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Appendix F

the Bayes Directory Organization

When the interface is started for the first time, it will define a “Bayes” directory in the user home directory. This home directory is the default location. This default can be changed on the Settings/Preferences menu. After using the software for a while, the home directory will accumulate various subdirectories and files. Here is a typical example of what is in a typical Bayes Home directory:

<table>
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<th>Bayes.Predefined.Spec</th>
<th>System.out.txt</th>
<th>exp4</th>
</tr>
</thead>
<tbody>
<tr>
<td>BayesAsciiModels</td>
<td>exp1</td>
<td>exp7</td>
</tr>
<tr>
<td>BayesManual.pdf</td>
<td>exp2</td>
<td>plugins</td>
</tr>
<tr>
<td>System.err.txt</td>
<td>exp3</td>
<td>resources</td>
</tr>
</tbody>
</table>

Here is a brief description of these files and what is contained in them:

**Bayes.Predefined.Spec** is used by the Metabolite package and contains copies of the system and user modified metabolite files. For a description of the metabolite package and the metabolite file formations, see Chapter 10.

**BayesAsciiModels** is a subdirectory that contains both system and user defined Ascii Models. Each model consists of at least two files, the Fortran or C code defining the model, and a parameter file that specifies among other things the prior probabilities for the parameter in the model, see Chapters 20, 22, 21, 28 and 29. Additionally, if the user happens to use the Magnetization Transfer Kinetics package, then a WaterViscosityTable will also be present in this directory. For details on this file, see Chapter 15.

**BayesManual.pdf** is your default copy of this manual. The default copy of the manual is located in your Bayes directory in home directory. This manual is distributed with the software and the user may download updated copies of this manual. Downloaded copies of the manual are written into the current Bayes Home directory.

**System.err.txt** is a file containing Java error messages and is used by us to assist in diagnosing problems, should they occur.

**System.out.txt** is a file containing Java console messages and is used by us to assist in diagnosing problems, should they occur.
exp1, exp2, exp4, exp4, and exp7 are the working directories defined in this Bayes directory. Working directories are work areas where an analysis is stored while it is being setup, run and analyzed. Working directories can have any names, and are not necessarily prefixed by “exp”.

plugins is a directory created and used by Java. Plugins are installed in this directory as needed.

resources is a directory containing the Java properties files. This file contains various settings that are remembered by the system. For example, it contains the list of servers, their names, IP address, port numbers, etc.

The Work Directories named exp1, exp2, etc. are users defined working directories. These directories are used by the interface to contain an analysis. Only a single analysis is contained in a given working directory. However, multiple working directories can be in use at any given time. Just as the Bayes home directory contained a number of files and subdirectories, so too, the individual working directories contain a number of files and subdirectories. However the contents of these subdirectories is very similar. Here is a typical example of what is found inside a working directory:

Bayes.model.fid   BayesOtherAnalysis  fid            images
BayesAnalyzeFiles dir.info   image.fid      model.compile

Each of these files and subdirectories are used by the interface for very specific purposes. Here is a very brief discussion of what these files and directories are used for:

Bayes.model.fid is written by packages that process fid data. For example, when the frequency finding program is run and a simulated model of the data is being viewed, that fid model is written into the Bayes.model.fid directory. This fid directory is in standard Varian fid file format and, consequently, the directory contains a fid, procpar and text file.

BayesAnalyzeFiles is a subdirectory contains outputs from the frequency finding package named Bayes analyze. For more on these files see Chapter 8.1.

BayesOtherAnalysis is a subdirectory that contains the inputs and outputs for most Ascii packages, i.e., exponential, enter Ascii, magnetization transfer, miscellaneous and histogram packages all use this directory to store inputs and outputs.

dir.info contains the current status of the analysis in this package. When the user leaves a directory for any reason, the interface writes this file and when the user rejoins this working directory the dir.info file is used to restore the analysis to its status at the time the user departed.

fid contains the current spectroscopic fid loaded into this working directory. This directory is in standard Varian fid file format.

image.fid contains the current image fid loaded into this working directory. This directory is in standard Varian image fid file format.

images contains the images and Abscissa currently loaded into this working directory. All images contained in this directory are in “4dfp” format, see Chapter G for a description of this file format.

model.compile is a subdirectory that is used whenever a model is built by the interface. This directory typically contains the last model built, a compile listing and if the compile was successful the executable.
Bibliography


[43] Metropolis, Nicholas, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller (1953), “Equation of State Calculations by Fast Computing Machines,” Journal of Chemical Physics. The previous link is to the American Institute of Physics and if you do not have access to Science Sitations you many not be able to retrieve this paper.


