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Acceptance Letter

Dear Sir/Madam,

I am pleased to inform you that your article entitled **"Modified Polyvinyl Alcohol Containing New Imides / Iron Oxide Nanoparticles :Synthesis , Characterization and Biological Evaluation"** authored by **Kawther Ayad Obead and Ruwaidah S. Saeed** has been accepted for publication in the **Iraqi Journal of Pharmaceutical Sciences**.

Thanks

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Modified Polyvinyl Alcohol Containing New Imides / Iron Oxide Nanoparticles :Synthesis , Characterization and Biological Evaluation

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Abstract

A series of new imides compounds[1-4] were synthesized from a reaction of tetrachlorophthalic anhydride , nitro phthalic anhydride , malic anhydride , Succinic anhydride with 4-amino benzene thiol under fusion conditions. Chloroacetic acid has been added after compounds [1-4] reacted to aqueous solution contain Na_2CO_3, producing compounds [5-8]. In benzene, compounds [5-8] also were reacted with the thionyl chloride to produce [9-12]. Poly (vinyl alcohol) was chemically modified by reacting PVA with compounds [9-12] and dimethyl formamide to produce compounds [13-16]. Iron oxide nanoparticles (IONPs) are mixed with modified PVA [13-16] to create nanocomposites [17-20]. Spectral and analytical data from synthesized compounds, such as ^{1}H-NMR, FTIR spectra and FESEM, were used to describe their structural characteristics. Molecular docking was studied, where used to predict the binding status of compound [9] with the enzyme(4ZGY) and to calculate the free energy (ΔG) of the synthesized compounds. Also, two different types of bacteria: *(G+) Bacillus cereus* and *E. coli (G-)* have been used to test the antibacterial activity. Additionally, the cytotoxicity activity of modified polyvinyl alcohol, modified polyvinyl alcohol with new imides and iron oxide NPs against the colon cancer cell line (HT29) was studied. MTT assay was utilized for estimating the cytotoxicity activity as well as comparing it to that of normal cells WRL-68 (the human hepatic cell line). The results showed nanocomposite [17] exhibited excellent inhibition rate higher of modified polyvinyl alcohol [13] against two types of bacteria and Colon Cancer Cell line (HT29).

Keywords: Biological Evaluation, Colon cancer cell line (HT29) , Iron Oxide Nanoparticles, Imide compounds, Modified PV

Introduction

Imides are compounds with a structural grouping of CO-NH-CO with a nitrogen atom attached to two carbonyl groups. In the realm of research and development, imides and their derivatives have drawn a lot of attention from chemists and pharmacists. These compounds are crucial to medicinal chemistry and the creation of new drugs. Researchers employed these substances as nerve conduction inhibiting, hypotensive, antibacterial, analgesic, muscle relaxant, anticancer, antitubercular, and antinociceptiv[(1)] .Polyvinyl alcohol is a water-soluble, non-toxic, biocompatible and biodegradable polymer, PVA has a wide range of uses in a variety of sectors, including materials for medication delivery systems and fibers for protective equipment films and membranes [(2-4)]. Yet, it needs to be physically and/or chemically crosslinked for being utilized in a crucial area [(5-7)]. The only vinyl polymer that bacteria could consume as carbon and energy source is the PVA. Also, the PVA could be degraded by 75% in a 46-day period when subjected to the bacterial and enzyme action[(8)], making it a bio-degradable polymer material type [(9)]. PVA polymer contain many hydroxyl groups as side chain and a carbon chain as main chain [(10-12)]. A significant method for creating novel materials with better qualities by the modification of traditional organic polymers [(13-15)]. PVA is helpful in the practical exploration of functional polymers since its hydroxyl group allows for simple modification[(16-20)]. Hydroxyl groups' esterification, acetalization, or etherification are the most frequent PVA modification reactions[(21,22)]. Due to its magnetic properties, biodegradability, biocompatibility, and non-toxic qualities, Iron Oxide Nanoparticles (IONPs) were majorly used as drug carriers [(23,24)]. For several therapeutic applications, such as cancer medication targeting and MRI, surface modification of IONPs brought further benefits [(25)]. They became particularly interested in cancer diagnosis and treatment due to iron oxide's selectivity in delivering medication to targeted sickness site with little side effects and its capacity to accumulate in a particular tissue in the case when exposed to an external magnetic field [(26)]. Additionally, the development of bacterial resistance to several antibiotics prompted

researchers to explore for a means of overcoming the resistance [27]. Gram-negative and Gram-positive bacteria were resistant to the broad-spectrum antibacterial activity of nano carriers, which were shown by the small size of IONPs and their capacity to alter bacterial metabolism [28-30].

Materials and Methods

Chemicals have been supplied from BDH and SCR. ^{1}H-NMR spectra have been performed by company: Ultra Shield 500MHz, Bruker , were done University of Tehran, Iran, solvent has been used DMSO, d6.Shimadzu FT-IR-8400 s, with FT-IR spectra between 400cm^{-1} and 4000cm^{-1}, were done University of Tabriz, Iran, performed FESEM.

Synthesis method Synthesis of compounds [1-4][31]

General procedure for Preparation of compounds [1-4]. A mixture of equimolar amounts (0.001 mol.) of commercially available tetrachlorophthalic anhydride , nitro phthalic anhydride , malic anhydride , Succinic anhydride were refluxed with 4-amino benzene thiol (0.001mol) in glacial acetic acid (15 ml) for five hrs. Aliquot of 25 ml. of ice distilled water was added to the reaction. The resulted precipitate was filtered and recrystallized from ethanol .

Analytical data for compounds [1-4] 4,5,6,7-tetrachloro-2-(4-mercaptophenyl) isoindoline-1,3-dione [1]

Color: Light yellow , percent of yields 79%, m.p:(260-262) °C .FT-IR (υ, cm^{-1}): 3039 (C-H aromatic), 2541 (SH),(1728,1780) C=O amide, 1599 (C=C aromatic) , 662 (C-S). ^{1}H NMR (δ ppm) of compound[1], 7.65-7.95 (4H, m, Ar-H), 3.34 δ (1H,s, SH).

2-(4-mercapto phenyl)-5-nitro isoindoline-1,3-dione[2]

Color: Orange, percent of yields 86 %, m.p: (220-222)°C .FT-IR (υ, cm^{-1}): 3034 (C-H aromatic), 2540 (SH) , (1734,1786) C=O amide., 1589 (C=C aromatic) , 640 (C-S).

1-(4-mercaptophenyl)-1H-pyrrole-2,5-dione[3]

Color : Yellow, percent of yields 76 %, m.p: (213-214)°C . FT-IR (υ, cm^{-1}): 3005(C-H aromatic) ,2550 (SH) , (1716,1734)C=O amide , 1585 (C=C aromatic) , 665 (C-S) .

1-(4-mercaptophenyl)pyrrolidine-2,5-dione [4]

Color : Yellow, percent of yields 87%, m.p : (248-250) °C .FT-IR (υ, cm^{-1}): 3086 (C-H aromatic) , 2543 (SH) , (1739,1786)C=O amide , 1595 (C=C aromatic) , 671 (C-S).

Synthesis of compounds [5-8][32]

Aliquots of one of the compounds [1-4] (0.01 mol) were combined with (0.02 mol) Na_2CO_3 in 15 mL of distilled water , and after that $ClCH_2COOH$ (0.01 mol) has been added. Conc.HCl was used to adjust the pH of the reaction mixture to 2 .Then the reaction mixture was reflux for six hrs. The result was filtered, then recrystallized from EtOH after being rinsed with water.

Analytical data for compounds [5-8]2-((4-(4,5,6,7-tetra chloro-1,3-dioxo Isoindolin-2-yl) phenyl) thio) acetic acid[5]

Color : Yellow, percent of yields 89%, m.p: (187-189) °C .FT-IR (υ, cm^{-1}) : 3400-2400 O-H, 3034 (C-H) arom. 2924,2883 (C-H) aliph. , 1699 (C=O) carboxlic , 1596C=C ,677C-S . ^{1}H NMR (δ ppm) : δ7.60- δ8.37(4H, m, Ar-H), 2.09(2H,s,CH_2) , 13.17(1H,s,COOH) .

2-((4-(5-nitro-1,3-dioxoisoindolin-2-yl) phenyl) thio) acetic acid [6]

Color : Off white , percent of yields 76%, m.p: (166-167) °C .FT-IR (υ, cm^{-1}) : (3400-2400) O-H, 3003 (C-H) aromatic, 2962,2802 (C-H) aliph. , 1678 (C=O) carboxlic , 1583(C=C) ,675(C-S) .

2-((4-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl) phenyl) thio) acetic acid [7]

Color : Yellow, percent of yields 81%, m.p: (194-195) °C .FT-IR (υ, cm^{-1}) : (3400-2400) O-H, 3053 (C-H) arom. 2972,2926 (C-H) aliph. , 1676 (C=O) carboxlic , 1598(C=C) ,653(C-S) .

2-((4-(2,5-dioxopyrrolidin-1-yl)phenyl)thio)acetic acid[8]

Color : Off white , percent of yields 65%, m.p: (163-165) °C .FT-IR (υ, cm^{-1}) : (3400-2400) O-H , 3050 (C-H) arom., 2958,2885 (C-H) aliph. , 1697 (C=O) carboxlic , 1566 (C=C) , 663(C-S) .

3.3.Synthesis of compounds[9-12] [33]

(0.01mol) of compound [5-8] has been reacted separately with $SOCl_2$ (0.01mol) in dry benzene (15mL) and refluxed for a period of 8 hours while the excess benzene and thionyl chloride have been expelled under vacuum.

Analytical data for compounds [9-12]

2-(4-(4,5,6,7),tetrachloro-1,3-dioxoisoindolin-2-yl) phenyl)thio)acetyl[9]

Color : Brown , percent of yields 67%, m.p: (147-149) °C .FT-IR (υ, cm^{-1}): 3058(C-H) arom., 2912,2809 (C-H) aliph. , 1762(C=O)Cl , 1579(C=C), 673(C-S.)

2-((4-(5-nitro-1,3-dioxoisoindolin-2-yl) phenyl) thio) acetylchloride[10]

Color : Red brown , percent of yields 75%, m.p: (120-122) °C .FT-IR (υ, cm^{-1}) : 3010 (C-H). arom.,2940,2910 (C-H) aliph. , 1766 (C=O)Cl , 1581(C=C) , 675 (C-S).

2-((4-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl) phenyl) thio) acetylchloride[11]

Color: Red, percent of yields 66%, m.p: (211-213) °C .FT-IR (υ, cm^{-1}): 3057 (C-H) arom. 2945,2901 (C-H) aliph. , 1759(C=O)Cl , 1597(C=C) , 653 (C-S).

2-((4-(2,5-dioxopyrrolidin-1-yl) phenyl) thio) acetylchloride [12]

Color: Brown , percent of yields 62%, m.p: (200-202)°C .FT-IR (υ, cm^{-1}): 3020(C-H) arom. 2920,2860 (C-H) aliph. , 1760 (C=O)Cl, 1590(C=C) ,663(C-S).

Synthesis of polymers [13-16][34]

In 20 ml of DMF, 1 mole of PVA and 1 mole of one of compounds [9-12] were added. The product has been poured in water and the precipitate was washed by a little sodium bicarbonate amount, water and after that washed with ethanol after the combination was often shaken for three hours. The product was purified through DMSO and re-precipitated from the ethanol.

Analytical data for polymers [13-16]

Polymer[13]: FT-IR (υ, cm^{-1}) :3266 (O-H) ,2946,2917 (C-H) aliph., 1732(C=O) ester,1134(C-O), 1588 (C=C) , ^1H NMR (δppm) : 7.61-8.77 (4H, m, Ar-H), 3.85 (2H,s,SCH_2) , 1.45 (2H,d, CH_2), 4.49(1H, t ,CH).

Polymer[14] :FT-IR (υ, cm^{-1}) :3390(O-H) ,2941,2914 (C-H) aliph., 1712(C=O) ester,1143(C-O), 1600(C=C).

Polymer[15] FT-IR (υ, cm^{-1}) :3352(O-H) ,2943,2916 (C-H) aliph., 1712(C=O) ester, 1145(C-O), 1587 (C=C) .

Polymer[16] FT-IR (υ, cm^{-1}) :3437(O-H) ,2926,2858 (C-H) aliph.,1724 (C=O) ester.1141(C-O), 1591(C=C).

Synthesis of Nanocomposites[17-20][35]

To bond The iron nanometal in blend matrix, 50mL of a 250 mg/L solution of iron oxide NPs was mixed with 100mg of dried modified PVA [13-16] with the use of hotplate stirrer for three hours.

Molecular docking study

The Complete Genetic Optimization of the British Cambridge Crystallographic Data Center (CCDC) (GOLD) Hermes 2021.2.0 (Build 327809) was used to perform molecular docking studies of compound[9] and visualize: protein, ligands, hydrogen bonding interactions, short contacts and bond length calculations.[36].The enzyme (4ZGY) proven through the Protein Data Bank (rcsb.org).

Biological activity

Modified PVA, modified PVA with iron oxide nanoparticle have been screened for antibacterial activities against (*Bacillus cereus* and *Escherichia coli*) using cup-plate agar diffusion method. Amoxicillin (50µg /ml) were used as a standard drug for antibacterial activity. These sterilized agar media were poured into petri dishes and allowed to solidify. Some of synthesized compounds (50µg /ml) were placed serially in the cavities with the help of micropipette and allowed to diffuse for 1 hr. DMSO was used as a solvent for all the compounds and as a control. These plates were incubated at 37°C for 24 hr for antibacterial activities. The zone of inhibition observed around the cups after respective incubation was measured in mm.

Cytotoxicity activity

The cytotoxic effect of modified polyvinyl alcohol [13] and nanocomposite[17] were investigated against Colon Cancer Cell line (HT29) and compared with normal liver cell line (WRL-68) .The MTT test was used in 96-well plates to investigate the cytotoxic impact of polymer (7). Cells were treated with polymer (7) after 24 hours or when a confluent monolayer was established. After 24 hours of treatment, cell viability was determined by removing the medium, µl/well solutions of MTT and incubating for 4 hr. at 37°C. Following the removal of the MTT solution, the crystals in the wells were solubilized by adding 200µL of DMSO (Dimethyl Sulphoxide) and incubating at 37 °C for 15 minutes with shaking. The absorbency was measured at 620 nm using a microplate reader [37]. Calculated cell growth inhibition rate granted to equations [38]

Inhibition rate

$$= \frac{\textit{mean of control} - \textit{mean of treatment}}{\textit{mean of control}} \times 100$$

Results and Discussion

The reactions carried out in this study are outlined in Schemes (1) and (2). The correct spectral and analytical data for compounds [1-4] validated their structure. The compound [1]'s FT-IR spectra revealed [39] bands at (1780,1728) cm^{-1} because of two (N-C=O) and 2541 cm^{-1} due to SH group.. Through reacting compounds [1-4] with chloroacetic acid in distilled water, compounds [5-8] were created in basic media. The compound [5]'s FT-IR spectra, revealed the elimination of SH at 2541 cm^{-1} and the emergence of bands at (3400–2400) cm^{-1} for (OH) of carboxylic acids, (1749,1734) cm^{-1} because of two (N-C=O) groups, and 1699 cm^{-1} for (C=O) of carboxylic acid. Compounds [9-12] through were refluxed in dry benzene for 7 hours with compounds [5-8] and thionyl chloride. Melting point and FT-IR spectra were used to describe compound [9]. FT-IR spectrum of compound [9], revealed [40] the presence of the band at 1762cm^{-1} connected to acyl chloride and the absence of the absorption bands at 1699 cm^{-1} and (3218) cm^{-1} because of (carbonyl, hydroxyl) group of carboxylic acid. Through reacting PVA with compounds [9-12] and dimethylformamide, Poly (vinyl alcohol)[13-16] was chemically modified. FT-IR spectra was used to identify the compounds [13-16]. FT-IR spectra of polymer [13] showed the presence of a significant peak at 3266cm^{-1}. This peak, which could be observed at 2917 cm^{-1} and 2946 cm^{-1} because of the asymmetric and symmetric stretching vibrations of C-H from alkyl groups[41], is related to O-H stretching from inter-molecular and intra-molecular hydrogen bonds. It had also shown the disappearance of the absorption band at 1762cm^{-1} because of the acyl chloride and the appearance of absorption band at 1732cm^{-1} because of the carbonyl group of an ester [42].

Nanocomposites [17-20] preparation of modified polyvinyl alcohol [12-16]with IONPs .FT-IR data of nanocomposites[17] , that the presence of peaks at

3265 cm^{-1} reveals to O-H stretching from the inter and intra-molecular hydrogen bonds and shifting asymmetric and symmetric stretching vibrational of C-H from alkyl groups at (2958, 2980) , 500 to 800 cm^{-1} iron-oxide bonding also supports the formation of particles. Also, a unique Fe-O band was visible in the band at 566 cm^{-1}.

Field Emission Scanning electron microscope studies (FESEM)

FESEM has been utilized in order to approve the morphology and size of modified PVA and nanocomposites. The modified PVA [13] figure (1) particles range in size from 389 to 495 nm on average. Iron NPs have been observed to have homogenous distributions on the surface of the matrix, their average nano size in nanocomposites [17] Figure (2) is between (45-56) nm for iron oxide NPs. Yet, a few of the agglomerations of NPs have been also discovered when the surface was slightly rough. The particles in nano-composite film have been found to have an almost spherical morphology [44-46]

Molecular Docking Study

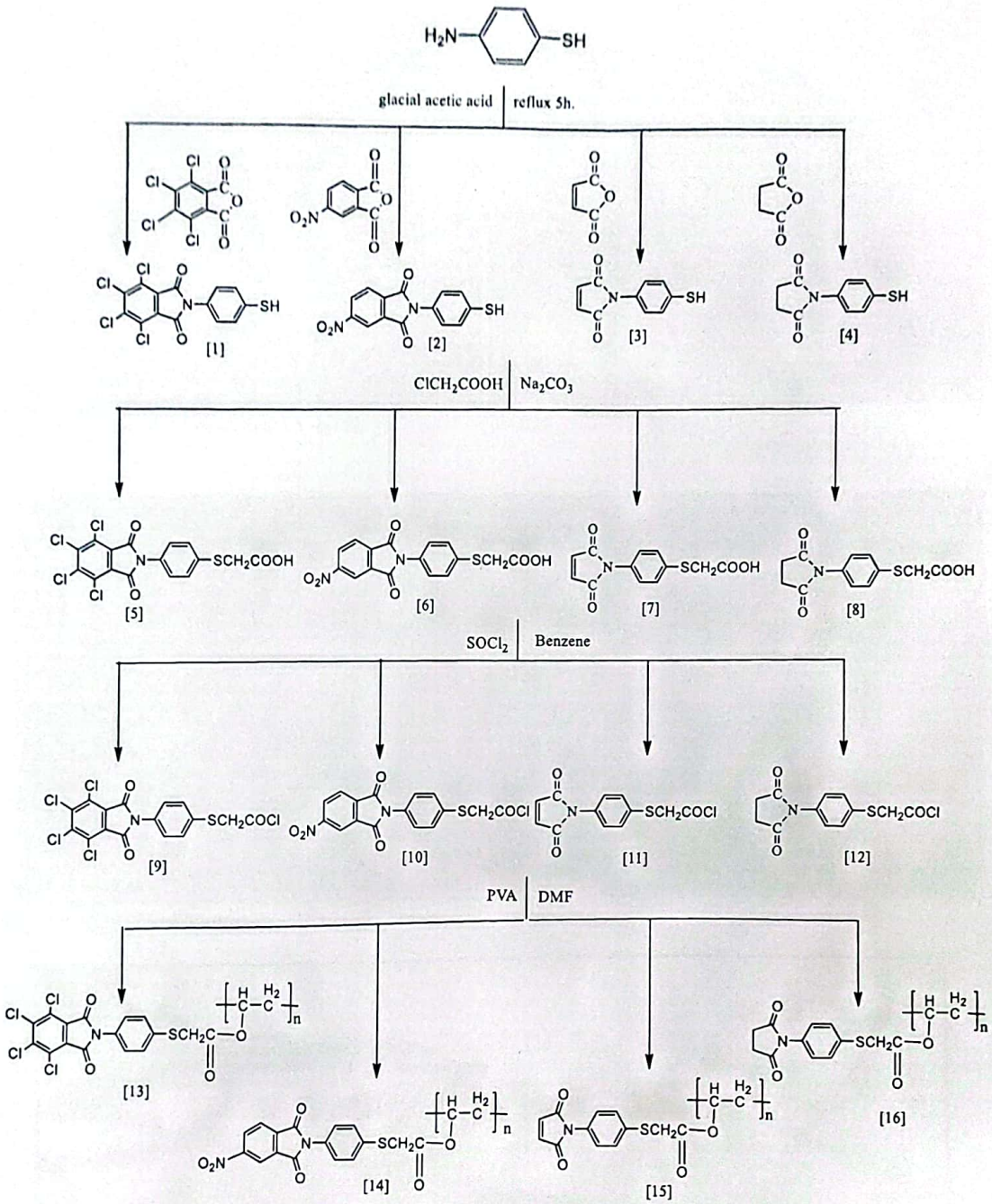
The synthesized compound (9) was tested for molecular docking study showed significant activities towards testing the stabilization of cancer cells in the enzyme (4ZGY) proven through the Protein Data Bank (rcsb.org) due to the interaction of hydrogen bonds with the main amino acids LYSINE (LYS69) VALINE (VAL198) GLYCINE(GLY201) ARGININE (ARG277). The prepared compound[9] proved to be more effective than the compound (PYRIDOXAL-5'-PHOSPHATE)being compared, and the binding energy with the enzyme was higher, reaching (62.15), while the binding energy of compound being compared with the enzyme was 47.43 due to the interaction of hydrogen bonds with the main amino acids (LYS69) (ARG277) (ASP332) as shown in Table1.

Biological activity

Modified PVA, modified PVA with iron oxide nanoparticle tested against two pathogenic bacteria types *(G+) Bacillus cereus* and *E. coli (G-)*, they all showed excellent inhibition rate, where the nanocomposites were the most activity comparable with Amoxicillin as standard antibiotic. Because of IONPs' great cell affinity and ease of uptake by immune cells, they can be delivered precisely to the site of infection, where they can inhibit and harm microbial pathogens. Because IONPs bind tightly to electron donor groups like nitrogen, sulfur, or oxygen in microbial cell walls and enter through the bacterial cell wall, they have an antibacterial impact. However, IONPs also produce free radicals, which can harm cells and perforate their membranes [47-51]. Recent research suggests that the ability of magnetic nano-particles to result in microbial toxicity is primarily caused by a series of interactions that compromise cell integrity due to the membrane depolarization, the development of oxidative stress, and the production of ROS, which in turn cause an inflammatory response. High ROS concentrations could harm cells by causing mitochondrial damage, lipid peroxidation, DNA oxidation, protein oxidation, and gene transcription regulation, which results in cell apoptosis [52–54].All of the polymers and their anti-bacterial activities have been listed in Table 2.

Cytotoxicity activity

The modified PVA [13] and nanocomposite[17] could selectively permeate cancer cells. Nanocomposite [17] exhibit good inhibition at concentration (20,50,75,100,200)µg/ml more than the modified PVA [13]. By increasing ROS levels and causing damage to the cellular components by intracellular oxidative stress and increase in glutathione oxidation IONPs could induce cytotoxicity [55]. In one of the recent studies, in *vivo* administration indicated their effectiveness as cytotoxic agents. Magnetic IONPs appears to mediate the DNA lesions in the tumor cells. Therefore, the anticancer activity of Nanocomposite[17] showed significant effects at concentration 100 µg /ml against HT29 cell line and IC50= 39.85 while IC50= 169.07 for (WRL-68) [56-58]



Scheme 1.Synthesis of compounds and modified PVA [1-16]

Modified PVA [13-16] —IONPs→ Nanocomposities [17-20]

Scheme2.Synthesis of nanocomposities [17-20]

Figure 1.FE SEM of modified PVA[13]

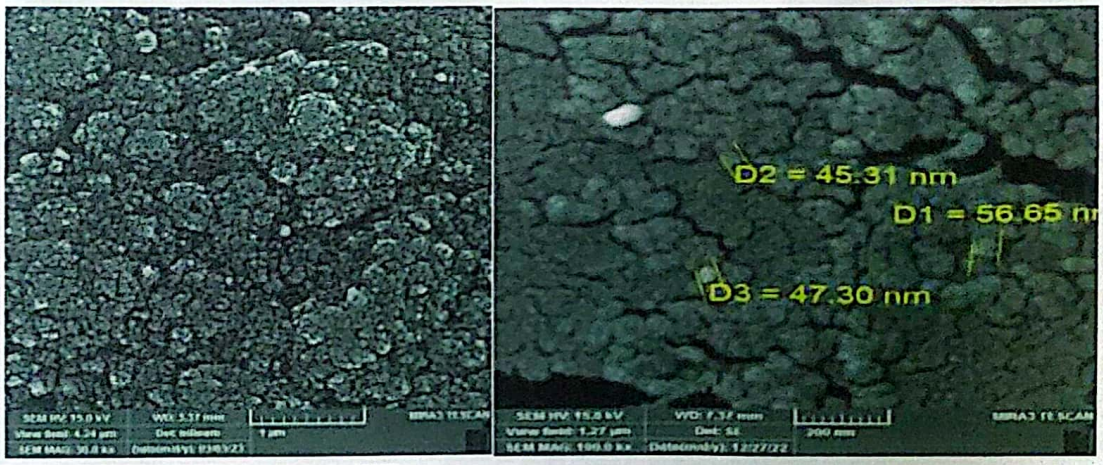


Figure2.FESEM of Nanocomposite [17]

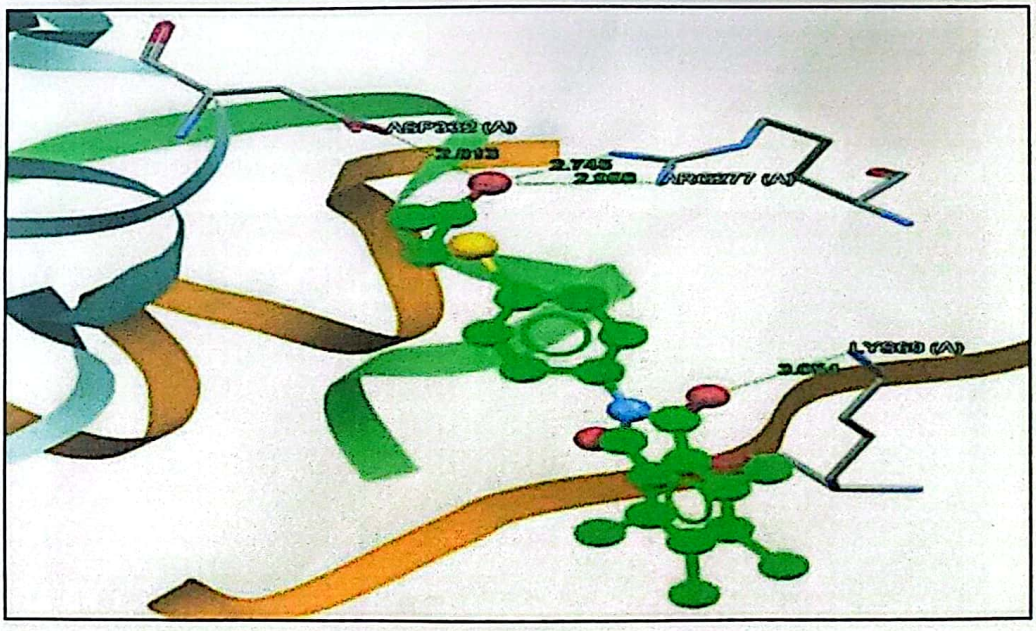


Figure3.molecular docking of compound[9]

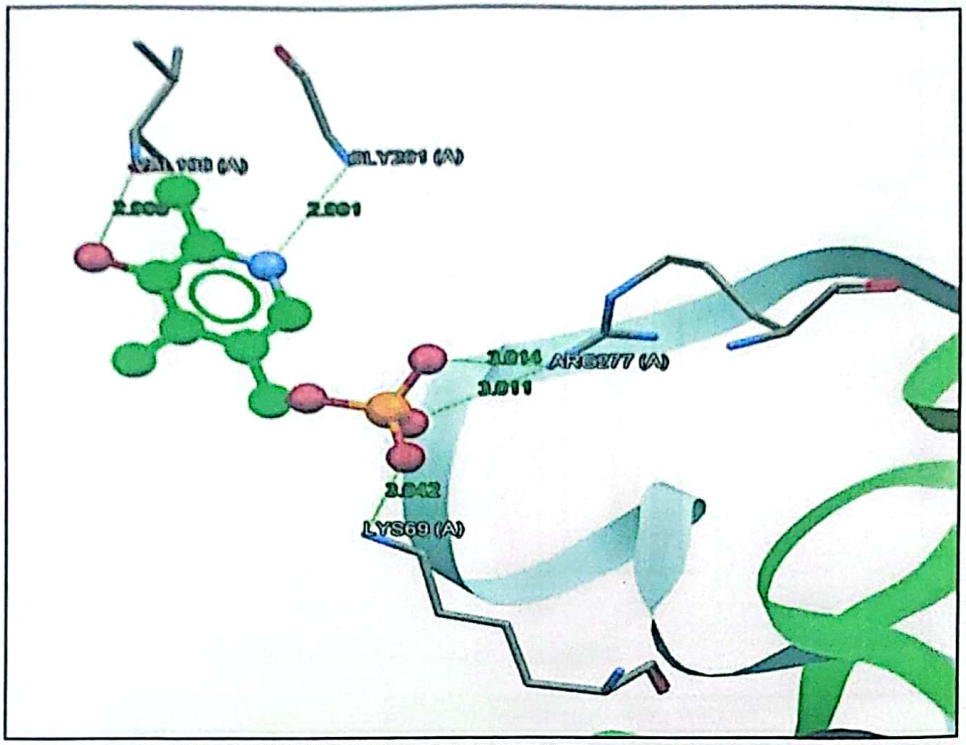


Figure4. molecular docking of PYRIDOXAL-5'-PHOSPHATE

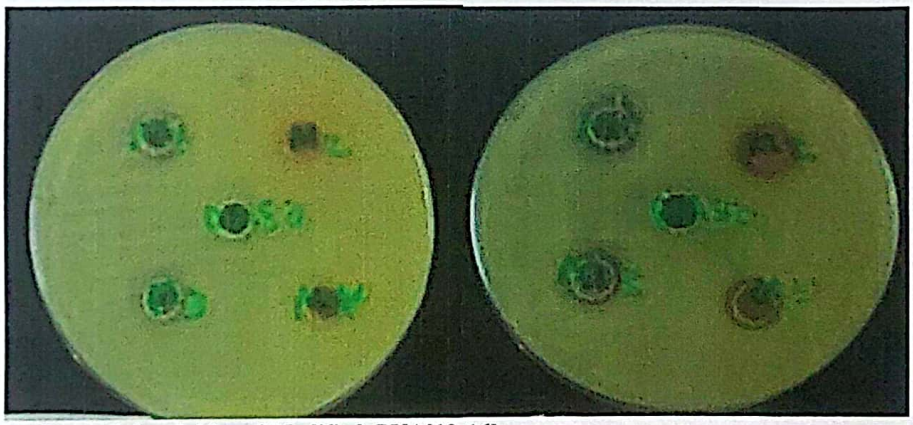


Figure5. Antibacterial activities of Modified PVA[13-16]

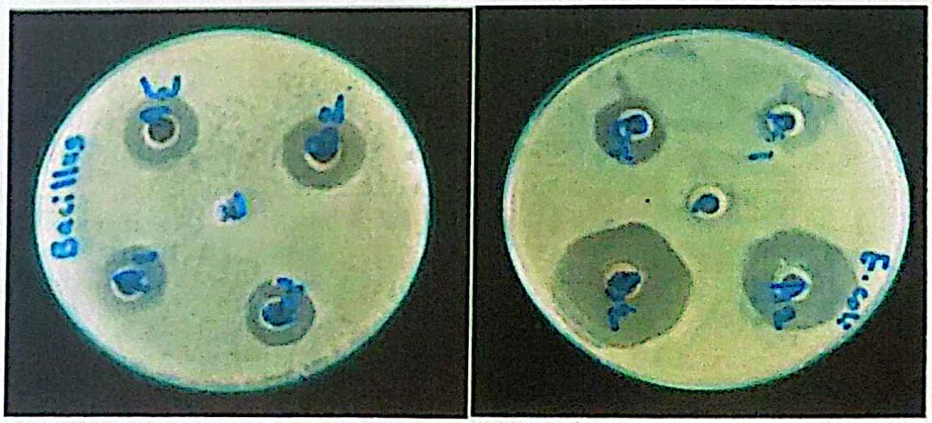


Figure6. Antibacterial activities of nanocomposities[17-20]

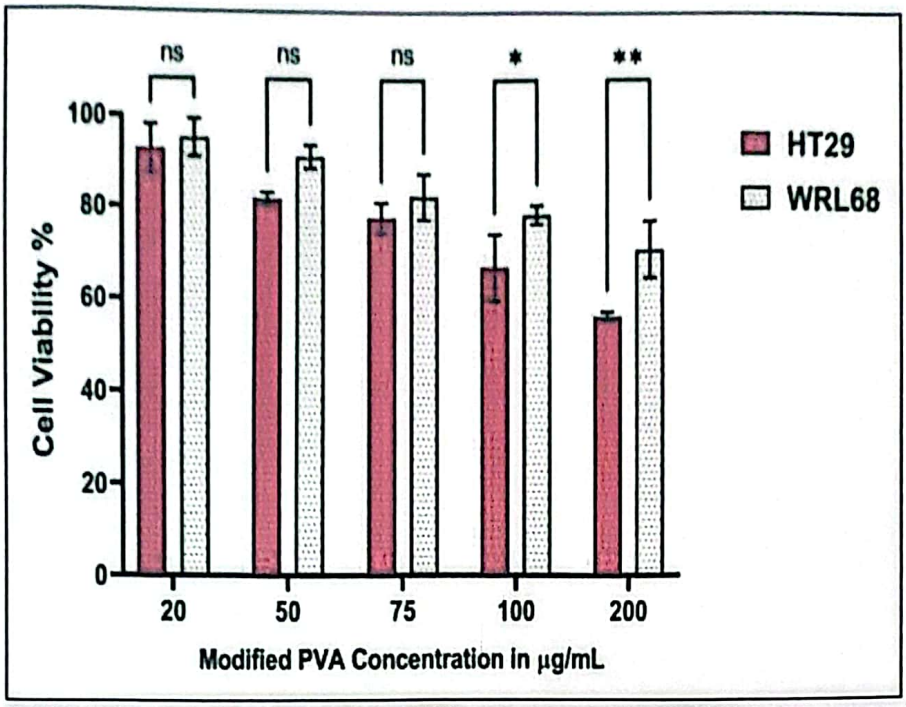


Figure7. Cell Viability of modified PVA[13] for HT29 and compare with WRL68

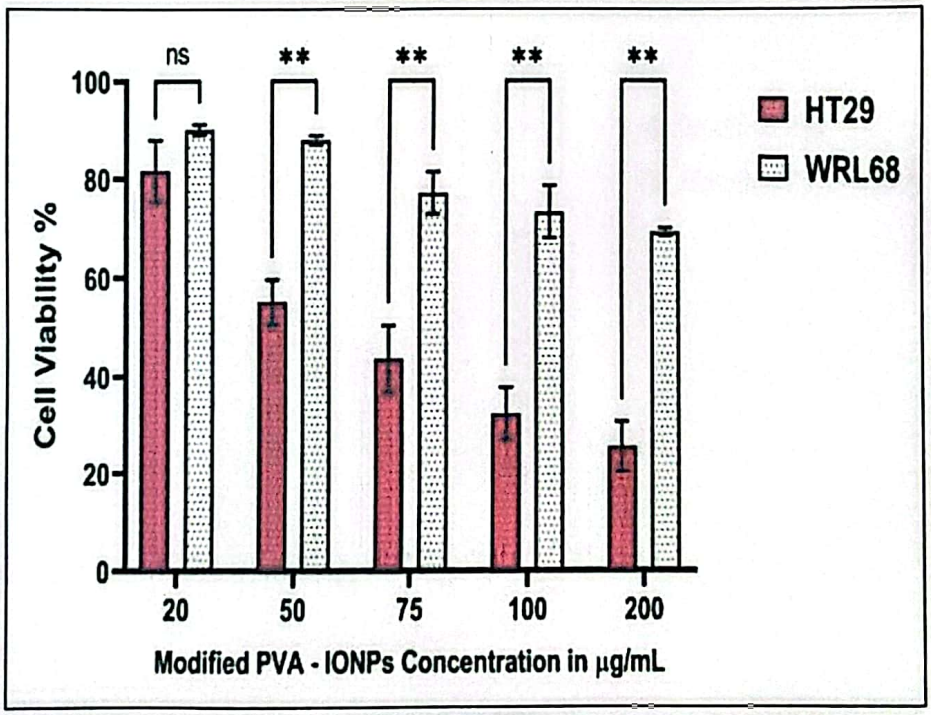


Figure8. Cell Viability of modified PVA-IONPs[17] for HT29 and compare with WRL68

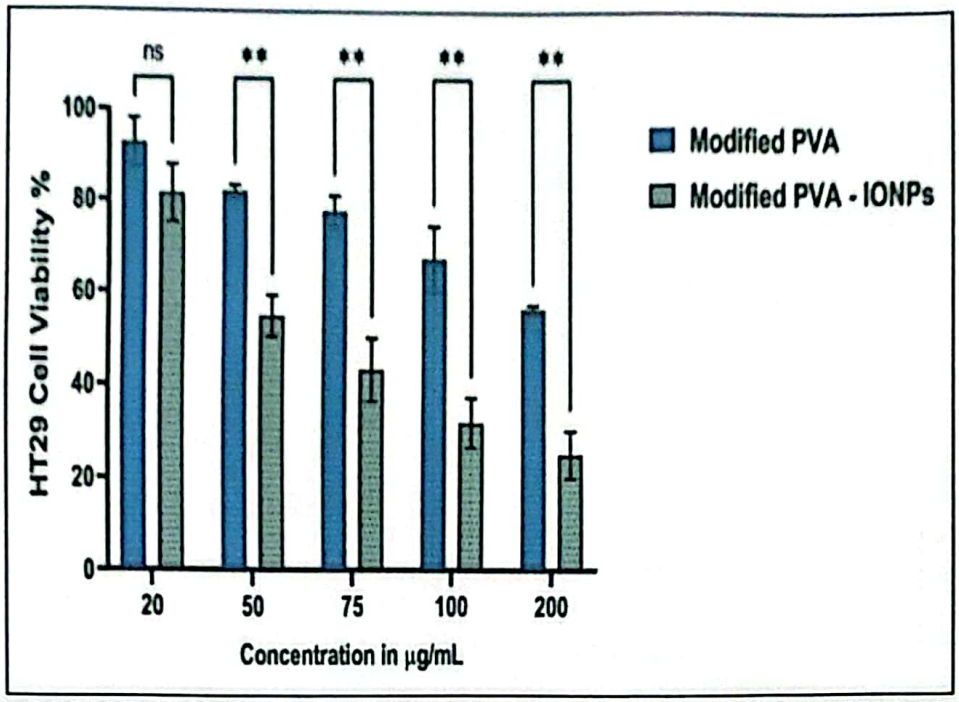


Figure9. Cell Viability of HT29 for modified PVA[13] and compare with modified PVA-IONPs [17]

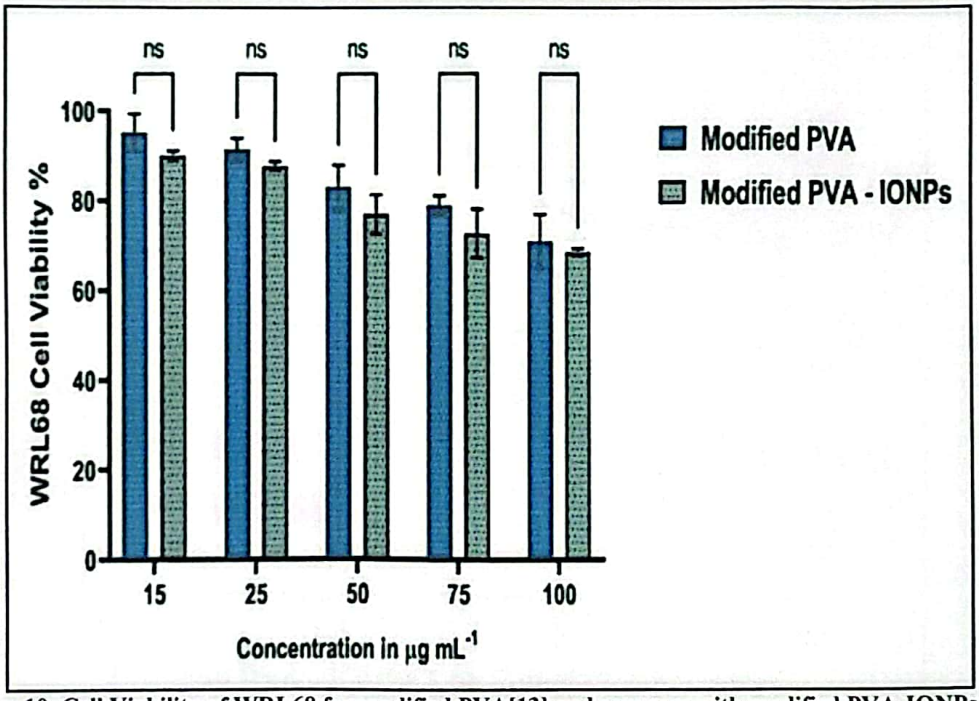


Figure10. Cell Viability of WRL68 for modified PVA[13] and compare with modified PVA-IONPs [17]

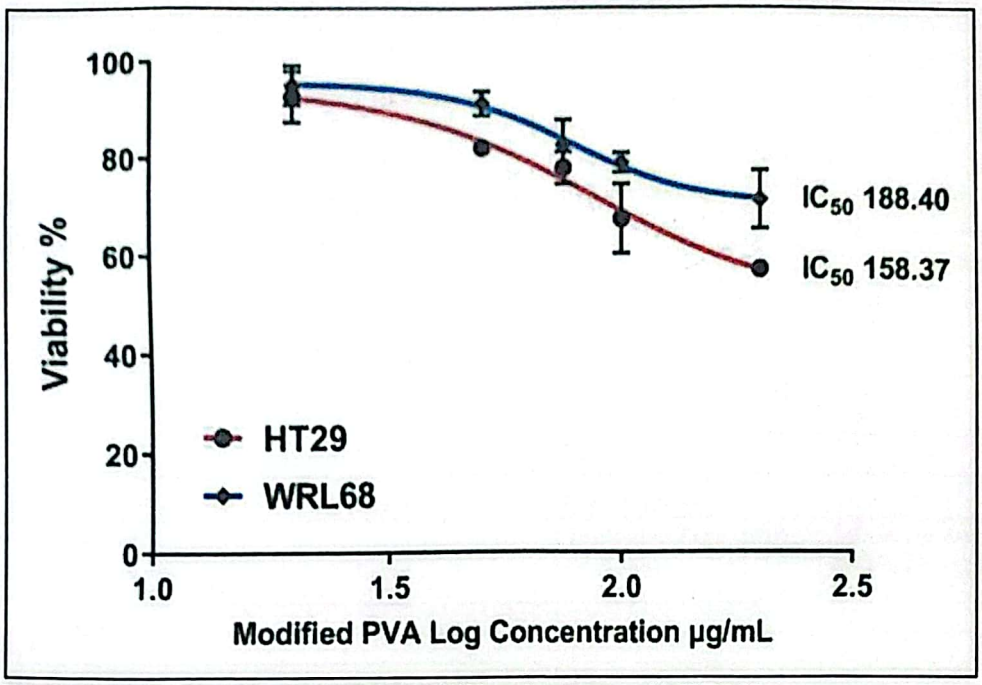


Figure11. IC50 of modified PVA[13] for HT29 and compare with WRL68

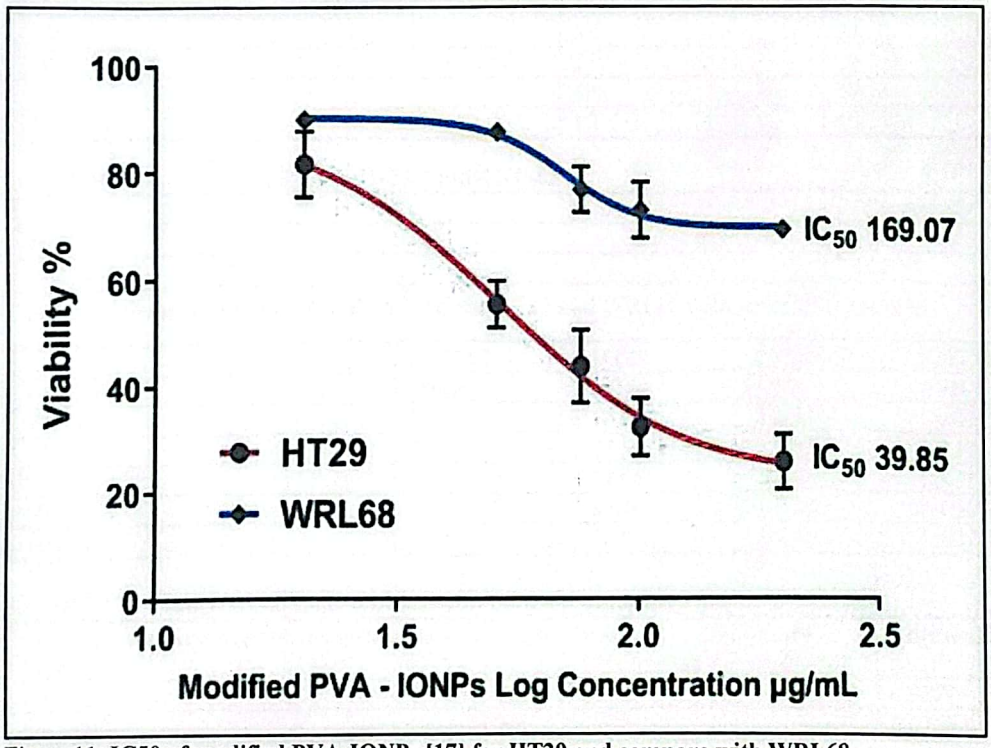


Figure11. IC50 of modified PVA-IONPs [17] for HT29 and compare with WRL68

Table1. Molecular docking of compound[9]and compare with PYRIDOXAL-5'- PHOSPHATE

Docking study (Anti colon cancer)					
Compounds	**Binding Energy (PLP Fitness) Kcal/Mol**	**No. of Amino Acids Included in H-bonding**	**Amino Acids Included in H-bonding**	**no. of bonding**	**power of bonding**
PYRIDOXAL-5'-PHOSPHATE	47.43	5	LYS69	1	3.042
			VAL198	1	2.909
			GLY201	1	2.991
			ARG277	2	3.011 3.014
[9]	62.15	4	LYS69	1	3.054
			ARG277	2	2.745 2.958
			ASP332	1	2.813

Table 2. Antibacterial screening data of some synthesized polymers.

Comp.No.	Inhibition Zone (mm) of *E .coli*	Inhibition Zone (mm) of *Bacillus cereus*
Amoxicillin	17	23
[13]	12	10
[14]	13	10
[15]	11	11
[16]	11	9
[17]	27	22
[18]	24	20
[19]	17	19
[20]	17	18

Table3. IC50 of modified PVA for HT29 andWRL-68

Cell Line	IC_{50} µg mL^{-1}
HT29	188.4
WRL-68	158.37

Table4 . Differences of modified PVA between HT29 and WRL68 with respect treatments

	WRL68	HT29	WRL68	HT29
Concen.	Mean	Mean	SD	SD
200	71.29	56.95	6.03	0.92
100	79.08	67.59	2.05	7.19
75	82.80	78.01	5.05	3.35
50	91.38	82.16	2.53	1.32
20	95.24	92.81	4.16	5.32

Table5 . HT29 and WRL68 Cells – Differences between Modified PVA

Šídák's multiple comparisons test HT29 - WRL68	Below threshold	Summary	Adjusted P Value
20	No	Ns	0.9677
50	No	Ns	0.0766
75	No	Ns	0.6416
100	Yes	*	0.0184
200	Yes	**	0.0028

Table6. IC50 of modified PVA -IONPs for HT29 andWRL-68

Cell Line	IC_{50} µg mL^{-1}
HT29	39.85
WRL-68	169.07

Table 7. Differences of modified PVA-IONPs between HT29 and WRL68 with respect to treatments

	HT29		WRL68	
Concen.	Mean	SD	Mean	SD
200	25.36	5.11	68.92	0.79
100	32.17	5.33	72.95	5.34
75	43.42	6.80	76.86	4.33
50	54.95	4.51	87.68	0.95
20	81.60	6.30	90.03	1.07

Table8 . HT29 and WRL68Cells – Differences between Modified PVA-IONPs

Šídák's multiple comparisons test HT29 - WRL68	Below threshold	Summary	Adjusted P Value
20	No	Ns	0.1676
50	Yes	**	< 0.0001
75	Yes	**	< 0.0001
100	Yes	**	< 0.0001
200	Yes	**	< 0.0001

Table9 . HT29 Cells – Differences between Modified PVA and Modified PVA - IONPs

Šídák's multiple comparisons test Modified PVA - Modified PVA – IONPs	Below threshold	Summary	Adjusted P Value
20	No	Ns	0.0639
50	Yes	**	<0.0001
75	Yes	**	<0.0001
100	Yes	**	<0.0001
200	Yes	**	<0.0001

Table10. WRL-68 Cells – Differences between Modified PVA and Modified PVA - IONPs

Šídák's multiple comparisons test Modified PVA - Modified PVA – IONPs	Below threshold	Summary	Adjusted P Value
20	No	Ns	0.4202
50	No	Ns	0.7467
75	No	Ns	0.2874
100	No	Ns	0.2588
200	No	Ns	0.9488

NS: Non-significant; * $p < 0.05$; ** $p < 0.01$

Conclusion

The aim of the research was to create nanocomposities by a series of reactions that began by the formation New Imides. Then modified of polyvinyl alcohol with new imides then modified polyvinyl alcohol reacted with Iron Oxide Nanoparticles. Prove the molecular docking of the prepared compound , It is more effective than the comparator compound and has greater enzyme binding energy .The antibacterial activity of most synthesized modified PVA and nanocomposities were tested in vitro. The modified PVA/IONPs exhibited very excellent antimicrobial activities comparable with modified PVA , cancer cell line(HT29) using MTT assay was used to estimate the cytotoxic effect of different concentrations of the created nanocomposities and compare with normal cell line (WRL68), the (modified PVA/AIONPs) exhibited very excellent Inhibition rate. Finally, study Toxicity Test for these nanocomposities, where it showed non-toxicity of these nanocomposities.

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Conflicts of Interest

Conflicts of Interest: None.

We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for re-publication attached with the manuscript.

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Ethics Statement

Ethical Clearance: The project was approved by the local ethical committee in University of Baghdad

Author Contribution

Study conception and design: Ruwaidah S. Saeed ; data collection: Kawther Ayad Obead ; analysis and inter pretation of results: Ruwaidah S. Saeed draft manuscript preparation R. S. S. All authors reviewed the results and approved the final version of the manuscript.

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بولي فينيل الكحول المحور الحاوي على إيميدات جديدة/جسيمات نانوية من أوكسيد الحديد: التحضير، التشخيص والتقييم البيولوجي

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الخلاصة

تم تحضير سلسلة من مركبات إلايميدات الجديدة[١-٤] من تفاعل رباعي كلورو فثاليك أنهيدريد, نيترو فثاليك أنهيدريد , الماليك أنهيدريد , السكسينيك أنهيدريد مع ٤-أمينو بنزين ثيول تحت ظروف الاندماج. تمت إضافة حمض الكلوروأسيتيك الى المحلول المائي للمركبات [١-٤] المحتوي على كاربونات الصوديوم لانتاج المركبات [٥-٨]. وفي البنزين، تم مفاعلة المركبات [٥-٨] مع كلوريد الثيونيل لإنتاج المركبات [٩-١٢]. تم تحوير البولي فينيل الكحول كيميائيًا عن طريق تفاعل PVA مع مركبات [٩-١٢] وثنائي ميثيل فورماميد لإنتاج مركبات [١٣-١٦]. يتم خلط جسيمات أوكسيد الحديد النانوية (IONPs) مع PVA المحور [١٣-١٦] لانتاج مركبات نانوية [١٧-٢٠]. تم استخدام البيانات الطيفية والتحليلية لتشخيص المركبات المصنعة، مثل أطياف ^{1}H-NMR وأطياف FTIR وFESEM، لوصف خصائصها الهيكلية. تمت دراسة الالتحام الجزيئي حيث يتم استخدام العمليات للتنبؤ بحالة ارتباط المركب [٩] بالإنزيم وحساب الطاقة الحرة (ΔG) للمركب المحضر. كما تم استخدام نوعين مختلفين من البكتيريا: *Bacillus cereus* (G+) and *E. coli* (G-) لاختبار النشاط المضاد للبكتيريا . بالإضافة إلى ذلك، تم استخدام اختبار MTT لتقدير النشاط السمي لبولي فينيل الكحول المحور مع إيميدات جديدة، لبولي فينيل الكحول المحور مع إيميدات جديدة وأوكسيد الحديد NPs ضد خط خلايا سرطان القولون (HT29). وكذلك مقارنته بنشاط الخلايا الطبيعية WRL-68 (خط الخلايا الكبدية البشرية). النتائج أظهرت أن المركب النانوي [١٧] لديه معدل تثبيط ممتاز اعلى من كحول البولي فينيل المحور[١٣] ضد نوعين من البكتيريا وخط خلايا سرطان القولون (HT29).

الكلمات المفتاحية: التقييم البيولوجي، خط خلايا سرطان القولون (HT29)، جزيئات أوكسيد الحديد النانوية، مركبات الإيميد، PVA المحور