Sodium Silicate, Potassium Silicate, and Copper Sulfate's Effectiveness *In Vitro* and *In Silico* against the Wood-decaying Fungus *Phanerochaete chrysosporium*

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Wood modification *via* silicon ingredients was investigated to increase its resistance to biological decay. Surfactant and desiccant features of derived products of silicates are considered the main contributors in wood resistance to decay. The detected fungus from decayed wood sample was identified as *Phanerochaete chrysosporium*. Inhibitory tests showed that sodium silicate (SS) was more effective than potassium silicate (PS) and copper sulfate (CS) against *P. chrysosporium* growth. The weight loss of infected wood with *P. chrysosporium* without treatment was 32.2%, while treatment by SS, PS, and CS reduced weight loss to 4.3%, 11.5%, and 14.3%, respectively, over 40 days. To ducument the effect of SS, PS, and CS on *P. chrysosporium,* molecular docking was used to evaluate the binding interactions of these compounds with the active site (Lignin peroxidase) of *P. chrysosporium* (PDB ID: 1QPA). Binding affinities were determined *via* docking scores, conformational energies, placement energies, and refinement parameters evaluation. SS exhibited the strongest docking scores (S = -6.17 to -5.83) and favorable interactions, including metal coordination and hydrogen bonding. PS and CS showed moderate to weak binding, with distinct interaction patterns. These computational results highlight SS as a potential candidate for further experimental validation in targeting the 1QPA protein.

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INTRODUCTION

Wood is naturally prone to biodegradation; thus, wood preservatives have been developed to extend wood's lifespan. Wood's rigidity and strength come from cellulose, lignin, and hemicellulose. Destructive behavior of wood decaying fungi have attracted numerous investigators to search for benefits or control of these types of fungi. At present, the wood protection is gaining significance due to the rising demand for timber, coupled with its restricted availability (Bari *et al*. 2022). One potential method to enhance decay resistance is the application of safe and efficient compounds, which can prove effective even with minimal amounts of active constituents. Wood can sustain structural damage from

white-rot fungi, which can break down lignin alone or in tandem with cellulose (Witomski *et al.* 2016). One of the main causes of wood product losses in outdoor use is decay *via* fungus-induced wood degradation.

The white-rot fungus *P. chrysosporium* has been employed to hydrolyse and delignify the biomass containing lignocellulose (Al-Rajhi *et al.* 2024a). The most well researched species, *P. chrysosporium*, produces a variety of hydrolytic and oxidative enzymes that may effectively break down any component of wood (Al-Rajhi *et al.* 2024c; Konan *et al.* 2024).

As the second most available element on Earth, silicon contributes between 0.1 and 10% of a plant's dry weight, which promotes healthy growth and increases resistance to diseases. Fungal fruit damage is prevented using potassium and sodium silicates after harvest (Zhou *et al.* 2018). Li *et al.* (2009) recorded strong activity of sodium silicate against growth of *Fusarium sulphureum* with strong deformation of hyphae and ultrastructures. George (2009) studied the action mechanism of sodium silicate toward *Gloeophyllum trabeum*, a brown-rot fungus and *Trametes versicolor* a white-rot fungus, and observed permeability disruption of cell membranes. According to Rayón-Díaz *et al.* (2021), the activity and proportion of phytopathogens were decreased by sodium silicate. Potassium silicate was applied to control the growth of *Rhizoctonia solani*, *Fusarium oxysporum*, *Pestalotiopsis clavispora*, and other fungi (Shen *et al.* 2017; Ritika and Gurdeep 2021). According to previous investigation, the treated wood by sodium silicate was characterized by several properties such as dimensional stability, resistance to decay, and flame resistance (Nguyen *et al.* 2019). As is well known, several OH groups are present in wood cellulose, and these groups can react with Si-based compounds, which is accompanied by the formation of Si–O–C construction (Popescu and Broda 2021).

Inorganic Cu formulations have been employed to suppress the pathogenic microorganisms, particularly fungi (Capinera and Dickens 2016). According to Farahat (2019), the fungus *Harpophora maydis* was inhibited *via* application of sodium silicate and copper sulfates. In the current decade, molecular docking interaction (MDI) represents one of the attractive techniques to discover, determine the action mechanism, and develop the active compounds in biological systems such as agriculture (Al-Rajhi *et al.* 2024b; Qanash *et al.* 2022, 2023). Therefore, MDI was applied in this study to better understand the role of the silicon or copper-based compounds against the development of wood-decaying fungus *P. chrysosporium*, as mentioned in similar studies that utilized MDI (Yahya *et al.* 2022; Alghonaim *et al.* 2023). Despite the wood protection progress documented, there is still a prerequisite for additional investigation on developing chemical preservatives that are silicon or copper-based but heavy metals-free. The goal of this investigation was to evaluate the influence of sodium silicate, potassium silicate, and copper sulfate on wood-decaying fungus *P. chrysosporium* with its evaluation via molecular docking interaction.

EXPERIMENTAL

Material Used

Three salts, namely sodium silicate, potassium silicate (Oxford production, India), and copper sulfate (El Nasr Pharm. Chem., Co. Production, Egypt), were utilized in the current study. Surfactant and desiccant features have been considered to explain the

effectiveness of silicate-derived compounds against wood resistance to decay. Moreover, several copper-linked compounds are inhibitors to pathogenic of fungi. Therefore, these salts were selected.

Fungus Isolation and Identification

Decayed wood of *Phonix dactyliphra* with apparent fungal mycelia was collected from farms, cultivated with dates in the Riyadh region, Saudi Arabia. The decayed wood was split into small pieces, then the fungal growth medium, namely Potato Dextrose Agar (PDA), was placed into petri dishes along with the decayed wood. For 7 days, the petri dishes were incubated at 30 °C. The visualized fungus was recultured for purification process, and then it was morphologically and microscopically identified according to identification keys (Burdsall 1998).

Effect of Sodium Silicate, Potassium Silicate, and Copper Sulfate on *P. chrysosporium* Growth

Specimens of amended PDA, treated individually with sodium silicate, potassium silicate, or copper sulfate at different concentrations of 25, 50, 100, and 200 mM, were cultivated by a disc (10 mm) of actively growing *P. chrysosporium* colony. The samples were left up to 10 days for an incubation period at 30 °C, and the growth was measured at each concentration every two days.

P. chrysosporium Growth on Wood Treated by Sodium Silicate, Potassium Silicate, and Copper Sulfate

The uninfected wood samples were cut into small pieces (1 to 3 cm) and individually sprayed with a solution of 100 mM sodium silicate, potassium silicate, or copper sulfate. The spraying process was accompanied by continuous stirring to ensure the complete dispersion of examined tested compounds on wood samples. A suspension of active growing *P. chrysosporium* (10-mm disc of colony /20 mL sterile distilled H_2O) was added to each sample of wood (100 g) in sterile plastic boxes. Then, they were incubated at 30 °C for 40 days. The appeared fungus mycelia were visualized. The extent of fungal attack was estimated by weight loss.

Docking Analysis

The molecular docking simulations were performed using Molecular Operating Environment (MOE) software (version 2019) developed by the Chemical Computing Group in Montreal, Quebec, Canada. The 1QPA protein structure was obtained from the Protein Data Bank (PDB) and prepared by protonation, energy minimization, and removal of water molecules and bound ligands. Ligands (sodium silicate, potassium silicate, and copper sulfate) were optimized using the MMFF94x force field. All ligands were placed at the site using the triangle matcher method, and the stiff receptor atoms were docked for 100 nanoseconds. The GBVI/WSA dG procedures were employed for rescoring, and the London dG served as a scoring function. Multiple poses were generated for each ligand-protein pair, and the top five ranked poses were selected for detailed analysis. Docking parameters included triangle matcher placement, London dG scoring for initial poses, and refinement *via* force field energy minimization. Key metrics, Key metrics (important parameters) such as rmsd_refine (root-mean-square deviation after refinement), interaction

distances, and energy scores (E_conf, E_place, E_score1, E_refine), were analyzed *via* same software of MOE. Interactions were visualized in 2D and 3D diagrams to assess binding modes.

RESULTS AND DISCUSSION

The visualized fungus on the wood collected sample (Fig. 1S) was isolated and identified as white-rot fungus, namely *P. chrysosporium*, according to morphological and microscopical features including color, structure of conidia, shape of hyphae, and chlamydospores formation. Numerous investigations recorded the presence of this fungus on various woods. The ability of this fungus to decay the woods may be due to secretion of hydrolytic enzymes. Several enzymes such as β-glucosidase, cellulase, lignin peroxidase, pectin methyltranseliminase, laccases, polygalacturonic acid transeliminase, and manganese peroxidase were produced by wood decaying fungi and represent the main factors in decaying process (Civzele and Mezule 2024; Al-Rajhi *et al*. 2025). *P. chrysosporium* was isolated from decayed woods according to other studies (Hervé *et al.* 2016; Schmerling *et al.* 2022; Al-Rajhi *et al*. 2024d). Different concentrations of sodium silicate, potassium silicate, and copper sulfate were applied to suppress the growth of *P. chrysosporium in vitro* at different days (Table 1). The low dose 25 mM of sodium silicate, potassium silicate, and copper sulfate induced the growth of *P. chrysosporium*, but at 50 and 100 mM, sodium silicate followed by potassium silicate reflected more inhibition than copper sulfate. In contrast, 200 mM copper sulfate addition showed the most effect on inhibiting *P. chrysosporium* growth compared to sodium silicate and potassium silicate. On the other hand, the positive control was Carbendazim ($C_9H_9N_3O_2$), which completely inhibited the fungal growth at 200 mM (data not tabulated). According to Ge *et al.* (2017), 100 mM of sodium silicate inhibited the growth of *Trichothecium roseum.* In a previous study, complete inhibition was observed on *T. roseum*, *Alternaria alternata*, and *Fusarium semitectum* (Bi *et al.* 2006). The current study's observations matched with an earlier study where potassium silicate at low concentration (5 mL/L) increased the *Fusarium oxysporum* growth, while 40 and 80 mL completely inhibited the fungus growth (Bekker *et al.* 2009). It is probable that sub-toxic doses of silicon could act as a nutrient enhancement and encourage faster fungal growth. In another investigation, sodium silicate (4 g/L) showed more activity against *Fusarium solani* with 80.0% inhibition compared to inhibition (72.2%) caused by potassium silicate (4 g/L). Also, *Rhizoctonia solani* was inhibited 61.1% using sodium silicate (2 g/L), while it was inhibited 55.6% using potassium silicate (Abd-El-Kareem *et al.* 2019). In an *in vitro* study on wood, the inoculated wood samples with *P. chrysosporium* (Fig. 1A) without any treatment showed heavy growth of the fungus with weight losses of 32.25±1.66%, while when treated with sodium silicate (Fig. 1B), potassium silicate (Fig. 1C), and copper sulfate (Fig. 1D) a low appearance of the fungus was observed with weight losses of 4.33±0.50%, 11.50±0.66%, and 14.26±1.0%, respectively (Fig. 2). The antifungal mechanisms of inorganic silicate salts involve buffering action (modifying pH) and osmotic pressure, which impede the activity of enzymes that facilitate cell wall solubilization and expansion (Ge *et al*. 2019). The buffering effect modifies the permeability and integrity of the membrane, as well as nutrients transport, resulting in cell inactivation and death, with the initial site of action is

the fungal wall and membrane. *In vitro* study by El-Abdean *et al.* (2020) showed that sodium silicate was more effective (29.02%) than potassium silicate (19.34%) in reducing the growth of *Macrophomina phaseolina.*

Table 1. *P. chrysosporium* Growth at Various Doses of Sodium Silicate (SS), Potassium Silicate (PS), and Copper Sulfate (CS), at Different Incubation Periods

Dose (mM)	*P. chrysosporium* Colony Radius (cm) at Various Incubation Periods (Day)														
	2			4			6			8			10		
	SS	PS	CS	SS	PS	CS	SS	PS	CS	SS	PS	CS	SS	PS	CS
0.0	1.50	1.50	1.50	3.00	3.00	3.00	5.50	5.50	5.50	7.50	7.50	7.50	7.50	7.50	7.50
25	1.66	2.00	2.50	3.25	3.66	3.75	6.00	6.25	6.00	7.66	7.70	7.66	7.70	7.80	7.80
50	1.33	1.46	1.40	2.66	2.66	3.00	3.20	3.33	4.50	3.75	3.80	4.60	3.86	3.86	4.66
100	0.0	0.0	0.0	0.0	0.0	0.0	1.25	1.50	2.25	2.00	2.20	2.30	2.10	2.30	2.33
200	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0

Fig. 1. Wood collected sample infected with white-rot fungus *P. chrysosporium* (S), inoculated wood samples with *P. chrysosporium* without any treatment (A), treated with sodium silicate (B), potassium silicate (C), and copper sulfate (D)

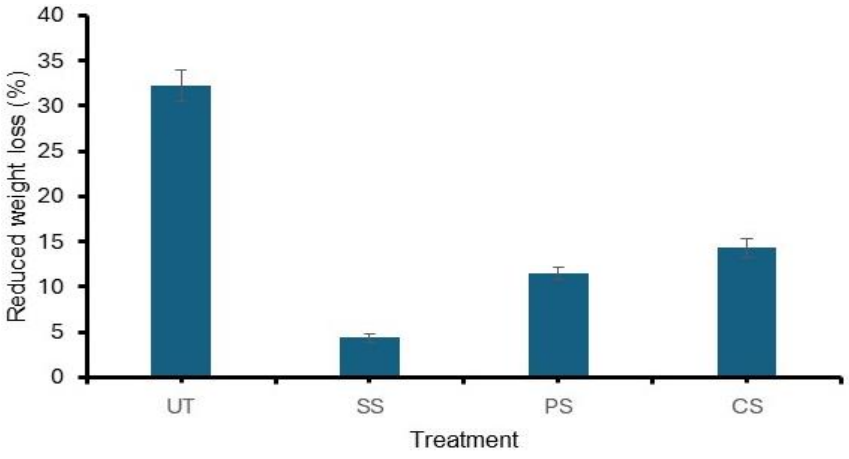

Fig. 2. Reduced weight loss infected with white-rot fungus *P. chrysosporium* without any treatment (UT), treated with sodium silicate (SS), potassium silicate (PS), and copper sulfate (CF)

A gradual decrease in *M. phaseolina* growth was linked with the applied concentration of sodium silicate (Siddiq *et al.* 2019). Nasser and Bhai (2022) found that the exogenous utilization of potassium silicate inhibited the post-harvest infection of ginger by *M. phaseolina.* The seeds of corn were preserved from the fungal infections by sodium silicate and copper sulfate for two seasons (Farahat 2019). Earlier investigation showed that infected wood by *Gloeophyllum trabeum* (brown-rot fungus) and *Trametes versicolor* (white-rot fungus) caused weight losses wood of 32.2 and 30.2%, while treated by sodium silicate caused weight losses of 3.4 to 5.2%, respectively (Chen 2009*). In vitro* and *in vivo* investigation showed that addition of cationic silica sol to malt-agar growth medium and woods inhibited the wood-decaying fungi *Trametes versicolor* and *Coniophora puteana* (Pries and Mai 2013).

Docking Interaction Study

Docking Scores: Sodium silicate showed the highest affinity (S = -6.17 to -5.83 kcal/mol), followed by potassium silicate (S = -3.26 to -2.69 kcal/mol) and copper sulfate (S = -2.38 to -1.73 kcal/mol) (Table 2).

Interactions: Sodium silicate formed metal bonds (Na–O/ASP183, distance = 2.71 to 2.96 Å) and H-acceptor interactions (O10–HIS47, -0.5 kcal/mol) (Table 3). Potassium silicate exhibited ionic and metal interactions with ASP183 (K–OD1/OD2, -1.3 to -5.4 kcal/mol). Copper sulfate displayed weaker H-acceptor (O6–ARG43) and metal (Cu–HIS176) interactions (Figs. 3-5).

Energy profiles: Sodium silicate had the lowest E_conf (-593.75 kcal/mol) and stable refinement (rmsd_refine = 1.52 to 2.54 Å), indicating robust binding. Copper sulfate showed higher E_refine values (19.04 to 30.84 kcal/mol), suggesting less stability.

The superior docking performance of sodium silicate correlates with its multiple metal coordination bonds and lower conformational energy, enhancing receptor-ligand stability. The ionic interactions of potassium silicate with ASP183, though energetically favorable, were less stable compared to sodium silicate's metal bonds. Copper sulfate's weaker binding may stem from fewer specific interactions and higher E_refine values, reflecting suboptimal pose refinement. The results align with the hypothesis that metal-coordinating ligands exhibit stronger affinity for 1QPA (1QPA: Lignin peroxidase, was investigated widely in white-rot fungi and their ability to degrade woods and dyes, plays a role in the biodegradation of lignin materials). The experimental verification is compatible with computational conclusions, which increases biological effectiveness.

The computational docking results reveal nuanced insights into the binding mechanisms of sodium silicate, potassium silicate, and copper sulfate with the 1QPA protein. In this clause, the authors delve deeper into the energetic, and geometrical variables that influence these interactions.

1. Energetic Stability and Conformational Preferences

Sodium silicate: Consistently low E_conf values (ranging from -593.75 to -578.20 kcal/mol) and small rmsd_refine (1.52–2.54 Å) suggest that sodium silicate adopts energetically favorable conformations with minimal deviation during refinement. This stability likely arises from its ability to form strong metal coordination bonds (*e.g.*, Na–O/ASP183 at 2.71 to 2.96 Å) and H-acceptor interactions (*e.g.*, O10–HIS47), which collectively reduce conformational strain.

Potassium silicate: While exhibiting moderate docking scores (S = -3.26 to -2.69), its higher rmsd_refine values (up to ~3.0 Å) imply greater pose flexibility or suboptimal binding precision. The reliance on ionic interactions (*e.g.*, K–OD1/OD2 of ASP183) rather than covalent metal bonds may contribute to this instability, as ionic bonds are typically weaker and more distance-dependent.

Copper sulfate: The unusually positive E_refine values (19.04 to 30.84 kcal/mol) indicate poor energetic convergence during refinement. This could stem from inaccuracies in modeling copper-ligand interactions within MOE's force field or challenges in optimizing the bulky sulfate group. Additionally, its weaker H-acceptor interactions (*e.g.*, O6–ARG43 at -0.8 kcal/mol) and less favorable metal coordination (Cu–HIS176 at -1.1 kcal/mol) highlight its inferior binding compared to silicates.

2. Residue-Specific Interactions and Receptor Compatibility

ASP183 Dominance: Both sodium and potassium silicates target ASP183, a residue with a negatively charged carboxylate group. This suggests a preference for metal/ionic coordination at this site, which aligns with the known role of aspartate residues in metal-binding motifs. Sodium's smaller ionic radius may enable tighter coordination compared to potassium, explaining its stronger binding sites of proteins, the coordinating atoms of oxygen (generated by carboxylate of aspartate amino acid residues).

Table 2. Docking Scores and Energies of Sodium Silicate (SS), Potassium Silicate (PS), and Copper Sulfate (CS) with Structure of *P. chrysosporium* (PDB ID: 1QPA)

Mol	S	rmsd_refine	E_conf	E_place	E_score1	E_refine	E_score2
SS	-6.16762	1.516398	-593.75	-53.7625	-7.11879	-25.3321	-6.16762
SS	-6.09203	1.972208	-591.694	-50.5791	-6.80009	-25.1321	-6.09203
SS	-6.00876	2.447731	-578.202	-50.9104	-8.14504	-20.8056	-6.00876
SS	-5.89268	2.541198	-591.717	-52.8131	-8.98554	-20.614	-5.89268
SS	-5.82826	2.003491	-593.022	-53.0122	-7.17624	-13.8558	-5.82826
PS	-3.25879	2.670632	-745.24	-27.7064	-4.92026	-7.7377	-3.25879
PS	-3.16222	1.069364	-744.358	-27.8243	-4.65085	-5.34101	-3.16222
PS	-2.97664	2.759199	-745.808	-33.9382	-5.40408	-8.10477	-2.97664
PS	-2.97458	2.988621	-745.418	-28.0316	-4.90306	-6.98352	-2.97458
PS	-2.68879	2.75981	-745.202	-29.6801	-6.30819	0.648402	-2.68879
CS	-2.38369	2.657192	-2073.77	-46.6141	-5.90849	19.0413	-2.38369
CS	-2.06461	2.752627	-2061.46	-43.0493	-5.81615	19.7757	-2.06461
CS	-2.0062	2.193118	-2070.4	-42.998	-6.1856	25.57064	-2.0062
CS	-1.73714	2.286763	-2054.3	-45.163	-6.00495	30.83545	-1.73714
CS	-1.7302	2.730402	-2061.17	-43.778	-5.65747	28.4482	-1.7302

HIS176 and ARG43: Copper sulfate's interactions with HIS176 (*via* Cu) and ARG43 (*via* H-acceptor) are weaker, potentially due to mismatched geometry or insufficient complementarity between copper's coordination sphere and the receptor's active site. However, HIS176 and ARG43 were the most crucial in binding of Lignin peroxidase of *P. chrysosporium* (PDB ID: 1QPA). The absence of strong acidic residues

near copper's binding site may further limit stabilization. To investigate the creation of active chemicals to inhibit pathogenic microorganisms and the target enzymes in charge of various metabolic processes, the role of docking in biological activities was documented (Alsalamah *et al.* 2023; Binsaleh *et al.* 2025). The relationship between bacteria and nano-silica particles was investigated *via* molecular docking was utilized (Tian *et al.* 2024). According to Al-Rajhi *et al.* (2025), the obtained bind energy -4.34457 and-4.46592 kcal/mol from the docking interaction of sodium silicate with cell wall degrading enzymes, namely pectin lyase and pectin methyltranseliminase of *Aspergillus flavus*, respectively, indicated the efficacy of sodium silicate.

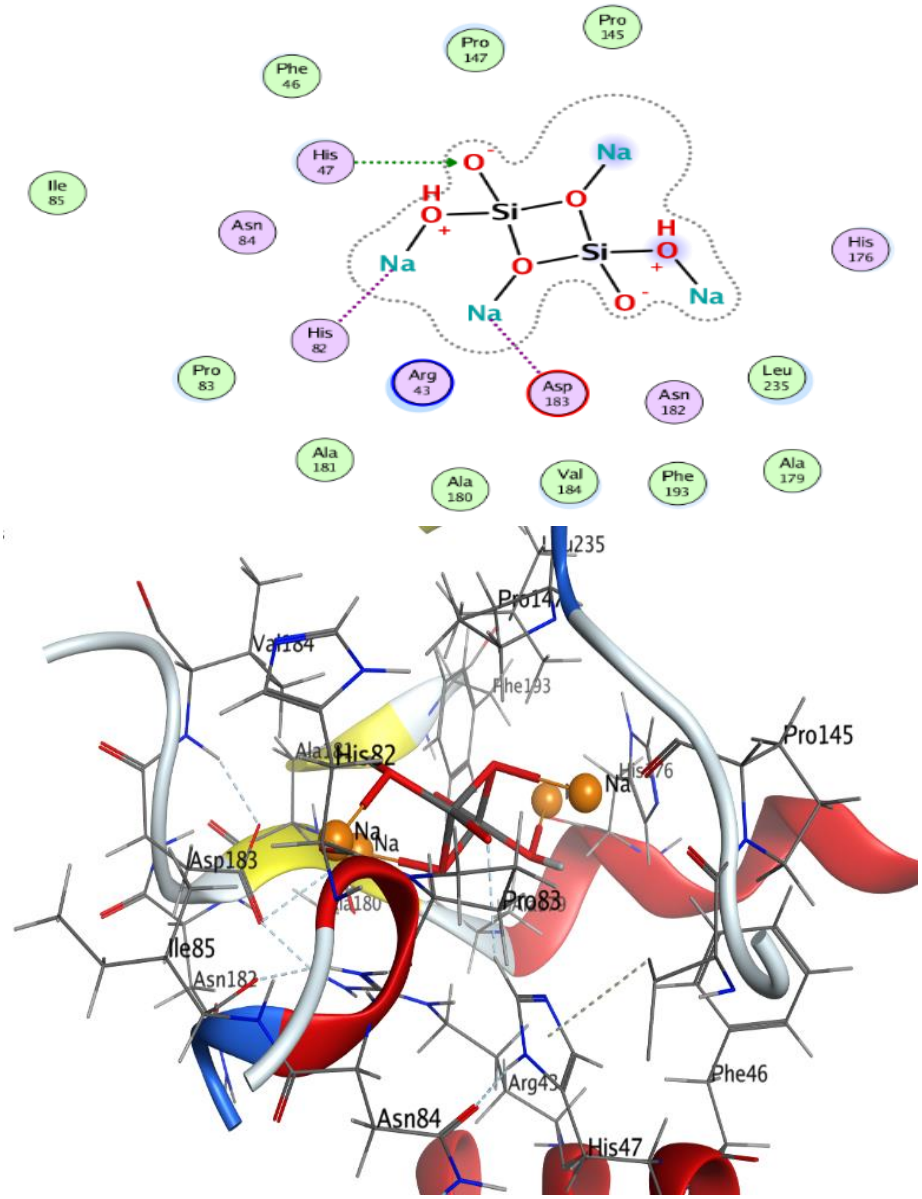

Fig. 3. Diagrams including 2D and 3D represent the interaction between sodium silicate and active sites of 1QPA protein of *P. chrysosporium* (PDB ID: 1QPA)

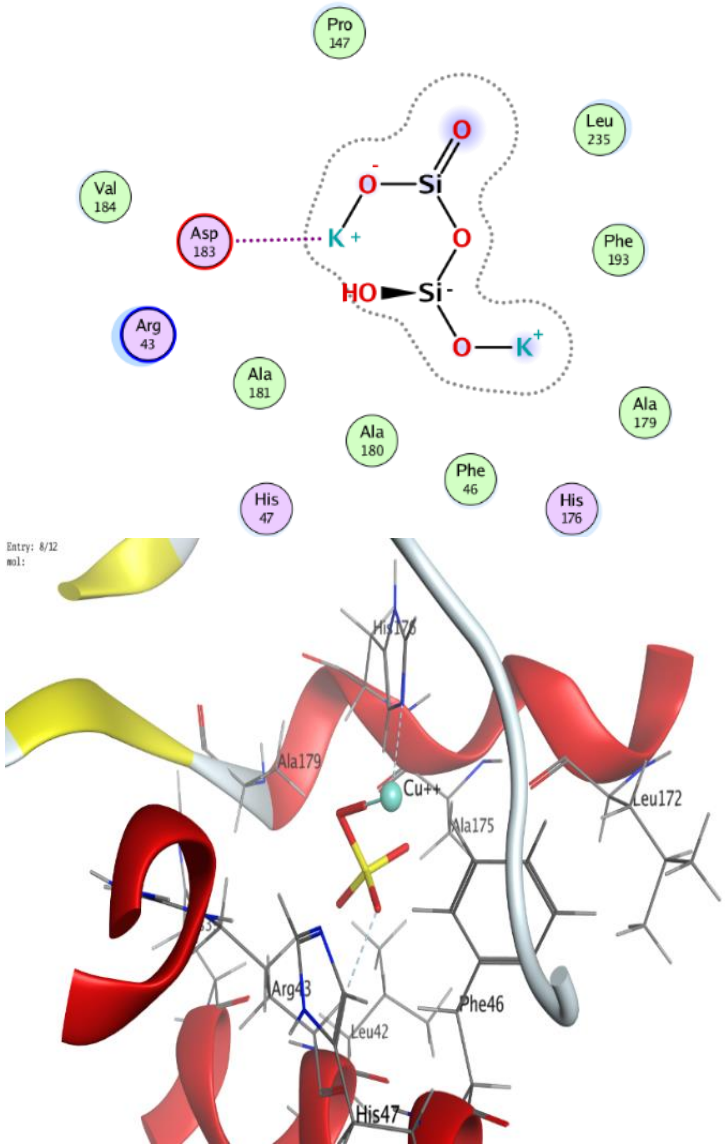

Fig. 4. Diagrams including 2D and 3D represent the interaction between potassium silicate and active sites of 1QPA protein of *P. chrysosporium* (PDB ID: 1QPA)

Table 3. Interaction of Sodium Silicate (SS), Potassium Silicate (PS), and Copper Sulfate (CS) with Structure of P. chrysosporium (PDB ID: 1QPA)

Mol	Ligand	Receptor	Interaction	Distance	E (kcal/mol)
SS	O 10	CE1 HIS 47 (A)	H-acceptor	3.44	-0.5
	Na 13	O HIS 82 (A)	Metal	2.71	-1.7
	Na 14	OD1 ASP 183 (A)	Metal	2.96	-0.8
PS	K 2	OD2 ASP 183 (A)	Metal	2.86	-2.0
	K 2	OD1 ASP 183 (A)	Ionic	3.67	-1.3
	K 2	OD2 ASP 183 (A)	Ionic	2.86	-5.4
CS	O 6	CA ARG 43 (A)	H-acceptor	3.24	-0.8
	Cu 1	NE2 HIS 176 (A)	Metal	2.62	-1.1

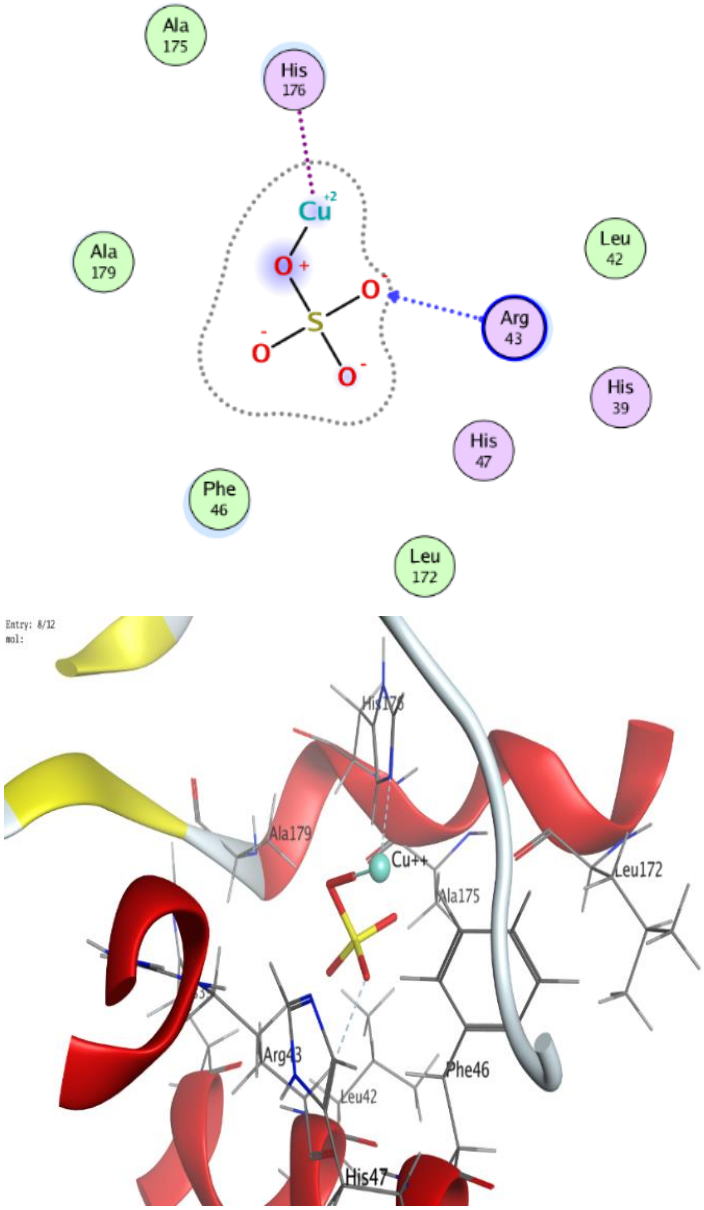

Fig. 5. Diagrams including 2D and 3D represent the interaction between copper sulfate and active sites of 1QPA protein of *P. chrysosporium* (PDB ID: 1QPA)

CONCLUSIONS

1. *Phanerochaete chrysosporium* was isolated from the decayed wood sample (this fungus is white-rot type). It follows that further investigation about broader utilization and enzymatic activities must be continued into this fungus.
2. *In vitro* and *in vivo* study revealed that sodium silicate was a more effective inhibitor than potassium silicate and copper sulfate for *P. chrysosporium*.

Furthermore, the outcoms of this investigation will support the application of these compounds in wood related materials.

3. From the docking interaction, sodium silicate demonstrated the highest potential for targeting the 1QPA protein of *P. chrysosporium*, driven by strong metal coordination and low energy scores. Potassium silicate and copper sulfate showed moderate interactions but lacked comparable stability, which is consistent with *in vitro* results and suggests sodium silicate as a possible option for a molecular inhibitor in targeting the 1QPA protein. In future studies sodium silicate, potassium silicate, and copper sulfate must be docked with more than one wood decaying fungus.

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