



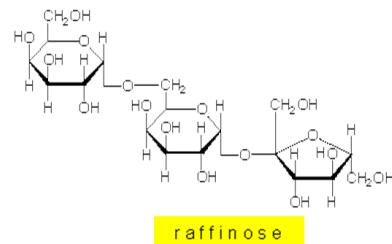
## Modélisation du comportement des $\alpha$ -galactosides/folates au cours du trempage-cuisson du niébé / Réduction de son pouvoir antinutritionnel



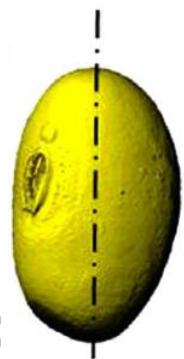
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# Présentation du modèle graine



- Niébé (*Wankoun*) = légumineuse d'Afrique de l'Ouest
- $\alpha$ -galactosides (verbascose, stachyose, raffinose) = oligo-saccharides fermentescibles dans le côlon => **flatulences**
- **Optimisation trempage-cuisson** permettrait de **réduire la teneur en  $\alpha$ -galactosides de la graine**
- **2 compartiments considérés dans le modèle:**
  - Graine supposée symétrique / composition homogène
  - Eau de trempage  $V(t)$  avec ratio eau-graine de 4:1 (m/m)
- **Phénomènes modélisés impliquant les  $\alpha$ -galactosides :**
  - Absorption ( $D$ ,  $\text{m}^2.\text{s}^{-1}$ ) d'eau de la graine
  - Diffusion ( $D$ ,  $\text{m}^2.\text{s}^{-1}$ ) de la graine vers l'eau trempage
  - Dégradabilité ( $k$ ,  $\text{s}^{-1}$ ) par voie enzymatique endogène ( $\alpha$ -galactosidase)
- **Températures de trempage étudiées:** 30 / 60 / 95°C

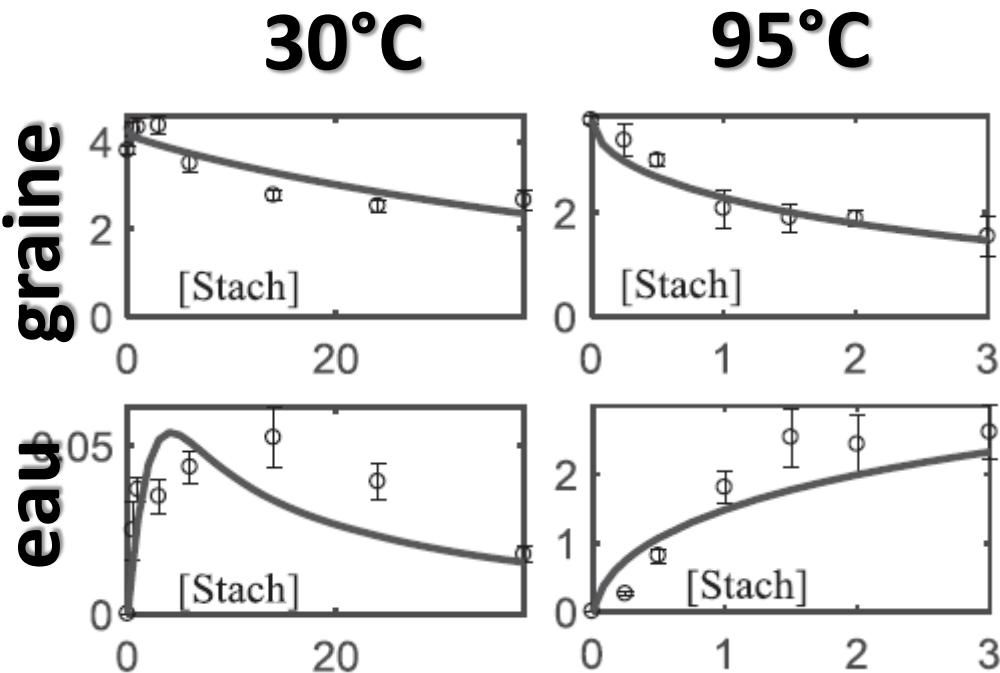


MATLAB®



# Transport vs Réactivité

- Comportement contrasté en fonction de la température: (ex; stachyose):



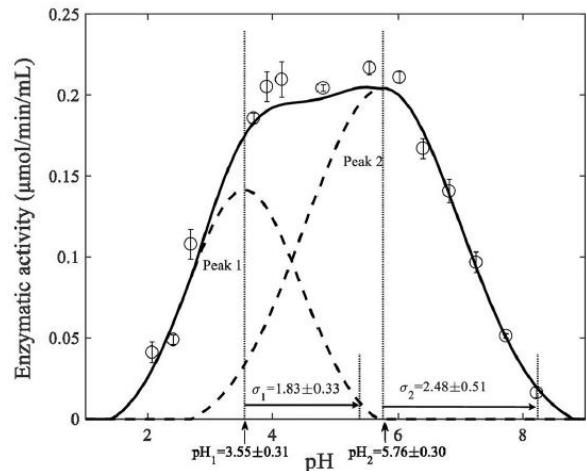
Stachyose:	30°C	95°C
Diffusivité $D$ ( $\text{m}^2.\text{s}^{-1}$ )	$2 \times 10^{-13}$	<u><math>4.3 \times 10^{-11}</math></u>
Dégradabilité $k$ ( $\text{s}^{-1}$ )	<u><math>2.9 \times 10^{-6}</math></u>	$0.0 \times 10^{-6}$

- À 30°C: activité enzymatique observée aussi bien dans graine que eau de trempage => caractérisation  $\alpha$ -galactosidase endogène

Coffigniez, F., Briffaz, A., Mestres, C., Alter, P., Durand, N., Bohuon, P., (2018). Multi-response modeling of reaction-diffusion to explain alpha-galactoside behavior during the soaking-cooking process in cowpea. Food Chemistry 242, 279-287.

# Modélisation du comportement enzymatique

- Identification des affinités et pH/T°C optimaux pour l'α-galactosidase endogène extraite du niébé:



Substrate	Michaelian parameters		RMSE <sup>§</sup> (mM)
	$v_{max}$ (μmol·min <sup>-1</sup> ·mL <sup>-1</sup> )	$K_m$ (mM)	
Verbascose	0.01 ± 0.01	0.25 ± 0.06 <sup>a</sup>	0.01
	0.21	15.9 ± 0.1 <sup>b</sup>	0.01
Stachyose	0.22 ± 0.06	4.1 ± 1.8 <sup>a</sup>	0.20
	0.21	3.6 ± 0.6 <sup>b</sup>	0.23
Raffinose	0.19 ± 0.01	1.2 ± 0.3 <sup>a</sup>	0.51
	0.21	1.7 ± 0.3 <sup>b</sup>	0.84

- Caractérisation (par ajouts dosés) des effets inhibiteurs de certains micro-constituants de la graine :

$$v = \frac{v_{max} [S]}{K_m^{app1} + [S]}$$
$$K_m^{app1} = K_m \left( 1 + \frac{[I]}{K_I} \right)$$

Michaelian parameters	Values	RMSE
$v_{max}$ for PNP (μmol·min <sup>-1</sup> ·mL <sup>-1</sup> )	0.21 ± 0.01	0.005 <sup>a</sup> μmol min <sup>-1</sup> mL <sup>-1</sup>
$K_m$ for PNP (mM)	0.40 ± 0.05	
$K_I$ galactose (mM)	0.28 ± 0.03	
$K_I$ galactinol (mM)	0.88 ± 0.02	0.06 <sup>b</sup> mM
$K_I$ myo-inositol (mM)	11.90 ± 0.20	0.06 <sup>b</sup> mM

Coffigniez, F., Briffaz, A., Mestres, C., Ricci, J., Alter, P., Durand, N., Bohuon, P., (2018). Kinetic study of enzymatic alpha-galactosidase hydrolysis in cowpea seeds. Food research international (Ottawa, Ont.) 113, 443-451.



# VITAMICOWPEA

**VITAMIn B9 (folate) study to Increase COwpea value  
chain sustainability in West Africa through Product  
and procESS innovAtion**

RFL2 / 10 October 2018  
Toulouse

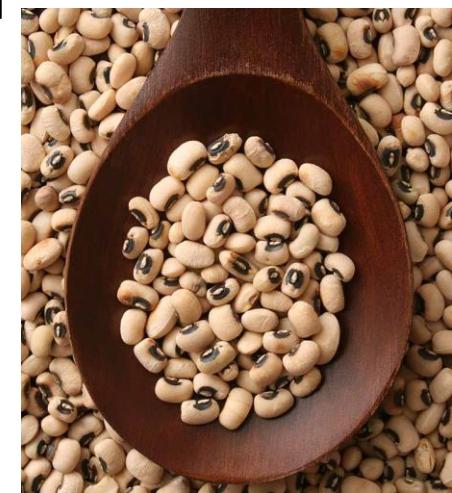
Dr Fanny Coffigniez (CIRAD/ QualiSud research unit, Montpellier (France)) PhD student

Prof. Michael Rychlik (Technical University of Munich), Fanny Supervisor

Dr Aurelien Briffaz (CIRAD/ QualiSud research unit, Montpellier (France)) Project Coordinator

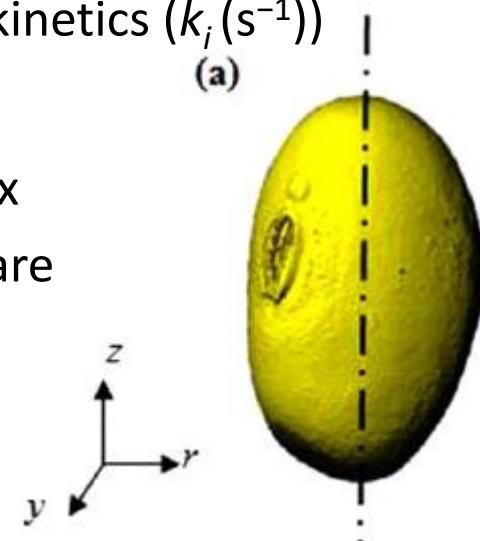
# Project objectives

- Investigate folate vitamer behaviour during cowpea soaking-cooking process and germination at 30°C/60°C/95°C.
- Develop a mathematical model describing transport and reactivity properties of folate vitamers during processing.
- Identify optimized processing pathways that could maximize folate retention in cowpea seeds.

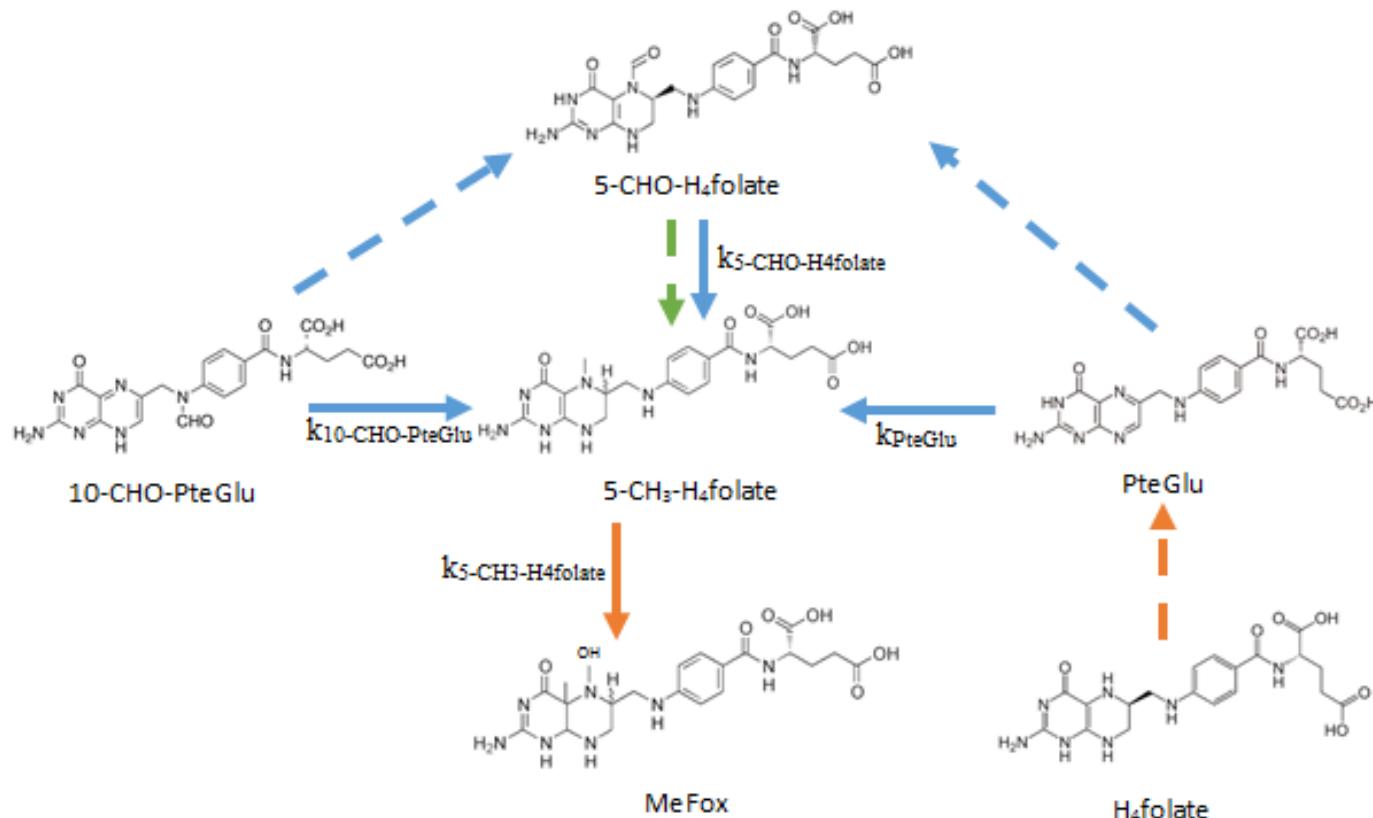


# Model presentation

- One single cowpea seed considered and being surrounded by a limited amount of water:
  - With a water-to-seed ratio of 4:1 (w/w) in the case of soaking
  - With a water-to-seed ratio of 1:1 (w/w) in the case of germination
- Investigated temperature: 30°C.
- Model assumptions:
  - Transport by means of molecular diffusion ( $D_i$  (m<sup>2</sup>.s<sup>-1</sup>), Fick's law)
  - Folate production/degradation assuming first-order kinetics ( $k_i$  (s<sup>-1</sup>))
- Model adjustments:
  - Minimization of the determinant of covariance matrix
  - Coupling of COMSOL Multiphysics and Matlab software



# Folate reaction scheme



— Enzymatic conversion

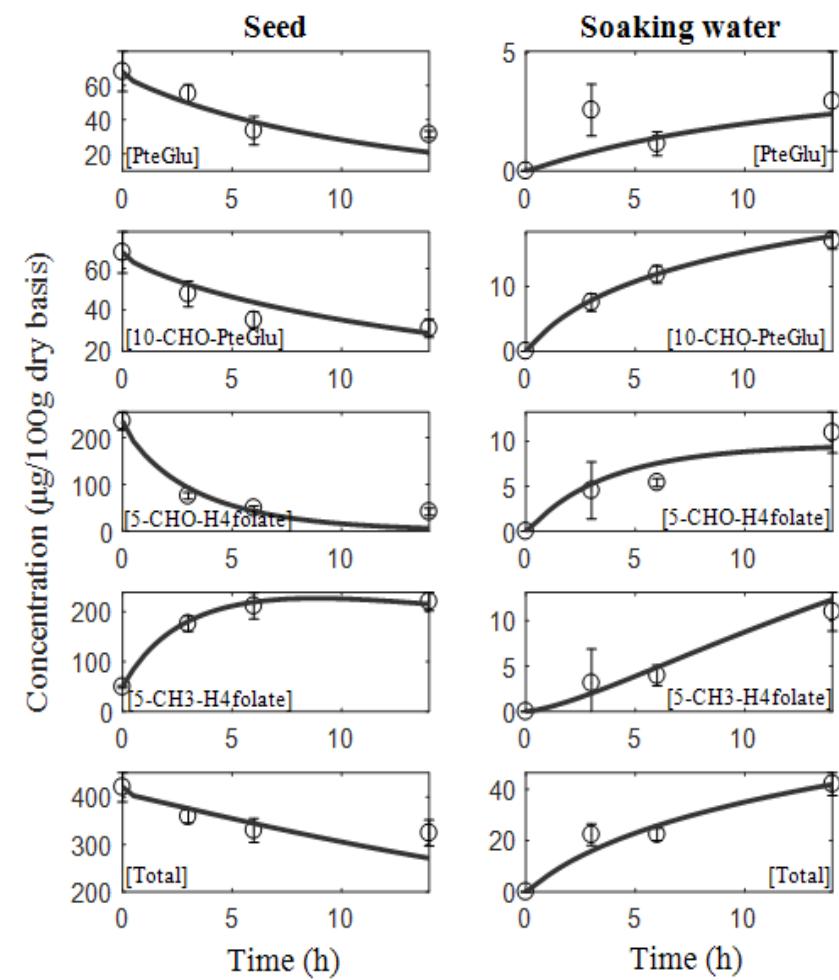
— Chemical conversion

— Thermal oxidation

Solid lines : modeled

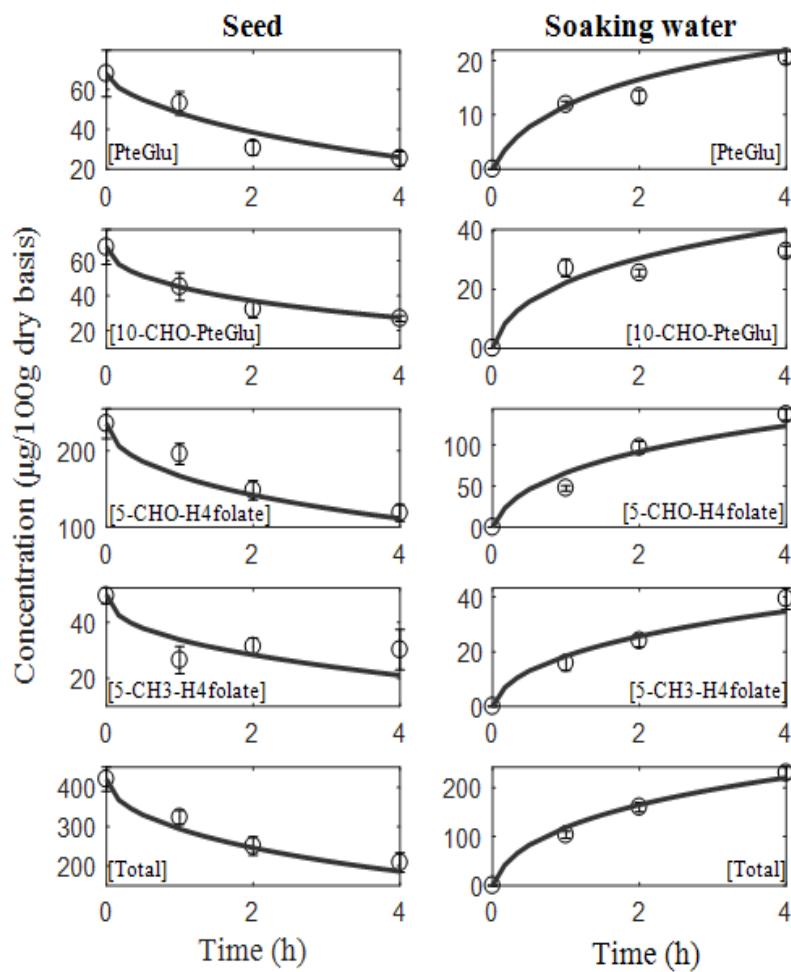
Dashed lines : Not modeled

# Soaking-cooking results 30°C (paper 1)



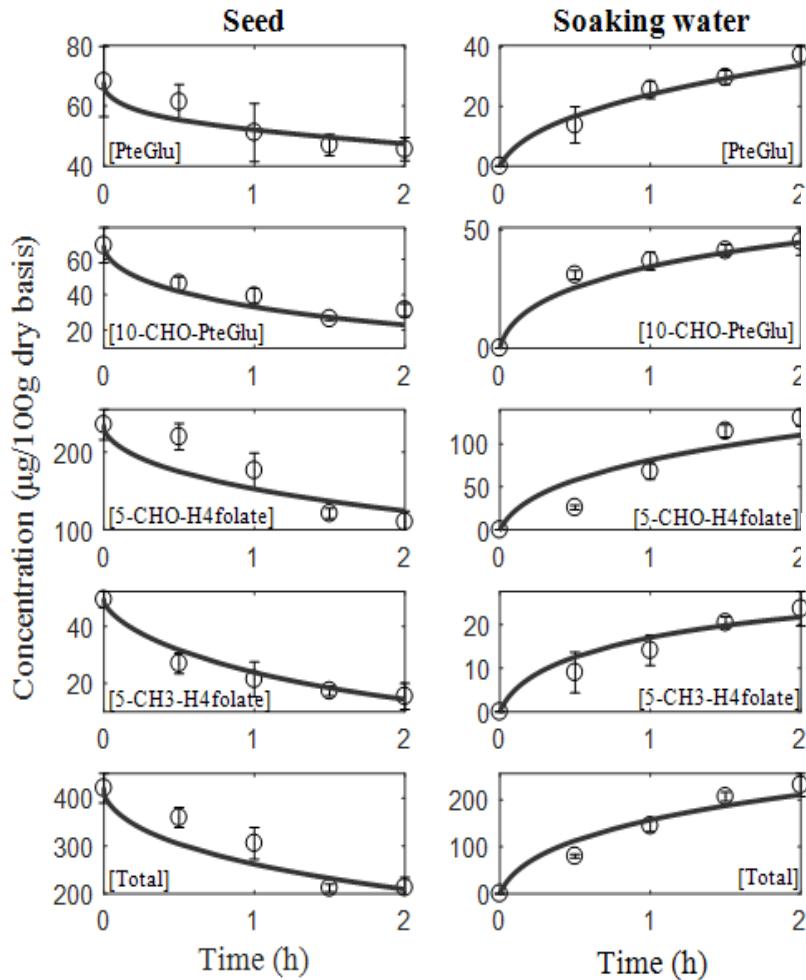
Vitamers <i>X</i>	<i>T</i> (°C)	<i>D<sub>X</sub></i> × 10 <sup>11</sup> ( <i>m</i> <sup>2</sup> <i>s</i> <sup>-1</sup> )	<i>k<sub>X,Ω<sub>s</sub></sub></i> × 10 <sup>5</sup> ( <i>s</i> <sup>-1</sup> )	RMSE*	
				In seed (S)	In soaking water (SW)
Folic acid	30	0.010 ± 0.001	2.21 ± 0.04	8.9	1.3
10-formyl-folic acid	30	0.181 ± 0.003	0.81 ± 0.01	8.3	1.3
5-formyl-H <sub>4</sub> folate	30	0.026 ± 0.001	8.0 ± 0.12	23.0	2.4
5-methyl-H <sub>4</sub> folate	30	0.014 ± 0.002	1.11 ± 0.02	17.1	1.4

# Soaking-cooking results 60°C (paper 1)



Vitamers $X$	$T(^{\circ}\text{C})$	$D_X \times 10^{11} (\text{m}^2\text{s}^{-1})$	$k_{X,\Omega_s} \times 10^5 (\text{s}^{-1})$	RMSE*	
				In seed (S)	In soaking water (SW)
Folic acid	60	0.81 $\pm$ 0.02	3.73 $\pm$ 0.06	7.2	1.4
10-formyl-folic acid	60	2.93 $\pm$ 0.05	0	6.3	5.2
5-formyl-H <sub>4</sub> folate	60	2.12 $\pm$ 0.04	0	20.1	12.4
5-methyl-H <sub>4</sub> folate	60	3.52 $\pm$ 0.07	3.39 $\pm$ 0.06	7.1	3.3

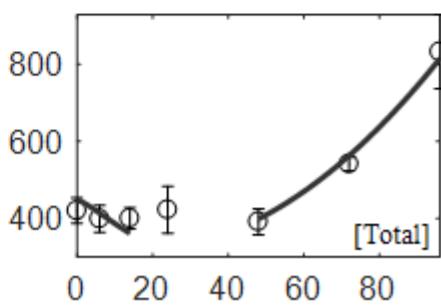
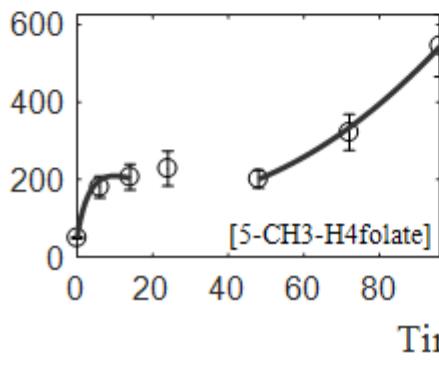
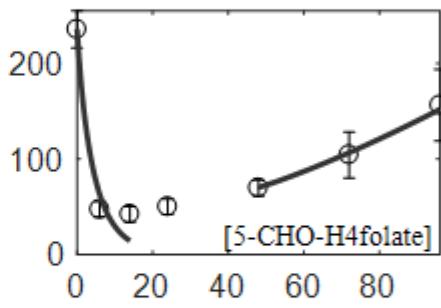
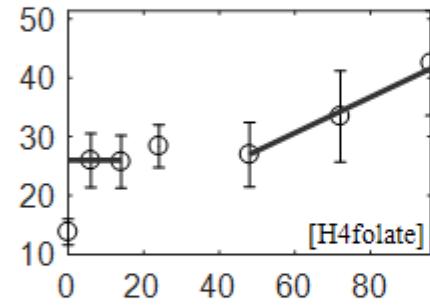
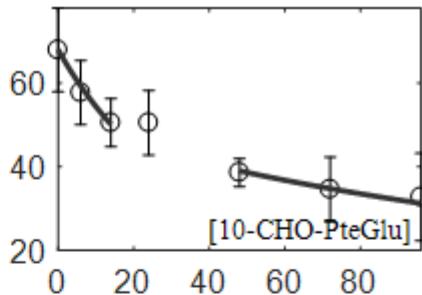
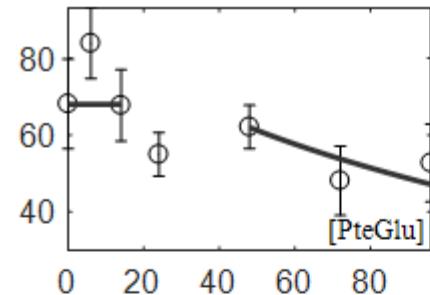
# Soaking-cooking results 95°C (paper 1)



Vitamers X	$T(\text{°C})$	$D_X \times 10^{11} (\text{m}^2 \text{s}^{-1})$	$k_{X,\Omega_S} \times 10^5 (\text{s}^{-1})$	RMSE*	
				In seed (S)	In soaking water (SW)
Folic acid	95	$3.12 \pm 0.06$	0	7.3	3.5
10-formyl-folic acid	95	$7.94 \pm 0.16$	0	6.6	4.4
5-formyl-H <sub>4</sub> folate	95	$3.23 \pm 0.05$	0	29.3	19.9
5-methyl-H <sub>4</sub> folate	95	$3.63 \pm 0.06$	$7.73 \pm 0.14$	4.2	3.4

# Germination results 30°C (paper 2)

Concentration ( $\mu\text{g}/100\text{g dry basis}$ )



<i>Species X</i>	<i>Process</i>	$k_{X,\Omega_s} \times 10^5 (\text{s}^{-1})$	$k_{pX,\Omega_s} \times 10^5 (\text{s}^{-1})$	RMSE*
Folic acid	S	$2.21 \pm 0.04$	0	8.9
	G1	0	0	12.5
	G2	$0.16 \pm 0.01$	0	8.8
10formyl-folic acid	S	$0.81 \pm 0.01$	0	8.3
	G1	$0.63 \pm 0.02$	0	7.6
	G2	$0.13 \pm 0.01$	0	6.7
5formyl-H <sub>4</sub> folate	S	$7.95 \pm 0.12$	0	23.0
	G1	$6.18 \pm 0.23$	0	22.6
	G2	$0.11 \pm 0.01$	$1.72 \pm 0.04$	21.4
5methyl-H <sub>4</sub> folate	S	$1.11 \pm 0.02$	0	17.1
	G1	$1.02 \pm 0.03$	0	21.5
	G2	0	$4.53 \pm 0.09$	12.7

\*RMSE: Root mean square error between experimental and predicted concentrations ( $\text{mg}/100\text{kg db}$ ).

S: soaking, G1: germination < 14 h; and G2: germination > 48 h

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