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Synthesis, antimicrobial activity, computational and modeling studies of some new organotellurium compounds containing azo moities

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ABSTRACT

A new series of organonotellurium compounds containing azo groups were prepared by new and convenient methods. Reaction of 1-(4-mercuric chloride-2,3-dichlorophenyl)-2-chloro diazine (4) with 8-hydroxyquinoline (5) gave the new organomercury compound 6 in good yield. Telluratio of compound 6 with tellurium tetrabromide in 1:1 and 1:2 mole ratio gave the *o*-tellurated azo compounds $ArTeBr_3$ (7) and Ar_2TeBr_2 (9), respectively. Reduction of both $ArTeBr_3$ and Ar_2TeBr_2 by hydrazine hydrate gave the ditelluride 8, and telluride 10, respectively. The synthesized compounds were screened for their antibacterial activity against *Staphylococcus aureus*, *Escherichia coli*, *Bacillus subtilis*, *Klebsiella pneumonia*, *Salmonella spp*., *Streptococcus spp*. and *Bacillus cereus*. Additionally, the prepared compounds were tested for antifungal activity against *Candida sp*., *Aspergillus multi* and *Aspergillus niger*. All compounds exhibited good antibacterial and antifungal activity. Computational study of the new compounds was calculated using Gaussian 09 program package. Molecular modeling studies were performed and showed hydrogen binding and hydrophobic interactions.

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1. Introduction

The pharmacological properties of organotellurium compound have attracted considerable attention as evidenced by several model studies on the antioxidant properties of synthetic organotellurium compounds [1-3]. Several tellurides showed antioxidative and immune modulating properties and antitumor activities [4-8], meanwhile clinical trials with a tellurane compound are presently underway [9,10]. The non-toxic tellurium compound ammonium trichloro(dioxo ethylene-*O*,*O*'-)tellurate, AS101 (**1**), has been recently shown to exert profound anti-inflammatory properties in animal models, associated with its Te(IV) redox chemistry [11], in addition, AS101 sensitizes tumors to chemotherapy by inhibiting the tumor interleukin 10 autocrine loop [12] as well as a potent immuno modulator (*in-vitro* and *in-vivo*) with a variety of potential therapeutic applications (Figure 1)[9,13]. Furthermore, the organotullraneRT-01 (**2**) has been reported to potent anticancer [4] and anti-leishmanial [14] agents. There is an increasing in the synthesis of aromatic organotellurium compounds containing electron donor nitrogen atom at position *ortho* to the tellurium atom [15,16]. Thus, azo compounds [17], Schiff bases [18,19], *N*,*N*-dimethylbenzyl amine [20] and *p*-substituted anilines [1] can be *o*-tellurated by various methods. Al-Rubaie *et al.* [21] have reported several organotellurium compounds containing amino group in an *ortho*position to tellurium atom, such as $ArTeBr_3$, Ar_2Te_2 and Ar_2Te by the reaction of the corresponding 2-amino aryl mercury chloride with tellurium tetrabromide in glacial acetic acid.

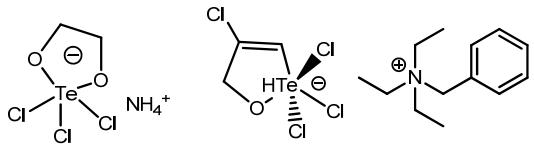

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Figure 1. Chemical structures of ammonium trichloro(dioxoethylene-*O*-*O*') tellurate (AS101) (**1**) and *N*-benzyl-*N*,*N*-triethylamonium 2,2,2,4-tetra chloro-2,5-dihydro-1,2-oxatellurate (**2**).

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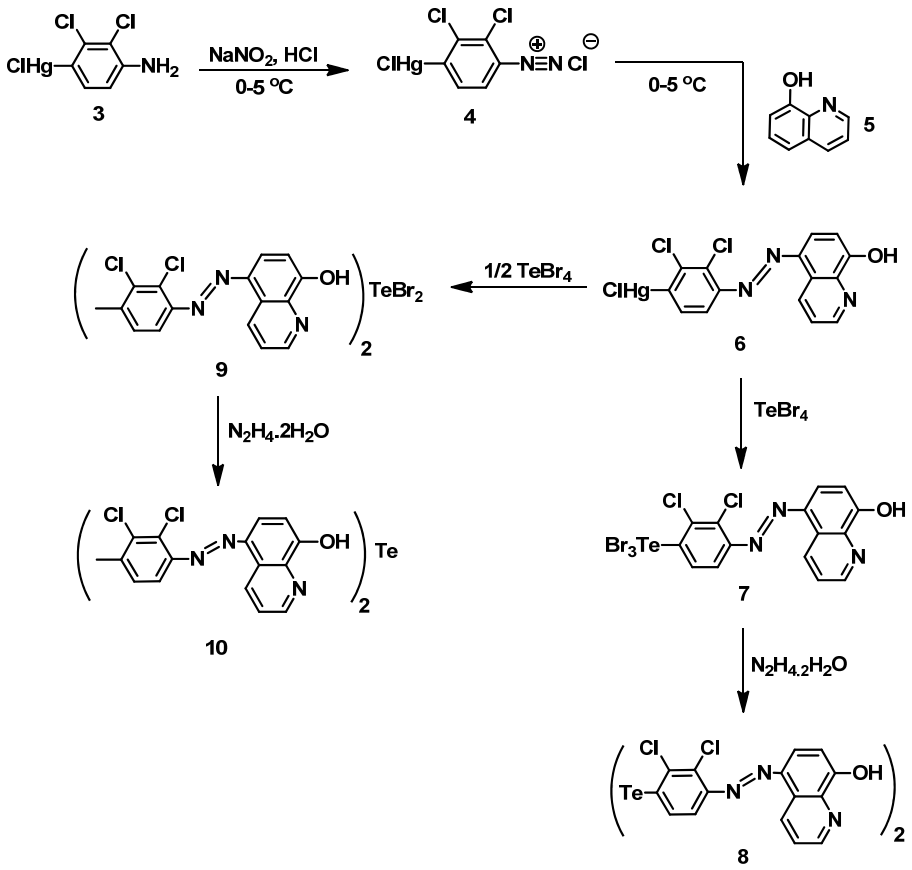

Scheme 1

Some organotellurium compounds containing azomethine and azo groups solutions have a non-linear optical properties [22], and for the production of living radical polymers [23,24], organotellurium-mediated living radical polymerization (TERP) using diphenylditelluride (DT-Ph) and di-*n*-butyl ditelluride (DT-Bu) in the presence of a binary azo initiator system [23].

Several organotellurium compounds containing azo group were prepared by reaction of the mercurated azo dyes with tellurium tetrabromide in 1:1 and 2:1 mole ratio using dry chloroform as a solvent to give the *o*-telluratedazo dyes compounds $ArTeBr_3$ and Ar_2TeBr_2, respectively [25].

In continuation of ongoing our work on tellurium chemistry [26], we report here the synthesis of some new organotellurium compounds containing azo moieties, and evaluation of their *in-vitro* antimicrobial activity, in addition to the computational and molecular modeling studies.

2. Experimental

2.1. Instrumentation

Melting points are uncorrected and were measured on a Philip Harris melting point apparatus and uncorrected. The IR spectra were recorded in the range 4000-200 cm^{-1} on a Pye-Unicam SP3-300 spectrometer using KBr disc. NMR spectra were spectra were recorded on 400 and 600 MHz (^1H) and on 150.91 MHz (^{13}C) spectrometers (Bruker, Germany) with TMS as an internal standard and on the δ scale in ppm. Mass spectra (EI, 70 eV) were recorded on MAT 8200 spectrometers (Finnegan MAT, USA).

2.2. Synthesis

2.2.1. Synthesis of (2,3-dichloro-4-((8-hydroxyquinolin-5-yl) diazenyl)phenyl)mercury(II) chloride (6)

To a cold stirred solution of (4-amino-2,3-dichlorophenyl) mercury(II) chloride (**3**) (1.98 g, 5.00 mmol) in conc. hydrochloric acid (20 mL) was added slowly sodium nitrite (0.45 M, 5.00 mmol). The mixture was stirred at 0-5 °C in an ice-bath for 30 min., then at room temperature for 2 h. A cold solution of 8-hydroxyquinoline (**5**) (0.73 g, 5.00 mmol) in 40% sodium hydroxide (20 mL) was added drop by drop to give a yellow solution of azo compound and the mixture was stirred for another 30 min with keeping the temperature under 5 °C. A reddish brown solid was obtained, filtered and washed several times with distilled water to yield compound **6** as reddish-brown solid (Scheme 1). Yield: 67%. M.p.: 238-240 °C. FT-IR (KBr, ν, cm^{-1}): 3452 (OH), 3049 (CH-Ar), 1624 (C=C), 1570 (N=N). ^1H NMR (400 MHz, DMSO-d_6, δ, ppm):9.40 (s, 1H, OH), 7.32-9.11 (m, 7H, Ar-H). MS (EI, *m/z* (%)): 553 [M^+, 41].

2.2.2. Synthesis of 2,3-dichloro-4-((8-hydroxyquinolin-5-yl) diazenyl)phenyltellurium(IV)tribromide (7)

A mixture of compound **6** (1.66 g, 3.00 mmol) and tellurium tetrabromide (1.34 g, 3.00 mmol) in 1,4-dioxane (50 mL) was heated under reflux for 6 h under argon atmosphere. On cooling, a white plates of a mixture of 2:1 of dioxane and mercuric(II) bromide was separated, removed by filtration. The filtrate was evaporated to dryness and the residue was recrystallized from a mixture of methanol and dichloro methane (2:1, *v*:*v*) to give compound **7** as a brown solid

(Scheme 1). Yield: 63 %. M.p.: 224-227 °C. FT-IR (KBr, ν, cm-1): 3412 (OH), 3062 (CH-Arom.), 1625 (C=C), 1587 (N=N). ^{1}H NMR (400 MHz, DMSO-d_6, δ, ppm): 9.43 (s, 1H, OH), 7.33-9.02 (m, 7H, Ar-H). MS (EI, *m/z* (%)): 684[M$^+$, 100].

2.2.3. Synthesis of bis[2,3-dichloro-4-((8-hydroxyquinolin-5-yl)diazenyl)phenyl]ditelluride (8)

To a solution of compound **7** (1.37, 2.00 mmol) in EtOH (20 mL) was added ethanolic solution of hydrazine hydrate (0.76 g, 15.00 mmol) very slowly and the solution was heated under reflux. Each addition was accompanied by a vigorous evaluation of nitrogen; meanwhile the tribromide was gradually dissolved. On completing the addition and no further nitrogen were evolved, the mixture was cooled. A dark red precipitate was formed and collected by filtration, washed with MeOH and dried under vacuum. Recrystallization from EtOH gave compound **8**, as a dark red solid (Scheme 1). Yield: 58 %. M.p.: 260-264 °C (Dec.). FT-IR (KBr, ν, cm-^{1}): 3335 (OH), 3055 (CH-Arom.), 1635 (C=C), 1577 (N=N). ^{1}H NMR (400 MHz, DMSO-d_6, δ, ppm):9.39(s, 2H, OH), 7.30-8.99 (m, 14H, Ar-H). MS (EI, *m/z* (%)): 891 [M$^+$, 99].

2.2.4. Synthesis of bis[2,3-dichloro-4-((8-hydroxyquinolin-5-yl)diazenyl)phenyl]tellurium(IV)dibromide (9)

A mixture of compound **6** (2.2 g, 4.00 mmol) and tellurium tetrabromide (0.89 g, 2.00 mmol) in 1,4-dioxane (25 mL) were heated under reflux for 6 h under argon atmosphere. The reaction mixture was filtered hot and the filtrate deposited, on cooling at room temperature, a 2:1 complex of HgClBr (Dioxane)$_2$ as a white plates. The white complex was filtered off. The filtrate was poured into 100 mL of ice-water during a brown precipitate was formed. The resulting product was recrystallized from a mixture of methanol and dichloro methane (2:1, *v:v*) twice to afford compound **9** as bright brown solid (Scheme 1). Yield: 64 %. M.p.: 198-200 °C. FT-IR (KBr, ν, cm-^{1}): 3545 (OH), 3049 (CH-Arom.), 1625 (C=C), 1552 (N=N). ^{1}H NMR (400 MHz, DMSO-d_6, δ, ppm): 9.51 (s, 2H, OH), 7.37-9.37 (m, 14H, Ar-H). MS (EI, *m/z* (%)): 923 [M$^+$, 63.5].

2.2.5. Synthesis of bis[2,3-dichloro-4-((8-hydroxyquinolin-5-yl)diazenyl)phenyl]telluride (10)

To a solution of compound **9** (1.84 g, 2.0 mmol) in ethanol (20 mL) was added dropwise ethanolic solution of hydrazine hydrate (1.00 g, 20 mmol) and the solution was heated under reflux until evolution of nitrogen was ceased. The mixture was cooled and filtered off. The product was twicely recrystallized from a mixture of ethanol and chloroform to give compound **10** as a brown solid (Scheme 1). Yield: 53 %. M.p.: 230-233 °C (Dec.). FT-IR (KBr, ν, cm-^{1}): 3400 (OH), 3062 (CH-Arom.), 1622 (C=C), 1493 (N=N). ^{1}H NMR (400 MHz, DMSO-d_6, δ, ppm): 9.38 (s, 2H, OH), 7.22-9.00 (m, 14H, Ar-H). MS (EI, *m/z* (%)): 761 [M$^+$, 84.1].

2.3. Computational study

The computations of the geometries and energies of the synthesis compounds **6-10** were done using density functional theory (DFT) with Gaussian 09 package [27]. The DFT was treated with hybrid functional Becke's three parameter and the Lee, Yang, Parr (B3LYP) [28] as a level of theory and LANL2DZ as a basis set [29,30].

2.4. Antimicrobial activity

The synthesized compounds were screened *in vitro* for their antibacterial activity against: *Klebsiella pneumonia*, *Escherichia coli*, *Salmonella spp*., *Staphylococcus aureus*, *Streptococcus sp*., *Bacillus subtilis*, *Bacillus cereus.* Additionally, the compounds were tested for antifungal activity against *Aspergillus niger*, *Aspergillus multi* and *Candida spp.* using the paper disc-agar diffusion technique on Muller Hinton agar as a culture media for antibacterial activity [31]. The test compounds were dissolved in DMSO solvent and recommended concentrations (50, 100 and 200 µg/mL) were used in the disc-agar diffusion technique. Antibiotic drug ampicillin and nystatin were used as control for bacteria and fungi, respectively. Petri plates containing 20 mL of Mueller Hinton Agar were used for all the bacteria tested. *Aspergillus niger*, *Aspergillus multi* and *Candida spp*. strains were cultivated in Sabouraud dextrose agar. Sterile Whatman No. 1 filter paper disks (6 mm in diameter) impregnated with the solution in DMSO of the test was placed on the Petri plates. A paper disk impregnated with dimethylsulfoxide (DMSO) was used as negative control. The plates were incubated for 24 h at 37 °C in the case of bacteria and 72 h that 27 °C for fungi. The inhibition zone diameters were measured in millimeters. The bacteria and fungi were supplied from department of Microbiology, College of Veterinary Medicine, University of Basrah, Iraq.

3. Results and discussion

3.1. Chemistry

Diazotization of (4-amino-2,3-dichlorophenyl)mercury(II) chloride (**3**) with sodium nitrite and conc. hydrochloric acid at 0-5 °C afforded the diazonium salt **4** which reacted, in situe, with 8-hydroxyquinoline (**5**) to afford the new organomercury compound **6** in 67% yield (Scheme 1). Tellurated of compound **6** with tellurium tetrabromide in 1:1 and 1:2 mole ratio gave the *ortho*-tellurated diazo compounds $ArTeBr_3$ (**7**) and Ar_2TeBr_2 (**9**) in 63 and 64% yield, respectively. The reduction of compound **7** and **9** by hydrazine hydrate gave the ditelluride**8** and **10** in 85 and 53% yield, respectively. The structures of the synthesized compounds were assigned by the IR and ^{1}H NMR and Mass spectra. The IR spectra displayed common features in certain regions and characteristic bands in the fingerprint and other regions. The spectra were characterized by the presence of broad strong bands in the rang 3545-3335 cm^{-1} attributed to ν(O-H), while the sharp bands at the region 1587-1493 cm^{-1} were assigned to the azo groups (N=N) stretching. In addition, the bands at the region 1635-1622cm^{-1} were assigned to the C=C aromatic group. In the ^{1}H NMR spectra of synthesized compounds, the hydroxy protons of 8-hydroxy quinoline were resonated as singlets at the regions δ 9.51-9.38 ppm and these values are in agreement with previously reported data [32]. The multiplet at the regions δ 7.22-9.11 ppm were attributed to the aromatic protons.

3.2. Antibacterial and antifungal activity

The synthesized compounds have been screened for their *in-vitro* antibacterial and antifungal activities, using the paper disc-agar diffusion technique [31] by measuring the inhibition zone in mm. The antibiotics, ampicillin and nystatin were used as a control against bacteria and fungi, respectively. The antibacterial activity of the synthesized compounds were tested against four Gram positive bacteria (*Staphylococcus aureus, Streptococcus sp.*, *Bacillus subtilis* and *Bacillus cereus*) and three Gram negative bacteria (*Klebsiella pneumonia*, *Escherichia coli* and *Salmonella spp.*) at a concentration of 50, 100 and 200 µg/mL using DMSO as a solvent, which not effected the growth of microbes. Mueller Hinton agar was used as culture media for antibacterial activity. The results of the antimicrobial activity are shown in Table 1 and 2. The prepared compounds had the highest activity against *S. aureus*, *Streptococcus sp*., *Klebsiella pneumonia*, *E. coli* and *Salmonella spp*., but inactive against *B. subtilis* and *B. cereus* except compound **8** which showed a moderate activity against *B.*

Table 1. Antibacterial activity of some tellurated compounds.

Compound	Diameter of inhibition zone in mm for different microbial species											
	Staphylococcus aureus			*Streptococcus sp.*			*Bacillus subtilis*			*Bacillus cereus*		
	50 µg/mL	100 µg/mL	200 µg/mL	50 µg/mL	100 µg/mL	200 µg/mL	50 µg/mL	100 µg/mL	200 µg/mL	50 µg/mL	100 µg/mL	200 µg/mL
6	8	9	26	12	20	21	-	-	-	-	-	-
7	9	10	26	8	10	20	-	-	-	-	-	-
8	-	10	20	-	7	20	6	7	16	-	-	8
9	8	8	22	12	20	24	-	-	-	-	-	-
10	7	8	24	17	20	22	-	-	-	-	-	-
Ampicillin	19			0			0			-	-	-

Table 2. Antibacterial activity of some tellurated compounds.

Compound	Diameter of inhibition zone in mm for different microbial species								
	Klebsiella pneumonia			*Escherichia coli*			*Salmonella spp.*		
	50 µg/mL	100 µg/mL	200 µg/mL	50 µg/mL	100 µg/mL	200 µg/mL	50 µg/mL	100 µg/mL	200 µg/mL
6	10	11	24	12	14	22	7	8 1	9
7	7	8	28	9	10	24	7	20	24
8	-	8	10	7	10	16	10	14	16
9	8	9	18	7	8	19	18	20	22
10	10	8	31	7	7	8	16	7	20
Ampicillin	16			20			9		

Table 3. Antifungal activity of some tellurated derivatives.

Compound	*Aspergillus niger*			*Aspergillus multi*			*Candida spp.*		
	50 µg/mL	100 µg/mL	200 µg/mL	50 µg/mL	100 µg/mL	200 µg/mL	50 µg/mL	100 µg/mL	200 µg/mL
6	6	7	11	8	17	28	7	10	20
7	6	7	8	7	10	30	12	16	16
8	-	-	-	-	-	-	8	20	26
9	-	6	7	7	14	16	7	8	17
10	-	-	10	7	8	11	-	-	-
Nystatin	15			13			12		

Table 4. Selected bond angles, bond angles and dihedral angles of the studied compounds

Compound	6	7	8	9	10	Experimental
Bond length (Å)						
C-Hg	2.243	-	-	-	-	2.065
Hg-Cl	2.430	-	-	-	-	2.326
N=N	1.276	1.277	1.259, 1.260	1.258, 1.256	1.260, 1.258	
C-Te	-	2.169	2.175, 2.172	2.187, 2.164	2.152, 2.161	2.158
Te-Br	-	2.701	-	2.716, 2.751	-	2.650
Te-Te	-	-	2.752	-	-	2.740
Angles bond (°)						
C-Hg-Cl	177.659	-	-	-	-	
C2-N1=N2	114.437	114.230	123.748, 124.562	124.870, 126.655	124.977, 125.510	
N1=N2-C3	115.065	115.344	124.517, 125.338	124.628, 125.784	125.758, 125.438	
C-Te-Te	-	-	100.406, 100.440	-	-	
C-Te-C	-	-	-	102.858	96.294	
Dihedral angles (°)						
C2-N1=N2-C3	178.708	179.419	-9.272, 14.753	16.184, 15.301	-8.064, 14.805	
C1-C2-N1=N2	171.449	179.664	142.538, -69.343	-138.704, -151.174	134.450, -69.144	
N1=N2-C3-C4	178.320	179.554	153.034, 150.421	-136.683, -160.302	-159.474, 155.815	
C-Te-Te-C	-	-	82.034	-	-	

subtilis and *B. cereus*. It is worth noting that all compounds have activity against both Gram positive and negative bacteria.

On the other hand, the antifungal activity of the synthesized compounds showed high-moderate activity towards all the fungal species such as *Aspergillus niger, Aspergillus multi* and *Candida spp*., except compounds **8** and **10** which exhibit no activity against all tested fungi and *Candida spp*., respectively (Table 3). Therefore, a plausible explanation of our results attributed to the chemical structure of the bacterial cells wall which provides important ligands for adherence and receptor sites for antibiotics and drugs.

3.3. Computational study

The calculations with use of DFT (Density function theory) B3LYP/LANL2DZ level of approximation has been successfully employed in a number of previous theoretical studies of organotellurium compounds [33]. The important structural parameters of the optimized geometries such as bonds lengths, bond angles and dihedral angles of the studied molecules **6**-**10**, (Figure 2) are summarized in Table 4. In the ArHgCl moiety, each mercury atom is linearly coordinated to a chloride and a carbon atom (angle C-Hg-Cl = 177.659 °) which is structurally fully characterized. From Table 4, there are in agreement between the calculated bonds lengths C-Hg, Hg-Cl, C-Te, Te-Br and Te-Te and their measured bonds lengths [34-37]. Generally there is no significant differences between the calculated bond lengths, however, only a slight decrease in the bond length N=N of compound **8**, **9** and **10**, might be due to the steric effects.

The lone pairs of electrons around tellurium should be stereochemically active according to VSEPR (Valence Shell Electron Pair Repulsion) theory [38], therefore the geometry of tellurium atom of compound **8** and **10** is related to the distorted *pseudo*-tetrahedral [39], where C-Te-C and C-Te-Te angles are 100.4 and 96.3 °. While the C-Te-Br and C-Te-C bond angles of compound **7** and **9** are 97.3 and 102.8 °, then they are significantly lower than the putative value of 120 ° for trigonal bipyramidal geometry [40].

In the ditelluride system (molecule **8**), the Te-Te bond is likely influence the repulsion between ion pairs [41].

Table 5. Values of total energy, binding energy and HOMO-LUMO energy gap for studied compounds.

Compound	Total energy (eV)	Binding energy (eV)	HOMO energy (eV)	LUMO Energy (eV)	ΔE, The difference LUMO-HOMO
6	- 560774.498	-160.795	-5.527	-3.736	1.791
7	- 437304.959	-164.970	-5.764	-4.325	1.439
8	- 454381.403	-318.824	-5.155	-3.555	1.600
9	-414484.720	-320.147	-5.447	-3.783	1.664
10	-274408.668	-316.560	-4.950	-3.593	1.357

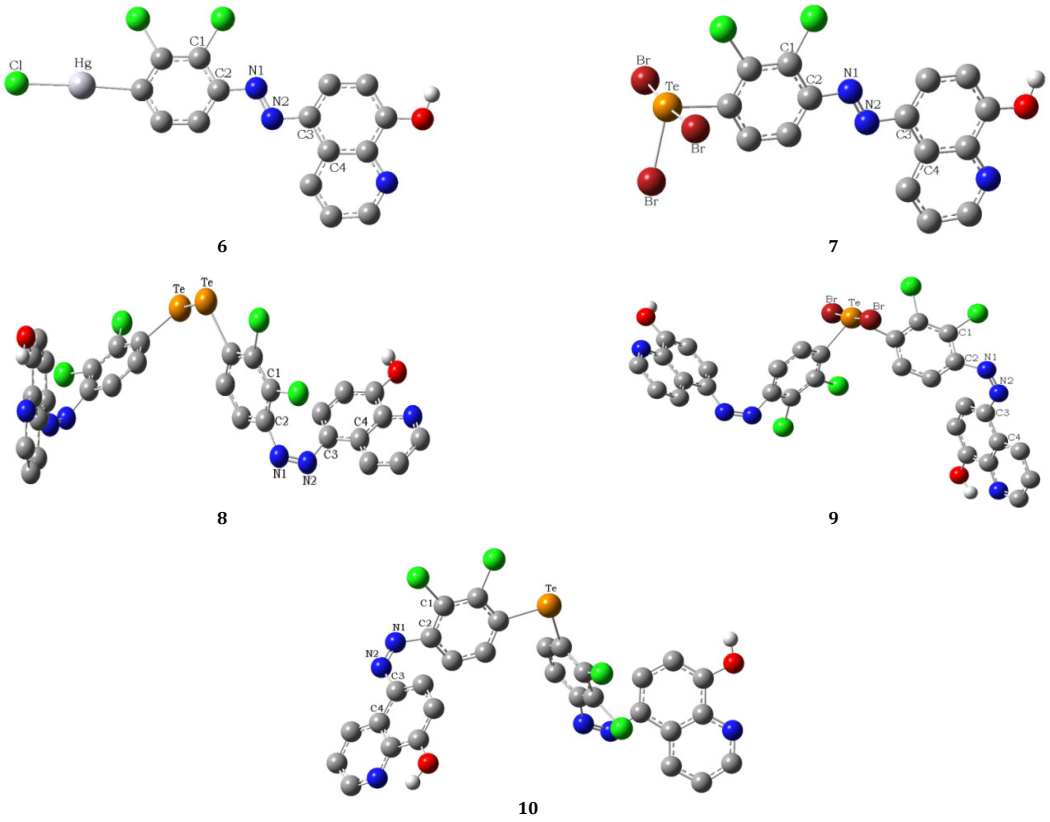

Figure 2. Optimization geometries structures of the studied molecules.

In addition, the steric interaction between aromatic rings is due to small C-Te-Te-C dihedral angles (82.034 °). This is a consequence of rotation around the C-Te bonds which take place because of the proximity of the phenyl rings to each other. From the dihedral angles measurement, we observed that compounds **6** and **7** are in a planar structure with a dihedral angle ≈ 180 ° (Table 4), meanwhile the other compounds have non planar structures (dihedral angles are from -8.064 to -160.302 °).

The total energy, binding energy and LUMO-HOMO energy gap are computed by using the same method and the basis set, which summarized in Table 5. The values of LUMO-HOMO energy gap and total energy of the organomercuric molecule **6** are: (ΔE LUMO-HOMO energy gap = 1.791 eV); (Total energy = -560774.498 eV), and these values are relatively large compared with corresponding organtellurium, indicating a high stability and high chemical hardness of this compound. The LUMO-HOMO energy gap showed also the lowest values of molecules **7** and **10** (1.439 and 1.357 eV), which reflected its relatively chemical reactivity compared with other synthesized compounds. Compound **5** revealed the lowest values of the total energy and LUMO-HOMO energy gap, which indicated that, is not stable, due to the steric disability of benzene rings. The HOMO and LUMO orbitals are depicted in Figure 3. The HOMO orbitals are localized mainly on tellurium, nitrogen and bromine atoms moieties in addition to some π orbitals of phenyl ring, meanwhile the LUMO of π nature are mostly located on the phenyl ring. The HOMO-LUMO transition implies an electron density transfer to the phenyl ring from tellurium atom.

3.4. Molecular modeling analysis

The molecular docking was performed using SYBYL-X 1.1 and the docking results were shown by PyMOL [42]. Our molecular docking analysis of the new analogues based on the modeling study which was performed to understand the binding mode of these analogues with the aspartate amino transferase (ATT) of *E. coli* [43]binding pocket (PDB code: 1ahg, [44]).

Compound **9** has been selected for the docking modeling study, since its binding energy score -11.9, with indicating a selectivity of 8-hydroxyquinoline and azo group in their binding to the enzyme pocket (Figure 4). As shown in Figure 4, the aromatic ring of compound **9** was fitted into an aromatic rich sub-pocket surrounded by the aromatic side chains of Phe217, in addition to two hydrogen bondings. The 8-hydroxyquinoline backbone was located in the middle of the binding pocket, anchoring the nitrogen atom of the azo group in a favourable position for hydrogen bonding with the NH_2 group of Lys246, in addition to a hydrogen bonding between the oxygen atom of OH group of 8-hydroquinoline with OH of

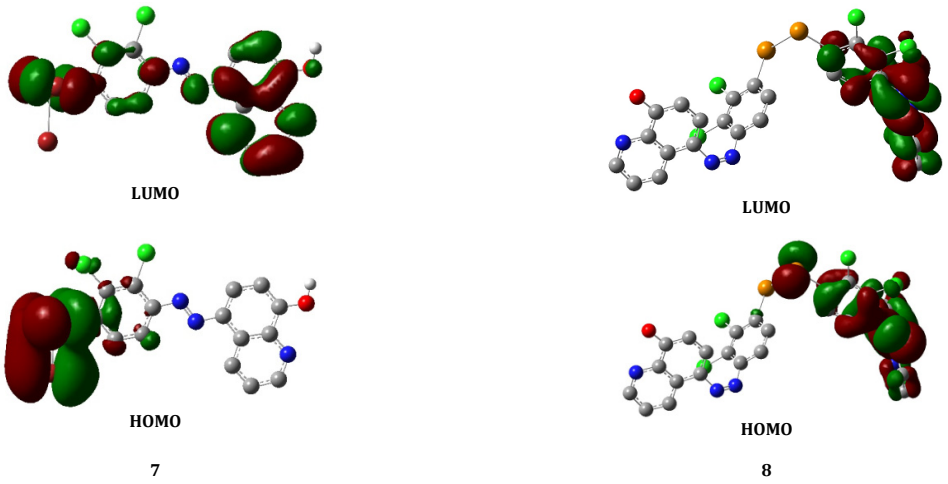

Figure 3. Representation of the HOMO and LUMO orbitals of molecules **7** and **8**.

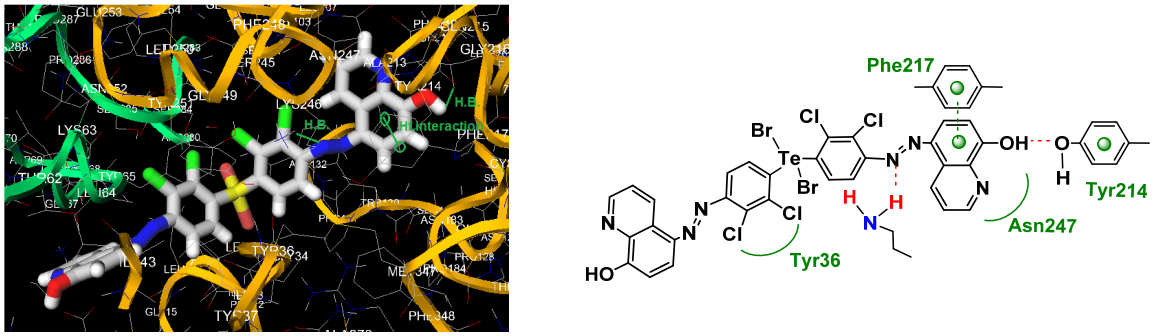

Figure 4. Docked conformation of compound **9** showing two hydrogen bonds: Tyr214 with OH of 8-hydroxyquinoline moiety, Lys246 with nitrogen atom of the azo group. It also exhibits hydrophobic interaction between phenyl ring of 8-hydroxyquinoline and Phe217 of reverse transcriptase (RT) enzyme residues.

Tyr214 of the aspartate aminotransferase (AAT) enzyme. Overall, the combination of hydrophobic interaction and π-stacking appears to govern the binding of compound **9** with AAT of *E. coli*.

4. Conclusion

In conclusion, a series of some new organomercury and organotellurium compounds containing azo group were prepared by convent method. Computational study of all compounds was calculated using Gaussian 09 program package. The antimicrobial activity was evaluated against seven bacterial strains and three fungal species. All the synthesized compounds exhibited good antibacterial and antifungal activities.

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