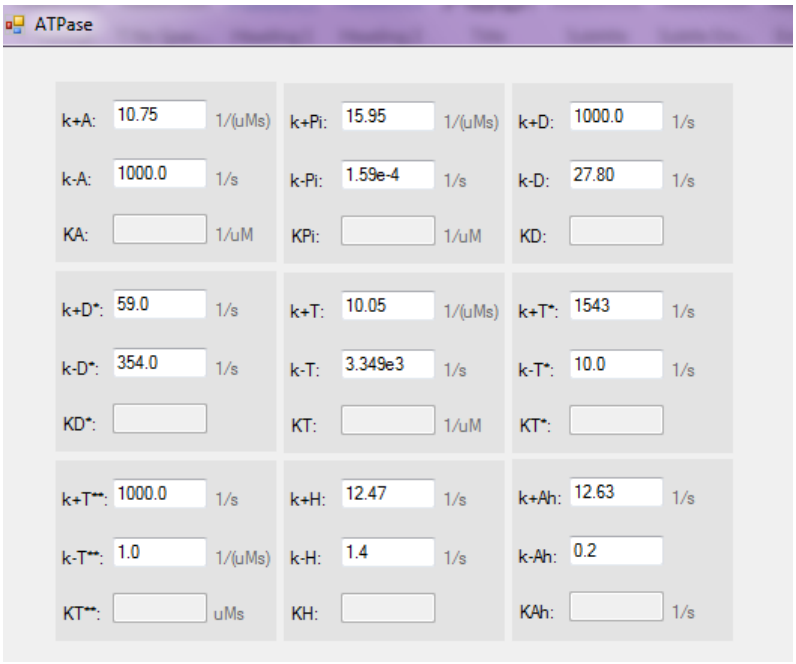
With our softer we are modeling the complete actin.myosin ATPase cycle. We can see the occupancy of each of the intermediates in the ATPase cycle for some values of rate constants at different actin concentration. Choosing a set of rate constants for study depends upon having a good estimate of the steady-state ATPase data and a complete set of the rate constants for the cycle depicted. Complete parameter estimation methods are described in Mijailovich et al., 2017.

For each equilibrium constant $K_i = k_i/k_{-i}$ we have k_i and k_{-i}, the forward and reverse rate constants. Defining any two of the three parameters experimentally is sufficient; the third can be calculated from the first two.

Follow these steps:

1) Set a values for all rate constants

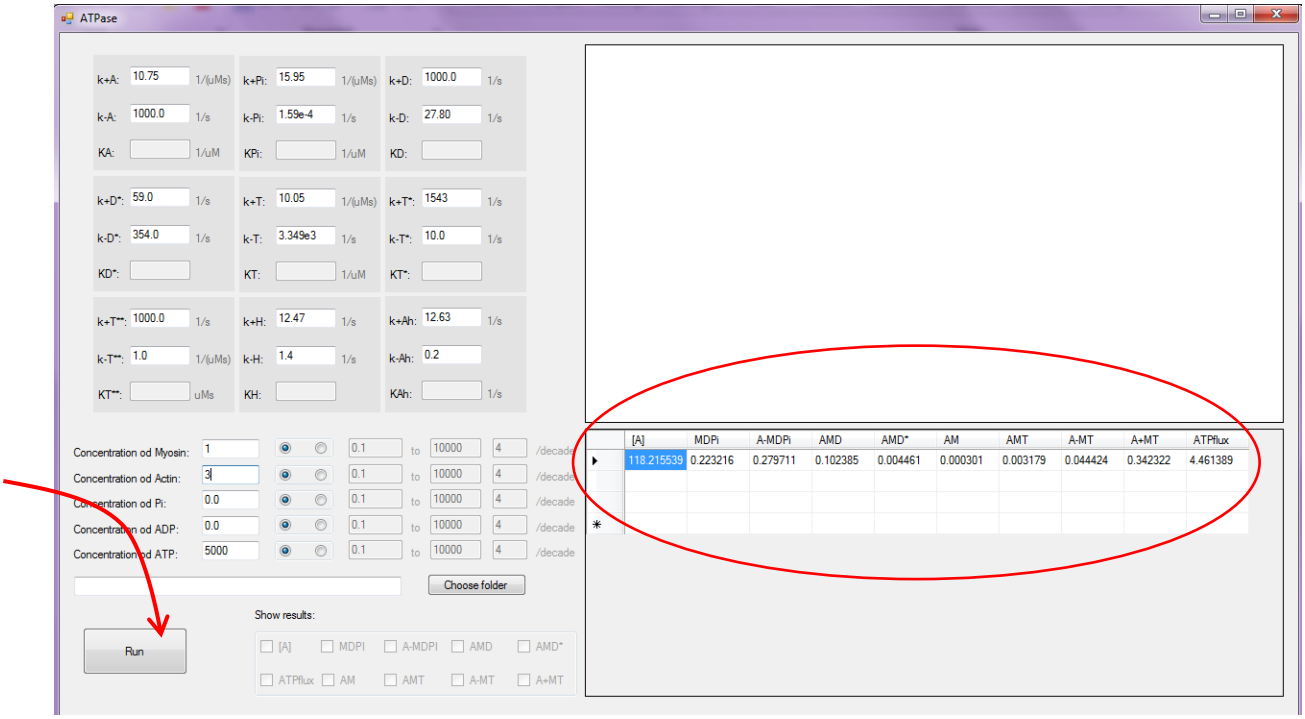


Rate Constants Used for Modeling the ATPase Cycle for HC-WT β-S1
(example from Mijailovich et al., 2017)

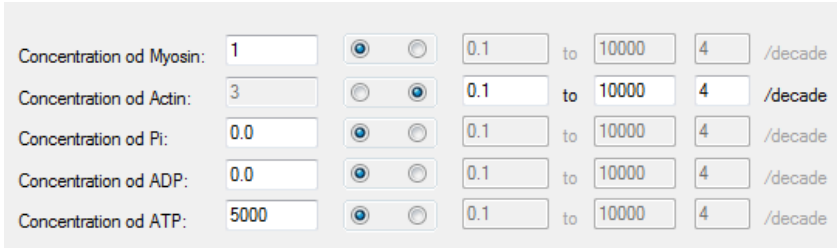
2) Set a values for all concentration

3) There is the option to select the folder that will be registered output files. If the folder does not indicate the output results will be stored in C: \ Users \ Documents \ ATPase Results

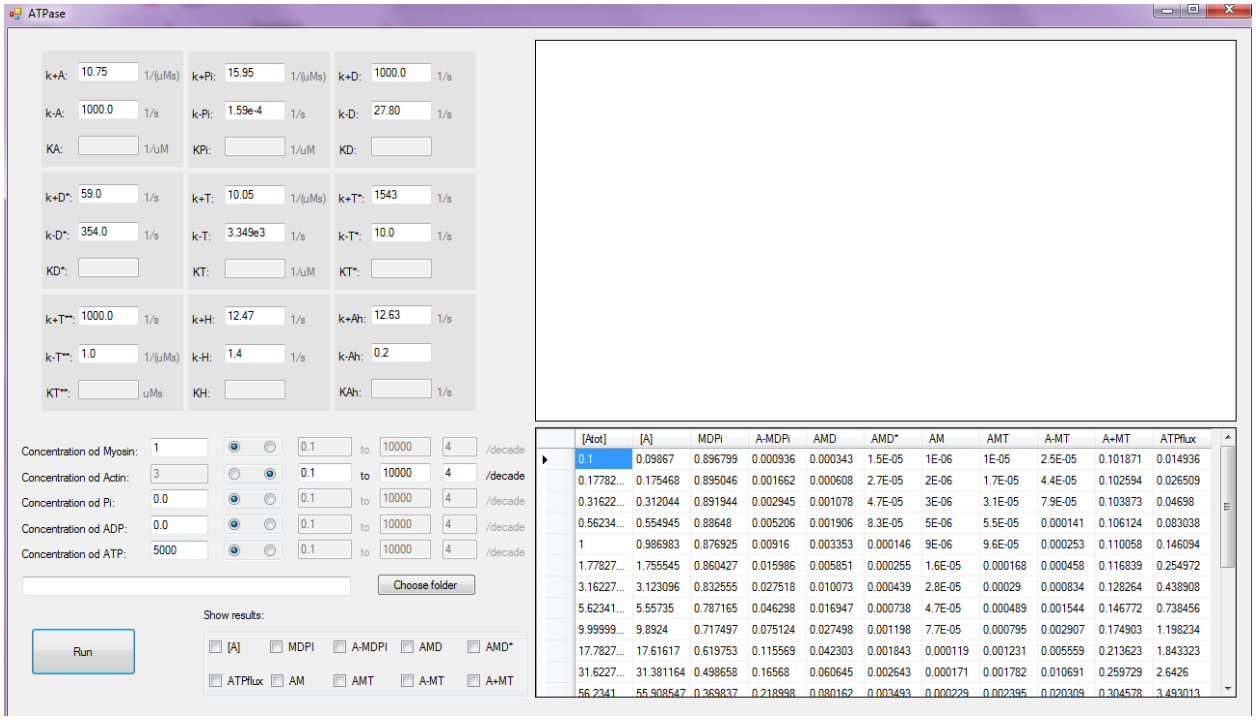
4) Also, the results will be shown in the table on the right side. Data in the table can be copied.



5) The results for fixed values of concentration cannot be drawn on charts. But we can use value range and number of points in the range for any concentration. For the beginning you can put for example [A tot] = = 0.1 μM to 100 mM, 4/decade, and [M tot] = 1 μM, [ATP] =5mM, [Pi]=[ADP] =0.



6) If we run simulation in the table will be display values for different concentrations of actin



7) Now we can display the results on a graph choosing what data we want. We can see the occupancy of each of the intermediates in the ATPase cycle for different values od actin concentration.