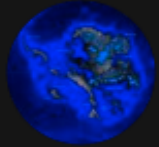


RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

User Perspectives of Metadata Use in Electronic Laboratory Notebooks

Cerys Willoughby, Jeremy Frey,
Emma Tonkin, Simon Coles,
and Colin Bird



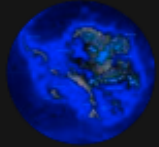
RDAP13

<https://www.asis.org/rdap/>

Research Data Access & Preservation Summit 2013



Why do we care about metadata?

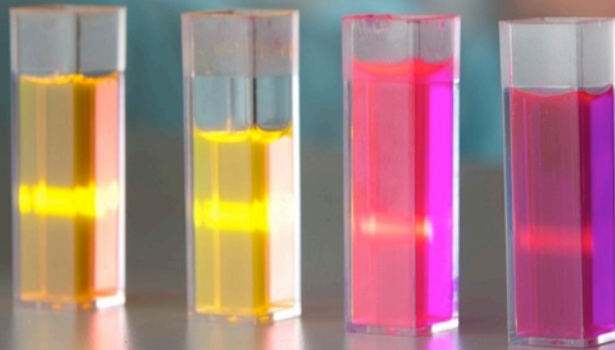


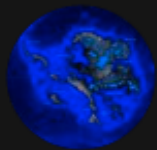
RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

Anatomy of an experiment

- Plan experiment
- Enact experiment
- Analyse results

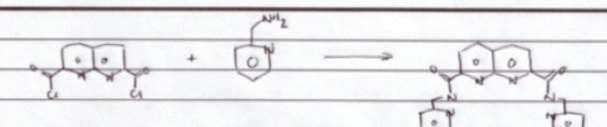


**RDAP13**<https://www.asis.org/rdap/>

Research Data Access & Preservation Summit 2013

Traditional recording

15/05/08 55



Name	Mass/Volume	Moles	Hazards
1,8-Naphthyridine-2,7-dicarbonyl dichloride MW = 255.1	1.10g	4.31mmol	Not known, Treat as toxic
2-(aminomethyl)pyridine MW = 108.14 g/mol d = 1.045 g/mL	0.97 mL	9.48mmol	Harmful if contact with skin and if swallowed Causes burns
Triethylamine	1.31 mL	9.48mmol	Highly Flammable Harmful by all routes Causes severe burns
Dichloromethane	50 mL	solvent	Limited evidence of a carcinogenic effect

Procedure

1,8-Naphthyridine-2,7-dicarbonyl dichloride (1.10g, 4.31mmol) was dissolved in DCM (50 mL) in a round bottom flask.

To this 2-(aminomethyl)pyridine (0.97 mL, 9.48mmol) was added to the reaction mixture by needle/syringe.

Following this triethylamine (1.31 mL, 9.48mmol).

56

Actual mass of 1,8 naphthyridine used = 1.1493g

- Dissolution of the solid in DCM gave a murky brown solution.
- On addition of the amine a white precipitate formed which dissolved again on addition of triethylamine.

After stirring overnight the reaction was TLC'd.



Eluent: 10% MeOH / DCM

- 18/35 UV active.

This shows the reaction to have formed some product. However it is hard to tell if the reaction has gone to completion due to polarity of the SM.

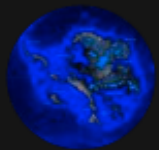
The workup proceeded as follows:

Reaction poured into water (50 mL) and separated.

The organic was washed with a further (2 x 50 mL) This separated red from the organic and leave a cloudy yellow solⁿ.

This organic was then washed with (50 mL) brine.

This removed the cloudiness and left a yellow solⁿ.

**RDAP13**<https://www.asis.org/rdap/>*Research Data Access & Preservation Summit 2013*

LabTrove
and
Automatic
capture of
metadata

Flexibility has
limitations..

ourexperiment
alpha

Enantioselective Hydrogenation of dehydro-PZQ and derivatives

Older Posts >>

Preparation of MNR40-2
10th July 2012 @ 03:29

MNR14 $\xrightarrow[180\text{ }^{\circ}\text{C}]{\text{sulphur}}$ MNR40

Compound	FW (g/mol)	mmol	Mass (g)	eq
MNR14	306.36	10.74	3.29	1.00
sulfur	32.07	21.48	0.69	2.00
MNR40-2	304.34			

Hazard and Risk Assessment:

HIRAC MNR37.pdf

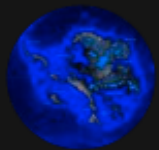
Procedure:
A mixture of recovered SM from MNR40-1 (3.29 g, 10.74 mmol) and sulfur (0.69 g, 21.48 mmol) under argon was heated at 190°C in a sand bath for 2 hours.

This Blog
[New Post](#)
[Timeline View](#)
[Exhibit View](#)
[Export Blog](#)

Archives
[July 2012 \(2\)](#)
[June 2012 \(1\)](#)
[May 2012 \(1\)](#)
[May 2011 \(1\)](#)
[April 2011 \(6\)](#)

Sections
[Experiments \(11\)](#)

Tools
[Show/Hide Keys](#)

**RDAP13**<https://www.asis.org/rdap/>*Research Data Access & Preservation Summit 2013*

LabTrove and User defined metadata

Section*
Analytical Procedures

Metadata

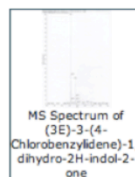
key	value
Substituent	Nitro
Spectroscopic	DSC

MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one

6th May 2012 @ 16:40

Spectroscopic Method: MS-ESI**Substituent:** Chloro

MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one:



The mass spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one has been obtained by positive electrospray ionization (ESI). The peak at $m/e = 256.2$ confirms the molecular mass of this compound as the molecular ion gains a proton.

Interpretation of MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one:

Peak Position	Diff. between mass and peak	molecular	Suspected molecules or ions	Inference
5=3			(M+H) ⁺ H(1)	Molecular ion gains a proton, ³⁷ Cl isotope present.
5=4			(M+He) ⁺ He(4)	Compound gains helium atom
5=33			(M+MeOH) ⁺ MeOH(32)	Molecular ion gains methanol, ¹³ C isotope present.
5=35			(M+H ₂ O+NH ₃) ⁺ H ₂ O(18), NH ₃ (17)	Molecular ion gains water and ammonia molecules
5=44			(M+CO ₂) ⁺ CO ₂ (44)	Compound gains carbon (IV) oxide molecule.
5=42			(M+Na+H ₂ O) ⁺ Na(23), H ₂ O(18)	Molecular ion gains water and sodium atom
5=18			(M+H ₂ O) ⁺	Compound gains water

This Post

Permalink
URI
URI Label
Revisions
Export:
XML (With Files)
PNG Image

This Blog

New Post
Timeline View
Exhibit View
Export Blog

Archives

June 2012 (1)
May 2012 (15)
March 2012 (29)

Sections

Analytical Procedures (8)
Condensation Products (5)
Experimental Procedure (1)
Spectroscopic Data (31)

Substituent

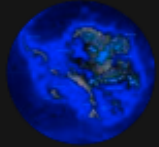
Nitro (8)
Methoxy (8)
Bromo (8)
Chloro (8)
Methyl (8)

Spectroscopic Method

DSC (5)
ATR-FT-IR (5)
HPLC (5)
MS-ESI (5)
PXRD (1)
H-NMR (5)
C-NMR (5)

Tools

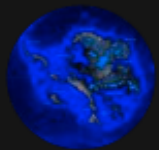
Show/Hide QR Code
Show/Hide Keys



RDAP13 <https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

What metadata might we expect?





RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

Metadata Survey

blogs@ChemTools

The thoughts of Chemists

blogs@BioLab

Open output from the BioLab

ALTC Enotebook

our experiment
alpha



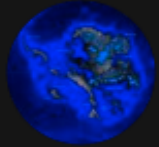
UNSW

THE UNIVERSITY OF NEW SOUTH WALES
SYDNEY • AUSTRALIA

enotebook

blogs@xray

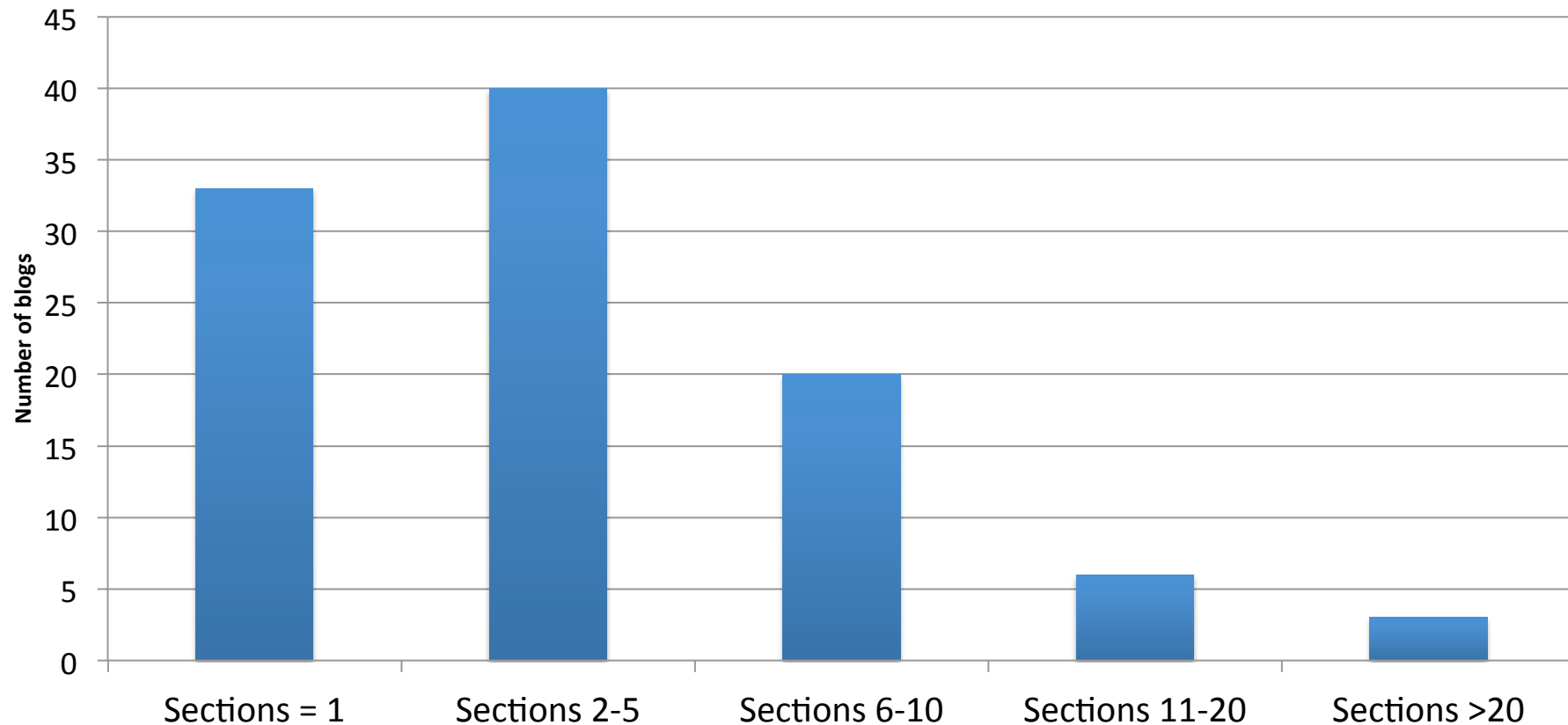
The thoughts of the ORC Xray Group

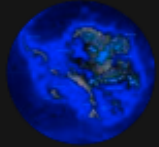


RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

Number of 'sections'



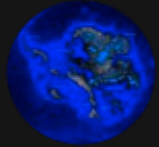


RDAP13

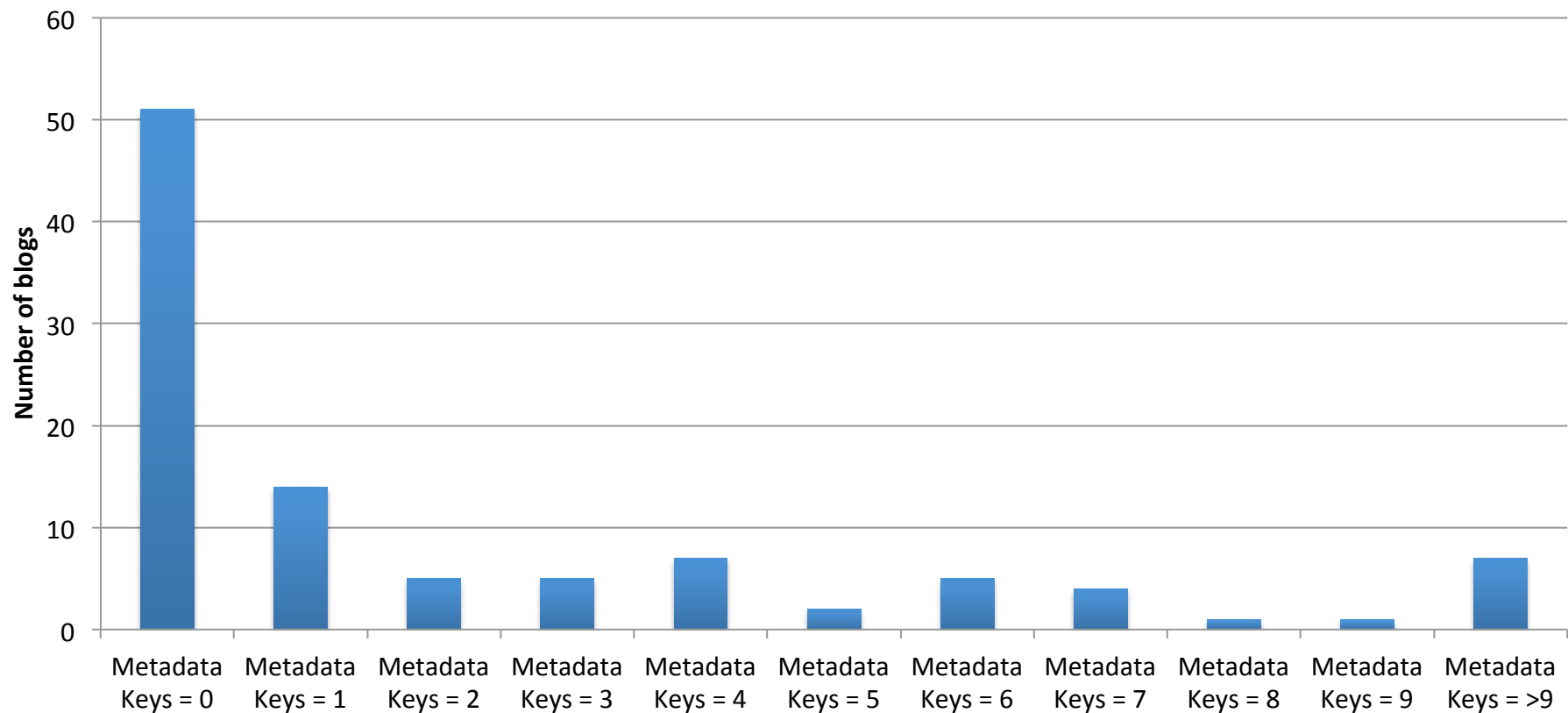
<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

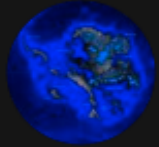
Values for section:

- Types of subject:
 - Experiment related
 - Project related
 - Blog related
- Top ten subjects:
 - Materials
 - Methods
 - Data
 - Experiments
 - Experiment stage
 - References
 - Samples
 - Instruments
 - Safety
 - Results



Number of 'Key value' pairs



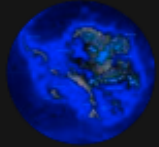


RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

Values for Keys:

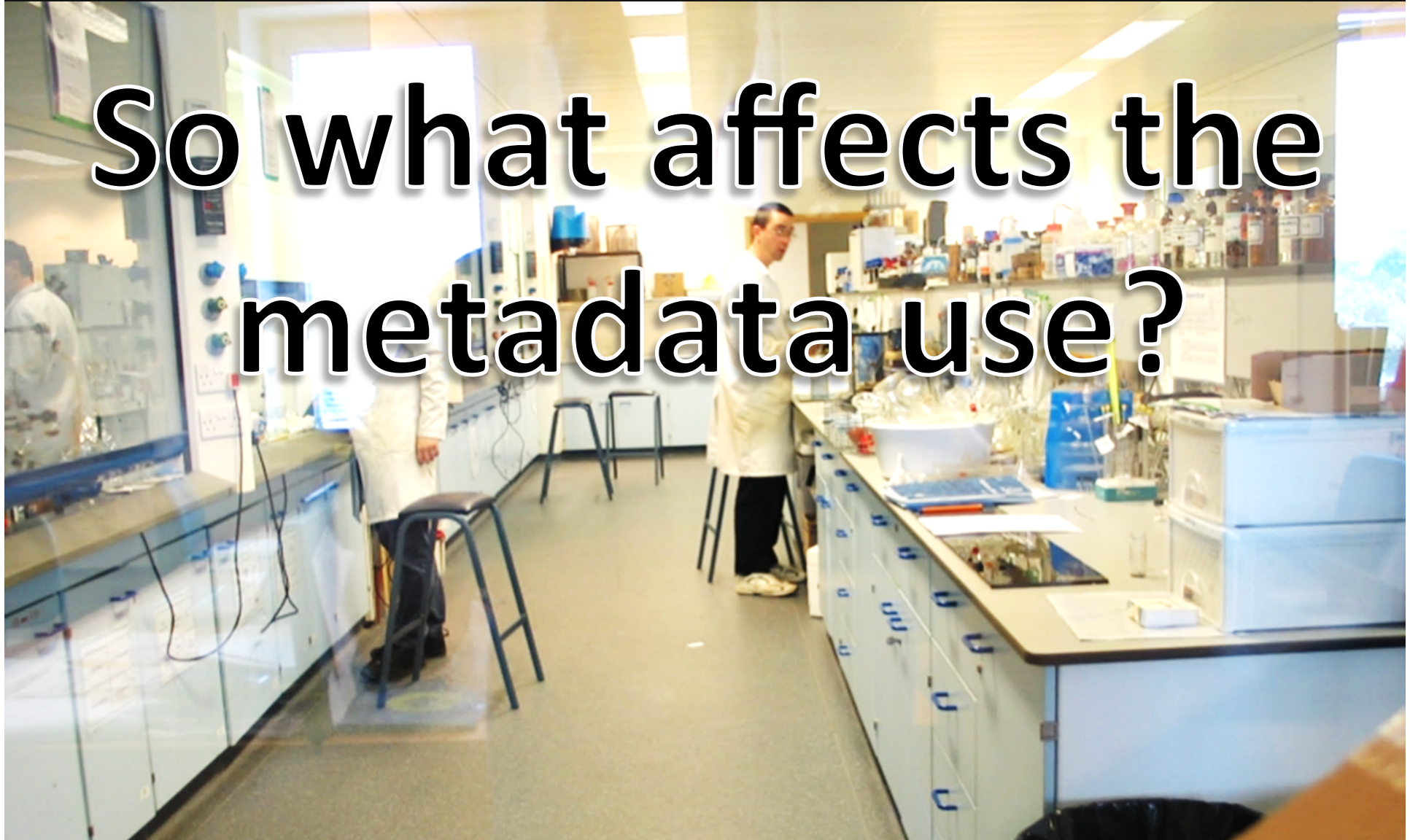
- Types of subject:
 - Experiment related
 - Project related
 - Blog related
 - the post type
 - the location of an instrument or experiment
 - a reference to a physical lab notebook (Ref/code)
 - the date of the experiment
 - the status of an activity or document
- Top ten subjects:
 - Materials
 - Instruments
 - Methods
 - Post type
 - Data
 - Experiments
 - Samples
 - References
 - Location
 - Ref/code

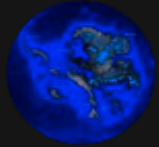


RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

So what affects the metadata use?

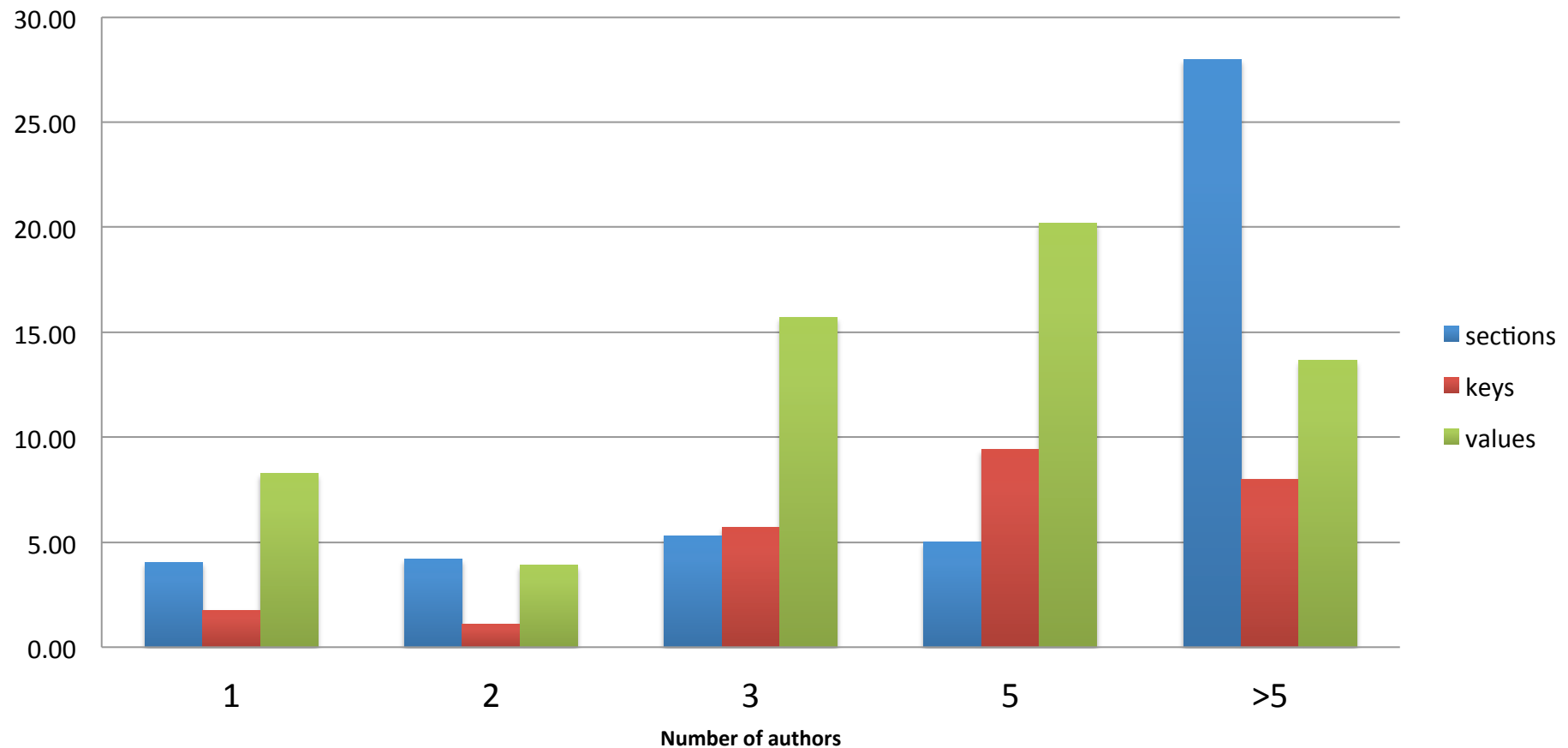


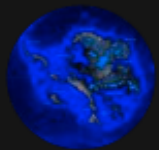


RDAP13

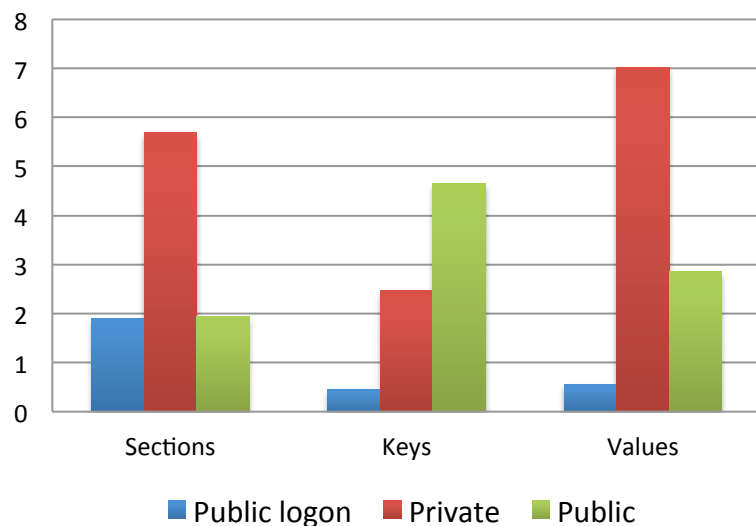
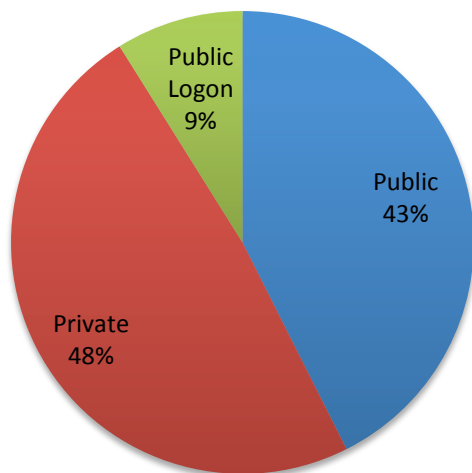
<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

Number of Authors?

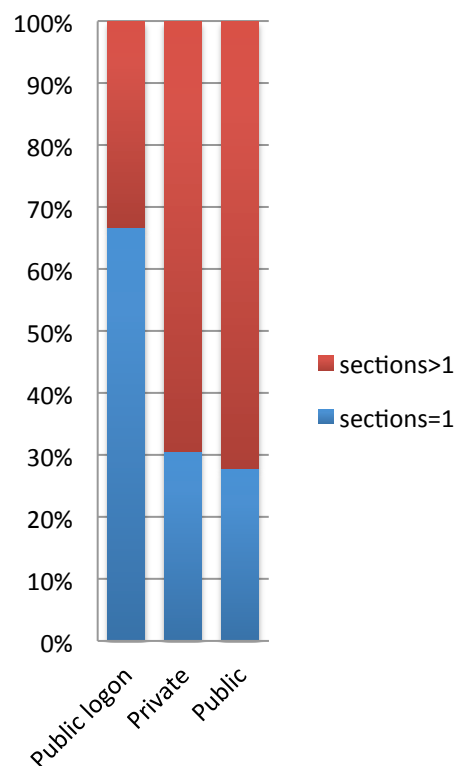




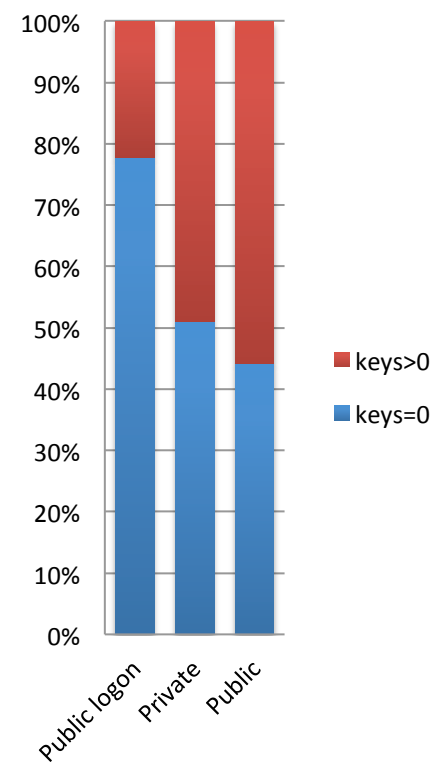
Public vs private?

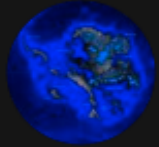


Sections by blog privacy



Keys by blog privacy





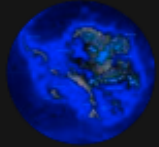
RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

User perspectives on metadata

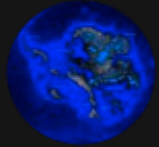
- User interviews
- User studies





RDAP13 <https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

What can we do about it?



RDAP13

<https://www.asis.org/rdap/>
Research Data Access & Preservation Summit 2013

Metadata is essential for
intelligent open access