On-line resources
to support NMR facilities

Freely accessible on-line info/tools

(beyond processing software)

Instrument booking sites

On-line calendars for instrument booking

- Faces
    - http://faces.ccrc.uga.edu/
    - *"Faces Scheduling System software is designed to facilitate the scheduling of scientific instruments and other resources in a research environment, and serves as a web accessible sign-up sheet."*
- Google Calendars/Docs
    - https://docs.google.com/a/bristol.ac.uk/spreadsheet/ccc?key=0AlRZSlSoOCBCdDdZc0pEd3VFVHhfWFNvMV9YRHNEU1E&hl=en_GB#gid=82
- Local web-based booking
    - e.g. developed from room-booking software
    - http://www.chem.ox.ac.uk/

v500a Booking Sheet ☆ ▨

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fx | Rule1: 4 hours max per user between 8am and 5pm

	A	B	C	D	E	F	G	H	I	J	K
1	Rule1: 4 hours max per user between 8am and 5pm										
2	Rule2: 6 hours max per user overnight unless discussed with Dr Butts										
3		Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday			
4	8am			va/sr			va/ga - pl				
5				va/sr			va/ga - pl				
6				va/sr			va/ga - pl				
7				va/sr			va/ga - pl				
8	9am						va/ga - pl				
9							va/ga - pl				
10				tg/nu			va/ga - pl				
11				tg/nu			va/ga - pl				
12	10am	cg/db	im/vd	tg/nu			va/ga - pl				
13		cg/db	im/vd	tg/nu			va/ga - pl				
14		cg/db	im/vd	tg/js		ad/tjm	va/ga - pl				
15		cg/db	im/vd	tg/js	cw/it	ad/tjm	va/ga - pl				
16	11am	cg/db	im/vd	tg/js	cw/it	ad/tjm	va/ga - pl	kb/jk			
17		cg/db	im/vd	tg/js	cw/it	ad/tjm	va/ga - pl	kb/jk			
18		cg/db	im/vd		cw/it	ad/tjm	va/ga - pl	kb/jk			
19		cg/db	im/vd		cw/it	ad/tjm	va/ga - pl	kb/jk			
20	12pm	cg/db	pp/sp	N2 FILL		ad/tjm	va/ga - pl	kb/jk			
21		cg/db	pp/sp	N2 FILL		ad/tjm	va/ga - pl	kb/jk			
22		cg/db	pp/sp	N2 FILL		jb/ms	va/ga - pl	kb/jk			
23		cg/db	pp/sp	N2 FILL	cr/lb	jb/ms	va/ga - pl	kb/jk			
24	1pm	va/jm	pp/sp		ad/tjm	ad/jc	va/ga - pl	kb/jk			
25		va/jm	pp/sp		ad/tjm	ad/jc	va/ga - pl	kb/jk			
26		va/jm	pp/sp		ad/tjm	ad/jc	va/ga - pl	kb/jk			
27		va/jm	pp/sp		ad/tjm	ad/jc	va/ga - pl	kb/jk			
28	2pm	va/jm			ad/tjm		va/ga - pl	kb/jk			
29		va/jm			ad/tjm		va/ga - pl	kb/jk			
30		va/jm			ad/tjm		va/ga - pl	kb/jk			
31		va/jm			ad/tjm		va/ga - pl	kb/jk			
32	3pm	va/jm	im/rm		cr/lb		va/ga - pl	kb/jk			
33		va/jm	im/rm		cr/lb		va/ga - pl	kb/jk			
34		va/jm	im/rm		cr/lb		va/ga - pl	kb/jk			
35		va/im	im/rm		cr/lb		va/ga - pl	kb/jk			

+ ≡ 29Apr-05May ▾ 06May-12May ▾ 13May-20May ▾ 20May-26May ▾ 27May-02Jun ▾ 03Jun-09Jun ▾ 10Jun-16Jun ▾ 17Jun-23Jun ▾ 24Jun-30Jun ◄ ►
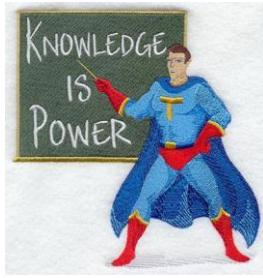
Supporting information

- NMR Facility web pages (our own!)
  - Primarily local user information
  - Information sheets etc that may be useful to others

- Vendor info:
  1) Main vendor *.com* sites for product information/software/buglists etc
  2) Support sites/forums/news/applications
  - http://www.theresonance.com/
  - http://www.spinsights.net/
  - http://nmrsupport.jeol.com/

- NMR Knowledge base:
  - http://www.spectroscopynow.com/
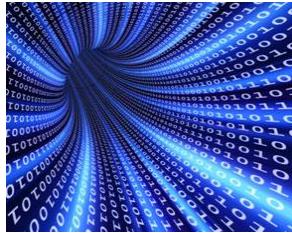
Databases

- BioMagRes:
  - http://www.bmrb.wisc.edu/
    - Data repository for biomolecules
- Spectral database of organic compounds:
  - http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng
    - Shifts, assignments, spectra
- NMR Shift DB:
  - http://nmrshiftdb.nmr.uni-koeln.de/
    - Shifts, assignments, spectra
- Human Metabolome Database:
  - http://www.hmdb.ca/
    - Data on small molecule metabolites found in the human body

Spectrum predictors

- ACD (RSC Chemical Database Service, *EPSRC funded*):
    - http://cds.rsc.org/
        - Free to academic users
        - Multinuclear spectrum prediction

- *Chemdraw* also has chemical shift prediction built-in (often widely available but less reliable/comprehensive).

- *Other commercial packages available*… NMR Predict (Mnova) comparable to ACD predictors, etc…?

NMR Wikipedia

"**NMR Wiki** is an effort to promote *sharing information, know-how and wisdom* among researchers working in the field of Magnetic Resonance"

- NMR wikipedia:
    - http://nmrwiki.org/wiki/index.php

- Also with the NMR Q&A forum:
    - http://qa.nmrwiki.org/

Networking sites

- *Linked-in* groups:
  - Magnetic resonance research
  - Nuclear magnetic resonance
  - NMR pulse sequences
  - SMASH NMR

UKMRM site?

- Would a site for UK managers be useful??
  - links to UK facility sites
  - info sheets
  - new or modified sequences
  - tips and tricks