APPLICATION NOTE: Building a Wobble Concentration Grid by Mixing Salts

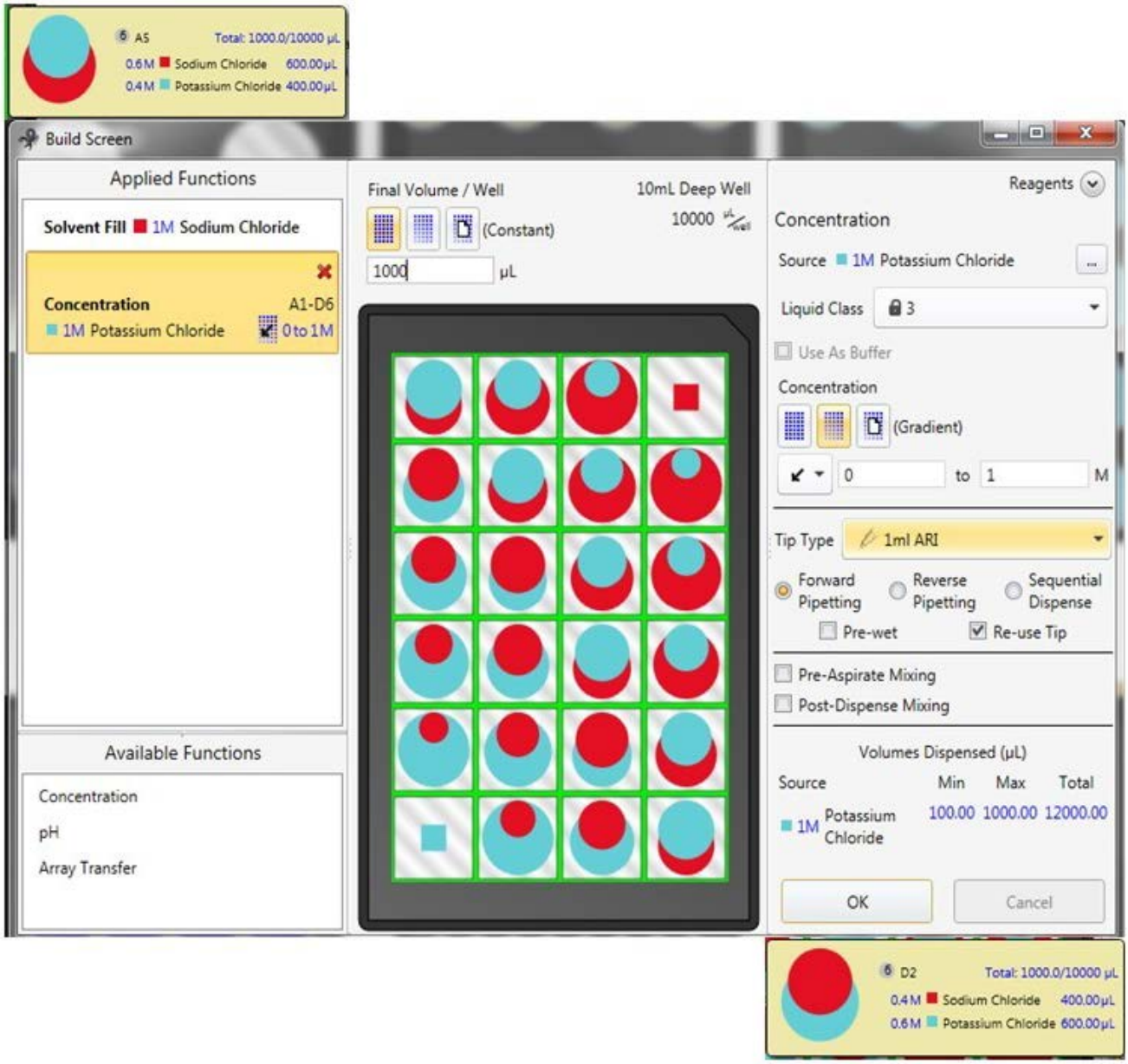
The Scorpion Screen Builder provides a powerful platform and suite of software tools to create new mixtures of reagents.

Description: Gradients can be formed in the vertical and horizontal directions in the Build Screen/Concentration/Gradient tab function by columns and rows respectively. The other tab, the "diagonal arrow" has a useful purpose as well. This function for gradient formation is what we can call a "wobble grid".

A wobble grid is the type of method explored when a user would like to test for the replacement of one component in a solution with another similar component that is being tested. Replacing one divalent salt with another like CaCl2 with MgCl2 is an example of this type of experiment. (You can hear scientists say things like we would like to test a more chaotropic salt reagent in the series for instance.) The diagonal concentration function produces a grid where the amounts of each component are added to one another in a reciprocal manner on the plate. It tests for the possibility that the mixture of these 2 salts in a certain ratio might favor better crystallogenesis.

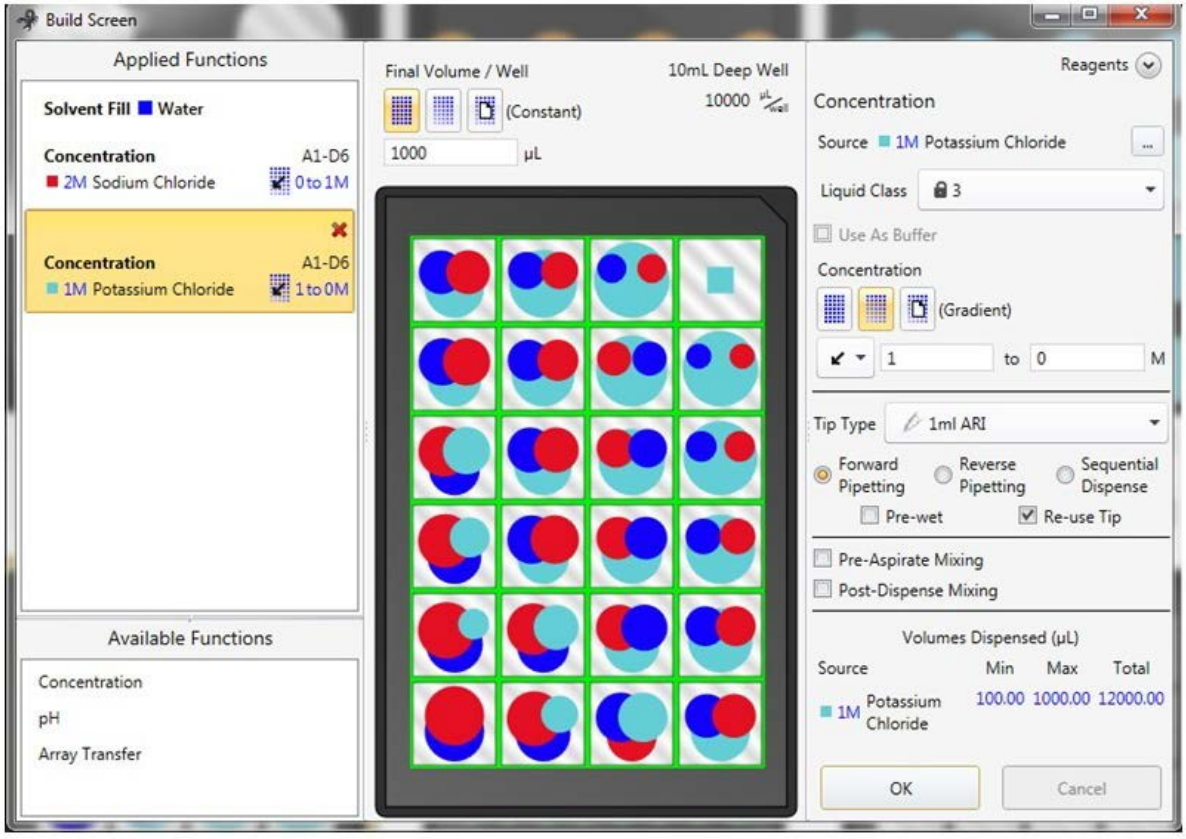
We can apply the diagonal arrow in 2 different approaches:

This first type of grid can be easily advised if you wanted to test replacing CaCl2 with MgCl2 as an example. This is accomplished by replacing the solvent (normally set to water) with the ingredient you want to test. So if you selected 1M CaCl2 as the "source" component that is in the crystal hit chemistry, then you would use the diagonal arrow replacing Water with 1M MgCL2 as the "solvent fill". In this method both of the salts must have the same starting molar concentrations. When added together by the diagonal arrow function, A1 is then pure 100% MgCl2 and D6 is pure 100% CaCL2. The other wells are then mixtures of these 2 salts with reciprocal proportions to one another throughout the plate. Often we find that there is a optimal mixture of the two salt components of interest to try in experiments going forward.



The diagram above shows how to set up the first method discussed above using NaCl and KCl as reagents. Note the reciprocal amounts of the 2 salts added as illustrated by the captions D2 and A5.

The second approach can use salts with different initial concentrations and is set up more conventionally as the gradient grid of the 2 components individually. When you select the diagonal arrow, first shift one of the salts from 0M to 1M and shift the other from 1M to 0M for instance. This will build a similar grid as described above with slightly different increments of each reagent.



This diagram shows a similar setup of the same reagents again using the diagonal gradient formation function. Now the starting reagents do not have to be the same concentration. The grid is formed somewhat differently, but accomlishes the same task of exchanging one salt for another in a sytematic manner.