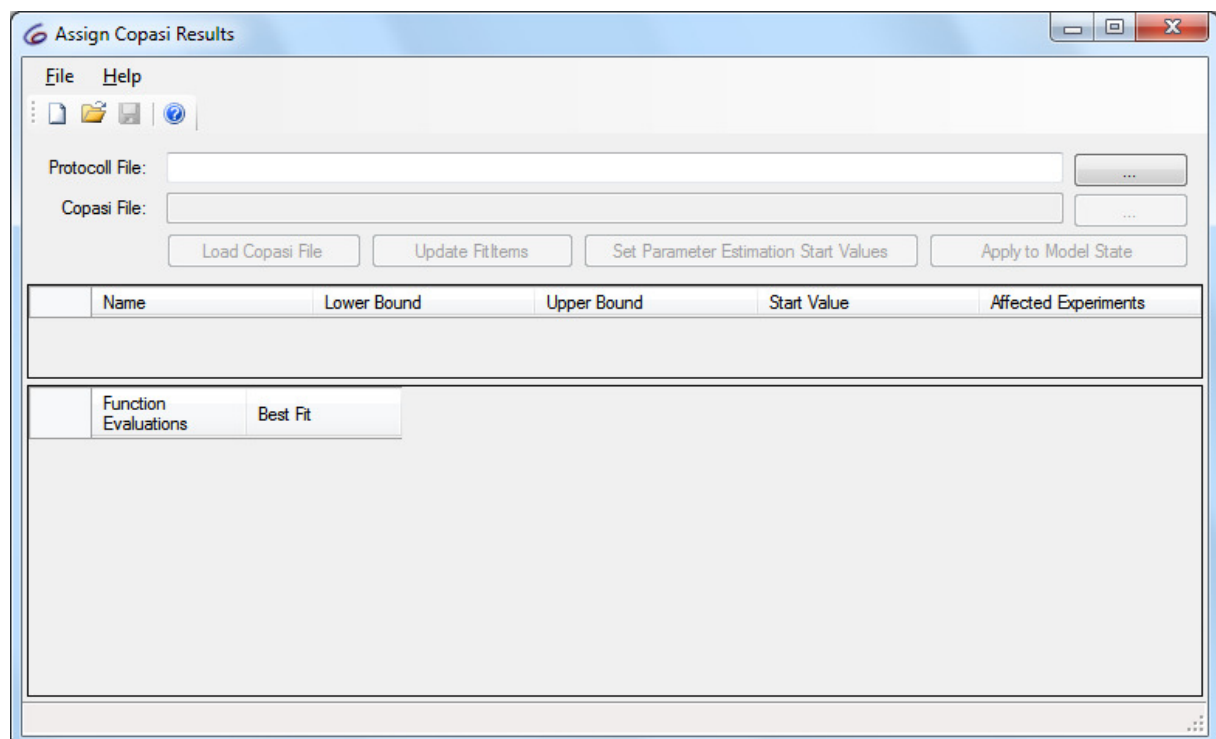


Applying COPASI Results

Frank T. Bergmann (fbergman@caltech.edu)

This document describes how to use the application for applying starting values for Parameter Estimation tasks from a previously recorded protocol. This is helpful if for example your parameter estimation task was cancelled for whatever reason, or you simply want to explore the parameter space visited during the fitting task at a later point in time.

The application



The main application screen is tiled into three areas:

- The area where you specify what protocol file to use and what COPASI file to load.
- The list of all currently defined parameters for the parameter estimation task
- The table of function evaluations, best fit and parameters of the protocol file.

The application is designed so as to only enable options when they are appropriate (for example you won't be able to save to a new COPASI file, before loading a protocol and selecting the new parameter set). At any point you are able to start over using File\New.

Installation

The current windows version is installed by simply double clicking the installer, and following the setup procedure.

Using the application

In order to use the application please follow the following steps:

1. Start the application
2. Open the protocol file (using the three dots in the first line you get to browse the file system, or you simply specify the full path).
3. Open the COPASI file that belongs to the model.

Name	Lower Bound	Upper Bound	Start Value	Affected Experiments
(05_HK).Vm	10	1000	299.592	Experiment_0, Experiment_1, Exp...
(05_HK).Vm	10	1000	299.592	Experiment_7
(06_PGI).Vf	50	1000	120.472	Experiment_0, Experiment_1, Exp...
(06_PGI).Vf	50	1000	120.472	Experiment_7

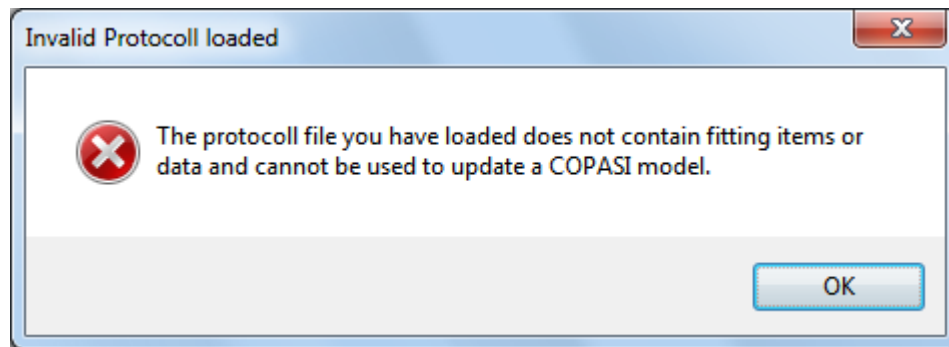
Function Evaluations	Best Fit	(05_HK).Vm	(05_HK).Vm	(06_PGI).Vf	(06_PGI).Vf	(07_PFK).Vm	(07_PFK).Vm	(08_ALD).Vf
3173	47.2198	118.769	37.9395	61.0734	79.5631	1922.78	1605.96	348.531
3290	41.4139	97.646	10	69.9422	100.711	2252.1	1202.67	630.406
3671	41.3872	97.6404	10	69.3347	101.398	2242.69	694.349	475.873
3743	41.2841	97.1783	201.943	92.021	95.7289	1176.04	947.393	3256.22
3771	40.9754	94.0689	10	70.2799	100.076	2285.49	511.363	783.075
3855	40.8346	103.601	10	65.8882	148.366	2405.81	1563.45	587.344
4390	40.1147	102.339	13.871	66.2053	129.894	1846.61	2067.72	492.559
4400	39.4574	113.085	10	69.5842	76.6324	1091.9	939.92	476.235
4698	39.356	103.244	18.3354	65.6866	172.178	1700.6	2064.3	480.809
4825	39.3315	104.742	10.2878	64.9594	220.362	1459.69	1637.07	418.044
4915	39.1013	112.299	50.6875	65.3167	125.517	1578.61	918.884	100.429
5038	38.9783	122.952	71.354	74.8596	92.0563	2462.15	2957.26	782.291

Number of Parameters: 234 Number of Rows: 37

4. At this point you would set the parameter estimation start values, by selecting first an entry from the list. Or you could apply the selected fit to the model initial state. In that case you will have to choose the priority order of the experiments used. (The parameter written to the model will be the one from the experiment with highest priority.)
5. Save the resulting COPASI file under a new filename.

Error Messages

The program will only work if the protocol file contains the fit items together with at least one recorded output step. Otherwise the following error message will be displayed:



Additionally, the COPASI file loaded has to have a parameter estimation task specified with the same number of parameters (and over the same variables). Otherwise the following error message will be displayed:

