Supporting Information

Eqation S1

$$F_c = F_m e^{(A_1+A_2)/2} \quad \text{(S1)}$$

Where F_c and F_m represent fluorescence intensity values for correction and determination, respectively. A_1 and A_2 represent quercetin's absorbance levels at fluorescence excitation and emission wavelengths, respectively.

Equations S2 – S4

$$\frac{1}{v} = \frac{K_m}{V_{max}}\left(1+\frac{[I]}{K_i}\right)\frac{1}{[S]} + \frac{1}{V_{max}}\left(1+\frac{[I]}{\alpha K_i}\right) \quad \text{(S2)}$$

$$\text{Slop} = \frac{K_m}{V_{max}} + \frac{K_m[I]}{V_{max}K_i} \quad \text{(S3)}$$

$$\text{Y-intercept} = \frac{1}{V_{max}^{app}} = \frac{1}{V_{max}} + \frac{1}{\alpha K_i V_{max}}[I] \quad \text{(S4)}$$

In these formulas, [I] represent inhibitor content, whereas [S] stands for substrate content; v and V_{max} represent enzymatic reaction rate and maximum catalytic reaction rate, respectively; K_m is the Michaelis–Menten constant; K_i and αK_i stand for the equilibrium constants of quercetin binding to the free AChE and AChE–substrate complex, and α is the apparent coefficient.

Equations S5

$$\frac{F_0}{F} = 1 + K_{SV}[Q] = 1 + K_q\tau_0[Q] \quad \text{(S5)}$$

In the formula, F_0 stands for system fluorescence intensity with AChE alone, whereas F indicates that with quercetin added, respectively, and K_{SV} stands for the Stern–Volmer quenching constant, which represents fluorescence quenching efficiency, [Q] denotes quercetin content, K_q indicates bimolecular quenching rate constant, whereas τ_0 denotes the average fluorophore lifetime, about 10^{-8} s.

Equations S6

$$\log\frac{F_0-F}{F}=n\log K_a-n\log\frac{1}{[Q_t]-\frac{(F_0-F)[P_t]}{F_0}} \quad \text{(S6)}$$

[Q_t] and [P_t] denote quercetin and AChE concentrations, respectively. F_0 and F are the same as in Equation S 5.

Equations S7 – S8

$$\log K_a=-\frac{\Delta H^\circ}{2.303RT}+\frac{\Delta S^\circ}{2.303R} \quad \text{(S7)}$$

$$\Delta G^\circ=\Delta H^\circ-T\Delta S^\circ \quad \text{(S8)}$$

where K_a and R suggest binding and gas (8.314 J mol^{-1} K^{-1}) constants, respectively. Temperature (T) was set to 25, 31, and 37 °C.

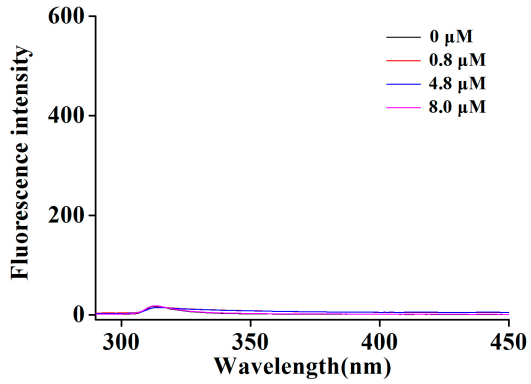

Figure S1. Fluorescence spectra of quercetin at varying concentrations (pH 7.6, T = 25 °C). *c*(quercetin) = 0, 0.8, 4.8 and 8.0 μM, respectively.

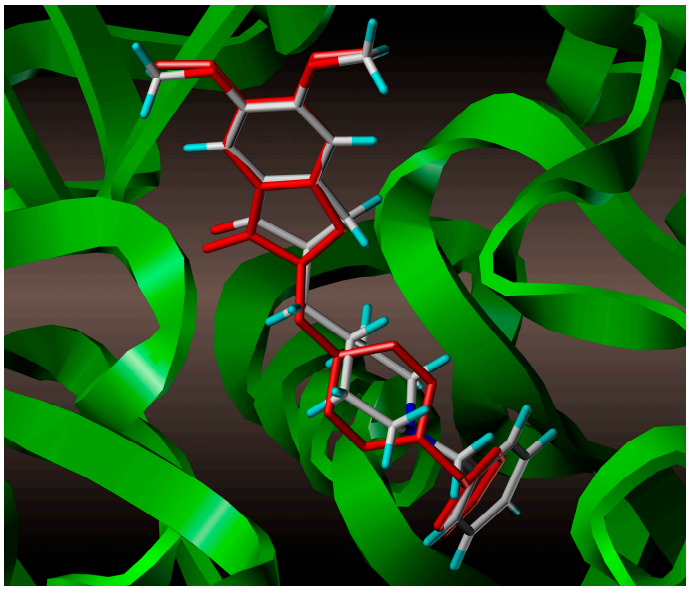

Figure S2. Docked conformer of donepezil (white) and original pose of co-crystallized donepezil (red).