**Highlights**

* The heteroatom and heterocyclic ring have important roles in promoting the antioxidant activity of Trolox.
* The NH2 and OH substituents in ortho position increase the antioxidant activity of Trolox.
* The derivatives ***e****,* ***c*** and ***d*** with NH, S and Se instead of O have higher antioxidant activity than Trolox.
* Obtained theoretical results about antioxidant activity of Trolox derivatives are in agreement with corresponding published experimental values.