

CUSTOMQ



- Provides an interface midway between these very basic choices and the first series of menus.
- The following interface allows anyone to successfully **setup** and **acquire** any desired set of experiments from the full suite of available choices.
- **Auto-locking** and appropriate **gradient shimming** are performed **automatically**

Location: SAMPLE: Solvent:

Experiment selection/setup

| | |
|------------------|------------------|
| H1 ONLY | C13 ONLY |
| H1&COSY | C13 & DEPT |
| H1&H1 Detected | C13&C13 Detected |
| H1& Selective 1D | H-C-P-F |
| F19 ONLY | P31 ONLY |

INSTRUCTIONS

1. Insert New Sample
[or enter location and "change"]
2. Select Solvent
3. Select Experiment "Group"
[Customize experiment during dialogs]
4. Check EXPLIST for time
5. Redo dialog, if necessary
[Do probe tuning, manual locking, and shimming now, if necessary]
6. Start Acquisition

 Dialog:

Acq & Obs
Decouplers
Sequence
Flags & Cond.
Process
Process2
Display
display2
LCNMR/STARS
Text
Spare
Setup EXP
CustomQ
Walkup



The Chempack Interface

(Foreground Operation)

Location: SAMPLE: Solvent:

Experiment selection/setup

| | |
|-------------------|------------------|
| H1 ONLY | C13 ONLY |
| H1&COSY | C13 & DEPT |
| H1&H1 Detected | C13&C13 Detected |
| H1 & Selective 1D | H-C-P-F |
| F19 ONLY | P31 ONLY |

EXPLIST Dialog:

INSTRUCTIONS

1. Insert New Sample
[or enter location and "change"]
2. Select Solvent
3. Select Experiment "Group"
[Customize experiment during dialogs]
4. Check EXPLIST for time
5. Redo dialog, if necessary
[Do probe tuning, manual locking,
and shimming now, if necessary]
6. Start Acquisition

Acq & Obs
Decouplers
Sequence
Flags & Cond.
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Process2
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display2
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Walkup



Lock, Shim, Save & Text Options

AutoLOCK: YES NO

AutoSHIM: YES NO

Directory:

Save As:

Text:

The initial dialog box in
Glide or Chempack experiments



1D and Experiment Options

PROTON Spectral Width (ppm):

Minimize SW?:

PROTON scans:

PROTON Relaxation Delay (sec):

PROTON Pulse Angle:

Select Experiments in addition to PROTON:

(more):

(more):

(more):

(more):

(more):



Individual Experiment Options

| | | | | |
|-----------------------------------|------------------------------|--------------------------------------|------------------------------|------------------------------|
| gCOSY scans per inc: | <input type="checkbox"/> 1 | <input type="checkbox"/> 2 | <input type="checkbox"/> 4 | <input type="checkbox"/> 8 |
| gCOSY number of inc: | <input type="checkbox"/> 128 | <input type="checkbox"/> 200 | <input type="checkbox"/> 256 | <input type="checkbox"/> 512 |
| <input type="text"/> | | | | |
| <input type="button" value="OK"/> | | <input type="button" value="Reset"/> | | |



Once setup, simply clicking the **Start ACQ** button begins the actual data acquisitions!

Dialog Menu

The Dialog menu allows a chemist to **modify parameters** and *add or remove* queued experiments at any time... **even after the chain of acquisitions have begun (!)**. As always, parameter modifications are posed in chemical terms so that the busy chemist does not have to learn a large set of complex underlying NMR commands.



gHSQC Scans per inc: 4 2 8 16 32

gHSQC number of inc: 128 200 256 512

Carbon Spectral Width (ppm): -10 -> 160 -10 -> 190 -15 -> 225 -20 -> 240

OK

Reset