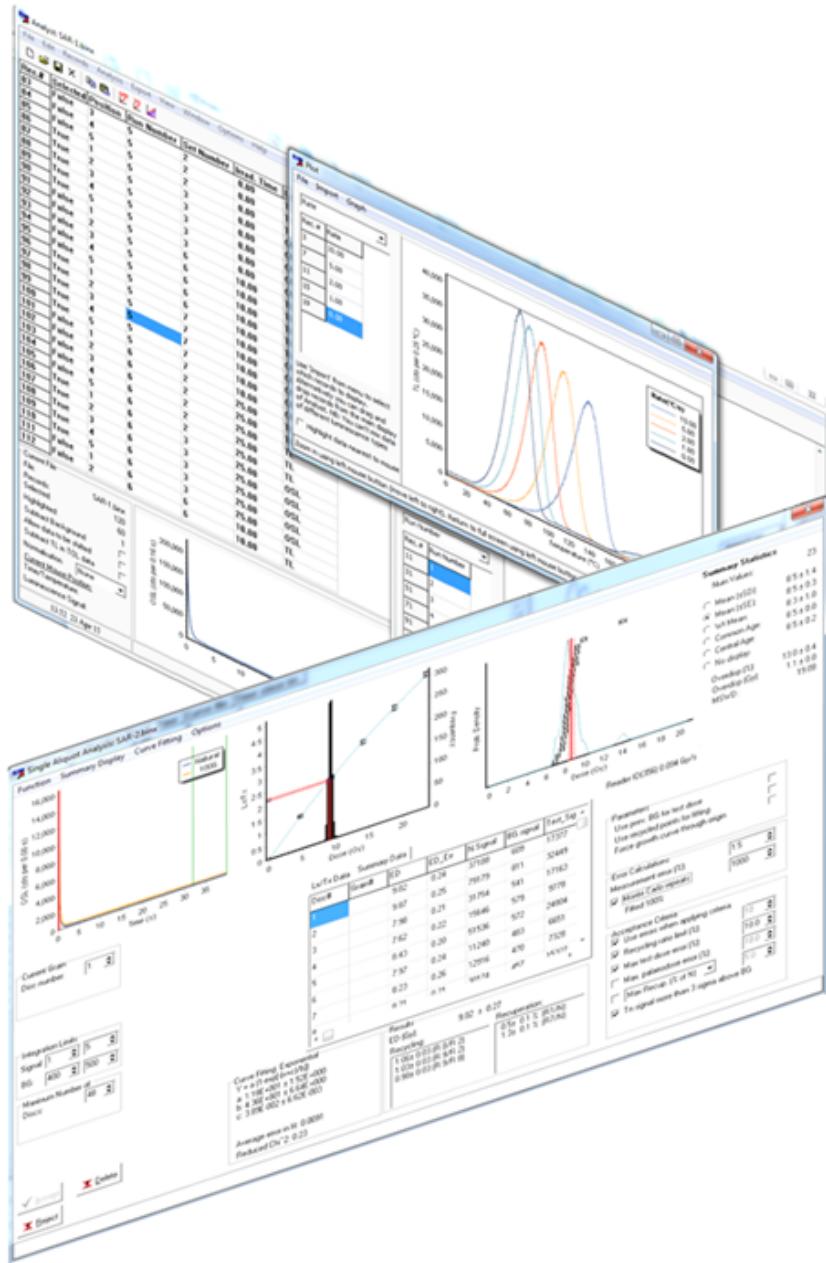


Analyst

v4.57

User Manual

November 2018



Geoff A.T. Duller
Aberystwyth Luminescence Research Laboratory
Aberystwyth University
users.aber.ac.uk/ggd

Table of Contents

1. Introduction	4
1.1 What's new.....	4
1.2 Installation of Analyst and Getting Started	5
1.3: Installation of R and the Luminescence Package	7
2. Main Analyst Window.....	9
2.1 Altering what information is displayed in the main window	10
2.2 Selecting and Highlighting Records.....	11
2.3 Front Panel Controls.....	14
2.4 Calculating Integrals	16
2.5 Graphs in Analyst	18
3. File Menu	21
3.1 New	21
3.2 Open.....	21
3.3 Save	21
3.4 Save As.....	22
3.5 Close	22
3.6 Exit	22
4. Edit Menu	23
4.1 Copy	23
4.2 Paste	23
4.3 Copy Selection & Data	24
4.4 Copy Selection & Data (transposed).....	24
5. Records Menu	25
5.1 Select	25
5.2 Unselect	25
5.3 Edit Current Record.....	25
5.4 Block Edit.....	27
5.5 Highlight All Records	28
5.6 Copy Highlighted Records.....	28
5.7 Paste Records	28
5.8 Delete Highlighted Records	28
5.9 Move Highlighted Records.....	29
5.10 New Record	29
6. Analysis Menu.....	30
6.1 Multiple Aliquot De	30
6.1.1 Integral De	30
6.1.2 Plateau test.....	32
6.2 SA Regeneration.....	33
6.2.1 Menus	37
6.2.1.1 Function menu	37
6.2.1.2 Summary Display menu	39
6.2.1.3 Curve Fitting menu	41
6.2.1.4 Options menu	43
6.2.2 Using SAR	46
6.2.2.1 Displaying the change in sensitivity (Tx/Tn).....	46
6.2.2.2 Calculation of uncertainty in De	47
6.2.2.3 Analysis of multiple equivalent dose values.....	49
6.2.2.4 Summary Statistics	51
6.2.2.5 Running R Scripts	52
6.2.2.6. Sample Camera.....	53
6.2.2 Single Grain Regeneration	53
6.3 Component Fitting.....	54
6.4 Fading Test	55
6.5 Display.....	59
6.5.1 Individual Curve Data	59
6.5.2 Plot Multiple Data	60
6.5.3 Flexi Plot	64
6.6 Deadtime correction	65
7. Export Menu.....	66
7.1 Current Data Display	67

7.2 Group Averages	67
8. View Menu	69
8.1 Classic View.....	69
8.2 Sequence View	69
9. Window Menu	73
10. Options Menu.....	73
10.1 Display Font.....	73
10.2 Change User.....	73
10.3 Group Definitions	73
10.4 Directories	75
10.4.1 Define RScript location.....	75
10.4.2 Define Script Library location	75
10.5 Manage R scripts.....	75
11. Help Menu	76
11.1 About	76
12. R support and use within Analyst.....	77
12.1 How to run R scripts.....	77
12.2 How to manage R for Analyst Libraries	80
12.3 How to get graphical output from R scripts.....	81
12.4 How to edit and create your own R in Analyst (RAN) scripts	81
12.4.1 Change the name of an R script.....	81
12.4.2 Edit an R script.....	82
12.4.3 Accessing data from Analyst in R	82
12.4.4 Using variables in 'R in Analyst' (RAN) scripts.....	83
12.5 How to export and import R for Analyst scripts	85
13. References	86
14. Appendices	89
14.1 Appendix A: BINX file format.....	89
14.2 Appendix B: Summary Data from single aliquot and single grain analysis	105

1. Introduction

Analyst is a Windows based program designed to allow you to view, edit and analyse luminescence data collected using a Risø automated TL/OSL reader. It offers a range of facilities, including equivalent dose determination. Additionally, since it is impossible for any analytical program to cater for every possibility it allows you to export the data in a variety of formats so that it can be transferred to other programs, including spreadsheets.

The basic file structure used by Analyst is the BINX file. This program has been designed to operate in conjunction with the Sequence Editor programme supplied by Risø for running the latest generation of automated TL/OSL readers. Older version of this software created BIN files, and these are compatible for this version of Analyst, but not all of the features described here are available with BIN files.

A detailed description of the format of this file type is given in [Appendix A](#). The important point to note at this stage is that by using this data format each luminescence measurement is stored in a 'record' that contains not only the numerical data from the luminescence measurement itself, but a wide range of additional information as well. This information can be grouped into three categories: sample characteristics, measurement conditions, and analytical data. Some of this information is automatically placed into the record when it is recorded by the TL/OSL system, some is set only if the user chooses to set it by using the 'Run Information' box in the Sequence Editor, while other parameters can only be set during processing. Analyst allows you to view, edit and use all of these parameters.

1.1 What's new

The main innovation in version 4.57 of Analyst is support for the use of [R scripts from within Analyst](#). This is designed to allow users to exploit some of the sophisticated modelling functions and graphing routines available within different packages in R, especially the package "Luminescence". In addition, a number of other changes have been made, some visible, some not:

- a) Loading and Saving BINX files is now faster
- b) In the summary page of the single aliquot and single grain section of Analyst, summary data are recorded for ALL aliquots that are measured. This includes those that pass criteria and those that do not. A toggle switch is available that allows users either to look at results for ALL aliquots, or just those aliquots that passed the acceptance criteria.
- c) A much greater range of data is now available in the summary data for each aliquot. This includes the Lx/Tx ratios for each regeneration point (up to a maximum of 15 regeneration points), along with the calculated uncertainty on that ratio.
- d) An option is now available to correct data for the deadtime of the PMT.

Previous version history

=====

Release version 4.43 included a number of minor additions as listed below. The main purpose for the release of version 4.43 is to provide compatibility with version of the BINX file format that was introduced in December 2015, to improve support for the new DASH head and to correct a number of minor bugs.

The changes in version 4.43 are:

- a) Analysis of multiple BINX files

The Single aliquot Regenerative dose (SAR) page was modified to make it possible to analyse multiple BINX files at once. This means that if different aliquots of a sample were measured in two or more sequences then it is now possible to analyse BOTH files at once, so that the distribution of D_e values from both files can be studied. The BINX files may also have been collected on different luminescence readers. In this case the analysis should be undertaken in Gy instead of seconds, to allow for the differences in the strength of the beta sources.

b) Reporting precision

A menu option has been created to allow users to adjust the precision with which Summary Statistics are displayed in the SAR page

c) Sample Camera

If visible images of discs have been acquired by a sample camera attached to the reader then these will be displayed on the single aliquot page

The new features added to version 4.31 of Analyst:

a) Online help

A manual and online help system have now been implemented for Analyst. While running Analyst context sensitive help can be obtained by pressing F1 at any time.

b) Ability to alter the appearance of graphs

All graphs in Analyst now offer the option to be able to change their appearance. This may include changing the scales of any axes, the font size of captions, whether to plot data on linear or logarithmic axes etc. In addition, there are now more options available for exporting data from graphs to other packages for further analysis.

c) Analysis of fading data

Measurement of g-values to characterise the anomalous fading of luminescence signals is now supported by Analyst. This is supported by the Sequence Editor that now automatically stores the time between irradiation and luminescence measurement.

d) Display of multiple luminescence data on the same graph

Analyst routinely shows data for an individual luminescence measurement, but sometimes it is useful to be able to plot the data from a series of measurements on the same graph. This has always been possible using the Viewer programme supplied by Risø but a similar functionality has now been included in Analyst. It is possible to have as many of these graphs open as the user wishes, so it is possible to compare data from different aliquots, or after different treatments simultaneously.

e) Sequence Display

As well as viewing the BINX file in the conventional way, it is now possible to see the original sequence that was used to collect the luminescence data, and use this to select or deselect data for analysis.

1.2 Installation of Analyst and Getting Started

The Analyst program may have been supplied as part of the Risø standard installation, or you may have downloaded it from my website (<http://users.aber.ac.uk/ggd>). You should have a setup program (SETUP.EXE) which will guide you through the process of installation in the manner usual for Windows software. It will install the Analyst program itself and a number of example data files. The program can be installed anywhere on your hard disk, but I would recommend that you place it

in a sub-directory of its own (e.g. C:\Program Files\Luminescence\Analyst). During the installation an icon will appear on your desktop that acts as a shortcut to the program.

If you wish to use R scripts with Analyst you will need to have R (<https://www.r-project.org/>) installed on your computer. When Analyst starts for the first time with R loaded on your computer it should detect it automatically and tell you that it has found it.

User Names

To start Analyst click on the short cut on your desktop created by the installation programme. On first running the program Analyst will appear along with a dialogue box asking you for a username (Figure 1.2(a)).

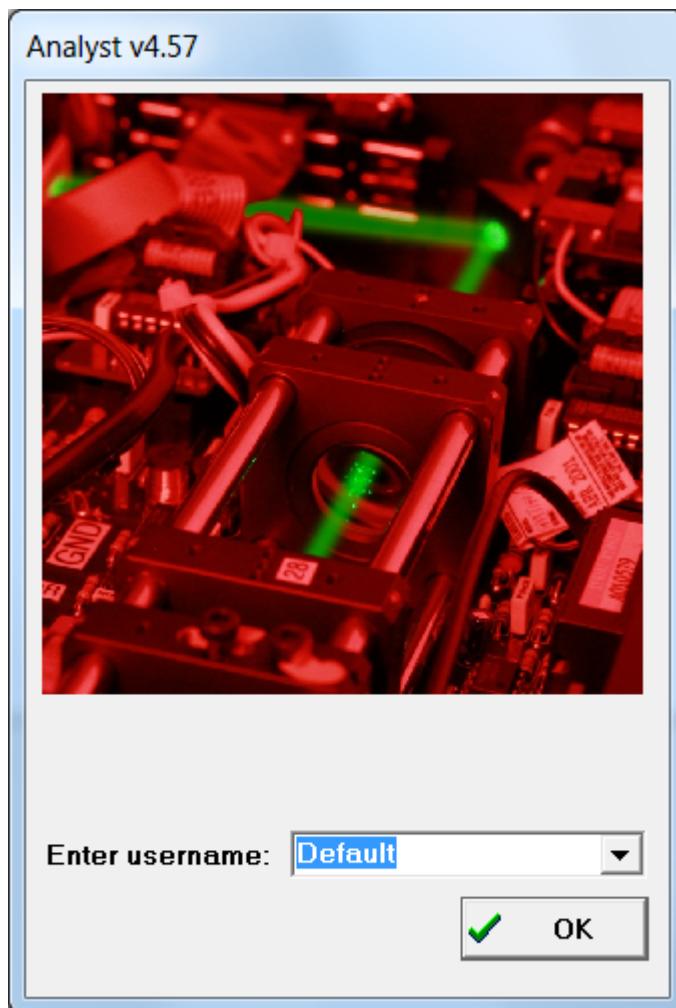
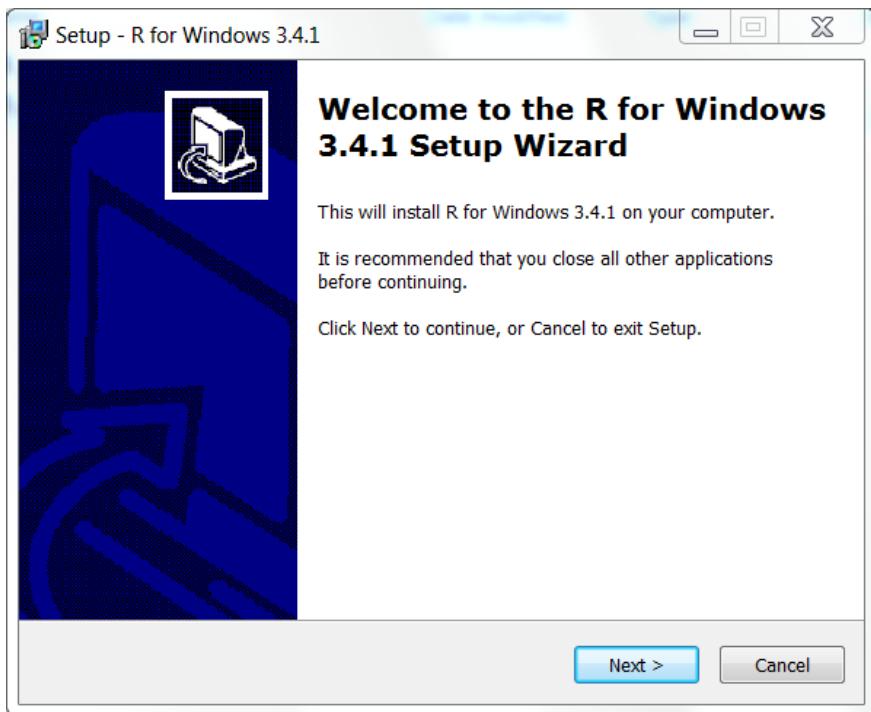


Figure 1.2(a): Selecting a user name. It is possible either to select an existing username, or type a new account name

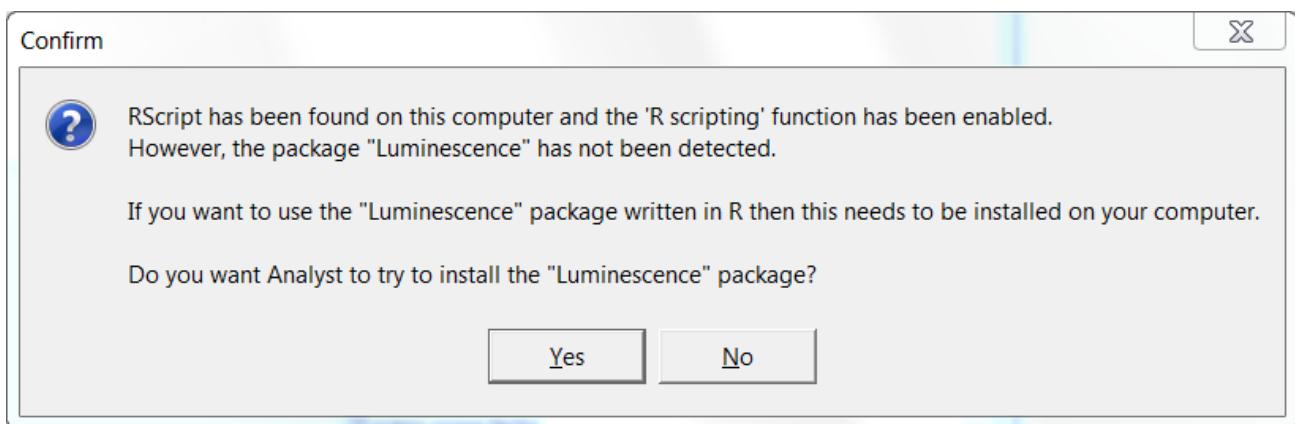
The purpose of having different user names is so that the system can be customised for more than one type of analysis. For instance, each user name can have a different default directory for your data, and set different integration limits for analysis. When you select a user name for the first time you are asked to confirm that you want to create a new user name, and Analyst will then set the default working directories to Documents\Analyst. As you use Analyst it will automatically remember the last directory that you used to open and save data files.

1.3: Installation of R and the Luminescence Package

If you wish to run R scripts from within Analyst then you need to install R on your computer. You can download R for free (<https://www.r-project.org/>). The default installation is sufficient for Analyst.



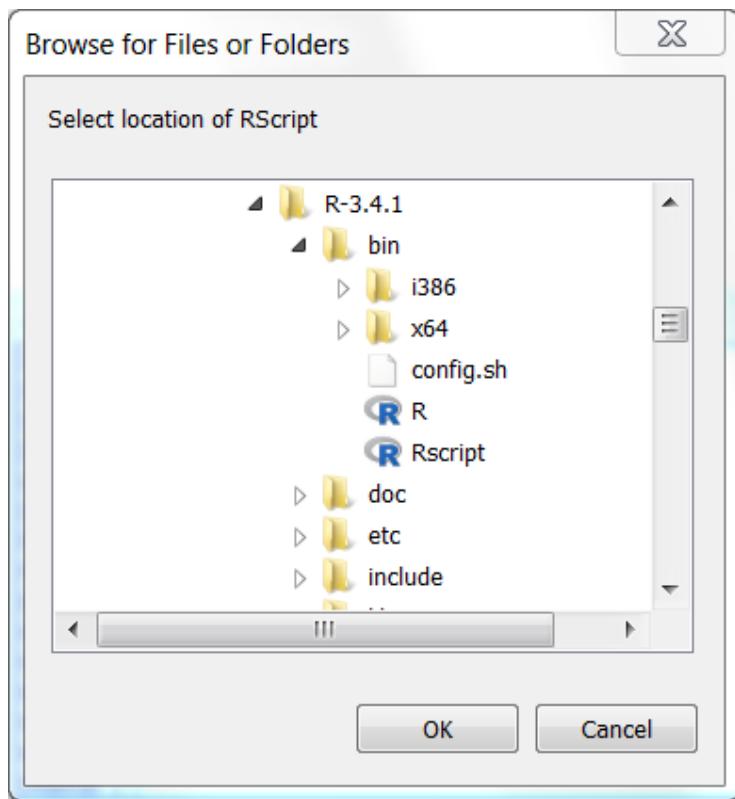
The first time that Analyst detects that R is installed you should receive a message telling you of this. In particular, Analyst is looking for "RScript.exe". When it first detects R present on your computer, Analyst also looks to see whether the R package Luminescence ([Kreutzer et al. 2012](#)) is installed. This powerful suite of routines are specifically designed to aid in the analysis of luminescence data and are constantly being updated ([R.Luminescence web site](#)). You do not have to install this package, but if you wish to use the R scripts included with Analyst then you will need it.



Analyst will automatically attempt to download the Luminescence package for you from one of the CRAN servers where these packages are stored. In order to do this, you need to have a working internet connection for this stage. Once the package is installed, there is no need for an internet connection.

If things go wrong

If you have R installed but for some reason Analyst is unable to recognise it, then you can manually find the RScript file that Analyst needs. Use the Options menu on the front page of Analyst and select the option "Define RScript location...". Analyst will try to locate RScript again, but if it cannot do this, then you need to tell it where RScript is located. Click on the file RScript and then press "OK".



If Analyst fails to download the Luminescence package then you can ask Analyst to try again by running a script. From the Options menu on the front page of Analyst select "Manage R scripts". In the window choose "Select Scripts" and select "Check Luminescence Package". This will load this script. You then need to run the script by pressing "Run Script" from the top menu, or using the shortcut "Ctrl-R". This will get Analyst to check whether the Luminescence package is installed or not. If it is not installed then it will try to download the package from the CRAN server and install it.

The screenshot shows the R Script window with the title bar "R Script". The menu bar includes "Select Script", "Run Script", and "Manage Scripts". The main area contains the following R script code:

```

#=====
# Name: Check_Luminescence_Package
#
# Purpose: Script to check whether Luminescence package
# has been installed on this computer. If the
# package is not found, then the script attempts to
# download it from CRAN and install it
#
# GAT Duller, August 2017
#=====

if!("Luminescence"%in%installed.packages()){
  message("Luminescence Package not installed - now installing...")
  r = getOption("repos")
  r["CRAN"] = "http://cloud.r-project.org"
  options(repos = r)
}

```

The status bar at the bottom of the window displays "RScript: Check_Luminescence_Package_Installation".

2. Main Analyst Window

When you first enter Analyst the screen should appear as shown in Figure 2(a). The layout of the program is a single row of menus along the top of the screen, a blank area in the middle of the screen that once a file has been opened will contain a list of the data records, and a set of summary and housekeeping information along the base of the screen. When there is no BINX file open, all of the menus along the top of the screen are inactive except **File**, **Options** and **About**.

To open a file, select the **File** menu and then **Open**. You will then be presented with a standard Windows file selection dialogue box. From here you can select the BINX or BIN file that you want to open. Initially I suggest that you select one of the BINX files provided with Analyst as an example (e.g. SAR_1.BINX).

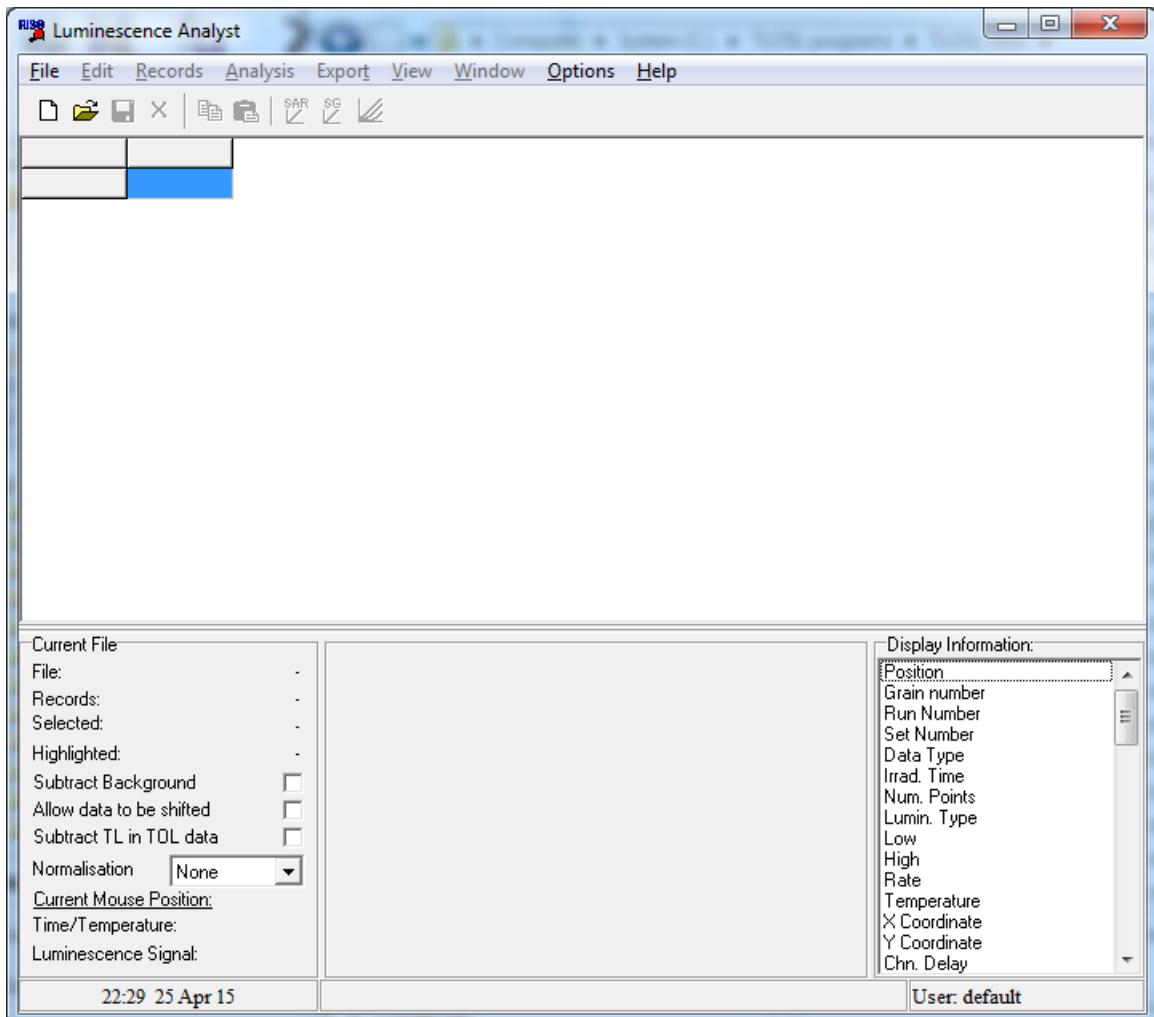


Figure 2(a): Analyst display when started

2.1 Altering what information is displayed in the main window

When Analyst is first displayed, the only information that is displayed about each record is the record number and whether it has been selected for data analysis or not. However you can elect to display any aspect of the BINX file that you choose. In the bottom left hand panel of Analyst is a list of all the different data stored in each record of the BINX file. You can select which data to display by clicking on this list. The full list of information in the BINX file is described in [Appendix A](#).

As an example of the type of data that you can display, scroll down through the list of 'Display Information' and select 'Position', 'Data Type' and 'Lumin. Type'. As you select each item a new column of data is added to the main display (Figure 2.1(a)). Lumin. Type displays the type of luminescence measurement that was made (TL, OSL, IRSL, etc), Position is the position of the sample disc on the carousel in the TL/OSL reader (1-24 or 1-48 depending on the size of carousel in your system), and Data Type is the treatment that you have given to the disc before it was measured. By default, Data Type is set to 'Natural'.

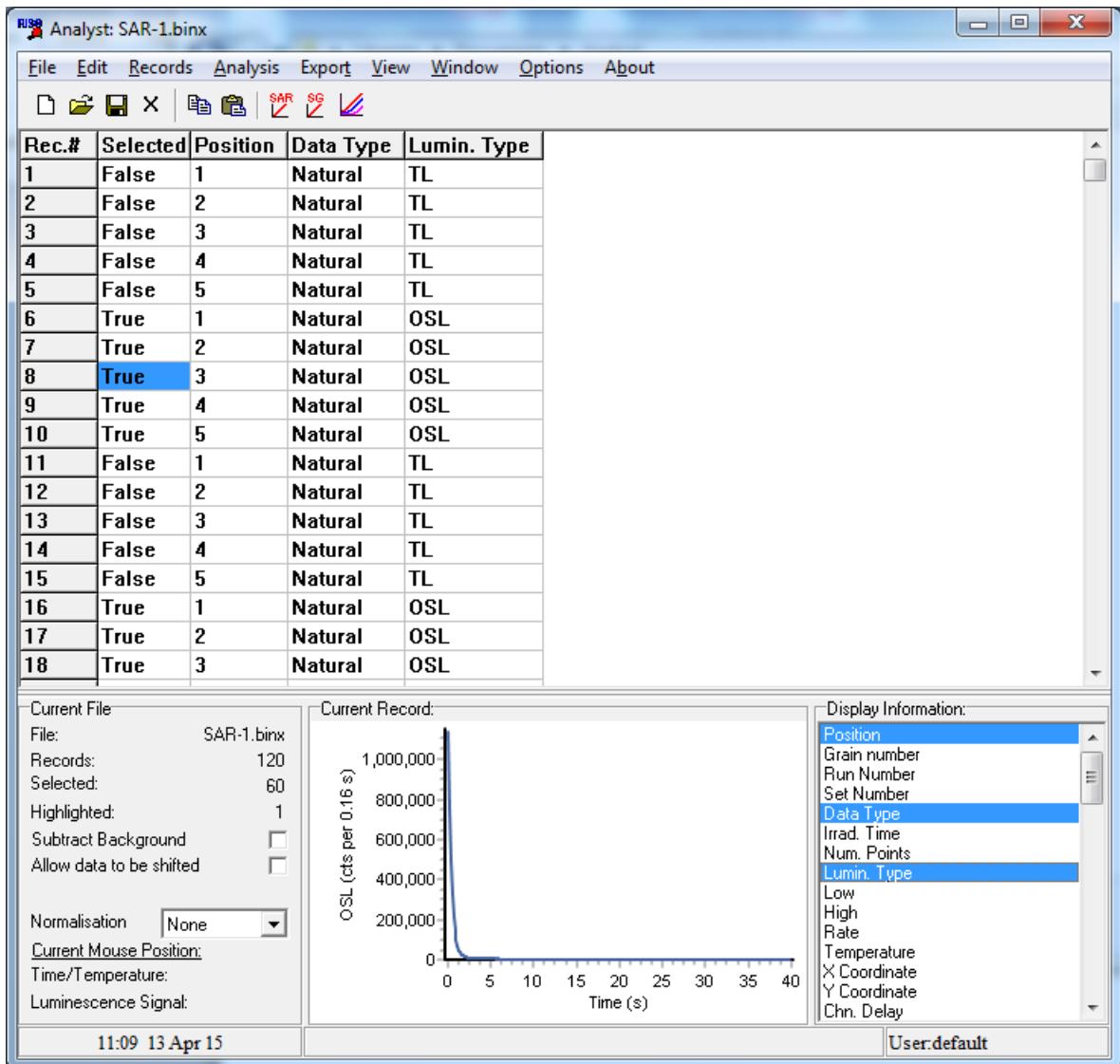


Figure 2.1(a): Altering the display of information in Analyst

2.2 Selecting and Highlighting Records

Once a BINX file is open, Analyst displays a list of the records in the main display area (Figure 2.2(a)). As well as showing the record number in the column on the far left of the display (headed 'Rec.#'), the second column (headed 'Selected') shows whether a given record is selected for analysis or not. When a BINX file is created, all the records are selected by default and thus will appear as 'True'. However, in many types of analysis it will be necessary to select only those records that are relevant. Analyst uses two ways of selecting which data to manipulate: **Selecting Data** and **Highlighting Data**. Understanding these two terms, and being familiar with how to highlight or select data is essential to maximise the use of Analyst.

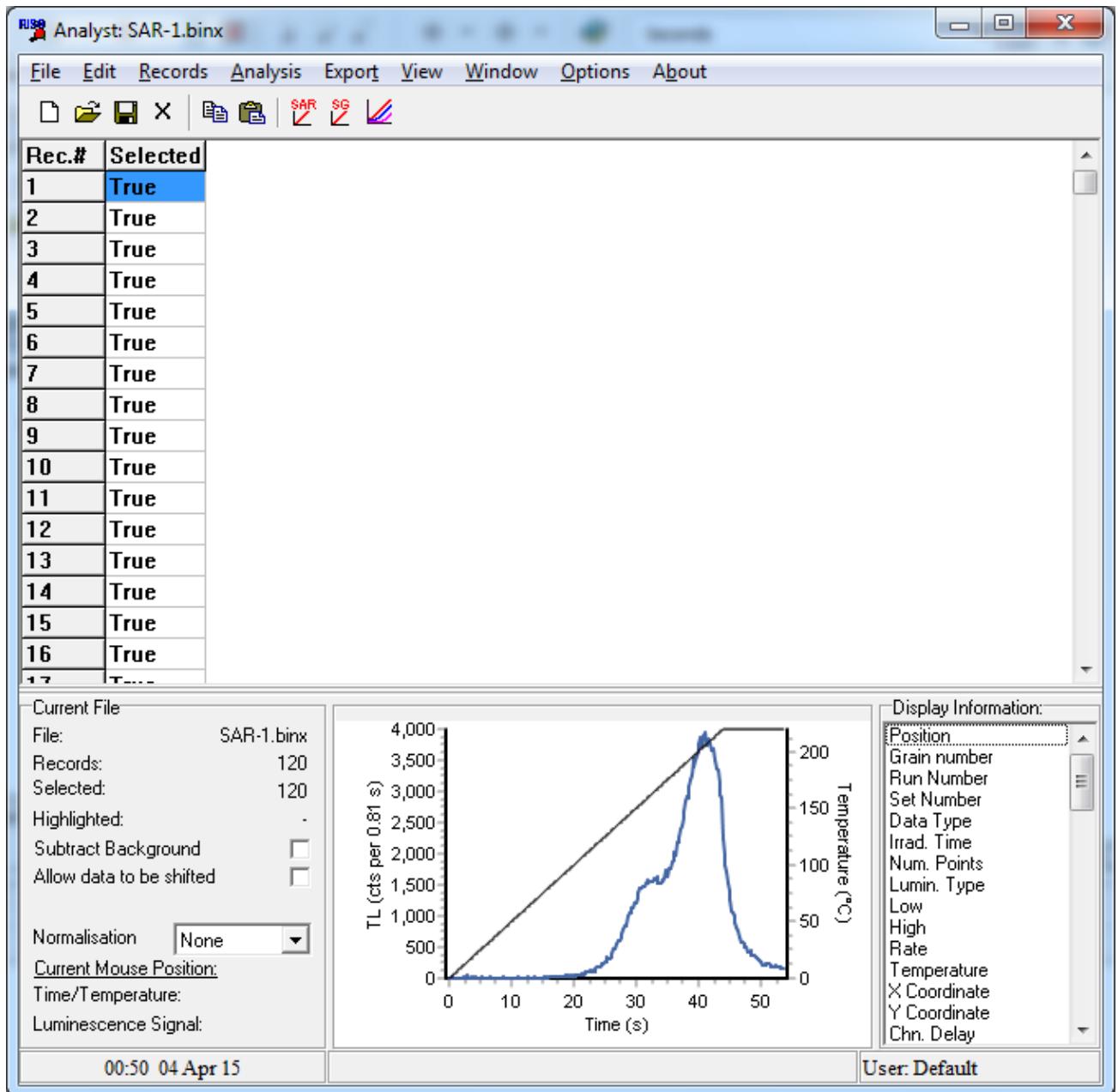


Figure 2.2(a):Initial display in Analyst when a file is opened.

Highlighting Data

Within the list of records in the main part of the display you can highlight one or more records. This is done using the mouse and the key pad in a standard Windows manner. You can select a single record by clicking in the main display area. Whichever record you select is highlighted by Windows and a graph of the data is displayed at the bottom of the screen. You can also select a group of records by holding the Shift key down and using the cursor keys to move up or down. Highlighting a set of records is useful if you want to undertake a [Block Edit](#) of all those records, or if you want to [copy](#), [move](#), or [delete](#) a group of records from the current BINX file. The number of highlighted records is constantly displayed in the bottom left hand panel of Analyst.

Selecting Data

The main display of what records are present in a BINX file always displays whether each record has been selected or not (this is shown as 'True' or 'False' in the second column of the main display). This is stored permanently in the BINX file structure. You can select or unselect records in a number of ways. The first is using keystrokes. Pressing the 'Insert' key will select the record

that is currently highlighted, and automatically move on to the next record. Pressing the ‘Delete’ key will unselect the record that is currently highlighted and move on to the next record. As you select or unselect records the number of records in the current BINX file that have been selected is displayed in the bottom left hand panel of Analyst.

The second way of selecting and unselecting data is from the main menu. If you choose **Records** from the main menu and then ‘[Select All...](#)’ you can choose to select ‘Every record’ in the current BINX file, to select just those records that you have currently got highlighted, or you can use ‘Records of type...’ to choose to select records depending upon a number of parameters. For instance, you may want to select all the IRSL data in your file. To do this, select Luminescence type from the first selection box (Figure 2.2(b)) and then type ‘IRSL’ into the last box. ‘[Unselect All...](#)’ works in the same manner.

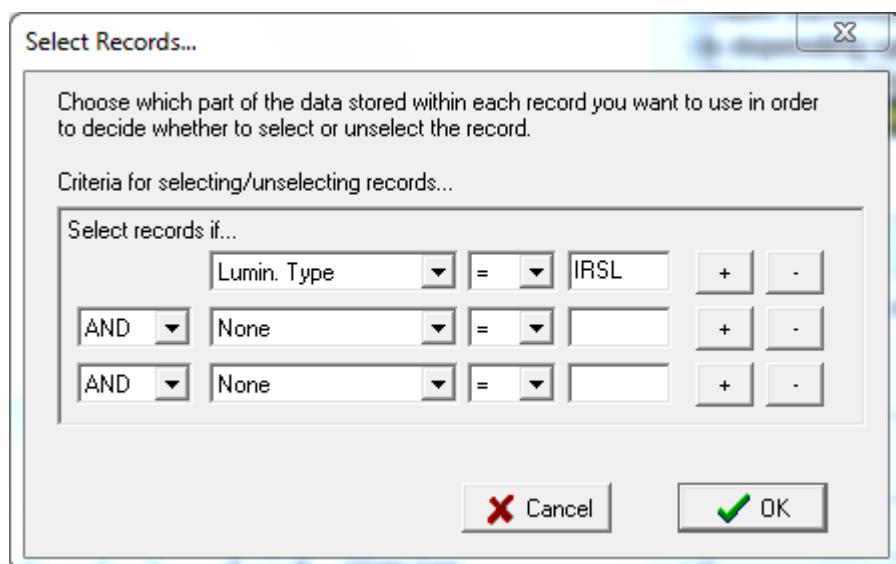


Figure 2.2(b): Selecting all records in the BINX file which were IRSL measurements.

You can undertake more complex decisions about which records you want to select by using multiple conditions. For instance, you may wish to select all the OSL records that were measured for samples in positions 2 to 4. This could be achieved using the combination of multiple criteria shown in Figure 2.2(c).

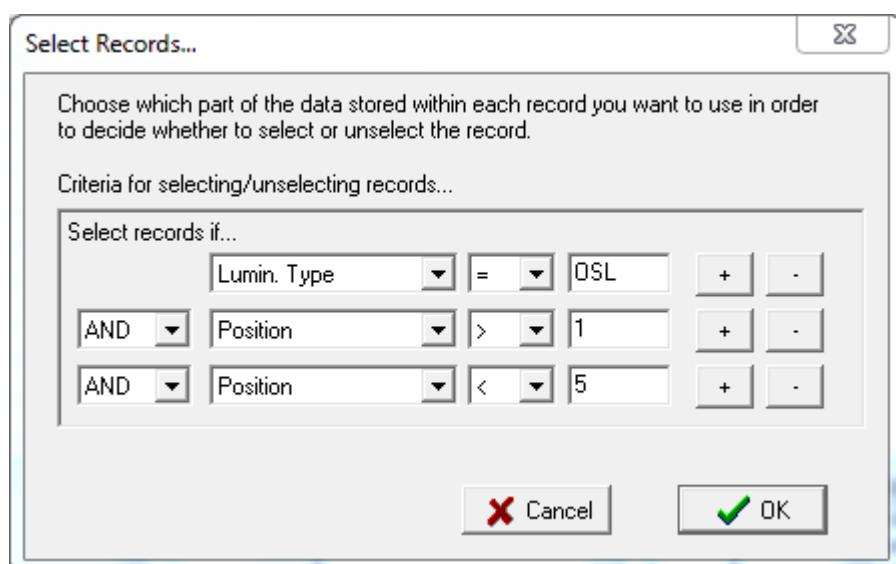


Figure 2.2(c): Using multiple criteria to select records in the BINX file

In this case, because the term 'AND' has been used between each criteria, all three criteria have to be met for a record to be selected. Alternatively the term 'OR' can be used if either criteria can be met for a record to be selected. If a larger number of criteria are needed, then any number can be added by clicking on the '+' symbol. Criteria can be removed by clicking the '-' symbol.

You can also select records when looking at your file using [Sequence View](#) which shows the sequence used to collect the BINX file.

2.3 Front Panel Controls

The front display of Analyst gives you a range of controls on how the data in the current BINX file is analysed. These are all displayed in the bottom left of the screen, and include the ability to subtract a background value of each record individually, to shift the data describing a record along the X axis (either to shift the temperature or time axes), and the ability to apply one of three normalisation values.

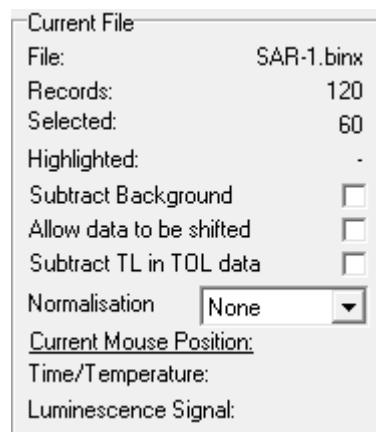


Figure 2.3(a): Front panel controls visible in Analyst

Background Subtraction

In almost all luminescence measurements there is some background component to the signal. This may be a dark count from the photomultiplier tube, breakthrough of the optical stimulation source, or some other source of background. One of the items of data stored as part of each data record in the BINX file is a background value. This is set to a value of zero by the Sequence Editor when it generates a BINX file, but you can input any value that you want (see [Edit Current Record](#)). This value may be the same for a whole suite of measurements (if you are simply subtracting the dark count of the photomultiplier tube), or it may be a different value for each record. The value that is entered into the data structure for record is the numerical value to subtract per channel.

By default Analyst does not take account of the background value. If you want this to be subtracted from the data then you must tick the box on the bottom left of the front display screen.

Shifting data

A second parameter that is included in the BINX file for each record is called 'Shift'. By default this is set to zero by the Sequence Editor. This is the number of channels that you want to translate the data along the X-axis during analysis. If the value is positive then the data are shifted to higher temperatures or times along the X-axis.

The main use for this type of editing of the data is if you are making TL measurements and they have been affected by thermal lag between the hotplate and the sample. This may occur if you have poor thermal conductivity between the heater plate and the sample disc, or between the sample disc and the grains of sample. In this case you may want to shift the data in order to align certain TL peaks.

By default, Analyst will not shift your data along the X-axis even if you have entered a value for the shift (see [Edit Current Record](#)). If you want Analyst to shift your data then you must tick the box marked 'Allow data to be shifted'.

Please note that this is a procedure that is controversial. Some practitioners are very adamant that data should never be shifted along the x-axis. Just because it is possible to do it in this program does not mean that it is necessarily endorsed.

Subtract TL in TOL data

One type of measurement possible with the Risø TL/OSL reader is TOL - thermo optical luminescence (shown in [Duller and Wintle 1991](#), Fig 1). This is where a sample is heated at a continuous rate (as would normally occur in TL measurements) and an optical stimulation source is periodically switched on for a short period of time. This provides a means of rapidly assessing the way in which the magnitude of an OSL signal varies with sample temperature. The signal measured whilst the optical stimulation is active will be a sum of the TL signal and any OSL signal. This option on the front page selects whether the graphs in Analyst should show the raw data (the box is unchecked) or if the TL component should be removed from the OSL measurements (box is checked). The signal subtracted during optical stimulation is based on the TL signals measured in the channel prior to optical stimulation and the channel after optical stimulation. If more than one channel of optical stimulation is used then the estimated TL intensity is interpolated.

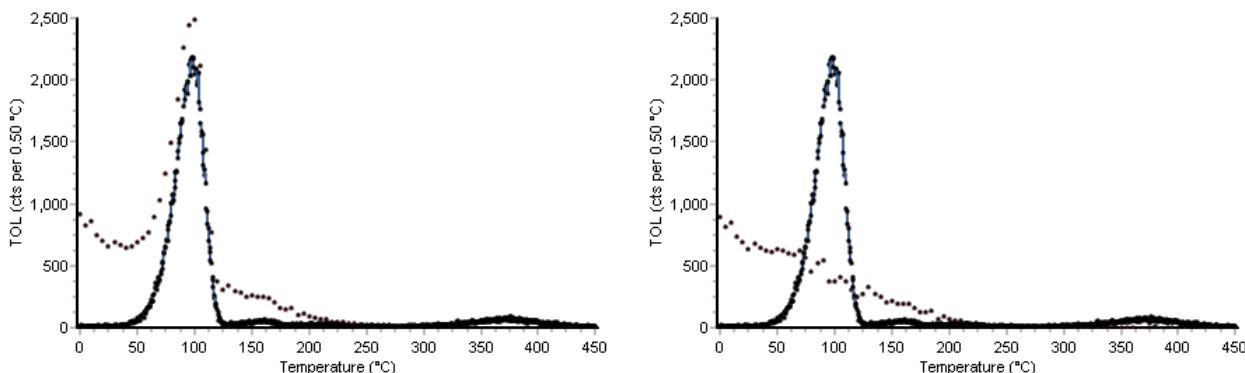


Figure 2.3(b): TOL data for an aliquot of quartz, without any TL subtraction (left), and with TL subtraction (right). The OSL signal (shown in brown) decreases monotonically after subtraction.

Normalisation

If you are attempting to compare two or more aliquots of a sample, you will often want to normalise the results in order to compensate for differences that are inherent to the sub-samples. For instance, you may have made 4 aliquots of a sample, but the mass of sample on each aliquot is very different (1.0, 1.5, 1.2, 2.0 mg). In this case you would not expect the OSL, or TL, signal from each aliquot to be the same. In fact you would expect that, all other things being equal, you would get twice as much signal from the fourth aliquot as you would from the first (since the mass is twice as much). To compensate for such differences you can enter a normalisation value for each aliquot. In this case we may enter the weights of the aliquots. When you display the data for these aliquots you will want to compensate for these differences.

You can store up to three normalisation values for a given record (you may derive one normalisation value from the mass of the sample, one from a short initial OSL measurement prior to any other measurements, and one from the response of the aliquot to a standard irradiation) in the parameters Norm1, Norm2 and Norm3. These can all be set using the [Edit Record](#) or [Block Edit](#) commands. By default Analyst does not perform any normalisation on your data, and the display box on the bottom left of the main panel is set to 'Normalisation: None'. To use one of the three normalisation values, change this display to 'Normalisation: Norm2', or whichever set of normalisation values you want to use. Analyst performs the normalisation by calculating the

average value of the normalisation figures for every record in the current BINX file that has been [selected for analysis](#). The data for any specific record is then scaled by the ratio of this average normalisation value divided by the normalisation value for the current record.

NB: If you have not selected any records for analysis then no average normalisation figure will be calculated, and the data for each record will be set to zero.

2.4 Calculating Integrals

In the bottom right hand corner, the list of parameters in the BINX file additionally shows 4 items called 'Integral 1', 'Integral 2', 'Integral 3' and 'Integral 4' (Figure 2.4(a)). These are for the user to use in any way they see fit. The idea is that one often wants to calculate the signal over a fixed integral for a single record, or a number of records.

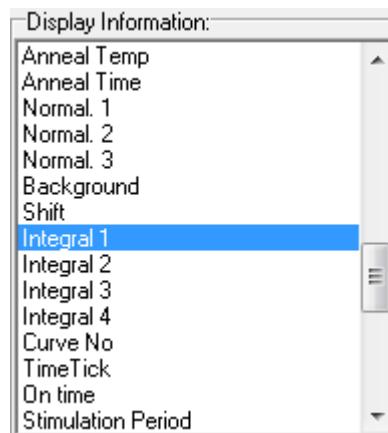


Figure 2.4(a): List of information stored in each record in a BINX file that can be displayed on the Analyst main screen

When you click on one of these integrals, a box pops up asking you to specify the channels that you want to integrate over. Note that the integration is defined by CHANNEL number, not by time (in the case of OSL) or temperature (in the case of TL). Furthermore there is no error checking in this section, so you may specify channels 1 to 2000 when only 250 channels of data were collected! In this instance the integral will be returned as zero.

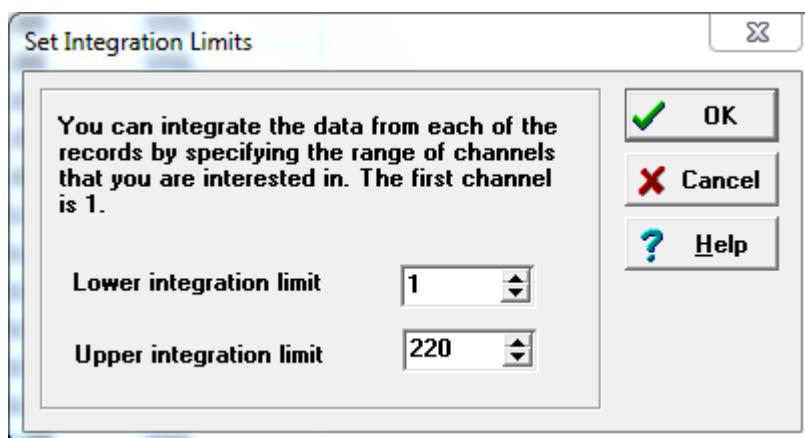


Figure 2.4(b): Window asking the user to specify the channels to integrate

Calculating integrals in this way can be useful for a variety of reasons, but one example would be to obtain normalisation values. For instance, you may want to compare the shape of a set of OSL decay curves that have different intensities. One approach would be to normalise each OSL curve to the intensity of the first channel. To achieve this you would use Integral 1 to calculate the signal in channel 1 (Lower integration limit = 1, Upper integration limit = 1). You would then highlight the

data for the records you want to normalise, select to [copy the data](#), and [paste](#) these values into one of the Normalisation columns.

Rec.#	Selected	Position	Set Number	Irrad. Time	Lumin. Type	Normal. 1	Integral 1
1	False	1	2	0.00	TL	0	6
2	False	2	2	0.00	TL	0	12
3	False	3	2	0.00	TL	0	6
4	False	4	2	0.00	TL	0	8
5	False	5	2	0.00	TL	0	1
6	True	1	3	0.00	OSL	0	727765
7	True	2	3	0.00	OSL	0	959894
8	True	3	3	0.00	OSL	0	1139737
9	True	4	3	0.00	OSL	0	861526
10	True	5	3	0.00	OSL	0	797959
11	False	1	6	10.00	TL	0	137
12	False	2	6	10.00	TL	0	795
13	False	3	6	10.00	TL	0	561
14	False	4	6	10.00	TL	0	765
15	False	5	6	10.00	TL	0	691
16	True	1	7	10.00	OSL	0	164678
17	True	2	7	10.00	OSL	0	222318
18	True	3	7	10.00	OSL	0	272037

Figure 2.4(c): Highlight the data that you want to use for mormalisation and Copy this to the clipboard

Rec.#	Selected	Position	Set Number	Irrad. Time	Lumin. Type	Normal. 1	Integral 1
1	False	1	2	0.00	TL	0	6
2	False	2	2	0.00	TL	0	12
3	False	3	2	0.00	TL	0	6
4	False	4	2	0.00	TL	0	8
5	False	5	2	0.00	TL	0	1
6	True	1	3	0.00	OSL	727765	727765
7	True	2	3	0.00	OSL	959894	959894
8	True	3	3	0.00	OSL	1139737	1139737
9	True	4	3	0.00	OSL	861526	861526
10	True	5	3	0.00	OSL	797959	797959
11	False	1	6	10.00	TL	0	137
12	False	2	6	10.00	TL	0	795
13	False	3	6	10.00	TL	0	561
14	False	4	6	10.00	TL	0	765
15	False	5	6	10.00	TL	0	691
16	True	1	7	10.00	OSL	0	164678
17	True	2	7	10.00	OSL	0	222318
18	True	3	7	10.00	OSL	0	272037

Figure 2.4(d): Paste the data into one of the columns for Normalisation values (in this case Norm1).

You then ensure that this normalisation value will be used by selecting Norm1 for Normalisation in the bottom left hand panel of Analyst.

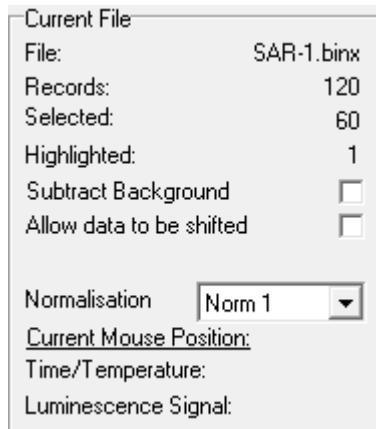


Figure 2.4(e): Front panel display (bottom left hand fo screen), showing 60 records selected from a total of 120 records

You can then plot the normalised OSL decay curves for all five aliquots using [Plot Multiple Data](#) (Figure 2.4(f)). The initial channel of all five aliquots will be identical after this normalisation and you can then visually compare the shape of the rest of the decay curve.

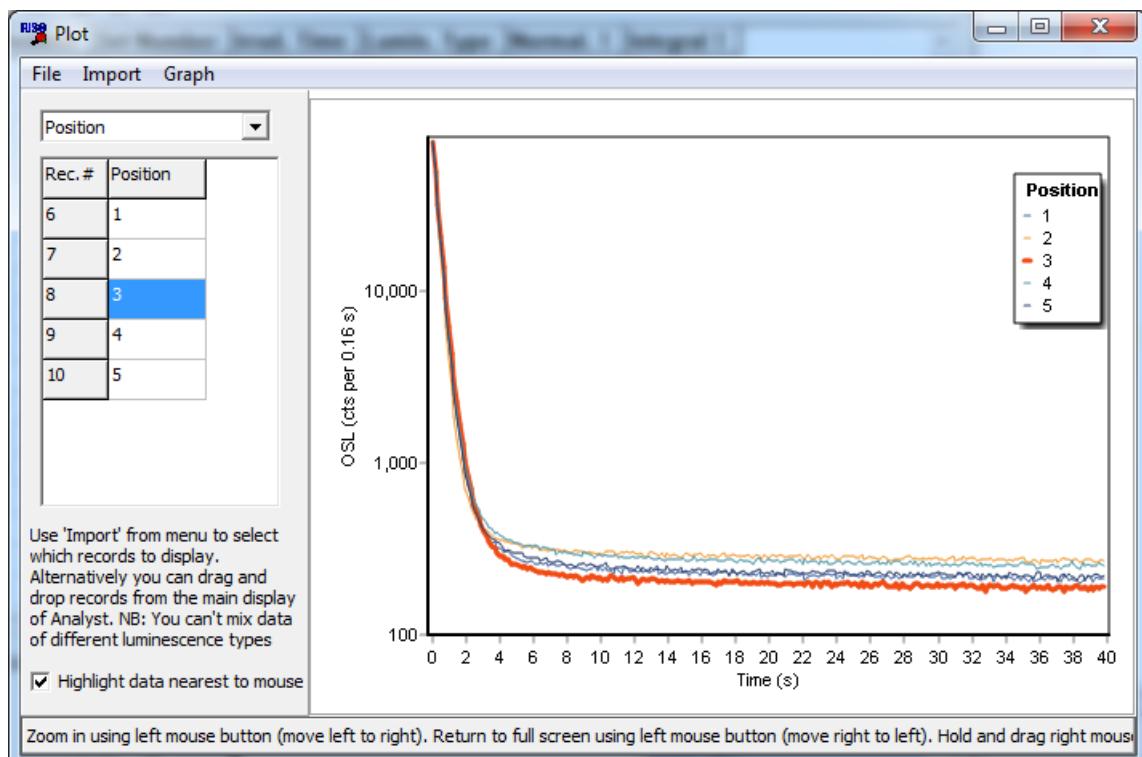


Figure 2.4(f): Graph showing 5 OSL decay curves

2.5 Graphs in Analyst

Graphs in Analyst are designed to offer a range of options to help the user explore their data, either visually, or by extracting data to analyse in other packages.

Scrolling and Zooming Graphs

You can **scroll** any graph by moving the mouse whilst holding the **right hand mouse button** down. You can **zoom** in to any part of the graph by clicking with the **left hand mouse button** and dragging to the **right** to define a region that you want to zoom into. When you release the left mouse button the graph will zoom into the region that you have just defined. To return to the original display, clicking with the left hand mouse button and drag it to the **left**.

Copying Data and Images from Graphs, and Editing Graphs

Almost all graphs in Analyst offer the ability to alter the way in which they appear. Clicking the right hand mouse button whilst over any graph will bring up a pop-up menu offering a number of options (Figure 2.5(a)). The number of options available may vary from one part of Analyst to another.

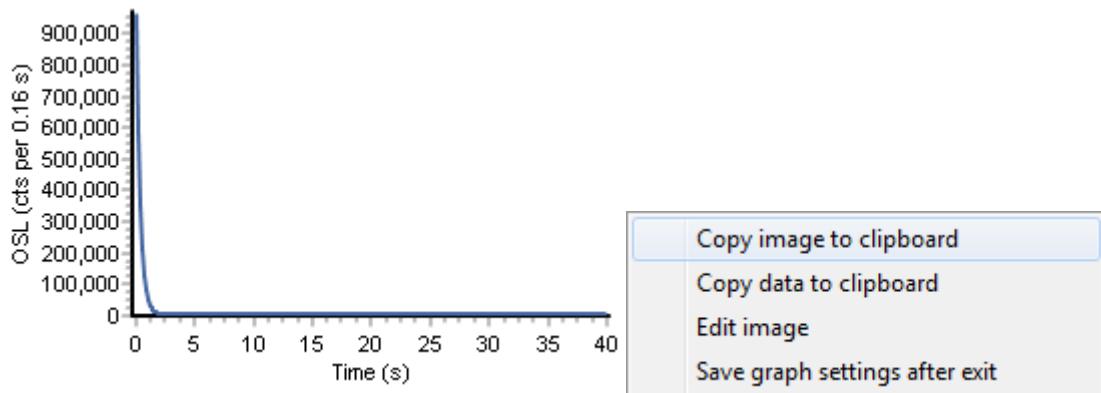


Figure 2.5(a): A typical graph in Analyst along with the popup menu that appears when you click on the right mouse button whilst over the graph

Copy Image to Clipboard

This option will copy the graph as it currently appears to the Windows clipboard. This image is then available to be pasted into other documents.

Copy Data to clipboard

This option will copy the data used to draw the current graph to the clipboard. The data is then available to be pasted into Excel or any other package capable of accepting numerical data in columns.

Edit Image

This option opens a new dialogue box that provides a very wide range of options for controlling the appearance of the graph (Figure 2.5(b)). A common change that users may wish to make is the way in which the axes are plotted. Each axis has a wide number of aspects which can be altered. In the figure below I have set the left hand axis (y-axis) to be logarithmic.

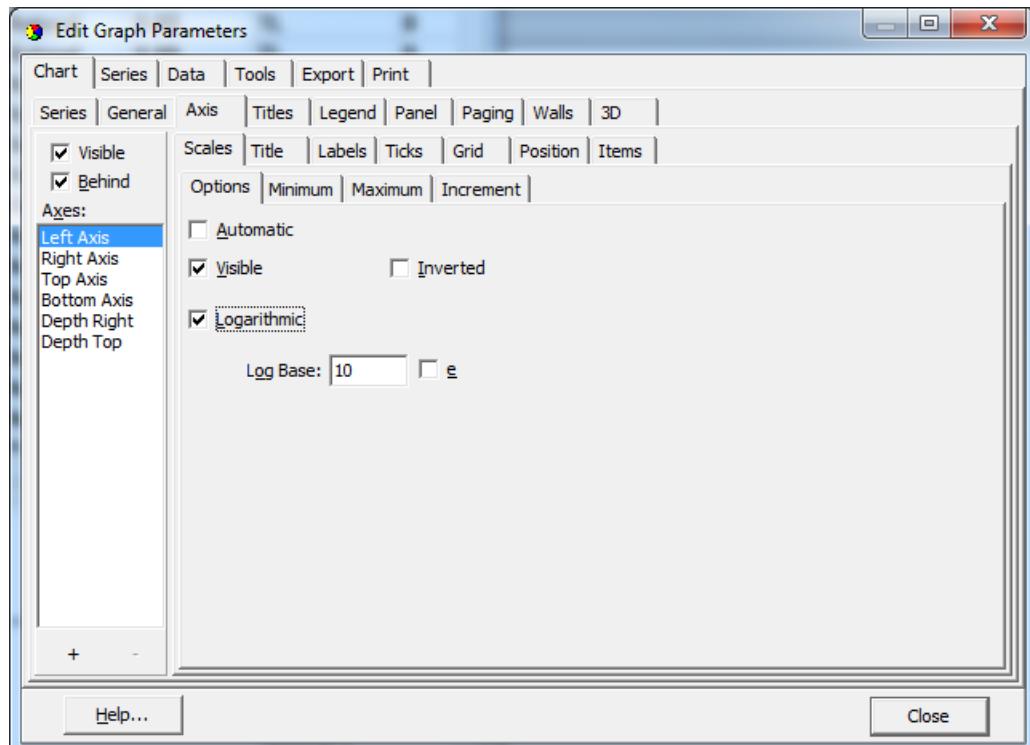


Figure 2.5(b): The Edit Graph option on the popup menu associated with graphs brings up a dialogue box containing a very wide range of options for controlling the appearance of the graph

There are a huge range of other parameters than can be altered (e.g. font size for labels, text to be used for axis labels, whether to show a grid on the graph, to give a title to the graph etc etc).

Note that unless you tick the option to 'Save graph settings after exit' any changes that you make will disappear when you close Analyst. Additionally, some parameters (such as the labels for the axes (e.g. "OSL (cts per 0.16 s)") are automatically set by Analyst every time it displays a new record, and thus changes that you make to that parameter will not be preserved. However, aspects such as the font size and colour will be preserved.

[Save graph settings after exit](#)

Any changes that you make to the appearance of a graph in Analyst will normally be lost when you exit the Window. However, if you wish to retain the settings for use next time you open Analyst then you can tick the option "Save graph settings after exit". This will save the settings and will automatically apply them next time you open Analyst. If you uncheck this menu option then the graph settings will not be saved, and when you next restart Analyst the default graph settings will be applied.

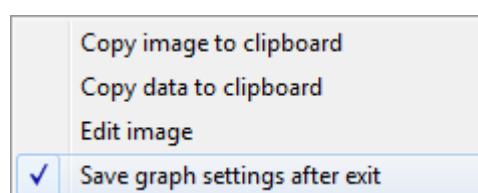


Figure 2.5(c): Popup menu associated with graphs in Analyst illustrating how it is possible to select to 'Save graph settings after exit'. Note that this option is not available on all graphs in Analyst.

3. File Menu

The File menu allows the user to create, open and save BINX (or BIN) data files for Analyst. Keyboard shortcuts and speed buttons are available for the most commonly used actions (New, Open, Save and Exit).

Note that most of the main menu items (e.g. Edit, Records etc) are not available until a BINX file is opened

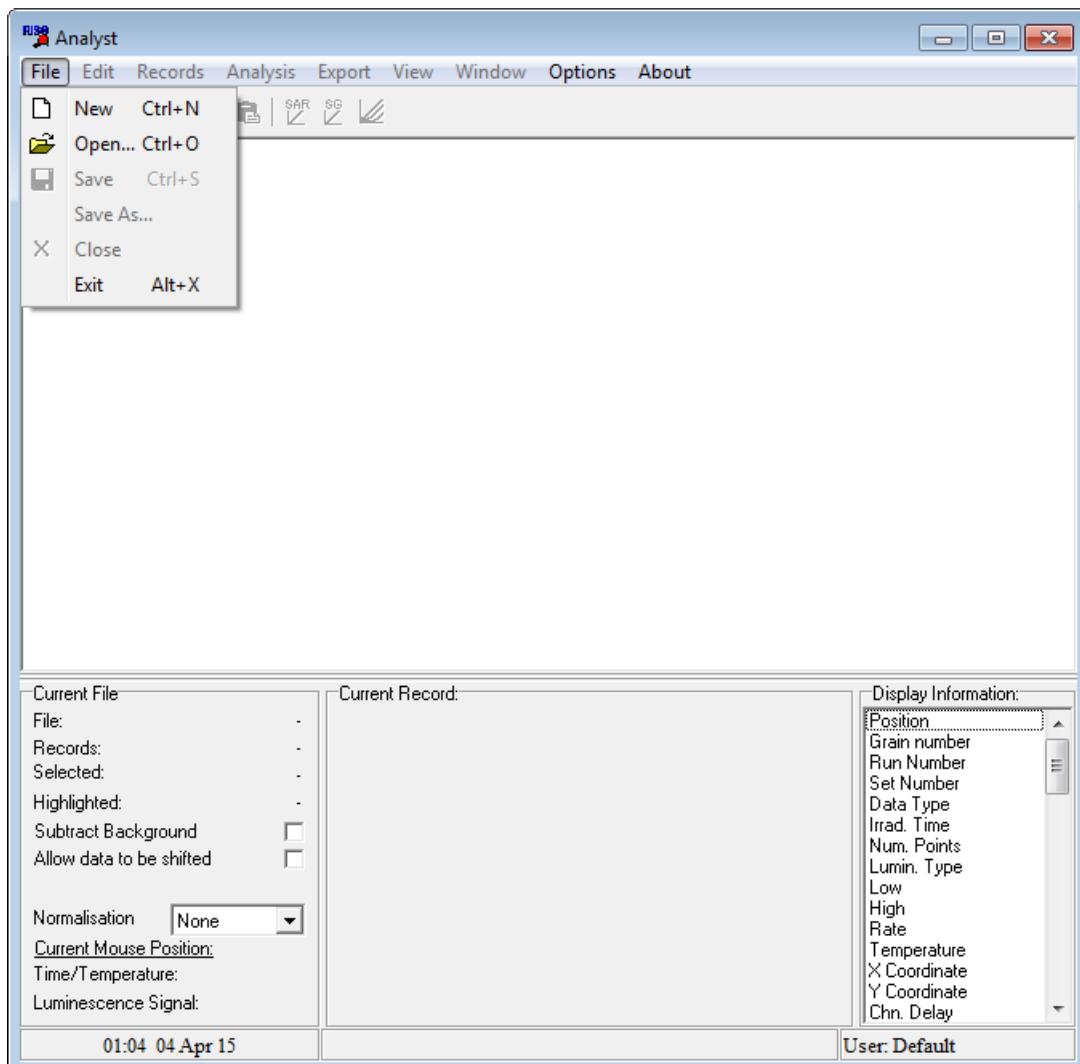


Figure 3(a): File menu in Analyst

3.1 New

It is unlikely that you will need to create a new BINX file since you will normally be working on data collected from the reader. However, sometimes you may wish to create a new BINX file so that you can [copy records](#) into it from other BINX files. The new BINX file will be given the default name 'NoName01.BINX'. You can have a maximum of 4 BINX files open at a time and can transfer records from one file to another using the '[Copy Highlighted Records](#)' command in the [Records](#) menu.

3.2 Open

Open an existing BINX or BIN file and display it. You can have a maximum of 4 BINX files open at any time and can switch between them using the [Window](#) menu.

3.3 Save

Save the current BINX file with its existing name, incorporating any changes that have been.

3.4 Save As

Save the current BINX file to a different file name or directory.

3.5 Close

Close the current BINX file. If the file has been edited since it was opened or since it was last saved then you will be asked whether you want to save the file before closing it. If you choose not to save the file then any changes are lost.

3.6 Exit

Close Analyst. If any BINX files are open then each is closed in turn, and if they have been modified then you will be asked whether you want to save them.

4. Edit Menu

The Edit menu contains a range of commands that allow you to copy and paste numerical data from the main display of Analyst either to another part of the Analyst display screen, or to another package within Windows (for instance a spreadsheet package). This facility makes it possible to undertake a range simple operations including [normalisation](#).

4.1 Copy

For any numeric variable in the records that are displayed within Analyst you can copy and paste from one set of records to another. For instance, suppose that you want to use the results of one set of OSL measurements as normalising factors for a second set of measurements on the same discs later in the sequence. To do this, you would ensure that the normalisation factor that you want to place the results in is visible on the screen (click on the ‘Display Information’ list to make sure it is there) and then integrate the OSL signal in the first set of measurements (say records 6-10) using the Integral option from the ‘Display Information’ list in the bottom right of the screen. This will create a column of data so that you can then select using the mouse or keyboard and then do ‘Copy Selection’. You can now select the area of the normalisation column where you want to paste the data to (say records 26-30), and use ‘Paste Selection’. If the two data sets are compatible then the data will be pasted into the appropriate records and the display updated. If the data is not compatible then no change will be made to the BINX file.

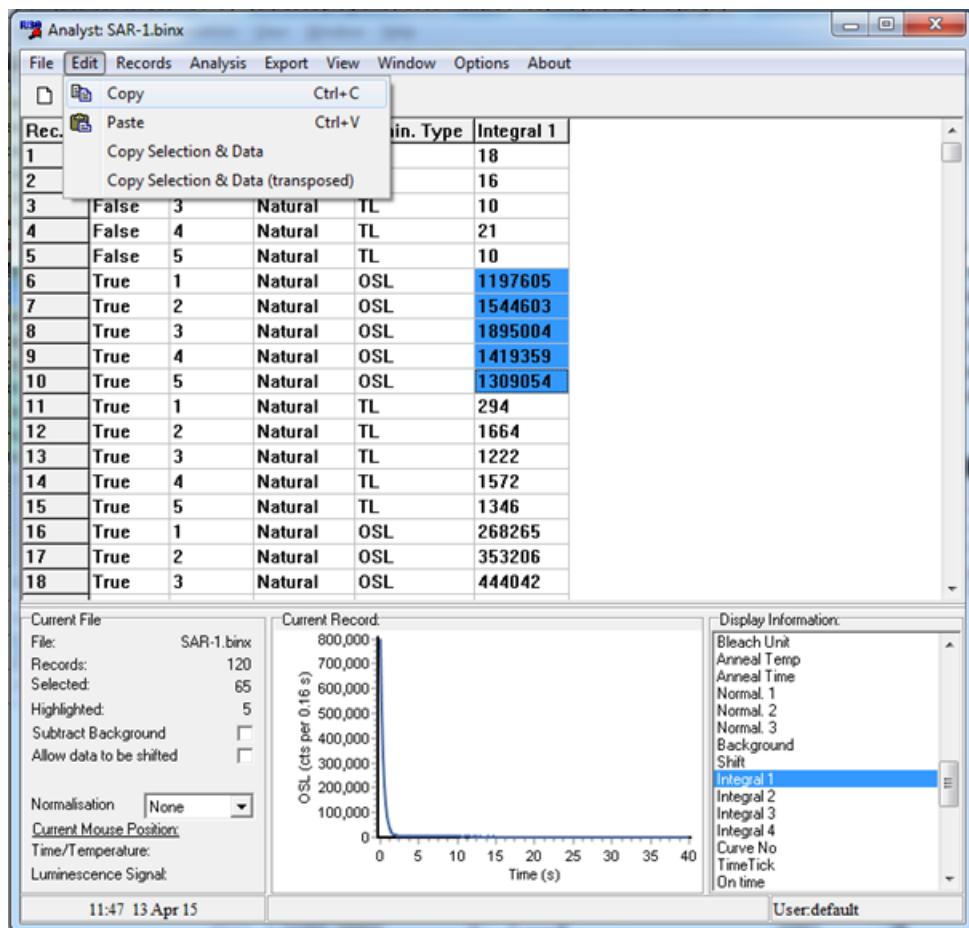


Figure 4.1(a): Selecting a column of data to copy

In addition, you can use the cut (and paste) operations to transfer data to and from other Windows applications such as the spreadsheet Excel. This makes it relatively easy to export data in a variety of forms.

4.2 Paste

See section on [copying a selection](#).

4.3 Copy Selection & Data

Utilising this option, you can copy the data that has been highlighted onto the Windows clipboard. This is the same as '[Copy selection](#)'. However, with 'Copy selection & Data' all of the data channels in the luminescence data are copied to the clipboard as well. This provides a short cut method of exporting data and an alternative to that described in [Current Data Display](#).

4.4 Copy Selection & Data (transposed)

This is identical to '[Copy selection & Data](#)' except that the data frame is transposed into columns instead of rows.

5. Records Menu

This menu offers a range of tools that allow you to manipulate whole records with a BINX file. Each TL, OSL, POSL etc measurement is a single record within a BINX file. You may wish to edit the parameters describing each record, or to copy records from one BINX file to another one.

5.1 Select

Selecting and unselecting records is a vital part of processing your data. Using ‘Select All...’ and ‘Unselect All...’ you can choose which records you want selected and which not. There are three sub-menu options – (a) You can choose to select **all the highlighted records**, (b) **every record** in the current BINX file, or (c) just those **records of a certain type**. This last option is the most flexible, and is particularly useful if you want to undertake analysis of a complex data file. You can use any of the parameters listed in the BINX file (see [Appendix A](#)) to filter which records you wish to select.

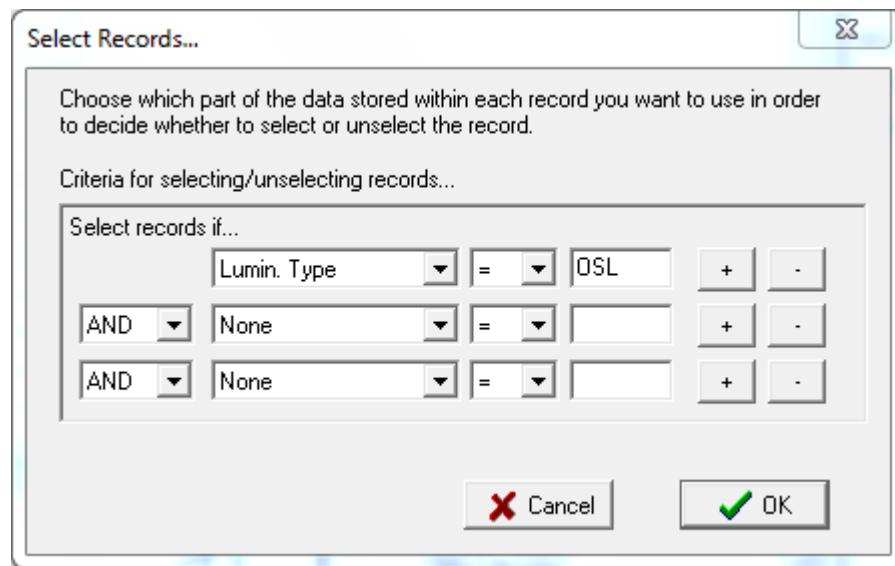


Figure 5.1(a): Selecting records based on the value of a specific variable within each record. In this case those records where the luminescence type is OSL will be selected.

A simple case is shown above where one wants to restrict analysis to the OSL data collected in the sequence. Another situation where this facility is useful is if you have undertaken a sequence with lots of regeneration doses, but you want to look at the dose response curve from a subset of these measurements. Another example is where you have used the post-IR IRSL method and have multiple IRSL measurements. Using the Select Records option you can select only those records that were IRSL measurements made at an elevated temperature. This can be done by using the Light Source or the Lumin. Type attributes of the records and the Set Number, or perhaps the Sample Temp attribute that records the temperature of the aliquot when the luminescence measurement was made.

Note that you can also use the ‘Insert’ key in the main display to select individual records. Simply move the cursor to the record that you want to select and then press the ‘Insert’ key on the keyboard.

5.2 Unselect

You can choose whether to unselect every record in the current BINX file, the records you have currently highlighted, or those of a specific type. See section on '[Select All](#)' for details. You can also use the ‘Delete’ key in the main display.

5.3 Edit Current Record

You can display all aspects of a record in the main display by [selecting](#) each item in the list in the bottom right hand panel of Analyst. You can also alter some parameters of the BINX header in this main display; those which are simple numeric values can be changed in the main display (e.g. irradiation time). However more complex parameters (e.g. Luminescence Type) can only be changed using 'Edit Current Record' to edit an individual record, or the [block edit](#) command for many records at the same time. The simplest way is using the 'Edit Current Record' command. This can be accessed either from the Records menu, or by pressing 'F2'. This will display a summary of all the information held in the BIN file about the record that is currently highlighted (Figure 5.3(a)).

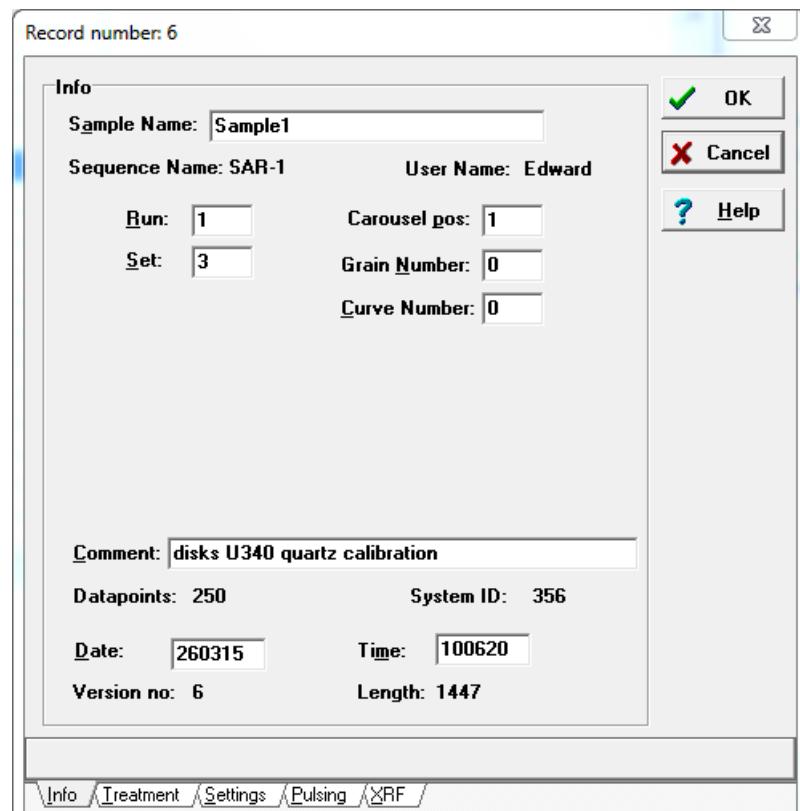


Figure 5.3(a): Display of record information obtained by pressing 'F2' on the main display, or clicking 'Edit Current Record' from the 'Records' menu

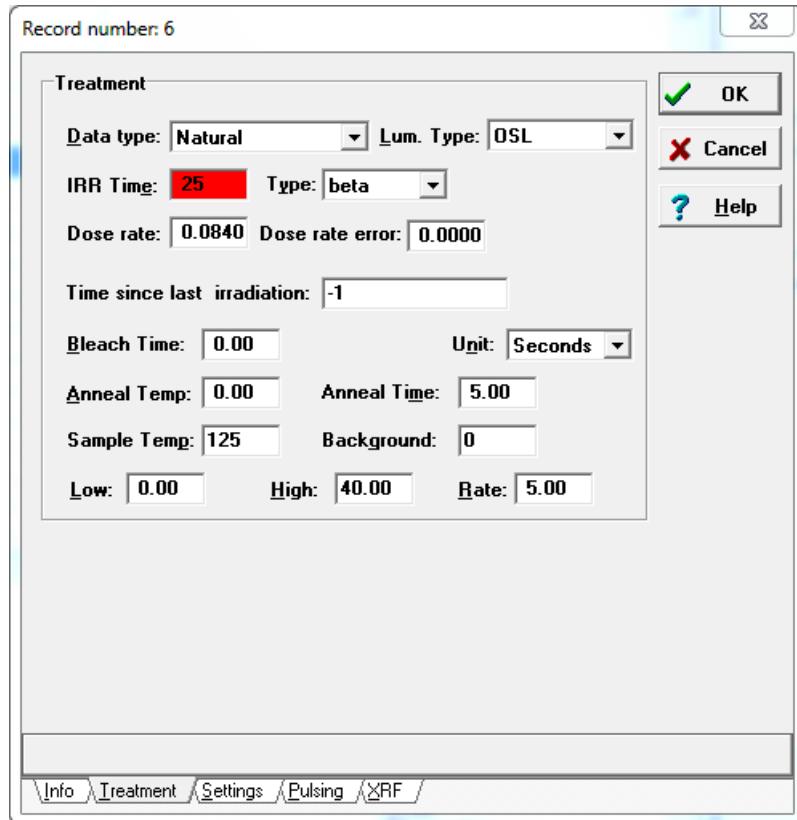


Figure 5.3(b): Record display while editing the irradiation time

This display is split into up to five sections, labelled 'Info', 'Treatment', 'Settings', 'Pulsing' and 'XRF' (NB: if you open older BINX files in Analyst then some of these pages may not be visible). You can switch between these different displays using the tabs at the bottom of the box. Most of the parameters may be edited, though there are some, such as the length of the record and the number of data points, which cannot be altered for obvious reasons. If you alter any of the parameters, the background to that entry will turn red indicating that a change has been made (see above). You can make as many changes as you like before pressing 'OK' to accept those changes. If you change your mind and do not want to save these changes then press 'Cancel'.

5.4 Block Edit

It is possible to edit the information associated with an individual record using [Edit Current Record](#). However you will often want to alter a particular parameter in many records. It is tedious to change each record in turn, so an alternative method is to use the Block Edit facility. This operates in the same way as the Edit Current Record command, except that whatever changes you make will be applied to all of the records that are currently [highlighted](#).

For instance, using the SAR-1.BINX file that was supplied with this program, you may want to make the comment parameter indicate where this file came from. In order to change the comment field of every record, highlight all the records in the file. You can highlight all the records either by starting from the first record and then pressing Page Down on your keyboard while holding down the shift key until all the records have been selected, or using the [Highlight All Records](#) command. Now select the Block Edit command from the Edit menu. This will display in the same format as for the Edit Record command, but instead of being for a single record this is a summary of all the records currently selected - in this case 120 records (see Figure 5.4(a)).

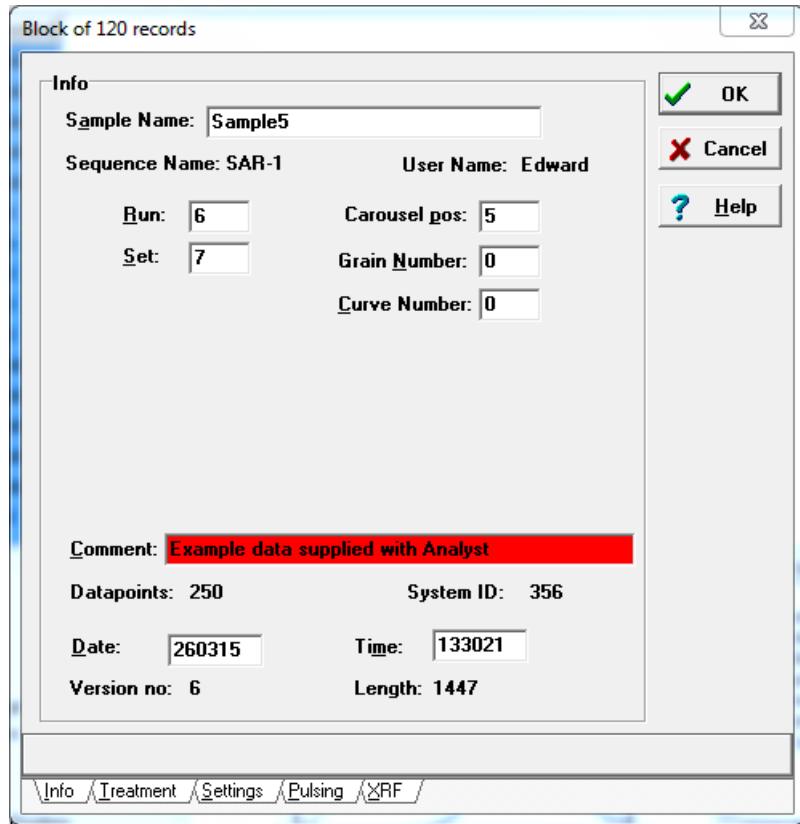


Figure 5.4(a): Block edit of the comment field

When you press 'OK' you will be asked to confirm that you want to alter all the highlighted records. The Block Edit command will only alter those parts of the records that you have edited - the ones marked with a red background. Any other aspects of the records will be left unaltered.

5.5 Highlight All Records

This command provides a useful shortcut to highlight all the records in the current BINX file. This can be useful if one wishes to make changes to all the records in a file using the [Block Edit](#) command. Alternative ways of highlighting records are described in the section on [Selecting and Highlighting records](#).

5.6 Copy Highlighted Records

You may often want to move records from one file to another. For instance, you may have made an initial set of measurements in one run on the TL/OSL reader, and a second set of measurements later. You can combine the data into a single BINX file by moving records from one data file to another using the Copy and Paste commands.

In order to copy one or more records you should have opened both the BINX file from which you want to copy records and the BINX file to which you want to copy them. Once this is done [highlight the records](#) and then select Copy Highlighted Records. Analyst will then copy these records to the clipboard (Note that the records are just copied, and not deleted from the source file). You can now switch to the BINX file that you want to copy the records to (using the [Window menu](#)), and then select [Paste Records](#). This will add the records on to the end of this BINX data file.

5.7 Paste Records

See [Copy Highlighted Records](#).

5.8 Delete Highlighted Records

You may at times want to remove a set of records from a BINX file. In order to do this simply [highlight the records](#) and select Delete Highlighted Records.

Note that once you have deleted records you cannot undo the operation.

5.9 Move Highlighted Records

Because some analyses within Analyst depend upon the order in which records appear in a BINX file, you may want to move a block of records from one position in a BINX file to another. Highlight the records that you wish to move, and then select this option. You will then be asked for the record number where you wish to place the records. The records will be put into the BINX file **after** the record number that you specify. For example, if you specify record number 10 then the first record will be pasted in as record number 11, the second as record number 12 etc. The other records in the BINX file will be moved to make space for these records.

5.10 New Record

You can create a new record within your BINX file using this option. You will be asked how many data channels you want in the record (N.B. you will not be able to change this value after you create the record), and you will then be shown the record header information (see [Edit Current Record](#)) allowing you to specify the type of data that this will be, and the various other parameters. After that, you will be shown the numerical data for each channel (see below) allowing you to type in the data.

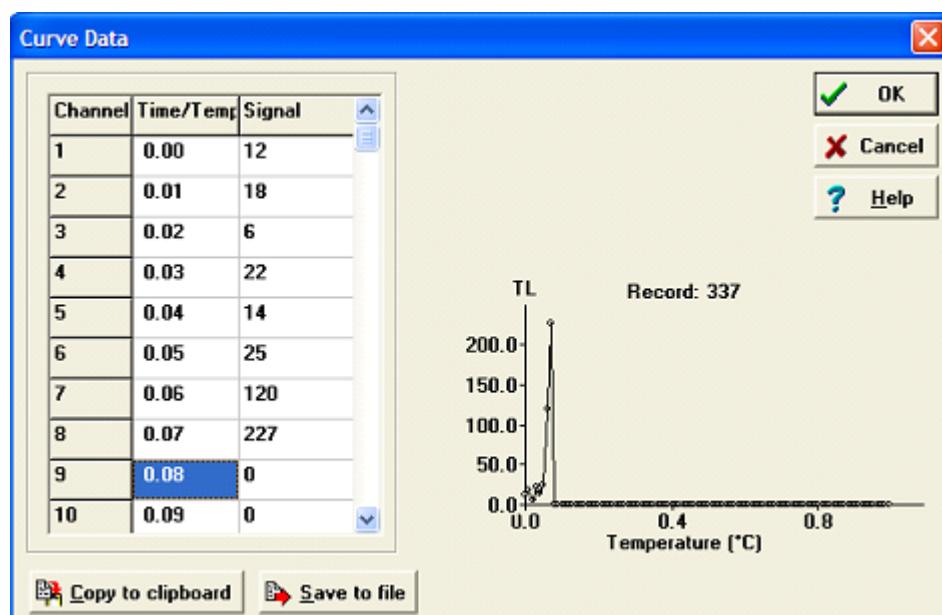


Figure 5.10(a): Typing in data for a new record within a BINX file

6. Analysis Menu

6.1 Multiple Aliquot De

Analyst can calculate an equivalent dose (D_e) from multiple aliquot luminescence data using either regeneration or additive dose procedures. In each case it is important that you set up the BINX file with the information that **Analyst** requires before attempting to calculate an D_e .

The most critical information is the treatment that each aliquot has been given prior to measurement. You must specify the data type (Data Type). For D_e determination the important data types are

- Natural - the natural signal with no dose added, and not bleached.
- Natural+Dose - an aliquot that retains its natural signal and has had laboratory radiation added.
- Bleach - an aliquot that has been bleached in the laboratory to define the residual luminescence level.
- Bleach+Dose - an aliquot that has been bleached in the laboratory and then irradiated in order to increase its luminescence signal.

To calculate a regeneration D_e you need to have one set of measurements that define the ‘Natural’ signal level, and at least two ‘Bleach+Dose’ sets, with different irradiation times. These ‘Bleach +Dose’ sets are used to define the luminescence growth curve, and the D_e is calculated by the intersection of the growth curve with the natural signal level.

To calculate an additive dose D_e you need to have at least two sets defining the growth curve. These may include one set for the ‘Natural’ and one or more sets for the additional doses (Natural +Dose). You can also have one set of residuals (Bleach) which will define the residual level to which the growth curve is extrapolated. If you do not include a residual level then the growth curve is extrapolated to zero luminescence intensity.

In addition to defining the data type (DType) you must also set the irradiation times (Irr_Time) in each record. Setting the bleaching times (Bl_Time) is less important.

Before you finally try to calculate a D_e there is one other important check. This is to make sure that whatever records you want to analyse have been selected (see section [2.2 Selecting and Highlighting records](#)).

See sections [6.1.1 Integral De](#) and [6.1.2 Plateau test](#) for more information about calculating multiple aliquot D_e values.

6.1.1 Integral De

The figure below shows the screen that is displayed when you select to calculate either an additive dose or regeneration D_e . File ‘Additive-1.BIN’ that is supplied with Analyst contains data that is suitable for analysis using the multiple aliquot additive dose procedure. This file has already had the correct data types and irradiation times set.

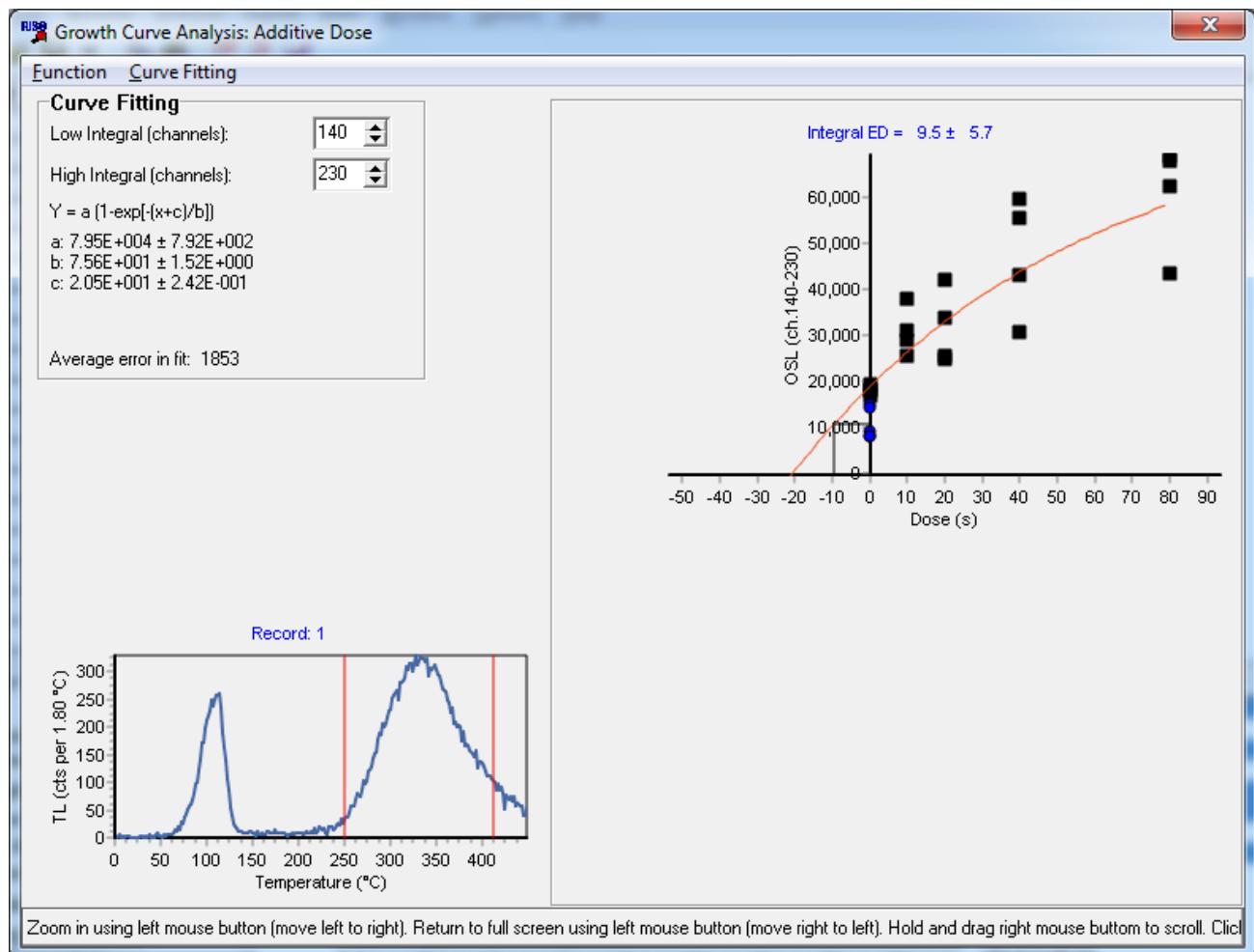


Figure 6.1.1(a): Additive dose growth curve for file Additive-1.BIN

The display shown above has not had any normalisation applied, and hence there is a large scatter between data points. In the sequence, two sets of normalisation factors were obtained, one prior to irradiation, and the second after measurement of the additive dose data set. After selecting to apply the Norm3 normalisation value on the front page of Analyst (see [Section 2.3 Front Panel Controls](#)) the scatter in the data is decreased as shown below.

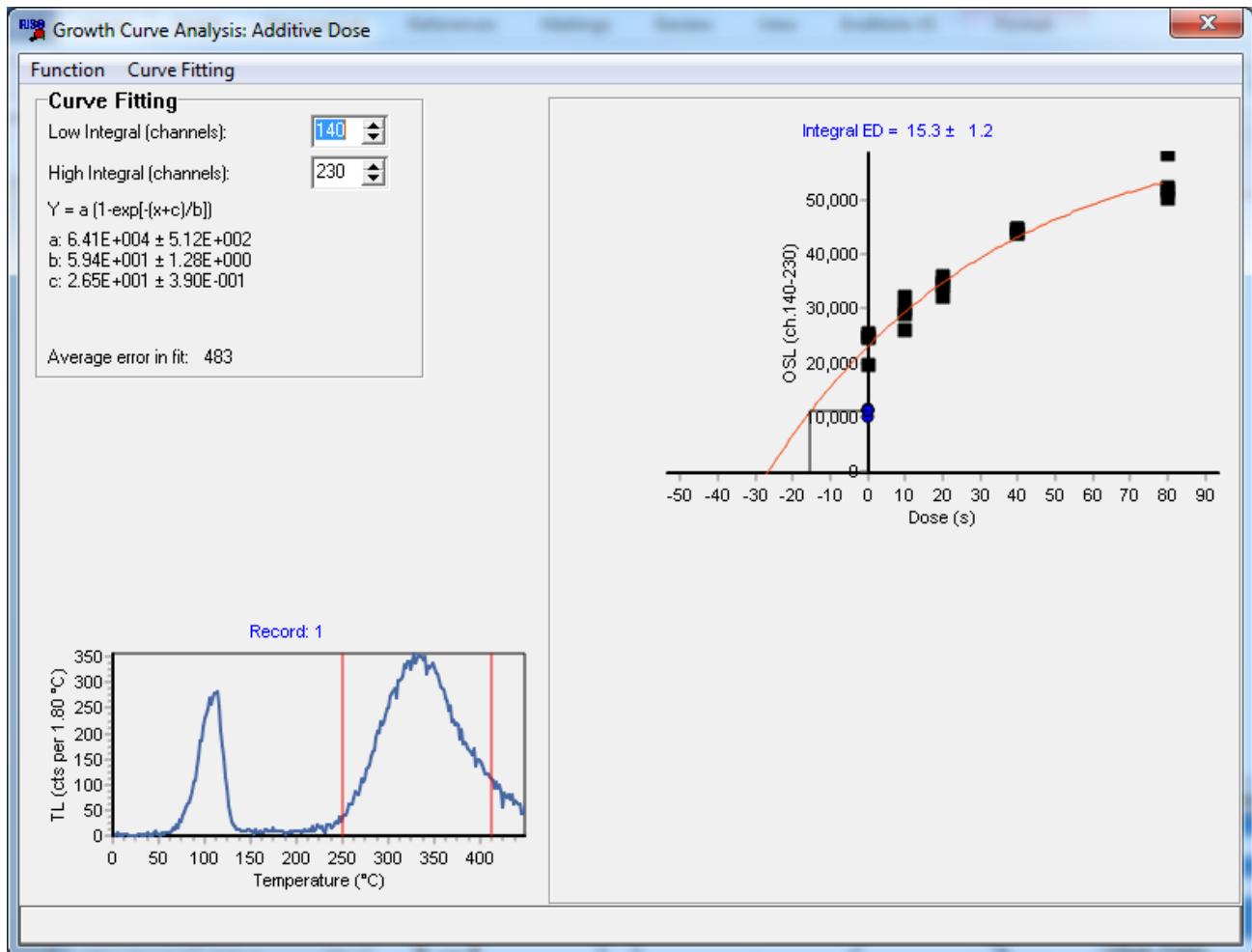


Figure 6.1.1(b): Additive dose growth curve using the same data as above, but with normalisation (Norm3).

The other type of normalisation data that is included with this file (Norm2) was obtained by making a short OSL measurement of each aliquot prior to any dosing or bleaching.

You will also need to select which type of equation you want to fit to the growth curve data. You can select from Linear, Quadratic, Cubic, Exponential, Exponential plus linear, and the sum of two exponentials under the 'Curve Fitting' menu at the top of the screen.

The individual data points are plotted on the growth curve in the upper right of the screen. When the mouse is clicked on a data point the TL glow curve (or OSL decay curve if appropriate) is displayed in the bottom left of the screen.

The equation that is currently being fitted to the growth curve is shown in the upper left of the screen. As well as the numerical values for the different parameters, the average error in the fit is given as well. This is the average deviation of the data points away from the fitted growth curve and is incorporated into the error calculation for the D_e .

As with all [graphs in Analyst](#), it is possible to alter the appearance of graphs, copy data from graphs to other packages, or copy an image of the graph to the clipboard.

If your BIN file has had the dose rate entries filled out then a menu 'Options' will be shown and you can select this to work in Gy instead of seconds.

6.1.2 Plateau test

When a multiple aliquot D_e is first calculated the display shows a single D_e determination that is obtained when integrating the individual luminescence records over a fixed time (or temperature) interval (see [section 6.1.1 Integral \$D_e\$](#)). However it is sometimes interesting to calculate the D_e at different temperatures (or times), and plot the D_e as a function of temperature - the ‘plateau test’.

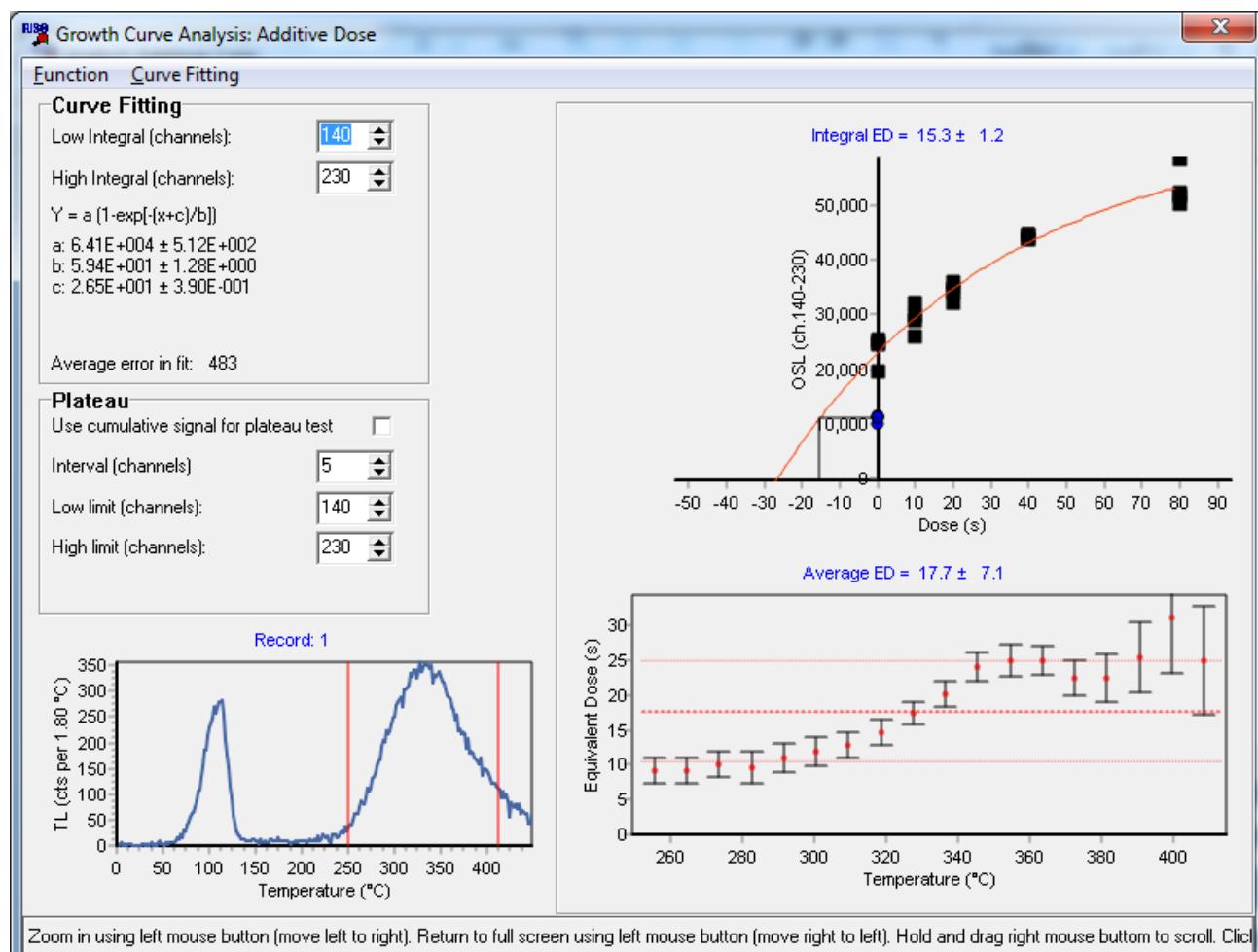


Figure 6.1.2(a): Plateau test for Additive-1.BIN

To plot a plateau test, select the item ‘Show plateau’ in the Function menu. This will then add an additional graph to the display (see Figure 6.1.2(a)) showing the D_e calculated as a function of temperature (or time). By default, the D_e is calculated between the intervals that you have set for the integral D_e , and calculating a D_e for every 5 data channels. If you alter the ranges used for the plateau test then a button marked ‘Recalculate Plateau’ will become visible, allowing you to recalculate the data once you are happy with the new parameters.

Analyst will automatically calculate the average D_e from a specific part of the plateau. The range of channels over which this average is calculated is specified at the bottom left of the display screen ('Low Limit' and 'High Limit'). The result of this calculation is displayed at the top of the lowermost graph. The value derived by this calculation is likely to be different from that derived by the integral D_e method since in one case the data from each channel is weighted evenly, while in the integral D_e method it is weighted according to the signal intensity.

6.2 SA Regeneration

Analyst has been set up to enable you to easily analyse data collected using the Single Aliquot Regeneration (SAR) protocol described by [Murray and Wintle \(2000\)](#) and reviewed by [Wintle and Murray \(2006\)](#). This is a very powerful procedure for determining the absorbed dose of a sample.

The protocol that was outlined by Murray and Wintle is designed to compensate for changes in luminescence sensitivity that may occur during a set of measurements. In short, the procedure involves repeated OSL measurement of an aliquot, initially to determine its natural OSL signal, and then subsequently to characterise its response to laboratory radiation. The OSL measurements evict the majority of the trapped charge within the sample, so the procedure is a regenerative one. However, the key element of the SAR described by Murray and Wintle is that after each OSL measurement (either of the natural signal or a regenerated dose) the aliquot is given a small radiation dose. The response of the aliquot to this ‘test dose’ is then measured. The test dose remains constant through the analysis of a given aliquot, and hence if no sensitivity changes occur the OSL response to the test dose should remain constant. In practice the response may vary, and this can be used to correct for sensitivity changes affecting the main regeneration measurements.

In practice this means that for each aliquot there are a series of pairs of OSL measurements. The first measurement is the Natural signal (L_N), while the second is the response of the aliquot (T_N) to the test dose that is administered. The third measurement is the response (L_X) of the aliquot to a regeneration dose, while the fourth is the response to the test dose once again (T_X).

Analyst can automatically process this data and generate growth curves. The program assumes that all the OSL records for a given aliquot will have the same ‘Position’ value (this is the position of the aliquot on the carousel). The position data is automatically put into the BINX file when the data file is written. You can check the position data by selecting this for display on the main Analyst screen. Additionally, Analyst assumes that the first record of a given aliquot within the BINX file will be the Natural signal, and the next measurement is the response to the test dose. After this each pair of measurements is the OSL after a regeneration dose and a test dose.

The file SAR-1.BINX that is supplied with Analyst is an example of a data file taken from the Risø reader that is in a format suitable for SAR analysis. In order to use the Single Aliquot Regeneration tool, ensure that:-

- 1/ All the records in the BIN file that you want to be used for the analysis have been [selected](#).
- 2/ That the regeneration doses given to the aliquots have been correctly entered into the ‘Irradiation Time’ entry in each data record. This may be done automatically by the Sequence Editor if you have selected this in the Sequence Options. You may also enter this at the time the data is collected by altering the ‘Run Info’ section of each OSL measurement in the Sequence Editor. Alternatively, you can use the [Edit Record](#) or [Block Edit](#) commands to set the irradiation times.

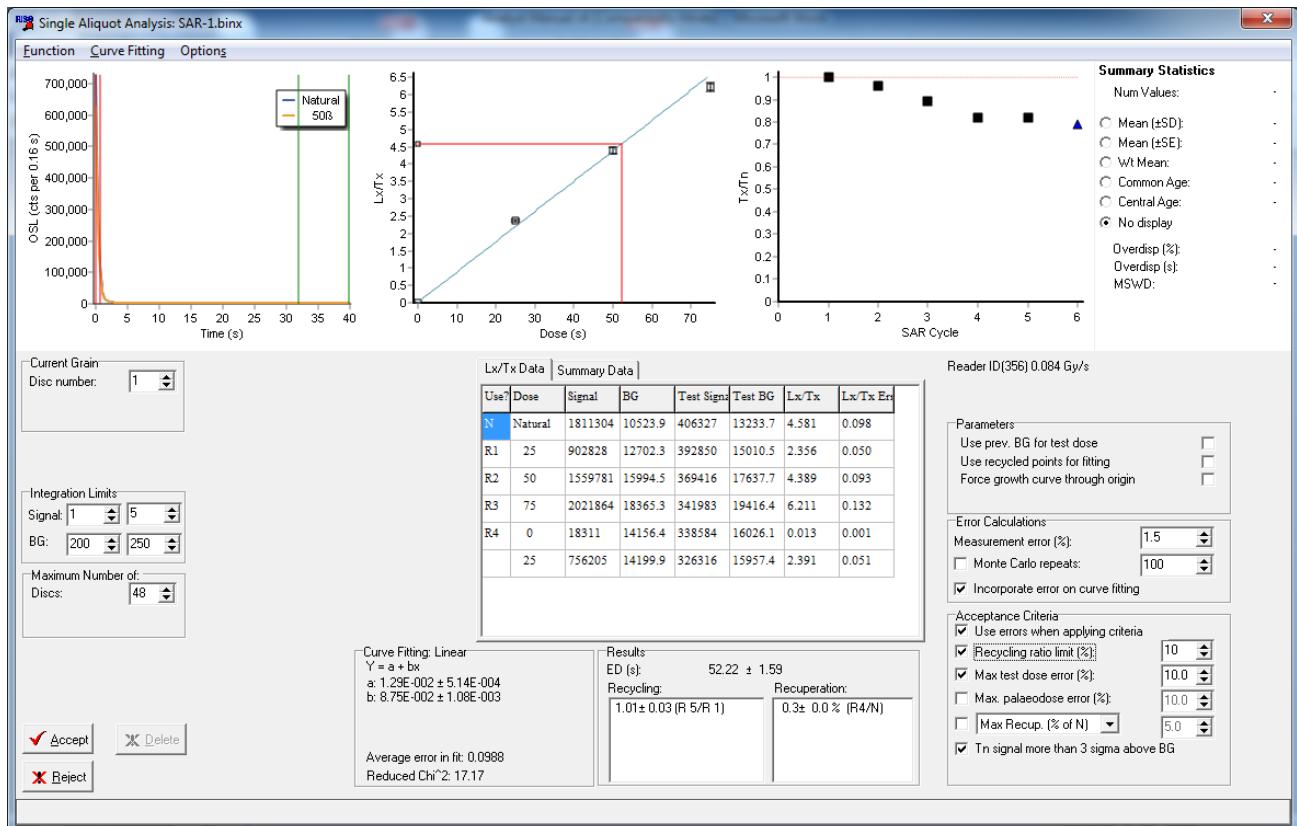


Figure 6.2.1(a): Initial display in the Single Aliquot regeneration analysis option

The single aliquot display presents a range of data about the OSL measurements for the current aliquot. In the upper left of the screen is the natural OSL decay curve for the sample (shown in blue). If an equivalent dose (D_e) has been calculated then a second decay curve is shown in orange. This is the OSL decay curve of the laboratory regeneration dose that is closest to the D_e (50 seconds of beta irradiation in the example shown above) and can be useful to visually inspect whether the OSL signal originating from natural and laboratory irradiation have a similar shape.

If you want to display other OSL decay curves for the same aliquot then click on whichever cell in the main summary table (in the middle of the display) refers to the measurement. For instance, to display the OSL decay curve that was measured for the test dose response following the natural signal, click on the column marked 'Test Signal' or 'Test BG' in the first row of data (corresponding to the Natural measurement). You can also display multiple OSL decay curves by selecting a single cell in the table of Lx/Tx data and then holding the Shift key down while using the cursor keys to move up or down.

A brief summary of the analytical results for the current aliquot is displayed at the bottom of the screen in the middle. If the SAR sequence contains two regeneration doses that are the same, then the recycling ratio will be calculated. In the example shown above, the 25 s dose was given twice (once as the first regeneration cycle R1 and again in the fifth regeneration cycle R5).

Integration limits

You must fix two sets of integration limits as part of the Single Aliquot regeneration analysis. The section headed 'Integration Limits' under 'Integration Limits' is used to fix the part of the decay curve that is used to define the range of channels that contain the dose dependent part of the signal. This is shown as two red lines on the decay curve in the top left of the screen. As you adjust the range of channels used, the data displayed in the main table in the centre of the screen will be updated. The same integration limits are used both for the first (the Natural and Regeneration doses - marked as 'Signal' on the table) and second (the test dose - marked as 'Test Signal' on the table) OSL

measurements. This is normally the first part of the OSL decay curve, and in general the best results are normally obtained by using a narrow integration range (possibly as little as one or two channels wide).

The second set of integration limits are used to define the 'BG' (Background) 'Integration Limits'. This integral is the part of the OSL curve that is used to define the background signal level - essentially the non-dose dependent part of the signal. This will normally be the last section of the OSL decay curve, though the use of early background methods have been proposed ([Cunningham and Wallinga, 2010](#)). The background value that is subtracted from the signals is calculated in the following way. The average signal within the range of channels defining the background integration is calculated, and this value is multiplied by the number of channels used to define the signal. This means that if you alter the number of channels used to calculate the background value, you should see little change in the value, but as you increase the number of channels used to define the signal component, the background value will also alter.

In some circumstances you may want to use the background value from the L_X OSL measurement as the background for the test dose response as well (this is discussed in [Murray and Wintle, 2000](#)) and this can be achieved by ticking the 'Use Prev. BG for test dose' option in the upper right of the screen.

Curve fitting options

The dose response curve data can be fitted using a variety of options selected from the Curve Fitting menu (see [Section 6.2.1.3](#)). The default setting is for a linear fit, but commonly one would want to use an exponential fit. The type of curve fitting is selected from the menu at the top of the screen, but additionally you can choose whether to force the growth curve through the origin using the check box on the right hand side of the screen ('Force growth curve through origin'). The equation being fitted to the data is shown at the bottom of the screen in the 'Curve Fitting' section, and the fitted values for the various parameters are also displayed here. Also shown in this section is the average error in the fit. This is a measure of the average deviation of the growth curve data from the equation that has been fitted. In the box entitled 'Error calculations' on the right hand side of the screen, one of these ('Incorporate error on curve fitting') is an option as to whether you want to incorporate this error term into your overall calculation of the error in D_E . This is described in the paper by [Duller \(2007\)](#) in Ancient TL

Numerical summary display and automated analysis

A summary of the numerical data extracted from the set of OSL measurements for the current aliquot is displayed in the centre of the screen. This displays the measurements for each regeneration dose on a separate line. The first line shows the data for the 'Natural' signal and the test dose measurement. The data are used to calculate a 'normalised OSL' value using the equation:-

$$\text{Norm. OSL} = \frac{(\text{Signal} - \text{BG})}{(\text{Signal} - \text{BG})} \quad \begin{array}{l} \text{[for the first OSL measurement]} \\ \text{[for the test dose measurement]} \end{array}$$

This value is displayed in the column marked ' L_X/T_X ', and the uncertainty in this ratio is displayed in the next column to the right. The uncertainty is calculated using the approach described in [Galbraith \(2002\)](#).

You can export the data for the current aliquot that is being analysed by using the 'Save' button. Alternatively you can use the mouse to highlight a block of data, and then click on the right mouse button to copy the highlighted data to the clipboard. This data can then be pasted into another Windows application such as a spreadsheet.

Normally you will have made more than one measurement of the palaeodose of a sample by running more than one aliquot. If this is the case then you can run through a data set to look at [multiple values of equivalent dose](#) using either an [automatic analytical procedure](#) or by hand.

Removing data points from the dose response curve

Prior to using the Single Aliquot Regeneration analysis you will normally have carefully selected which data from the BINX file you want to use for analysis (see first section on this page and [Section 2.2 Selecting and Highlighting Records](#)). However, there may be times when you are interested to see what would happen to a dose response curve if you removed one or more of the data points. You can do this by double clicking on the entries 'R1', 'R2', 'R3' etc in the panel showing the Lx/Tx data. Double clicking again will restore those data points.

Parameters and Error Calculations

On the right hand side of the screen there are a number of options regarding the way in which Analyst deals with the data in your BINX file. The first value that you can set under "Error Calculations" is entitled 'Measurement error (%)'. This is a parameter that is an estimate of the ability of the luminescence reader to measure an OSL signal reproducibly. Experience has shown that even with samples where the OSL intensity is very bright, there is scatter in the OSL measurement from one SAR cycle to the next ([Armitage et al 2000](#); [Thomsen et al 2005](#)). It is thought that this reflects the inherent uncertainty in the intensity of the OSL stimulation source, the positioning of the aliquot relative to the beta source and heating of the sample. In practice the combined effect is to produce a 'Measurement error' of approximately 1.5% for standard multiple grain measurements. There is also an option in this box that allows you to decide whether you want to incorporate the average uncertainty in the curve fitting procedure into the estimate of D_e .

A new option is to use a Monte Carlo approach for estimating the uncertainty in the D_e value and is described elsewhere (see [Section 6.2.1.6 Calculation of Uncertainty in \$D_e\$](#)).

Under the heading "Parameters" the first option is labelled 'Use prev. BG for test dose'. If this entry is ticked then Analyst will use the background value for the first OSL decay curve of each pair as the background both for that measurement, AND for the subsequent OSL measurement which monitors the aliquots response to a test dose. If the entry is not ticked then the background is calculated for each OSL measurement separately. By default this entry is ticked.

The second option is whether to use the recycled regeneration data points as part of the data set that is fitted by Analyst.

The third option allows you to force the growth curve through the origin. When you select this option you will see that the form of the equation that is fitted with alter accordingly (this is shown in the box near the bottom of the screen entitled "Curve Fitting").

6.2.1 Menus

6.2.1.1 Function menu

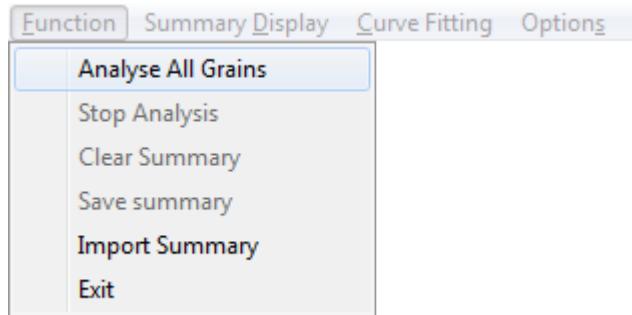


Figure 6.2.1.1(a): Options available in the 'Function' menu

Analyse All Grains

This menu provides options that allow you to automatically calculate D_e values (see [Section 6.2.1.7](#)) for a large number of aliquots (or single grains). The function 'Analyse All Grains' will step through the BINX data file starting from the current position (marked by the entries in the boxes on the left hand side of the screen; Figure 6.2.1.1(b)), and running until it reaches the maximum number of aliquots allowed (marked in the box below). In the example shown below the data for disc number 8, grain number 1 is being viewed on screen. If 'Analyse All Grains' is selected now, then Analyst will step through all the grains for discs 8, 9, 10, 11 ... 36.

Figure 6.2.1.1(b): Current disc number and grain number being viewed. These values can be changed manually and 'Analyse All Grains' will start automatic analysis from this point in the datafile.

Figure 6.2.1.1(c): Parameters setting up the maximum number of discs. This is set to 48 by default, but can be set to a lower value if one wants to restrict 'Analyse All Grains' to analysis of a smaller number of aliquots.

The results from an aliquot or a grain will be accepted if the luminescence data pass all of the Acceptance Criteria selected. In the example shown below (Figure 6.2.1.1(d)), data will only be accepted if the recycling ratio is within 10% of unity (within uncertainties calculated for the recycling ratios), and if the uncertainty on the measurement of the signal resulting from the test dose following the natural is between 0 and 10%.

Criteria	Value
Use errors when applying criteria	Checked
Recycling ratio limit (%)	10
Max test dose error (%)	10.0
Max palaeodose error (%)	10.0
Max Recup. (% of N)	5.0
Tn signal more than 3 sigma above BG	Checked

Figure 6.2.1.1(d): Box containing the acceptance criteria that can be used to automatically filter single aliquot or single grain data

Stop Analysis

The automated analysis can be stopped by selecting 'Stop Analysis' at any time.

Clear Summary

The automated analysis described above stores results in the "Summary Data" table. This menu option will clear all the data from that Summary Data table.

Save Summary

The results stored in the "Summary Data" table can be saved using this option. A file with a .ANR extension is created. This is a comma separated (CSV) ASCII file where the first line is the BINX file being analysed, and then the analytical results from the Summary Data table are listed (see [Appendix B](#) for full details). This .ANR file can be read by Excel (as a CSV) or it can be imported back into Analyst at a later date (see below).

Import Summary

If you have previously undertaken analysis of this BINX file then you can import that analysis back into Analyst using this option. Note that whilst the ANR file remembers a lot about your analysis (e.g. [the signal integration used, the type of curve fitting, and the fitting options that you used](#)), it does not remember how you set up the BINX file, or if you deselected some regeneration points.

6.2.1.2 Summary Display menu

As you build up a set of analyses on separate aliquots, the data is displayed visually in the top-middle of the screen. The data may be displayed using three different graphical methods. The default display is a radial plot, but you can also use a histogram or a weighted histogram (sometimes known as a probability density function). The Summary Display menu appears at the top of the Single Aliquot analysis page once data have been accumulated either by pressing the 'Accept' button and manually selecting which D_e values to use, or after using the 'Analyse all grains' option in the Function menu (see [Section 6.2.1.1 Function Menu](#) and also [Section 6.2.1.7 Analysis of multiple equivalent dose values](#)).

In addition to the visual display of D_e data, a [statistical summary](#) is given in the upper right hand corner of the Single Aliquot Regeneration analysis page.

A brief comment is made below on the different types of visual display possible in Analyst. A very thorough review of the analysis and display of multiple D_e determinations is given by [Galbraith and Roberts \(2012\)](#).

Histogram

Histograms are a convenient, and easily understood means of displaying data so that the distribution of the data can be seen. There are some drawbacks with histograms, including the fact that their visual appearance can radically change depending upon the class interval that is used, and that they weight all data points equally (regardless of their relative precision). In Analyst the class interval (bin width) is set as the mean of the uncertainties of the D_e values being plotted.

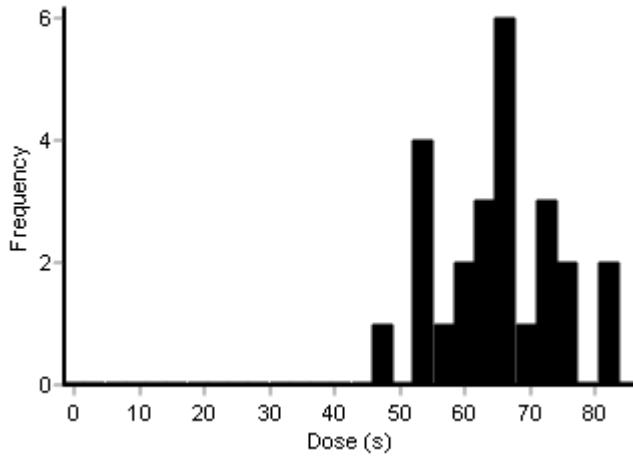


Figure 6.2.1.2(a): Histogram from the Summary Diagram on the single aliquot regeneration page

Weighted Histogram (Probability Density Function)

A weighted histogram represents each data point as a Gaussian curve, whose mid-point is the value being plotted, and whose width is related to the precision with which the value is known. The area of the Gaussian representing each data point is kept constant, so that a poorly known value is represented by a low, flat, Gaussian, while a precisely known value is shown as a high, narrow, Gaussian curve. For a population of values, the individual Gaussian curves are summed to give a distribution (hence the term probability density function).

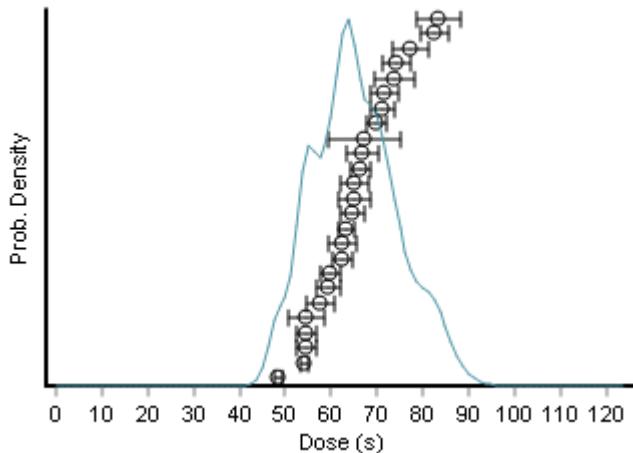


Figure 6.2.1.2(b): Weighted histogram from the Summary Display on the single aliquot regeneration page showing the same data as for the histogram above

Radial Plot

Radial plots were introduced by [Galbraith \(1990\)](#) specifically for the display of data whose individual values were known with different precisions. He has argued against the use of histograms and weighted histograms ([Galbraith 1998](#)). In essence the plot is a two-dimensional one, with the precision of an individual data point plotted on the x-axis, and the difference between the central value for that point and some mean value for the whole population plotted on the y-axis. The difference plotted on the y-axis is expressed as the number of standard deviations of that individual data point away from the mean value for the population. The third 'radial' scale plotted on the right hand side is a derived scale, and can be plotted only because it is a mathematical property

of a radial plot that all the points plotted on a radial line from the origin have the same central value (in this case the same D_e).

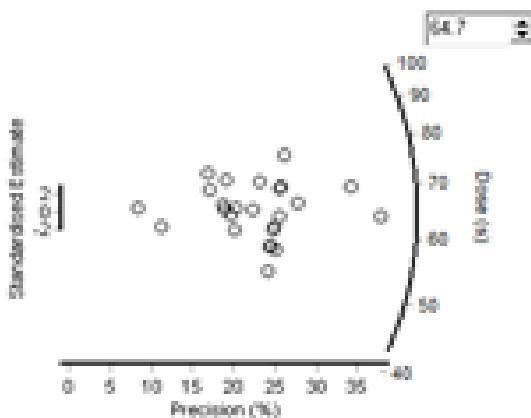


Figure 6.2.1.2(c): Radial plot from the Summary Diagram on the single aliquot regeneration page of the same data as for the histogram above

The reference value for the radial plot shown above is 64.7, but this can be set to any value simply by editing the value in the box on the diagram. The quality of these diagrams is not sufficient for publication, but is only meant as a tool for data exploration.

If a [summary statistic](#) is selected from the display on the right hand side of the screen then this is shown on the summary displays. Figure 6.2.1.2(d) shows the mean and standard deviation plotted on the weighted histogram.

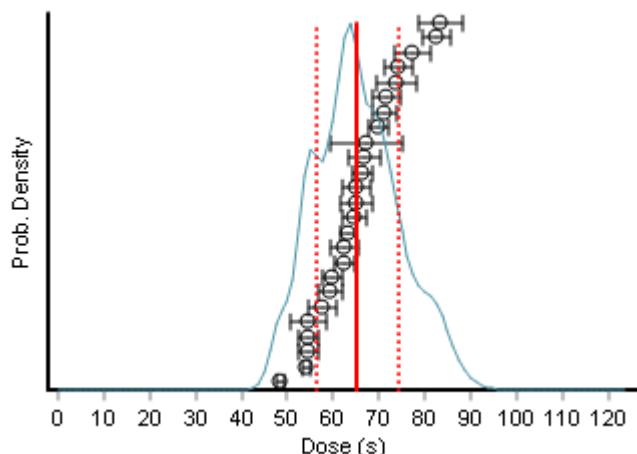


Figure 6.2.1.2(d): Weighted histogram showing the mean (solid vertical red line) and standard deviation (dashed vertical red lines) for a suite of D_e values

6.2.1.3 Curve Fitting menu

Analyst offers a range of options for how to fit the single aliquot regenerative dose (SAR) data to generate a dose response curve and calculate an equivalent dose (D_e).

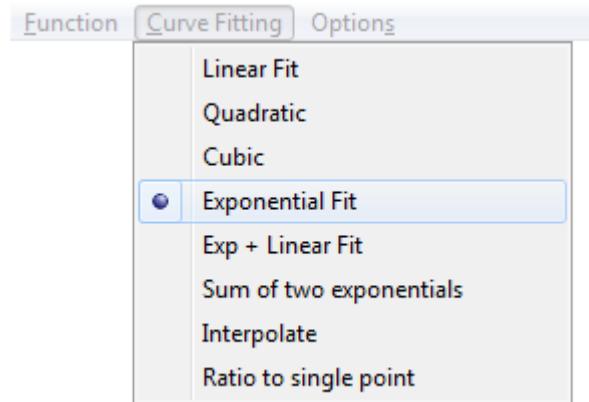


Figure 6.2.1.3(a): Curve fitting menu

When the SAR page is first opened the curve fitting is 'Linear Fit' by default. The first six options for curve fitting are mathematical functions to fit to the entire dose response data set. The last two options ('Interpolate' and 'Ratio to single point') do not involve any mathematical fitting.

The equations fitted are listed below. A Levenberg-Marquardt method is used to fit the selected equation to the dose response curve data, and the fitted parameters are given in the box entitled 'Curve fitting' at the bottom of the page. Note that if you select 'Force growth curve through origin' in the 'Parameters' listed on the right hand side of the SA screen then the constants are removed from the equations below.

Linear Fit

$$y = a + bx$$

Quadratic

$$y = a + bx + cx^2$$

Cubic

$$y = a + bx + cx^2 + dx^3$$

Exponential

$$y = a \left(1 - e^{-\frac{x+c}{b}}\right)$$

Exponential plus linear

$$y = a \left(1 - e^{-\frac{x+c}{b}}\right) + gx$$

Sum of two exponentials

$$y = a \left(1 - e^{-\frac{x}{b}}\right) + c \left(1 - e^{-\frac{x}{d}}\right) + g$$

An example of a dose response curve fitted with the sum of two exponentials is given in Figure 6.2.1.3(b), along with the numerical parameters for the fit in Figure 6.2.1.3(c). The reduced chi squared value given at the bottom of the fitted parameters (Figure 6.2.1.3(c)) may be used to help decide which type of curve fitting is appropriate for the current data.

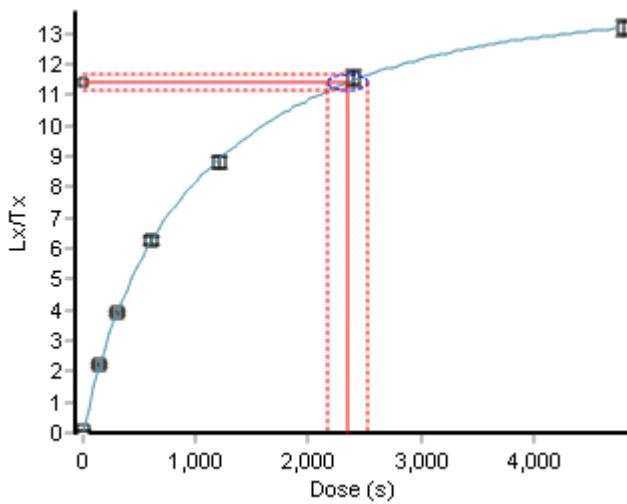


Figure 6.2.1.3(b): Example of a dose response curve fitted with the sum of two exponentials

The parameters of the equation fitted to the dose response curve are saved as part of the Summary Data table when the 'Accept' button is pressed in the bottom left hand side of the screen. Further information about the data saved in the Summary Data table is given in [Appendix B](#).

Curve Fitting: Sum of two exponentials

$$Y = a(1-\exp[-x/b]) + c(1-\exp[-x/d]) + g$$
a: 3.66E+000 ± 2.16E+000
b: 3.44E+002 ± 1.26E+002
c: 9.96E+000 ± 1.76E+000
d: 1.57E+003 ± 4.81E+002
g: 3.73E-002 ± 2.22E-003
Average error in fit: 0.0150
Reduced Chi^2: 0.31

Figure 6.2.1.3(c): Parameters for the dose response curve shown in Figure 6.2.1.3(b)

6.2.1.4 Options menu

The options menu provides the following facilities:

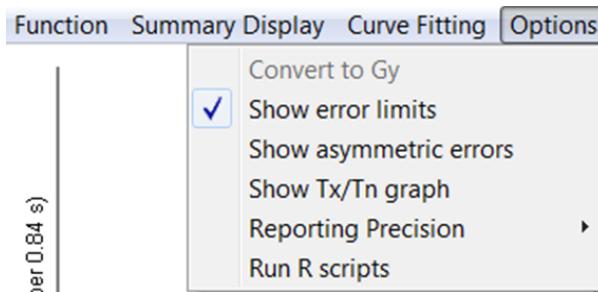


Figure 6.2.1.4(a): Options menu in the single aliquot regeneration function

Convert to Gy

The BINX file header has an entry for the Dose Rate of the radiation source used to irradiate aliquots. In more recent versions of the Sequence Editor the user can set the dose rate of the beta source so that it is automatically inserted into BINX files when measurements are made. Alternatively the user can set the Dose Rate using the [Block Edit](#) command.

If the current BINX file has had the Dose Rate set then this will appear immediately below the T_x / T_N graph on the right hand side of the screen, and the Convert to Gy menu item will be available. If the dose rate has not been set then the menu item is greyed.

If the Convert to Gy option is selected then the Dose Rate is used to convert all the regeneration doses from seconds to Gray. The x-axis of the dose response curve is then plotted in Gy, and the equivalent dose is expressed in Gy.

Show error limits

Checking this option will show the uncertainties on the L_n/T_n ratio and interpolate these onto the dose response curve and the dose axis.

Show asymmetric errors

Analyst normally expresses the uncertainty on each equivalent dose as a symmetric value, but as samples approach saturation this approximation becomes less appropriate (Figure 6.2.1.4(b)). Selecting this option will yield asymmetric uncertainties, with the symmetric positive and negative uncertainty on the L_n/T_n ratio extrapolated to yield asymmetric uncertainties in D_e .

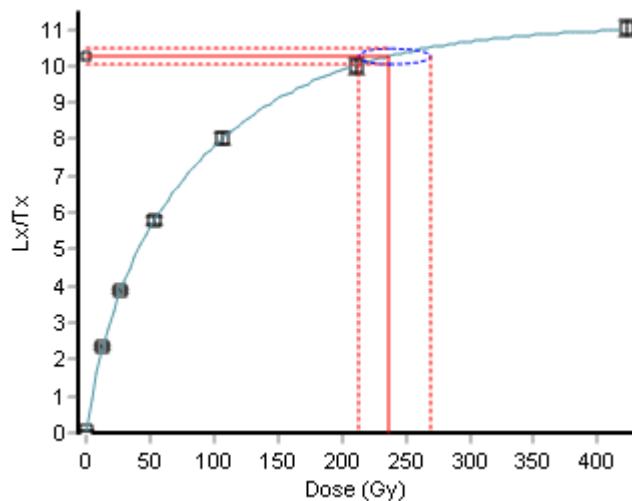


Figure 6.2.1.4(b): Dose response curve showing the best estimate of the D_e (solid red line), and the calculated uncertainties (dashed red lines). In this case the error limits are asymmetric because of the curvature of the dose response curve

Note that these asymmetric errors are shown on the screen, but the symmetrical errors are used when [combining \$D_e\$ values](#).

Show Tx/Tn graph

Checking this option forces the [Tx/Tn graph](#) to be shown on the right hand side of the screen (Figure 6.2.1.4(c)). This can be useful if a [Summary Diagram](#) is currently being shown.

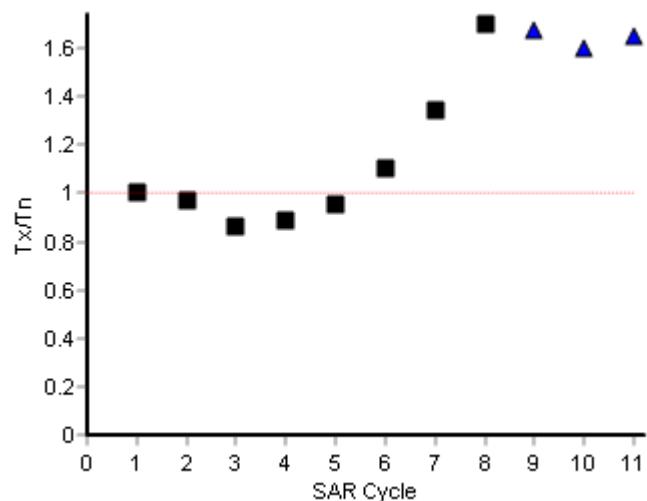


Figure 6.2.1.4(c): Tx/Tn graph showing the change in apparent sensitivity of the aliquot (or grain) through the SAR sequence

Reporting precision

You can select how many decimal places (0, 1, 2, or 3) you want to use when displaying data in the [Summary Statistics panel](#).

Run R scripts

Select this option to open a window in which you can run R scripts. This menu option is only available when you have accepted some data using the "Accept" button, or used "Analyse all grains" on the "Function" menu of this page. When you select to run R scripts the data from the "Summary data" panel in the middle of the SAR page is exported to a file called "AnalystDeData.txt" and this can then be read into the R script. Further details of using R scripts is given in the section on [R support](#).

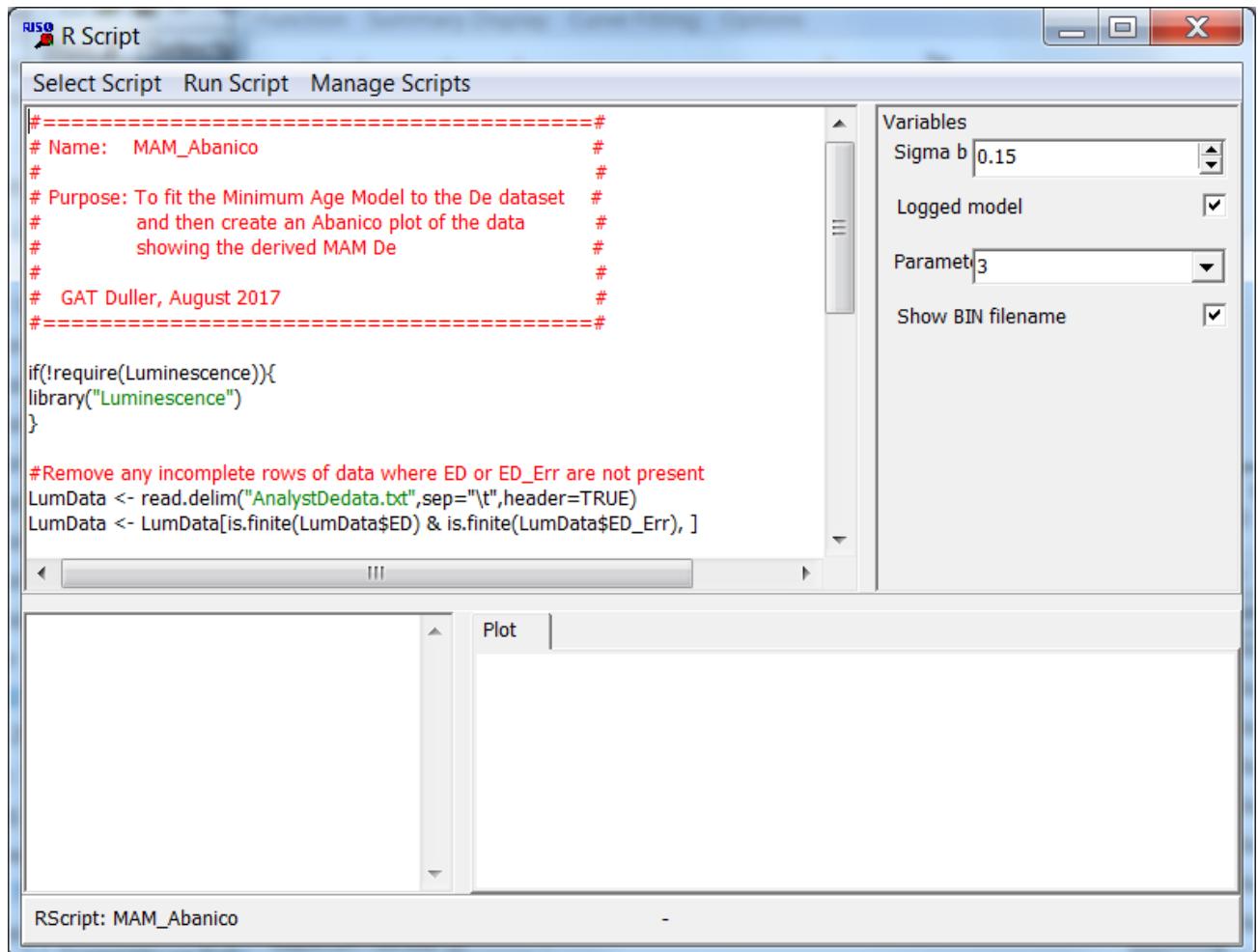


Figure 6.2.1.4(d): R script window providing users with the ability to run R scripts to analyse their data

6.2.2 Using SAR

6.2.2.1 Displaying the change in sensitivity (Tx/Tn)

The change in sensitivity of the aliquot through the SAR sequence is defined by changes in the response to the test dose (e.g. [Armitage et al. 2000](#)). A graph of this variation is shown on the upper right hand side of the screen. This space is also used to display a summary plot if multiple De values have been calculated. The plot of the change in sensitivity can always be restored using the 'Show Tx/Tn graph' from the [options menu](#).

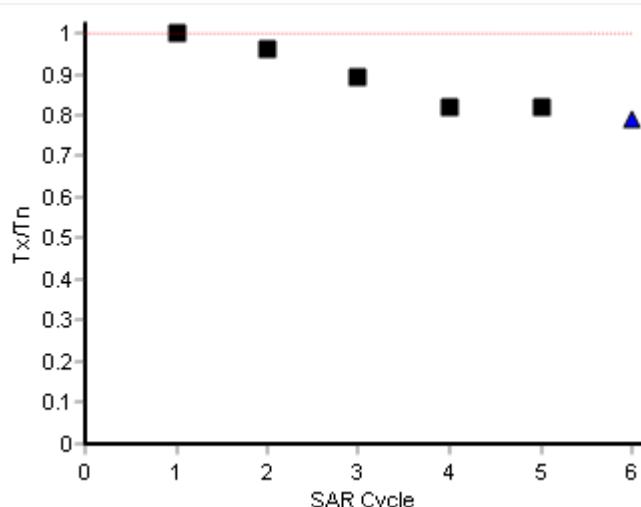


Figure 6.2.1.5(a): Change in the ratio of T_x/T_n for a single aliquot during a SAR sequence

The graph plots the test dose for each cycle in the SAR sequence, normalised to the signal from the first (natural) cycle (see figure 6.2.1.5(a)), and thus starts from unity by definition. A horizontal dotted red line marks the value of 1.00 which would indicate no sensitivity change.

6.2.2.2 Calculation of uncertainty in D_e

The default option for Analyst to use to calculate the uncertainty on an equivalent dose (D_e) when fitting any of the mathematical equations selected from the [Curve Fitting menu](#) is to use a combination of the counting statistics and the quoted measurement error (see [Section 6.2.1](#)) to derive the uncertainty on the L_N/T_N ratio, and, if selected, to combine this in quadrature with the average deviation from the curve.

An alternative approach to estimating the uncertainty on the D_e is to use a Monte Carlo method, with the widths of the Gaussians for each point being defined by the error in the ratios of L_x/T_x as defined above. To use the Monte Carlo approach for estimating the error, tick the check box, and select the number of repeat fits that are required. Suitable values would typically be 1000. When this option is selected, a histogram is superimposed on the SAR growth curve showing the distribution of D_e values determined. The final error quoted at the bottom of the screen (1.45 seconds in the example shown in Figure 6.2.1.6(a)), is the standard deviation of this distribution, whilst the D_e value given (52.34 seconds in the example below) is the best fit to the data, and is not derived from the Monte Carlo results.

Note that since the Monte Carlo approach is based on a stochastic sampling of the L_x/T_x ratios, the error vary slightly each time the Monte Carlo routine is run. For most samples, there is relatively little difference in the uncertainty in D_e determined using the two methods described above. The paper by [Duller \(2007\)](#) describes comparisons of these two approaches on a limited number of example data sets. The Monte Carlo method is probably the most rigorous. Additionally, at high doses the Monte Carlo approach will correctly give an asymmetric distribution of calculated D_e values. Analyst will still take the standard deviation of such asymmetric distributions, but if users wish to undertake their own analysis of these distributions then result of each iteration of the Monte Carlo approach can be obtained by clicking on the right hand mouse button while pointing at the histogram of D_e values and selecting to “Copy data to clipboard”.

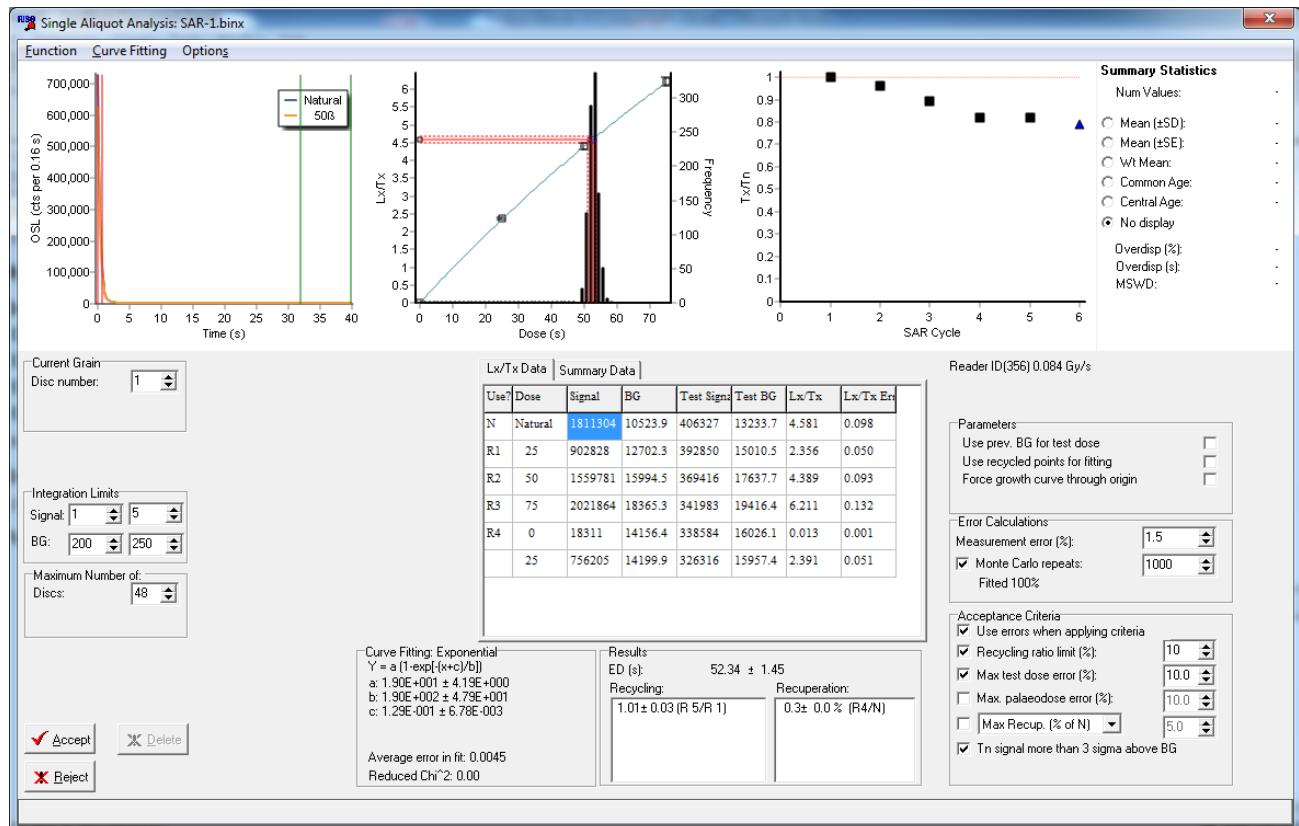


Figure 6.2.1.6(a): Single aliquot regeneration using a Monte Carlo method for estimating the error in the D_e .

Calculating the uncertainty when calculating D_e from a ratio, or by interpolating between two points

As well as fitting a mathematical function to the growth curve data, you can also [calculate a \$D_e\$ by taking the ratio](#) of $L_N/T_N (=R_N)$ to $L_x/T_x (R_x)$ for the regeneration dose (D) that most closely matches the natural.

In this case the error in D_e (excluding systematic errors) is given by the following equation:

$$S_{D_e} = D_e \sqrt{\left(\frac{S_{R_N}}{R_N} \right)^2 + \left(\frac{S_{R_1}}{R_1} \right)^2}$$

Another alternative is to [calculate the \$D_e\$ by interpolating](#) between the two regeneration points whose L_x/T_x ratios straddle that obtained during measurements of the natural. In this case the D_e and error are given by the expressions from [Thomsen et al \(2005\)](#).

$$D_e = \frac{(R_N - R_1)}{(R_2 - R_1)} (D_2 - D_1) + D_1$$

$$S_{D_e} = \sqrt{\left(\frac{D_2 - D_1}{R_2 - R_1}\right)^2 \left\{ S_{R_N}^2 + \left(\frac{1}{R_2 - R_1}\right)^2 \left[(R_N - R_2)^2 S_{R_1}^2 + (R_N - R_1)^2 S_{R_2}^2 \right] \right\}}$$

A summary of these various options for calculating D_e and the uncertainty on the D_e are given in [Duller \(2007\)](#).

6.2.2.3 Analysis of multiple equivalent dose values

It is normal to make measurements on a number of different single aliquots and hence make replicate measurements of equivalent dose. There are two methods for undertaking this, either by hand or automatically.

To analyse a set of single aliquot results by hand, set the Disc Number (on the left hand side of the screen) to the first aliquot (normally 1). This will display the growth curve and palaeodose for this aliquot. If you accept this result then press the 'Accept' button at the bottom of the screen. This will save the analytical results for that aliquot, display a [summary diagram](#) (either in the form of a histogram, a weighted histogram, or a radial plot) of all the current analyses in the upper middle part of the screen, and automatically move on to the next aliquot position. Continue either pressing the 'Accept' or 'Reject' buttons. As you do so, the histogram in the middle of the screen will build up and the average palaeodose value is displayed.

You can switch the data shown in the middle panel between displaying the " L_x/T_x Data" for the current aliquot and the "Summary Data" of the results of the aliquots that you have accepted so far. Either data set can be exported using the 'Save' button. Additionally, the "Summary Data" can be saved using the option on the [Function Menu](#). The "Summary Data" for each aliquot is described in Appendix B

You can also undertake the same analysis automatically. Once again, set the Current Disc Number to the first aliquot. You should also set the 'Number of Disc Positions' (on the left hand side of the screen) to the value of the maximum position that you want to be analysed (e.g. if you want to analyse discs 1 to 18, then set this value to 18) (see [Section 6.2.1.1](#)). Select 'Function| Analyse all grains', and Analyst will automatically step through each disc position trying to calculate a palaeodose. Certain criteria are used to decide whether to accept or reject a given aliquot. The criteria are listed on the right hand side of the screen, and you can choose whether to use these or not by checking or clearing the tick boxes:-

- Recycling Ratio limit - a common check that is made as part of the Single Aliquot Regeneration procedure is to measure one of the regeneration doses twice. If the SAR method is working correctly then the normalised OSL value for both sets of measurements should be similar. Setting the threshold recycling value allows you to automatically reject an aliquot if the recycled point is not the same as the first measurement of that dose within the specified percentage.
- Max Test Dose Error – the uncertainty in the test dose is a good measure of how bright an aliquot is since the same dose is given to all samples. The error is calculated using the approach of [Banerjee et al. \(2000\)](#). You can select a threshold value, which an aliquot must exceed to be accepted. Note that any aliquots where the test dose error is zero or negative (i.e. the background of the test dose signal is equal to or greater than the test dose signal) are rejected.
- Max. palaeodose error – if the percentage error on the palaeodose exceeds the threshold specified on the right hand side of the screen, then the aliquot is rejected.
- Max. Recuperation - if the response to a zero regeneration dose has been made then this will be used to calculate an estimate of the recuperation. If this recuperation value exceeds the threshold

then the aliquot is rejected. The recuperation can be calculated in one of three ways. The default method ('Max Recup (% of N)') is by expressing the Lx/Tx ratio measured from the zero dose point as a percentage of the Lx/Tx for the natural signal. The second method ('Max Rec (% of largest R)') is to express the Lx/Tx ratio from the zero dose as a percentage of the Lx/Tx obtained from the largest regeneration dose in the current data set. The third method ('Max Recup. (seconds)') uses the dose response curve fitted to the current data set, extrapolates this to determine the intercept with the x-axis and uses this as the apparent 'recuperated dose'.

- Tn Signal more than 3 sigma above BG – if the net signal from the natural (minus the BG level) is less than three times the standard deviation of the background signal then the aliquot is rejected.

If an aliquot fails one of these criteria then the check box is highlighted in red. Before starting an automatic analysis you will have to clear the summary display using the menu entry, 'Function|Clear Summary'.

Reviewing and editing the summary data

Once you have compiled a list of equivalent doses in the 'Summary Data' grid, using either the manual or automated approaches described above, you can review this data. Ensure that the 'Summary Data' grid is visible by clicking on the tab in the middle of the screen. Then use the mouse or the arrow keys to move from the results of one aliquot to another. As you highlight the results from each aliquot the growth curve will be shown on the display.

If you decide that you want to remove an equivalent dose from the 'Summary Data' grid and from the summary display, simply highlight that result and press the 'Delete' key on your keyboard.

In the example shown in the figure below the data is displayed as a weighted histogram. As with all of the graphs within **Analyst** the scales on the graph can be [stretched or modified](#), or the data can be extracted for plotting in other software.

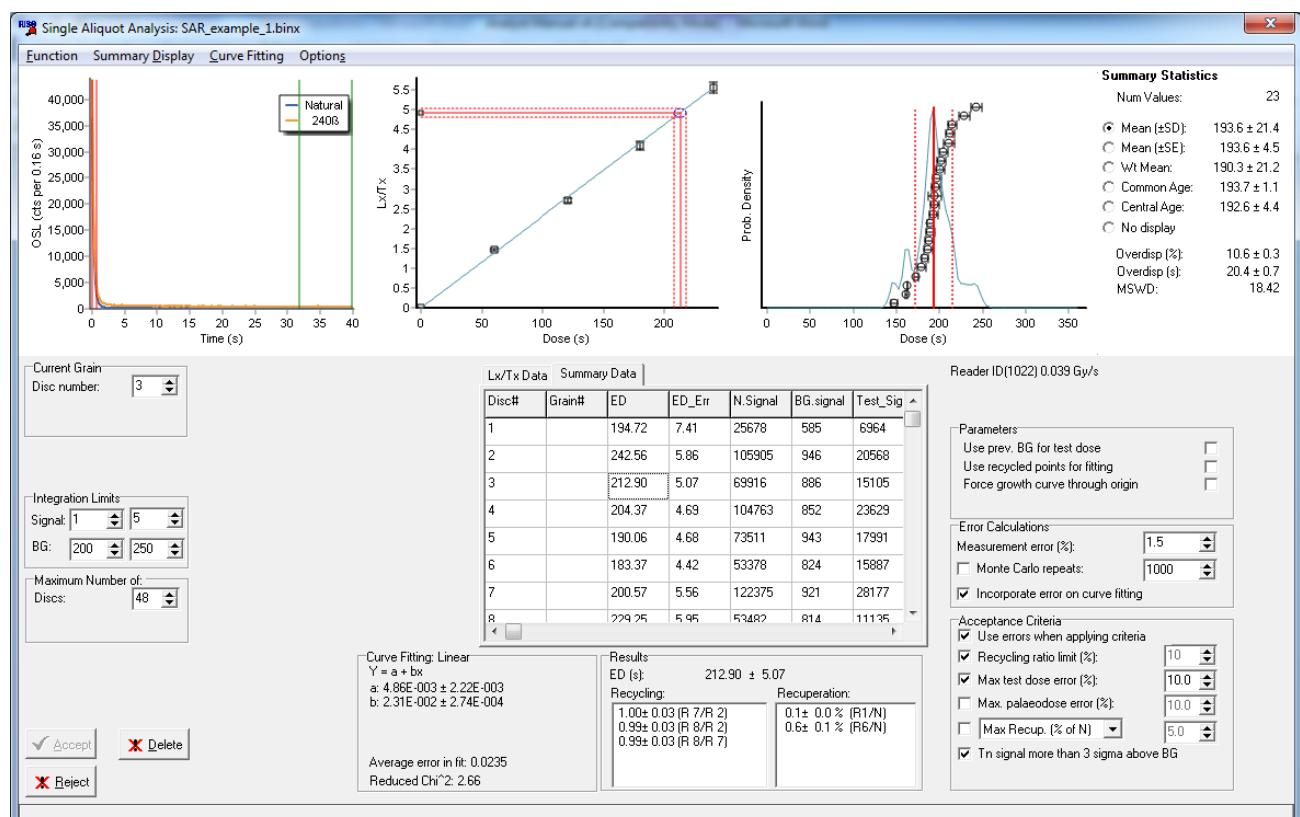


Figure 6.2.1.7(a): Summary data display having accepted 23 aliquots. Clicking on the ED for aliquot 3 (212.9 seconds) has prompted Analyst to display that growth curve.

6.2.2.4 Summary Statistics

If a number of D_e values have been calculated then summary statistics of those D_e values is shown in the upper right hand side of the screen. Selecting one of the radio buttons next to some of these values allows the summary value to be shown on the [summary display](#) (e.g. histogram or weighted histogram). The number of decimal places used to display the summary statistics can be altered using the "Reporting Precision" menu under the ["Options"](#) heading.

Summary Statistics	
Num Values:	25
<input checked="" type="radio"/> Mean ($\pm SD$):	65.3 \pm 8.9
<input type="radio"/> Mean ($\pm SE$):	65.3 \pm 1.8
<input type="radio"/> Wt Mean:	62.9 \pm 8.4
<input type="radio"/> Common Age:	64.5 \pm 0.5
<input type="radio"/> Central Age:	64.7 \pm 1.7
<input type="radio"/> No display	
Overdisp (%):	12.6 \pm 0.4
Overdisp (s):	8.1 \pm 0.3
MSWD:	10.43

Figure 6.2.1.8(a): Panel showing the summary statistics routinely displayed when multiple D_e estimates are available.

The mean (\bar{x}) and standard deviation (σ) of the data are calculated from the individual D_e estimates (x_i) and their associated uncertainties (σ_i) as:

$$\bar{x} = \frac{1}{N} \sum x_i$$

$$\sigma = \sqrt{\frac{1}{N-1} \sum (x_i - \bar{x})^2}$$

The standard error on the mean is calculated using the equation:

$$\text{Standard error} = \frac{\sigma}{\sqrt{N}}$$

The weighted mean and the uncertainty on the weighted mean are calculated as:

$$\bar{x} = \frac{\sum \left(\frac{x_i}{\sigma_i^2} \right)}{\sum \frac{1}{\sigma_i^2}}$$

$$\sigma = \sqrt{\left[\frac{\sum \left(\frac{x_i^2}{\sigma_i^2} \right)}{\sum \frac{1}{\sigma_i^2}} - (\bar{x})^2 \right] \times \frac{N}{N-1}}$$

The Common Age model of [Galbraith et al \(1999\)](#) is calculated following the method outlined in that paper. Note that since this calculation works with the natural log of the De values, any zero or negative De values will be ignored.

$$\ln(\text{Common Age}) = \frac{\sum \frac{\ln x_i}{\left(\frac{\sigma_i}{x_i} \right)^2}}{\sum \frac{1}{\left(\frac{\sigma_i}{x_i} \right)^2}}$$

The Central Age Model of [Galbraith et al \(1999\)](#) is calculated using the iterative method described on page 359 of that article, to find a solution for the CAM and the overdispersion of the data set. As with the Common Age Model, the calculation uses the natural log of the De values, so any zero or negative De values are ignored.

The MSWD (Mean Square of Weighted Deviates) is calculated using the equation:

$$MSWD = \frac{1}{(N-1)} \sum \frac{(x_i - \bar{x})^2}{\sigma_i^2}$$

Further details about measures of central tendency are given in [Bevington and Robinson \(1992\)](#).

6.2.2.5 Running R Scripts

R scripts can be run from within the SAR area of Analyst providing that at least one De value has been accepted and is shown in the summary data panel.

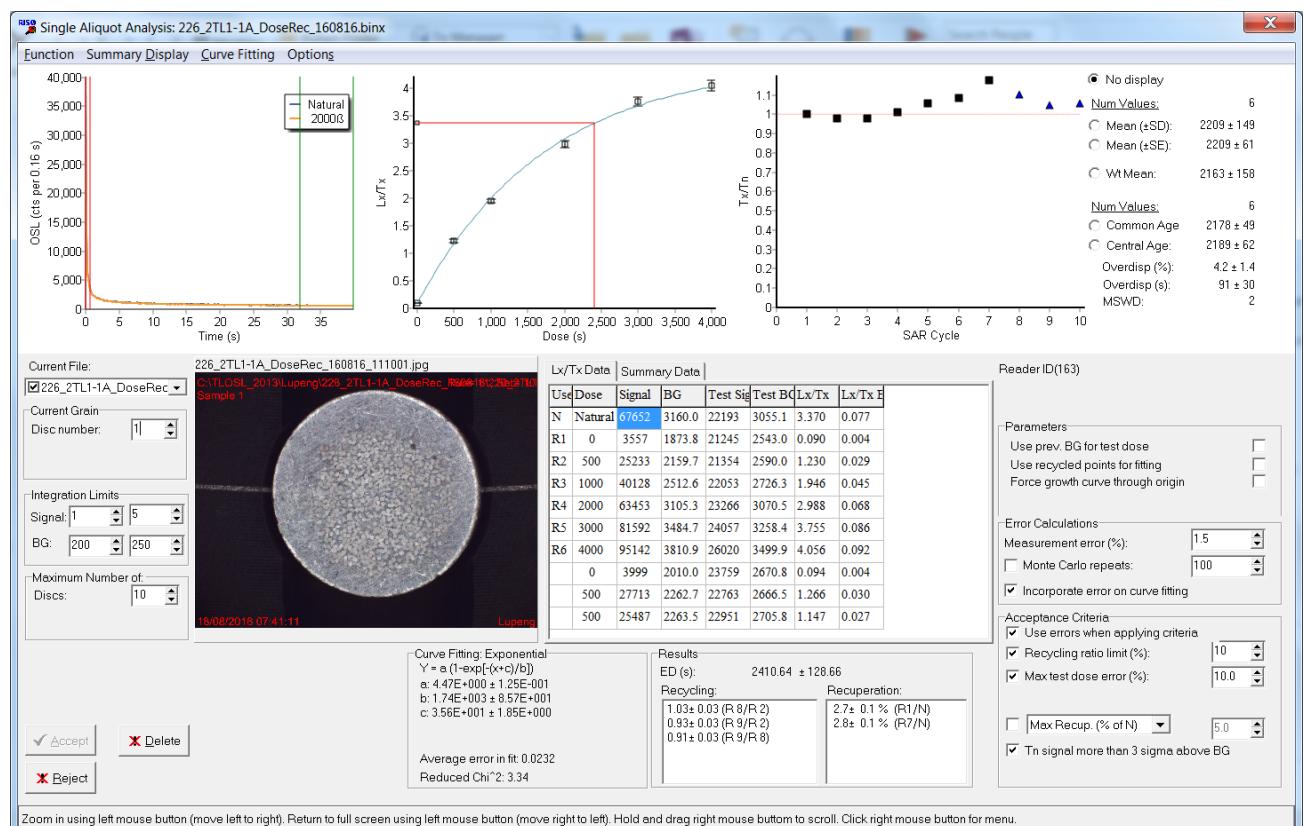
Lx/Tx Data		Summary Data		<input checked="" type="checkbox"/> Only show those that pass criteria					
#	Selected	Pass_Cr	Filename	Disc#	Grain#	ED	ED_Err	N.Signal	More
1	TRUE	TRUE	105_KB2	1	1	32.53	3.90	2170	More
3	TRUE	TRUE	105_KB2	1	3	17.70	2.23	301	More
4	TRUE	TRUE	105_KB2	1	4	12.62	1.42	456	More
6	TRUE	TRUE	105_KB2	1	6	17.78	1.71	905	More
8	TRUE	TRUE	105_KB2	1	8	17.06	3.11	425	More
10	TRUE	TRUE	105_KB2	1	10	14.44	1.12	564	More
12	TRUE	TRUE	105_KB2	1	12	7.33	1.08	377	More
13	TRUE	TRUE	105_KB2	1	13	10.70	0.73	1054	More
17	TRUE	TRUE	105_KB2	1	17	224.09	15.34	8372	More
19	TRUE	TRUE	105_KR2	1	19	140.83	15.72	3953	More

Figure 6.2.2.5: Summary data panel on the SAR page listing accepted analyses

Details of how to run and edit R scripts in Analyst are given in [section 12](#).

6.2.2.6. Sample Camera

If your instrument is equipped with a Sample Camera and you have collected a photograph of an aliquot as part of the sequence used to collect the BINX file, the image of the aliquot currently being analysed will be displayed.



6.2.2 Single Grain Regeneration

Analysis of single grain data uses procedures that are almost identical to those used for multiple grain [single aliquot regenerative dose \(SAR\)](#) measurements. A number of additional controls become visible when undertaking single grain measurements. These are (1) a control allowing the grain number to be selected (below the disc number on the left hand side of the screen), and (2) an additional entry in the [Options menu](#) entitled "Sum all grains". When this is selected,

mathematically combines the OSL signals from all 100 grains from each disc and thus treats the single grain disc as a multiple grain aliquot (containing 100 grains). This allows the analysis of synthetic aliquots.

6.3 Component Fitting

Quartz OSL decay curves are thought to consist of a number of different components, each of which decays exponentially ([Bailey et al. 1997](#)). This option provides the opportunity to fit up to a maximum of three exponentially decaying components to a CW-OSL decay curve. The equation is of the form:

$$y = a + [n_1 \cdot b_1 e^{-b_1 t}] + [n_2 \cdot b_2 e^{-b_2 t}] + [n_3 \cdot b_3 e^{-b_3 t}]$$

where a is a constant that will include the dark count and any very slow components, and for each of the three components, n_X is the number of trapped charges and b_X is the detrapping probability. The detrapping probability is the product of the photoionisation cross-section (σ) and the stimulation light intensity (I_0).

The 'Component Fitting' menu option will only be available when the cursor on the front window of Analyst is on a CW-OSL record. When the option is selected, the data for that OSL decay curve is shown both numerically (on the left hand side of the screen) and graphically. The user then selects how many components to fit and presses the Fit button. The example shown below is for record 6 of the SAR-1.BINX example file provided with Analyst.

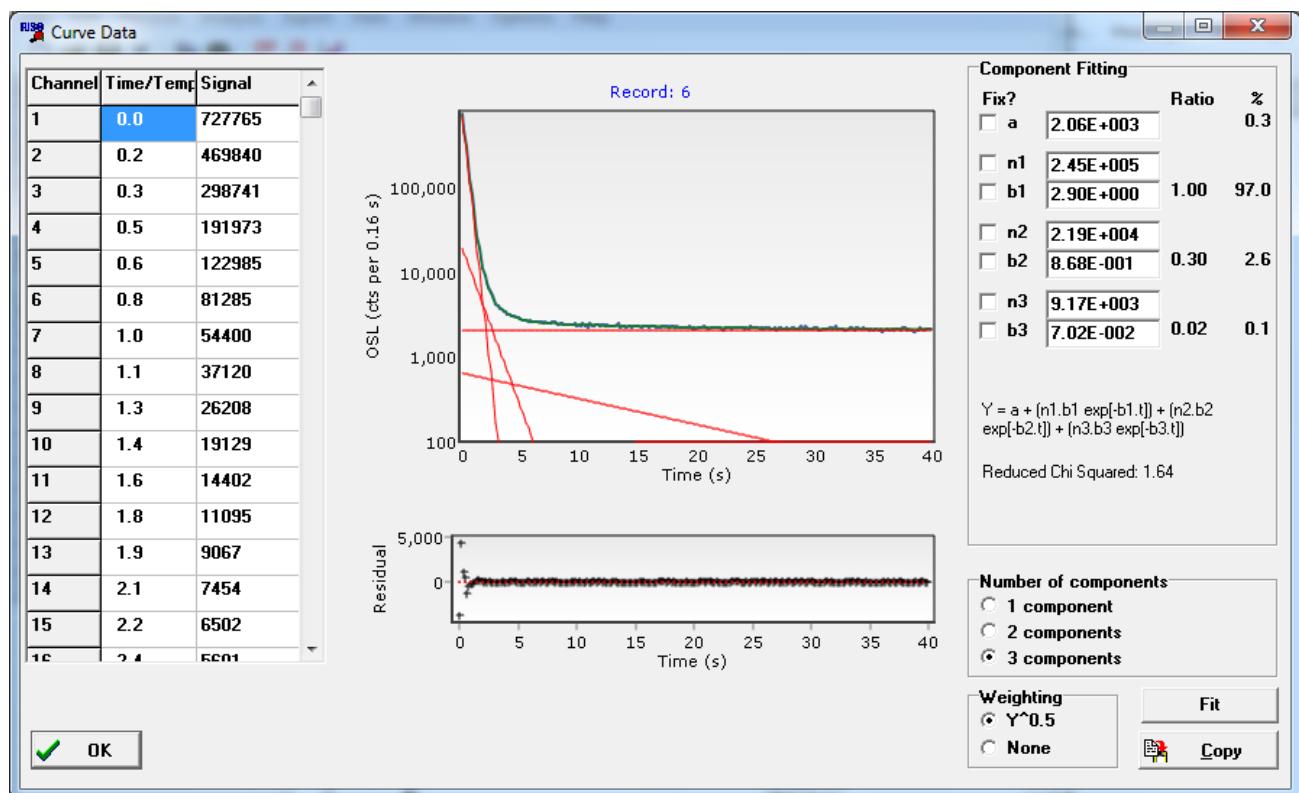


Figure 6.3(a): Example of using the component fitting tool to analyse a CW-OSL decay curve

Each individual component is shown on the main graph as a red line (these are straight in the example shown above since the y-axis is logarithmic by default) and the sum of these three individual components is shown as a green line (this is often difficult to see because it tracks the raw data closely and this is shown in black). The residuals (the difference between the fitted data and the measured data) are shown in the graph panel at the bottom of the page.

The numerical values of the fitted parameters are given in the panel on the right hand side of the screen (at present, Analyst does not provide uncertainties on these parameters). You can copy these parameters to the clipboard by pressing the 'Copy' button. This makes it straightforward to then paste the results into Excel or some other package. In addition to giving the values for the parameters, there are two columns to the right of the parameters labelled 'Ratio' and '%'. The values in the column marked 'Ratio' give the ratio of the b values to one another. Thus in the example shown above, the detrapping probability of the second component (b2) is 0.30 times the value of b1 and the detrapping probability of the third component (b3) is 0.02 times b1. The values in the column marked '%' looks at the values of signal intensity associated with each of the components (and the constant). Thus in the example above, 97.0% of the initial signal originates from the first component, 2.6% of the signal from the second component, and only 0.1% from the third component and 0.3% from the constant. The percentage (P) of the total signal at time ($t=0$) that originates from component i is calculated using the equation below:

$$P_{i(t=0)} = 100 \times \frac{n_i \cdot b_i}{[a + [n_1 \cdot b_1] + [n_2 \cdot b_2] + [n_3 \cdot b_3]]}$$

Altering the initial parameter estimates

When the Component Fitting window is shown, Analyst makes initial estimates of all of the parameters (a, b1, n1, b2, n2 etc) based on the data for that OSL decay curve (these estimates are simply made as a starting point for the fitting procedure). When the data are fitted, the Levenberg-Marquardt method optimises all of the parameters to best characterise the data. However, there will be sometimes when the LM method is unable to find a good fit starting from the initial value estimates determined by Analyst. In these circumstances you can alter the initial values of any of the parameters simply by typing new values into the boxes on the right hand side of the screen. Then press 'Fit' to see whether the LM method can find an appropriate mathematical solution.

Fixing parameter values

To the left of each of the parameters is a check box with the label 'Fix?' at the top of the column. By default these boxes are unchecked, meaning that the value for that parameter will not be fixed and that it will be optimised by the Levenberg-Marquardt method when the user presses the Fit button. However, there may be times when you want to fix an individual parameter. Perhaps you want to fix the values of b1 and b2 for a set of OSL data so that you can compare the n1, n2 etc values. Once you check the 'Fix?' box then the value for that parameter will not be altered by the LM fitting method.

Note:

- a) If the CW-OSL data was collected with a number of channels collected BEFORE optical stimulation was switched on and then some channels collected AFTER optical stimulation was switched off then the fitting will be applied only to the data collected whilst optical stimulation was active.
- b) At present it is not possible to undertake component fitting on LM-OSL data.

6.4 Fading Test

The measurement of anomalous fading outlined by Huntley and Lamothe (2001) is well suited to a single aliquot method. Analyst provides the opportunity to analyse a series of Lx/Tx values obtained after administering the same regeneration dose, but with the period of time between irradiation and measurement being varied.

The critical piece of information used to calculate the fading rate is the period of time between irradiation and measurement. This is stored in the BINX header in the parameter called 'Time since irr' and is the period of time between the start of an irradiation command and the start of the measurement command. This is set by Sequence Editor when the irradiation and the luminescence measurement are made in the same sequence.

For calculating the g-value the approach outlined in Auclair et al (2003) is used. The value t^* is used to denote the time since irradiation, and takes into account the fact that irradiation takes a finite period of time. The value of t^* is calculated using the equation below, with the values of t_1 and t_2 defined as shown in the diagram below taken from Auclair et al. (2003).

$$t^* = 10^{\left[\left\{ \frac{(t_2 \log t_2 - t_1 \log t_1)}{(t_2 - t_1)} \right\} - \frac{1}{\ln 10} \right]}$$

The diagram fits the change in L_x/T_x as a function of t^* to obtain the slope and hence the g-value. The g-value is normalised to a t_C of 2 days (Huntley and Lamothe 2001).

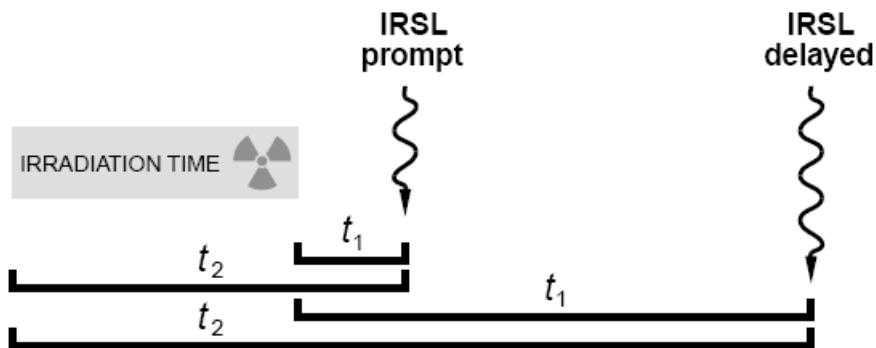


Figure 6.4(a): Illustration of time relationships relevant for calculating t^* (from Auclair et al. 2003).

In order to obtain the most accurate g-values it is useful to collect data spanning as many decades of time as possible. Thus a series of measurements with short storage times are made (for instance the prompt measurement shown above), and then longer periods of storage are used to increase the magnitude of the change in signal that is seen. Prompt measurements, and measurements with delay times of tens of hours, are easily done within a single sequence of measurements. However, making measurements for longer storage as part of an automated sequence on the Risø reader becomes wasteful of instrument time. Thus it is common to make the short measurements with a single sequence, and then irradiate aliquots before taking them out of the reader and storing them externally for days, weeks or months. After storage the IRSL delayed signal is read out in a second sequence, thus generating a second BINX file. To generate g-values using the combined data sets (both prompt and long storage), the two BINX files (or more if you make multiple long storage times) can be combined in Analyst to create a single BINX file. The 'Time Since Irr' entry in the second BINX file, and the irradiation time will not be set automatically since the instrument has no way of knowing this information. Thus the user has to enter this data manually. An example of this is shown below using data sets included with Analyst.

Example of fading analysis

In the example data sets included with Analyst are three data files demonstrating the use of the fading calculation (Fading_Prompt+1hr+10hr_delay.BINX and Fading_100hr+Prompt+1hr.BINX along with their associated .SEC files). The sequence file has been set up to run 'one at a time' so that the period between irradiation and measurement can be as short as possible for the prompt measurements. The sequence is to measure the IRSL₅₀ and the post-IR IRSL₂₂₅ signals.

In the first instance we may wish to look at records in the data file Fading_Prompt+1hr+10hr_delay.BINX for the post-IR IRSL₅₀ signal. We could [select which records to use for analysis](#) a number of ways, but a convenient way is to use the 'Temperature' parameter in the BINX files to

select only those records that were measured at 50°C. After opening the datafile, using '[Unselect all](#) | Every record' to set all the records to false. Then use 'Select all | Records of type...' and select 'Temperature = 50'.

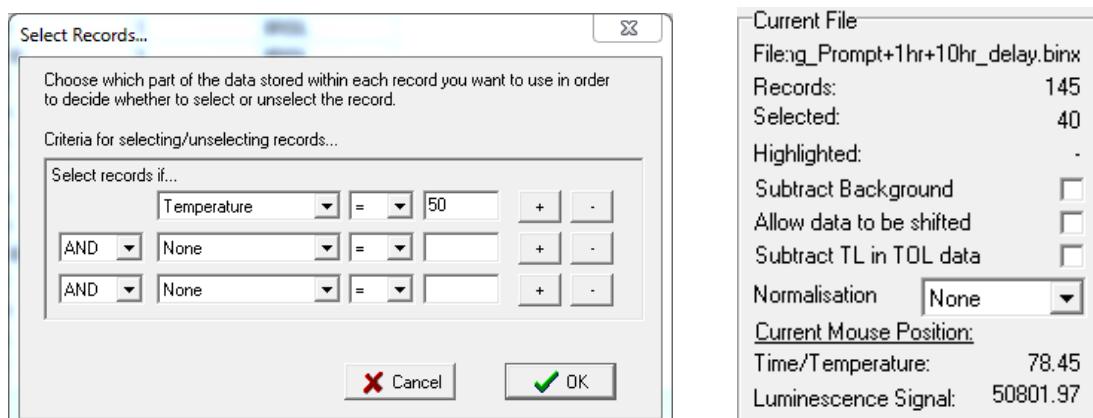


Figure 6.4(b): Left: Selecting records which were measured whilst holding the sample at 50°C.

The correct data is now selected (there should be 40 records selected, and this should be shown on the bottom left of the main Analyst screen, see above). This data can now be used to look at fading for the 5 aliquots measured. The results for aliquot is position 1 are shown below.

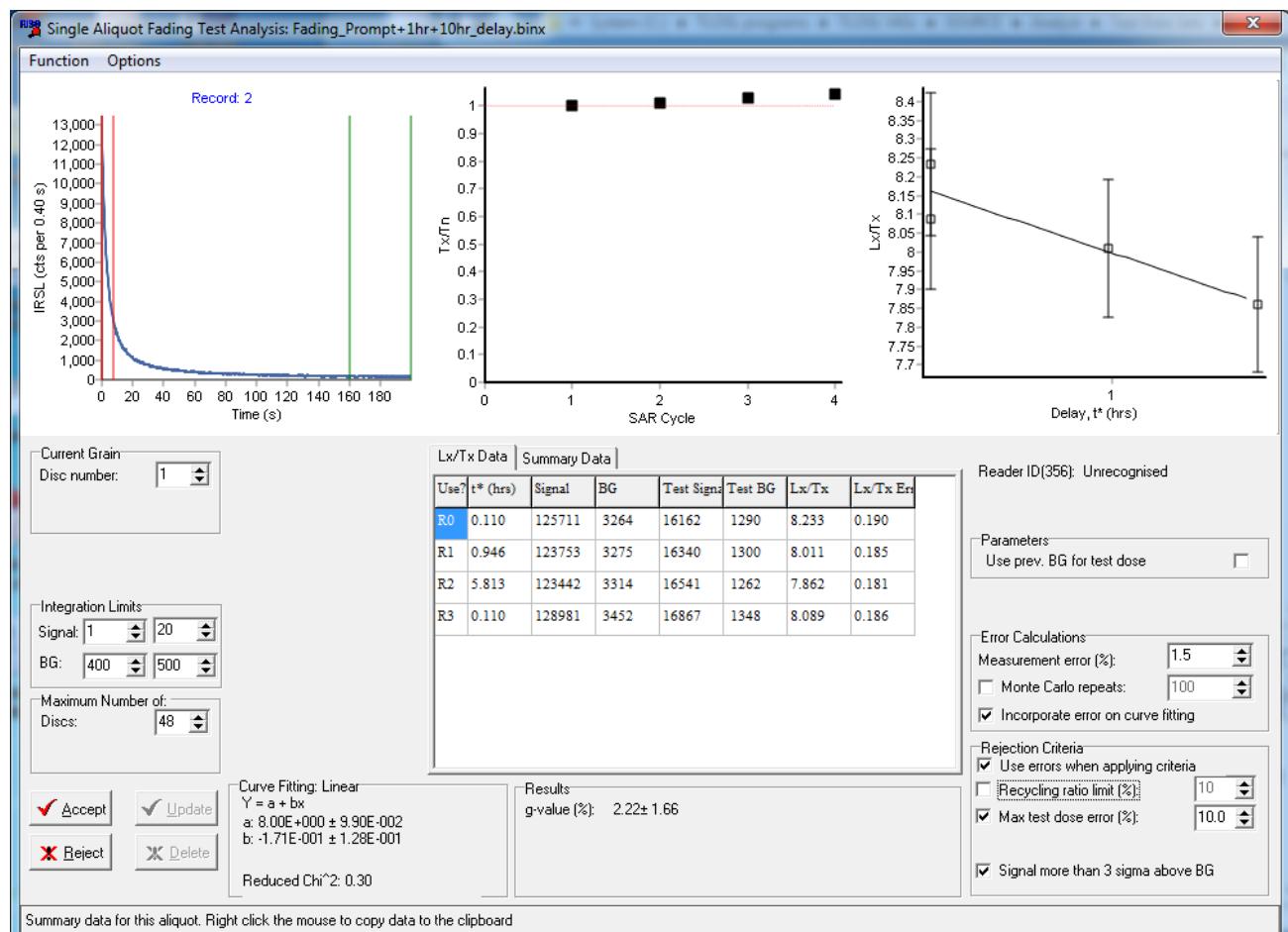


Figure 6.4(c): Fading data for one aliquot from the example data set provided with Analyst.

Better estimates of the fading rate could be made by extending the duration of storage, and the second BINX file (Fading_100hr+Prompt+1hr.BINX) has such data. At the end of the first sequence (Fading_Prompt+1hr+10hr_delay.SEC) the last operation was to irradiate the five aliquots for

460 seconds and preheat them (Set 7). The aliquots were then taken out of the reader and stored externally. They were replaced into the reader ~4 days later and the second sequence run (Fading_100hr+Prompt+1hr.SEC).

The first step in the analysis is to combine the two BINX files using the [Copy Highlighted Records](#) and [Paste Records](#) commands. Open the two BINX files that you wish to combine, then [highlight all](#) the records in the second BINX files (Fading_100hr+Prompt+1hr.BINX) and selected to [Copy Highlighted Records](#). Using the [Window menu](#), switch to the first BINX file (Fading_Prompt+1hr +10hr_delay.BINX), and then use the [Paste Records](#) command to add the data to this file. I would recommend that you then save this combined BINX data file with a different filename with the [Save As](#) command so that you have your original data sets intact. After combining the two data sets, you need to select only those records that you wish to analyse (in this example the IRSL signal measured at 50°C). The way of doing this was described above.

The second step in combining these two BINX data files is to set the time since irradiation and irradiation time for the measurements made in the second BINX file after the external storage (Set 1, Run 4 and Run 5). Because these were measured in a separate sequence, the Sequence Editor had no way of knowing what previous irradiation had been administered, or when. Thus the user has to add this information into the BINX file. The irradiation time is 460 seconds, so setting this value is straightforward. The time since irradiation has to be calculated by the user, and users will presumably maintain their own records. Information about the time of the last irradiation in the first sequence can be gained from the TL measurements made for preheating in Set 7 - in the example here, the last TL measurement for aliquot 1 (record number 141) occurred at 11:42 of 14th May 2014. The first IRSL measurement in the second BINX file was recorded at 15:25 on 18th May 2014. The time between those two measurements is 4 days, 3 hours and 43 minutes (358,980 seconds, or ~100 hours). The time since irradiation that should be entered in Analyst should also include the period of irradiation (460 seconds, making a total of 359,440 seconds) to make it comparable with the value automatically set by Sequence Editor (see start of this section).

The time since irradiation and irradiation time parameters can be set either using [Edit Record](#), or by typing directly into the main screen of Analyst as shown below for record 146.

Rec.#	Selected	Position	Run Number	Set Number	Irrad. Time	Lumin. Type	Temperature	Time since Irr.
139	False	9	9	6	50.00	IRSL	225	504
140	False	9	10	6	50.00	IRSL	290	802
141	False	1	2	7	460.00	TL	250	538
142	False	3	2	7	460.00	TL	250	538
143	False	5	2	7	460.00	TL	250	538
144	False	7	2	7	460.00	TL	250	538
145	False	9	2	7	460.00	TL	250	538
146	True	1	4	1	460	IRSL	50	359440
147	True	1	5	1	0.00	IRSL	225	-1
148	True	1	7	1	50.00	TL	250	128
149	True	1	8	1	50.00	IRSL	50	239
150	True	1	9	1	50.00	IRSL	225	503
151	True	1	10	1	50.00	IRSL	290	802
152	True	3	4	1	0.00	IRSL	50	-1
153	True	3	5	1	0.00	IRSL	225	-1
154	True	3	7	1	50.00	TL	250	128
155	True	3	8	1	50.00	IRSL	50	240
156	True	3	9	1	50.00	IRSL	225	504

Figure 6.4(d): Setting the Irradiation Time and Time Since Irradiation values for record 146 directly on the main Analyst screen

The same process would need to be done for the post-IR IRSL₂₂₅ measurement for aliquot 1 in record 147, and then the other 4 aliquots that were measured (records 152 and 153, 158 and 159, 164 and 165, and 170 and 171). In the BINX file supplied with Analyst that combined these two data sets, the time since irradiation has been set the same for all five aliquots. This is a rough approximation and users may prefer to be more precise about these calculations.

After combining the two BINX files, the data for aliquot 1 with the longer storage time (100 hrs) is shown below (Figure 6.4(e)). Also included are replicate measurements of the prompt and 1 hour measurement. Including data for this longer storage time has reduced the uncertainty on the g-value that was seen when using only the shorter storage times (Figure 6.4(c)).

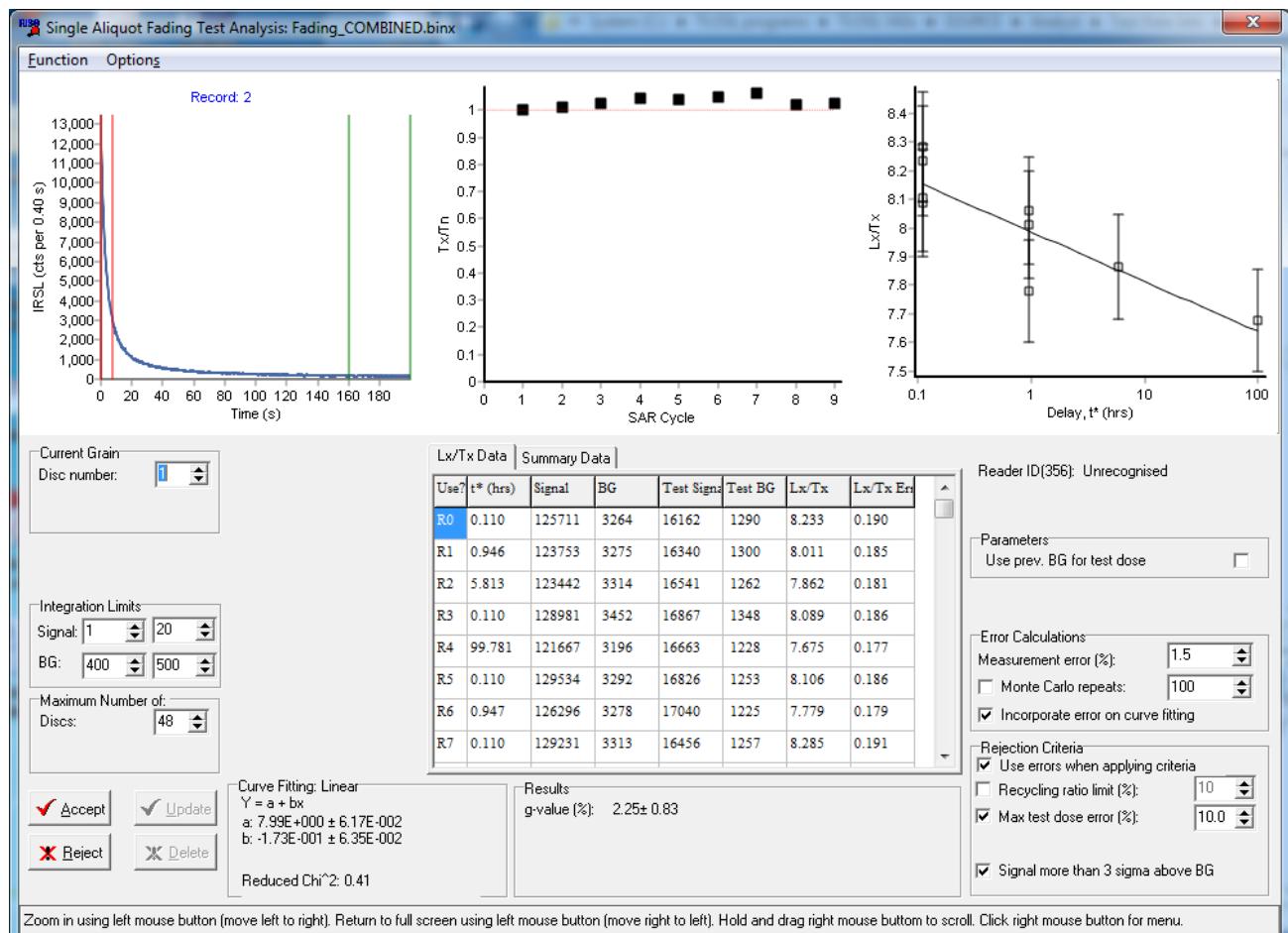


Figure 6.4(e): Fading data for the same aliquot as shown in Fig 6.4(c), but now with the additional data from the second BINX file.

6.5 Display

This menu provides a number of different options for visualising data from your BINX file.

6.5.1 Individual Curve Data

The numerical data for a single OSL decay curve or TL glow curve can be viewed in the 'Individual Curve data' option of the ['Analysis|Display'](#) menu. This option also offers the option to export the data to an ASCII file (see Figure 6.5.1(a)). This will display a list of the data for whichever record in the BIN file is currently highlighted. **Analyst** will display the channel number, the time or temperature represented by each channel, and the numerical data. **NB: This data is NOT normalised, temperature shifted, or background subtracted, regardless of what is currently set on the main display panel.**

To save the data to an ASCII file, click on the 'Save to file' button.

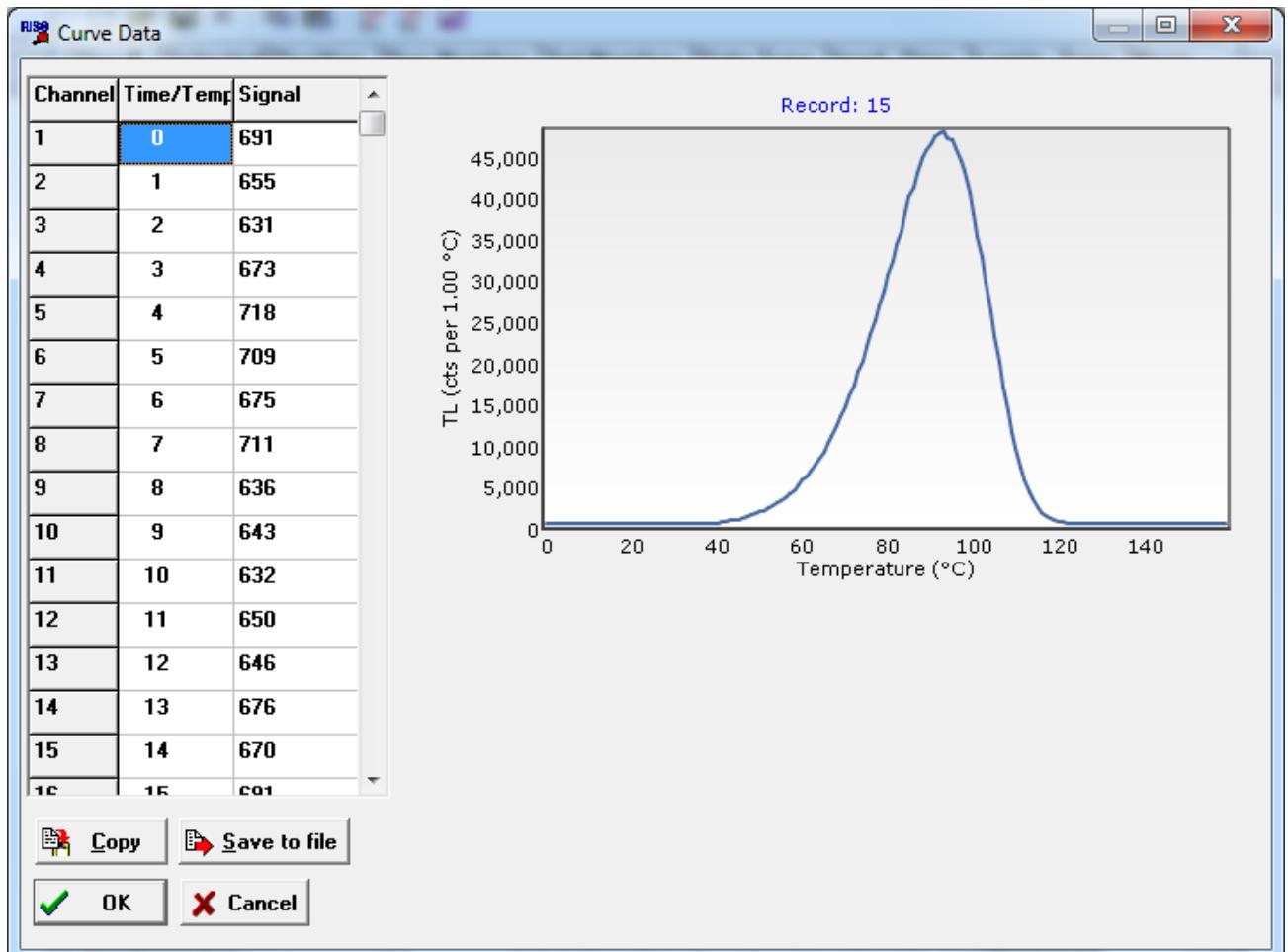


Figure 6.5.1(a): Outputting numerical data for a single TL glow curve

6.5.2 Plot Multiple Data

This option allows the user to create any number of graphs displaying multiple luminescence records. For instance one may wish to display all the TL glow curves collected for a single aliquot during a SAR run to check for the reproducibility of the heating. It is possible to have as many graphs open at a time as you like. Note that in this graph you can only display data of the same type (e.g. TL data). You cannot mix TL and OSL data, or other data types.

When first displayed, no data are shown. There are TWO ways of adding records to be display in this graph (A: Drag and Drop, or B: Import Records) and these are described below.

A) Drag and Drop

The first method for adding records to be shown in this diagram is to drag and drop a record from the main Analyst display. Select the record you want to move by clicking the left mouse button, and whilst holding the button down, drag the mouse to the graph. When you release the mouse button the record should appear in the display. The display below shows TL data from the SAR-1.BINX data file supplied with Analyst.

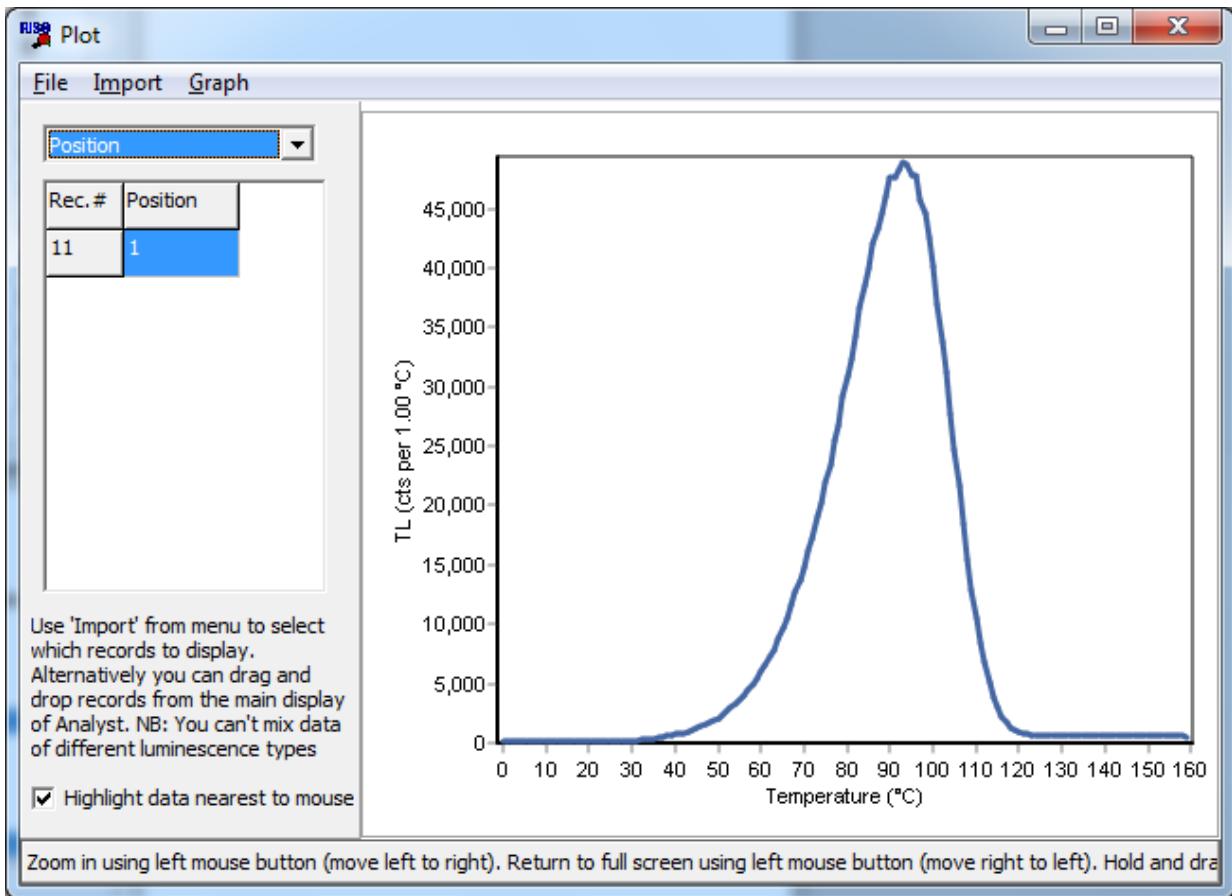


Figure 6.5.2(a): Plot option showing a single TL record

Additional TL records can be added. In the example below TL data from five different aliquots have been added. The default display is to show a legend displaying the carousel Position. However, any parameter from the BINX file can be selected using the drop down menu in the upper left of the screen.

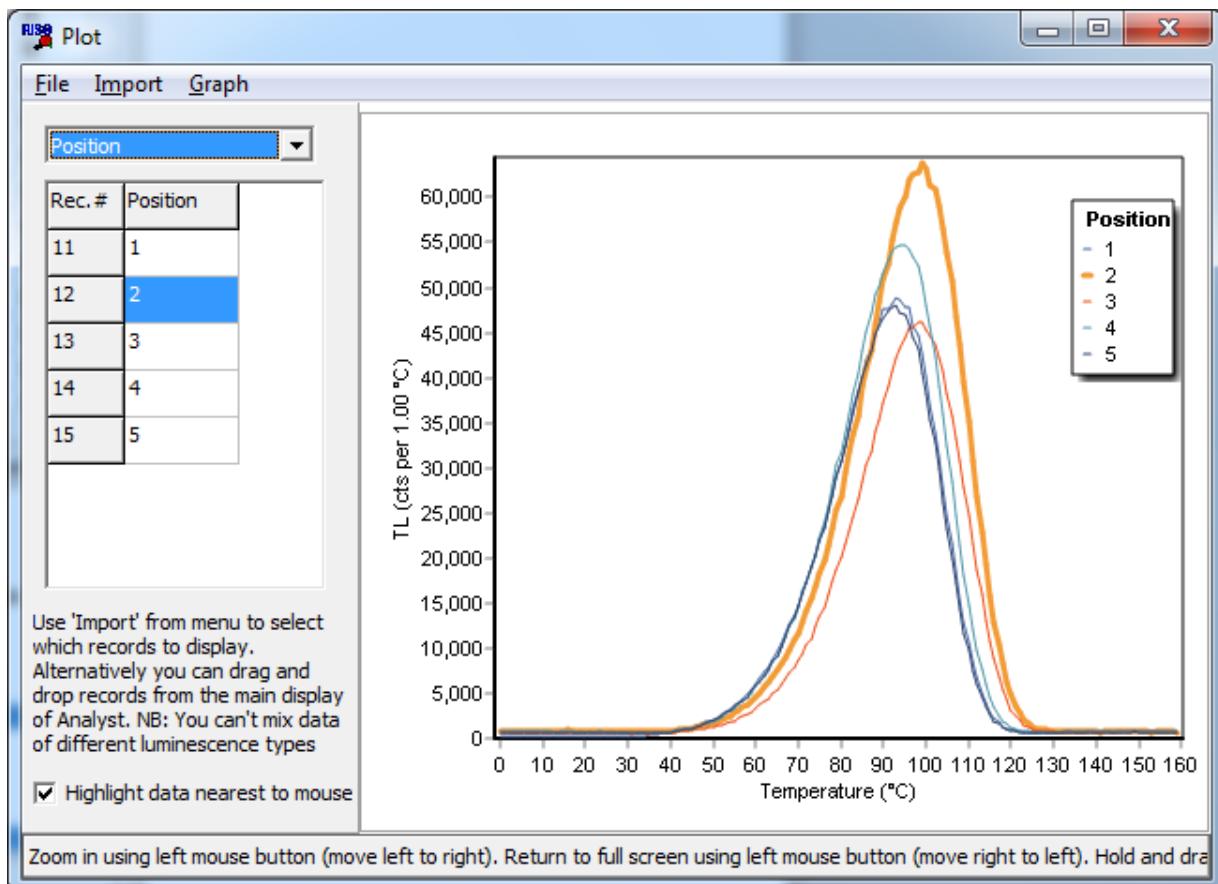


Figure 6.5.2(b): The plot page showing five TL glow curves for different aliquots

B) Import Records

Sometimes it may be easier to get Analyst to import records that match certain criteria. For instance in the SAR-1.BINX example file it may be useful to look at the TL measurements made on a disc after each of the test doses. These are in set number 6 (as can be seen using the [Sequence View](#)). Starting with a new graph, click on the 'Import' menu at the top of the screen and select to import records that have a Set number of 6, and are from Position 1.

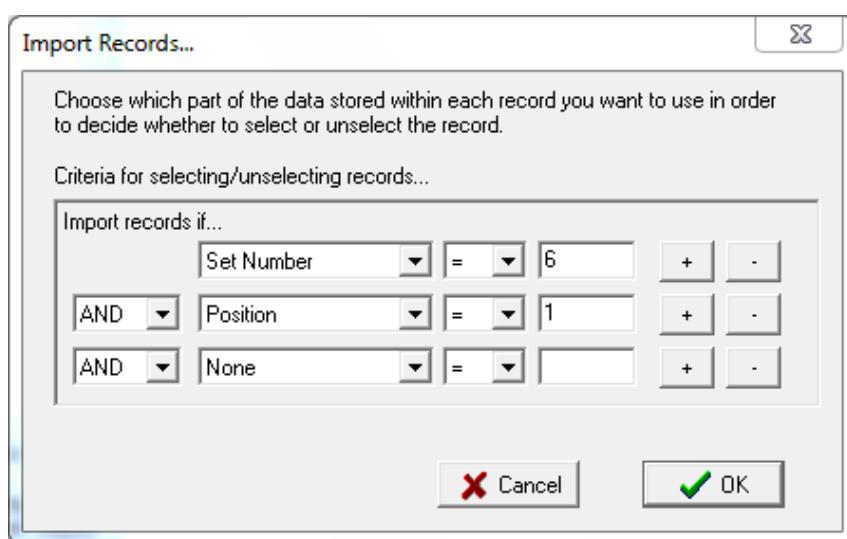


Figure 6.5.2(c): Selecting which records to import from the current BINX file

This will import 6 records. They will all have the same position number, so the legend will not be very useful. A more useful legend may display the Run Number. Change this using the drop down menu in the upper left hand of the screen.

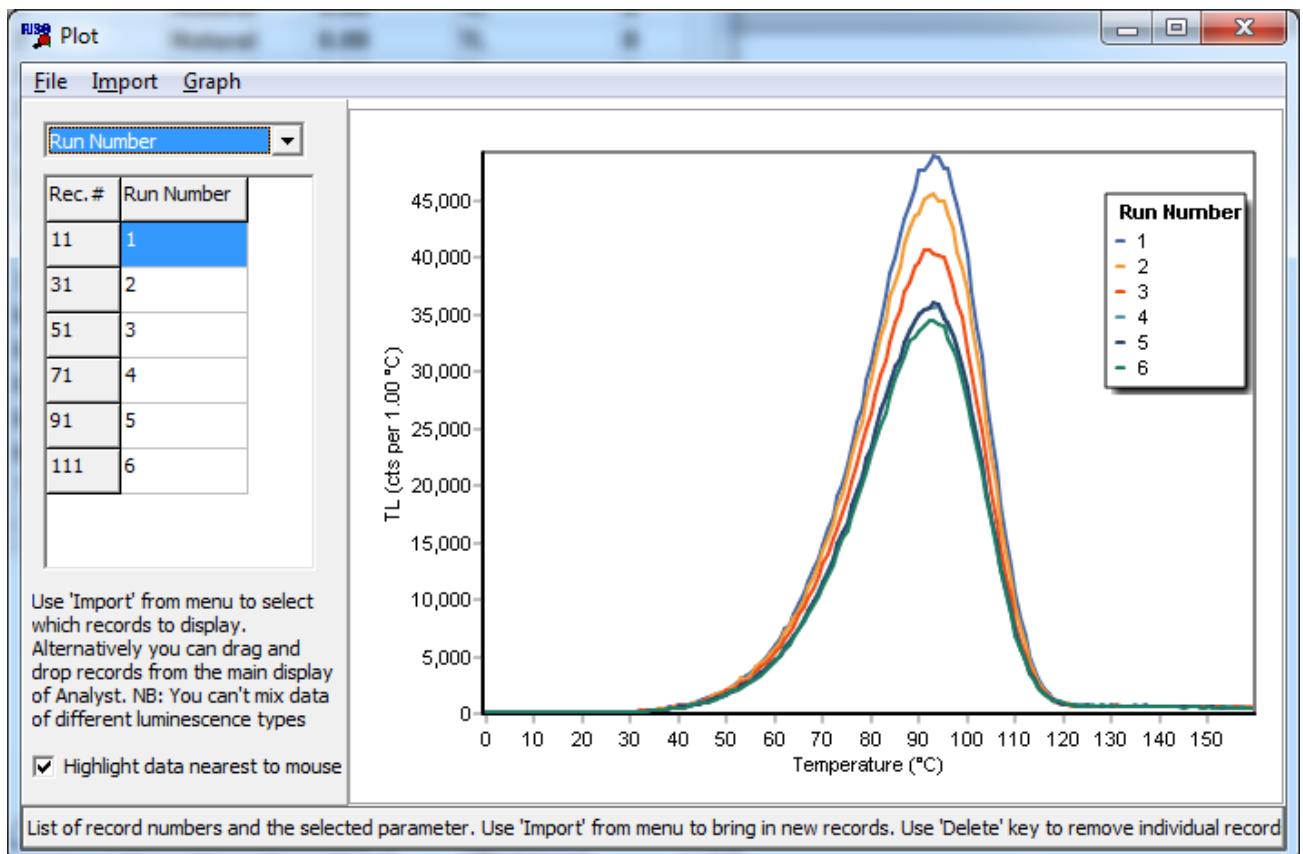


Figure 6.5.2(d): The graph produced from importing data using the criteria shown in the previous figure

Deleting Data

Individual data records can be deleted from the graph using the list of records displayed on the left hand side of the screen. Highlight a record (or many records) and press the 'Delete' key to remove these records from the display.

Saving and Recalling Chart Formats

Like other graphs in Analyst, the format of individual graphs can be altered. For instance you may want to display the luminescence data on a log scale (Figure 6.5.2(e)). If this is a format that you may want to use frequently then you can save this chart format to a file using the 'File|Save Chart Format' menu option. When you create another graph at a later date and want to use the same format you can then use the 'File|Open chart format' option to read the chart format back again.

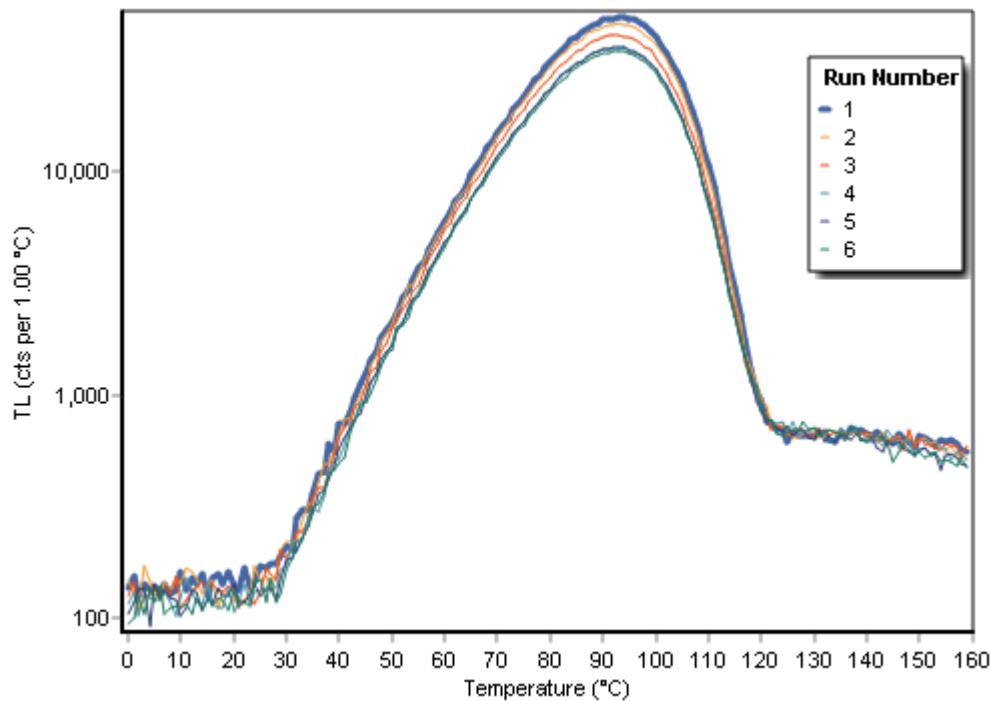


Figure 6.5.2(e): Many options are available for altering the way in which the graph displays data. In this case a logarithmic Y-axis has been used

6.5.3 Flexi Plot

This is the most flexible form of display. It allows you to plot a combination of any four parameters that are stored in the BINX file as a histogram (if you only select a variable to display on the X-axis and leave the Y-axis variable as 'None', or as a scatter plot (if you select a variable for both the X-axis and the Y-axis).

You can also select whether you want to plot all the data, or just that from certain records. For instance you can integrate data from two parts of a decay curve (say the first 2 seconds and the last 2 seconds), and then use FLEXI to plot these two integrals against each other.

6.6 Deadtime correction

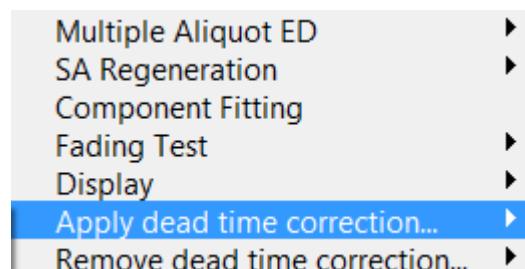
Photomultipliers used for the majority of luminescence measurements are only able to detect a single photon at a time. After a photon hits the photocathode a pulse is generated, and until this pulse ends, the tube is unable to register a second photon. The time interval during which the pulse is generated and the tube unable to register a second photon is known as the deadtime, and for the tubes typically used on Risø instruments, deadtime is between 20 and 30 nanoseconds (ns). The impact of this deadtime is that at high photon fluxes (i.e. as seen for bright signals) the PMT will undercount the true photon rate. The problem becomes more severe at higher count rates. For a PMT with a typical deadtime of ~25 ns the Riso manual recommends that count rates are kept below 5 million counts per second.

As described in the Risø user manual, it is possible to measure the deadtime for each PMT, and then to correct for deadtime mathematically. This allows measurements to be made to count rates of up to 20 million counts per second. The measured count rate (N_m measured in counts per second) in each channel of the luminescence data can be corrected for a deadtime (τ measured in seconds) to give the corrected count rate (N_c) for that channel using the following equation:

$$N_c = \frac{N_m}{1 - (N_m \times \tau)}$$

Within the [BINX file format](#), there are two entries in the header relevant to deadtime correction. 'DeadTime' is the value of tau (τ measured in seconds) for the PMT used to collect the data in a particular record. Typical values are bewteen 2.0e-8 and 3.0e-8 (20 to 30 ns). The other relevant entry in the header is 'DTEnabled'. If this has a value of zero then it indicates that the luminescence data have not been corrected for deadtime. If the value is 1 (or any other value) then this indicates that the luminescence data in this record have been corrected for the deadtime specified in 'DeadTime'.

Analyst provides the ability to apply, or remove, a deadtime correction to data in a BINX file. This can be applied to all the records in a BINX file, or just those highlighted by the user. To apply a deadtime correction the deadtime of the PMT has to be specified for each record (i.e. set the value for 'DeadTime' in the header of each record). This can be done various ways, as described in the sections on [Edit Current Record](#) or [Block Edit](#).

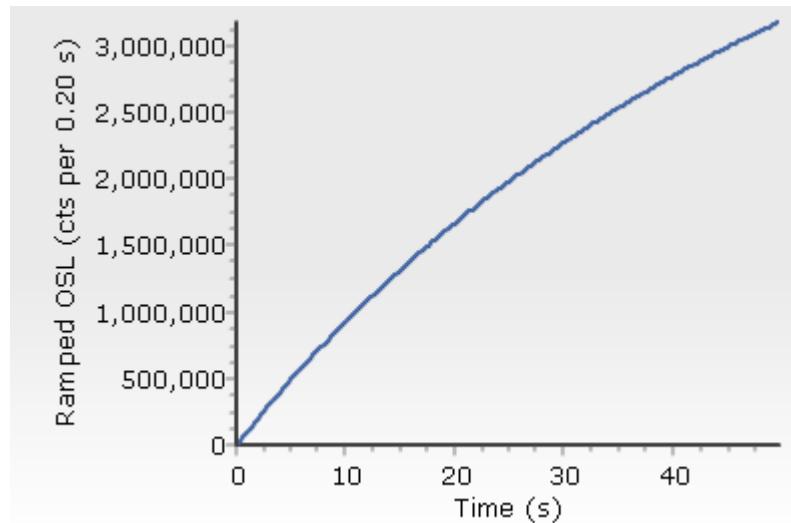


If you wish to remove the deadtime correction from a record, or group of records, then this can be done as well. The removal of the deadtime correction uses the following equation:

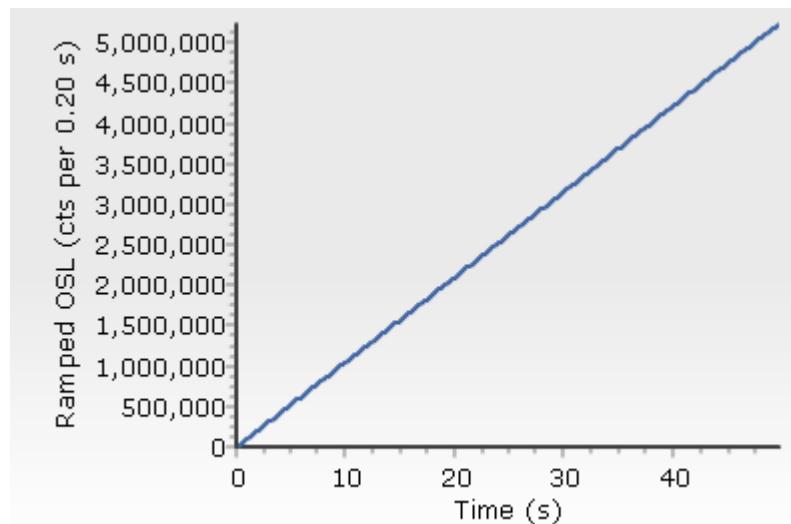
$$N_m = \frac{N_c}{1 + (N_c \times \tau)}$$

Note that luminescence data are stored as integer values, but the two equations described above will result in floating point values. The results of these calculations are rounded so that they can be stored as integers in the BINX format. Deadtime correction will therefore lead to a small amount of rounding. This will normally be negligible, but users are not advised to repeatedly apply and then remove the deadtime correction as this may lead to errors.

The impact of deadtime correction can be seen in the example below. Here an LM-OSL measurement was undertaken with blue LED stimulation and an NG9 filter in front of the PMT. Thus what is being observed is a small proportion of the blue light, not luminescence. The count rates here are high (3,000,000 counts per 0.2s, so 15,000,000 counts per second) and so the effect of the deadtime is substantial.



After applying the deadtime correction the data appear as follows. The linear increase in intensity of the blue LEDs that we would expect is now seen.



7. Export Menu

Two items under this menu heading allow you to take data out of Analyst for further analysis or graphing. These are '[Current Data Display](#)' to export data as it is displayed on the main Analyst

page and '[Group Averages](#)' allowing you to calculate the mean and standard deviation of groups of records as defined by the [Group Definitions](#).

7.1 Current Data Display

The most flexible method for exporting data is provided by the 'Current Data Display' option. Essentially, this allows you to export whatever you are currently displaying on the main screen.

Select whatever part of the BINX file records you want to export using the list of 'Display Information'. Once you are happy that you have the correct data displayed, select the 'Export| Current Data Display' menu item. This will give you a number of options as shown below.

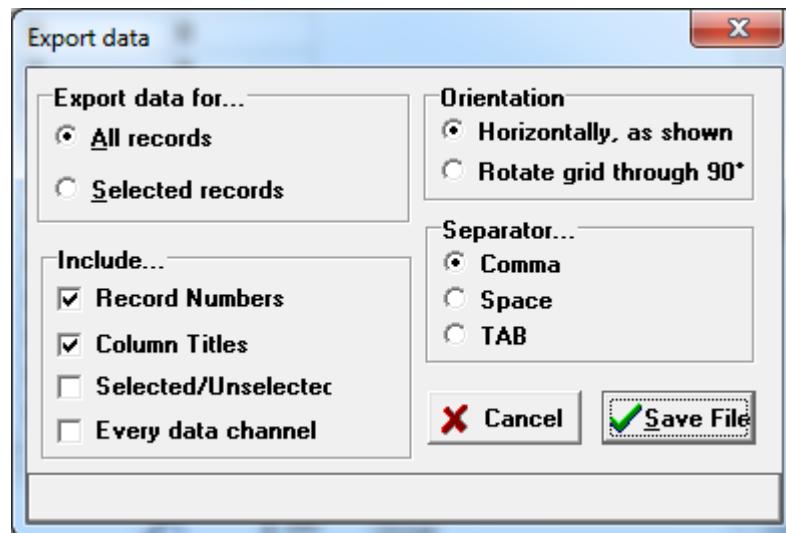


Figure 7.1(a): Export Current Data is the most flexible method of exporting data

7.2 Group Averages

Using the '[Group definition..](#)' option in the Options menu you can make Analyst assign each record to a specific group, based on the characteristics of the record (e.g. its irradiation time, data type, position on the carousel etc). This is useful for a wide range of operations. However, you may also want to calculate the integral luminescence signal from each group of records. This can be done using the 'Group Averages' command in the Export menu.

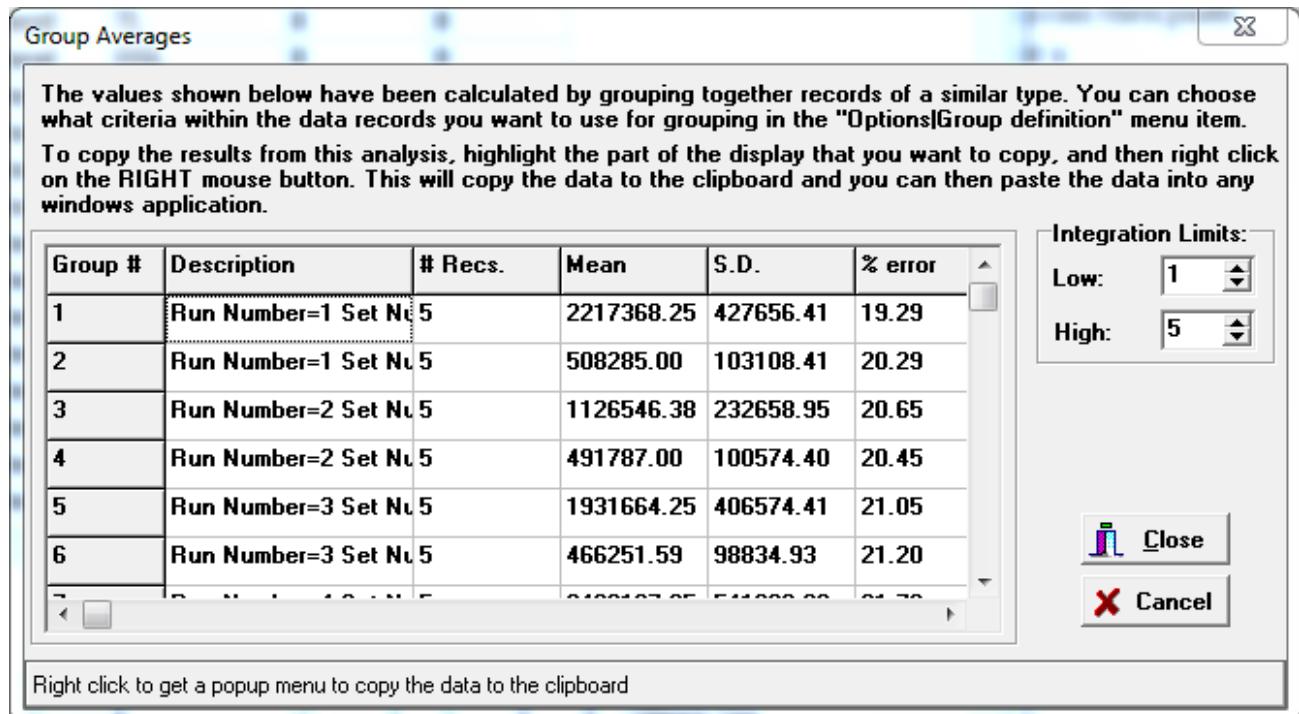


Figure 7.2(a): Calculating the integrals for each group of records

You can alter the range of channels over which you want to integrate the data using the boxes on the right of the screen. If you try to integrate beyond the range for which data are available then the integrals will be set to zero.

You can copy the data to the clipboard by highlighting the part of the display that you want to copy using the left mouse button and dragging the cursor, and then clicking on the right mouse button. This will copy the data to the clipboard and you can then paste the data directly into any Windows program such as a word processor or a spreadsheet.

8. View Menu

There are two ways in which it is possible to display luminescence data in Analyst: [Classic View](#) and [Sequence View](#).

8.1 Classic View

The normal display of data in Analyst is as a simple list, with each row of the display corresponding to a record in the BINX data file. The records are numbered sequentially and shown in the column on the furthest left of the display. As described earlier ([Section 2.1 Altering what information is displayed](#)), the choice of which details about each record (e.g. the carousel position, the type of luminescence etc) is made by selecting from list in the bottom right hand corner of the screen.

Whether a record has been selected for analysis or not is shown in the second column, and the data for the current record is shown in a graph at the bottom of the page.

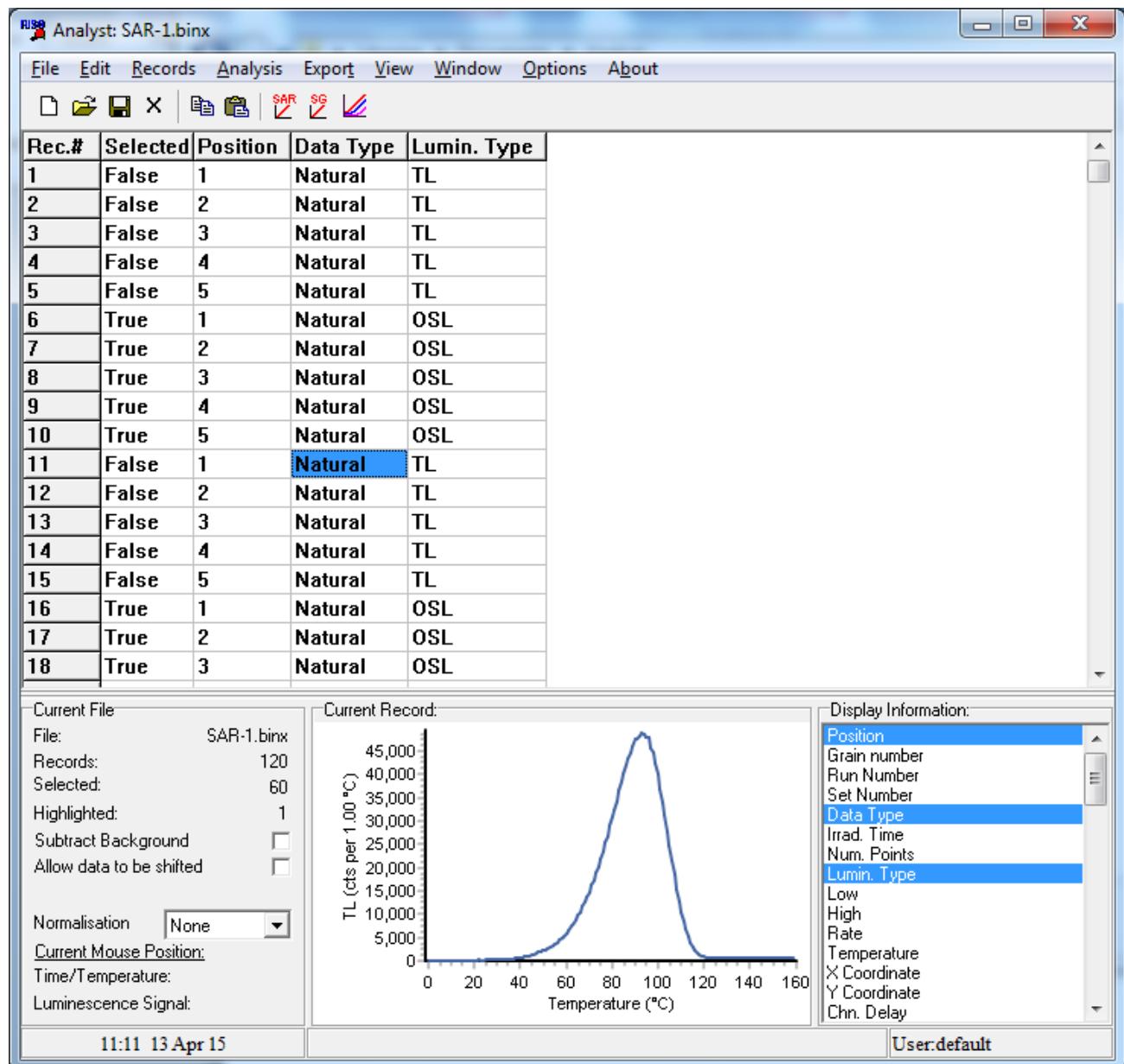


Figure 8.1(a) Main display shown in Analyst in 'Classic View'

8.2 Sequence View

It is sometimes clearer to visualise the BINX file that has been collected (and the data in it), but looking at the sequence used to collect the data. When the Sequence Editor is used to collect data, it creates a copy of the sequence file with a file ending .SEC (Sequence Copy). To use Sequence View you must have the SEC file and the BINX file for your data in the same directory. If Analyst is able to find the SEC file then the Sequence View option is available. When it is selected, the name of the sequence file is shown in the title of the Analyst window (SAR-1.SEC in the example shown below). If Analyst cannot find the SEC file then this option is greyed out and unavailable.

The sequence view is designed to look very like the view in Sequence Editor with sets running down the left hand side of the screen, and the run number along the top of the screen.

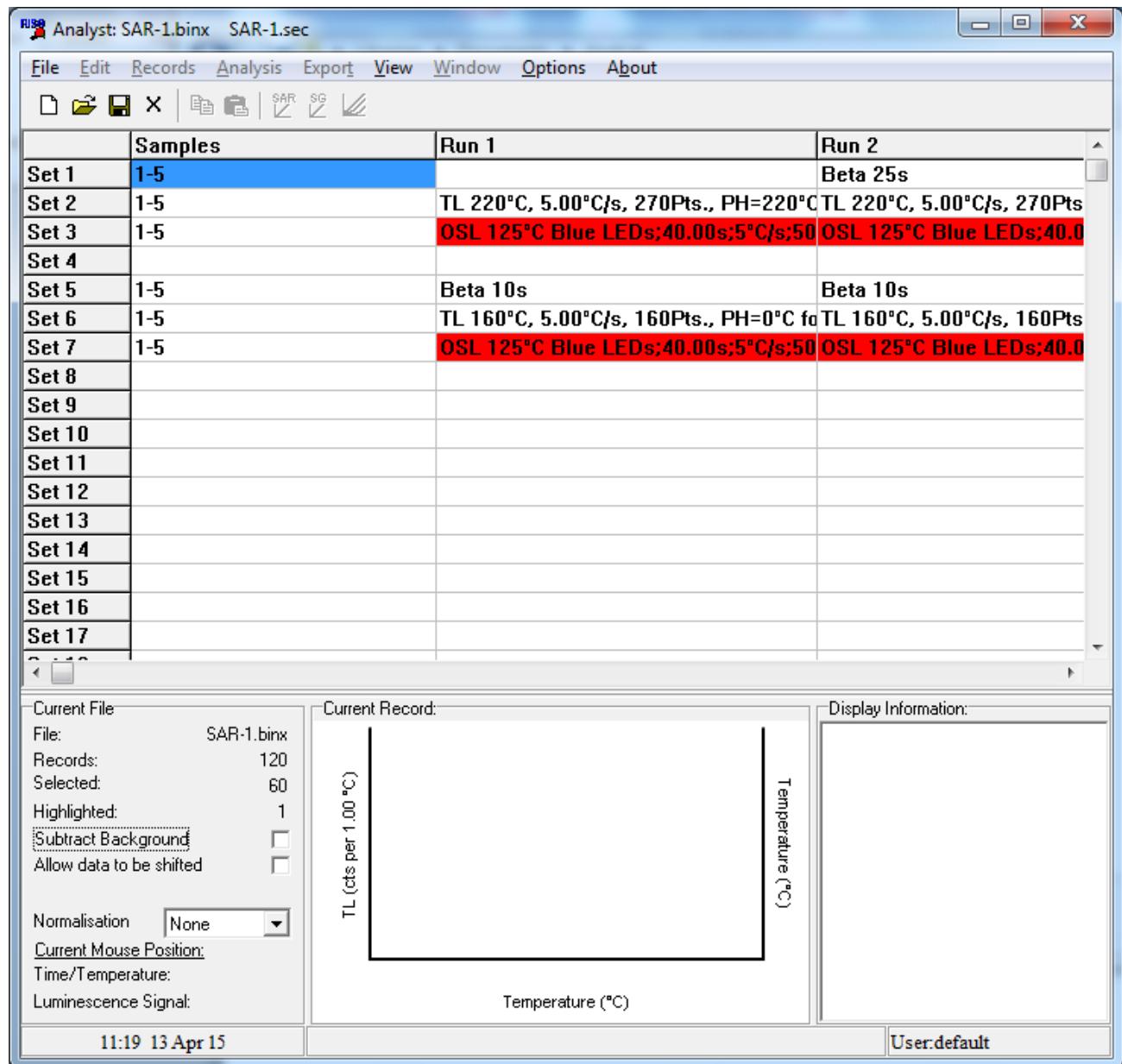


Figure 8.2(a): Analyst main display when the user switches to 'Sequence View'

When a cell is selected which did not collect any data in the sequence then the graph at the bottom of the screen and the box beside it, are blank. This is shown above where the selected cell is the list of samples for set number 1. When a cell is clicked on that collected some data (e.g. Set 7, Run 1), then the display changes as shown below. In the box in the lower right hand side of the screen is a list of all the data collected by this operation. In this case TL was measured for Disc 1, 2, 3, 4 and 5. By default the first data from this list is shown in the graph at the bottom of the page. Other data can be displayed on the graph by clicking on the names 'Disc 2', 'Disc 3' etc.

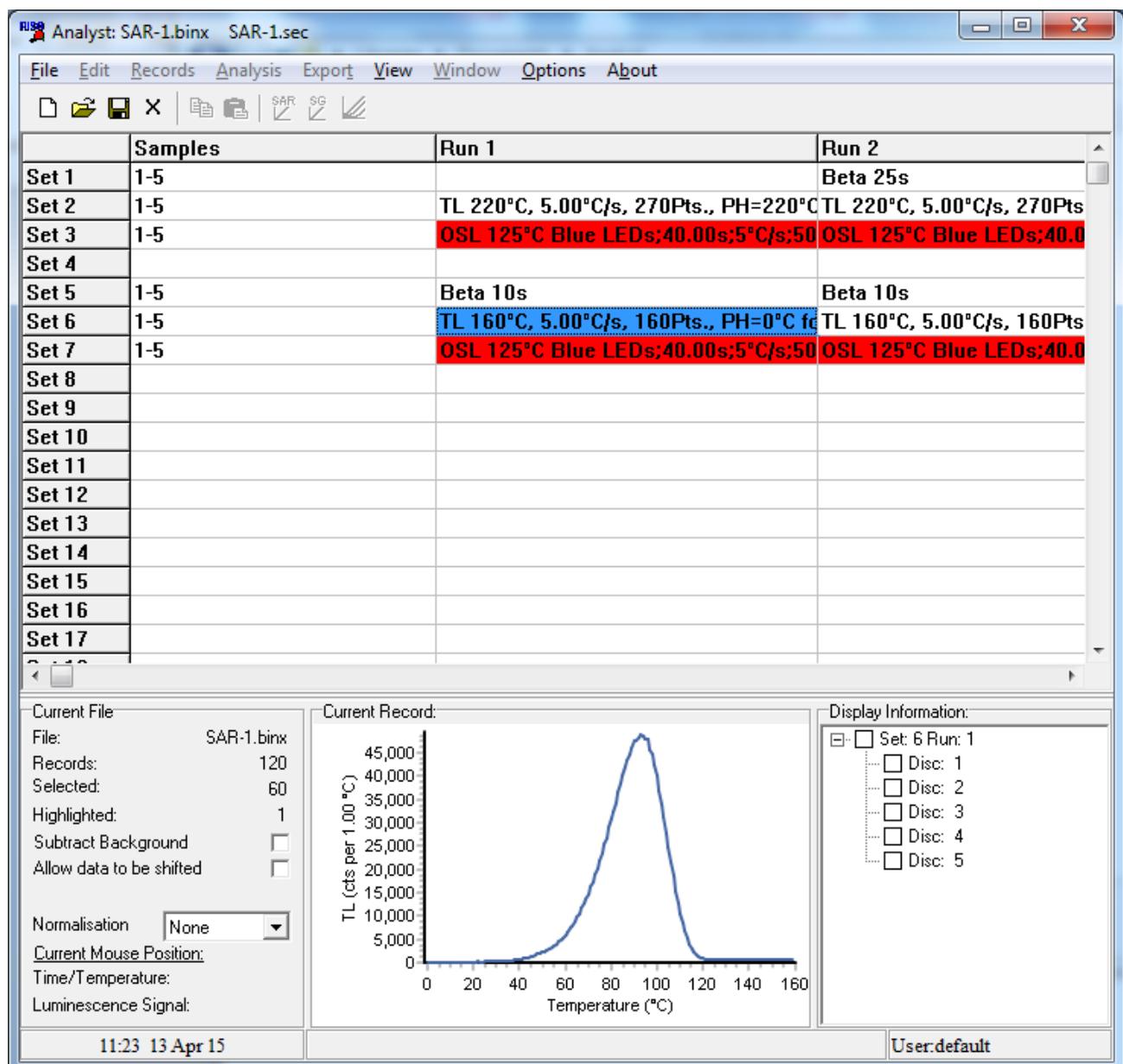


Figure 8.2(b): Sequence view - when a cell is highlighted that resulted in data being collected, a list of aliquots which were measured is given in the box in the lower right hand side of the screen (in this case discs 1, 2, 3, 4 and 5).

Selecting and Deselecting data

The Sequence View shows which data are selected for analysis by colour coding the display. Where a box is red (e.g. Set 3, Run 1) then at least some of the data collected in that operation have been selected. Where the box is uncoloured (e.g. Set 6, Run 1) then none of the records are selected for Analysis.

You can alter whether data are selected for analysis or not in two different ways using the Sequence view. To select or unselect individual records you can check or uncheck the boxes in the lower right hand side of the screen (e.g. discs 3 and 5 are selected below).

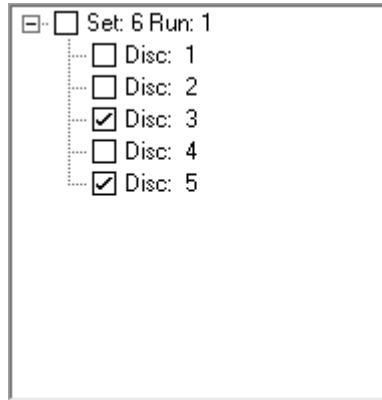


Figure 8.2(c): Using the box in the lower right hand side of the screen to select individual data records (shown with a tick in this figure)

To select or unselect all of the records that were produced by a command in the sequence, highlight the cell in the Sequence display and press the 'Insert' key on your keyboard to select all the records, or the 'Del' key to unselect them all.

Note that you need to return to [Classic View](#) in order to activate most of the menu options in Analyst.

9. Window Menu

You can open a maximum of 4 BINX files at any one time in Analyst. The files that are currently open are displayed if you select the Window menu. You can switch between the different files that are currently open by clicking on the appropriate filename.

10. Options Menu

This menu is always available to allow the user to alter a number of options for Analyst. The options are: '[Display Font](#)', '[Change User](#)', '[Group Definitions](#)', '[Define RScript location](#)', and '[Manage R scripts](#)'.

10.1 Display Font

The colour, size and font used to display information in the main part of Analyst can be altered using the Display Font option in the Options menu. The default font is 'System', Bold, font size 10.

10.2 Change User

You can change to a different user name during a session. This allows you to change the display format in a controlled manner. For instance you may set up one user name so that the main display in Analyst shows the irradiation time, data type and luminescence type, while another user name displays the position on the carousel, the time when data were collected and a series of other system parameters.



Figure 10.2(a): Window showing current user and allowing a choice of a different user

10.3 Group Definitions

An important facility within **Analyst** is the ability to assign records to a number of different groups. This is useful because often you will have made more than one measurement of a particular treatment etc. For instance, you may be undertaking a bleaching experiment where you want to expose samples to a particular light source for different periods of time. In this case you would use the [Edit Record](#) or [Block Edit](#) commands in order to set up the Bleaching Time parameter in the different records in the BINX file to whatever values you have used (0, 1, 2, 5, 10, 20, 50, 100 s for instance). Normally you will have measured more than one aliquot with each treatment. Therefore you may want to group together the aliquots which have had a similar treatment and look

at the behaviour of the group as a whole rather than individual aliquots. To do this, select 'Group Definitions...' (see below).



Figure 10.3(a): Window listing all the parameters available in a BINX file (see [Appendix A](#)) and which can be used to build groups

You are given a list of all of the parameters that are stored in each record of a BINX file. Initially all these boxes will not be selected. In order to define the groups according to the bleaching time, check the box marked 'Bleach Time' and press 'OK'.

Note that a record is only included in a group if the record has been [selected for analysis](#).

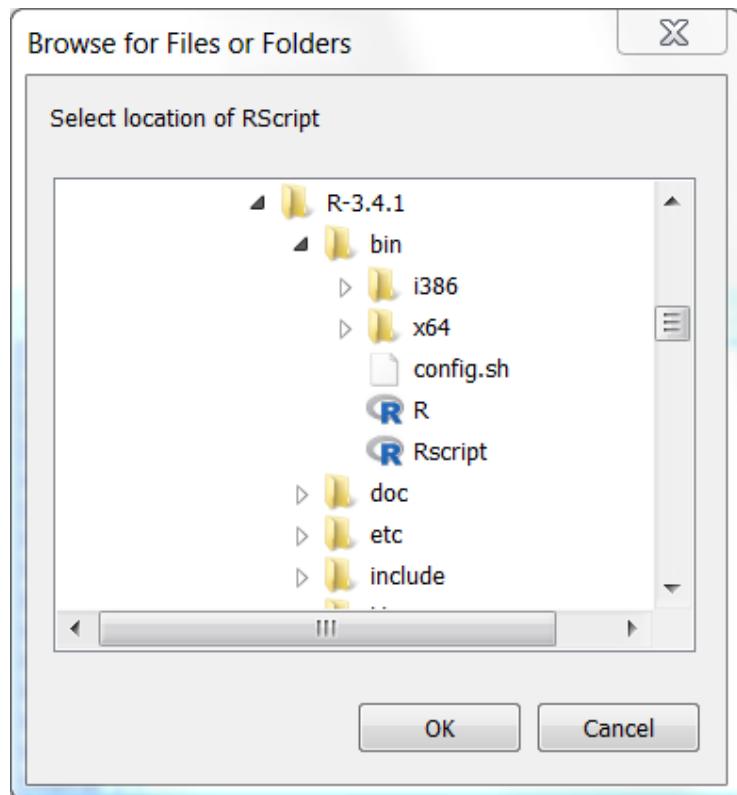
You can use the group definitions in a number of the analytical tools within Analyst, including [displaying the mean and standard deviation of an integral of a group](#).

10.4 Directories

This option allows you to define the directories used by some of the R functionality in Analyst

10.4.1 Define RScript location

You should not need to use this option. Analyst should automatically detect if R is installed on your computer. However, if this does not work then you can use this dialogue box to show Analyst where R is installed. The specific file that Analyst needs to find is "RScript.exe". Select that file and then press "OK" in the dialogue box below.



10.4.2 Define Script Library location

By default the file containing all the R scripts for Analyst is installed in your 'My Documents' folder under a folder called 'Analyst/RScripts'. However, if there is a problem with your installation, or if you wish to have multiple R libraries then you can define the location of the R Library (.rlb file) to be used by the current user of Analyst with this menu. Further information is given in the section on [How to manage R for Analyst Libraries](#).

10.5 Manage R scripts

This launches the R script interface window. From this window you can view, edit, delete or run scripts. Further information is given in the section on [R support](#).

The screenshot shows the R Script window with the title bar "R Script". The menu bar includes "Select Script", "Run Script", and "Manage Scripts". The main area contains the following R script code:

```
#=====
# Name: List_SAR_data_fields
#
# Purpose: List the data fields exported from SAR in Analyst
# so it is clear what data fields are available
# An explanation of what data is in these fields is
# in the Analyst manual (available by pressing F1)
#
# GAT Duller, August 2017
#=====
#
# Read data file exported by Analyst
LumData <- read.delim("AnalystDedata.txt",sep="\t",header=TRUE)

# Show the structure of the object, listing the names of the
# variables exported by Analyst, their type and some example values
str(LumData)
```

The right side of the window has a "Variables" panel. Below the main area is a "Plot" pane which is currently empty. At the bottom left, there is a status bar with the text "RScript: List_SAR_data_fields".

11. Help Menu

11.1 About

You can check the version number and the build date in this menu. Please include this information if you make any enquiries about this programme.

12. R support and use within Analyst

R provides enormous flexibility in the analysis and presentation of data. Analyst is now able to run R scripts to take advantage of this flexibility and power. The implementation is designed to be simple to use, but to have enough flexibility to enable powerful analyses to be undertaken.

A script is simply a list of instructions for the R interpreter to undertake. It may be a single instruction (and hence a single line of text), or it may be many tens of hundreds of instructions covering many lines of text. These commands allow manipulation, analysis and plotting of data.

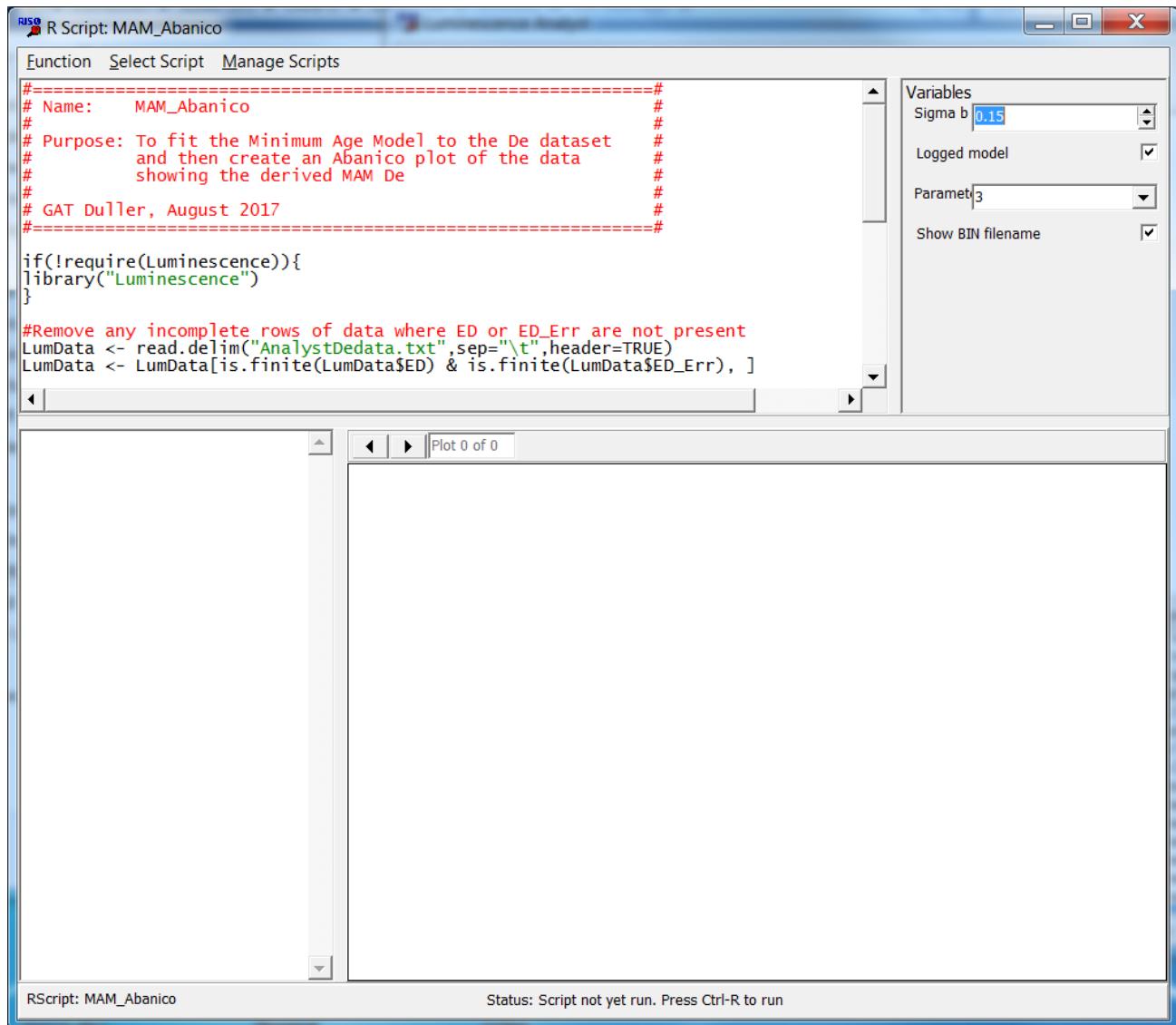
A number of simple R scripts are included with Analyst and should be available to all users if they have used a Setup.exe file to install Analyst.

The example script files take advantage of a range of functions written by the R.Luminescence group (http://www.r-luminescence.de/en/plot_en.html) which are bundled together in the package "Luminescence" that is available on R servers such as CRAN. Other R packages can also be used.

[Installation of R and the Luminescence package](#) have already been discussed in this manual.

12.1 How to run R scripts

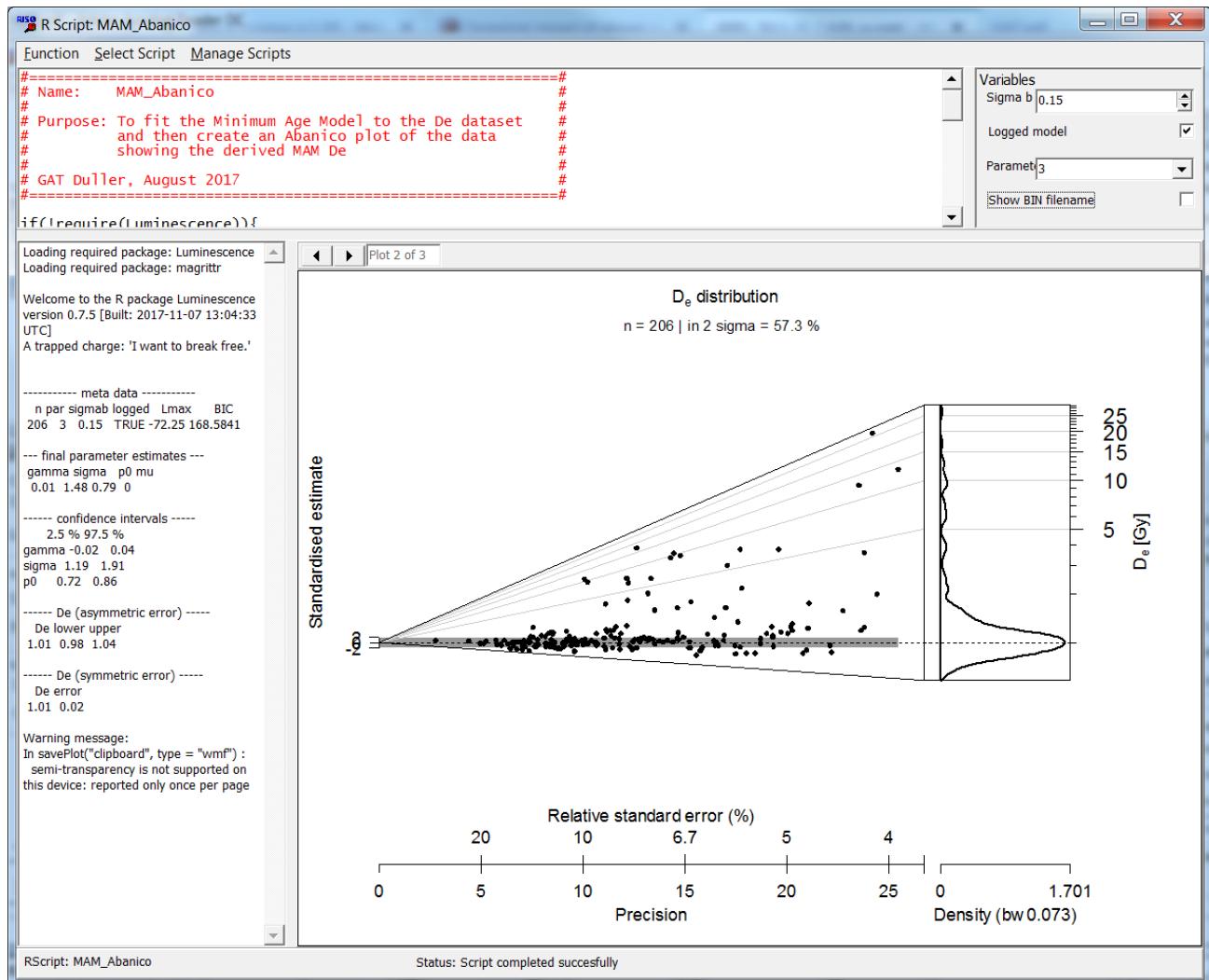
R scripts are run from the script window. This automatically shows the last script that has been used (in this case it is called "MAM_Abanico", shown in the bottom of the window). The list of available scripts is given in the "Select script" menu at the top of the window. Clicking on the name of the script will automatically load it into the script window.



In the script window, simple colour coding is used to make reading of the scripts easier. The "#" symbol is used to mark a comment (and which is ignored by R when running the script), and any text in a comment is highlighted in red. Extensive use of comments is encouraged to clarify the purpose of each section of the script. Items in green are text strings rather than instructions.

Running the script is very simple. Once the script that you want to run is loaded from the "Select script" menu, pressing the "Function" menu and then the "Run script" menu item will send the script to R. A shortcut of "Ctrl-R" will also do the same thing. When the script is running, a message will appear to that effect at the bottom of the window, and output from the script will appear in the panel in the lower left hand of the screen.

A graphical window may appear temporarily, but you can ignore that. The final graphical output will appear in the "plot" window in the bottom right of the screen.



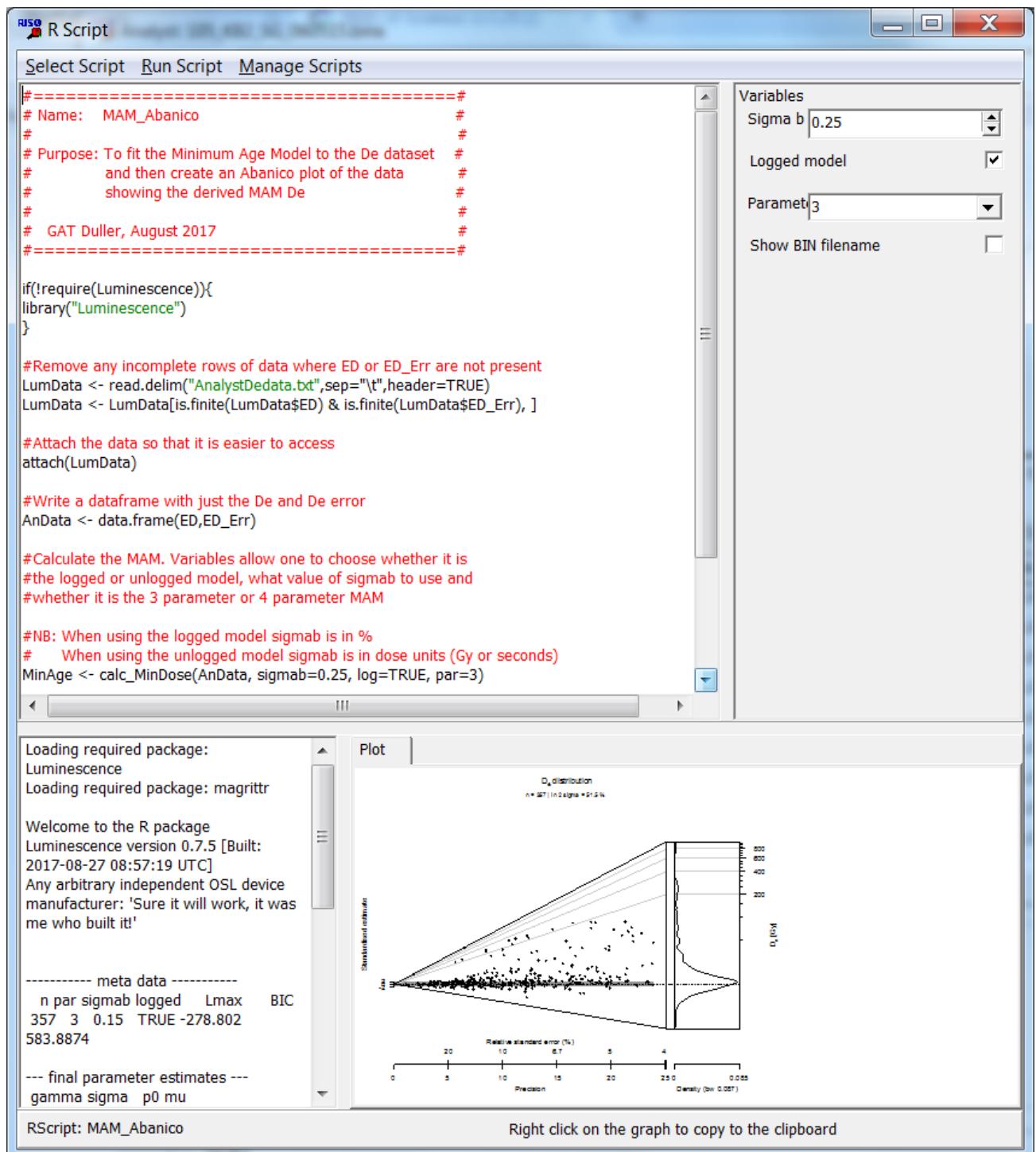
This script has run the 3-parameter minimum age model of Galbraith et al. (1999) using a sigma-b value of 0.15. The calculated MAM D_e value is 1.01 ± 0.02 Gy (shown in the lower left hand panel). The script has also plotted the D_e data on an Abanico plot ([Dietze et al. 2016](#)). When you first run the script the graphical output may appear to small. You can resize the window to enlarge the plot with no loss of quality in the graphics. You can copy the graphical output to the clipboard by right clicking the mouse while you are over the plot window. This will put a Windows Metafile (WMF) copy of the plot onto the clipboard and this can be pasted into many other packages.

Variables

A feature of R scripts in Analyst is the ability to define variables. This gives users a simple way to vary aspects of the script that are changed very often, without having to directly edit the script. In the example shown above, four variables have been defined (see [How to edit and create your own scripts](#) for details of how to define your own variables) and these are shown in the upper right of the window. The first variable has the title "Sigma b" and has been given the value 0.15 above. For the MAM, the value of sigma_b used for fitting is critical, and often it is interesting to see what impact varying sigma b has upon the final D_e. In this case the value 0.15 can be edited by the user in the upper right of the screen to any other value (e.g. 0.25) and as the value is changed in the upper right of the screen, the value is changed in the script - in this case about 20 lines down, in the last line of code visible here:

```
MinAge <- calc_MinDose(AnData, sigmab=0.25, log=TRUE,par=3)
```

The script can then be rerun by pressing Ctrl-R, or selecting "Run script" to see what the result is of using a different sigma b value.



In this example script the other variables control whether the logged or unlogged minimum age model is used, whether the 3-parameter or 4-parameter model are used, and whether the name of the BIN file is displayed on the plot.

12.2 How to manage R for Analyst Libraries

The R scripts available within Analyst are stored in a R Library file (with a .rlb extension). The default library is called RScripts.rlb and is normally installed in your 'My Documents' folder under a subfolder called 'Analyst/RScripts'. If there is a problem with your installation, or you want to place a library in a different location then you need to show Analyst where the R Library file is located. This

is done using the Options menu on the front page of Analyst, and the option under 'Directories' to '[Define R script library location](#)'.

Analyst allows you to either use the same library of R scripts for all of your projects, or to have different sets of R scripts that are used for different user names. To create a new R Library (.rlb) file, use the 'Option | Directories | Define R script library location' function and choose the directory and filename that you want to use for a new R Library. This will create a new library, populating the library with a set of basic scripts (you can delete these if you do not want them). You can either write new R scripts here, or if you want to transfer scripts from other libraries you can [export individual scripts](#) as .RAN files and then import them into the new library.

12.3 How to get graphical output from R scripts

One of the powerful aspects of R is the rich variety of graphical tools available for visualising data. In Analyst the graphical output produced by a script is easily available as a series of pages. You can switch between each page using the arrow buttons. Scripts are also provided with Analyst that show how to export graphical output to a file, either as a JPEG or PNG file.

12.4 How to edit and create your own R in Analyst (RAN) scripts

It is very likely that you will want to make changes to the scripts that are supplied by Analyst, or that you get from other researchers. To edit an existing scripy you should select the script from the "Select Script" menu. Then choose the "Edit script" option from the "Manage scripts" menu. This will copy the script to a new window "R Script Editor" where you are able to edit the script, and the variables. If you wish to create an entirely new script then you can select the "Create script" option.

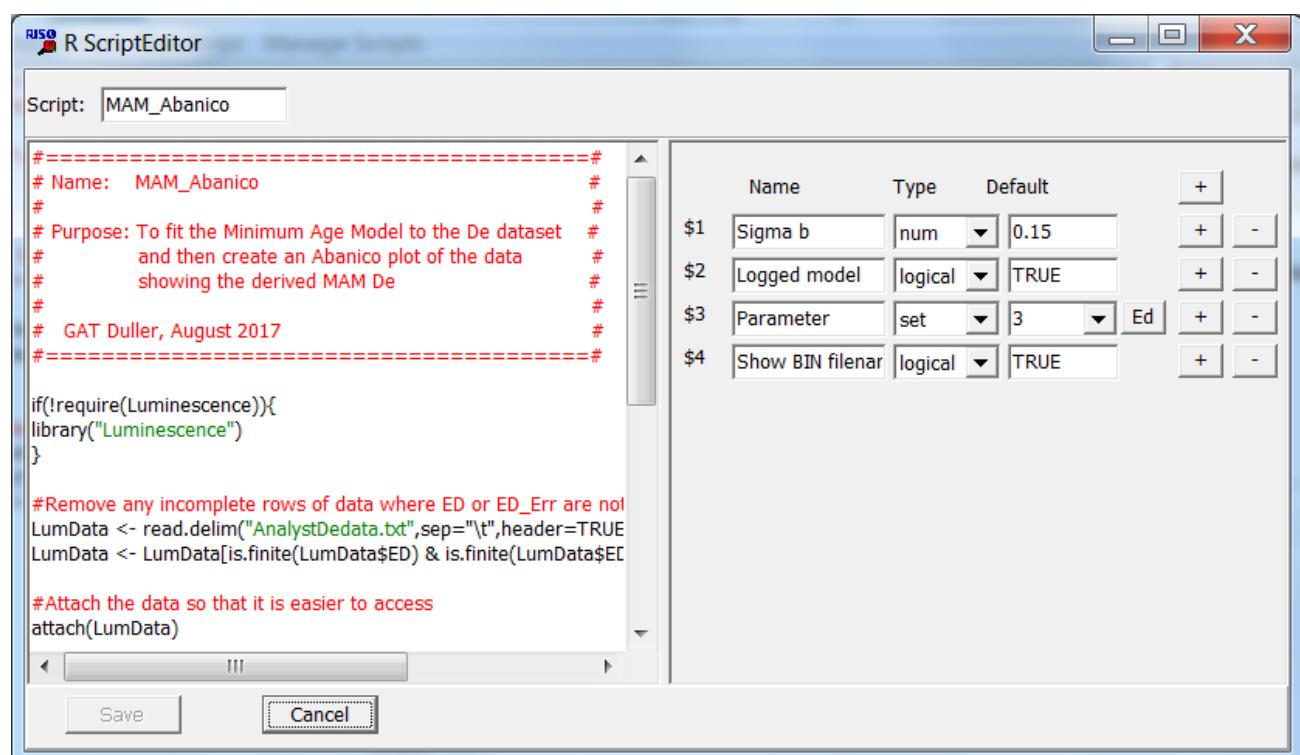


Figure 12.4: The R script editor, showing the MAM_Abanico script, and the variables that have been defined for use in this script.

12.4.1 Change the name of an R script

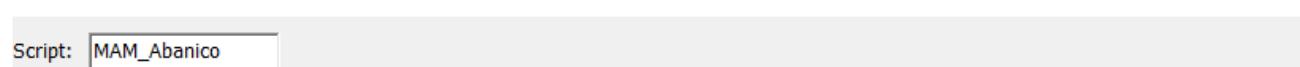
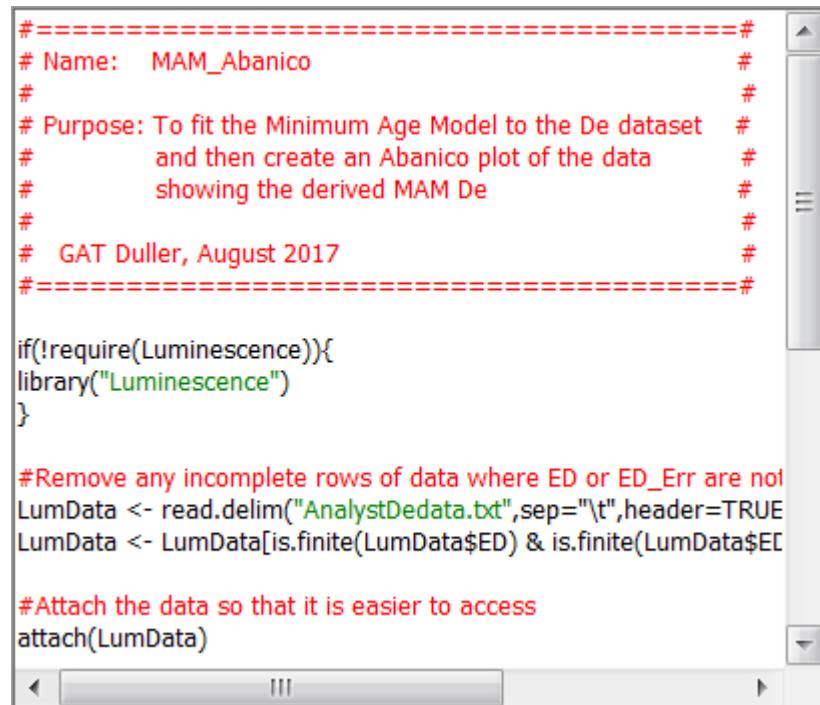


Figure 12.4.1: Text box to edit the name of the R script

To change the name of the script, simply edit the text in the box shown in the upper left of the window.

12.4.2 Edit an R script



The screenshot shows the Analyst software's editor window. The code in the editor is as follows:

```
#=====#
# Name: MAM_Abanico #
#
# Purpose: To fit the Minimum Age Model to the De dataset #
#           and then create an Abanico plot of the data #
#           showing the derived MAM De #
#
# GAT Duller, August 2017 #
#=====#
if(!require(Luminescence)){
library("Luminescence")
}

#Remove any incomplete rows of data where ED or ED_Err are not
LumData <- read.delim("AnalystDedata.txt",sep="\t",header=TRUE
LumData <- LumData[is.finite(LumData$ED) & is.finite(LumData$ED

#Attach the data so that it is easier to access
attach(LumData)
```

Figure 12.4.2: The editor window

To alter the script itself, simply type in the box on the left of the screen. As you type, colour formatting will be applied. Note that unlike environments like RStudio, there is no autocomplete, or context sensitive help. If you wish to develop complex scripts then this is much better achieved in dedicated R environments such as RStudio.

Help can be found on the web at a number of sites, including at <https://www.rdocumentation.org/>. If you type "Luminescence" you will get help on this package and a list of the functions available.

12.4.3 Accessing data from Analyst in R

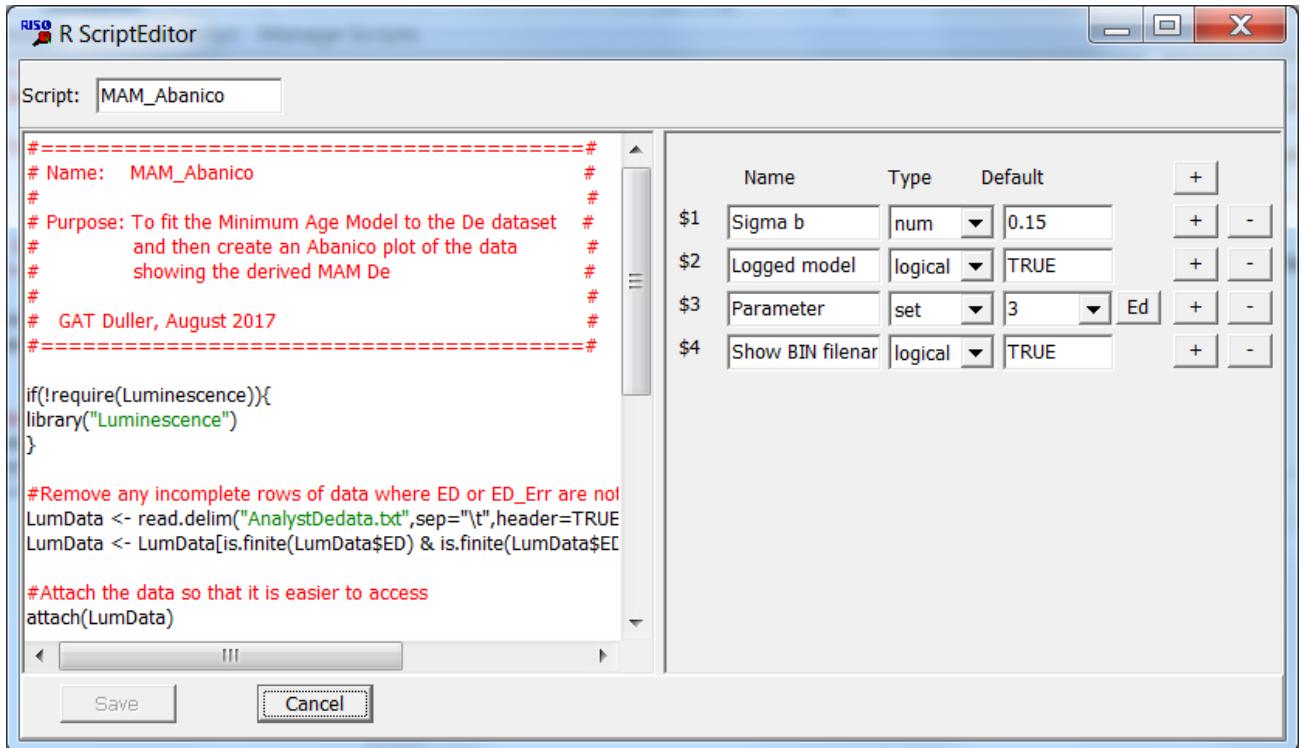


Figure 12.4.3: The R script editor, showing the MAM_Abanico script, and the variables that have been defined for use in this script.

Analyst exports data to an ASCII text file to make it available to R scripts. Thus most R scripts will start by reading this data file into R. The data file produced by Analyst containing the summary data from the SAR section is called "AnalystDeData.txt". Before running a users script, Analyst sets the working directory for RScript to the directory where this file is saved. Thus there is no need for any path information when opening the AnalystDeData.txt file.

The text file contains all the fields displayed in Analyst (e.g. ED, ED_Err, Test_Signal etc). A list of these is given in [Appendix B](#), and a script called 'List_SAR_data_fields' is included in Analyst which when it is run will give a list of the data fields that are available.

12.4.4 Using variables in 'R in Analyst' (RAN) scripts

One of the differences bewteen standard R scripts and 'R in Analyst' (RAN) scripts is the ability to include variables in the script, making it easy to change values at run time without the need to edit the script. Variables can be created or edited in the 'R Script editor' window.

Name	Type	Default	+	-
\$1	Sigma b	num	0.15	+ -
\$2	Logged model	logical	TRUE	+ -
\$3	Parameter	set	3	+ -
\$4	Show BIN filenar	logical	TRUE	+ -

Figure 12.4.4: The panel showing the currently defined variables in a script

Variables are added or deleted by pressing the "+" or "-" symbols respectively. Note that there is no "undo" on this, so undertake this carefully. Variables in the script are called \$1, \$2, \$3, \$4. Wherever this text appears in your code, it will be replaced by the value defined at run time. For instance, in the panel above, the first variable (\$1) is given the default value 0.15. When you write your script, you can put the variable \$1 in, and when you view the script in the [R script window](#) the value \$1 will be replaced by whatever is typed into the text box for that variable (the default will be 0.15).

You may type into the R Script editor:

```
MinAge <- calc_MinDose(AnData, sigmab=$1, log=$2, par=$3)
```

When this is viewed in the R script window, the 3 variables will be replaced by their values and the script will appear as follows. This is the script that will be run in R.

```
MinAge <- calc_MinDose(AnData, sigmab=0.15, log=TRUE, par=3)
```

Defining variables

Each variable has four elements to it: variable number, name, type, and default value

Variable number	e.g. \$1, \$2, \$3. Users have no control over this numbering. Analyst will automatically number variables sequentially. If you delete a variable (e.g. \$2 from the list in Fig 12.3.4, then variables with a higher value will decrease by one. Hence what is currently defined as \$3 and called "Parameter" above, would now be \$2. Your code would need to be changed to reflect this change.
-----------------	---

Name	When you define a variable, the first column you need to define is the "name" (Fig 12.3.4). This value is what will appear in the R Script window and
------	---

so should be chosen to make it clear to the user what this variable is. The name of it is not used in any other way.

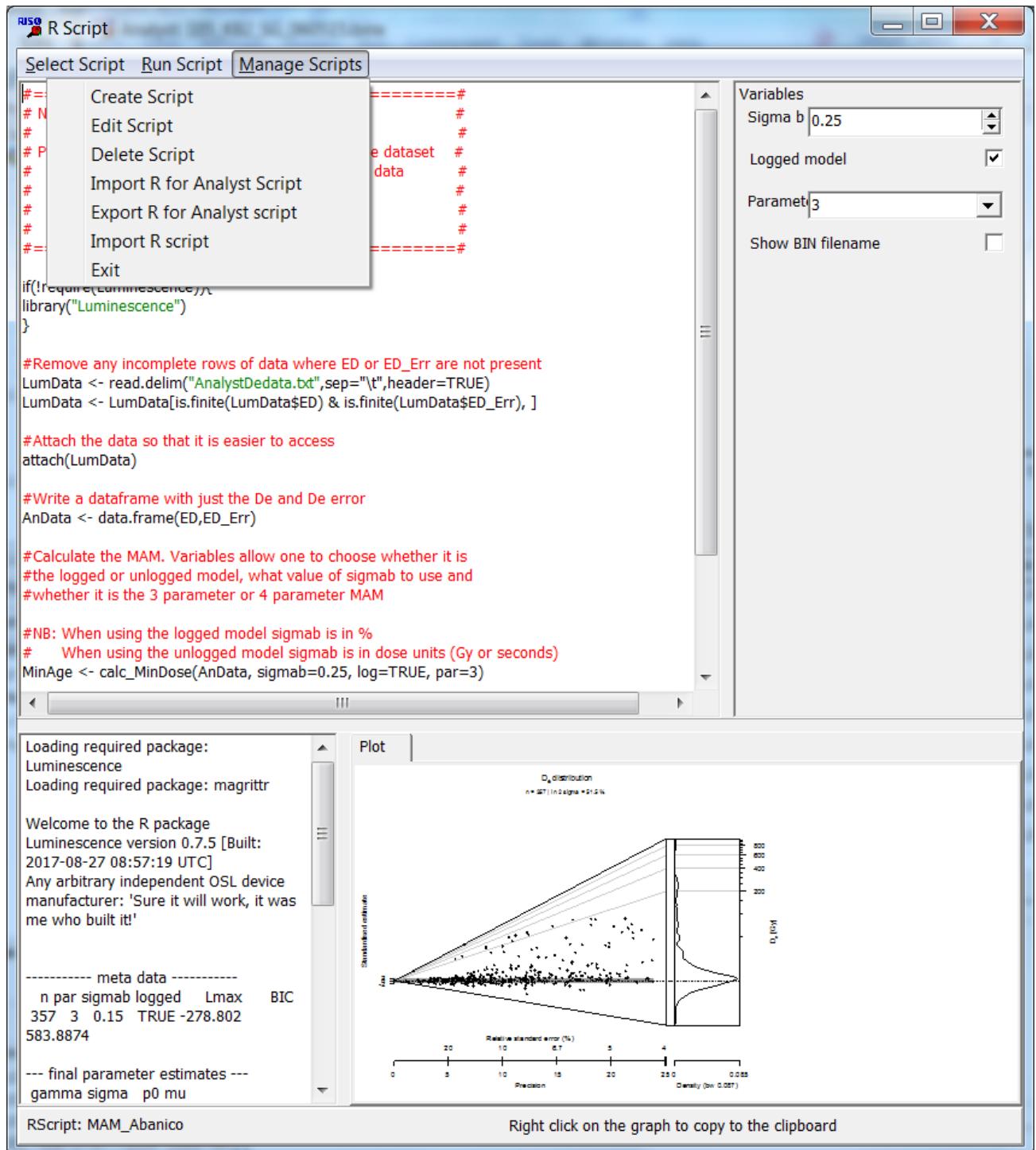
Type	Four types of variables can be defined, num, character, logical and set. These are mostly self explanatory: - num is any numeric value - character is any text value - logical is a boolean value and will return TRUE or FALSE - set allows users to select a value from a predefined list of options (e.g. 2,3,4 or blue,green,red). These options are any ASCII characters, so can be numeric or text.
Default value	Each variable should be given a default value. This is the value that will appear when the script is opened in the R script window. The user can then change this value, but it will make using variables much easier if the default is set carefully.

12.5 How to export and import R for Analyst scripts

When you install Analyst a small number of scripts are automatically installed to illustrate how this aspect of the software works. However, it is likely that users will write many other scripts for specific tasks. These will automatically be saved to the version of Analyst the user is working on. It is possible to export the R scripts written in Analyst to a file, so that these can be archived along with a data set, transferred to another computer, or distributed to other researchers.

Exporting R for Analyst scripts

In the R script window, a series of functions are available from the "Manage Scripts" menu. To export a script so that it can be imported into Analyst, you should select "Export R for Analyst script" - this will create a file with the extension RAN (short for R for Analyst). The file is a simple text file and can be opened by any text editor. The format includes information about the variables defined in the script, and hence cannot be run directly in R (e.g. RStudio). If do you want to run your code in R or RStudio directly, then the simplest approach is probably to right click on the script and choose select all and copy the text to the clipboard.



Importing R for Analyst scripts

Files produced by the export function can be imported using this option. If a script of the same name already exists then you will be asked to provide a different name. Note that this function will only import RAN files produced by Analyst. If you wish to import an R script (which is a simple text file), then you should use the Import R script option. This will import a text file and simply paste it into the script window.

13. References

This page contains a set of references that have been used in this manual.

- Armitage, S.J., Duller, G.A.T. and Wintle, A.G. (2000). Quartz from southern Africa: sensitivity changes as a result of thermal pretreatment. *Radiation Measurements* **32**(5-6): 571-577.
- Auclair, M., Lamothe, M. and Huot, S. (2003). Measurement of anomalous fading for feldspar IRSL using SAR. *Radiation Measurements* **37**: 487-492.
- Bailey, R.M., Smith, B.W. and Rhodes, E.J. (1997). Partial bleaching and the decay form characteristics of quartz OSL. *Radiation Measurements* **27**: 123-136.
- Bevington and Robinson (1992) *Data reduction and error analysis for the physical sciences*. 2nd edition. McGraw-Hill.
- Cunningham, A.C. and Wallinga, J. (2010). Selection of integration time-intervals for quartz OSL decay curves. *Quaternary Geochronology* **5**: 657-666.
- Dietze, M., Kreutzer, S., Burow, C., Fuchs, M.C., Fischer, M., Schmidt, C. (2016). The abanico plot: Visualising chronometric data with individual standard errors *Quaternary Geochronology* **31**: 12-18.
- Duller, G.A.T. (2007). Assessing the error on equivalent dose estimates derived from single aliquot regenerative dose measurements. *Ancient TL* **25**: 15-24.
- Duller, G.A.T. and Wintle, A.G. (1991). On infrared stimulated luminescence at elevated temperatures. *Nuclear Tracks and Radiation Measurements* **18**: 379-384.
- Galbraith, R.F. (1990). The radial plot: graphical assessment of spread in ages. *Nuclear Tracks and Radiation Measurements* **17**: 207-214.
- Galbraith, R.F. (1998). The trouble with "probability density" plots of fission track ages. *Radiation Measurements* **29**: 125-131.
- Galbraith, R.F. (2002). A note on the variance of a background-corrected OSL count. *Ancient TL* **20**(2): 49-51.
- Galbraith, R.F. and Roberts, R.G. (2012). Statistical aspects of equivalent dose and error calculation and display in OSL dating: An overview and some recommendations. *Quaternary Geochronology* **11**: 1-27.
- Galbraith, R.F., Roberts, R.G., Laslett, G.M., Yoshida, H. and Olley, J.M. (1999). Optical dating of single and multiple grains of quartz from Jimmum rock shelter, northern Australia: Part I, Experimental design and statistical models. *Archaeometry* **41**: 339-364.
- Huntley, D.J. and Lamothe, M. (2001). Ubiquity of anomalous fading in K-feldspars and the measurement and correction for it in optical dating. *Canadian Journal of Earth Sciences* **38**: 1093-1106.
- Kreutzer, S., Schmidt, C., Fuchs, M.C., Dietze, M., Fischer, M., Fuchs, M. (2012). Introducing an R package for luminescence dating analysis *Ancient TL* **30**: 1-8.
- Murray, A.S. and Wintle, A.G. (2000). Luminescence dating of quartz using an improved single-aliquot regenerative-dose protocol. *Radiation Measurements* **32**(1): 57-73.
- Thomsen, K.J., Murray, A.S. and Bøtter-Jensen, L. (2005). Sources of variability in OSL dose measurements using single grains of quartz. *Radiation Measurements* **39**: 47-61.

Wintle, A.G. and Murray, A.S. (2006). A review of quartz optically stimulated luminescence characteristics and their relevance in single-aliquot regeneration dating protocols. Radiation Measurements **41**: 369-391.

14. Appendices

14.1 Appendix A: BINX file format

The following information is taken from the Sequence Editor manual supplied by Risø.

The results from a run of a Risø TL/OSL sequence are stored in a BINX file.

For all versions of the BINX files, the version number is stored in the first 2 byte of the header.

V.8

The file format V.8 is used by Sequence editor V.4.40 and later

Description	Name	Type	Length (bytes)
<i>Header size and structure</i>			
Data format version number	Version	Small Integer	2
Length of this record ^(†)	Length	Long Integer	4
Length of previous record ^(†)	Previous	Long Integer	4
Number of data points	NPoints	Long Integer	4
Record type ^(§)	RecType	Byte	1
<i>Sample characteristics</i>			
Run number	Run	Small Integer	2
Set Number	Set	Small Integer	2
Carousel position	Position	Small Integer	2
Grain Number	GrainNumber	Small Integer	2
Curve number (for multiple curve operations)	CurveNo	Small Integer	2
X position of a single grain	XCoord	Small Integer	2
Y position of a single grain	YCoord	Small Integer	2

Sample name	Sample	String @	21
Comment	Comment	String @	81

Instrument and sequence characteristics

System ID	SystemID	Small Integer	2
File name (.SEC, .BINX etc.)	FName	String @	101
User name	User	String @	31
Data collection time (hh-mm-ss)	Time	String @	7
Data collection date (dd-mm-yy)	Date	String @	7

Analysis

Data type #	DType	Byte	1
Bleaching time	BL_Time	Single	4
Bleaching unit (mJ, J, secs, mins, hrs)	BL_Unit	Byte	1
Normalisation factor (1)	Norm1	Single	4
Normalisation factor (2)	Norm2	Single	4
Normalisation factor (3)	Norm3	Single	4
Background level	BG	Single	4
Number of channels to shift data	Shift	Small Integer	2
Tag	Tag	Byte	1
Reserved for internal use			20

Measurement characteristics

Luminescence type ‡	LType	Byte	1
Light Source *	LightSource	Byte	1
Optical Stimulation Power	LightPower	Single	4
Low (temperature, time, wavelength)	Low	Single	4
High (temperature, time, wavelength)	High	Single	4
Rate (heating rate, scan rate).	Rate	Single	4
Sample temperature	Temperature	Small Integer	2

Measured temperature	MeasTemp	Small Integer	2
Preheating temperature	An_Temp	Single	4
Preheating time	An_Time	Single	4
TOL 'delay' channels	Delay	Small Integer	2
TOL 'on' channels	On	Small Integer	2
TOL 'off' channels	Off	Small Integer	2
Irradiation time	IRR_Time	Single	4
Irradiation type (alpha, beta or gamma)	IRR_Type	Byte	1
Irradiation dose rate (Gy/s)	IRR_DoseRate	Single	4
Irradiation dose rate error (Gy/s)	DoseRateErr	Single	4
Time since last irradiation (s)	TimeSinceIrr	Long Integer	4
Time unit (time tick) for pulse parameters (s)	TimeTick	Single	4
On-time for pulsed stimulation (in time ticks)	OnTime	Long Integer	4
Stimulation period (on+off time in time ticks)	StimPeriod	Long Integer	4
PMT signal gating enabled	GateEnabled	Byte	1
Start of gating (in time ticks from start of on pulse)	GateStart	Long Integer	4
End of gating (in time ticks from start of on pulse)	GateEnd	Long Integer	4
Photon Timer enabled	PTenabled	Byte	1
PMT dead time correction enabled	DTenabled	Byte	1
PMT dead time (s)	DeadTime	Single	4
Stimulation power corresponding to 100% (mW/cm ²)	MaxLPower	Single	4
XRF acquisition time (s)	XrfAcqTime	Single	4
XRF X-ray high voltage (V)	XrfHV	Single	4

XRF X-ray current (uA)	XrfCurr	Long Integer	4
XRF dead time fraction	XrfDeadTimeF	Single	4
Detector ID	DtID	Byte	1
Lower filter ID	Fl1ID	Small Integer	2
Upper filter ID	Flt2ID	Small Integer	2
Excess Noise factor	ExNoiseF	Single	4
Marker position 1 to 3	Mrk.X, Mrk.Y	6xSingle	24
Extraction start	ExtrStart	Single	4
Extraction end	ExtrEnd	Single	4
Reserved for internal use		Byte	42

Length of header 507

Data

Data array of NPOINTS Long Integers (Record type=0, 1) DPoints Long Integer 4x
NPoints

or

Region Of Interest definitions (Record type=128) 504 x
NPoints

One ROI definition (504 bytes):

Number of points in definition	NofPoints	Integer	4
Samples the ROI is used for	UsedFor	Byte	48 x 1
Samples the ROI is shown for	ShownFor	Byte	48 x 1
The colour the ROI is drawn with	Color	Integer	4
X Coordinates (in ref coordinate system)	X	Single	50 x 4
Y Coordinates (in ref coordinate system)	Y	Single	50 x 4

Notes:

- § Record type is introduced so the bin file may hold other data than signal data.
- 0: identifies ordinary count data acquired by the Sequence Editor

1: identifies count data for Region Of Interests (ROIs) extracted by e.g. the Viewer+ program
 128: identifies ROI definitions. In This case “number of data points” means number of ROIs

† The records are of a variable length since the number of data points recorded (NPOINTS) may vary from one to 9,999 (this may be expanded in the future). A record with a single data point in it will be $507 + (1 \times 4)$ = 517 bytes long, while one with 2000 data points will be $507 + (2000 \times 4) = 8507$ bytes long. Thus there is a considerable saving of disc space by having semi-variable length records. However, once created the length of the record is fixed (it does not make sense to be able to delete or add single data points) and is recorded in the variable LENGTH. This allows the program to be able to step through from one record to another without having to search for specific end of record markers. In order to be able to move UP through a file the length of each previous record is also stored in a record (this will be zero in the first record).

@ Strings are stored in Pascal format. That is with an additional byte used to define the length of the string. Thus the number of bytes used to store the string is one byte longer than the string itself. Thus the Date is stored as a 6 character string (ddmmyy), but this requires 7 bytes.

‡ The different types of luminescence that can be specified are as follows:-

Value	LTYPE	Description	Associated device
0	TL	Thermoluminescence	-
1	OSL	Optically stimulated luminescence	OSL lamp / Blue diodes
2	IRSL	Infrared stimulated luminescence	IR diode array or IR laser
3	M-IR	Infrared monochromator scan	IR monochromator
4	M-VIS	Visible monochromator scan	Visible monochromator
5	TOL	Thermo-optical luminescence	Any optical stimulation
6	TRPOSL	Time Resolved Pulsed OSL	Any optical stimulation
7	RIR	Ramped IRSL	IR diode array or IR laser
8	RBR	Ramped Blue LEDs	Blue diodes
9	USER	User defined	-
10	POSL	Pulsed OSL	Blue or IR diode arrays
11	SGOSL	Single Grain OSL	Green or IR laser
12	RL	Radio Luminescence	Beta irradiation source
13	XRF	X-ray Fluorescence	X-ray unit

The various data types specified by DTYPY are primarily designed for use when calculating equivalent doses. The different data types are as follows.

Value	Data Type	Irr.	Bl.
0	Natural		
1	N+dose	x	
2	Bleach		x
3	Bleach + dose	x	x

4	Natural (Bleach)		x
5	N+dose (Bleach)	x	
6	Dose	x	
7	Background		

* The values for the light source are as follows:

Value	Light Source
-------	--------------

0	None
1	Lamp
2	IR diodes / IR Laser
3	Calibration LED
4	Blue Diodes
5	White light
6	Green laser (single grain)
7	IR laser (single grain)

V.7 and V.6 (file extension: binx)

The file format V.7 is used by Sequence editor V.4.30 to 4.39

The file format V.6 is used by Sequence editor V.4.20 to 4.29

Description	Name	Type	Length (bytes)
-------------	------	------	-------------------

Header size and structure

Data format version number	Version	Small Integer	2
Length of this record ⁽⁺⁾	Length	Long Integer	4
Length of previous record ⁽⁺⁾	Previous	Long Integer	4
Number of data points	NPoints	Long Integer	4

Sample characteristics

Run number	Run	Small Integer	2
Set Number	Set	Small Integer	2

Carousel position	Position	Small Integer	2
Grain Number	GrainNumber	Small Integer	2
Curve number (for multiple curve operations)	CurveNo	Small Integer	2
X position of a single grain	XCoord	Small Integer	2
Y position of a single grain	YCoord	Small Integer	2
Sample name	Sample	String @	21
Comment	Comment	String @	81

Instrument and sequence characteristics

System ID	SystemID	Small Integer	2
File name (.SEC, .BINX etc)	FName	String @	101
User name	User	String @	31
Data collection time (hh-mm-ss)	Time	String @	7
Data collection date (dd-mm-yy)	Date	String @	7

Analysis

Data type (#)	DType	Byte	1
Bleaching time	BL_Time	Single	4
Bleaching unit (mJ, J, secs, mins, hrs)	BL_Unit	Byte	1
Normalisation factor (1)	Norm1	Single	4
Normalisation factor (2)	Norm2	Single	4
Normalisation factor (3)	Norm3	Single	4
Background level	BG	Single	4
Number of channels to shift data	Shift	Small Integer	2
Tag	Tag	Byte	1
Reserved for internal use			20

Measurement characteristics

Luminescence type (#)	LType	Byte	1
Light Source (*)	LightSource	Byte	1
Optical Stimulation Power	LightPower	Single	4
Low (temperature, time, wavelength)	Low	Single	4
High (temperature, time, wavelength)	High	Single	4
Rate (heating rate, scan rate).	Rate	Single	4
Sample temperature	Temperature	Small Integer	2
Measured temperature	MeasTemp	Small Integer	2
Preheating temperature	An_Temp	Single	4
Preheating time	An_Time	Single	4
TOL 'delay' channels	Delay	Small Integer	2
TOL 'on' channels	On	Small Integer	2
TOL 'off' channels	Off	Small Integer	2
Irradiation time	IRR_Time	Single	4
Irradiation type (alpha, beta or gamma)	IRR_Type	Byte	1
Irradiation dose rate (Gy/s)	IRR_DoseRate	Single	4
Irradiation dose rate error (Gy/s)	DoseRateErr	Single	4
Time since last irradiation (s)	TimeSinceIrr	Long Integer	4
Time unit (time tick) for pulse parameters (s)	TimeTick	Single	4
On-time for pulsed stimulation (in time ticks)	OnTime	Long Integer	4
Stimulation period (on+off time in time ticks)	StimPeriod	Long Integer	4
PMT signal gating enabled	GateEnabled	Byte	1
Start of gating (in time ticks from start of on pulse)	GateStart	Long Integer	4

End of gating (in time ticks from start of on pulse)	GateEnd	Long Integer	4
Photon Timer enabled	PTenabled	Byte	1
PMT dead time correction enabled	DTenabled	Byte	1
PMT dead time (s)	DeadTime	Single	4
Stimulation power corresponding to 100% (mW/cm ²)	MaxLPower	Single	4
XRF acquisition time (s)	XrfAcqTime	Single	4
XRF X-ray high voltage (V)	XrfHV	Single	4
XRF X-ray current (uA)	XrfCurr	Long Integer	4
XRF dead time fraction	XrfDeadTimeF	Single	4
Detector ID ^x		Byte	1
Lower filter ID ^x		Small Integer	2
Upper filter ID ^x		Small Integer	2
Excess Noise factor ^x		Single	4
Reserved for internal use		Byte	15 / (24 ^x)

Length of header 447

Data

Data array of NPOINTS Long Integers	DPoints	Long Integer	4x NPoints
-------------------------------------	---------	--------------	---------------

Notes:

^x These parameters are only stored in V.7 and not in V.6. The header size is unchanged from V.6 to V.7 and therefore the bytes reserved for internal use are different from V.7 to V.6.

[†] The records are of a variable length since the number of data points recorded (NPOINTS) may vary from one to 9,999 (this may be expanded in the future). A record with a single data point in it will be 423+(1x4) = 427 bytes long, while one with 2000 data points will be 423+(2000x4) = 8423 bytes long. Thus there is a considerable saving of disc space by having semi-variable length records. However, once created the length of the record is fixed (it does not make

sense to be able to delete or add single data points) and is recorded in the variable LENGTH. This allows the program to be able to step through from one record to another without having to search for specific end of record markers. In order to be able to move UP through a file the length of each previous record is also stored in a record (this will be zero in the first record).

@ Strings are stored in Pascal format. That is with an additional byte used to define the length of the string. Thus the number of bytes used to store the string is one byte longer than the string itself. Thus the Date is stored as a 6 character string (ddmmyy), but this requires 7 bytes.

‡ The different types of luminescence that can be specified are as follows:-

Value	LTYPE	Description	Associated device
0	TL	Thermoluminescence	-
1	OSL	Optically stimulated luminescence	OSL lamp / Blue diodes
2	IRSL	Infrared stimulated luminescence	IR diode array or IR laser
3	M-IR	Infrared monochromator scan	IR monochromator
4	M-VIS	Visible monochromator scan	Visible monochromator
5	TOL	Thermo-optical luminescence	Any optical stimulation
6	TRPOSL	Time Resolved Pulsed OSL	Any optical stimulation
7	RIR	Ramped IRSL	IR diode array or IR laser
8	RBR	Ramped Blue LEDs	Blue diodes
9	USER	User defined	-
10	POSLOSL	Pulsed OSL	Blue or IR diode arrays
11	SGOSL	Single Grain OSL	Green or IR laser
12	RL	Radio Luminescence	Beta irradiation source
13	XRF	X-ray Fluorescence	X-ray unit

The various data types specified by DTYPY are primarily designed for use when calculating equivalent doses. The different data types are as follows.

Value	Data Type	Irr.	Bl.
0	Natural		
1	N+dose		
2	Bleach		

3	Bleach + dose
4	Natural (Bleach)
5	N+dose (Bleach)
6	Dose
7	Background

* The values for the light source are as follows:

Value	Light Source
0	None
1	Lamp
2	IR diodes / IR Laser
3	Calibration LED
4	Blue Diodes
5	White light
6	Green laser (single grain)
7	IR laser (single grain)

V.4 (file extension: bin)

The file format us used by Sequence editor V.4.00 to V.4.12

Description	Name	Type	Length (bytes)
Data format version number	Version	Small Integer	2
Length of this record ⁽⁺⁾	Length	Small Integer	2
Length of previous record ⁽⁺⁾	Previous	Small Integer	2
Number of data points	NPoints	Small Integer	2
Luminescence type ^(#)	LType	Byte	1
Low (temperature, time, wavelength)	Low	Single	4
High (temperature, time, wavelength)	High	Single	4

Rate (heating rate, scan rate).	Rate	Single	4
Sample temperature	Temperature	Small Integer	2
X position of a single grain	XCoord	Small Integer	2
Y position of a single grain	YCoord	Small Integer	2
TOL 'delay' channels	Delay	Small Integer	2
TOL 'on' channels	On	Small Integer	2
TOL 'off' channels	Off	Small Integer	2
Carousel position	Position	Byte	1
Run number	Run	Byte	1
Data collection time (hh-mm-ss)	Time	String	7
Data collection date (dd-mm-yy)	Date	String	7
Sequence name	Sequence	String	9
User name	User	String	9
Data type (#)	Dtype	Byte	1
Irradiation time	IRR_Time	Single	4
Irradiation type (alpha, beta or gamma)	IRR_Type	Byte	1
Irradiation unit (Gy, Rads, secs, mins, hrs)	IRR_UNIT	Byte	1
Bleaching time	BI_Time	Single	4
Bleaching unit (mJ, J, secs, mins, hrs)	BI_Unit	Byte	1
Annealing temperature	An_Temp	Single	4
Annealing time	An_Time	Single	4
Normalisation factor (1)	Norm1	Single	4
Normalisation factor (2)	Norm2	Single	4
Normalisation factor (3)	Norm3	Single	4
Background level	BG	Single	4
Number of channels to shift data	Shift	Small Integer	2

Sample name	Sample	String	21
Comment	Comment	String	81
Light Source (*)	LightSource	Byte	1
Set Number	Set	Byte	1
Tag	Tag	Byte	1
Grain Number	Grain	Small Integer	2
Optical Stimulation Power	LightPower	Single	4
System ID	SystemID	Small Integer	2
Reserved for internal use			20
Curve number (for multible curve operations)	CurveNo	Small Integer	2
Time unit for pulse parameters	TimeTick	Single	4
On-time for pulsed stimulation (in time ticks)	OnTime	Long Integer	4
Stimulation period (on+off time in time ticks)	StimPeriod	Long Integer	4
PMT signal gating enabled	GateEnabled	Byte	1
Start of gating (in time ticks from start of on pulse)	GateStart	Long Integer	4
End of gating (in time ticks from start of on pulse)	Gateend	Long Integer	4
Photon Timer enabled	PTenabled	Byte	1
Reserved			10
<i>Length of header</i>			272
Data array of NPOINTS Long Integers	DPoints	Long Integer	4 x NPOINTS

V.3 (file extension: bin)

The file format us used by Sequence editor V.3.xx

Description	Name	Type	Length (bytes)
Data format version number	Version	Small Integer	2
Length of this record ⁽⁺⁾	Length	Small Integer	2
Length of previous record ⁽⁺⁾	Previous	Small Integer	2
Number of data points	NPoints	Small Integer	2
Luminescence type ^(‡)	LType	Byte	1
Low (temperature, time, wavelength)	Low	Single	4
High (temperature, time, wavelength)	High	Single	4
Rate (heating rate, scan rate).	Rate	Single	4
Sample temperature	Temperature	Small Integer	2
X position of a single grain	XCoord	Small Integer	2
Y position of a single grain	YCoord	Small Integer	2
TOL 'delay' channels	Delay	Small Integer	2
TOL 'on' channels	On	Small Integer	2
TOL 'off' channels	Off	Small Integer	2
Carousel position	Position	Byte	1
Run number	Run	Byte	1
Data collection time (hh-mm-ss)	Time	String	7
Data collection date (dd-mm-yy)	Date	String	7
Sequence name	Sequence	String	9
User name	User	String	9
Data type ^(#)	Dtype	Byte	1
Irradiation time	IRR_Time	Single	4

Irradiation type (alpha, beta or gamma)	IRR_Type	Byte	1
Irradiation unit (Gy, Rads, secs, mins, hrs)	IRR_UNIT	Byte	1
Bleaching time	Bl_Time	Single	4
Bleaching unit (mJ, J, secs, mins, hrs)	Bl_Unit	Byte	1
Annealing temperature	An_Temp	Single	4
Annealing time	An_Time	Single	4
Normalisation factor (1)	Norm1	Single	4
Normalisation factor (2)	Norm2	Single	4
Normalisation factor (3)	Norm3	Single	4
Background level	BG	Single	4
Number of channels to shift data	Shift	Small Integer	2
Sample name	Sample	String	21
Comment	Comment	String	81
Light Source (*)	LightSource	Byte	1
Set Number	Set	Byte	1
Tag	Tag	Byte	1
Grain Number	Grain	Small Integer	2
Optical Stimulation Power	LightPower	Single	4
System ID	SystemID	Small Integer	2
Reserved for internal use			36
On-time for pulsed stimulation (s) (#)	OnTime	Single	4
Off-time for pulsed stimulation (s) (#)	OffTime	Single	4
Enable flags (PMT Gating and Photon Timer enable) (#)	EnableFlags	Byte	1
On-gate delay (s) (#)	OnGateDelay	Single	4
Off-gate delay (s) (#)	OffGateDelay	Single	4
Reserved			1

Length of header 272

Data array of NPOINTS Long Integers	DPoints	Long Integer	4 x NPOINTS
-------------------------------------	---------	--------------	----------------

Notes:

The pulsing parameters are only stored from Sequence Editor V.3.30 and onwards

14.2 Appendix B: Summary Data from single aliquot and single grain analysis

During single aliquot or single grain analysis it is normal to generate multiple equivalent dose (D_e) values. As described in [Section 6.2.1.7](#) and [Section 6.2.1.1](#) a summary of this data is produced. This Summary Data can be reviewed on screen, copied to the clipboard for export to some other package, it may be saved to a Summary File (see [Section 6.2.1.1](#)), or it may be used by R routines (see [Section 12](#)) for further data processing.

This appendix describes the data produced in this Summary Data.

Column	Title	Description
1	Selected	Whether the aliquot has been selected for inclusion in summary data
2	Pass_Criteria	True or False - whether the aliquot passes the acceptance criteria specified by the user
3	Filename	Name of the BINX file used
4	Disc#	The disc number for the aliquot
5	Grain#	Grain number for the single grain. Left blank if this is a single aliquot
6	ED	Equivalent dose either in seconds or Gy. Parameter XX indicates which unit is used.
7	ED_Err	The uncertainty calculated for the equivalent dose given above
8	N.Signal	The gross natural signal (L_n) integrated over the channels defined in parameters 29 and 30
9	BG.signal	The background signal that is subtracted from the value above to give the net L_n signal. Note that this value has been corrected to take into account any differences in the number of channels used to define the signal (parameters 29 and 30) and the background (parameters 31 and 32)
10	MCarlo_Cycles	How many repeats were used if a Monte Carlo approach was used for error calculation
11	Test_Signal	The same as parameter 5, but for the test dose measured following the natural
12	BG.T_Signal	The same as parameter 6, but for the test dose measured following the natural
13	TD_Err	Uncertainty in the test dose measured following the natural calculated from the counting statistics and instrumental uncertainty. The value is expressed as a percentage.

14	Test_Dose	The test dose used for SAR measurements (in seconds of irradiation)
15	Test_Signal_Change	The ratio of the response to the test dose in the last cycle of the SAR sequence to the response to the test dose following the natural. This gives some impression of the amount of sensitivity change that occurs during the SAR sequence
16	Residual_Signal	If the response to zero regenerative dose has been measured then this is the luminescence signal measured (integrated over the channels defined in parameters 29 and 30)
17	RR1	The first recycling ratio calculated for this aliquot (or grain)
18	RR1_Err1	The uncertainty on the first recycling ratio
19	RR2	As above
20	RR2_Err2	As above
21	RR3	As above
22	RR3_Err3	As above
23	RR4	As above
24	RR4_Err4	As above
25	RR5	As above
26	RR5_Err5	As above
27	Recup1	The first recuperation value calculated for this aliquot (or grain)
28	Recup_Err1	The uncertainty on the recuperation value
29	Recup2	As above
30	Recup_Err2	As above
31	Recup3	As above
32	Recup_Err3	As above
33	Recup4	
34	Recup_Err4	
35	Recup5	
36	Recup_Err5	
37	Sig1	The first channel used to define the signal
38	Sig2	The last channel used to define the signal

39	BG1	The first channel used to define the background
40	BG2	The last channel used to define the background
41	Ln/Tn	The Ln/Tn ratio for this grain or aliquot
42	Ln/Tn error	Uncertainty in the Ln/Tn ratio
43	Fit	Numeric value indicating the Curve Fitting used to calculate this equivalent dose: 1 = Linear; 2 = Quadratic; 3 = Cubic; 4 = Exponential; 5 = Exponential plus linear; 6 = Sum of two exponentials; 7 = Interpolated; 8 = Ratio to single point
44	Options	<p>This numeric value encodes a variety of options for the curve fitting. The values given below are added if the option is true:</p> <ul style="list-style-type: none"> 1 Use previous BG for test dose 2 Use recycled points for fitting 4 Force growth curve through origin 8 Not currently used 16 Incorporate error on curve fitting 32 Use Monte Carlo method for error estimation <p>Additional options may be incorporated in the future.</p>
45	R_Chi_Sq	Reduced chi squared for the dose response curve used to calculate the equivalent dose
46	Param1	The value of the first parameter in the equation used for the dose response curve
47	Error1	The uncertainty on the value of the first parameter
48	Param2	As above
49	Error2	As above
50	Param3	As above
51	Error3	As above
52	Param4	As above
53	Error4	As above
54	Param5	As above
55	Error5	As above
56	Param6	As above
57	Error6	As above
58	Param7	As above

59	Error7	As above
60	Dose_Rate	The dose rate for the irradiation source used during the single aliquot measurements (Gy/s)
61	DR_Error	Uncertainty on the dose rate of the irradiation source
62	ED_in_Gy	"True" if the ED and doses are given in Gy; "False" if the values are in seconds
63	Not Used	Not currently used in this version of Analyst.
64	Not Used	As above
65	Not Used	As above
66	Not Used	As above
67	UseLxTx01	Whether 1st regeneration point is used for curve fitting
68	Dose01	1st Regeneration dose
69	LSig01	Signal from Lx (counts)
70	LBG01	Background signal from Lx (counts)
71	TSig01	Signal from Tx (counts)
72	TBG01	Background signal from Tx (counts)
73	LxTx01	Lx/Tx ratio for Dose01
74	Unc01	Uncertainty in the Lx/Tx ratio for Dose01
75	UseLxTx02	As above, but for 2nd regeneration dose
76	Dose02	As above, but for 2nd regeneration dose
77	LSig02	As above, but for 2nd regeneration dose
78	LBG02	As above, but for 2nd regeneration dose
79	TSig02	As above, but for 2nd regeneration dose
80	TBG02	As above, but for 2nd regeneration dose
81	LxTx02	As above, but for 2nd regeneration dose
82	Unc02	As above, but for 2nd regeneration dose
83-186	Dose, LxTx and Unc	Values for dose, Lx/Tx and uncertainty for doses 3-15