



What's NEW In ICONNMR

Mike Brown
03012012

Sample Express is now controlled with Ethernet



SampleXpress

ICONNMR 4.6

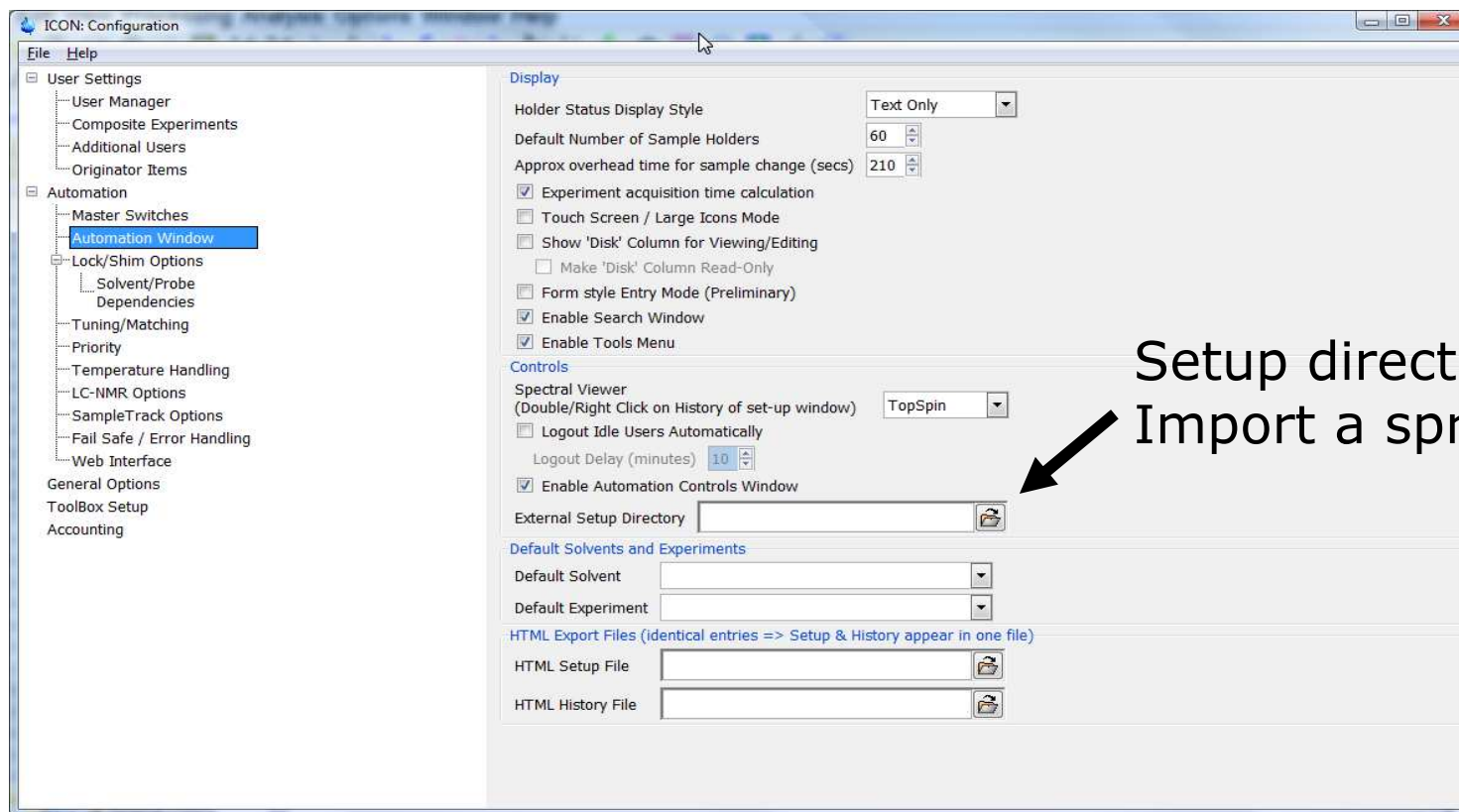


- A new IconNMR controlled command 'isx' is available inside TopSpin for direct Sample Changer (BACS/SampleXpress/SampleJet) operation, independently of IconNMR.
- Solvents/Experiments names containing spaces are now allowed.
- Variables may be used as Originator Items and/or Title. The following variables are available: \$NAME, \$EXPNO, \$DISK, \$SOLVENT \$EXPERIMENT etc.
- Experiments may be submitted, cancelled with <Alt-s>, <Alt-c> etc. in the Sample Holder Overview window.
- Assure System for Testing of Raw Materials for Adulterants*. See www.bruker.com/assure for more details

ICONNMR 4.6



Automation window reads spreadsheets in .xls/.xlsx format for import of experiment and sample lists with support for different workspaces.



Setup directory here
Import a spread sheet

ICONNMR 4.6



- Individual columns in Automation window may be hidden/displayed as required.

IconNMR: Automation May02-2012-2057-BBIOUS-meb

File Run Holder View Find Parameters Options Tools Help

Start [Play] [Pause] [Stop] [Refresh] [Info]

Experiment Queue

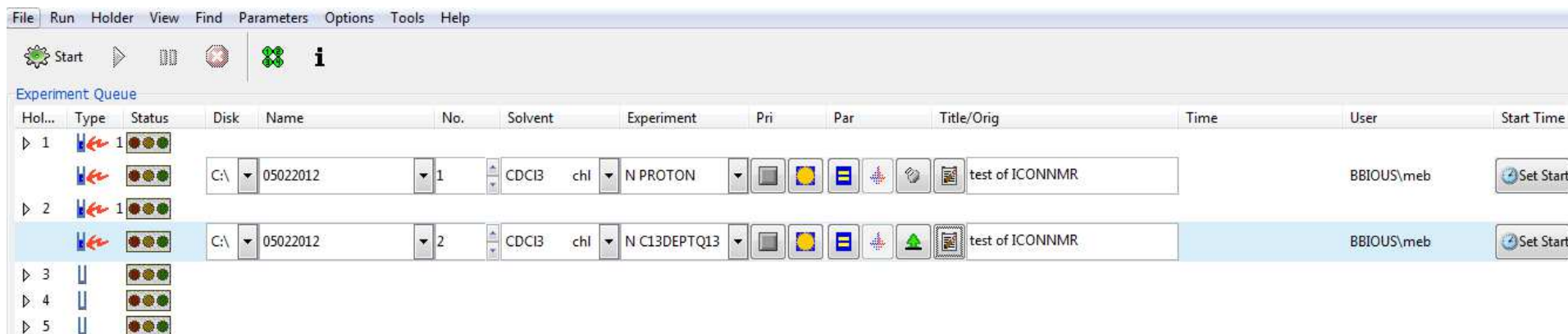
Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
Show all columns													
1	4	[Icons]											
[Icons]		[Icons]		05022012	1	CDCB3 chl	N PROTON	[Icons]	[Icons]	test			
[Icons]		[Icons]		05022012	2	CDCB3 chl	N C13DEPTQ13	[Icons]	[Icons]	test			
[Icons]		[Icons]		05022012	3	CDCB3 chl	C HSQCEDETGP	[Icons]	[Icons]	test			
	F2	[Icons]		05022012	1								
	F1	[Icons]		05022012	2								
[Icons]		[Icons]		05022012	4	CDCB3 chl	C COSYGPSW	[Icons]	[Icons]	test			
	F2	[Icons]		05022012	1								
	F1	[Icons]		05022012	1								
2		[Icons]											
3		[Icons]											

Submit [Cancel] [Edit] [Delete] Add 1 Copy 1

ICONNMR 4.6



You can turn off (or on) printing for each individual experiment



You can also choose to process or not to process the experiments

ICONNMR 4.6



It is much easier to set up Composite Experiments

- Designate the preparation experiments
- Then create the 2D or even 3D experiment
- Then test it

Composite Experiments

Name	Comment
FAB5	PROTON, C13DEPTQ135, HSQCED, COSYGP, HMBC
FAB4	PROTON, C13DEPTQ135, HSQCED, COSYGP
C13MULT	C13 Multiplicity Analysis
COSY45SW	sw opt. COSY45 (magn. mode)
COSY90SW	sw opt. COSY90 (magn. mode)
COSYGPSW	Gradient selected COSY
COSYGSSW	sw opt. COSY with gradients (magn. mode)
COSYDQFPHSW	sw opt. COSY with dq filter (States-TPPI)
COSYGPDPHPSW	Gradient selected double quantum filtered phase sensitive COSY
COSYGPMFSW	sw opt. COSY with gradients and dq filter (magn. mode)
MLEVPHSW	Phase sensitive TOCSY
MLEVPHPR	Phase sensitive TOCSY with solvent suppression
NOESYPHPR	Phase sensitive NOESY with solvent suppression
NOESYPHSW	Phase sensitive NOESY
ROESYPHSW	Phase sensitive ROESY
ROESYPHPR	Phase sensitive ROESY with solvent suppression
ROESYPHPREASY	Phase sensitive 'EASY' ROESY with solvent suppression
HMQCGP	sw opt. HMQC with gradients (magn. mode)
HMBCGP	sw opt. HMBC with gradients, low pass J-filter, no decoupling
HMBCETGPL3ND	1H-13C HMBC with gradient selection using 3-fold low pass filter for better 1J
HSQC GP	sw opt. HSQC sens. improved with gradients (e/a TPPI)
HSQCEDETGP	sw opt. edited HSQC with gradients (e/a TPPI)
HSQCEDETGPSISP_ADIA	1H-13C multiplicity edited HSQC with gradient selection BF1 >= 700 MHz
HSQCEDETGPSISP	1H-13C multiplicity edited HSQC with gradient selection 600 MHz >= BF1
HMQCGPML	sw opt. HMQC-TOCSY with gradients (magn. mode)
HMQCBI	sw opt. HMQC using BIRD pulse (magn. mode)
HMQCBIPH	sw opt. HMQC using BIRD pulse (States-TPPI)
HMQC	sw opt. HMQC (magn. mode)

Add new Modify Delete Save to User(s)

Component Experiments

Experiments	F2 Reference	F1 Reference
a PROTON		
b C13DEPTQ135		
c HSQCEDETGP	a PROTON	b C13DEPTQ135
d COSYGPSW	a PROTON	a PROTON
e HMBCLPND	a PROTON	b C13DEPTQ135

ICONNMR 4.6



- Updated and improved IconWeb look and feel
- You can see which experiments are done
- You can add experiments to the queue

The screenshot displays the Bruker IconWeb interface. At the top, it shows the system status: "Automation - Running - Busy until: Mon 12:27 - Day Experiments: 02:15 - Night Experiments: 00:00". Below this is a navigation menu with options like "Help", "Logoff", "Stop Run", and "Pause".

The main area contains a table of experiments with columns for Holder, Type, Status, Disk, Process Data, Name, No., Solvent, Experiment, Par, Title/Orig, Pri, Time, User, and Start Time. The table lists several experiments, some in 'Running' status and others 'Completed' or 'Queued'.

An "Add Experiment" dialog box is open, showing the following details:

- Plot-Title:** ASA in DMSO-d6
- Disk:** C:\Bruker\DATA\ICONNMR
- Expno:** 10
- Experiment:** C CHHANDRA PROTON, C13DEPTQ135, HSQC
- Lock Program:** LOCK.#Default
- Select Data Set Names:** 04232012
- Name:** 04232012
- Solvent:** DMSO dimethylsulfoxide-d6
- Shim Program:** GRADSHIM ;#Start Gradshim

Below the dialog box, there are several parameter settings, each with a "Default" button:

- rd Size of fid
- o1p Observe Frequency (in PPM)
- o2p Decouple Frequency (in PPM)
- si Size of spectra
- ns Number of scans
- p1 Pulse
- plw1 Power level in Watt
- ite Required Sample temperature
- cust11 Read pulse for DEPTQ
- cust13 LP filter for HMBC (8->10Hz)
- d9 TOCSY Mixing Time (80 ms)
- d8 NOESY Mixing Time (300 ms)
- p15 ROESY Mixing Pulse
- vdlist Variable delay list

At the bottom of the dialog, there are checkboxes for "Priority", "Night", and "Print", and buttons for "Add Experiment" and "Close Window".

ICONNMR 4.6



Web Server Settings

Enable Web Interface

Enable Standard Web Server

Access Standard Web Server as follows

(Mobile Devices)

Enable SSL Web Server

Access SSL Web Server as follows

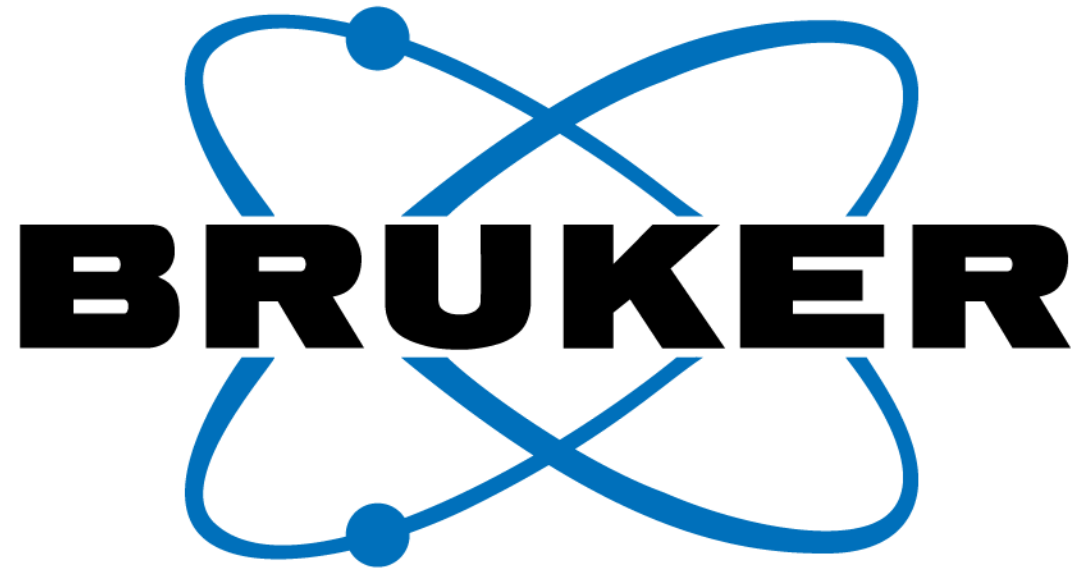
(Mobile Devices)

Web users can view spectra as PDF

- You can use SSL Certificates or a standard normal Web interface. Such Firefox, or Chrome
- You can use a mobile device
- You can also set it so that the users can view the spectra as a pdf



Are there any questions?



www.bruker-biospin.com