

Video S1. The π - π interaction between Biochanin-A ring C and superoxide acts like sigma scavenging on H(hydroxyl) of ring A



Biochanin_ringC_vd
W_piO2Rad_GoesSl

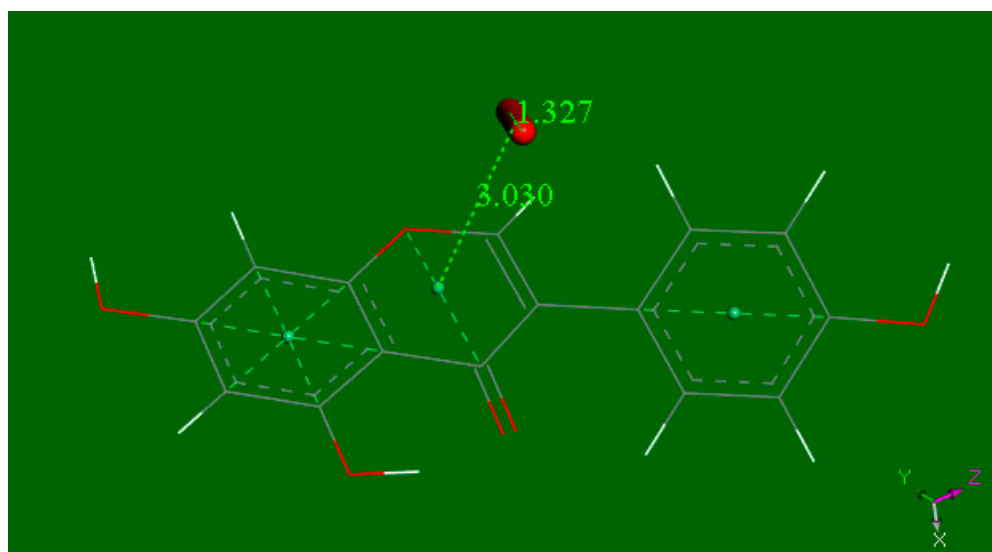


Figure S2. DFT minimization of superoxide π - π posed over genistein ring C forms a superoxide- η -genistein complex.

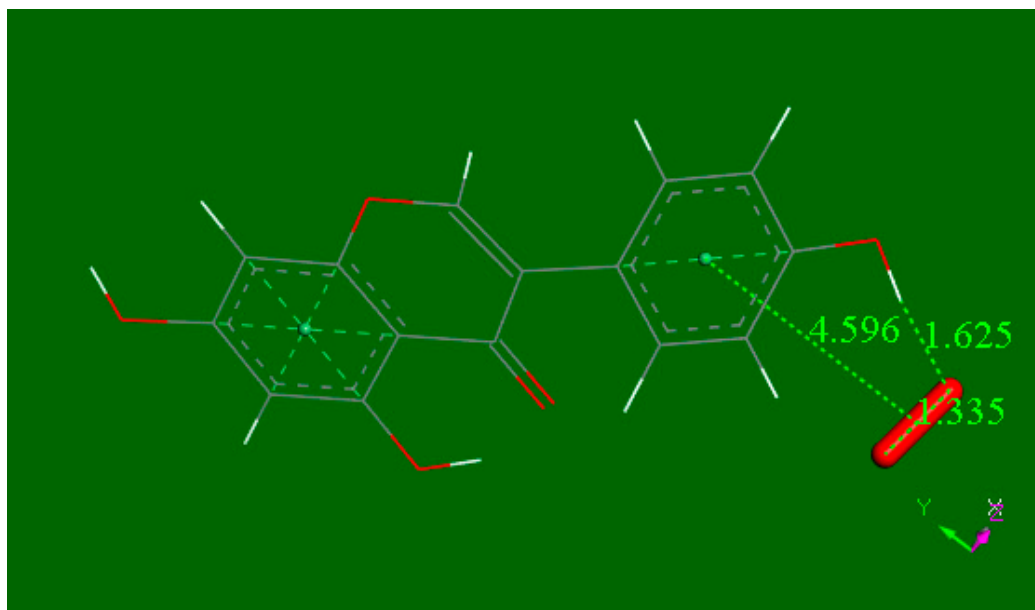


Figure S3. DFT minimization of superoxide π - π posed over genistein ring B forms a H-bond with H4'(hydroxyl).

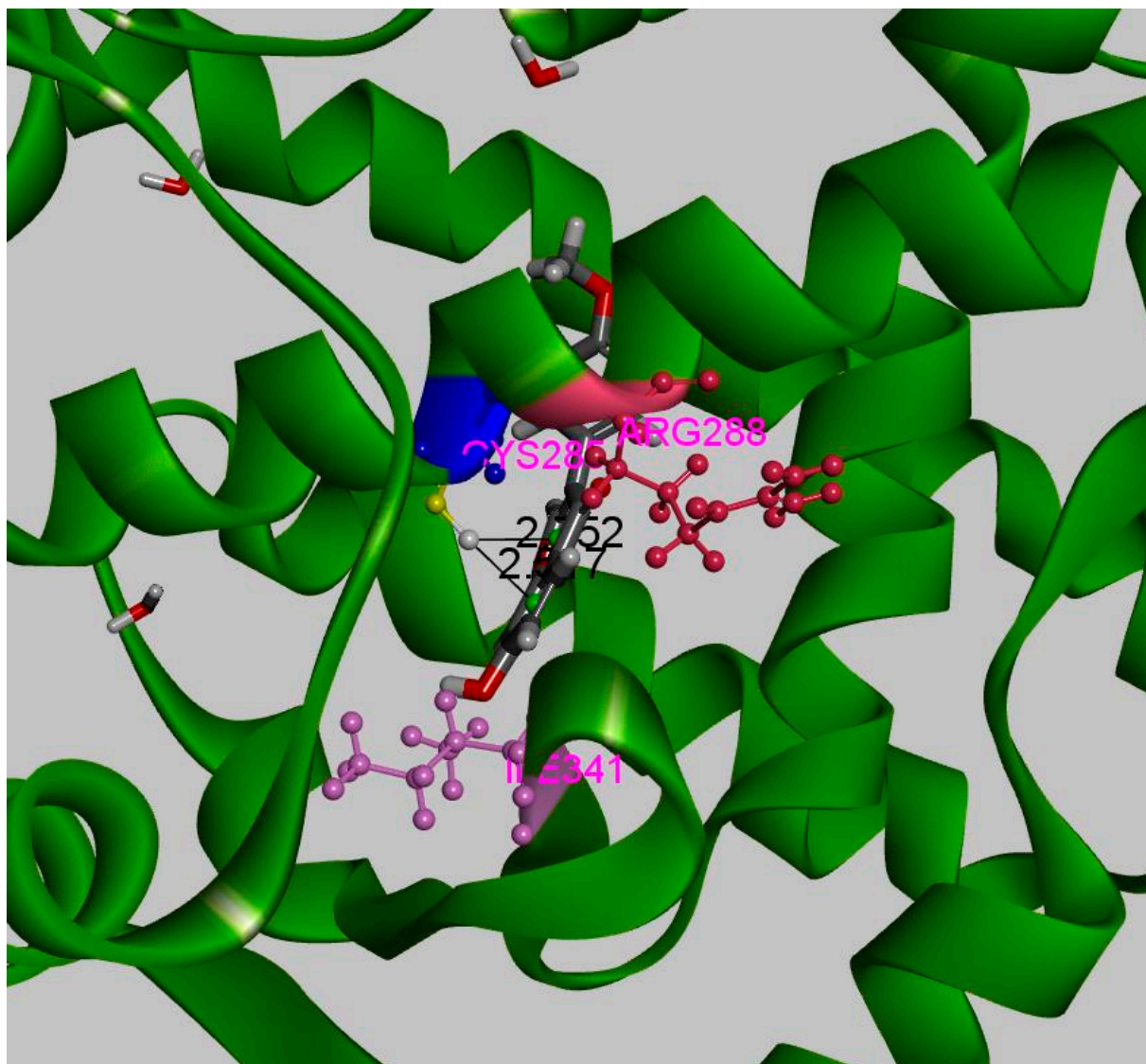


Figure S4. Calculating binding energy (-22.1 Kcal/mol) for a partial view of 5UGM protein including FMNT pose 5 (stick style) after dynamic cascade. Amino acid Cys285 (blue) has its S in yellow and its associated H atom in white. Arg288 (copper) and Ile341 (cyan) are also displayed as a ball style. H(Cys285) separation from ring centroids is 2.517 Å (ring A) and 2.572 Å (pyrone ring).