## A very quick guide to using AMDIS.

**This guide is meant to be followed step by step. At the end you will have run through most of the important things that AMDIS can do. Once done, you can find out more about AMDIS, but please go through the guide at least once.**

The package is supplied with two data files for Agilent (HP) instruments.

The working assumption of AMDIS is that retention index data will be established by external standards - by default the straight chain hydrocarbons (C-series) - run once a day. These standards will establish a correspondence between time and retention index. The retention times in data files are then converted to retention indices using the linear correlation of van der Dool and Kratz.

When you first start up AMDIS after it has been installed, it will ask you to select the default format of your GC/MS data. For the purpose of this demonstration, select Agilent Files and click **OK** (it can always be changed to your actual file format later using the "Data file format" parameter on the **Instrument** tab in the dialog of the **Analyze** menu's **Settings** command).

The screen that will be shown next has a **File** menu, which you should click and then click **Open** on its menu. From the default AMDIS directory you should select TUTORIAL (a subdirectory) and then ALK3.D (also a subdirectory, but because of the way Agilent stores files this is the target for the analysis) and finally click the **Open** button. NOTE: All the data files for this quick guide are in this subdirectory.

The program will bring up a chromatography file and more menu selections will become available. Click **Analyze**, and then **Analyze GC/MS Data**. A dialog box will come up.

- The first line in the box will show the name of your GC/MS Data file.
- The second line is the type of analysis. Using the arrow tab on the side, bring down the selection and select **RI Calibration/Performance**.
- The third line is now the RI Calibration Library. Click the RI **Calib/Stds. Lib.** button. You will be shown a tabbed dialog box with RI Calibration/Standards Library highlighted. Click the **Select New** button and you will be given a file selection box. The Calibration Library you are looking for is in a subdirectory called TUTORIAL under the AMDIS32 directory if you used the default install conditions. It is entitled ALKANES.CSL. Select this, click **Open** and then click **Save** at the bottom of the tabbed dialog; which will close it. You may if you want change the name of the calibration file by clicking the **RI Calib. Data** button, but it is not necessary.
- Now click **Run**.
- Click **OK** to the box that appears next, which may warn you that "Previous RI calibration data will be replaced".

Depending on the speed of your computer you will normally get the results within a few seconds.

You have now had AMDIS build a correspondence table for converting RT (retention time) to RI (retention index). AMDIS will use this to convert retention times to RI values.

Since this is a quick guide, we will not cover all the features of the program. You can see the results by selecting the various compounds identified using your mouse in the list. To see what data was retained by the program for the calibration click the **Info** button on the button bar below the menu bar. In the tabbed dialog box that appears, click **Standards**. You will see the data that will be used to convert retention times (RT) to retention indices (RI). When you are finished click the **Done** button.

Now you are ready to analyze data.

Got back to the **Analyze** menu selection. Click **Analyze GC/MS Data** again.

- In the first line select a new file. Find the file CARD5P.D, select it and click **Open**. A dialog asks what you want to do with the current result files. For the purposes of this guide you can click either **Delete** or **Keep**.
- In the second line choose the analysis type as **Use Retention Index Data**
- In the third line choose PESTPLUS.MSL as the target library and return to this dialog.
- Notice that the last line contains the same name you used in the previous run for the calibration data. Now click **Run**.

Again the results will appear in about the same amount of time as the previous run.

Try selecting different target compound names or retention times in the lists on the right hand side of the screen and notice that the Component and Match list box values change for the selection. In many cases there is data about the difference between the RI observed and the RI in the library; RI-RI(lib) value. If this number is too large there is a penalty applied to the match factor.

Both of these experiments were run under similar chromatographic conditions. Typically a GC/MS is very stable for several days, but since it is normal good laboratory practice to do a quality control run each day, the same quality control run can be used to establish the calibration file for the day.

There is a lot more that you can do with AMDIS, but you have now completed a "standard" analysis with retention index calibration.

This is a quick start up. The help file will give aid in doing other tasks.
Chapter 2 of the Help file has a far more extensive discussion of these examples.