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Diffraction Data in Context

Metadata approaches

Simon Coles (s.j.coles@soton.ac.uk)

Director, UK National Crystallography Service

What can structures be used for?

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- We don't capture valuable information from every part of the "study"
- Good crystallographic practice requires information about the experiment not covered wholly by CIF
- Cant predict how a structure might be used in the future – measure AND CATALOGUE everything you possibly can!

- Data management is key: its all about context and linking…

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Why bother?

- Scientific rigour, reproducibility, long-term preservation
- Enable reuse
  - Amongst collaborators
  - For teaching & software development
  - New science
- Reanalysis as new techniques develop

- Some case studies/examples…

Operating a Service

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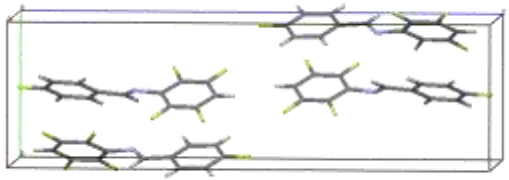

Proposal

Approval

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ncs | UK National Crystallography Service

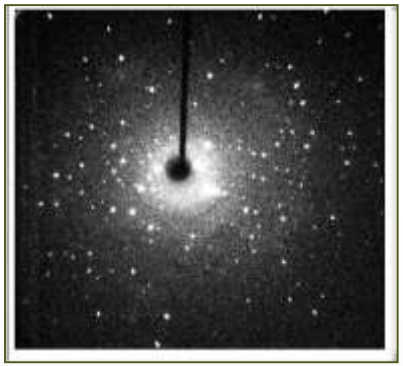
Publication

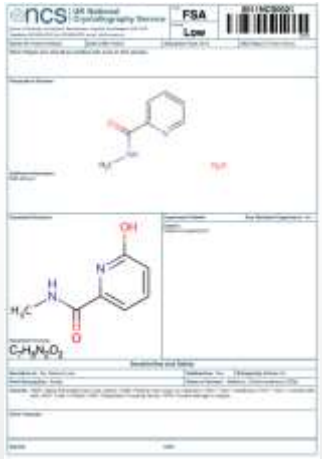
Submission

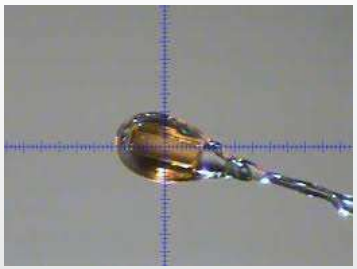
Reporting

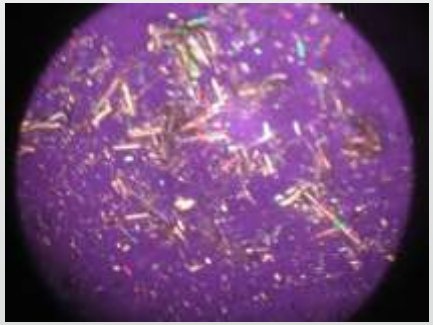
Analysis

Experiment









In-house Management

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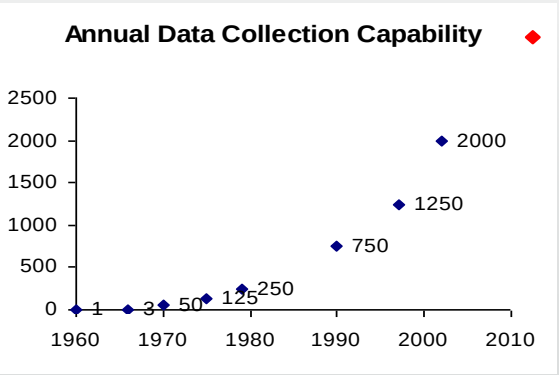
- Average publication lead-in time = 3 years
- 80% not published



Working Across Facilities

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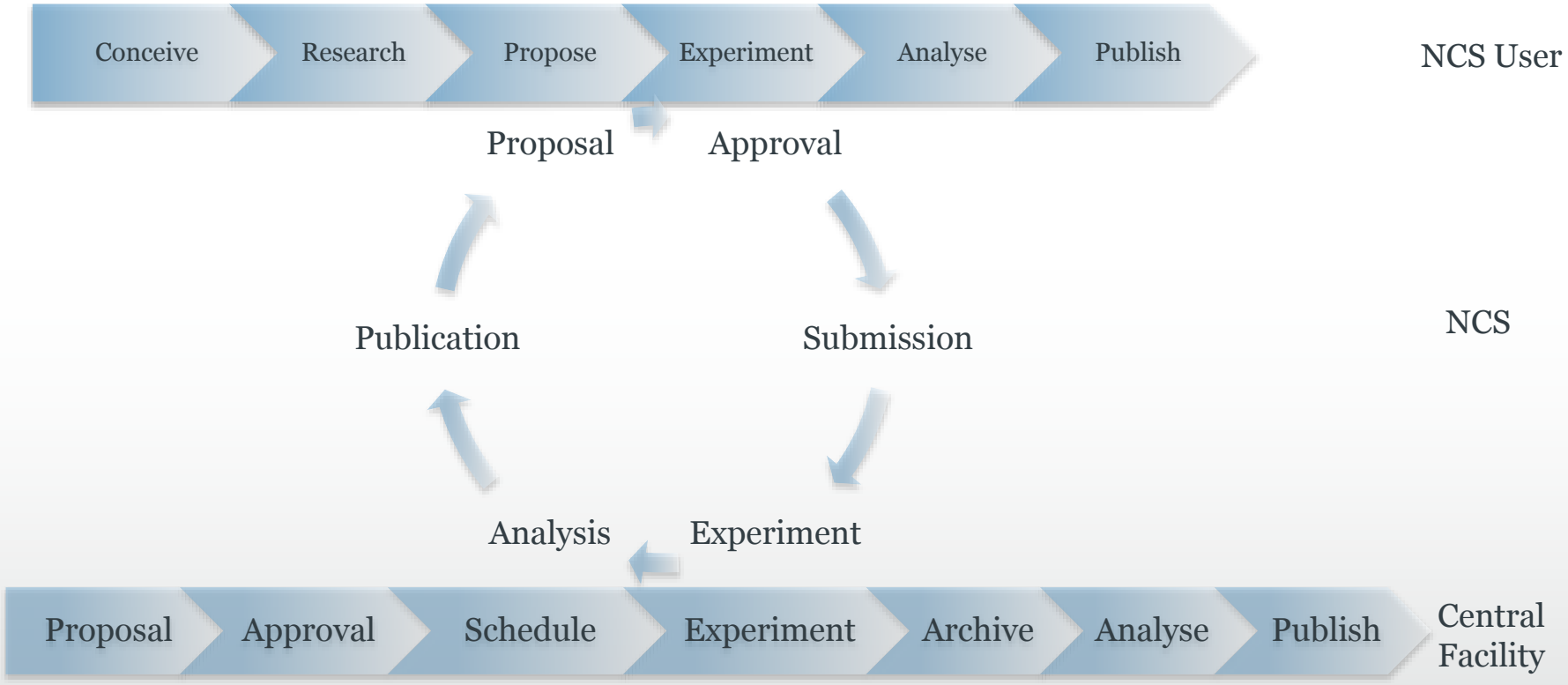

Availability & Reuse

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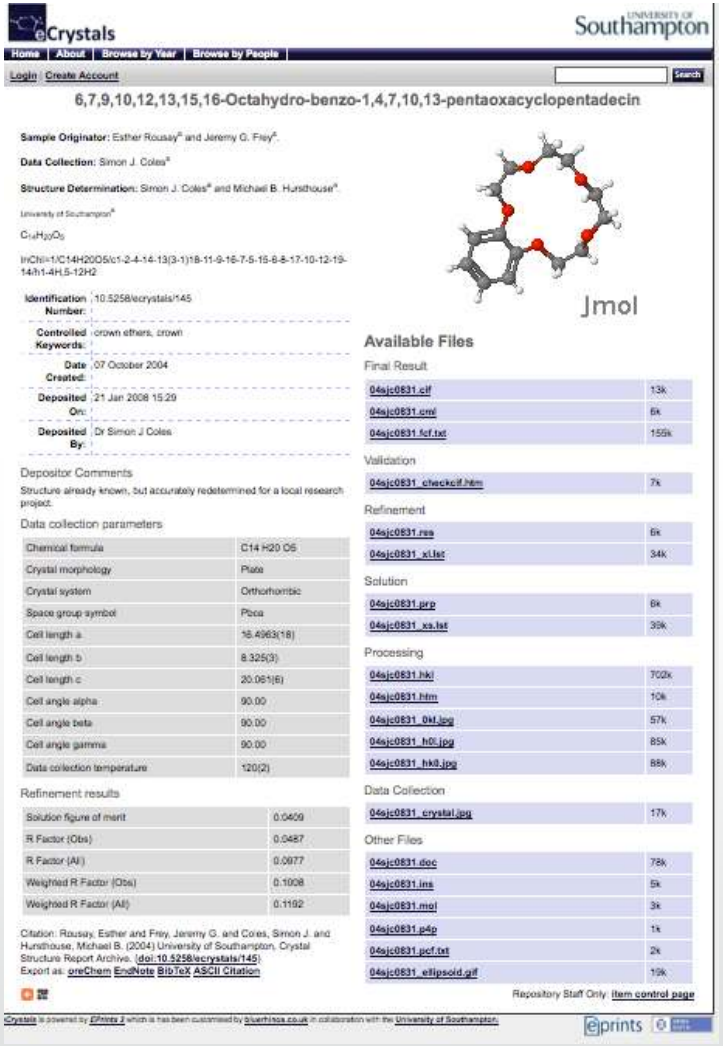
- Cant publish everything in the traditional way
- WWW alternative route
- Data needs to 'speak for itself'
- Provide enough raw data & metadata so that
  - Error understood
  - Reproducible
  - Reanalysis possible
  - Reuse facilitated



http://ecrystals.chem.soton.ac.uk

Supporting future reanalysis

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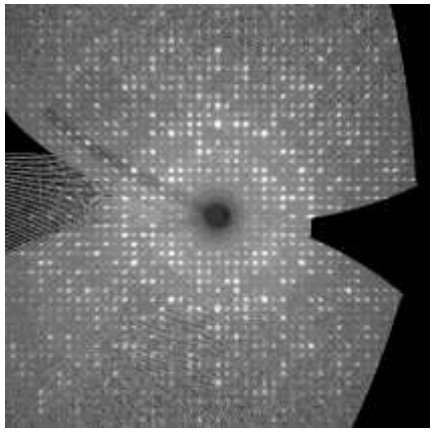
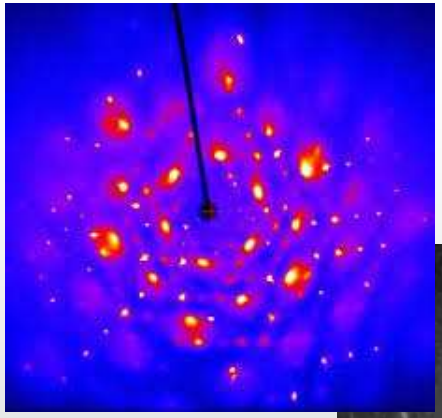
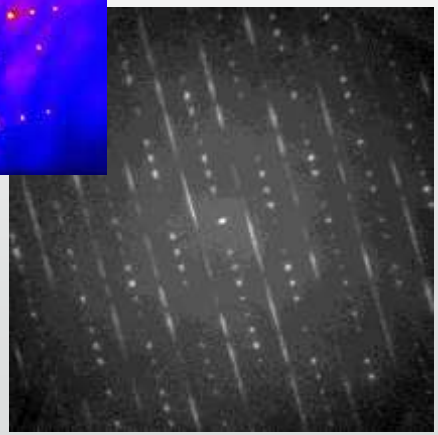
- Model unclear – need to come back to the raw data later
  - (Z' = 30, 60, 120 or 360?!?)
- What's going on in the system – unstudied non-Bragg regions
  - Disorder
  - No long range order
  - Solvent effects
  - Phase transitions







Approaches in the Future

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- What is structural information and what is background? Contributions to a reflection can only really be understood when we have a structural model! Second cycle of extracting structure factors once the model is complete…?
- The next generation will be addressing the information that we collect that is not Bragg scattering.
- Cant necessarily just do the experiment again
  - Interesting samples synthesised now may not be available in the future…
  - Facilities time difficult to get
  - Experiments performed on current equipment which may not be easily available in the future

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But what about process and context?

Detail behind the diffraction experiment itself.

Motivation behind the study as a whole.

Results in terms of the bigger scientific picture.

Getting Mobile in the Lab

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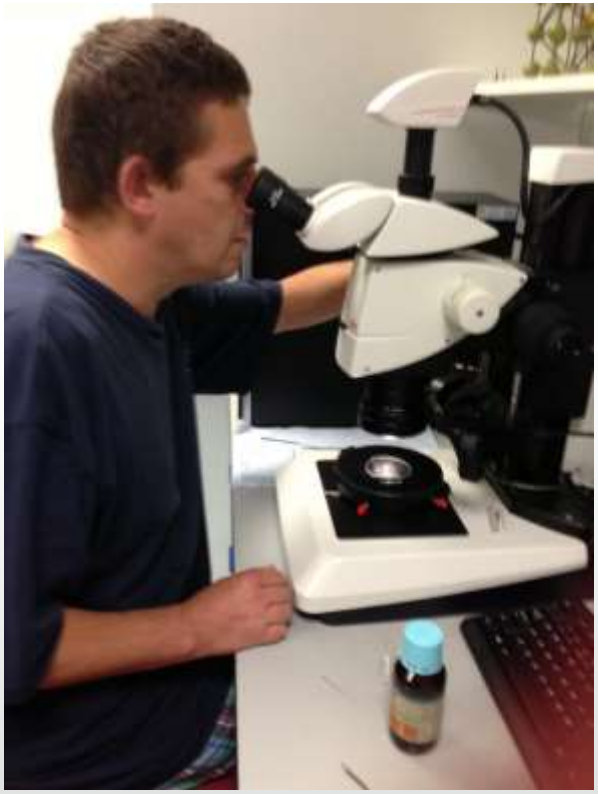
- Every crystallographic experiment has ‘unstructured’ data



Getting Mobile in the Lab

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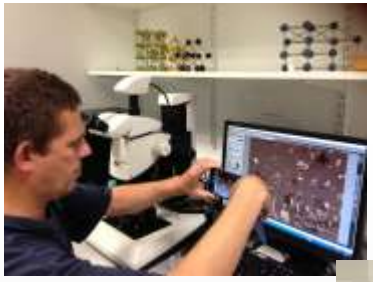
Package & Sample Tube




Bulk Sample & Manipulation



Mounted Sample

Trial Diffraction Pattern

Getting Mobile in the Lab

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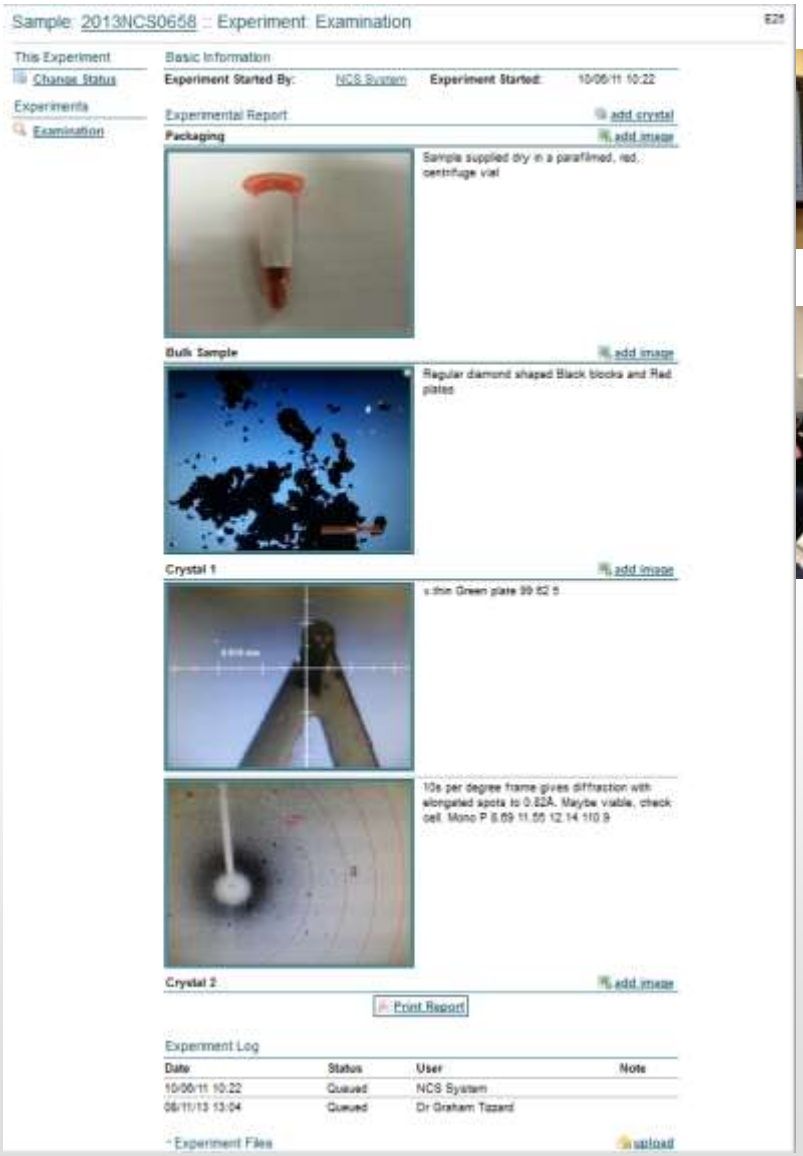

Rationale for the crystallography

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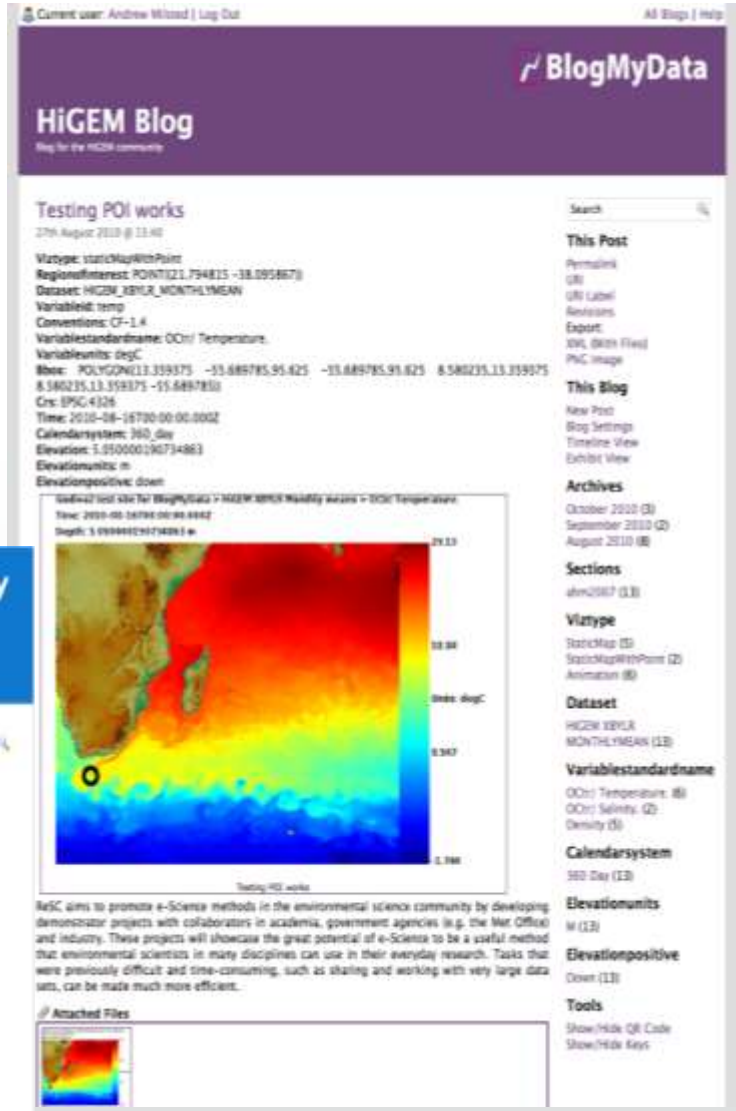

Rationale for the crystallography

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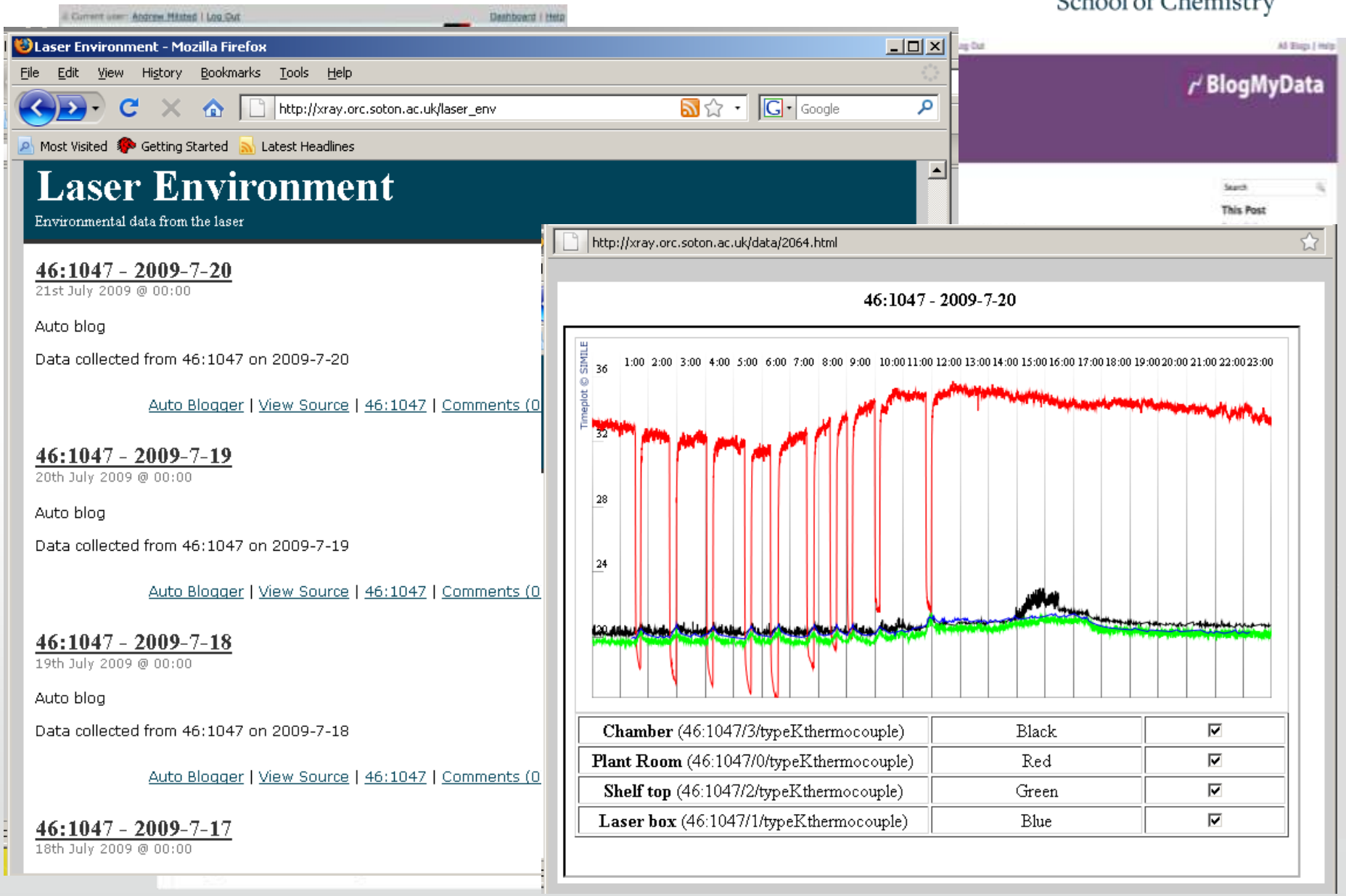

Rationale for the crystallography

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UltraFast Xray Group

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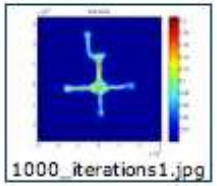
Reconstructing the new data

3rd August 2011 @ 22:52

Just a quick post to show some pictures from the reconstructions of the latest data and update everyone on progress.

Looking at data taken on 2nd August - the old 2um sample taken with a single wavelength. The diffraction patterns look v clean, with good detail right out to the edge - haven't worked out the resolution yet.

Tried to get Ben's CDI routine working, but it broke badly, and I couldn't fix it immediately, so i went back to my old routines (from 2 years ago! can't believe it's been that long) and got 'hio6.m' working. This is running on Boxer under Windows, but not using anything clever.



1000_iterations1.jpg

This one is a very plain HIO reconstruction, 1000 iterations after binning the data to 512x512. Shrinkwrapping every 100 (I think - notes at work right now). You can see that it reconstructs beautifully, and this happens every time - no need for multiple phases to get it to work.

(Once I'd remembered to background-subtract properly, of course - before that it all failed

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April 2011 (17)

Rationale for the crystallography

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Transformation of plasmid JRH4712/66 into BW25141 by electroporation

11th December 2006 @ 14:31

Transformations were set up according to the following protocol:
LB Ampicillin arabinose plates and SOC medium were warmed to 37 °C briefly before the arabinose plates were spread with X-glu (80 µL, 1:1 X-glu and LB) and allowed to continue warming.

BW25141 cells, plasmid JRH4712/66, p042, and electroporator cuvettes were cooled on ice. Items were added to the cuvettes as follows

-	1	+ve ctrl	-ve ctrl
BW25141	40 µL	40 µL	40 µL
plasmid 4712/66	4 µL	0 µL	0 µL
p042	0 µL	4 µL	0 µL

Cuvettes were electroporated at 1.75 kV, immediately had SOC medium (950 µL) added and the transformant transferred to eppendorf. The transformants were incubated at 37 °C for one hour with shaking. The transformants were diluted 1 in 20 with LB and 100 µL added to LB amp arabinose plates and incubated at 37 °C overnight.

Data

Jennifer Hale | Beta-glucuronidase | Comments (3)

Archives

January 2007 (24)
December 2006 (11)
November 2006 (5)

Sections

beta-galactosidase preparation and assays (18)

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Data

Test digestions to check the activity of two batches of EcoRI and NcoI

22nd January 2007 @ 11:57

Lab Book Ref: jrh4712-89
Sample Parent: jrh4712-80_blue
Sample Parent2: jrh4712-80_white
Digestions were set up as follows:

-	1	2	3	4	5	6	7	8	9	10	11
4712/80 blue	8 µL	-	-	8	-	-	-	8 µL	-	-	-
4712/80 white	-	8 µL	-	-	8 µL	-	-	-	8 µL	-	-
p042	-	-	5 µL	-	-	5 µL	5 µL	-	-	5 µL	5 µL
water	7.5 µL	7.5 µL	10.5 µL	7.5 µL	7.5 µL	10.5 µL	10 µL	7.5 µL	7.5 µL	10.5 µL	10 µL
EcoRI buffer	2 µL	2 µL	2 µL	-	-	-	2 µL	2 µL	2 µL	2 µL	2 µL
NEB buffer 4	-	-	-	2 µL	2 µL	2 µL	-	-	-	-	-
BSA	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL
EcoRI (a)	0.5 µL	0.5 µL	0.5 µL	-	-	-	0.5 µL	-	-	-	-
NcoI	-	-	-	0.5 µL	0.5 µL	0.5 µL	0.5 µL	-	-	-	0.5 µL
EcoRI (b)	-	-	-	-	-	-	-	0.5 µL	0.5 µL	0.5 µL	0.5 µL

EcoRI (a) assay date 2/05
EcoRI (b) assay date 7/05

Digestions were incubated in a waterbath at 37 °C for 3 hours.

Archives

January 2007 (24)
December 2006 (11)
November 2006 (5)

Sections

beta-galactosidase preparation and assays (18)
Beta-glucuronidase (18)
Data (Formatting) (1)
Software discussions (2)
Starting materials and reagents (1)

Lab Book Ref

JRH4712-63 (1)
JRH4712-64 (2)
JRH4712-66 (1)
jrh4712-76 (1)
jrh4712-77 (1)
jrh4712-78 (1)
jrh4712-80 (1)
jrh4712-81 (1)
jrh4712-83 (1)
jrh4712-82 (1)
jrh4712-84 (1)
jrh4712-85 (1)
4712-88 (1)
jrh4712-89 (1)
4712-86 (1)
jrh4712-87 (1)
4712-90a (1)

Product

jrh4712-74 (1)
jrh4712-76 (1)
jrh4712-76a (1)

jrh4712-76a (1)
jrh4712-77 (1)

April 2011 (17)

Rationale for the crystallography

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Open Source Malaria

Looking for New Medicines – Project Lab Notebooks

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Lab Notebooks

- TCMDC_ArylPyrrole (Paul Ylioja)
- TSP Synthesis of TCMDC Aryl Pyrrole Analogues (Laura White)
- TCMDC Near Neighbours (Zoe Hungerford)
- Biological Evaluation of Compounds (Matthew Todd)
- CDRI Synthesis of TCMDC Aryl Pyrrole Analogues (Soumya Bhattacharyya)
- Amino-thienopyrimidine Series (James Cronshaw)
- Triazolourea Singleton (James Cronshaw)
- In Silico Target Prediction of Actives (Matthew Todd)
- Grad Dip Arylpyrrole (Matin Dean)
- Pyrazole analogues (Paul Ylioja)
- CDRI synthesis of Pyrazole analogues (B.Harikrishna)
- Experimental Procedures (OSDD Malaria)
- Pharmacophore Modelling of OSM Compounds (Murray Robertson)

Project Admin

- OSM Online Project Meetings (OSDD Malaria)
- OSM Shared Data (OSDD Malaria)
- OSM Logos and Templates (Open Source Malaria)

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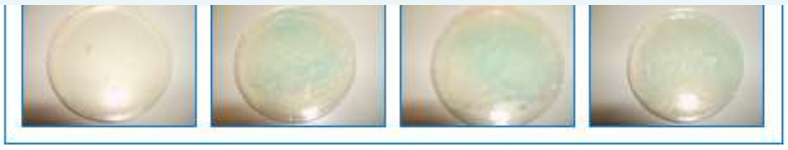


Jennifer Hale | Beta-glucuronidase | Comments (3)

*Eco*RI (b)

*Eco*RI (a) assay date
*Eco*RI (b) assay date

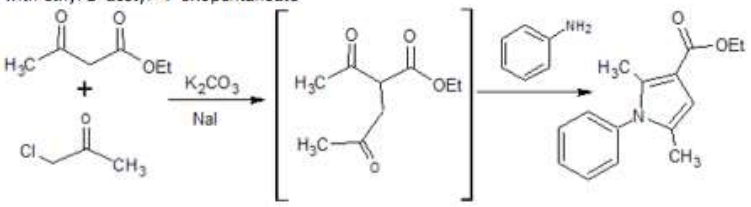
Digestions were inc

jrh4712-76a (1
jrh4712-77 (1)

Synthesis of ethyl 2,5-dimethyl-1-phenyl-1*H*-pyrrole-3-carboxylate (LMW 8)

20th November 2011 @ 06:41

Synthesis of ethyl 2,5-dimethyl-1-phenyl-1*H*-pyrrole-3-carboxylate from condensation of aniline with ethyl 2-acetyl-4-oxopentanoate



Ethyl acetoacetate (6 mL,47 mmol, 1 equiv.) and K_2CO_3 (8.45 g, 61.1 mmol, 1.3 equiv.) were mixed in MeCN (55 mL). NaI (7.05 g, 47 mmol, 1 equiv.) and Chloroacetone (4.8 mL, 51.7 mmol, 1.1 equiv.) were added and mixture heated to 80°C in an oil bath. TLC at 2 hours showed reaction at completion. Reaction was allowed to cool to room temperature. Mixture washed with EtOAc (2 x 20 mL), water (2 x 20 mL), 1:1 water:brine (2 x 20 mL) and brine (2 x 20 mL) and dried with MgSO4 and concentrated under reduced pressure to form a yellow oil. Ethyl 2-acetyl-4-oxopentanoate intermediate (2 mL, 10.7 mmol, 1 equiv.) was added to Aniline (1.17 mL, 12.89 mmol, 1.2 equiv.) and heated at 80°C in an oil bath for 1.25 hrs. TLC at 1 hour showed reaction at completion and reaction was allowed to cool to room temperature. Product was washed with EtOAc (2 x 20 mL), 10% citric acid (3 x 20 mL), water (20 mL) and brine (2 x 20 mL) and then concentrated under reduced pressure to form a dark brown oil. Product was purified by chromatography on silica (2-15% EtOAc in petrol - *suggest a lower % EtOAc*). Product containing fractions concentrated under reduce pressure to produce a yellow oil (952 mg, approximate yield 37%). Product did not crystallise.

Collected data: ethyl 2,5-dimethyl-1-phenyl-1*H*-pyrrole-3-carboxylate

mpt: n/a
***m/z* (APCI+):** 244 $[M+H]^+$, 100%
^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.41-7.50 (qn, 2H), 7.15, 7.18 (m, 2H), 6.38 (s, 1H), 4.20-4.32 (sx, 2H), 2.29 (s, 3H), 1.97 (s, 3H), 1.27-1.36 (qn, 3H)
^{13}C-NMR (75 MHz, $CDCl_3$): δ 165.72, 137.76, 136.16, 129.39, 129.19, 128.93, 128.68, 128.53, 128.18, 111.49, 107.55, 59.21, 14.59, 12.64, 12.37
IR: 696.57, 770.6, 1072.8, 121.34, 1411.26, 1693.25, 2978.29

For data files, refer to Synthesis of ethyl 2,5-dimethyl-1-phenyl-1*H*-pyrrole-3-carboxylate (LMW 8-1) and Synthesis of ethyl 2-acetyl-4-oxopentanoate intermediate. (LMW 7-1)

References:
doi: 10.1016/0040-4020(80)80102-5

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Attached Files

Laura White | View Source | Procedures | Comments (0)

Rationale for the crystallography

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Synthesis of 4-substituted methylidene oxindoles

Project E-Lab Notebook for the synthesis of five 4-substituted methylidene oxindole from oxindole and their corresponding aromatic aldehydes.

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Single Crystal X-ray crystallography

27th June 2012 @ 23:09

Single-crystal X-ray diffraction analyses were performed using a Bruker APEXII CCD diffractometer mounted at the window of a Bruker FR591 rotating anode (MoKα = 0.71073 Å) and equipped with an Oxford Cryosystems cryostream device. Data were processed using the Collect package and unit cell parameters were refined against all data. An empirical absorption correction was carried out using SADABS . The structures were solved by direct methods using SHELXS-97 and refined on Fo^2 by full-matrix least-squares refinements using SHELXL-97. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were added at calculated positions and refined using a riding model with isotropic displacement parameters based on the equivalent isotropic displacement parameter (Ueq) of the parent atom. Figures were produced using OLEX2

Graham Tizzard | View Source | Analytical Procedures | Comments (0)

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

6th May 2012 @ 18:16

Spectroscopic Method: MS-ESI
Substituent: Nitro
MS Spectrum of (3E)-3-(4-Nitrobenzylidene)-1,3-dihydro-2H-indol-2-one:

The mass spectrum of (3E)-3-(4-Nitrobenzylidene)-1,3-dihydro-2H-indol-2-one has been obtained by negative electrospray ionization (ESI). The peak at m/e = 265.2 confirms the molecular mass of this compound as the molecular ion gains a proton.

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

Peak Position	Diff. between molecular mass and peak	Suspected molecules or ions	Inference
265.2	265 - 264 = 1	$(M+H)^+$	Parent compound plus a proton

Nicola Knight | View Source | Spectroscopic Data | Comments (0)

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

Spectroscopic Method
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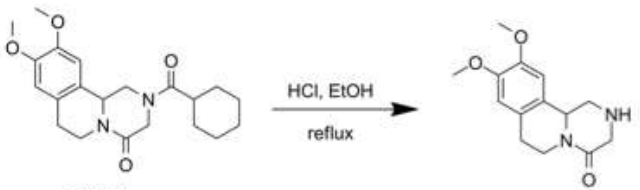
Hydrolysis of MNR11-18 to give MNR26-7

23rd April 2013 @ 01:09

Mnr: 21-30
As for
Hydrolysis of MNR11-16 to MNR26-4
Hydrolysis of MNR11-17 to MNR26-5
Starting material from
Synthesis of MNR11-18



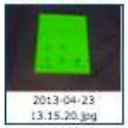
MNR11 MNR26

Compound	FW (g/mol)	Density (g/mL)	mmol	Mass (g)	Volume (mL)	eq	conc. (mmol/mL)
MNR11-18	372.48		10.63	3.96		1.00	
1M HCl		0.97	106.32		110	10.00	
EtOH					21		0.50
MNR26-7	262.30						

Hazard and Risk Assessment:

Procedure:
MNR11-8 (3.96 g, 10.63 mmol) was dissolved in EtOH (21 mL) and HCl (1M) (110 mL) and heated to reflux for 2.5 hours. The solution was allowed to cool to room temperature then cooled in an ice bath, basified with NaOH pellets (approx 8 g, pellets used to minimise volume of aqueous material) to pH 12-13 and extracted with DCM (4 x 100 mL). The organic fractions were combined, dried over magnesium sulphate, filtered and concentrated under reduced pressure to give an orange crispy solid (1.008 g).

TLC
Reaction mixture after 2.5 hours ran in 100% EtOAc



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1-10 (5)

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Structures in the context of ‘traditional’ publishing

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- ELN as Supplementary Information for conventional publication (*Chemistry Central Journal* 2013, 7:182)

Structures in the context of 'traditional' publishing

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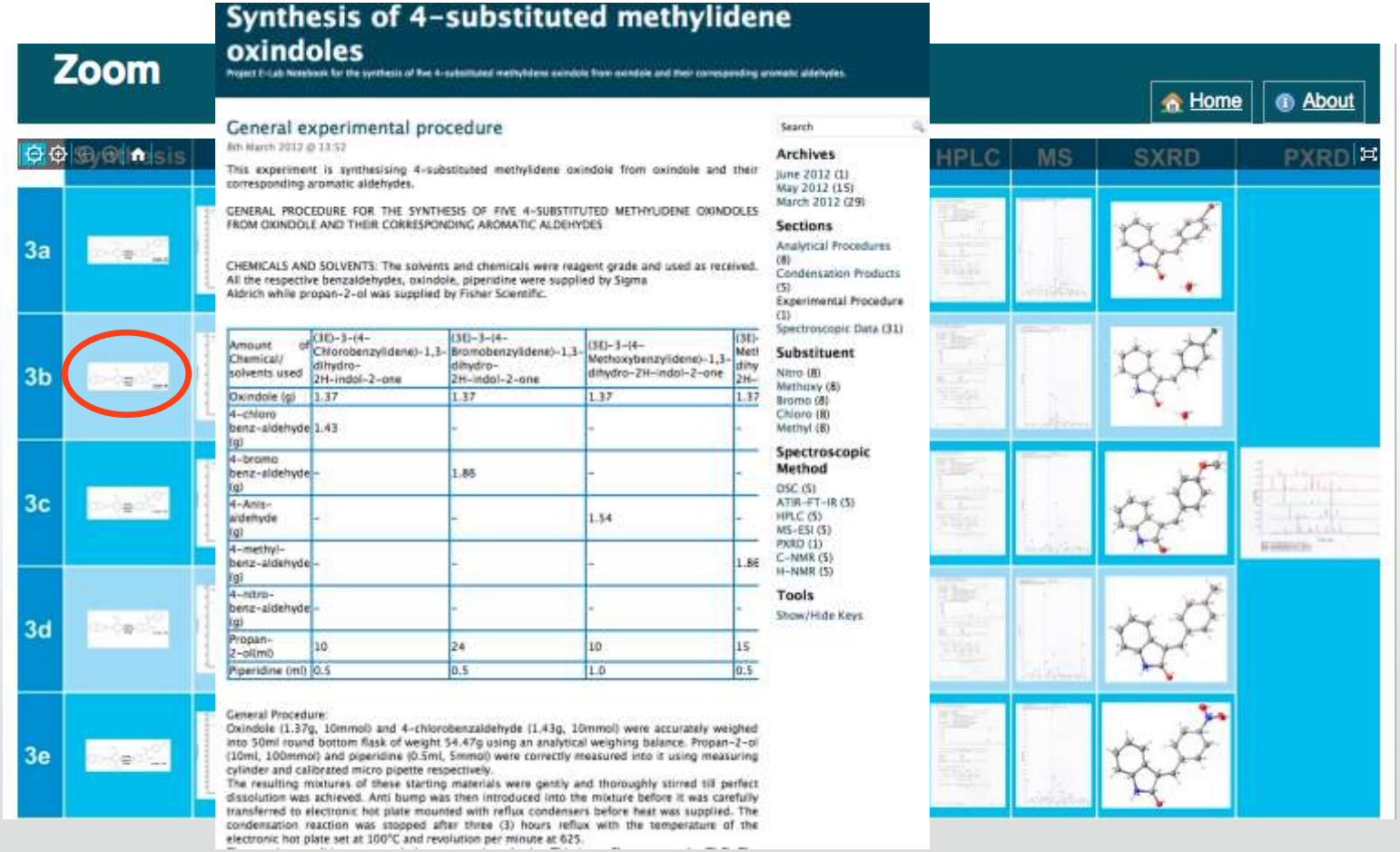
- ELN as Supplementary Information for conventional publication (*Chemistry Central Journal* 2013, 7:182)



Structures in the context of 'traditional' publishing

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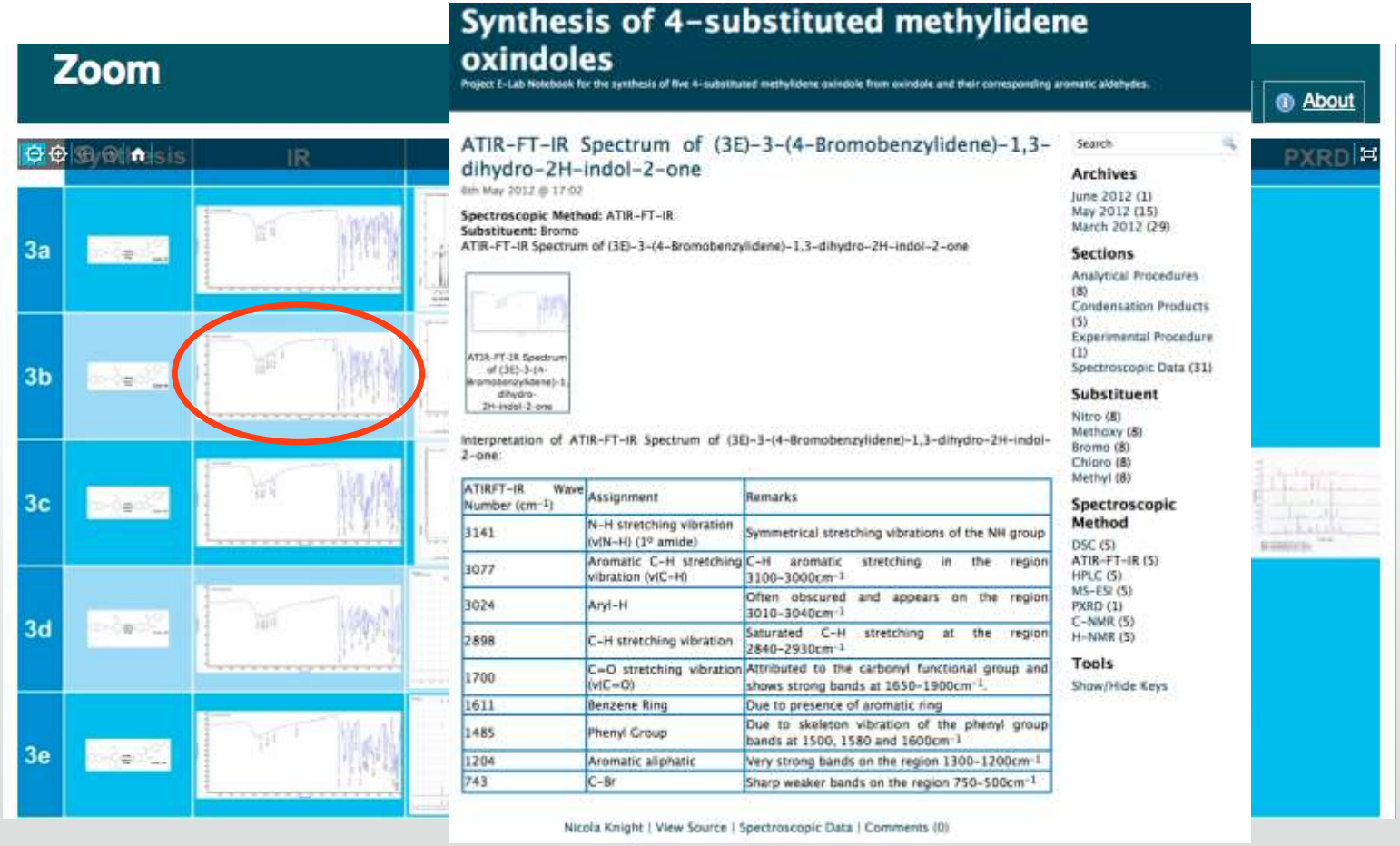

Structures in the context of ‘traditional’ publishing

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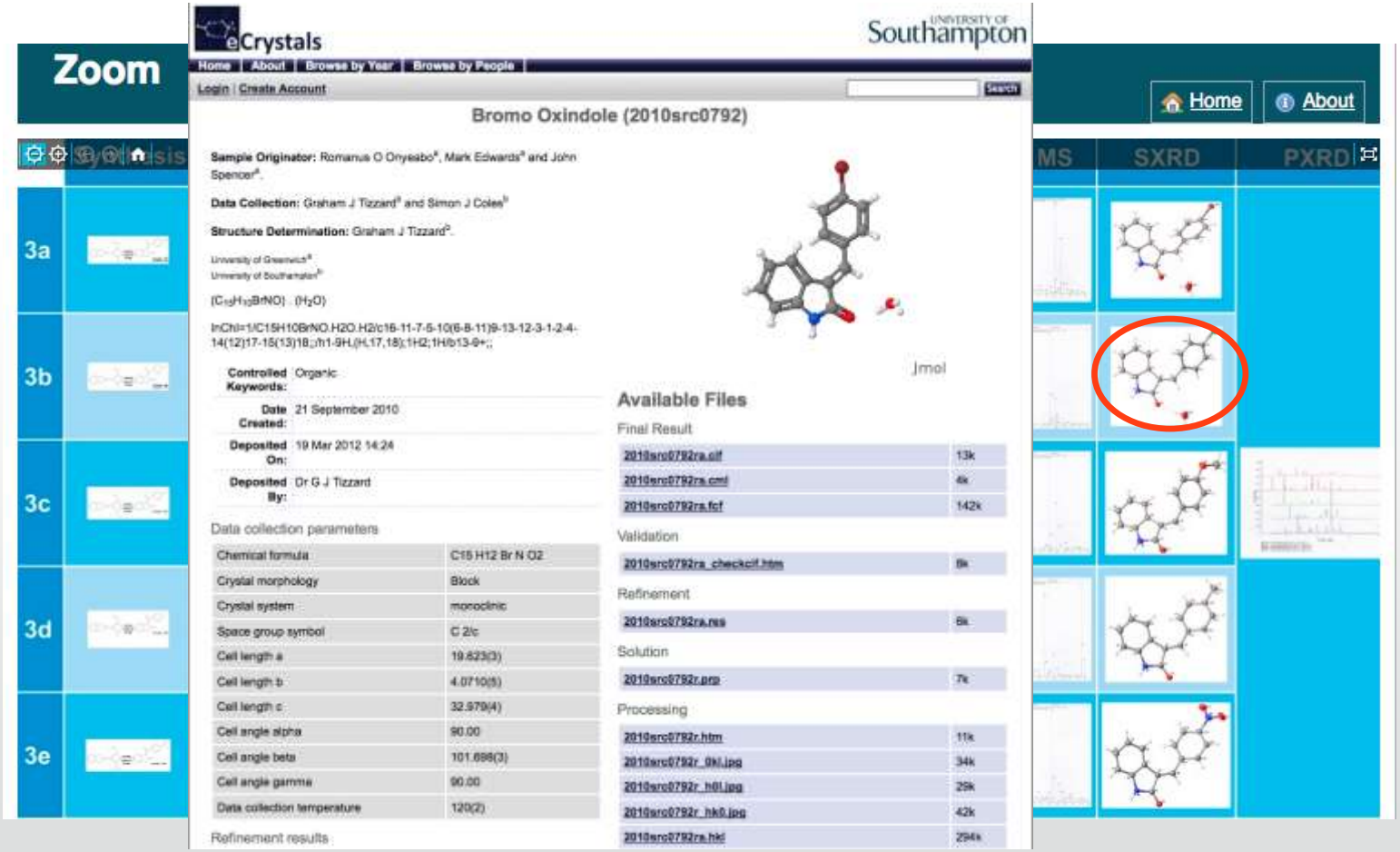

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Metadata support for solutions.

Invariably the context for a crystal structure

Or

The context a crystal structure has to fit into!

Datastores, ICAT & CSMD

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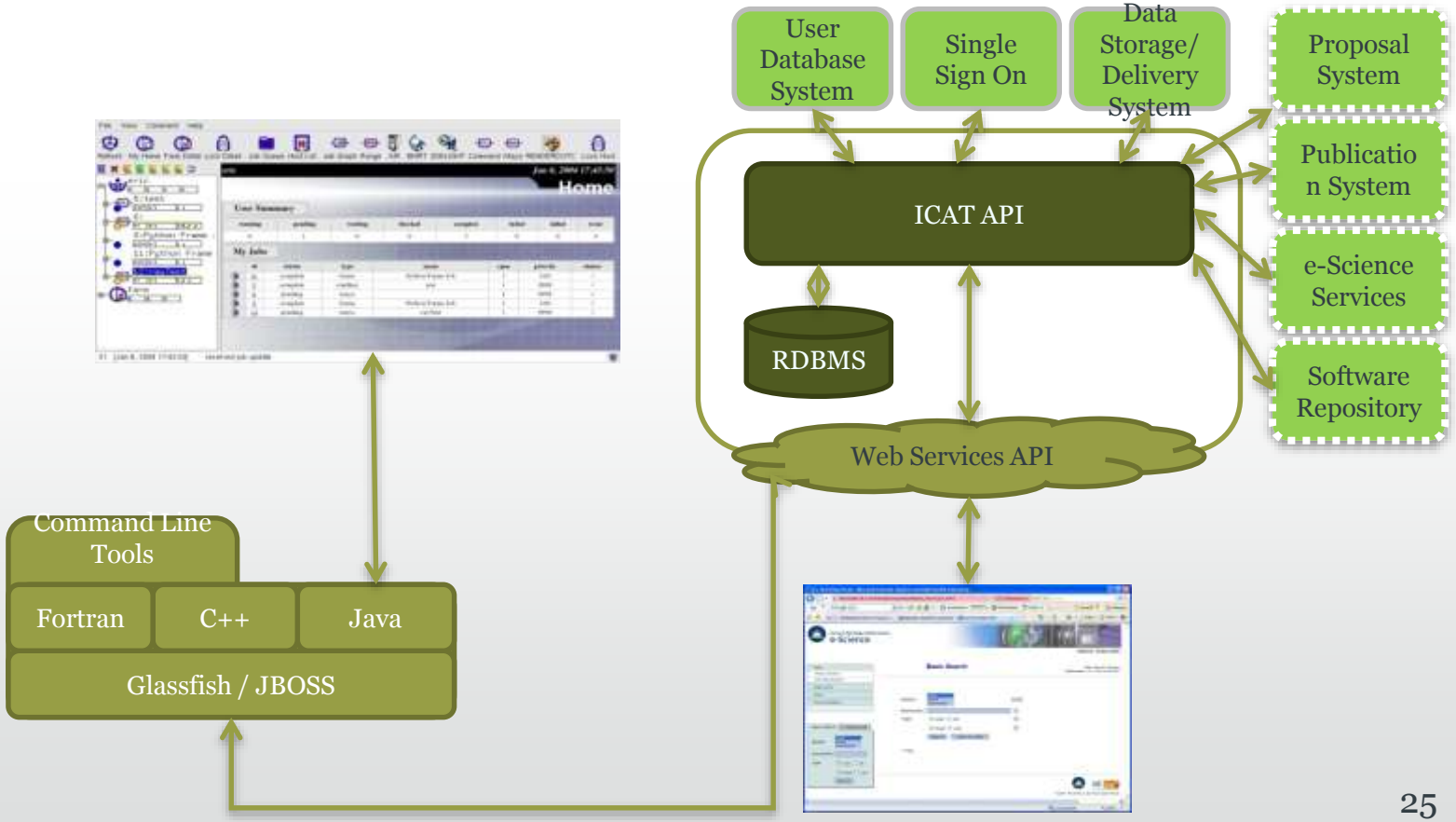
The Core Scientific Metadata model forms the information model for ICAT & is designed to describe facilities-based experiments



CSMD as a Starting Point

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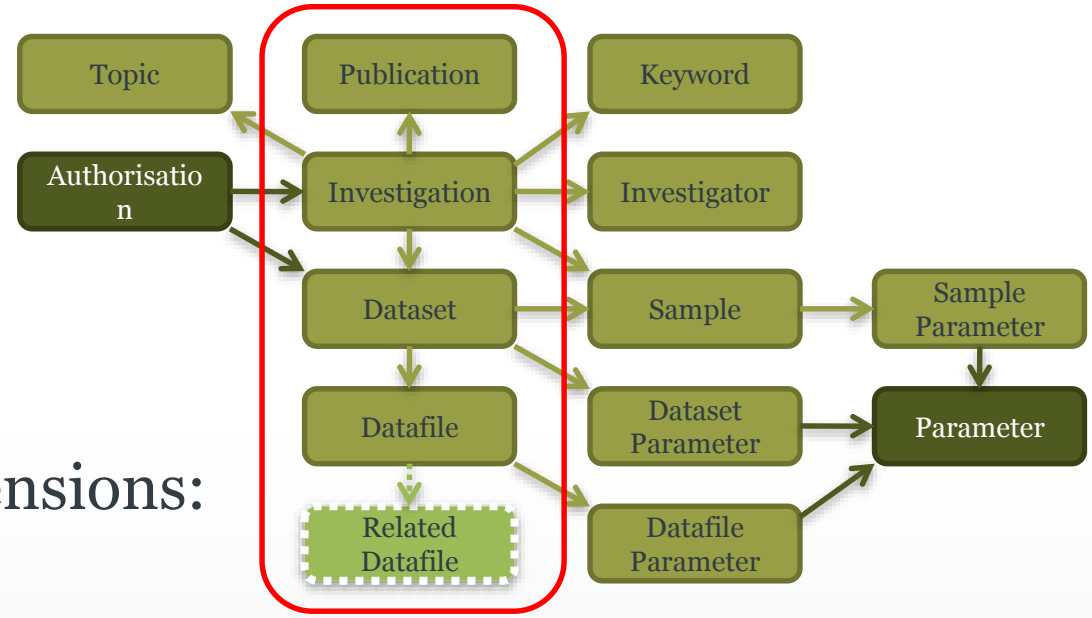

- Doesn't cover all, but…
- Forms the basis for extensions:
  - To derived data
  - To laboratory based science
  - To secondary analysis data
  - To preservation information
  - To publication data

Recording process

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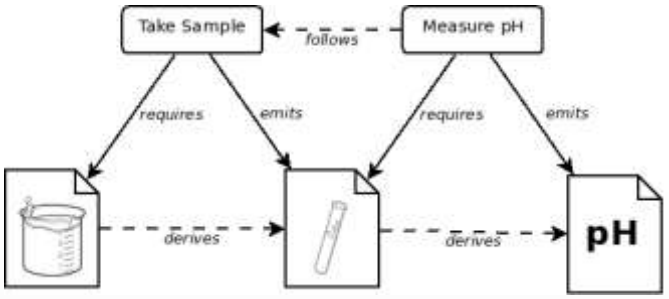
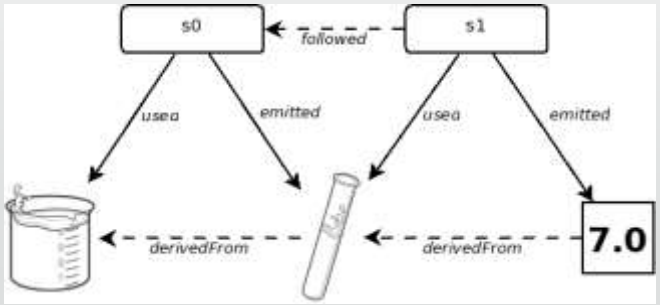
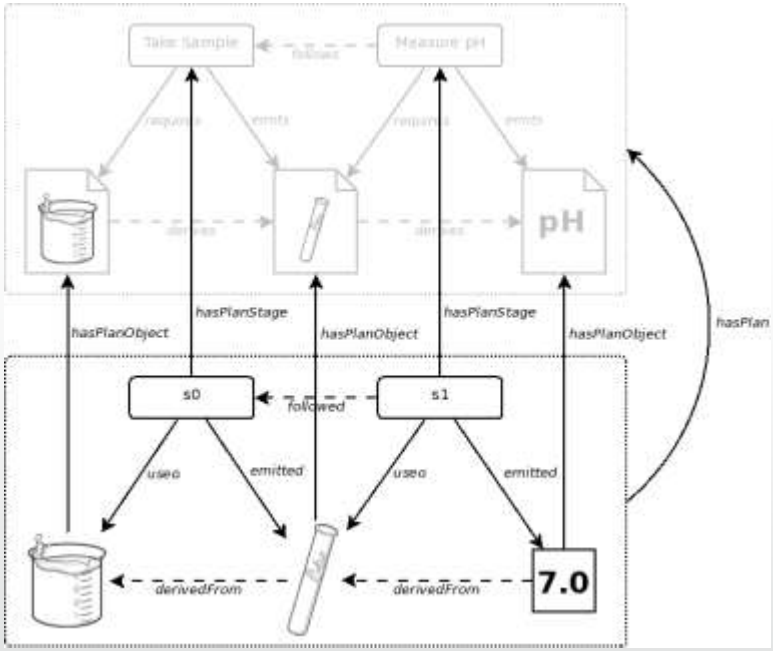
- Plan (Prospective provenance)



- Enactment (Retrospective provenance)



- Realisation



oreChem Plan for eCrystals

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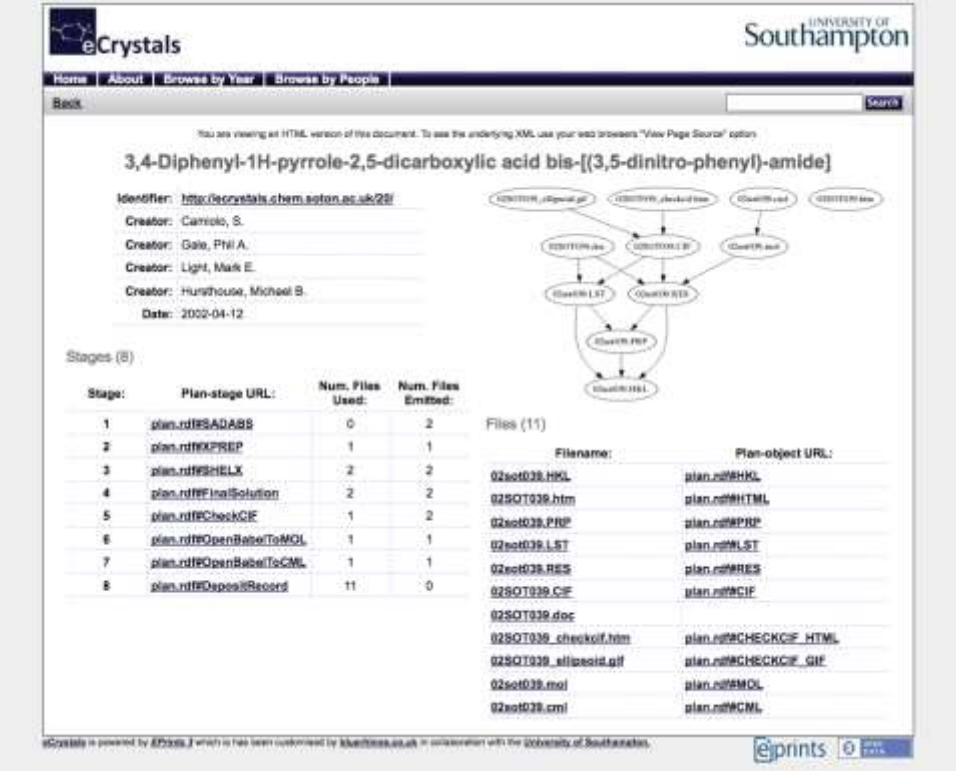
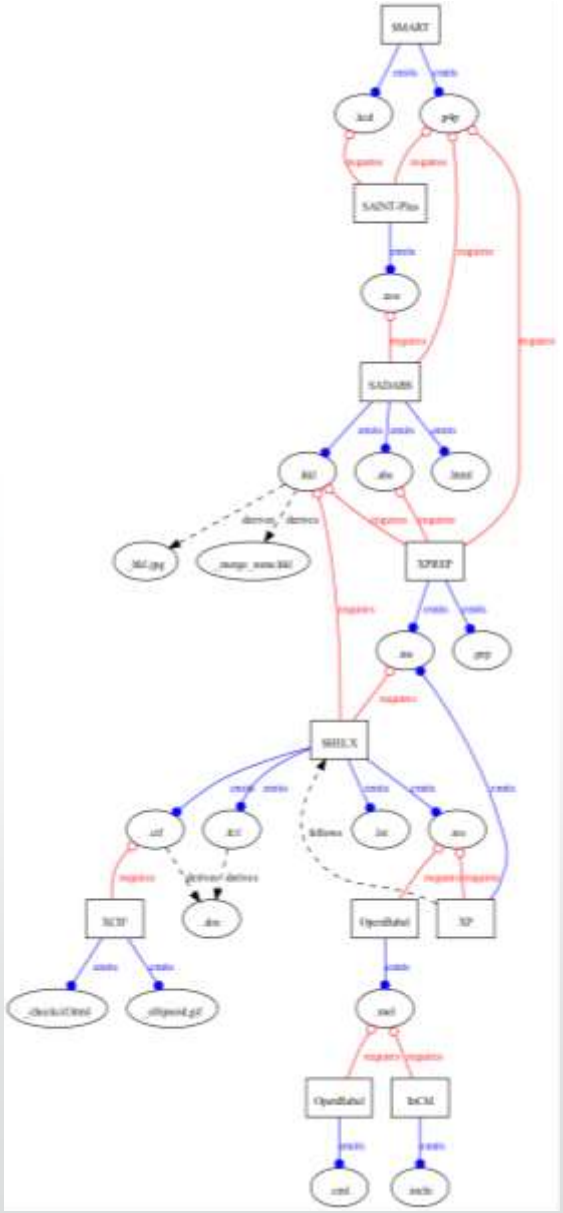
- Machine-readable representation of methodology
- Describes requirements for software and data products





SIMS:
Sample Information Management System

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- A standard/format for crystallographic sample and experiment data management and archival
- Supported by CrystalClear and NCS Portal, providing interaction between facility, instruments and CIF, ImgCIF etc

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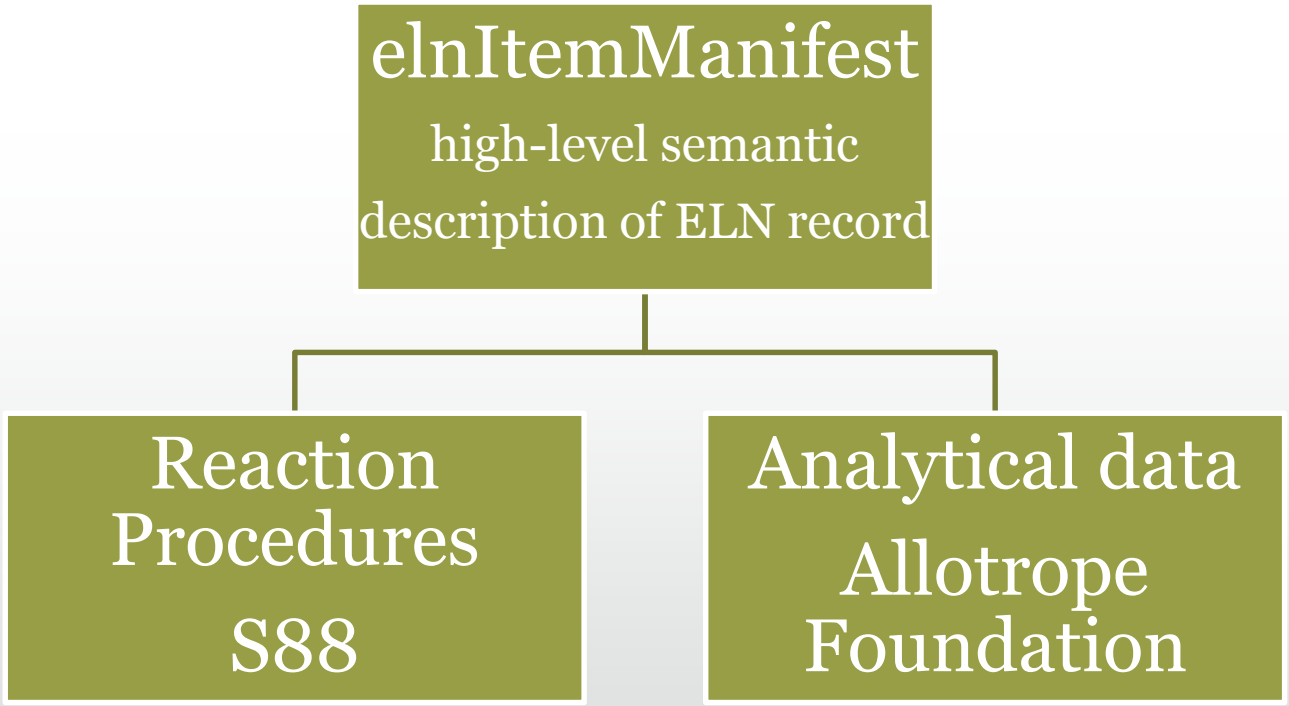
A semantic framework for chemistry

- Describes and relates different types of process information



elnItemManifest

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- Layered metadata model for description, export & packaging
- This is the first (information) layer – leads into knowledge
- Published through Dial-a-Molecule athttp://wp.me/p2JoQ6-xF & in J. ChemInf 2013, **5**:52

```
<?xml version="1.0"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema">

<xs:annotation>
  <xs:documentation>Change history</xs:documentation>
  <xs:documentation>==============</xs:documentation>
  <xs:documentation>15 June 2012 - [CLB] Created from enDataDescription prototype</xs:documentation>
</xs:annotation>

<xs:annotation>
  <xs:documentation>Definitions of data types used in the manifest of the ELN item</xs:documentation>
  <xs:documentation>-------------------------------------------------------------</xs:documentation>
</xs:annotation>

<xs:complexType name="keywordSet">
  <xs:annotation>
    <xs:documentation>A list of terms</xs:documentation>
  </xs:annotation>
  <xs:sequence>
    <xs:element name="keyword" type="xs:string" minOccurs="0" maxOccurs="unbounded"/>
  </xs:sequence>
</xs:complexType>

<xs:complexType name="identifierSet">
  <xs:sequence>
    <xs:element name="primaryLocalIdentifier" type="xs:string">
      <xs:annotation>
        <xs:documentation>Primary string, URI, or item in any other format that enables</xs:documentation>
        <xs:documentation>this record to be located uniquely in the originating system</xs:documentation>
      </xs:annotation>
    </xs:element>
    <xs:element name="otherLocalIdentifier" type="xs:string" minOccurs="0" maxOccurs="unbounded">
      <xs:annotation>
        <xs:documentation>[Optional] Alternative means of locating record in the originating system</xs:documentation>
      </xs:annotation>
    </xs:element>
    <xs:element name="accessIdentifier" type="xs:anyURI" minOccurs="0">
      <xs:annotation>
        <xs:documentation>[Optional] URI that provides a direct link to the content.</xs:documentation>
        <xs:documentation>If included, must be a 'linked data' URI giving open access</xs:documentation>
      </xs:annotation>
    </xs:element>
  </xs:sequence>
</xs:complexType>
```

```
<xs:complexType name="contentInformation">
  <xs:annotation>
    <xs:documentation>Text that describes what the item is, with a descriptor of the</xs:documentation>
    <xs:documentation>digital type, or "undefined" if no corresponding MIME format</xs:documentation>
  </xs:annotation>
  <xs:sequence>
    <xs:element name="description" type="xs:string"/>
    <xs:element name="mimeType" type="xs:string" default="undefined"/>
  </xs:sequence>
</xs:complexType>

<xs:complexType name="relatedID">
  <xs:annotation>
    <xs:documentation>Nature of the related information, for example, publication or related work</xs:documer
    <xs:documentation>Id can be any string, but DOI preferred if the related item is a publication</xs:docume
  </xs:annotation>
  <xs:sequence>
    <xs:element name="relationship" type="xs:string"/>
    <xs:element name="id" type="xs:string"/>
  </xs:sequence>
</xs:complexType>

<xs:complexType name="relatedItemSet">
  <xs:annotation>
    <xs:documentation>Zero or more item(s) of related information</xs:documentation>
  </xs:annotation>
  <xs:sequence>
    <xs:element name="item" type="relatedID" minOccurs="0" maxOccurs="unbounded"/>
  </xs:sequence>
</xs:complexType>

<xs:complexType name="contributorInformation">
  <xs:annotation>
    <xs:documentation>For example, Author, Funding Body, PI, institution, ...</xs:documentation>
    <xs:documentation>Plain text, but name ideally complemented by unique identifiers</xs:documentation>
  </xs:annotation>
  <xs:sequence>
    <xs:element name="role" type="xs:string"/>
    <xs:element name="name" type="xs:string"/>
  </xs:sequence>
</xs:complexType>

<xs:complexType name="contributorSet">
  <xs:annotation>
```

Standards for reactions: S88

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- Group arising from Dial-a-Molecule consisting of Mettler Toledo, Pfizer, GlaxoSmithKline, AstraZeneca, Johnson & Johnson, Southampton University, NextMove, Royal Society of Chemistry looking to:
  - Provide guidance for S88 implementations for synthetic organic chemistry reaction procedures
  - Provide example set
  - Agree on controlled vocabularies for elements
  - Generate a schema
  - IUPAC uptake?

Standards for reactions: S88

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```
<?xml version="1.0" encoding="utf-8"?>
<Experiment Name="SJH-01-227" StartTime="2014-04-11T09:00:00Z" Duration="00:??:??" User="sam" NetworkAddress="???.??.??.???" DNSName="????????????.??.??.?????"
Application="RscDataRepository" ApplicationVersion="1.0.0.0" ExperimentId="ReactionRunIDFromDataRepositoy" ExperimentStatus="?????" FormatVersion="1.0">
 <LinkedExperiment>
   <Experiment Name="SJH-01-211" Description="Another run of the same reaction"/>
   <Experiment Name="SJH-01-211" Description="The previous step in the reaction which created &lt;b&gt;16&lt;&#47;b&gt; as a product"/>
 <LinkedExperiments/>
 <Process>
   <ProcessStage>
   <ProcessOperation Name="Reaction">
     <ProcessAction Name="Start Experiment" Description="Add &lt;b&gt;16&lt;&#47;b&gt; (0.101 g, 0.132 mmol) to a round bottom flask.">
       <ProcessParameter Name="&lt;b&gt;16&lt;&#47;b&gt;.TotalMass" Value="0.101" Unit="g"/>
       <EquipmentUnit UnitId="1"/>
     </ProcessAction>
     <ProcessAction Name="Add Cu(OTf)&lt;sub&gt;2&lt;&#47;sub&gt;" Description="Add Cu(OTf)&lt;sub&gt;2&lt;&#47;sub&gt; (0.006 g, 0.01 mmol) under a N&lt;sub&gt;2&lt;&#47;sub&gt;
atmosphere" >
       <ProcessParameter Name="Cu(OTf)&lt;sub&gt;2&lt;&#47;sub&gt;.TotalMass" Value="0.006" Unit="g"/>
       <ProcessParameter Name="Atmosphere" Value="N&lt;sub&gt;2&lt;&#47;sub&gt;"/>
       <EquipmentUnit UnitId="1"/>
     </ProcessAction>
     <ProcessAction Name="Dissolve &lt;b&gt;2&lt;&#47;b&gt; in C&lt;sub&gt;2&lt;&#47;sub&gt;H&lt;sub&gt;4&lt;&#47;sub&gt;C1&lt;sub&gt;2&lt;&#47;sub&gt;" Description="In a separate
vial, dissolve &lt;b&gt;2&lt;&#47;b&gt; (0.155 g, 0.753 mmol) in C&lt;sub&gt;2&lt;&#47;sub&gt;H&lt;sub&gt;4&lt;&#47;sub&gt;C1&lt;sub&gt;2&lt;&#47;sub&gt; (1.3 mL)">
       <ProcessParameter Name="&lt;b&gt;2&lt;&#47;b&gt;.TotalMass" Value="0.155" Unit="g"/>
       <ProcessParameter Name="&lt;b&gt;2&lt;&#47;b&gt;.TotalVolume" Value="1.3" Unit="mL"/>
       <EquipmentUnit UnitId="2"/>
     </ProcessAction>
     … etc …
   </ProcessOperation>
  </ProcessStage>
 </Process>
 <Unit UnitId
 </Unit>
 <Unit UnitId
 </Unit>
</Experiment
```


16 (0.101 g, 0.132 mmol) and $Cu(OTf)_2$ (0.006 g, 0.01 mmol) were added to a round-bottom flask under a N_2 atmosphere. In a separate vial, **2** (0.155 g, 0.753 mmol) was dissolved in $C_2H_4Cl_2$ (1.3 mL) and transferred to the reaction flask. CF_3CO_2H (0.030 mL, 3 equiv) was added to the reaction mixture, which was refluxed at 100 ° C for 1 h. The reaction mixture was washed with saturated $NaHCO_3$ (15 mL) and extracted with $C_2H_4Cl_2$ (3 x 5 mL). The organic fractions were collected, dried ($MgSO_4$), and filtered to give a dark red solution. The solvent was removed, and the product was purified by column chromatography (SiO_2, 30:70 CH_2Cl_2 : hexane) to yield 17 as a pale yellow powder (0.096 g, 68% yield).

Allotrope Foundation

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- Standards for analytical process in (pharma) industry

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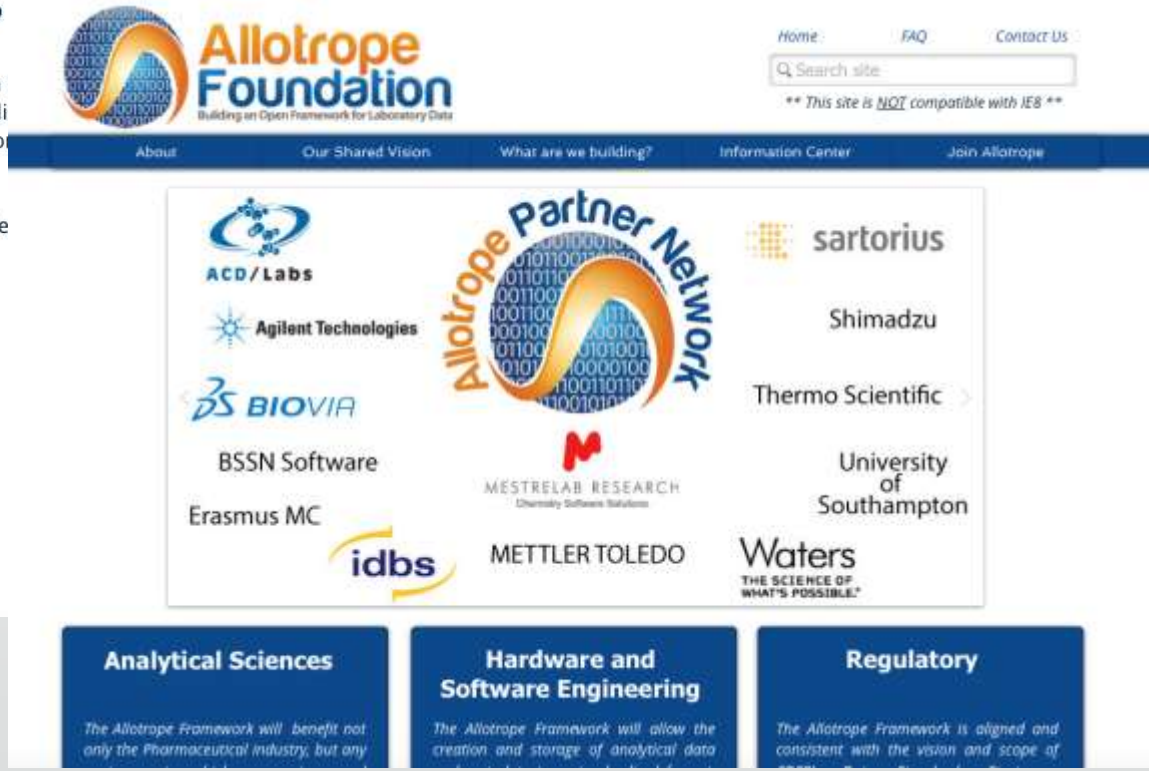
Current Allotrope Foundation members include

- AbbVie
- Amgen
- Baxter
- Bayer
- Biogen
- Boehringer Ingelheim
- Bristol-Myers Squibb
- Eli Lilly
- Genentech/Roche
- GlaxoSmithKline
- Merck & Co.
- Pfizer



Allotrope Foundation

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The tasks and deliverables to achieve the goals of Allotrope Foundation are carried out by Working Groups who work in close collaboration with our Framework Architect. These groups include:

- **Core team** – Coordinates activities within the working groups, ensuring the forward progress of the project.
- **Architecture & Development** – Responsible for defining the architecture, underlying data model, and specifications for the software components of the Allotrope project built by our Framework Architect.
- **Business Model Development** – Develops business strategies and business models for the project both near- and long-term.
- **Communications** – Develops and implements communication strategies to ensure consistent, timely and efficient messaging to all relevant audiences, both internal and external.
- **Membership** – Reaches out to potential new members to support expansion of the project base through increasing Allotrope membership
- **Proof-of-Concept (PoC) Delivery** – Gathers requirements for integrating the Allotrope Framework into a member company's daily business practices.
- **Quality and Compliance** – Ensures that quality, validation, and other regulatory-relevant requirements and best practices are "built-in" at all levels during the development of the Allotrope Framework.
- **Regulatory Affairs** – Interacts with regulatory agencies regarding activities of Allotrope Foundation in order to educate, to provide a means for the Allotrope Foundation to gain a better appreciation of the regulatory perspective and to provide a channel for regulators to offer feedback and influence the development of the Framework
- **Standards (Document Standards, Metadata, and Test Data)** – This group, along with subject matter experts from our Framework Architect evaluates existing data standards, and defines appropriate controlled vocabularies and ontologies to use with the Framework. Provides real and simulated test datasets for use in Framework development, and in close collaboration with our Framework Architect maps the metadata associated with the test data to existing standard definitions.

Allotrope Foundation

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Allotrope Foundation
Building an Open Framework for Laboratory Data

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What are we building?

- Open Document Standards
- Metadata Repositories
- Class Libraries
- Proofs-of-Concept
- What is out of scope?

Metadata Repositories

The Metadata Repository provides a single location for maintaining accurate, pre-approved metadata that applications will use as input to drive scientific and business processes. The controlled vocabulary in the Metadata Repository allows for the standardization of input to software applications, thus ensuring that complete, correct, and consistent metadata enters the system from the very start. This eliminates the need to clean up, reconcile, or rename metadata values after data creation and enables many more possibilities for downstream automation in the analytical laboratory than exist today.

The controlled vocabularies used by the Framework will be defined using Document Standards. The Allotrope public domain vocabulary facilitates interoperable exchange of laboratory data; Vendor vocabularies will allow for application-, technique-, or platform- specific data that are not strictly vendor neutral, and Enterprise vocabularies will provide enterprise specific data.

CREAM:

Collaboration for Research Enhancement using Active Metadata

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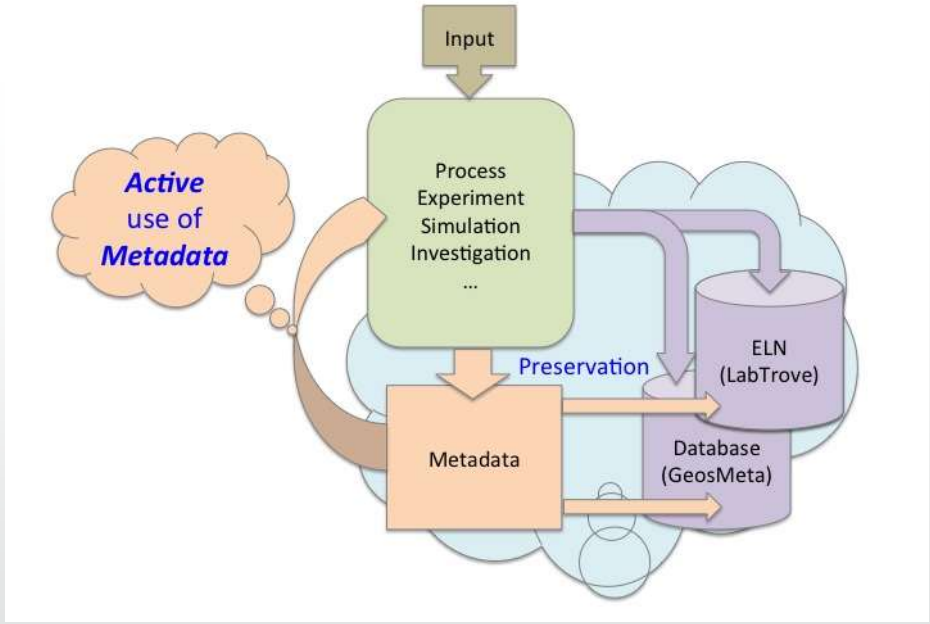
- How to collect and ***use metadata actively*** to capture tacit information
- Active metadata: assemblage of metadata and annotations used actively within the process that generates it (capable of being reused by another process).
- Central Facilities; Chemistry; Geosciences; Art; Music…
- Uptake: CODATA; Research Data Alliance



https://blog.soton.ac.uk/cream/

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Research Data Alliance

- Chemistry data interest group
- Joint RDA/IUPAC Charter drafted
  - Characterise chemical data types
  - Leverage to establish standards
  - Examine workflows in disciplines interacting with chemistry
  - Cultivate a sharing culture
- Inaugral meeting: Paris Sept 23rd September 2015 (hosted by Ian Bruno, Richard Kidd and Dave Martinsen)