

Mechanisms of Herb-Drug Interactions Involving Cinnamon and Cytochrome P450 2A6:
Focus on Time-dependent Inhibition by Cinnamaldehyde and 2-Methoxycinnamaldehyde

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Supplemental Table 1 Rate constants defined using the numerical method

Table S1a. Microrate constants and errors parameterized with the EII-MIC-M-IL model 2 for CA.

Rate constant	Values \pm SE
k_1 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_2 (min^{-1})	4050.0 (fixed)
k_3 (min^{-1})	52.0 ± 0.31
k_4 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_5 (min^{-1})	16449 ± 4998
k_6 (min^{-1})	0.08 ± 0.01
k_7 (min^{-1})	0.04 ± 0.003
k_8 (min^{-1})	0.002 (fixed)
k_{10} (min^{-1})	0.0024 (fixed)
k_{11} (min^{-1})	0.033 ± 0.008
k_{13} (min^{-1})	204 ± 45.3

Table S1b. Microrate constants and errors parameterized with the MIC-EII-M-IL model 1 for CA.

Rate constant	Values \pm SE
k_1 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_2 (min^{-1})	4050.0 (fixed)
k_3 (min^{-1})	52.1 ± 0.31
k_4 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_5 (min^{-1})	16386 ± 4986
k_6 (min^{-1})	0.085 ± 0.02
k_7 (min^{-1})	0.044 ± 0.005
k_{10} ($\mu\text{M}^{-1} \text{min}^{-1}$)	27366 ± 24377
k_{11} (min^{-1})	0.034 ± 0.01
k_{13} (min^{-1})	210.8 ± 46.82

Table S1c. Microrate constants and errors parameterized with the PI-M-IL model for CA.

Rate constant	Values \pm SE
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k_1 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_2 (min^{-1})	4050.0 (fixed)
k_3 (min^{-1})	51.98 ± 0.24
k_4 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_5 (min^{-1})	10109 ± 1119.3
k_6 (min^{-1})	0.11 ± 0.01
k_7 ($\mu\text{M}^{-1} \text{min}^{-1}$)	24.9 ± 0.43
k_8 (min^{-1})	554.0 ± 48.85

Table S1d. Microrate constants and errors parameterized with the MIC-M-IL model for MCA.

Rate constant	Values \pm SE
k_1 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_2 (min^{-1})	4050.0 (fixed)
k_3 (min^{-1})	41.6 ± 0.22
k_4 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_5 (min^{-1})	10414 ± 3409
k_6 (min^{-1})	0.25 ± 0.07
k_7 (min^{-1})	0.092 ± 0.015
k_8 (min^{-1})	0.033 ± 0.005
k_{10} (min^{-1})	422 ± 92.2

Table S1e. Microrate constants and errors parameterized with the PI-M-IL model for MCA.

Rate constant	Values \pm SE
k_1 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_2 (min^{-1})	4050.0 (fixed)
k_3 (min^{-1})	41.57 ± 0.2
k_4 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_5 (min^{-1})	7244 ± 2243
k_6 (min^{-1})	0.27 ± 0.06
k_7 (min^{-1})	17.09 ± 0.5
k_8 (min^{-1})	942 ± 192

Table S1f. Microrate constants and errors parameterized with the EII-PI-M-IL model for MCA.

Rate constant	Values \pm SE
k_1 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)
k_2 (min^{-1})	4050.0 (fixed)
k_3 (min^{-1})	40.9 ± 0.20
k_4 ($\mu\text{M}^{-1} \text{min}^{-1}$)	270.0 (fixed)

k_5 (min ⁻¹)	28265 ± 7445
k_6 (min ⁻¹)	0.71 ± 0.15
k_7 (μM ⁻¹ min ⁻¹)	18.0 ± 0.33
k_8 (min ⁻¹)	3715 ± 516
k_{10} (μM ⁻¹ min ⁻¹)	1350 (fixed)
k_{11} (min ⁻¹)	0.11 ± 0.02