receptor and thiochromene (PDB Code: 8IOM). (b) A three-dimensional illustration of how the amino acids surround and interact with the most stable conformer.

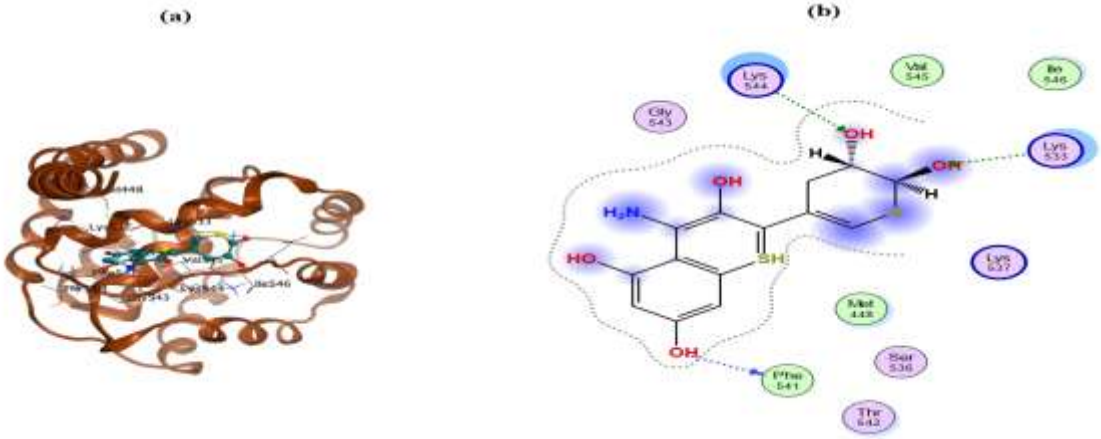

Figure 10: Representations of Molecular Docking standard (a) The binding site from the top-ranked conformer from the docking simulation between the A. baumannii receptor and thiochromene (PDB Code: 8IOM). (b) A three-dimensional illustration of how the amino acids surround and interact with the most stable conformer.

Conclusion

The Sodium 4-amino-2-(2,3-dioxido-2H-thiopyran-5-yl)-4H-hiochromene-3,5,7-tris(olate) compound was

extracted from garlic (Allium sativum), and the chemical structure of the extracted compound was proven using the NMR and GC-Mass techniques and FT-IR techniques. The biological activity against Acinetobacter baumannii bacteria was studied, and the compound proved to be highly effective in killing this type of bacteria, as was proven practically.

Acknowledgments: We, the authors, extend our sincere thanks to the College of Pharmacy and the College of Science/Department of Biology at the University of Basra, for their assistance in completing this research.

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