Electronic Supplementary Material (ESI) for Food & Function.

Supplementary Information

The influence of acylation, metal binding and natural antioxidants on the thermal stability of red cabbage anthocyanins in neutral solution

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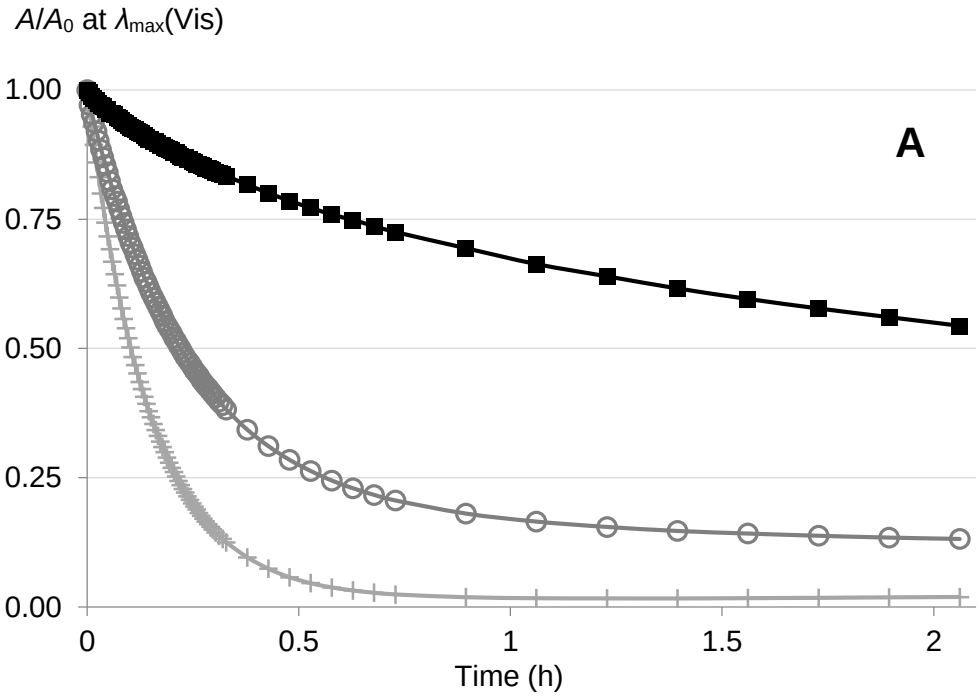

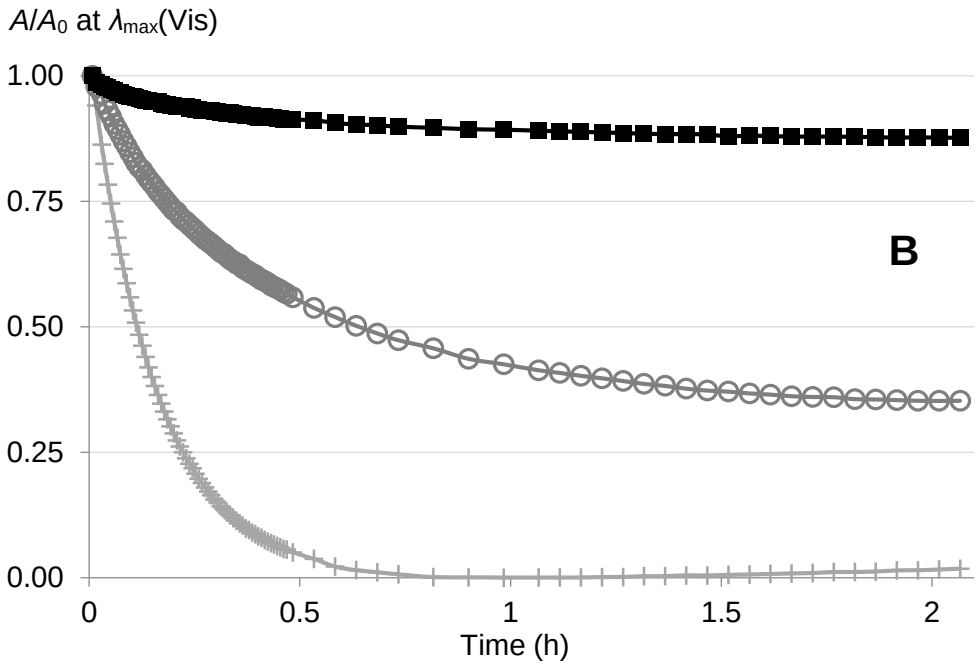

Fig. 1-SI Spectroscopic monitoring of color loss at pH 7, 50°C. **A:** Pigment A (+), P1 (○), P4 (■), **B:** same pigments in the presence of 0.6 equiv. Fe^{2+}.

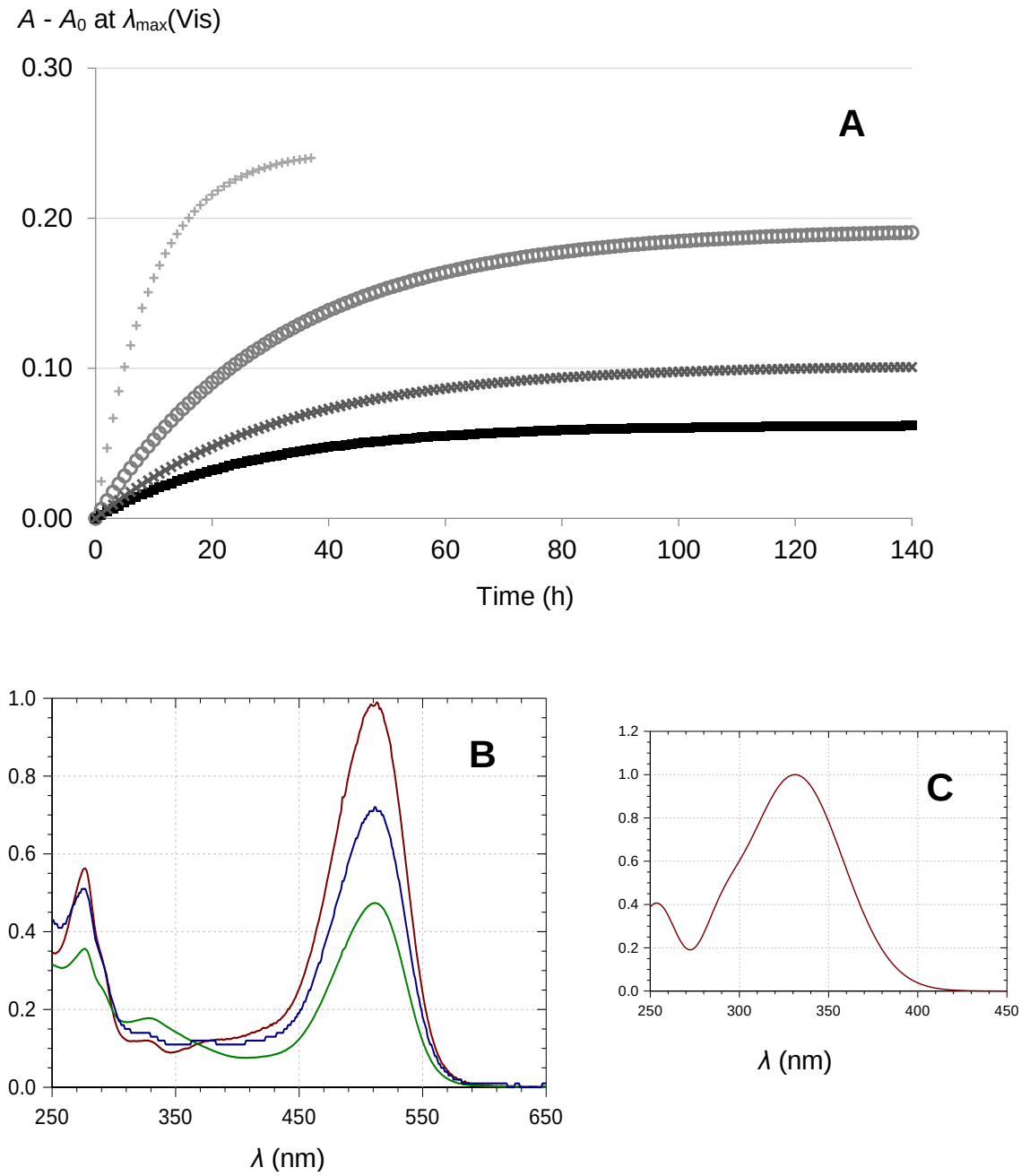

Fig. 2-SI **A:** The slow conversion of the *trans*-chalcone to flavylium ion (25°C) after acidification to pH 1-2 of samples uptaken after a 2h period of thermal treatment at pH 7, 50°C. A_0 = absorbance immediately after acidification. PA (+), P1 (○), P4 (■), RCE (X). First-order curve fitting gives: k_{obs} (x10^{-3}, h^{-1}) = 106.0 ± 2.3 (PA), 31.7 ± 0.1 (P1), 37.4 ± 0.6 (P4) and 31.4 ± 0.7 (RCE). **B:** —: intact pigment A (control, pure flavylium), —: sample immediately after acidification (flavylium + Ct + degradation products), —: sample after incubation for 48h (flavylium + degradation products). **C:** Normalized spectrum of the *trans*-chalcone deduced from the spectra of part B.

Simulation	k_{DA} / h^{-1}	k_{DB} / h^{-1}	k_h / h^{-1}	k_{-h} / h^{-1}	Q_h
1	0.5	0	10	1	10
2	0.5	0.5	10	1	10
3	0.5	0.05	10	0.1	100

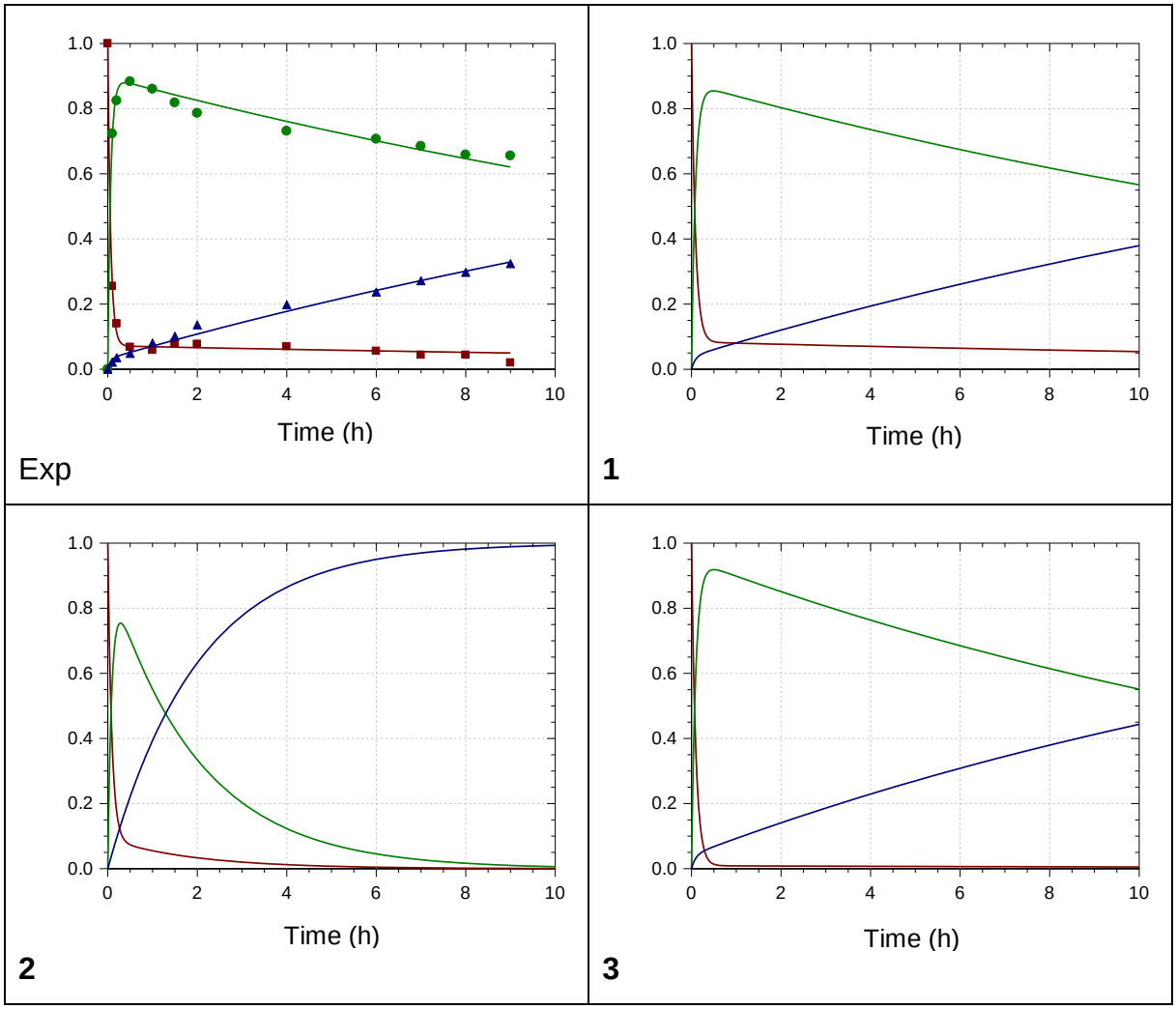

Fig. 3-SI Kinetic simulations for the degradation of pigment A at pH 7, 50°C. First graph: curve-fitting of the experimental data. Graphs 1-3: simulations from parameters reported in Table. X_n: —, X_h: —, X_d: —.

Simulation	k_{DA} / h^{-1}	k_{DB} / h^{-1}	k_h / h^{-1}	k_{-h} / h^{-1}	Q_h
1	0.08	0	0.14	0.2	0.7
2	0.08	0.08	0.14	0.2	0.7
3	0.08	0.008	0.08	0.01	8

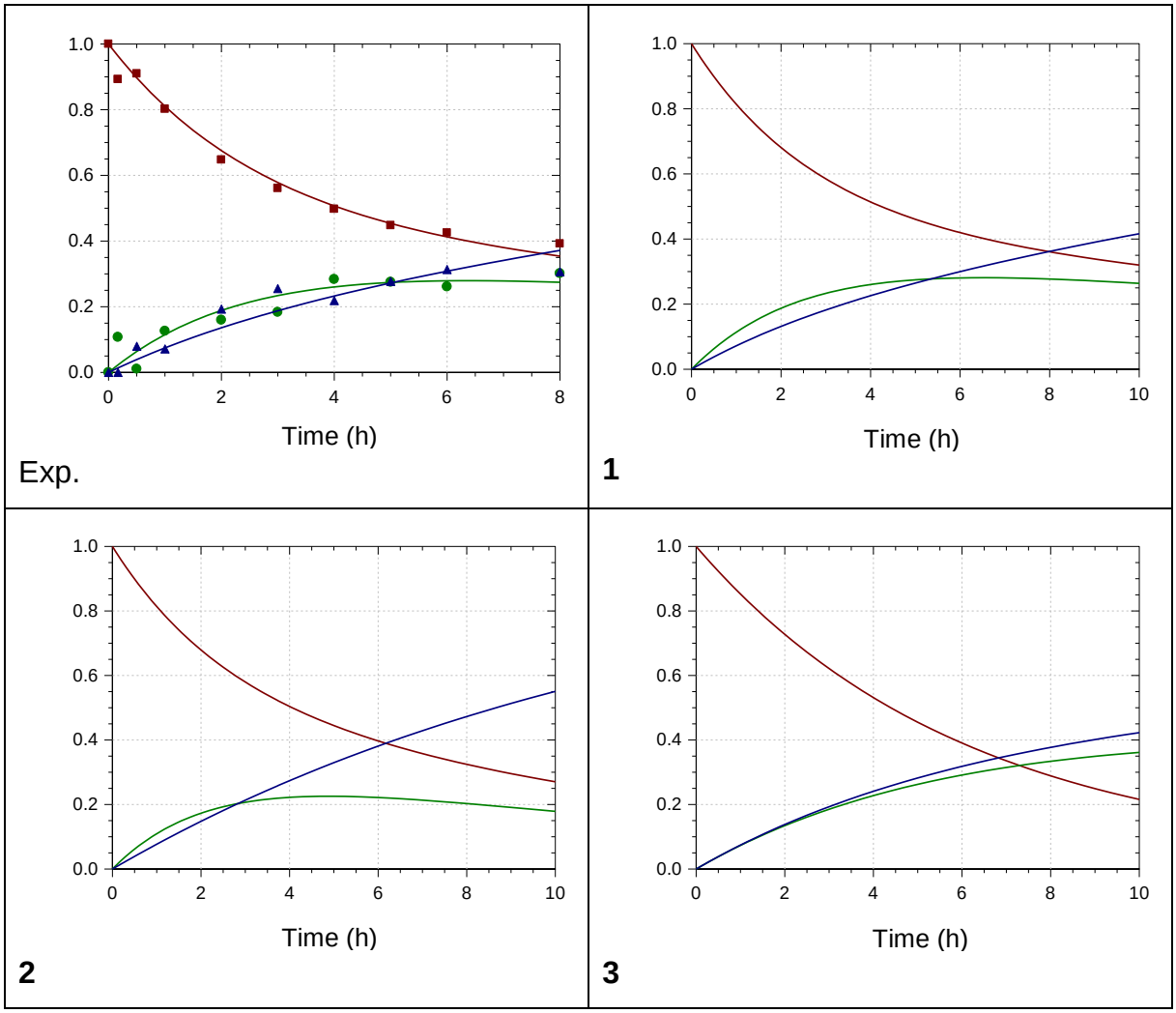

Fig. 4-SI Kinetic simulations for the degradation of P4 at pH 7, 50°C. First graph: curve-fitting of the experimental data. Graphs 1-3: simulations from parameters reported in Table. X_n: —, X_h: —, X_d: —.

Table 1-SI Apparent rate constants and amplitudes of color loss at pH 7 deduced from mono- or biexponential curve-fitting ($r > 0.999$).

	Pigment A	**P1**	**P4**
k_{obs} (h^{-1}), 25°C	-	1.42 (± 0.06) [a] 0.11 (± 0.03)	0.32 (± 0.02) [a] 0.04 (± 0.01)
ΔA, 25°C	-	0.66 (± 0.02) 0.12 (± 0.02)	0.199 (± 0.009) 0.35 (± 0.01)
k_{obs} (h^{-1}), 50°C	6.89 (± 0.01)	4.05 (± 0.03)	0.80 (± 0.02) 8.1 (± 0.5)
ΔA, 50°C	0.98 (± 0.01)	0.85 (± 0.01)	0.49 (± 0.01) 0.06 (± 0.01)
k_{obs} (h^{-1}), Fe^{2+} (0.6 equiv.), 50°C	6.19 (± 0.04)	2.55 (± 0.02)	-
ΔA, Fe^{2+} (0.6 equiv.), 50°C	*ca*. 1	0.64 (± 0.01)	*ca*. 0.1

[a] Calculated k_{obs} values (pure hydration) at 25°C = 0.195 (P1) and 0.064 (P4) h^{-1}.