

Hormone Overview

Version 2.000

Copyright Michael L. Johnson, 2006

All Rights Reserved

Acknowledgments

The use of the following names and trademarks is acknowledged : Microsoft, Windows, Windows 95, Windows 98, Windows Me, Windows NT, Windows 2000, Windows XP, DOS, IBM, DEC, Digital, HP-GL, HP-GL/2, PCL, Lahey, Fujitsu, LF95, PostScript, Adobe Systems, Acrobat, CalComp, Motif, Excel, Redhat, Linux, Intel, and Winteracter.

Copyright

This document and software are copyrighted 2004 by Michael L. Johnson. It may not be copied in any form whatsoever without the prior written permission of the copyright holder.

Disclaimer

While every effort is made to ensure the accuracy of the information in this manual, Michael L. Johnson cannot be held responsible for any errors therein. The software described in this manual is subject to constant improvement. The right is reserved to revise this document and the associated software without notice. Michael L. Johnson makes no warranty about the functionality of this software.

Conditions of Use

Use of this package will be in accordance with the following License Agreement.

License Agreement

Software is furnished to the Licensee free, or for a nominal charge, and may only be copied, in whole or in part, for use by the Licensee and his/her employees. The Licensee acknowledges that copyrights exist on this software. The licensee shall not provide or otherwise make available the software or any part or copies thereof in any form to any third party, except as may be permitted in writing by the Licensor. No title to or ownership of the software or any modified or unmodified parts is hereby transferred to the Licensee. The Licensor shall have the right to terminate the license if Licensee fails to comply with these license terms and Licensee agrees, upon notice of such termination, to return immediately or destroy the software and all portions and copies thereof.

The Licensee further agrees that this software will not be used for profit by anyone. This license is extended to allow corporate (i.e., for profit) users to use the software for internal research purposes only. It does not allow for the resale of the software.

This software is supplied with no stated or implied warranties as to its functionality. The Licensor cannot be held responsible, or liable, for any damages, including but not limited to special, indirect, or consequential, arising out of, or in connection with, the use or performance of the software. This agreement will be governed by and interpreted according to the laws of the Commonwealth of Virginia.

NO WARRANTIES ARE EITHER EXPRESSED OR IMPLIED

Technical Support

Technical support directions are available on the software website (<http://mljohnson.pharm.virginia.edu/support.html>). You may be able to resolve your problem by reading through the information provided there. If you are still experiencing difficulties, please feel free to post an inquiry on the website or to email our support technician. Be sure to provide enough information to enable other users or developers to reproduce your problem. Simply sending an email or posting a message stating that “it did not work” is a waste of your time and ours. PLEASE DO NOT USE THE TELEPHONE!!!

Conventions Used in This Document

Throughout this document buttons and check boxes will be typeset in a bold, sans-serif font. For example, you start the calculation by clicking on the **Calculate** button. Menus are listed in the same font as buttons, but separated by an arrow. For example, to exit the application choose **File → Exit**. User input will be typeset in a fixed-width typewriter font. For example, to change your current directory to the root, type `cd C:\`. Data supplied by the user will be surrounded by less than and greater than symbols. For example, to change directory to your documents folder run `cd C:\Documents and Settings\<username>\My Documents`.

Table of Contents

| | |
|--------------------------|----|
| Preface | 5 |
| Introduction | 6 |
| Main Menu | 9 |
| File Menu | 10 |
| Algorithms Menu | 10 |
| Results Menu | 10 |
| Tools Menu | 11 |
| Data_Select Menu | 11 |
| Graphics Menu | 11 |
| Help Menu | 12 |
| Text Editor Window | 13 |

Preface

This manual provides an overview of the Hormone.EXE user interface of this version of the University of Virginia suite of Hormone Pulse Analysis (PULSE_XP) software. It presupposes that the reader already has an existing familiarity with a previous version of this software and wants to quickly learn the new user interface.

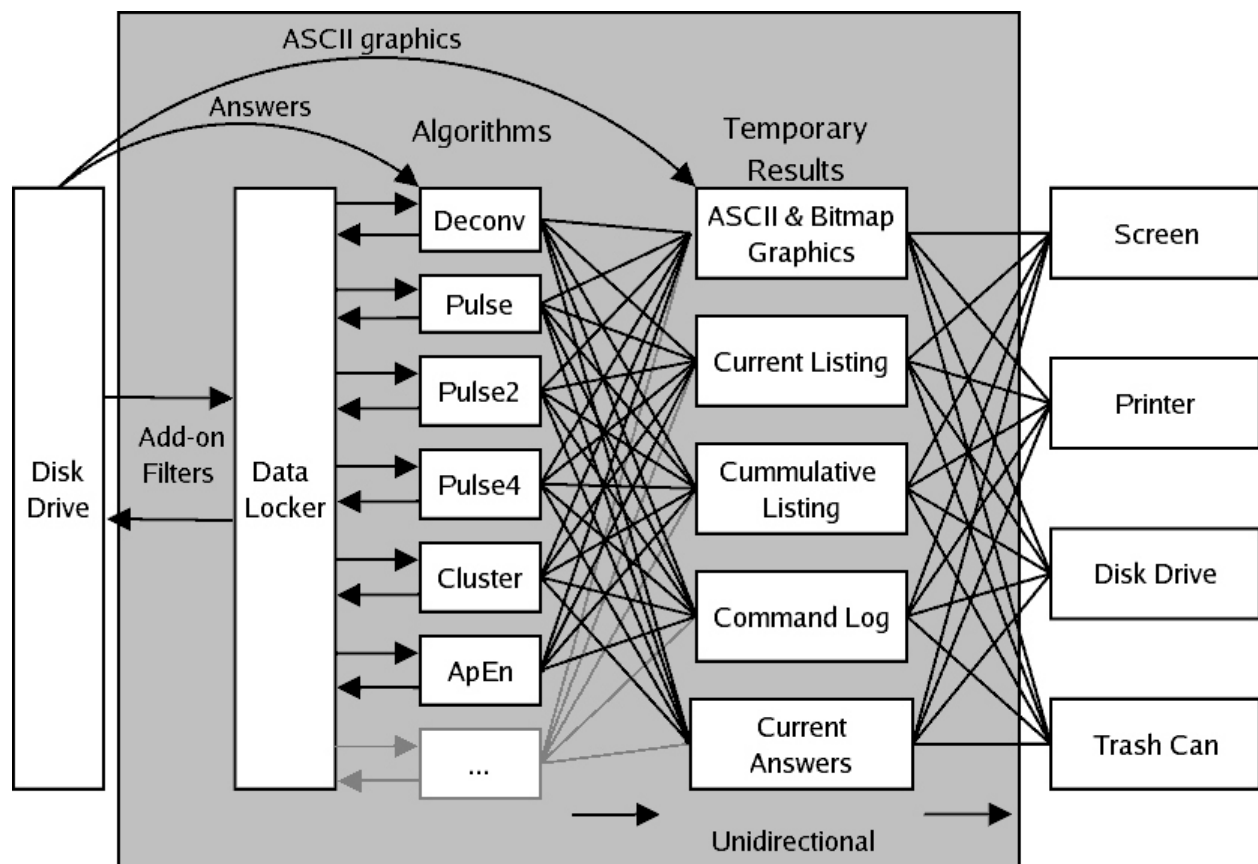
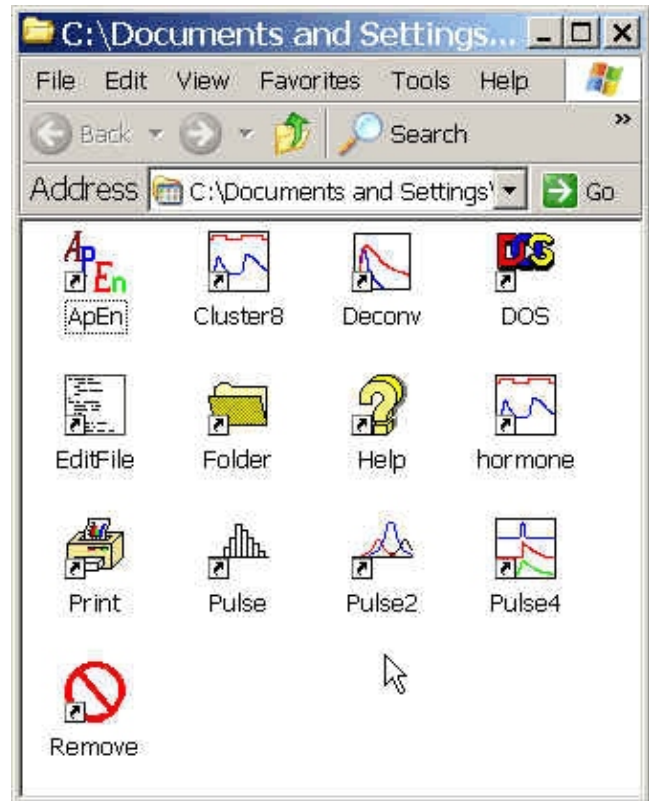
It is highly recommended that users that are new to this suite of software begin with the User's Guide and/or the original published articles.

Introduction

The Pulse_XP package incorporates most of the functionality of the previous version of the University of Virginia Hormone Pulse Analysis Package into a single program, Hormone.EXE. This program has several modes that mimic previous versions of the software.



The installation procedure creates a link on the user's Desktop like the one shown at the left. This link takes you to a folder with the same shortcuts as a link in the Start Menu. The default folder is shown on the right. With the exception of "Remove" and "Help", all of these shortcuts are pointing to the same program, Hormone.EXE, but invoke the program in different modes. These shortcuts are discussed in more detail in the Tutorial and the Users Guide. The advantage of

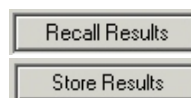


combining all of the software into a single unit is that it allows for a uniform user interface and for the easy transfer of information between the individual algorithms.

The overall schematic of the software is shown on the previous page. The program consists of two main parts: the Data Locker and a series of numerical algorithms such as Deconv, Pulse, Pulse2, Pulse4, Cluster, and ApEn.

While the program is executing, the Data Locker provides many administrative functions [such as checking our web site for software updates] and provides a dynamic file storage location that can be accessed by each of the algorithms. With the start of any of the algorithms, a fresh copy of the data is first retrieved from the data locker. This minimizes the possibility of unwanted interaction between the algorithms.

By clicking on **Recall Results** the user can always obtain a fresh copy of the data set with any algorithm. The current results may also be saved into the Data Locker with the **Store Results** command. The combination of these two buttons allows the user to change parameter values and ask “what if” questions. For example, while the current results look good, the user may still wish to try a different hormone elimination half-life. This can be accomplished by clicking on **Store Results** and then entering the modified half-life value in the grid and clicking **Calculate** again. If the user decides that the prior results are more appropriate, those previous results may now be retrieved with **Recall Results**.



A second use of **Store Results** is to make the results of one algorithm available to a different algorithm. For example, the Deconv algorithm functions optimally with an initial set of secretion peak positions, amplitudes, half-lives, etc. These can either be entered directly by the user or they can be estimated by another algorithm and then made available to the Deconv algorithm by clicking on **Store Results** and retrieving them when initiating the new algorithm.

When the program executes it creates several general types of temporary disk files:

- ASCII and binary graphics file;
- A current listing file;
- A cumulative listing file;
- A command log (i.e. a history) file;
- In most cases, a current answer file.

These files are temporary and will be deleted unless the user specifically instructs the program to save them. Deleting these files prevents the computer's disk from being quickly filled with unwanted files. Each of these files can be displayed on the computer screen, printed, saved as a disk file, or automatically deleted by the program. Most of the ASCII files are displayed with a text editor that is integral to the program.

All of the graphics created by this suite of software is created in a two step process. Firstly, an ASCII graphics file (*.GRF) is created that contains all of the information about how the graph is to be drawn. Secondly, this ASCII file is then translated into the appropriate screen,

printer, or binary disk file. An ASCII file can be easily edited with standard editors such as Notepad (a text editor that is part of MS Windows). Since these ASCII files can be read and altered by the user, they can be customized in almost any desired way with ease. The details of the ASCII graphics file are described in the File Format document.

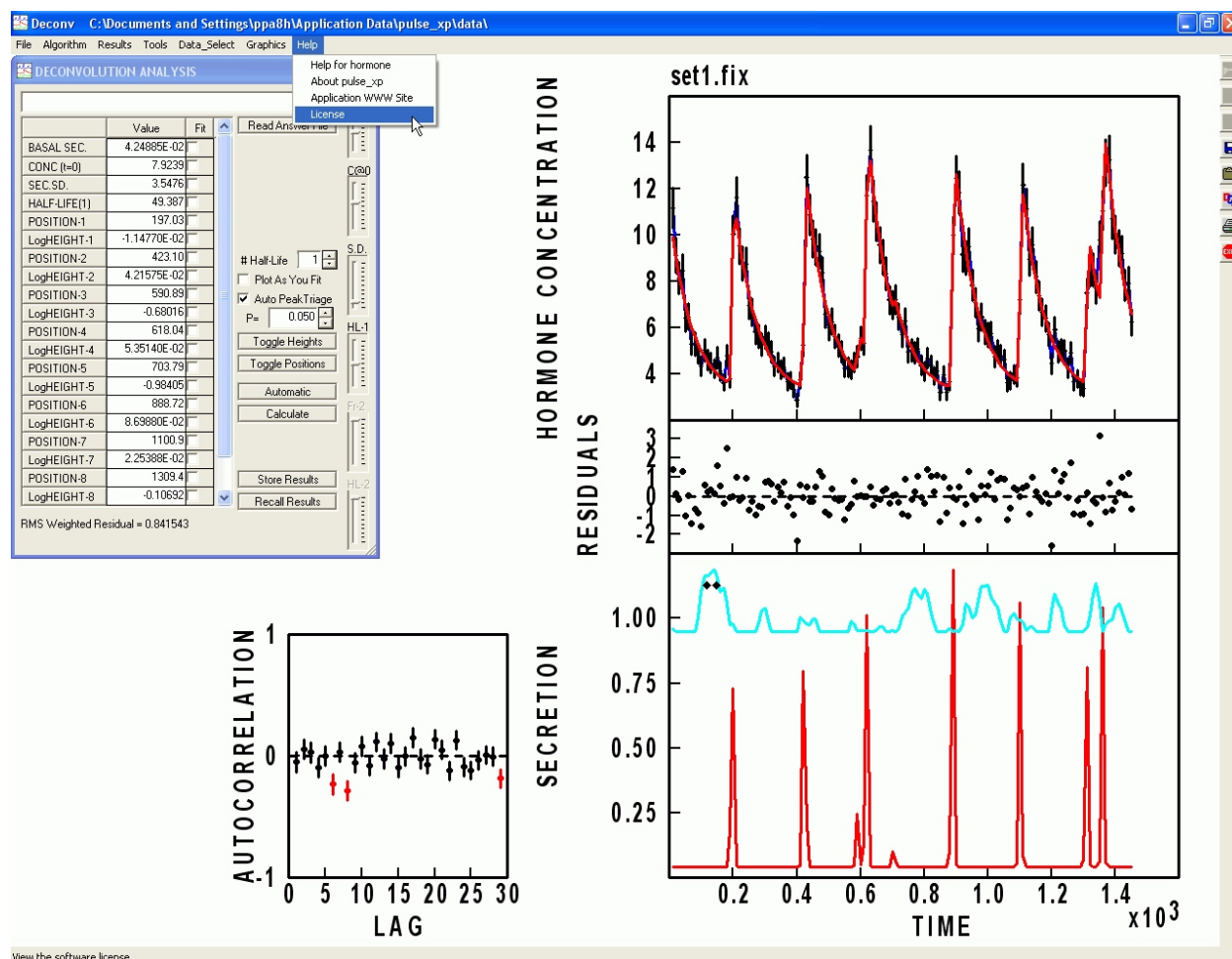
When any of the algorithms performs a calculation an ASCII Current Listing file is created. This file can then be printed with **Print Results** or edited with the integral text editor by clicking **View Results**. This editor allows for the printing of selected portions of the file. The software also maintains a cumulative listing file that can be viewed, stored or printed with the **Results** option of the programs main menu.



Although most of the algorithms also create a Current Answer file, not all do. This Current Answer file is the BST file created by the previous version of this software. Its primary purpose is to supply the initial values for the weighted nonlinear least-square parameter estimation algorithm that is incorporated in the Deconv algorithm. This file also can be viewed, stored or printed with the **Results** option of the programs main menu.

Main Menu

The image below is a typical screen from the HORMONE.EXE program.



The software consists of a main menu, a graphics engine, and a set of individual algorithms. The top row of the screen shows the currently selected algorithm, Deconv being the example here. The bottom line provides a help message for the currently selected item. The Toolbar on the descending top right allows the user to manipulate the displayed image.

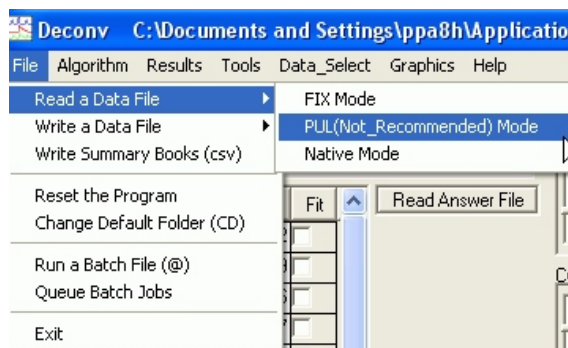
The upper panel of the above image contains the hormone concentration data as vertical black error bars. The data points are connected with the blue line. The red line in the upper panel is the estimated concentration profile based upon the secretion pattern which is shown in the lower right panel as a red line. The specific numerical results from this analysis are shown in the grid on the left. The right middle panel contains a plot of the residuals (i.e., the variance weighted differences between the data points and the calculated concentration profile). Note that these residuals should be random and follow a Gaussian, or bell shaped, distribution. The lower left panel contains the autocorrelation of these residuals for lags from 1 to 30. The three red autocorrelation values indicate that these are significantly ($P=0.05$) non-zero. One or two apparently non-random autocorrelations are expected at a 0.05 probability cutoff level.

Note that if the mouse cursor is placed on the graphics image without clicking any buttons, an information panel will report the current coordinates of the graphics cursor in the lower left of the screen. In this example, the mouse cursor is indicating a time of 1321.0 minutes and a hormone concentration of 9.3608.



File Menu

The **File** menu allows the user to read and write data files in several formats (see the Data File Format manual) and to change the default folder location of the data files. It also has an option to run a batch file and even to queue batch jobs. A prototype batch file is created whenever the software is executed and can be examined with the Results, Command History options. Resetting the program simply re-initializes the software without the need of exiting/ restarting the program.

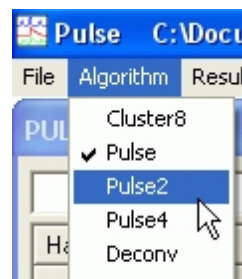


The Change Folder (CD) option is also available in the File Sub Menu and from the Start Menu and Desktop icons (at right).



Algorithms Menu

The user can use one algorithm and then switch to another algorithm by simply selecting a different algorithm with the **Algorithms** menu. A check mark is displayed next to the selected algorithm. In the image on the right, **Pulse** is the currently selected algorithm.



Each of the algorithms is also available from Start Menu and Desktop icons, as seen at right.



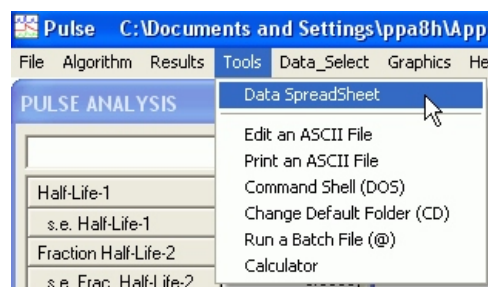
Results Menu

As mentioned, when executed, this program creates several types of temporary disk files that can be accessed with **Results**. These include the Log File (i.e., the cumulative listing file), the Command History file (i.e., command log), the current answer file (or BST file), and the ASCII Current Graph file. Each of these can be viewed and edited within an ASCII Editor Window, saved to a disk file, or printed from the Results menu.



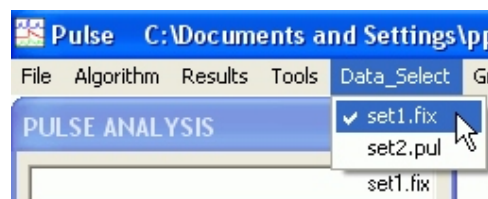
Tools Menu

The **Tools** menu has several functions such as allowing the user to edit and/or print any ASCII file on the computer. Additionally, the menu permits the user to open a command shell to use MS-DOS commands, change the default data folder (i.e., directory), execute a batch file, or display the standard MS-Windows calculator.



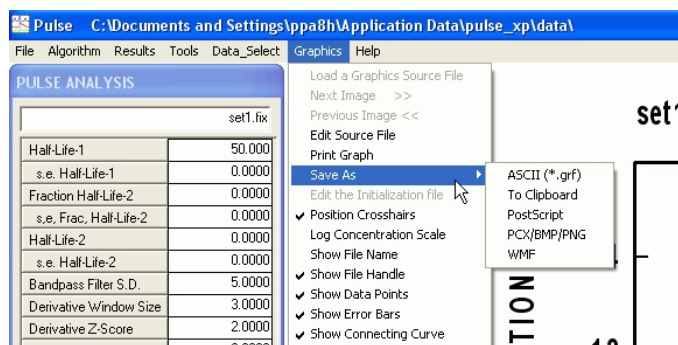
Data_Select Menu

Multiple data sets can be simultaneously read into the software's Data Locker. The **Data_Select** menu provides the user with a method to rapidly switch between several data sets. In the present example, the Data Locker contains two data sets with set1.fix being the currently selected data set.



Graphics Menu

This menu controls all graphic output. The software forms all of its images by creating an ASCII graphics file and then converting that file to an image file. The current ASCII graphics file can be edited, printed, and saved in various formats. A number of options that can be easily controlled by the user are available. For example, the user can remove the plot of the residuals by deselecting **Graphics** → **Show Residuals**.

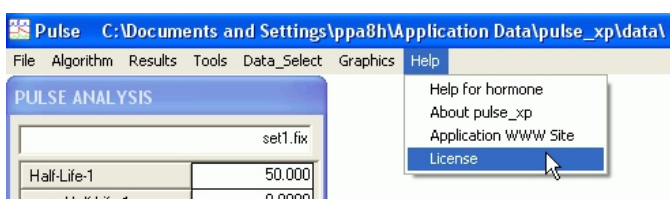


The software can also be used to create a wide variety of graphs by entering the ASCII graphics information into a file. This file can be read into the graphics engine from the **Graphics** menu even if the Data Locker does not contain any data sets (e.g., such as after a Reset command). This file can then be edited, modified, displayed and printed. The format of the ASCII graphics file is described in the File Formats manual. This option is also available with the GrfView icon which is shown at right.



Help Menu

Several types of help are available from



the Help menu. A PDF reader (such as Adobe Acrobat Reader) is needed to view some of the help files and publications. If you do not have the software, you can download Adobe Acrobat PDF reader free of charge from www.adobe.com.

The manuals are also accessible from the Start Menu and Desktop icons.



Text Editor Window

When the user views or edits an ASCII file, the software opens a full featured text editor in a new window. Note that this editor window must be closed before you can resume using the software.

The following figure presents an example of one of the software's editor windows. This

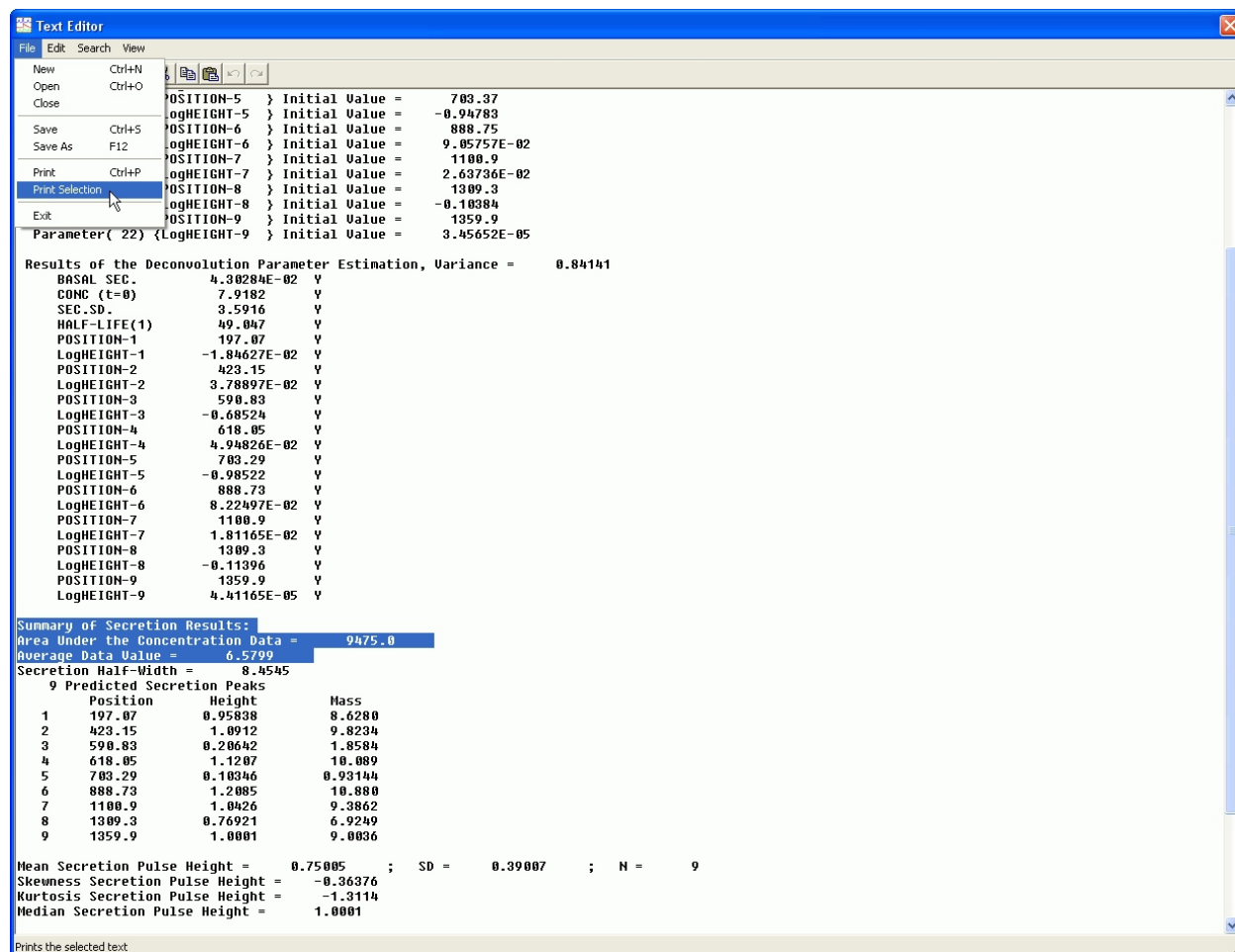


figure presents an example of the text editor viewing a Current Listing File created by the Pulse4 algorithm. To print a selection of the file, highlight the desired text with the mouse and click on **File → Print Selection**. All of the features of a standard editor are available within the editor window.

The text editor is also available with the EditFile icon.



Index

| | |
|----------------------------|----|
| Acknowledgments | 2 |
| Algorithms Sub Menu | 10 |
| ASCII Editor | 13 |
| Conditions of Use | 2 |
| Copyright | 2 |
| Data_Select Sub Menu | 11 |
| Disclaimer | 2 |
| Editor | 13 |
| File Sub Menu | 10 |
| Graphics Sub Menu | 11 |
| Help Sub Menu | 12 |
| Introduction | 6 |
| License Agreement | 2 |
| Main Menu | 9 |
| Preface | 5 |
| Results Sub Menu | 10 |
| Table of Contents | 4 |
| Technical Support | 3 |
| Tools Sub Menu | 11 |