ABSTRACT: Imines are multipurpose pharmacophores, simply accessible compounds, and have a broad range of usage in several areas of chemistry especially in medicine. Two novel compound imines, (E)-4-methyl-2-((o-tolylimino)methyl)phenol (1) and (E)-2-(((4-methoxybenzyl)imino)methyl)-4-methylphenol (2), were synthesized with effective product via reported protocol in the literature. Single crystal X-ray diffraction (SCXRD) was employed for structural exposition, disclosing that both compounds are orthorhombic. To optimize the newly designed imines, a B3LYP functional with a basis set 6-31G(d,p) was mainly considered. DFT results were utilized to check correlation between the data recovered from SCXRD outcomes and also to measure the energy difference. Hirshfeld surface study was done to demonstrate the intermolecular contacts along the percentage of interaction in the overall crystalline compound. Molecular operating environment program was tested against AChE and BChE enzymes to perform a modeling study of the compounds. The docking score and binding affinity of the compounds revealed that 2 showed comparatively more inhibition than 1. In silico ADMET studies exposed the physiochemical nature of these novel compounds, and it also unveiled that both compounds behaved as drug-like candidates.

1. INTRODUCTION

Imines are now well recognized by the name of Schiffs bases. Amines are reacted by a condensation process with derivatives of aldehydes and ketones to give imines. Dyes and coordination polymers are synthesized using Schiff bases on a large scale. Imine based ligands are considered the most reliable ligands owing to the lesser efforts required for their synthesis and notable versatility. Transition metals formed various types of stable complexes with these ligands and consequently played an extensive part in the advancement of coordination chemistry.

The condensation process of diamines with salicylaldehyde yields imine based ligands that have [N2O2] donor sets and are available for formation of stable coordination compounds. The biological activity of salicylaldehydes and their derivatives was studied.

The process of biosynthesis of an ergosterol is inhibited by using a derivative of benzylamine that was also prescribed to cure not only tinea pedis and tinea corporis but also tinea cruris. Transition metals form a very stable complex assembly with salicylaldehyde that is used as an antimalarial. The cell toxicity of imines was determined by a LDH cell toxicity test, and antiproliferative activity was determined by means of MTT cell proliferation.

Schiff bases are known as an imperative class of carbon-based compounds with extensive biological applications. Synthesis of novel therapeutic imines is now under an important consideration of pharmaceutical researchers for treatment of several illnesses. A number of studies have discussed the biotic actions of imines, together with their herbicidal, anticancer, and antimycotic activities.

Molecules with an active site of receptors can be studied by molecular modeling which also supports the analysis of the structure–activity relationship (SAR) of compounds. Modeling studies also exhibit the binding energies, contact approach, and locations of interactions. The interactions of molecules fitted with receptor protein are helpful in examining the nonhydrophilic interaction, hydrogen bonding, and binding energy.
Density Functional Theory (DFT) was accomplished to minimize the energy of those solids molecules having large numbers of electrons. In the past, DFT was used just for calculations of bond structure and properties of solids molecules; however, now DFT calculations are carried out for quantum chemical analysis. The best methodology to devise DFT is given by Kohn and Sham in which they explained a practical approach for measuring the energy properties. The Thomas Fermi approximation which considers the energy and density relationship and its effects supports much of the DFT studies. DFT is also helpful in order to determine the strength of the bond, electron affinities, and ionization energies.

Molecular assembly directs the various electrochemical parameters as well as the contact of drug molecular binding sites. Hence, the foundation of in silico study is mainly the assessment of the lowest most energy value of a molecule. DFT is used for computation of relative conformational energies.

A neurodegenerative syndrome often known as Alzheimer’s disease (AD) is common among old age people and develops as continuous memory loss and cognitive failure. The lower level of acetylcholine (Ach) concentration in the brain is the foremost cause of AD. A number of reported methods have been observed for improvement of cholinergic neurotransmission, including the rise of acetylcholine synthesis, presynaptic acetylcholine release, and lessening the synaptic acetylcholine’s degradation with cholinesterase inhibitors. The inhibitors of acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) are well thought as significant targets for therapeutic plans of AD. In a current study new salicylaldehyde derived imines have been synthesized with imperative biological activity. The structure of their compounds has been elucidated by means of SCXRD and their computational studies have been performed by density functional theory.
functional theory, molecular modeling, adsorption, distribution, metabolism, excretion, and toxicity (ADMET).

2. MATERIALS AND METHODS

In this work the chemicals used were ethanol, amine, aromatic aldehyde, and others reagents/solvents. They were of analytical grade and purchased from Merck (Germany).

2.1. Synthesis of (E)-4-methyl-2-((o-tolylimino)methyl)phenol imine (1) and (E)-2-(((4-methoxybenzyl)imino)methyl)-4-methylphenol imines (2). Imines were designed by the stated method with some modifications.\(^{20}\) (E)-4-methyl-2-((o-tolylimino)methyl)phenol 1 and (E)-2-(((4-methoxybenzyl)imino)methyl)-4-methylphenol 2 were synthesized in ethanol (20 mL) by refluxing o-toluidine (0.02 mmol), (4-methoxyphenyl)methanamine (0.02 mmol), respectively, with 2-hydroxy-5-methylbenzaldehyde (0.02 mmol) in ethanol (20 mL). Crystal materials were attained after the mixture was stirred up to 5 h under reflux, washed with ethanol, and dried at room temperature. The synthetic route for 1 and 2 is given in Scheme 1.

2.2. Single Crystal Structure Analysis. The image plate diffractometer STOE IPDS II was run up to 296 K to obtain the SCXRD. The structural assemblies of compounds were elucidated by SHELXT as a direct method\(^{21}\) and processed completely via full-matrix least-squares process along with the WinGX program\(^{22}\) associated also with the SHELXL module.\(^{23}\) The chief parameters of anisotropic displacement were added to refine the non-hydrogen atoms. The crystallographic tools were PLATON,\(^{24}\) ORTEP-3,\(^{25}\) and MERCURY,\(^{26}\) utilized for the structural demonstration along the evaluation of consequences.

2.3. Density Functional Theory. A density functional theory (DFT) study was positively led by means of Gaussian 09 using B3LYP as a functional method along the 6-31G(d,p) basis

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Table 2. Comparison of Bond Lengths for 1

| atom | atom | XRD/Å | DFT/Å | atom | atom | XRD/Å | DFT/Å |
|------|------|-------|-------|------|------|-------|-------|
| O1   | C14  | 1.369(3) | 1.36269 | C7   | C2   | 1.406(3) | 1.41684 |
| N1   | C6   | 1.429(3) | 1.41726 | C7   | C6   | 1.390(3) | 1.40752 |
| N1   | C8   | 1.291(3) | 1.30560 | C7   | C13  | 1.389(3) | 1.40376 |
| C9   | C10  | 1.401(3) | 1.41379 | C2   | C3   | 1.391(4) | 1.40183 |
| C9   | C14  | 1.405(3) | 1.42294 | C2   | C1   | 1.515(4) | 1.51024 |
| C9   | C8   | 1.456(3) | 1.44639 | C2   | C12  | 1.384(4) | 1.39024 |
| C10  | C11  | 1.393(3) | 1.39265 | C6   | C5   | 1.386(4) | 1.39629 |
| C11  | C12  | 1.400(4) | 1.41536 | C3   | C4   | 1.373(4) | 1.39968 |
| C11  | C15  | 1.516(3) | 1.51293 | C5   | C4   | 1.376(4) | 1.39857 |

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Figure 2. A close crystal assembly of 1.

Figure 3. A single crystal structure of 2.
set to minimize the energy of compounds.\textsuperscript{26–28} The B3LYP method mainly comprises Becke’s three-parameter (B3) exchange functional in conjunction with the Lee Yang and Parr (LYP) associated functional.\textsuperscript{29} Gauss View 5.0 software was run to calculate the energy gap measurement of the synthesized compounds and other outcomes of the DFT studies.\textsuperscript{30} 

**Figure 4.** A close crystal assembly of 2.

**Table 3. Comparison of Bond Angles for 1**

| atom | atom | atom | XRD deg | DFT       | atom | atom | atom | XRD deg | DFT       |
|------|------|------|---------|-----------|------|------|------|---------|-----------|
| C8   | N1   | C7   | 119.3(2)| 122.80    | O1   | C14  | C13  | 119.0(2)| 119.18    |
| C10  | C9   | C14  | 118.7(2)| 118.86    | C13  | C14  | C9   | 119.7(2)| 119.49    |
| C10  | C9   | C8   | 119.2(2)| 120.43    | N1   | C8   | C9   | 112.6(2)| 121.91    |
| C14  | C9   | C8   | 122.1(2)| 120.70    | C7   | C2   | C1   | 120.6(2)| 120.90    |
| C11  | C10  | C9   | 122.4(2)| 122.03    | C3   | C2   | C7   | 117.5(2)| 118.16    |
| C10  | C11  | C12  | 117.0(2)| 117.70    | C3   | C2   | C1   | 121.9(2)| 120.92    |
| C10  | C11  | C15  | 121.2(3)| 121.66    | C12  | C13  | C14  | 120.2(2)| 120.07    |
| C12  | C11  | C15  | 121.8(2)| 120.63    | C13  | C12  | C11  | 121.9(2)| 121.83    |
| C2   | C7   | N1   | 118.2(2)| 117.86    | C5   | C6   | C7   | 120.3(2)| 120.57    |
| C6   | C7   | N1   | 121.5(2)| 121.98    | C4   | C3   | C2   | 122.4(3)| 121.66    |
| O1   | C14  | C9   | 121.3(2)| 121.31    | C3   | C4   | C6   | 120.1(3)| 119.73    |

**Table 4. Comparison of Bond Lengths for 2**

| atom | atom | length/Å | length/Å |
|------|------|----------|----------|
| O1   | C2   | 1.349(2) | 1.36418  |
| O2   | C13  | 1.369(3) | 1.39087  |
| O2   | C16  | 1.427(3) | 1.45136  |
| N1   | C8   | 1.270(3) | 1.29816  |
| N1   | C9   | 1.469(3) | 1.47542  |
| C7   | C6   | 1.397(3) | 1.41150  |
| C7   | C2   | 1.406(3) | 1.42516  |
| C7   | C8   | 1.459(3) | 1.45195  |
| C5   | C6   | 1.385(3) | 1.39386  |
| C5   | C4   | 1.399(3) | 1.41432  |
optimize compounds, the input records were obtained from the crystal assembly data of the corresponding compound in order to get good coherence using the empirical data.

2.4. Hirshfeld Surfaces Analysis. Hirshfeld surface analysis (HS) was executed to explore and determine the involvement of the various interactions in a crystalline environment. Crystal Explorer 17.5 software was used to calculate two-dimensional (2D) fingerprint plots for analysis of surface contact on a Hirshfeld surface. The $\text{d}_{norm}$ is known as normalized contact distance that depends upon $d_e$ and $d_i$ that are measured from a standard equation.

2.5. Molecular Modeling Studies. Compounds 1 and 2 were docked by Molecular Operating Environment (2016.08) software. In molecular modeling two PDB files 1EVE and 1P0I, the first one for AChE (acetylcholinesterase) and the second for BChE (butyrylcholinesterase) enzymes, were chosen. The 2D molecule-receptor interactions were exhibited by means of MOE. The docking outcomes, contacts of ligand, and surface contact on a Hirshfeld surface are shown in Figure 6.

Table 5. Comparison of Bond Angles for 2

| atom | atom | atom | XRD/deg | DFT/deg | atom | atom | atom | XRD/deg | DFT/deg |
|------|------|------|---------|---------|------|------|------|---------|---------|
| C13  | O2   | C16  | 117.40(17) | 118.77  | C10 | C15 | C14 | 122.14(19) | 121.38  |
| C8   | N1   | C9   | 119.75(19) | 120.34  | C3  | C4  | C5  | 121.7(2)  | 121.80  |
| C6   | C7   | C2   | 118.67(17) | 119.01  | C15 | C14 | C13 | 119.2(2)  | 119.33  |
| C6   | C7   | C8   | 120.39(16) | 120.59  | O2  | C13 | C14 | 124.2(2)  | 124.39  |
| C2   | C7   | C8   | 120.94(18) | 120.39  | O2  | C13 | C12 | 116.67(19) | 115.52  |
| C8   | C5   | C4   | 117.12(19) | 117.66  | C12 | C13 | C14 | 119.1(2)  | 120.08  |
| C6   | C5   | C1   | 121.39(19) | 121.63  | C15 | C10 | C11 | 117.6(2)  | 118.31  |
| C4   | C5   | C1   | 121.5(2)  | 120.70  | C15 | C10 | C9  | 120.9(2)  | 120.93  |
| C5   | C6   | C7   | 122.47(18) | 122.01  | C11 | C10 | C9  | 121.4(2)  | 120.72  |
| O1   | C2   | C7   | 121.33(18) | 121.46  | C4  | C3  | C2  | 120.77(19) | 120.12  |
| O1   | C2   | C7   | 119.45(17) | 119.16  | C11 | C12 | C13 | 120.7(2)  | 119.78  |
| C3   | C2   | C7   | 119.23(19) | 119.36  | C12 | C11 | C10 | 121.3(2)  | 121.09  |
| N1   | C8   | C7   | 121.94(18) | 122.005 | N1  | C9  | C10 | 109.66(17) | 111.58  |

Figure 5. DFT energy minimized structures of the synthesized 1 and 2.

Figure 6. Correlation determination for bond lengths of 1.

Figure 7. Correlation determination for bond angles of 1.

Figure 8. Correlation determination for bond lengths of 2.
analyses were viewed by means of the Discovery Studio program.

2.6. In Silico Adsorption, Distribution, Metabolism, Excretion, and Toxicity. The evaluation profile of the ADMET is significant for newly discovered drugs and assessment of their pharmacodynamic activities. ADMET deals with promising parameters as physiochemical properties, pharmacokinetics, synthetic accessibility, drug likeness, and lipophilicity of newly synthesized compounds. At present, a number of sources are available as online and offline to check the drug-like potential of synthesized compounds.35 In the current study, in silico analysis was done using the admetSAR online available prediction tool (http://lmmd.ecust.edu.cn:8000/).

3. RESULTS AND DISCUSSION

3.1. SCXRD Assessment of 1 and 2. Compounds were synthesized by the reported protocol with good yield and recrystallized just on the slow rate of solvent evaporation at room temperature. The reaction completion was analyzed via thin layer chromatography (TLC). The structure elucidation of 1 and 2 was done by single crystal X-ray diffraction analysis. X-ray diffraction assessment of 1 was accomplished and the outcomes are arranged in Table 1. The geometry of the crystallized compound is orthorhombic, with formula unit $Z = 4$, $C_{15}H_{15}NO$, and also having space group $P 2_12_12_1$. The structure of the compound is illustrated in Figure 1 that also displays the intramolecular (O1–H1···N1) H-bonding. However, intratomic distances in the molecular structure $C_{15}H_{15}NO$ are 1.291(3) Å and 1.429(3) Å between $C8$–$N1$ and $N1$–$C7$ groups, respectively. In a unit cell, the crystal assembly of the compound is exhibited in Figure 2. In the case of X-ray analysis data are also given in Table 1. Data have revealed that the compound crystallized in orthorhombic form, with formula unit $Z = 4$, $C_{16}H_{17}NO_2$ and also has $P 2_12_12_1$ space group. The structure of the compound, shown in Figure 3, also possesses intramolecular (O1–H1···N1) H-bonding, although the intratomic distances in the structure of $C_{16}H_{17}NO_2$ are 1.469(3) Å and 1.270(3) Å between $N1$–$C9$ and $N1$–$C8$, respectively. The crystal assembly of 2 in a unit cell is exhibited in Figure 4.

3.2. HOMO-LUMO Analysis. Gaussian 09 software was used to optimize the newly prepared imine based compounds using the B3LYP functional and with basis set of 6-31G (d,p). The energy minimized structures of 1 and 2 were illustrated in Figure 5. To compare DFT and XRD outcomes, optimized values of bonds (length and angle) were attained. It has depicted...
from evaluation of experimental and theoretical results that there is a strong coherence found as shown in Tables 2–5. Moreover, agreement in DFT and XRD estimations were also expressed on the basis of correlation coefficient ($R^2$). In 1, $R^2$ values measured both for bond length and bond angle are 0.9581 and 0.6454, respectively, also shown in Figures 6 and 7. In 2, $R^2$ values are 0.9861 (bond length) and 0.9424 (bond angle) as presented in Figures 8 and 9. These consequences determined that the electrochemical parameters were approximately the same; therefore, the correlation coefficient is near to 1.0. An inconsequential variance in 1 was due to the different design phase of both studies. The HOMO, HOMO−1, LUMO, and LUMO+1 energy orbitals and their energy gaps between the different orbitals were also determined by DFT. The calculated
energy gap in HOMO and LUMO of 1 was 0.14361, although for HOMO−1 and LUMO+1 it was 0.2296 as given in Figure 10. The energy gap for the HOMO and LUMO of 2 was 0.1592 and in the same way for HOMO−1 and LUMO+1 was 0.21745 (Figure 11). The energy gap in 1 and 2 is relatively satisfactory to stabilize the compounds.36

3.3. Hirshfeld Surface Analysis. In crystalline molecules, Hirshfeld surface (HS) analysis is done to check the intermolecular contacts and also explain the surface features of the molecules. Crystal Explorer is run by loading up CIF files as input files for Hirshfeld analysis. The HS is diagrammed by means of distinctive colors (blue, white, and red), and is

Figure 14. 2D fingerprint plots of interactions along their corresponding percentages for 2.
primarily governed by radii distances. Molecular surfaces are transparent to show the imagining in a similar alignment, wherever this was determined. The $d_{\text{norm}}$ surface is valuable representing adjacent interactions and its values start from the negative side to the positive end. The more negative values denote a closer interaction as compared to standard $r_{\text{vdW}}$ (van der Waals radii) and vice versa for positive values, although, a reference surface resolution was considered to exhibit a HS along the 3D $d_{\text{norm}}$ with the set range ($-0.25$ to $1.3$ Å). The red spots represent nearer contacts ($d_{\text{norm}}$ value: negative), white spots seemed due to an alike variation around the zero value, and blue colors displayed extended contacts ($d_{\text{norm}}$ value, positive). The HS illustration of 1 and 2 is given in Figure 12 in $d_{\text{norm}}$ fashions.

To study the contacts between atoms, 2D fingerprint plots of 1 and 2 are plotted in Figures 13 and 14. It was revealed from all interactions that $\text{H} \cdots \text{H}$ contacts are mostly considered in the prepared compounds. $\text{H} \cdots \text{H}$ interactions were seen as $56.2\%$ and $54.4\%$ of all interactions in 1 and 2, respectively. After hydrogen interactions, $\text{C} \cdots \text{H}/\text{C} \cdots \text{H}$ contacts were nearly $32.3\%$ in 1 and $30.1\%$ in 2. The $\text{H} \cdots \text{O}/\text{H} \cdots \text{O}$ contacts were about $5.6\%$ for 1, whereas they were $13.0\%$ for 2. In 1 other interactions are $1.8\%$ for $\text{N} \cdots \text{H}/\text{N} \cdots \text{H}$ and $1.1\%$ for $\text{C} \cdots \text{C}/\text{C} \cdots \text{C}$. Compound 2 also has $1.7\%$ for $\text{N} \cdots \text{H}/\text{N} \cdots \text{H}$ and $0.4\%$ for $\text{C} \cdots \text{N}/\text{C} \cdots \text{N}$. These interactions played a major role in stabilizing the crystal assembly of both compounds.

### 3.4. Molecular Modeling Studies

To check the enzyme inhibition potential of synthesized imines, molecular modeling was accomplished. The binding affinity and docking score values exposed that 2 executed effective inhibition as compared to 1. For inhibition of AChE and BChE, the docking score values for 1 were $-14.5496$ and $-16.5711$ and also binding affinity values $-13.0807$ and $-15.0943$, respectively. Compound 2 exhibited contacts on AChE with docking score $-19.2255$ and binding affinity $-14.2516$, although the BChE $-19.2986$ docking score and $-15.9512$ binding affinity values are also listed in Table 6. The true docked posture of 1 and 2 with AChE and BChE are shown in Figures 15, 16, 17, and 18. Compound 1 exhibited interaction (Figure 15) with the binding position of AChE as $\pi \cdots \pi$ interactions with Tyr334, Phe330, and Trp279.

$\pi \cdots \pi$ contacts with His440, Tyr334, Phe330, and Tyr121 and conventional interaction by Asp72 were also seen with 1. Similarly, Trp279, Tyr121, Tyr334, Asp72, Phe330, and His440 are amino acid positioned on the binding furrow, 2 showed various interactions (Figure 16) with these residues. $\pi \cdots \pi$ stacked interaction with Tyr121, Tyr334, and Phe330 through $\pi \cdots \pi$-alkyl interactions were shown by Trp279, Phe330, and His440. The newly synthesized compounds also showed intermediate types of interaction with the I1POI receptor site. Compound 1 displayed $\pi \cdots \pi$ connections with Trp82 and Phe329. Compound 1 also had $\pi \cdots \pi$-alkyl contacts with Leu286 and Phe329 and conventional contact with Gly116. (Figure 17). The contacts of BChE (Figure 18) were also presented with Trp82 and Leu286 by means of $\pi \cdots \pi$-alkyl and $\pi \cdots \pi$ interactions with Leu286 but conventional contacts with Gly116.

#### 3.5. In Silico ADME Evaluation

Currently, various parameters associated to drug properties of formulated compounds have been determined by in silico ADMET studies using the Swiss online available AdmetSAR tool. Most of the parameters discussed are lipophilicity, water-solubility, drug likeness, pharmacokinetics, and medicinal chemistry. These distinctive characteristics explain that either the formulated compounds exhibit drug-likeness or not. According to the Lipinski rule, the values of log $P_{\text{o/w}}$ (LogP) for both synthesized 1 and 2 were 2.41 and 2.83, respectively. Similarly, the solubility log S (ESOL) values were $-3.90$ and $-3.60$, respectively for 1 and 2. These prepared compounds also showed Lipinski zero violation. The synthetic accessibility of compounds was in good range and 2 gave a higher value of 2.59 for it. The gastrointestinal absorption rate is also high in both compounds. Compounds 1 and 2 showed inhibition of cytochrome as CYP2C19 and CYP1A2, while 2 also inhibited CYP2D6 and CYP3A4. The physicochemical parameters of the compounds are presented in Tables 7–12.

### 4. CONCLUSIONS

To treat the existing and new diseases, a number of research efforts were carried out to synthesize novel therapeutical agents.

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**Table 6. Docking Outcomes of Synthesized 1 and 2**

| Enzymes | AChE docking score | AChE binding affinity (kcal/mol) | BChE docking score | BChE binding affinity (kcal/mol) |
|---------|---------------------|---------------------------------|---------------------|---------------------------------|
| 1       | $-14.5496$          | $-13.0807$                      | $-16.5711$          | $-15.0943$                      |
| 2       | $-19.2255$          | $-14.2516$                      | $-19.2986$          | $-15.9512$                      |

Figure 15. Docking view of 1 with AChE.
Nitrogen-based compounds have attracted the attention of pharmaceutical chemists toward the designing of innovative chemical agents against several diseases. In the present study, two active imines were synthesized starting from different
The Supporting Information is available free of charge at

**ASSOCIATED CONTENT**

**Supporting Information**

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.2c00102.

- Compound 1 (CIF)
- Compound 2 (CIF)

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