

# Project Prospect

Introducing semantics into chemical science publishing

Richard Kidd

# Aims of Project Prospect

- Preserve authors' science
- Capture the science as XML
- Apply ontologies to find meaning
- Make it part of the publishing process
- Provide new views to readers
- Computer-readable chemistry

# Meaningful searches

Why is it hard for chemistry?

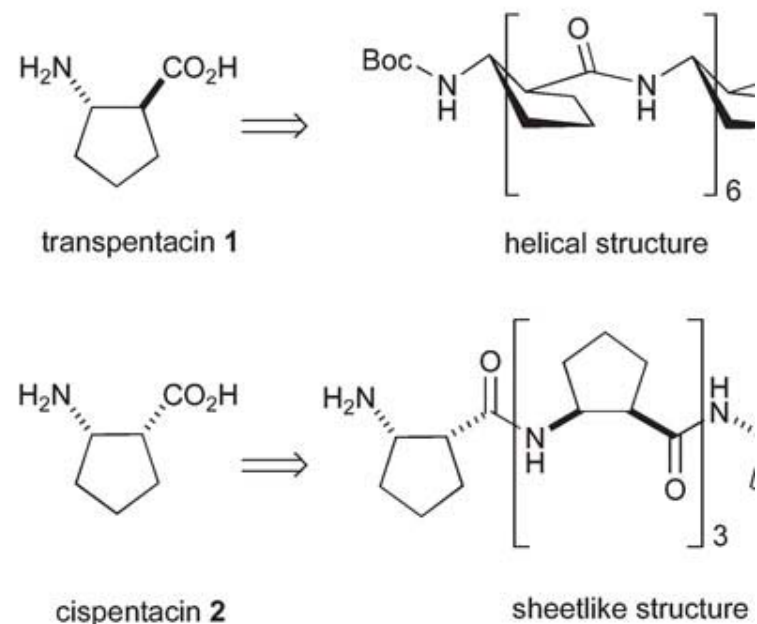
- Searching
  - Free text or proprietary
- Related articles
  - No standards

## Introduction

The generation of bespoke pseudopeptide sequences that exhibit highly ordered secondary and tertiary structures in both solution and solid phase has developed into a highly competitive field of research in recent years, with the ability to predict the conformation of a given peptide sequence from knowledge of its primary structure an elusive goal. While much effort has been directed towards understanding the factors that control the secondary structure of  $\alpha$ -peptides, the utility of peptides incorporating the  $\beta$ -amino acid structural motif has recently been investigated widely, most notably by Seebach<sup>1</sup> and Gellman.<sup>2</sup> For instance, Gellman *et al.* have shown that  $\beta$ -peptides derived from *trans*-2-aminocyclopentanecarboxylic acid (transpentacin) **1** adopt a helical structure in both the solid state and in solution,<sup>3</sup> while Fülop *et al.* have shown that homo-oligomers of *cis*-2-aminocyclopentanecarboxylic acid (cispentacin) **2** form a sheetlike secondary structure in solution (Fig. 1).<sup>4</sup> The ability of mixed  $\alpha,\beta$ -peptides containing both  $\alpha$ -amino and  $\beta$ -amino acid derivatives to adopt a preferred conformation in solution has also been reported recently.<sup>5</sup>

We have shown extensively that the conjugate addition of lithiumamides derived from  $\alpha$ -methylbenzylamine to  $\alpha,\beta$ -unsaturated acceptors may be used for the asymmetric synthesis of  $\beta$ -amino acid derivatives.<sup>6</sup> This methodology has recently been utilised for the synthesis of (1*R*,2*S*,3*R*)-3-methylcispentacin **5** in >98% de and 98  $\pm$  1% ee and (1*S*,2*S*,3*R*)-3-methyltranspentacin **7** in >98% de and 97  $\pm$  1% ee by the kinetic resolution of *tert*-butyl (*RS*)-3-methylcyclopentene-1-carboxylate **3** with lithium (*S*)-*N*-benzyl-*N*- $\alpha$ -methylbenzylamide (Scheme 1).<sup>7</sup>

The protocol that we use to understand fully the stereoselectivity observed in these kinetic resolution reactions



**Fig. 1** Secondary structure of poly homo-pe

requires an initial evaluation of the level of offered by the chiral  $\alpha,\beta$ -unsaturated ester unjugate addition, which is achieved through the achiral lithium amide to the ester. If the  $\alpha,\beta$ -uns shows high facial selectivity upon conjugate add of enantiorecognition between the chiral  $\alpha,\beta$ -uns and a chiral lithium amide is evaluated through kinetic resolution [addition of (*RS*)-ester to ar (*RS*)-lithium amide]. In this approach,<sup>8</sup> the ef action are eliminated, allowing the maximum st factor (*E*) for the reaction to be calculated inde reaction conversion, as it is identical to the diast observed in the reaction.<sup>9</sup> If high enantiorecog between the reacting partners in a mutual kine then efficient kinetic resolution may be expec

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# Systematic name

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We have shown extensively that the conjugate addition of lithiumamides derived from  $\alpha$ -methylbenzylamine to  $\alpha,\beta$ -unsaturated acceptors may be used for the asymmetric synthesis of  $\beta$ -amino acid derivatives.<sup>6</sup> This methodology has recently been utilised for the synthesis of (1*R*,2*S*,3*R*)-3-methylcispentacin **5** in >98% de and 98  $\pm$  1% ee and (1*S*,2*S*,3*R*)-3-methyltranspentacin **7** in >98% de and 97  $\pm$  1% ee by the kinetic resolution of *tert*-butyl (*RS*)-3-methylcyclopentene-1-carboxylate **3** with lithium (*S*)-*N*-benzyl-*N*- $\alpha$ -methylbenzylamide (Scheme 1).<sup>7</sup>

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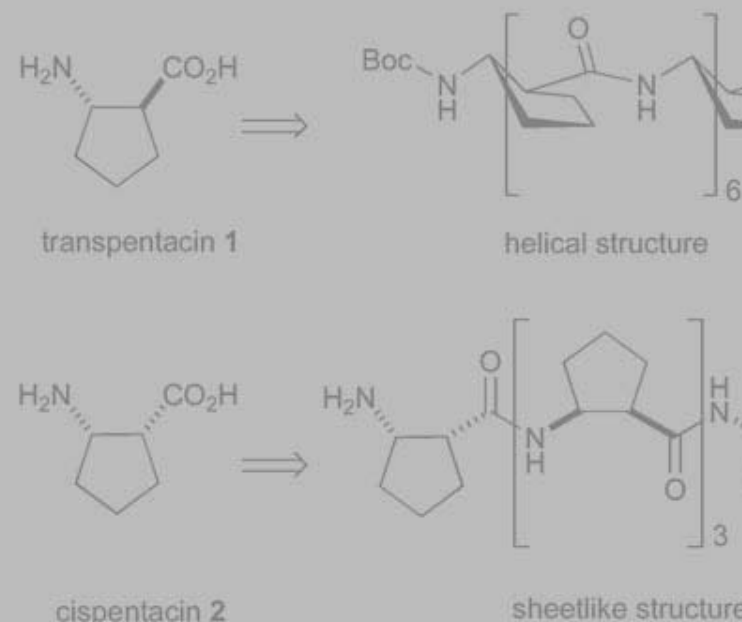


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## Introduction

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We have shown external lithiumamides derived from  $\alpha,\beta$ -unsaturated acetoacetates of  $\beta$ -amino acids can be used as chiral auxiliaries in the kinetic resolution of  $\beta$ -amino acids.

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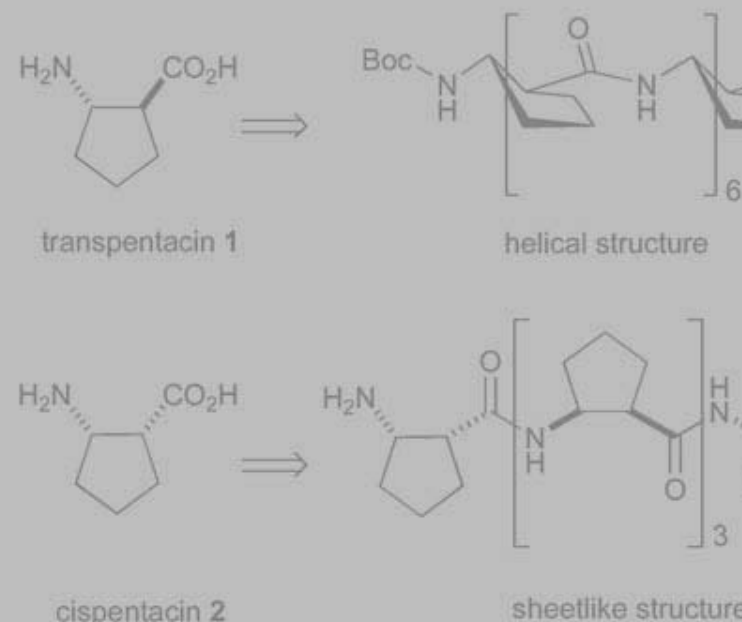


Fig. 1 Secondary structure of poly homo-peptides

requires an initial evaluation of the level of stereocontrol offered by the chiral  $\alpha,\beta$ -unsaturated ester unit. The kinetic resolution of the  $\beta$ -amino acid is achieved through the addition of the  $\beta$ -amino acid to the lithium amide to form the  $\beta$ -amino acid lithium amide. If the  $\alpha,\beta$ -unsaturated ester unit offers high facial selectivity upon conjugate addition, then the  $\beta$ -amino acid lithium amide is evaluated through the kinetic resolution [addition of (*RS*)-ester to an (*RS*)-lithium amide]. In this approach,<sup>8</sup> the effect of the  $\beta$ -amino acid on the reaction are eliminated, allowing the maximum stereocontrol factor (*E*) for the reaction to be calculated independent of reaction conversion, as it is identical to the diastereoselectivity observed in the reaction.<sup>9</sup> If high enantioselectivity is observed between the reacting partners in a mutual kinetic resolution, then efficient kinetic resolution may be expected.

Trivial name

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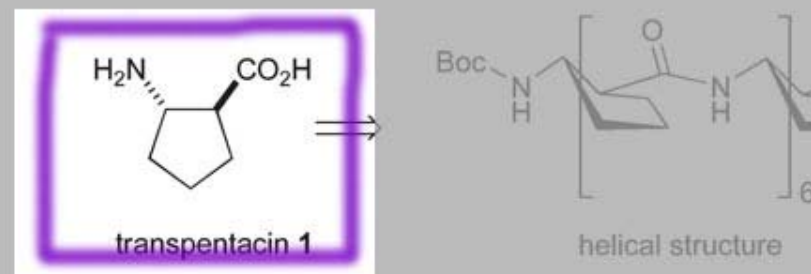
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# 2D structural diagram

*cis*-pentacin **2**

sheetlike s

Fig. 1 Secondary structure of poly homo-pe

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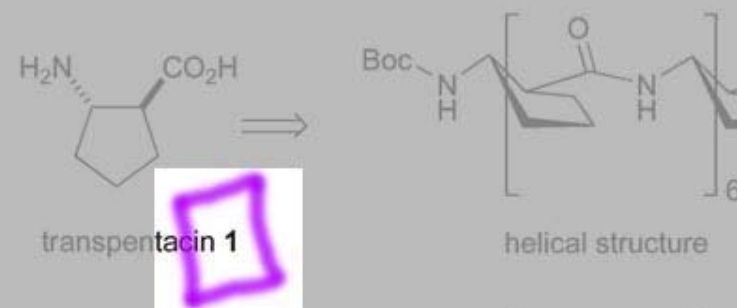
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# boldface numbers

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# The Prospect model

- Enhance existing publications
- Build straight into existing workflow
- Reduce problems with introducing separate product
- Marked small molecule libraries...  
...lysyl oxidase in zebrafish notochord  
morphogenesis

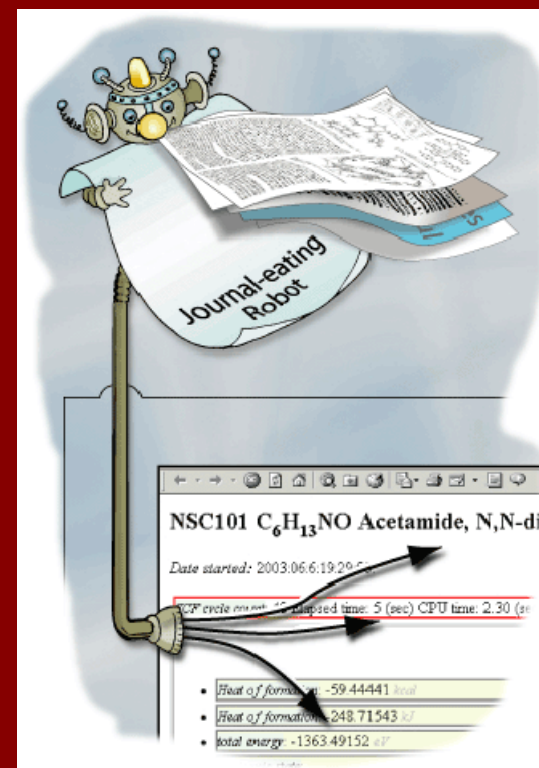
# How?

- Collaborations
  - Unilever Centre/Computer Lab
  - Others
- Technology
  - OSCAR text mining
  - Standards
  - Workflow
  - RSS feeds

# OSCAR text mining

## Open Source Chemical Analysis Routines

- University of Cambridge:  
Chemistry (Unilever Centre)  
–Computer Lab collaboration
- SciBorg
- Analyses single words and short chemical-looking phrases to determine structure
- Attaches structures to text
- Extended to subjects





# InChI

- IUPAC International Chemical Identifier
- InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3
- Machine readable
- InChIkey  
RYYVLZVUVIJVGH-UHFFFAOYAW

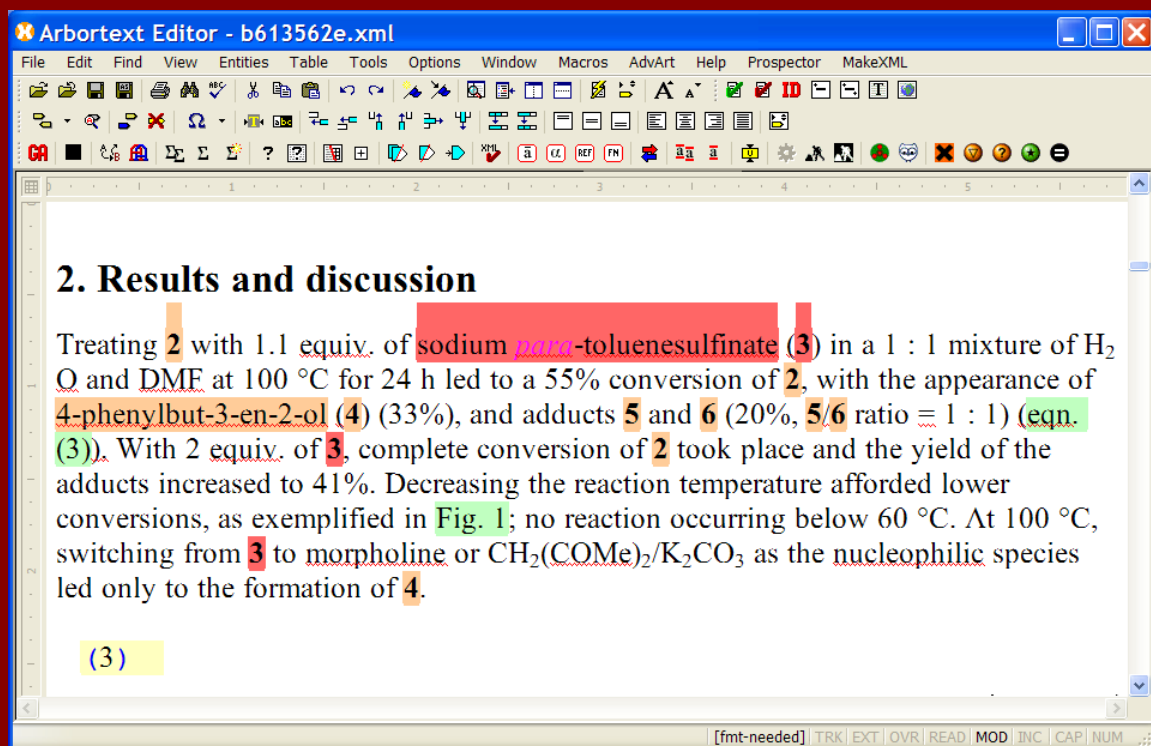


# Subject terms

- Open Biomedical Ontologies
  - Gene Ontology (GO)
  - Sequence Ontology (SO)
  - Cell Ontology (CL)
- IUPAC Gold Book
  - Dictionary of chemical terminology

# RSC Publishing process

- Editing
- Mining
- Add & Tidy





# Enhanced RSS feeds

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- Others (392)
- RSC (191)
- RSC Journals (1102)
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  - RSC - Annu. Rep. Prog. Chem., Sect. A: Inorg. Ch...
  - RSC - Annu. Rep. Prog. Chem., Sect. B: Org. Chem...
  - RSC - Annu. Rep. Prog. Chem., Sect. C: Phys. Chem...
  - RSC - Chem. Commun. latest articles (218)
  - RSC - Chem. Soc. Rev. latest articles (30)
  - RSC - Chemical Biology Virtual Journal latest article
  - RSC - Dalton Trans. latest articles (127)
  - RSC - Green Chem. latest articles (30)
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  - RSC - J. Environ. Monit. latest articles (36)
  - RSC - J. Mater. Chem. latest articles (109)
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  - RSC - Mol. Biosyst. latest articles (21)
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- Software (970)
- Technology (229)
- test (434)


RSC - Photochem. Photobiol. Sci. latest articles (25)

R	Headlines	Received dates	Published dates
	Picosecond time-resolved infrared study of 2-...	24/05/2007 15:58	24/05/2007 00:00
	Novel emission properties of melem caused b...	23/05/2007 16:16	23/05/2007 00:00

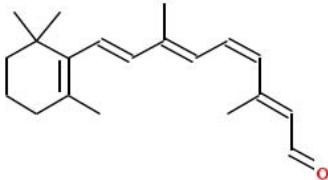
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**Chlorophyll derivatives as visual pigments for super vision in the red**



Ilyas Washington, Jilin Zhou, Steffen Jockusch, Nicholas J. Turro, Koji Nakanishi, Janet R. Sparrow  
(Paper from Photochem. Photobiol. Sci.)  
Ilyas Washington, Photochem. Photobiol. Sci., 2007, DOI: 10.1039/b618104j  
To cite this article before page numbers are assigned, use the DOI form of citation above.  
**Ontology Terms:** photoreceptor cell; crystallin accumulating cell; visual perception; response to blue light; photoreceptor activity; response to red light  
**Primary Compounds:**  
11-cis-retinal:



Done

# Problems?

- Significant manual QA required
  - and old data even harder
- Ontology development required in many areas
- Wider adoption and interlinking required to maximise benefits

# New data standards

- Experimental data checker
  - Validation
  - Visualisation
- Role for society publishers

2-Methyl-2-hydroxymethyl-2,5-dihydrofuran **9** (50 mg, 0.51 mmol) was oxidised using OsO<sub>4</sub>, TMEDA to yield the crude products [6 : 1 (*syn* : *anti*) by <sup>1</sup>H NMR]. The resulting oil was purified by flash chromatography (petrol-EtOAc, 4 : 1) to afford the pure title compound as a colourless oil (116 mg, 83%);  $\nu_{\max}$  (film)/cm<sup>-1</sup> 2977, 2929, 1746, 1374, 1230, 1046<sup>[a]</sup>;  $\delta_{\text{H}}$  (300 MHz; CDCl<sub>3</sub>) 5.43 (1H, q, *J* 5), 5.17 (1H, d, *J* 5), 4.26-4.09 (3H, m), 3.89 (1H, dd, *J* 10 and 5), 2.10 (6H, s), 2.08 (3H, s), 1.36 (3H, s)<sup>[a]</sup>;  $\delta_{\text{C}}$  (75 MHz; CDCl<sub>3</sub>) 170.6, 169.8, 169.5, 80.8, 76.2, 71.2, 68.9, 65.3, 22.3, 20.6, 20.4, 18.3<sup>[a]</sup>. Found (CI) 292.1392, C<sub>12</sub>H<sub>22</sub>NO<sub>7</sub> + NH<sub>4</sub> requires 292.1396.

## ***anti*-2-Methyl-2-(acetoxymethyl)tetrahydrofuran *anti*-15**

2-Methyl-2-hydroxymethyl-2,5-dihydrofuran **9** (50 mg, 0.51 mmol) was oxidised using UpJohn conditions to yield the crude products [2 : 1 (*anti* : *syn*) by <sup>1</sup>H NMR]. The resulting oil was purified by flash chromatography (petrol-EtOAc, 4 : 1) to afford the product mixture as a colourless oil (110 mg, 79%) as an inseparable mixture of isomers (*anti* major compound);  $\nu_{\max}$  (film)/cm<sup>-1</sup> 2989, 2944, 1746, 1379, 1232, 1046<sup>[a]</sup>;  $\delta_{\text{H}}$  (300 MHz; CDCl<sub>3</sub>) 5.46-5.39 (1H, m), 5.26 (1H, d, *J* 6), 4.26-3.85 (4H, m), 2.11 (3H, s), 2.10 (6H, s), 1.26 (3H, s)<sup>[a]</sup>;  $\delta_{\text{C}}$  (75 MHz; CDCl<sub>3</sub>) 170.4, 169.8, 169.6, 81.2, 72.7, 71.9, 69.3, 67.9, 20.7, 20.5, 20.4, 18.3<sup>[a]</sup>. Found (CI) 292.1400, C<sub>12</sub>H<sub>22</sub>NO<sub>7</sub> requires 292.1396.

## ***syn*-1,2,4-Triacetoxycyclohexane *syn*-16**

Cyclohex-3-en-1-ol **11** (50 mg, 0.51 mmol) was oxidised using OsO<sub>4</sub>, TMEDA to yield the crude mixture of products [3 : 1 (*syn* : *anti*) by <sup>1</sup>H NMR]. The resulting oil was purified by flash chromatography (EtOAc) to afford a colourless oil (121 mg, 92%) as an inseparable mixture of isomers; mixture:  $\nu_{\max}$  (film)/cm<sup>-1</sup> 2953, 1745, 1370, 1235, 1028<sup>[a]</sup>; *syn*-**16**  $\delta_{\text{H}}$  (300 MHz; CDCl<sub>3</sub>) 5.17-5.11 (1H, m), 4.84-4.72 (2H, m), 2.04 (3H, s), 1.98 (3H, s), 1.86 (3H, s), 2.05-1.45 (6H, m);  $\delta_{\text{C}}$  (75 MHz; CDCl<sub>3</sub>) 170.1, 170.0, 169.9, 69.5, 69.3, 67.9, 31.4, 25.3, 24.7, 21.1, 20.9, 20.8<sup>[a]</sup>; *anti*-**16**;  $\delta_{\text{H}}$  (300 MHz; CDCl<sub>3</sub>) 5.08-5.01 (1H, m), 4.81-4.67 (2H, m), 1.99 (9H, s), 2.05-1.45 (6H, m)<sup>[a]</sup>;  $\delta_{\text{C}}$  (75 MHz; CDCl<sub>3</sub>) 170.3, 170.2, 170.1, 69.7, 68.8, 68.6, 31.8, 25.9, 25.3, 23.6, 21.1, 20.9<sup>[a]</sup>; mixture Found (CI) 276.1437, C<sub>12</sub>H<sub>22</sub>NO<sub>6</sub> requires 276.1447.

## ***anti*-1,2,4-Triacetoxycyclohexane *anti*-16**

Cyclohex-3-en-1-ol **11** (50 mg, 0.51 mmol) was oxidised using UpJohn conditions to yield the crude mixture of products [1 : 1 (*syn* : *anti*) by <sup>1</sup>H NMR]. The resulting oil was purified by flash chromatography (EtOAc) to afford the product mixture as a colourless oil (115 mg, 88%) as an inseparable mixture of isomers; All data are consistent with *syn*- and *anti*-**16** prepared previously.

## ***syn*-1,2,4,5-Tetraacetoxycyclohexane *syn*-17**



*"My first forays show [Project Prospect is] **brilliant**. [It's] great to see the compounds and have machine readable SMILES and InChIs"*

*"Your new system is **very impressive**, I am sure it will become very useful to a large community"*

*•It is **great and exciting!!** Just from the very few minutes I looked into it I realized its great potential and immediately ran to show it to my students!"*

*"This is **a fantastic resource** for the community, and a great use of the GO and SO. Nice work"*

*"I have ... found it **very intuitive/straightforward** to use.[I] believe that it will make the manuscript even more appealing to readers."*

*“It is fantastic.  
I’ve just seen the  
future of the journal”*

Ed Pentz

*Executive Director, CrossRef*

# What's unique?

- Technology
  - Semantic enrichment
    - Compounds
    - Ontology terms
  - Enhanced RSS feeds
- Implementation across existing portfolio
  - Incorporation into workflow
  - Shows the possibilities for structured science

# Future for RSC Project Prospect

- Experimental data
- Linguistics
- Extensive linking
- Other subject areas
- E-books, databases and backfile
- Peer review
- Prospect services



# Project Prospect

Introducing semantics into chemical science publishing

Richard Kidd