SUPPORTING INFORMATION

Theoretical Insights into the Antioxidant Activity of Moracin T

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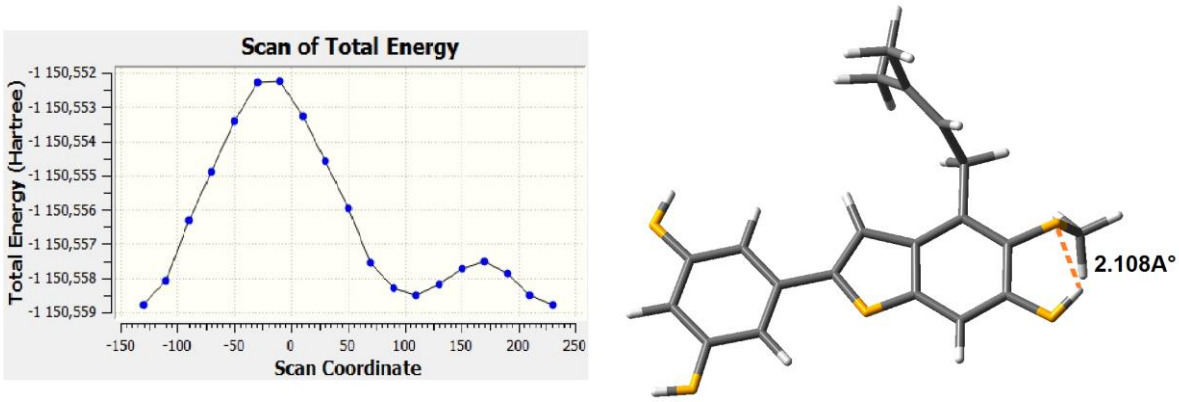

Figure S1. Potential energy profile for Moracin T as a function of torsion angle between the allyl group and the benzofuran ring (left), as well as optimized molecular geometry with intramolecular hydrogen bond (right).

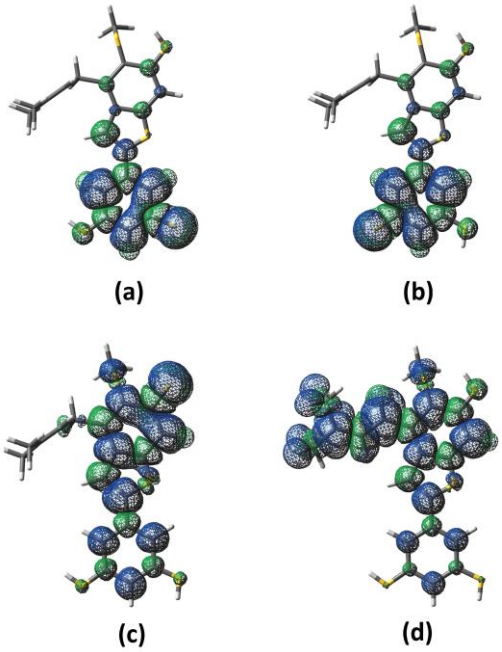

Figure S2. Spin density distribution of Moracin T after abstracting of a proton from 1-OH (a), 2-OH (b), 3-OH (c) and CH (d).

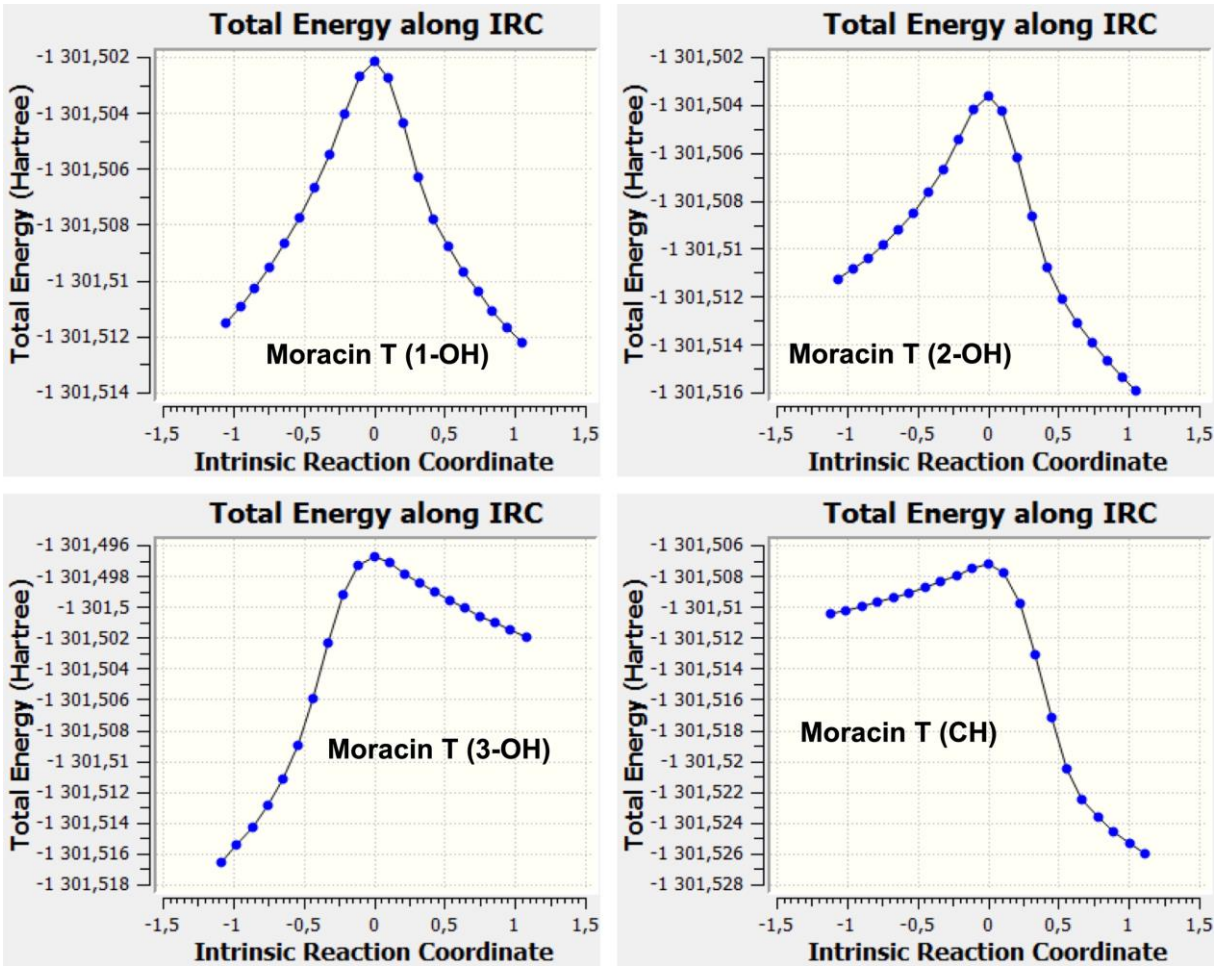

Figure S3: IRC plots for all transition states related to the reaction of HOO• radical with Moracin T in the gas-phase calculated at B3LYP/6-311G(d,p) level of theory.