

Short GCMS Instructions: GCMS-TQ8040 NX

1. Log onto the computer and sign in on the **Excel** sheet.
2. Cancel ECOLOGY mode.
3. Put dilute samples into the autosampler. The samples should be in a low boiling solvent and free of dust and particulates. The numbering system on the autosampler is hard to read.
4. Check the fluid level of the syringe/needle wash vials. Fill as needed. A = hexanes, B = chloroform, C = isopropyl alcohol
5. Two programs are used to collect and analyze data. **Realtime Analysis** runs the experiments. **Post Run Analysis** is where you look at the data. The path to collecting data starts by creating a **Batch File** in **Realtime Analysis**, saving it, running it, then analyzing the data in **Post Run Analysis**. A sample **Batch** file is attached to the end of these instructions.
6. Open **Realtime Analysis**. Locate the **Assistant Bar**, (the vertical window, on the left side of the monitor). To create a Batch file, choose **Batch Processing** then **File** then **New File** then **Batch Table Template with switching Methods**. The first line tells the GC to switch from standby nitrogen to helium. The last line tells the instrument to switch from helium to nitrogen and standby. The first line takes 12 minutes. Insert rows between the first and last rows as needed.
7. **Batch File** details:
 - a) Sample Name and Sample ID should be used to describe your sample. Do **not** describe your sample in the data file name.
 - b) The format for **method files**: C:\Methods\lab director\method name.qgd
For example: C:\Methods\Yoon\SNGMethodMidRangeEarlyCollect.qgm
 - c) The format for **data files**: C:\Data\lab director\name\yymmdd_01.qgd
For example: C:\Data\Yoon\Lacker\230403_06.qgd
 - d) Make sure there is a **tune** file in each row of the **batch** file.

TIP: In Batch File window: [File Search → Methods (or Data) → Browse for Folder]
8. Save **Batch** file. C:\Data\2023\April\230403
[To run a second Batch File on a given day: C:\Data\2023\230403a]
9. Go to **Settings** on the **Assistant Bar** to tell the GC which row it should start with.

10. **Start.** The computer will calculate how long it will take to run the samples. This tells you
 - a) when to pick up the samples and take them back to your lab, and
 - b) when to make sure the GCMS is in standby.
11. To **edit a batch file** while it is running, click in the pause button at the top of the screen. It'll let you edit the batch and then start it back up again.
12. If nobody else is signed up to use the GCMS after you, start **ECOLOGY** mode by clicking on the round green **ECO** button in the lower right side of the monitor.
13. After a sample is run, go to **Post Run Analysis** and open the file. The triple headed arrow button at the top of the screen is very useful.

DO NOT exit **Realtime Analysis** software as it is controlling the GCMS. The mass spec is under vacuum so it stays on. A small flow of nitrogen runs through the GC column when it is not being used. Turning off the controller/computer is **UNACCEPTABLE** (“a no no”).

TIPS: To write a new Method, start with an old Method, “save as” to the name of your new Method. Make the changes you need and “save” them. Make sure the starting GC column temperature is above the boiling point of the sample solvent.

See training handouts for more details.

<u>solvent</u>	<u>boiling point</u>
CHCl ₃	61.2° C
hexanes	69° C
iPrOH	82.5° C
MeOH	64.7° C
EtOAc	77.1° C
CH ₃ CN	82° C
THF	66° C
CH ₂ Cl ₂	39.6° C

