The presence of endocrine interferents such as 17 beta-estradiol, natural estrogen present in hormone replacement therapies, and 17 alpha-ethinylestradiol, synthetic estrogen used in contraceptive pills, can cause adverse effects in an organism or its descendants [1]. Several studies have already been carried out showing adverse effects associated with estradiol compounds, such as feminization of male fish, reduction in sperm count, among others [2]. Most of these endocrine disruptors when excreted go directly to the water bodies, and new technologies are required for the removal / degradation of this compound in the sewage treatment station area [3].

In this way, this work evaluate the structural and electronic properties of the interaction of graphene nanoribbon (armchair and zigzag) with 17 beta-estradiol and 17 alpha-ethinylestradiol. It was analyzed the nature of the physical or chemical interaction that occurs between the systems in order to know the potential of the nanostructure for the removal of the endocrine interferents present in the wastewater. The methodology used is based on the ab initio Density Functional Theory that makes use of the SIESTA code [4].

The results obtained show that the most stable configuration of the zigzag graphene nanoribbon interacting with beta-estradiol [alpha-ethynylestradiol] has a binding energy of 1.21 [1.19] eV with metallic character. The most stable configuration for the armchair nanoribbon interacting with beta-estradiol [17 alpha-ethinylestradiol] presents a binding energy of 1.03 [1.15] eV and a band gap of 0.76 [0.74] eV. These results indicate a physical adsorption process that corroborates theoretical and experimental studies of JAURIS et al [5] for similar molecules and show the possible use of this nanomaterials for pollutants removal in wastewater.