Free Cation Tool

Computational Bioengineering Group
Medical College of Wisconsin

Abstract

This document is used to describe the usage of the **Free Cation Tool** demo for calculation of the free cation in physiological buffer. All functions codes are written in MATLAB®. All original reference binding constant and thermodynamical data are from NIST database.

Authors: Feng Qi Ph.D., Ranjan Dash Ph.D., Daniel A. Beard Ph.D.
Software engineer: Yu Han.

Contents

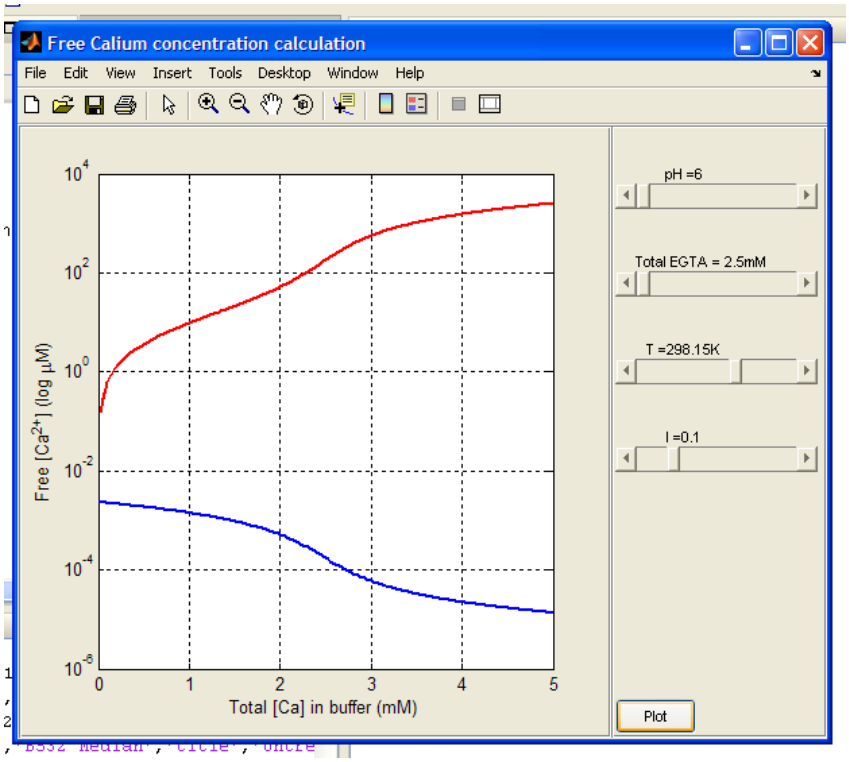

Figure 1: The main interface for the tool.

1 GUI interface and Usage

1.1 GUI interface

The main GUI interface will look like the figure shown in Figure 1. There are on button, one axes, and four sliders. The plot gives the free [Ca] concentration (red) and free [EGTA] concentration (blue) v.s. the total [Ca] concentration in the buffer. The range of the total [Ca] concentration is from 0 to 5 mM.

The four sliders are corresponding pH, total EGTA, temperature and ionic strength. The default values for those have been set as pH = 6.0, Total EGTA = 2.5mM, temperature = 298.15, and ionic strength = 0.1.

The plot given on the GUI is log (μM) scale. The range for pH is from 6.0 to 8.0. The range for temperature is from 273.15K to 313.15K. The range for ionic strength is from 0.0 to 0.5. The range for total EGTA concentration is from 0.1mM to 5.0mM.

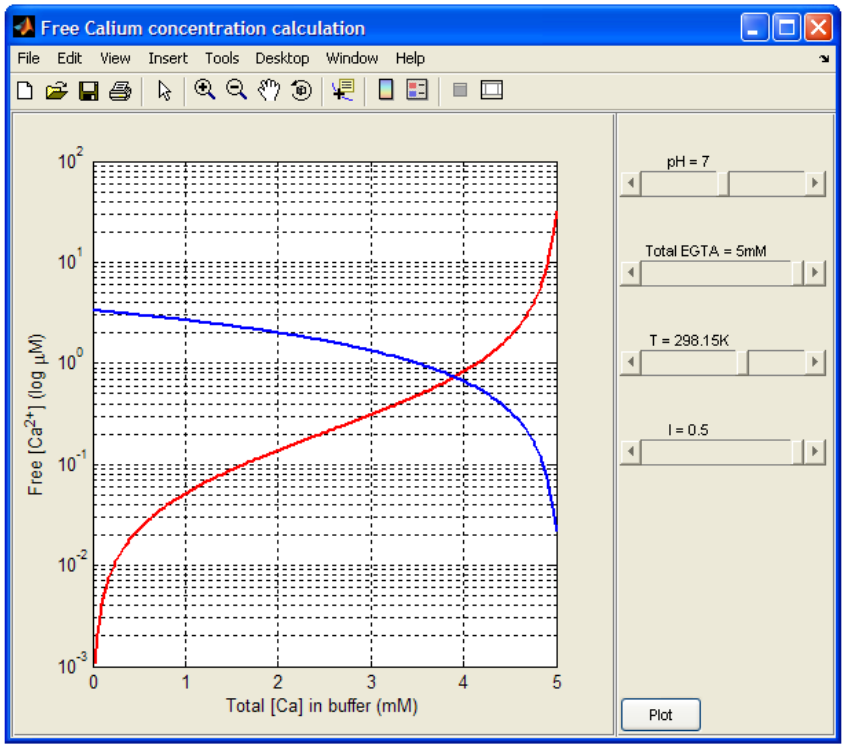

Figure 2: A example result plot when setting a new condition.

1.2 Usage

To run the program, input 'Main' in MATLAB command, the GUI interface will show up, click the plot button, the program will produce the plot corresponding to the default set conditions. User can change any slides to desired value, the plot will regenerate the new curve automatically.

Figure 2 give a example when setting pH = 7.0, total EGTA = 5mM and ionic strength = 0.5.

2 Functions List

2.1 Main.m

Main script to set up the GUI interface and call sub-functions in the package.

2.2 get_freeCa_square.m

Function to calculate the free Ca and EGTA concentration given conditions.(Analytical solution)

Usage:
[Ca EGTA] = get_freeCa_square(EGTA_tot, Ca_total, pH, ionic, temperature)

Input:
EGTA_tot – Total EGTA concentration
Ca_total – Total Ca concentration
pH – pH value
ionic – Ionic strength
temperature – Temperature

Output:
Ca – Free Ca concentration
EGTA – Free EGTA concentration

Also see:
get_EGTA_K.m

2.3 get_EGTA_K.m

Function used to calculate the dissociation constants for EGTA given ionic strength and temperature.

Usage:
[K] = get_EGTA_K(T_new, I_new)

Input:
T_new – Temperature
I_new – Ionic strength

Output:
K – Array of the dissociation constant
K(1): HEGTA; K(2): H2EGTA; K(3): H3EGTA; K(4) H4EGTA; K(5): MgEGTA; K(6): CaEGTA; K(7): KEGTA; K(8): CaHEGTA; K(9): MgHEGTA.

Also see:
get_dH_I0.m, get_gama.m

2.4 get_dH_I0.m

Function used to calculate the δH at the I = 0.

Usage:
[dH] = get_dH_I0(dH_old, I, z_p, z_r)

Input:
dH_old – δH at I
I – Ionic strength
z_p – charge array for product
z_r – charge array for reactant

Output:
dH – δH at I = 0

2.5 get_gamma.m

Function used to calculate the γ given temperature(T), ion strength(I) and charge

Usage:
[gamma] = get_gamma(T, I, z)

Input:
T - temperature
I - ionic strength
z - charge

Output:
gamma – γ at T and I.