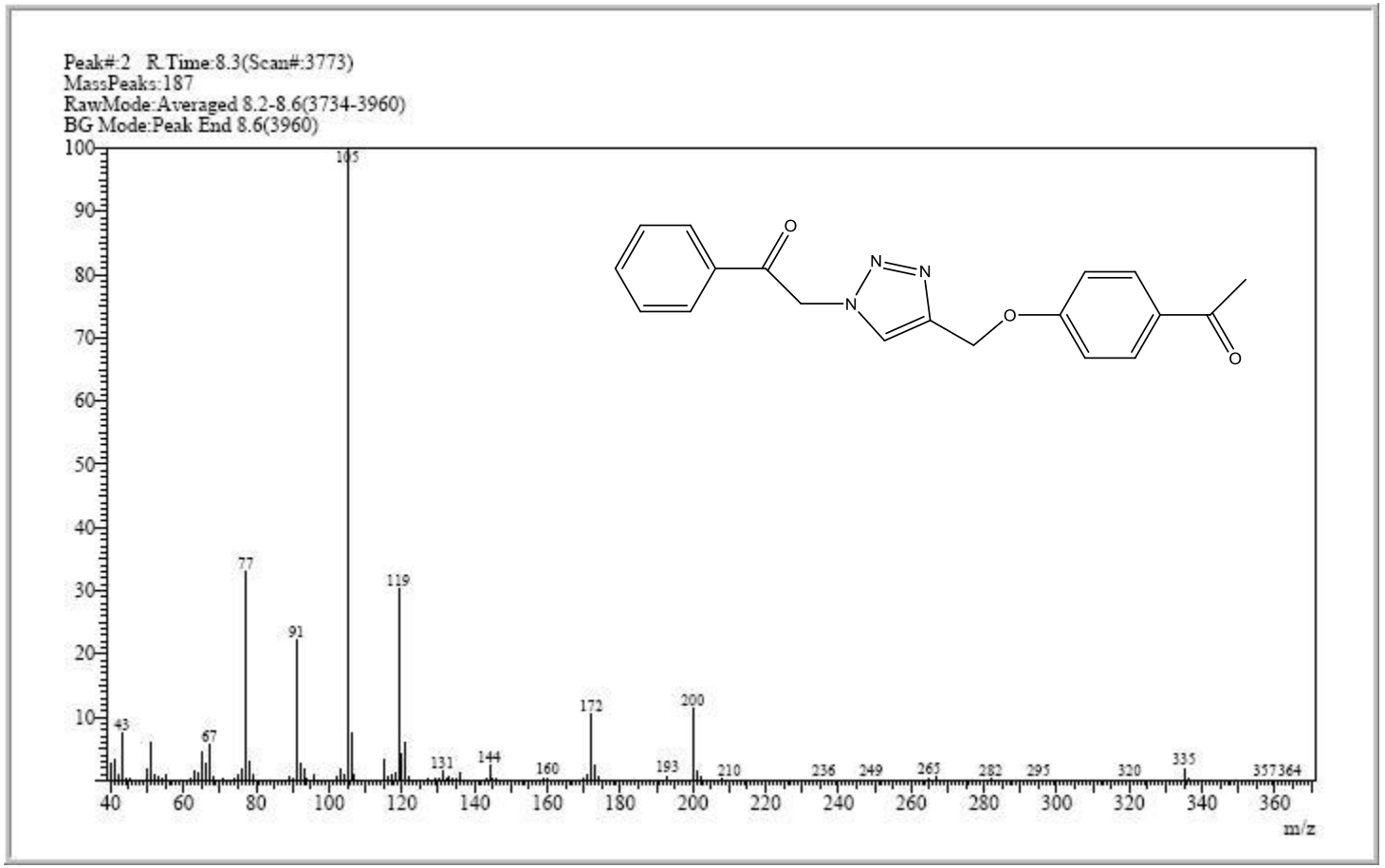
How to Process GCMS Data

After you run the GCMS to collect data for your sample, you need to get the mass spectrum of your product.

You will use a copy of the GCMS software that *is <u>not</u> attached to the instrument* to print your data.



Load the CASPiE Instrument Site

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

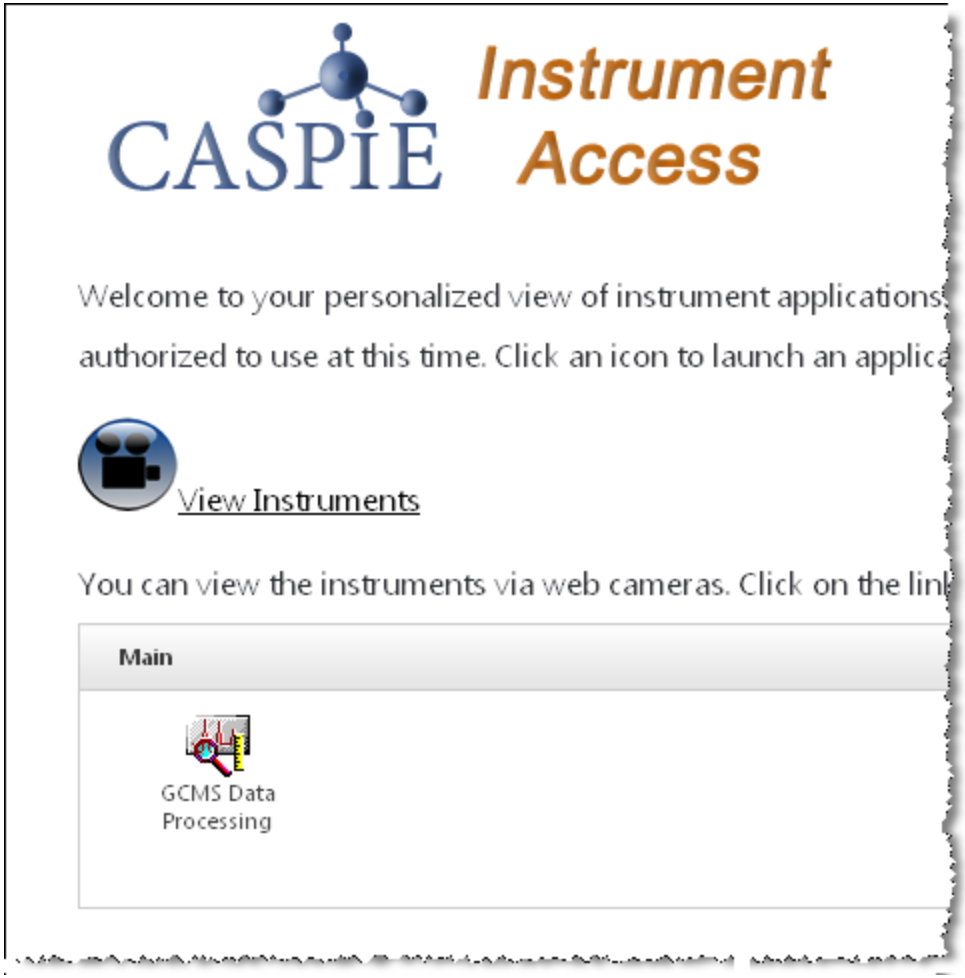
The GCMS Data Processing Software

You will use a copy of the GCMS software that *is <u>not</u> attached to the instrument* to process your data files.

The stand alone version of the software called 'GCMS Data Processing'.

You will always have access to the GCMS data processing software during a CASPiE module. You will only have access to the GCMS <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 GCMS Data Processing Software

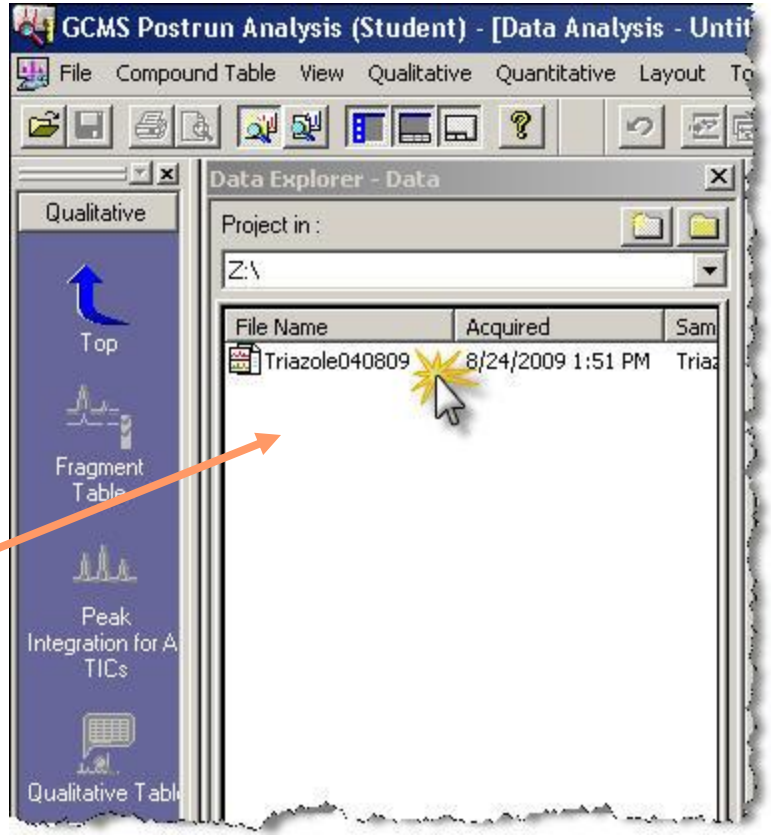
- **You should see the *GCMS Data Processing* icon in the Applications box. Launch the software by clicking once on the icon (a). If the *GCMS Data Processing* icon is not present ask your TA for help.**
- **A login window will appear (b). Use the user ID '<u>Student</u>.'** ***No password is required*.**

(a)

Open Data File

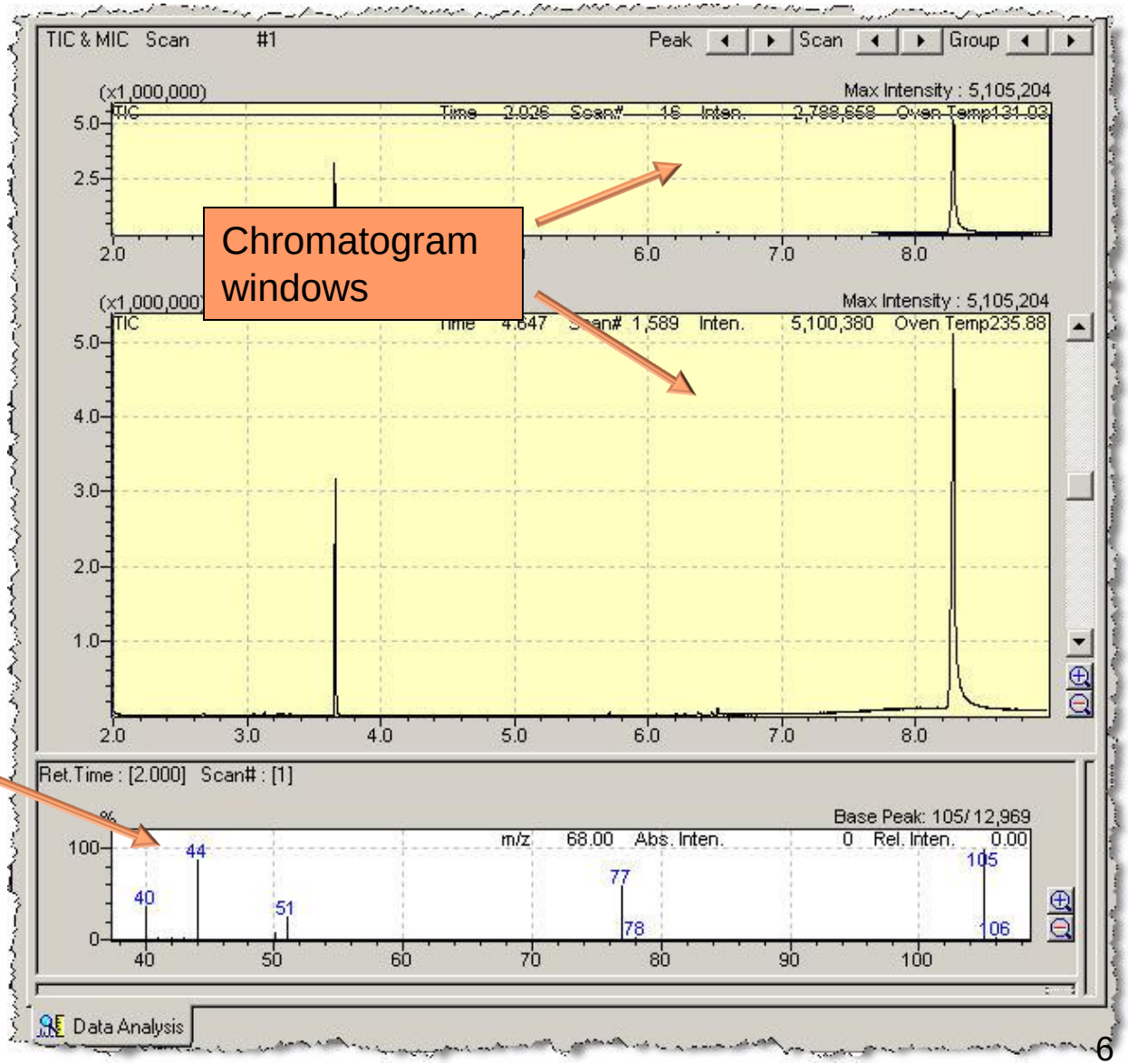
- **The data analysis application that opens is called *GCMS Postrun Analysis.***
- **In the Data Explorer window, double-click your data file to open the file.**

Data Explorer window



Data Display

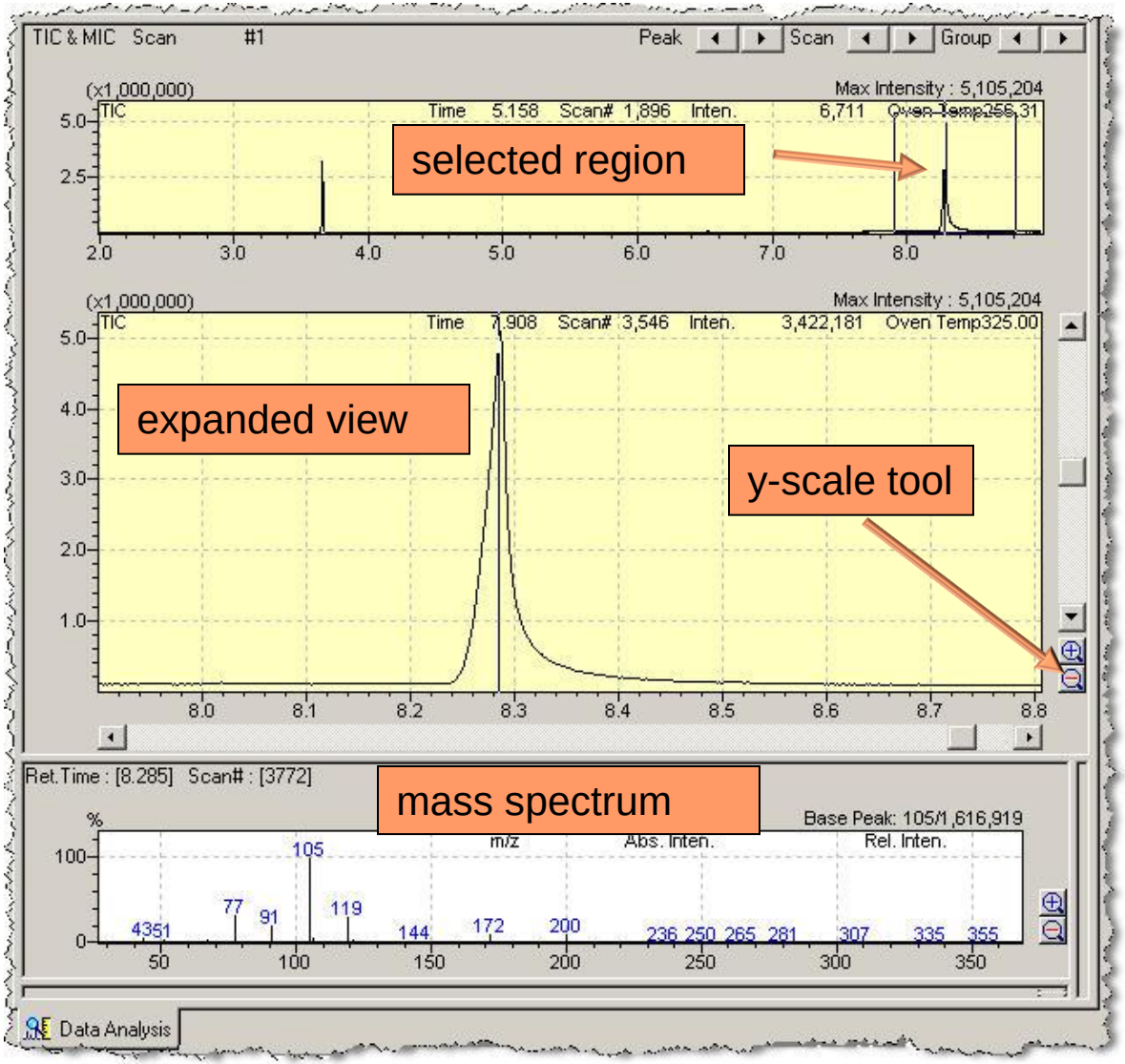
- **The data display has three windows, two chromatogram windows and the mass spectrum window.**



mass spectrum window

Chromatogram Windows

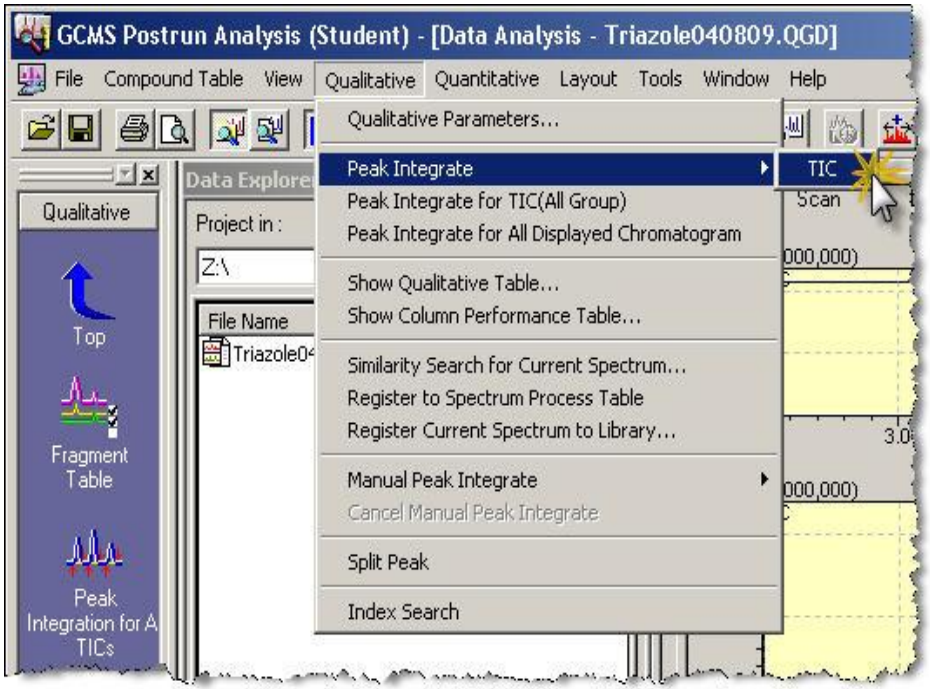
- **The bottom chromatogram window can display an expanded view of the chromatogram.**
- **In the top window click and drag around the region of interest. The expanded view of the selected region will be shown in the lower window.**
- **You can adjust the y-scale of the chromatogram using the tools shown.**
- **Double click on any point in the chromatogram to display the mass spectrum at that retention time.**



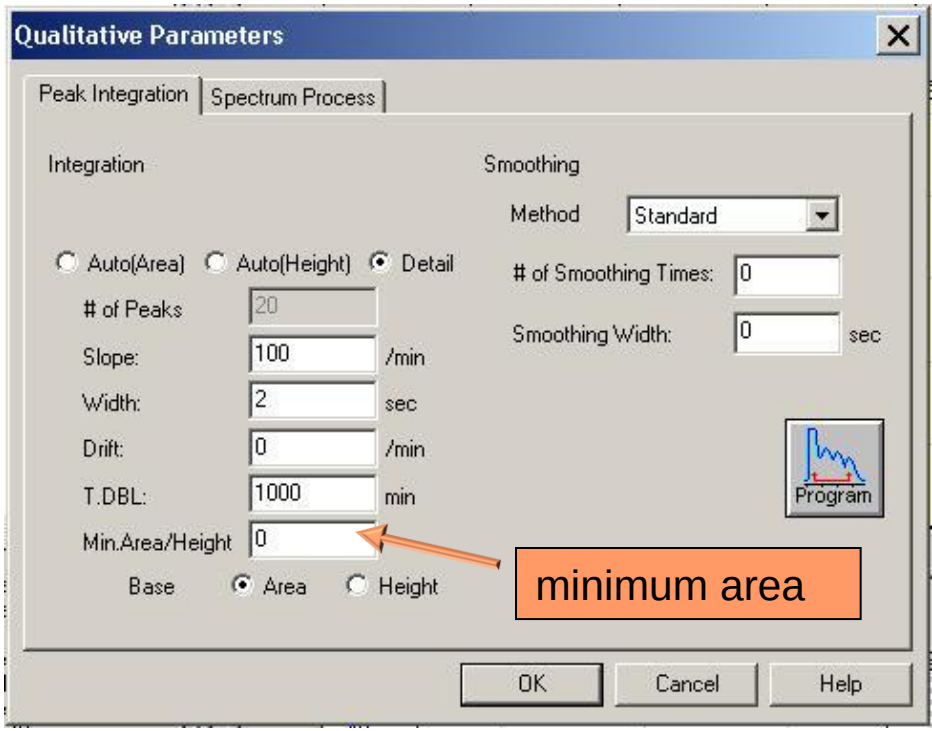
Integrate Peaks

- **In order to produce a quality spectrum of your peak(s), you must integrate the chromatographic peaks first.**
- **Select 'Qualitative| Peak Integrate| TIC' (a) from the menu.**
- **The Qualitative Parameters window will open (b).**
- **Change the minimum area to 100,000 and click OK. Keep the other default values.**

(a)

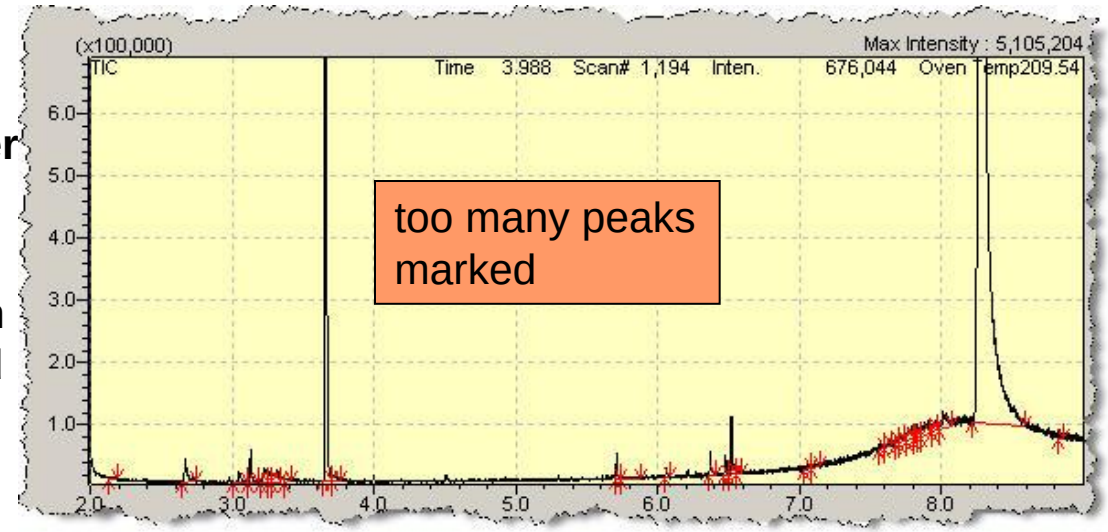


(b)

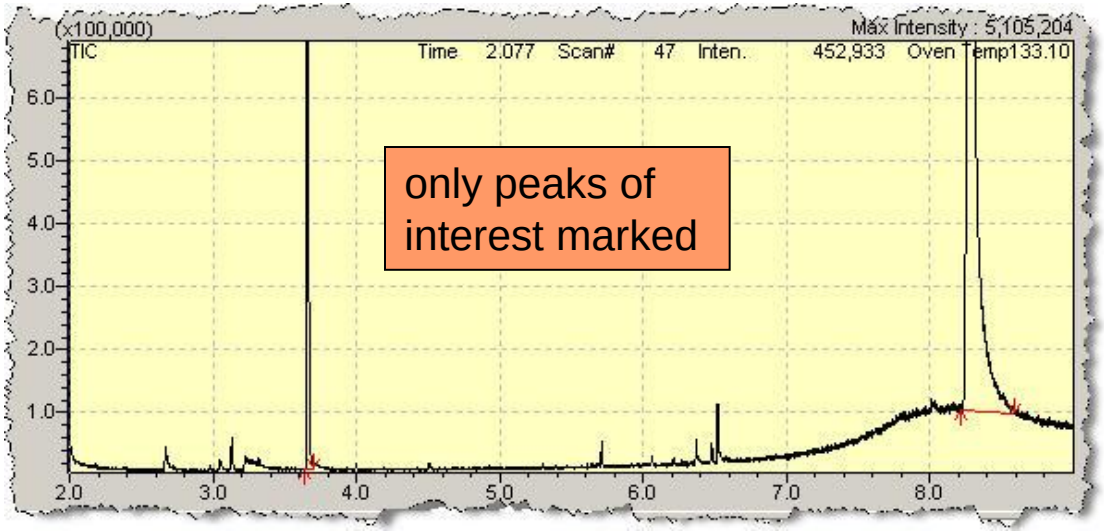


Optimize Integration

- **If there are too many peaks marked (lots of red arrows) change the minimum integration area to a larger number.**
- **Select 'Qualitative| Peak Integrate| TIC' again and change the minimum area by one order of magnitude and re-integrate by clicking OK.**
- **Repeat this process, increasing the minimum peak area until you get only the peaks of interest marked by red arrows. Make sure all the large peaks are marked.**



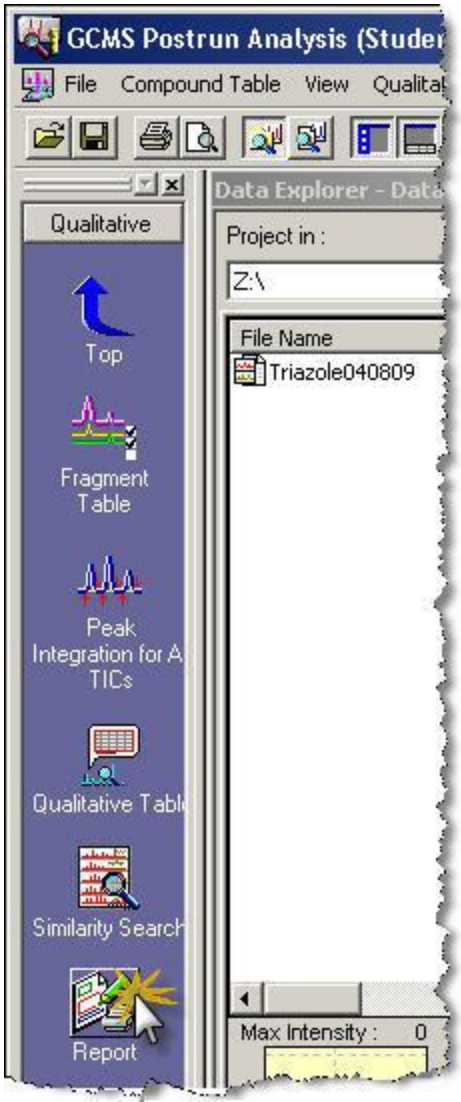
- **How many peaks you mark is up to you. Generally, the very small peaks are not of interest (insufficient concentration to be significant).**



Launch Report Template

- **To print the chromatogram and peak spectra you must create a report.**
- **Click on the 'Report' icon on the left (a).**
- **The report template file will be displayed in the Data Explorer window (b).**
- **Double click on the 'Antiviral' file to open the report template (b).**

(a)

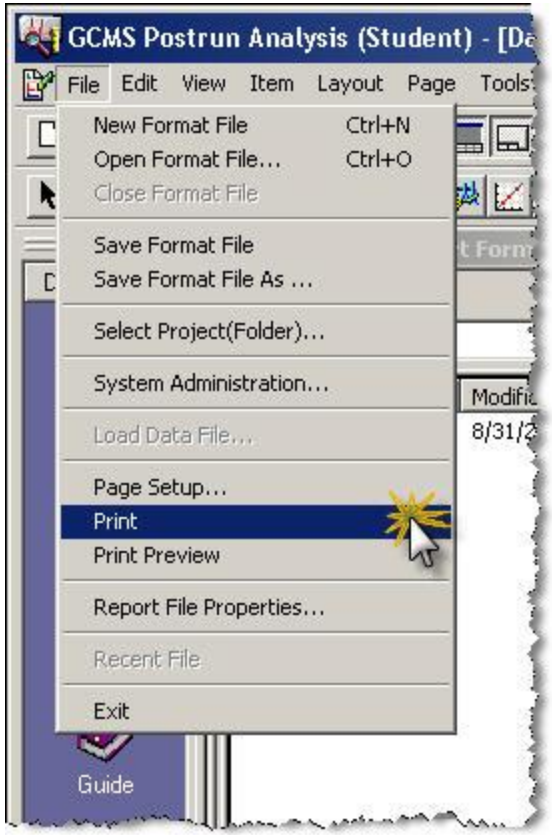


(b)

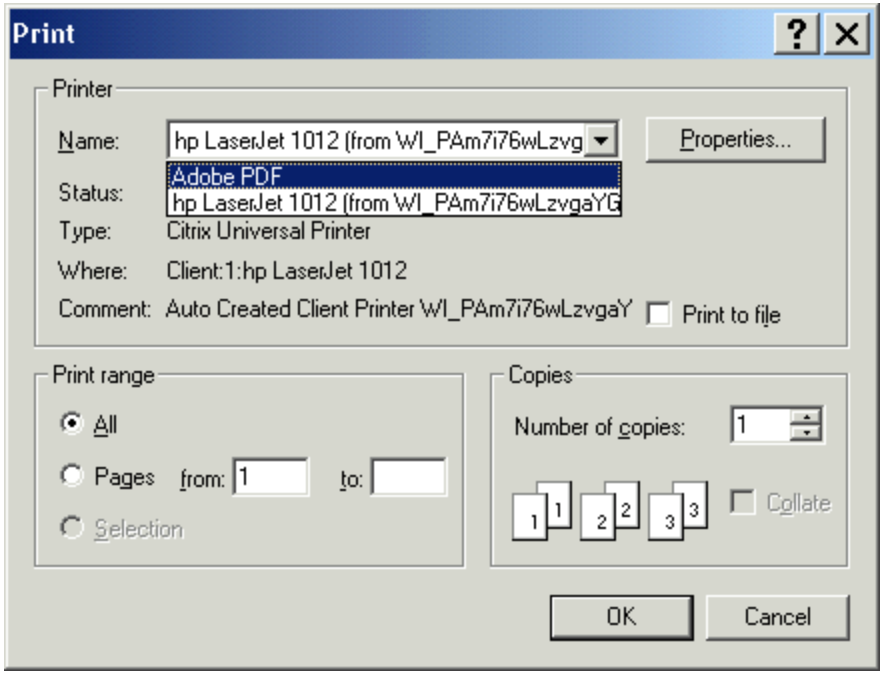
Print Report

- **To print the report select File |Print (a).**
- **Your local printer and an Adobe PDF printer should be listed in the print window (b).**
- **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 14.**

(a)



(b)



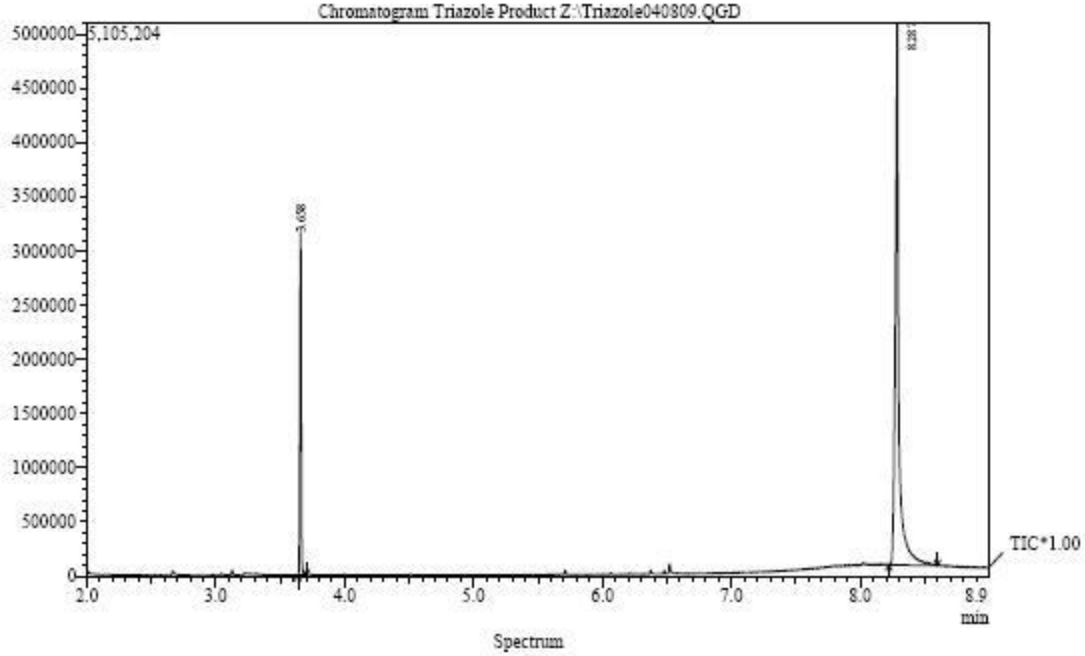
The Report

- **The report includes sample information, the chromatogram, and mass spectra of all integrated peaks.**

Sample Information

Analyzed by	: Student
Analyzed	: 8/24/2009 1:51:49 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Triazole Product
Sample ID	: Triazole Product
Vial #	: 1
Injection Volume	: 1.000
Data File	: Z:\Triazole040809.QGD
Method File	: Z:\Antiviral.qgm
Tuning File	: C:\GCMSsolution\System\Tune1\EI090619.qgt

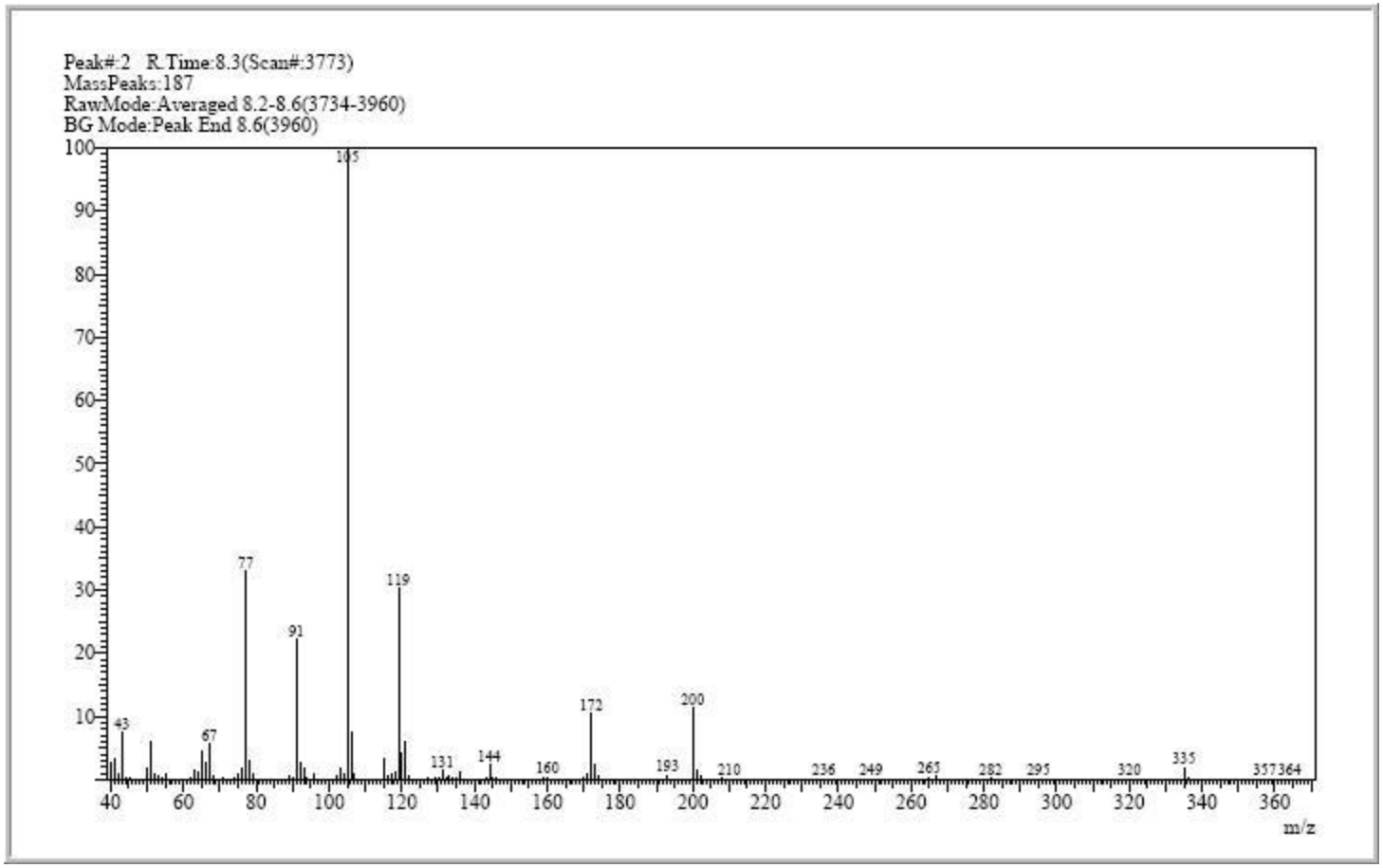
Chromatogram Triazole Product Z:\Triazole040809.QGD



Spectrum

The Report

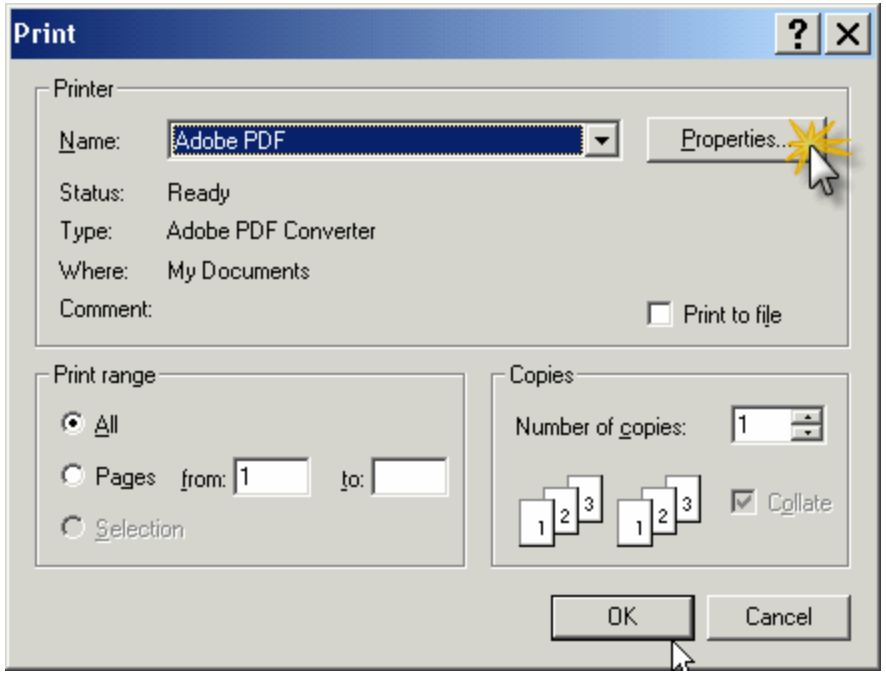
- **The printed mass spectrum is the peak average minus a background spectrum.**



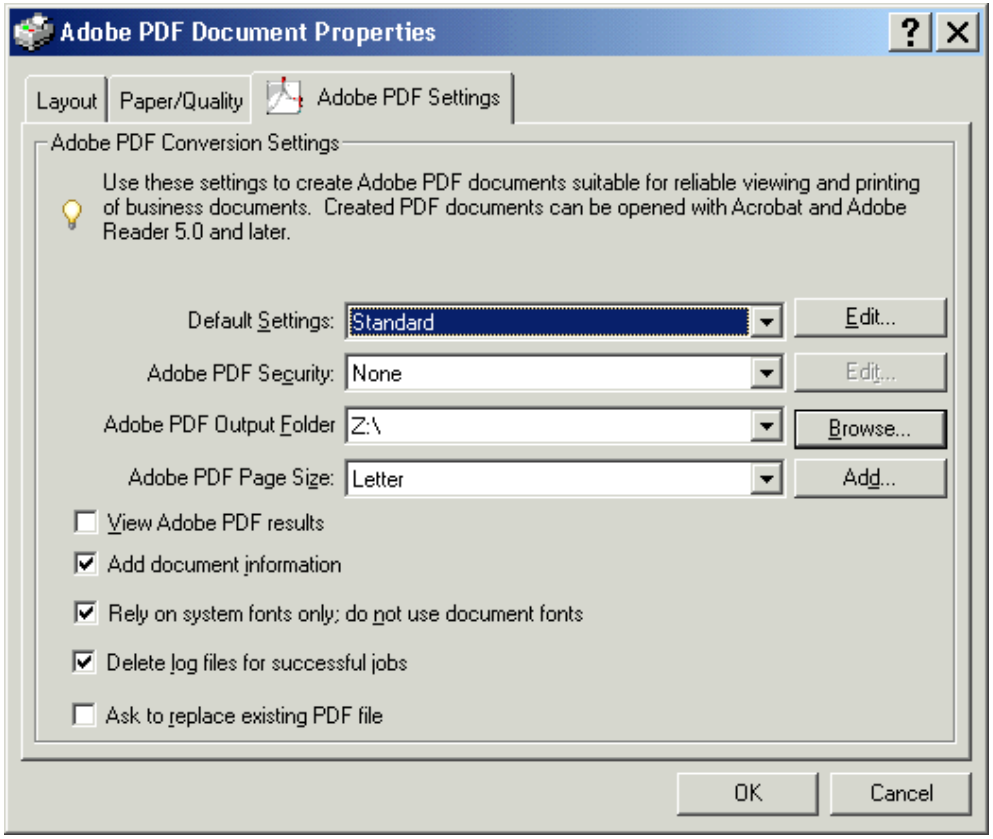
Optional PDF Printing

- **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)

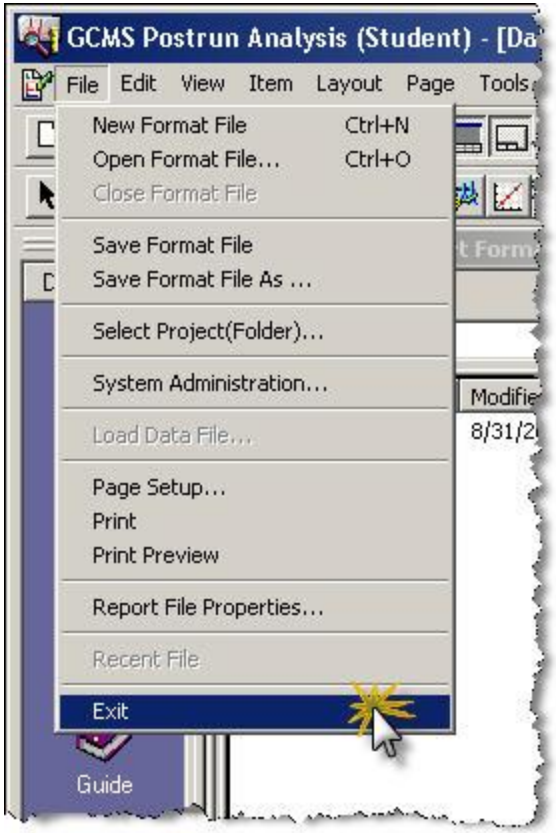


(b)



Close Windows

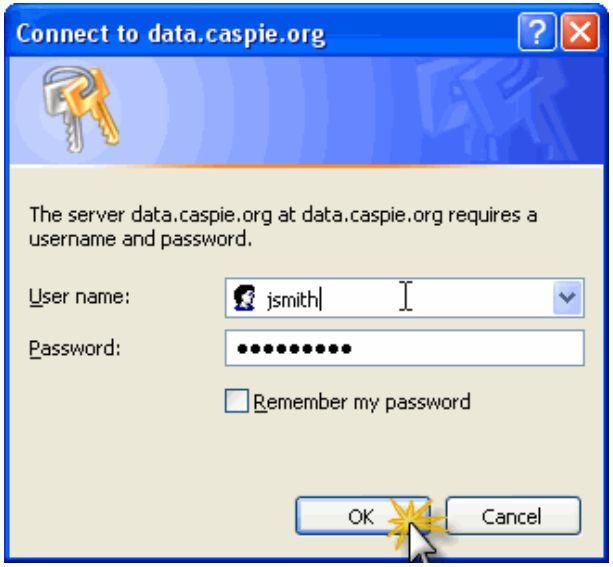
When you have finished printing exit the GCMS software.



External Access to Data Files

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

(a)



(b)