

IN VITRO EVALUATION OF COPPER-CHELATING PROPERTIES OF FLAVONOIDS

SUPPLEMENTARY DATA

6 pages

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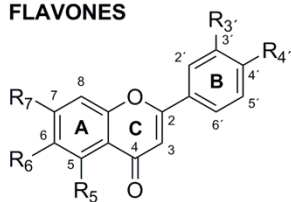
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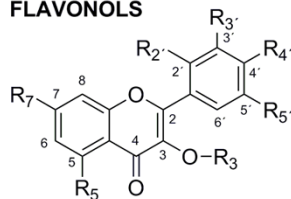
Heyrovského 1203

FLAVONES



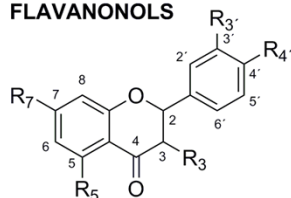
	R ₅	R ₆	R ₇	R _{3'}	R _{4'}
flavone	H	H	H	H	H
5-hydroxyflavone	OH	H	H	H	H
7-hydroxyflavone	H	H	OH	H	H
chrysin	OH	H	OH	H	H
apigenin	OH	H	OH	H	OH
luteolin	OH	H	OH	OH	OH
luteolin-4'-O-Glc	OH	H	OH	OH	O-Glc
mosloflavone	OH	OCH ₃	OCH ₃	H	H
negletein	OH	OH	OCH ₃	H	H
baicalein	OH	OH	OH	H	H
baicalin	OH	OH	O-Glu	H	H
diosmin	OH	H	O-Glc-Rha	OH	OCH ₃

FLAVONOLS



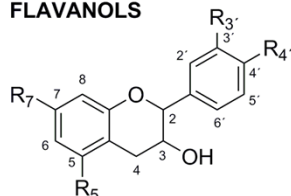
	R ₃	R ₅	R ₇	R _{2'}	R _{3'}	R _{4'}	R _{5'}
3-hydroxyflavone	H	H	H	H	H	H	H
kaempferol	H	OH	OH	H	H	OH	H
quercetin	H	OH	OH	H	OH	OH	H
morin	H	OH	OH	OH	H	OH	H
myricetin	H	OH	OH	H	OH	OH	OH
rutin	Glc-Rha	OH	OH	H	OH	OH	H
troxerutin	Glc-Rha	OH	O-C ₂ H ₄ -OH	H	O-C ₂ H ₄ -OH	O-C ₂ H ₄ -OH	H

FLAVANONES/ FLAVANONOLS



	R ₃	R ₅	R ₇	R _{3'}	R _{4'}	configuration
naringenin	H	OH	OH	H	OH	2RS
naringin	H	OH	O-Glc-Rha	H	OH	2RS
hesperetin	H	OH	OH	OH	OCH ₃	2S
hesperidin	H	OH	O-Glc-Rha	OH	OCH ₃	2S
taxifolin	OH	OH	OH	OH	OH	2R, 3R

FLAVANOLS



	R ₅	R ₇	R _{3'}	R _{4'}	configuration
(-)-epicatechin	OH	OH	OH	OH	2R, 3R
(+)-catechin	OH	OH	OH	OH	2R, 3S

Fig. S1 Chemical structures of the tested flavonoids. Glc: glucose, Glu: glucuronic acid, Rha: rhamnose.

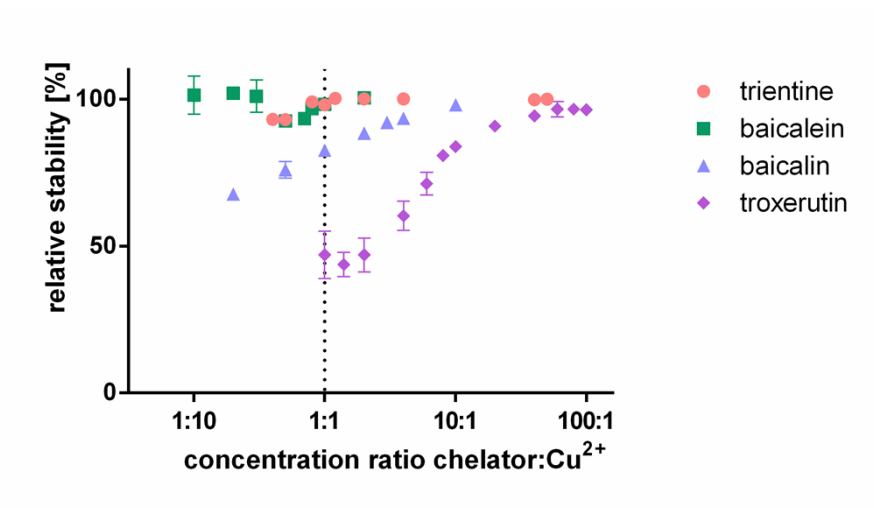


Fig. S2 The representative examples of stable (trientine, baicalein) and unstable (baicalin, troxerutin) copper-chelator complexes, evaluated by the hematoxylin method. The values express mean per cent relative stability of flavonoids at all tested pH conditions and that of trientine at pH 6.8 and 7.5 due to instability of its complexes under acidic conditions.

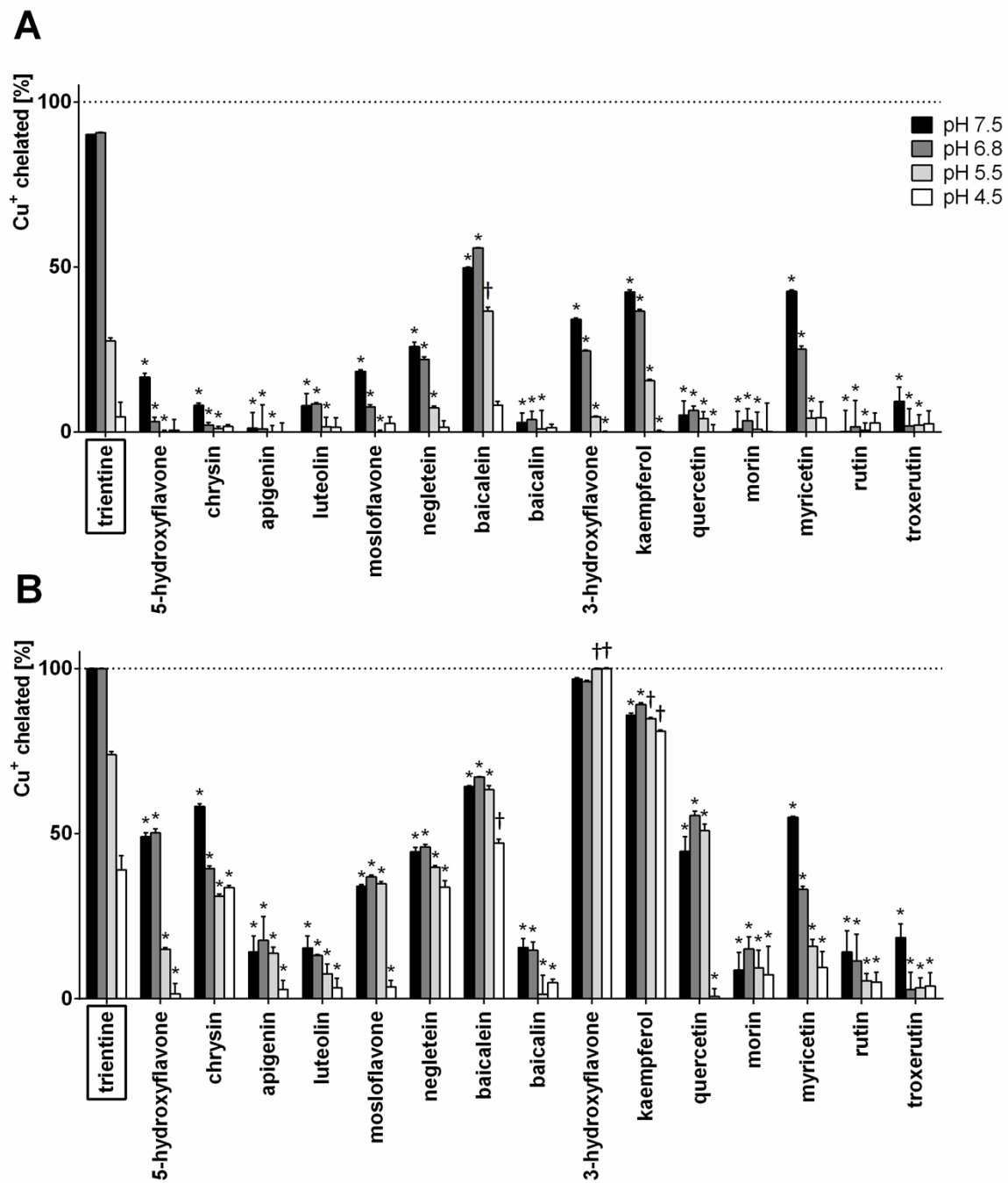


Fig. S3 The chelation of cuprous ions by flavonoids, compared with trientine, at the ratios of 1:1 (A) and 10:1 (B) (flavonoid:copper). * Less potent than trientine, † more potent than trientine ($p < 0.05$).

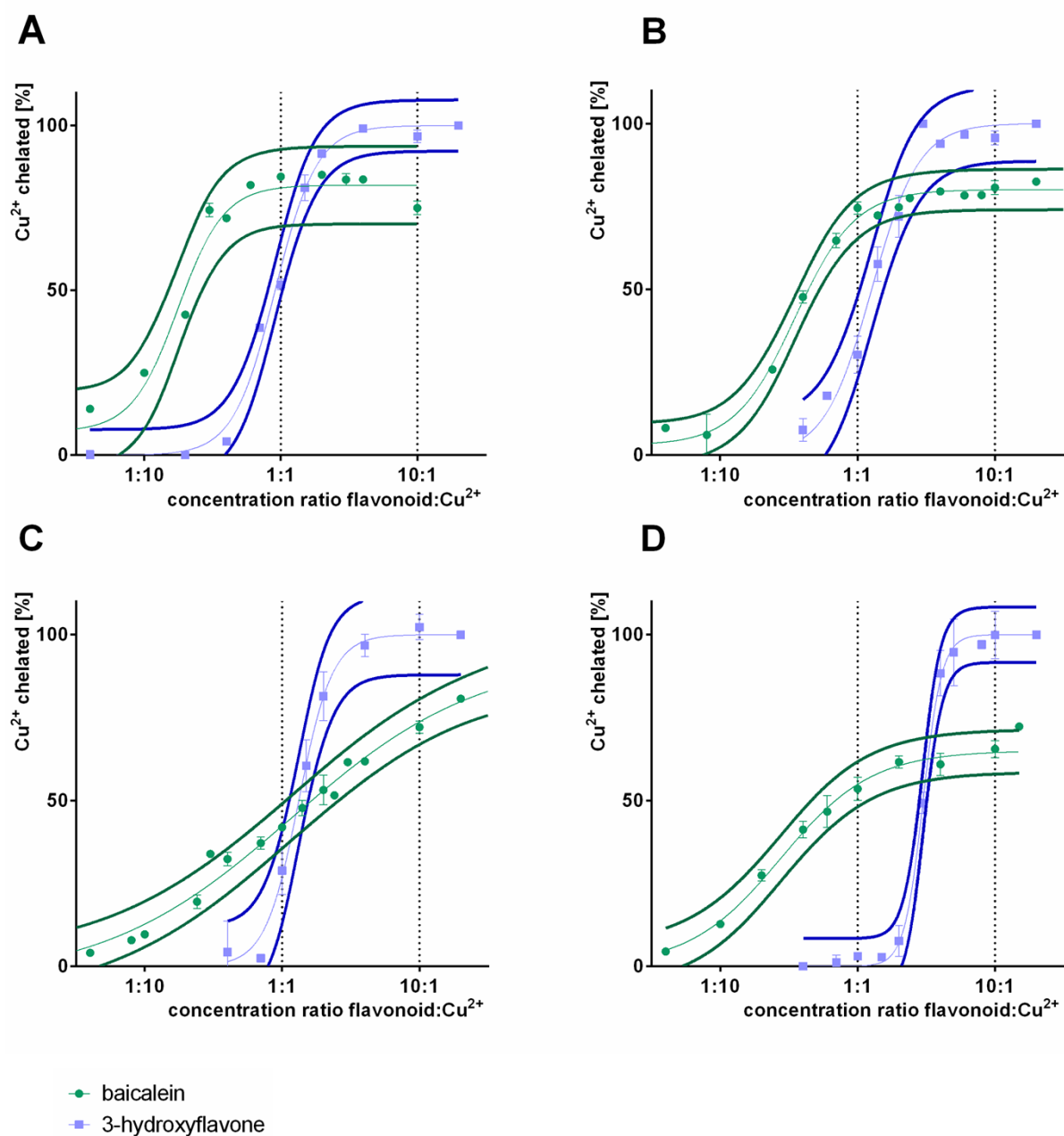


Fig. S4 The comparison of cupric chelation properties of baicalein and 3-hydroxyflavone according to the pH conditions: pH 7.5 (A), 6.8 (B), 5.5 (C), and 4.5 (D). Different character of chelation curves was observed: while the chelation by baicalein reached a plateau at the concentration ratio of 1:1, flavonoid to copper, respectively, in most cases, the chelation of 3-hydroxyflavone increased up to 100% between the concentration ratios of 1:1 and 10:1.

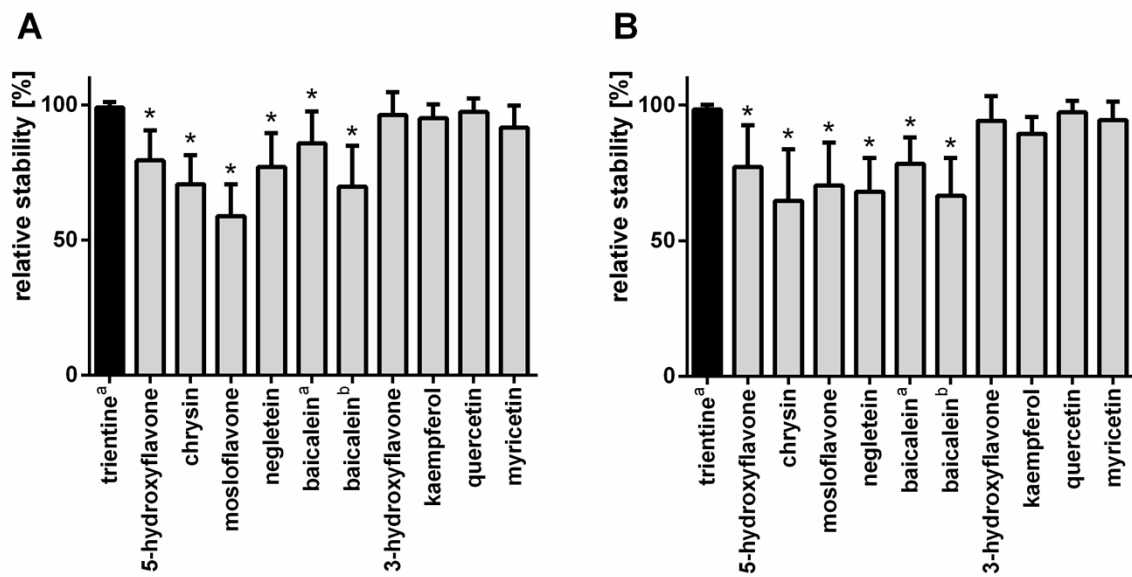


Fig. S5 The relative stability of complexes compared with those of trientine. (A) Cupric ions, (B) cuprous ions, ^a pH 6.8 and 7.5, ^b pH 4.5 and 5.5. * Less stable than the complexes of trientine ($p < 0.05$).