Anticancer activities of acetylacetone coordinated Re(I) tricarbonyl complexes: a single crystal investigation, spectroscopic, DFT studies, and in-silico molecular docking.

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Over 50% of malignancies are treated with platinum-based drugs (cisplatin, carboplatin, and oxaliplatin), either alone or as a combination. While platinum resistance and severe side effects associated with chemotherapy have become common, new anticancer medications are still actively being researched [1]. The past few decades have seen the development of a number of highly effective anticancer therapies containing organometallic compounds, or molecules with at least one metal-carbon link. A variety of ligands can be designed for organometallic complexes, as well as a variety of mechanisms of action. [2]. Compared to some widely studied organometallic complexes such as those based on ruthenium, rhenium organometallic compounds are relatively rare, but many studies describing the potential of such compounds have lately been reported [3]. In recent years, several studies have described these rhenium compounds' potential [4]. Organometallic compounds containing rhenium (Re) have numerous properties that are useful for developing anticancer medications. It is often possible to use ⁹⁹mTc in conjunction with ¹⁸⁶Re and ¹⁸⁸Re due to the similar coordination chemistry between these group 7 congeners [5]. Therefore, Re complexes may be used as radio-imaging agents, therapeutic agents and luminous probes as well as multimodal molecules. Furthermore, "hot" analogs can be used to study in-vivo biodistribution and pharmacokinetics, both of which are essential for developing new medications. Based on these inherent properties of rhenium complexes, and the various inimical increasing cancer reports, this study presents, the synthesis, spectroscopic characterization, molecular crystal structures as seen in Figure 1, DFT, and in-silico anticancer activities of fac-[Re(Acac)(CO)₃(1,2-DiCH₃Im)] (Re-1) and fac-[Re(Acac)(CO)₃(2-CH₃Im)] (Re-2) is investigated in detail.

Figure 1. Molecular structures of Re-1 and Re-2. Thermal ellipsoids are plotted at a 50% probability level.