

Synthesis, Biological Activity and Computational Study of Some New Unsymmetrical Organotellurium Compounds Derived from 2-Amino-5-carboxyphenyl Mercury(II) Chloride

Abstract

The reaction of 2-amino-5-carboxyphenyl mercury(II) chloride under argon atmosphere with tellurium tetrabromide gave 2-amino-5-carboxyphenyl tellurium(VI) tribromide (1) in good yield. Reaction of 1 with 4-hydroxyphenyl mercury(II) chloride under argon atmosphere gave 4-hydroxyphenyl-2-amino-5-carboxyphenyl tellurium(VI) dibromide (2). Reduction of compound 2 by hydrazine hydrate gave new unsymmetrical compound 4-hydroxyphenyl-2-amino-5-carboxyphenyl telluride (3). The synthesized compounds were characterized by elemental analysis (CHN), FT-IR, ^1H NMR, ^{13}C NMR and mass spectra. *in vitro* antitumor activity of compounds was tested against two types of human tumor cells (Prostate cells Pc-3 and Bladder cells T24), compound 1 has higher activity than other compounds. *in vitro* antioxidant activity of synthesized compounds was tested by using DPPH method, all compound showed the antioxidant activity. The three molecules 1-3 were modeled and optimized by using density functional theory, DFT/B3LYP method and LANL2DZ as a basis set. Calculated descriptor, the HOMO, LUMO energy gap was used to interpret the biological activity of the compounds. The results showed that compound 1 has higher biological activity than compounds 2 and 3.