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The study of antimicrobial activity and molecular dockingsimulation of treated cotton fabric with fire retardancy phosphorous-PMMA/modified MMT nanocomposites

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Abstract

In this study, Scanning Electron Microscope (SEM) was used to investigate the morphology of untreated and treated cotton fabric, SEM-EDX and mapping were used to prove the presence of phosphate in treated cotton fabric CF. The antimicrobial study of the untreated and treated CF with fire retardancy phosphorous-polymethylmethacrylate (PMMA)/modified montmorillonite (MMT) nanocomposites with diffferent concentrations was done on unicellular fungi (*C. albicans*), two types of bacteria (*L. monocytogenes and S. aureus*) as Gram-positive and on another two types of bacteria (*Salmonella sp. and E. coli*) as Gram-negative. by measuring the inhibition zone diameter. Antimicrobial effect of treated and untreated CF were applied through disc diffusion method. The results showed a good efficiency of treated CF samples with the most of microorganisms than untreated CF. The antimicrobial activity also showed the highest inhibition zone for treated CF with P3 (7 %) of fire retardant phosphorous-PMMA/modified MMT nanocomposites was recorded against *L. monocytogenes* and *Salmonella sp.* Also, the molecular docking simulation was investigated to treated CF which showed that the treated CF had high efficiency than pencelien g against positive bacteria and methicillin against negative bacteria**.** On the other hand, the treated CF showed high efficiency than fluconazole against *candida alibicans.*

Keywords: Antimicrobial activity, molecular docking, untreated and treated cotton fabric.

1. Introduction

In recent years, technical textiles have found rapid growth and demanddue to the imparting novel properties of added value to textiles and the awareness for healthy life style has increased multifold creating demand for health and hygiene products. The antimicrobial finishing to textiles has applied by the ancient Egyptians through means of herbal extracts and spices to preserve mummies. There is a great scope for production of textiles and apparel that provide protection against microbes [1-5].

Adding of antimicrobial properties to textiles by treating with chemicals or natural extracts for inhibition the growth of microbes such as fungi, virus and bacteria [6,7]. Research has been intensive in antibacterial material containing untreated and treated cotton fabric with fire retardancy phosphorous-PMMA/modified MMT nanocomposites with diffferent concentrations of phosphoric acid. The use of phosphorous-PMMA/modified MMT nanocomposites as a developement technique to give cotton fibers antibacterial qualities is a creative and successful way that made it possible to first report the use of antimicrobial for cellulosic fibers like cotton, an emerging class of antibiotics that is particularly effective against resistant bacteria.

The most interest application for polymer materials in the fields of textiles' products through improved by increasing their flame retardant for producing protective work clothes, firefighter uniforms, protective clothing for use in welding and related procedures, and protection against heat and flames. Another important application of polymer materials is improved the textiles products through increasing in antimicrobial efficiency. One of the most important fabrics is cotton fabrics that support the growth of microorganisms especially in moisture, nutrients and temperature. Since cotton fabrics contain carbohydrates that represent energy sources for the growth of microorganisms. This growth of microorganisms on textiles raised the risk of infection [8]. So, it's necessary applying treatment for textiles to increase the microbial resistance. Cotton is a common dressing used in wound care because it has a higher gas permeability than occlusive dressings. In hospitals and nursing homes, cotton gauze is still a successful long-term wound care option for extremely exudative wounds that require regular dressing changes [9].

By predicting how two molecules would interact, a computational technique called molecular docking may create a binding model. A protein and a ligand is an example of the kind of docking that is done in many drug development applications. More recently, docking is also applied to predict the binding model between two

macromolecules, for instance protein-protein docking [10].

The aim of this work is to study the antimicrobial activity and molecular docking simulation of untreated and treated cotton fabric with fire retardancy phosphorous-PMMA/modified MMT nanocomposites of different concentrations P1-P5 (3%-11%).

2. Experimental and characterization techniques

2. 1. Materials

In this work distilled water was used. Montmorillonite (MMT) was obtained from the international company for mining and investment, Egypt. Methyl methacrylate (MMA) was purchased from (Merck, India) and Phosphoric acid was obtained with percent (85 %) from (Merck, India).

2. 2. Cotton Fiber (CF)

Unbleached 100 % cotton fabric (area density 550 g/m^2) was supplied from Misr for Control and Instrumentation (MCI) Egypt Company.

2.3. Methods

2. 3. 1. Preparation of cotton fabric (CF)

Cotton fabric was cut into pieces with dimension 5 cm ×15 cm before use. The fabrics were rinsed with distilled water, In2% non-ionic detergent, the fabrics were scoured at pH 7, dried at 90 ºC for 20 min in an oven and then kept in drier for storage [11,12].

2.3.2. Fabrication process of phosphorous-PMMA/modified MMT nanocomposite flame-retardant (FR) binding of CF

Pad-dry-cure methodis the standard method using for the treating of fibers. In brief, CF was first immersedfor 3-4 min in a petri dish containing a phosphorous-PMMA/modified MMT nanocomposite solution with (different concentrations of phosphoric acid of 3% (P1), 5% (P2), 7% (P3), 9% (P4) and 11% (P5)). After the fabric was completely saturated time with the solution, it was dried for another 3 minat 90 ºCin an ovenand then curing for 2.5 min at 160-180 ºC[13].

The weight gain (WG) of amount FR loaded on CFscan be determined as the total amount of dry FR material added.In order to accurate determination, untreated and treated CF samples were dried until weight becomes constant. The value of WG % was calculated as follows:

$$WG\ (\%) = \frac{W_2 - W_1}{W_1} \times 100\ \%$$

Where W1 and W2, respectively, are the weights of the untreated and treated CF samples.

2. 4. Characterization Techniques

2. 4. 1. The morphology

Using JEM-1230 electron microscopy (SEM, FEI Inspect S, Oxford USA) of acceleration beam of (25–30) k.v under vacuum pressure 60 Pa, the morphology of both treated and untreated fabrics was examined. This micrscope provide a spot size of (5–6). Also, SEM-EDX and mapping was investigated for untreated and treated CF samples at chemical lab, Egypt army, Nasr city, Egypt.

2. 4. 2. Antimicrobial studies

The antimicrobial efficiency of the untreated and treated CF was investigated on unicellular fungi (*Candida albicans* ATCC 10231), two types of bacteria (*Listeria monocytogenes* ATCC 7646 and *Staphylococcus aureus* ATCC 6538) as Gram-positive and on another two types of bacteria (*Salmonella sp.* ATCC 14028 and *Escherichia coli* ATCC 25922) as Gram-negative. The tests were applied through disc diffusion method, which a samples of untreated and treated CF were poured into wells in agar plates that containing fungi and bacteria in form of squares. Then, for 24 h at 37 °C and for 48 h at 30 °C, respectively, the bacterial and fungal plates were incubated. The inhibition zone diameter was determined in mm.

2. 4. 3. Molecular Docking study

Using a notebook with a specification AMD Ryzen 3 3250U 2.6 GHz dual-core hp, Windows 10 Home 64-bit RAM 8GB DDR4 2400 MHz. The software used Molecular Operating Environment (MOE 2015.10; Chemical Computing Group, Montreal, Canada) as the computational software. The materials used in this study were the PI3K protein database, the chemical structure of treated CF. Some data sources included: Protein Data Bank (GDP) (http://www.rscb.org/pdb/), NCBI database, and Pubchem (http://pubchem.ncbi.nlm.nih.gov/).

3. Result and Discussion

3.1. Morphology of untreated and treated CF with phosphorous-PMMA/modified MMT nanocomposite

The morphology of untreated CF and treated ones with different concentrations of phosphorous-PMMA/modified MMT nanocomposites P1-P5 (3%-11%) was studied by SEM technique as shown in **Fig. 1**. The untreated CF was flat in comparison with treated ones which are fuller. The surface of treated fabrics byphosphorous-PMMA/modified MMT nanocomposites becomes more smooth that permeated phosphorous-PMMA/modified MMT nanocomposites into the fabrics. Where a clear bubble was generated on the treated fiber surface, that indicating the formation

of layer from phosphorous-PMMA/modified MMT nanocomposites on the treated fabrics. The SEM-EDX and mapping spectrum with SEM images of untreated cotton fabric and treated ones with different concentrations of phosphorous-PMMA/modified MMT nanocomposites was also studied **Fig.(2-7)**, to prove the presence of phosphate in treated fabric. PMMA/modified MMT nanocomposites were shown to have permeated the cotton fabric based on the images, which also showed the homogeneous distribution of phosphate element with other elements of the untreated fabric [14].

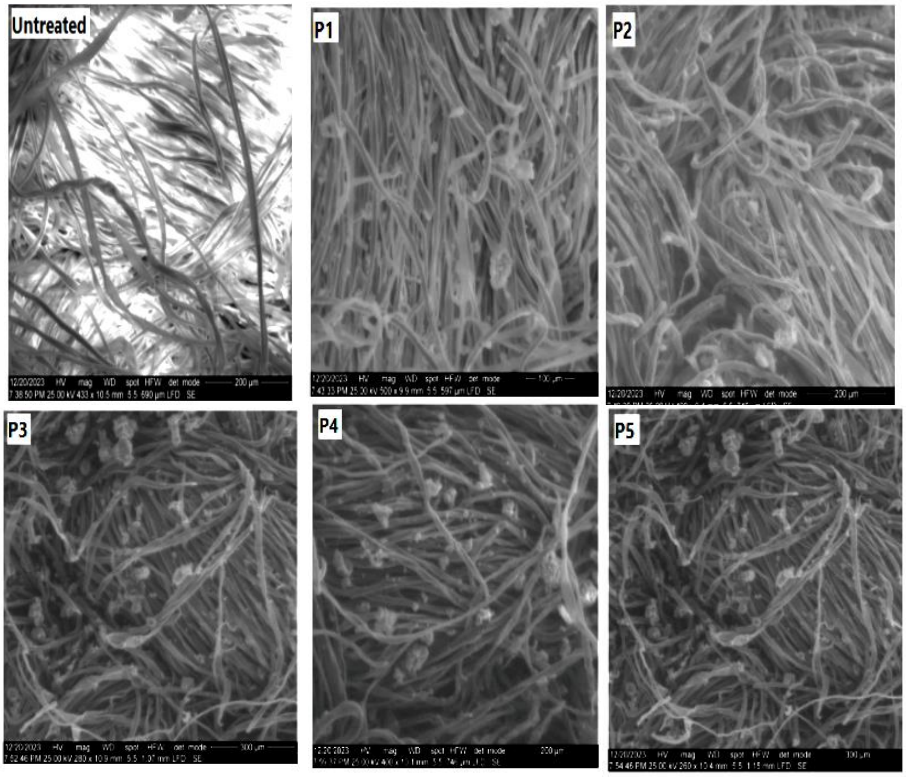


Fig.1. SEM images of untreated and treated cotton fabric

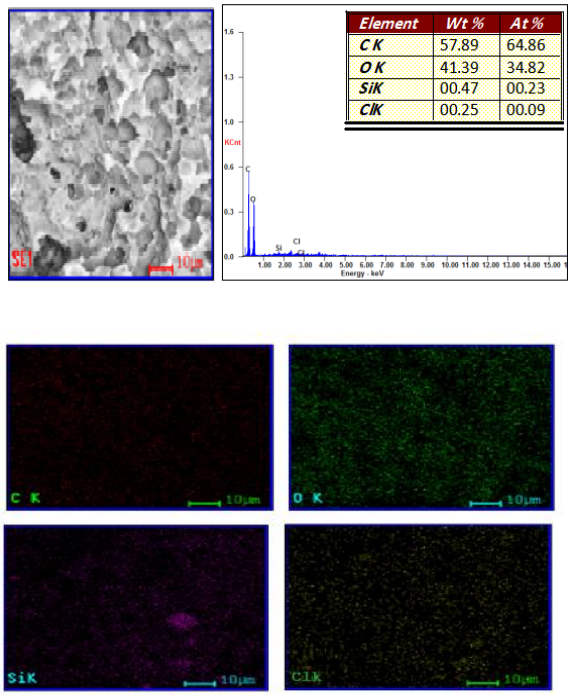


Fig.2. SEM-EDX and mapping spectra of untreated CF.

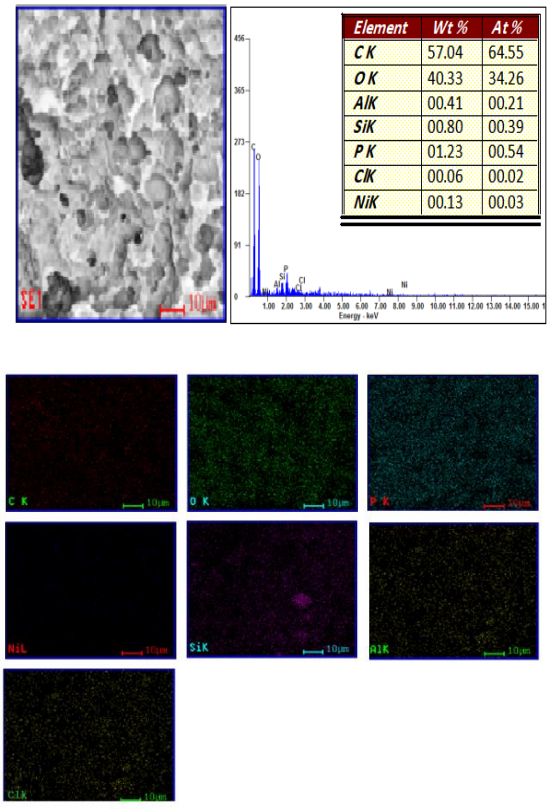


Fig.3. SEM-EDX and mapping spectra of treated CF with phosphorous-PMMA/modified MMT nanocomposite P1 (3%).

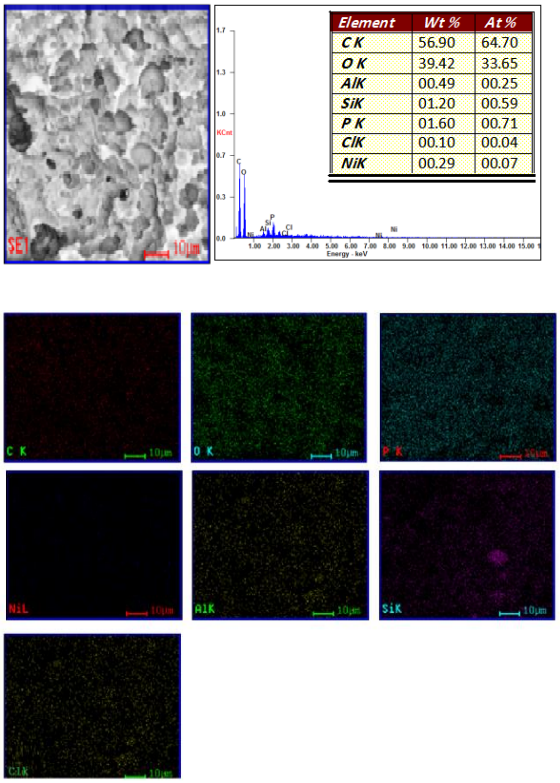


Fig.4. SEM-EDX and mapping spectra of treated CF with phosphorous-PMMA/modified MMT nanocomposite P2 (5%).

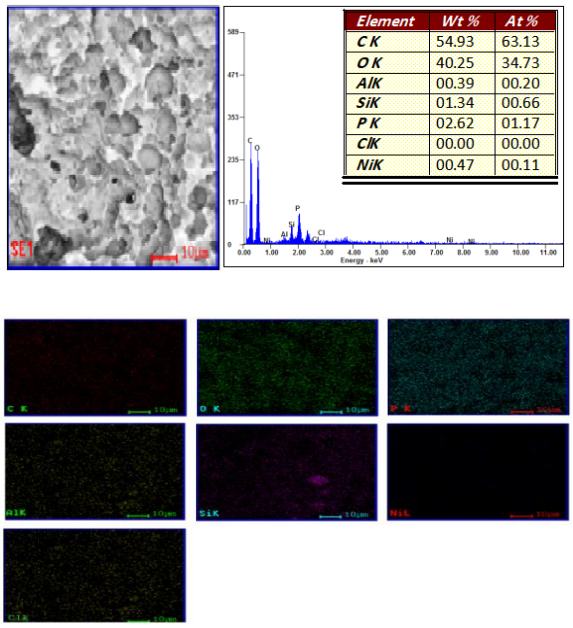


Fig.5. SEM-EDX and mapping spectra of treated CF with phosphorous-PMMA/modified MMT nanocomposite P3 (7%).

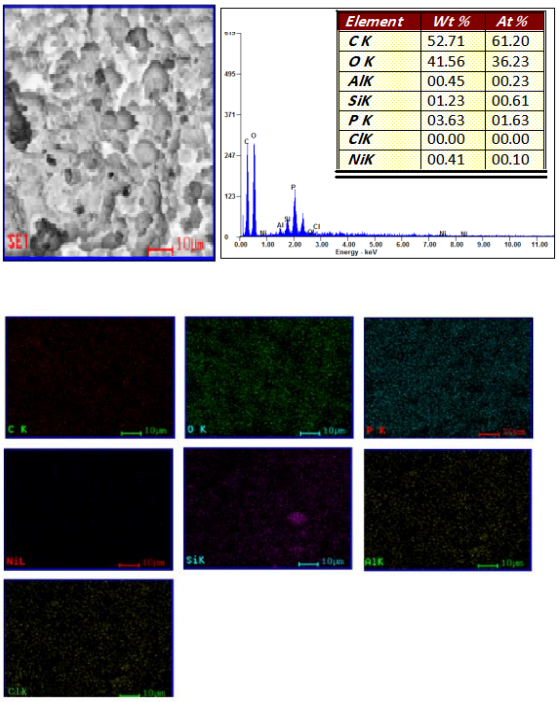


Fig.6. SEM-EDX and mapping spectra of treated CF with phosphorous-PMMA/modified MMT nanocomposite P4 (9%).

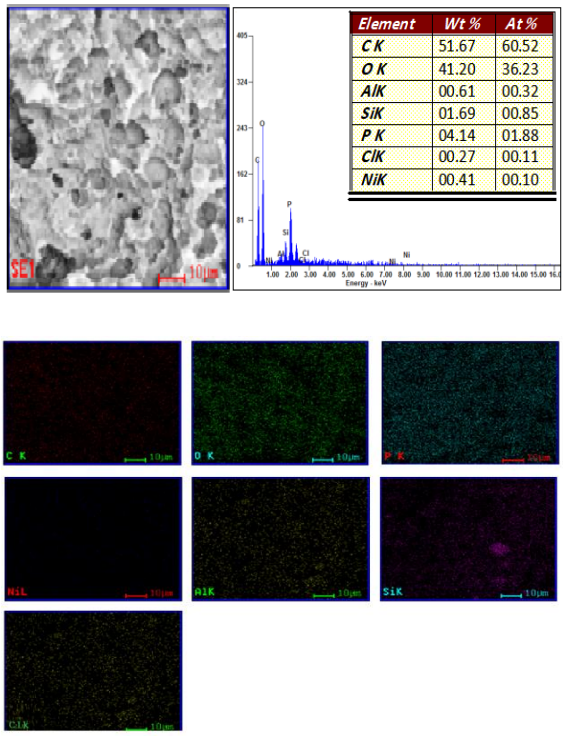


Fig.7. SEM-EDX and mapping spectra of treated CF with phosphorous-PMMA/modified MMT nanocomposite P5 (11%).

3. 2. Antimicrobial studies

The antimicrobial efficiency of the untreated, treated CF was investigated against some of microorganisms. In order to determine the antimicrobial activity, the resulting inhibition zone diameters were measured in mm. The antimicrobial efficiencies are represented numerically in terms of inhibition zone diameters in **Table (1)** and shown graphically in **Fig's (8 and 9)**. The results showed better efficiency for the treated CF samples with phosphorous-PMMA/modified MMT nanocomposites of different concentrations P1-P5 (3%-11%) against all the microorganisms than the untreated sample. Also, the results obtained showed that among the treated CF samples, the sample P3 (7%) showed the highest bacterial and fungal activities followed by the sample P4 (9%). In general, the inhibition efficiency fall, more or less, in the order P3 > p4 > p2 > p1 ≥ p5 as shown in Fig.8. Last but not least, the use of phosphorous-PMMA/modified MMT nanocomposites. as a developement technique to give cotton fibers antibacterial qualities is a creative and successful way that made it possible to first report the use of antimicrobial for cellulosic fibers like cotton, an emerging class of antibiotics that is particularly effective against resistant bacteria.

Table (1): Antimicrobial activities of untreated CF, treated CF with phosphorous-PMMA/modified MMT nanocomposites of different concentrations as measured by inhibition zone diameter (mm).

Organism		Untreated CF	P1	P2	P3	P4	P5
Gram (-)	*E.coli*	0	15	15	23	18	15
	Salmonella sp.	0	15	16	24	18	14
Gram (+)	*L. monocytogenes*	0	12	13	24	16	14
	S. aureus	0	17	18	22	17	16
Fungi	*C. albicans*	0	13	13	22	15	14

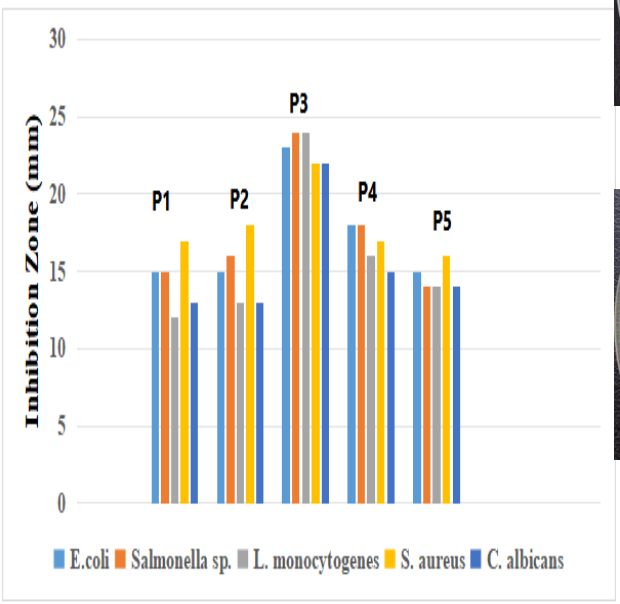
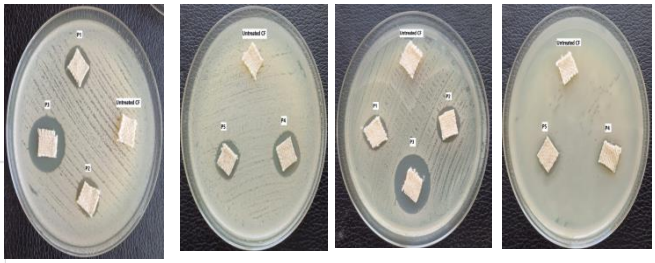
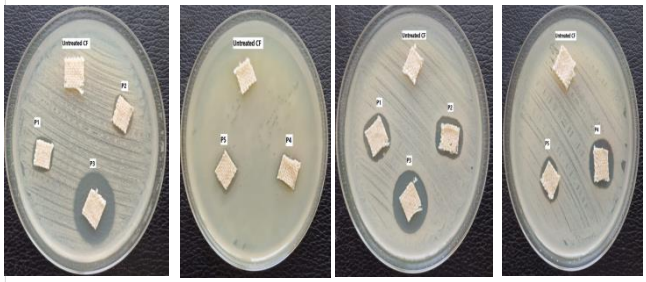


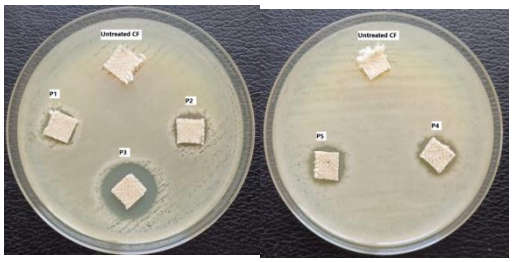
Fig. 8. Inhibition zone for untreated and treated CF with phosphorous-PMMA/modified MMT nanocomposites of different concentrations



E. coli *Salmonella sp.*



L. monocytogenes *S. aureus*



C. albicans

Fig. 9. Inhibition zone images of the untreated and representative treated CF, against some of the microorganisms

3.3. Molecular docking simulation

When molecules are coupled to one another to create a stable complex, computational techniques such as molecular docking predict the preferred orientation of one molecule to a second[10]. The preferred orientation Knowledge may be used to predict the strength of association or binding affinity between two molecules using, for example, scoring functions. In this work, docking studies have been applied to explore the ability of the treated CF with phosphorous-PMMA/modified MMT nanocomposites to pencelien g [15-17], methicillin [18] and fluconazole [19] and to bind with A-DNA of negative bacteria as *E. coli*(PDB code: 1HNJ) [20] and *salmonella* (PDB code: 9iwq) [21] and the positive bacteria like *Staphylococcus* (PDB code: 2dhn) [22], *Listeria Monocytogeness* (PDB code: 5hu4) [23] and the *candida albicans* (PDB code: 4yde) [24].

3.3.1. Docking on the active site of treated CF and pencelien G with positive bacteria like *Staphylococcus* (PDB code: 2dhn),*ListeriaMonocytogeness* (PDB code: 5hu4)

Using the antimicrobial experiments of MOE programto examine the binding mode between the pencelieen G as a treatment care of positive bacteria as *Staphylococcus*(PDB code: 2dhn) which formedone intermolecular bond formed between S1 N and ALA 83 through intermolecular distance 3.32 Å with bending energy score -6.0690 as shown in **Fig. (10,11)** and **Table (2).**

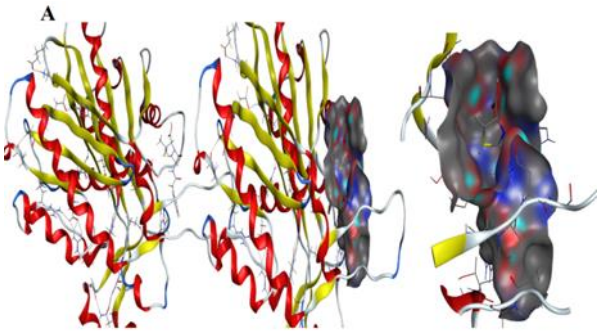


Fig. 10.3D interactions of the Pencelien g with the active sites of amino acid residues of protein *Staphylococcus* (PDB code: 2dhn).

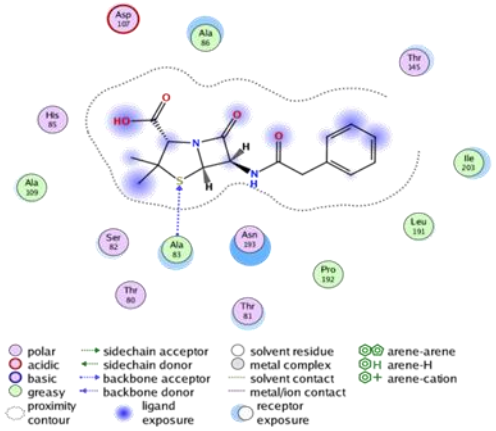


Fig. 11.2D interactions of the Pencelien g with the active sites of amino acid residues of protein Staphylococcus (PDB code: 2dhn).

The treated CF formed three intermolecular bonds with *Staphylococcus aureus*. The first intermolecular bond formed between O 3 NH2 and ARG 97 through intermolecular distance 3.04 Åand second intermolecular bond formed between O 15 NH2 and ARG 97 through intermolecular distance 2.85 Å. The third intermolecular bond formed between O 50 OG1 and THR 99 through intermolecular

distance 2.90Å with bending energy score -6.5327 as shown in **Fig. (12,13)** and **Table (2).**

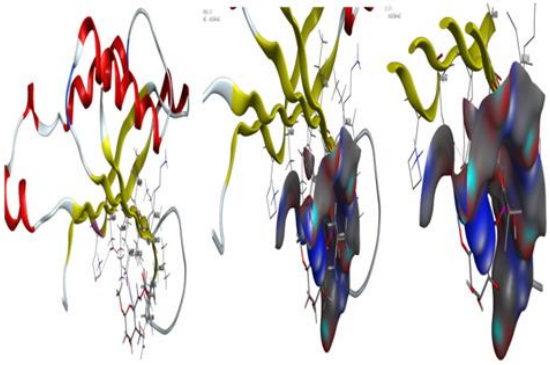


Fig.12.3D interactions of treated CF with the active sites of amino acid residues of protein *Staphylococcus* (PDB code: 2dhn).

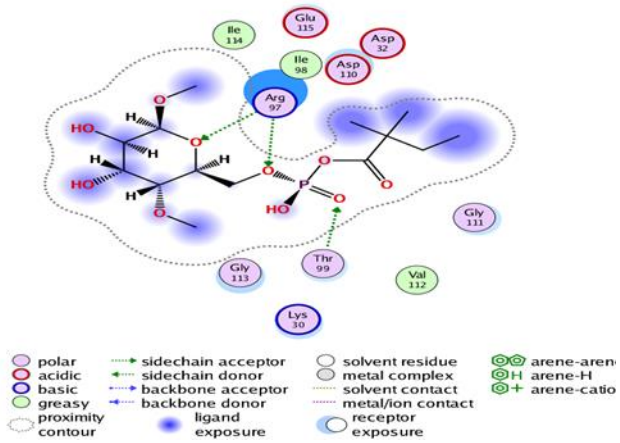


Fig.13.2D interactions of treated CF with the active sites of amino acid residues of protein *Staphylococcus* (PDB code: 2dhn).

While the binding mode between the Listeria Monocytogeness(PDB code: 5hu4)and treated CF which formed two intermolecular bonds. The first intermolecular bond formed between O 18 O and GLU 98 through intermolecular distance 3.09 Åand second intermolecular bond formed between O3 NE and ARG 126 through intermolecular distance 2.92 Å with bending energy score -6.9227 as shown in Fig. (14,15) and Table (2).

The molecular docking showed a comparison of the scores of treated CF and Pencelien g with positive bacteria to explain whether a compound was potent or not. The molecule with the lowest docking score (minus score) showed a good stability affinity [25] so, the treated CFshowed high efficiency than pencelien g against positive bacteria.

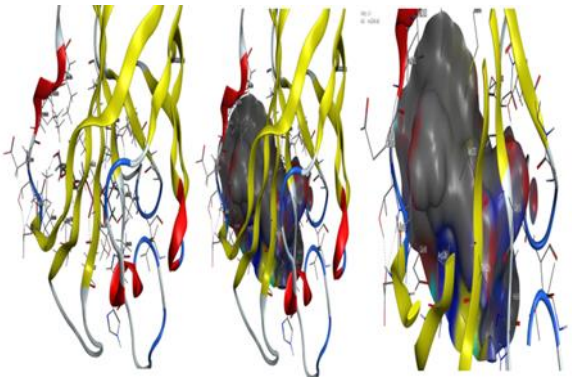


Fig. 14.3D interactions of treated CF with the active sites of amino acid residues of protein *Listeria Monocytogeness* (PDB code: 5hu4).

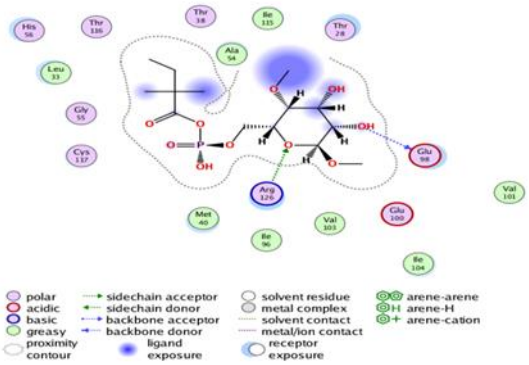


Fig. 15.2D interactions of treated CF with the active sites of amino acid residues of protein *Listeria Monocytogeness* (PDB code: 5hu4).

Table (2): The molecular docking data fortreated CF and Pencelien g against positive bacteria (Staphylococcus aureus and Listeria Monocytogeness) using MOE 2015.08 software.

No.	Compound	Binding site	Receptor	Interaction	Distance Å	E (kcal/mol)	The binding energy score (S)
1	Pencelien g	S 1 N	ALA 832	H-acceptor	3.32	-2.1	-6.0690
2	*Staphylococcus aureus*	O 3 NH2	ARG 97	H-acceptor	3.04	-2.5	-6.5327
		O 15 NH2	ARG 97	H-acceptor	2.85	-1.1	
		O 50 OG1	THR 99	H-acceptor	2.90	-2.3	
3	*Listeria Monocytogeness*	O 18 O	GLU 98	H-donor	3.09	-1.3	-6.9227
		O 3 NE	ARG 126	H-acceptor	2.92	-2.3	

3.3.2. Docking on the active site of treated CF and methicillin compound with negative bacteria as *Escherichia coli* (PDB code: 1HNJ) and *salmonella* (PDB code: 9iwq)

Using the antimicrobial experiments of MOE program to examine the binding mode between the methicillin as a treatment care of *Escherichia coli*(PDB code: 1HNJ) which formed three bonds two of them hydrogen bond and the third one intermolecular bond. The first one formed between S 1 ND2 and ASN 193 through intermolecular distance 3.38 Å and the second hydrogen bond formed between O 5 CA and SER 82 through intermolecular distance 3.50 Å. The second intermolecular bond formed between 6-ring CG2 and THR 145 through intermolecular distance 4.08 Å with bending energy score -6.0744 as shown in**Fig. (16,17)** and **Table (3).**

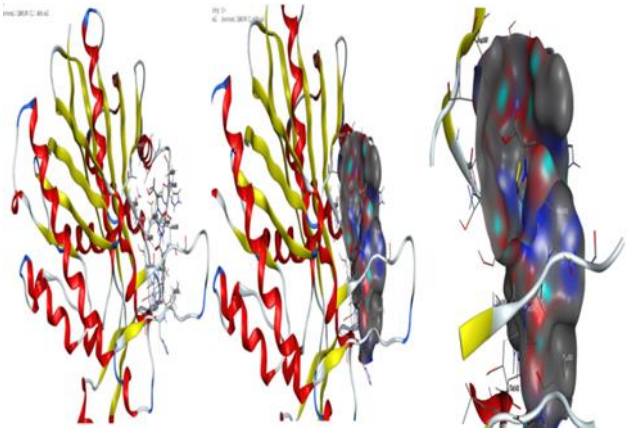


Fig. 16.3D interactions of the methicillin with the active sites of amino acid residues of protein *Escherichia coli* (PDB code: 1HNJ).

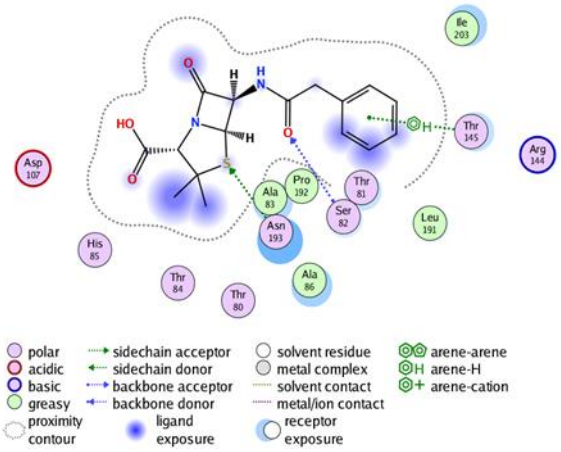


Fig.17.2D interactions of the methicillin with the active sites of amino acid residues of protein *Escherichia coli* (PDB code: 1HNJ).

The treated CF formed two hydrogen bonds with *Escherichia coli*(PDB code: 1HNJ).The first hydrogen bond formed between O 51 O and ALA 83 through intermolecular distance 2.97Åand second hydrogen bond formed between O 16 ND2 and ASN 193 through intermolecular distance 2.97 Å while, the third intermolecular bond formed between O 16 ND2 and ASN 193 through intermolecular distance 3.08 Å with bending energy score -7.3972 as shown in **Fig. (18,19)** and **Table (3).**

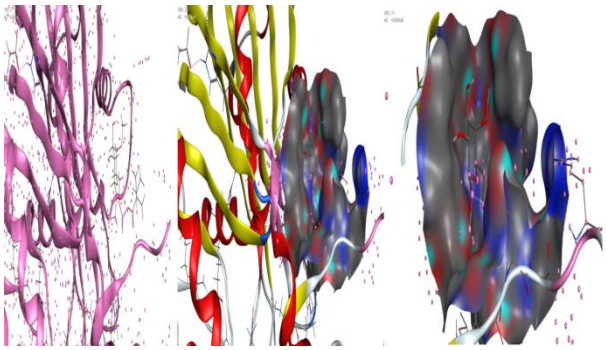


Fig. 18.3D interactions of treated CF with the active sites of amino acid residues of protein *Escherichia coli* (PDB code: 1HNJ).

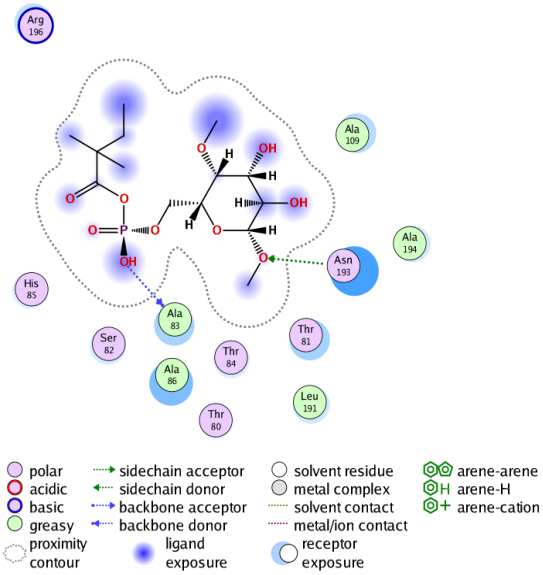


Fig. 19.2D interactions of treated CF with the active sites of amino acid residues of protein *Escherichia coli* (PDB code:1HNJ)

The treated CF formed three intermolecular bonds with *salmonella* (PDB code: 9iwq). The first intermolecular bond formed between O 16 NZ and LYS 177 through intermolecular distance 3.14 Åand second intermolecular bond formed between O 20 N and GLY 365 through intermolecular distance 3.14 Å. The third intermolecular bond formed between O 50 N and TYR 331 through intermolecular distance 3.08 Å with bending energy score -7.9227 as shown in **Fig. (20,21)** and **Table (3).**

The molecular docking showed a comparison of the scores of treated CF and methicillinwith negative bacteria to explain whether a compound was potent or not. The molecule with the lowest docking score (minus score) showed a good stability affinity [25] so, the treated CF showed high

efficiency than methicillin against negative bacteria**.**

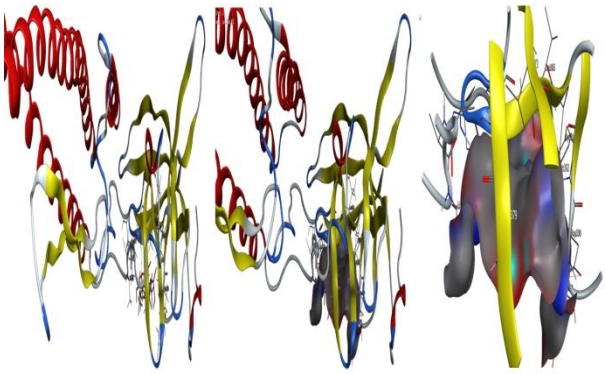


Fig. 20.3D interactions of treated CF with the active sites of amino acid residues of protein *salmonella* (PDB code: 9iwq).

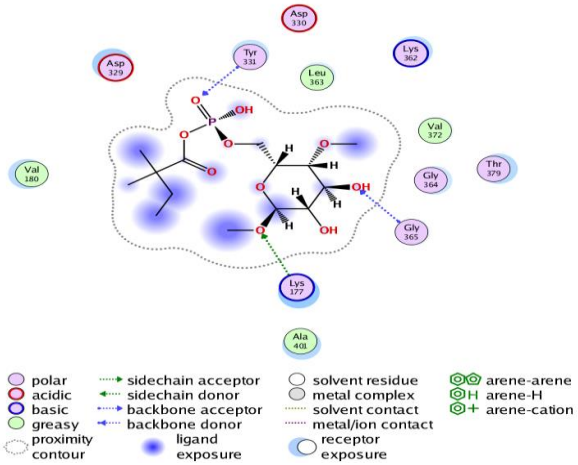


Fig. 21. 2D interactions oftreated CF with the active sites of amino acid residues of protein *salmonella* (PDB code: 9iwq).

Table (3)The molecular docking data for treated CF and methicillin compound against negative bacteria (Escherichia coli, aureus and Salmonella) using MOE 2015.08 software.

No.	Compound	Binding site	Receptor	Interaction	Distance Å	E (kcal/mol)	The binding energy score (S)
1	methicillin	S 1 ND2	ASN 193	H-acceptor	3.38	-2.7	-6.0744
		O 5 CA	SER 82	H-acceptor	3.50	-0.7	
		6-ring CG2	THR 145	pi-H	4.08	-0.6	
2	*Escherichia coli*	O 51 O	ALA 83	H-donor	2.97	-3.1	-7.3972
		O 16 ND2	ASN 193	H-acceptor	3.08	-1.6	
3	*Salmonella*	O 16 NZ	LYS 177	H-acceptor	3.14	-3.4	-7.0101
		O 20 N	GLY 365	H-acceptor	3.14	-1.6	
		O 50 N	TYR 331	H-acceptor	3.08	-3.0	

3.3.3. Docking on the active site of treated CF and fluconazole compound with *candida alibicans* (PDB code: 4yde)

Using antimicrobial experiments of MOE program to examine the binding mode between the fluconazole as a treatment care of *Candida albicans* (PDB code: 4YDE) which formed three hydrogen bond. The first one formed between C 11 O and CYS 294 through intermolecular distance 3.49 Å and the second hydrogen bond formed between N 8 NZ and LYS 193 through intermolecular distance 3.41 also, the third hydrogen bond formed between 5-ring OG and SER 351 through intermolecular distance 3.99 Å with bending energy score -4.7614 as shown in **Fig. (22,23)** and **Table (4).**

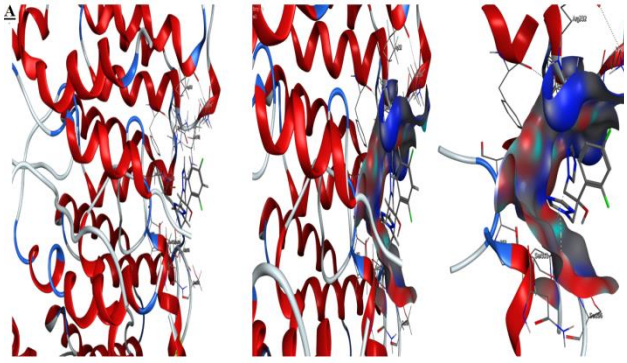


Fig. 22.3D interactions of the fluconazole with the active sites of amino acid residues of protein *Candida albicans* (PDB code: 4YDE).

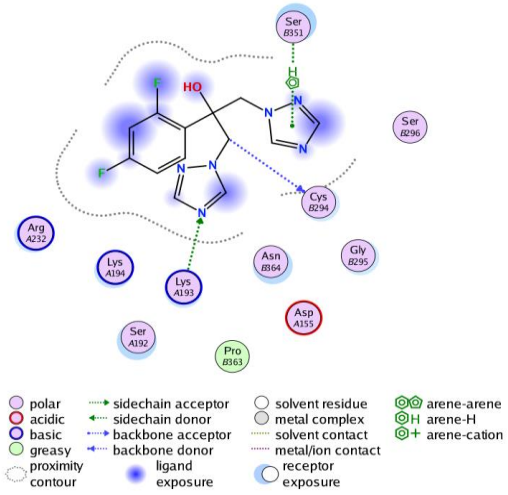


Fig. 23.2D interactions of the fluconazolewith the active sites of amino acid residues of protein *Candida albicans* (PDB code: 4YDE).

The treated CF formed three intermolecular bonds with *candida alibicans*. The first intermolecular bond formed between O 51 OD1 and ASN 364 through intermolecular distance 2.89 Å and second intermolecular bond formed between O 20 NZ and LYS 193 through intermolecular distance 2.97 Å. The third intermolecular bond formed between O43 OG and SER 351 through intermolecular distance 3.22 Å with bending energy score -7.3972as shown in **Fig. (24,25)** and **Table (4).**

The molecular docking showed a comparison of the scores of treated CF and fluconazole to wards *candida alibicans* to explain whether a compound was potent or not. The molecule with the lowest docking score (minus score) showed a good stability affinity [25] so, treated CF showed high efficiency than fluconazoleagainst *candida alibicans*.

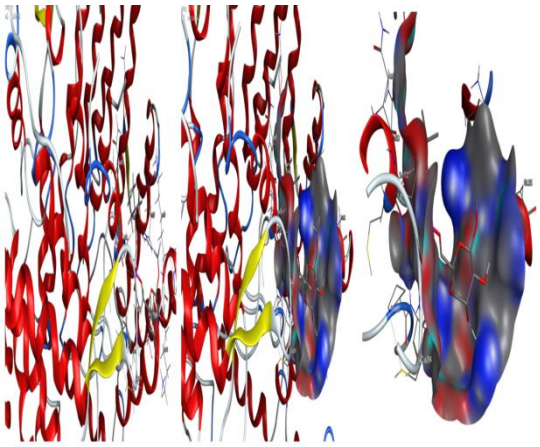


Fig. 24.3D interactions of treated CF with the active sites of amino acid residues of protein *candida alibicans* (PDB code: 4yde).

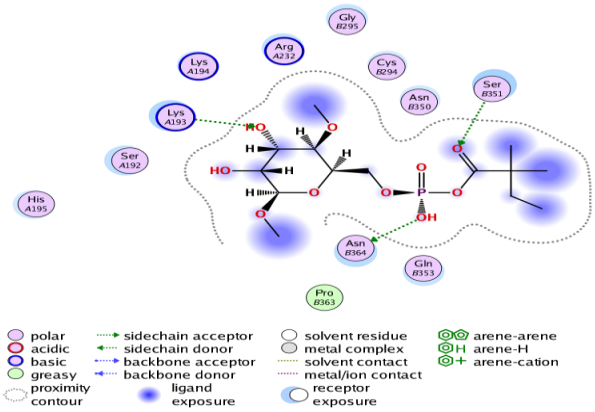


Fig. 25.2D interactions of treated CF with the active sites of amino acid residues of protein *candida alibicans* (PDB code: 4yde).

Table (4) The molecular docking data for treated CF and fluconazole compound against *candida alibicans* using MOE 2015.08 software.

No.	Compound	Binding site	Receptor	Interaction	Distance Å	E (kcal/mol)	The binding energy score (S)
1	fluconazole	C 11 O	CYS 294	H-donor	3.49	-0.7	-4.7614
		N 8 NZ	LYS 193	H-acceptor	3.41	-4.7	
		5-ring OG	SER 351	pi-H	3.99	-1.0	
2	*candida alibicans*	O 51 OD1	ASN 364	H-donor	2.89	-1.0	-7.3972
		O 20 NZ	LYS 193	H-acceptor	2.97	-6.2	
		O 43 OG	SER 351	H-acceptor	3.22	-0.7	

4. Conclusion

The fabricated process of phosphorous-PMMA/modified MMT nanocomposite flame-retardant binding to the cotton fabric (CF) was investigated the morphology, antimicrobial activity and molecular docking simulation of untreated and treated CF. The morphology showed that the surface of untreated CF was flat in comparison with treated ones which are fuller. The SEM-EDX and mapping spectra proved the presence of phosphate in treated CF. The antimicrobial activity and molecular docking were investigated against unicellular fungi (*C. albicans*), two types of bacteria (*L. monocytogenes and S. aureus*) as Gram-positive and on another two types of bacteria (*Salmonella sp. and E. coli*) as Gram-negative. The antimicrobial activity showed a good efficiency of treated CF samples with the most of microorganisms than untreated one and the treated CF samples showed the highest inhibition zone for treated CF with P3 (7 %) of fire retardant phosphorous-PMMA/modified MMT nanocomposites was recorded against *L. monocytogenes* and *Salmonella sp.* Also, The results of molecular docking showed that the treated CF had high efficiency than pencelien g against positive bacteria and methicillin against negative bacteria**.**Also, treated CF showed high efficiency than fluconazole against *candida alibicans*.

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