

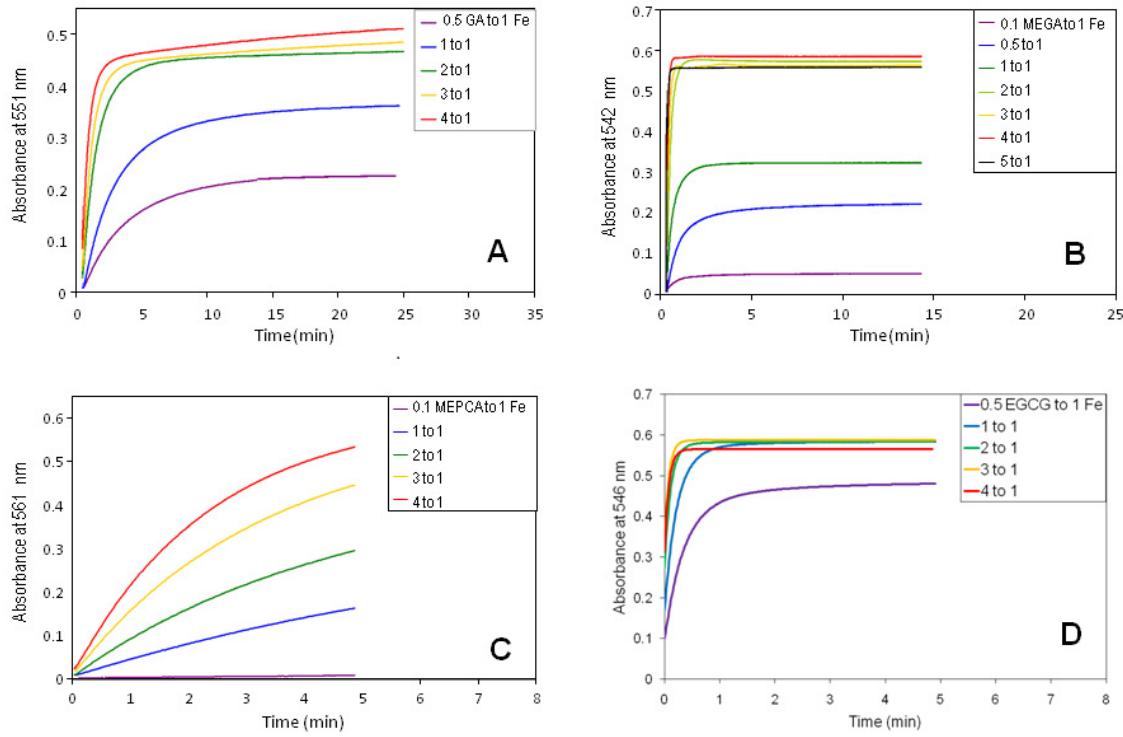
# Electronic Supplementary Information (ESI) for

## Kinetics of iron oxidation upon polyphenol binding

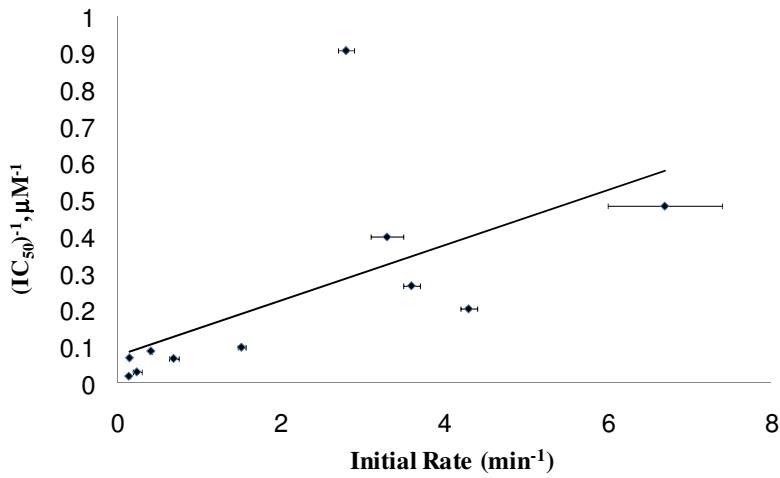
Nathan R. Perron, Hsiao C. Wang, Sean N. DeGuire, Michael Jenkins, Mereze Lawson, and Julia L. Brumaghim\*

### Table of Contents

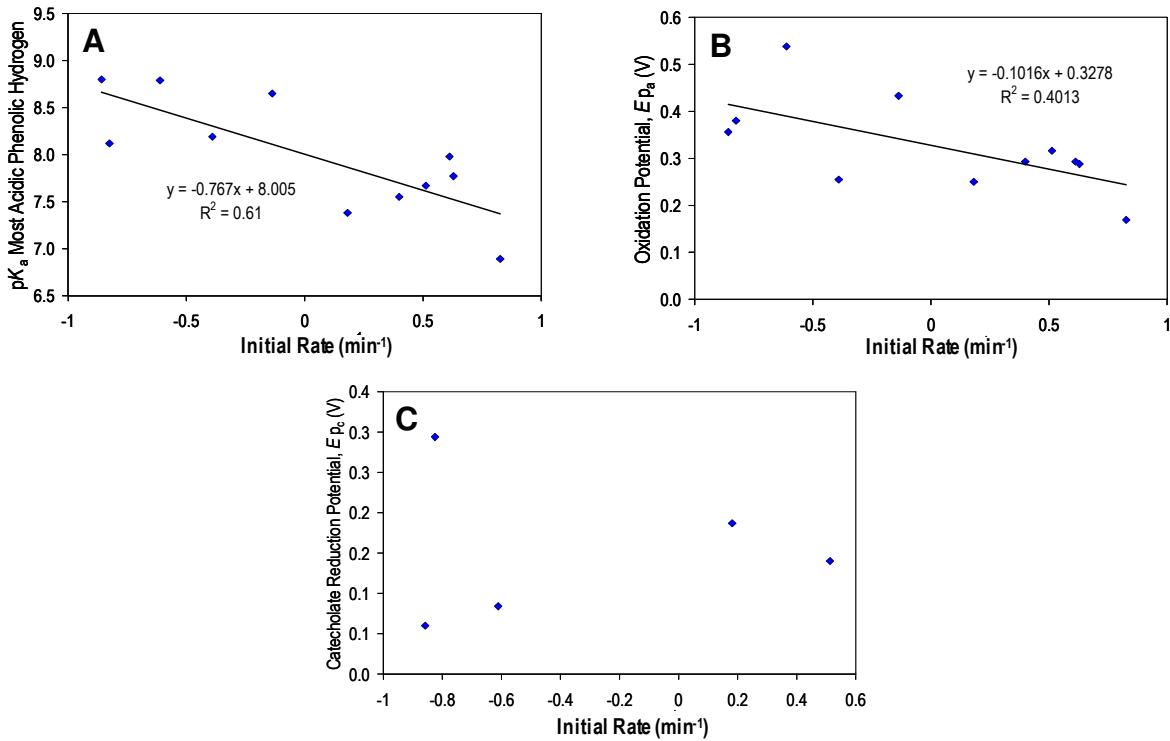
<b>Fig. S1</b> Absorbance vs. time graphs for variation of A) gallic acid (GA) to Fe <sup>2+</sup> molar ratio; B) methyl 3,4,5-trihydroxybenzoate (MEGA) to Fe <sup>2+</sup> molar ratio; C) methyl 3,4-dihydroxybenzoate (MEPCA) to Fe <sup>2+</sup> molar ratio; and ; and D) (-)-epigallocatechin-3-gallate (EGCG). .....	2
<b>Fig. S2</b> A graph showing the relationship between initial rates and IC <sub>50</sub> values for all eleven compounds (solid line, R <sup>2</sup> = 0.35). Error bars for rates are the standard deviations from three experiments. .....	2
<b>Fig. S3</b> Plots of initial rates as a function of A) polyphenol pK <sub>a</sub> (most acidic phenolic hydrogen); B) polyphenol oxidation potential (E <sub>p,a</sub> ); and C) catecholate compound reduction potential (E <sub>p,c</sub> ). .....	3
<b>Fig. S4</b> Graph showing the linear relationship between Fe <sup>2+</sup> oxidation reaction rate and concentration of A) gallic acid (GA; y = 0.2306x); B) epicatechin (EC; y = 0.0473x); and C) (-)-epigallocatechin-3-gallate (EGCG); y = 0.8204x + 0.5499). For all compounds, Fe <sup>2+</sup> autoxidation is first order with respect to polyphenol ligand (solid line, R <sup>2</sup> = 0.99, 0.99, and 0.97, respectively). Error bars for rates represent standard deviations.....	3
<b>Fig. S5</b> Graphs showing the relationships between Fe <sup>2+</sup> oxidation reaction rate and concentration of Fe <sup>2+</sup> for samples of A) gallic acid (GA; y = 0.1969x); B) epicatechin (EC; y = 0.2578x); and C) (-)-epigallocatechin-3-gallate (EGCG; y = 13.083x + 0.4032). For all compounds, Fe <sup>2+</sup> autoxidation is first order with respect to polyphenol ligand (solid line, R <sup>2</sup> = 0.97, 0.98, and 0.95, respectively). Error bars represent the standard deviations.....	4



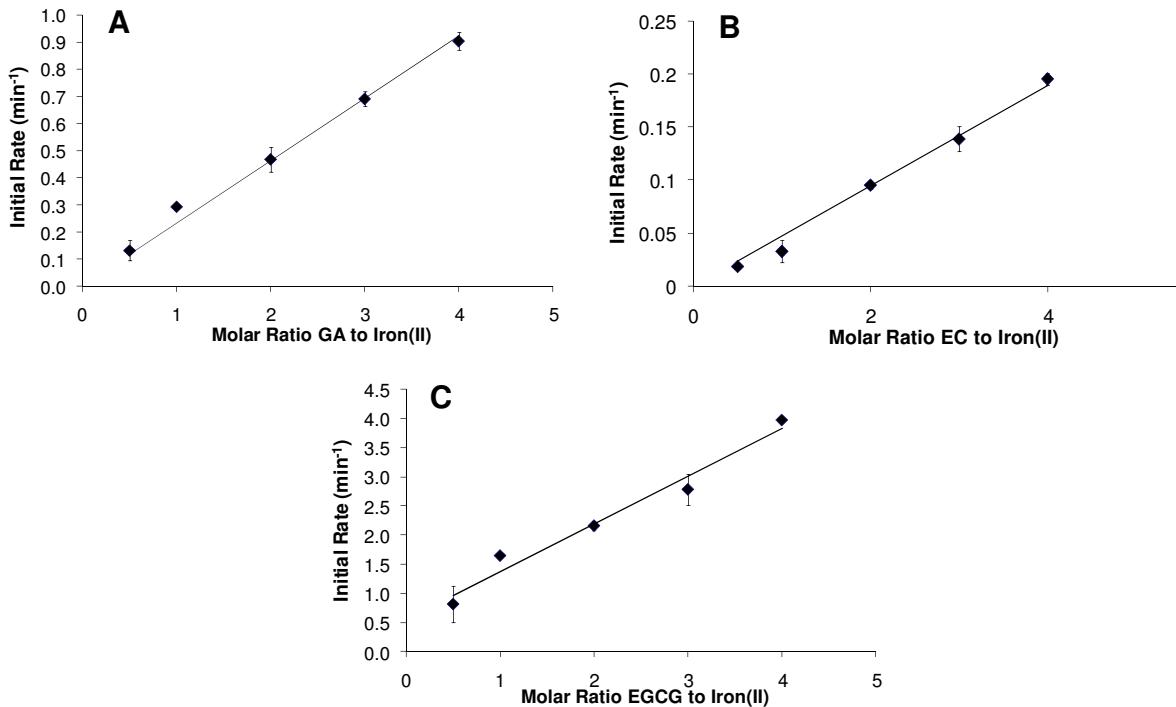
**Fig. S1** Absorbance vs. time graphs for variation of A) gallic acid (GA) to  $\text{Fe}^{2+}$  molar ratio; B) methyl 3,4,5-trihydroxybenzoate (MEGA) to  $\text{Fe}^{2+}$  molar ratio; C) methyl 3,4-dihydroxybenzoate (MEPCA) to  $\text{Fe}^{2+}$  molar ratio; and D) (-)-epigallocatechin-3-gallate (EGCG).



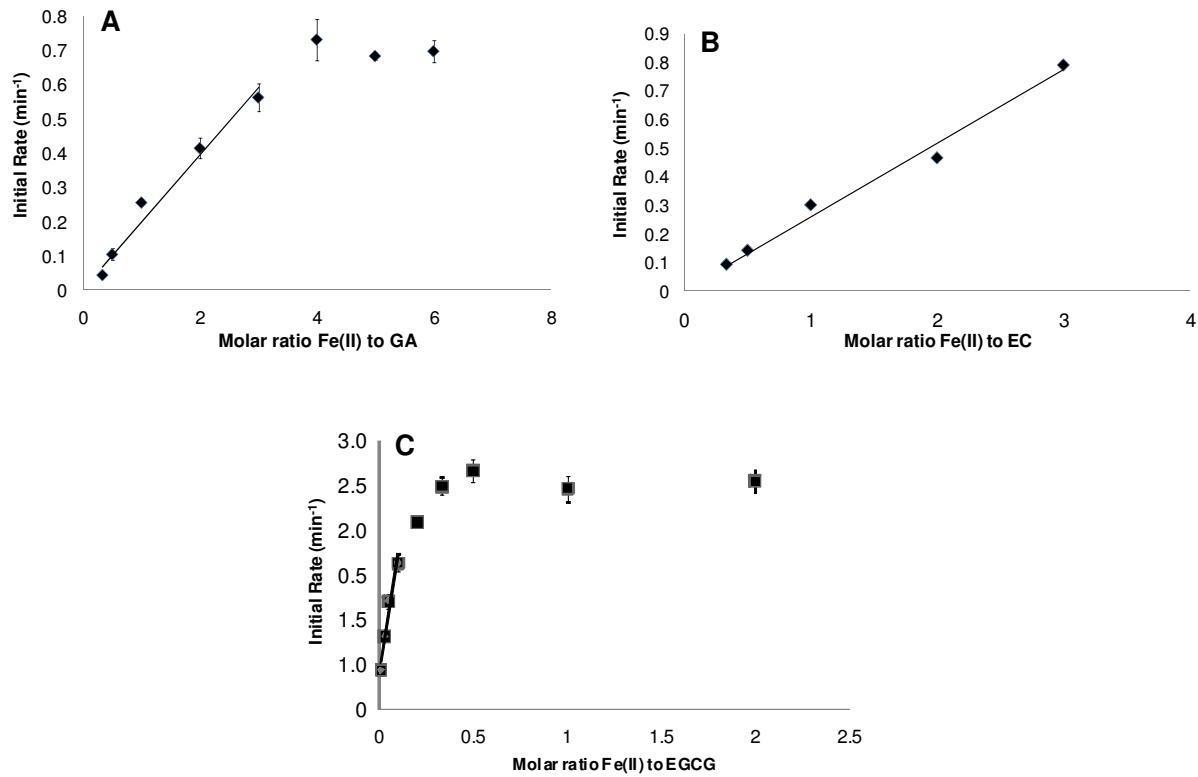
**Fig. S2** A graph showing the relationship between initial rate and  $\text{IC}_{50}$  values for all eleven compounds (solid line,  $R^2 = 0.35$ ). Error bars for rates are the standard deviations from three experiments.



**Fig. S3** Plots of initial rate as a function of A) polyphenol  $pK_a$  (most acidic phenolic hydrogen); B) polyphenol oxidation potential ( $E_{P_a}$ ); and C) catecholate compound reduction potential ( $E_{P_c}$ ).



**Fig. S4** Graphs showing the linear relationship between  $\text{Fe}^{2+}$  oxidation reaction rate and concentration of A) gallic acid (GA;  $y = 0.2306x$ ); B) epicatechin (EC;  $y = 0.0473x$ ); and C) (-)-epigallocatechin-3-gallate (EGCG;  $y = 0.8204x + 0.5499$ ). For all compounds,  $\text{Fe}^{2+}$  autoxidation is first order with respect to polyphenol ligand (solid line,  $R^2 = 0.99$ ,  $0.99$ , and  $0.97$ , respectively). Error bars represent standard deviations.



**Fig. S5** Graphs showing the relationships between  $\text{Fe}^{2+}$  oxidation reaction rate and concentration of  $\text{Fe}^{2+}$  for samples of A) gallic acid (GA;  $y = 0.1969x$ ); B) epicatechin (EC;  $y = 0.2578x$ ); and C) (-)-epigallocatechin-3-gallate (EGCG;  $y = 13.083x + 0.4032$ ). For all compounds,  $\text{Fe}^{2+}$  autoxidation is first order with respect to polyphenol ligand (solid line,  $R^2 = 0.97$ ,  $0.98$ , and  $0.95$ , respectively). Error bars represent the standard deviations.