

BUSINESS TECHNOLOGY



ChemInformatics in SharePoint: A Big Pharma Perspective

Location: ChemAxon UGM, Budapest, Hungary

Date: 19th May 2010

Presenter: Luke Bullard



Pfizer Internal Use

What's all the fuss about ???



**“The answer is SharePoint..... Now,
what’s your question?”**



To understand “why”, one must understand what SharePoint is and how it is used in a company like Pfizer.

In the past project teams have traditionally used many methods to “run” the project:

- Specialized apps for Chem & Bio Informatics (e.g. Instant JChem, Accord for Excel etc..)
- E-Mail for “current thinking”
- Network shares & personal hard disks to store working documents such as target lists, patents of interests etc..
- No obvious central location for project information e.g. Top five promising compounds

Combine web based collaboration features
(Microsoft SharePoint) with desktop
productivity application (Microsoft OneNote)

The combination is known in Pfizer as
“OnePoint”.

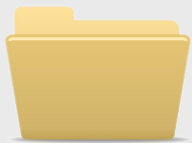
Note: You can view the Microsoft Case Study and Video showing the use of OnePoint in Pfizer
here : http://www.microsoft.com/casestudies/Case_Study_Detail.aspx?casestudyid=4000004505

What is SharePoint ?



SharePoint powers Team Sites

SharePoint 2007 provides a broad collection of tools for team collaboration and document management.



Store files

Store and share all of your Word, Excel, PowerPoint and OneNote files



Create lists

Create team to-do, resource, issue, risk or any other type of tracking list



Manage Permissions

Control exactly what users can see and do within your site



Calendar

Create team calendars – view in traditional calendar view or as a list



Discussion Boards

Host online discussion and bulletin board forums and blogs



Workflow

Create custom workflows to identify the steps required to complete tasks

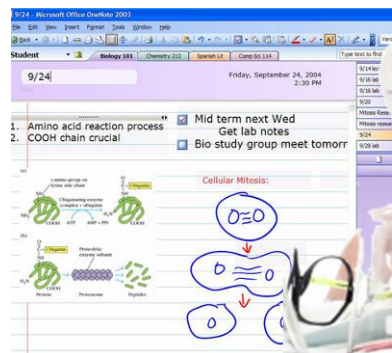
What is OneNote ?



OneNote Shared Notebook

Microsoft OneNote facilitates free-form information gathering and multi-user collaboration.

“An easy-to-use note-taking and information-management program where you can capture ideas and information in electronic form. Insert files or Web content in full-colour, searchable format or as icons that you can click to access.” [Microsoft](#)



Capture notes

Capture notes as you would in a paper journal.



Work together

OneNote 2007 introduced the concept of *shared notebooks!*



Attach or embed files

Drop files directly onto the page...and automatically have them stored in SharePoint



Synchronization

Work online. Work offline. Work on a shared notebook. OneNote takes care of all the synchronization!



OCR

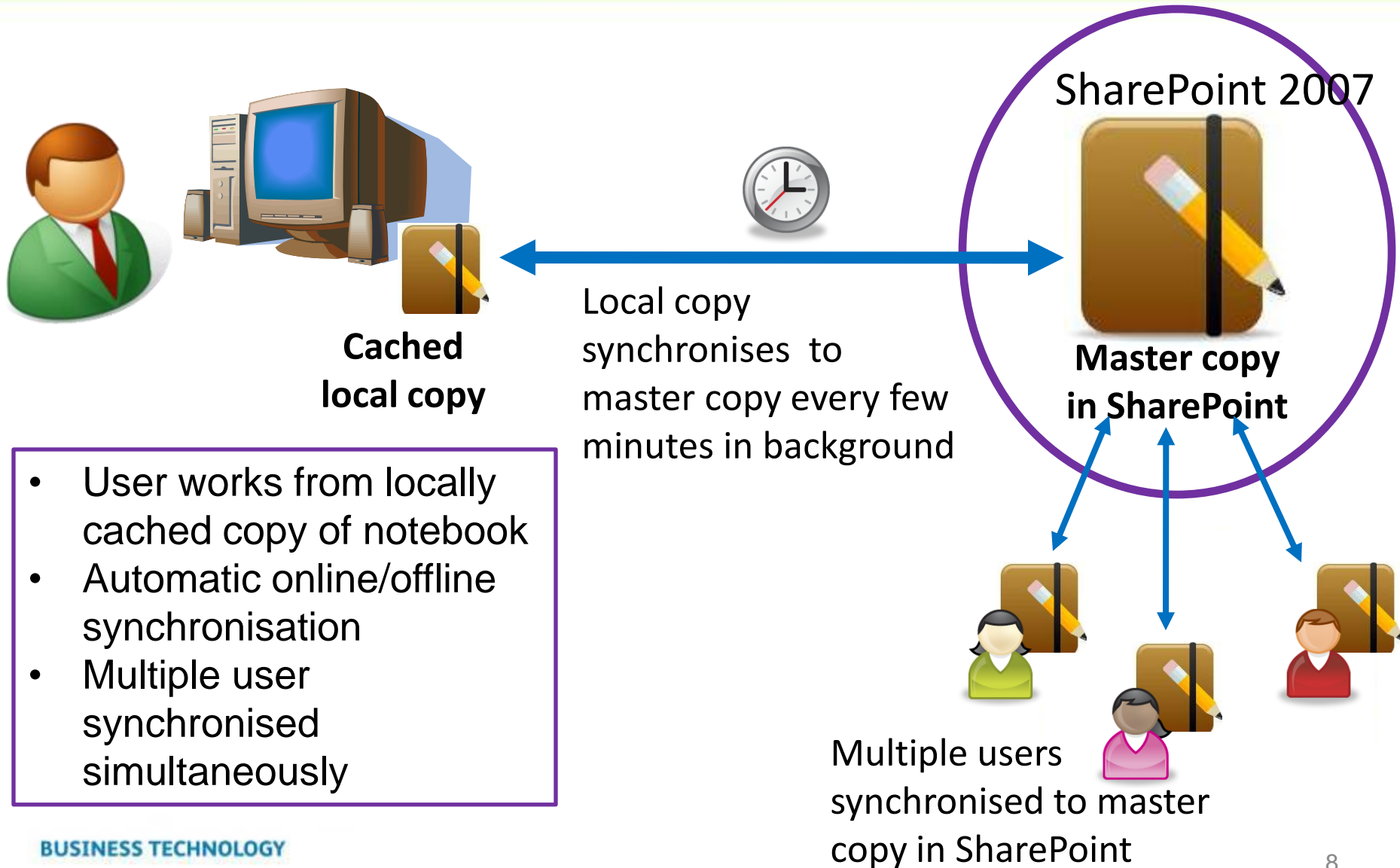
Take screen clippings or insert images – automatics OCR!



Sharepoint

OneNote can be used in conjunction with Sharepoint.

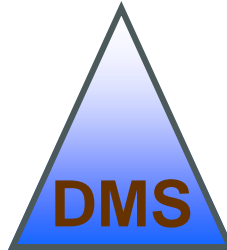
OnePoint = OneNote + SharePoint



Where does it fit in Pfizer ?

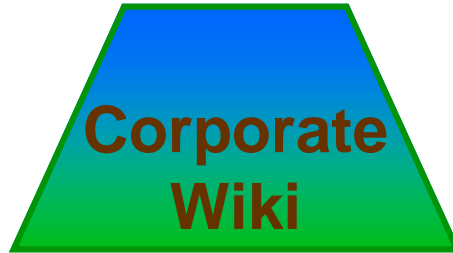


External world



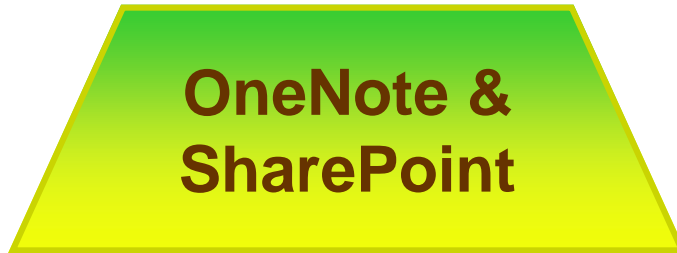
- Historic record of key events
- Static snapshots i.e. Stage gates
- Validated documentation

Corporate



- Current progress
- Structured format
- Living document

Team



- Project team centric
- Idea evaluation
- Transient information

Individual



- Idea capture
- Unstructured
- Transient

SharePoint is much more than just a place to put files.

List creation is a very powerful mechanism for team members to solve collaborative problems.

For example

- Lab equipment booking system
- Synthesis target recording and resource management

Announcements are useful for things like structural alerts.

Blogs can be used for things like synthetic problem solving (“I need help with this.....”)

Nice Team Site Example



Sandwich Research > Research Units > Allergy & Respiratory > Operations > COPD POC/POM LDT

Welcome Haque, Nuzul | My Site | My Links | Email Site URL | Add Site to Favorites

COPD POC/POM LDT

This Site: COPD POC/POM LDT

COPD POC/POM LDT

- View All Site Content
- Discussions**
 - COPD Post Board
- Documents**
 - Document Library
 - OneNote Library
- Lists**
 - Action Tracker
 - Literature References
 - Meetings
 - Team Members
- Sites**
 - Recycle Bin

COPD Proof of Concept (POC) and Proof of Mechanism (POM) Limited Duration Team

For information about this Project please contact: [Click here to email Steve directly](#)

Announcements

Unbiased review of the efficacy and safety of [redacted] in COPD 05/03/2010 13:37
by [redacted]
This review is worth a read as it compares the impact of [redacted] on exacerbation frequency with that of ICS and ICS/beta-agonist combinations.

New meta-analysis of Treatment effect on COPD Exacerbations from [redacted] 15/01/2010 17:16
by [redacted]

Draft Slide Set Results and Recommendations of COPD POM/POC Team 13/01/2010 15:33
by [redacted]
An early draft slide set (updated from 13/1/10 meeting) compiled from team minutes and slide sets can be found in the Documents and Files area. Team members, please review and provide feedback. The slide set is short on recommendations so far, but as...

Inhibitor Whole Lung LPS Slide Set 25/11/2009 17:15
by [redacted]
The slide set showing the effects of the [redacted] inhibitor [redacted] in human whole lung LPS challenge has been posted in the documents folder.

Impressive efficacy of triple therapy in AJRCCM article in press @ 12/08/2009 10:26
by [redacted]
Please find attached a paper from AZ describing triple therapy with [redacted] added to it. Efficacy in the study impressive and claim significant reduction in exacerbation, although study period relatively short (12 weeks). High hurdle for...

Add new announcement

Literature References

Reference Title	Created By
Antibiotics and reduced risk of COPD re-exacerbations.	[redacted]
Antibiotics for exacerbations of chronic obstructive pulmonary disease.	[redacted]
Antibiotics for exacerbations of chronic obstructive pulmonary disease.	[redacted]
[redacted] in chronic obstructive pulmonary disease: evidence from large trials.	[redacted]
[redacted] in chronic obstructive pulmonary disease: evidence from large trials.	[redacted]

Add new link

Documents and Files

Click on icon to access the Document Library to View and Upload Content that is **NOT associated specifically to LDT meetings**

Post Board

Click on icon to access the Discussion Forum To post Questions and read Answers

Useful Links

- Pfizer Official Public A&R webpage
- Journal of Allergy

Add new link

Lists are really cool...



Sandwich Research > Research Units > Allergy & Respiratory > Exploratory > NHLI Collaboration

Welcome Haque, Nuzrul | My Site | My Links



NHLI Collaboration

This List: Toolbox compo

NHLI Collaboration

NHLI Collaboration > Toolbox compound list

Toolbox compound list

New Actions Settings

PF-Number Structure Target Pathway eric Target location Cytotoxicity IC50 (µM) Compound properties Primary/whole cell literature data It link Selectivity profile

		Akt	Inhibitor; Allosteric	Intracellular	to be tested				Yes
--	--	-----	--------------------------	---------------	--------------	--	--	--	-----



		Akt	Inhibitor; Allosteric	Intracellular	9.7				Yes
--	--	-----	--------------------------	---------------	-----	--	--	--	-----



		Akt	Inhibitor	Intracellular	to be tested				Yes
--	--	-----	-----------	---------------	--------------	--	--	--	-----



View All Site Content

Discussions

Documents

- Clinical Documents
- OneNote Library
- Pre-Clinical Documents

Lists

- NHLI Onenote
- R-gate
- Team Calendar
- Toolbox compound list

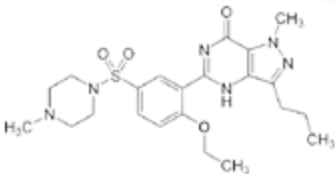
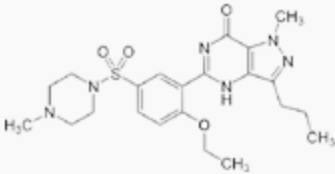
Sites

- Recycle Bin

Compound List Filtering



View: Lab work

PF-Number	Target Pathway	Compound properties	Cytotoxicity IC50 (uM)	Inventory	lit link	Primary/whole cell literature data	Structure	Target location
	Akt	Clear Filter from Cytotoxicity IC50 (uM)	(Empty)	135 mg				Intracellular
	Akt		>100	435 mg				Intracellular

to be tested

Ok, so what's the big problem ?



Problem #1

The “structure” is a common currency within the Chemistry discipline, however as yet we do not have a simplistic way to use this data type in SharePoint.

Problem #2

If you embed structural assets in documents & lists (assuming you fix problem #1!) etc.. within SharePoint, you must provide a way to search for these assets.

What we have now...



Sandwich Research > Research Units > Allergy & Respiratory > Exploratory > NHLI Collaboration

Welcome Haque, Nuzrul | My Site | My Links



NHLI Collaboration

This List: Toolbox compo

NHLI Collaboration

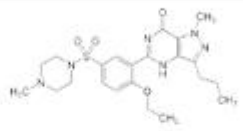
NHLI Collaboration > Toolbox compound list

Toolbox compound list

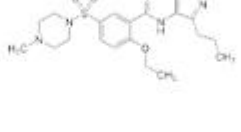
New Actions Settings

PF-Number Structure Target Pathway Target location Cytotoxicity IC50 (µM) Compound properties Primary/whole cell literature data It link Selectivity profile

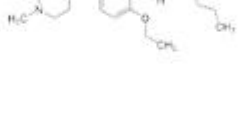
  Akt Inhibitor; Allosteric Intracellular to be tested Yes



  Akt ALLOSTERIC to be tested Yes

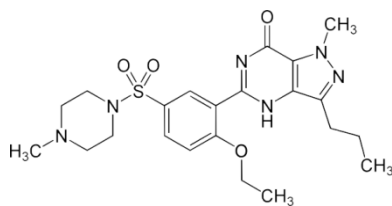


  Akt Inhibitor Intracellular to be tested Yes

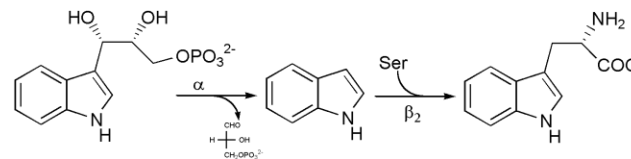
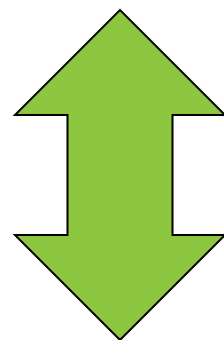


Structures in Lists etc.. are actually images that cannot be manipulated or searched !

“What chemists really want is the ability to use SharePoint like they currently use Word/PowerPoint/Excel.”



Single compounds



Reaction schemes

Rich Text Areas

Lists

Blogs

Announcements

Wikis

- Calculated properties available as extra columns on list where a structure has been defined
- Intra-list structural filtering nice but not essential

Bad News

- Traditional SharePoint search doesn't provide for complex data type queries
- Structures can be embedded within documents in Document Libraries, Lists/Blogs/Wikis etc (assuming problem #1 is fixed) but then cannot be surfaced
- Surfacing structure based search results needs thinking through to be effective
- Additional overhead of structure analysis can adversely effect SP performance

Good News

- However, search complexity can be reduced as the full range of options are not needed.

Structure Search Results Mock-up



Pfizer Welcome Bullard, Luke

Search Center My Home My Profile PfizerWorld

All Sites People GO-Search

Find documents with... **By Structure**

All of these words:

The exact phrase:

Any of these words:

None of these words:

Narrow the search...

Only the language(s): French German Japanese Spanish

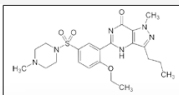
Result type:

Add property restrictions...

Where the Property... Equals

Working together for a healthier world™

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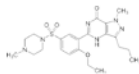


Pfizer Welcome Bullard, Luke

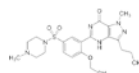
Search Center My Home My Profile PfizerWorld



All Sites People GO-Search

Results 1-10 of about 1,536. Your search took 0.98 seconds. [Results by Relevance](#) | [View by Modified Date](#) | [Alert Me!](#) [RSS](#) Processed 300 results | Not cached

 **ChemaAxon User Group meeting Test Document.doc**
This section usually represents the summarised data from the file that was found as a result of the search.
<http://ecf.pfizer.com/sites/sandwichinformatics/ChemAxonUGM/Test.doc>
19/05/2010, 2KB

[+ 2 others](#)

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19/05/2010, 2KB

Content Type

- PDF (65)
- PowerPoint (58)
- HTML (42)
- Word (33)
- Event (21)
- ...

Language

- English (290)
- French (1)
- German (2)
- Indonesian (1)
- Italian (4)
- ...

- Same drawing rules as corporate tools
- Automatic structural resolution of both corporate id's and SMILES/INCHI text (Name2Structure as well !)
- Exact match & substructure should be supported.
 - Functional groups not really critical
- Basic filtering should be available, i.e:
 - Stereo chemistry
 - Mol Weight
- Search result metadata important for quick sifting

Implementation of SharePoint is more important than the deployment.

Use SharePoint as a summarisation tool for project data, and don't try to replicate Instant JChem !

Encourage self-service behaviours – i.e. use Lists to self manage resources in project teams.

Live structures are a **MUST** have

Search becomes much more important as project teams embrace using SharePoint

Thanks to the following for supplying various slide decks for me to steal from...



• Ben Gardner – ben.gardner@pfizer.com



• Nuz Haque - nuz.haque@pfizer.com



• Simon Revell – simon.revell@pfizer.com

Questions

