Experimental and Theoretical Investigation of Antioxidant Activity and

Capacities of Thiosemicarbazones Based on Isatin Derivatives

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**Supplemental Materials**

The optimized HOMO, LUMO, and electron density of H25MI3PT and H25MI3ClPT for neutral, anionic, cationic, and radical forms are given in Fig. S 1. The HOMO mainly consists of an isatin group and a S atom for H25MI3PT, but for H25MI3ClPT, the HOMO is distributed over the whole of the molecule. The LUMO mainly consists of an isatin group for the neutral form. The optimized HOMO, LUMO, and electron density of DPPH for neutral, radical, anionic, and cationic forms are shown in Fig. S2.

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**Figure S 1:** Optimized form, HOMO, LUMO and Electron density of H25MI3ClPT and H25MI3PT molecules for neutral radical anionic and cationic form

 

**Figure S 2:** Optimized form, HOMO, LUMO and Electron density of DPPH molecule for neutral radical anionic and cationic form