Routine 3D shimming through automation

Problem: Regularly shimming magnets running in automation is time consuming

Solution: get iconNMR to do it for you

Implementation:

1. Copy your favourite shim file: ‘wsh shim.icon’
2. In the iconNMR Lock/Shim Options -> Solvent/Probe Dependencies set the shim file for all solvents to ‘shim.icon’
3. Download the au_make_shim.icon file from http://nmr.chemistry.manchester.ac.uk (downloads/AU programs) and save it in /opt/topspin/exp/stan/nmr/au/src/user/. or equivalent
4. Create a standard ^{1}H experiment and set the automation acquisition AU program ‘AUNM’ to au_make_shim.icon
5. Save the parameter set
6. Add the parameter set to your admin user in iconNMR
7. Put in a 90 % H_2O/10 % D_2O sample
8. Submit the experiment using iconNMR

What the program does:

1. Insert sample and lock
2. Wait 5 minutes for equilibration
3. Tune and match
4. 1D (z) gradient shimming
5. 3D gradient shimming
6. Save shim to shim.‘todays_date’
7. Save shim to shim.icon
8. Acquire a ^{1}H spectrum

Takes 15-20 mins

Should run a separate line shape experiment afterwards

Generates a log of shims over time

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```
/* au_make_shim.icon
Usage:
Use a 90:10 H2O:D2O sample
Equilibrates the sample then runs 3d shim and save a file to shim.icon and shim.todays_date
type XAUA au_make_shim.icon, or copy the 'PROTON' parameter set and replace "au_zg" with "au_make_shim.icon“
*/

#include <stdio.h>
#include <time.h>
                time_t rawtime;
                struct tm *info;
                char buffer[80];
                time( &rawtime );
                info = localtime( &rawtime );
                strftime(buffer,80,"wsh shim.%Y%m%d", info);

/* equilibration time (seconds) five minutes should be enough*/
#define EQUILIBTIME 300

#define COMMAND1 ATMA
#define COMMAND2 XCMD("topshim tuneb tunea")
#define COMMAND3 XCMD("topshim 3d")
#define COMMAND4 XCMD(buffer)
#define COMMAND5 XCMD("wsh shim.icon")
#define COMMAND6 RGA
#define COMMAND7 ZG

/* Start of AU program */
GETCURDATA
i1 = ssleep (EQUILIBTIME);
COMMAND1
COMMAND2
COMMAND3
COMMAND4
COMMAND5
COMMAND6
COMMAND7

QUIT
```