We have included two zipped folders of different sets of XML input files for DESSA 2.0 that were used for separate simulation studies analyzing the effects of RNA on CCMV capsid assembly:

1. [2014.CCMV.RNA.XML.FILES.zip](https://github.com/rsschwartz/Dessa2.0/blob/master/2014.CCMV.RNA.XML.FILES.zip)

XML Input Files for DESSA 2.0 that simulate CCMV capsid assembly under different combinations of studied RNA effects. File format is of the form:

CCMV1\_156\_xx\_abcd.xml

This XML file calls for the simulation of CCMV capsid assembly producing 1 capsid at parameters fit to experimental data found at 15.6 µL. xx reflects the percentage of simulation space filled by crowding agents (for these xml files, xx = 00). abcd reflects the four individual RNA effects calculated. Each letter reflects a binary value of 0 or 1 depending on if that RNA effect is "turned on" for that particular set of inputs. For example, \_0101 would suggest that the second and fourth RNA effects are turned on, while the first and third are turned off.

2. [CCMV.Grid.Search.XML.Files.zip](https://github.com/rsschwartz/Dessa2.0/blob/master/CCMV.Grid.Search.XML.Files.zip)

XML input files for DESSA 2.0 to produce a grid search of rate parameter modifications to the standard input file CCMV1\_156\_00\_0000.xml.

A file named CCMV1\_156\_00\_0000-1000-0005 means that on rates are multiplied by 1000\*.1 = 100 and off-rates are multiplied by 5\*.1 = .5 compared to the standard input file. Files with -00025 for the off rate modification mean off-rates are multiplied by .25. The files CCMV\_156\_00\_0000.xml and CCMV\_156\_00\_0000-0010-0010.xml are equivalent.

There is also a standard XML file for assembly of a single CCMV capsid with rate parameters fit to experimental light scattering data included within the DESSA 2.0 zip file named CCMV1\_156\_00\_0000.xml