Supporting Materials

Theoretical and Experimental Investigation of the Antioxidation Mechanism of Loureirin C by Radical Scavenging for Treatment of Stroke

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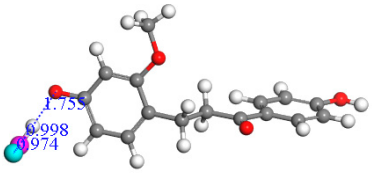
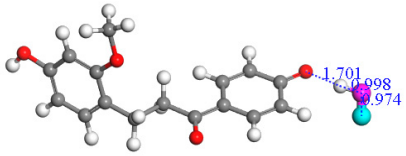
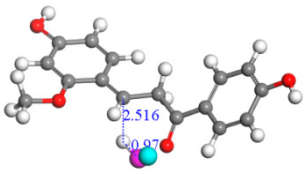
Figure S1. Optimized structures of LC+OH• Pradical in water; (a) near to the OH of A ring (left) of LC; (b) near to the OH of B ring(light) of LC; (c) near to H21; (d) near to H23 and H24; (e) near to H28 and H30; (f) near to H29 and H31 and (g) near to H25 and H27. The energy difference between the LC+OH• complex and two reactants and the distances (Å) between the oxygen atom of OH• and the hydrogen atom of LC, between the hydrogen atom of LC and its neighbor, C, and between the two atoms of OH• radical are shown. The Hirshfeld charges of O and H atoms of OH• were showed at the top of Fig. S1 (d), (e), (f), (g).



(a) −0.0753 Ha



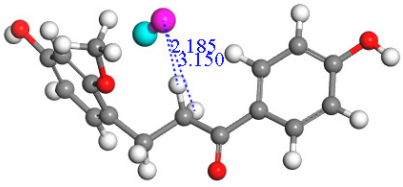
(b) −0.0706 Ha



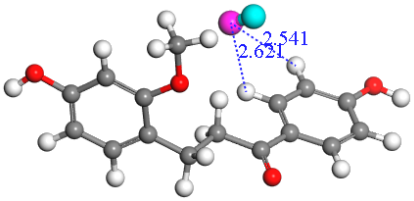
(c) −0.0648 Ha

H: 0.0783e; O: −0.4163e

H: 0.096087e; O: −0.4719e



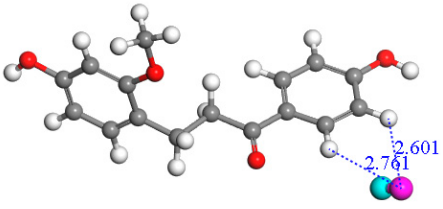
(d) −0.02752Ha



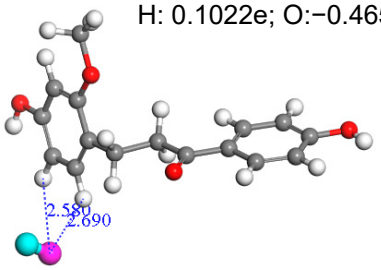
(e) −0.02420 Ha

H: 0.0902e; O:−0.4828e

H: 0.1022e; O:−0.4650e

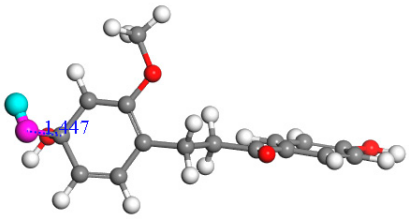


(f) −0.02414 Ha

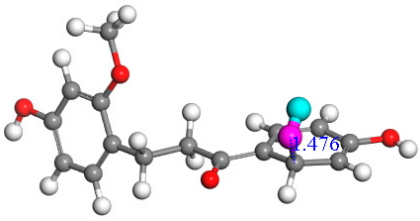


(g) −0.02359 Ha

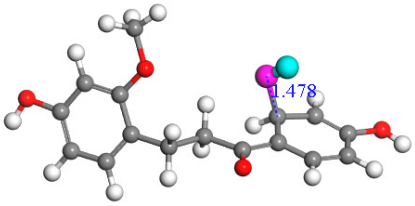
Figure S2: Optimized structures of LC+OH$^{\bullet}$ in water. OH$^{\bullet}$ was added on C14(a), C7(b), C13(c) sites of LC (A ring, left); on the site of C8 of the C=O double bond (d), on the C16(e), C15(f), C19 (g), C18(h) sites of LC (B ring, right). The energy difference between the LC+OH$^{\bullet}$ adduct and two reactants and the distances (Å) between the oxygen atom of OH$^{\bullet}$ and the C atom of LC are shown.



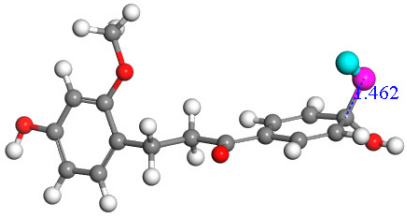
(a) C14+OH$^{\bullet}$(−0.0397 Ha)



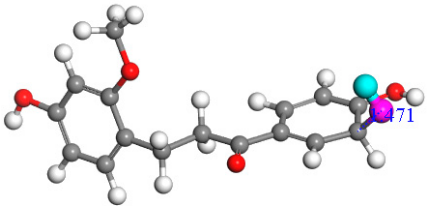
(b) C16+OH$^{\bullet}$(−0.0406 Ha)



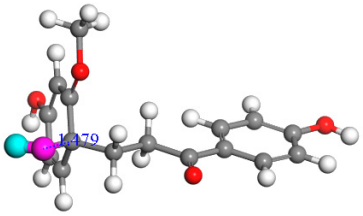
(c) C15+OH$^{\bullet}$(−0.0399 Ha)



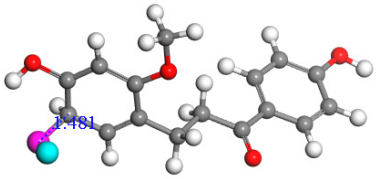
(d) C19+OH$^{\bullet}$(−0.03999 Ha)



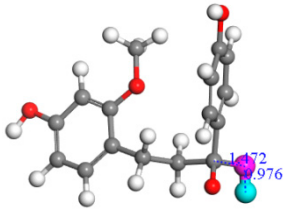
(e) C18+OH$^{\bullet}$(−0.03886 Ha)



(f) C7+OH$^{\bullet}$(−0.04576 Ha)



(g) C13+OH$^{\bullet}$(−0.04370 Ha)



(h) C8+OH$^{\bullet}$(−0.04145 Ha)

Figure S3: IC50 of LC

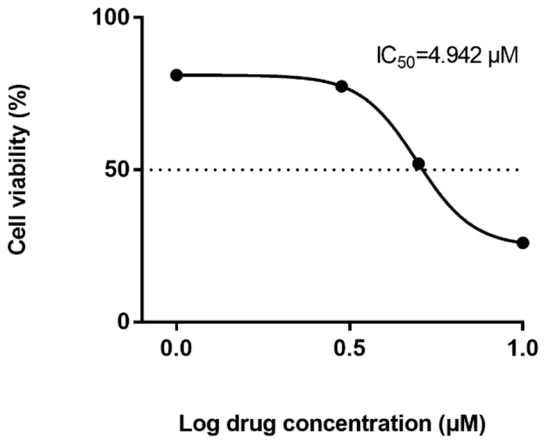


Figure S4： Chromatogram of LC