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:

(1) $Fe(II) + 3\ FZ = Fe(II)\cdot FZ_3$; $K_b = [Fe(II)\cdot FZ_3]_e/[Fe(II)]_e \times [FZ]_e^3$;

(2) $Fe(II) + DfTf = Fe(II)\cdot DfTf$; $K_c = [Fe(II)\cdot DfTf]_e/[[Fe(II)]_e \times [DfTf]_e$;

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 ferrozin and Fe(II) and DfTf, respectively; and $[...]_e$ is the equilibrium concentration of each species.

The ratio of the binding constants is expressed as:

$K_b/K_c = ([Fe(II)\cdot FZ_3]_e/[Fe(II)\cdot DfTf]_e) \times ([DfTf]_e/[FZ]_e^3) \Rightarrow$

$K_c = K_b \times ([FZ]_e^3/[DfTf]_e) \times ([Fe(II)\cdot DfTf]_e/[Fe(II)\cdot FZ_3]_e)$.

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

In the case that equal amounts of [Fe(II)·DfTf] and [Fe(II)·FZ_3] complexes are formed, we obtain:

$[Fe(II)\cdot FZ_3]_e \approx [Fe(II)\cdot DfTf]_e \approx 50 \times 10^{-6}$ M; $[DfTf]_0 = 404.75 \times 10^{-6}$ M (the initial concentration of DfTf was found by interpolating the graph on Fig. 4);

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

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

$[FZ]_e \approx [FZ]_0 - 3 \times [\ Fe(II)\cdot FZ_3]_e = 333 \times 10^{-6}\ M - 3 \times 50 \times 10^{-6}\ M = 183 \times 10^{-6}$ M.

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