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Synthesis, Single Crystal XRD and Molecular Docking of 3-α-Carboxy Ethyl Rhodanine

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The crystal product of 3-α-carboxy ethyl rhodanine was confirmed by single crystal XRD analysis. Furthermore, to examine the binding interactions of 3-α-carboxy ethyl rhodanine with the Bcr AblT315I tyrosine kinase and HPV 16 E2 protein molecular docking study was carried out. The results showed reasonable docking scores and displayed good interactions, thereby suggesting that 3-α-carboxy ethyl rhodanine may be used as a template for the further development of anticancer drugs.

Keywords: 3-α-Carboxy ethyl rhodanine, SXRD, Bcr AblT315I tyrosine kinase, HPV 16 E2 protein, Molecular docking.

INTRODUCTION

Owing to the excellent properties of rhodanine based molecules are one of the bioactive heterocyclic compounds and are used in various applications in industry, biochemistry and coordination chemistry. Rhodanine and their derivatives have broad industrial applications and widely used as intermediates in the syntheses of dyes, extreme-pressure lubricants and as brightening additives in silver electroplating. They also exhibit antioxidant properties as well as pharmacological [1] and biological activities including antibacterial [2], antiviral [3] and antidiabetical [4] properties. Due to their strong ability in donating electrons to metal ions, make them strong ligands in coordination compounds [5]. A rapid development in rhodanine chemistry was observed because of their use as inhibitors for protein mannosyl transferase-1 [6], phosphodiesterase-4 [7], protease [8], JSP-1 [9], UDP-N-acetylmuramate-L-alanine ligase [10], antimalerials [11], HIV-1 integrase [12-15] and β-lactamase [16]. Rhodanine nucleus containing commercial drug Epalrestat is used as aldose reductase inhibitor in some Asian countries [17,18]. In our earlier study reported that the *in vitro* cytotoxicity of a series of rhodanines found that 3-α-carboxy ethyl rhodanine was found to be more active against HeLa cell lines (IC_{50} = 10 μg/mL). The present work, we have reported the single crystal XRD of the active molecule 3-α-carboxy ethyl rhodanine for the first time. Further we have carried out *in silico* molecular docking studies against human cervical cancer oncoproteins HPV 16 E2 and a tyrosine kinase Bcr-Abl T315I protein to explore the possibility of using it as a lead molecule against cancers.

EXPERIMENTAL

The commercially available chemicals used were of reagent grade and used without further purification. The single crystal X-ray diffraction data were obtained at 293 K on a Bruker SMART APEX2 CCD diffractometer.

Synthesis of 3-α-carboxy ethyl rhodanine (3ACER): 3-α-Carboxy ethyl rhodanine (3ACER) was prepared (**Scheme-I**) according to the method previously reported [19] and used for the single crystal XRD study.

Preparation of protein molecule and ligand: The trans-activation domain (TAD) receptor of human papillomavirus type 16 E2 protein (PDB ID: 1DTO) and the Bcr-Abl T315I (PDB ID: 2V7A) were retrieved from protein databank PDB [www.rcsb.org/pdb]. The obtained receptor was energy minimized by using Swiss PDB Viewer after adding hydrogen bond in AutoDock. 3ACER was constructed using ChemDraw Ultra 8.0 and 3-D structure was generated and optimized using AutoDock to acquire proper geometry.

RESULTS AND DISCUSSION

Crystal structure description of 3ACER: The asymmetric unit of 3ACER molecule structure comprises of 3-α-carboxy ethyl rhodanine molecule, an isolated sulphur atom and a water molecule, as shown in Fig. 1. The single X-crystal data of the