

In silico exploration of selected coumarin derivatives as potential antioxidant: Insights from DFT, NBO, Hirshfeld surface, ADMET profiling, Molecular docking and Dynamics simulations

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Supplementary Data

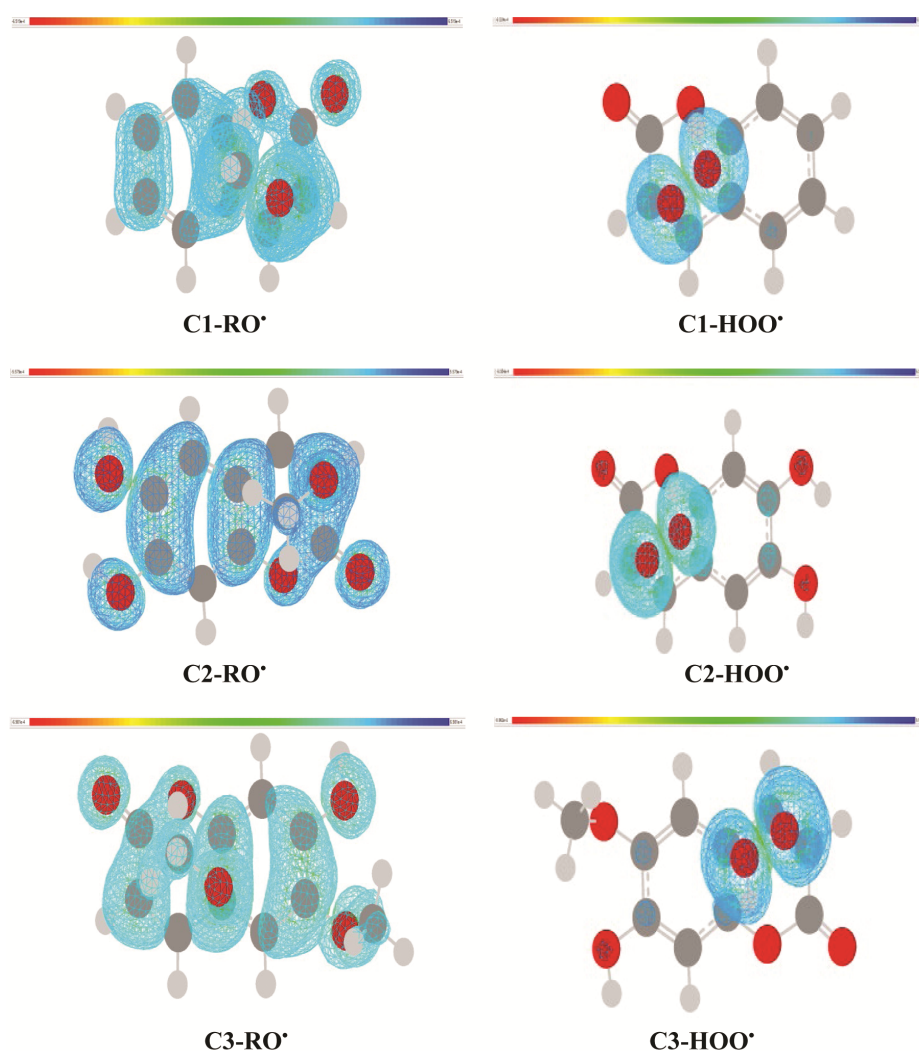


Fig. S1 — Spin density distribution map for C1- RO[•]/HOO[•], C2- RO[•]/HOO[•] and C3- RO[•]/HOO[•] Antioxidant-radical complexes

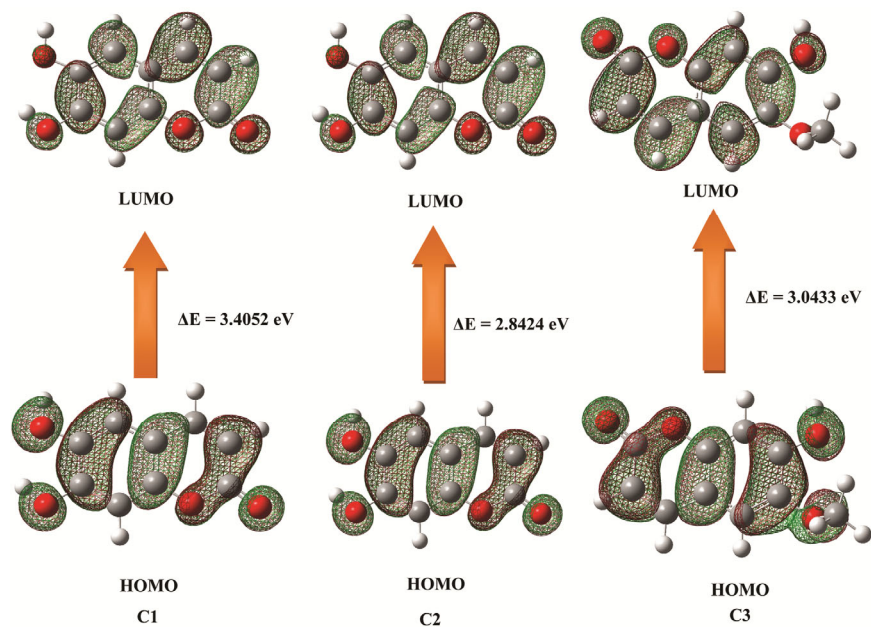


Fig. S2 — HOMO-LUMO plots of Antioxidants C1, C2 and C3

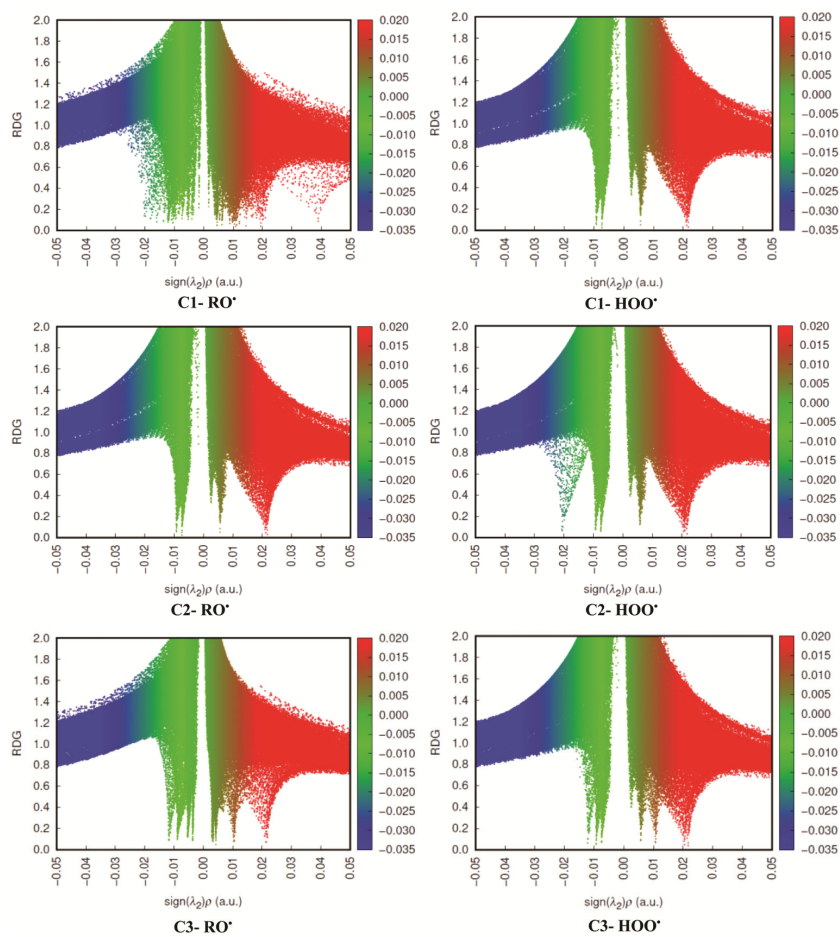


Fig. S3 — NCI plots of the minimized models of C1, C2 and C3 with RO'/HOO' Antioxidant-radical complexes

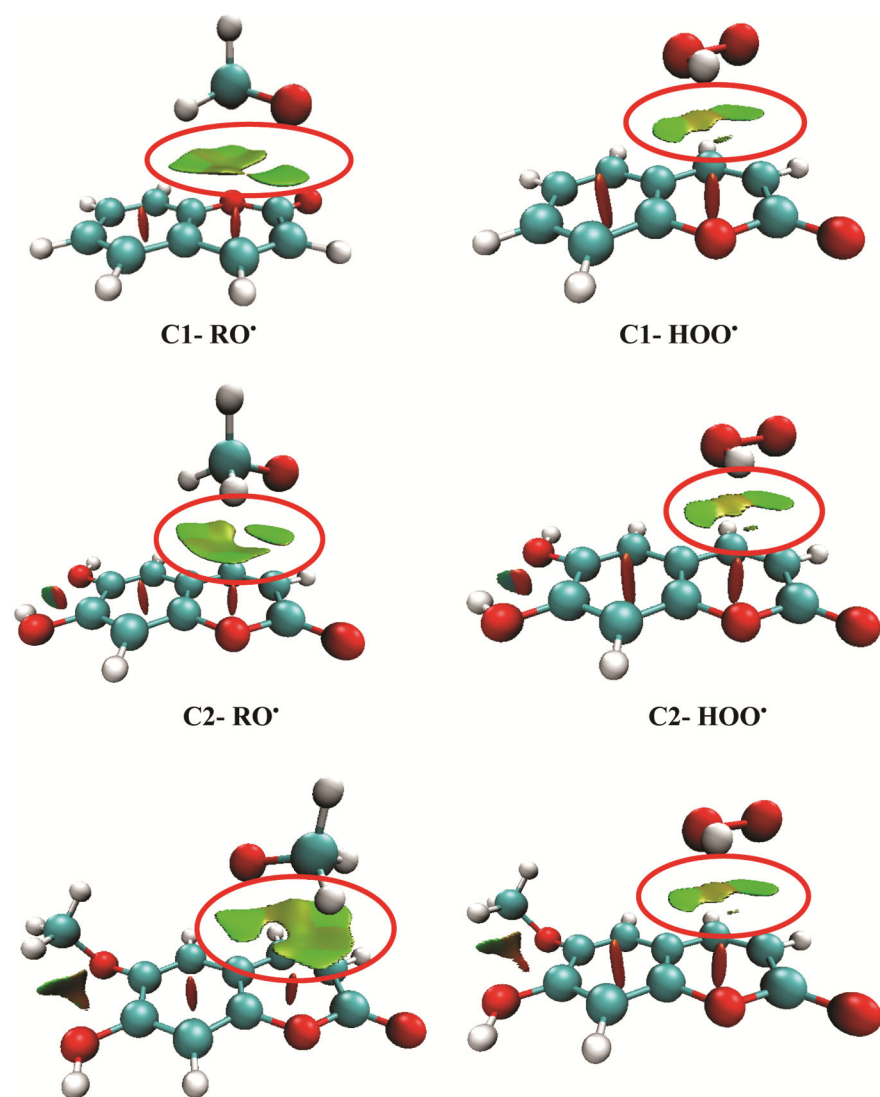


Fig. S4 — VMD plots of the minimized models of C1, C2 and C3 with RO•/HOO•Antioxidant-radical complexes