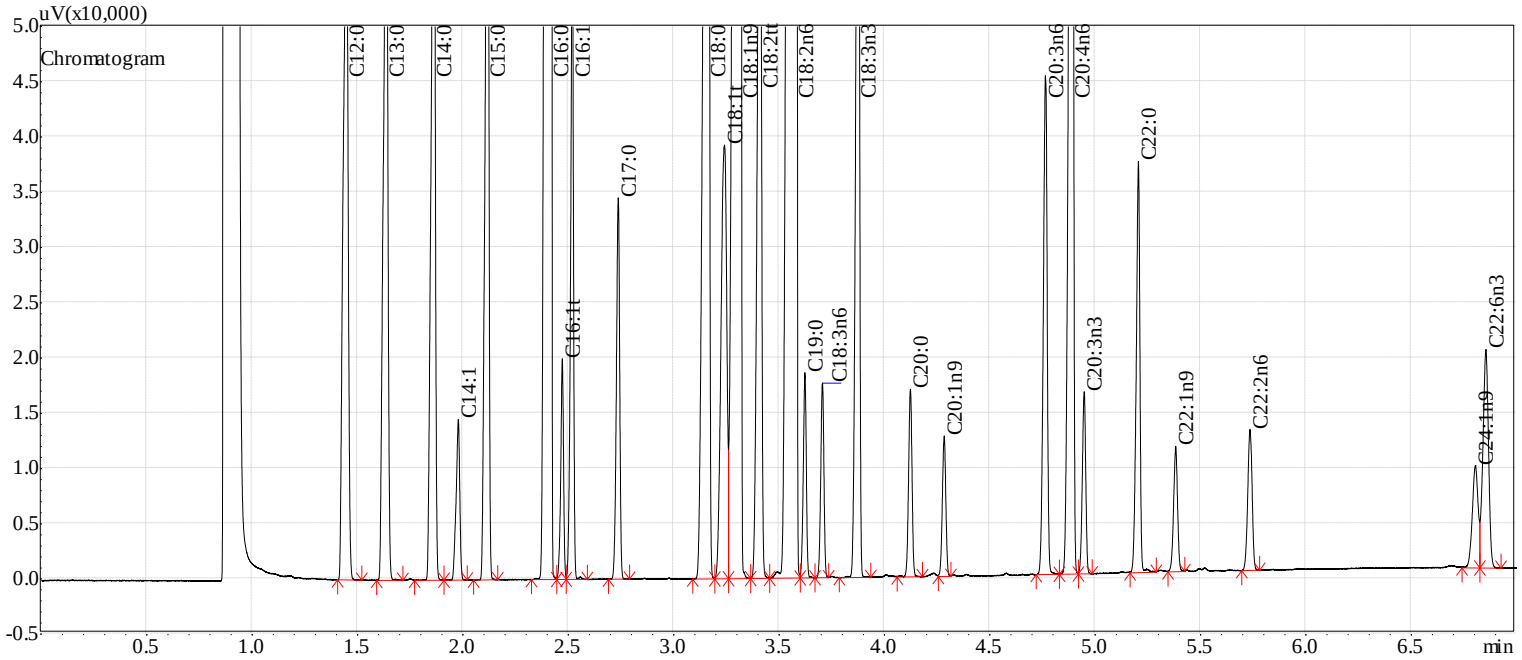
How to Process GC Data

After you run the GC to collect chromatograms for your samples you need to get information from the data.

The information you need is the identity and area percent concentration of each FAME peak.

You will use a copy of the GC software that *is <u>not</u> attached to the instrument* to identify and quantify the peaks in your chromatograms.



Peak Table

Sample peak identification is based on retention time comparison with a 'GLC 87' FAME standard chromatogram. Retention time is the amount of time a compound takes to travel from the GC injection port to the FID detector. Each FAME compound has a different retention time.

Sample concentration is determined by taking the ratio of a given peak area to the total area of all peaks in the chromatogram. This is called 'Area %'.

The peak table contains both Area % and the identification based on retention time.

GLC 87 FAME Standard Peak Table

Area%

Peak ID

Peak#	Ret. Time	Area	Height	Conc.	Units	Compound
1	1.446	103164	63947	2.65	Area %	C12:0
2	1.636	104198	70012	2.68	Area %	C13:0
3	1.861	108960	84196	2.80	Area %	C14:0
4	1.977	17591	14216	0.45	Area %	C14:1
5	2.116	110755	95250	2.85	Area %	C15:0
6	2.416	730749	511488	18.79	Area %	C16:0
7	2.471	18331	18345	0.47	Area %	C16:1t
8	2.518	54840	55599	1.41	Area %	C16:1
9	2.737	37525	33309	0.97	Area %	C17:0
10	3.16	252214	144953	6.49	Area %	C18:0
11	3.24	75134	38686	1.93	Area %	C18:1t
12	3.314	644506	359094	16.58	Area %	C18:1n9
13	3.409	113337	87172	2.91	Area %	C18:2tt
14	3.577	929507	465460	23.90	Area %	C18:2n6
15	3.622	18482	17994	0.48	Area %	C19:0
16	3.706	18464	16401	0.47	Area %	C18:3n6
17	3.874	115279	97877	2.96	Area %	C18:3n3
18	4.123	19323	16656	0.50	Area %	C20:0
19	4.283	14618	12435	0.38	Area %	C20:1n9
20	4.764	57361	44226	1.48	Area %	C20:3n6
21	4.889	192696	139838	4.96	Area %	C20:4n6
22	4.947	18577	16195	0.48	Area %	C20:3n3
23	5.204	44782	35313	1.15	Area %	C22:0
24	5.382	14811	10985	0.38	Area %	C22:1n9
25	5.734	18497	12456	0.48	Area %	C22:2n6
26	6.804	17922	9186	0.46	Area %	C24:1n9
27	6.854	36769	19566	0.95	Area %	C22:6n3

Load the CASPiE Instrument Site

- **To open the GC software launch your web browser and navigate to the CASPiE instrument website at https://instruments.caspie.org.**
- **Enter your account information to login.**

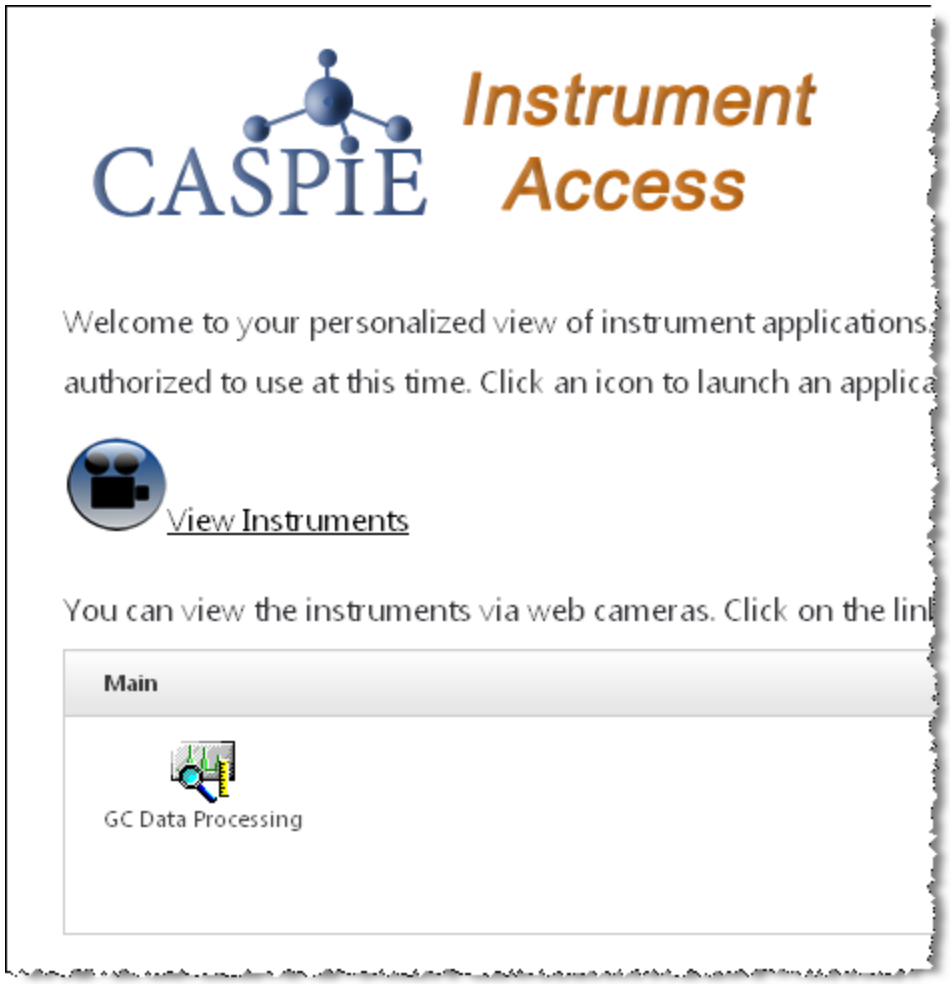
The GC Data Processing Software

You will use a copy of the GC software that *is <u>not</u> attached to the instrument* to process your data files. It is the same version used to create the GC batch file.

The version of the software not attached to an instrument is called 'GC Data Processing'.

You will always have access to the GC data processing software during a CASPiE module. You will only have access to the GC <u>instrument</u> for remote control during your scheduled hours.

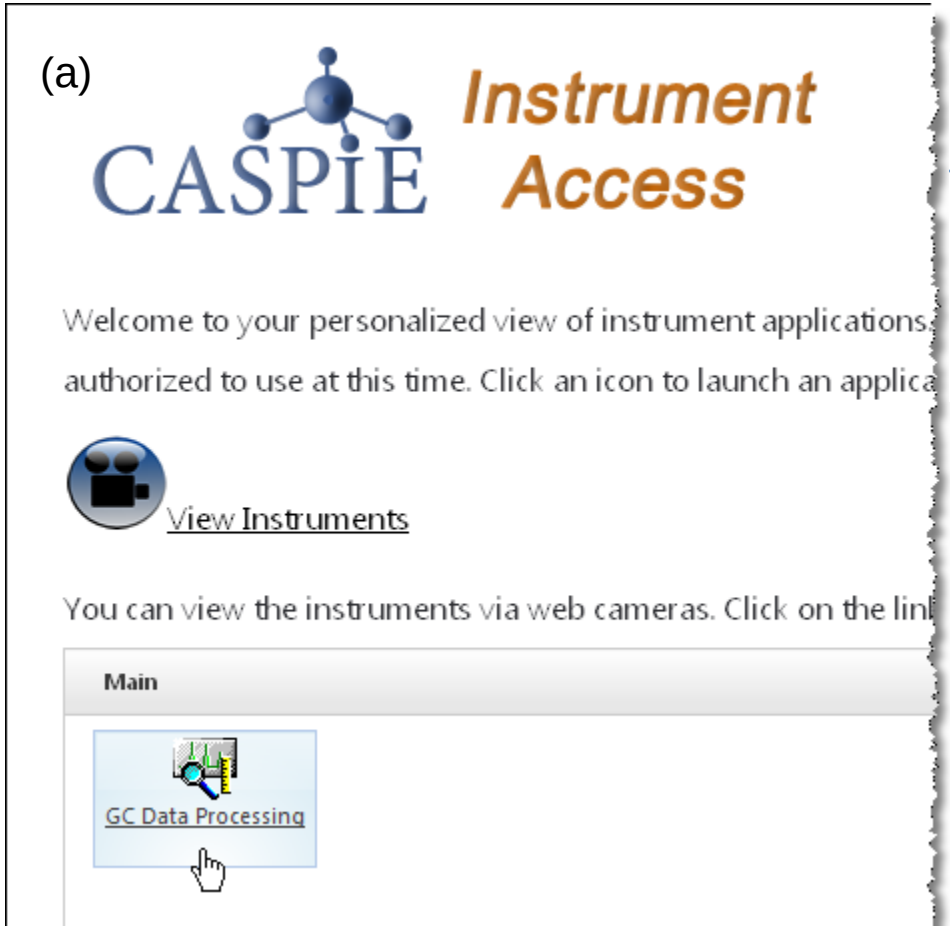
Important Note:
You <u>must</u> have the Citrix client installed on your computer to proceed!



Launch GC Data Processing Software

- **You should see one icon in the 'Applications" box. Launch the GC data processing software by clicking once on the icon (a).**
- **If the 'GC Data Processing' icon is not present ask your TA for help.**
- **A login window will appear (b). Use the user ID 'Student.' No password is required.**

(a)



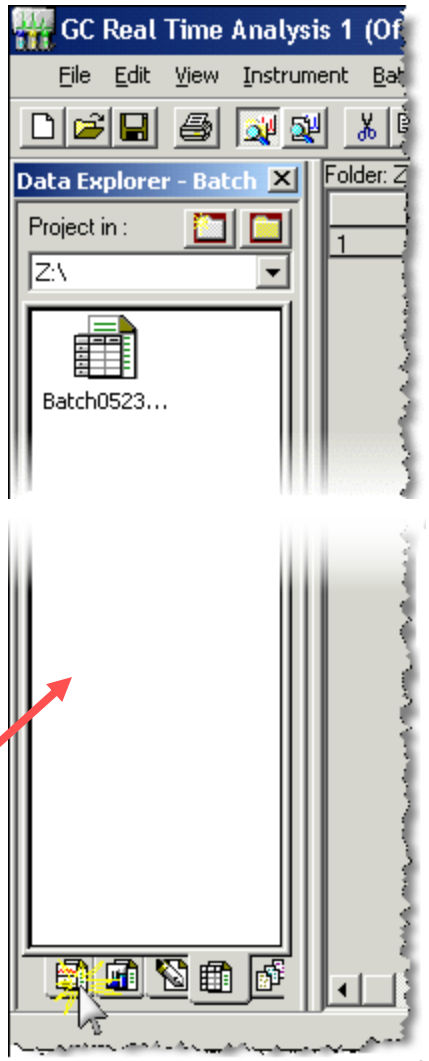
(b)

Open Data Window and Data File

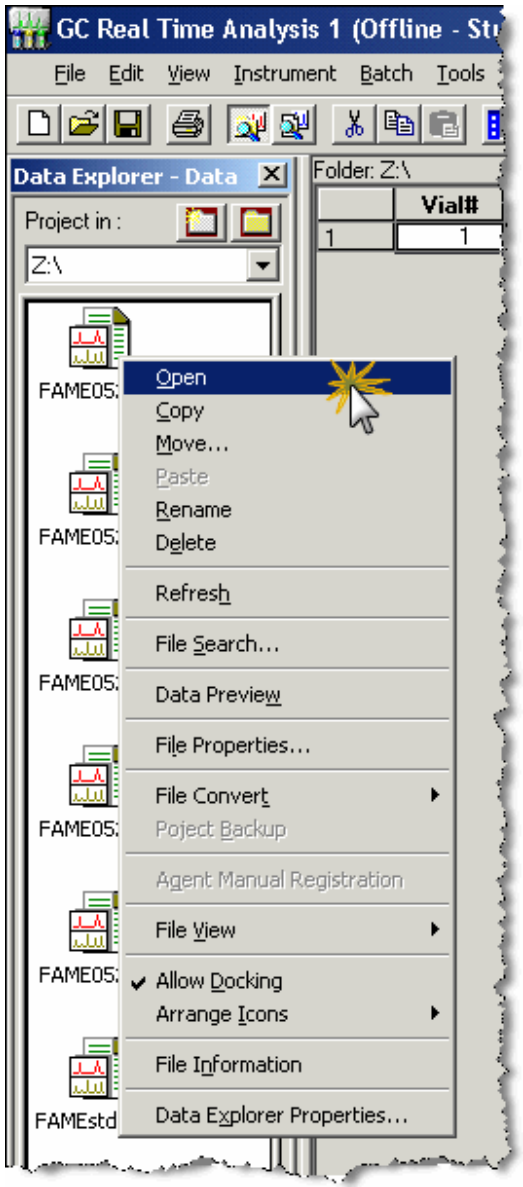
- **Display your data files in the Data Explorer window by clicking on the ‘Data’ tab at the bottom of the Data Explorer (a).**
- **Right click on one of the data files and open the file (b).**
- **A new application will open called ‘GC Postrun’.**

Data Explorer window

(a)

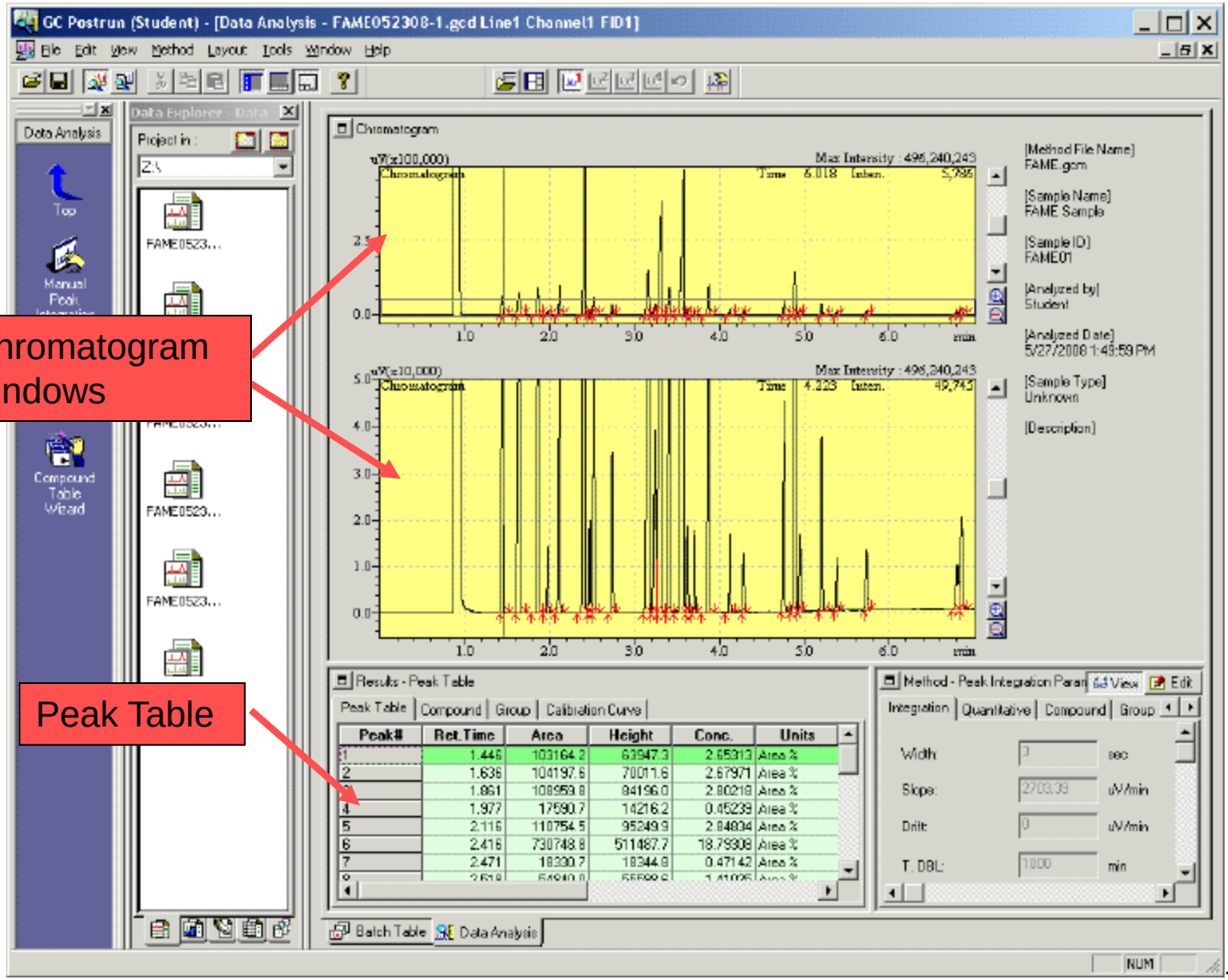


(b)



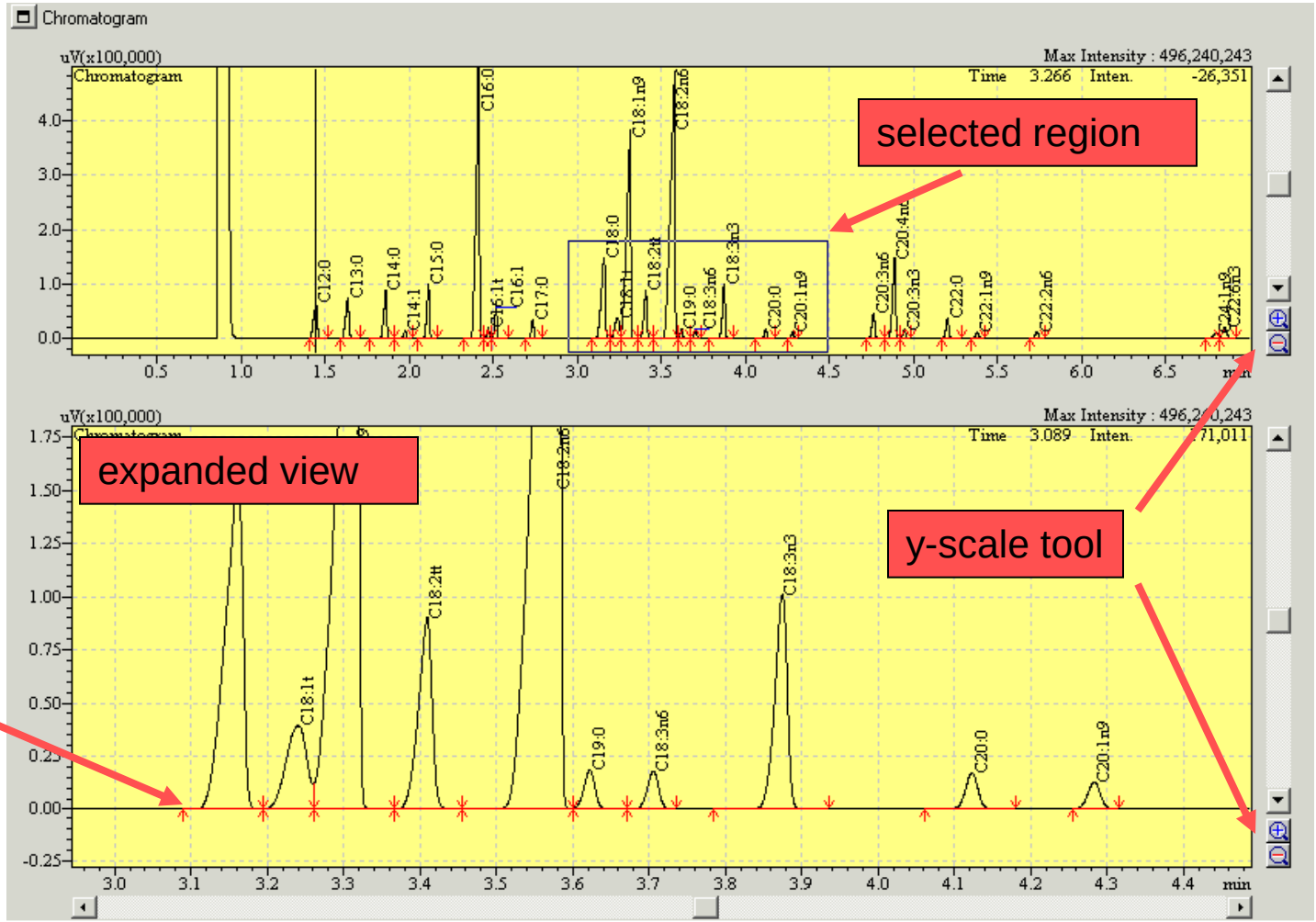
GC Postrun Software

- **The Postrun software has three important windows, two chromatogram windows and the Results-Peak Table windows.**



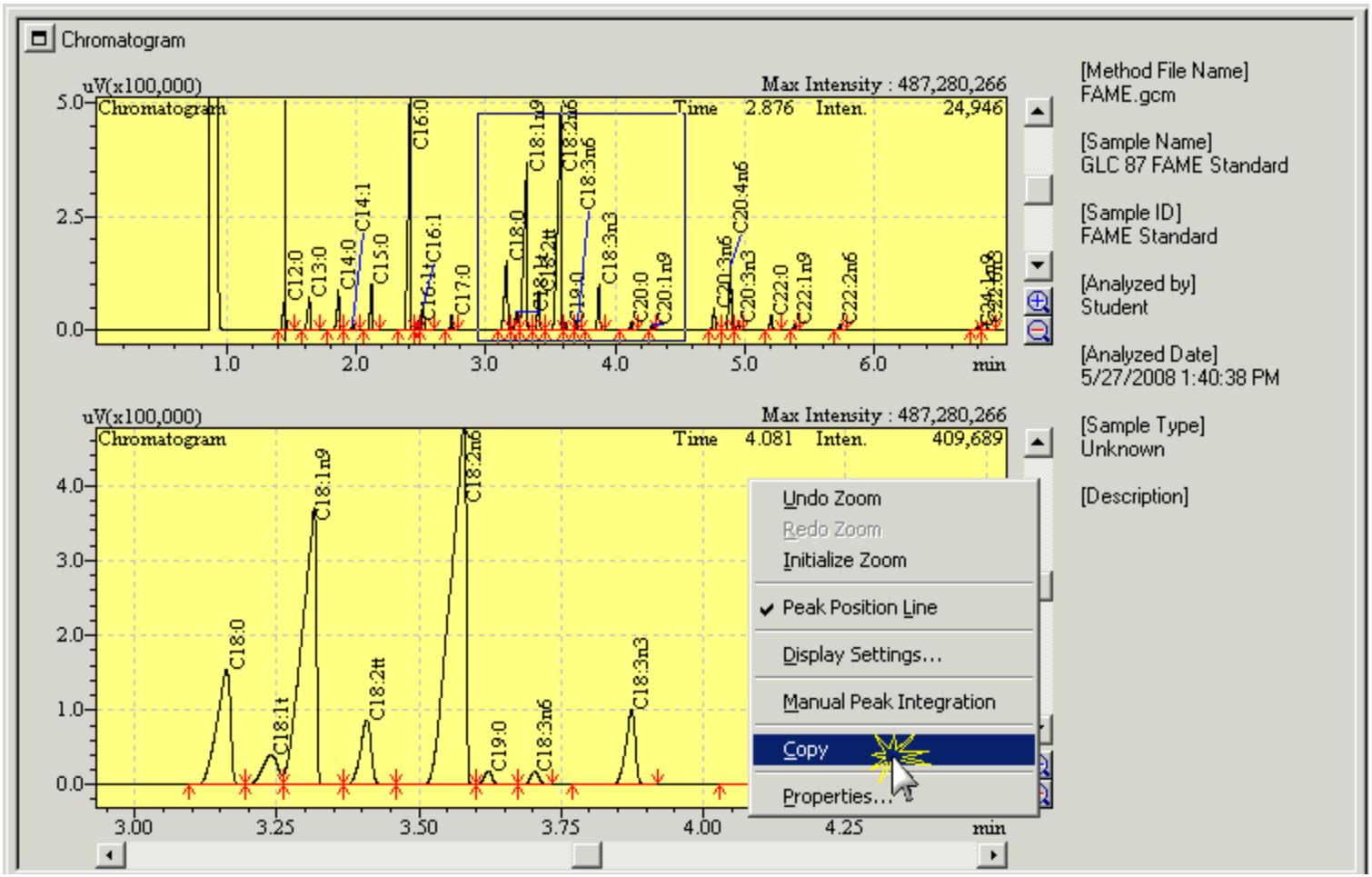
Chromatogram Windows

- **The bottom chromatogram window will show an expanded view of the chromatogram.**
- **In the top window click and drag a region of interest. The expanded view of the selected region will be shown in the lower window.**
- **You can move the position of a peak baseline point by clicking it and dragging it where you want.**
- **You can adjust the y-scale using the tools shown.**



Copy Chromatogram

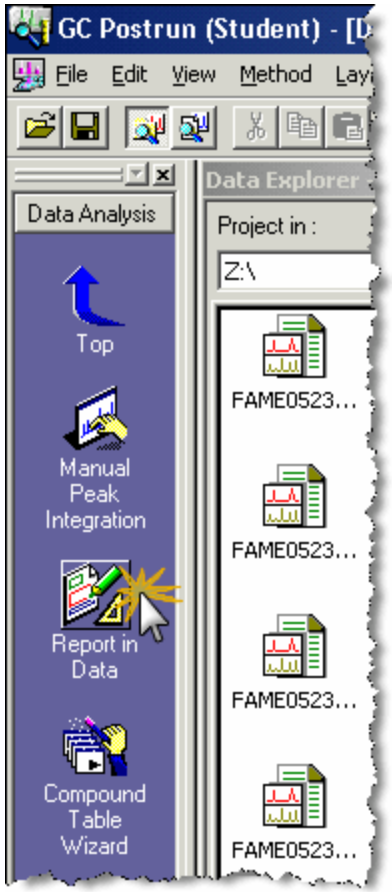
- **If you want to copy the chromatogram to another document, right click on the chromatogram and select ‘Copy’. This will place the chromatogram on the clipboard so you can paste it into Word or other document.**



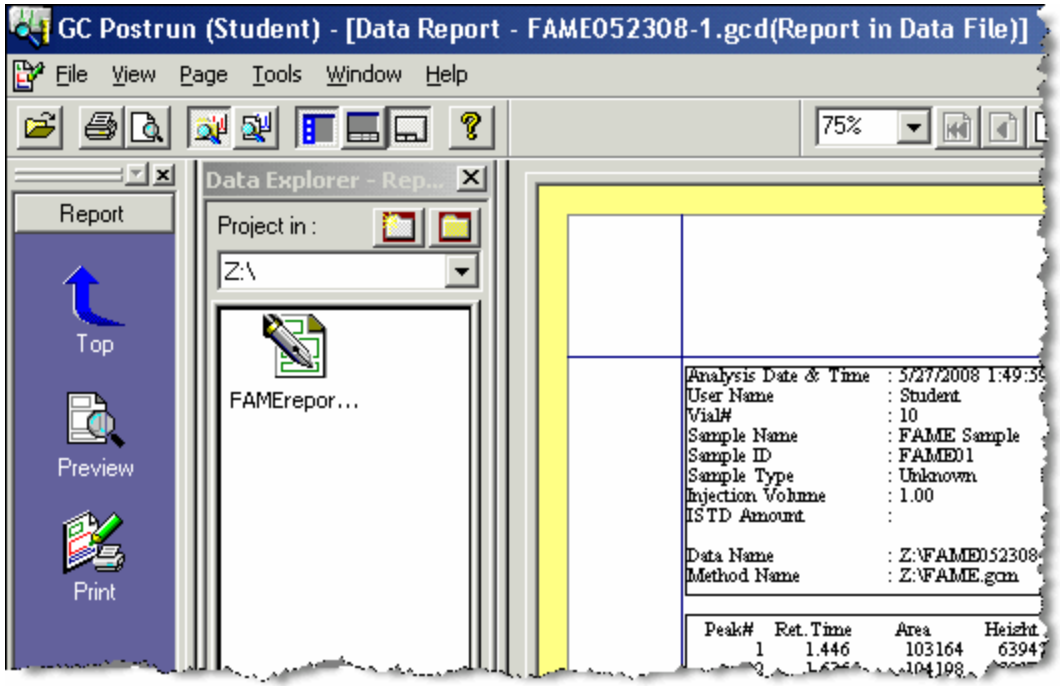
Open Report Window

- **To create a report of your data click on the 'Report in Data' icon on the left side of the GC Postrun window (a).**
- **The Data Report window will open displaying the data for the selected chromatogram in a report template (b). The report template file (FAMEreport.gcr) is shown in the Data Explorer window.**

(a)



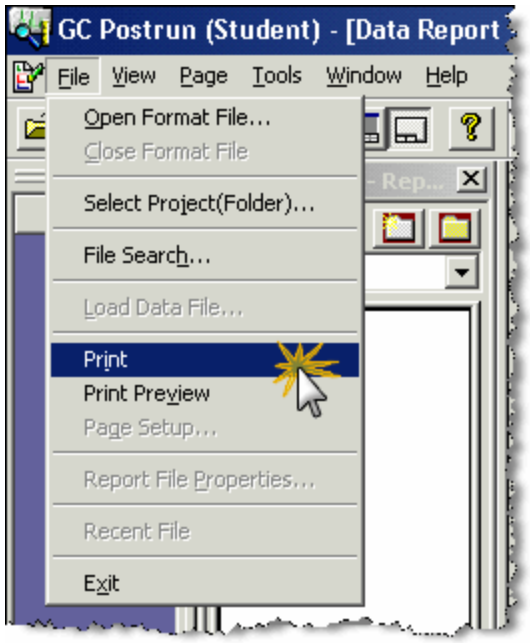
(b)



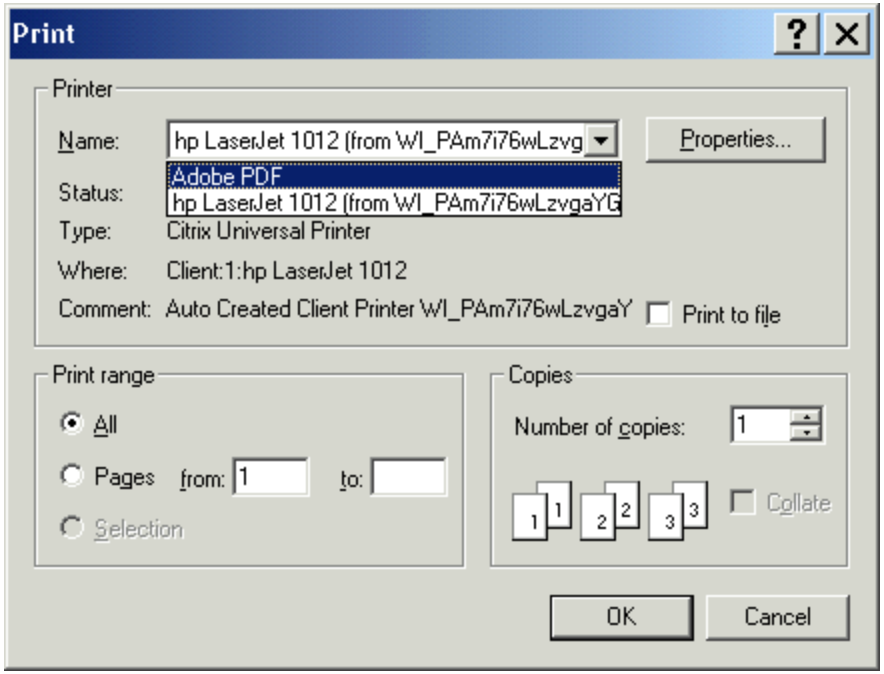
Print Report

- **To print the report select File |Print (a).**
- **In the print window your local printer and an Adobe PDF printer should be listed (b). Only your default printer will be displayed.**
- **You can print directly to your printer or create a PDF file.**
- **If you want to create a PDF file select the Adobe PDF printer and follow the directions on the page 13.**

(a)



(b)



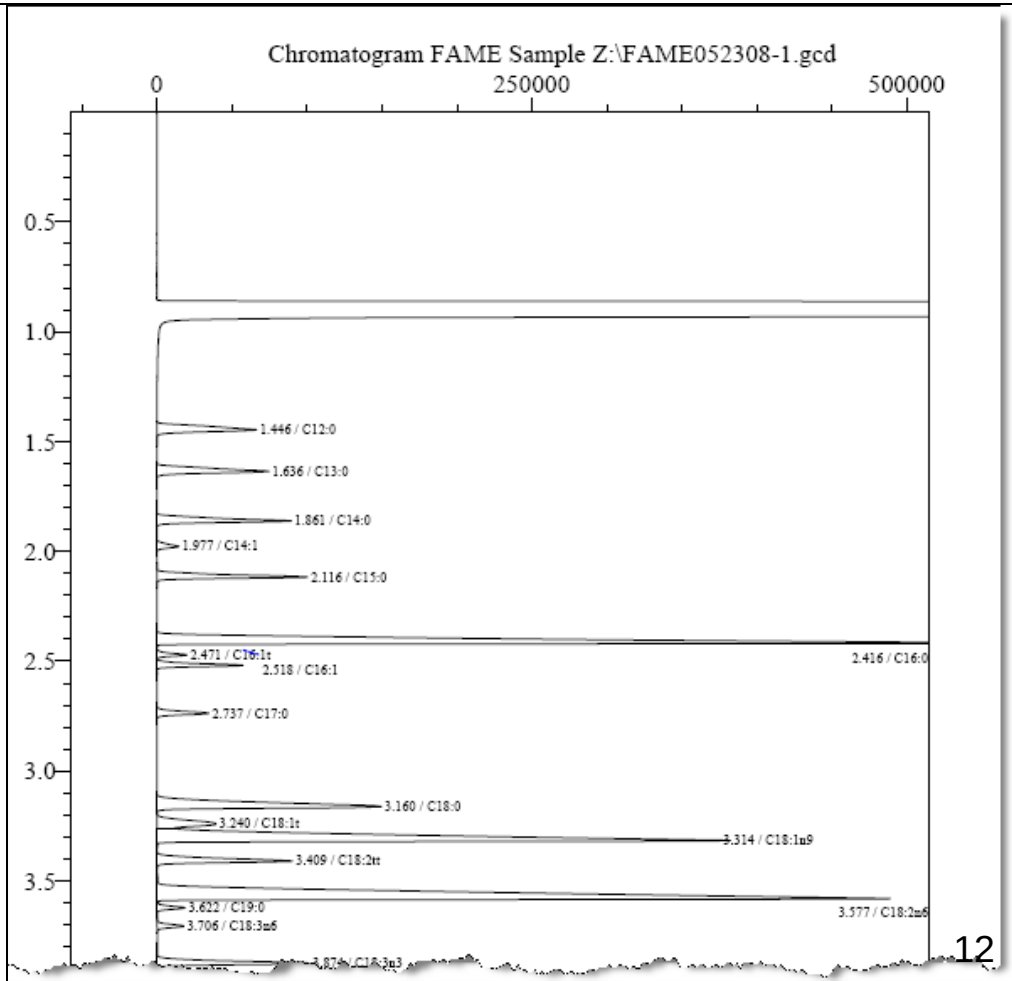
The Report

- **The two-page printed report will look like this. The peak table is on page one, the chromatogram is on page two.**

Analysis Date & Time : 5/27/2008 1:49:59 PM
User Name : Student
Vial# : 10
Sample Name : FAME Sample
Sample ID : FAME01
Sample Type : Unknown
Injection Volume : 1.00
ISTD Amount :

Data Name : Z:\FAME052308-1.gcd
Method Name : Z:\FAME.gcm

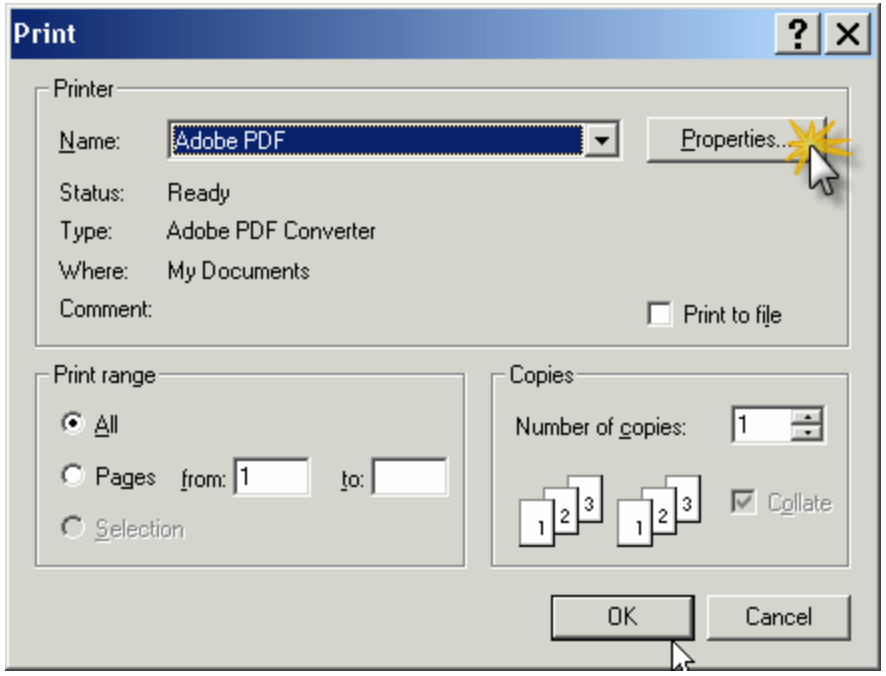
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.446	103164	63947	2.653	Area		1	C12:0
2	1.636	104198	70012	2.680	Area		2	C13:0
3	1.861	108960	84196	2.802	Area	V	3	C14:0
4	1.977	17591	14216	0.452	Area	V	4	C14:1
5	2.116	110755	95250	2.848	Area		5	C15:0
6	2.416	730749	511488	18.793	Area		6	C16:0
7	2.471	18331	18345	0.471	Area	V	7	C16:1t
8	2.518	54840	55599	1.410	Area	V	8	C16:1
9	2.737	37525	33309	0.965	Area		9	C17:0
10	3.160	252214	144953	6.486	Area		10	C18:0
11	3.240	75134	38686	1.932	Area	V	11	C18:1t
12	3.314	644506	359094	16.575	Area	V	12	C18:1n9
13	3.409	113337	87172	2.915	Area	V	13	C18:2tt
14	3.577	929507	465460	23.905	Area	V	14	C18:2n6
15	3.622	18482	17993	0.475	Area	V	15	C19:0
16	3.706	18464	16401	0.475	Area	V	16	C18:3n6
17	3.874	115279	97877	2.965	Area	V	17	C18:3n3
18	4.123	19323	16656	0.497	Area	V	18	C20:0
19	4.283	14618	12435	0.376	Area	V	19	C20:1n9
20	4.764	57361	44226	1.475	Area		20	C20:3n6
21	4.889	192696	139838	4.956	Area	V	21	C20:4n6
22	4.947	18577	16195	0.478	Area	V	22	C20:3n3
23	5.204	44782	35313	1.152	Area	V	23	C22:0
24	5.382	14811	10985	0.381	Area	V	24	C22:1n9
25	5.734	18496	12456	0.476	Area		25	C22:2n6
26	6.804	17922	9186	0.461	Area	V	26	C24:1n9
27	6.854	36769	19566	0.946	Area	V	27	C22:6n3
Total		3888391	2490854					



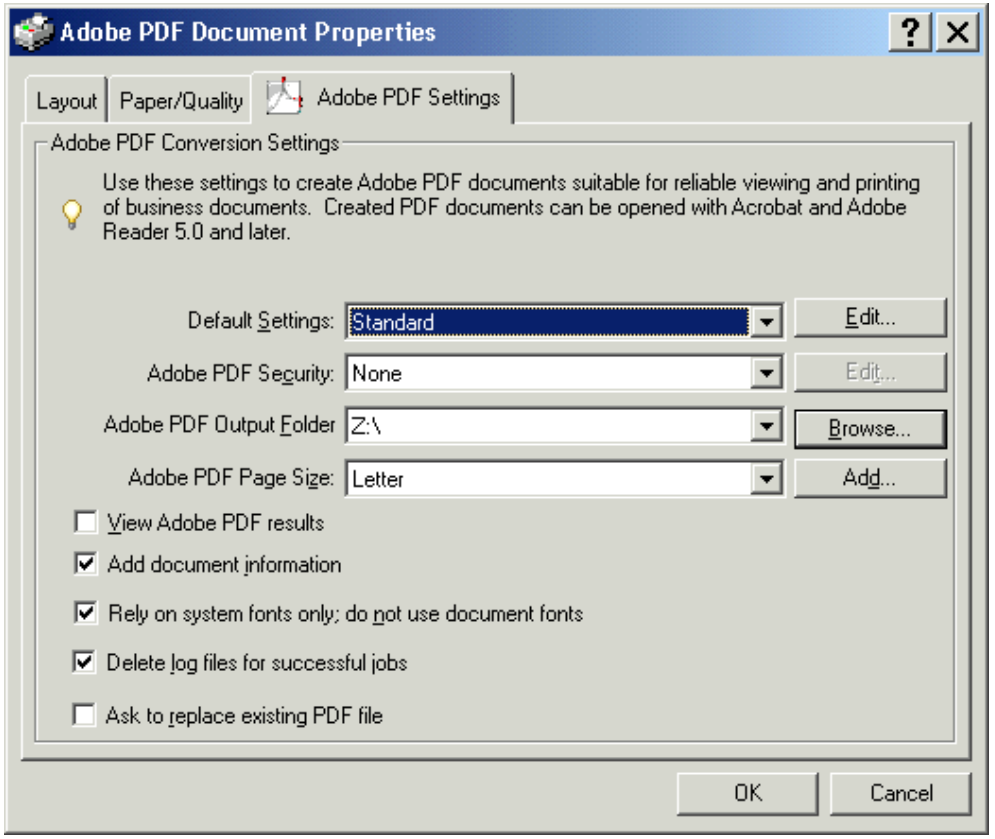
Optional PDF Printing

- **If you want to create a PDF file select File| Print and select the ‘Adobe PDF’ printer. Then click on the PDF printer properties button (a).**
- **On the ‘Adobe PDF Settings’ tab click on the ‘Browse’ button next to the ‘Adobe PDF Output Folder’ box. Select the Z:\ drive folder. This is your folder on the CASPiE file server.**
- **The rest of the settings should be as shown.**

(a)

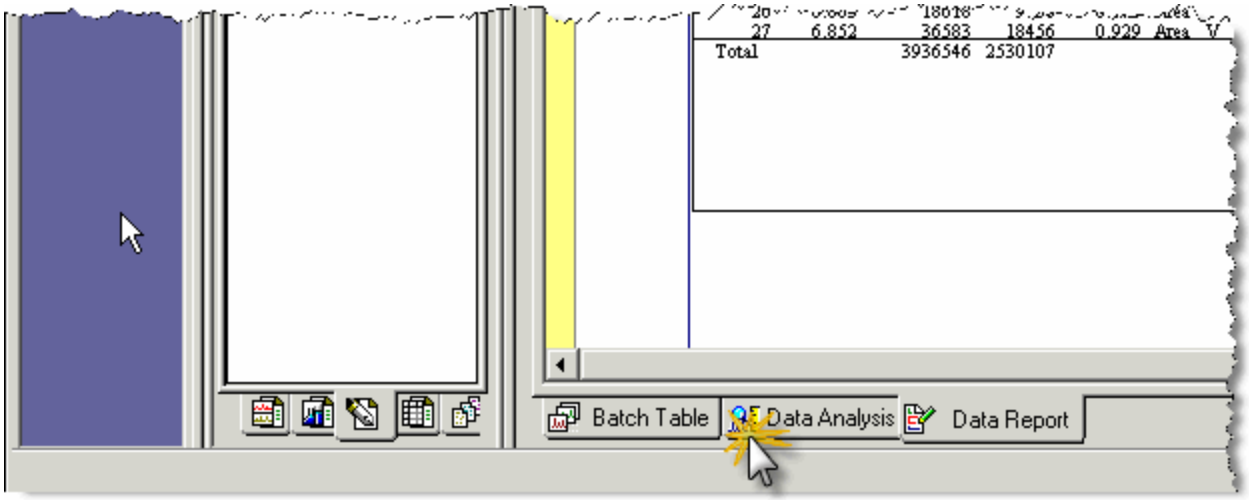


(b)



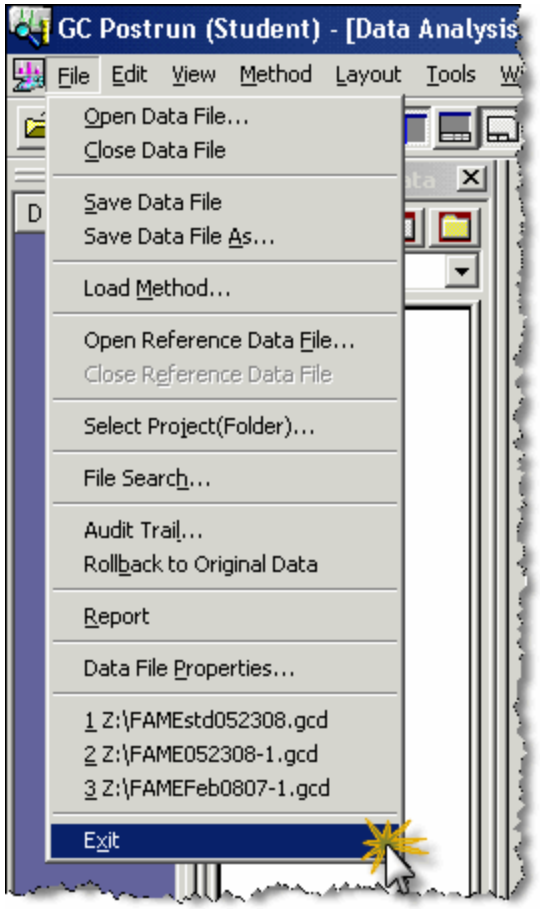
Print Remaining Chromatograms

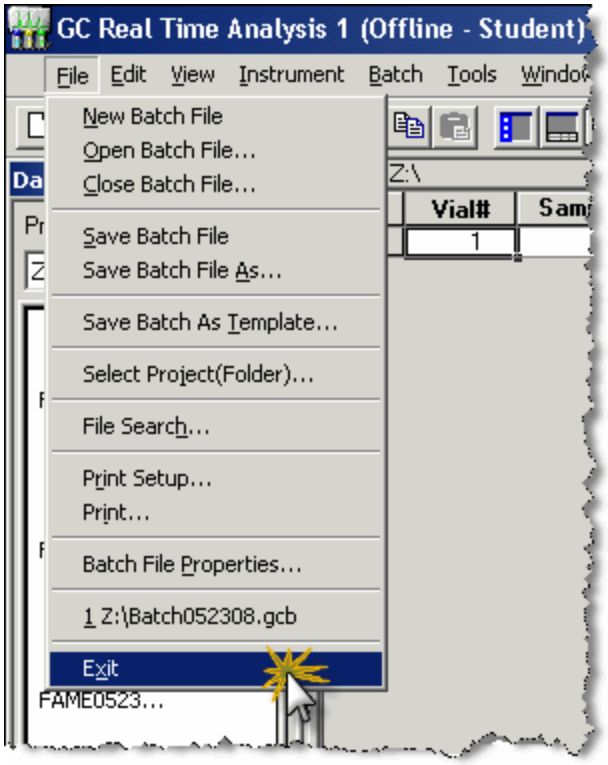
- **Return to the Data Analysis window by clicking on the Data Analysis tab at the bottom of the window (see below).**
- **Select another chromatogram and repeat the directions on pages 10-11. Repeat until all your chromatograms are printed.**



Close Windows

When you have finished printing exit all GC software windows.





External Access to Data Files

- **You can access your data files without the GC software. To do this use your browser to navigate to https://data.caspie.org.**
- **Login with your user name and password to display the data in your CASPiE folder (a).**
- **You can download any pdf file you may have created by right clicking on the file and selecting 'Save Target As…. (b).**

(a)

(b)