

## Running the NMRFAM Bruker Nanostar Using Scripts

The Bruker Nanostar software has a command line function that allows you to run the instrument entirely using scripts. Here you can move the stage, open the shutter, change the temperature, etc. without having to click anything. A major advantage of running the instrument using scripts is that there is little room for human error if you repeat the experiment over and over. Here you can just change the file names in the script to continue repeating the same experiment.

Every time you run on the Nanostar, the instrument records all of the operations you carry out into the frame.slm file. Here you can find the commands to carry out any desired operation that you've done by clicking. Scripts can be created by inserting a string of commands into a text file with the .slm extension.

### How to run a script

1. In the menu click special, then select "command mode".
  - You will notice that you can no longer click any of the menu items
  - When in the command mode type **menu** and push enter to exit command mode and re-active the menu bar.
2. If you have a script you want to run such as "A.slm" type **@A.slm** into the command prompt and press enter. The Nanostar will now run the script.
  - It's a good idea to always put the menu command at the end of each script so that the command mode is exited when the script is complete.

### Example Temperature Titration Script

In the NMRFAM SAXS manual directory there is a script for running temperature titrations "SAXSTemperaturescript.slm". Below is a description of each command in the script:

```
GONIOMETER /TEMP 40 /RAMP=6.0 /HOLD=450 /WAIT
```

This changes the temperature stage to 40 degrees Celsius with a ramp rate of 6 degrees/minute. The instrument will then wait 450 seconds after the temperature has reached 40 degrees.

```
GONIOMETER /DRIVE 35.5 30.0 36.000 0.000 0.000
```

This moves the stage out of the way with coordinates of X= 35.5, Y= 30.0, Wheel = 36 degrees.

```
ADD 5 /CLEAR /COUNTS=10000000 /DISPLAY=15 /REALTIME /RESET=0 /SHUTTER &  
/SLAM=$null /BARTIME=0.0 /SLAM=$null  
SAVE 14_04_11_GCCRiscUbuff_40_frame_1 /TITLE="New frame" /DISPLAY=0
```

```
SPATIAL /UNWARP 14_04_11_GCCRIscUbuff_40_frame_1.gfrm 1 frame_u_0_000  
/DISPLAY=16
```

```
SAVE 14_04_11_GCCRIscUbuff_40_frame_1 /TITLE="New frame" /DISPLAY=0
```

Next a 5 second shot of glassy carbon is recorded to normalize the data based on beam intensity. Key features: "Add 5" tells the instrument to collect for 5 seconds. The file names will be "14\_04\_11\_GCCRIscUbuff\_40\_frame\_1". The Unwarp and Saves are automatically done when you manually collect a single scan using the user interface.

***\*\*Ultimately all you need to change is the Add time and File Name.***

```
GONIOMETER /DRIVE 35.5 72.6 10.000 0.000 0.000
```

The sample is moved into the path of the beam with X= 35.5, Y=72.6, and wheel = 10 degrees.

```
ADD 3600 /CLEAR /COUNTS=10000000 /DISPLAY=15 /REALTIME /RESET=0 /SHUTTER  
&
```

```
/SLAM=$null /BARTIME=0.0 /SLAM=$null
```

```
SAVE 14_04_11_IscUbuff_40_frame_1 /TITLE="New frame" /DISPLAY=0
```

```
SPATIAL /UNWARP 14_04_11_IscUbuff_40_frame_1.gfrm 1 frame_u_0_000 /DISPLAY=16
```

```
SAVE 14_04_11_IscUbuff_40_frame_1 /TITLE="New frame" /DISPLAY=0
```

Data is recorded for 3600 seconds. This is followed in the script by two more 1 hour frames.

menu

At the end of the script is the menu command that exits the command mode.