

Figure S2: Determining the Number of  $bc_1$  Complexes: Average Master Score

Average master score of the best 100 (out of a total of 840) parameter sets vs. the number of  $bc_1$  complexes  $N_{bc1}$  for the single flash experiment used to determine  $N_{bc1}$ . This value of  $N_{bc1}$  was later employed for the optimization of the rate constants. The black points show the result from the first set of optimizations that considered  $\Delta\Phi::\epsilon_M$ ,  $\Delta\Phi::\Delta\Phi_0$ , and  $bc_1::\Phi_0$ . In the second set (red points), PR::pK was included, too.