

ModSpace

Promoting
dissemination and
reuse of models
and modeling
results

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The Problem

- While groups are few and small, communication is easy to maintain
- But as groups grow and become more diffuse, must find another solution



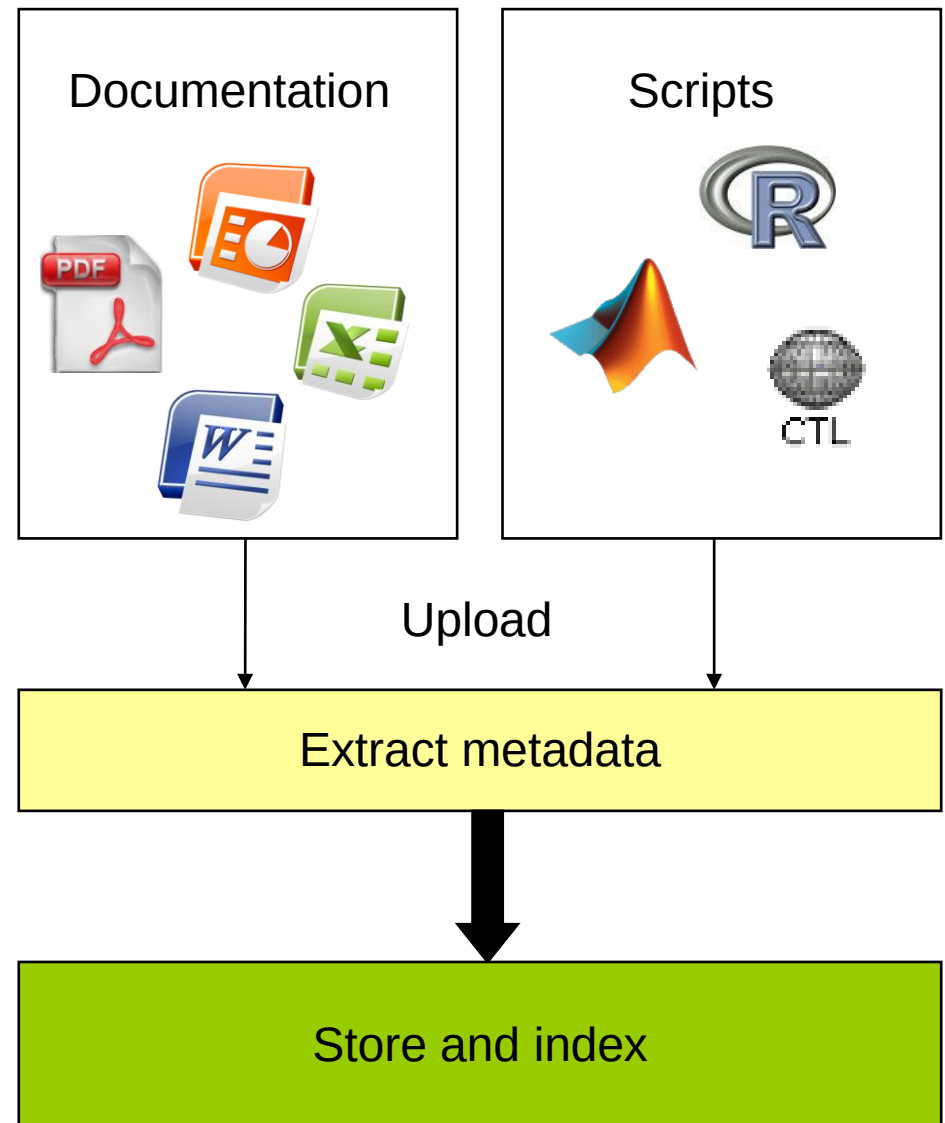
A Drug and Disease Model library

- A searchable repository of ordered, tagged information
- Repository contains:
 - Completed modeling projects
 - Templates for new model
 - Standard scripts and toolboxes
 - External literature



Adding an entry

- Import from local file system or SVN
- Extract metadata
- Fill in any missing metadata
- Publish



Extract and display metadata

- Coding standards define headers
- ModSpace reads and parses files to extract and match metadata
- Specific to the type of file being added (R, NONMEM, etc.)

```
% [DESCRIPTION]
% The function reads in the NONMEM c
% dosing times and amounts + the PK info
clc; clear all; close all

% CHANGE TO THE CORRECT FOLDER
cd('P:\ABC123\indication1
```

```
[NAME]
Chemokine XYZ target summit

[DESCRIPTION]
This folder contains MATLAB code and associated
The target was a soluble protein, a small chemo
The receptor was not modelled. We considered a
fibronectin, and aptamer based drug.

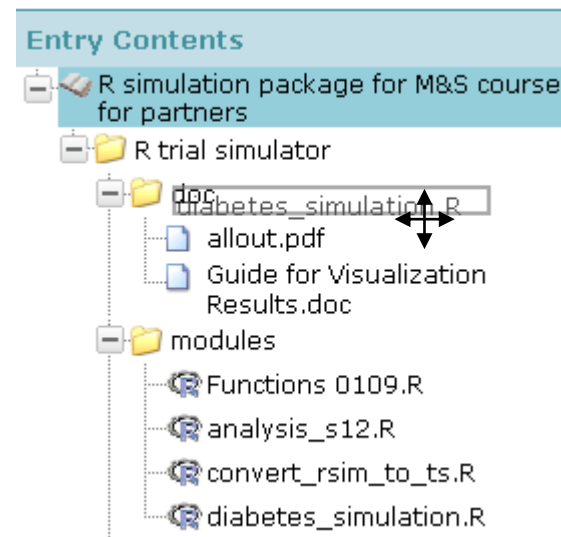
[KEYWORDS]
target summit, matlab, early biologics
```

[DISEASE]	Overview	File Preview	History
Inflammato	Overview of 'additiv		
Filename:	additive.nmctl		
Problem:	Fitting a two compartment model		
Problem Count:	1		
Subroutines:	ADVAN3 TRANS4		
Table Outputs:	C, ID, TIME, RATE, AMT, LCT, PD1,		
Table Filenames:	inf2.tab		
Input Data:	DOG1.CSV		
Thetas:	4 (Theta1,Theta2,Theta3,Theta4)		
Omegas:	1 (Omega1)		
Sigmas:	0		

Entry content

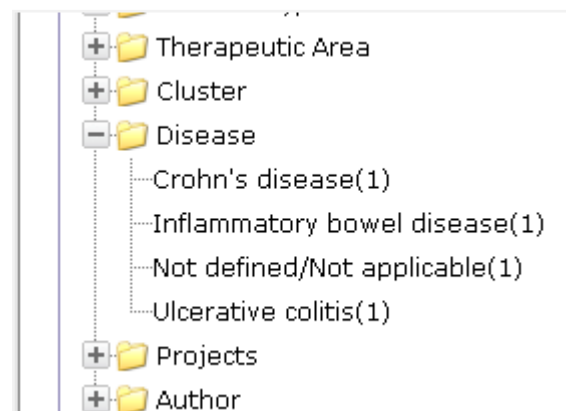
- In place editing, setting and suggesting metadata
- Complete control over entry structure
 - Add/Remove files
 - Drag and drop content
- *All configurable*
 - Possible values, fields

Drug Type:	Biologics
Disease: (Look up and select)	he
	Heart failure
	Helicobacter pylori infection
	Hematologic Malignancies
	Hepatitis C (H CV)
	Hereditary Angioedema
Mechanism:	
Cluster:	Cardiovascular Medicine
Language:	R



Search

- Search on:
 - Metadata
 - E.g. Disease, language, libraries used
 - Content
 - Word, PDF, PowerPoint
- Filtering
 - Is “smart”
- Based on Lucene



	Name	Last Modified	Sc
	<u>Calculating individual weighted residuals correctly with different error models</u> This document describes how to code a NONMEM model in order to be able to calculate individual weighted residuals correctly. The document includes code examples and explanations for NONMEM only, but ... IWRES , individual weighted residuals , NLME , nonlinear mixed effects , NONMEM , MONOLIX , error models Liam Shields , Helene Karcher , Roland Fisch	05 Oct 2009	
	<u>Chemokine XYZ target summit</u> This folder contains MATLAB code and associated documentation used for target summit modeling		

Helping users search

- Did you mean?

Search Results

No results found
Your search **pratform** did not match any results.
Did you mean?
[platform](#)
[perform](#)
[reform](#)

d

diabetes

- disease:
- drugtype:
- description:

- Suggestions

MODSPACE

Advanced Search

disease:"inflammatory"

Find entries that have:

fields that contain these values:

all these words:

this exact word or phase:

one or more of these words:

But don't show entries that have:

any of these unwanted words:

disease inflammatory

author

platform

OR

- Advanced

Viewing entries

- Browsers can view metadata and history
- Logged in users can
 - Preview
 - Download

The screenshot displays a web interface for viewing file entries. At the top, there are three tabs: 'Overview', 'File Preview', and 'History'. The 'File Preview' tab is active, showing a code snippet in R. The code includes a description, setup paths, and a random number generator seed. Below the code, there is a table with columns 'Name', 'Author', and 'Description'. The table contains one entry: 'R simulation package for M&S course' by 'Oliver Sander'. The description states: 'This package contains the R-simulation package for partners. This is, ..., the content of the package is stored with the simulation package in the root directory. The code is not finished. For more information, please contact Oliver to provide more details. Once we have a decision, we should change the package name to ... any suggestion is welcome. The package name should be "MOOGLE.txt" or "MODSPACE.txt" or "MODSPACE.txt"?'.

Overlaid on the interface are two dialog boxes. The first is a 'Ready for download' dialog with a question mark icon and the text 'File size is 23.60MB. Continue?'. It has 'Yes' and 'No' buttons. The second is a 'Preparing file(s)' dialog with a progress bar and the text 'Please wait...'. It has a 'Cancel' button.

```
## [Description]
## This can be run by using source() or by copying and pasting
## an R Console. MAKE SURE TO SET THE WORKING DIRECTORY BEFORE
## The working directory needs to contain the R files for the
## especially (as they are sourced):
##   - modules/diabetes_simulation.R
##   - modules/convert_rsim_to_ts.R
##   - modules/Functions_0109.R
## The output of the simulation will be stored in the subdirectory
##
VERBOSE = 1
#####
# Setup paths
#####

## Set random number generator seed
set.seed(1)
```

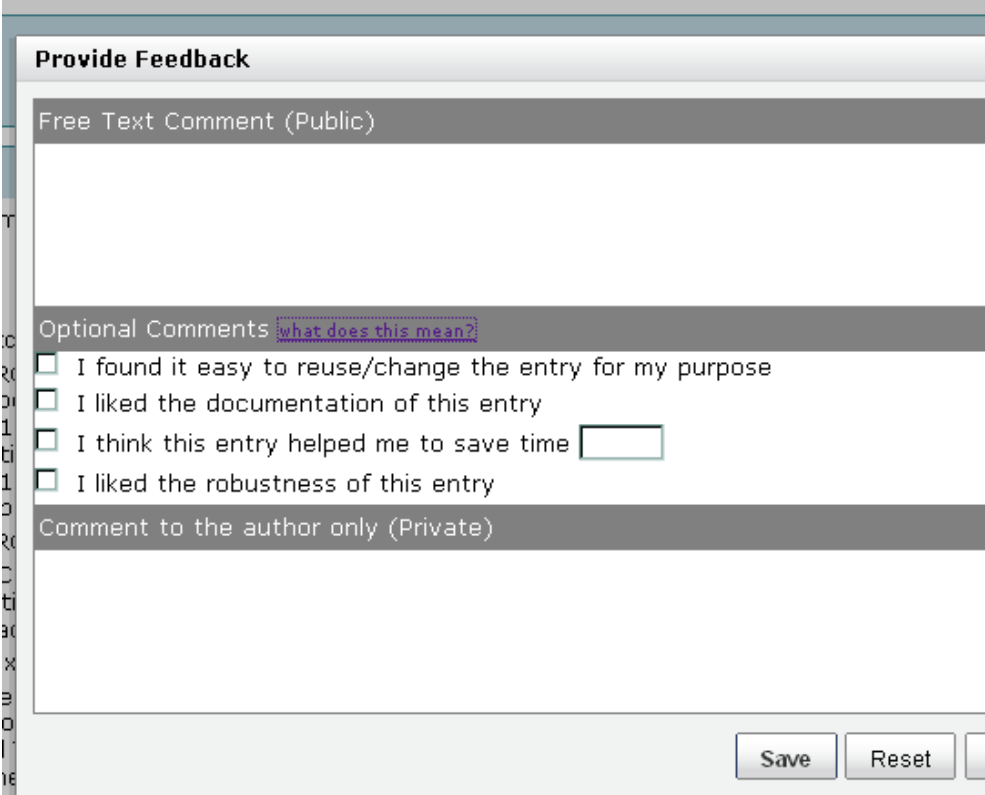
Name	Author	Description
R simulation package for M&S course	Oliver Sander	This package contains the R-simulation package for partners. This is, ..., the content of the package is stored with the simulation package in the root directory. The code is not finished. For more information, please contact Oliver to provide more details. Once we have a decision, we should change the package name to ... any suggestion is welcome. The package name should be "MOOGLE.txt" or "MODSPACE.txt" or "MODSPACE.txt"?

Ready for download
File size is 23.60MB. Continue?
Yes No

Preparing file(s)
Please wait...
Cancel

Feedback

- Downloaders reminded to give feedback
- Public and private comments
- Provides metrics about the quality of the entries



The screenshot shows a web form titled "Provide Feedback". It contains three main sections: a "Free Text Comment (Public)" section with a large text area; an "Optional Comments" section with four checkboxes and their corresponding text: "I found it easy to reuse/change the entry for my purpose", "I liked the documentation of this entry", "I think this entry helped me to save time" (with a small input box), and "I liked the robustness of this entry"; and a "Comment to the author only (Private)" section with another text area. At the bottom right, there are "Save" and "Reset" buttons.

Provide Feedback

Free Text Comment (Public)

Optional Comments [what does this mean?](#)

☐ I found it easy to reuse/change the entry for my purpose

☐ I liked the documentation of this entry

☐ I think this entry helped me to save time

☐ I liked the robustness of this entry

Comment to the author only (Private)

Save Reset

Groups

- A collection of entries that share a theme or address a particular group of problems
- Has own metadata

The screenshot displays a web interface for a group. On the left, under the heading "Group Contents", there is a tree view showing a folder named "R scripts". Inside this folder, there are three items: "Analysis scripts", "R simulation package for M&S course for partners", and "Graphics scripts". On the right, there is a tabbed interface with tabs for "Overview", "News", "History", and "Members". The "Overview" tab is selected, showing a table of metadata for the "R scripts" group.

Overview	
Name	R scripts
Description	A collection of R scripts for gen
Keywords	boxplot, tornado plot
Therapeutic Area	Not applicable
Drug Type	Not applicable
Target Categories	Not applicable
Cluster	Cardiovascular Medicine
Language	R

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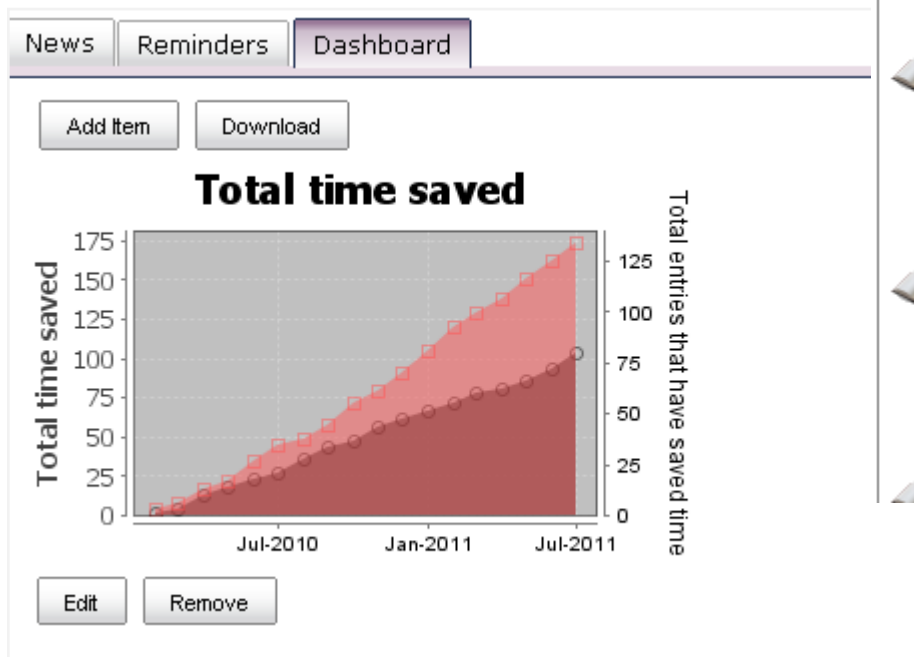
Contents		
R simulation package for M&S course for partners	dbrowne	Open

Home page

- Bookmarks
- News feed
- Reporting dashboard

Bookmarks

- + Unpublished Items (2)
- My Bookmarks
 - Calculating individual weighted residuals correctly with different error models
- My Entries
 - Model of I κ B-NF κ B signaling in wild type cells
 - wbailey 20091005 18:54:47
- + My Groups
- + Recently Viewed



 Feedback : Chemokine XYZ target summit
This model is really interesting, but the documentat
✓ *I think this entry helped me to save time (4 hrs)*
Warren Bailey, 05-Oct-09 01:18

 Update : Model of I κ B-NF κ B signaling in wild type cell type cells
The model is based on the following paper: Science :
IkappaB-NF-kappaB signaling module: temporal cont
Hoffmann A, Levchenko A, ...
Updated link to paper
Warren Bailey, 05-Oct-09 12:58

 New : Calculating individual weighted residuals corre
Calculating individual weighted residuals correctly wi
This document describes how to code a NONMEM mo
individual weighted residuals correctly. The documen
explanations for NONMEM only, but...
Initial version
Liam Shields, 05-Oct-09 12:55

 New : Model of I κ B-NF κ B signaling in wild type cells :

Reporting

- Evidence that the system is providing value
 - Growth in usage
 - Number of entries
 - Size of groups
 - Downloads
 - Collaboration
 - Quality of entries
 - Quantify the feedback
 - Expose popular/useful entries
 - “Related entries”





Questions?

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