

Open Access Laboratories in Industry

Evaluation and Adjustments in Open Access NMR Environments

The Lilly logo is written in a red, cursive script font.

Answers That Matter.

The Environment

NMR spinners in magnet without tubes

NMR tubes in magnet without spinners

< you fill in the blank >

What can happen when procedures are ignored?

... another super-con that can be donated
for educational purposes. ☹



Open Access Experiences

Pharmacia – Kalamazoo

- Six Open Access Bruker NMR systems running automation
- Transitioned toward basic web-based instrument status and NMR data searching

Eli Lilly – Indianapolis

- Eight Open Access Varian NMR systems running automation
- Expanding suite of web-tools for central Open Access System Administration

Evaluation

Geographically Diverse

- Seven instrument locations (chemist clusters) in four buildings on two campuses

Automation Partially Developed

- Seven Open Access NMR instruments had daily web-scheduled walkup capabilities, two of which had evening automation

How should time be best spent? How could the chemists spend theirs?

What needs to be accomplished? What's enjoyable to do?

“The most important question in performance evaluation becomes not, “How well did you perform your job since we last met?” but, “How much did you change it?”” – from General Colin Powell, Chairman (Ret) Joint Chiefs of Staff “A Leadership Primer” – Lesson 10

1st Round of Adjustments

We created Web Tools for history, status, etc.

- Explogs with e-mail links, Automation History & links to saved console logs, Queue times, Service Event scheduling on 24/7 NMRs

The first screenshot shows the 'NMR Automation Queue History' for Wed Mar 22 08:01:30 EST 2006. It features a table with columns for INSTRUMENT, SAMPLE STATUS, and CONSOLE LOG. The second screenshot shows the 'NMR Automation Queue Status' for Wed Mar 22 07:59:58 EST 2006, with two tables: one for overall queue status and another for detailed instrument status including NIGHT AUTOMATION, TOTAL QTime, USED QTime, FREE QTime, and PERCENT FREE. The third screenshot shows the 'NMR Automation Console Log' for autolog06032201.ct on bigburn, displaying automation parameters like SAMPLES, USER, MACRO, EXPDIR, LOGDIR, SOLVENT, TEXT, SampleDir, Archive, USEDIR, EMAIL, EMAILwhen, DATA, and STATUS.

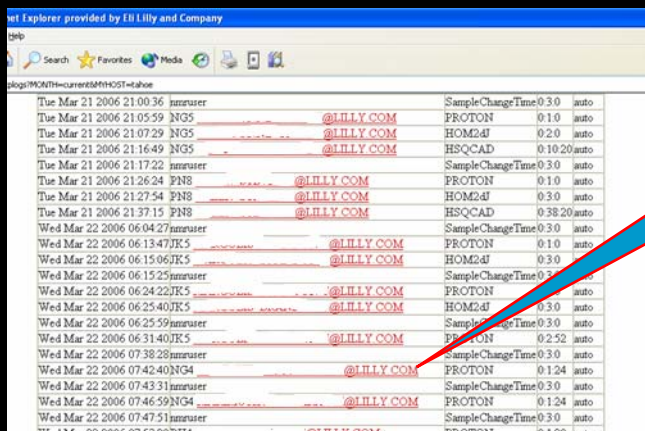
Identified and trained local chemist contacts

- Leverage local assistants for anomaly correction (< 5 min each instance; < 3 times per month)

1st Round Results

Enhanced CSINMR (Crime Scene Investigation NMR)

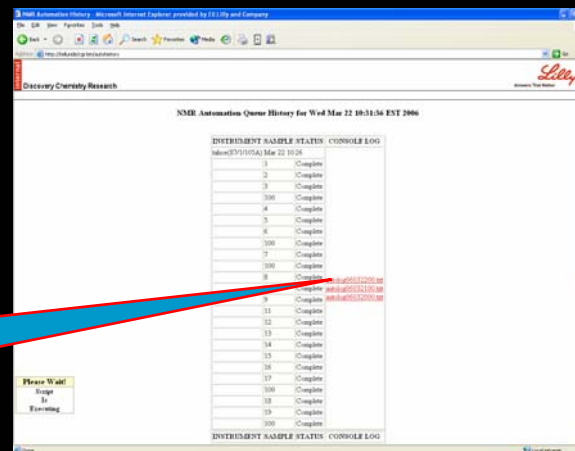
- Proactively address issues sometimes before chemists were aware of them
- We were able to communicate with the cluster before addressing the issue



Date/Time	User	Sample	Change Time	Mode
Tue Mar 21 2006 21:00:36	innruser	PROTON	0:30	auto
Tue Mar 21 2006 21:05:59	NG5	HOM2dJ	0:10	auto
Tue Mar 21 2006 21:07:29	NG5	HOM2dJ	0:20	auto
Tue Mar 21 2006 21:16:49	NG5	HSQCAD	0:10:20	auto
Tue Mar 21 2006 21:17:22	innruser	SampleChangeTime	0:30	auto
Tue Mar 21 2006 21:26:24	PN8	PROTON	0:10	auto
Tue Mar 21 2006 21:27:54	PN8	HOM2dJ	0:30	auto
Tue Mar 21 2006 21:37:15	PN8	HSQCAD	0:38:20	auto
Wed Mar 22 2006 06:04:27	innruser	SampleChangeTime	0:30	auto
Wed Mar 22 2006 06:13:47	JK5	PROTON	0:10	auto
Wed Mar 22 2006 06:15:06	JK5	HOM2dJ	0:30	auto
Wed Mar 22 2006 06:15:25	innruser	SampleChangeTime	0:30	auto
Wed Mar 22 2006 06:24:22	JK5	PROTON	0:30	auto
Wed Mar 22 2006 06:25:40	JK5	HOM2dJ	0:30	auto
Wed Mar 22 2006 06:25:59	innruser	SampleChangeTime	0:30	auto
Wed Mar 22 2006 06:31:40	JK5	PROTON	0:25:52	auto
Wed Mar 22 2006 07:38:28	innruser	SampleChangeTime	0:30	auto
Wed Mar 22 2006 07:42:40	NG4	PROTON	0:1:24	auto
Wed Mar 22 2006 07:43:31	innruser	SampleChangeTime	0:30	auto
Wed Mar 22 2006 07:46:59	NG4	PROTON	0:1:24	auto
Wed Mar 22 2006 07:47:51	innruser	SampleChangeTime	0:30	auto
Wed Mar 22 2006 07:53:20	BE4	PROTON	0:1:20	auto

E-Mail
address links

Console log
links



INSTRUMENT	SAMPLE	STATUS	CONSOLE LOG
1		Complete	
2		Complete	
3		Complete	
4		Complete	
5		Complete	
6		Complete	
7		Complete	
8		Complete	
9		Complete	
10		Complete	
11		Complete	
12		Complete	
13		Complete	
14		Complete	
15		Complete	
16		Complete	
17		Complete	
18		Complete	
19		Complete	
20		Complete	

Enhanced Time Management

- Were able to manage the decommissioning, moving, and reinstallation of eleven NMR instruments in 2005
- Were able to roll-out 24/7 automation in new Open Access Labs during moves

2nd Round of Adjustments

We increased automation capacity/increased software capabilities

- Converted all systems for evening automation w/ e-mail notification
- Started 24/7 automation in three locations w/ e-mail notification
- Flexible automation parameter setting with Chempack 3.1
- Creating web-based program so chemist can track all their OA samples from submission to completion

Hardware upgrades in progress to support our direction

- Standardizing on INOVA consoles
- Transitioning to Linux PCs for VJ/Chempack 3.1 automation interface
- Retraining SMS accessories for 100 sample capacity

2nd Round Results

A Café-like NMR experience in 24/7 Open Access labs

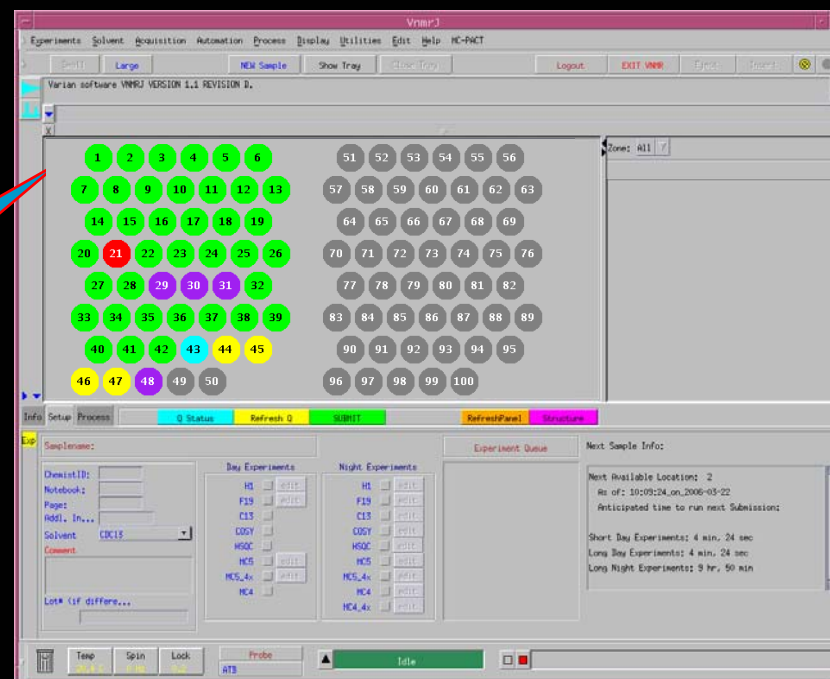
- Chemists appreciate quick visits to local OA lab several times/day to queue up new experiments while pickup/drop-off samples and hardcopy plots
- Chemists utilize remote access of NMR data
- Chemists spend more time in their lab

Providing an intuitive VJ/Chempack 3.1

Open Access Interface

Coming Soon!

Colors signify status of sample



Intentional chemist interaction

- Choose to prioritize chemist relationships

3rd Round Considerations

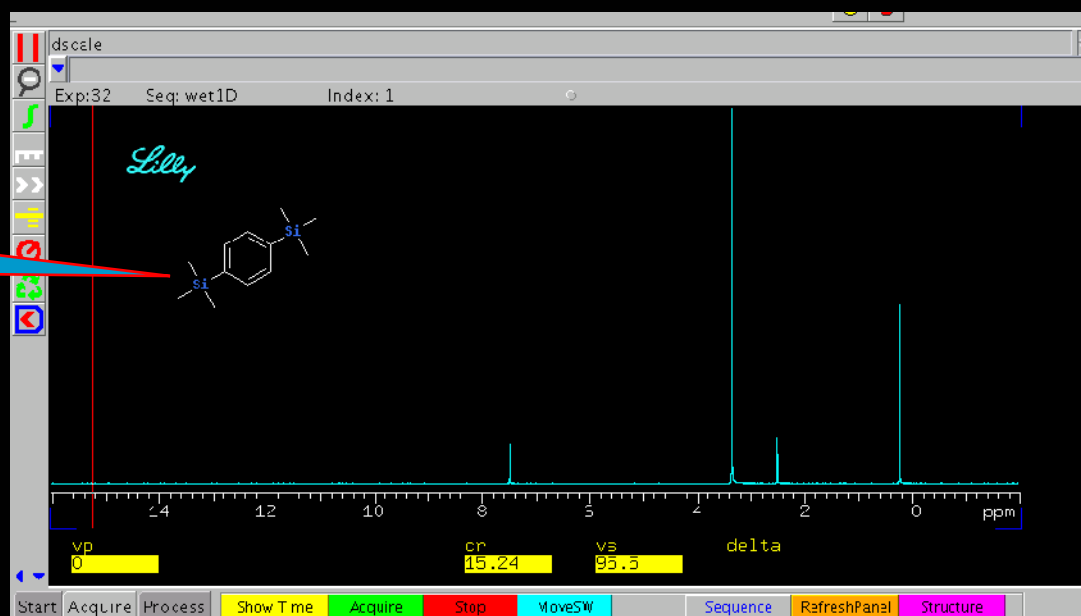
We interface e-notebook efforts with worklist submissions to OANMR

- minimizes transcription errors and save chemist's time

Utilize structure display capabilities of VJ for chemist's post-acquisition tasks

- Increase tools placed in the chemist's hands

Structure



3rd Round Considerations

We enhance multiple venues for NMR training opportunities

- Continue to grow the chemist's NMR capabilities creatively
 - CBT (Computer Based Training), Lunch-time Learning, etc.
 - Instant Messaging & VNC Servers help real-time NMR assistance

Alter Open Access Labs to be ergonomically updated to reflect a cafe environment

- 24/7 submissions at a bar height workspace, bar stools, etc

Chemists/Students
initial vision of
café NMR



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