

Relating the Research Workflow and the Publication Workflow

Wendy White, Simon Coles
20 June 2014

Blueprint context for innovation & service

- Evidence – cross disciplinary survey of research RDM practice (questionnaire, interviews)
- Governance – roles, decision making, steering developments (DCC AIDA audit tool, policy iteration)
- Resources – business modelling (explore options e.g. Princeton pay once store forever)
- Case studies – (disciplinary and thematic)
- Vision – 10 year roadmap (framework, goal setting)

LabTrove Lab Notebooks

- Live collaborative data environment
- Automatic capture from instruments
- Provides added semantics and templates

Research article

Open Access

Synthesis and solid-state characterisation of 4-substituted methyldene oxindolesGraham J Tizzard^{1*}, Simon J Coles¹, Mark Edwards², Romanus Oforbike Onyeabo², Mark Allen² and John Spencer³* Corresponding author: Graham J Tizzard Graham.Tizzard@soton.ac.uk

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For all author emails, please [log on](#).*Chemistry Central Journal* 2013, **7**:182

doi:10.1186/1752-153X-7-182

The electronic version of this article is the complete one and can be found online at:

<http://journal.chemistrycentral.com/content/7/1/182>

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Published: 20 December 2013

**Aim: enriched approach to publishing
supplementary information****Crystallography context: agreed process and
protocols for presenting data – good platform**<http://journal.chemistrycentral.com/content/7/1/182>

Experimental

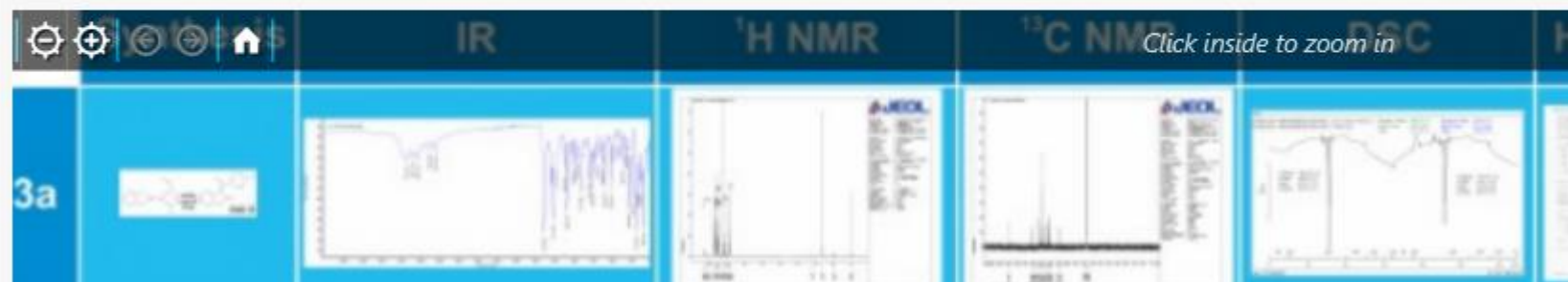
Synthesis

The general reaction scheme outlined below (Scheme 1) was followed, with specific details of the synthesis procedures of all the derivatives of 3 available at http://poc.labtrove.soton.ac.uk/synth_methyl_oxin/group/Condensation%20Products [webcite](#).

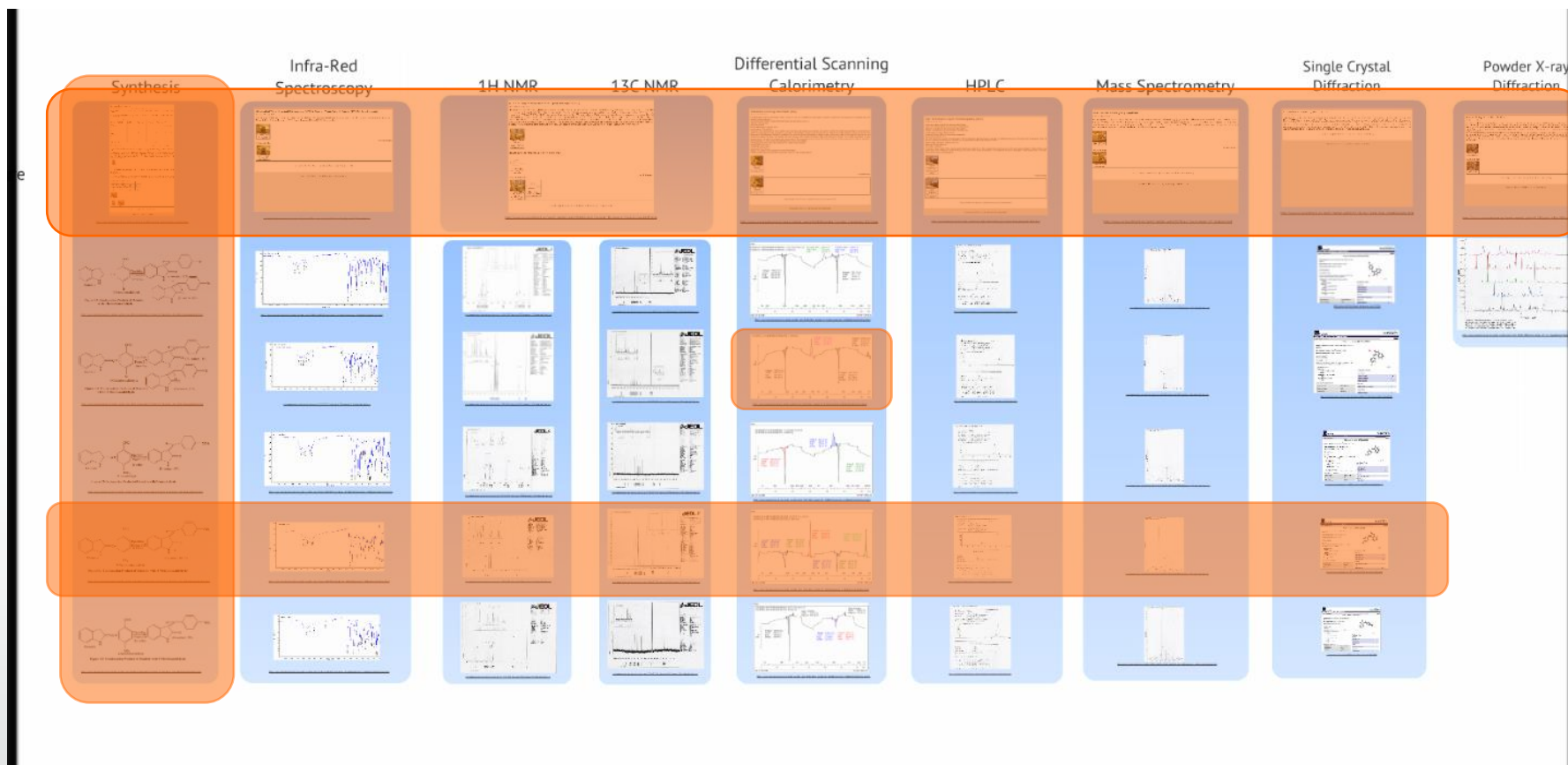
35 cells can replace 35 paras of text – navigable image layer provides bridge between lab notebook and article.

Additional file 1. DeepZoom: 4-methylidene oxindole synthesis and characterization. Microsoft Silverlight plug-in is required to view this. Use + and - buttons or scroll wheel to zoom in and out of image to view individual spectra. Use home button to reset view to full image. Click table cells to follow link to relevant section of electronic lab notebook for full supporting data (spectral assignments etc).

Format: ZIP Size: 37.1MB [Download file](#)



Each compound a cell, full characterization & downloadable spectra



3d: doi:10.5258/poc/lt/r/4 <http://dx.doi.org/10.5258/poc/lt/r/4> [webcite](#) Yellow solid; yield: 1.61g, 6.84mmol, 68%; mp: 187.0°C IR (ν_{\max} , cm^{-1}) 1690 (C=O stretch); ^1H (DMSO- d_6): 2.43 (3H, s), 6.87-6.92 (2H, m), 7.25-7.29 (2H, m), 7.52 (2H, d, J=7.9), 7.60 (2H, d, J=7.9), 7.82 (1H, s), 8.23 (1H, s). ^{13}C (CDCl_3): 21.5, 110.2, 121.7, 121.8, 122.9, 123.9, 129.1, 129.4, 129.5, 129.6, 131.9, 132.2, 137.8, 140.1, 141.5, 170.7; ESIMS (positive mode) (m/z): 236.3 [M+H] $^+$, 471.5 [2M+H] $^+$.

3e: doi:10.5258/poc/lt/r/5 <http://dx.doi.org/10.5258/poc/lt/r/5> [webcite](#) Red solid; yield: 1.80g, 6.76mmol, 68%; mp: 247.0°C (ν_{\max} , cm^{-1}) 1697 (C=O stretch); ^1H (dms o - d_6): 6.81-6.91 (2H, m), 7.21 (1H, pseudo tr, J=7.5), 7.39 (1H, ps tr, J=7.5), 7.68 (1H, s), 7. (2H, d, J= 8.6), 8.34 (2H, d, J=8.6), 10.70 (1H, brs). ^{13}C (dms o - d_6): 110.7, 121.5, 122.9, 123.8, 129.9, 130.9, 132.4, 141.9, 143.3, 147.7, 161.1, 169.1 (some quaternaries missing, poor solubility); ESIMS (positive mode) (m/z): 265.2 [M+H] $^+$.

Full details of characterisation techniques and data for 3a-e are available at

http://poc.labtrove.soton.ac.uk/synth_methyl_oxin/group/Analytical%20Procedures [webcite](#) and http://poc.labtrove.soton.ac.uk/synth_methyl_oxin/group/Spectroscopic%20Data [webcite](#).

Each compound with characterisation and synthesis data linked together as a primary static dataset and assigned a DOI

3a doi:10.5258/ecrystals/1505 <http://dx.doi.org/10.5258/ecrystals/1505> [webcite](#)

3b doi:10.5258/ecrystals/1326 <http://dx.doi.org/10.5258/ecrystals/1326> [webcite](#)

3c doi:10.5258/ecrystals/1327 <http://dx.doi.org/10.5258/ecrystals/1327> [webcite](#)

3d doi:10.5258/ecrystals/1324 <http://dx.doi.org/10.5258/ecrystals/1324> [webcite](#)

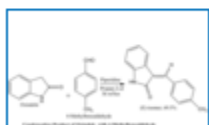
3e doi:10.5258/ecrystals/1325 <http://dx.doi.org/10.5258/ecrystals/1325> [webcite](#)

Table 1. Crystallographic data for 4-substituted methylidene oxindoles

Reports

(3E)-3-(4-Methylbenzylidene)-1,3-dihydro-2H-indol-2-oneGraham Tizzard, Nicola Knight
13th June 2013 | doi:10.5258/poc/lt/r/4

Condensation Product of Oxindole with 4-Methylbenzaldehyde

Substituent: MethylCondensation
Product of Oxindole
with 4-
Methylbenzaldehyde**This Report**

Print view

Availability

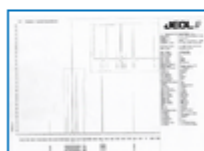
Currently:

Public (Googleable)

Make:

Private (Just For You)

Notebook Users only

¹³C NMR Spectrum of (3E)-3-(4-Methylbenzylidene)-1,3-dihydro-2H-indol-2-one**Spectroscopic Method:** C-NMR**Substituent:** Methyl¹³C NMR Spectrum of (3E)-3-(4-Methylbenzylidene)-1,3-dihydro-2H-indol-2-one**DOI View**Snapshot report in
LabTrove
Title, attribution,
timestamp¹³C NMR Spectrum
of (3E)-3-(4-
Methylbenzylidene)-
dihydro-2H-indol-
2-one¹³C NMR Spectrum
of (3E)-3-(4-
Methylbenzylidene)-
dihydro-2H-indol-
2-one PDF¹³C NMR Spectrum
of (3E)-3-(4-
Methylbenzylidene)-
dihydro-2H-indol-
2-one ascii data¹³C NMR Spectrum
of (3E)-3-(4-
Methylbenzylidene)-
dihydro-2H-indol-
2-one Jeol Delta
data¹³C NMR Spectrum
of (3E)-3-(4-
Methylbenzylidene)-
dihydro-2H-indol-
2-one JCAMP-DX
data

Synthesis of 4-substituted methyldene oxindoles

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

Attenuated Total Internal Reflectance (ATIR) Fourier Transform Infrared (FT-IR) Spectroscopy

8th March 2012 @ 14:00

The presence of elements in each of these five methyldene oxindoles synthesized was analyzed qualitatively by using a Perkin-Elmer Paragon 1000 Attenuated Total Internal Reflectance (ATIR) Fourier Transform Infrared (FT-IR) Spectrometer.



Varian Excalibur
(ATIR FT-IR)
Spectrometer

Attached Files

LabTrove View

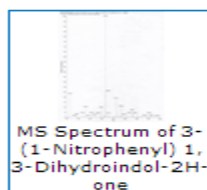
MS Spectrum of (3E)-3-(4-Nitrobenzylidene)-1,3-dihydro-2H-indol-2-one

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:



MS Spectrum of 3-(1-Nitrophenyl)-1,3-Dihydroindol-2H-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

Further developments

- Microsoft Silverlight Deep Zoom proprietary, but proof of concept and raw data files underpin visualisation
- Layering of files for visualisation for this article 2 days of time, look to reduce this
- Negotiation with reviewers on balance between new presentation and traditional layout – this is a compromise
- Aim for audio-visual one stop shop to non-linear data access
- RSC developer embedded in Soton group, looking at recommended file exchange formats and ELNs at scale in the cloud

ePrints Soton data repository

- Supports all data with no appropriate disciplinary repository
- Uses ReCollect plug-in developed by Essex
- Integrated as tab option next to publication deposit – one-stop-shop

Preparing and depositing data – journal

3. Results and discussion

The isotherm maps presented in this paper provide a striking visual depiction of summer air temperature development over the landmass of northwest Europe during the Lateglacial–early Holocene transition. In this discussion we will first highlight the major gradients and trends apparent in the C-IT data and discuss the likely mechanisms driving these temperature developments. Second, we will contrast and compare the C-IT against the B-MCR data and discuss likely reasons for any major differences between these data. Third, we will consider the reliability of the data we present and discuss the reasons for any major shortfalls. Finally, we will use the maps to identify gaps in the geographical and temporal coverage of our data in order to prioritise the locations for new summer temperature records. The data and maps shown in Figs. 3 and 4 can be downloaded from the University of Southampton eprints: <http://dx.doi.org/10.5258/SOTON/361991> (Langdon et al., 2014).



Quaternary International

Available online 5 March 2014

In Press, Corrected Proof — Note to users




Summer temperature gradients in northwest Europe during the Lateglacial to early Holocene transition (15–8 ka BP) inferred from chironomid assemblages

Stephen J. Brooks^a,  , Peter G. Langdon^b

Show more

<http://dx.doi.org/10.1016/j.quaint.2014.01.034> 

 Get rights and content

Langdon, Peter, Riddy, Liam and Brooks, Steve (2014) Summer temperature gradients in northwest Europe during the Lateglacial to early Holocene transition (15-8 ka BP) inferred from chironomid assemblages.
[doi:10.5258/SOTON/361991](https://doi.org/10.5258/SOTON/361991) [dataset]

Download



Archive (ZIP) (Lateglacial (pre 14700 years BP to 11700 years BP) summer temperature data inferred from chironomids for NW Europe) - Data
 Available under License [Creative Commons Attribution](#).
[Download \(2391Kb\)](#)



Archive (ZIP) (Holocene (11000 years BP to 8000 years BP) summer temperature data inferred from chironomids for NW Europe) - Data
 Available under License [Creative Commons Attribution](#).
[Download \(4Mb\)](#)



Other (GIS layer file) - Data
 Available under License [Creative Commons Attribution](#).
[Download \(14Kb\)](#)



PDF (Instructions. Read before uploading and accessing the datasets) - Documentation
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Archive (ZIP) (Holocene) - Additional metadata
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Archive (ZIP) (Lateglacial) - Additional metadata
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[Download \(59Kb\)](#)

Description/Abstract

The raster temperature data was interpolated from site temperature data estimated from Chironomid records using Kriging. Temperatures are in Degrees Centigrade. The dataset covers all of Northern Europe including Iceland and Scandanavia.

Further developments

- Draft institutional DOI policy endorsed, will work with BL, UKDA and others on issues before final approval e.g. use of DataCite DOIs for theses, granularity of files and standard presentation of suffixes
- Consultations with depositors - learning a lot, but will need to adapt to scale
- Raising awareness of service as part of publication offer and importance of considering some issues at early stage of workflow e.g. ethics approval

3D imaging - Computed Tomography

- Multidisciplinary – Engineering, Bio-Sci, Archaeology, Environmental Sci
- multiscale, high volume, TBs
- Keen to look at data availability as part of workflow and set up system

Developments

- Would like DOIs to bolster attribution and citation
- Working on pilot to support data files on request, with ePrints Soton landing page
- On request linked to size so will also look at range of options for file delivery
- Hard to snapshot data for publications, desire to make large raw data files available for transparency
- Query with Royal Society about data availability policy

Portus MOOC – Archaeology

- Opportunities to make data available to support MOOC
- Can look at teaching and impact aspects, not just about research workflow

Franco, Pina (2012) *African amphorae from Portus. University of Southampton, School of Humanities, Doctoral Thesis , 864pp.*

WEEK 3

TOPIC	CHAPTER/PAGES	STEP
Roman Empire in the later second century		3.2
Emperor Septimius Severus and policies of the Severan emperors.	Chapter 1, pp5–6 (Direct link to page 5)	
Olive oil traded to Portus. On the importance of the link between Portus, Leptis Magna and Septimius Severus, and between Portus and other identified commercial North	Chapter 8, pp 308–354 (Chapter 8 is very important)(Direct link to page 308)	

7.4). Tripolitania in particular supplied Portus-Rome with wine, carried in the Mau 35, fish sauce, transported in the Tripolitana 2, and olive oil in Tripolitana 1 and 1/3. All Mau 35 occur in Tripoli fabric, with the exception of two vessels, which may have originated from Djerba. Wine may have also been imported from Djerba, where kiln sites of Dressel 2-4 were uncovered (Fentress 2001).

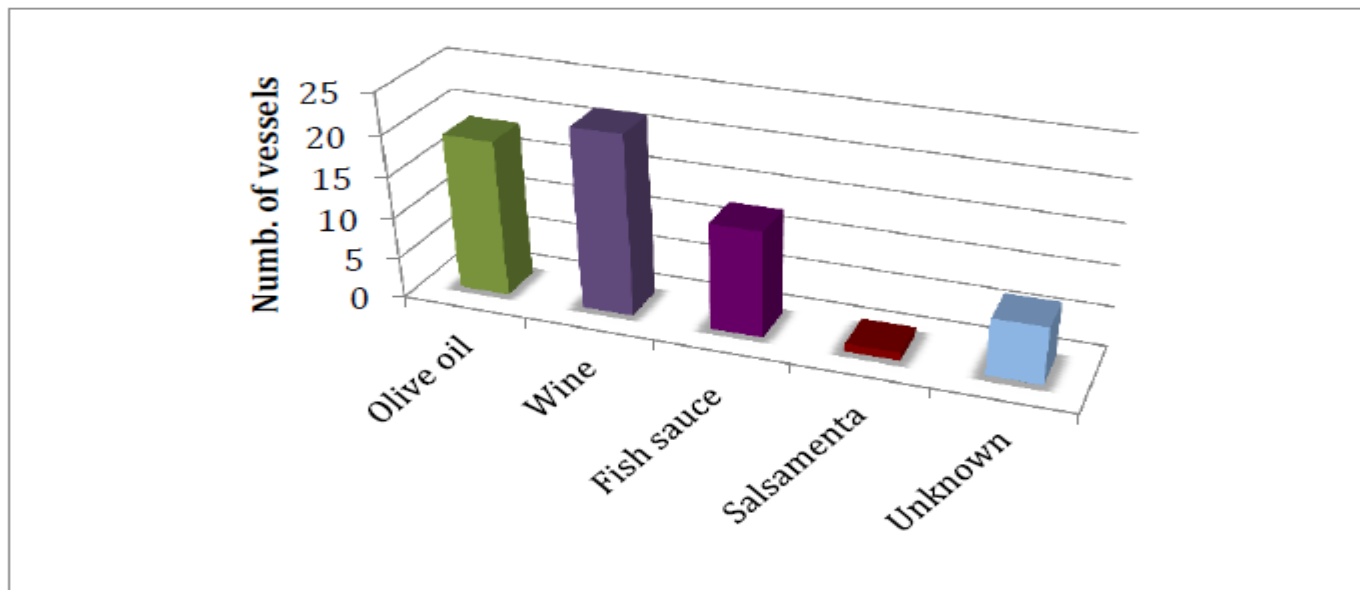


Fig. 7.4 Share of African produce at Portus in the Early-Imperial period

Developments

- Incentive of download and analytics stats to show engagement – crude but important to demonstrate usage
- Taking data from text of thesis and providing raw and rich data files
- Have piloted data availability as part of upgrade process for PhD – then part of workflow and progress review
- Optional data deposit now formal part of PhD deposit process, general support to make this mandatory after initial period

E-thesis deposit form

I understand that the metadata including the abstract of the thesis deposited in ePrints Soton will be available immediately. According to my wishes below, the full text of the thesis and accompanying research data (where applicable) will be made available immediately after any stated embargo period and will be accessible to a wide variety of people and institutions - including automated agents - via the World Wide Web. I also agree and understand that any accompanying research data I deposit will be used by the University as set out in its Research Data Management Policy.

[Link between process and RDM policy](#)

Encourages embedding link to data in the text of the thesis,
metadata records will also be linked

3. Research Data


You may deposit research data associated with and/or underpinning assertions within a thesis as a separate deposit in ePrints Soton where this may facilitate a fuller description than might be permitted within the thesis record¹.

Your data should be deposited in agreement with your supervisor. Timing of the deposit and its release should also be agreed.

You will be able to incorporate links in your thesis to the underlying data, where appropriate, by creating a data record in advance. Adding data to your work area in ePrints Soton will create the record and necessary URI for inclusion in your thesis. Data held in your work area are not publically available. At the appropriate time the data and/or data record can be made public as previously agreed with your supervisor.

Prior to deposit it is essential to consider whether there are any reasons that might require that access to your data is restricted in the short or longer-term. Reasons

Visualisation of the flow and force distribution around a self propelled container ship in head waves

 Share

Windén, Björn (2014) Visualisation of the flow and force distribution around a self propelled container ship in head waves. [doi:10.5258/SOTON/365546](https://doi.org/10.5258/SOTON/365546) [dataset]

Download



Archive (ZIP) (.zip archive containing all animations as well as an explanatory report) - Data
[Download \(50Mb\)](#)

Description/Abstract

This data set contains animations showing the development of quantities relating to powering performance over one period of encounter in head waves Korean Container Ship (KCS.)

The data set consists of:

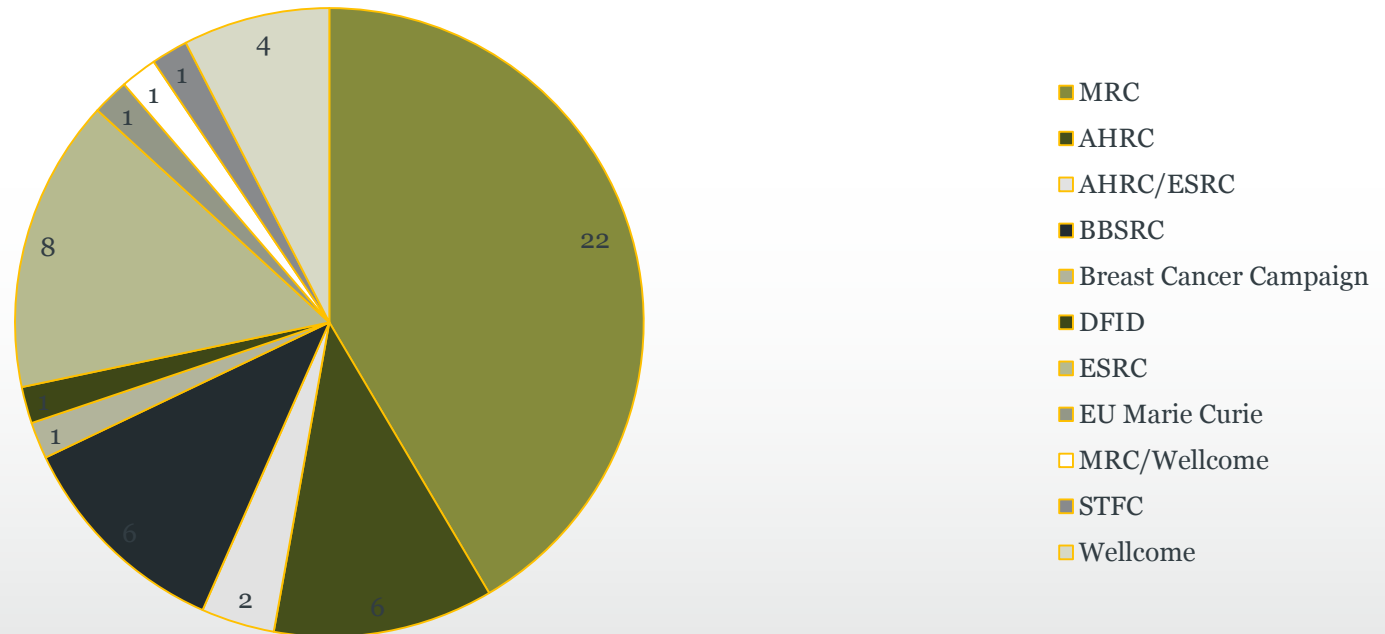
- *Animation of the unsteady wave pattern around the hull
- *Animations of pressure and viscous force distributions on the underwater body. Both the total and the surge components are shown
- *Animations of axial velocity in and around the propeller plane
- *Animations of transverse velocity in and around the propeller plane

A report is also attached which explains the colour scales and the quantities shown in the animations.

Developing culture of publication as integral part of workflow

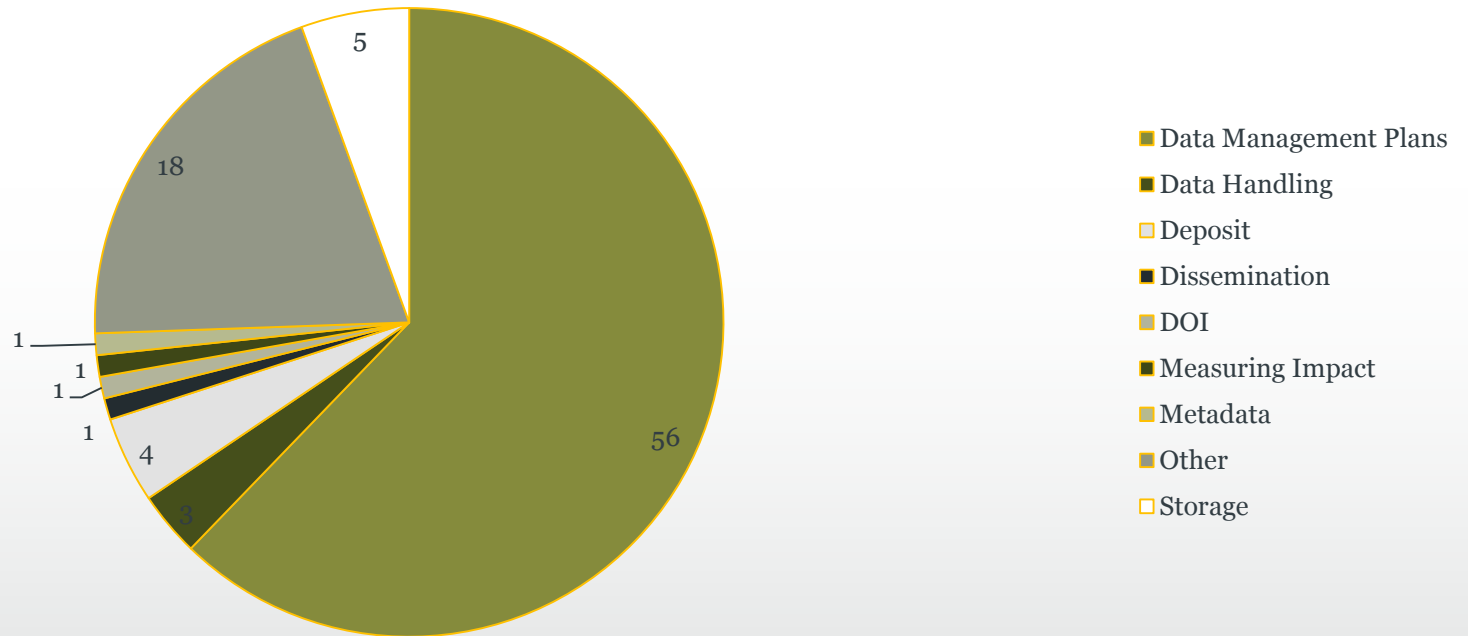
Data Management Planning

Number of Data Management Plans by Funder



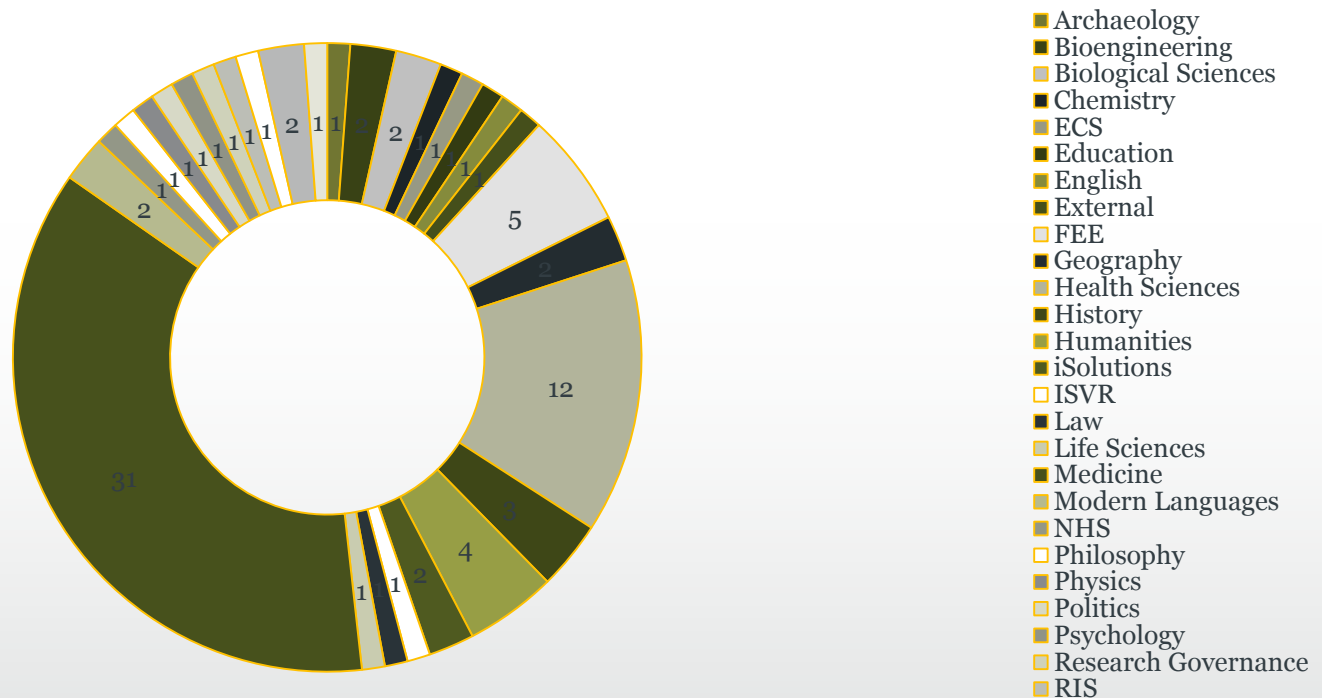
DMP only part of service

Number of Data Enquiries



Wide discipline spread for data enquiries

Total Enquiries by Discipline



Training

- On demand group sessions on preparing DMPs by Faculty/disciplinary centre
- Embedded PGR training as part of Researcher Development Graduate Centre programme “RDM 101” – first principles and case study exemplar
- Co Library and PGR/ECR led
- RDGC just funded 2 year continuation for PGR input and production of some supporting podcasts to supplement case study guide

Expanding case study approach – looks at workflows

Introducing Research Data



Aimed at those about to start some research work, this useful guide is an introduction to the various forms that research data can take; provides examples from a number of disciplines; sections on the importance of looking after data and some helpful tips on best practice.



<http://library.soton.ac.uk/researchdata>

Next steps

Partnership approach to engagement

- Learn by engaging with workflows - 2 EPSRC IT as a Utility funded embedding of academic liaison librarians in research groups, Chemistry and National Centre for Research Methods
- Work with National Agreements, National Centres and shared services opportunities to support curation and storage and seamless signposting
- Balancing institutional requirements and research practice e.g. researchers can't sign away rights to data owned by the University

Shared Service Engagement

