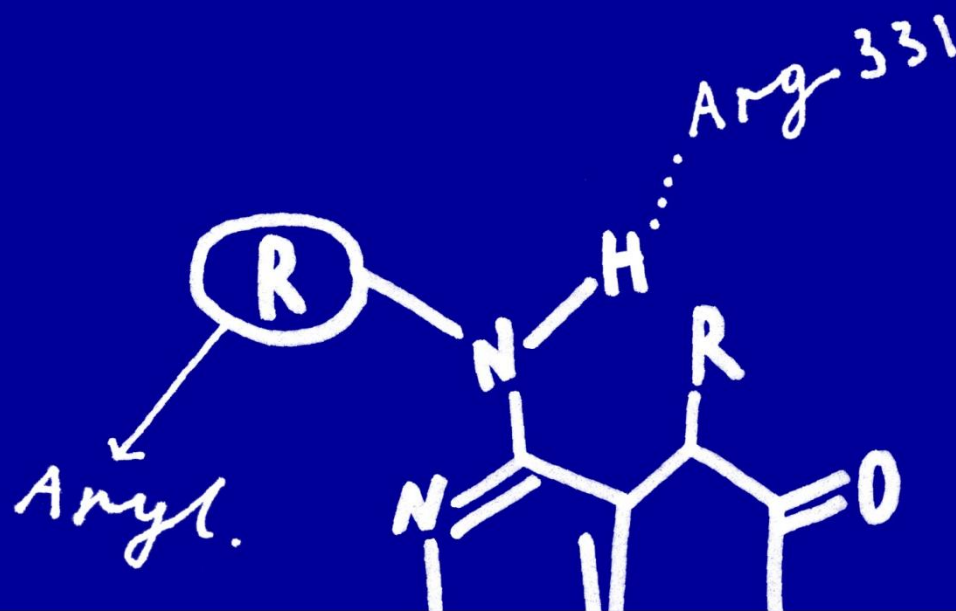


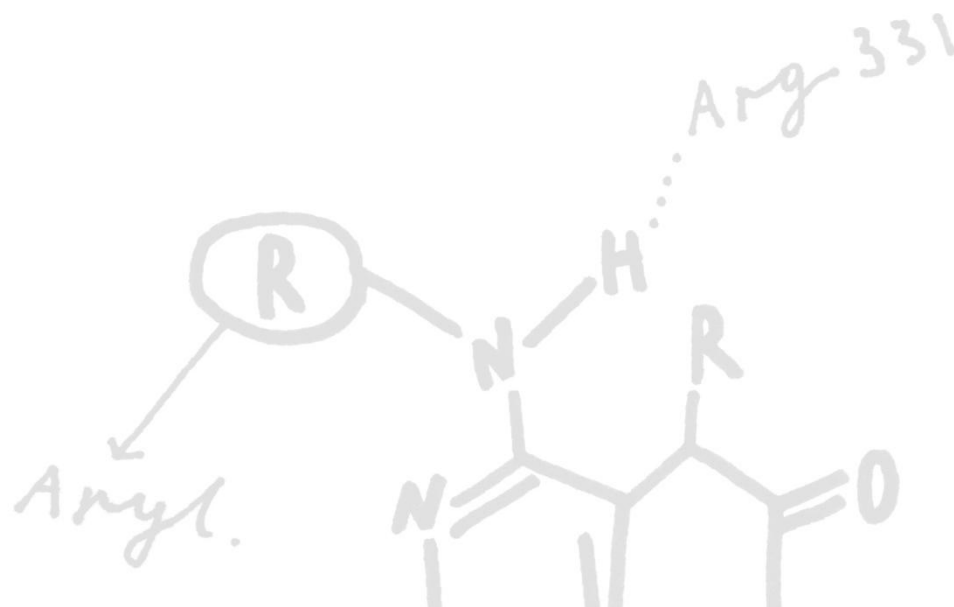
# Cheminformatics in SharePoint



## Agenda

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- **What's the (Share)Point?**
- Out of the box “cheminformatics”
- What we really want to do!
- What are the options?
- Conclusions



## What's the (Share)Point?

Many, many things or perhaps just one?



**Sites**  
SharePoint 2010 Sites provides a single infrastructure for all your business Web sites. Share documents with colleagues, manage projects with partners, and publish information to customers.

**Communities**  
SharePoint 2010 Communities delivers great collaboration tools—and a single platform to manage them. Make it easy for people to share ideas and work together the way they want.

**Composite**  
SharePoint 2010 Composites offers tools and components for creating do-it-yourself business solutions. Build no-code solutions to rapidly respond to business.

**Content**  
SharePoint 2010 Content makes content management easy. Set up compliance measures "behind the scenes"—with features like document retention, automatic content classification, and more. Work naturally in the cloud.

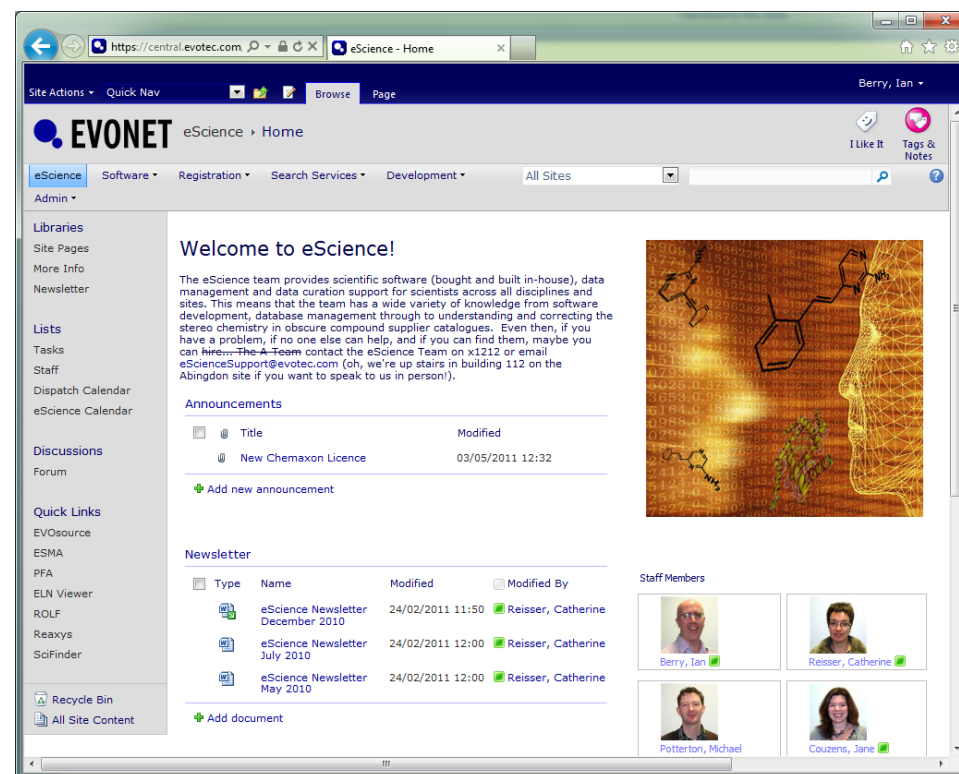
**Insights**  
SharePoint 2010 Insights gives everyone access to the information in databases, reports, and business applications. Help people locate the information they need to make good decisions.

**Search**  
SharePoint 2010 Search cuts through the clutter. A unique combination of relevance, refinement, and social cues helps people find the information and contacts they need to get their jobs done.

**It is a PLATFORM for doing whatever you want!**

# What's the (Share)Point?

- In its simplest form, SharePoint is a web portal – you can use it as an intranet
- At a higher level, it can be a document storage system – you can use it to replace your shared drives but have more information than ever about those files with Metadata!
- In its most complex form its anything you want – anything you do in a web application you can “do” in SharePoint
- SharePoint is a great tool but is not for the faint-hearted! You need to clearly define its role and stick to it.
- Good governance is key



The screenshot shows a SharePoint site for EVONET eScience. The page title is "Welcome to eScience!". The main content area contains a welcome message, an "Announcements" section with a table, and a "Newsletter" section with a table. The "Announcements" table has one entry: "New Chemaxon Licence" dated 03/05/2011 12:32. The "Newsletter" table has three entries: "eScience Newsletter December 2010", "eScience Newsletter July 2010", and "eScience Newsletter May 2010", all dated 24/02/2011 12:00 and modified by "Reisser, Catherine". The right sidebar shows "Staff Members" with four profile pictures: Berry, Ian; Reisser, Catherine; Potterton, Michael; and Couzens, Jane. The left sidebar contains navigation links like "Libraries", "Site Pages", "More Info", "Newsletter", "Lists", "Tasks", "Staff", "Dispatch Calendar", "eScience Calendar", "Discussions", "Forum", "Quick Links", "EVOsource", "ESMA", "PFA", "ELN Viewer", "ROLF", "Reaxys", "SciFinder", "Recycle Bin", and "All Site Content".

## Collaboration

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### Sharing in projects and with clients

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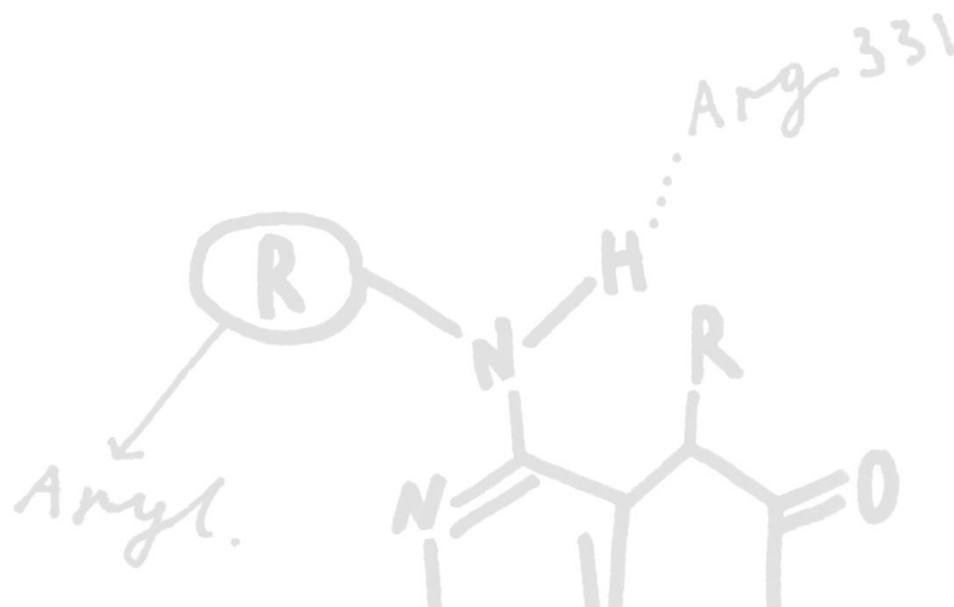
- SharePoint has replaced our old Intranet – its been live for 1.5 months – so still developing and growing
- SharePoint will be the collaboration tool for all projects at Evotec at all sites
- Next year, we will also make aspects of it available to our clients for them to access some of their data directly through a single interface (e.g. ELN PDFs, analytical results, etc.) so that they can have an up to date picture on how their projects are proceeding



## Agenda

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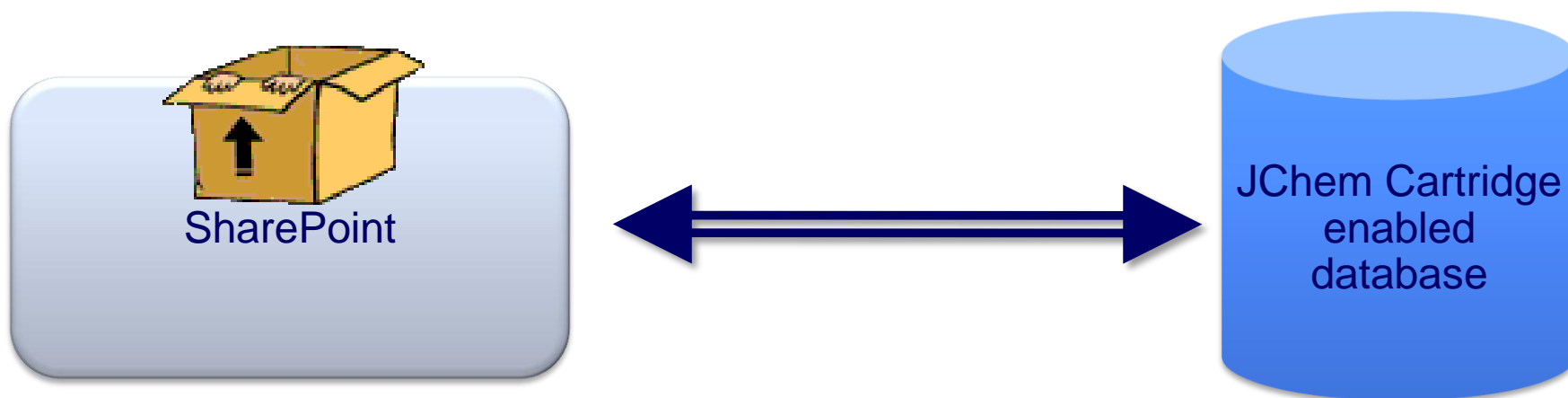
# Out of the Box Cheminformatics

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Simple but useful

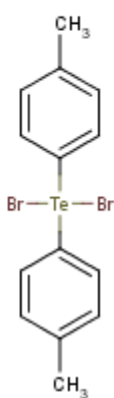
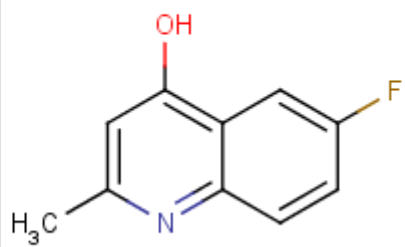
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- Handle lists of data
- Connect to databases and extract data (SQL / calls to PL/SQL – e.g. Cartridge functions)
- Create forms to query & filter lists and database connections (SQL / PL/SQL do the processing)
- Do simple calculations in columns of lists of data



# Out of the Box

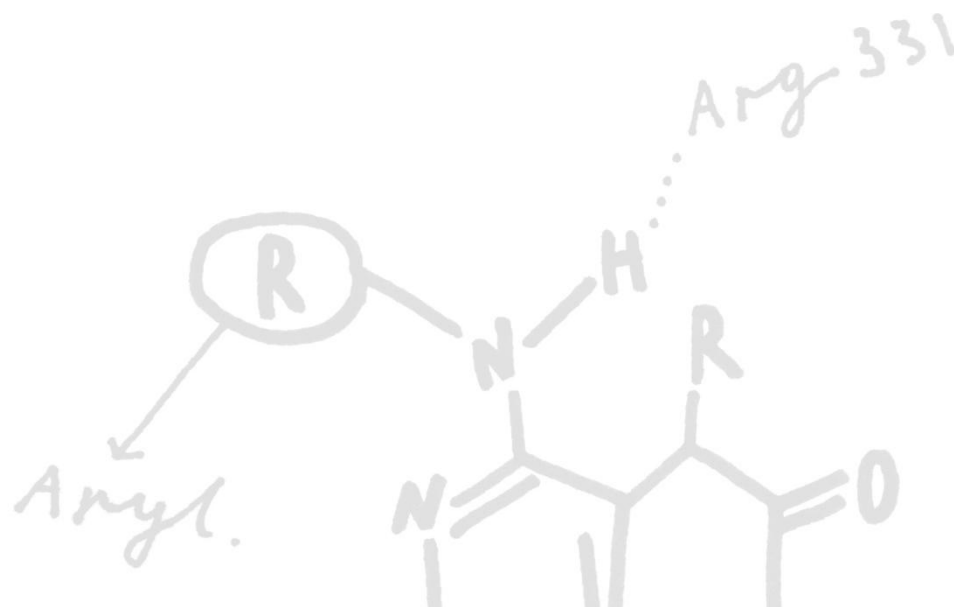
With a little help...

dev	All Sites			
	Smiles	Mol Wt	Mol Formula	Ifs Part Id
Intranet Questionnaire		469.67	C14H14Br2Te	257731
Libraries				
Site Pages				
CAF v2				
structures				
Lists				
Phone Call Memo				
Staff				
testlinks		177.175	C10H8FNO	15739
Holidays				
Time Card				
CAF v1				
Compounds				
Discussions				

## Agenda

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# What we really want to do

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Collaboration with structures!

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- Be able to draw structures in
  - Lists
  - Libraries
  - discussion groups
  - wikis
- Calculate properties
- Naming
- Plugins (our own calculators!)
- Structure search in...
  - Lists
  - Libraries (i.e. inside documents)
  - Existing databases (cartridge or JChem Base)
- Visualization
  - Like IJC Viz (simple plots) (3<sup>rd</sup> party tools!)



## Use Cases

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Some examples

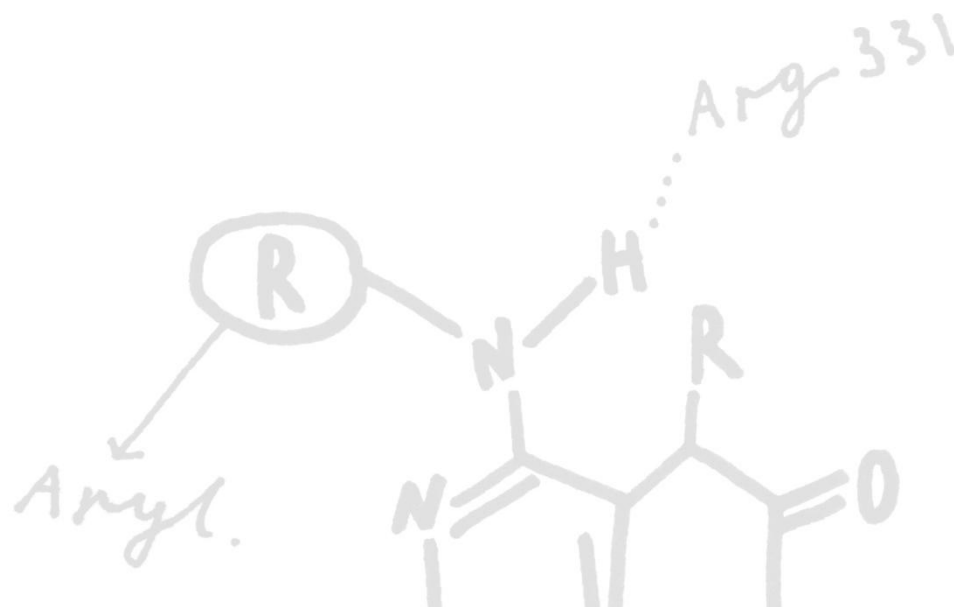
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- Find out how a compound was synthesized when a hit is found in a screening run (requires structure search through a lot of word documents)
- In projects where the chemistry done in UK and India, each week, they look through an Excel Spreadsheet of compounds chosen by the client and each chemist will choose what to synthesize next. In SharePoint this could be achieved by “checkin out a compound”
- Saving ourselves and our clients the cost of e-rooms - with the advantage that they are chemistry aware
- Building knowledge centres of chemistry for particular targets
- Searching through existing PowerPoints for relevant chemistry when preparing proposals for new clients
- Devolved access control – easier for PMs to manage who sees what (chemistry)!
- Less duplication of files
- One place for Wikis, help files, discussion groups, etc. for all applications, etc.

## Agenda

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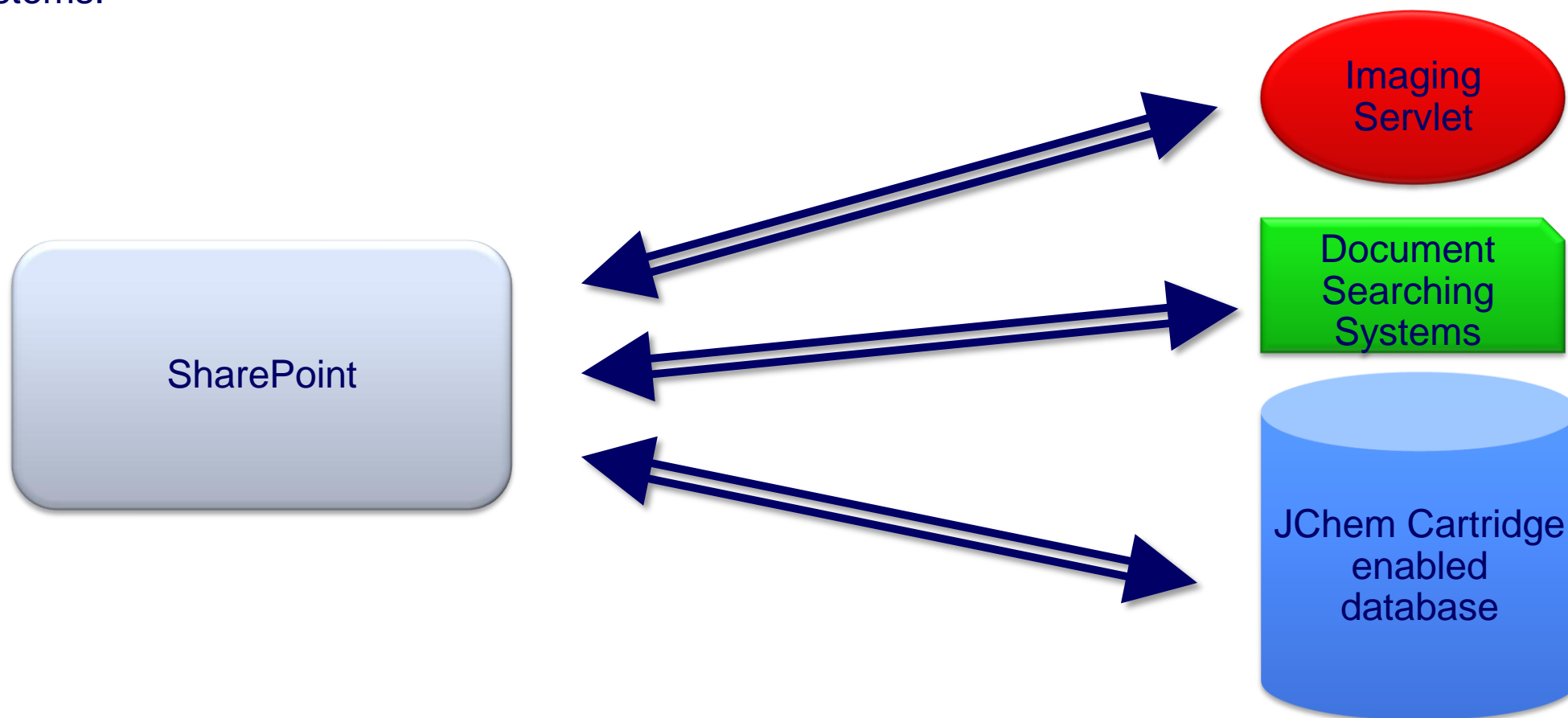
- What's the (Share)Point?
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# Hacks, Hacks and more hacks!

Utilising all resources

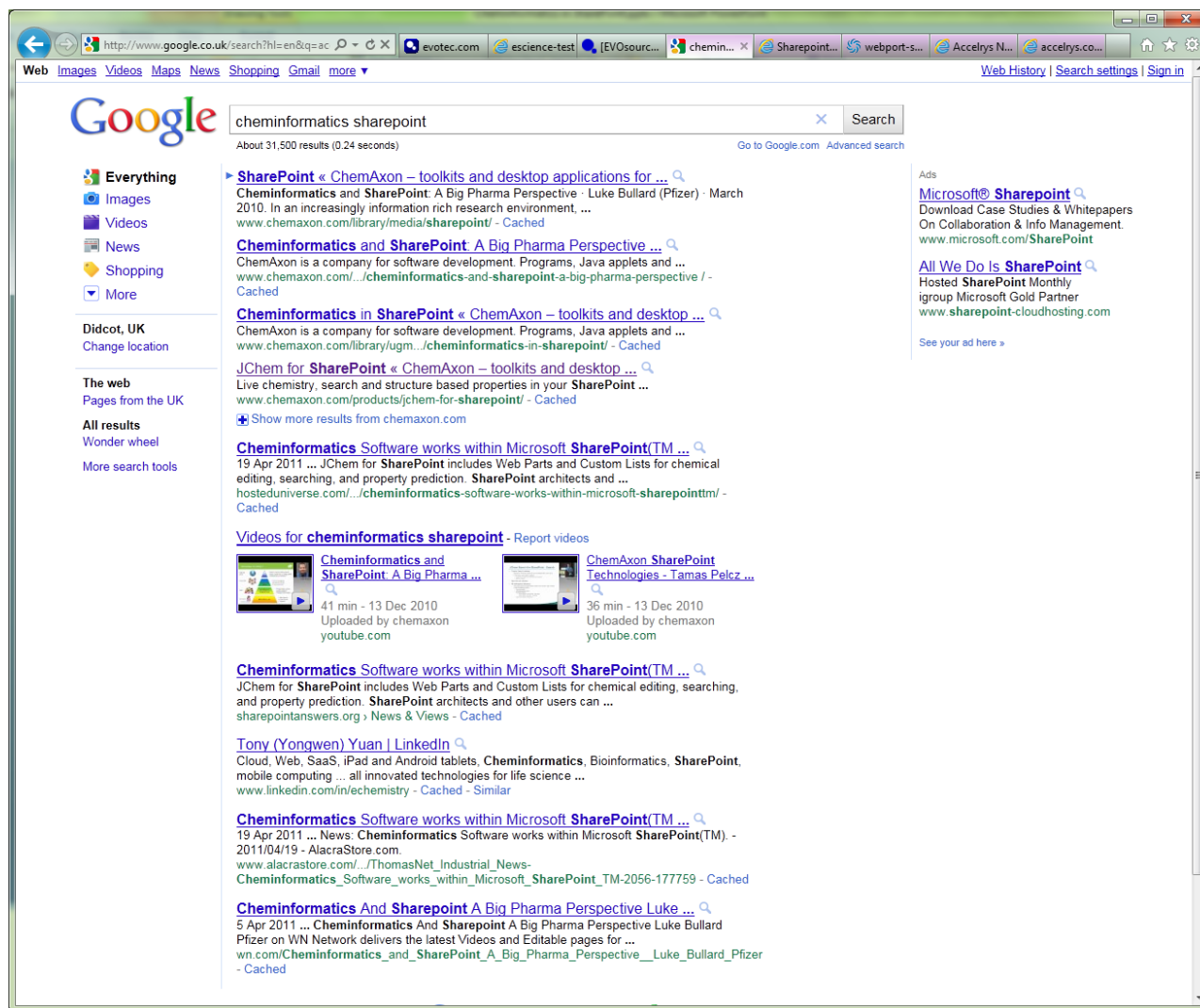
- There is always a way to do what you want, but it mostly will include hacks and links to other systems.



# Others have seen the potential

But we won't discuss those here!

- ChemAxon makes the first page and a half of Google results...
- The others only make the second page!
  - Isentris for SharePoint
  - Pipeline Pilot
  - etc.



# JChem for SharePoint

Showing the possibilities!


cxn > NCI100

## NCI100

NCI100 Custom List





Select a list: NCI100

Select a molecule field: Structure

Search Type: Substructure 

Apply Filter Clear Filter

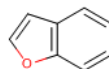
New Actions Settings View: All Items

Structure	logP	IUPAC Name
	2.153693549	2-chloro-4,6-dinitrophenol
	1.906019194	7-chloroquinolin-4-amine
	4.550064919	(4-chlorophenyl)(4-methylphenyl)methanone
	2.371364015	7-chloro-3-nitroquinolin-4-ol

Template > ChemAxon Wiki > Benzofuran

## Benzofuran

**Benzofuran** is the [heterocyclic compound](#) consisting of fused [benzene](#) and [furan](#) rings. compounds with more complex structures. For example, [psoralen](#) is a benzofuran deriv



Last modified at 5/5/2010 4:58 PM by System Account

ChemAxon Demo > Markush > (no title) > Edit Item

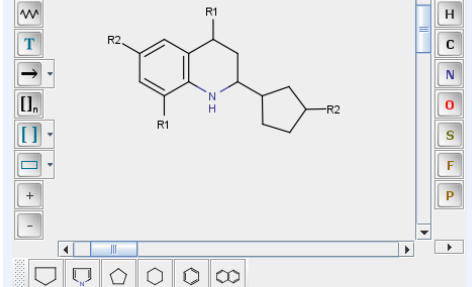
## Markush: (no title)

Attach File Delete Item

Structure

Molecule Editor

File Edit View Insert Atom Bond Structure Tools Help



Structure Field

Enumeration Count

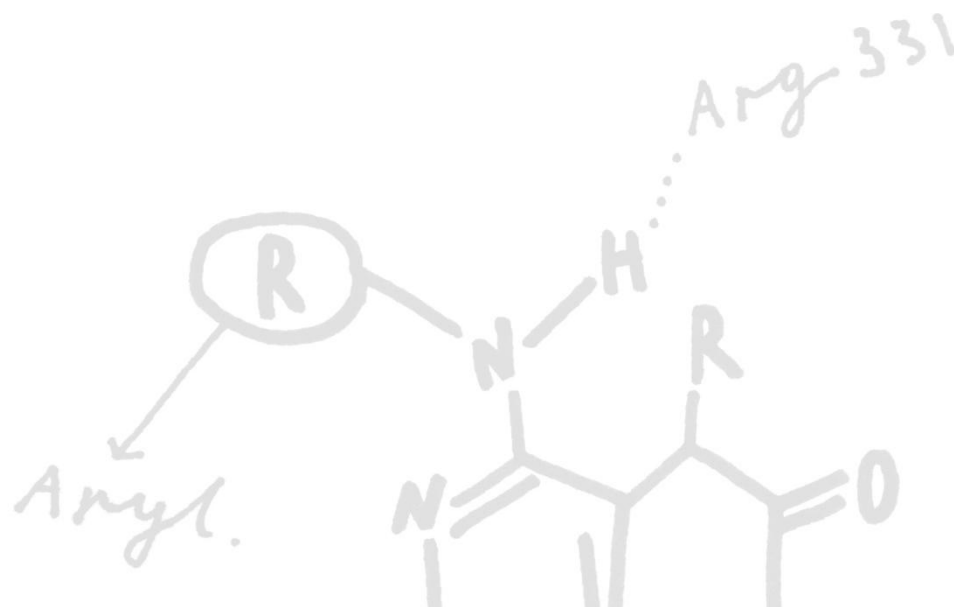
Chemical Term - Enumeration Count

Created at 4/30/2010 12:10 PM by System Account  
Last modified at 4/30/2010 12:10 PM by System Account

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## Conclusion

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### Changing quotes

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- At the 2010 EU UGM, Luke Bullard (Pfizer) stated:

**The answer is SHAREPOINT,  
Now what's your question?**

- I propose a slight change to...

**The answer is SHAREPOINT,  
Now what do you want to do?**



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