

## Description of Codes for Chapter 5: Chemical Reaction Systems, Thermodynamics and Chemical Equilibrium

### Section 5.7.1: Equilibrium of a biochemical reaction

The biochemical equilibrium analysis of Section 5.7.1 can be obtained by running the script 'CK1.m'. This script inputs the data from Table 5.2, computes the estimated free ion concentrations, and finally produces the plot of observed equilibrium mass action ratio versus free magnesium ion concentration. This script calls the function 'CK\_mb', which computes the mass balance error at a given input free  $[Mg^{2+}]$ ,  $[K^+]$ , pH, and total input concentrations.

### Section 5.7.2: Standard enthalpy of a biochemical reaction

The biochemical equilibrium analysis of Section 5.7.2 can be obtained by running the script 'CK2.m'. This script inputs the data from Table 5.5, computes the estimated free ion concentrations, and finally produces the plot of observed equilibrium mass action ratio versus  $1/T$ . Here, the analysis uses the chemical equilibrium constant, which is estimated from the estimated mass action ratio of species concentrations,  $K_{eq}$ . This mass action ratio is computed by the script 'CK\_Keq.m'. (This script calls the function 'CK\_mb', which computes the mass balance error at a given input free  $[Mg^{2+}]$ ,  $[K^+]$ , pH, and total input concentrations.)