

# Model-Based Analysis of Coupled Equilibrium-Kinetic Processes: Indirect Kinetic Studies of Thermodynamic Parameters Using the Dynamic Data

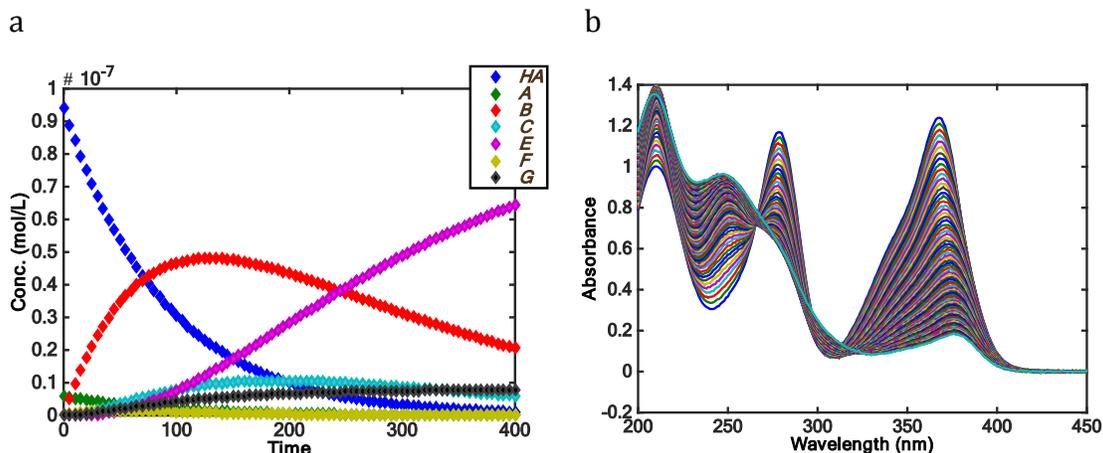
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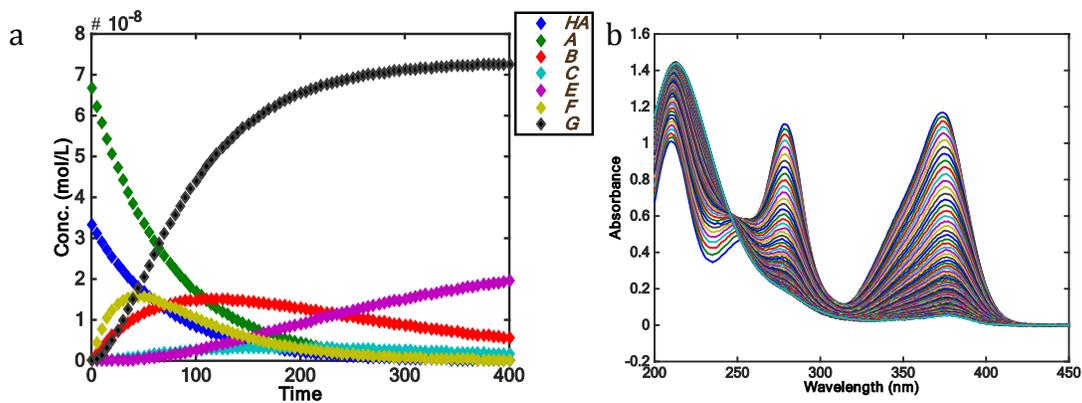
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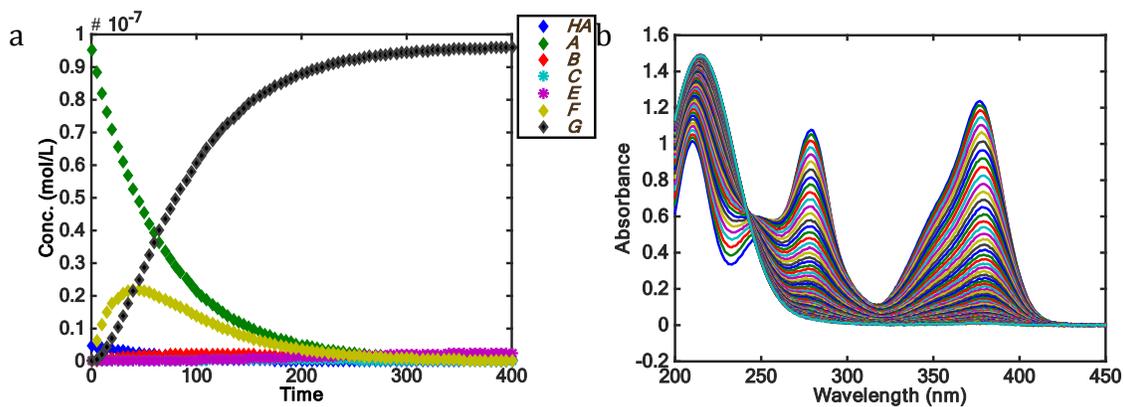
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**Figure S1.** (a) Simulated concentration profiles for  $C_{AML}^0 = 1.00 \times 10^{-7}$  M and  $pH = 7.50$  with  $K_a^{AML} = 2.00 \times 10^{-9}$ ,  $k_1 = 1.10 \times 10^{-2}$  s<sup>-1</sup>,  $k_2 = 5.00 \times 10^{-3}$  s<sup>-1</sup>,  $k_3 = 2.10 \times 10^{-2}$  s<sup>-1</sup>,  $k_4 = 1.50 \times 10^{-2}$  s<sup>-1</sup> and  $k_5 = 3.50 \times 10^{-2}$  s<sup>-1</sup>; (b) Simulated dataset.



**Figure S2. (a)** Simulated concentration profiles for  $C_{AML}^0 = 1.00 \times 10^{-7}$  M and  $pH = 9.00$  with  $K_a^{AML} = 2.00 \times 10^{-9}$ ,  $k_1 = 1.10 \times 10^{-2} \text{ s}^{-1}$ ,  $k_2 = 5.00 \times 10^{-3} \text{ s}^{-1}$ ,  $k_3 = 2.10 \times 10^{-2} \text{ s}^{-1}$ ,  $k_4 = 1.50 \times 10^{-2} \text{ s}^{-1}$  and  $k_5 = 3.50 \times 10^{-2} \text{ s}^{-1}$ ; **(b)** Simulated dataset.



**Figure S3. (a)** Simulated concentration profiles for  $C_{AML}^0 = 1.00 \times 10^{-7}$  M and  $pH = 10.00$  with  $K_a^{AML} = 2.00 \times 10^{-9}$ ,  $k_1 = 1.10 \times 10^{-2} \text{ s}^{-1}$ ,  $k_2 = 5.00 \times 10^{-3} \text{ s}^{-1}$ ,  $k_3 = 2.10 \times 10^{-2} \text{ s}^{-1}$ ,  $k_4 = 1.50 \times 10^{-2} \text{ s}^{-1}$  and  $k_5 = 3.50 \times 10^{-2} \text{ s}^{-1}$ ; **(b)** Simulated dataset.