

Antibacterial and Molecular Study of Thiourea Derivative Ligand and its Dimethyltin(IV) Complex with the Superior of its Copper(II) Complex as a Hepatocellular Antitumor Drug

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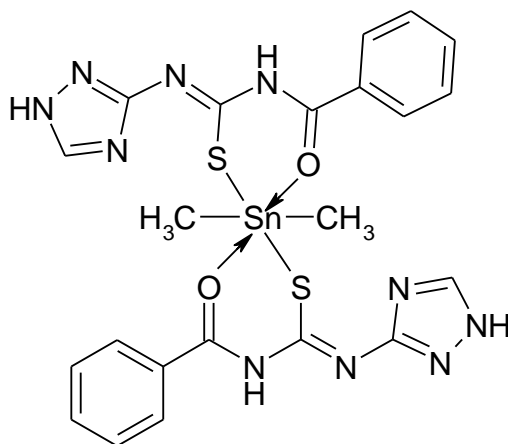


Figure 1. The suggested structure for $\text{Me}_2\text{Sn(IV)} (\text{BTThU})_2$ complex

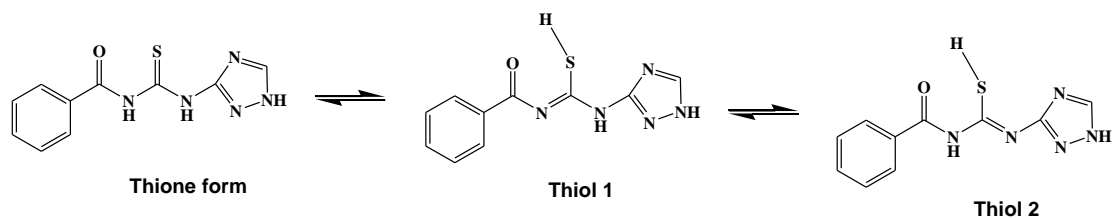


Figure 2. Tautomers of BTThU

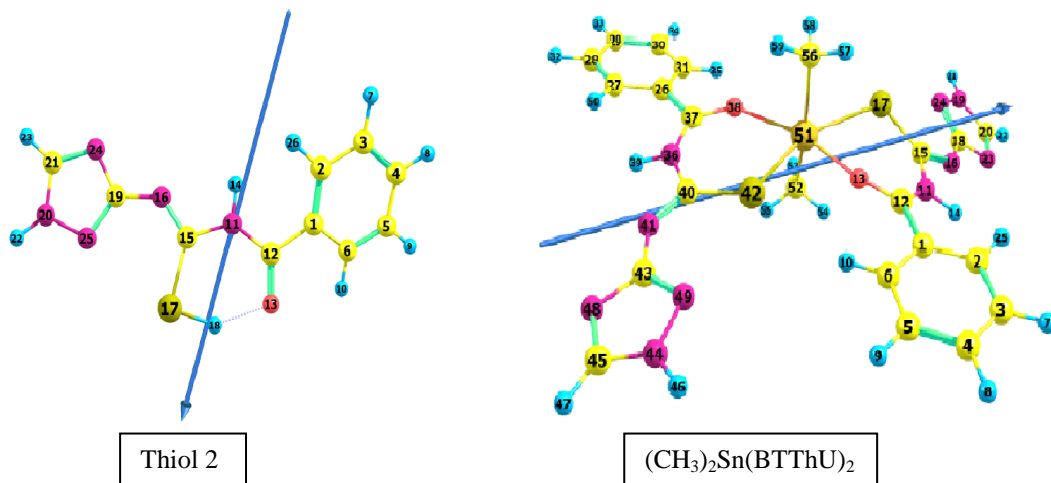


Figure 3. (a) Optimized geometry with the arrows representing the dipole moments

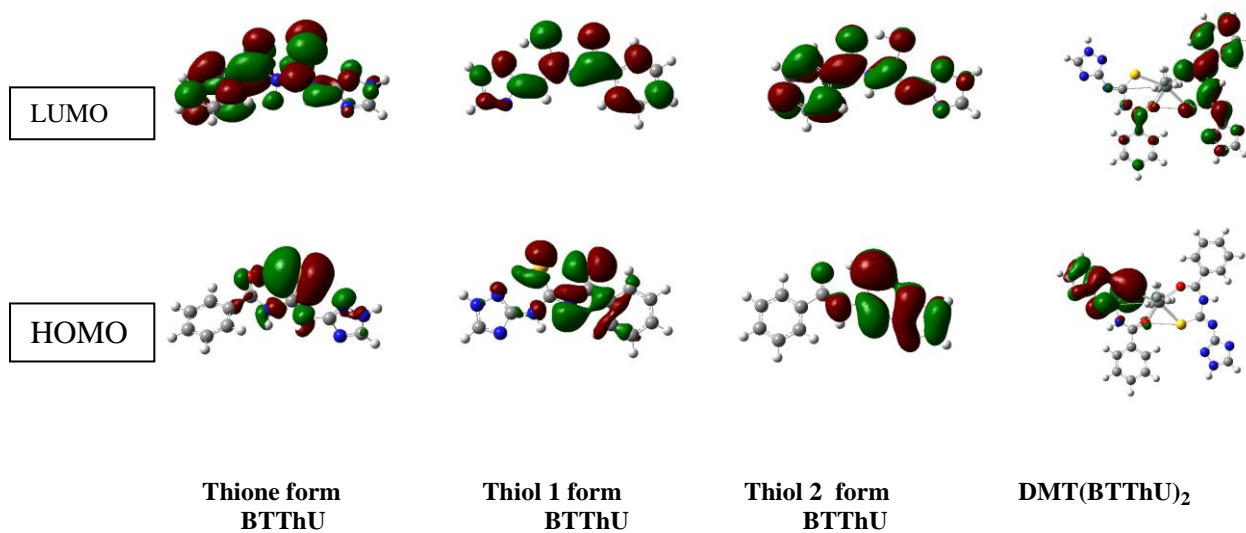


Figure 3. (b) Highest occupied molecular orbitals and lowest unoccupied molecular orbitals

Molecular graphs of BTThU and DMT(BTThU)₂

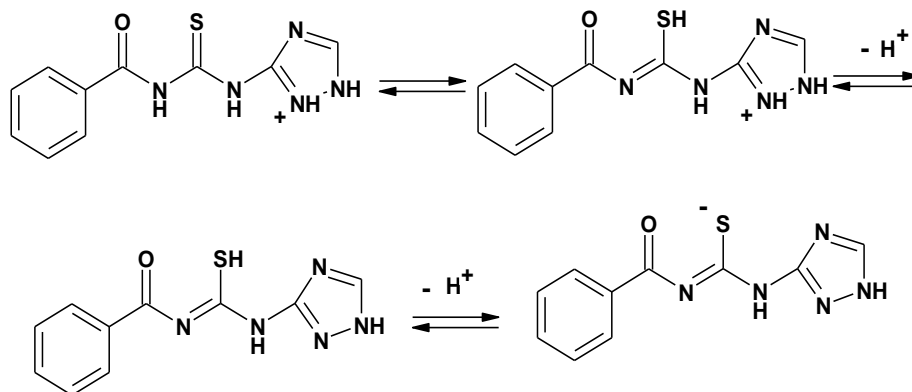


Figure 4. The acid dissociation constants of 1-benzoyl(1,2,4-triazol-3-yl)thiourea [BTThU] (H_2L^+)

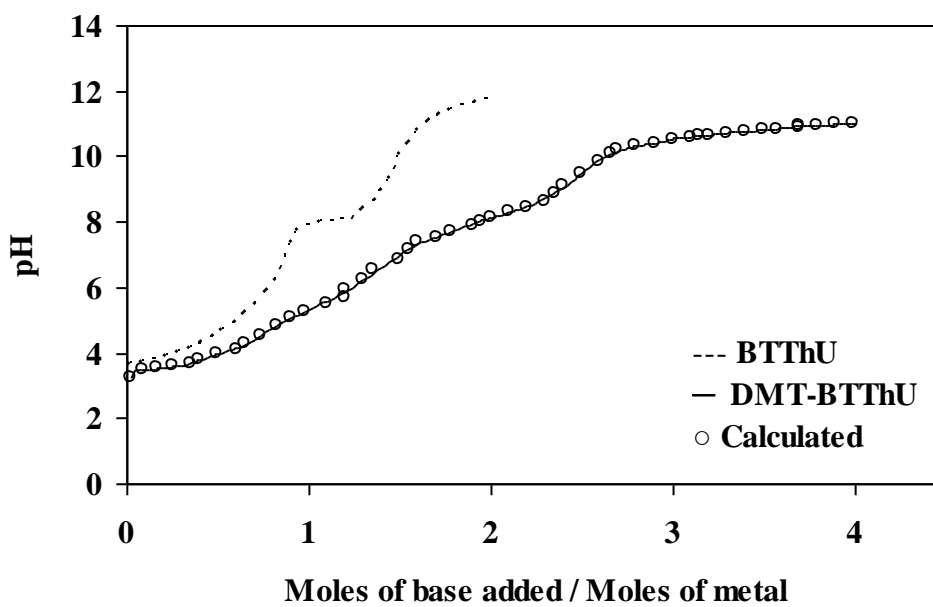


Figure 5. Potentiometric titration curve of 0.05 mmoles of [(Methyl)₂Sn(IV)- BTThU] complexes at 25°C.

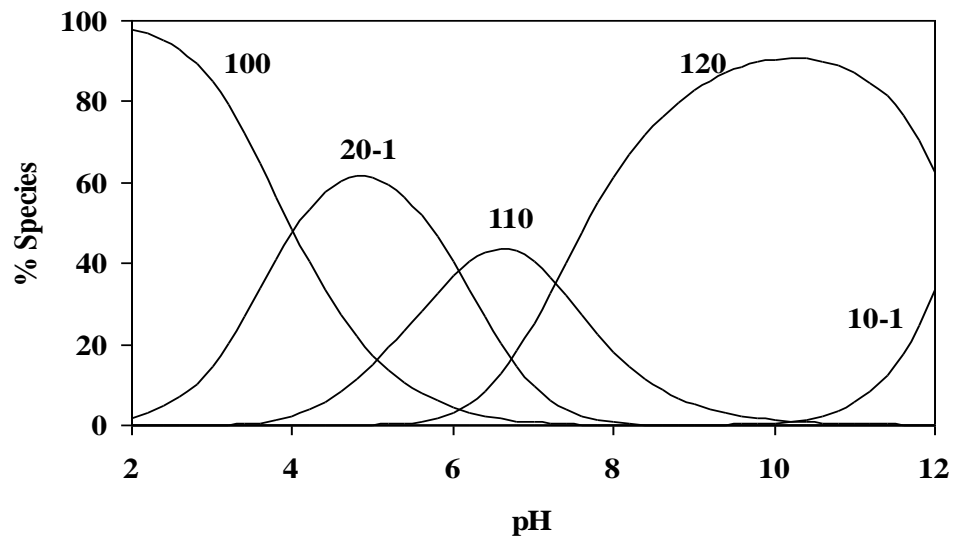


Figure 6. Speciation distribution of DMT- BTThU system as a function of pH at 25 °C with concentration of 1.25 mmole/liter for DMT and 2.5 mmole/liter for BTThU.

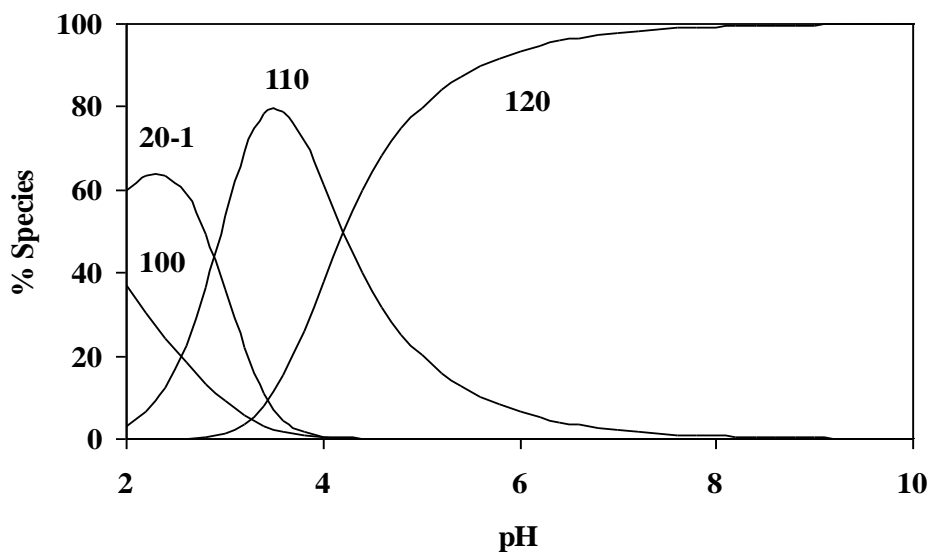


Figure 7. Speciation distribution of DBT- BTThU system as a function of pH at 25 °C with concentration of 1.25 mmole/liter for DBT and 2.5 mmole/liter for BTThU.

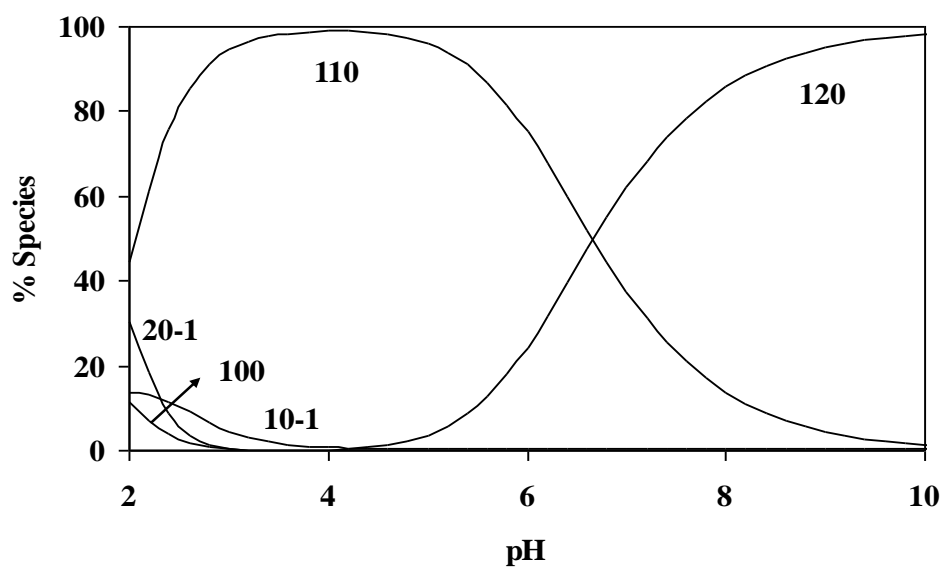


Figure 8. Speciation distribution of DPT- BTThU system as a function of pH at 25 °C with concentration of 1.25 mmole/liter for DPT and 2.5 mmole/liter for BTThU.

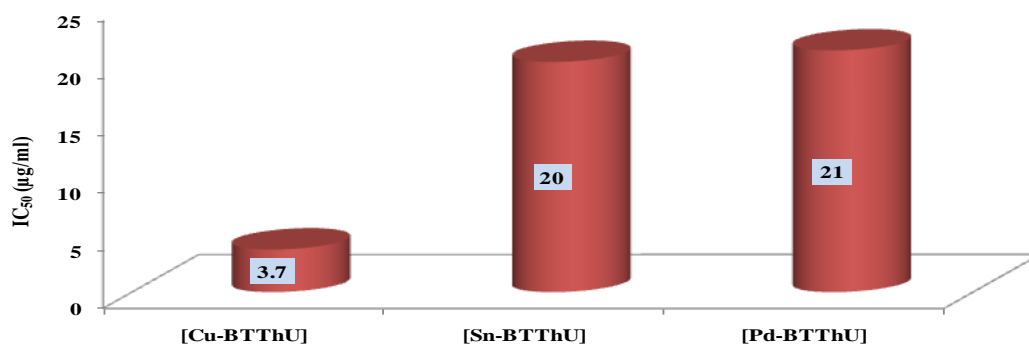
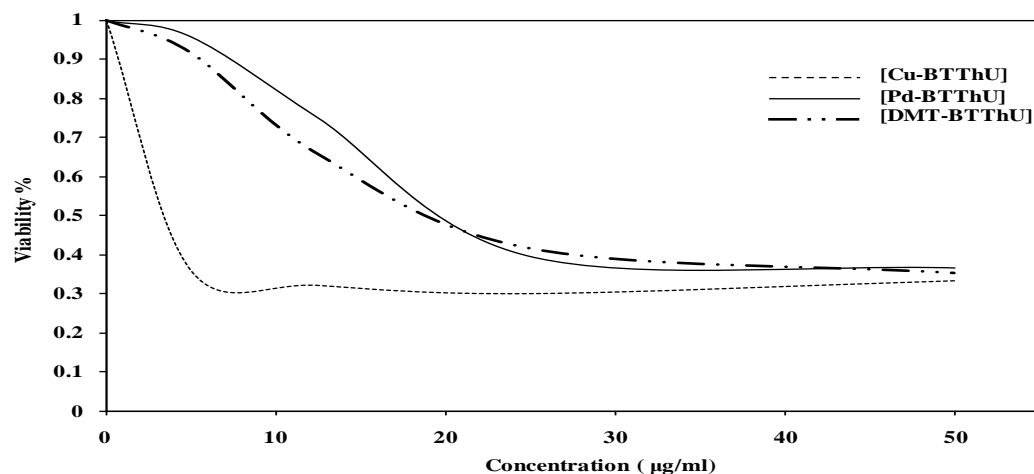


Figure 9. The cell viability (HepG2 human liver cancer) with the concentration change of the suggested drugs complexes. IC₅₀ values of the suggested complexes.

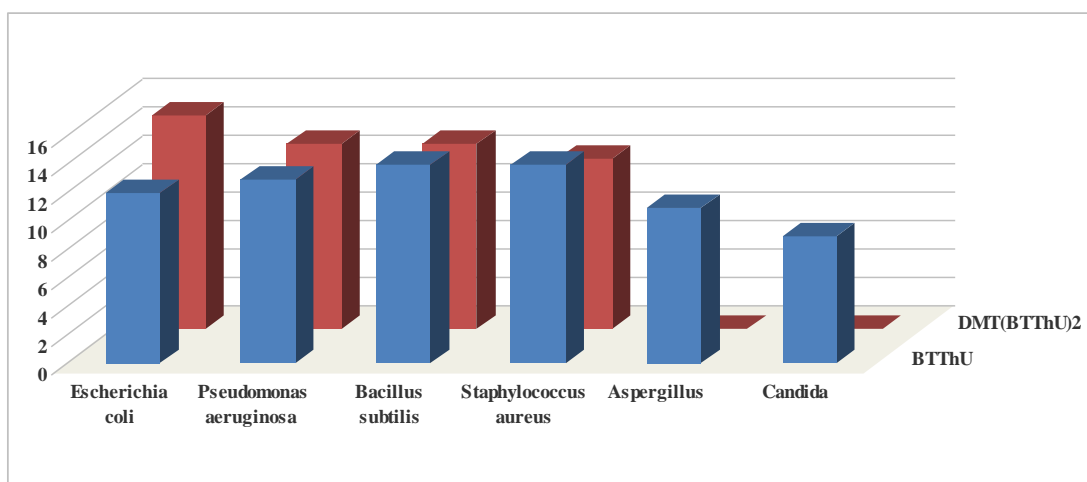


Figure 10. Biological activity of the DMT(BTThU)₂ complex towards different types of bacterial and antifungal strain.

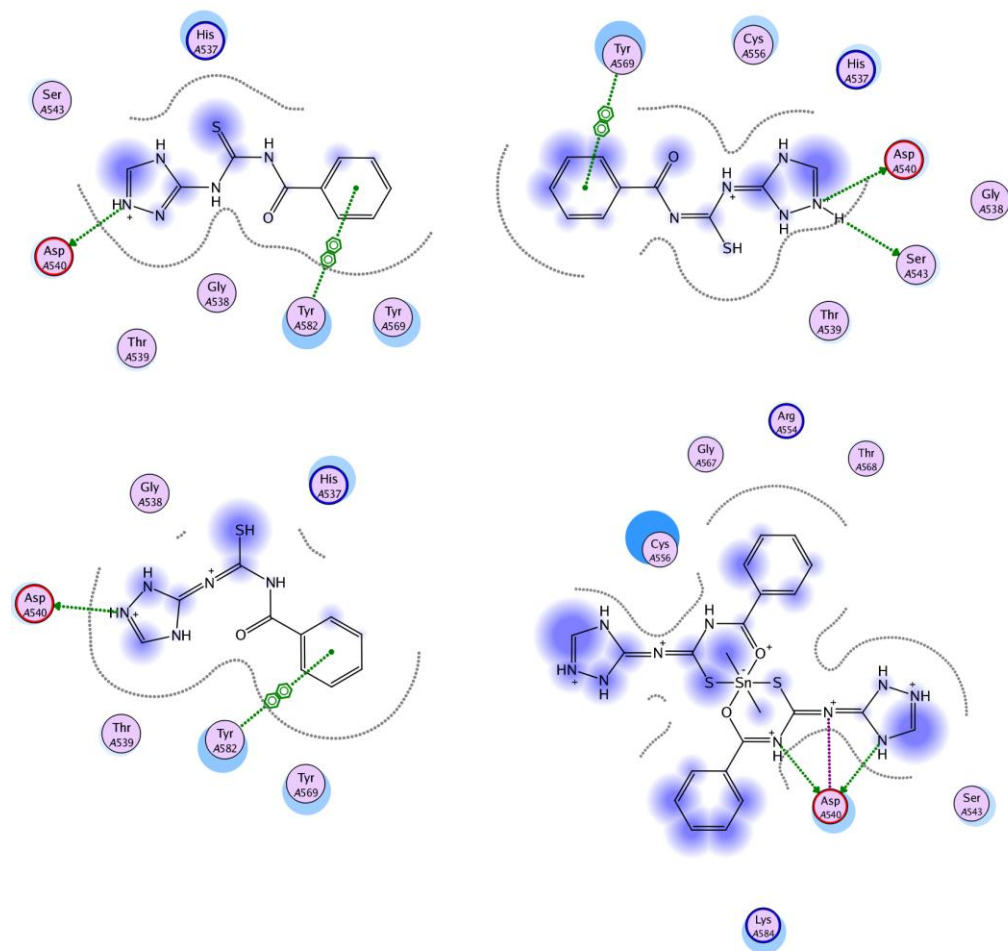


Figure 11. Docking results of BTThU and DMT(BTThU)₂