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Proton-Coupled Electron Transfer of Catechin in Tea Wine: The Enhance Mechanism of Anti-Oxidative Capacity

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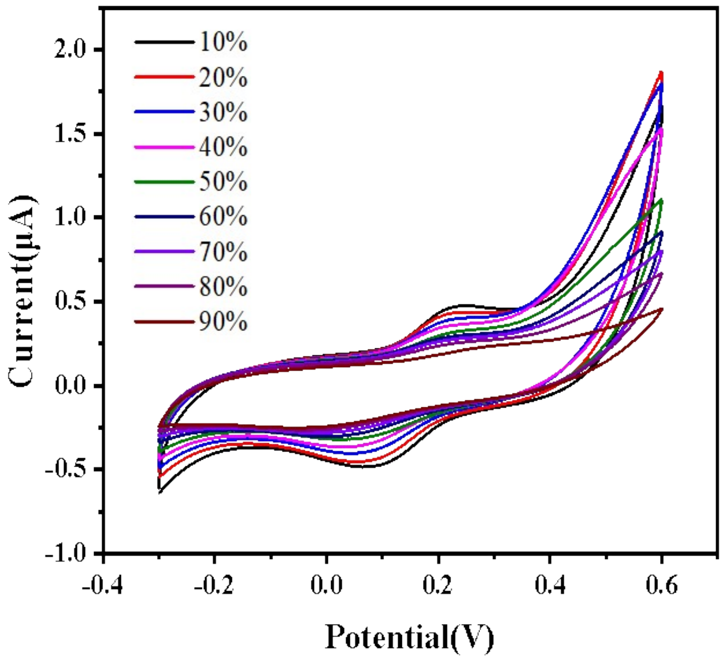


Figure S1. The cyclic voltammograms of 1 mM catechin in the presence of ethanol (10% - 90%), respectively. Scan rate: 0.1 V·s^{-1}.

Table S1. The oxidation peak current and diffusion coefficient obtained from Figure S1.

Ethanol concentration	10%	20%	30%	40%	50%	60%	70%	80%	90%
I_p / μA	0.32	0.30	0.26	0.24	0.17	0.14	0.10	0.08	0.06
D / 10^{-9} $cm^2 \cdot s^{-1}$	1.76	1.61	1.19	1.02	0.51	0.35	0.18	0.11	0.06

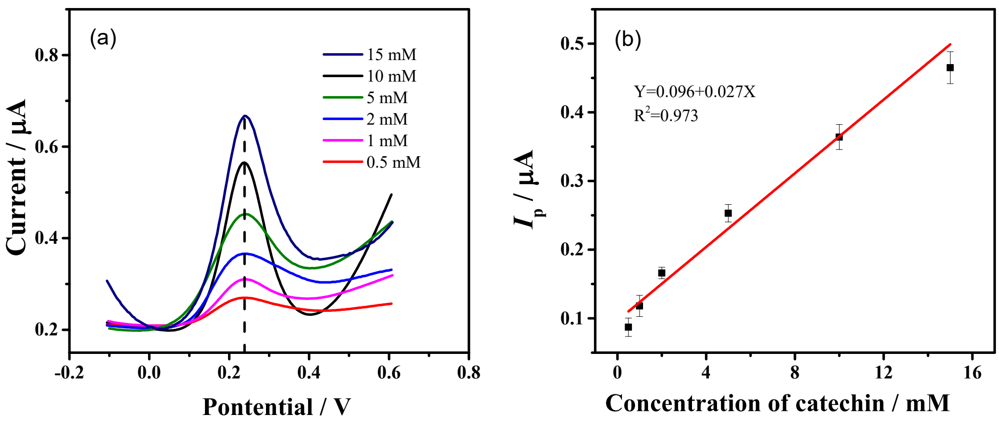


Figure S2. (a) The differential pulse voltammograms of different concentration of catechin in 10% ethanol, respectively. (b) The plot of oxidative peak current versus catechin concentration.

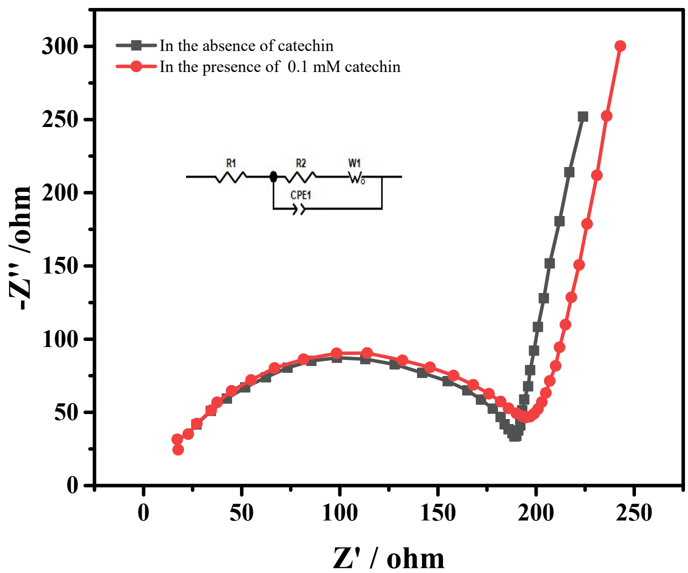


Figure S3. Electrochemical impedance spectroscopy of 1.0 mM $Fe(CN)_6^{3-/4-}$ on mercaptoethanol self-assembled monolayer electrode in the absence of catechin and in the presence of 0.1 mM catechin, respectively. The insert is the Randles equivalent circuit.

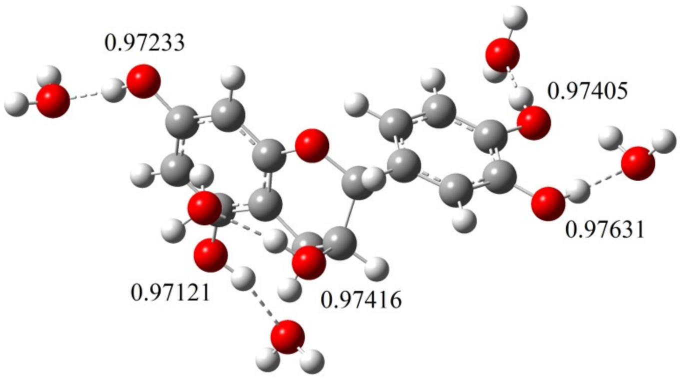
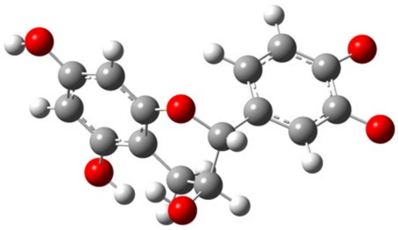


Figure S4. The optimized geometry of catechin-water cluster.

(a)

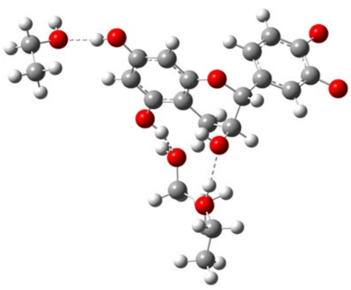


Structure B, Charge: -2,
E_B= -1030.373838 hartree

(b)

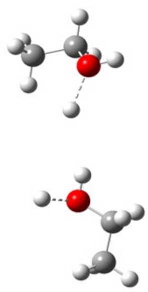
Structure C, H, Charge: +1,
E_B= 0.170720 hartree

(c)



Structure E, Charge: -2,
E_E= -1495.697104 hartree

(d)



Structure F, Charge: +2,
E_F= -310.404231 hartree

Figure S5. Optimized geometries, charge and electron energy of surtcture B, C, E and F.

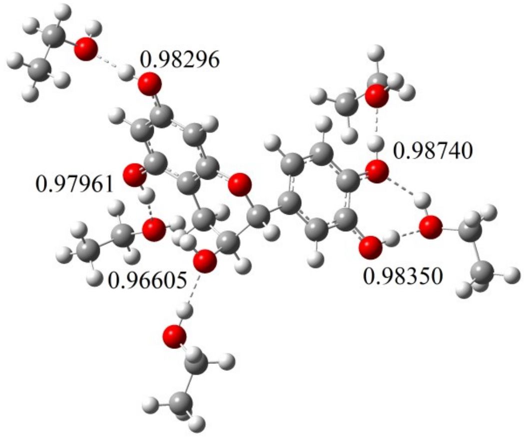


Figure S6. The optimized geometry of catechin-ethanol-water cluster in water environment.