**Abstract**

This thesis comprises four chapters. The first one is an introduction which consists of a brief literature survey about different methods to synthesize thieno[3,2-*d*]pyrimidine and thieno[3,4-*d*]pyrimidine containing compounds in addition to an account on their cytotoxic activities.

The second chapter clarifies the objectives of the work and the Schemes designed for the preparation of the new required target compounds.

The third chapter deals with the theoretical discussion of the experimental work for the preparation of the starting materials **Ia&b**, **IIa-d** and the key intermediates **IIIa-d**, **XVa&b**, in addition to the target new compounds **I**V**a-d**, **Va&b**, **VIa&b** and the new hydrazides **VIIa&b** which on condensation with aromatic aldehydes furnished **VIIIa-f**. Reacting the key intermediates **IIIa-d** with orthoesters, formamide, cyclohexanone and aromatic aldehydes afforded **IXa-f**, **XIIa&b**, **XIIIa&b** and **XIVa-f**, sequentially. Moreover, reaction of **IXa&b** with hydrazine hydrate gave **Xa&b** that underwent cyclization to triazole derivatives **XIa-d** upon treatment with different orthoesters.

Reacting **XVa&b** either with the suitable alkyl halide or POCl3 yielded **XVIa-g** and the chloro derivatives **XVIIa&b**, respectively.The latter compounds converted to **XVIIIa&b** which, in turn, cyclized with SOCl2 to afford **XIXa&b**. The structure elucidation of the new compounds was supported by element analysis, IR, 1H-NMR and mass spectral data.

Additionally, a brief account on the docking study was explained through the binding conformations in comparison with the experimental results.

The fourth chapter consists of the experimental part of this thesis which contains the detailed procedures used for the synthesis of the starting compounds **Ia&b** and **IIa-d**,the key intermediates **IIIa-d** and **XVa&b** in addition to the target new compounds **I**V**a-d**, **Va&b**, **VIa&b**, **VIIa&b**, **VIIIa-f**, **IXa-f**, **Xa&b**, **XIa-d**, **XIIa&b**, **XIIIa&b**, **XIVa-f**, **XVIa-g**, **XVIIa&b**, **XVIIIa&b** and **XIXa&b**.This chapter clarifies the physical properties in addition to the detailed data obtained from element and spectral analysis of the newly synthesized compounds. It also includes the *in-vitro* anticancer activity of fifteen compounds of the novel target compounds compared with doxorubicin as a reference anticancer agent. The results revealed that nine of the test compounds showed enhanced anticancer activity than doxorubicin. Finally, this chapter demonstrates the correlation between the results of the molecular docking study and the anticancer evaluation.  
 Indeed, compound **XIIa** showed the highest energy score (-26.43 Kcal/mol) and exhibited the most potent *in-vitro* cytotoxic activity with IC50 = 2.04 µM.