

Electronics and
Computer Science



JISC

Archiving research data and research publications.

Dr Leslie Carr, Intelligence, Agents Multimedia, University of Southampton

Dr Simon Coles, School of Chemistry, University of Southampton

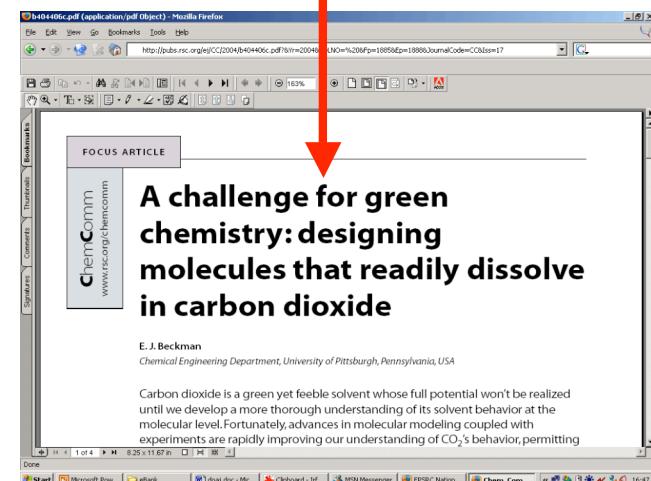
Dr Liz Lyon, UKOLN, University of Bath

Overview

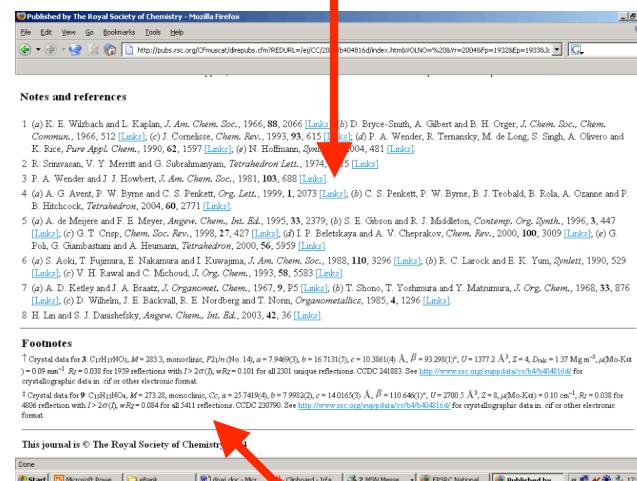
- In an Open Access environment
 - scientific outputs are openly available
 - described by appropriate metadata
 - in Institutional Repositories
 - harvestable by OAI protocols
- Scientists can use the same infrastructure
 - (here eprints.org software and an existing scientific portal service)
 - to provide maximal open access
 - to all their data, as well as their published articles
 - raw data, intermediate calculations, final results
 - in a searchable, accessible form
- BUT this is subject to ongoing investigation.

Current chemistry publishing protocols

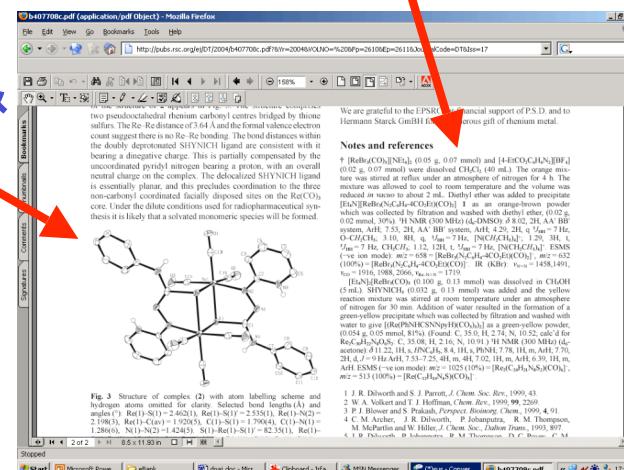
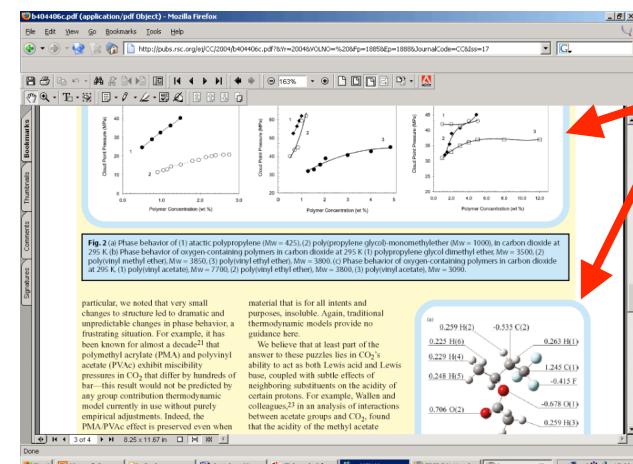
Ideas and interpretations

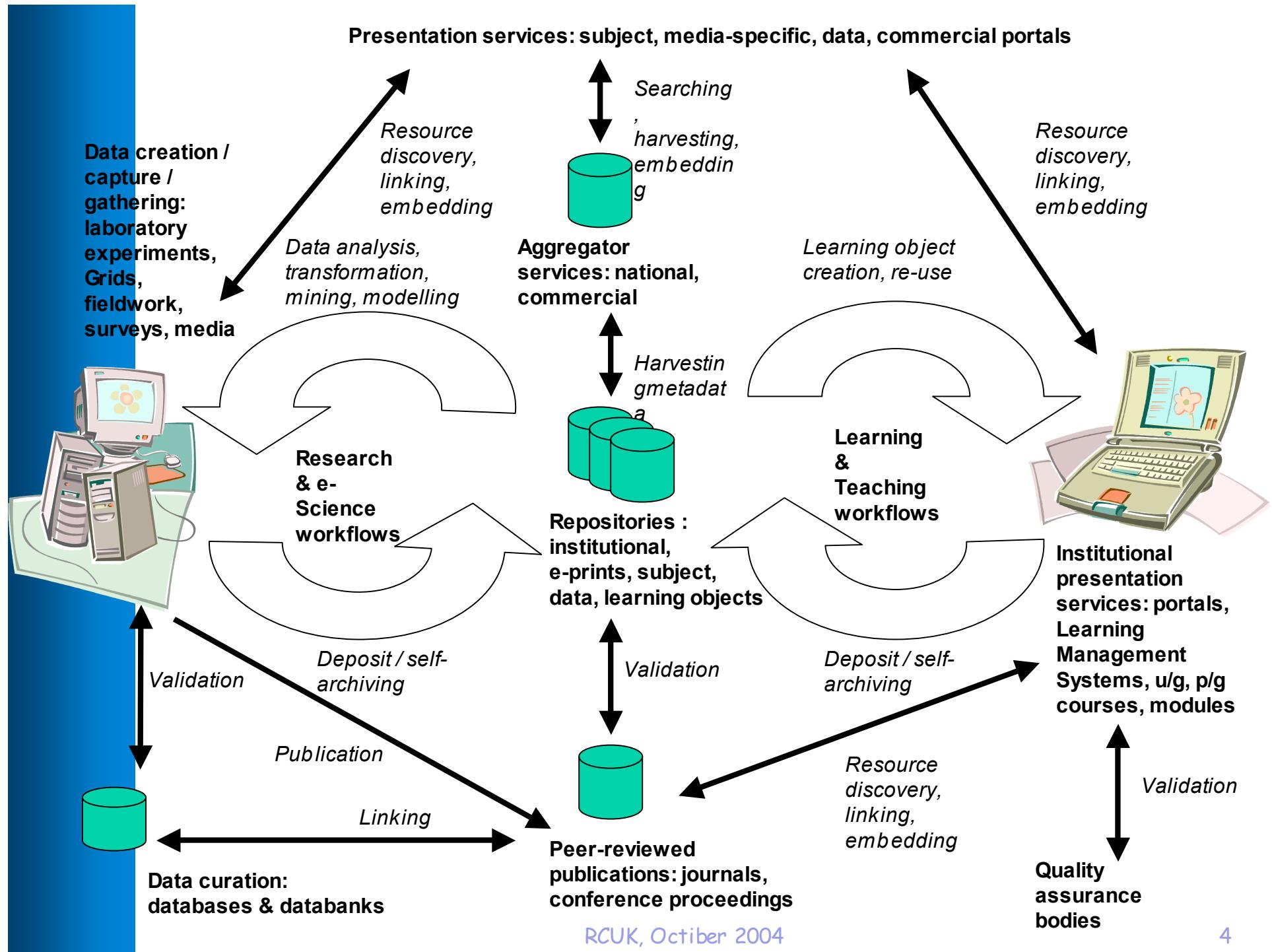


Hooks into the literature

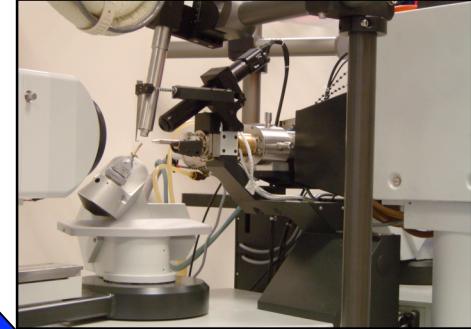
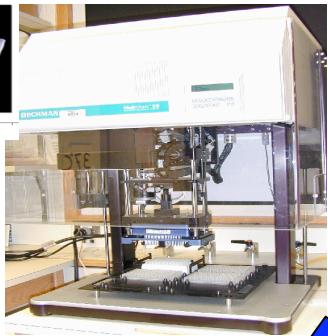


Results & derived data





The data deluge



Data
Overload!

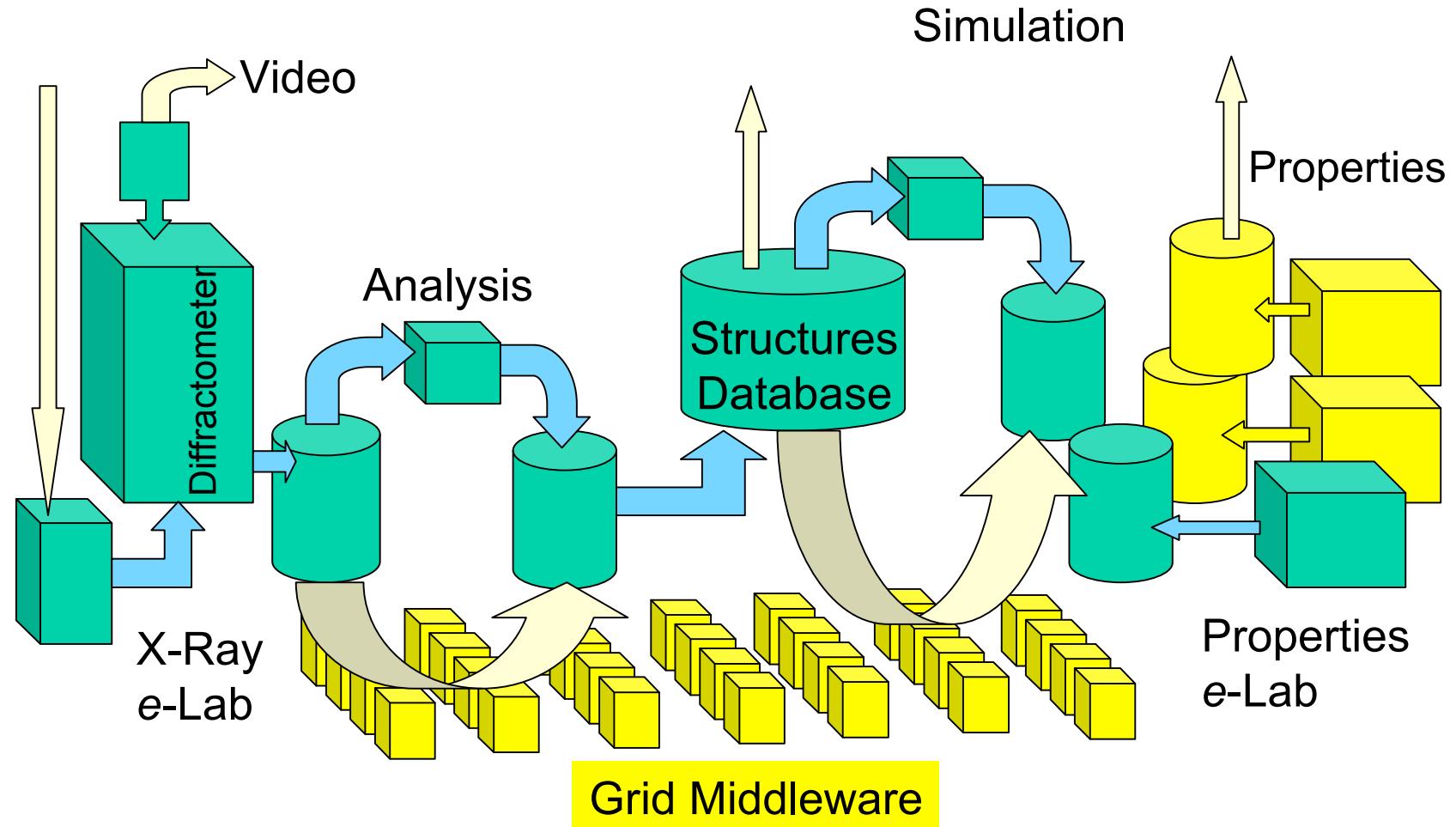


EPSRC National
Crystallography
Service

How do we
disseminate?

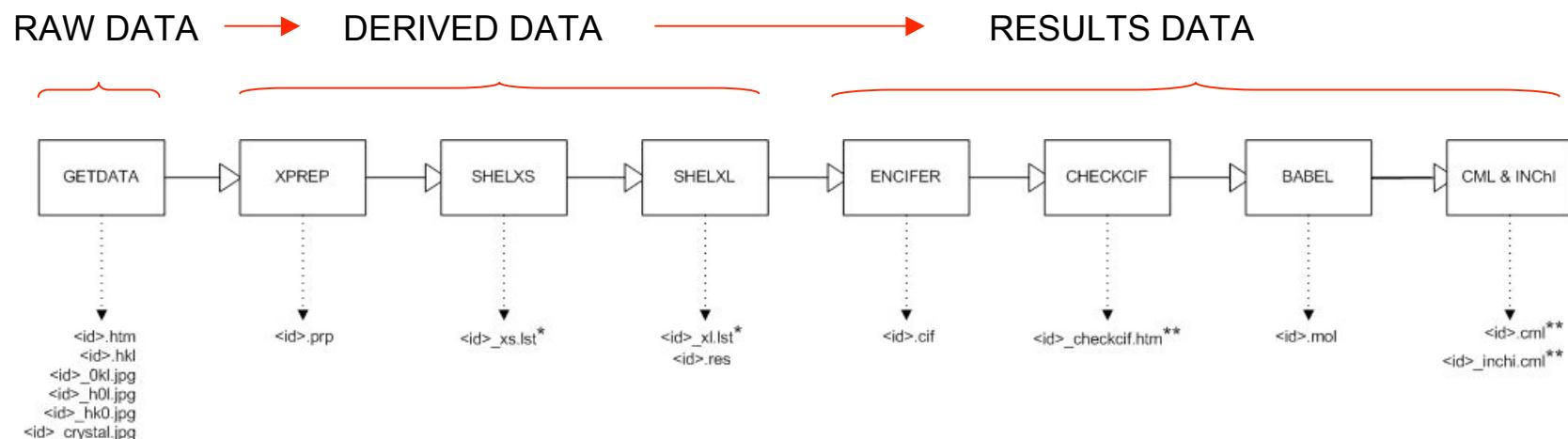


CombeChem: An EPSRC pilot project

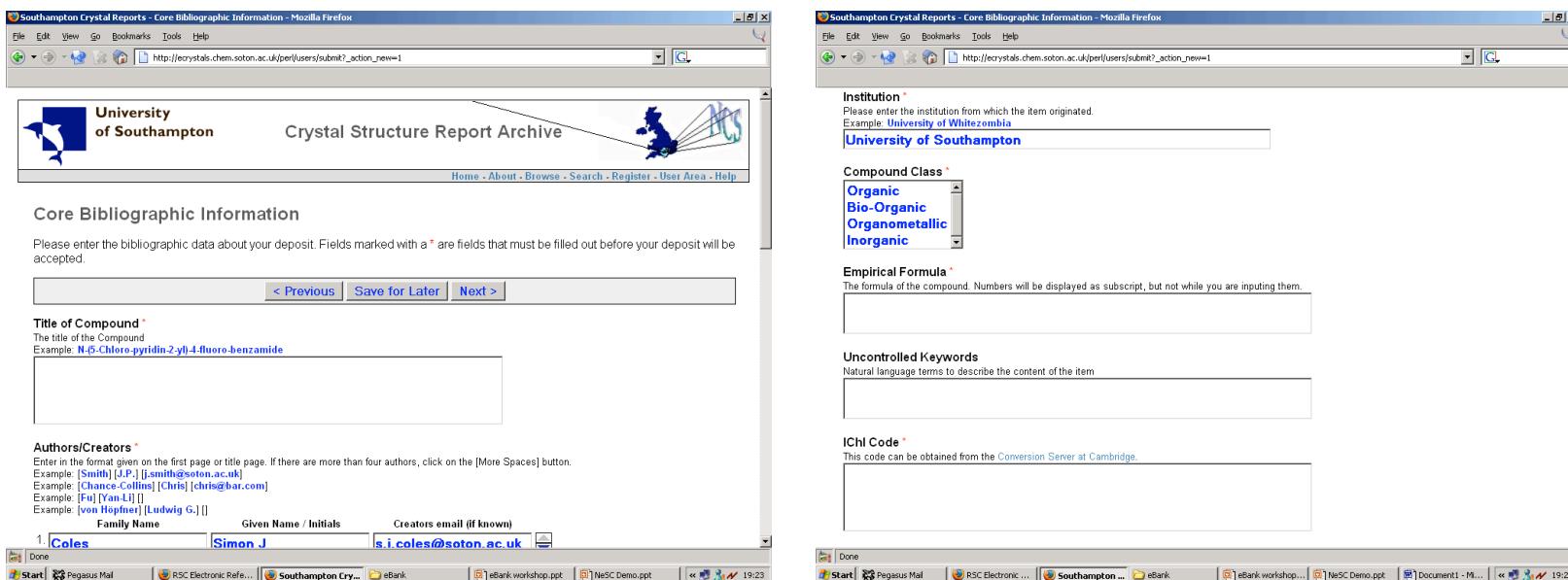


Crystallography workflow

- **Initialisation:** mount new sample on diffractometer & set up data collection
- **Collection:** collect data
- **Processing:** process and correct images
- **Solution:** solve structures
- **Refinement:** refine structure
- **CIF:** produce CIF (Crystallographic Information File format)
- **Report:** generate Crystal Structure Report



Deposition into the archive



Southampton Crystal Reports - Core Bibliographic Information - Mozilla Firefox

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http://ecrystals.chem.soton.ac.uk/perl/users/submit?_action_new=1

University of Southampton Crystal Structure Report Archive

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Core Bibliographic Information

Please enter the bibliographic data about your deposit. Fields marked with a * are fields that must be filled out before your deposit will be accepted.

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Title of Compound *

The title of the Compound
Example: [N-\(5-Chloro-pyridin-2-yl\)-4-fluoro-benzamide](#)

Authors/Creators *

Enter in the format given on the first page or title page. If there are more than four authors, click on the [More Spaces] button.
Example: [Smith] [J.P.] [j.smith@soton.ac.uk]
Example: [Chance-Collins] [Chris] [chris@bar.com]
Example: [Fu] [Yan-Li] []
Example: [von Hophner] [Ludwig G.] []

Family Name Given Name / Initials Creators email (if known)

1 Coles Simon J s.i.coles@soton.ac.uk

Done Start Pegasus Mail RSC Electronic Refe... Southampton Cry... eBank eBank workshop.ppt NeSC Demo.ppt 19:23

Southampton Crystal Reports - Core Bibliographic Information - Mozilla Firefox

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http://ecrystals.chem.soton.ac.uk/perl/users/submit?_action_new=1

Institution *

Please enter the institution from which the item originated.
Example: [University of Whitezombia](#)

University of Southampton

Compound Class *

Organic Bio-Organic Organometallic Inorganic

Empirical Formula *

The formula of the compound. Numbers will be displayed as subscript, but not while you are inputting them.

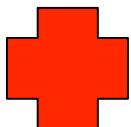
Uncontrolled Keywords

Natural language terms to describe the content of the item

ICCh Code *

This code can be obtained from the [Conversion Server at Cambridge](#).

Done Start Pegasus Mail RSC Electronic ... Southampton ... eBank eBank workshop... NeSC Demo.ppt Document1 - M... 19:23



id.zip

An Archive entry

EBank Southampton - 2-(N-Ferrocenylmethylcarbamoyl)-5-(methoxycarbonyl)-3,4-diphenylpyrrole - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://eprints.ebank.ecs.soton.ac.uk/archive/00000025/

University of Southampton Crystal Structure Report Archive

Home - About - Browse - Search - Register - User Area - Help

2-(N-Ferrocenylmethylcarbamoyl)-5-(methoxycarbonyl)-3,4-diphenylpyrrole

Susanne L. Huth, Michael B. Hursthouse, Simon J. Coles, Mark E. Light, Peter N. Horton, Phil A. Gale, G. Denuault and C. N. Warriner.

University of Southampton

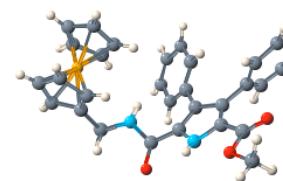
C₃₀H₂₆FeN₂O₃

CCDC Code: XUZSUG
ICChI Code: C30H26FeN2O3,1H3-36-20(35)18-16(14-10H-6H-3H-7H-11H-14)15(13-8H-4H-2H-5H-9H-13)17(33H-18)19(34)32H-12H-30-28H-26H-27H-29H(30)31(26,27,28,30)21H-22H(31)24H(31)25H(31)23H(21)31
Compound Class: Organometallic
Keywords: Supramolecular Chemistry
Creation Date: 31 May 2002
Deposited By: Susanne L. Huth
Deposited On: 10 May 2004

Applet jmol started

Start Pegasus Mail WinGX v1.6... ISSC-XIII - M... EBank Sout... Windows Mes... eBank ISSC a... ECM22EPrint..

ecrystals.chem.soton.ac.uk



Data collection parameters

Chemical formula	C ₃₀ H ₂₆ FeN ₂ O ₃
Crystallisation Solvent	
Crystal morphology	
Crystal system	Orthorhombic
Space group symbol	Pbca
Cell length a	6.0816(4)
Cell length b	24.8503(16)
Cell length c	31.120(3)
Cell angle alpha	90.00
Cell angle beta	90.00
Cell angle gamma	90.00
Data collection temperature	120(2)

Refinement results

Solution figure of merit	
R Factor (Obs)	0.0573
R Factor (All)	0.1185
Weighted R Factor (Obs)	0.1046
Weighted R Factor (All)	0.1243

Available Files

Final Result

02sot064.CIF	19k
02sot064.cml	8k
02sot064_checkcif.html	14k

Refinement

02sot064.RES	9k
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Solution

02sot064.PRP	5k
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Processing

02SOT064.HTM	6k
02sot064.HKL	338k

Other Files

02sot064.DOC	113k
02sot064.LST	49k

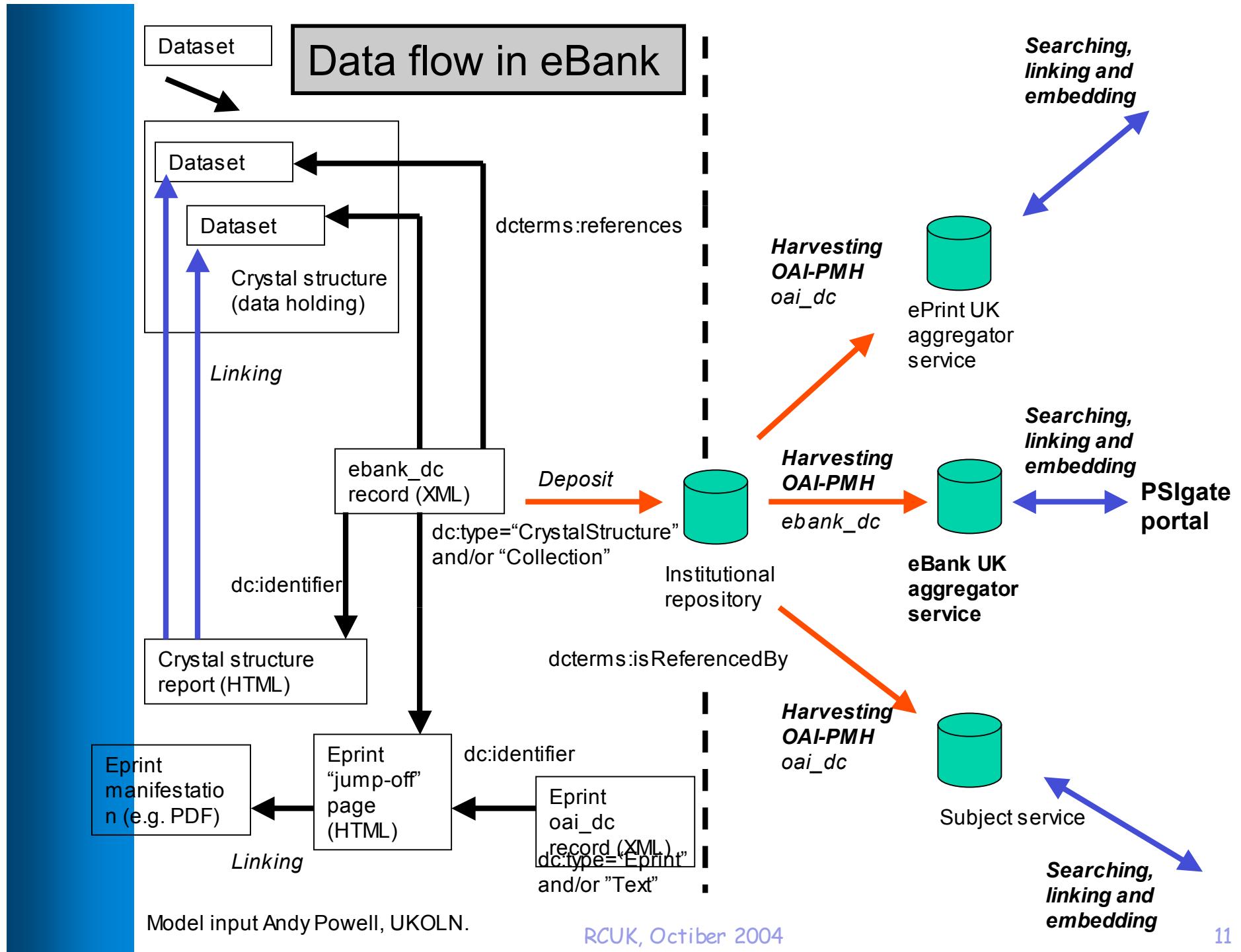
All the way back to the underlying data...

The figure displays the ESRF Data Processing Pipeline interface. The main window is titled 'Available Files' and shows a hierarchical list of files:

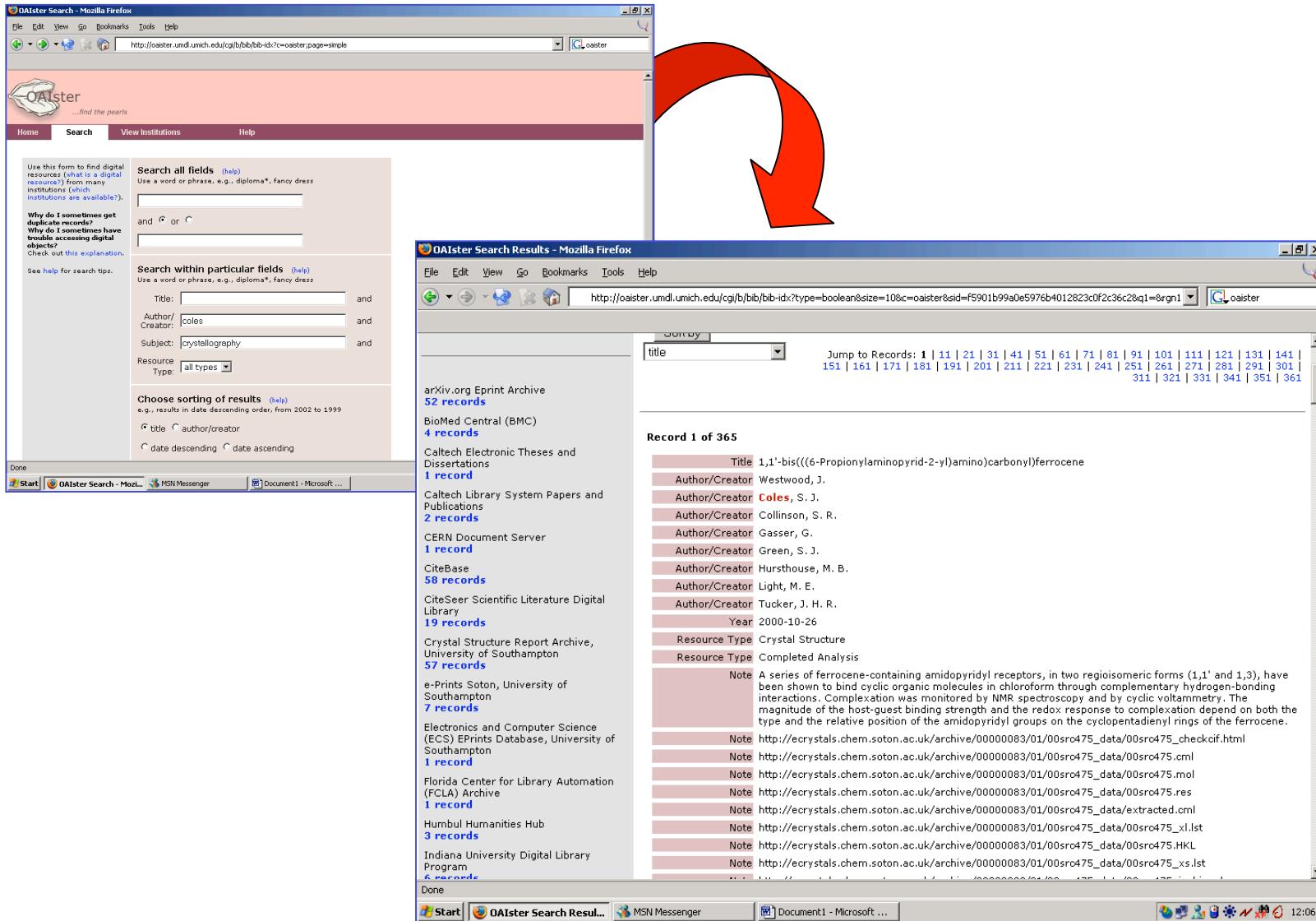
- Final Result**:
 - 02sot064.CIF (19k)
 - 02sot064.cml (8k)
 - 02sot064_checkcif.html (14k)
- Refinement**:
 - 02sot064.RES (9k)
- Solution**:
 - 02sot064.PRP (5k)
- Processing**:
 - 02SOT064.HTM (6k)
 - 02sot064.HKL (338k)
- Other Files**:
 - 02sot064.DOC (113k)
 - 02sot064.LST (49k)

Red arrows point from the 'Final Result' and 'Refinement' sections to a separate window titled 'checkCIF/PLATON report (full structural check)'. This window shows the CIF file content and a detailed report of the structural check results.

Below the main window, a separate window shows a 2D intensity image of the diffraction pattern.



Harvesting: OAster



The image shows two side-by-side screenshots of the OAster search interface. The left screenshot is the search interface, and the right is the results page. A large red arrow points from the search interface to the results page, indicating the flow of the harvesting process.

Search Interface (Left):

- Header: OAster Search - Mozilla Firefox
- Address bar: <http://oaster.umdl.umich.edu/cgi/b/bib-bib-id?c=oaster;page=simple>
- Logo: OAster
- Navigation: Home, Search, View Institutions, Help
- Search Form:
 - Search all fields (help): Use a word or phrase, e.g., diploma*, fancy dress
 - Search fields: and, or, and, or, and
 - Search within particular fields (help): Use a word or phrase, e.g., diploma*, fancy dress
 - Search fields: Title: [] and, Author/Creator: [Coles] and, Subject: [crystallography] and, Resource Type: [all types]
 - Choose sorting of results (help): e.g., results in date descending order, from 2002 to 1999
 - title
 - author/creator
 - date descending
 - date ascending
- Footer: Done, Start, OAster Search - Mozilla Firefox, MSN Messenger, Document1 - Microsoft ...

Results Page (Right):

- Header: OAster Search Results - Mozilla Firefox
- Address bar: <http://oaster.umdl.umich.edu/cgi/b/bib-bib-id?type=boolean&size=10&c=oaster&sid=f5901b99a0e5976b40128230f2c36c2&q1=8&gn1>
- Summary: title
- Jump to Records: 1 | 11 | 21 | 31 | 41 | 51 | 61 | 71 | 81 | 91 | 101 | 111 | 121 | 131 | 141 | 151 | 161 | 171 | 181 | 191 | 201 | 211 | 221 | 231 | 241 | 251 | 261 | 271 | 281 | 291 | 301 | 311 | 321 | 331 | 341 | 351 | 361
- Record 1 of 365:
 - Title: 1,1'-bis(((6-Propionylaminopyrid-2-yl)amino)carbonyl)ferrocene
 - Author/Creator: Westwood, J.
 - Author/Creator: Coles, S. J.
 - Author/Creator: Collinson, S. R.
 - Author/Creator: Gasser, G.
 - Author/Creator: Green, S. J.
 - Author/Creator: Hursthorne, M. B.
 - Author/Creator: Light, M. E.
 - Author/Creator: Tucker, J. H. R.
 - Year: 2000-10-26
 - Resource Type: Crystal Structure
 - Resource Type: Completed Analysis
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/00sro475_checkcif.html
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/00sro475.cml
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/00sro475.mol
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/00sro475.res
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/extracted.cml
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/00sro475_xl.lst
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/00sro475_HKL
 - Note: http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sro475_data/00sro475_xs.lst
- Footer: Start, OAster Search Result..., MSN Messenger, Document1 - Microsoft ...

Linking and aggregating: Search & discover

eBank UK Demo

This is a prototype interface for the [eBank UK](#) JISC-funded project. It demonstrates an OAI-PMH aggregator service which cross searches a small sample of metadata records describing crystallography experiments (provided by the National Crystallography Service at the University of Southampton), and a small number of metadata records describing articles from the Crystallography literature (made available for use in this demo only by IUCr.) Links to the crystallography data sets and to the articles online at the IUCr website are available in the search results.

Search for entries matching all the following:

Author =

CCDC Code =

IUPAC name =

Empirical Formula =

Compound Class =

General keywords =

Date released =

OR published in the last

Search within: Data Reports Publications e.g. journal articles

eBank UK Demo

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Empirical Formula =

Compound Class =

General keywords =

Date released =

OR published in the last

Search within: Data Reports Publications e.g. journal articles

Linking and aggregating: Hit browsing

The image displays two side-by-side screenshots of the eBank UK Demo interface, illustrating the linking and aggregating of search results for crystal structure data reports and publications.

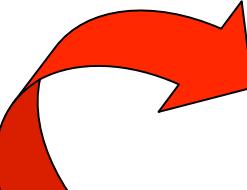
Left Screenshot (Top): This screenshot shows a search result for a crystal structure report. The title is "Crystal Structure Report of 5alpha-cholestane". The report is authored by Coles, Simon J., Hursthouse, Michael B., and Frampton, C. S. It was released on 23/05/2004. The empirical formula is C27H48. The IUPAC name is 5alpha-cholestane. The CCDC code is ZZKG101. The compound class is Organic. A related article is linked to the report. The report is available as a CIF file, processing Dataset, refinement Dataset, and solution Dataset.

Left Screenshot (Bottom): This screenshot shows a search result for a publication. The title is "Crystal Structure Report of 2-(N-Ferrocenylmethylcarbamoyl)-5-(N-phenylcarbamoyl)-3,4-diphenyl pyrrole". The report is authored by Hursthouse, Michael B., Light, Mark E., Coles, Simon J., Horton, Peter N., Gale, Phil A., Denault, G., and Warner, C. N. It was released on 23/05/2004. The empirical formula is C35H29FN3O2. The IUPAC name is 2-(N-Ferrocenylmethylcarbamoyl)-5-(N-phenylcarbamoyl)-3,4-diphenyl pyrrole. The CCDC code is XUZSU. The compound class is Organic. General keywords are Supramolecular Chemistry. A related article is linked to the report. The report is available as a CIF file, processing Dataset, refinement Dataset, and solution Dataset.

Right Screenshot (Top): This screenshot shows a search result for a publication. The title is "5alpha-Cholestane". The report is authored by Coles, S. J., Hursthouse, M. B., and Frampton, C. S. It was released on 23/05/2004. The empirical formula is C27H48. The IUPAC name is 5alpha-cholestane. The CCDC code is ZZKG101. The compound class is Organic. A related dataset is linked to the publication. The publication is available as a CIF file, processing Dataset, refinement Dataset, and solution Dataset.

Right Screenshot (Bottom): This screenshot shows a search result for a publication. The title is "Crystal Structure Report of 2-(N-Ferrocenylcarbamoyl)-5-(methoxycarbonyl)-3,4-diphenylpyrrole". The report is authored by Hursthouse, Michael B., Coles, Simon J., Light, Mark E., Horton, Peter N., Gale, Phil A., Denault, G., and Warner, C. N. It was released on 23/05/2004. The empirical formula is C29H24FeN2O3. The IUPAC name is 2-(N-Ferrocenylcarbamoyl)-5-(methoxycarbonyl)-3,4-diphenylpyrrole. The CCDC code is XUZSOA. The compound class is Organometallic. General keywords are Supramolecular Chemistry. A related article is linked to the report. The report is available as a CIF file, processing Dataset, refinement Dataset, and solution Dataset.

And finally... eBank embedded in a science portal



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Your search returned 28 data reports and 4 publications. Viewing 1 to 10

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Crystal Structure Data Reports

[Crystal Structure Report of 2-\(N-Ferrocenylmethylcarbamoyl\)-5-\(N-phenylcarbamoyl\)-3,4-diphenyl pyrrole](#)

Creator(s): Hursthouse, Michael B., Light, Mark E., Coles, Simon J., Horton, Peter N., Gale, Phil A., Denuault, G., Warriner, C. N.

Date released: 23/05/2004

Empirical Formula: C35H29FeN3O2

IUPAC name: 2-(N-Ferrocenylmethylcarbamoyl)-5-(N-phenylcarbamoyl)-3,4-diphenyl pyrrole

Compound Class: Organic

General keywords: Supramolecular Chemistry

Related article: [?A URL citation?](#)

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