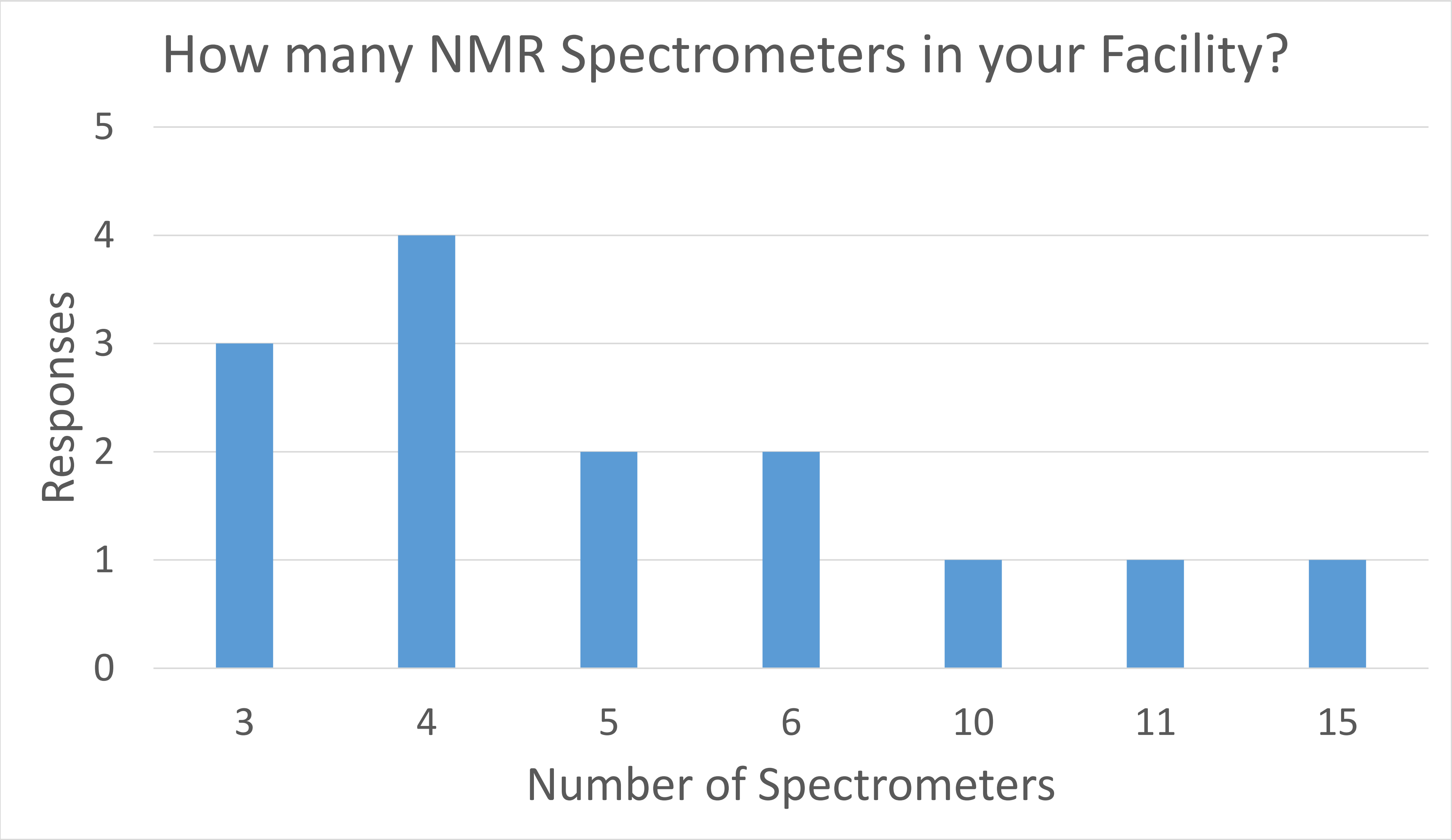
Teaching and Training Survey

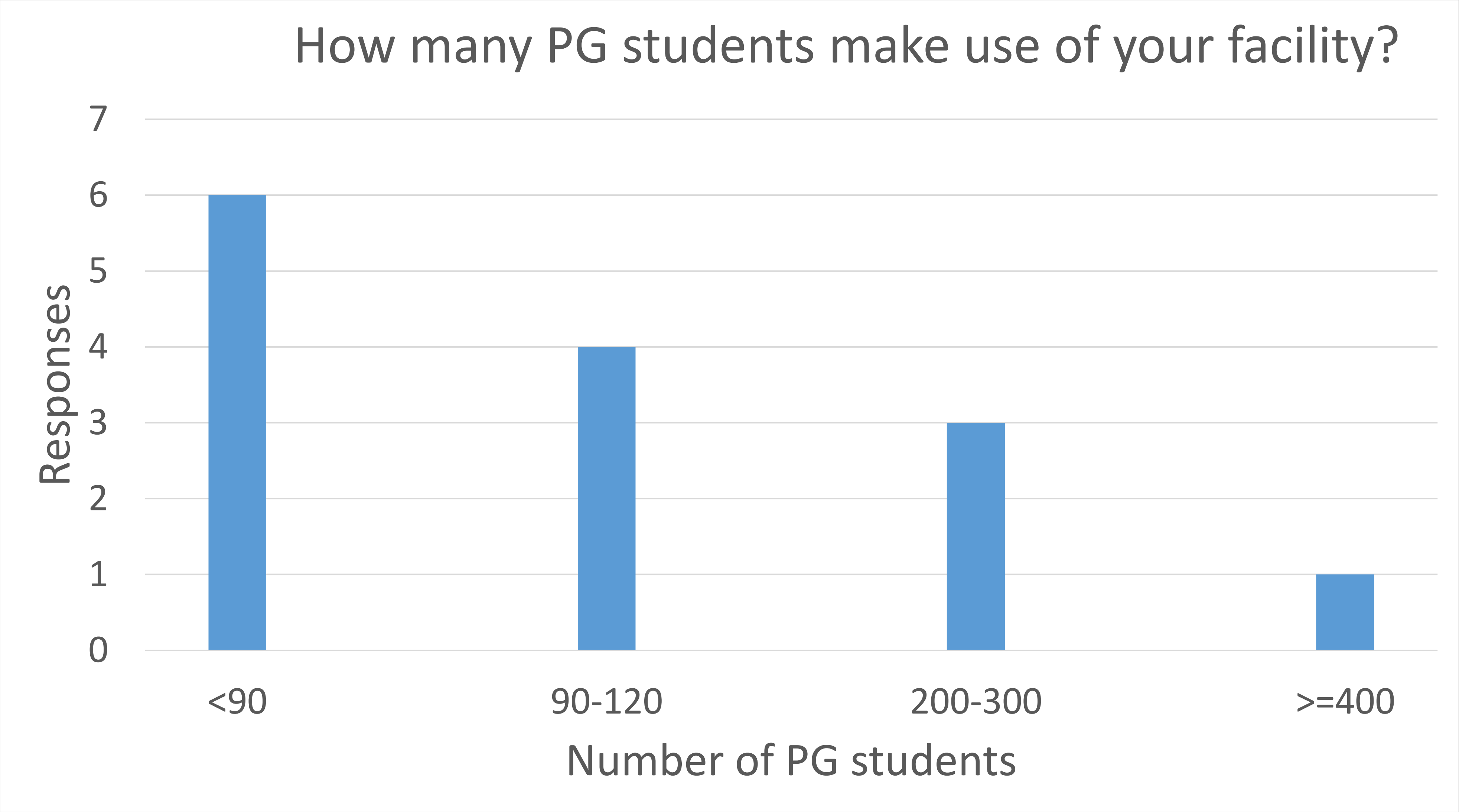
UKMRM 2017

Adrienne Davis, University of Nottingham

Facility Size



Facility Size

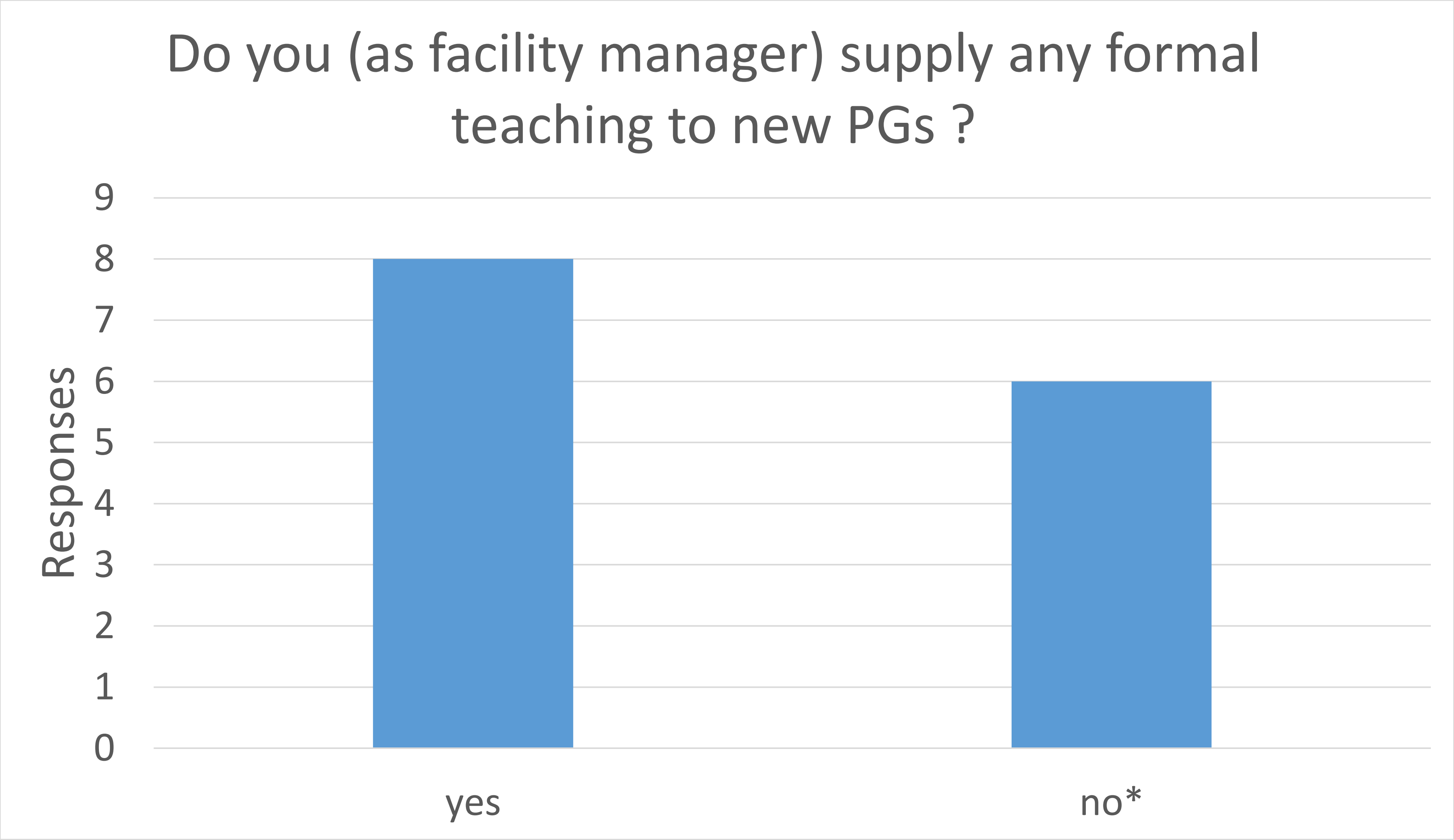


What typical level of understanding of NMR do your new PG students have?

Category	No. of Responses
full knowledge of 2Ds, NOEs	0
awareness of 2Ds can analyse 1Ds competently*	12
some familiarity with 1D interpretation*	2
would struggle to explain the proton coupling pattern and integrals of ethanol	0
what's NMR?	0

* Some comments that there is quite a wide variation in prior knowledge.

Teaching

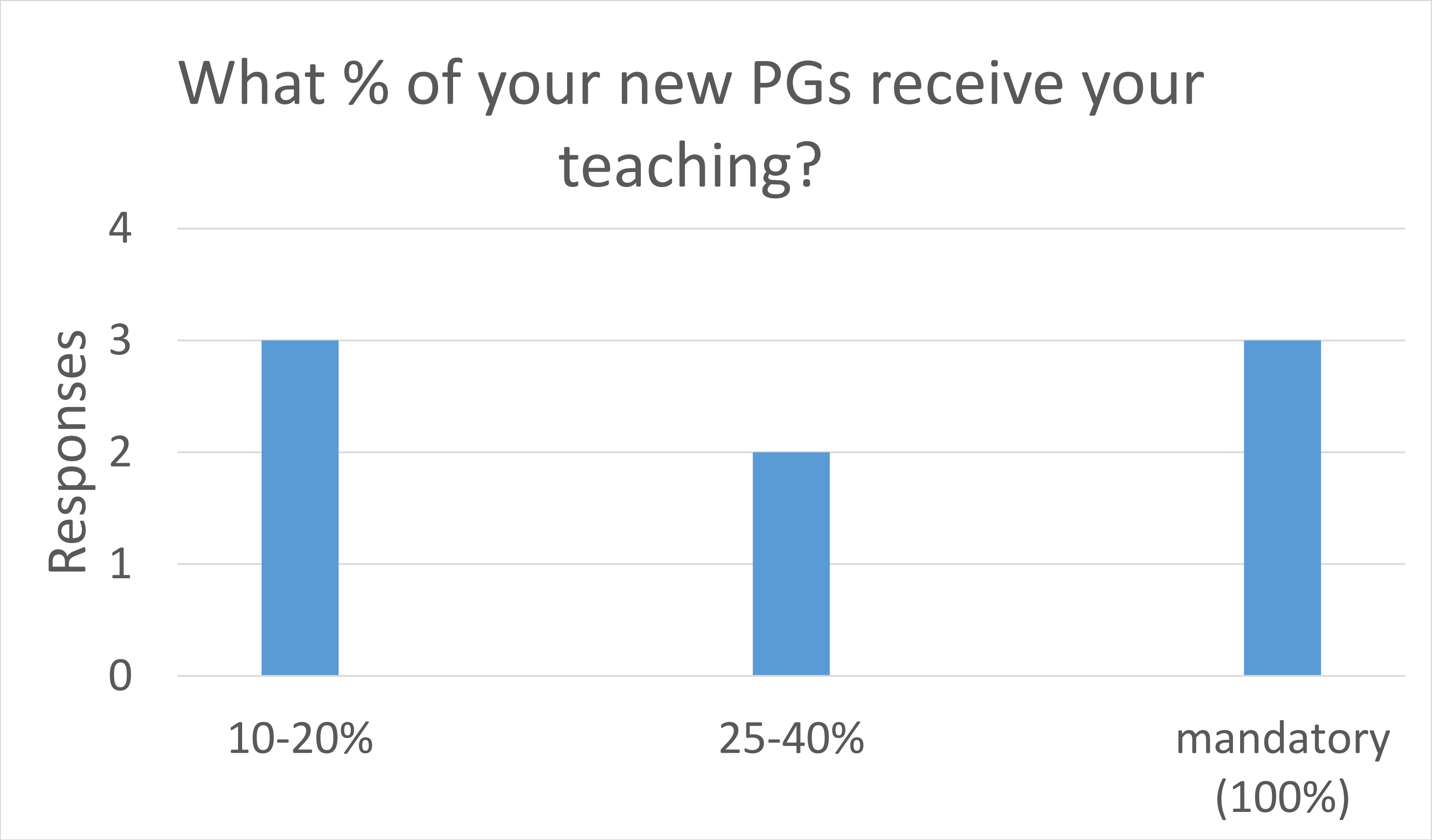


* I included the response ‘occasionally’ in the no category.

Teaching: if you (as facility manager) do not supply formal teaching, what is the reason?

Category/Response	No.
'done by an academic member of staff'	1
'students are taught informally by supervisors‘	4
Teaching is not required	0
Other Reason	0

Teaching: attendance



This question is not well-designed since I haven't properly distinguished between 'all' PhDs and those who are facility users…at Nottingham attendance is mandatory for those that use the facility (i.e. we are one of the 100%-ers)

Teaching: what form does it take?

Response
6 x 1hr lectures, 1 x 2hr processing workshop, 1 homework problem
15 lectures
mostly 1hr lectures
12 x 1hr lectures
4 x 1hr lectures, 4 x 3h problem solving
8 x 1hr lectures
7 x 1hr lecture, 1 x 2hr processing lecture, 4 x 1hr problem solving
‘individual’
‘continuous discussion’

How valuable do you believe the problem solving sessions are? Do students engage?

Teaching: what subjects do you cover?

Physical principles of NMR
Principles and applications of multi-pulse NMR
Other topics: dynamics and 2nd order coupling

Very basic Undergraduate introduction to organic and multinuclear NMR.

Intro, interpretation of ^{1}H/^{13}C/DEPT, diastereotopicity, 2nd order spectra, other nuclei (inc quadrupolar nuclei), intro to dynamic NMR, 2D chemical shift correlation experiments (COSY, TOCSY, HSQC, HMBC), relaxation, quantitative NMR, NOE theory, 1D and 2D NOESY/ROESY

General NMR intro, NMR interpretation, processing, NMR theory (to vector model level), experimental methods, 2D methods/theory, diffusion, relaxation/NOE, complex NMR problems, NMR hardware

- Relaxation (in a very general sense) and its implications for quantitation
- Basic 1D and 2D NMR experiments and their interpretation
- Some heteronuclear NMR (mainly spin-½ nuclei that are relevant to organic chemists as they are my largest audience)
- Diastereotopicity
- NOE
- VT NMR and fluxionality
- Reporting NMR spectra

1D proton, 2D COSY, 2D HMQC, 2D HMBC, sel-TOCSY, sel-nOe, 19F, 31P.

NOEs, J(CH) coupling, Karplus, relaxation

We have basic introduction to facilities, basic strategies for structure elucidation, how to process your data with Topspin …

Introducing Modern NMR– historical context, basic elements of NMR, sensitivity, relaxation, repetition, quantification
1D NMR methods– optimising 1D data, decoupling, pure shift NMR, sensitivity enhancement (INEPT), spectrum editing (DEPT and DEPTQ)
2D NMR methods I– homonuclear correlation spectroscopy (COSY and variants), total correlation spectroscopy (TOCSY), carbon–carbon correlations (INADEQUATE/ADEQUATE)
2D NMR methods II– heteronuclear correlation spectroscopy– one-bond correlations (HSQC and HMQC), editing HSQC, long-range correlations (HMBC and H2BC), measuring and using $^{n}J_{CH}$ couplings (HSQMBC), hybrid methods (HSQC-TOCSY)
the nuclear Overhauser effect– equilibrium *vs* transient NOEs, 1D and 2D nOe spectroscopy (NOESY), rotating-frame nOes (ROESY), heteronuclear nOes (HOESY)
Methods for studying molecular interactions– diffusion NMR spectroscopy (DOSY), protein-small molecule (ligand) interactions (STD, WaterLOGSY etc),
Dynamic effects in NMR– Chemical exchange processes, NMR timescales– fast, intermediate and slow exchange, exchange decoupling, rate constants from lineshape analysis and magnetisation transfer experiments, 2D exchange (EXSY), kinetics and thermodynamics of exchange, protein–ligand binding and exchange.
How NMR works: The spectrometer, signal selection (phase cycling and pulsed field gradients), selective excitation, solvent suppression, inside the spectrometer.

Teaching: what subjects do you cover…

- Diffusion: 2 mentions
- Quantitative NMR: 3 mentions
- NMR hardware: 2 mentions
- More ‘exotic’ nuclei: 1 mention (or 3 if you include ^{19}F, ^{31}P, other spin ½ as ‘exotic’)
- J(CH) couplings: 2 mentions
- Reporting data: 1 mention
- Protein-ligand interactions/methods: 1 mention
- NMR Processing: 2 mentions

It is a big subject, how do we decide what is a priority to cover?

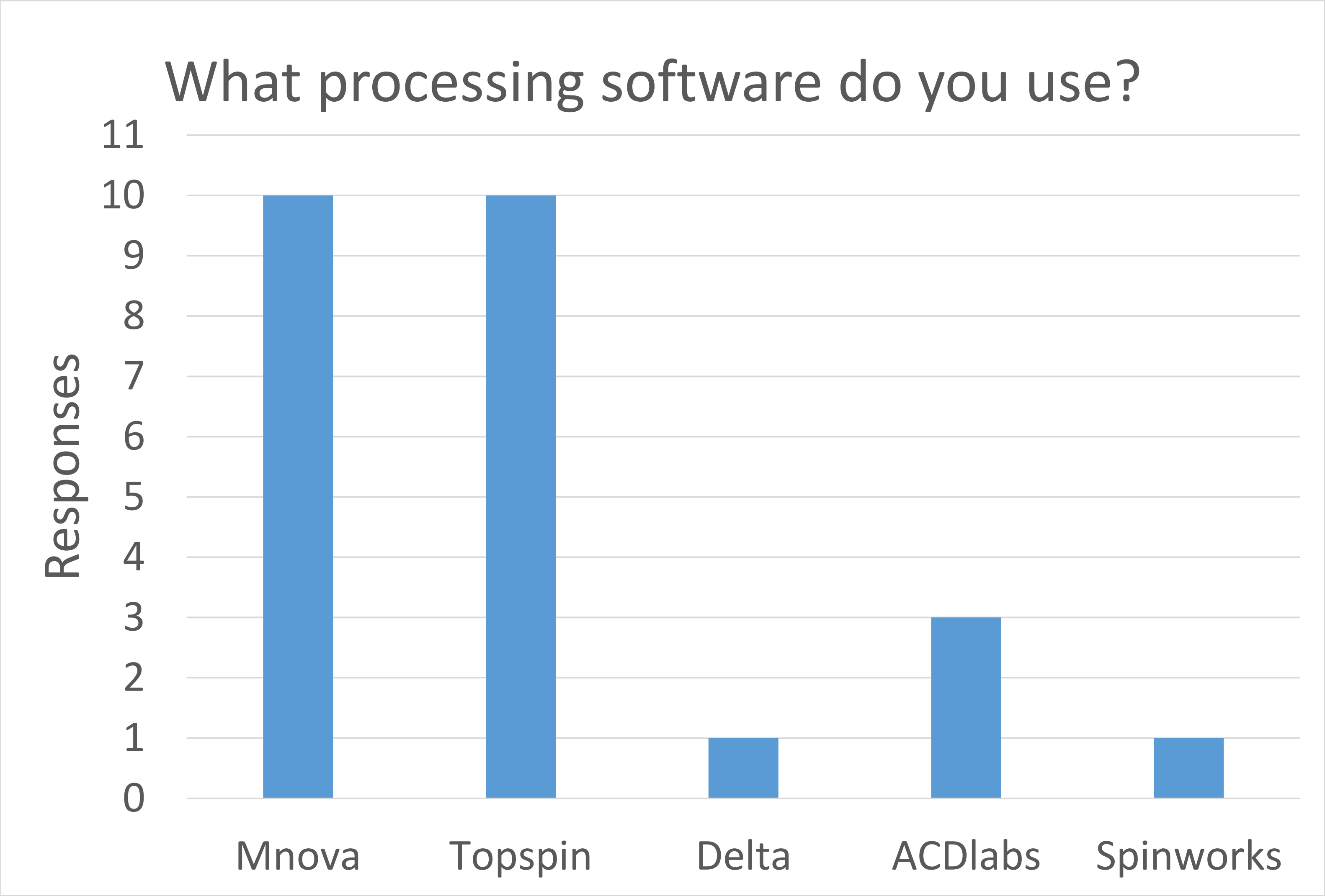
Teaching: How much do you think your PGs appreciate the NMR teaching they receive (as PGs)

Category	Responses
Very much	2
A fair bit	7
Not much	0
Not at all	0

I find quite a lot of variation in my teaching feedback, do you?

“why is there a lot of unnecessary information I will never use”
“too theoretical”
“your module helped me a lot with my viva”
“great notes”

Training: Software



Training: Software – do you supply formal training, how much?

Response
no reponse (x2)
ad hoc only
10-20 mins
1 hr + ad hoc
1 hr + ad hoc
1 hr intro
1 hr lecture plus ad hoc
Topspin 1-2h plus ad hoc
2h workshop
2hr (Topspin), (notes Mnova)
2 hr lecture and ad hoc
during biannual training course
no formal training, screen capture videos on the VLE

Do we believe this is sufficient in an ideal world? Would students prefer more than this?

Training: Hands on access – what proportion of your PG user-base have full hands-on access to the instruments?

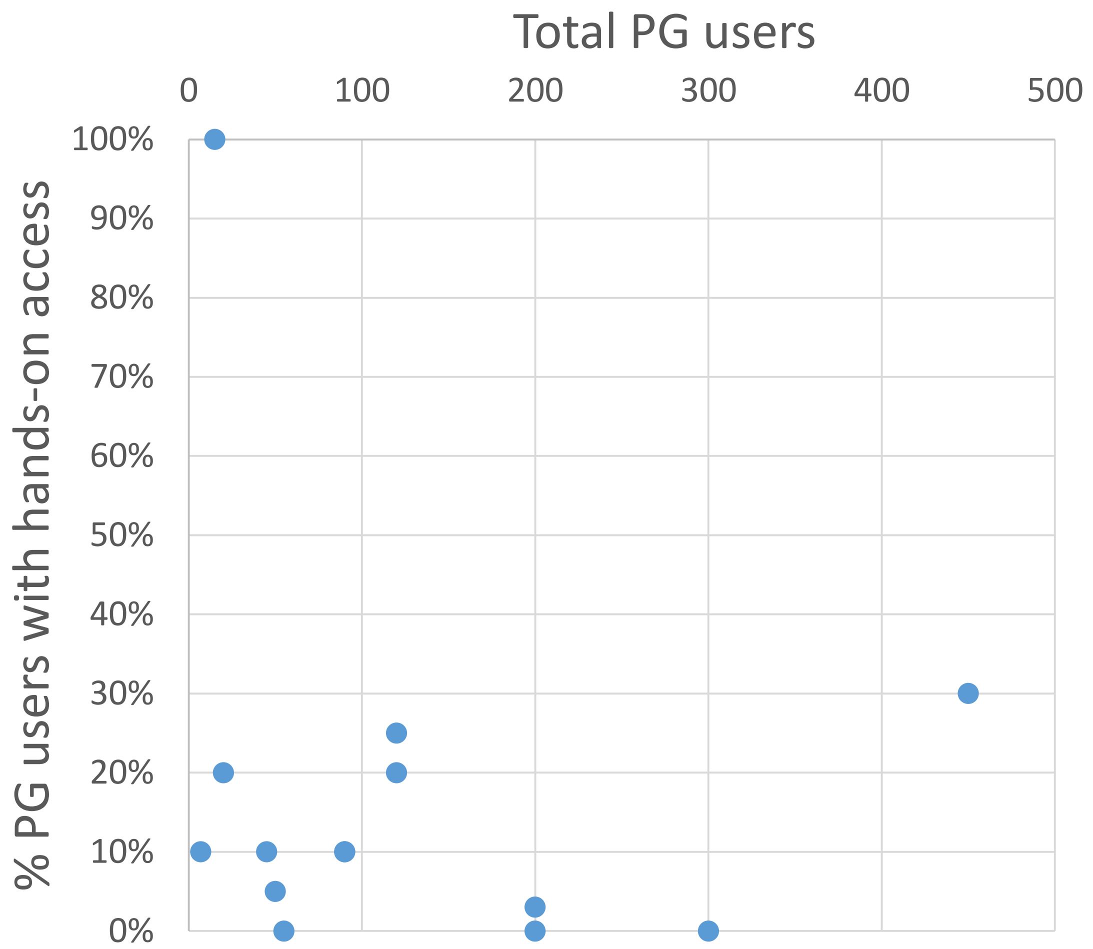
Hands-on access (%) [Not including Icon-nmr and an autosampler]	What form does training take?
100	1-2 hrs individual
30	1-2 hrs intro then as required
25	2hrs plus customisation
20	typically 2 hrs
20	typically 2 x 1 hr
10	personalised
10	informal - as required
10	one week or more if necessary (e.g. solids)
10	1-2-1 as required
5-7	2 hrs - days/weeks as required (bio)
5	several hrs 1-2-1
<5	mainly Bio-NMR: 1-2 afternoons then as required
0	N/A
0	N/A

Training: Hands on access

- Very large variation in the proportion of students trained/competent for hands-on access.

- The variations cannot be accounted for by facility size.

What is the reason for these differences and do we care?



Training: Hands-on access – what % of your PG cohort have these privileges:

UKMRM member	1	2	3	4	5	6	7	8	9	10	11	12	13	14
choose predefined parameter sets, amend O1, D1, NS	100	100	100	100	5	100	50	10	5	10	100	100	100	15 (on req)
high VT	5	10	25	100	7	10	0	10	5	5	50	100 (icon)	10	<5
low VT	0	10	25	50	1	10	0	0	5	5	50	10 (BCU-X Icon)	10	<1
amend parameters of 'fraught' experiments:	0	<10	10	10	1	10	0	0	0	2	10	0	2	1
set-up new experimental protocols from scratch:	0	0	0	10	1	0	0	0	0	0	0	0	0	0

What (NMR-related) difficulties do your PG students have?

Problem	Responses
Sample Preparation (length, weighing)	4
Force fitting of data/correct problem solving technique	2
Correct experiment selection (direct observe *vs* inverse)	3
Diastereotopicity	1
Understanding 'external' chemical shift referencing	1
Dynamic NMR	1
NOE theory	1
Processing diffusion data	2
Data Reporting	1

Final Thoughts

- NMR is a big (and fast-moving) subject.

- Giving our PhD students the information they need, without overdoing it, is a fine balance.

How many here have done any teacher training?
Is it necessary/desirable?