# How to use

Required parameters for a given drug are the following:

- Concentration
- $IC_{50}$ on $I_{Kr}$ (coordinate x)
- $IC_{50}$ on $I_{CaL}$ (coordinate y)
- $IC_{50}$ on $I_{Ks}$ (coordinate z)
- $IC_{50}$ on $I_{NaL}$ (coordinate z')

First, calculate x, y, z and z' as written in the *Description section*, rounding to the first decimal. Use -3 when drug-channel interaction does not exist or is unlikely to happen. Resulting Coordinates can be outside the ranges that were provided. In that case, use the nearest value in the range (either maximum or minimum).

Then, search for the nearest coordinate values in each Excel file to obtain the value of the desired biomarker. Note that each Excel file has 3 coordinate columns and a column corresponding to the biomarker. Those 3 columns are the currents that were considered to be affected by the drug to obtain the given biomarker.

*Example compound*: consider compound D such as concentration (could be therapeutic or just test concentrations) of 1 nM, $IC_{50}$ $I_{Kr}$ of 1 nM, $IC_{50}$ $I_{CaL}$ of 10 nM, $IC_{50}$ $I_{Ks}$ of 10000 nM, and $IC_{50}$ INaL of 100 nM. Coordinates would be x=0, y=-1, z=-4 and z'=-2. The third coordinate should be transformed to -3, the nearest value in the simulated range. Here are the results of searching into the files for those coordinates.

- "Tx matrix KrKsCaL.xlsx" = 0.11
- "Tx matrix KrNaLCaL.xlsx" = 0.11
- "TqNet matrix KrKsCaL.xlsx" = 0.316
- "TqNet matrix KrNaLCaL.xlsx" = 0.395
- "Ttirang matrix KrKsCaL.xlsx" = 3.340
- "Ttriang matrix KrNaLCaL.xlsx" = 3.275