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Synthesis, characterization, and DFT study of a Pd(II) Schiff base complex: Exploration of its catalytic efficacy in the Suzuki cross-coupling reaction and its antibacterial activity

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RESEARCH ARTICLE



doi: 10.5155/eurjchem.17.3.258-267.2799

Received: 21 April 2026
 Received in revised form: 30 July 2026
 Accepted: 14 August 2026
 Published online: 30 September 2026
 Printed: 30 September 2026

ABSTRACT

A Schiff base ligand (H₂L) was synthesized by condensation of 3,3'-methylenedianiline with 2-hydroxy-1-naphthaldehyde under reflux conditions. Subsequently, the corresponding palladium(II) complex was prepared by reacting the ligand with palladium(II) acetate in a 1:1 molar ratio. The structures of both the ligand and its Pd(II) complex were characterized by elemental analysis, NMR, mass spectrometry, UV-vis spectroscopy, and FT-IR spectroscopy. Density functional theory calculations were performed to optimize the molecular structure and evaluate its electronic properties, providing further insight into the stability of the complex. The catalytic performance of the Pd(II) complex was investigated in the Suzuki cross-coupling reaction conducted in an aqueous medium. In addition, the *in vitro* antibacterial activities of the free ligand and the Pd(II) complex were evaluated against *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli*, and *Klebsiella pneumoniae*. Molecular docking was used to explore possible protein-complex interaction modes; these calculations were not treated as independent confirmation of the antibacterial results.

KEYWORDS

DFT
 Schiff base
 Catalytic activity
 Molecular docking
 Antibacterial activity
 Suzuki cross-coupling reaction

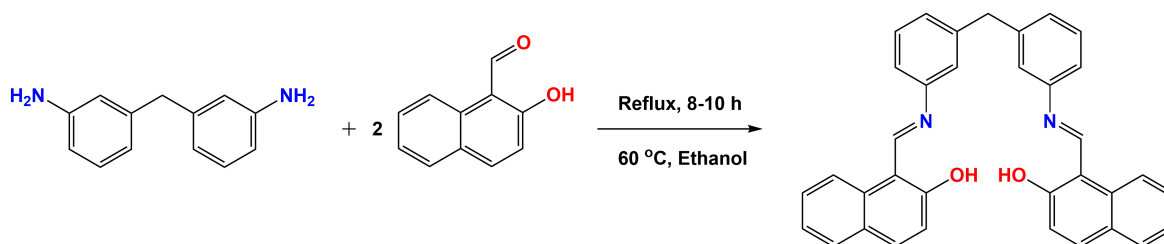
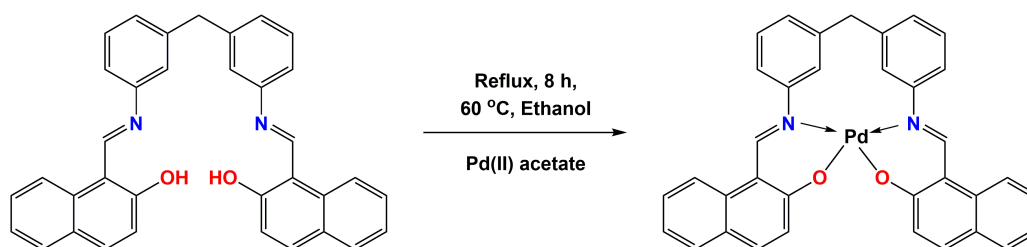
Cite this: *Eur. J. Chem.* 2026, 17(3), 258-267

Journal website: www.eurjchem.com

1. Introduction

In recent years, Schiff base ligands have attracted considerable research interest because of their distinctive structural features and wide range of physicochemical properties. These properties have led to an extensive investigation of their potential applications [1-4]. Their utility also comes from their ability to stabilize a variety of metal complexes in different oxidation states [5,6]. Furthermore, they serve an important function in influencing the behavior of metals for a variety of significant transformations. The extensive literature demonstrates that the organometallic chemistry of these substances is a crucial factor in their biological activity, demonstrating the importance of metals as catalysts [7-14]. The planarity and donor character of the C=N functionality facilitate coordination to metal centers. When used as a reactant in cycloaddition, ring closure, and substitution processes, this kind of material greatly advances inorganic biochemistry and produces a variety of physiologically active chemicals [15-17].

Palladium is a significant precious metal with several applications in the contemporary industry due to its favorable characteristics, such as its remarkable ability to resist corrosion, its constant thermoelectric performance, and its extremely active catalytic nature. It is widely used in organic synthesis, automotive catalytic converters, dental and medical device manufacture, electronics, and hydrogenation and dehydrogenation processes. Around half of the global production of palladium is thought to be consumed each year in the manufacture of automobile catalysts [18]. The extensive use of palladium in modern industries has led to a notable increase in the environmental emissions of the metal [19]. Palladium is believed to go through methylation processes in aquatic environments and could build up in the food chain, providing risks to the environment and the general public health depending on certain conditions, such as the redox potential and pH [20,21]. Therefore, it is crucial to create an easy, exceptionally sensitive, and selective method to measure the trace amounts of palladium in water samples. However, the low or even very low concentration of palladium combined with

Scheme 1. Reaction scheme for the synthesis of the ligand (H₂L).

Scheme 2. Reaction scheme for the synthesis of the Pd(II) complex.

matrix effects can make it impossible to determine the metal directly using established analytical techniques. One of the best solutions to these problems is preconcentration and separation combined with incredibly sensitive technologies.

In coordination chemistry, Schiff base ligands provide a versatile platform for the construction of ligand systems with tunable metal-ion binding properties [22-24]. From the standpoint of catalytic activity, this particular group of ligands may be able to stabilize metals in various oxidation states and promote stability in homogeneous and heterogeneous catalysts [25]. The medical sciences, catalysis, and molecular magnetism are just a few of the fields of study that have found use for metal complexes made from Schiff bases [26]. Catalysis using palladium compounds facilitates a multitude of C-C bond forming processes, including Heck and Suzuki coupling. In the past ten years, new phosphorus-free palladium catalysts have drawn a great deal of attention because of their enhanced activity, stability, and substrate tolerance, all of which enable reactions to be carried out under more secure conditions.

Computational methods provide valuable tools to evaluate the electronic structure and stability of metal complexes [27]. The gap between the HOMO and the LUMO, electrostatic potential (ESP) maps, Mulliken charge distribution, and reduced density gradient (RDG) are among the electronic characteristics that were determined through computational simulations using density functional theory (DFT) to determine the stable geometry of the complex.

In this work, a Schiff base ligand and its palladium(II) complex were synthesized and characterized. DFT calculations were used to support the structural and electronic interpretation, while catalytic studies evaluated the complex in the Suzuki cross-coupling reaction. The *in vitro* antibacterial activities were evaluated against two Gram-positive bacteria (*B. subtilis* and *S. aureus*) and two Gram-negative bacteria (*E. coli* and *K. pneumoniae*) using the disc diffusion method. The interaction between the palladium (II) complex and the crystal structure receptors of *B. subtilis* (2BH0), *E. coli* (1XFF), *K. pneumoniae* (2GCX), and *S. aureus* (5ZH8) was anticipated using molecular docking. The ligand was selected because its N₂O₂ donor set and extended π -conjugated framework favor stable Pd coordination and provide an electronically tunable platform for catalytic and biological evaluation.

2. Experimental

2.1. Materials

3,3'-Methylenedianiline and 2-hydroxy-1-naphthaldehyde were purchased from Sigma-Aldrich (Germany). Ethanol, chloroform, CDCl₃, and palladium(II) acetate were purchased from SD Fine Chemicals in India. Solvents were distilled according to the procedures of the literature prior to use [28].

2.2. Instrumentation

A Perkin-Elmer 240 elemental analyzer was used to perform elemental analyses (C, H, and N %). NMR spectra were recorded on a Bruker 400 MHz FT-NMR instrument. Additionally, the UV-vis spectra of the isolated compounds were recorded using a Jasco V-530 spectrophotometer. Infrared spectra were recorded on a PerkinElmer RX-I FT-IR spectrometer in the range 400-4000 cm⁻¹ using KBr pellets. The specific conductance of the resulting compound in DMSO at room temperature was measured using TDS-308 India. The purity of the obtained compounds was confirmed by thin-layer chromatography. The open capillary approach was used to determine the melting points of the ligand and its metal complex.

2.3. Synthesis of the Schiff base ligand H₂L

3,3'-Methylenedianiline (0.1 mmol) and 2-hydroxy-1-naphthaldehyde (0.2 mmol) were dissolved in ethanol and gradually mixed under stirring. The reaction mixture was refluxed at 60 °C for 8-10 h using a 1:2 molar ratio of diamine to aldehyde (Scheme 1). Upon completion of the reaction, the resulting yellow precipitate was collected by filtration using Whatman No. 41 filter paper, washed thoroughly with cold ethanol, and dried under vacuum over anhydrous calcium chloride for 24 h.

1,1'-((1E,1'E)-((methylenebis(3,1-phenylene))bis(azaneylylidene))bis(methanelylidene))bis(naphthalen-2-ol): Color: Yellow. Yield: 81%. M.p: >200 °C. FT-IR (KBr, ν , cm⁻¹): 3513-3149 (O-H), 1641 (C=N), 1403 and 1109 (phenolic C-O). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 15.444 (s, 2H, OH), 9.286-9.282 (s, 2H, CH=N-), 7.038-8.047 (m, 20H, Ar-H), 4.106-4.156 (s, 2H, CH₂). ¹³C NMR (100 MHz, CDCl₃, δ , ppm): 171.188 (C-OH), 154.609 (CH=N), 108.969-145.555 (Ar-C), 41.921 (CH₂). UV-

Vis (CHCl₃, 1×10^{-5} M, λ_{max} , nm): 323 and 425. MS (EI, m/z): 506 (nominal molecular-ion peak), 505 (base peak). Anal. calcd. for C₃₅H₂₆N₂O₂: C, 82.98; H, 5.17; N, 5.53. Found C, 82.55; H, 5.15; N, 5.50%.

2.4. Synthesis of palladium(II) complex

A solution of the Schiff base ligand (0.1 mmol) was added dropwise to a heated solution of palladium(II) acetate (0.1 mmol) in a 1:1 molar ratio. The reaction mixture was refluxed at 60 °C for approximately 8 h, resulting in the formation of a turmeric yellow precipitate (Scheme 2). The resulting solid was collected by filtration and dried under vacuum in a desiccator for several days.

Pd(II) complex: Colour: Turmeric yellow. Yield: 72%. M.p: >240 °C. FT-IR (KBr, ν , cm⁻¹): 1578 (C=N), 1399 (C-O), 673 (Pd-O), 618 (Pd-N). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 7.992 and 7.835 (s, 2H, CH=N), 6.940–7.832 (m, 20H, Ar-H), 4.160 (s, 2H, CH₂). ¹³C NMR (100 MHz, CDCl₃, δ , ppm): 166.194 (coordinated C-O), 155.660 (CH=N), 111.888–141.143 (Ar-C), 39.991 (CH₂). UV-Vis (CHCl₃, 1×10^{-5} M, λ_{max} , nm): 318, 375, 440, and 460 (sh). MS (EI, m/z): 609 (low-intensity peak in the nominal molecular-ion region). Anal. calcd. for C₃₅H₂₄N₂O₂Pd: C, 68.80; H, 3.96; N, 4.58%. Found: C, 68.72; H, 3.91; N, 4.13%.

2.5. Computational study

Density functional theory (DFT) calculations were performed using the Gaussian 16 software package [29] to optimize the geometry of the Pd(II) complex at the B3LYP level of theory. The LANL2DZ effective core potential and basis set were used for the Pd atom, while the 6-31G(d,p) basis set was used for all non-metal atoms (C, H, O, and N) [30,31]. Subsequently, frequency calculations were carried out to confirm that the optimized geometry corresponded to a true minimum on the potential energy surface, as evidenced by the absence of imaginary frequencies [31]. The same computational methodology was also employed to investigate the electronic properties of the complex, including Mulliken charge distribution, molecular electrostatic potential (MEP) maps, frontier molecular orbitals (HOMO-LUMO) and reduced density gradient (RDG) analyses [32,33].

2.6. Antibacterial study

The antibacterial activity of the synthesized compounds was evaluated using the Bauer disc diffusion method using Mueller–Hinton agar medium (MH) (HiMedia) [34]. The medium was prepared by dissolving 38.0 g of MH agar in 1000 mL of double distilled water, followed by autoclaving at 121 °C for 30 min. Overnight-grown cultures of two Gram-positive bacteria (*Bacillus subtilis* and *Staphylococcus aureus*) and two Gram-negative bacteria (*Escherichia coli* and *Klebsiella pneumoniae*) were standardized to a 0.5 McFarland turbidity standard. Subsequently, 300 μ L of each standardized bacterial suspension was inoculated into each plate. After being cooled to 50°C, the sterile medium was poured into sterile Petri plates under aseptic conditions and allowed to solidify. The synthesized ligand and its metal complex were dissolved in dimethyl sulfoxide (DMSO) at concentrations of 5, 10, 15, 20, and 30 mg/mL. Sterile filter paper discs (5 mm in diameter) were immersed in the tested solutions and placed onto the inoculated agar plates. Plates were incubated at 37 °C for 24 h. Following incubation, the complete inhibition-zone diameter was measured across the centre of each disc. The reported value was calculated by subtracting the 5 mm disc diameter from the complete measured diameter. All experiments were performed independently in triplicate ($n = 3$).

2.7. Molecular docking

Molecular docking studies were performed to investigate the interactions of the Pd(II) complex with selected bacterial protein targets using the iGEMDOCK software package [35]. These calculations were carried out to examine possible binding modes and to complement the experimentally observed antibacterial activities. Prior to docking, all protein structures were retrieved from the Protein Data Bank (PDB). The protein structures were prepared by removing cocrystallized ligands, water molecules, and any non-essential heteroatoms, followed by the addition of polar hydrogen atoms. The prepared proteins were then used as rigid receptors for the docking simulations. The iGEMDOCK software was used for all docking calculations, providing an integrated platform for virtual screening and interaction analysis. Binding affinities were evaluated using the iGEMDOCK fitness score, defined by the empirical scoring function: Fitness = vdW + H-bond + electrostatic, where vdW, H-bond, and electrostatic terms represent van der Waals, hydrogen bonding, and electrostatic interaction energies, respectively. Docking simulations were performed with a grid spacing of 1 Å. The grid box dimensions ($X \times Y \times Z$) were set to $40 \times 46 \times 48$ Å for *Escherichia coli* (PDB ID: 1XFF, chain A), $40 \times 44 \times 40$ Å for *Klebsiella pneumoniae* (PDB ID: 2GCX, Model 1, chain A), $62 \times 58 \times 60$ Å for *Staphylococcus aureus* (PDB ID: 5ZH8, chain A), and $56 \times 54 \times 40$ Å for *Bacillus subtilis* (PDB ID: 2BH0, chain A).

3. Results and discussion

3.1. Characterization of the Pd(II) complex of the ligand

The synthesized compounds were characterized using spectroscopic and analytical techniques, including mass spectrometry, FT-IR spectroscopy, and ¹H NMR spectroscopy. The physical and analytical data presented in the Experimental section support the formation of a mononuclear palladium complex with a 1:1 metal-to-ligand ratio [36].

3.2. Molar conductance

Both the ligand and its Pd(II) complex were soluble in chloroform and DMSO. At room temperature, the Pd(II) complex exhibited a molar conductance value of 12.06 S cm² mol⁻¹ in a 1×10^{-3} M DMSO solution, consistent with its classification as a non-electrolyte [37].

3.3. Infrared spectroscopy

The FT-IR spectra of the synthesized compounds were recorded over 4000–400 cm⁻¹. The band at 1641 cm⁻¹ for the ligand represents the azomethine ν (C=N) group [37]. The complex shows a band shifted to lower wavenumber at 1578 cm⁻¹, indicating the bond between the metal ion and the N atom of the azomethine group [38]. The ligand spectrum showed a broad band at 3513–3149 cm⁻¹ assigned to the phenolic OH group. This band disappeared in the spectrum of the complex, indicating deprotonation of the phenolic group and coordination of its oxygen atom to Pd(II) [39]. The band at 1109 cm⁻¹ was also assigned to the phenolic group of the ligand. The ligand ν (C–O) stretching band shifts from 1403 to 1399 cm⁻¹ during complexation, providing additional proof of the coordination between metal ions and phenolic oxygen. The appearance of two bands at 673 and 618 cm⁻¹, which are induced by ν (Pd–O) and ν (Pd–N), confirms the existence of phenolic O and azomethine N in complexation. Taken together, these spectroscopic changes are consistent with coordination through the imine nitrogen and phenolate oxygen atoms and with the proposed square-planar coordination geometry around Pd(II) [40–42].

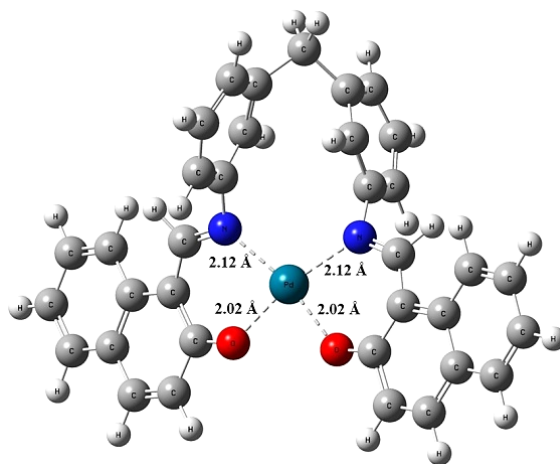


Figure 1. DFT-optimized molecular structure of the synthesized Pd(II) complex.

3.4. Mass spectrometry

The EI mass spectrum of the Schiff base ligand ($C_{35}H_{26}N_2O_2$) showed an ion at nominal m/z 506 in the expected molecular ion region, while m/z 505 was observed as the base peak. The EI mass spectrum of the Pd(II) complex ($C_{35}H_{24}N_2O_2Pd$) showed a low-intensity ion at nominal m/z 609 in the molecular-ion region. Additional ions were observed at nominal m/z 503 and 459; however, definitive elemental composition and fragmentation assignments would require high-resolution MS/MS data. Thus, the mass-spectral features are consistent with, but do not independently confirm, the proposed structures. The coordination of the azomethine nitrogen and phenolate oxygen atoms with Pd(II) is supported primarily by the combined FT-IR and NMR results.

3.5. 1H and ^{13}C NMR spectral analysis

The resonance frequency of a nucleus is compared to a reference value to determine the absorption peak in an NMR spectrum. $CDCl_3$ was used as the 1H NMR spectra of the solvent to obtain the ligand and Pd(II) complex. The azomethine protons of the ligand ($-CH=N-$) were observed at δ 9.286 and 9.282 ppm [43]. Following coordination, the corresponding signals of the Pd(II) complex appeared at δ 7.992 and 7.835 ppm. The existence of a hydroxyl ($-OH$) proton in the ligand was indicated by an additional signal at δ 15.444 ppm. This signal was absent from the spectrum of the complex, indicating deprotonation of the O-H group during complex formation. For the ligand, the aromatic and methylene proton signals appeared at δ 7.038–8.047 and 4.106–4.156 ppm, respectively. In the Pd(II) complex, the corresponding signals were observed at δ 6.940–7.832 and 4.160 ppm, respectively.

^{13}C NMR data of the Schiff base ligand and its Pd(II) complex were compared to evaluate the spectral changes accompanying coordination. Peaks for aromatic carbons were found in the ligand's ^{13}C spectra at δ 108.97–145.55 ppm and for CH_2 at δ 41.92 ppm. The peak at δ 154.61 ppm is due to the ($-CH=N-$) group, while the $-C-OH$ group shows a peak at δ 171.19, which also shows the formation of the Schiff base ligand. The ^{13}C NMR spectrum of the Pd(II) complex shows signals at δ 166.19 (coordinated C-O), 155.66 ($CH=N$), 111.89–141.14 (aromatic carbons), and 39.99 ppm (CH_2). Relative to the ligand signals at δ 171.19, 154.61, and 41.92 ppm, respectively, these shifts are consistent with the coordination of the phenolate oxygen and azomethine nitrogen with Pd(II).

3.6. Electronic absorption study

At ambient temperature, the electronic spectra of the Pd(II) complexes, obtained at 1×10^{-5} M in chloroform, revealed strong absorption in the UV-vis band. The Schiff base ligand spectra showed that the absorption bands at 325 nm were attributed to a phenyl ring $\pi \rightarrow \pi^*$ transition, while the bands at 370–445 nm were linked to an $n \rightarrow \pi^*$ transition that was connected to the azomethine chromophore ($-CH=N$) [44]. These absorption bands change to blue, but are still present in the Pd(II) complex spectra. Palladium(II) Schiff base complexes are formed when the ligand coordinates with the Pd(II) ion, as evidenced by shifts in the spectrum of the produced complex. Furthermore, a band in the 440–465 nm region was observed in the Pd(II) complex due to the metal-ligand charge transfer (LMCT) transition [45–47].

3.7. Electronic properties study using DFT

The optimal structure is shown in Figure 1. The Pd center is coordinated by the nitrogen and oxygen donor atoms of the ligand. Bond distances between 2.02–2.12 Å indicate strong binding. The bond distance values reflect that the oxygen atom has a stronger interaction with Pd than with nitrogen. The compact structure of the complex is further supported by data from the Mulliken charge analysis (Figure 2). Strong bonds exist between the negative N and O (red) and the positive Pd (green).

The ESP study (Figure 3) illustrates the complex's surface charge. Red regions near the oxygen atoms indicate areas of relatively negative electrostatic potential. According to the RDG analysis, van der Waals and attractive interactions contribute to the stabilization of the complex, as indicated by the green and blue regions in Figure 4. The RDG analysis indicates that the repulsive steric interaction (shown in red) is minor. The RDG analysis visualizes the calculated noncovalent interaction regions within the optimized complex; it does not independently establish experimental synthesis or stability. The calculated HOMO-LUMO energy gap of the complex is 3.1 eV (Figure 5). The relatively small calculated HOMO-LUMO gap and the frontier orbital distribution around the Pd coordination environment are consistent with the electronic accessibility of the metal center and may facilitate substrate activation; this qualitative correlation does not establish the catalytic mechanism by itself.

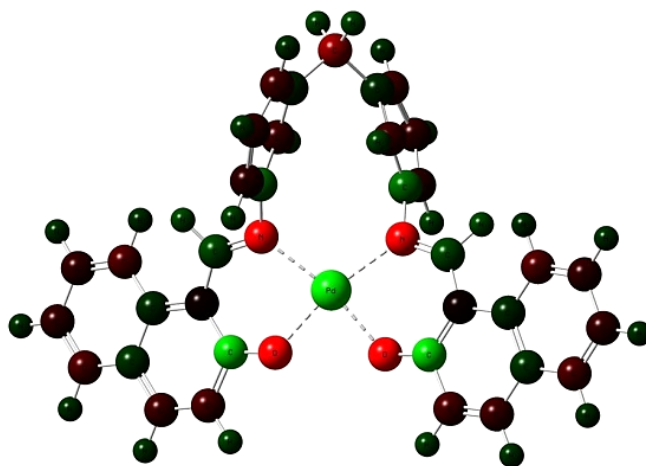


Figure 2. Mulliken charge distribution of the synthesized Pd(II) complex (charge range: -1.056 to $+1.056$).

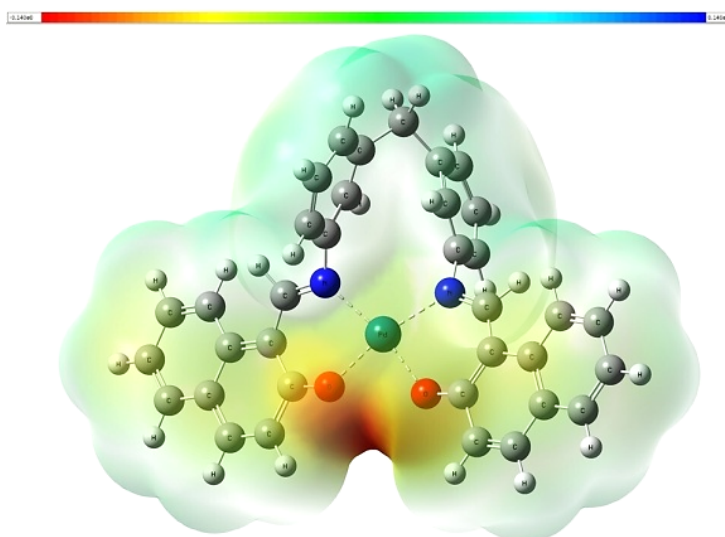


Figure 3. Molecular electrostatic potential (MEP) map of the synthesized Pd(II) complex

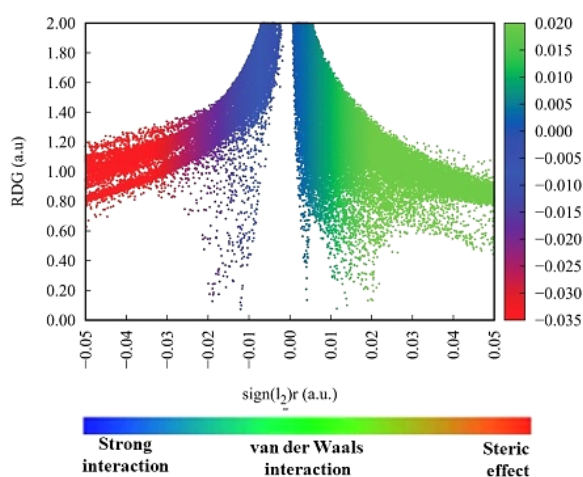
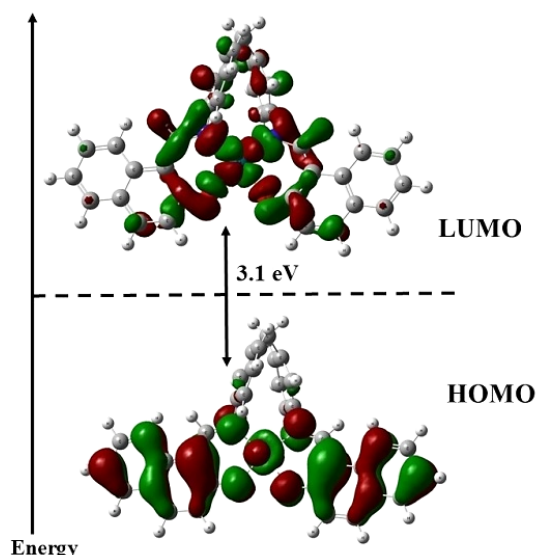
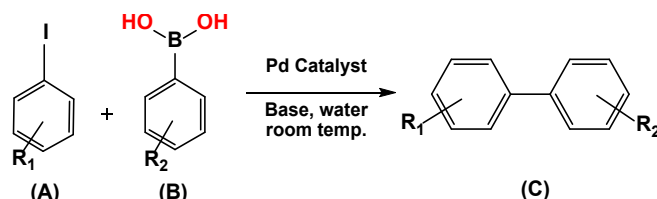


Figure 4. Reduced density gradient (RDG) analysis of the synthesized Pd(II) complex

Table 1. Suzuki cross-coupling reaction catalysed by the complex in aqueous medium.

Entry	Catalyst amount (mol %)	Base	Yield (%)
1	0.1	Et ₃ N	60
2	0.1	NaOH	62
3	0.1	K ₂ CO ₃	68
4	0.5	K ₂ CO ₃	78
5	1.0	K ₂ CO ₃	80
6	2.0	K ₂ CO ₃	84
7	4.0	K ₂ CO ₃	85

**Figure 5.** HOMO and LUMO molecular orbital distributions and the corresponding energy gap.**Scheme 3.** Reaction conditions: A (1.00 mmol), B (1.2 mmol), Pd Catalyst (mole %), base (1.5 mmol), deionized water (3 mL), 16 h of stirring, room temperature. (R₁=R₂=H)

3.8. Suzuki cross-coupling reaction catalysis

The effects of base identity and catalyst loading on the Suzuki cross-coupling reaction were evaluated. A model reaction between iodobenzene and phenylboronic acid was used to optimize the reaction conditions. Scheme 3 summarizes several experimental reaction circumstances and outcomes. At room temperature, the optimum conversion with a good to high yield of biphenyl is achieved using K₂CO₃ as the base and 2 mol% of catalyst (Table 1, Entry 6). A control experiment performed with phenylboronic acid alone under the optimized conditions did not produce biphenyl after 16 h, indicating that phenylboronic acid homocoupling was not detectable under these conditions. For the representative optimized reaction (Table 1, entry 6), the calculated TON and TOF were 42 and 2.63 h⁻¹, respectively, based on a reaction time of 16 h. The catalytically active species is plausibly generated by in situ reduction of Pd(II) to Pd(0), followed by oxidative addition, transmetalation, and reductive elimination; this mechanistic proposal was not independently verified in the present study.

A good yield was also obtained with the 1 mol% catalyst. Some catalyst was recovered during the standard work-up; however, catalyst recycling was not investigated because the objective was to evaluate catalytic activity in the Suzuki cross-coupling reaction. The catalyst was optimally loaded at 2 mol% for the Suzuki cross-coupling reaction. Several aryl iodide and

arylboronic acids were used as substrates to test the catalyst's efficacy in the Suzuki cross-coupling reaction in the aqueous phase. The optimized method was applied to substituted iodobenzenes and arylboronic acids, affording the corresponding products in good to excellent yields [48] (Scheme 4).

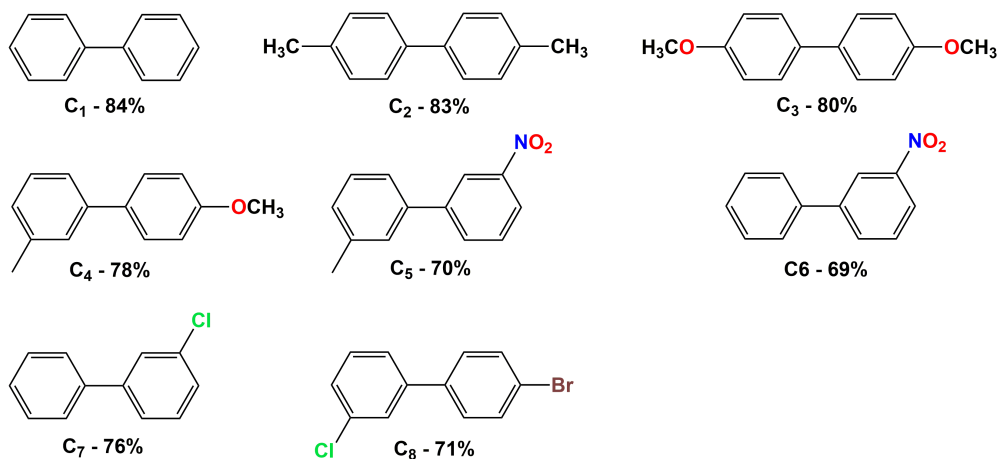
Scheme 4 shows the findings of an investigation into the efficacy of a recently designed Pd catalyst in the Suzuki cross-coupling reaction in the aqueous phase utilizing various aryl halide and arylboronic acids as substrates. In comparison to that for iodobenzene under the same reaction circumstances, the reaction for chloro and bromobenzene takes longer to complete and yields less. The identical approach has also been used for substituted aryl halides that have groups that donate or withdraw electrons. Groups that donate electrons proportionately increase the product's percentage (Scheme 4, entries C2–C4). Whereas the rate of yield decreases in the presence of an electron-withdrawing group present in both aryl moieties (Scheme 4, entries- C-5, C-6, C-7, and C-8). Different substituted iodobenzenes and arylboronic acids reacted to produce corresponding coupled products with excellent yields (69–84%). Solvent extraction using hexane and ethyl acetate made it easy to separate different coupling products from the aqueous phase, which contained the catalyst.

Table 2. Results of antibacterial susceptibility testing of the ligand and Pd(II) complex using the paper-disc diffusion method at concentrations of 5, 10, 15, 20, and 30 mg/mL.

Compound	Pd(II) complex					Ligand				
	5	10	15	20	30	5	10	15	20	30
<i>E. coli</i> (-ve)	2 mm	7 mm	9 mm	10 mm	11 mm	2 mm	2 mm	3 mm	10 mm	11 mm
<i>K. pneumoniae</i> (-ve)	3 mm	6 mm	7 mm	10 mm	12 mm	1 mm	1 mm	3 mm	6 mm	7 mm
<i>S. aureus</i> (+ve)	2 mm	2 mm	2 mm	3 mm	3 mm	1 mm	2 mm	2 mm	2 mm	3 mm
<i>B. subtilis</i> (+ve)	2 mm	8 mm	9 mm	10 mm	12 mm	2 mm	2 mm	7 mm	8.5 mm	10 mm

Table 3. Molecular docking interaction profile and docking scores of the Pd(II) complex.

Protein name	PDB ID	Docking score				Amino acid residues
		iGMDOCK	vDW	H-Bond	Elec	
Glutamate (<i>Escherichia coli</i>) with the glutaminase domain of glucosamine 6-phosphate synthase complexed	1XFF	-97.69	-95.36	-2.33	0	GLY99, GLY175, TYR156, SER176, TRP74, THR76, ASN98, ARG73, ILE100, CYS1, ARG26, ALA155, HIS71, HIS86, THR124, THR122, HIS97, ASP123
The structure of the ferrous iron transport protein A (FeoA) found in <i>Klebsiella pneumoniae</i>	2GCX	-98.52	-93.86	-4.67	0	HIS50, VAL59, ARG61, PRO48, LYS63, ASP47, LYS62, GLY46
FmtA Crystal Structure from <i>Staphylococcus aureus</i> at 2.58 Å	5ZH8	-90.41	-89.35	-1.07	0	ASN390, THR391, TYR389, VAL396, GLN397, HIS318, THR313, ASN314, LEU317, GLN303, TYR305, ASP357, PRO310
At 2.5 Å, the crystal structure of a SeMet derivative of <i>Bacillus subtilis</i> EXPA	2BH0	-97.53	-97.53	-	0	ALA2, TYR44, TYR3, ARG178, ILE177, ALA50, VAL138, ASP176, GLY45, VAL47, THR175, LYS140

**Scheme 4.** Suzuki cross-coupling reaction of various substituted substrates catalysed by the newly developed Pd catalyst in aqueous medium.

The substrate scope of the optimized Suzuki cross-coupling reaction was investigated using different aryl halides and arylboronic acids. Product C1 was obtained from iodobenzene and phenylboronic acid; C2 from 1-bromo-4-methylbenzene and (4-methylphenyl)boronic acid; C3 from 1-bromo-4-methoxybenzene and (4-methoxyphenyl)boronic acid; C4 from 1-bromo-4-methoxybenzene and (3-methyl-phenyl)boronic acid; C5 from 1-bromo-3-nitrobenzene and (3-methylphenyl) boronic acid; C6 from 1-bromo-3-nitrobenzene and phenylboronic acid; C7 from 1-bromo-3-chlorobenzene and phenylboronic acid; and C8 from 1-chloro-3-iodobenzene and (4-bromophenyl)boronic acid. All reactions were completed within 50 min, and the corresponding isolated yields are presented in Scheme 4. The products were purified by silica-gel column chromatography using petroleum ether/ethyl acetate (90:10, v/v) as the eluent and characterized by NMR spectroscopy and, where applicable, by comparison with previously reported spectral data.

3.9. Antibacterial activity

Both compounds tested exhibited antibacterial activity, as indicated by inhibition zones after 24 h of incubation. The diameters of the inhibition zone (mm) of the ligand and its Pd(II) complex, expressed as the mean of three independent measurements, are presented in Table 2. Two Gram-positive bacteria (*S. aureus* and *B. subtilis*) and Gram-negative bacteria (*E. coli* and *K. pneumoniae*) were utilized to assess the

antibacterial activity of the ligand and complex. In *Klebsiella pneumoniae* and *Bacillus subtilis* assays, the Pd(II) complex (1) showed the largest inhibition zone of 12 mm, while *Staphylococcus aureus* produced the least inhibition zone. The Pd(II) complex generally produced inhibition zones equal to or larger than those of the ligand; however, equal values were observed for several organism–concentration combinations, including *E. coli* at 30 mg/mL [49]. Also, three replicates were done for each organism.

3.10. Molecular docking

iGEMDOCK software was used to analyze the complex for interactions with various bacteria, as shown in Figure 6a–d. The docking results provide a computational description of possible protein–complex interactions, as summarized in Table 3; they should not be interpreted as experimental binding affinities or as independent confirmation of the disc diffusion results. The receptor proteins of *Escherichia coli* (1XFF), *Klebsiella pneumoniae* (2GCX), *Staphylococcus aureus* (5ZH8) and *Bacillus subtilis* (2BH0) were used to molecularly bind the complex. According to reports, the binding scores for the Pd(II) complex were -97.69, -98.52, -90.41 and -97.53, respectively. Negative iGEMDOCK fitness scores indicate favorable poses within the applied scoring function; however, these calculated scores are not experimental binding affinities and do not establish a causal relationship with the observed inhibition zones.

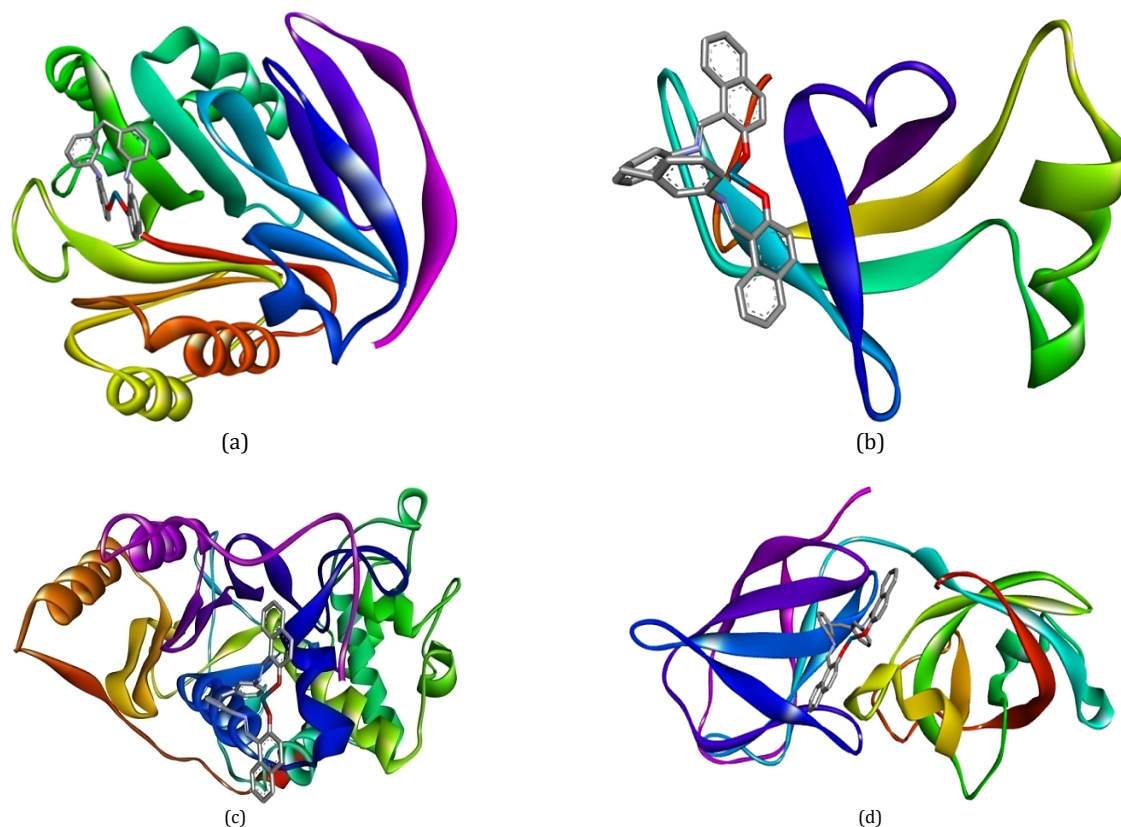


Figure 6. Three-dimensional (3D) binding poses of the Pd(II) complex with target proteins of (a) *Escherichia coli* (PDB ID: 1XFF), (b) *Klebsiella pneumoniae* (PDB ID: 2GCX), (c) *Staphylococcus aureus* (PDB ID: 5ZH8) and (d) *Bacillus subtilis* (PDB ID: 2BH0).

4. Conclusions

In this study, a Schiff base ligand and its Pd(II) complex was synthesized and characterized. The stability and electronic properties of the complex were further supported by density functional theory (DFT) calculations. The catalytic performance of the Pd(II) complex was evaluated in the Suzuki cross-coupling reaction under aqueous conditions. The catalyst exhibited useful catalytic activity, affording good to excellent yields across the tested substrate scope. Notably, the reactions proceeded in an aqueous medium under mild conditions without a phase-transfer catalyst. These results demonstrate useful catalytic performance; however, a claim of superiority over previously reported systems would require a systematic comparison under equivalent conditions. Although some catalyst was recovered during the process, recyclability was not evaluated; therefore, no conclusion regarding reuse or long-term catalytic stability can be drawn from the present study.

Acknowledgements

The authors would like to acknowledge the Departmental Special Assistance Scheme under the University Grants Commission, New Delhi (SAP-DRS-III, No. 540/12/DRS/2013) and University of North Bengal, Government of West Bengal for financial and instrumental support.

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Conceptualization: Uttam Kumar Singha; Methodology: Uttam Kumar Singha, Kingkar Ghosh; Software: Tanmoy Dutta; Validation: Biswajit Sinha; Formal Analysis: Sudarshan Pradhan; Investigation: Uttam Kumar Singha, Sudeshna Nandi, Malay Bhattacharya; Data Curation: Tanmoy Dutta, Sudarshan Pradhan, Pritika Gurung; Writing - Original Draft: Uttam Kumar Singha; Writing - Review and Editing: Biswajit Sinha; Visualization: Uttam Kumar Singha, Pritika Gurung, Biswajit Sinha; Supervision: Biswajit Sinha; Project Administration: Biswajit Sinha.

Disclosure statement

Conflict of interest: The authors declare that they have no conflict of interest. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethical approval: Not applicable. This study did not involve human participants or animals.

Sample availability: Samples of the compounds are available from the author. Availability of data and materials: Data supporting the findings of this study are available from the corresponding author on reasonable request. Additional raw experimental and computational data will be provided where required.

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