# Efficacy of Sodium Silicate on *Aspergillus flavus* and its Action on Cell Wall Degrading Enzymes with Molecular Docking Studies

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The extent of spoilage of fruits and vegetables increases post harvest, and fungal attack is one of the greatest causes. The effect of sodium silicate on *Aspergillus flavus* and its cell wall degrading enzymes, namely polygalacturonic acid transeliminase (PGTE), pectin methyltranseliminase (PMTE), and pectin lyase (PL), was investigated *via* molecular docking. On the 4th day, 100 mM of sodium silicate completely inhibited *A. flavus*, while it reflected 79.70, 61.16, 56.82, and 37.23% inhibition at 6, 8,10, and 12 days, respectively. The PGTE (369.33 ± 2.08 U/mL) showed maximum activity at the 8th day in the medium without sodium silicate. Also at 20 to 80 mM sodium silicate, their maximum activity was recorded at the 8th day, while it reached to maximum at the 10th day in the medium with 100 mM sodium silicate. The PMTE recorded the highest activity at the 6th day (414.00 ± 1.73 U/mL) without sodium silicate, at the 8th day when sodium silicate ranged from 20 to 80 mM, and at the 10th day (97.67 ± 1.25 U/mL) with 100 mM sodium silicate. The maximum PL activity was recorded on day 8. Sodium silicate demonstrates potent interaction with the active sites of the studied proteins, suggesting its potential as a molecular inhibitor of studied enzymes.

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## INTRODUCTION

Fungi are among the most significant factors that contribute to the deterioration of fresh vegetables and fruit. Various products of nutrition, including vegetables, seeds, and dry and fresh fruits are affected by *Aspergillus flavus* and their toxins, which are known as aflatoxins (Segura-Palacios *et al.* 2021). Such toxins are potent carcinogens, and they are extensively controlled in numerous countries (Samaila *et al.* 2018; Zakaria *et al.* 2024).

To create a complex network and colonize the plant tissues, the pathogen typically needs to break through the cell walls of the plant. Certain fungal pathogens release cell wall degrading enzymes (CWDEs) during this process to break down the elements of plant cell walls, facilitating the pathogen's entry into the cell (Xue *et al.* 2018; Zhang *et al.* 2021). Fruit softening is regulated by CWDEs, including endo-1,4-$\beta$-D-endoglucanase (EGase), xyloglucan endotransglucosylase (XET), $\beta$-galactosidase ($\beta$-gal), cellulase (Cx), polygalacturonase (PG), pectin methylesterase (PME), polygalacturonic acid transeliminase (PGTE), pectin methyltranseliminase (PMTE), and pectate lyase (PL). Both PGTE and PMTE remove the hydrogen at C5 by cleaving the α-1,4-linkage between the methylgalacturonides in the pectin molecule. While PMTE targets methylated polygalacturonic acid or pectin in the cell wall, PGTE specifically cleaves the α-1,4-glycosidic bond within the pectinate molecule. Research has demonstrated that fungi including *Colletotrichum gloeosporioides* and *Botrytis cinerea* secrete a variety of CWDEs, such as PG, PME, and PL. The mechanisms used by fungi to regulate the secretion of CWDEs have not been well documented.

Silicon is the second major element on Earth, representing 0.1 to 10% in plant's dry weight and impacts disease resistance in plants. Applying sodium silicate after harvest inhibits fungal fruit deterioration (Zhou *et al.* 2018). However, knowledge of its exact mode of action regarding the induction of plants to suppress fungal pathogens is still limited. Si contributes to the host-pathogen interaction metabolically by boosting the activities of plant defense enzymes, which increases the accumulation of defensive compounds such as phytoalexins and phenolics, thus strengthening the plants' resistance to biotic and abiotic stressors (Reynolds *et al.* 2016). The composition of soil fungal and bacterial communities was also altered by sodium silicate ($Na_2SiO_3$); in particular, it reduced the relative abundances of microbial taxa that contained plant pathogens while increasing those that had potential benefits for plants (Zhou *et al.* 2018; Rayón-Díaz *et al.* 2021). Zhang *et al.* (2021) recorded the inhibitory action of both sodium silicate and chitosan individually against *Alternaria alternata*, but their combination proved more effective than chitosan alone. Moreover, the natural rate of rotting of winter jujube by *A. alternata* was decreased as a result of sodium silicate and chitosan. Currently, an important and accessible form of computational chemistry is molecular docking. It is beneficial to look at a specific drug candidate's potential action mechanism and target interactions (Al-Rajhi *et al.* 2022a, 2022b; Qanash *et al.* 2022; Yahya *et al.* 2022; Alghonaim *et al.* 2023; Qanash *et al.* 2023; Al-Rajhi *et al.* 2024). The purpose of this study was to evaluate the influence of sodium silicate on decaying fungus of apple fruits, as well as their effect on CWDEs activity *via* molecular docking studies.

## EXPERIMENTAL

### Fungus Isolation and Identification

Apple fruits exhibiting spoilage were collected from fruit markets of Riyadh region, Saudi Arabia. Small segments of spoiled fruit were sterilized employing hypochlorite (1%) for 2 min (for killing the spores on the fruit surface from air but not killing the invaded fungal mycelia within the tissues). Then, the segments were placed on the surface of potato dextrose agar (PDA) medium, followed by incubation at 30 °C. The fungus was

recultivated for purification process at the same conditions of the isolation process. The purified fungus was identified according to Raper and Fennell (1973) and Samson *et al.* (1995), depending on the morphological and microscopical features including shape, color, texture of colonies, diameter, and form of conidiospores, hyphae, and phialide.

### Growth of *A. flavus* at Different Doses of Sodium Silicate

Supplemented PDA (SPDA) medium with different doses 20, 40, 60, and 100 mM of sodium silicate was prepared. Active discs (6 mm radius) from cultivated PDA with *A. flavus* for 5 days were transferred to the center of plate containing SPDA, followed by incubation up to 12 days. The diameter of the developed colony was detected at each period of incubation.

### Preparation of Crude Enzyme Extracts of *A. flavus*

Czapek's-Dox broth medium containing sodium silicate (80 mM) was inoculated with *A. flavus.* The culture was incubated at 30 °C under shaking condition (120 rpm) for a period between 4 to 12 days**.** The control was applied using medium lacking sodium silicate. At the end of the incubation period, the broth medium was centrifuged for 25 min, at 4 °C and at 10,000 g. The supernatant functioned as the crude enzymes.

### Assay CWDE Activities of *A. flavus*

With minor changes, according to Yang *et al.* (2012), the activities of polygalacturonic acid transeliminase (PGTE) and pectin methyltranseliminase (PMTE) were recorded. The required substrates for PGTE and PMTE were polygalacturonic acid and pectin, respectively. The following contents 0.3 mL of 1 mg/mL polygalacturonic acid or pectin, 1 mL of 3 mM $CaCl_2$, 4 mL of Gly–NaOH (50 mM, pH 9) buffer, and crude enzyme (100 μL) were mixed to start the enzymes reaction. At 30 °C, the mixture was incubated for 5 min. The activities of enzymes were expressed as U/mL. With minor changes, according to Jia *et al.* (2009), the activities of pectin lyase (PL) were recorded. The contents of the reaction mixture were 0.5 mL of crude enzyme and 2.0 mL of 0.5 mg/mL pre-incubated pectin at 40 °C for 5 min. Then, the reaction mixture was kept for 10 min at 40 °C. For ending the reaction, 7.5 mL of HCl (10 mM) was added.

### Molecular Docking

Molecular docking was performed to investigate the affinity of sodium silicate against pectin lyase, pectin methyltranseliminase, and polygalactronase. The chemical structure of sodium silicate was drawn using ChemDraw Ultra 15.0. The 3D structures of the target proteins pectin lyase (PDB ID: 1IDJ), pectin methyltranseliminase (PDB ID: 3OQB), and polygalacturonase (PDB ID: 1K5C) were obtained from the Protein Data Bank (PDB). The following steps were carried out to prepare the protein structures:

1. All non-protein components, such as water molecules and bound ligands, were removed.
2. Hydrogen atoms were added, and protonation states were adjusted according to physiological pH.
3. The structures were energy-minimized to relieve any steric clashes.
4. The site finder created the active binding sites, which served as the binding pocket's dummy sites.

*Preparation of ligand (sodium silicate)*

1. The ligand structure was created and optimized to achieve a low-energy conformation.
2. Partial charges were assigned, and the geometry was optimized using a molecular mechanics force field.

*Docking Procedure*

Sodium silicate was placed at the site using the triangle matcher method, and the stiff receptor atoms were docked for 100 ns. 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.

The 2D and 3D interaction diagrams were generated to visualize the binding modes of sodium silicate within the active sites of each protein. These visualizations highlighted specific interactions, such as hydrogen bonds and metal-ligand interactions.

The docked complexes were analyzed to determine the interactions between sodium silicate and the active site residues of the proteins. Hydrogen bonds, hydrophobic interactions, and metal coordination were identified. Key interaction parameters, such as bond distances and interaction energies, were recorded.

## Statistical Analysis

The findings were offered as mean ± standard deviation (SD) by Microsoft Excel 365 and SPSS v.25.

## RESULTS and DISCUSSION

The isolated fungus from decayed fruits of apple was identified as *A. flavus*. This fungus has been isolated previously from various fruits, vegetables, grains, and seeds (Mailafia *et al.* 2017; Samaila *et al.* 2018; Abdelghany *et al.* 2020; Al-Rajhi *et al.* 2023; Zakaria *et al.* 2024). The application of different doses of sodium silicate evidently inhibited *A. flavus* growth with larger inhibitory action at high doses. The colony development of *A. flavus* treated by 100 mM of sodium silicate was completely inhibited up to the 4$^{th}$ day, and showed 12.25, 25.50, 30.60, and 45.26 mm at 6, 8,10, and 12 days with inhibition levels 79.70, 61.16, 56.82, and 37.23% (Table 1). Moreover, from Table 1, as the incubation period increased, the resistance of *A. flavus* to sodium silicate increased. At 60 and 80 mM of sodium silicate, there was no growth on the 2$^{nd}$ day, but it appeared afterwards. Sodium silicate was applied previously to control the fungal growth such as *Fusarium sulphureum* (Li *et al.* 2009), *Trametes versicolor* (George 2009), and *Harpophora maydis* Farahat (2019). Remarkable changes appeared in the structures of *A. flavus* exposed to sodium silicate, where the diameter of conidial head, vesicle, and hypha, besides the length of phialides, were decreased with increasing dose of sodium silicate (Table 2). This outcome was consistent with the examination of Li *et al.* (2009) and Ge *et al.* (2017). They observed that sodium silicate at 100 mM completely prevented the *Fusarium semitectum* and *Trichothecium roseum* growth, respectively. Additionally,

sodium silicate showed a suppressed effect on *Geotrichum citri-aurantii* growth (causing sour rot of citrus fruit) (Li *et al.* 2019).

**Table 1.** Growth of *A. flavus* under Different Concentrations of Sodium Silicate and Incubation Periods

| Dose (mM) | Incubation Period (Day) | | | | | |
|---|---|---|---|---|---|---|
| | 2 | 4 | 6 | 8 | 10 | 12 |
| **0.0** | 15.66 | 35.50 | 50.33 | 65.66 | 70.87 | 72.10 |
| **20** | 8.33 | 20.22 | 30.50 | 45.50 | 60.55 | 70.50 |
| **40** | 10.25 | 15.53 | 25.57 | 40.50 | 55.23 | 68.50 |
| **60** | 0.0 | 10.50 | 25.25 | 30.20 | 52.89 | 65.76 |
| **80** | 0.0 | 10 | 15.50 | 38.67 | 50.53 | 65.70 |
| **100** | 0.0 | 0.0 | 12.25 | 25.50 | 30.60 | 45.26 |

**Table 2.** Morphological Characterization of *A. flavus* at Different Doses of Sodium Silicate

| Dose (µm/L) | Conidial Head Diameter (µm) | Vesicle Diameter (µm) | Phialide Length (µm) | Spore Diameter (µm) | Hypha Diameter (µm) |
|---|---|---|---|---|---|
| **0** | 272.13 ± 7.81a | 175.37 ± 5.55a | 45.36 ± 1.22a | 13.30 ± 0.53b | 31.50 ± 1.65a |
| **20** | 144.00 ± 13.00b | 87.00 ± 25.5b | 32.66 ± 2.59b | 15.06 ± 0.34a | 25.94 ± 2.37bc |
| **40** | 160.00 ± 12.00 ± b | 91.00 ± 6.50b | 30.00 ± 2.70b | 13.30 ± 0.85ab | 27.86 ± 1.94b |
| **60** | 155.12 ± 12.00 ± b | 87.20 ± 2.50b | 27.00 ± 0.50b | 13.11 ± 0.52ab | 27.15 ± 1.22b |
| **80** | 139.00 ± 11.20b | 66.50 ± 3.81b | 22.98 ± 0.85c | 13.50 ± 1.00b | 20.63 ± 1.59c |
| **100** | 132.00 ± 11.20b | 60.50 ± 3.64b | 18.98 ± 0.82c | 12.22 ± 1.00b | 15.66 ± 1.65c |
| Means followed by the same letters are not significantly different | | | | | |

From Table 3, the maximum activity of PGTE was recorded at the 8$^{th}$ day in the medium without sodium silicate (369.33 ± 2.08 U/mL) and the medium with sodium silicate ranged from 20 to 80 mM, while it reached maximum at day 10 in the medium with 100 mM sodium silicate and then decreased with increasing period of incubation. Their activity level at the 8$^{th}$ day under 100 mM of sodium silicate regarding the control (100%) was 33.1%. Additionally, the activity of PMTE increased with an increase in the period of incubation up to 6 days for the control (414.00 ± 1.73 U/mL), 8 days for the specimen supplemented with sodium silicate from 20 to 80 mM (363.00 ± 3.00 to 136.33 ± 0.58 U/mL), and 10 days for medium supplemented with 100 mM sodium silicate (97.67 ± 1.25 U/mL) (Table 4). Their activity level at the 8$^{th}$ day under 100 mM of sodium silicate regarding the control (100%) was 14.0%. At the 8$^{th}$ day, the maximum activity of PL was detected in the medium without (787.67 ± 2.31 U/mL) or with different concentrations of sodium silicate (Table 5).

**Table 3.** Activity of PGTE (U/mL) at Different Doses of Sodium Silicate and Different Incubation Periods

| Dose (mM) | Incubation Period (Day) | | | | | |
|---|---|---|---|---|---|---|
| | 2 | 4 | 6 | 8 | 10 | 12 |
| 0.0 | 53.33 ± 2.89 | 100.33 ± 5.77 | 277.67 ± 2.52 | 369.33 ± 2.08 | 361.33 ± 4.16 | 353.33 ± 2.89 |
| 20 | 52.33 ± 2.31 | 88.67 ± 1.15 | 267.67 ± 2.08 | 374.33 ± 4.04 | 354.33 ± 1.15 | 346.67 ± 1.53 |
| 40 | 45.33 ± 1.15 | 80.00 ± 1.73 | 233.33 ± 5.03 | 354.33 ± 3.51 | 301.67 ± 1.53 | 277.00 ± 2.65 |
| 60 | 20.67 ± 1.15 | 59.33 ± 2.31 | 201.67 ± 2.89 | 177.67 ± 0.58 | 172.67 ± 3.51 | 170.67 ± 1.15 |
| 80 | 0.0 ± 0.00 | 46.67 ± 1.15 | 156.67 ± 7.64 | 131.33 ± 1.15 | 129.33 ± 4.51 | 111.33 ± 1.15 |
| 100 | 0.0 ± 0.00 | 0.0 ± 0.00 | 76.33 ± 0.58 | 122.33 ± 2.08 | 124.33 ± 1.15 | 110.00 ± 3.46 |

**Table 4.** Activity of PMTE (U/mL) at Different Doses of Sodium Silicate and Different Incubation Periods

| Dose (mM) | Incubation Period (Day) | | | | | |
|---|---|---|---|---|---|---|
| | 2 | 4 | 6 | 8 | 10 | 12 |
| 0.0 | 100.67 ± 2.08 | 219.67 ± 2.08 | 414.00 ± 1.73 | 408.67 ± 5.51 | 404.67 ± 0.58 | 330.67 ± 5.03 |
| 20 | 89.33 ± 4.16 | 201.33 ± 1.53 | 368.33 ± 9.71 | 363.00 ± 3.00 | 360.17 ± 0.29 | 320.00 ± 1.73 |
| 40 | 66.33 ± 1.15 | 178.00 ± 1.00 | 224.33 ± 0.58 | 221.67 ± 2.08 | 212.50 ± 0.50 | 197.33 ± 1.15 |
| 60 | 0.0 ± 0.00 | 175.33 ± 0.58 | 177.67 ± 0.58 | 166.67 ± 1.25 | 150.17 ± 0.29 | 131.00 ± 1.73 |
| 80 | 0.0 ± 0.00 | 91.0 ± 1.73 | 131.83 ± 4.86 | 136.33 ± 0.58 | 119.67 ± 0.58 | 100.83 ± 1.44 |
| 100 | 0.0 ± 0.00 | 0.0 ± 0.00 | 35.17 ± 0.29 | 57.33 ± 0.29 | 97.67 ± 1.25 | 88.33 ± 1.15 |

**Table 5.** Activity of PL (U/mL) at Different Concentrations of Sodium Silicate and Different Incubation Periods

| Dose (mM) | Incubation Period (Day) | | | | | |
|---|---|---|---|---|---|---|
| | 2 | 4 | 6 | 8 | 10 | 12 |
| 0.0 | 598.50 ± 0.50 | 650.17 ± 0.29 | 710.33 ± 0.58 | 787.67 ± 2.31 | 781.67 ± 2.89 | 730.67 ± 2.08 |
| 20 | 546.00 ± 1.73 | 557.67 ± 1.53 | 600.67 ± 5.51 | 670.00 ± 4.00 | 565.00 ± 0.87 | 532.67 ± 1.53 |
| 40 | 511.83 ± 0.29 | 554.33 ± 1.15 | 589.33 ± 1.15 | 659.67 ± 5.51 | 545.50 ± 0.50 | 521.33 ± 2.31 |
| 60 | 0.0 ± 0.00 | 511.83 ± 2.75 | 502.00 ± 2.65 | 525.00 ± 1.73 | 489.33 ± 0.58 | 470.83 ± 2.75 |
| 80 | 0.0 ± 0.00 | 420.00 ± 1.80 | 421.33 ± 0.58 | 456.17 ± 0.29 | 434.33 ± 2.31 | 405.33 ± 0.58 |
| 100 | 0.0 ± 0.00 | 0.0 ± 0.00 | 345.00 ± 1.73 | 385.50 ± 0.87 | 377.83 ± 0.29 | 367.83 ± 2.75 |

Their activity level on the 8$^{th}$ day under 100 mM of sodium silicate regarding the control (100%) was 48.9%. Generally, the activity of CWDEs, namely PGTE, PMTE, and PL, was affected by sodium silicate at all incubation periods. Such enzymes (CWDEs) are regarded as pathogenicity agents that participate in fruit and vegetable decay caused by

several fungi. According to Ge *et al.* (2017), sodium silicate possesses inhibitory action on the activity of CWDEs. González-Jiménez *et al.* (2023) mentioned that sodium silicate controlled the citrus fruit decaying *via* their effects on CWDEs.

The docking study focused on the interaction of sodium silicate with three specific proteins: Pectin Lyase (PDB ID: 1IDJ), Pectin Methyl transeliminase (PDB ID: 3OQB), and Polygalacturonase (PDB ID: 1K5C), as illustrated in Fig. 1. The key docking parameters, including docking scores, interaction types, binding energies, and distances, were analyzed to evaluate binding affinities and interaction mechanisms, as presented in Tables 6 and 7.

## Docking Scores and Binding Energies

**1IDJ (Pectin Lyase)** showed docking scores ranging from -3.69269 to -4.34457, with energy contributions highlighting a mix of hydrophobic and electrostatic interactions.

**3OQB (Pectin Methyltranseliminase)** exhibited scores from -3.80886 to -4.04268, suggesting strong stability in binding.

**1K5C (Polygalacturonase)** had scores from -3.81369 to -4.46592, indicating slightly stronger binding compared to 3OQB.

All proteins demonstrated favorable energy contributions, especially from E_conf and E_place, emphasizing stable conformations upon docking.

## Interaction Analysis

**1IDJ**: Sodium silicate formed hydrogen bonds and metal interactions with Aspartate (ASP 154) and Valine (VAL 101), showing short interaction distances (2.78 to 3.07 Å) with low binding energies (-0.7 to -1.5 kcal/mol).

**3OQB**: Strong hydrogen bonding and metal coordination were observed with residues, such as Arginine (ARG 185) and Glutamate (GLU 113), with distances ranging from 2.77 to 2.95 Å and energies as low as -4.9 kcal/mol.

**1K5C**: Interactions were observed with Lysine (LYS 228) and Aspartate (ASP 153, ASP 173), having distances of 2.65 to 2.92 Å and binding energies ranging from -1.0 to -3.1 kcal/mol.

The docking results highlight that sodium silicate exhibits significant binding affinity and stability across all three enzymes. The strong binding of sodium silicate can be attributed to the following:

1. **Energy Contributions**:
   The favorable E_place and E_conf values underscore the ability of sodium silicate to fit well into the active sites of these proteins.
   The binding energies, particularly those involving hydrogen bonding and metal coordination, are indicative of specific and strong interactions with catalytic residues.
2. **Specific Interactions**:
   Residues such as ASP and GLU are crucial in stabilizing sodium silicate because of their ability to coordinate metal ions effectively.
   The low RMSD_refine values (< 4 Å for most configurations) suggest minimal structural deviations post-docking, confirming stable complexes.

3. **Comparative Binding Strength**:
   **Polygalacturonase (1K5C)** exhibited the highest binding score (-4.46592), which may be due to more favorable metal interactions compared to other proteins.

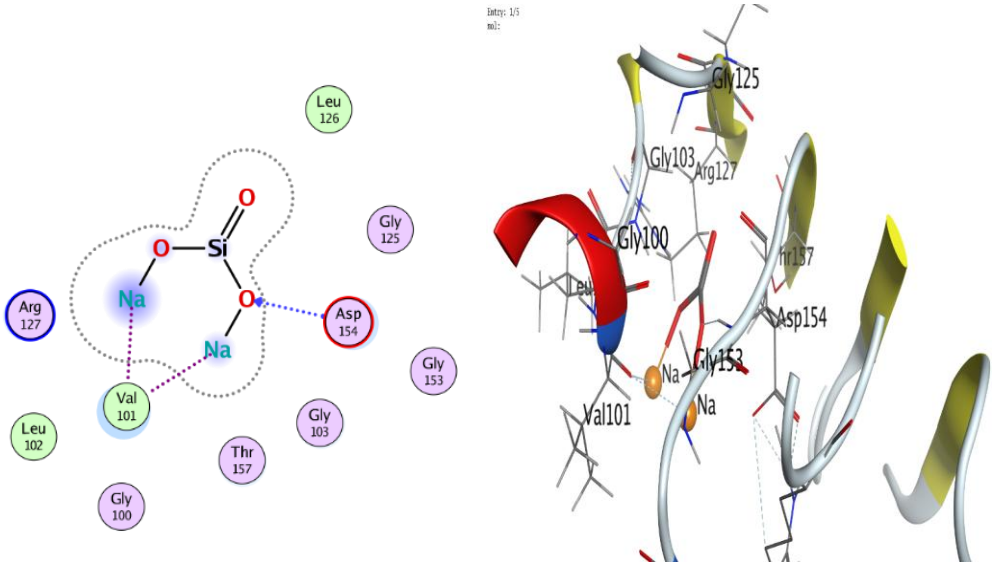
The interaction energy for **Pectin Methyltranseliminase (3OQB)** was notable, especially for ARG 185, indicating its critical role in stabilization. The role of docking in biological activities was recorded to explore the development of active compounds to suppress pathogenic microorganisms, as well as to inhibit the target enzymes responsible for several metabolic activities (Alsalamah *et al*. 2023; Le Thanh *et al*. 2023; Binsaleh *et al*. 2025).

**Table 6.** Docking Scores and Energies of Sodium Silicate with Structure of Pectin Lyase (PDB ID: 1IDJ), Pectin Methyltranseliminase (PDB ID: 3OQB), and Polygalacturonase (PDB ID: 1K5C)

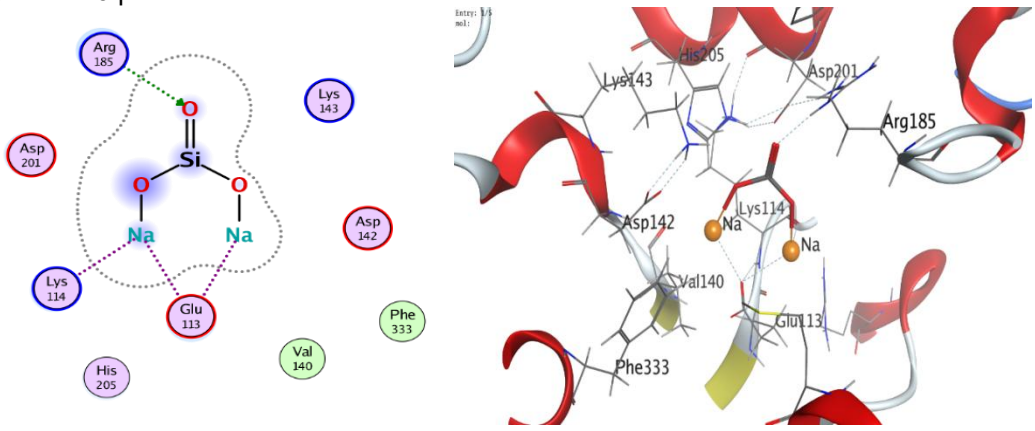
| Mol | Protein | S | rmsd_refine | E_conf | E_place | E_score1 | E_refine | E_score2 |
|---|---|---|---|---|---|---|---|---|
| Sodium silicate | 1IDJ | -4.34457 | 2.643072 | -141.867 | -24.6458 | -2.95106 | -14.2176 | -4.34457 |
| Sodium silicate | 1IDJ | -4.16547 | 1.317401 | -146.955 | -22.3478 | -1.58472 | -7.10574 | -4.16547 |
| Sodium silicate | 1IDJ | -4.15926 | 4.019346 | -141.988 | -20.226 | -3.15415 | -7.9195 | -4.15926 |
| Sodium silicate | 1IDJ | -3.88469 | 3.411921 | -146.289 | -38.958 | -3.75654 | -11.6563 | -3.88469 |
| Sodium silicate | 1IDJ | -3.69269 | 3.513837 | -141.817 | -27.0546 | -3.66119 | -10.4341 | -3.69269 |
| Sodium silicate | 3OQB | -4.04268 | 2.575892 | -142.013 | -31.044 | -3.28293 | -6.13246 | -4.04268 |
| Sodium silicate | 3OQB | -3.92105 | 0.966468 | -146.402 | -32.8135 | -4.15845 | -13.7671 | -3.92105 |
| Sodium silicate | 3OQB | -3.90118 | 2.26121 | -146.408 | -21.1867 | -3.73405 | -10.6435 | -3.90118 |
| Sodium silicate | 3OQB | -3.86792 | 1.64772 | -146.495 | -34.5449 | -3.16511 | -13.0887 | -3.86792 |
| Sodium silicate | 3OQB | -3.80886 | 2.121973 | -141.907 | -23.1249 | -3.28093 | -12.9622 | -3.80886 |
| Sodium silicate | 1K5C | -4.46592 | 2.910793 | -142.027 | -25.5122 | -3.74031 | -17.5517 | -4.46592 |
| Sodium silicate | 1K5C | -4.13442 | 2.061158 | -145.877 | -29.7785 | -3.94353 | -10.6491 | -4.13442 |
| Sodium silicate | 1K5C | -3.94879 | 1.253019 | -147.698 | -32.2905 | -2.87534 | -9.07095 | -3.94879 |
| Sodium silicate | 1K5C | -3.83257 | 3.382757 | -146.502 | -30.5791 | -3.48259 | -11.0874 | -3.83257 |
| Sodium silicate | 1K5C | -3.81369 | 5.926071 | -147.566 | -26.4578 | -2.57928 | -6.72188 | -3.81369 |

**Table 7.** Interaction of Sodium Silicate with Structure of Pectin Lyase (PDB ID: 1IDJ), Pectin Methyltranseliminase (PDB ID: 3OQB), and Polygalacturonase (PDB ID: 1K5C)

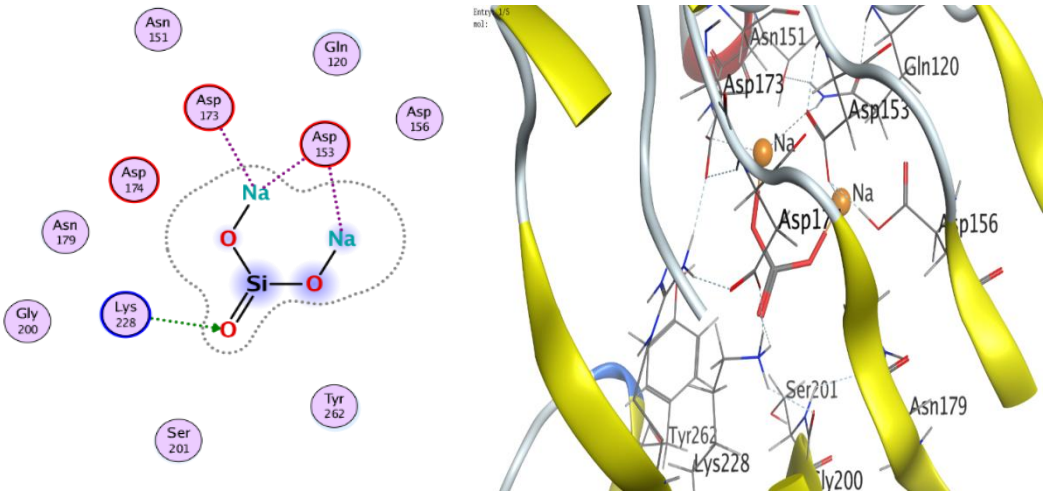
| Mol | Protein | Ligand | Receptor | Interaction | Distance | E (kcal/mol) |
|---|---|---|---|---|---|---|
| Sodium silicate | 1IDJ | O 3 | N ASP 154 (A) | H-acceptor | 3.07 | -0.7 |
| | | Na 5 | O VAL 101 (A) | Metal | 2.88 | -0.8 |
| | | Na 6 | O VAL 101 (A) | Metal | 2.78 | -1.5 |
| Sodium silicate | 3OQB | O 4 | NE ARG 185 (A) | H-acceptor | 2.95 | -4.9 |
| | | Na 5 | OE1 GLU 113 (A) | Metal | 2.77 | -2.7 |
| | | Na 6 | OE1 GLU 113 (A) | Metal | 2.82 | -0.8 |
| | | Na 6 | O LYS 114 (A) | Metal | 2.82 | -1.5 |
| Sodium silicate | 1K5C | O 4 | NZ LYS 228 (A) | H-acceptor | 2.92 | -2.2 |
| | | Na 5 | OD1 ASP 153 (A) | Metal | 2.65 | -3.1 |
| | | Na 5 | OD2 ASP 173 (A) | Metal | 2.68 | -1.0 |
| | | Na 6 | OD2 ASP 153 (A) | Metal | 2.83 | -1.3 |



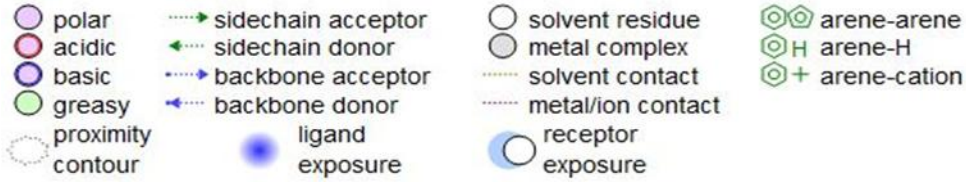

2D and 3D diagrams show the interaction between sodium silicate and active sites of Pectin Lyase 1IDJ protein




2D and 3D diagrams show the interaction between sodium silicate and active sites of pectin methyltranseliminase 3OQB protein




2D and 3D diagrams show the interaction between sodium silicate and active sites of Polygalacturonase 1K5C protein




The representative key for the types of interaction between sodium silicate and selected protein receptors

**Fig. 1.** Interaction between sodium silicate and active sites of enzymes

## CONCLUSIONS

1. Sodium silicate showed inhibitor activity on *A. flavus* growth and their cell wall degrading enzymes.
2. The inhibitor activity of sodium silicate depending on their concentration and period of fungus incubation
3. The molecular docking interaction demonstrated the activity of sodium silicate on the studied cell wall degrading enzymes

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## REFERENCES CITED

Abdelghany, T. M., Hassan, M. M., El-Naggar, M. A., and Abd El-Mongy, M. (2020). "GC/MS analysis of *Juniperus procera* extract and its activity with silver nanoparticles against *Aspergillus flavus* growth and aflatoxins production," *Biotechnology Reports* 27, article ID e00496. DOI: 10.1016/j.btre.2020.e00496

Alghonaim, M. I., Alsalamah, S. A., Alsolami, A., and Ghany, T. A. (2023). "Characterization and efficiency of *Ganoderma lucidum* biomass as an antimicrobial and anticancer agent," *BioResources* 18(4), 8037-8061. DOI: 10.15376/biores.18.4.8037-8061

Al-Rajhi, A. M. H., Mashraqi, A., Al Abboud, M. A., Shater, A.-R. M., Al Jaouni, S. K., Selim, S., and Abdelghany, T. M. (2022b). "Screening of bioactive compounds from endophytic marine-derived fungi in Saudi Arabia: Antimicrobial and anticancer potential," *Life* 12(8), article ID 1182. DOI: 10.3390/life12081182

Al-Rajhi, A. M. H., Qanash, H., Almuhayawi, M. S., Al Jaouni, S. K., Bakri, M. M., Ganash, M., Salama, H. M., Selim, S., and Abdelghany, T. M. (2022a). "Molecular interaction studies and phytochemical characterization of *Mentha pulegium* L. constituents with multiple biological utilities as antioxidant, antimicrobial, anticancer and anti-hemolytic agents," *Molecules* 27(15), article ID 4824. DOI: 10.3390/molecules27154824

Al-Rajhi, A. M., Ganash, M., Alshammari, A. N., Alsalamah, S. A., and Abdelghany, T. M. (2024). "*In vitro* and molecular docking evaluation of target proteins of lipase and protease for the degradation of aflatoxins," *BioResources* 19(2), 2701-2713. DOI: 10.15376/biores.19.2.2701-2713

Al-Rajhi, A. M., Salem, O. M., Mohammad, A. M., and Ghany, T. M. (2023). "Mycotoxins associated with maize wastes treated with comprised capsule of *Spirulina platensis* biomass," *BioResources* 18(3), 4532-4542. DOI: 10.15376/biores.18.3.4532-4542

Farahat, G. A. (2019). "Potential impacts of copper sulfate and sodium silicate salts of maize late wilt disease and synthase of anti-defense compounds," *Env. Biodiv. Soil Security* 3, 269-282. DOI: 10.21608/jenvbs.2020.21138.1079

Ge, Y., Chen, Y., Li, C., Wei, M., Lv, J., and Meng, K. (2017). "Inhibitory effects of sodium silicate on the fungal growth and secretion of cell wall-degrading enzymes by *Trichothecium roseum*," *Journal of Phytopathology* 165(9), 620-625. DOI: 10.1111/jph.12600

George, C. (2009). "Treatment of wood with polysilicic acid derived from sodium silicate for fungal decay protection," *Wood and Fiber Science* 41(3), 220-228.

González-Jiménez, V., Moscoso-Ramírez, P. A., Ortíz-García, C. F., Sánchez-Soto, S., and Lara-Viveros, F. M. (2023). "Preventive and curative antifungal activity of the

sodium silicate on postharvest crown rot in banana cv. Enano Gigante," *Silicon* 15(15), 6683-6693. DOI: 10.1007/s12633-023-02547-8

Li, L., Tang, X., Ouyang, Q., and Tao, N. (2019). "Combination of sodium dehydroacetate and sodium silicate reduces sour rot of citrus fruit," *Postharvest Biology and Technology* 151, 19-25. DOI: 10.1016/j.postharvbio.2019.01.006

Li, Y. C., Bi, Y., Ge, Y. H., Sun, X. J., and Wang, Y. (2009). "Antifungal activity of sodium silicate on *Fusarium sulphureum* and its effect on dry rot of potato tubers," *Journal of food Science* 74(5), M213-M218. DOI: 10.1111/j.1750-3841.2009.01154.x

Li, Y. C., Bi, Y., Ge, Y. H., Sun, X. J., and Wang, Y. (2009). "Antifungal activity of sodium silicate on *Fusarium sulphureum* and its effect on dry rot of potato tubers," *Journal of Food Science* 74(5), M213-M218. DOI: 10.1111/j.1750-3841.2009.01154.x

Mailafia, S., Okoh, G. R., Olabode, H. O. K., and Osanupin, R. (2017). "Isolation and identification of fungi associated with spoilt fruits vended in Gwagwalada market, Abuja, Nigeria," *Vet World* 10(4), 393-397. DOI: 10.14202/vetworld.2017.393-397

Qanash, H., Alotaibi, K., Aldarhami, A., Bazaid, A. S., Ganash, M., Saeedi, N. H., and Abdelghany, T. A. (2023). "Effectiveness of oil-based nanoemulsions with molecular docking of its antimicrobial potential," *BioResources* 18(1), 1554-1576. DOI: 10.15376/biores.18.1.1554-1576

Qanash, H., Yahya, R., Bakri, M. M., Bazaid, A. S., Qanash, S., Shater, A. F., and Abdelghany, T. M. (2022). "Anticancer, antioxidant, antiviral and antimicrobial activities of Kei Apple (*Dovyalis caffra*) fruit," *Scientific Reports* 12, article ID 5914. DOI: 10.1038/s41598-022-09993-1

Raper, K. B., and Fennell, D. I. (1973). *The Genus Aspergillus*, Lippincott Williams & Wilkins, Philadelphia, PA, USA.

Rayón-Díaz, E., Birke-Biewendt, A. B., Velázquez-Estrada, R. M., González-Estrada, R. R., Ramírez-Vázquez, M., Rosas-Saito, G. H., and Gutierrez-Martinez, P. (2021). "Sodium silicate and chitosan: An alternative for the *in vitro* control of *Colletotrichum gloeosporioides* isolated from papaya (*Carica papaya* L.)," *Revista bio Ciencias* 8, article ID e1059. DOI: 10.15741/revbio.08.e1059

Reynolds, O. L., Padula, M. P., Zeng, R., and Gurr, G. M. (2016). "Silicon: Potential to promote direct and indirect effects on plant defense against arthropod pests in agriculture," *Frontiers in Plant Science* 7, article 744. DOI: 10.3389/fpls.2016.00744

Samaila, Y., Kankara, S. L., and Yusuf, M. (2018). "Isolation and identification of fungi from some selected vegetables in Kankara Local Government Area, Katsina State," *UMYU Journal of Microbiology Research (UJMR)* 3(1), 76-80. DOI: 10.47430/ujmr.1831.012

Samson, R. A., Hoekstra, E. S., Frisvad, J. C., and Filtenborg, O. (eds.). (1995). *Introduction to Food-borne Fungi* (No. Ed. 4, pp. 322). ISBN (Hardback): 978-90-70351-27-4.Publisher: Centraalbureau voor Schimmelcultures (CBS)

Segura-Palacios, M. A., Correa-Pacheco, Z. N., Corona-Rangel, M. L., Martinez-Ramirez, O. C., Salazar-Piña, D. A., Ramos-García, M. L., and Bautista-Baños, S. (2023). "Use of natural products on the control of *Aspergillus flavus* and production of aflatoxins in vitro and on tomato fruit," *Plants* (*Basel*) 10(12), article 2553. DOI: 10.3390/plants10122553

Xue, C. Y., Zhou, R. J., Li, Y. J., Xiao, D., and Fu, J. F. (2018). "Cell-wall-degrading enzymes produced in vitro and in vivo by *Rhizoctonia solani*, the causative fungus of peanut sheath blight," *PeerJ.* 6, article 5580. DOI: 10.7717/peerj.5580

Yahya, R., Al-Rajhi, A. M. H., Alzaid, S. Z., Al Abboud, M. A., Almuhayawi, M. S., Al Jaouni, S. K., Selim, S., Ismail, K. S., and Abdelghany, T. M. (2022). "Molecular docking and efficacy of *Aloe vera* gel based on chitosan nanoparticles against *Helicobacter pylori* and its antioxidant and anti-inflammatory activities," *Polymers* 14, article ID 2994. DOI: 10.3390/polym1415299

Zakaria, L. (2024). "An overview of *Aspergillus* species associated with plant diseases," *Pathogens* 13(9), article 813. DOI: 10.3390/pathogens13090813

Zhang, J., Cheng, X., Chang, L., Zhang, L., and Zhang, S. (2021). "Combined treatments of chitosan and sodium silicate to inhibit *Alternaria alternata* pathogens of postharvest winter jujube," *Food Science and Biotechnology* 30(4), 589-597. DOI: 10.1007/s10068-021-00890-3

Zhou, X., Shen, Y., Fu, X., and Wu, F. (2018). "Application of sodium silicate enhances cucumber resistance to fusarium wilt and alters soil microbial communities," *Frontiers in Plant Science* 9, article 624. DOI:10.3389/fpls.2018.00624

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