RESEARCH PAPER

Design, Synthesis, Molecular Docking, ADMET Prediction and Biological Evaluation of Novel 1,4,5-Triphenyl-Substituted Pyrrole Derivatives as Potential Anti-inflammatory and Anticancer Agents

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ABSTRACT
Pyrrole based heterocyclic compounds constitute an important class of pharmacologically active molecules owing to their broad spectrum of biological activities and favorable structural characteristics. In the present study, a series of novel 1,4,5-triphenyl-substituted pyrrole derivatives were designed and synthesized using both conventional reflux and microwave-assisted synthetic methodologies. Microwave-assisted method significantly reduced the reaction time and enhanced product yield compared to the traditional protocol. The synthesized compounds were characterized by Fourier-transform infrared spectroscopy (FT-IR), proton nuclear magnetic resonance (1H NMR), carbon-13 nuclear magnetic resonance (13C NMR) and mass spectrometry which confirmed the formation of desired pyrrole derivatives. The biological potential of the synthesized molecules was investigated by molecular docking against cyclooxygenase (COX; PDB ID: 6COX) and antibacterial target protein (PDB ID: 3G75). The compound B (-8.4 kcal/mol) showed the best binding affinity towards COX receptor which is very close to diclofenac while compound E (-7.1 kcal/mol) showed the highest interaction towards antibacterial target which is similar to streptomycin. The experimental biological evaluation also indicated significant anti-inflammatory activity especially for the o-chloroaniline derivative with 78.77% inhibition of protein denaturation at 1000 µg/mL. Antimicrobial screening revealed moderate activity against Staphylococcus aureus where compound E exhibited the largest zone of inhibition (21 mm). The in vitro anticancer evaluation against MDA-MB-4355 cells revealed that compound C was the most potent derivative with 65% growth inhibition comparable to 5-fluorouracil. ADMET prediction revealed good gastrointestinal absorption, good bioavailability and promising drug-likeness for most of the synthesized compounds.
Keywords: Pyrrole derivatives; Microwave-assisted synthesis; Molecular docking; Anti-inflammatory activity; Anticancer activity; ADMET; Medicinal chemistry.
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1. Introduction

Heterocyclic compounds represent one of the most important structural classes in medicinal chemistry, accounting for a large proportion of currently marketed pharmaceuticals. Among these, pyrrole-containing molecules have attracted considerable attention because of their unique aromatic electronic structure and their presence in numerous biologically important natural products, including heme, chlorophyll, vitamin B12, and bile pigments. Their remarkable structural versatility enables interaction with diverse biological targets, making pyrrole derivatives valuable scaffolds in modern drug discovery [1,2].

Pyrrole derivatives have shown a wide range of pharmacological activities like antimicrobial, anti-inflammatory, anticancer, antiviral, antioxidant, anticonvulsant and enzyme inhibitory activities.

Several clinically approved drugs such as sunitinib, atorvastatin and tolmetin, containing pyrrole or

pyrrole-related pharmacophores further emphasize the therapeutic importance of this heterocyclic nucleus. Further, the biological activity of pyrrole compounds can be enhanced by suitable structural modifications especially by introducing electron withdrawing or electron donating substituents which can affect receptor binding, lipophilicity and metabolic stability [3,4,5].

Conventional methods for the synthesis of pyrroles, such as Knorr and Paal-Knorr reactions, usually require long reaction times, harsh conditions and provide moderate yields [6,7]. Microwave-assisted organic synthesis is a new and efficient alternative that offers rapid heating, shortened reaction time, improved energy efficiency and higher product yields. Hence, the microwave-assisted methods have attracted increasing interest for the synthesis of biologically active heterocyclic compounds [8,9,10,11].

Along with synthetic chemistry, computational techniques including molecular docking and in silico ADMET prediction have become essential tools in early drug discovery [12]. These methods permit the prediction of protein-ligand interactions, pharmacokinetic properties and drug-likeness, reducing experimental costs and speeding up lead optimization. Integration of computational and experimental evaluation provides a holistic approach to identify promising therapeutic candidates [13,14].

On the basis of these considerations, the present work was aimed to the design and synthesis of a new library of 1,4,5-triphenyl substituted pyrrole derivatives by both conventional and microwave-assisted methods. The synthesized compounds were characterized in detail by FT-IR, 1H NMR, 13C NMR and mass spectrometry. Further, molecular docking, ADMET prediction, anti-inflammatory, antimicrobial and anticancer studies were carried out to screen potential lead compounds for future drug development.

2. Materials & Methods

2.1 Reagents and Chemicals

All the chemicals and solvents used in this study were analytical reagent (AR) grade and were used as received without any further purification. Commercially available benzoin, substituted aniline derivatives, malononitrile, hydroxylamine hydrochloride, sodium acetate, pyridine, triethyl orthoformate (TEOF), sodium hydroxide, concentrated hydrochloric acid, ethanol and other laboratory grade reagents were purchased from various commercial sources. Thin-layer chromatography (TLC) was performed using silica gel 60 F254 precoated aluminum plates, and reaction progress was monitored under ultraviolet light (254 nm). Melting points were determined by the open capillary method and are reported without correction.

2.2 Synthesis of 1,4,5-Triphenyl Pyrrole Derivatives by conventional method

The target 1,4,5-triphenyl pyrrole derivatives were synthesized via a conventional multistep protocol. Initially, benzoin and substituted aniline were refluxed in ethanol under acidic conditions to afford the corresponding aminoketone intermediate, which was subsequently cyclized with malononitrile in pyridine to yield 2-amino-4,5-diphenyl-1-substituted-1H-pyrrole-3-carbonitrile.

This key intermediate was further functionalized through reactions with hydroxylamine hydrochloride, alcoholic sodium hydroxide, or triethyl orthoformate to obtain the corresponding oxime, acetamide, and ethoxymethylene derivatives, respectively. The progress of each reaction was monitored by thin-layer chromatography (TLC), and the products were isolated by precipitation, purified by recrystallization from ethanol, and characterized by standard spectroscopic techniques.

2.3 Synthesis of 1,4,5-Triphenyl Pyrrole Derivatives by Microwave method

Microwave-assisted synthesis was performed in a sealed microwave reaction vessel. Benzoin (0.01 mol) and substituted aniline (0.01 mol) were dissolved in ethanol with a catalytic amount of concentrated hydrochloric acid and irradiated at 120-140°C (300-500 W) for 5-10 min to obtain intermediate compounds. Subsequently, the intermediates were reacted with malononitrile in pyridine under microwave irradiation at 130-150°C (300-500 W) for 5-8 min. After cooling, the reaction mixtures were poured into ice cold water and were purified by recrystallization from ethanol. The microwave irradiation provided shorter reaction time and higher product yield compared to the traditional synthesis.

2.4 Characterization of 1,4,5-Triphenyl Pyrrole Derivatives

2.4.1 Fourier Transform infrared (FTIR):-The synthesized substituted 1,2,4-triazole derivative were characterized by FTIR spectroscopy for identification of characteristic functional groups and structural confirmation. FTIR spectra were recorded using a shimadzu FTIR spectrophotometer in the range of 4000-400cm-1 employing the potassium bromide pellet method [15].

2.4.2 NMR Spectra :- The structural elucidation of the synthesized compound was further carried out using proton nuclear magnetic resonance (H1 NMR) spectroscopy. The spectra were recorded on brukeravance NMR spectrometer operating at 400 MHz using Dimethyl sulfoxide-d6 (DMSO-d6) as the solvent and tetramethylsilane (TMS) as the internal reference standard. Chemical shift were expressed in parts per million (ppm) the H1 NMR spectra were interpreted on the basis of chemical shift values, multiplicity, coupling patterns, and integration of proton signals. Characteristic signals corresponding to aromatic protons, amino protons,

triazole N-H protons and other substituent groups were analyzed to confirm the molecular structure of the synthesized derivatives. Residual solvent peaks and exchangeable proton signals were also identified during spectral interpretation.

2.4.3 Mass spectroscopy:- Mass spectrometric analysis of the synthesized substituted 1,2,4-triazole derivatives was performed to determine their molecular weights and fragmentation patterns. The spectra were recorded using an LC-MS/MS mass spectrometer equipped with an electrospray ionization source operating in positive ion mode.

2.5 Molecular Docking Study

Molecular docking studies were performed to explore the binding interactions of the synthesized compounds with biologically relevant protein targets. The anti-inflammatory activity was checked by cyclooxygenase (COX; PDB ID: 6COX) as the receptor and antibacterial activity was tested by the bacterial target protein (PDB ID: 3G75). Protein structures were obtained from the Protein Data Bank and prepared by removing crystallographic water molecules and co-crystallized ligands, followed by hydrogen atom addition and energy minimization. The synthesized ligands were geometry optimized before docking.

Docking calculations were performed using standard molecular docking software and the binding affinity values were shown as kcal/mol. The docking poses with the lowest binding energies were chosen for the analysis of the interactions. The protein–ligand interactions were visualized using molecular visualization software to identify the hydrogen bonds, hydrophobic contacts, and π-π interactions responsible for ligand stabilization in the active site.

2.6 Anti-inflammatory Activity in Vitro

The protein denaturation assay was used to determine the anti-inflammatory activity of synthesized compounds. The synthesized compounds were incubated with the protein solution in different concentrations (200-1000 µg/mL) under controlled experimental settings. The standard reference was diclofenac sodium. The absorbance of each sample was measured spectrophotometrically and the percentage of inhibition of protein denaturation was calculated compared to the untreated control. All experiments were carried out in triplicate and results are shown as mean values.

2.7 Antibacterial activity

Agar well diffusion method was used to test the antibacterial activity against Staphylococcus aureus. Fresh bacterial cultures were grown on nutrient agar plates and compounds synthesized were loaded into the agar wells. Streptomycin was used as positive control. The antibacterial activity was characterized by the measurement of the zone of inhibition (mm) diameter after incubation. All experiments were performed in triplicate and averages were reported.

2.8 Anticancer Activity

In Vitro The cytotoxic in vitro activity of the synthesized compounds against the human breast cancer cell line MDA-MB-4355 was determined by the Sulforhodamine B (SRB) assay. Cells were grown in L-15 medium supplemented with fetal bovine serum and antibiotics in standard culture conditions. The synthesized compounds were screened at a concentration of 20 µg/mL and 5-fluorouracil (5-FU) was used as a reference standard. Cell viability was measured spectrophotometrically and the percentage inhibition of cell growth was calculated with respect to untreated control cells.

2.9 In Silico ADMET Prediction

Drug-likeness and pharmacokinetic properties of the synthesized compounds were evaluated using computational ADMET prediction tools. Parameters including gastrointestinal absorption, blood–brain barrier permeability, skin permeability (Log Kp), aqueous solubility, molecular weight, and bioavailability score were predicted. These properties were analyzed to estimate the pharmaceutical suitability and oral drug potential of the synthesized pyrrole derivatives.

3. Results and Discussion

3.1 Physiochemical Properties

The synthesized substituted 1,4,5-Triphenyl Pyrrole derivative were obtained with moderate to excellent yields. Microwave assisted synthesis resulted in higher percentage yield (80-90%) compared to the conventional reflux method (62-74%) as shown in table 1 indicating improved reaction efficiency and reduced reaction time

Table 1 The physical data of substituted aroyl hydrazide acid By Conventional and microwave method.

Sr no.	Compound code	Molecular formula	Molecular weight	M.P ^{0}C	Percentage yield		Rf value	Mobile phase
					Conventional	Microwave		
1	A	$C_{25}H_{23}N_3O_2$	397.47	218-222	62-68%	80-88%	0.58	Ethyl acetate: N-hexane
2	B	$C_{24}H_{20}CLN_3O$	401.89	212-216	65-70%	82-88%	0.62	Ethyl acetate: N-hexane
3	C	$C_{24}H_{21}CLN_3O^+$	402.90	198-202	68-74%	85-92%	0.64	Ethyl acetate: N-hexane
4	D	$C_{24}H_{20}FN_3O$	385.44	198-202	68-72%	85-90%	0.58	Ethyl acetate: N-hexane
5	E	$C_{24}H_{20}N_4O_3$	412.44	228-230	62-68%	82-88%	0.60	Ethyl acetate: N-hexane
6	F	$C_{25}H_{21}N_3O_3$	411.46	242-246	65-72%	82-90%	0.62	Ethyl acetate: N-hexane
7	G	$C_{24}H_{20}N_4O_3$	412.44	198-202	58-65%	78-88%	0.62	Ethyl acetate: N-hexane
8	H	$C_{30}H_{24}N_6O_6$	564.55	238-242	65-70%	85-90%	0.62	Ethyl acetate: N-hexane

3.2 Structural Characterization

3.2.1 FT-IR Study

The chemical structures of the synthesized pyrrole derivatives were initially confirmed by FT-IR spectroscopy. Representative compounds B **a**nd E exhibited the characteristic absorption bands corresponding to the expected functional groups, including N-H stretching (3416 and 3451 cm^{-1}), aromatic C-H stretching (3058-3060 cm^{-1}), amide carbonyl (C=O) stretching (1652-1679 cm^{-1}), and aromatic C=C skeletal vibrations (1500-1595 cm^{-1}), the spectrum are shown in figure 1 and 2 and their value are shown in table 2 and 3. These spectral features collectively verified the successful incorporation of the amino, amide, aromatic, and pyrrole moieties, confirming the successful synthesis of the target pyrrole derivatives.

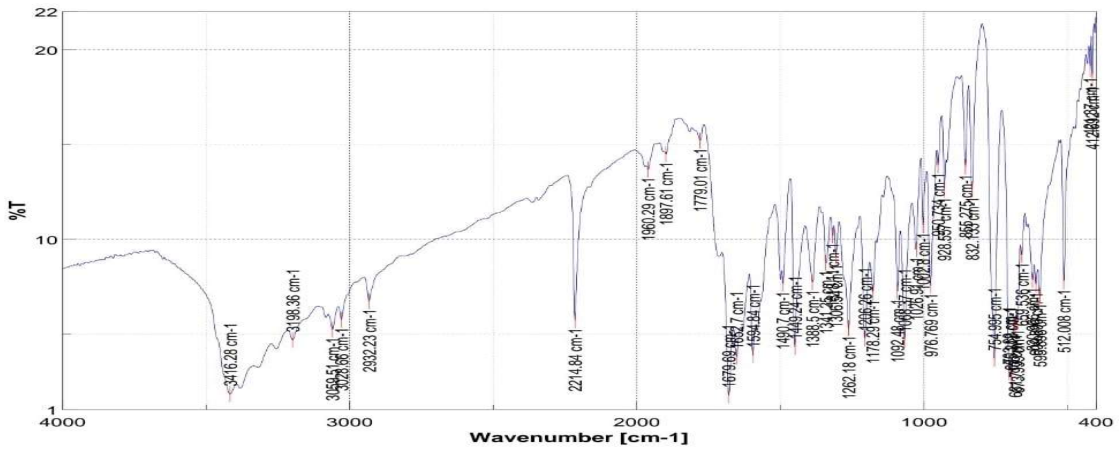


Figure1:- IR spectrum of compound B

Table2 :- IR spectrum value of compound B

Sr no.	Wave number (cm^-)	Vibration type	Functional group assignment
1	3416.28	N-H stretching	Amine / amide (N-H)
2	3058.51	Aromatic C-H stretching	Aromatic ring (C-H)
3	2932.23	Aliphatic C-H stretching	Alkane
4	2214.84	Hydrogen bonded N-H	Hydrogen bonded amine
5	1679.69	C=O stretching	Amide carbonyl (-CONH-)
6	1594.84	C-C stretching	Aromatic ring (C=C)

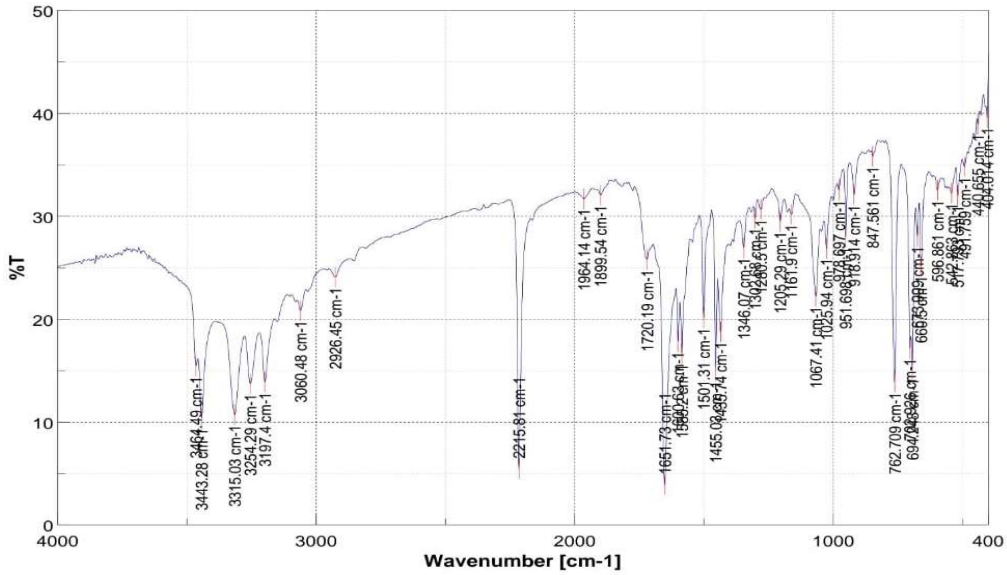


Figure 2:- IR spectrum of compound E

Table 3:- IR spectrum value of compound E

Sr no.	Wave number (cm^-)	Vibration type	Functional group assignment
1	3451.49	N-H stretching	Amine / amide (N-H)

2	3060.48	Aromatic C-H stretching	Aromatic ring (C-H)
3	2926.45	Aliphatic C-H stretching	Alkane
4	1651.73	C=O stretching	Amide carbonyl (-CONH-)
5	1590.28 / 1582.64	C-C stretching	Aromatic ring (C=C)
6	1501.31 / 1455.02	Aromatic skeletal vibrations	Aromatic ring

3.2.2 NMR spectra

The 1H NMR spectra (Figures 3 and 4; Tables 4 and 5) exhibited the characteristic chemical shifts expected for the synthesized pyrrole derivatives. The amide N-H proton resonated in the downfield region at 8.5-9.5 ppm, while the aromatic protons appeared as multiplets between 7.0-8.2 ppm. The amino protons were observed at 6.5-7.2 ppm, and the pyrrole ring protons resonated at 6.2-6.8 ppm. In addition, the methyl substituent of compound B appeared as a singlet at 2.0-2.5 ppm. These characteristic resonance signals were consistent with the proposed molecular structures and confirmed the successful synthesis of the target pyrrole derivatives.

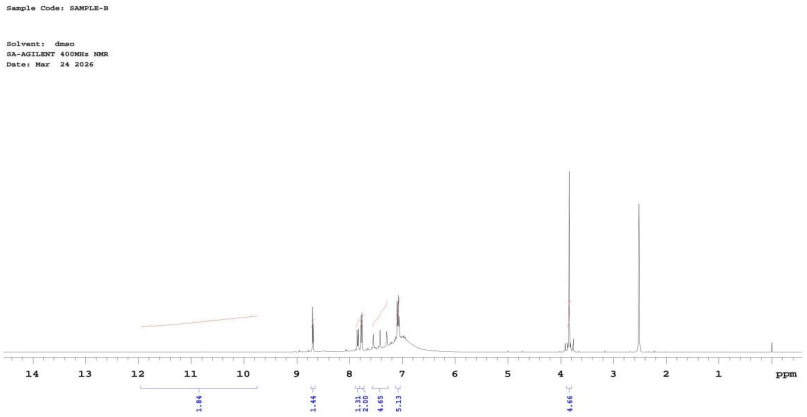


Figure 3: - NMR spectrum of compound B

Figure 4: - NMR spectrum value of compound B

Sr no.	Chemical shift	Proton assignments
1	8.5-9.5	CONH (Amide NH)
2	7.0-8.2	Aromatic proton (phenyl + substituted benzene)
3	6.5-7.2	-NH_2(aniline)
4	6.2-6.8	Pyrrole ring proton
5	3.5-4.2	$CONH_2$(amide NH_2)
6	2.0-2.5	-CH_3(attached to pyrrole ring)

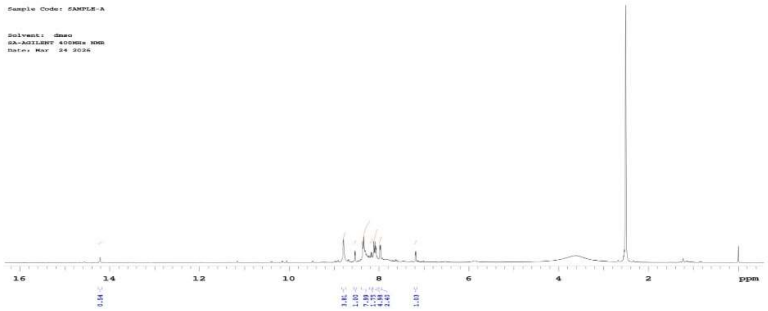


Figure 4: - NMR spectrum of compound E

Figure 5: - NMR spectrum value of compound E

Sr no.	Chemical shift	Proton assignments
1	11.0-12.0	CONH (Amide NH)
2	9.0-10.0	Pyrrole NH
3	7.0-8.2	Aromatic proton (phenyl + substituted phenyl rings)
4	6.8-7.2	Aromatic proton (adjacent to $–NH_2$ group)
5	4.0-4.5	NH_2(amine)
6	2.1-2.5	$-CH_3$(methyl on pyrrole ring)

3.2.3 Mass Spectral Analysis

The mass spectra (Figures 5 and 6; Tables 6 and 7) confirmed the molecular masses of the synthesized pyrrole derivatives. The protonated molecular ion peaks $[M+H]^+$ corresponding to the expected molecular weights were observed for all compounds. Characteristic fragmentation patterns involving amide cleavage, pyrrole ring fragmentation, and substituted aromatic moieties were consistent with the proposed molecular structures. The observed molecular ion and fragment ions collectively validated the successful synthesis and structural integrity of the target pyrrole derivatives.

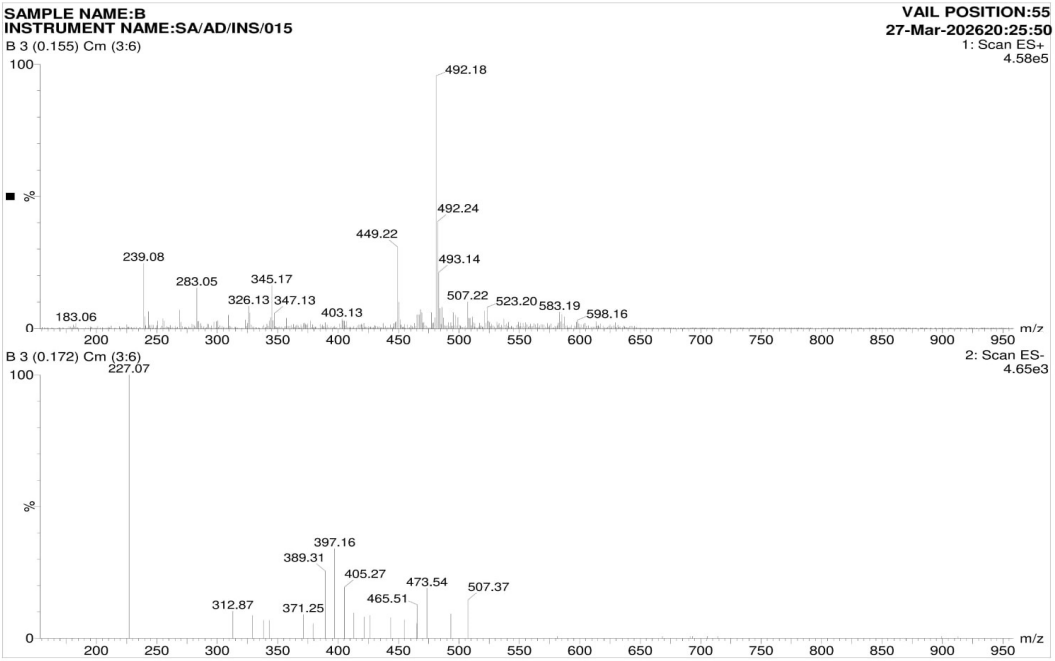
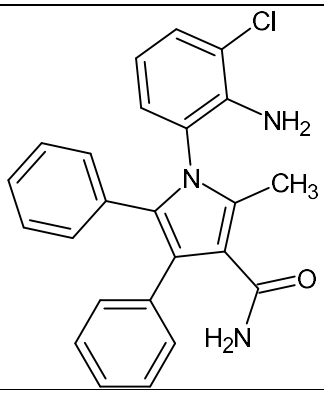
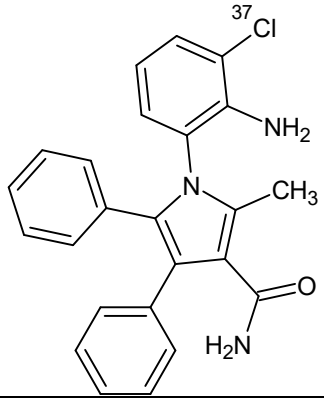
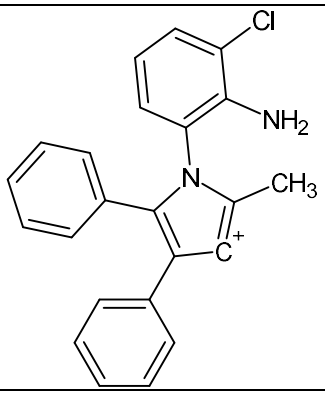
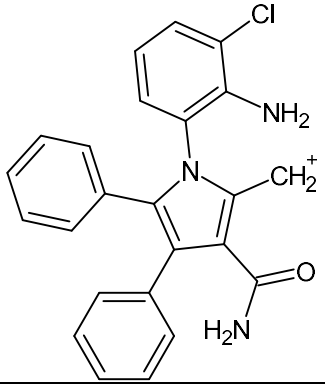
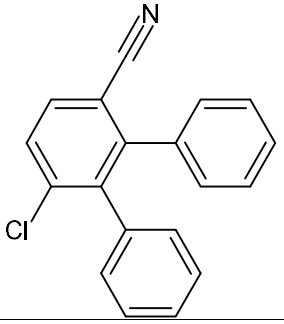


Figure 5: - Mass spectrum of compound B

Table 6: - Mass spectrum of compound B

Sr no.	Structural change	Structural formula of fragment	Structures	Actual m/z	Observed m/z
1	Molecular ion	$C_{24}H_{20}CLN_3O$		401	403.13
2	Isotopic peak (M+2) due to cl	Cl isotope fragment		403	405.27

4	Loss of $CONH_2$ group	Amide cleavage		358	371.25
6	Loss of CH_3 group	M – CH_3		388	397.16
7	Pyrrole ring fragmentation	Ring cleavage		300	312.87

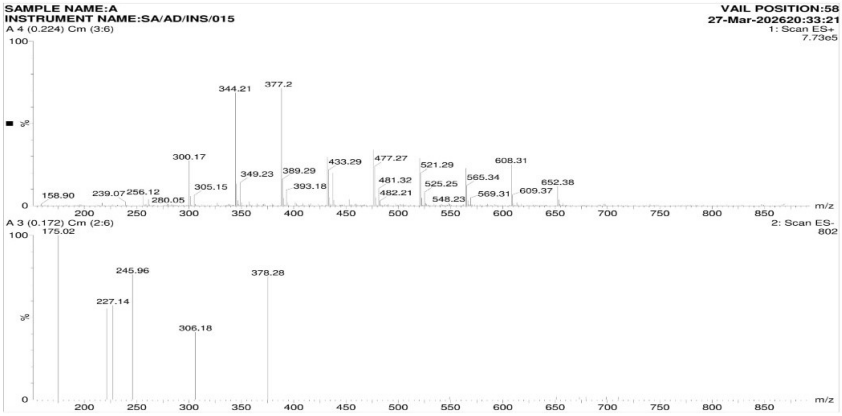
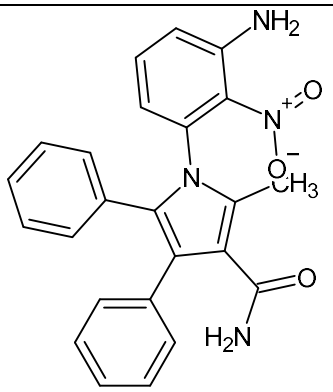
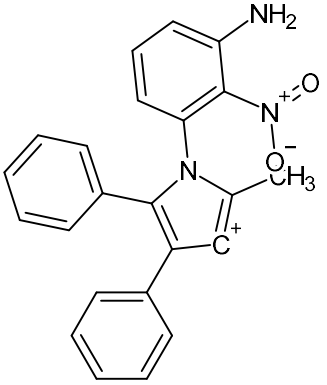
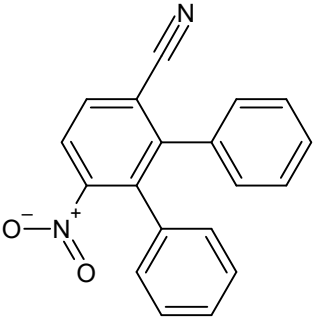
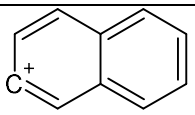
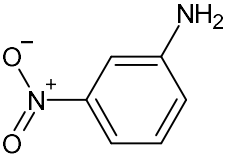
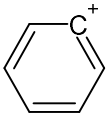


Figure 6: - Mass spectrum of compound E

Table 7: - Mass spectrum of compound E

Sr no.	Structural change	Structural formula of fragment	Structures	Actual m/z	Observed m/z
1	Molecular ion	$C_8H_6N_6O_4^+$		412	413.29
2	Loss of $CONH_2$ group	Amide cleavage		369	389.29
3	Pyrrole ring fragmentation	Ring rearrangement		300	300.17
4	Diphenyl fragment formation	$C_{12}H_9^+$		165	158.90
5	Nitroaniline fragment	$C_6H_6N_2O_2^+$		154	159.07

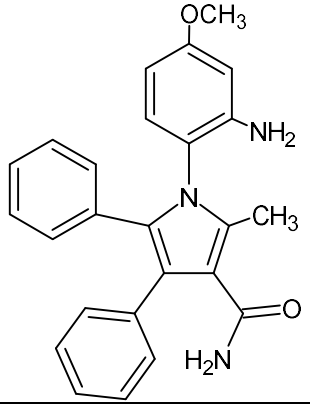
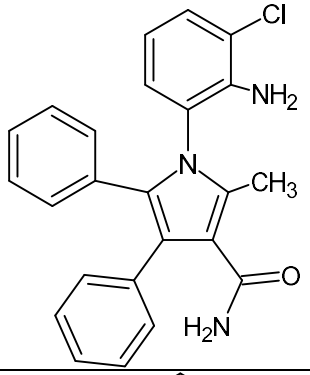
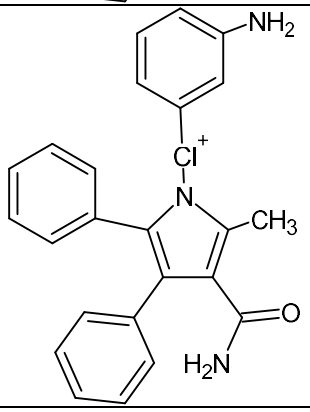
6	Aromatic cation fragment	Phenyl cation		77	76.12

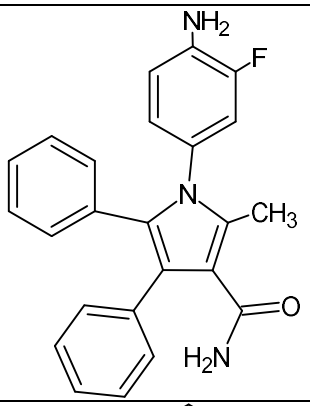
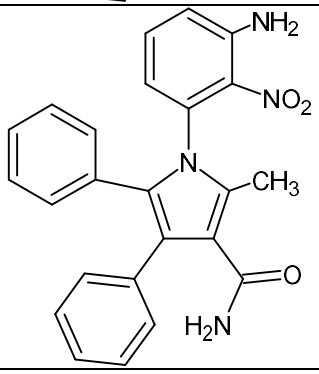
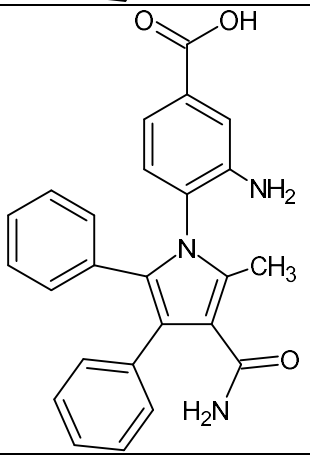
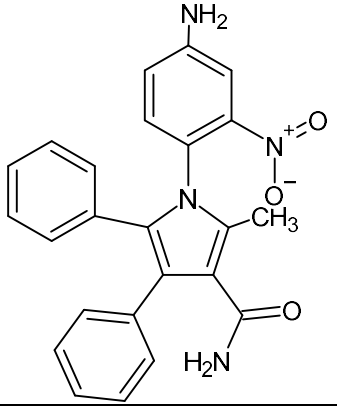
3.3 Molecular Docking Studies

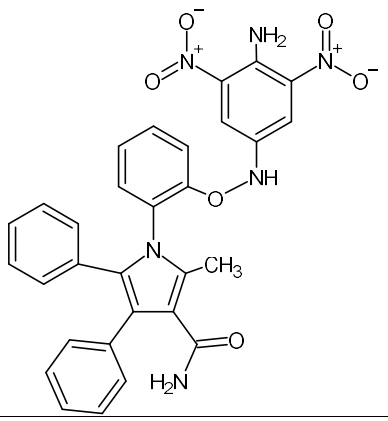
3.3.1 Anti-inflammatory Target (6COX)

The synthesized pyrrole derivatives were initially evaluated for their anti-inflammatory potential by molecular docking against cyclooxygenase (COX; PDB ID: 6COX). Most compounds exhibited favorable binding affinities toward the COX active site, with compound B showing the strongest interaction (-8.4 kcal/mol), comparable to the reference drug diclofenac sodium (-9.2 kcal/mol) as shown in table 8. Compounds A, D, E, and F also demonstrated promising binding energies (-7.8 to -8.1 kcal/mol), whereas C, G, and H displayed relatively weaker interactions. Notably, compound B adopted a binding mode similar to diclofenac, forming hydrogen-bonding and hydrophobic interactions within the active site, highlighting chlorinated pyrrole derivatives as promising COX inhibitors.

Table 8:- Anti-inflammatory activity results of molecular docking studies by binding affinity (6COX)

Sr.no	Compound name	Structure of Compound	Binding Affinity
1	A		-8.1
2	B		**-8.4**
3	C		-3.1

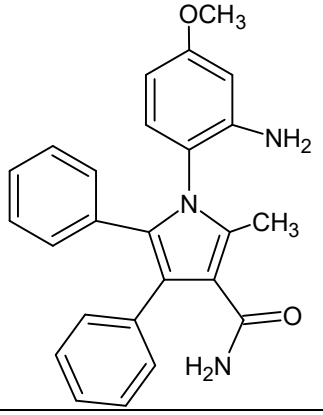
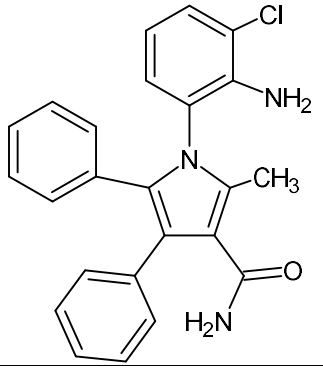
4	D		-7.9
5	E		-7.8
6	F		-7.8
7	G		-4.4

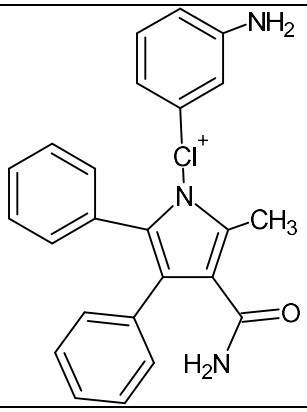
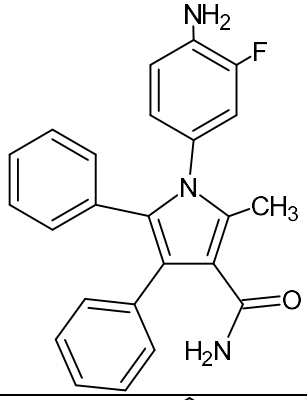
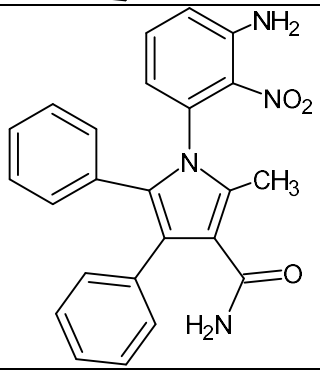
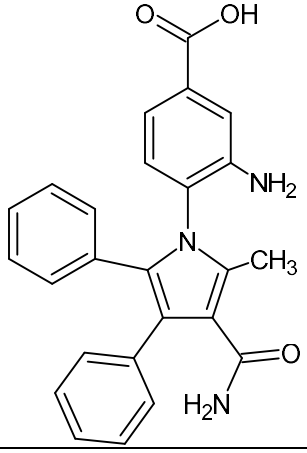
8	H		-5.1

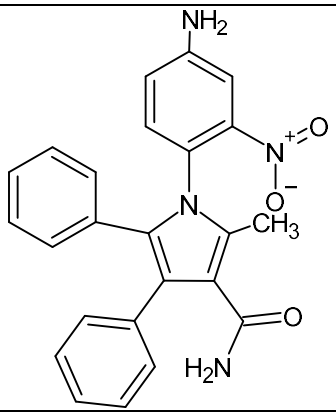
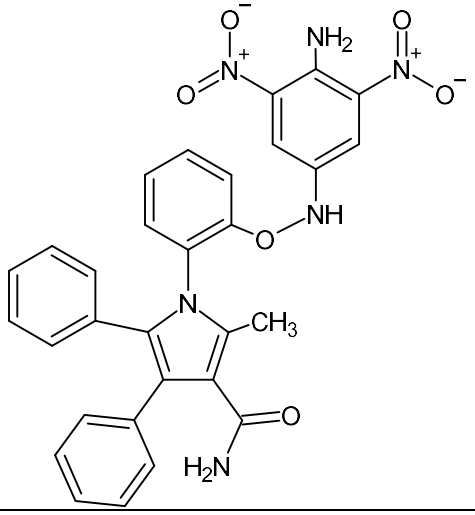
3.3.2 Antibacterial Target (3G75)

The antibacterial potential of the synthesized pyrrole derivatives was evaluated by molecular docking against the bacterial target protein (PDB ID: 3G75). Compound E exhibited the highest binding affinity (-7.1 kcal/mol), comparable to the reference antibiotic streptomycin (-7.6 kcal/mol), while compounds B and F also demonstrated favorable docking scores (-7.0 kcal/mol) as shown in table 9. In contrast, compounds C, G, and H showed relatively weaker interactions. The enhanced binding profile of compound E suggests that nitro substitution promotes favorable hydrogen-bonding and electrostatic interactions within the enzyme active site, highlighting its potential as a promising antibacterial lead.

Table 9: - Antimicrobial activity results of molecular docking studies by binding affinity (3G75)

Sr.no	Compound name	Structure of Compound	Binding Affinity
1	A		-6.6
2	B		-7.0

3	C		-2.4
4	D		-6.4
5	E		**-7.1**
6	F		-7

7	G		-3.7
8	H		-3.8

3.5 Antimicrobial Activity

The antibacterial activity of the synthesized pyrrole derivatives was evaluated against *Staphylococcus aureus* using the agar well diffusion assay. Compound E exhibited the highest antibacterial activity with a zone of inhibition of 21 mm**,** followed by compounds D and F (18 mm), compound B (17 mm), and compound A (15 mm), whereas streptomycin produced the largest inhibition zone (25 mm). Compounds C and G displayed comparatively weaker antibacterial activity. The superior performance of compound E was consistent with its molecular docking results, indicating that nitro substitution enhances its interaction with the bacterial target and contributes to improved antibacterial efficacy as shown in table 10.

Table 10 Antibacterial activity of synthesized pyrrole derivatives against *Staphylococcus aureus*

Sr no.	Compound code	Concentration	Zone of inhibition
1	A	25	15
2	B	25	17
3	C	25	9
4	D	25	18
5	E	25	21
6	F	25	18
7	G	25	11
8	H	25	13
Standard	Streptomycin	25	25

3.6 Anticancer Activity

The antiproliferative activity of the synthesized pyrrole derivatives was evaluated against MDA-MB-4355 human breast cancer cells using the sulforhodamine B (SRB) assay. Compound C exhibited the highest cytotoxic activity **(**65%**),** comparable to the reference drug 5-fluorouracil **(**68.33%**),** whereas compounds F, E, and B demonstrated moderate antiproliferative effects (50.0%, 48.33%, and 43.33%, respectively). In contrast, compound H showed the lowest activity (16.66%) as shown in table 11. These findings indicate that the electronic nature of substituents on the pyrrole scaffold plays a critical role in modulating antiproliferative activity.

Table 11 Anticancer activity against MDA-MB-4255 Cells

Compound	% inhibition
A	33.33
B	43.33
C	65.00
D	31.66
E	48.33
F	50.00
G	31.66
H	16.66

3.7 ADMET Prediction

Computational ADMET analysis revealed that the synthesized pyrrole derivatives possess favorable drug-like and pharmacokinetic properties. Most compounds exhibited high gastrointestinal absorption, acceptable bioavailability scores (~0.55), moderate aqueous solubility, and no predicted blood–brain barrier permeability. Compounds with molecular weights below ~450 Da displayed the most balanced pharmacokinetic profiles, whereas the higher molecular weight of compound H was associated with reduced solubility and bioavailability as represent in table 12. Overall, these findings indicate that the synthesized derivatives have promising ADMET profiles suitable for further optimization and drug development.

Table 12 In silico ADMET and pharmacokinetic profiles of the synthesized pyrrole derivatives

Sr. No	Compound code	Mol.Wt (g/mol)	Solubility	GI Absorption	Log Kp (cm/sec)	BBB Permeability	Bioavailability
1	A	397.47	Moderately soluble	High	-5.76	No	0.55
2	B	401.89	Moderately soluble	High	-5.32	No	0.55
3	C	402.90	Moderately soluble	High	-5.08	No	0.55
4	D	384.45	Moderately soluble	High	-6.08	No	0.55
5	E	411.45	Moderately soluble	High	-6.44	No	0.55
6	F	440.45	Moderately soluble	Low	-6.47	No	0.56
7	G	412.44	Moderately soluble	Low	-5.95	No	0.55
8	H	564.55	Poorly soluble	Low	-5.30	No	0.17

4. Conclusion

In the present work, a novel series of 1,4,5-triphenyl-substituted pyrrole derivatives have been efficiently designed, synthesized and biologically evaluated through an integrated medicinal chemistry approach. The target molecules were obtained efficiently by both conventional reflux and microwave assisted synthetic approaches although microwave irradiation led to a notable reduction in reaction time with improved product yields, which demonstrates the advantages of microwave irradiation as a environmentally benign and energy efficient synthetic approach. The structures of all the target compounds were unambiguously confirmed by FT-IR, 1 H NMR, 13 C NMR and mass spectrometry analysis.

Molecular docking studies revealed favorable interactions of some of the synthesized compounds with the anti-inflammatory (6COX) and antibacterial (3G75) targets . In particular, compound B had the highest affinity for cyclooxygenase and compound E had the highest affinity for the antibacterial target. These computational observations were confirmed by experimental biological studies, where compound B exhibited a potent anti-inflammatory activity and compound E exhibited the highest antibacterial efficacy among the synthesized molecules. In addition, compound C showed excellent antiproliferative activity on MDA-MB-4355 breast cancer cells comparable to the reference drug.

The ADMET analysis showed that most of the compounds have good pharmacokinetics such as

high gastrointestinal absorption and acceptable bioavailability, indicating promising drug-like properties. The structure–activity relationship analysis also revealed that the presence of electron-withdrawing substituents, especially chloro and nitro groups, dramatically increased the biological activity by increasing the interactions with the targets .

In conclusion, the present study identifies the triphenyl-substituted pyrrole derivatives as promising lead scaffolds for the design of new anti-inflammatory and anticancer agents. Further preclinical development would be possible with future studies focusing on molecular optimization, enzyme inhibition studies, molecular dynamics simulation, toxicity profiling and in vivo pharmacological evaluation.

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