Supporting Information

Anti-Cancer and Electrochemical Properties of Thiogenistein—New Biologically Active Compound

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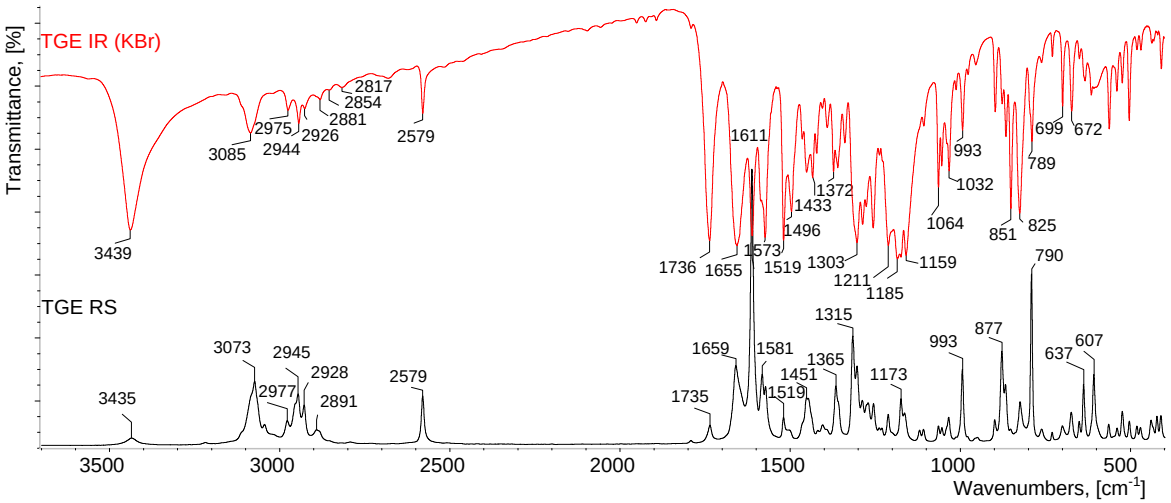

Fig. S1. IR (red) and Raman spectra (blue) of TGE.

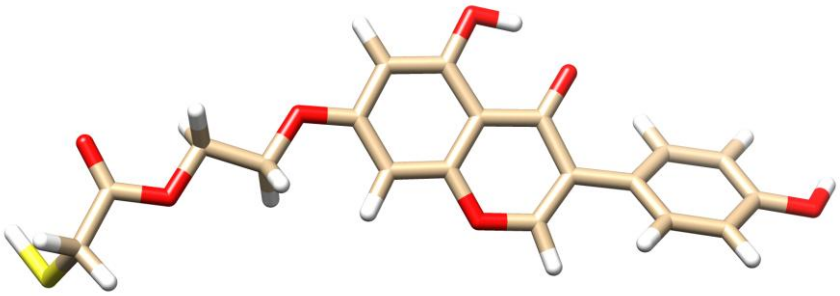

Fig. S2. The optimal geometry of the TGE molecule with the intramolecular hydrogen bond C(4)=O•••HO-C(5) following the B3LYP/6-311++G(d,p) calculations. The H(O at C-5)-O(at C-4) distance is 1.70 Å. Colors of atoms: H-white, C-gold, O-red, S-yellow.

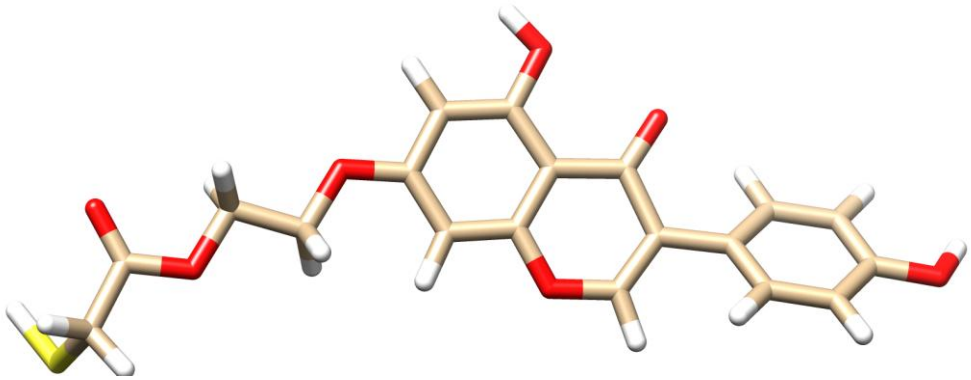

Fig. S3. The optimal geometry of the TGE molecule where the intramolecular hydrogen bond does not appear. The H(O at C-5)-O(at C-4) distance is 3.63 Å. Colors of atoms and the method of calculations as in the Figure S2.

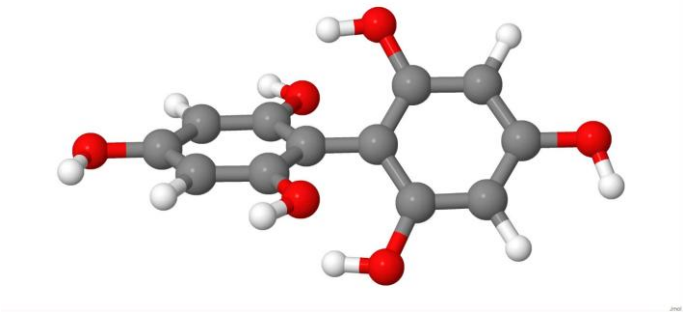

Fig. S4. The optimal geometry of the adduct of the 1,3,5-trihydroxybenzene linked by the C-C bond, following the B3LP/6-311++G(d,p) calculations.

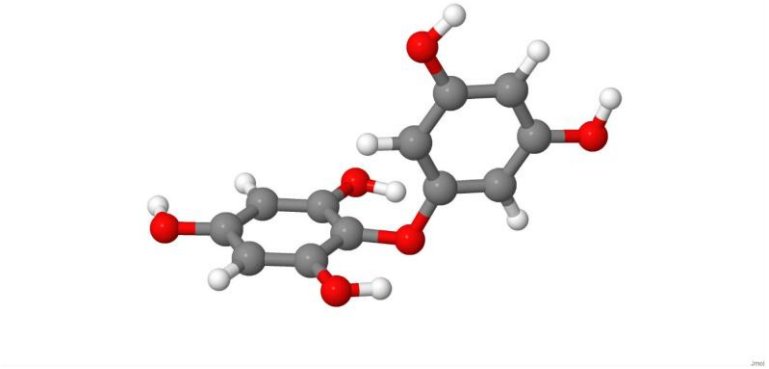

Fig. S5. The optimal geometry of the adduct of the 1,3,5-trihydroxybenzene linked by the C-O-C bond, following the B3LP/6-311++G(d,p) calculations.