Datasets – the role of the Publisher

June 2011 Philippe Terheggen Senior Vice President, Journals, ELSEVIER

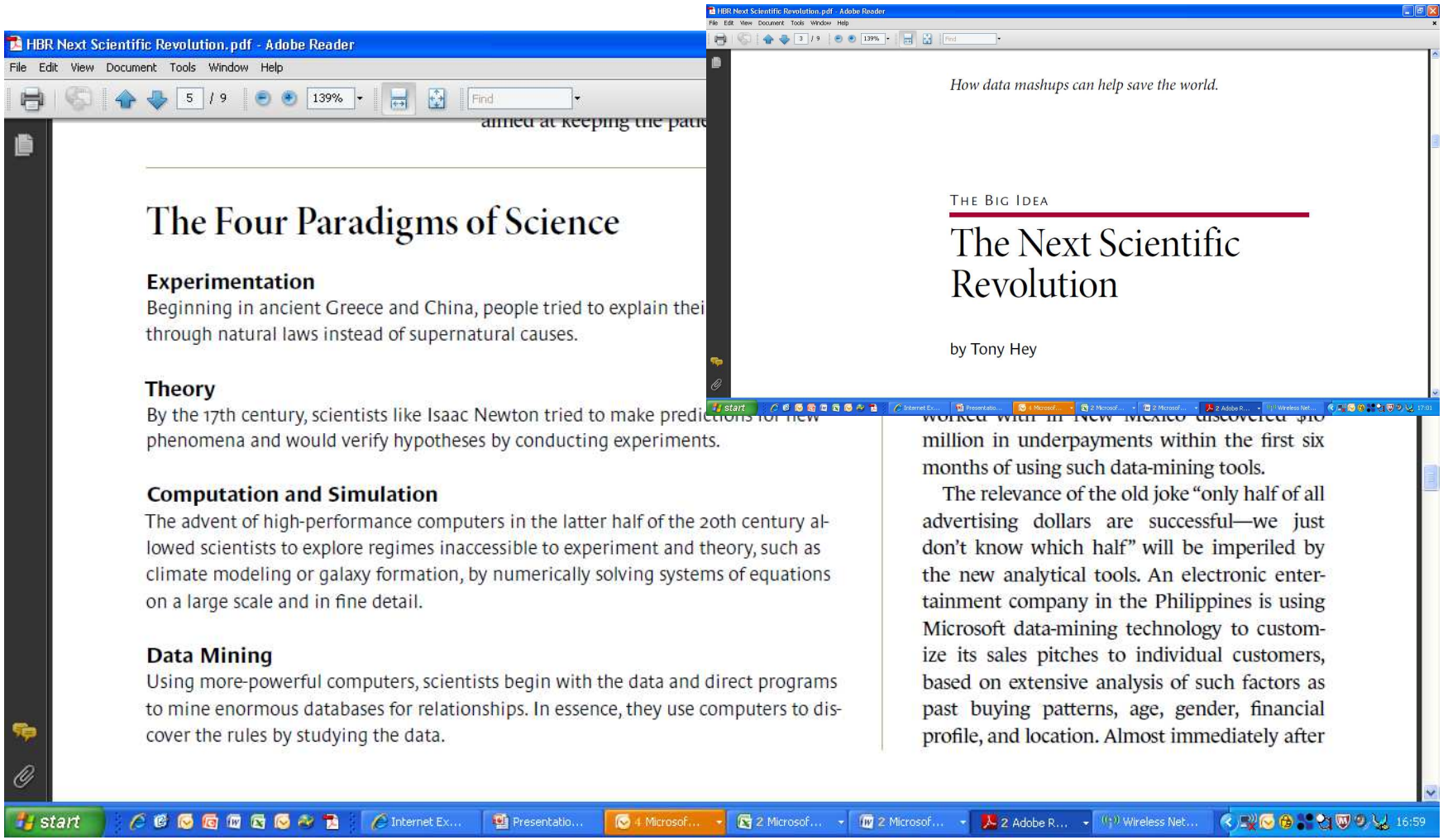
ELSEVIER

Early innovation

- 1638 Elzevir published Galileo Galilei's greatest work
- Galileo published his "*Discorsi e dimostrazioni matematiche, intoro a due nuoue scienze*" with Elzevir despite being banned by the Inquisition.

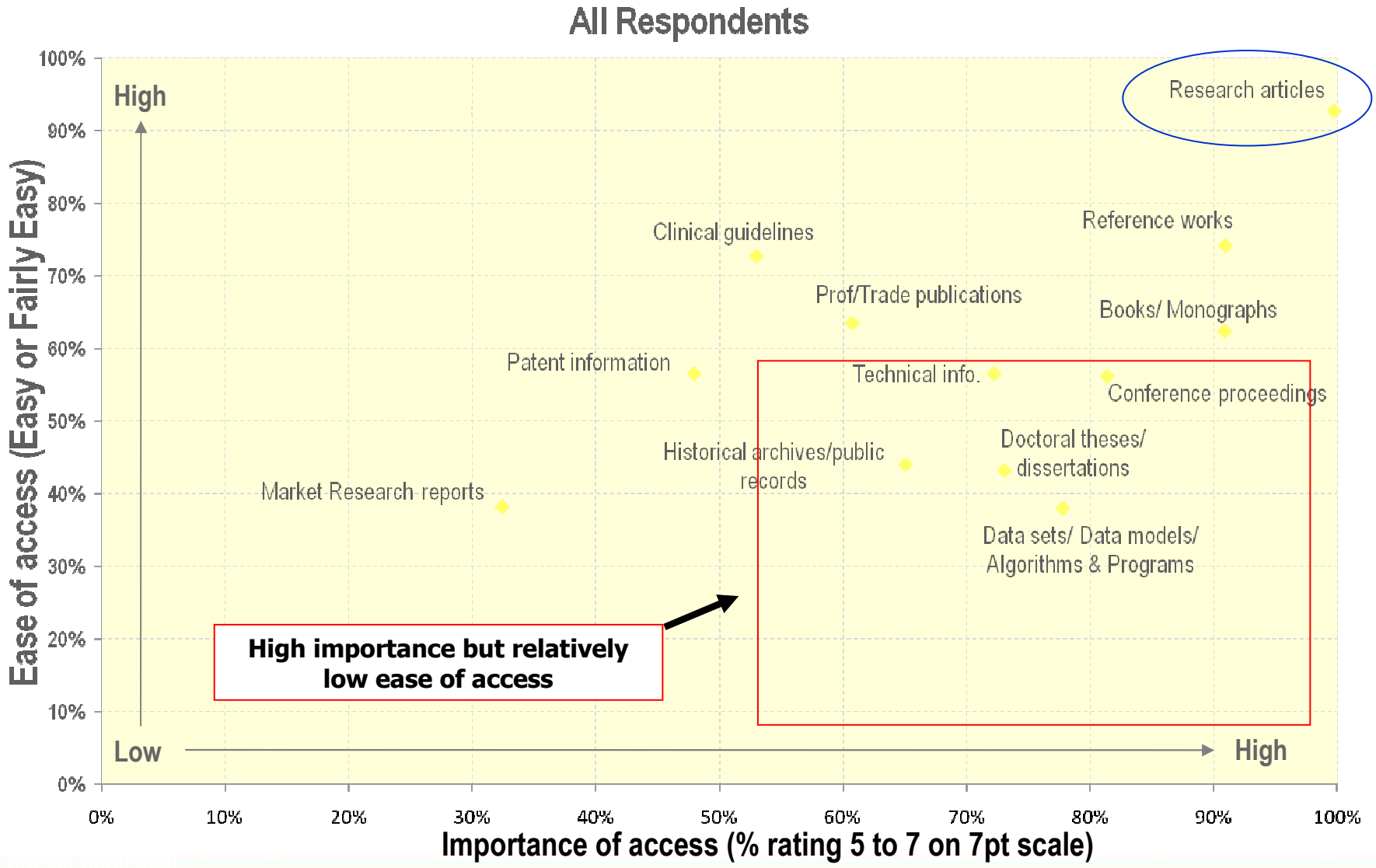
''An elsevier'' was a trademark for any book with a certain portable format.

Why data are relevant



Harvard Business Reviews. Toney Hey, 2010

Access vs. Importance (4109 respondents)



Topics

1. Overview of existing collaborations.
2. Our perspective on datasets
3. Our open invitation to collaborate further

Data enrichment in publications

1. Supplemental data
2. Article linking
   - PANGAEA, CCDC, EarthChem, ...
3. Entity linking
   - Genes, Proteins, CCDC Structures, Arabidopsis, ...
4. Embedded applications
   - Reaxys, PANGAEA, Protein Viewer, Google Maps, ...

Our efforts on article linking are part of much wider initiative on article innovation...

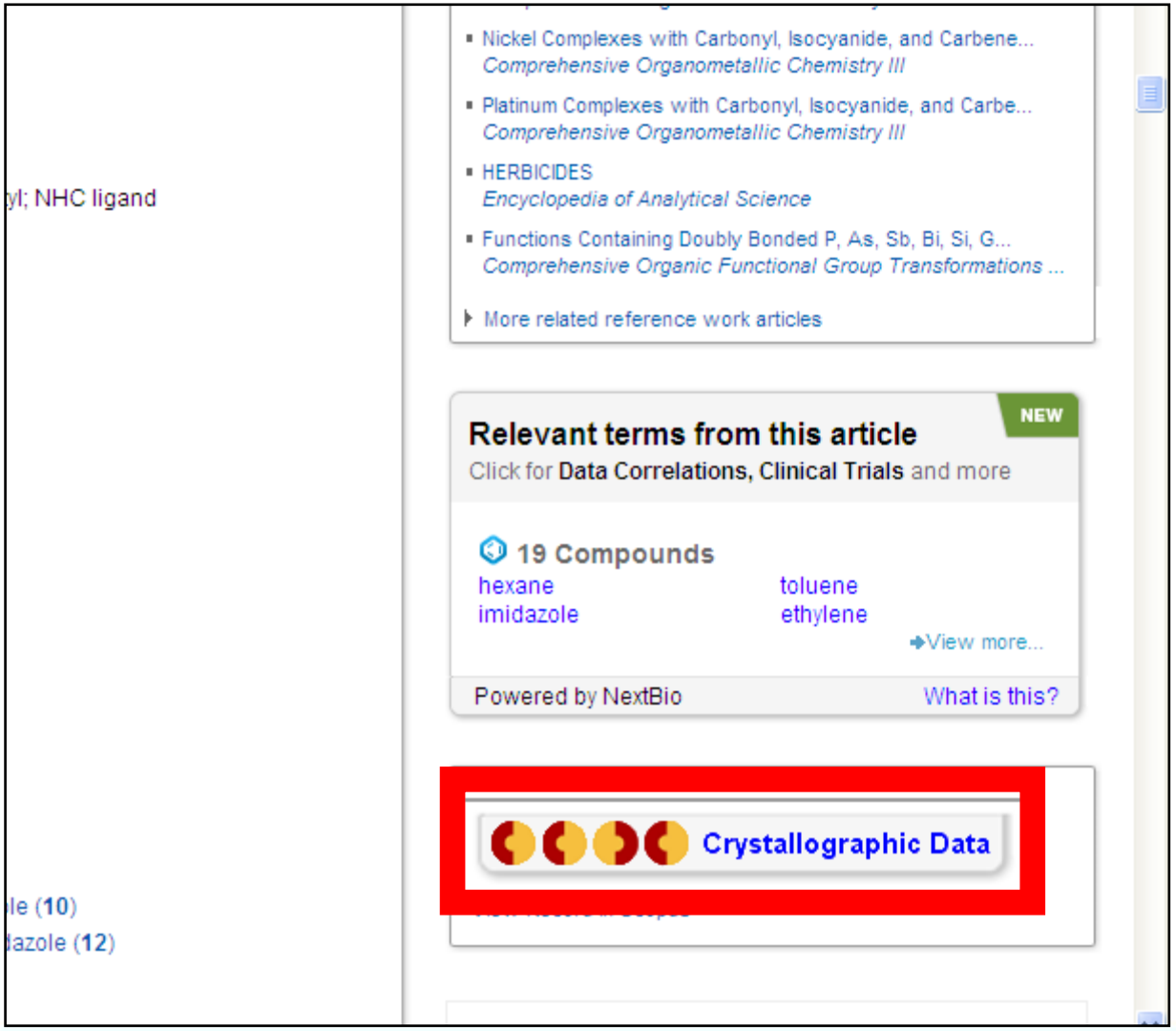
1. Supplemental data – current situation

- Elsevier receives more and more supplemental materials in different formats to publish next to articles (40% 4-yr CAGR)
- The types of supplemental material vary widely per discipline (e.g. methods/protocols, datasets, executable codes, videos of experiments, etc) and vary also in importance to support the argument made in the article

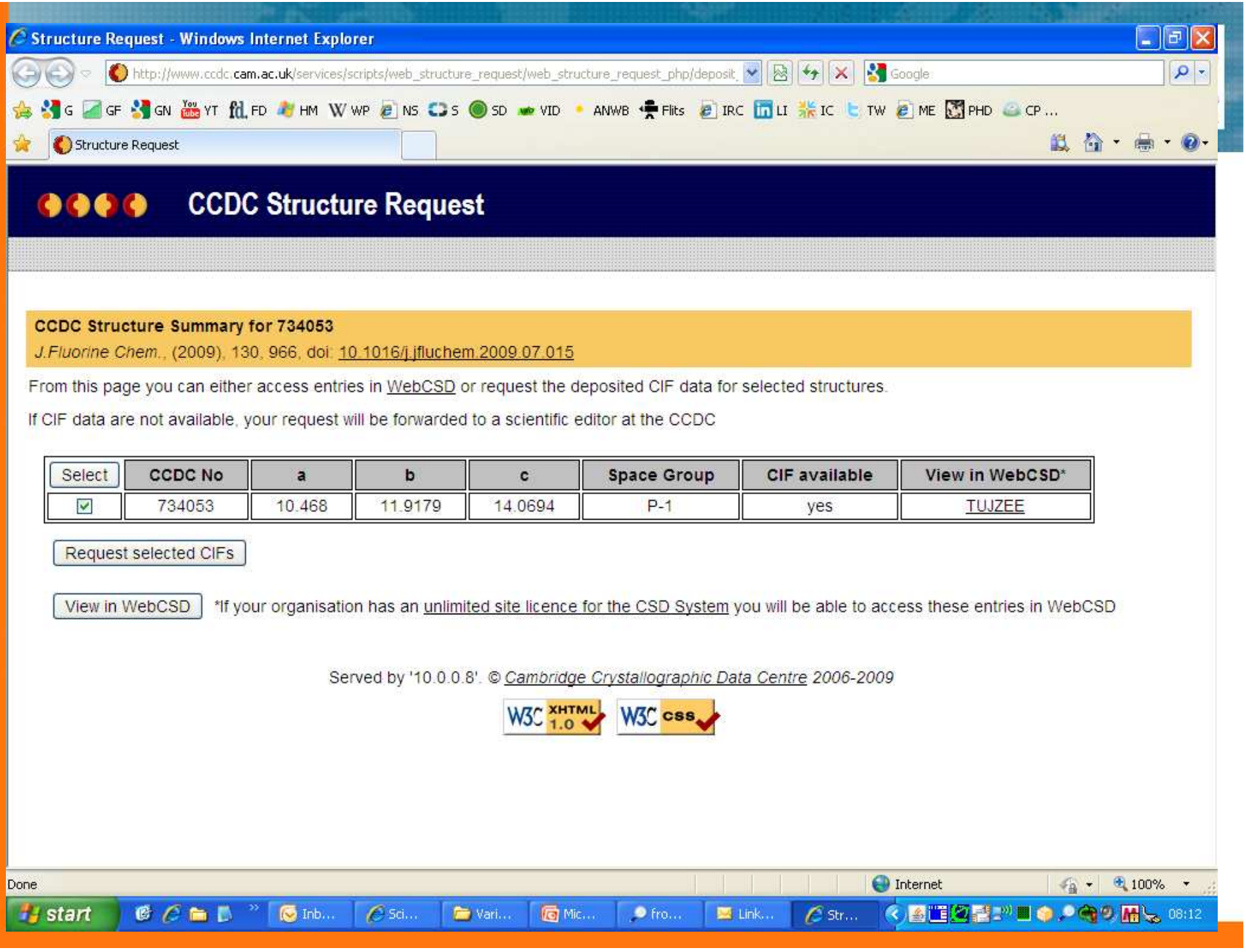
	2005	2006	2007	2008	2009	CAGR
Applications*	7,499	12,670	17,217	23,492	29,349	41%
Audio	20	76	96	51	137	62%
Images	3,009	5,154	6,339	9,579	13,331	45%
Video	1,890	2,513	3,400	3,908	4,749	26%
Total	12,418	20,413	27,052	37,030	47,566	40%

* Applications: .pdf, .csv, .txt, .tar, .zip, .doc, .rtf, .xls, .ppt

2. Article Linking



- Author posted
- Automatic connection between Elsevier and repository


Structure Request - Windows Internet Explorer
http://www.ccdc.cam.ac.uk/services/scripts/web_structure_request/web_structure_request_php/deposit
Google
Structure Request
CCDC Structure Request
CCDC Structure Summary for 734053
J.Fluorine Chem., (2009), 130, 966, doi: 10.1016/j.jfluchem.2009.07.015
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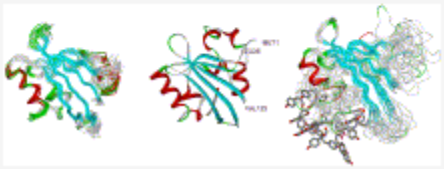
3. Entity Linking

Upon irradiation at 446 nm, the chromophore switches to the cis form, and the protein partially unfold
[33] and [34] (Fig. 1). In the dark, the trans folded state is regained in seconds to minutes, depending o
experimental conditions.[35] Several studies have shown that the N-terminal section (residues 1–25) o
PYP undergoes an almost complete unfolding upon irradiation, exposing a hydrophobic patch on the
protein.[36], [37], [38], [39] and [40] The N-terminally truncated protein (Δ1–25) is still fully functional, albe
with a slower photocycle.[33]



Full-size image (72K)
High-quality image (755K)

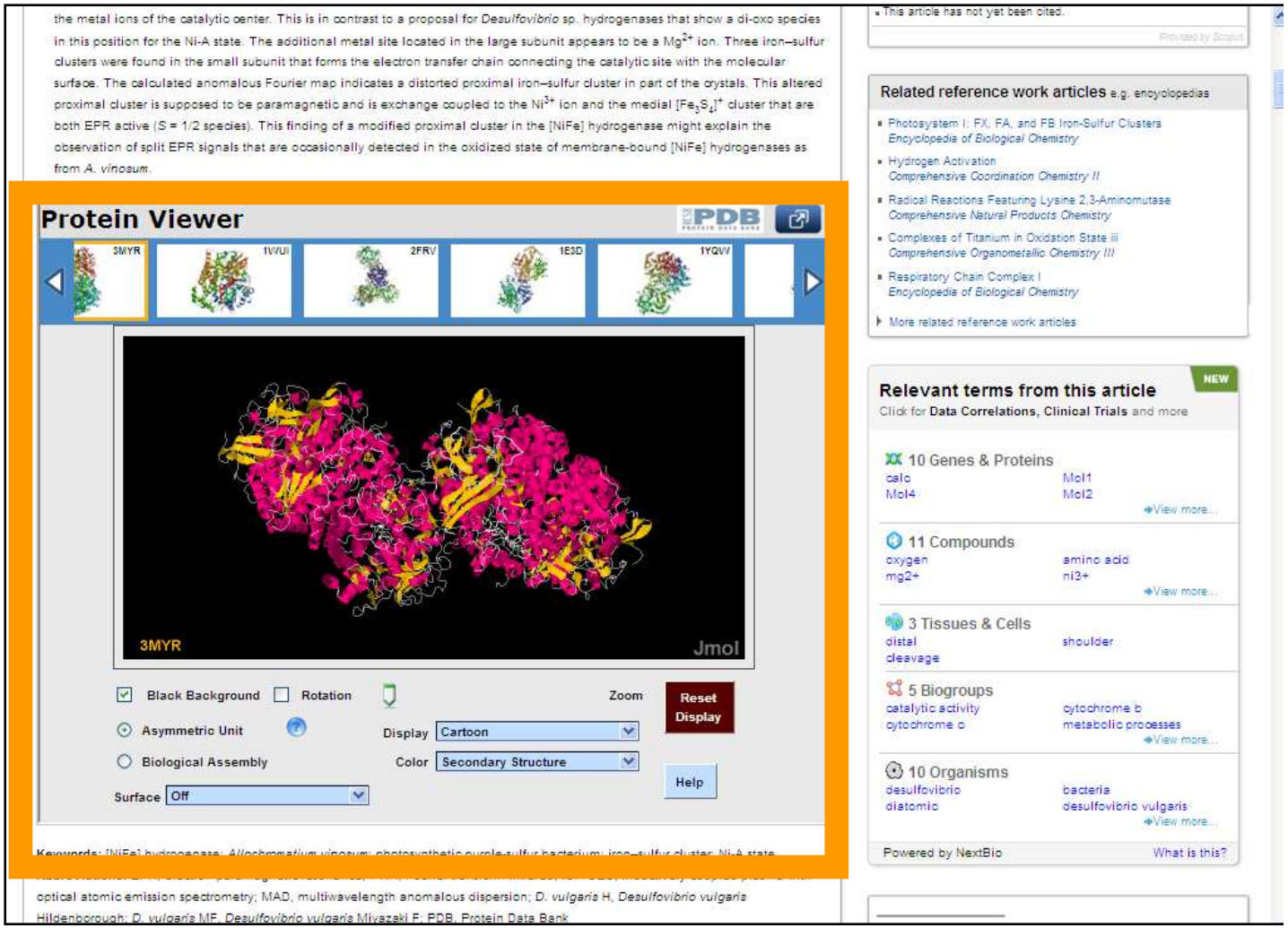
Fig. 1.
Structures of PYP under various conditions. (a) NMR solution structure of dark-adapted Δ25PYP (PDB code 1XFN).[33] (b) X-ray crystal structure of dark-adapted full-length wild-type PYP (the N-terminal ca B code 1NWZ).[32] (c) NMR solution structure of light-adapted Δ25PYP (P code 1XFQ).[33]

Our approach to using PYP as a photoswitch aims to use the folded state of PYP to sterically prevent interaction, which is then allowed to occur in the flexible light-adapted form. It has been suggested tha such a mechanism may explain how PYP interacts with its putative partner protein *in vivo*.[36] We wish to explore the possibility of designing a genetically encoded photoswitchable DNA binding protein by fusing PYP to the prototypical leucine-zipper-type DNA binding protein GCN4-bZIP. The bZIP domain i

- Automatic or author-tagged
- Automatic linked to data:
  - External
  - Selectable
  - Personal preference

4. Embedded Applications: PDB

- Author-tagged
- Data from PDB
- 3D Visualisation
  - Select
  - Zoom
  - Rotate
- All inside article



RCSB Protein Data Bank - Structure Summary for 1XFQ - structure of the blue shifted intermediat - Windows Internet Explorer

http://www.rcsb.org/pdb/explore.do?structureId=1XFQ

RCSB Protein Data Bank - Structure Summary for 1XF...

RCSB PDB PROTEIN DATA BANK

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An Information Portal to Biological Macromolecular Structures

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structure of the blue shifted intermediate state of the photoactive yellow protein lacking the N-terminal part

1XFQ

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DOI:10.2210/pdb1xfq/pdb

Primary Citation

The solution structure of a transient photoreceptor intermediate: Delta25 photoactive yellow protein.

Bernard, C., Houben, K., Derix, N.M., Marks, D., van der Horst, M.A., Hellingwerf, K.J., Boelens, R., Kaptein, R., van Nuland, N.A.

Journal: (2005) STRUCTURE **13:** 953-962

PubMed: 16004868
DOI: 10.1016/j.str.2005.04.017

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PubMed Abstract:

The N-terminally truncated variant of photoactive yellow protein (Delta25-PYP) undergoes a very similar photocycle as the corresponding wild-type protein (WT-PYP), although the lifetime of its light-illuminated (pB) state is much longer. This has allowed determination of the structure of both...

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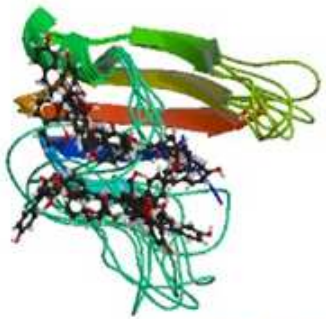
Structure Image



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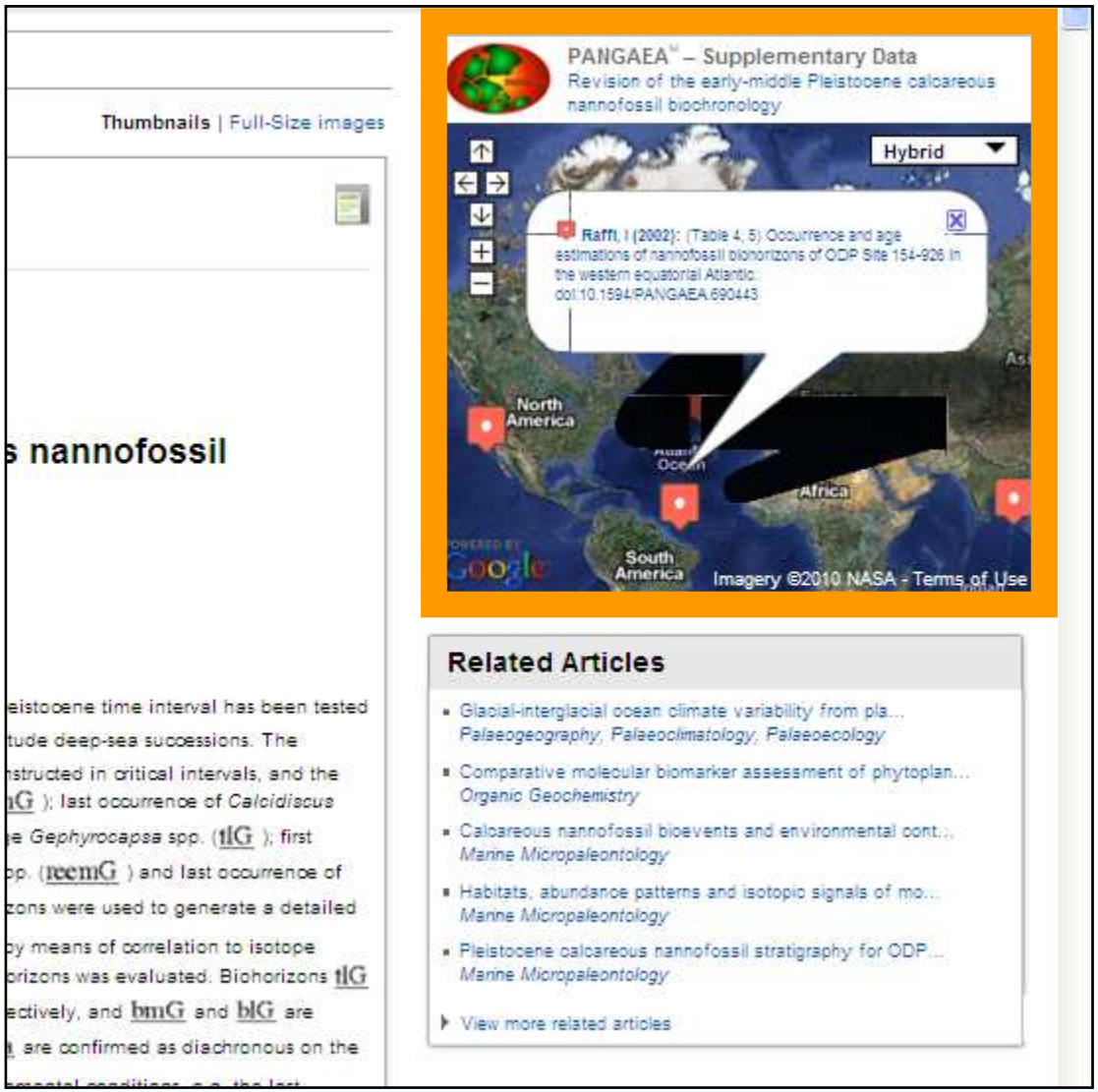
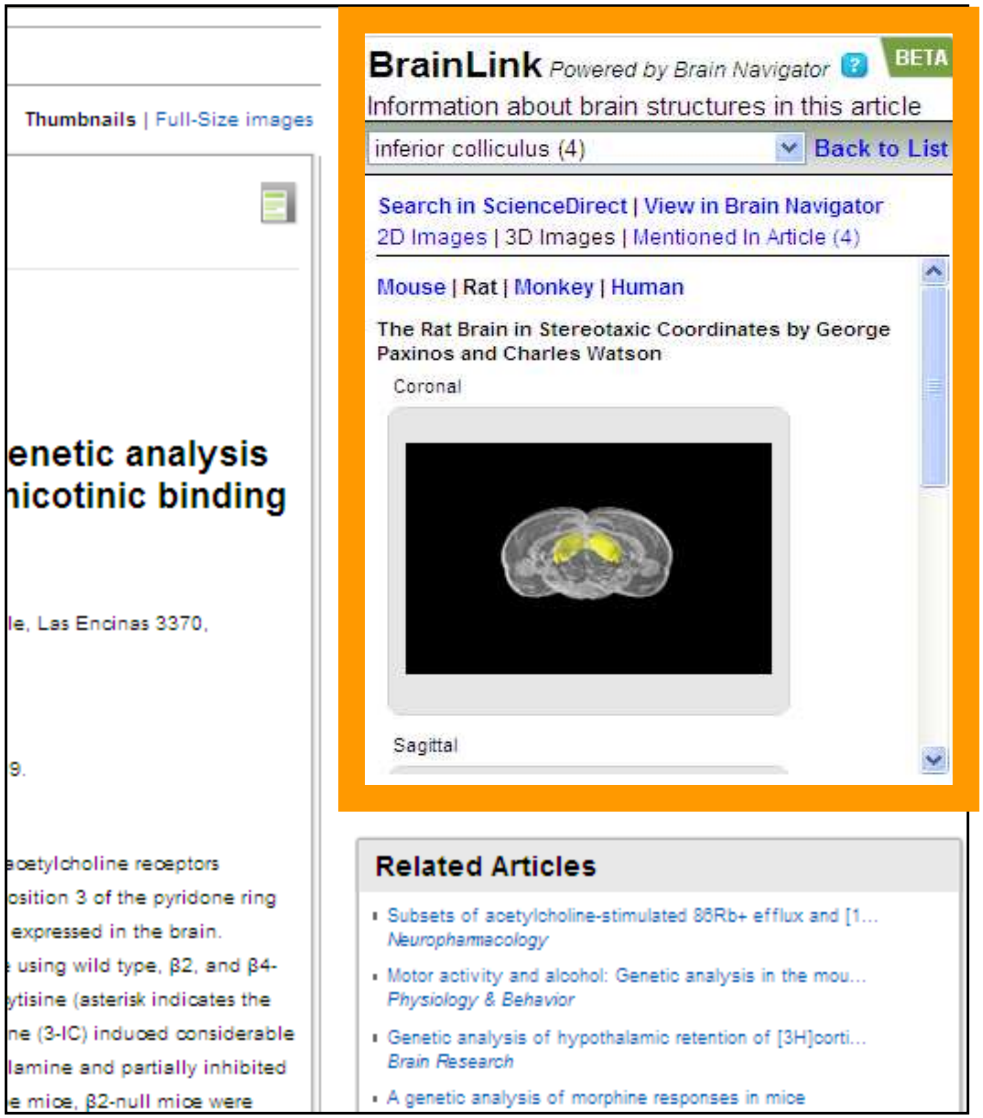
Embedded Application in: PANGAEA

- Author-posted
- PANGAEA-hosted
- Real-time match
- Full Google Maps functionality
- Links to PANGAEA
- All inside article



Embedded Application: BrainLink

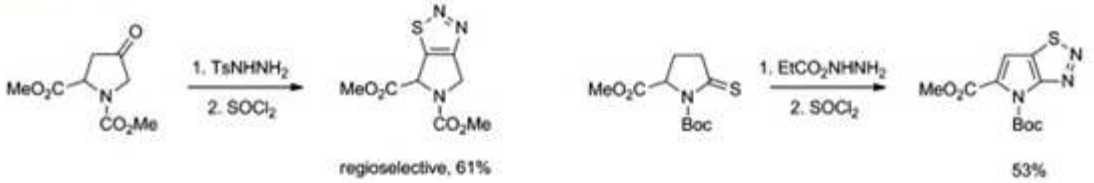
- Automatically generated
- Text-mining and linking to structures
- Lists and displays all structures:
  - Occurrences
  - 2D, 3D images
  - Rat, mouse, monkey, human views
- Again inside article
- Links to more data at BrainNavigator



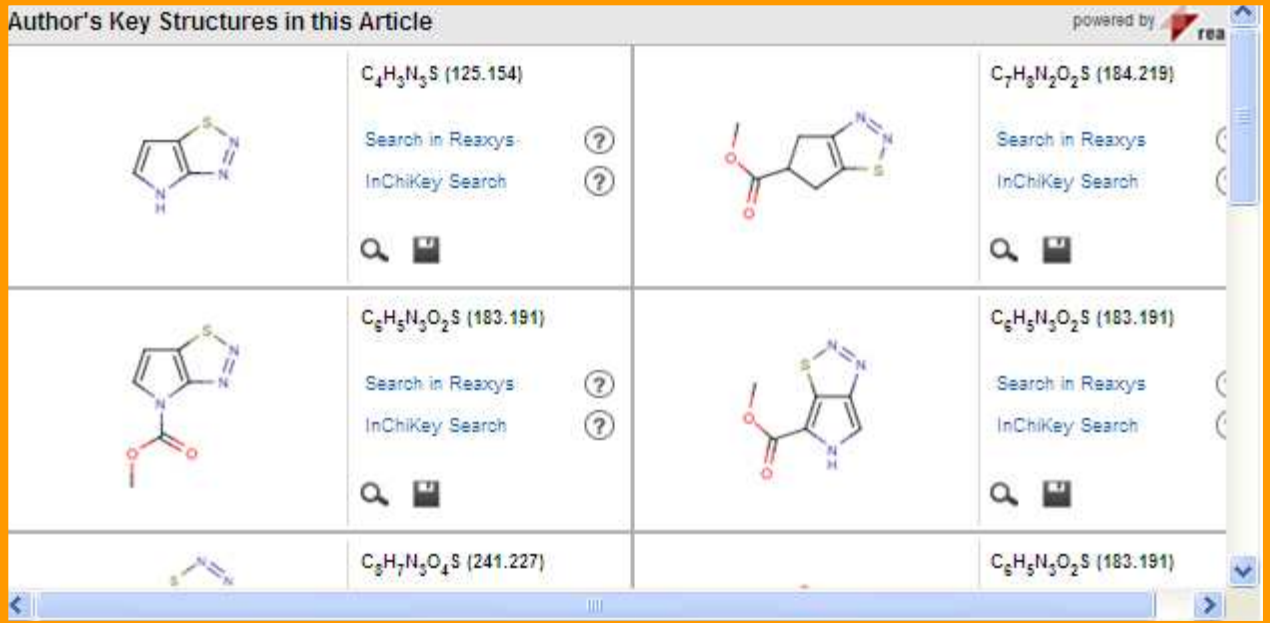
Embedded Application: chemistry

cyclization direction to afford bicyclic 1,2,3-thiadiazoles. Effects promoting and disfavoring the reaction have also been investigated to guide the synthesis of scaffolds of this type.

Graphical abstract



Author's Key Structures in this Article



Keywords: Annelated heterocycle; Cyclization; Protecting group; Regioselectivity; Systemic acquired resistance
BKEJQHMFJCUTKL-UHFFFAOYSA-N; TYPJSLXIPNEPES-UHFFFAOYSA-N; LSLFJEGXOZLMIB-UHFFFAOYSA-N;

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General

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