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Synthesis, characterization and antibacterial effect of diarylmethylamine-based imines

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ABSTRACT

Firstly, starting from benzoic acid the diarylmethanone compound was synthesized. The diarylmethanone was converted to the corresponding oxime and then reduced to the diarylmethylamine compound. Four different imine compounds were obtained from the condensation of the diarylmethylamine compound with four different salicylaldehyde derivatives. Antimicrobial activities against Gram (+) and Gram (−) microorganisms (*Staphylococcus aureus, Bacillus cereus* as the Gram (+); *Escherichia coli and Salmonella typhimurium* as the Gram (−); and *Candida albicans* as the fungi) were investigated.

1. Introduction

In our days, the source of many active pharmaceutical agents are laboratories. It has even become possible to synthesize many drugs that can be obtained naturally. Pharmaceutical companies prefer this way when it is cost effective. While the first drugs used medically are simple molecules [1], it is now seen that more complex active substances are used today [2,3]. Misuse of the active substances has led to the increasing resistance of some microbes to drugs [4–6]. In addition to combating harmful microbes, such active substances should not cause any side effects in the body. In order to overcome this situation, synthesis of new drug candidate molecules has gained importance [7–10]. Human beings are exposed to very different chemicals in daily life. These chemical compounds can themselves be toxic or become toxic compounds as a result of biotransformation within the organism [11]. It is thought to cause mutation by making covalent bonds with proteins containing −SH, $-NH_2$ or −OH groups and macromolecules such as RNA and DNA [12–15].

Diarylmethylamines are important compounds because of their pharmacological properties and easy availability [16]. In recent years, diarylmethylamines have attracted attention due to their high activity against tuberculosis, various viruses and HIV [17–19]. Also, many of the molecules containing the diarylmethylamine skeleton are currently used as pharmaceutical drugs. Examples include Levocetirizine, Zyrtec, Solifenacin, Meclozin, etc. Found. Moreover, the diarylmethylamine based compounds have been shown to possess antimicrobial properties [20a]. Schiff base ligands and metal complexes are used successfully in many fields such as agricultural chemistry, medicine, optical and electrochemical sensors [20b]. Imine derivatives and metal complexes are extremely important compounds because of these effective properties. All of these advantages emphasize that Schiff bases are pioneering compounds in the pharmaceutical industry [21–25]. Nowadays, the first step of pharmaceutical studies is the synthesis of target molecule(s). 2-Hydroxybenzaldehyde and its derivatives are widely used for the synthesis of novel imine derivatives [26–28].

The aim of this study was to investigate the synthesis, structural characterization and antimicrobial effects of new imine compounds which could be drug candidate molecules. In order to investigate the antimicrobial properties, diarylmethylamine-based imine compounds (Scheme) have been synthesized. The hydroxy and methoxy substitute groups on the phenyl ring have been found to affect the biological properties of the Schiff base compounds. The effect of the substitute groups on the antimicrobial activity was also examined. The single crystals of the ligands **7a** and **7d** were obtained from ethanol (**7a**) and ethylacetate/hexane (**7d**) solution by the slow evaporation at room temperature and their molecular

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structures were examined by the X-ray diffraction studies. The antimicrobial and antifungal properties of all compounds were investigated.

2. Experimental

2.1. Materials and measurements

All reagents and solvents were of reagent-grade quality and obtained from commercial suppliers (Aldrich or Merck) and used as received, unless otherwise noted. Elemental analyses (C, H, N) were performed using a Costech ECS 4010 (CHN). Infrared spectra were obtained using KBr disc (4000-400 cm^{-1}) on a PerkinElmer Spectrum 100 FT-IR. ^1H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz instrument and TMS was used as an internal standard.

2.2. General method for the synthesis of imine compounds (7a-d)

The synthesis of diarylmethanon **3**, oxime **4** and diarylmethylamine **5** were carried out using a method available in the literature [29–31]. Phenyl (*p*-tolyl) methanamine (4 g; 20.27 mmol) was dissolved in CH_2Cl_2 (30 mL). To this solution, potassium carbonate (4 g; 29 mmol), 2-hydroxy-3-methoxy benzaldehyde (3.08 g; 20.27 mmol) and sodium sulfate (4 g; 28 mmol) were added respectively, and stirred under nitrogen gas at room temperature for 24 h. The progress of the reaction was controlled by TLC. The solids in the reaction media were removed by filtration. After removal of the solvent, the oily residue was filtered over silica gel (10 g) with ethylacetate/hexane (1:9). The solvents were removed and the product was crystallized from ethanol.

7a: Yield 4.60 g (69%), color: Yellow. melting point:91–93 °C. FTIR: (ν_{max}, cm^{-1}): 3423, 3025, 2956, 1624, 1460, 1381, 1334, 1253, 1081, 1048, 969, 838, 800, 775, 733, 694, 545.^1H NMR (400 MHz, $CDCl_3$, δ ppm): 14.20 (s, 1H, phenolic OH), 8.65 (s, N=CH, 1H), 7.33–7.40 (m, 4H, ArH), 7.26–7.28 (m, 3H, ArH), 7.17 (d, J = 8.0 Hz, 2H, ArH), 6.97 (dd, J = 7.8, 1.5 Hz, 1H, ArH), 6.92 (dd, J = 7.8, 1.5 Hz, 1H, ArH), 6.85 (t, J = 7.8 Hz, 1H, ArH), 5.63 (s, 1H, HC=N), 3.95 (s, 3H, OCH_3), 2.35 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):164.84, 151.60, 148.47, 142.75, 139.64, 137.12, 129.40, 128.69, 127.34, 123.19, 118.76, 118.18, 114.23, 76.25, 56.13, 21.07. Anal. Calcd for $C_{22}H_{21}NO_2$: C, 79.73; H, 6.39; N, 4.23. Found C, 79.68; H, 6.41; N, 4.26.

7b: Yield 4.8 g (72%), color: Light yellow. melting point: 122–124 °C. FTIR: (ν_{max}, cm^{-1}): 3435, 2963, 2928, 2847, 1625, 1574, 1512, 1443, 1399, 1376, 1288, 1204, 1168, 1114, 1043, 1025, 963, 840, 813, 735, 700, 650, 524.^1H NMR (400 MHz, $CDCl_3$, δ ppm) 14.10 (s, 1H, phenolic OH), 8.37 (s, N=CH, 1H), 7.38 (d, J = 4.4 Hz, 4H, ArH), 7.26–7.32 (m, 3H, ArH), 7.16–7.20 (m, 3H, ArH), 6.53 (d, J = 2.3 Hz, 1H, ArH), 6.47 (dd, J = 8.5, 2.4 Hz, 1H, ArH), 5.60 (s, 1H, HC=N), 3.85 (s, 3H, OCH_3), 2.37 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):164.22, 163.94, 163.58, 142.93, 139.81, 137.05, 132.90, 129.38, 128.66, 127.45, 127.29, 112.71, 106.52, 101.17, 75.78, 55.40, 21.09. Anal. Calcd for $C_{22}H_{21}NO_2$: C, 79.73; H, 6.39; N, 4.23. Found C, 79.71; H, 6.32; N, 4.18.

7c: Yield 5.35 g (84%), color: Orange, melting point: 113–115 °C. FTIR: (ν_{max}, cm^{-1}):3429, 3020, 2919, 2857, 1630, 1463,1380, 1273, 1205, 1084, 1045, 843, 800, 777, 724, 700, 537.^1H NMR (400 MHz, $CDCl_3$, δ ppm): 8.40 (s, N=CH, 1H), 7.16–7.42 (m, 11H, ArH and ArOH), 7.04 (dd, J = 7.7, 1.6 Hz, 1H, ArH), 6.84 (dd, J = 7.9, 1.5 Hz, 1H, ArH), 6.77 (t, J = 7.8 Hz, 1H, ArH), 5.71 (s, 1H, HC=N), 2.39 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 164.71, 151.64, 145.62, 142.05, 138.91, 137.44, 129.54, 128.82, 127.60, 127.46, 126.90, 122.37, 118.13, 117.53, 116.96, 74.93, 21.11. Anal. Calcd for $C_{21}H_{19}NO_2$:C, 79.47; H, 6.03; N, 4.41. Found C, 79.31; H, 6.24; N, 4.46.

7d: Yield 4.30 g (66%), color: orange, melting point: 167–169 °C. FTIR: (ν_{max}, cm^{-1}): 3435, 3021, 2917, 1632, 1583, 1503, 1469, 1368, 1281, 1229, 1172, 1122, 621.^1H NMR (400 MHz, $CDCl_3$, δ ppm): δ 8.02 (s, 1H), 7.26–7.37 (m, 5H, ArH), 7.22 (d, J = 8.1 Hz, 2H, ArH), 7.16 (d, J = 8.0 Hz, 2H, ArH), 6.92 (d, J = 8.6 Hz, 1H, ArH), 6.44 (d, J = 2.2 Hz, 1H, ArH), 6.30 (dd, J = 8.6, 2.3 Hz, 1H, ArH), 5.63 (s, 1H, HC=N), 2.34 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 168.73, 163.28, 163.05, 163.04, 141.75, 138.59, 137.43, 134.16, 129.53, 128.81, 127.60, 127.41, 111.57, 107.87, 104.19, 72.93, 21.07. Anal. Calcd for $C_{21}H_{19}NO_2$:C, 79.47; H, 6.03; N, 4.41. Found C, 79.35; H, 5.93; N, 4.37.

2.3. X-ray crystallography

X-ray crystallographic data for the compounds **7a** and **7d** were collected at 293 (2) K on a Bruker D8 QUEST diffractometer using Mo-$K\alpha$ radiation (λ = 0.71073 Å). Data reduction was completed using Bruker SAINT [32]. SHELXT 2018/2 was used to solve and SHELXL-2018/3 to refine the structures [33]. The structures were solved by direct methods and refined on F^2 using all the reflections. All the non-hydrogen atoms were refined using anisotropic atomic displacement parameters and hydrogen atoms bonded to carbon, nitrogen and oxygen atoms were inserted at calculated positions using a riding model and refined with temperature factors. The crystal data and refinement details are given in Table 1 and the rest of the crystallographic data are given in the supplementary documents (Tables S1–S12).

2.4. Preparation and cultivation of bacterial strains

The imine compounds were evaluated *in vitro* antibacterial and antifungal activity against the *Staphylococcus aureus, Bacillus cereus* as the gram (+); *Escherichia coli* and *Salmonella typhimurium* as the gram (−); and *Candida albicans* as the fungi. Antibiotics (Gentamicin and amikacin) were used as positive control groups. The susceptibility of a microorganism to antimicrobial agents and antibiotics was determined by assay plates incubated at 37 °C for 18–24 h for bacteria and 25 °C for three days for yeasts. In the antimicrobial activity studies, Malt Extract Agar (MEA) for the yeast strain and Müeller Hinton Agar (MHA) for bacteria was used as a stock medium. Bacteria standardized with 0.5 McFarland standard was inoculated to sterile prepared petri dishes and incubated for 1 h at 37 ± 1 °C [30,31]. DMSO was used as control. Amikacin (AK: 30 μg) and Gentamicin (CN: 10 μg) were used as standards. The antimicrobial activity of the imine compounds was determined using Kirby-Bauer Disk Diffusion Method [34,35]. The imine compounds (12.50 mg/mL) were dissolved in 10% DMSO and impregnated with disks at a concentration of 25 μL to discs made of blank sterile whatman papers of 6 mm diameter. Prepared discs were placed on the cultivation of bacteria in the MHA. Discs were placed on planted cultures of bacteria in MHA and yeast strains in MEA. Discs were incubated at 37 ± 1 °C for 18–24 ± 2 h to determine inhibition zones [34–39]. The study was performed in three replicates and the mean values were given.

The samples (**7a-d**) were 12.5 mg/mL, 1.25 mg/mL and 0.125 mg/mL dissolved in 10% DMSO to determine the minimum inhibitory concentration (MIC) against Gram positive (+), Gram negative (−) bacteria and yeast strains and the value was determined.

3. Results and discussion

In the current work, four different imine compounds were synthesized in order to investigate biological activities. The synthesis of diaryl methylamine, which is the key molecule for the synthesis of four new imine compounds, was carried out from benzoic acid (**Scheme**). For this purpose, benzoic acid was first converted to benzoyl chloride and then the corresponding ketone

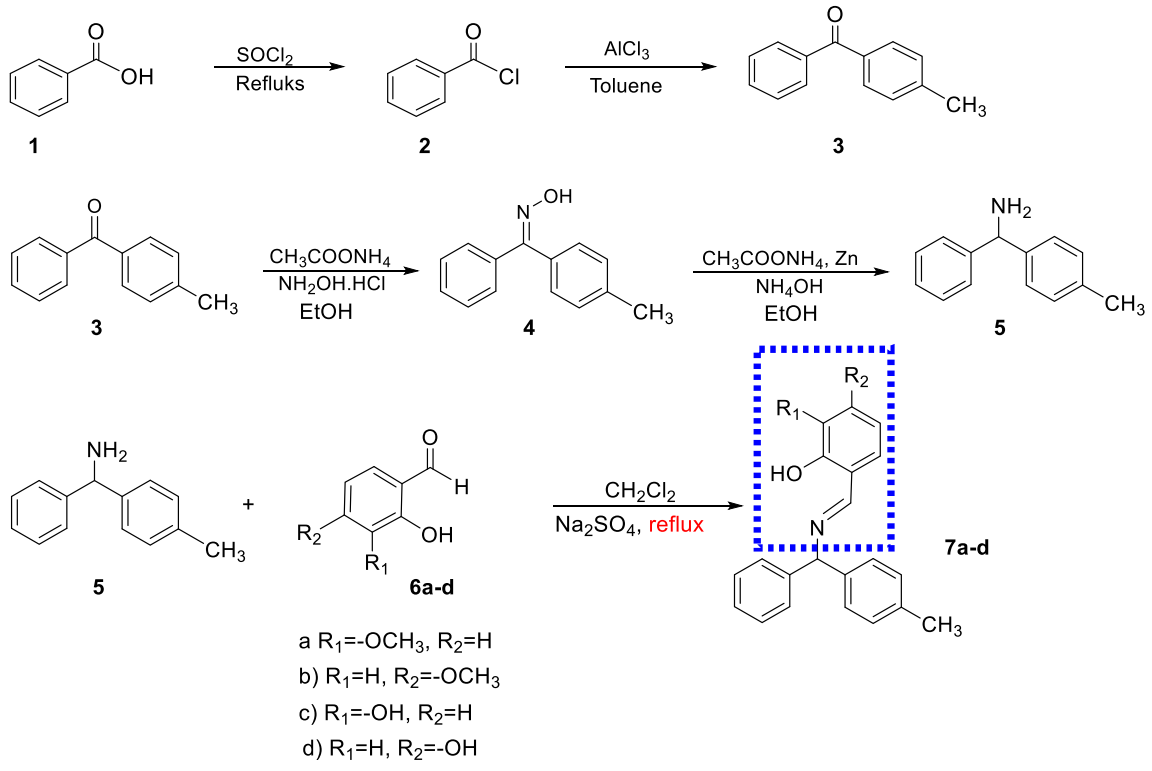
Table 1
X-ray crystallographic data for compounds **7a** and **7d.**

Compound	7a	7 d
Formulae	$C_{22}H_{21}NO_2$	$C_{21}H_{19}NO_2$
Molecular weight	331.40	317.37
Temperature	293 (2) K	293 (2)
Wavelenght	0.71073 Å	0.71073 Å
Crystal system	*Orthorhombic*	*Triclinic*
Crystal color	Yellow	Orange
Space group	$P2_12_12_1$	*P-1*
Unit cell parameters	a = 6.2645 (5) Å α = 90° b = 16.1190 (15) Å β = 90° c = 18.0294 (16)Å γ = 90°	a = 9.7556 (7) Å α = 88.664 (7)° b = 11.8979 (10) Å β = 78.304 (7)° c = 15.3674 (14) Å γ = 89.548 (6)°
Volume ($Å^3$)	1820.6 (3)	1746.2 (3)
Z	4	4
Density (calc.) (Mg/m^3)	1.209	1.207
Absorption coefficient (mm^{-1})	0.077	0.077
Crystal size (mm^3)	0.16 × 0.11 x 0.09	0.18 × 0.12 x 0.10
Ref. collected	7271	11,280
Indepent ref.	4101 [R_{int} = 0.0837]	7511 [R_{int} = 0.0261]
Final R values [I > 2 sigma(I)]	R_1 = 0.0796, wR_2 = 0.1073	R_1 = 0.0955, wR_2 = 0.2177
R indices (all data)	R_1 = 0.3036, wR_2 = 0.1702	R_1 = 0.1610, wR_2 = 0.2574
Completeness to θ = 25.242°	99.7%	99.0%
CCDC Number	1,973,960	1,973,961

compound was synthesized with the aid of $AlCl_3$/toluene. The targeted phenyl (*p*-tolyl) methanamine molecule was synthesized by converting the diarylmethanone compound to oxime and followed by reduction to corresponding amine. The condensation of **5** with salicylaldehyde derivatives, (2-hydroxy-3-methoxybenzaldehyde, 2-hydroxy-4-methoxybenzaldehyde 2,3-dihydroxybenzaldehyde, and 2,4-dihydroxybenzaldehyde), gave four new imine compounds (**7a-d**). After required purification, the structure of each molecule was characterized using analytical and spectroscopic methods. The elemental analysis data of the synthesized compounds are consistent with the calculated values of the proposed structures. (Scheme 1).

3.1. Spectroscopic characterization of the imine compounds

FT-IR spectra of the imine compounds were carried out and the data are given in the experimental section. FT-IR spectra of the compounds were given in the supplementary documents (Figs. S1–S4). The broad peaks around 3400-300 cm^{-1} are due to the ν(OH) stretchings. The bands observed at 1623, 1619, 1628 and



Scheme 1. Synthesis route of Schiff base ligands.

Table 2
Selected bond lengths (Å) and angles (°) for **7a** and **7d**.

	7a	7 d
N1–C14	1.279 (9)	1.304 (5)
O1–C20	1.352 (9)	1.305 (4)
C14–C15	1.417 (10)	1.404 (5)
O3–C41	–	1.295 (4)
N2–C35	–	1.309 (4)
C8–C7–C6	110.4 (8)	114.9 (4)
N1–C14–C15	122.4 (9)	123.5 (4)
C14–N1–C7	117.6 (7)	127.1 (4)

1627 cm^{-1} are characteristic signals of the imine groups. The absence of the carbonyl group stretchings of the starting salicylaldehyde derivatives also confirmed the formation of the imine compounds.

In the ^{1}H NMR spectra of synthesized compounds (Figs. S5–S8), especially the expected *ortho* and *meta* interactions in the salicylaldehyde ring can be seen very clearly. When the ^{1}H NMR spectra of the new imine compounds were examined; Singlets for **7a,7b**, **7c** and **7d** observed at 8.49, 8.37, 8.40 and 8.02 ppm respectively are the proton signals of the characteristic azomethine group (CH=N). Singlets observed at 5.63, 5.60, 5.71 and 5.63 ppm in the spectra of all ligands are dibenzylic proton signals adjacent to the imine group, respectively. The methyl group in the structure of imine compounds resonated as singlet at 2.35, 2.37, 2.39 and 2.34 ppm, respectively. Singlets, which are seen at 3.95 and 3.80 ppm in **7a** and **7b** spectra respectively, belong to OMe protons.

The ^{13}C NMR spectra of the ligands appear to be in complete agreement with the proposed structures. The characteristic imine carbons resonated at 164.84, 163.94, 164.85 and 163.28 ppm, respectively. The other carbon atoms of **7a-d** compounds resonated between 168.07 and 21.07 ppm.

3.2. X-ray structure solution and refinement of 7a and 7 d

The single crystals of the compounds suitable for X-ray diffraction experiments were obtained from slow evaporation of

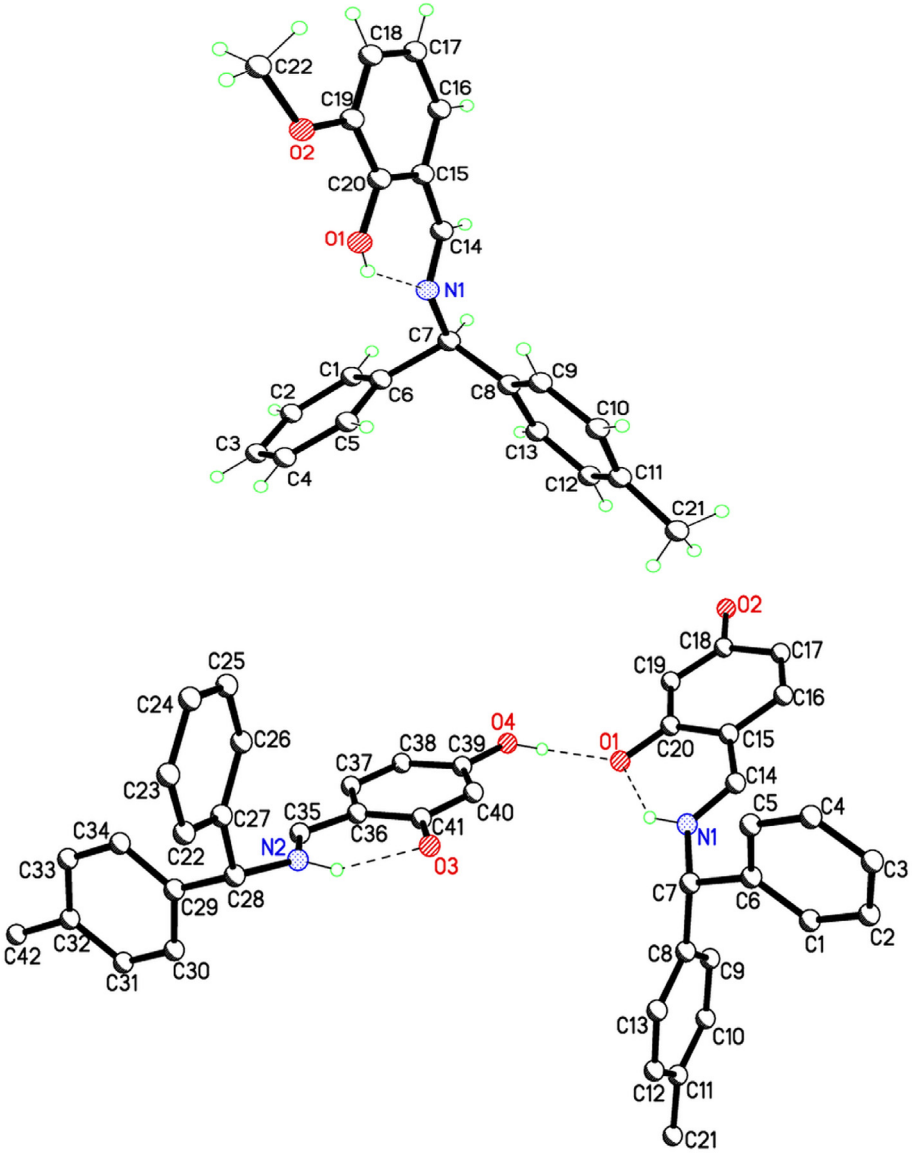


Fig. 1. Molecular structures of **7d** and **7a** with atom numbering. Hydrogen bonds are shown as dashed lines. The hydrogen atoms bonded to carbon atoms are not shown for clarity in **7d**.

Table 3
Hydrogen bond parameters for **7a** Ligand.

Compound	D-H … ·A	d (D-H)	d (H … ·A)	d (D … ·A)	<(DHA)
7a	O (1)–H (1) … ·N (1)	0.82	1.86	2.564 (9)	143.7
7d	O (2)–H (2) … ·O (3)^{i}	0.82	1.76	2.579 (4)	173.8
	N (1)–H (1) … ·O (1)	0.86	1.90	2.591 (4)	135.8
	O (4)-H (4A) … ·O (1)	0.82	1.74	2.552 (4)	172.8
	N (2)-H (2B) … ·O (3)	0.86	1.93	2.604 (4)	134.0

Symmetry transformations used to generate equivalent atoms: *i*: x-1,y,z.

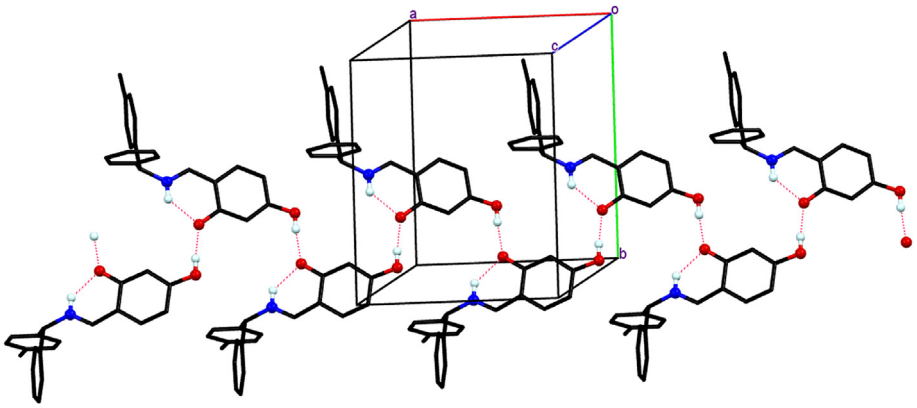


Fig. 2. Packing diagram of **7d** showing 1D OH … ·O hydrogen bond chain.

ethanol for **7a** and ethyl acetate-hexane mixture for **7d**. Crystallographic data of are given in Table 1 and the selected bond lengths and angles are given in Table 2. The X-ray data showed that compound 7a crystalizes in the *orthorhombic* crystal system and P_{212121} space group, while compound 7 d is in the *triclinic* crystal system and *P-1* space group. Perspective view of the compounds are given in Fig. 1. The asymmetric unit of **7d** contains two crystallographically independent molecules. The two independent molecules show similar bond lengths and angles with different dihedral angles between the phenyl rings. In the structure of **7a**, the imine (N1–C14) bond distance of 1.279 (9) Å is within the range of characteristic carbon nitrogen double bond (C=N). The compound **7a** favors the phenol-imine tautomeric form in the solid state. However, in the structure of **7d** the imine bond [N1–C14 and

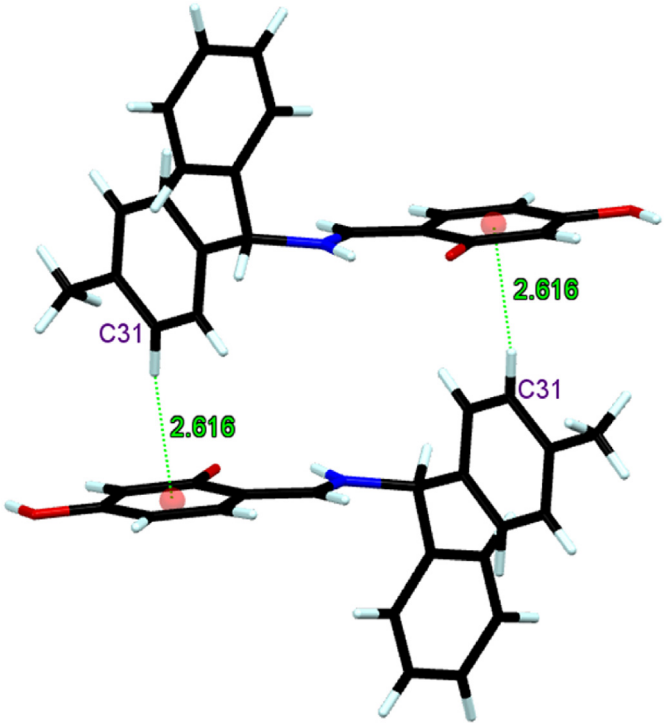


Fig. 3. CH … ··π interactions in **7d**.

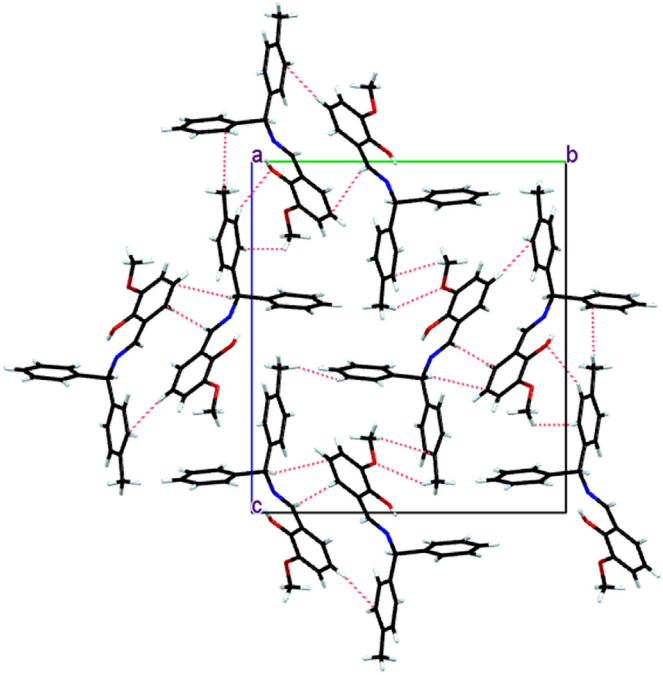
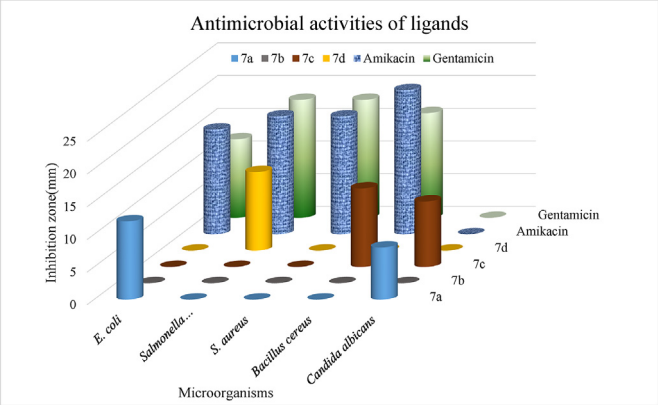


Fig. 4. Packing diagram of **7a** showing CH … ··π and CH … ··O interactions.

Table 4
Antimicrobial activity values of the bacteria and fungi (mm).



N2—C35] distances are longer than those characteristic C═N distances and phenolic [C20—O1 and C41—O3] bond distances are shorter than phenolic C—O bond distances (Table 2). This suggests that the compound **7d** favors the keto-enol tautomeric form in the solid state.

The compounds showed an expected phenol-imine and keto-amine intramolecular hydrogen bonding. The compound **7d** contains second hydroxyl group which is involved in intermolecular hydrogen bonding with the phenolic oxygen of an adjacent molecule. The hydrogen bond parameters for **7a** and **7d** are listed in Table 3. The intermolecular hydrogen bond contacts form a 1D hydrogen bond chains as shown in Fig. 2. In the structure of **7d**, no phenyl-phenyl stacking interactions were observed and instead CH … ••π interactions stabilize the structure of the compound (Fig. 3). The molecules of **7a** are linked by CH … ••π and CH … ••O interactions. Packing diagram of **7a** is shown in Fig. 4.

3.3. Biological activity findings

In the *in vitro* antimicrobial activity studies, we used the *Staphylococcus aureus and Bacillus cereus* as the Gram (+); *Escherichia coli and Salmonella typhimurium* as the Gram (−); and *Candida albicans* as the fungi. The antimicrobial activities of the ligands (**7a-d**) used in the study were investigated by disc diffusion method against Gram (+), Gram (−) bacterial strains and *Candida albicans* fungi. The results were compared with the standard antibiotics amikacin and gentamicin. The observed antimicrobial activities of the ligands are shown in Table 4. According to the findings, **7a** ligand showed significant activity against *Escherichia coli* and *Candida albicans* strains, **7c** ligand against *Bacillus cereus* and *Candida albicans* strains and **7d** ligand against *Salmonella typhimurium* strain. It was determined that ligand **7b** showed no zone of inhibition against the microorganisms used in the study. According to the findings, an important point is that antifungal effect of **7a** and **7c** ligands against *Candida albicans* fungus (see Table 4). Compounds **7a** and **7b** are isomers differing only in the position of the methoxy groups on the phenol ring. The change of position of the methoxy groups cause significant change in the activity of the compounds. While compound **7a** exhibits significant activity against *Escherichia coli,* compound **7b** has very low activity against the all microorganisms studied. This may be due to the cell permeation properties of these compounds that may be changed with the position of the methoxy group. Similar results were observed for compounds **7c** and **7d**. Although compound **7c** inhibits the bacterial growth of *Bacillus cereus* and *Candida albicans* strains, the change of the position of the hydroxy group in compound **7d** results in a sharp decline in the activity towards the same microorganisms. However, compound **7d** has considerable antimicrobial activity against *Salmonella typhimurium* when compared to the standard antibiotics (amikacin and gentamicin). All compounds are almost no-toxic towards *Staphylococcus aureus* at the concentration studied (12.50 mg/mL).

4. Conclusion

Four imine compounds (**7a-d**) were prepared by the Schiff base condensation reaction of phenyl (*p*-tolyl) methanamine and 2-hydroxy-3-methoxybenzaldehyde (for **7a**), 2-hydroxy-4-methoxybenzaldehyde (for **7b**), 2,3-dihydroxybenzaldehyde (for **7c**) and 2,4-dihydroxybenzaldehyde (for **7d**) in dichloromethane. Molecular structure of compounds**7a** and **7d** were determined by single crystal X-ray diffraction study. In the solid state, compound **7d** exists in keto-amine tautomeric form. Antimicrobial activity studies of the imine compounds were studied using the *E. coli, S. typhimurium, S. aureus, B. cereus*, as bacteria and *C. albicans* as fungi. Imine **7a** showed the high activity against to the *E. coli*, **7c** *B. cereus* and **7d** *S. aureus* while the ligand **7b** do not showed the activity towards the bacteria and fungi. Compound **7a** and **7c** showed the good activity against to the *C. albicans.*

CRediT authorship contribution statement

Sultan Onur: Investigation. **Muhammet Köse:** Data curation, Software, Writing - review & editing. **Ferudun Koçer:** Investigation. **Ferhan Tümer:** Supervision, Project administration, Writing - original draft.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.molstruc.2020.128150.

Authors declare no conflict of interests for this article.

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