

MATLAB programming developed and implemented to obtain theoretical progress curves considering 1%, 5%, and 10% of substrate depletion threshold:

Function definition	Script Matlab
Define the M_i exclusive integrated function when two inhibitors are mutually exclusives	<pre>function [t]=MIexclus(St,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2) t=(-1/Vmax)*(Km * (S0/Kic1 + I1/Kic1 + I2/Kic2 + 1) * log(St/S0) + (1 - Km/Kic1 + S0/Kiu1 + I1/Kiu1 + I2/Kiu2) * (St-S0) - (1/(2*Kiu1)) * (St.^2 - S0.^2)); end</pre>
Define the initial values for parameters	<pre>function [slopes] = results(Sinicial,incremento,Sfinal,ficheiro) % close all % equation: MI Vmax= 0.12; Km = 500; Kiu1 = 50; Kiu2 = 5; Kic1 = 100; Kic2 = 5; I1 = 0; % inibidor 1 time zero I2 =10; % inibidor 2 time zero %S0 = 100;</pre>
Define a file “xls” where the result variables will be presented	<pre>file = append(file, '.xls'); parameters = {'Vmax',Vmax,' ', 'Km',Km}; writecell(parameters, file); parameters = {'Kiu1',Kiu1,' ', 'Kiu2',Kiu2}; writecell(parameters, file,'WriteMode','append') parameters = {'Kic1',Kic1,' ', 'Kic2',Kic2}; writecell(parameters, file,'WriteMode','append') parameters = {'I1',I1,' ', 'I2',I2}; writecell(parameters, file,'WriteMode','append') col_header = {'S0','1%','5%','10%'}; writecell(col_header,file,'WriteMode','append')</pre>
Define the model to be used and the increments	<pre>for S0 = Sinicial:incremento:Sfinal St=0:0.01:S0; % product tt = MIexclus(St,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2);</pre>
Define a graph simulation, Making a new figure and not delete the previous ones and keeps the chart open to include more information	<pre>figure(3) plot(tt,S0-St) hold on</pre>
Define in the XX and YY axis the points where we want to draw the tangent for 1%, 5% and 10% of product reaction in the plot, and marks with a red dot.	<pre>X0=S0 X1=S0*0.99; X5=S0*0.95; X10=S0*0.90; Y0 = MIexclus(X0,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2); Y1 = MIexclus(X1,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2); Y5 = MIexclus(X5,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2); Y10 = MIexclus(X10,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2); plot(Y0,S0-X0,'r.',MarkerSize=10) plot(Y1,S0-X1,'c.',MarkerSize=10) plot(Y5,S0-X5,'k.',MarkerSize=10) plot(Y10,S0-X10,'b.',MarkerSize=10)</pre>
Sets the slope of the secant line to the graph of the function at 0 and X_0	<pre>m1 = (MIexclus(X1,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2)-MIexclus(X0,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2))/(X1-X0); m5 = (MIexclus(X5,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2)-MIexclus(X0,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2))/(X5-X0); m10 = (MIexclus(X10,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2)-MIexclus(X0,S0,Vmax,Km,Kic1,Kic2,Kiu1,Kiu2,I1,I2))/(X10-X0); mline1 = -1/m1; mline5 = -1/m5; mline10 = -1/m10; slopes = [S0,mline1, mline5, mline10];</pre>
Sets the secant line to the graph of the function at X_0 and draws the plot	<pre>zz1=m1*(St-X1)+Y1; zz5=m5*(St-X5)+Y5; zz10=m10*(St-X10)+Y10; plot(zz1,S0-St,'c') plot(zz5,S0-St,'k-.') plot(zz10,S0-St,'color', [0.9290 0.6940 0.1250],'linestyle',':')</pre>
Sets the axes labels and title, close the graph, write the results to the “xls” file, and ends.	<pre>legend('MIexclus','ponto (0)','ponto (1)','ponto (5)','ponto (10)','reta secante (1)','reta secante (5)','reta secante (10)','Location','southeast') xlabel('t') ylabel('S_0-St=P') title('MIexclus - secantes') writematrix(declives,ficheiro,'WriteMode','append') end end</pre>