ORIGINAL ARTICLE

In silico modeling, synthesis, and *in vitro* anti-tubercular activity of some novel thiazolidine-2-one derivatives

S. Karthika[1], B. Sathya[2], E. Punitha[3], S. Anbazhagan[1]

[1]Department of Pharmaceutical Chemistry, Surya School of Pharmacy, The Tamil Nadu Dr. M.G.R. Medical University, Chennai, Tamil Nadu, India, [2]Department of Pharmacology, Surya School of Pharmacy, The Tamil Nadu Dr. M.G.R. Medical University, Chennai, Tamil Nadu, India, [3]Department of Pharmaceutics, Surya School of Pharmacy, The Tamil Nadu Dr. M.G.R. Medical University, Chennai, Tamil Nadu, India

Abstract

Background: Tuberculosis, caused by *Mycobacterium tuberculosis*, remains a major global health concern despite available treatments and vaccination. The pathogen's ability to evade immune responses and establish latent infection complicates disease control. **Objectives:** The study investigates *in silico* design, synthesis, physicochemical characterization, and *in vitro* anti-tubercular activity of some novel Thiazolidine-2-one derivatives that were synthesized by a conventional method. **Methods:** All the newly synthesized derivatives were characterized by determining their melting point, retention factor from thin-layer chromatography, and spectral methods (infrared, ^{1}H nuclear magnetic resonance spectroscopy, ^{13}C nuclear magnetic resonance spectroscopy, and mass spectroscopy) and evaluated for their *in vitro* anti-tubercular activity. **Results:** Thiazolidine-2-one derivatives have been synthesized and characterized using physical and spectral methods. *In vitro* anti-tubercular study revealed that compounds **1c** and **2c** have shown promising anti-tubercular activity at 50 µg/mL and 100 µg/mL. Compounds **1a** and **2a** have shown moderate anti-tubercular activity at 100 µg/mL against the H37Rv strain. **Conclusion:** From the results, it can be concluded that compounds **1c** and **2c** showed more potent *in vitro* anti-tubercular activity.

Key words: H37Rv strain, *in silico* design, *in vitro* anti-tubercular activity, thiazolidine-2-one derivatives

INTRODUCTION

Tuberculosis (TB) is a serious infectious disease caused primarily by *Mycobacterium tuberculosis*, which most commonly affects the lungs but can involve multiple organ systems.[1] TB is classified into latent TB infection and active TB disease. Latent TB is asymptomatic and non-infectious, while active TB is symptomatic and transmissible. The pathogenesis of TB involves inhalation of airborne droplets containing the bacilli, which are then phagocytosed by alveolar macrophages. A complex immune response, including the activation of T lymphocytes and the formation of granulomas, attempts to contain the infection.[2] However, in some individuals, especially those with compromised immune systems, the bacteria can multiply and spread. TB is a major global health concern due to its association with high morbidity and mortality, particularly in low- and middle-income countries. Current treatment regimens for TB include first-line anti-tubercular drugs such as isoniazid, rifampicin, ethambutol, and pyrazinamide. For drug-resistant TB, second-line drugs including fluoroquinolones (levofloxacin, moxifloxacin) and injectable agents such as amikacin or capreomycin are used.[3]

Thiazolidine-2-one, a five-membered heterocyclic scaffold containing both sulfur and nitrogen atoms, has emerged as a privileged structure in medicinal chemistry due to its broad spectrum of biological activities. This moiety

Address for correspondence:
Dr. S. Karthika, Department of Pharmaceutical Chemistry, Surya School of Pharmacy, The Tamil Nadu Dr. M.G.R. Medical University, Chennai, Tamil Nadu, India. Mobile: +91-9789286976.
E-mail: karthikaselvam1990@gmail.com

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serves as a core structure in numerous synthetic derivatives exhibiting antimicrobial, anti-inflammatory, antidiabetic, and anticancer properties. Recent studies have underscored the importance of structural modifications at the 4 and 5 positions of the thiazolidine-2-one ring, enabling the fine-tuning of pharmacokinetic and pharmacodynamic profiles. The structural versatility and drug-likeness of thiazolidine-2-one derivatives continue to make them attractive candidates for the development of novel therapeutic agents across a range of clinical applications.[4-6]

MATERIALS AND METHODS

Materials

All reagents and solvents used in the synthesis were of analytical grade and obtained from Sigma-Aldrich. They were employed as received without further purification. Melting points of the synthesized compounds were determined using an electrically heated melting point apparatus via the open capillary method and are reported uncorrected in degrees Celsius. Reaction progress and product purity were monitored by thin layer chromatography (TLC) using silica gel-G as the stationary phase and Ethyl acetate: Methanol (5:5) as the mobile phase, and spots were detected by ultraviolet chamber ^{1}H nuclear magnetic resonance (^{1}H NMR) spectra were recorded on a Bruker AC-F 400 MHz Fourier-transform (FT)-NMR spectrometer. Spectra were acquired in deuterated chloroform with tetramethylsilane as the internal standard (δ = 0.00 ppm), at room temperature. FT infrared (FT-IR) spectra were obtained using an FT-IR-6600 type spectrometer. Samples were prepared as potassium bromide pellets and analyzed in the range of 4000–350 cm^{-1}. Mass spectra were recorded using a Shimadzu liquid chromatography-mass spectrometry system.

Methods

Chemical structures, including organic compounds, organometallics, and polymers, were designed and analyzed using ACD/Labs ChemSketch version 12.0.[7] This software also facilitated the estimation of various molecular properties. To visualize molecular structures encoded in SMILES or SD file formats and assess key molecular descriptors, as well as predict potential bioactivity against key drug targets, the molinspiration molecular viewer was employed.[8]

Pharmacokinetic Profiling using Software

Swiss absorption, distribution, metabolism, and excretion (ADME) was utilized to predict the ADME characteristics of the lead compound. The platform also provided insight into drug-likeness and other physicochemical parameters through computational models, including the BOILED-Egg diagram for gastrointestinal (GI) absorption and brain access [Figure 1], iLOGP for lipophilicity, and the Bioavailability Radar [Figure 2] for overall drug-likeness evaluation.[9-11]

Molecular Docking

The docking studies of the synthesized compounds were carried out using the AUTODOCK tools version 1.5.6 working system. The synthesized molecules were tested for their binding affinities toward the target protein (PDB ID: 4HZR).[12-15]

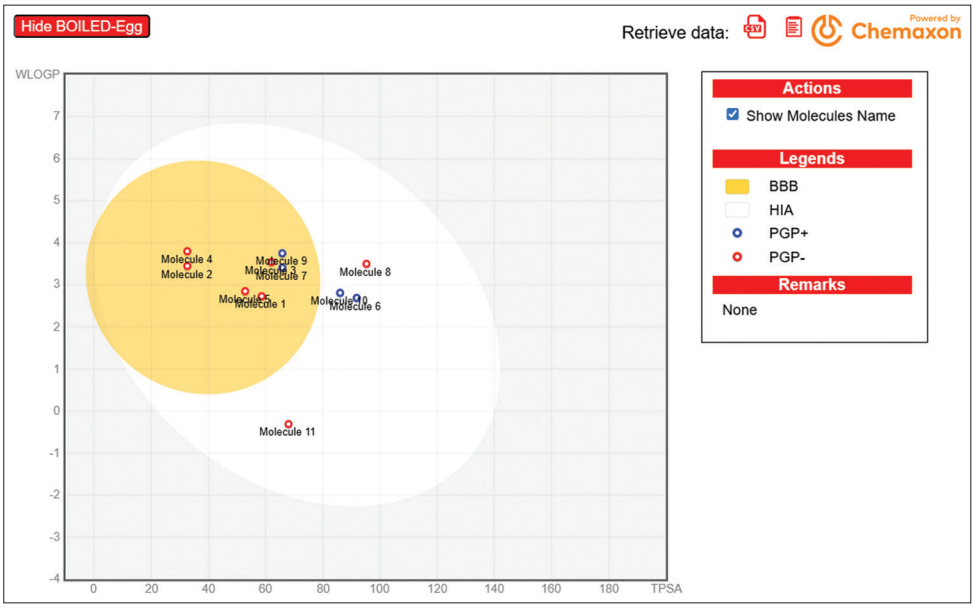


Figure 1: BOILED Egg model to predict passive diffusion by Swiss absorption, distribution, metabolism, and excretion

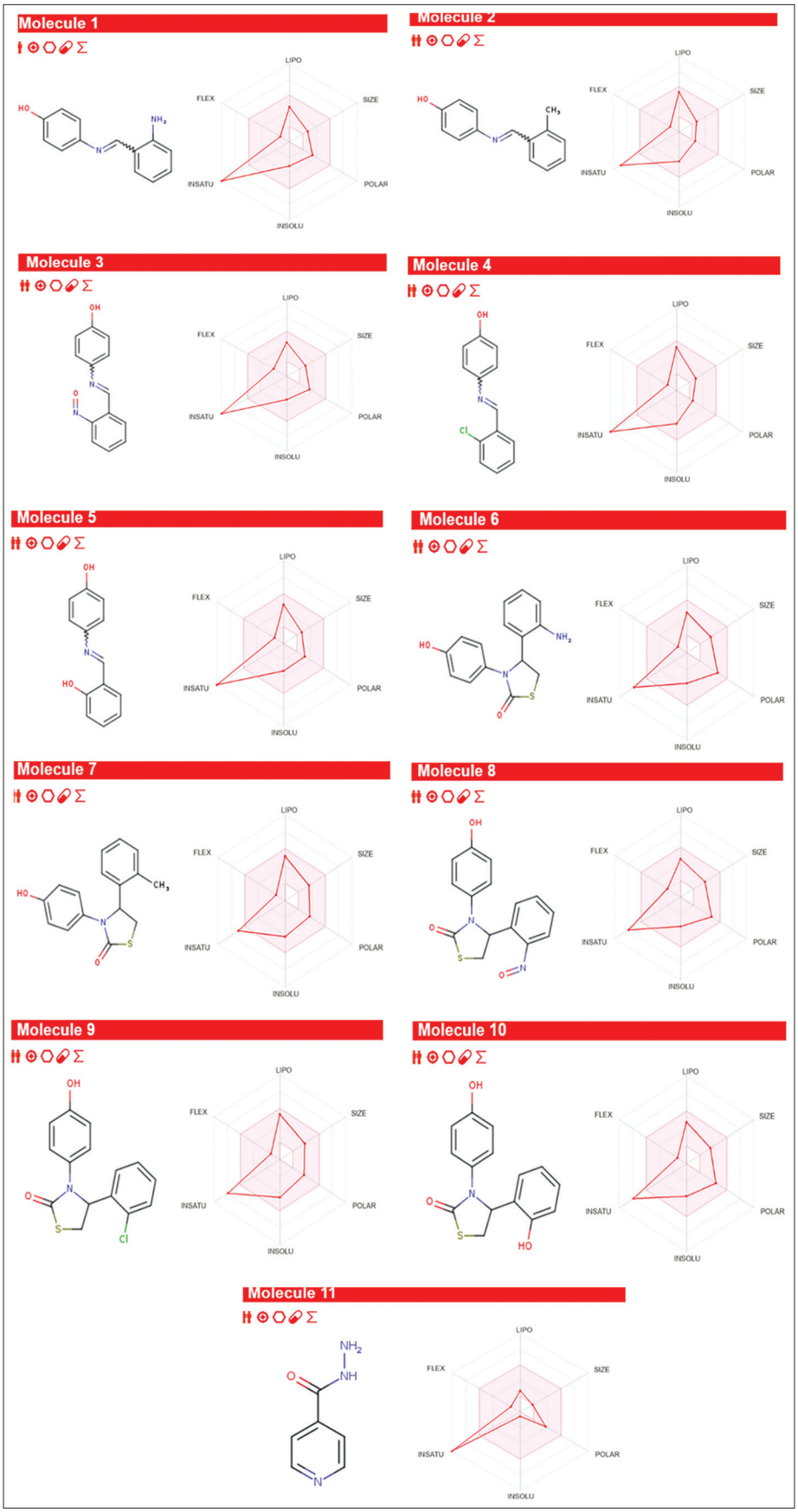


Figure 2: Bioavailability radar of the synthesized compound with standard drug

Synthetic Procedure

General preparation for the synthesis of Schiff's base (1a-e)

About 10 g of substituted benzaldehyde (0.05 mol) and 6 g of 4-aminophenol (0.05 mol) were mixed with 40 mL of ethanol and refluxed for 5 h. The crude product obtained was recrystallized from ethanol.

General preparation for the synthesis of thiazolidine-2-one derivatives (2a-e)

About 1.33 g of synthesized Schiff's base (0.05 mol), 25 mL of benzene, and 4.3 mL of 2-mercaptoacetic acid were taken in a 250 mL R.B. flask. The mixture was refluxed on a water bath using the Stark and Dean apparatus for 12 h. After refluxing, the mixture was cooled and poured into ice water. The upper organic layer was washed successively with aqueous sodium bicarbonate and water. The organic layer is dried and concentrated. The crude product obtained was recrystallized from ethanol.

The synthetic scheme is given below:

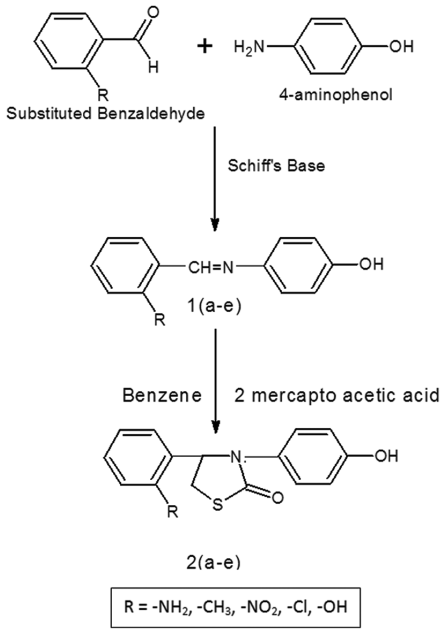


Table 1: Analysis of Lipinski's rule of five by molinspiration

Compound code	mi log P	TPSA	n atoms	n ON	n OHNH	n rotb	Volume
1a	2.43	58.62	16	3	3	2	198.02
1b	3.39	32.59	16	2	1	2	203.29
1c	2.90	78.42	18	5	1	3	210.06
1d	3.62	32.59	16	2	1	2	200.27
1e	2.93	52.82	16	3	2	2	194.75
2a	2.45	66.56	20	4	3	2	247.44
2b	3.82	40.54	20	3	1	2	252.72
2c	3.33	86.36	22	6	1	3	259.49
2d	4.05	40.54	20	3	1	2	249.69
2e	2.89	60.77	20	4	2	2	244.17

Table 2: Drug-likeness score evaluation by molinspiration

Compound code	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
1a	0.07	0.13	0.10	−0.36	−0.41	0.05
1b	−0.11	0.03	0.09	−0.40	−0.54	0.08
1c	−0.02	0.12	0.27	−0.18	−0.49	0.07
1d	−0.11	0.12	0.12	−0.29	−0.60	0.12
1e	−0.11	−0.19	−0.05	−0.17	−0.19	−0.04
2a	−0.04	−0.19	−0.01	−0.19	−0.30	−0.06
2b	−0.10	−0.12	−0.01	−0.19	−0.22	−0.04
2c	−0.01	−0.17	0.03	−0.17	−0.19	−0.06
2d	0.12	−0.12	0.05	−0.18	−0.22	−0.08
2e	0.02	−0.15	0.21	−0.34	−0.19	−0.12

GPCR: G Protein-Coupled Receptor.

Anti-tubercular Activity

The anti-tubercular activity was carried out by Middlebrook 7H9 agar medium against the H37Rv Strain. Middlebrook 7H9 contains different derivatives, standard drugs, as well as controls. Middlebrook 7H9agar medium was incubated with *M. tuberculosis* H37Rv strain. The incubated bottles were incubated at 37°C for 4 weeks they were checked for growth. Standard drug, streptomycin, was used.[16-23]

RESULTS AND DISCUSSION

In view of our ongoing research focused on the development of new synthetic novel Thiazolidine-2-one derivatives, the present study aims to design, synthesize, and *in silico* studies of a novel series of substituted thiazolidin-2-one derivatives were prepared from the corresponding Schiff bases and 2-mercaptoacetic acid in benzene. The estimation of molecular descriptors and pharmacokinetic parameters of

Table 3: Pharmacokinetic study by SWISS**ADME**

Compound code	GI absorption (high/low)	BBB permeant (Yes/No)	P-gp Substrate (Yes/No)	PAINS (alert)
1a	High	Yes	No	0
1b	High	Yes	No	0
1c	High	Yes	No	0
1d	High	Yes	No	0
1e	High	Yes	No	0
2a	High	No	Yes	0
2b	High	Yes	Yes	0
2c	High	No	No	0
2d	High	Yes	Yes	0
2e	High	No	Yes	0

GI: Gastrointestinal, ADME: Absorption, distribution, metabolism, and excretion, BBB: Blood–brain barrier

Table 4: Docking score of synthesized compounds with protein 4HZR

Compound code	H-bond interaction	Vdw interacting residues	Binding energy (Kcal/mol)
1a	VALA292:H	LEUA302, PHEA294, PROA293, SERA301, VALA292, CYSA293, ARGA305, PHEA30, META286, LYS291	**–7.14**
1b	CYSA119:O	ASPA146, ALAA147, CYSA119, ASPA125, TRPA145, ILEA121, GLYA122, PROA148, HISB182, THRB118, LEUA120	–4.11
1c	ARGB290:H	PHEB294, LYSB291, LEUB302, ARGB290, VALB292, SERB301, ARGB305, PHEB307, METB286, CYSB297	**–8.47**
1d	GLUB329:H TRPB331:O ILEB332:O	GLUB329, TRPB331, ILEB332, TRPB321, PROB351, GLN328, PROB330, LEUB350	–5.53
1e	VALA292:H	LEUA302, PHEA294, CYSA297, SERA301, VALA292, ARGA305, PHEA307, META286, LYSA291	–5.28
2a	VALA292:H	LEUA302, PHEA294, PROA293, SERA301, VALA292, CYSA293, ARGA305, PHEA30, META286, LYS291	**–7.23**
2b	CYSA119:O	ASPA146, ALAA147, CYSA119, ASPA125, TRPA145, ILEA121, GLYA122, PROA148, HISB182, THRB118, LEUA120	–6.23
2c	ARGB290:H	PHEB294, LYSB291, LEUB302, ARGB290, VALB292, SERB301, ARGB305, PHEB307, METB286, CYSB297	**–8.53**
2d	GLUB329:H TRPB331:O ILEB332:O	GLUB329, TRPB331, ILEB332, TRPB321, PROB351, GLN328, PROB330, LEUB350	–6.60
2e	VALA292:H	LEUA302, PHEA294, CYSA297, SERA301, VALA292, ARGA305, PHEA307, META286, LYSA291	–5.84

Bold values indicate the lowest binding energy (kcal/mol) for each ligand–receptor complex, representing the most favourable binding affinity as predicted by molecular docking.

the proposed derivatives was done by ACD Lab Chemsketch version. 12.0 and Molinspiration Online Software, respectively. From all these parameters are enlisted in Table 1, the compounds obeying Lipinski's rule of five were selected for docking studies. The drug-likeness score, which is used to determine their affinity toward certain receptors, is shown in Table 2.

Pharmacokinetic prediction of the synthesized derivatives by Swiss ADME is represented in Table 3. All the derivatives exhibited high GI absorption. All the derivatives were found to be permeant of the blood–brain barrier except compounds **2a**, **2c,** and **2e,** and zero alert for PAINS.

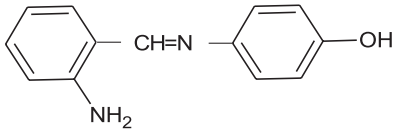
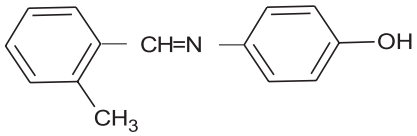
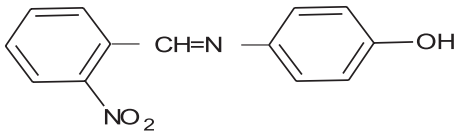
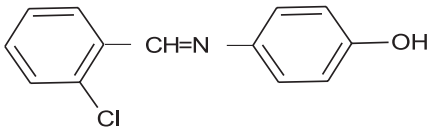
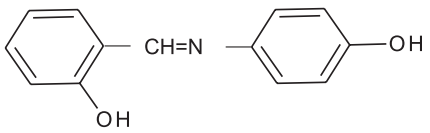
Docking results revealed a high negative docking score, as illustrated in Table 4. It indicates very good interaction and affinity with the binding site of protein 4HZR. All the synthesized compounds exhibit hydrogen bonding with the receptor and show binding in the active site between −4.11 and −8.53 Kcal/mol.

The characterization of synthesized derivatives carried out by TLC and melting point determination is presented in Table 5. Spectral characterization was done by Infrared, ^{1}H NMR, ^{13}C NMR, and mass spectroscopy. The results are shown in Tables 6-8.

Table 5: Physical characterization of synthesized compounds

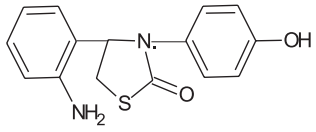
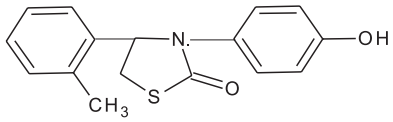
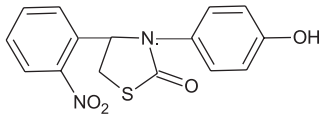
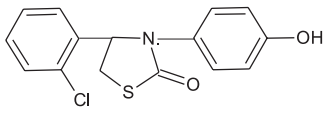
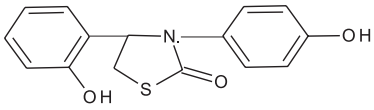
Compound code	Molecular formula	Melting point (°C)	Rf-value
1a	$C_{13}H_{12}N_2O$	98–102	0.65
1b	$C_{14}H_{13}NO$	107–109	0.69
1c	$C_{13}H_{10}N_2O_3$	113–115	0.72
1d	$C_{13}H_{10}ClNO$	123–125	0.75
1e	$C_{13}H_{11}NO_2$	121–124	0.60
2a	$C_{15}H_{12}SN_2O_2$	129–131	0.66
2b	$C_{16}H_{13}SNO_2$	130–132	0.78
2c	$C_{15}H_{10}SN_2O_4$	133–135	0.73
2d	$C_{15}H_{10}ClSNO_2$	142–145	0.72
2e	$C_{15}H_{11}SN_2O_4$	139–141	0.70

Table 6: Characteristic IR peaks of synthesized compounds

Compound code	Structure and IUPAC name	IR (KBr υ/cm)
1a	 4-(2-benzylidene diamino)phenol	3354.32N-H (stretch), 1469.81C=C, 1342.50C-N, 1618.33C=N, 1701.27 C-OH
1b	 4-(2-methylbenzylidene amino)phenol	3285.18C-H (aromatic), 1577.38C=C 608.12 Aliphatic C-H stretch, 1597.11C=N,1338.94C-N, 1577.32 -OH
1c	 4-(2-nitrobenzylidene amino)phenol	3132.21 (Ar-CH str), 3245.23 (CH=CH str), 2843.43 (CH2 str), 1684.39 (C-OH str), 742.23(C-C-str), 3457.54 (NH-str), 1264.32 cm-1 (C-Nstr)
1d	 4-(2-chlorobenzylidene amino)phenol	3169.76 (Ar-CH str), 2876.87 (CH2 str), 1687.54 (C=O str), 1034.56 (C-O-C str), 1598.89(C=N-str), 865.43 (Ar-C-Cl), 3467.98 (NH-str),1257.85 cm-1 (C-N-str)
1e	 4-(2-hydroxybenzylidene amino)phenol	3124.32 (Ar-CH str), 2832.12 (CH2 str), 1685.34 (C=O str), 1034.53 (C-O-C str), 1567.32(C=N-str), 845.32 (C-C-str), 3467.32 (NH-str),1256.34 cm-1 (C-N-str)

(Contd...)

Table 6: *(Continued)*

Compound code	Structure and IUPAC name	IR (KBr υ/cm)
2a	 (2-(2amino-phenyl)-3-(4-hydroxy phenyl)thiazolidin-2-one)	3198.36, 1309.01 CC stretch, 2591.86 ArSH stretch, 1557.24 CO stretch, 1663.3 C=N stretch, 710.25 CSC stretch, 1264.83 CN stretch, 3316.54 ArN stretch
2b	 (2-(2methyl-phenyl)-3-(4-hydroxy phenyl)thiazolidin-2-one)	2922.59 Aliphatic CH stretch, 1658.48 Aromatic CH stretch, 1611.23 C=N stretch, 3200.29 NH stretch, 740.03 CSC stretch, 3061.44 NH stretch (2º amine), 1430.92 C=C stretch, 905.41 CC stretch
2c	 (2-(2nitro-phenyl)-3-(4-hydroxy phenyl)thiazolidin-2-one)	1371.14 C-H bending, 2894.66 Ar-SH stretch, 1283.63 C-Ostretch, 938.54 C-C stretch, 755.07 C-S-C stretch, 1638.23 C=C stretch, 1589.06 Ar-NO2
2d	 (2-(2chloro-phenyl)-3-(4-hydroxy phenyl)thiazolidin-2-one)	1591.95 Aromatic C=C stretch, 1810.24 NNstretch, 1655.04Ar C=N stretch, 1310.26 CO stretch, 2919.7 Aliphatic CH stretch, 696.08 CSC stretch, 3198.36 ArNH stretch, 848.64 ArCl stretch
2e	 (2-(2hydroxy-phenyl)-3-(4-hydroxy phenyl)thiazolidin-2-one)	1507.20 C=C stretch 1589.06 C=N stretch, 1112.32 C-Ostretch, 957.23 Aromatic C-C stretch, 1857.4 N-N stretch, 1265.81 C-N stretch 637.8 C-S-C stretch, 3192.58 N-H stretch 1265.81 C-O stretch

IR: Infrared, IUPAC: International Union of Pure and Applied Chemistry

Table 7: ^{1}H NMR & ^{13}C NMR spectral values of synthesized compounds

Compound code	^{1}H NMR (ppm)	^{13}C NMR (ppm)
2a	7.418 (d, ArH, 1H), 7.421 (t, ArH, 1H), 7.830 (d, ArH, 1H), 7.752 (d, ArH, 1H), 4.161 (s, SCH2, 2H), 4.263 (s, NH2, 2H), 7.850 (t, NH, 1H)	a (122.281C, s), b (128.951C, s), c (152.871C, s), d (135.381C, s), e (165.271C, s), f (36.111C, s), g (153.171C, s), h (159.171C, s), i (52.141C, s), j (135.141C, s), k (121.831C, s), l (128.951C, s), m (129.071C, s)
2b	7.936 (t, Ar-H, 1H), 7.825 (d, Ar-H, 1H), 7.440 (d, Ar-H, 1H), 7.409 (d, Ar-H, 1H), 4.441 (s, S-CH2,2H), 9.579 (d, S-H, 1H)	a (121.831C, s), b (126.931C, s), c (152.911C s), d (135.201C, s), e (165.471C, s), f (35.371C, s), g (158.791C, s), h (161.371C, s), i (40.391C, s), j (40.591C, s), k (27.201C, s), l (39.341C, s)
2c	7.803 (d, ArH, 2H), 7.337 (d, ArH, 2H), 4.153 (s, SCH2, 2H), 4.441 (s, SCH2, 2H), 2.264 (d, ArC, 4H),3.370 (d, ArC, 4H)	a (122.351C, s), b (126.931C, s), c (152.891C s), d (135.351C, s), e (165.481C, s), f (34.891C, s), g (158.841C, s), h (180.581C, s), i (50.091C, s), j (40.551C, s), k (66.621C, s
2d	7.312 (d, ArH, 2H), 7.804 (d, ArH, 2H), 4.150 (s, SCH2, 2H), 4.466 (s, SCH2, 2H), 7.993 (s, NH, 1H), 6.925 (d, ArH, 2H), 6.998 (d, ArH, 2H), 2.166 (s, ArCH3, 3H)	a (122.181C, s), b (128.951C, s), c (152.871C, s), d (135.141C, s), e (165.271C, s), f (36.111C, s), g (159.171C, s), h (148.171C, s), i (52.141C, s), j (135.381C, s), k (119.081C, s), l (129.071C, s), m (147.511C, s), n (27.111C, s)
2e	7.012 (d, ArH, 2H), 7.194 (d, ArH, 2H), 4.218 (s, SCH2, 2H), 4.473 (s, SCH2, 2H), 8.113 (s, NH, 1H), 7.79 (d, ArH, 2H), 8.071 (d, ArH, 2H)	a (119.451C, s), b (131.761C, s), c (147.851C, s), d (131.961C, s), e (66.991C, s), f (39.301C, s), g (107.701C, s), h (67.111C, s), i (40.551C, s), j (111.961C, s), k (116.441C, s), l (116.231C, s), m (147.231C, s)

^{1}H NMR: ^{1}H Nuclear magnetic resonance

Table 8: Mass spectral values of synthesized compounds

Compound code	Molecular mass	Molecular ion peak
1c	242.23	242.31
2c	316.34	316.37

Table 9: Anti-tubercular activity of synthesized compounds

Compound code	Concentration		
	25 µg/mL	50 µg/mL	100 µg/mL
1a	R	R	S
1b	R	R	R
1c	R	S	S
1d	R	R	R
1e	R	R	R
2a	R	R	S
2b	R	R	R
2c	R	S	S
2d	R	R	R
2e	R	R	R
Std. Streptomycin	S	S	S

R: Resistant, S: Sensitive

Anti-tubercular Evaluation

The anti-tubercular activity results presented in Table 9 reveal that compounds 1c and 2c demonstrated strong inhibitory effects at both 50 µg/mL and 100 µg/mL against the H37Rv strain. Compounds 1a and 2a, however, showed only moderate activity at 100 µg/mL.

CONCLUSION

The present study was conducted by *in silico* modeling and synthesis of substituted thiazolidin-2-one derivatives. These derivatives were characterized using physical and spectral analytical studies. All the derivatives were evaluated for *in vitro* anti-tubercular activity.

Compounds 1c and 2c demonstrated significantly higher *in vitro* anti-tubercular activity compared to other tested derivatives. This enhanced potency suggests that the specific structural modifications present in these compounds may play a critical role in improving their biological efficacy.

These modifications could potentially enhance cell permeability or promote stronger and more specific interactions with the bacterial target, contributing to their superior activity. Further studies are warranted to elucidate the exact mechanisms underlying their improved performance and to explore their potential as lead compounds for anti-tubercular drug development.

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