



Research article

Extraction of bioactive compounds from yerba mate (*Ilex paraguariensis* St.-Hil.) leaves by packed-bed extractor using hot water as solvents: Kinetics study and mathematical modeling

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Supplementary file

Table S1. Statistical analysis of bioactive compounds extraction from yerba mate using central composite design (CCD)*.

Parameters	Effect	Std. Err.	Coeff.	Std. Err. Coeff	p**
Total phenolic content (TFC)					
Mean	760.36	4.31	760.87	4.31	2.46×10^{-20}
Temperature (1)	541.75	9.64	520.52	4.82	7.03×10^{-15}
Feed flow rate (2)	24.09	9.64	2.86	4.82	0.03
1by2	-67.26	9.64	-88.49	4.82	2.30×10^{-5}
Theobromine					
Mean	37.04	0.41	37.04	0.41	3.20×10^{-17}
Temperature (1)	29.46	0.92	14.73	0.46	3.20×10^{-11}
Feed flow rate (2)	0.88	0.92	0.44	0.46	0.36
1by2	-3.08	0.92	-1.54	0.46	6.45×10^{-3}
Caffeine					
Mean	186.30	2.58	186.30	2.58	4.55×10^{-16}
Temperature (1)	154.95	5.78	77.47	2.89	2.25×10^{-11}
Feed flow rate (2)	6.84	5.78	3.42	2.89	0.26
1by2	-18.11	5.78	-9.06	2.89	9.49×10^{-3}
Chlorogenic acid					
Mean	243.04	1.70	243.04	1.70	2.45×10^{-19}
Temperature (1)	198.13	3.80	99.07	1.90	1.14×10^{-14}
Feed flow rate (2)	6.40	3.80	3.20	1.90	0.12
1by2	-20.89	3.80	-10.45	1.90	1.87×10^{-4}
Caffeic acid					
Mean	107.46	0.59	107.46	0.59	1.57×10^{-20}
Temperature (1)	90.08	1.31	45.04	0.65	7.53×10^{-1}
Feed flow rate (2)	2.79	1.31	1.40	0.65	0.06
1by2	-9.23	1.31	-4.62	0.65	2.10×10^{-5}
Rutin					
Mean	81.97	1.00	81.97	1.00	1.57×10^{-20}
Temperature (1)	84.59	2.25	42.30	1.12	7.53×10^{-1}
Feed flow rate (2)	3.22	2.25	1.61	1.12	0.06
1by2	-8.51	2.25	-4.26	1.12	2.10×10^{-5}
Quercetin					
Mean	0.68	3.53×10^{-3}	0.68	3.53×10^{-3}	8.78×10^{-21}
Temperature (1)	0.37	7.99×10^{-3}	0.19	3.94×10^{-3}	4.95×10^{-14}
Feed flow rate (2)	4.70×10^{-2}	7.99×10^{-3}	2.37×10^{-2}	3.94×10^{-3}	8.88×10^{-5}
1by2	-8.37×10^{-2}	7.99×10^{-3}	-4.19×10^{-2}	3.94×10^{-3}	4.05×10^{-7}

*: Analysis of Variance (ANOVA) for the cumulative concentration of bioactive compounds obtained from the packed-bed extraction process after 60 min.

** : Significant at $p < 0.05$.

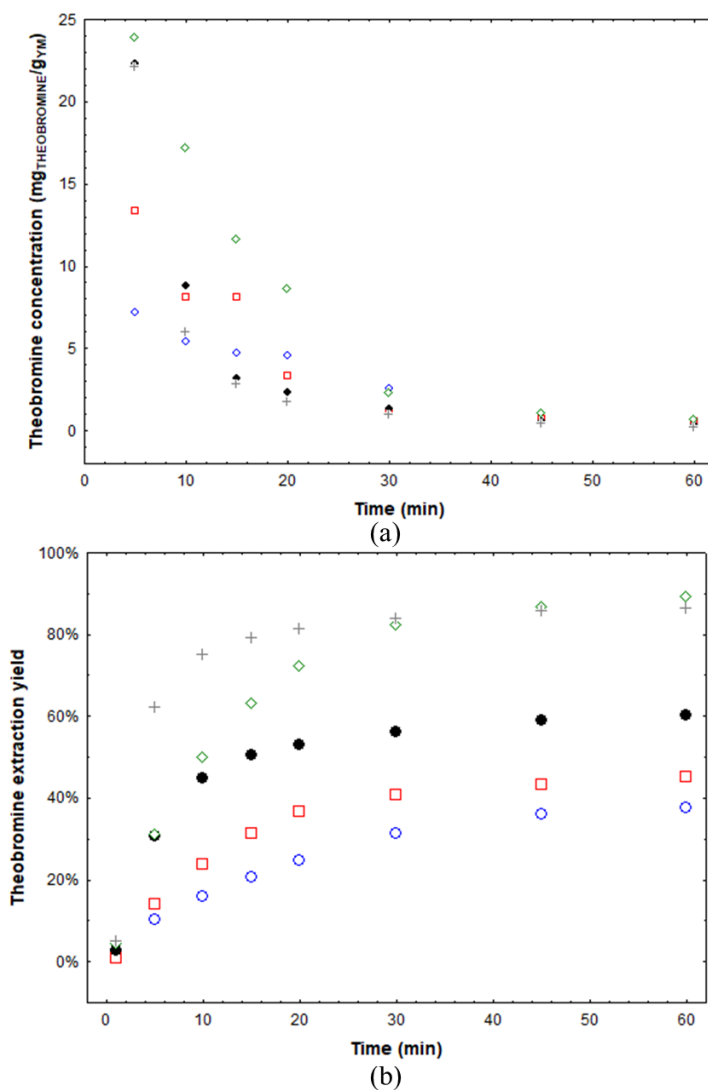


Figure S1. Kinetic of packed-bed extraction process for theobromine. (a) Theobromine concentration, (b) Theobromine extraction yield. \circ $T = 50\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$; \square $T = 50\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$; \bullet $T = 60\text{ }^{\circ}\text{C}$, $Q = 15\text{ cm}^3/\text{min}$; \diamond $T = 70\text{ }^{\circ}\text{C}$, $Q = 10\text{ cm}^3/\text{min}$; $+$ $T = 70\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$.

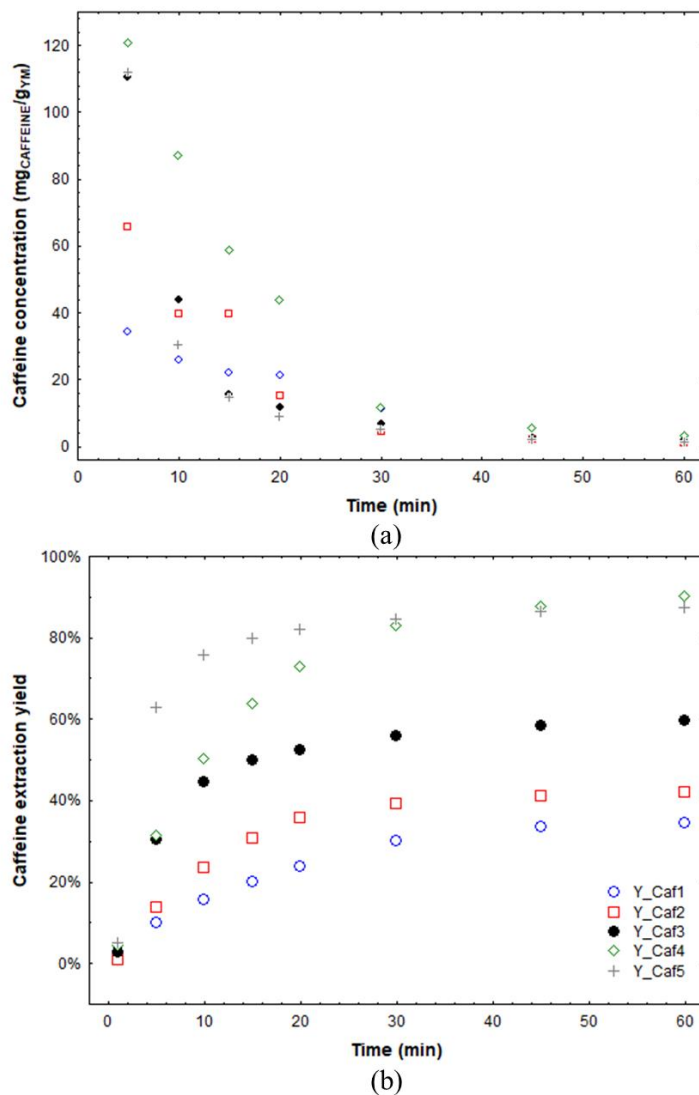


Figure S2. Kinetic of packed-bed extraction process for caffeine. (a) Caffeine concentration, (b) Caffeine extraction yield. \circ $T = 50\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$; \square $T = 50\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$; \bullet $T = 60\text{ }^{\circ}\text{C}$, $Q = 15\text{ cm}^3/\text{min}$; \diamond $T = 70\text{ }^{\circ}\text{C}$, $Q = 10\text{ cm}^3/\text{min}$; $+$ $T = 70\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$.

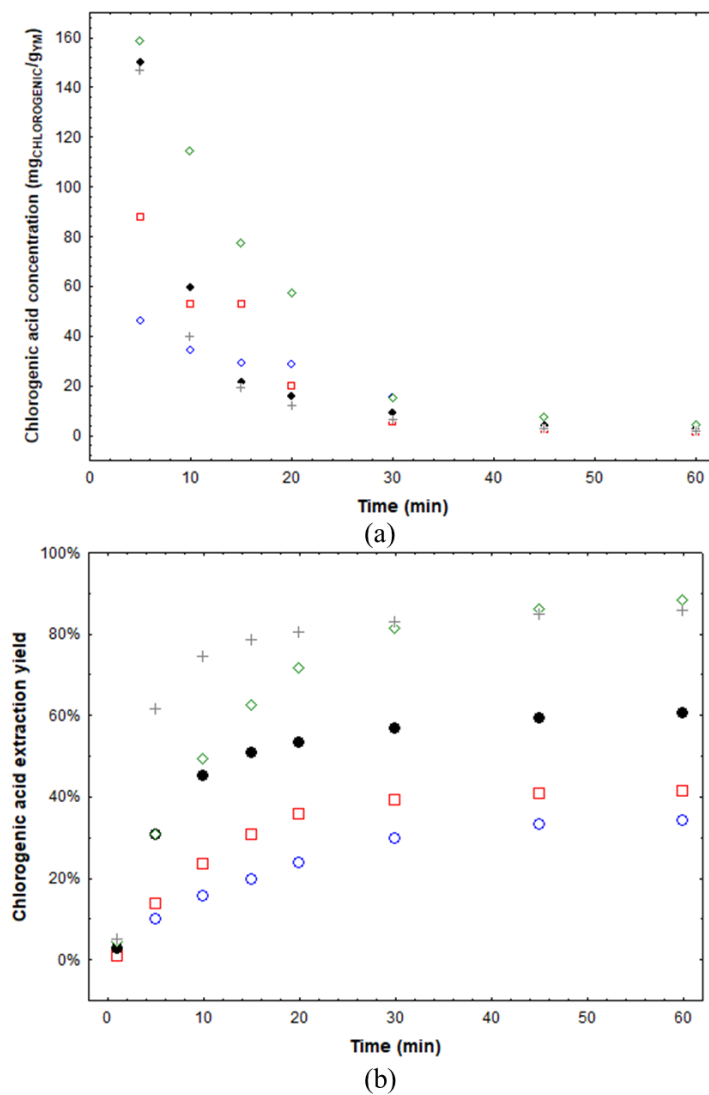


Figure S3. Kinetic of packed-bed extraction process for chlorogenic acid. (a) Chlorogenic acid, (b) Chlorogenic acid extraction yield. ○ T = 50 °C, Q = 20 cm³/min; □ T = 50 °C, Q = 20 cm³/min; ● T = 60 °C, Q = 15 cm³/min; ◇ T = 70 °C, Q = 10 cm³/min; + T = 70 °C, Q = 20 cm³/min.

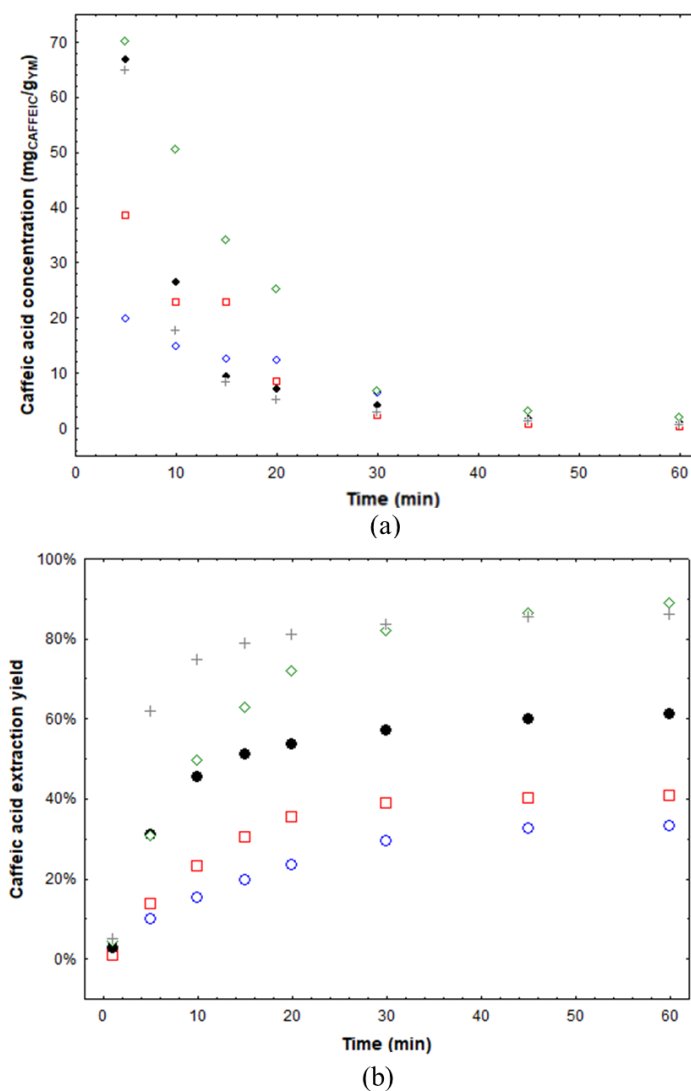


Figure S4. Kinetic of packed-bed extraction process for caffeic acid. (a) Caffeic acid concentration, (b) Caffeic acid extraction yield. \circ $T = 50\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$; \square $T = 50\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$; \bullet $T = 60\text{ }^{\circ}\text{C}$, $Q = 15\text{ cm}^3/\text{min}$; \diamond $T = 70\text{ }^{\circ}\text{C}$, $Q = 10\text{ cm}^3/\text{min}$; $+$ $T = 70\text{ }^{\circ}\text{C}$, $Q = 20\text{ cm}^3/\text{min}$.

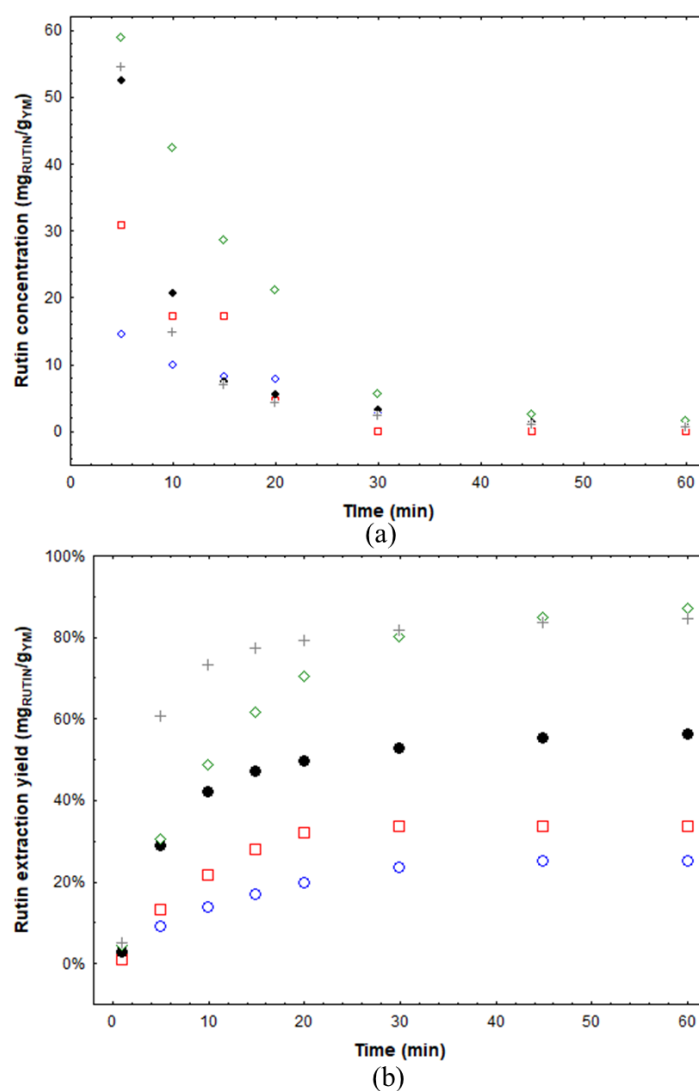


Figure S5. Kinetic of packed-bed extraction process for rutin. (a) Rutin concentration, (b) Rutin extraction yield. \circ T = 50 °C, Q = 20 cm³/min; \square T = 50 °C, Q = 20 cm³/min; \bullet T = 60 °C, Q = 15 cm³/min; \diamond T = 70 °C, Q = 10 cm³/min; $+$ T = 70 °C, Q = 20 cm³/min.

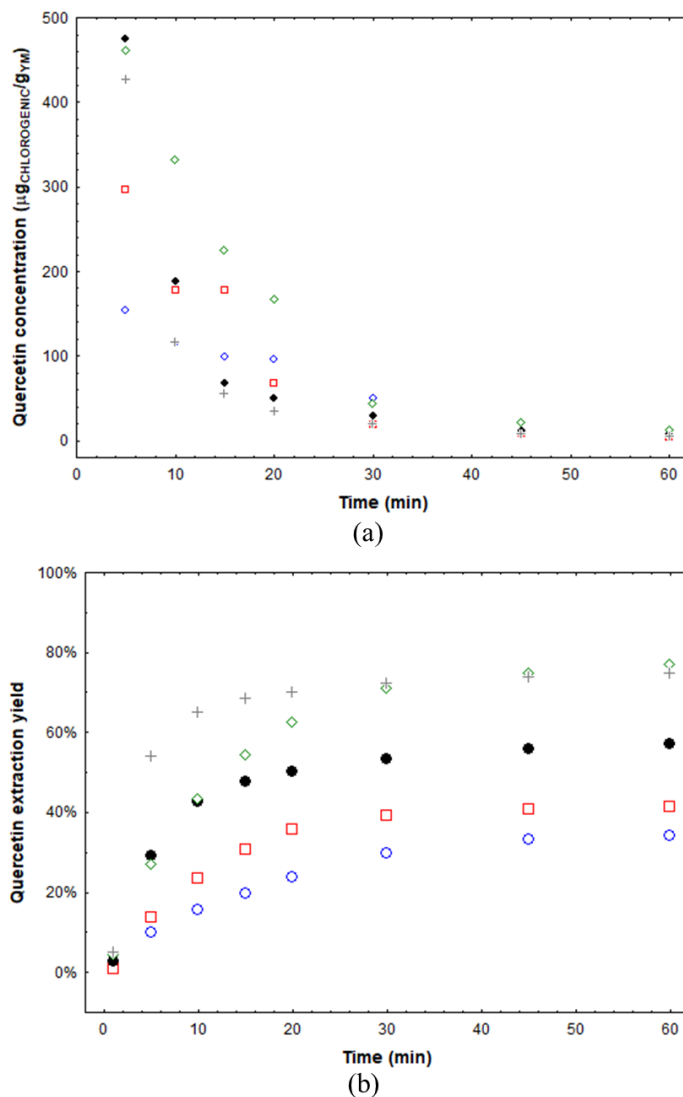


Figure S6. Kinetic of packed-bed extraction process for quercetin. (a) Quercetin concentration, (b) Quercetin extraction yield. ○ T = 50 °C, Q = 20 cm³/min; □ T = 50 °C, Q = 20 cm³/min; ● T = 60 °C, Q = 15 cm³/min; ◇ T = 70 °C, Q = 10 cm³/min; + T = 70 °C, Q = 20 cm³/min.



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