

## **Presentation of a web-based ELN system**

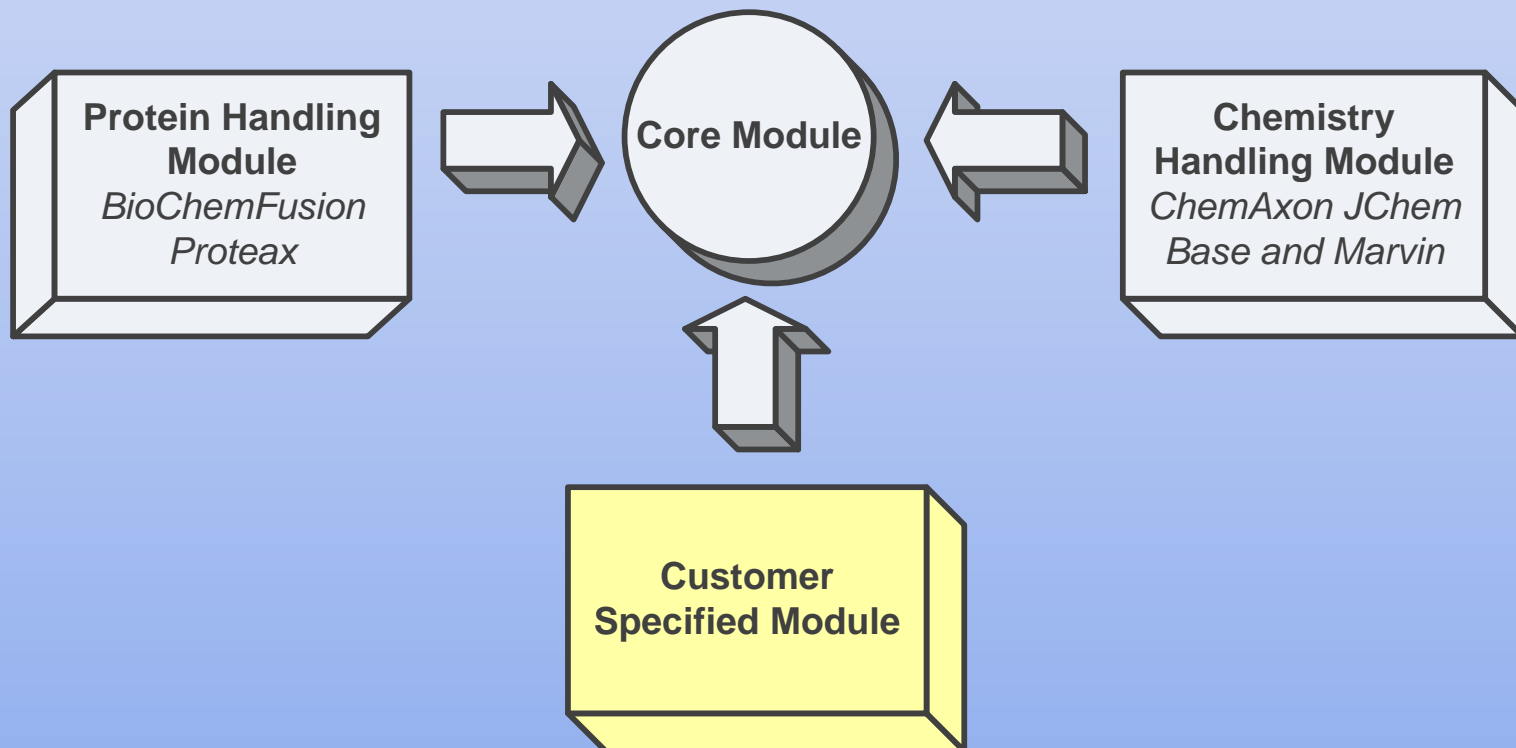
## Concept of Sysment Notebook

- ❑ **hostable, web-based electronic laboratory notebook**
- ❑ **browser and database independent**
- ❑ **unique combination of traditional medicinal chemistry and biopharmaceuticals**

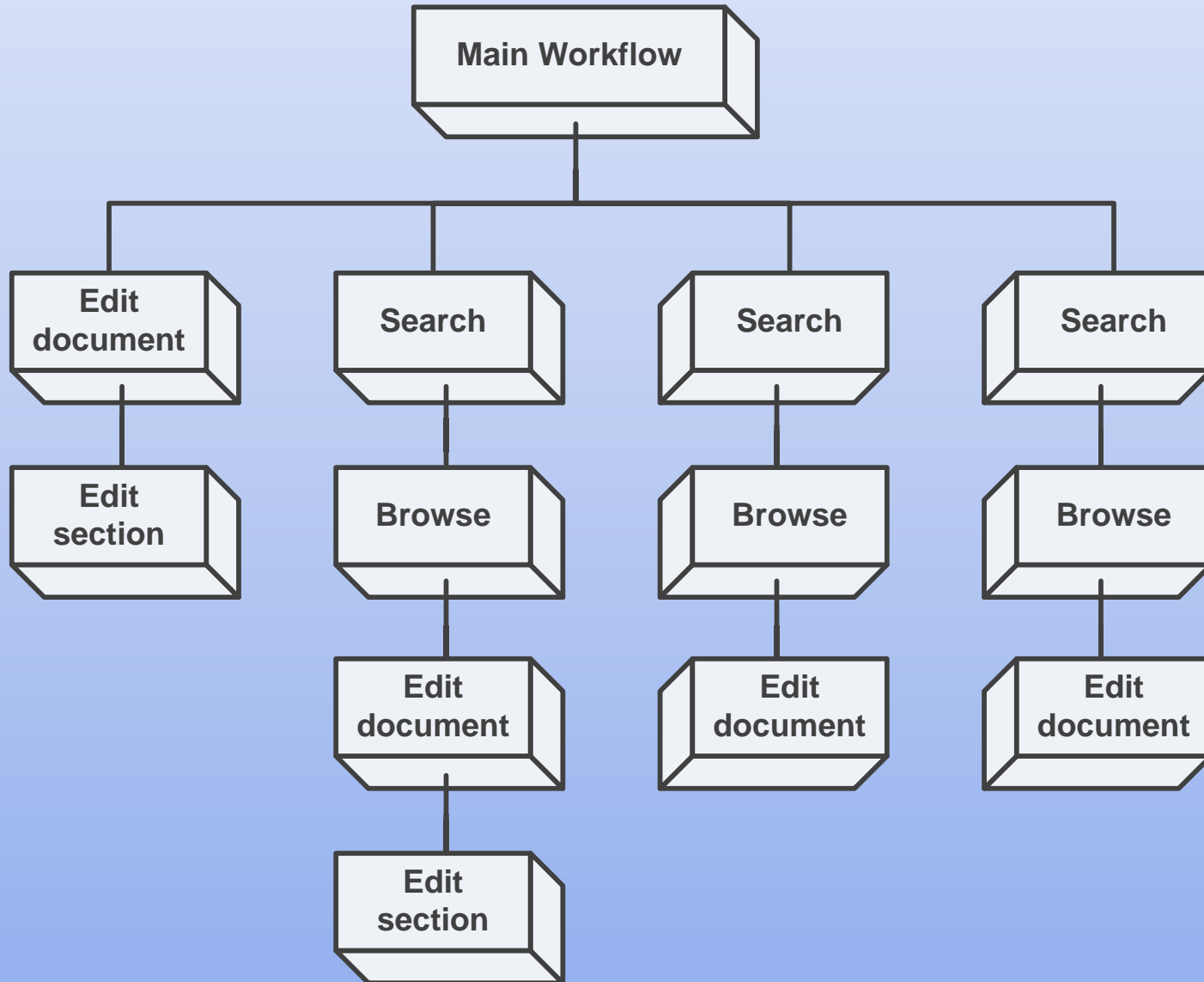


## Modularity

- well-equipped and configurable core software with basic functionality prepared for many plug-in modules



# Workflow handling



# The document

- fundamental unit and entry point in the ELN application

The screenshot shows the 'MainPage' in Mozilla Firefox. The browser address bar shows 'http://30.0.0.246:82/Default.aspx'. The page title is 'MainPage'.

**document header**: A callout points to the 'Document Header' section, which includes 'Document Number: NUM:00014', 'Projects: 0025: insulin project', and 'Keywords: insulin'.

**add a new section to the document**: A callout points to the 'Available Section Types' sidebar, which lists: 'New Reaction', 'Add File Attachments', 'New Html Section', and 'New Text Section'.

**sections – logical paragraphs in the document**: A callout points to the main content area, which shows a section titled 'Synthesis of ε-NB29-dehydrocholyl insulin' with a 'Include in Extract' checkbox checked. Below the title is a sequence alignment diagram showing the amino acid sequence: 1 GIVEQCCTSI C SLYQLENYC, 21 N FVNQHL CGS H LVEALYLV C, 41 G E R G F F Y T P K T. A chemical structure of a peptide fragment is shown between the 21st and 41st residues. Below the alignment is an 'Experimental description' section with a 'Include in Extract' checkbox checked. The text reads: 'In this work, a novel acylated insulin, ε-NB29-dehydrocholyl insulin was prepared by covalent linkage of dehydrocholic acid (DHC) to porcine insulin without acrylamide gel electrophoresis (PAGE), reversed phase high performance liquid chromatography (RP-HPLC) and matrix-assisted laser desorption/ionization mass spectrometry (MALDI-TOF-MS). The activated amide was reacted with unprotected insulin and showed free amino groups on insulin in the mixture of water and N-methyl-2-pyrrolidone at pH above 10 in the presence of a group of LysB29 was dominant at pH over 10.'

**links for the existing sections**: A callout points to the 'Existing Sections' sidebar, which lists: 'Synthesis of ε-NB29-dehydrocholyl insulin', 'Experimental description', and 'Analysis results'.

At the bottom right of the page, there are buttons for 'Save', 'Save & Close', and 'Cancel'. The status bar at the bottom left shows 'Done'.

# Integrated Marvin structure editor

The screenshot shows the Marvin structure editor interface within a Mozilla Firefox browser window. The interface includes a menu bar (File, Edit, View, History, Bookmarks, Tools, Help), a navigation pane on the left, a central workspace for drawing chemical structures, and a properties panel on the right. A chemical structure of a complex steroid-like molecule is shown in the workspace. Three callout boxes provide instructions:

- role and name of the component:** A callout points to the 'Component Role' dropdown menu in the Properties panel, which is currently set to 'Reactant', and the 'Component Name' field, which contains 'Activated amide deriv:'.
- decide if the component should appear in the reaction sketch or not:** A callout points to the 'Display in Sketch' checkbox in the Properties panel, which is checked.
- transfer the component to the reaction editor form:** A callout points to the 'OK' button at the bottom right of the Properties panel.

The Properties panel also shows 'Component Name: Activated amide deriv:' and a checked 'Display in Sketch' option. The workspace contains a complex chemical structure with a steroid-like core and a side chain ending in a benzimidazole ring system. The interface also features a 'Navigation' pane on the left with options like 'Create New Document', 'New Search', 'Browse', 'Search List', and 'Saved Browse Lists'. The status bar at the bottom shows 'Done'.

# Protein editor

MainPage - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://30.0.0.246:82/Default.aspx

MainPage

**Protein**

Protein Text: ID HUMAN\_INSUL STANDARD; PRT; 51 AA.  
 DE Human Insulin  
 FT CHAIN 1 21 Chain A  
 FT CHAIN 22 51 Chain B

N-terminal C-terminal

A R N D C E Q G H I L K M F P S T W Y V U

Molecule:  
 Zoom (+) Zoom (-)

**Properties**

Component Role: Reactant

Component Name: Human Insulin

Display in Sketch

Render as Protein

OK Cancel

Done

# Reaction editor with the complete reaction

title of the reaction

roles and names of the reaction components

decide if the reaction should appear in the document extract or not

save the reaction section

MainPage - Mozilla Firefox  
 File Edit View History Bookmarks Tools Help  
 http://30.0.0.246:82/Default.aspx  
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**Reaction Section**

Title: Synthesis of ε-NB29-dehydrocholyl insulin  
 Include in Extract:

Reaction Cal...

Components	
Component Name	Role
Human Insulin	Reactant
Activated amide derivative of dehydrocholic acid	Reactant
ε-NB29-dehydrocholyl insulin	Product

1 G I V E Q C C T S I C S L Y Q L E N Y C  
 21 N F V N Q H L C G S H L V E A L Y L V C  
 41 G E R G F F Y T P K T + C1=CC=C2C(=C1)C(=O)N(C2)C → 1 G I V E Q C C T S I C S L Y Q L E N Y C  
 21 N F V N Q H L C G S H L V E A L Y L V C  
 41 G E R G F F Y T P K T

Add molecule in Delete Edit  
 Import Reaction  
 Ok Cancel

Done

# Calculations

MainPage - Mozilla Firefox  
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 MainPage

Aspirin

unit selection

Reaction Calculations

Mol Unit: mmol Weight Unit: mg Volume Unit: ml

Generate Reaction Table

Reaction Table

Is Leading	Role	Name	MolFormula	MW [g/mol]	D [g/ml]	Mol [ratio]	n [mmol]	W [mg]	V [ml]	Yield [%]	Action
<input checked="" type="checkbox"/>	Reactant	Salicylic acid	C7H6O3	138.121		1	4.625	638.808			
<a href="#">Set</a>	Reactant	Acetic anhydride	C4H6O3	102.089		1	4.625	472.160			
	Product	Acetyl salicylic acid	C9H8O4	180.157		1	2.775	499.937		60	
	Product	Acetic acid	C2H4O2	60.052		1	2.775	166.644		60	

Add Row

Ok Cancel

Done

calculated values

# File attachments

The screenshot shows a web browser window with the URL `http://30.0.0.246:82/Default.aspx`. The page title is "MainPage". On the left, there is a "Navigation" sidebar with a "Menu" containing: "Create New Document", "New Search", "Browse", "Search List", and "Saved Browse Lists". At the bottom of the sidebar are "Opened Searches", "Opened Documents", and "Help" sections, each with a "+" button. The main content area is titled "File Attach" and contains a form with the following fields: "Title:" (with the value "est results"), "Include in Extract:" (with a checked checkbox), and "Attached Files". The "Attached Files" section is a table with two columns: "Original Filename" and "Action".

Original Filename	Action
Test results 1.xlsx	[-] [v]
Test results 2.xlsx	[-] [v]
Test methods.docx	[-] [v]

Below the table is a "File" section with the following fields: "Original Filename:" (with the value "Test methods.docx"), "Comment:" (with a text area containing "Description of test methods"), and "File:" (with a text box containing "C:\TestFiles\Test methods.docx" and a "Browse..." button). A "Save" button is located below the "File" section. At the bottom right of the page are "Add new", "Ok", and "Cancel" buttons.

Three callout boxes provide instructions:

- "list of the attached files" points to the "Attached Files" table.
- "add a new file with comment" points to the "File" section.
- "delete and download an attached file" points to the "Action" column of the "Attached Files" table.

Search

**available search fields**

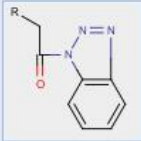
- chemistry data
- administrative data
- joint data

**user defined search layout**

The screenshot shows a web browser window titled 'MainPage - Mozilla Firefox'. The browser's address bar and menu bar are visible. The main content area is divided into two panels: 'Search Fields' on the left and 'Search Criteria' on the right.

**Search Fields Panel:** Contains a tree view with two main categories: 'Chemistry Fields' and 'Document Fields'. Under 'Chemistry Fields', there are 'Product Structure' and 'Reactant Structure'. Under 'Document Fields', there are 'Document Number', 'Document Title', 'Document Owner', 'Creation Date', and 'Project Name'. At the bottom of this panel are buttons for 'Expand All', 'Collapse All', and 'Add Condition'.

**Search Criteria Panel:** Contains three rows of search conditions, each with a 'Clear' and 'Remove' button.

Field	Operator	Value	Buttons
Document Owner	<input type="checkbox"/> Not equals	Zsolt	Clear, Remove
Document Title	<input type="checkbox"/> Not like	insulin	Clear, Remove
Reactant Structure	<input type="checkbox"/> Not substructure		Clear, Remove

At the bottom of the 'Search Criteria' panel, there are buttons for 'Clear All' and 'Remove All', followed by a 'Search title:' field containing 'Insulin project related search' and a 'Save Search' button.

**Annotations:** A callout bubble points to the 'Chemistry Fields' section in the 'Search Fields' panel. Another callout bubble points to the 'Search Criteria' panel. A third callout bubble points to the 'Save Search' button.

The status bar at the bottom of the browser window shows 'Done'.

**save search**

Search

Close

**Browse**

list of documents

extract of the selected document

list handling functions

- open
- delete
- clone

save list

MainPage - Mozilla Firefox  
http://30.0.0.246:82/Default.aspx

Most Visited Getting Started

MainPage

**List**

Search by Document Number:  Search and Open

Document Number	Title	Creation Date	Owner
NUM:00017	Synthesis of the activated amide derivative of de	5/8/2011 2:23:04 PM	ZSOLT
NUM:00018	Total synthesis of human insulin	5/8/2011 2:33:09 PM	ZSOLT
NUM:00019	Synthesis of e-NB29-dehydrocholyl insulin	5/8/2011 2:44:47 PM	ZSOLT
NUM:00020	Purification of the e-NB29-dehydrocholyl insulin	5/8/2011 2:46:24 PM	ZSOLT

open  
 delete  
 clone

Open Document Clone Document Delete Document

**List save**

List title:  Save List

**Extract**

**Synthesis of e-NB29-dehydrocholyl insulin** (NUM:00019)

**Synthesis of e-NB29-dehydrocholyl insulin**

Include in Extract

1 G I V E Q C C T S I C S L Y Q L E N Y C  
21 N F V N Q H L C G S H L V E A L Y L V C  
41 G E R G F F Y T P K T

**Experimental description**

Include in Extract

In this work, a novel acylated insulin, e-NB29-dehydrocholyl insulin was prepared by covalent linkage of dehydrocholic acid (DHC) to porcine insulin without protecting agents and analyzed by polyacrylamide gelelectrophoresis (PAGE), reversed phase high performance liquid chromatography (RP-HPLC) and matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF-MS). The activated amide was reacted with unprotected insulin and showed a selective acylation of one of the three free amino groups on insulin in the mixture of water and N-methyl-2-pyrrolidone at pH above 10 in the presence of TEA. Generally, the acylation of LysB29 was dominant at pH over 10.

Back to Search Close

Done

# Saved lists

The screenshot shows a web application interface with the following components:

- Navigation Menu:** Create New Document, New Search, Browse, Search List, Saved Browse Lists.
- Browse List Table:**

Browse Title	Creation Date
Insulin project browse list	5/8/2011 3:15:26 PM
Aspirin project browse list	5/8/2011 3:15:43 PM
GLP-1 project browse list	5/8/2011 3:16:36 PM
- List Logic Panel:**
  - Browse List A:** Insulin project browse list
  - Browse List B:** GLP-1 project browse list
  - Logic Options:**  A u B,  A n B,  A \ B,  B \ A
  - Buttons:** Add / Modify, Execute List Logic
- Callouts:** "saved browse lists" points to the table; "list logic function" points to the logic configuration area.

## Possibilities and features under implementation

- dedicated section type for certain file types (Excel, JChem for Excel, Word, PDF etc...) with preview
- import reactants and reagents from external databases
- direct compound and batch registration
- reactor module
- reporting and printing
- export to SharePoint

## Key features

- ❑ web-based, self-hostable or hosted by Sysment
- ❑ browser and database independent
- ❑ extendable by plug-ins
- ❑ supports multiple opened documents
- ❑ handling of traditional medicinal chemistry and biopharmaceuticals together

**Thank you for your attention!**

**[www.sysment.hu/notebook](http://www.sysment.hu/notebook)**