

Creating context for the experiment record: user- defined metadata

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16 March 2014

LabTrove



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ourexperiment

Pictet–Spengler route to Praziquantel

Synthesis of intermediates and derivatives of PZQ

Older Posts >>

Continuation: Acid-catalyzed Pictet–Spengler reaction with methanesulfonic acid (MW56–9 to MW56–12)
17th March 2011 | 0:07:14

Acid-catalyzed Pictet–Spengler using methanesulfonic acid in various concentrations

Continuation of Acid-catalyzed Pictet–Spengler reaction with methanesulfonic acid (MW56–5 to MW56–8)

Archives

- March 2011 (3)
- February 2011 (8)
- August 2010 (3)
- July 2010 (3)
- June 2010 (14)
- May 2010 (3)

Sections

- Experiments (26)

Tools

- Show/Hide Keys

LabTrove enables the formation of a Smart Research

La LabTrove
labtrove

labtrove Public Blog Post: Synthesis of amine-linked analogue of TCMDC-123812 via reductive aminatio...
<http://t.co/Bla5hWbb> #malaria #drugdesign
yesterday · reply · retweet · favorite

labtrove Public Blog Post: Synthesis of ether-linked analogue of TCMDC-123812 (PMY 37-1) <http://t.co/XhqyRb8i> #malaria #drugdesign
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labtrove Public Blog Post: Synthesis of 2-Ethoxycarbonylthiolan-3-one
<http://t.co/m9mUBQKS> #malaria

Metadata in LabTrove

Automatic capture of metadata

Flexibility could mean a lack of context..

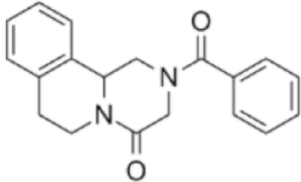
ourexperiment
alpha

Enantioselective Hydrogenation of dehydro-PZQ and derivatives

Older Posts >>

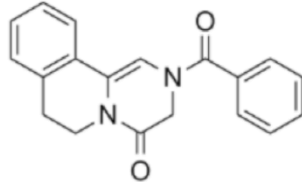
Preparation of MNR40-2

10th July 2012 @ 03:29



MNR14


→ sulphur
180 °C



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.

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- [New Post](#)
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Archives

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

Sections

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

Tools

- [Show/Hide Keys](#)

LabTrove and User defined metadata

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:



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

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

(3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one has been analyzed by mass spectrometry (ESI). The peak at $m/e = 256.2$ confirms the molecular ion gains a proton.

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

Molecular Ion	Suspected molecules or ions	Inference
273.2	(M+H) ⁺ H(1)	Molecular ion gains a proton, ³⁷ Cl isotope present.
274.2	(M+He) ⁺ He(4)	Compound gains helium atom
299.2	(M+MeOH) ⁺ MeOH(32)	Molecular ion gains methanol, ¹³ C isotope present.
300.2	(M+H ₂ O+NH ₃) ⁺ H ₂ O(18), NH ₃ (17)	Molecular ion gains water and ammonia molecules
317.2	(M+CO ₂) ⁺ CO ₂ (44)	Compound gains carbon (IV) oxide molecule.
273.2	(M+Na+H ₂ O) ⁺ Na(23), H ₂ O(18)	Molecular ion gains water and sodium atom
273.2	(M+H ₂ O) ⁺	Compound gains water

Attached Files



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

Section*

Analytical Procedures

Metadata

key

value

Substituent

Nitro

Spectroscopic

DSC

Metadata Survey

blogs@ChemTools

The thoughts of Chemists

blogs@BioLab

Open output from the BioLab

ALTC Enotebook

our experiment
alpha



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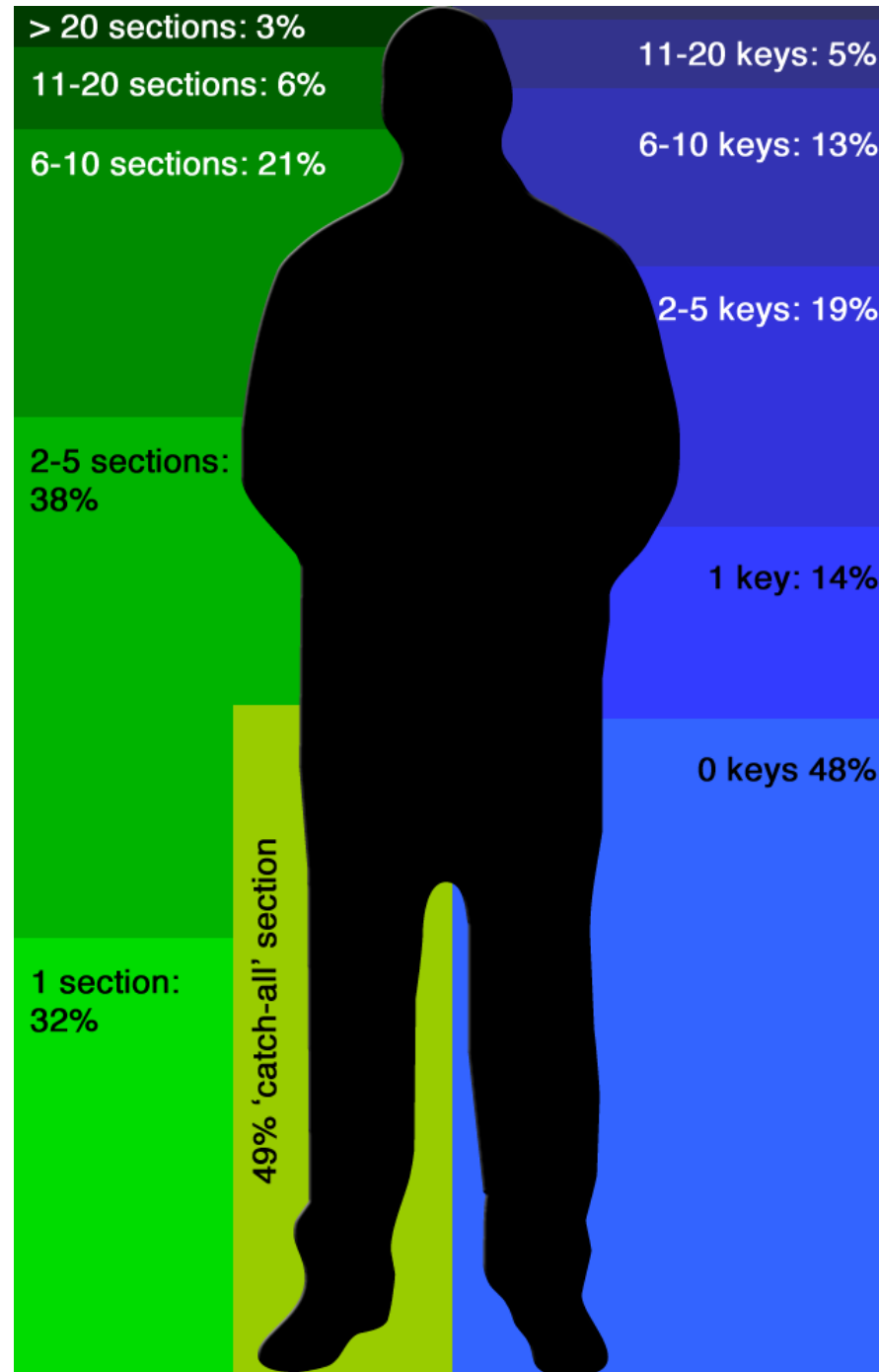
enotebook

blogs@xray

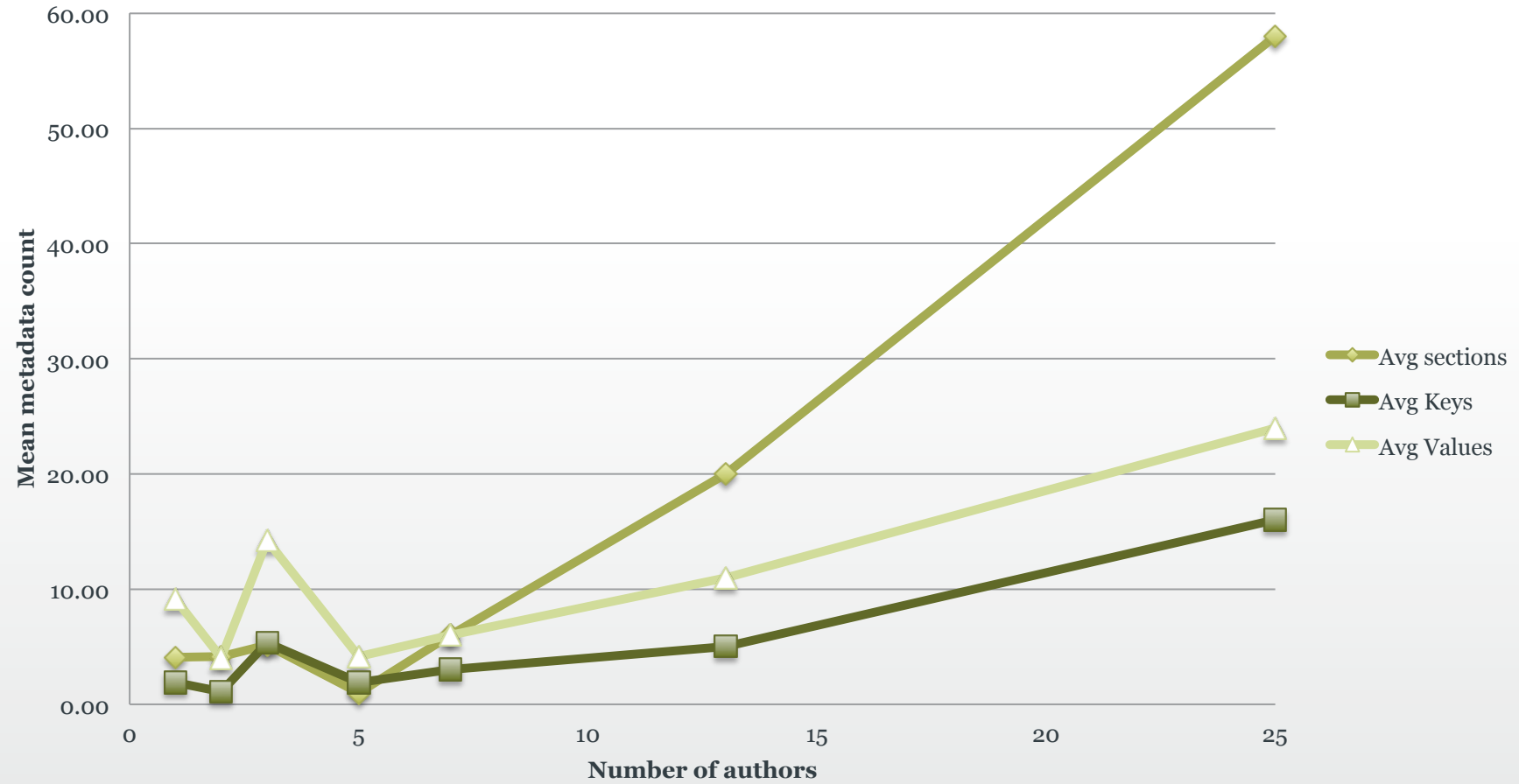
The thoughts of the ORC Xray Group

104 blogs

A big proportion
of our users are
not really adding
metadata!

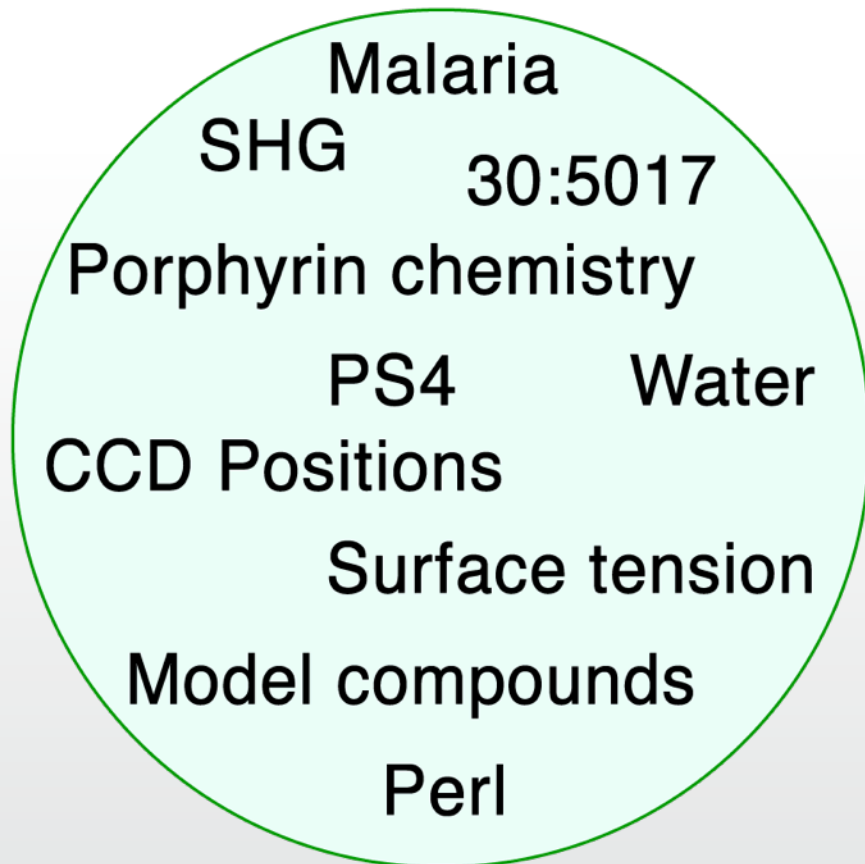


Number of authors



Most metadata is high-level not specific

Specific



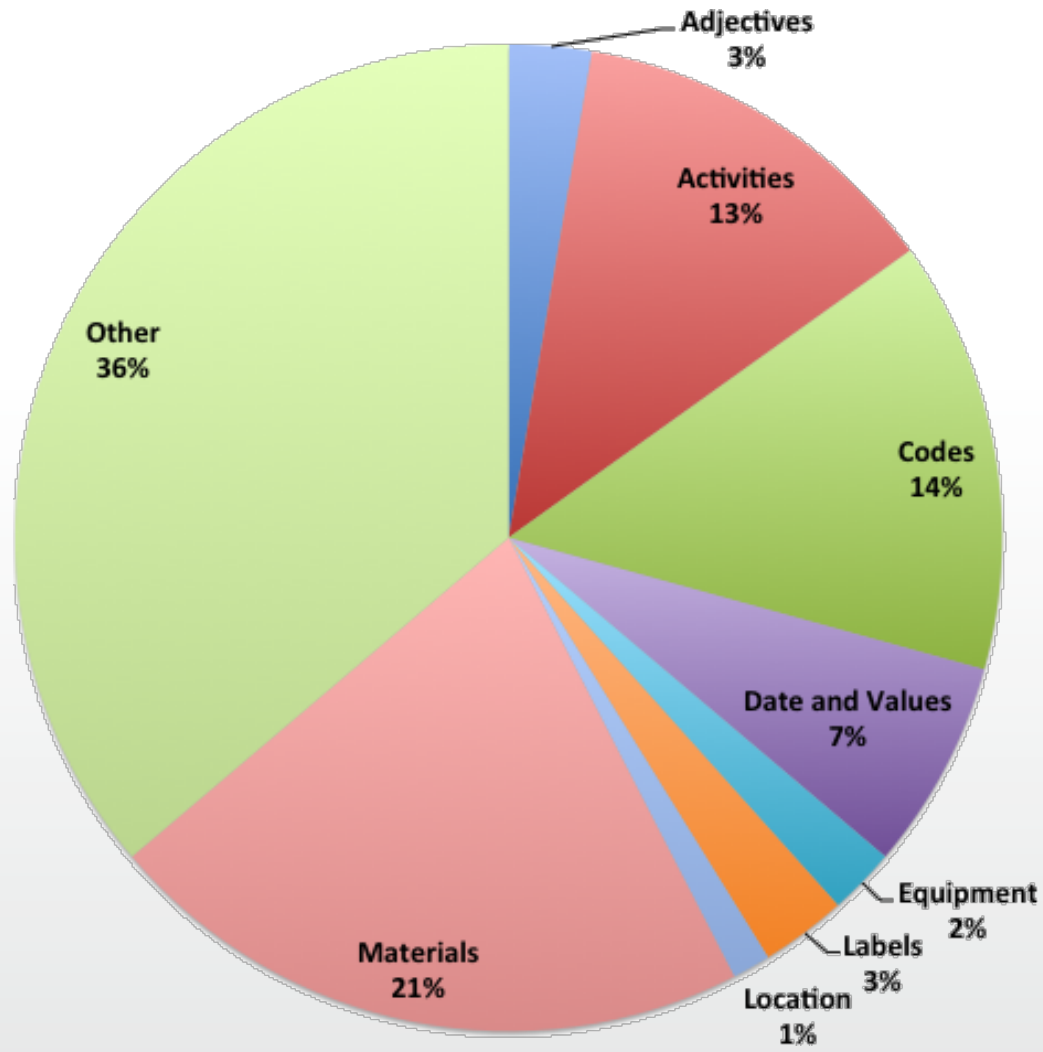
High-level



Sections as labels



Values



Metadata anxiety and other problems



- ‘Blank canvas’ effect
- Consistency
- Duplication
- Mistakes
- Inappropriate metadata

A preference for ‘things’ over ‘activities’?

	Nouns	Verbs	Adjectives
Sections	513	15	3
Keys	263	4	1
Values	893	40	26

Nominalization:

making a noun from a verb or adjective

“zombie nouns”

Categorizing 'activity' nouns

A photograph of a study desk. On the left, a row of five large, bound volumes of a dictionary stands upright. The spines are light brown with dark labels that read 'LEXICON PARALLEL' followed by Roman numerals I, II, III, IV, and V. Each volume has a small red label at the bottom. In the center, a brass lamp with a glass chimney sits on the desk. To the right, two more volumes are lying flat. In the foreground, one of the volumes is open, showing two pages of dense text with columns and headings. The desk is made of dark wood.

I'll come back to
classifying activities
later..

Is LabTrove metadata different?

- Flickr
- NASA blogs
- Chemistry-related blogs
- myExperiment



flicker

Editing 1 photo:

On the bike

Add a description

Add tags


Separate tags with a space


Add people

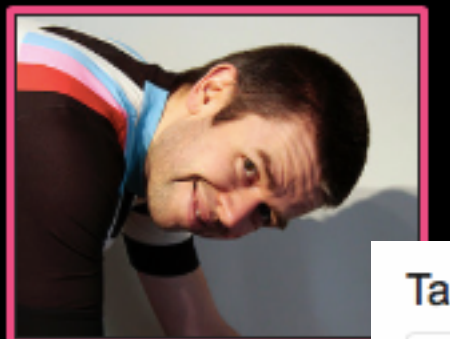
Add to sets

Add to groups

Owner settings ▾

 None (All rights reserved)

 Visible to everyone



On the bike

Add a description

Tags

click a tag: [2012](#) [animals](#) [archaeology](#) [autumn](#) [berlin](#) [bw](#) [cats](#) [cleveland](#) [dig](#) [dinnington](#) [doodle](#) [eb](#) [eb2008](#) [eclipse](#) [england](#) [expo](#) [extremeblue](#) [f1](#) [florida](#) [flower](#) [flowers](#) [g7](#) [gardens](#) [green](#) [hampshire](#) [hilliers](#) [history](#) [honeymoon](#) [hursley](#) [hursley50](#) [iphone](#) [japan](#) [july](#) [keukenhof](#) [kimahri](#) [landscape](#) [lego](#) [legoland](#) [macro](#) [marwell](#) [may](#) [me](#) [moscow](#) [nature](#) [niigata](#) [ohio](#) [orlando](#) [panto](#) [paris](#) [phil](#) [picnic](#) [pink](#) [portrait](#) [red](#) [roman](#) [sc7](#) [silverstone](#) [spring](#) [sunset](#) [sydney](#) [team](#) [tree](#) [ut](#) [utpicnic](#) [villa](#) [water](#) [wedding](#) [winchester](#) [windsor](#) [xmas](#) [yellow](#)

[get more of your tags](#) | [get all of your tags](#)

Separate each tag with a space: *cameraphone urban moblog*. Or to join 2 words together in one tag, use double quotes: *"daily commute"*.

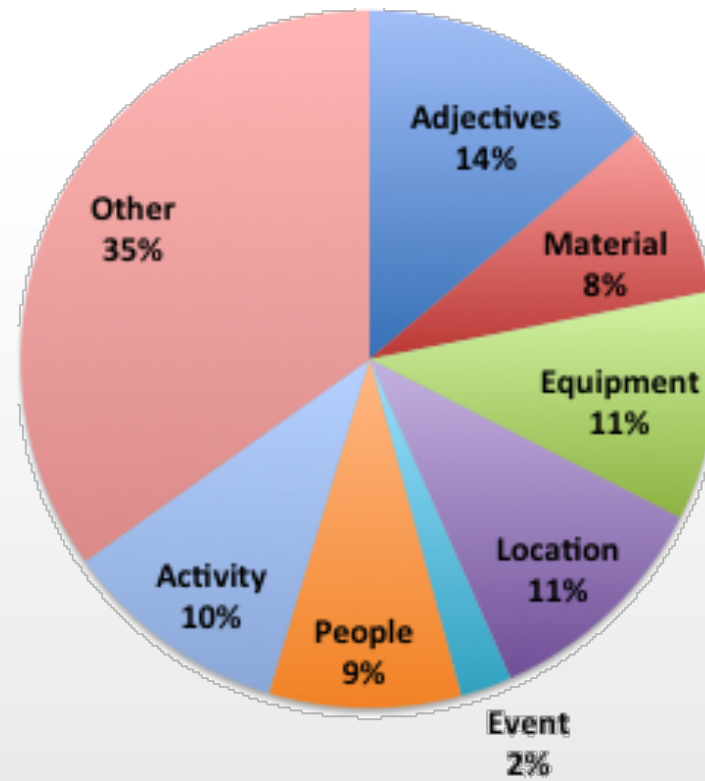
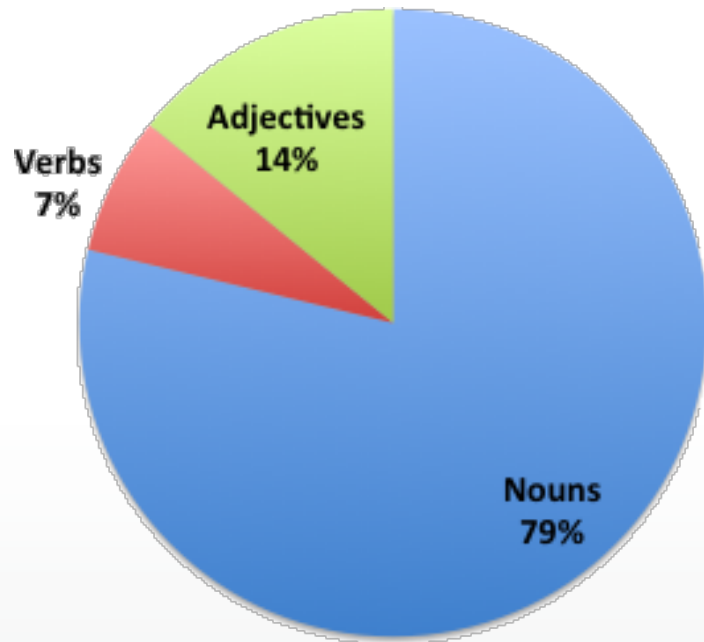
Flickr results

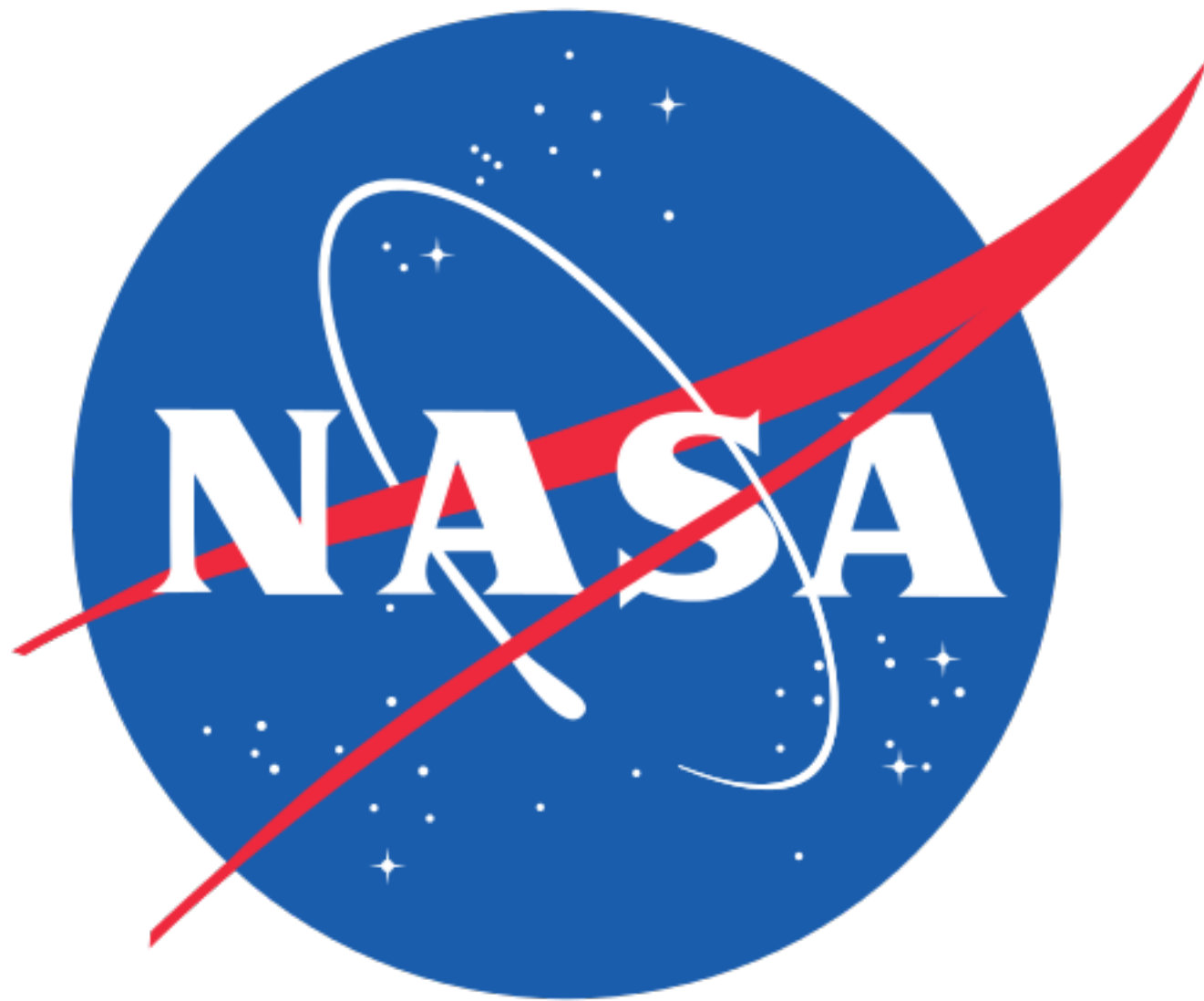
1381 tags



Top 500 most interesting photos tagged
with 'chemistry' and 'experiment'

Flickr results





when were on the plane and were doing the set-up and startup, I was really “uber-focussed” on the payload and not on myself for the first few cycles. When things started to get into a rhythm around Parabola #5 I had no idea we were 1/5th of the way done. Wow.



“That was short. That was very short.” My comments after the very first parabola, which was a Martian (0.33 G) scenario. This image shows our team’s positions in between parabola 1 & 2. We did not have space enough to fully lay down so we reclined against the side of the aircraft. Left to right is Con Tsang, myself (monitoring a payload via a table), Cathy Olkin, and Alan Stern (face not visible). The photo is taken via Go-Pro camera on the head of Dan Durda who was across the way. Eric Schindhelm, who rounded out our team, was next to Dan and not in this view.

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Authors

[Brian Glass](#)

[Jennifer L Dungan](#)

[Jessica Culler](#)

[Kimberly Ennico](#)

[Maria Navarro](#)

[Max Spolaor](#)

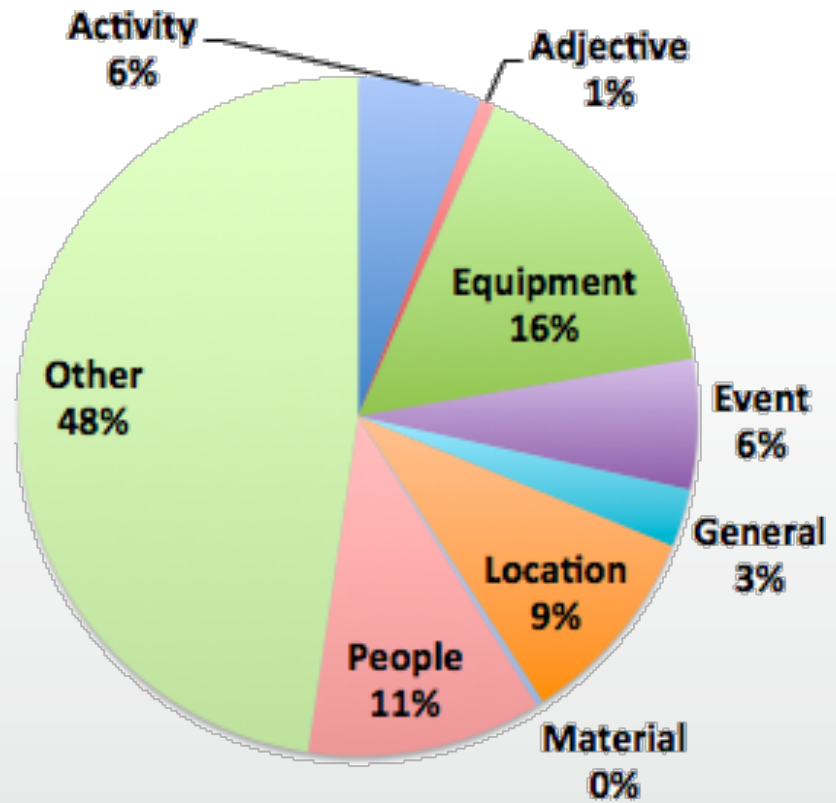
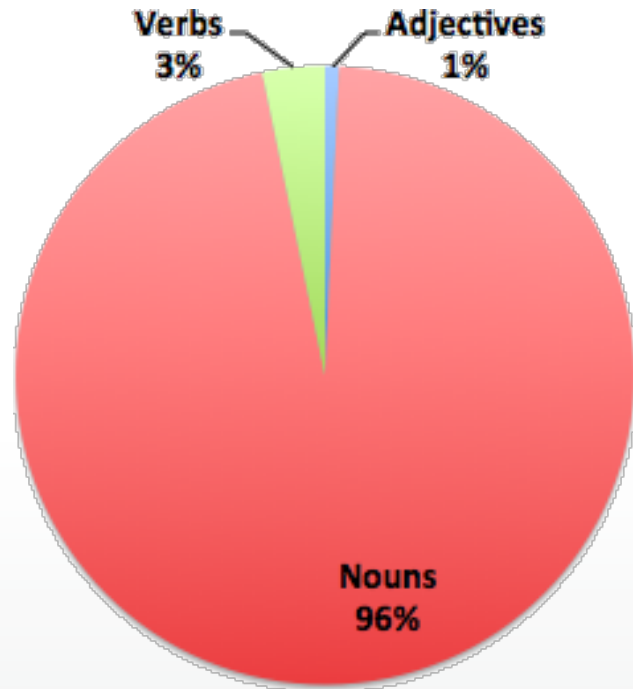
[Melissa Pandika](#)

NASA results



53 NASA blogs – 1226 ‘tags’

Nasa results





WORDPRESS



Tags

Separate tags with commas

[Choose from the most used tags](#)

[accessibility](#) [agile](#) [blogging](#) [cat](#)
[comic](#) [cool](#) [data](#) [design](#)
[documentation](#) [doodle](#)
[eclipse](#) [f1](#) [f1_cars](#) [food](#) [game](#)
[help](#) [information](#) [architecture](#)
[interfaces](#) [iOS](#) [iPad](#) [iPhone](#) [iso](#)
[lego](#) [managers](#) [mark](#) [webber](#) [message](#)
[broker](#) [photography](#)
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Categories

All Categories [Most Used](#)

- accessibility
- blogging
- comic
- f1
- Featured
 - Photography
 - Reviews
- information architecture

[+ Add New Category](#)

Tagging

Click on a suggested tag to add it to your post:

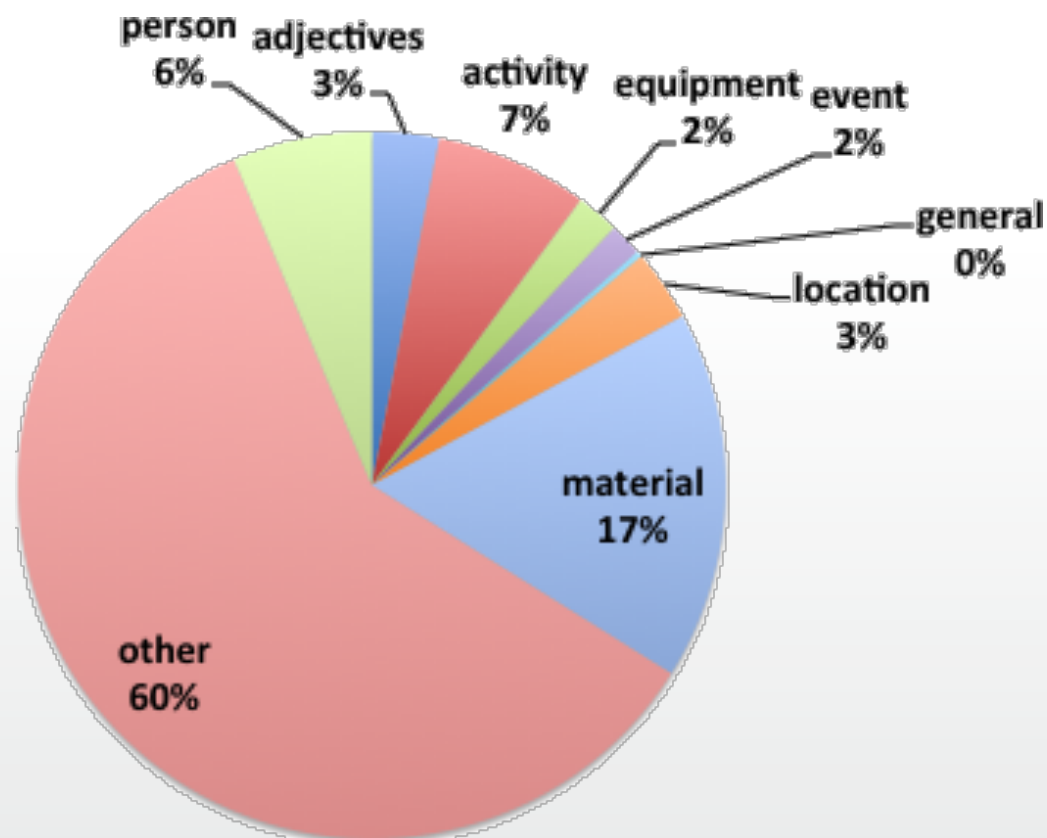
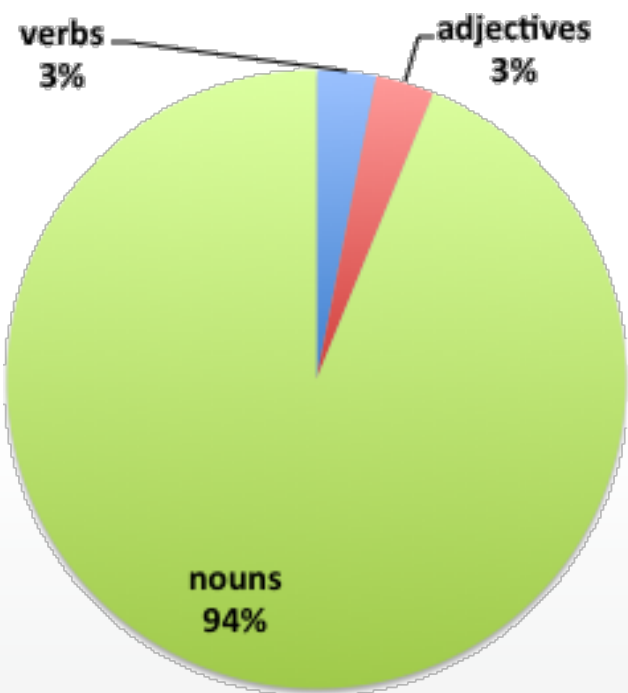
Post settings

Labels

Separate labels with commas

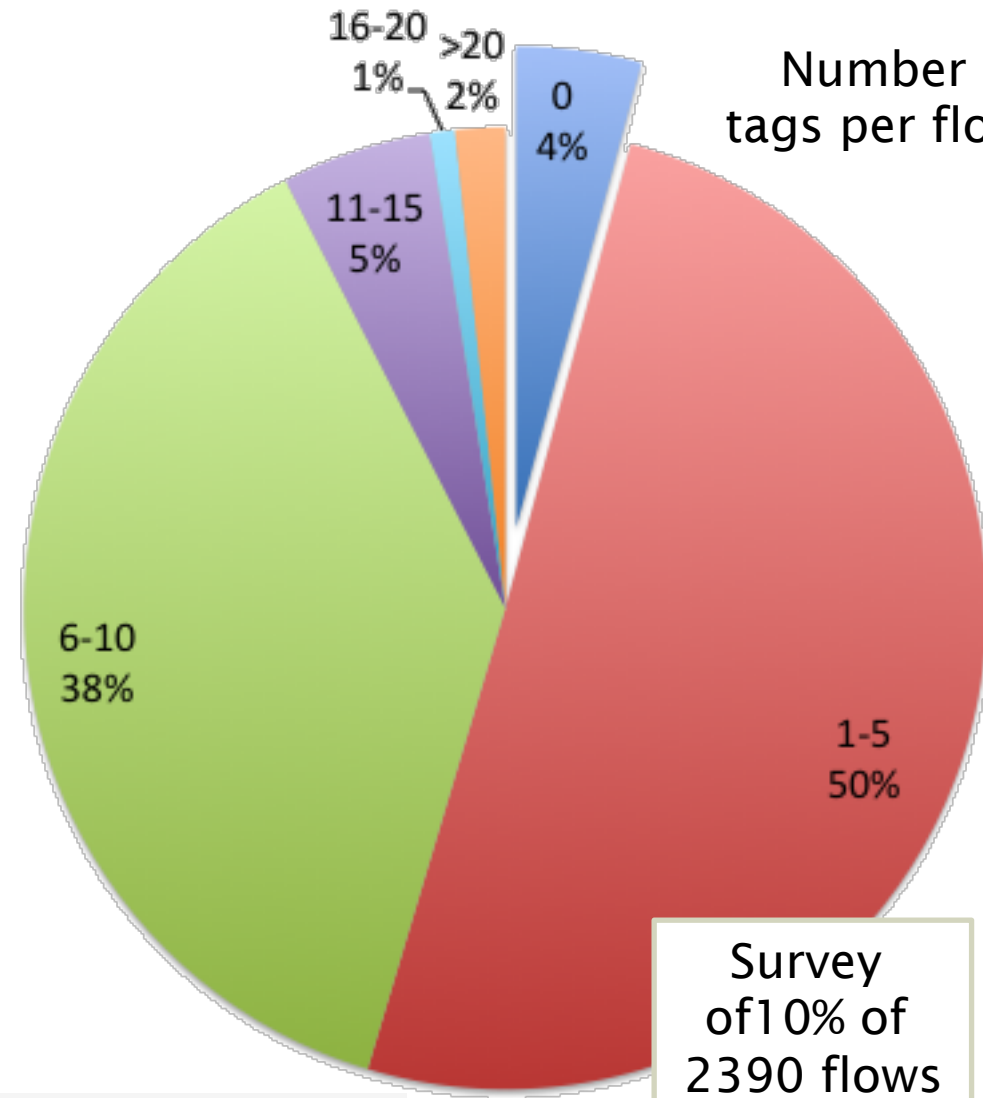
[bananas](#), [blogger](#), [blogging](#), [conference](#), [pancakes](#), [posting](#), [testing](#)

Chemistry Blog results



my experiment

Number of tags per flow



Survey of 10% of 2390 flows

Tags (7)

Original Uploader tags

cme | hec | **heliophysics** | lasco | propagation | solar | wsd

Add Tags

(use commas to separate different tags)

Add

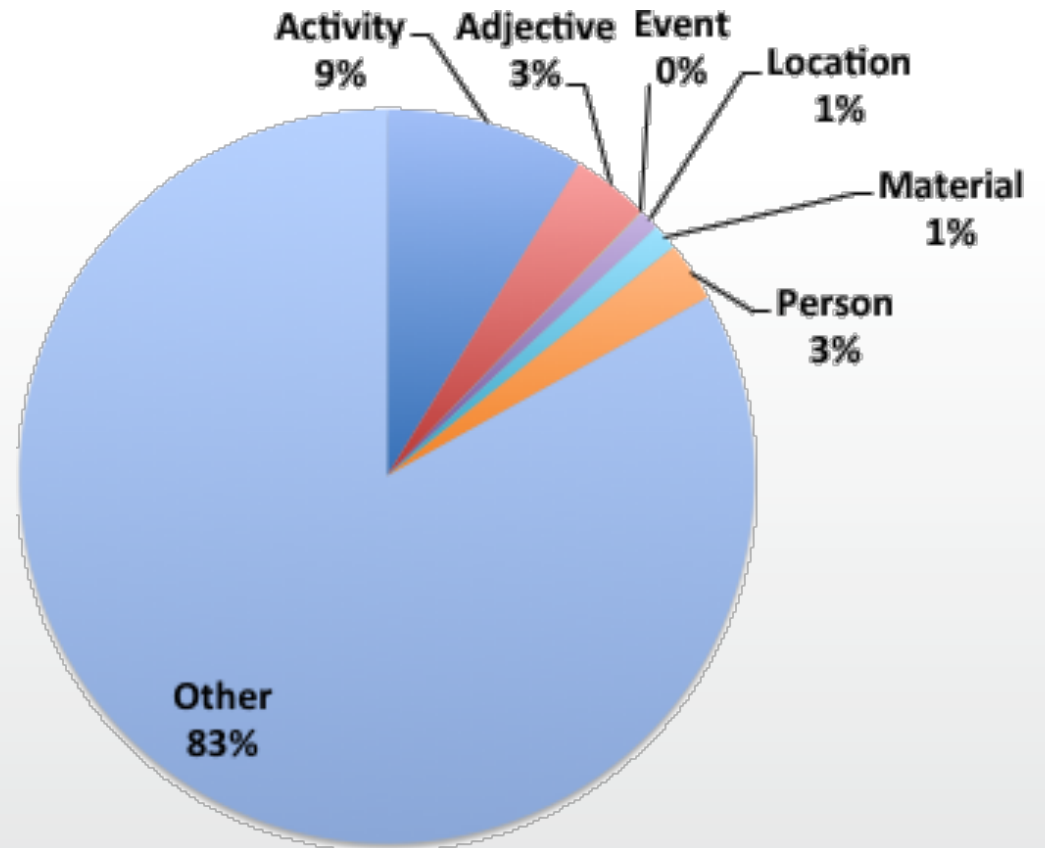
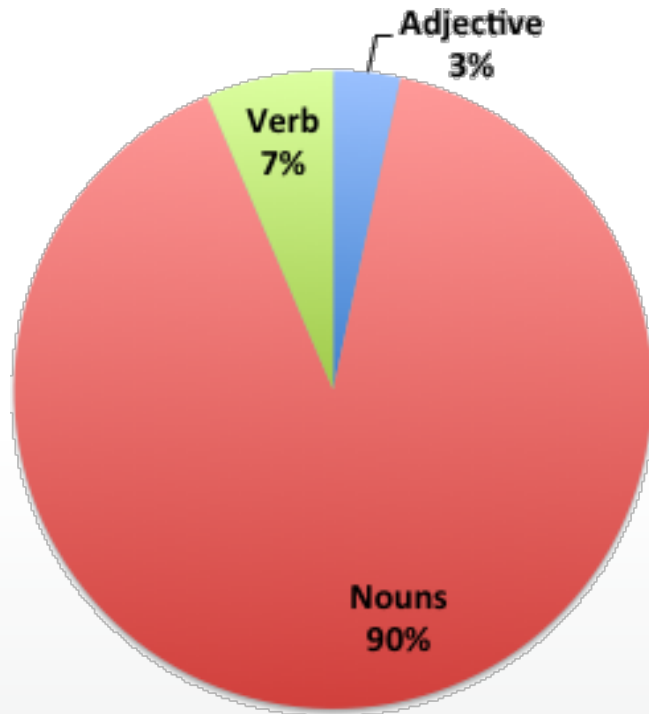
Tags (7):

d-grid | example | gwes | gworkflowd | loop | structured loop | workflow pattern

This Workflow has no tags!

myExperiment results

2349 tags



Classifying activities

- Potential to differentiate between action, activity, process, and technique
- But need to understand who is doing the activity or to what the activity is being done: person, material, or data?
- Intent is difficult to determine from ‘activity-related’ metadata

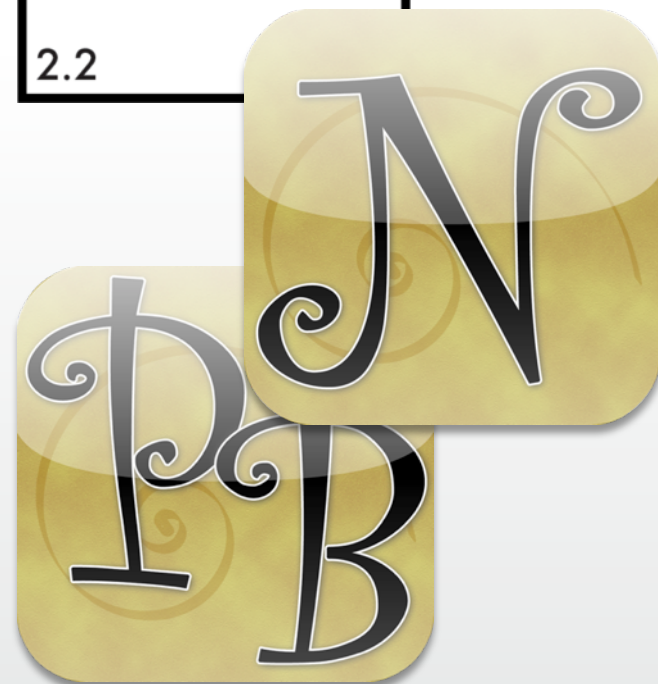
Summary

- Metadata has to be present to be useful!
- Common mistakes and “sense-making”
- Tells us about the interests and needs of the communities
- Users will use predefined values if they are available
- A number of possible strategies to encourage better use (and user experience) of metadata in ELNs



Futures

- Our findings have already had an influence on our ELN developments
- Considerations for our ELN interface designs in the future
- Links to our current research on how we can use cues to influence what students and researchers record..



Metadata Study

<http://sites.google.com/site/cmetastudy/>



