

# Correction to “New Procedure to Calculate All Equilibrium Constants in Flavylum Compounds: Application to the Copigmentation of Anthocyanins”


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ACS Omega 2019, 4 (7), 12058–12070. DOI:10.1021/acsomega.9b01066

 Cite This: ACS Omega 2020, 5, 25476–25476

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We detected an error in eq 59 of the original article concerning the transcription of the mole fractions and consequently in the final formula. When  $\text{pH} \leq 1$  the flavylum cation is the sole species of the multistate. Considering the 1:1 complex



$$C_0 = [\text{AH}^+] + [\text{AH}^+\text{CP}] = [\text{AH}^+](1 + K_{\text{AH}^+\text{CP}}[\text{CP}]) \quad (2)$$

$$\chi_{\text{AH}^+} = \frac{[\text{AH}^+]}{C_0} = \frac{1}{1 + K_{\text{AH}^+\text{CP}}[\text{CP}]} \text{ and}$$

$$\chi_{\text{AH}^+\text{CP}} = \frac{[\text{AH}^+\text{CP}]}{C_0} = \frac{K_{\text{AH}^+\text{CP}}[\text{CP}]}{1 + K_{\text{AH}^+\text{CP}}[\text{CP}]} \quad (3)$$

$$A_\lambda = \varepsilon_{\text{AH}^+}C_0\chi_{\text{AH}^+} + \varepsilon_{\text{AH}^+\text{CP}}C_0\chi_{\text{AH}^+\text{CP}} \quad (4)$$

Substituting the mole fractions in eq 4 gives the correct equation:

$$A_\lambda = \frac{\varepsilon_{\text{AH}^+}C_0 + \varepsilon_{\text{AH}^+\text{CP}}C_0K_{\text{AH}^+}[\text{CP}]}{1 + K_{\text{AH}^+}[\text{CP}]}$$

$$= \frac{A_0 + A_fK_{\text{AH}^+}[\text{CP}]}{1 + K_{\text{AH}^+}[\text{CP}]} \quad (5)$$

with

$$A_0 = \varepsilon_{\text{AH}^+}C_0 \text{ and } A_f = \varepsilon_{\text{AH}^+\text{CP}}C_0 \quad (6)$$

This eq 5 is the correct expression and not the one reported in eq 59 in the original manuscript (also give below):

$$A_\lambda = \frac{A_0 + A_f(1 + K_{\text{AH}^+}[\text{CP}])}{1 + K_{\text{AH}^+}[\text{CP}]} \quad (7)$$

The constants  $K_{\text{AH}^+\text{CP}}$  in Table 3 and in Table 5 are correct because they were calculated with the right equation. We apologize to our readers for this mistake.

Received: September 14, 2020

Published: September 24, 2020

