

Supplemental File

Quantifying the Binding Interactions Between Cu(II) and Peptide Residues in the Presence and Absence of Chromophores

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Equations

$$(1) \quad Abs_{normalized} = \frac{(V_{initial} + V_{Cu(II)}) \times Abs_{buffer \text{ subtracted spectrum}}}{V_{initial}}$$

$$(2) \quad Abs_{normalized} = \frac{(V_{initial} + V_{peptide}) \times Abs_{buffer \text{ subtracted spectrum}}}{V_{initial}}$$

$$(3) \quad [phen]_{free} = [phen]_{initial} - (3 \times [Cu(phen)_3^{2+}])$$

$$(4) \quad [peptide]_{free} = \frac{[peptide]_{stock} \times V_1}{V_2} - [Cu^{2+} - peptide]$$

$$(5) \quad K_{ex} = \frac{[Cu^{2+} - peptide][phen]_{free}}{[Cu(phen)_3^{2+}][peptide]_{free}}$$

$$(6) \quad K_{d,Cu(II)-peptide} = \frac{K_{d,[Cu(phen)]^{2+}}}{K_{ex}}$$

$$(7) \quad c - value = n \times K_{ITC} \times [sample \ cell]$$

Instrumental parameters

Electronic absorption spectrophotometer

Scanning range:	200–900 nm
Ave time (s):	0.100
Data interval (nm):	1.000
Scan rate:	200 nm/s
Y Mode:	Absorbance

Isothermal titration calorimetry

Stir rate (RPM):	150
Temperature set point (°C):	25
Syringe concentration (mM):	1.00
Cell concentration (mM):	0.100
Injection interval (s):	300
Volume (μL):	2.5