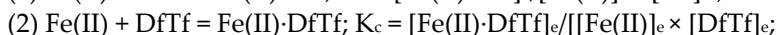
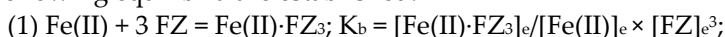


Supporting Information for Comparison of Antioxidant Properties of a Conjugate of Taxifolin with Glyoxylic Acid and Selected Flavonoids

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For a mixture containing two compounds that compete for binding to iron(II) ions, the following equilibria are established:



where FZ is ferrozine; DfTf is a conjugate of taxifolin with glyoxylic acid; K_b and K_c are the binding constant of Fe(II) and ferrozine and Fe(II) and DfTf, respectively; and $[...]_e$ is the equilibrium concentration of each species.

The ratio of the binding constants is expressed as:

$$K_b/K_c = ([\text{Fe(II)} \cdot \text{FZ}_3]_e / [\text{Fe(II)} \cdot \text{DfTf}]_e) \times ([\text{DfTf}]_e / [\text{FZ}]_e^3) \Rightarrow$$

$$K_c = K_b \times ([\text{FZ}]_e^3 / [\text{DfTf}]_e) \times ([\text{Fe(II)} \cdot \text{DfTf}]_e / [\text{Fe(II)} \cdot \text{FZ}_3]_e).$$

where $K_b = 3.65 \times 10^{15} \text{ M}^{-2}$ [56]

In the case that equal amounts of $[\text{Fe(II)} \cdot \text{DfTf}]$ and $[\text{Fe(II)} \cdot \text{FZ}_3]$ complexes are formed, we obtain:

$[\text{Fe(II)} \cdot \text{FZ}_3]_e \approx [\text{Fe(II)} \cdot \text{DfTf}]_e \approx 50 \times 10^{-6} \text{ M}$; $[\text{DfTf}]_0 = 404.75 \times 10^{-6} \text{ M}$ (the initial concentration of DfTf was found by interpolating the graph on Fig. 4);

Thus, $[\text{DfTf}]_e \approx [\text{DfTf}]_0 - [\text{Fe(II)} \cdot \text{DfTf}]_e = 404.75 \times 10^{-6} \text{ M} - 50 \times 10^{-6} \text{ M} = 354.75 \times 10^{-6} \text{ M}$.

Taking into account that the initial concentration of ferrozine ($[\text{FZ}]_0$) was $333 \times 10^{-6} \text{ M}$, we have:

$$[\text{FZ}]_e \approx [\text{FZ}]_0 - 3 \times [\text{Fe(II)} \cdot \text{FZ}_3]_e = 333 \times 10^{-6} \text{ M} - 3 \times 50 \times 10^{-6} \text{ M} = 183 \times 10^{-6} \text{ M}.$$

Thus, $K_c = 6.3 \times 10^7 \text{ M}^{-1}$.