Using the Plant Pharmacokinetic Modeling Software

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**File Setup:**

Download (Plant\_Code.zip) and unzip. The included files are listed below.

Code:

 Plant\_control\_akc.py

constants.h

find\_MAT\_akc.h

find\_MAT\_akc.c

fit\_sv\_akc.h

fit\_sv\_akc.c

get\_tac\_akc.h

get\_tac\_akc.c

parse\_in\_akc.h

parse\_in\_akc.c

Plant\_main\_akc.c

struct\_ROI.h

struct\_TAC\_in.h

write\_data\_akc.h

write\_data\_akc.c

Makefile

Data:

 **Input File:** RBO019Input.txt

 **ASIPro output file (TACs):** 2011\_06\_14\_c\_RBO019\_18F\_60m\_20x1\_x5m\_rawATNSC\_

alpha\_07242013\_FINAL.csv

**Cleaned ASIPro output file:** 2011\_06\_14\_c\_RBO019\_18F\_60m\_20x1\_x5m\_rawATNSC\_

alpha\_07242013\_FINAL\_cleaned.csv

Output:

 **Output File:** RBO019input\_out\_20140507\_1350.txt

 **Linear Regression File:** RBO019input \_out\_20140507\_1350.png

**Graphed TAC:** RBO019input \_out\_20140507\_1350\_cor\_43.png

**Graphed TAC:** RBO019input \_out\_20140507\_1350\_cor\_44.png

**Graphed TAC:** RBO019input \_out\_20140507\_1350\_cor\_45.png

**Graphed TAC:** RBO019input \_out\_20140507\_1350\_cor\_46.png

**Graphed TAC:** RBO019input \_out\_20140507\_1350\_cor\_47.png

**Graphed TAC:** RBO019input \_out\_20140507\_1350\_cor\_48.png

**Software Details:**

The McKay Plant model was programmed on a VirtualBox Linux virtual machine running Ubuntu 11.10. Code functionality on alternate systems is not guaranteed, and these instructions are specific to the specified system

The Plant model software Plant\_control\_akc.py uses command line input. Each option is described below:

0 – Perform McKay Modeling

1 – Linear Regression of MAT and Position

2 – Graph TACs

3 – Clean ASIPro File

4 – Exit

0 – Perform McKay Modeling:

This command is used to run the modeling code. A file chooser window asks the user to select an input file. The command automatically creates a new file named on the format of: oldfile\_out\_YYYYMMDD\_HHMM.txt. This file contains the model-generated free and trapped activity curves and the calculated mean arrival time of each ROI. This output file is used as input to the 1 – Linear Regression of MAT and Position and 2 – Graph TACs commands.

1 – Linear Regression of MAT and Position:

This command is used to fit a linear regression line to the data in the output file generated by command 0 – Perform McKay Modeling. A file chooser window asks the user to select one of these output files. The command automatically saves a file named on the format of: outputFile.png, where outputFile is named as described above.

2 – Graph TACs:

This command is used to graph the Time Activity Curve (TAC) used to calculate the model and the model-generated trapped, free, and trapped + free curves, which are stored in the output file generated by the command 0 – Perform McKay Modeling. A file chooser window asks the user to select one of these output files. The command automatically saves a file named on the format of: outputFile\_ROIName.png, where outputFile is described above.

3 – Clean ASIPro File:

This command is used to strip the TAC-containing file of extra punctuation that is added when ASIPro saves the file. The command automatically saves a file named on the format of: scanName\_cleaned.csv

4 – Exit

This command is used to exit the model.

**Input File Details**

The three input files provided are listed below:

RBO019input.txt

This is a formatted input file as shown below. Notes are listed following “//” marks and should not be included in the actual input file.

Subject // Subject identifier

RBO019

scan // Scan identifier

2011\_06\_14\_c\_RBO019\_18F\_60m\_24\_20x1\_x5m\_rawATNSC\_alpha.img

comment

Testing

administered activity // Total activity administered during scan

3180000 // in same units used for TACs

ASIPro Tacs File: // CLEANED file containing TAC data

2011\_06\_14\_c\_RBO019\_18F\_60m\_20x1\_x5m\_rawATNSC\_alpha\_07242013\_FINAL\_cleaned.csv

nROIs: // Total number of ROIs

6

MAT UB: // Upper bound frame for integral to calculate MAT

12

nFrames: // Total frames

28

n60Frames: // Number of 60-second frames at start

20 // See find\_MAT\_akc.c for more information

ROIs: // All ROI names

cor\_48

cor\_47

cor\_46

cor\_45

cor\_44

cor\_43

Xi(mm): // All ROI Positions; calculated using slice thicknesses

3.78 // Position 0 is at slice where cut petiole meets stem

5.67 // Position in list corresponds to position of ROI in list

7.56 // i.e. ROI cor\_50 is at position 0 mm, cor\_49 at 1.22 mm

9.45

11.34

13.23

Slice Thickness (mm):// Slice thickness of ROI

1.89

Areas (cm2): // Area of each ROI

0.827488482

0.758531094

0.804502666

0.78151685

0.804502666

0.712559462

Times: // Midpoint of each frame

30

90

150

210

270

330

390

450

510

570

630

690

750

810

870

930

990

1050

1110

1170

1350

1650

1950

2250

2550

2850

3150

3449.94

2011\_06\_14\_c\_RBO019\_18F\_60m\_20x1\_x5m\_rawATNSC\_alpha\_07242013\_

FINAL.csv

The version of the data file generated by ASIPro. This file contains data about each Region of Interest (ROI) that is used to generate the model.

2011\_06\_14\_c\_RBO019\_18F\_60m\_20x1\_x5m\_rawATNSC\_alpha\_07242013\_

FINAL\_cleaned.csv

The version of the data file used by the program. This ‘cleaned’ file has been stripped of extra punctuation and is parse-able by the program.

**Running the Software:**

1. Open the command line and navigate to the folder containing the code files.

2. Compile the McKay plant code into an executable file using the make command.

3. The C modeling code uses a Python front end. Run the Python front end using the command python ./Plant\_control\_akc.py

4. Enter a choice in the command line. If a file window opens, choose an appropriate file as described above. If running the software for the first time, use the following choice order. Only the number should be typed in to the command line:

**3 - Clean ASIPro File**

Choose file: 2011\_06\_14\_gc\_RBO019\_18F\_60m\_20x1\_x5m\_rawATNSC\_alpha\_07242013\_

FINAL.csv

**0 - Perform McKay Modeling**

Choose file: RBO019input.txt

**1 - Linear Regression of MAT and Position**

Choose file: RBO019input\_out\_YYYYMMDD\_HHMM.txt

**2 - Graph TACs**

Choose file: RBO019input\_out\_YYYYMMDD\_HHMM.txt

To verify the software is working correctly, compare those outputs to the sample outputs listed in the output section.

5. When finished graphing, select 4 – Exit to exit the program.