Synthesis, Spectroscopic Characterization, Antibacterial Screening, and Computational (DFT and *In-silico* Docking) studies of Novel Organotellurium (IV) Pyrrolidine Dithiocarbamates

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Abstract

Template condensation reaction between organotellurium (IV) iodides R_2TeI_2 [$R_2 = C_4H_8$, $C_4H_7(CH_3)$, C_5H_{10}] and silver salts of pyrrolidine dithiocarbamate $AgS_2CNC_4H_8$ in dichloromethane, resulted in six (6) novel disubstituted and monosubstituted dithiocarbamate derivatives of the type $R_2Te[S_2CN(C_4H_8)]_2$ and $R_2TeI[S_2CN(C_4H_8)]$ [$R_2 = C_4H_8$, C_5H_{10} and $C_4H_7(CH_3)$. The characterisation of these novel compounds was done with the help of elemental analysis, (IR, ^{1}HNMR,^{13}CNMR & UV) spectroscopic studies and conductance measurements. Synthesis, characterisation, and *in vitro antibacterial activity* have been discussed. In silico docking studies were also performed for these compounds to evaluate the binding free energy of the present inhibitor within the macromolecule. Protein preparation was done by Autodock 4.2. Optimized geometry of all six molecules has been proposed by employing the first-principles calculations based on density-functional theory simulations (DFT). The important parameters, such as binding energy, root mean square deviation, hydrogen bond interaction, HOMO-LUMO gaps, electron affinity, ionization potentials and electronegativities were also investigated in this study.

Keywords: Dithiocarbamates, Pyrrolidine, Organotellurium (IV), Molecular docking, Protein, Antibacterial activities. DFT & GGA,

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1. Introduction

Foss[1] has studied organotellurium dithiocarbamates of the type [$(p\text{-}OCH_3C_6H_4)Te(dtc)$]. Organotellurium (IV) N,N dialkyl dithiocarbamates [2-5] have been the subject of several investigations. Our group[4] investigated the synthetic features as well as spectral (IR, ^{1}H-NMR) analyses of $R_2Te(R'dtc)_nX_{2-n}$ [where $R_2=(CH_3)_2$, C_4H_8, $(C_6H_5)_2$, $(p\text{-}CH_3C_6H_4)_2$, $(p\text{-}OCH_3C_6H_4)_2$; X= Cl or I; n=1 or 2 and R'dtc = diethyl]. There are numerous reports [1-18] on N,N-dialkyl dithiocarbamates that function as 1,1-dithio ligands. Our group [16,17] also reported many dithiocarbamate derivatives of heterocyclic organotellurium dihalides of the type $C_5H_{10}Te(R')_2$ [$R'=S_2CN(C_2H_5)_2$, $S_2CNC_5H_{10}$, $S_2CNC_4H_8O$, $S_2CNHC_6H_5$. The synthesized compounds were analyzed by IR, (^{1}H, ^{13}C) NMR, and single-crystal X-ray diffraction studies. Dakternieks[18] et al. studied organotellurium complexes viz. $C_8H_8Te[S_2CN(C_2H_5)_2]$, $C_8H_8Te[S_2P(OC_2H_5)_2]_2$, and $C_8H_8Te[S_2CO(C_2H_5)_2]_2$ and characterized them with their crystal/molecular structures and NMR data. However, the chemistry of monothiocarbamate complexes of cyclic organotellurium[19] compounds is less explored, whereas reports on monothiocarbamate complexes of 1-iodo-1-N,-dialkyl dithiocarbamate-1,2,3,4,5-hexahydro tellurophene are available in the literature. The coordination chemistry of ligands[20-22] with dialkyl dithiocarbamate and their self-assembly due to (i) reaction of complexes with a wide range of transition metals and organometals leading to the formation of supramolecular arrays and (ii) the optical and electrochemical properties of the dithiocarbamate have also been reported[23-25].

The use of *cis*-diamine dichloroplatinum (II) and related compounds for chemotherapeutic purposes has several undesirable side effects, including nephrotoxicity, which is thought to be produced principally by the inactivation of enzymes caused by Pt(II) coordination to thiol groups[26]. Diethyl dithiocarbamate (Et_2NCS_2) ion [27-29], containing soft sulfur atoms, is used as a competitive "rescue agent" to protect these thiols. Dithiocarbamates are a class of metal-chelating, antioxidant compounds that have a variety of medical applications, including the treatment of bacterial and fungal infections, as well as the potential treatment of AIDS[30]. In continuation of expanding our previous work[31] on dithiocarbamates and due to the wide range of applications of organotellurium dithiocarbamate derivatives in biological fields[32 -37], we have undertaken the task of exploring some new monosubstituted and disubstituted compounds derived from three tellurocycles with pyrrolidine dithiocarbamate ligands. To predict the activity of the compounds, computational methods have been applied to study the activities of the synthesized compounds. The *in-vitro* antibacterial activities of synthesised compounds were investigated against Gram-negative species such as *E. coli* and Gram-positive species such as *Bacillus subtilis*, as well as antifungal activity against *Candida albicans*.

2. Experimental

2.1. General methods:

The synthetic method for the synthesis of Organotellurium (IV) pyrrolidine derivatives is displayed in **Scheme 1**.$C_4H_8TeI_2$[38], $C_4H_7(CH_3)TeI_2$[39], and $C_5H_{10}TeI_2$[40] were synthesised using the methods described in the literature. The tellurium percentage of every compound was determined in the laboratory as per literature[41]. The reported method [42] was used to synthesise the sodium salt of pyrrolidine dithiocarbamates. The silver salt of pyrrolidine dithiocarbamates ($AgS_2CNC_4H_8$) was made by mixing equimolar amounts of $AgNO_3$ and the corresponding sodium salt of pyrrolidine dithiocarbamate. The resulting white solid was filtered and dried. The solvents and other general reagents, used in this study, were freshly distilled and purified according to standard procedure before use. Elemental analysis for C, H, and N was carried out using an Elementar Vario EL III (accuracy: ±5%). Shimadzu 8210 PC FTIR spectrometer was used to record IR spectra in the frequency range 4000-350 cm^{-1} with samples in KBr discs. ^1H and ^{13}C NMR spectra of the complexes were recorded in $CDCl_3$ on Varian VXR 3005 spectrometer. The UV spectral data of the complex solutions in $CDCl_3$ were collected using a Labtronics L.T. 2900 spectrophotometer with a 10 mm path length. Molar conductivity was also measured using an ESICO model 1601 microprocessor-based conductivity/TDS metre. Melting points were determined using a Brannan Immersion Glass Thermometer.

*2.2 Synthesis of complexes: preparation of **1** and **2**, and **3***

1,1,2,3,4,5-Hexahydro-1,1-diiodotellurophene ($C_4H_8TeI_2$) **(1)** was prepared using literature methods[38] and re-crystallized in benzene to obtain its bright red prism (m.p.149-150°C) crystals. 2-methyl-1,1-diiodo-1-telluracyclopentane [$C_4H_7(CH_3)TeI_2$] **(2)** was prepared using literature methods[39] and was re-crystallised with dimethyl formamide (DFM) and kept in a petri dish to obtain orange colour crystalline compound (m.p.70°C). 1,1,2,3,4,5,6-Heptahydro-1,1-diiodotellurane ($C_5H_{10}TeI_2$) **(3)** was synthesised using the literature method[40] and re-crystallised twice from acetone to yield an orange-brown prism-shaped (m.p.135-136°C) crystal. The reported method[42] was used to synthesise the sodium salt of pyrrolidine dithiocarbamates. The silver salt of pyrrolidine dithiocarbamates ($AgS_2CNC_4H_8$) was made by mixing equimolar amounts of $AgNO_3$ and the corresponding sodium salt of pyrrolidine dithiocarbamate. The resulting white solid was filtered and dried.

Compounds (**1-3**) and (**4-6**) were synthesised in a similar manner using a 1:2 and 1:1 molar ratio of diiodo tellurocycle dithiocarbamate, respectively. In each case, the diiodo tellurocycle was dissolved in dichloromethane (30 ml), and the corresponding silver salt of the pyrrolidine dithiocarbamate ligand was added. The reaction mixture was stirred at room temperature for 3 hours. Filtration was carried out to remove the unidentified material from the reaction mixture. The filtrate was concentrated to 15 ml and then coated with pet-ether (40-60°C). It was kept overnight. The crystalline solid obtained was filtered, dried, and weighed.

2.2.1 Synthesis of 1,1,2,3,4,5-Hexahydro-1,1-bis-Pyrrolidine dithiocarbamate tellurophene $C_4H_8Te(S_2CNC_4H_8)_2$ ***(4)***

The reaction of [$C_4H_8TeI_2$] (0.7g, 1 mmol) and silver salt of pyrrolidine dithiocarbamate (0.81g, 2 mmol) in 30 ml of dichloromethane yielded compound **(4)**. The result was orange-coloured crystals with a melting point of 118°C and a yield of 0.76g (80%). Elemental Anal. Calc for $C_{14}H_{24}N_2S_4Te$: Found C= 35.27, H=4.97, N=5.85, S=26.79, Te=26.16%. Calculated C=35.32, H=5.05, N=5.90, S=26.91, Te=26.82%. IR (cm^{-1}): 1435 (s), 1398 (s) (ν CN); 1018 (s), 980 (m) (ν CS); s 546 (νTeCH$_2$). ^{1}HNMR (CDCl$_3$, δ ppm): 2.68 (m, 1H, Te-CH$_2$), 2.00 (m, 3H, Te-C-CH$_2$), 3.81 (t, 2H, N-CH$_2$), 2.01 (m, 3H, N-CCH$_2$); ^{13}CNMR (100.60 MHz, CDCl$_3$, δ ppm): 39.21 (s, Te-CH$_2$), 21.34, (s, Te-CCH$_2$), 202.71 (s, S$_2$CN), 51.45 (s, N-CH$_2$), 25.21 (s, N-CCH$_2$). UV/ Vis: 355 nm (ε = 22375 M^{-1} cm^{-1}), 322 nm (ε = 27598 M^{-1} cm^{-1}), 287 nm (ε = 26745 M^{-1} cm^{-1}) and 253 nm (ε = 48927 M^{-1} cm^{-1}).

2.2.2 Synthesis of 1,1,2,3,4,5,6-Heptahydro-1,1-1,1-bis-Pyrrolidine dithiocarbamate tellurane $C_5H_{10}Te(S_2CNC_4H_8)_2$ ***(5)***

The reaction of [$C_4H_8TeI_2$] (1.16g, 1 mmol) and silver salt of pyrrolidine dithiocarbamate (1.3g, 2 mmol) in 30 ml of dichloromethane resulted in compound **(5)**. The result was yellow crystals with a melting point of 146°C and a yield of 0.70g (73%). Elemental Anal. Calc for $C_{15}H_{26}N_2S_4Te$: Found C=36.60, H=5.20, N=5.67, S=26.00, Te=25.52%. Calculated C=36.76, H=5.31, N=5.72, S=26.15, Te=26.06%. IR (cm^{-1}): 1429 (s),1378 (m) (ν CN);1034 (s),960 (m) (ν CS); 563 (s) (νTeCH$_2$). ^{1}HNMR (CDCl$_3$, δ ppm): 2.71 (m, 1H, Te-CH$_2$), 1.62 (m, 3H, Te-CCH$_2$), 1.62 (m, 3H, Te-CCCH$_2$) ,3.81 (t, 2H, N-CH$_2$), 2.01 (m, 3H, N-CCH$_2$); ^{13}CNMR (100.60 MHz, CDCl$_3$, δ ppm): 39.67 (s, Te-CH$_2$), 26.38 (s, Te-CCH$_2$), 32.30 (s, Te-CCCH$_2$), 202.25 (s, S$_2$CN), 51.45 (s, N-CH$_2$), 25.21 (s, N-CCH$_2$). UV/ Vis: 360 nm (ε = 22246 M^{-1} cm^{-1}), 324 nm (ε = 27655 M^{-1} cm^{-1}), 285 nm (ε = 28738 M^{-1} cm^{-1}) and 255 nm (ε = 49621 M^{-1} cm^{-1}).

2.2.3 Synthesis of 2-methyl-1,1-bis-Pyrrolidine dithiocarbamate Telluracyclopentane $C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$ ***(6)***

The reaction of [$C_4H_7(CH_3)TeI_2$] (1.3g, 1 mmol) and silver salt of pyrrolidine dithiocarbamate (1.3g, 2 mmol) in 30 ml of dichloromethane resulted in compound **(6)**. The result was yellow crystals with a melting point of 100°C and a yield of 0.50g (52%). Elemental Anal. Calc. for $C_{15}H_{26}N_2S_4Te$: Found C=36.68, H=5.28, N=5.70, S=26.00, Te=25.52%. Calculated C=36.76, H=5.31, N=5.72, S=26.15, Te=26.06%. IR (cm^{-1}):1444 (s), 1382 (m) (ν CN); 1067 (s), 964 (m) (ν CS); 521 (s) (νTeCH$_2$). ^{1}HNMR (CDCl$_3$, δppm): 2.95 (m, 1H, Te-CH), 2.65 (m, 1H, Te-CH$_2$), 1.76 (m, 1H, Te-CCH$_2$), 1.24 (d, 6H, Te-CCH$_3$), 3.81 (t, 2H, N-CH$_2$), 2.01 (m, 3H, N-CCH$_2$). ^{13}CNMR (100.60 MHz, CDCl$_3$, δ ppm): 56.12 (s, Te-CH), 42.46 (s, Te-CH$_2$), 29.75, 19.41 (s, Te-CCH$_2$), 19.22 (s, Te-CCH$_3$), 203.56 (s, S$_2$CN), 51.45 (s, N-CH$_2$), 25.21 (s, N-CCH$_2$). UV/ Vis: 367 nm (ε = 22034 M^{-1} cm^{-1}), 321 nm (ε = 27698 M^{-1} cm^{-1}), 283 nm (ε = 28576 M^{-1} cm^{-1}) and 248 nm (ε = 50432 M^{-1} cm^{-1}).

2.2.4 Synthesis of 1,1,2,3,4,5-Hexahydro-1-Iodo,1-Pyrrolidine dithiocarbamate tellurophene $C_4H_8TeI(S_2CNC_4H_8)$ ***(7)***

The reaction of [$C_4H_8TeI_2$] (1.5g, 1 mmol) and silver salt of pyrrolidine dithiocarbamate (0.87g, 1 mmol) in 30 ml of dichloromethane resulted in compound **(7)**. The result was yellow crystals with a melting point of 120°C and a yield of 1.0g (55%). Elemental Anal. Calc. for $C_9H_{16}INS_2Te$: Found C=23.59, H=3.47, N=3.05, S=13.98, I=27.75, Te=26.84%. Calculated C=23.66, H=3.50, N=3.07, S=14.02, I=27.80, Te=27.95%. IR (cm^{-1}): 1421 (s), 1375 (m) (ν CN); 1084 (s), 940 (m) (ν CS); 576 (s) (νTeCH$_2$). ^{1}HNMR (CDCl$_3$, δ ppm): 3.14 (m, 1H, Te-CH$_2$), 2.01 (m, 3H, Te-CCH$_2$), 3.81 (t, 2H, N-CH$_2$), 2.01 (m, 3H, N-CCH$_2$); ^{13}CNMR (100.60 MHz, CDCl$_3$, δ ppm): 48.34 (s, Te-CH$_2$), 21.79, (s, Te-CCH$_2$), 200.55 (s, S$_2$CN), 51.45 (s, N-CH$_2$), 25.21 (s, N-CCH$_2$). UV/ Vis: 365 nm (ε = 22276 M^{-1} cm^{-1}), 331 nm (ε = 27132 M^{-1} cm^{-1}), 290 nm (ε = 28633 M^{-1} cm^{-1}) and 245 nm (ε = 51287 M^{-1} cm^{-1}).

2.2.5 Synthesis of 1,1,2,3,4,5,6-Heptahydro-1-Iodo,1-Pyrrolidine dithiocarbamate tellurophene $C_5H_{10}TeI(S_2CNC_4H_8)$ ***(8)***

The reaction of [$C_5H_{10}TeI_2$] (1.5g, 1 mmol) and silver salt of pyrrolidine dithiocarbamate (0.84g, 1 mmol) in 30 ml of dichloromethane resulted in compound **(7)**. The result was yellow crystals with a melting point of 130°C and a yield of 1.11g (60%). Elemental Anal. Calc. for $C_{10}H_{18}INS_2Te$: Found C=23.59, H=3.47, N=3.05, S=13.98, I=27.75, Te=26.84%. Calculated C=23.66, H=3.50, N=3.07, S=14.02, I=27.80, Te=27.95%. IR (cm^{-1}): 1407 (s), 1390 (m) (ν CN); 1060 (s), 965 (m) (ν CS); 542 (s) (νTeCH_2). ^{1}HNMR ($CDCl_3$, δ ppm): 2.70 (m, 1H, Te-CH_2), 1.65 (m, 3H, Te-CCH_2), 1.62 (m, 3H, Te-$CCCH_2$), 3.81 (t, 2H, N-CH_2), 2.01 (m, 3H, N-CCH_2); ^{13}CNMR (100.60 MHz, $CDCl_3$, δ ppm): 42.50 (s, Te-CH_2), 26.70, (s, Te-CCH_2), 201.75 (s, S_2CN), 51.45 (s, N-CH_2), 25.21 (s, N-CCH_2). UV/ Vis: 374 nm (ε = 22464 M^{-1} cm^{-1}), 327 nm (ε = 27179 M^{-1} cm^{-1}), 287 nm (ε = 28373 M^{-1} cm^{-1}) and 249 nm (ε = 51287 M^{-1} cm^{-1}).

2.2.6 Synthesis of 2-methyl-1-Iodo,1-Pyrrolidine dithiocarbamate Telluracyclopentane $C_4H_7(CH_3)TeI(S_2CNC_4H_8)$ **(9)**

The reaction of [$C_4H_7(CH_3)TeI_2$] (1.3 g, 1mmol) and silver salt of pyrrolidine dithiocarbamate (0.73g, 1 mmol) in 30 ml of dichloromethane resulted in compound **(8)**. The result was an orange-colored amorphous solid with a melting point of 128°C and a yield of 0.96g (51%). Elemental Anal. Calc. for $C_{10}H_{18}INS_2Te$: Found C=25.47, H=3.75, N=2.90, S=13.53, I=26.91, Te=26.16%. Calculated C=25.50, H=3.83, N=2.98, S=1.60, I=26.97 Te=27.12%. IR (cm^{-1}): 1439 (s), 1381 (m) (ν CN); 1086 (s), 955 (m) (ν CS); 535(s) (νTeCH_2). ^{1}HNMR ($CDCl_3$, δ ppm): 3.00 (m, 1H, Te-CH), 3.00 (m, 1H, Te-CH_2), 1.80 (m, 1H, Te-CCH_2), 1.20 (d, 6H, Te-CCH_3), 3.81 (t, 2H, N-CH_2), 2.01 (m, 3H, N-CCH_2). ^{13}CNMR (100.60 MHz, $CDCl_3$, δ ppm): 61.77 (s, Te-CH), 51.89 (s, Te-CH_2), 29.85, 19.73 (s, Te-CCH_2), 19.73 (s, Te-CCH_3), 202.01 (s, S_2CN), 51.45 (s, N-CH_2), 25.21 (s, N-CCH_2). UV/ Vis: 365 nm (ε = 22464 M^{-1} cm^{-1}), 331 nm (ε = 27421 M^{-1} cm^{-1}), 287 nm (ε = 28373 M^{-1} cm^{-1}) and 251 nm (ε =49875 M^{-1} cm^{-1}).

3 Biological assay

3.1 Test Microbial Strains:

Three microbial strains were chosen for antibacterial and antifungal testing: one Gram-positive bacterium (*Bacillus subtilis*), one Gram-negative bacterium (*Escherichia coli*), and one fungal strain (*Candida albicans*).

3.2 Antimicrobial Potency

The antimicrobial activity of all compounds was assessed using the agar well diffusion method[43]. For the inoculation of bacterial and fungal strains, Luria Bertani and Potato Dextrose agar plates were prepared. The test organisms were evenly distributed on the agar plates. Wells were punched into the agar plates after spreading and filled with 100 l (80 mg/ml) samples. For comparison, standard antibiotics such as *Ciprofloxacin* and *Amphotericin-B* (to which the test organisms were sensitive) were used. All the plates were incubated and stored overnight at 37°C (for bacteria) and 25°C (for yeast) (for fungal strain). Plates were observed for bacterial and fungal growth after incubation. For determining the zone of inhibition, the CLSI (Clinical and Laboratory Standards Institute, USA) guidelines were used. Dimethyl sulfoxide (DMSO) was used as negative control.

4. Computational studies

4.1 Molecular docking:

Molecular docking studies were performed on the crystal structures of Cyclooxygenase-2 (Prostaglandin Synthase-2) and Alpha-haemolysin from *Staphylococcus Aureus* at active sites to determine the possible binding mode and predominant binding interactions. Autodock was used for molecular docking studies to determine the inhibitor's binding free energy inside the target molecule. The protein was prepared using Autodock 4.2. For energy minimization, the ligands $R_2Te(dtc)_2$ and $R_2TeI(dtc)$ were modelled using ChemDraw software and CS Chem. 3D. Three parameters were determined: binding energy, RMSD, and non-covalent interaction (hydrogen bond and hydrophobic interaction).

4.2 Preparation of target compounds for docking:

In-silico interaction analysis of Cyclooxygenase-2 (prostaglandin synthase-2) complexed with a selective inhibitor, SC-558, in the i-222 space group (PDB id: 6COX) as target and representative compound ($C_4H_8Te(S_2CNC_4H_8)_2$ as ligand[44] was performed using Autodock 4.2. Autodock 4.2 was used to initiate protein preparation, with Kollaman charge of -30.00, non-polar H of 11, number of rotatable bonds of 2, and aromatic carbons of 16. Following the preparation of the protein, the ligand was prepared by a total of eight torsions. The size of the grid box was chosen to be 60, 60, 60, with the centre of the grid box for the x, y, and z axes being analysed on a scale of co-ordinate dimension of (24.714*23.857*36.961). Docking preparations include the generation of 27000.

Autodock 4.2 was used once more for the *in-silico* interaction analysis of *Staphylococcus aureus* alpha-haemolysin (PDB id: 7AHL) as target and representative compound ($C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$ as ligand[44]. Autodock 4.2 was used to start the protein preparation, and the

Kollman charge was -29.15, the number of rotatable bonds was 2, and the aromatic carbons were 16. Following the preparation of the protein, the ligand was prepared with a number of torsions as 8. The size of the grid box was set to 90, 70, 70 as the centre of the grid box for the x, y, and z axes, and the scale of co-ordinate dimension was set to (51.064*26.600*48.189). Docking preparations include the generation of 27000.

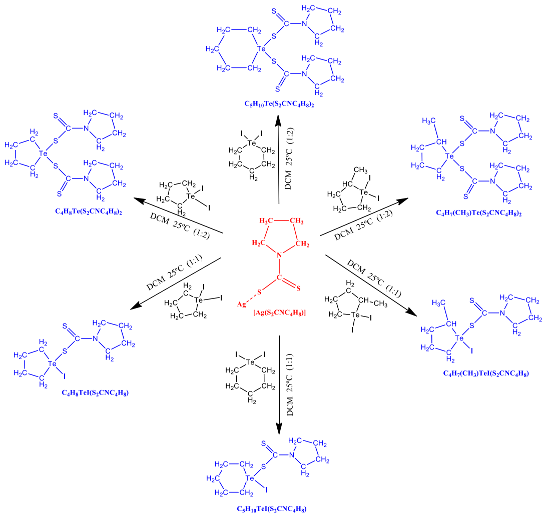
4.3 Identification and confirmation of binding sites: The binding pockets present in the complex, i.e. protein taken, are extremely important in docking for providing a site for the ligand to bind. Literature was used to equate these binding pockets. Following docking, the protein-ligand interactions were investigated with the help of two programmes: Pymol and protein-ligand interaction profiler.

4.4 Density-functional Theory (DFT) simulations

DFT simulations are employed to calculate the optimized geometry, HOMO-LUMO, band gap, electron affinity, electronegativities, and relative stabilities of the synthesized molecules. To find the optimized geometry, we have employed first-principles calculations based on density functional theory within a generalized gradient approximation (GGA). For greater reliability in our results, we use the Perdew–Burke–Ernzerhof [1]45 form of the GGA with quantum espresso package [2]46 based on ultrasoft pseudopotentials [3]47and a plane wave basis. Local minima of the energy landscape are obtained through structural relaxation starting with different initial structures and using Hellman–Feynman forces and stresses [4]48. The kinetic energy cutoff for wavefunctions was 40 Ry, and a gamma-only k-mesh was used in sampling Brillouin zones. Around 20 Å vacuum space was chosen to avoid any interaction between the periodic images.

5. Results and Discussion

The reactions of 1,1,2,3,4,5-Hexa-hydro-1,1-diiodo tellurophene, 1,1,2,3,4,5,6-Hepta-hydro-1,1-diiodo tellurane, and 2-Methyl-(1,1,2,3,4,5-Hexahydro-1,1-diiodo tellurophene) with the silver salts of pyrrolidine dithiocarbamate in dichloromethane produced the corresponding disubstituted compounds: $C_4H_8Te[S_2CN(C_4H_8)_2]$ **(4)**, $C_5H_{10}Te[S_2CN(C_4H_8)_2]$ **(5)**, and $C_4H_7(CH_3)Te[S_2CN(C_4H_8)_2]$ **(6)** and mono-substituted compounds: $C_4H_8TeI[S_2CN(C_4H_8)]$ **(7)**, $C_5H_{10}TeI[S_2CN(C_4H_8)]$ **(8)** and $C_4H_7(CH_3)TeI[S_2CN(C_4H_8)]$ **(9)**. All the compounds were solids and were soluble in common organic solvents such as $CHCl_3$, $(C_2H_5)_2O$, and C_6H_6. All the compounds were stable at room temperature. Furthermore, while these compounds are stable as solid samples for long periods of time, they decompose slowly in solution. IR, multinuclear NMR (^1H and ^{13}C), and U.V spectroscopy were used to characterize the compounds. At room temperature, the molar conductance values of the synthesised complexes in DMSO ranged from 1.13 to 1.28 ohm^{-1} cm^2 mol^{-1}, indicating that they are non-electrolytes. Isolated yields, melting points, analytical data, and molar conductance for the newly synthesised complexes are listed (Table 2). The reactions involved in the synthesis are depicted in the diagram below **(Scheme 1)**.



Scheme 1. Synthetic route of Dithiocarbamate compounds

Table 2. Characterization data of Organotellurium dithiocarbamates

Comp.	Molecular formula	Colour	m. w.	Yield (%)	m.p. (ºC)	Elemental analysis (%) : found (calculated)						Molar conductivity
						C	H	N	S	I	Te	
4	$[C_4H_8Te(S_2CNC_4H_8)_2]$	Orange	475.6	80 %	118 ºC	35.27 (35.32)	4.97 (5.05)	5.85 (5.90)	26.79 (26.91)		26.16 (26.82)	1.19
5	$[C_5H_{10}Te(S_2CNC_4H_8)_2]$	Yellow	489.6	73 %	146 ºC	36.60 (36.76)	5.20 (5.31)	5.67 (5.72)	26.00 (26.15)		25.52 (26.06)	1.13
6	$[C_4H_7(CH_3)Te(S_2CNC_4H_8)_2]$	Yellow	489.6	52 %	100 ºC	36.68 (36.76)	5.28 (5.31)	5.70 (5.72)	26.00 (26.15)		25.52 (26.06)	1.20
7	$[C_4H_8TeI(S_2CNC_4H_8)]$	Yellow	456.5	55 %	120 ºC	23.59 (23.66)	3.47 (3.50)	3.05 (3.07)	13.98 (14.02)	27.75 (27.80)	26.84 (27.95)	1.28
8	$[C_5H_{10}TeI(S_2CNC_4H_8)]$	Orange	470.5	60 %	130 ºC	25.47 (25.50)	3.75 (3.83)	2.90 (2.98)	13.53 (1.60)	26.91 (26.97)	26.16 (27.12)	1.25
9	$[C_4H_7(CH_3)TeI(S_2CNC_4H_8)]$	Orange	470.5	51 %	128 ºC	25.47 (25.50)	3.75 (3.83)	2.90 (2.98)	13.53 (1.60)	26.91 (26.97)	26.16 (27.12)	1.27

5.1 Spectroscopic Studies

5.1.1 IR Spectroscopy:

The IR (KBr) spectra of the reported compounds **(4-9)** were assigned by comparing them to similar compounds reported in the literature [49-53] (**Table 3**). The spectra of all newly synthesized organotellurium dithiocarbamates show sharp absorptions in the range 1375-1444 cm^{-1}, which is associated with the $N-CS_2$ stretching mode, indicating the shifting of the C-N of the NCS_2 group towards higher energies due to strong delocalization of electrons in the dithiocarbamate moiety. The presence of a C-S absorption band is a feature of the dithiocarbamate ligand's coordination mode[51]. Two signals of medium intensity were observed in the reported compounds **(4-9)** due to the stretching mode of the νC-S bonds in the regions 960±20 cm^{-1} and 1052±34 cm^{-1}, respectively. The difference in wave numbers between these two bands is greater than 20 cm^{-1}, indicating that the dithiocarbamate ligands are monodentately coordinated to tellurium.[53] The $\nu(TeCH_2)$ of the C_4H_8Te group appears in their standard positions.

Table 3. IR Spectroscopy data of Organotellurium dithiocarbamates

S. No	Complex	υ(C-N) in cm^{-1}	υ(C-S) cm^{-1}	υ(Te-CH_2) cm^{-1}
4	$[C_4H_8Te(S_2CNC_4H_8)_2]$	1435 (s) 1398 (s)	1018 (s) 980(m)	546(s)
5	$[C_5H_{10}Te(S_2CNC_4H_8)_2]$	1429 (s) 1378 (s)	1034 (s) 960(m)	563(s)
6	$[C_4H_7(CH_3)Te(S_2CNC_4H_8)_2]$	1444 (s) 1382 (s)	1067 (s) 964(m)	521(s)
7	$[C_4H_8TeI(S_2CNC_4H_8)]$	1421 (s) 1375 (s)	1084 (s) 940(m)	576(s)
8	$[C_4H_7(CH_3)TeI(S_2CNC_4H_8)]$	1407 (s) 1390 (s)	1060 (s) 965(m)	542(s)
9	$[C_4H_7(CH_3)TeI(S_2CNC_4H_8)]$	1439 (s) 1381 (s)	1086 (s) 955(m)	535(s)

5.1.2 ^{1}H-NMR Spectroscopy:

The absorption and integration of the tellurocycle group and the dithiocarbamate ligands observed in the ^{1}H-NMR spectra of the synthesised novel organotellurium compounds (**Table 4**), correspond to what is expected for mono and disubstituted compounds. The chemical shifts for $\delta(Te-CH_2)$ and δ $(Te-C-CH_2)$ were detected as multiplets in the ^{1}H-NMR spectra of compounds **(4-8)**. The signals corresponding to $\delta(Te-CH_2)$ appear in the range of 2.65 to 3.14 ppm, while the signals corresponding to δ $(Te-C-CH_2)$ appear in the range of 1.62 to 2.01 ppm. Furthermore, the signals corresponding to δ $(N-CH_2)$ appear as a 3.81 ppm triplet, and the signals corresponding to $\delta(N-C-CH_2)$ appear as a multiplet with a single value of 2.01 in all compounds. The signals corresponding to δ $(Te-C-C-CH_2)$ were spotted as a 1.62 ppm multiplet in compound **(5,8)**, and the signals corresponding to δ (Te-CH) appeared as a multiplet in the range 2.95 to 3.00 ppm in compounds **(6,9)**, and the signals corresponding to $\delta(Te-C-CH_3)$ appeared as a doublet in the range 1.20 to 1.24 ppm.

Table 4.^{1}HNMR spectral data of Organotellurium dithiocarbamates

S. No	Complex	δ(Te-CH) (ppm)	δ(Te-CH₂) (ppm)	δ(Te-C-CH₂) (ppm)	δ(Te-C-CH₃) (ppm)	δ(Te-C-C-CH₂) (ppm)	δ(N-CH₂) (ppm)	δ(N-C-CH₂) (ppm)
4	$[C_4H_8Te(S_2CNC_4H_8)_2]$		2.68 (m)	2.00 (m)			3.81 (t)	2.01 (m)
5	$[C_5H_{10}Te(S_2CNC_4H_8)_2]$		2.71 (m)	1.62 (m)		1.62 (m)	3.81 (t)	2.01 (m)
6	$[C_4H_7(CH_3)Te(S_2CNC_4H_8)_2]$	2.95 (m)	2.65 (m)	1.76 (m)	1.24 (d)		3.81 (t)	2.01 (m)
7	$[C_4H_8TeI(S_2CNC_4H_8)]$		3.14 (m)	2.01 (m)			3.81 (t)	2.01 (m)
8	$[C_5H_{10}TeI(S_2CNC_4H_8)]$		2.70 (m)	1.65 (m)		1.62 (m)	3.81 (t)	2.01 (m)
9	$[C_4H_7(CH_3)TeI(S_2CNC_4H_8)]$	3.00 (m)	3.00 (m)	1.80 (m)	1.20 (d)		3.81 (t)	2.01 (m)

*5.1.3 ^{13}**C-NMR Spectroscopy**:*

Furthermore, the ^{13}C-NMR spectra of compounds **(4-9)** (**Table 5**) show a signal of the nitrogen atom attached to the methylene carbons δ (N-CH_2) as a singlet at 51.[44] ppm. The signals corresponding to δ (N-C-CH_2) appear as a singlet at 25.21 ppm. Furthermore, signals corresponding to δ (Te-CH_2) and δ (Te-C-CH_2) were detected as singlets, with δ (Te-CH_2) ranging from 39.21 to 51.89 ppm and δ (Te-C-CH_2) ranging from 19.41 to 29.85 ppm, respectively. In comparison to the remaining signals, the signals corresponding to δ (S_2CN) carbon atoms are relatively weak and appear as a singlet in the range 200.55 to 203.56 ppm. The signals corresponding to δ (Te-C-C-CH_2) were detected as a 32.30 ppm singlet in compound **(5, 8)**. Furthermore, the signals corresponding to δ (Te-CH) and δ (Te-C-CH_3) were detected as a singlet in compounds **(6,9)**. The signals for δ (Te-CH) appear between 56.12 and 61.77 ppm, and for (Te-C-CH_3) between 19.22 and 19.73 ppm.

Table 5.^{13}CNMR spectral data of Organotellurium dithiocarbamates

S. No	Complex	δ(Te-CH₂) (ppm)	δ(Te-C-CH₂) (ppm)	δ(S₂-CN) (ppm)	δ(Te-CH) (ppm)	δ(Te-C-CH₃) (ppm)	δ(Te-C-C-CH₂) (ppm)	δ(N-CH₂) (ppm)	δ(N-C-CH₂) (ppm)
4	$[C_4H_8Te(S_2CNC_4H_8)_2]$	39.21 (s)	21.34 (s)	202.71 (s)				51.45 (s)	25.21 (s)
5	$[C_5H_{10}Te(S_2CNC_4H_8)_2]$	39.67 (s)	26.38 (s)	202.25 (s)			32.30 (s)	51.45 (s)	25.21 (s)
6	$[C_4H_7(CH_3)Te(S_2CNC_4H_8)_2]$	42.46 (s)	29.75 (s) 19.41 (s)	203.56 (s)	56.12 (s)	19.22 (s)		51.45 (s)	25.21 (s)
7	$[C_4H_8TeI(S_2CNC_4H_8)]$	48.34 (s)	21.79 (s)	200.55 (s)				51.45 (s)	25.21 (s)
8	$[C_5H_{10}TeI(S_2CNC_4H_8)]$	42.50 (s)	26.70 (s)	201.75 (s)			32.30 (s)	51.45 (s)	25.21 (s)
9	$[C_4H_7(CH_3)TeI(S_2CNC_4H_8)]$	51.89 (s)	29.85 (s) 19.73 (s)	202.01 (s)	61.77 (s)	19.73 (s)		51.45 (s)	25.21 (s)

5.1.4 UV-Vis Spectroscopy:

When the electronic spectra of the novel organotellurium dithiocarbamate are compared to the corresponding sodium salts of dithiocarbamic acid, it was found that the absorption around 250 nm in the spectra of the compounds, is due to the transition located in the CS_2 group of the ligand.[55-57] The presence of a single intense absorption at 250±5 nm in the spectra of all novel dithiocarbamate derivatives **(4-9)** (**Table 6**) suggests that dithiocarbamate groups are monodentate.

Table 6. U-V spectroscopy data of Organotellurium compounds

Comp.	Complex	Wavelength (λ) (nm)	Absorbance(A) (A.U.)	$\varepsilon_{max} = (A / c\,l)$ (M^{-1} cm^{-1})
4	$[C_4H_8Te(S_2CNC_4H_8)_2]$	x_1= 253 x_2= 287 x_3= 322 x_4= 355	y_1= 4.8927 y_2= 2.6745 y_3= 2.5798 y_4= 2.2375	$\varepsilon_{1\,max}$ = 48927 $\varepsilon_{2\,max}$ = 26745 $\varepsilon_{3\,max}$ = 2.5798 $\varepsilon_{4\,max}$ = 2.2375
5	$[C_5H_{10}Te(S_2CNC_4H_8)_2]$	x_1= 255 x_2= 285 x_3= 324 x_4= 360	y_1= 4.9621 y_2= 2.8738 y_3= 2.7655 y_4= 2.2246	$\varepsilon_{1\,max}$ = 49621 $\varepsilon_{2\,max}$ = 28738 $\varepsilon_{3\,max}$ = 27655 $\varepsilon_{4\,max}$ = 22246
6	$[C_4H_7(CH_3)Te(S_2CNC_4H_8)_2]$	x_1= 248 x_2= 283 x_3= 321 x_4= 367	y_1= 5.0432 y_2= 2.8576 y_3= 2.7698 y_4= 2.2034	$\varepsilon_{1\,max}$ = 50432 $\varepsilon_{2\,max}$ = 28576 $\varepsilon_{3\,max}$ = 27698 $\varepsilon_{4\,max}$ = 22034
7	$[C_4H_8TeI(S_2CNC_4H_8)]$	x_1= 245 x_2= 290 x_3= 331 x_4= 365	y_1= 5.1287 y_2= 2.8633 y_3= 2.7132 y_4= 2.2276	$\varepsilon_{1\,max}$ = 51287 $\varepsilon_{2\,max}$ = 28633 $\varepsilon_{3\,max}$ = 27132 $\varepsilon_{4\,max}$ = 22276
8	$[C_5H_{10}TeI(S_2CNC_4H_8)]$	x_1= 249 x_2= 281 x_3= 327 x_4= 374	y_1= 4.9001 y_2= 2.7924 y_3= 2.7179 y_4= 2.2560	$\varepsilon_{1\,max}$ = 49001 $\varepsilon_{2\,max}$ = 27924 $\varepsilon_{3\,max}$ = 27179 $\varepsilon_{5\,max}$ = 22560
9	$[C_4H_7(CH_3)TeI(S_2CNC_4H_8)]$	x_1= 251 x_2= 287 x_3= 331 x_4= 365	y_1= 4.9875 y_2= 2.8373 y_3= 2.7421 y_4= 2.2464	$\varepsilon_{1\,max}$ = 49875 $\varepsilon_{2\,max}$ = 28373 $\varepsilon_{3\,max}$ = 27421 $\varepsilon_{5\,max}$ = 22464

5.2 Antimicrobial Potency Studies:

In this study, three synthesized compounds **(4-6)** were evaluated against *Bacillus subtilis, Escherichia coli* and *Candida albicans* for their antimicrobial potency. All the tested compounds showed good antibacterial activities. Standard commercial drugs *Ciprofloxacin* and *Amphotericin-B* were used to compare the antibacterial activities and antifungal activities shown by the synthesized complexes (**Table-7**). $[C_4H_8Te(S_2CNC_4H_8)_2]$ **(4)** showed good activity against Gram-negative bacteria (*E. Coli*) and the diameter of the inhibition zone were studied as 14 (mm)^a and $[C_5H_{10}Te(S_2CNC_4H_8)_2]$ **(5)** showed good activity against (*Bacillus subtilis*), and the diameter of inhibition were noted as 16 (mm)^a. The good activity of synthesized compounds can be explained based on the diffusion of the metal complexes into the bacterial cells, thus stopping the unknown metabolic pathway. The good activity may also be defined in terms of increased lipophilicity. None of the compounds was found to be effective against the fungal stain *Candida albicans.*

Table 7. Zone of inhibition shown by the synthesized complexes and standard drugs

S. No.	Complex Name	Diameter of inhibition zone (mm)^a		
		Gram -ve Bacteria	Gram +ve Bacteria	Fungal Strain
		Escherichia coli	*Bacillus subtilis*	*Candida albicans*

4.	$C_4H_8Te(S_2CNC_4H_8)_2$	14	14	NT
5.	$C_5H_{10}Te(S_2CNC_4H_8)_2$	12	16	NT
6.	$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$	10	15	NT
Amphotericin-B		-	-	26
Ciprofloxacin		18	20	-

5.3 Molecular Docking

5.3.1 Docking result of [$C_4H_8Te(S_2CNC_4H_8)_2$]:

Autodock 4.2 docking findings for cyclooxygenase-2 (prostaglandin synthase-2) (PDB id: 6COX) with [$C_4H_8Te(S_2CNC_4H_8)_2$] **(4)** have been given in Table 8. Run 4 had the lowest binding energy of -7.78 kcal/mol and the smallest RMSD of 55.94 of the top ten runs. The image depicts the hydrogen and hydrophobic bond interactions of cyclooxygenase-2 (prostaglandin synthase-2) with ligands (PDB id: 6COX) (**Figure 7**). The interaction of the ligand with the oxygen atom of methionine and the N of the ligand with 3.06 distances clearly indicated the H-bond. All the amino acids, viz., valine, leucine, tyrosine, and alanine have been found to have hydrophobic interactions.

Table 8. The Binding energy values of [$C_4H_8Te(S_2CNC_4H_8)_2$] as ligand and cyclooxygenase-2 (prostaglandin synthase-2) (Pdb id: 6COX) as target protein were obtained via a docking study.

Sr. No.	Run	Binding energy score	RMSD
1	1	-5.14	51.37
2	2	-4.07	54.05
3	3	-4.51	62.39
4	4	-7.78	55.94
5	5	-4.08	52.87
6	6	-6.36	53.34
7	7	-4.74	53.02
8	8	-7.70	43.96
9	9	-5.86	53.91
10	10	-7.44	43.86

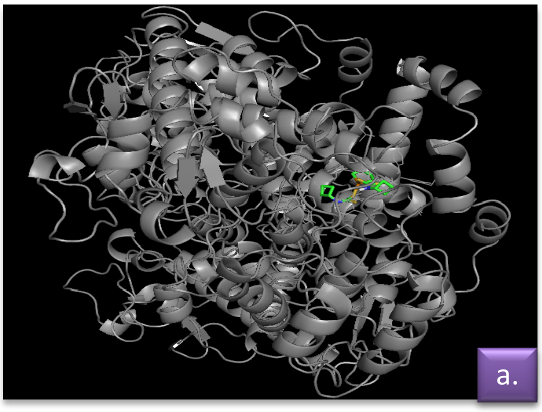


Fig 7 (a) Cyclooxygenase-2 binding pose with [$C_4H_8Te(S_2CNC_4H_8)_2$] (Pdb id: 6 COX) (b) Cyclooxygenase-2 (prostaglandin synthase-2) (Pdb id: 6 COX) 2-D Interaction diagram with [$C_4H_8Te(S_2CNC_4H_8)_2$]

5.3.2 Docking result of [$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$]:

The docking findings of Alpha-Haemolysin from *Staphylococcus Aureus* (Pdb id: 7AHL) with [$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$] **(6)**, as determined by Autodock 4.2, are presented in the table 9. With binding energy of 6.01 kcal/mol and RMSD of 73.40, Run 7 was found to be the best among the best 10 runs. The interaction of Alpha-Haemolysin from *Staphylococcus Aureus* (Pdb id: 7AHL) with ligands via hydrogen and hydrophobic bonding is described in the figure 8. The results show that the H-bond with oxygen atom of aspartic acid and N of ligand has 2.90, the H-bond with the O atom of valine has a distance of 2.34, the H-bond with O atom of glutamine has a distance of 2.10, and another H-bond with the O atom of Asparagines has a distance of 3.62 & 3.45. Thus, the amino acids threonine, phenylalanine, and asparagines have a hydrophobic interaction with the ligand. These interactions show that the ligand has a high affinity for the receptor.

Table 9. The binding energy values of [$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$ as ligand and Alpha-Haemolysin from *Staphylococcus Aureus* (Pdb id: 7AHL) as target protein were obtained via docking study.

Sr. No.	Run	Binding energy score	RMSD
1	1	-4.70	83.27
2	2	-3.19	79.63
3	3	-3.55	74.72
4	4	-4.45	65.23

5	5	-3.86	72.35
6	6	-3.23	82.44
7	7	-6.01	73.40
8	8	-4.84	87.21
9	9	-3.76	83.62
10	10	-3.96	80.33

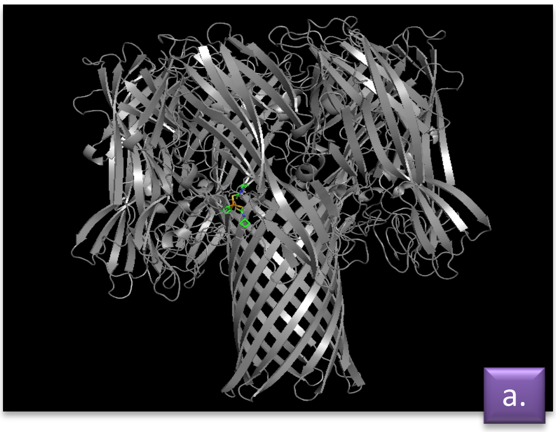


Fig 8. (a) *Staphylococcus Aureus* Alpha Haemolysin binding pose with [$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$ (Pdb id: 7AHL) (b) *Staphylococcus Aureus* Alpha Haemolysin (Pdb id: 7AHL) 2-D interaction diagram with [$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$]

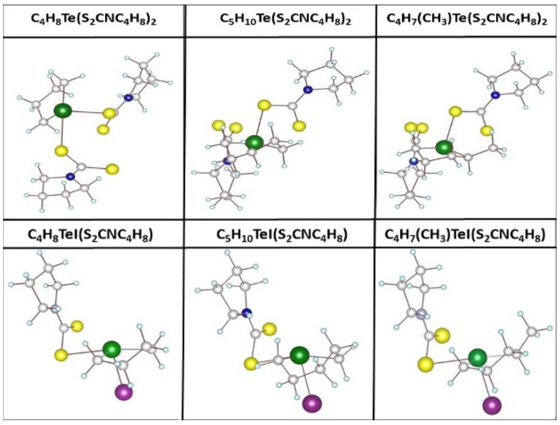


Figure 9: The optimized structure of the compounds as found using the DFT calculations.

Molecule/Bond	Te-S (P)	Te-S (S)	Te-C	C-N (C)	(S) C-N	C-H	C-S	C-S (Te)	Te-I	Energy/atom (Ry)
[$C_4H_8Te(S_2CNC_4H_8)_2$]	2.601(2.611)	4.179(4.324)	2.229 (2.269)	1.513 (1.527)	1.423 (1.426)	1.133	1.668	1.793 (1.796)	NA	-21.55
[$C_5H_{10}Te(S_2CNC_4H_8)_2$]	2.639	4.110(4.438)	2.236 (2.256)	1.523 (1.532)	1.429 (1.437)	1.137	1.670 (1.672)	1.787	NA	-20.64
[$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$]	2.639(2.645)	4.160(4.264)	2.293 (2.252)	1.532 (1.535)	1.430 (1.438)	1.132	1.673 (1.679)	1.780 (1.786)	NA	-20.64
[$C_4H_8TeI(S_2CNC_4H_8)$]	2.537	3.833	2.228 (2.253)	1.523	1.426	1.133	1.674	1.783	2.938	-37.47
[$C_5H_{10}TeI(S_2CNC_4H_8)$]	2.841	3.205	2.248 (2.280)	1.527	1.422	1.134	1.719	1.726	2.862	-33.56
[$C_4H_7(CH_3)TeI(S_2CNC_4H_8)$]	2.624	3.926	2.228 (2.326)	1.523 (1.525)	1.418	1.125 (1.136)	1.679	1.78	2.913	-33.56

The I-containing molecules seem more stable compared to their no-I counterparts. The bond-lengths of bonds are roughly the same in similar compounds.

5.3.3 DFT Results

The relaxed geometry of the molecules is shown as Figure 9, and the bond lengths of various bonds is shown as Table 1. Our DFT calculations clearly indicate the formation of one primary (P) and one secondary (S) bond between Te and S.

Green, magenta, navy blue, white, yellow and blue balls are representing Te, I, N, C, S and H atoms

Table 10: Bond-length of bonds between various elements in the molecule. As the molecules contain more than one bond between same elements, the maximum and minimum bond-lengths given in the table. Total energy per atom for each molecule is also presented in the Table 10.

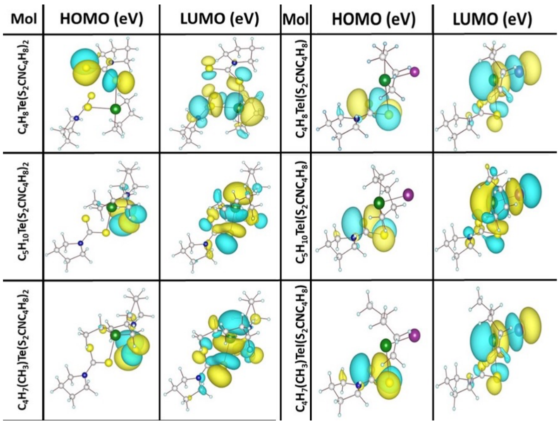


Figure 10: The HOMO and LUMO of synthesized compounds.

Furthermore, the energies of HOMO and LUMO are found (Figure 10), and the band gap E_g is calculated as the difference between HOMO and LUMO. Electronegativity and electronic affinity can be calculated respectively from the two relationships (2) and (3)[58,59]

$$E_g = E_{HOMO} - E_{LUMO} \quad (1)$$

$$X = \frac{E_{HOMO-}E_{LUMO}}{2} \quad (2)$$

Our results show that the HOMO energies follow the trend of increasing energy for compounds
6 > 4 > 5 > 8 > 9 > 7,
whereas the LUMO energies for compounds can be arranged as follows:
5 > 6 > 4 > 9 > 8 > 7,
the band-gap for the compounds increases in order 7 > 9 > 8 > 5 > 6 > 4, and electronegativity decreases as 4 > 5 > 6 > 7 > 9 > 8.
According to Koopman's theory, the following Eq. (3) and (4)[60] can express the ionization potential and electron affinity, as shown in Table -11.

$$I.P = - E_{HOMO} \quad (3)$$

$$E.A = E_{LUMO} \quad (4)$$

Our results show the highest I.P for 5, whereas the lowest value is shown by 8. From Eq. (3), it is clear that E. A will follow the same trend as shown by E_{LUMO}.

Table 11: For synthesized molecules the electronic states, i.e. E_{HOMO}, E_{LUMO}, and E_g are given in eV.

S.No	Synthesized Compound	E_{HOMO} (eV)	E_{LUMO} (eV)	E.A (eV)	I.P (eV)	X = (E_{HOMO} +E_{LUMO})/2	E_g= (E_{HOMO} - E_{LUMO})
4	$C_4H_8Te(S_2CNC_4H_8)_2$	-3.6499	-3.3738	-3.3738	3.6499	-3.5809	0.2761
5	$C_5H_{10}Te(S_2CNC_4H_8)_2$	-3.7683	-3.3101	-3.3101	3.7683	-3.5392	0.4582
6	$C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$	-3.6145	-3.3363	-3.3363	3.6145	-3.5119	0.2782
7	$C_4H_8TeI(S_2CNC_4H_8)_2$	-3.1766	-2.5468	-2.5468	3.1766	-2.8617	0.6298
8	$C_5H_{10}TeI(S_2CNC_4H_8)_2$	-3.0095	-2.4119	-2.4119	3.0095	-2.7107	0.5976
9	$C_4H_7(CH_3)TeI(S_2CNC_4H_8)_2$	-3.0317	-2.4073	-2.4073	3.0317	-2.7195	0.6244

The Electron affinity (E.A), Ionization potentials (I.P) and electronegativity (X) are also given for the organotellurium compounds.

5. Conclusion

Six novel organotellurium dithiocarbamates were synthesised with good yields using silver dithiocarbamate salts. The synthesis of the expected monosubstituted and disubstituted novel organotellurium dithiocarbamates was confirmed by elemental, structural and spectral analysis. The dithiocarbamate moiety in all these novel tellurium complexes exhibits monodentate chelating ligand behaviour. In biological studies, none of the synthesised organotellurium dithiocarbamate complexes were found to be effective against the fungal stain *Candida albicans*; however, some of the complexes exhibited good antibacterial activity. *In-silico* molecular docking studies of the synthesised organotellurium dithiocarbamate $[R_2Te(S_2CNC_4H_8)_2]$ & $[R_2TeI(S_2CNC_4H_8]$ (where R=C_4H_8, C_5H_{10}, & $C_4H_7(CH_3)$) with cyclooxygenase-2 (prostaglandin synthase-2) and Alpha-Haemolysin was also carried out in this research. The compounds were evaluated based on their RMSD values and binding energies. In general, RMSD values are used to analyze protein stability and predict protein conformational changes. The binding interaction and energy between protein and ligand influence the RMSD values. Furthermore, the optimized protein has the lowest RMSD values.

We therefore, conclude that among the six novel synthesized organotellurium dithiocarbamates, $C_4H_8Te(S_2CNC_4H_{10})_2$ **(4)** with cyclooxygenase-2 (prostaglandin synthase-2) and $C_4H_7(CH_3)Te(S_2CNC_4H_8)_2$ **(6)** with *Staphylococcus Aureus* Alpha-Haemolysin gives the best binding energies and RMSD values. The supramolecular associations formed by the cooperative participation of intramolecular Te----S and intermolecular Te----S secondary bonds containing pyrrolidine dithiocarbamate groups may be useful as ‘‘rescue agents." Furthermore, based on a comparison of supramolecular associations of organotellurium (IV) pyrrolidine dithiocarbamates (Table-12), it appears that any change in the organic group (e.g., in the current investigation from $C_4 \rightarrow C_5$ system) attached to tellurium most likely determines the nature and pattern of the supramolecular associations present in these organotellurium (IV) complexes.

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Conflict of Interest

The authors declare that there is no conflict of interest regarding this manuscript

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