



Instant JChem

**INFORMATICS
MATTERS**

Informatics solutions for drug discovery



Topics

- **Background**
- **Aims**
- **Architecture**
- **Current status**
- **Demo**
- **Future**

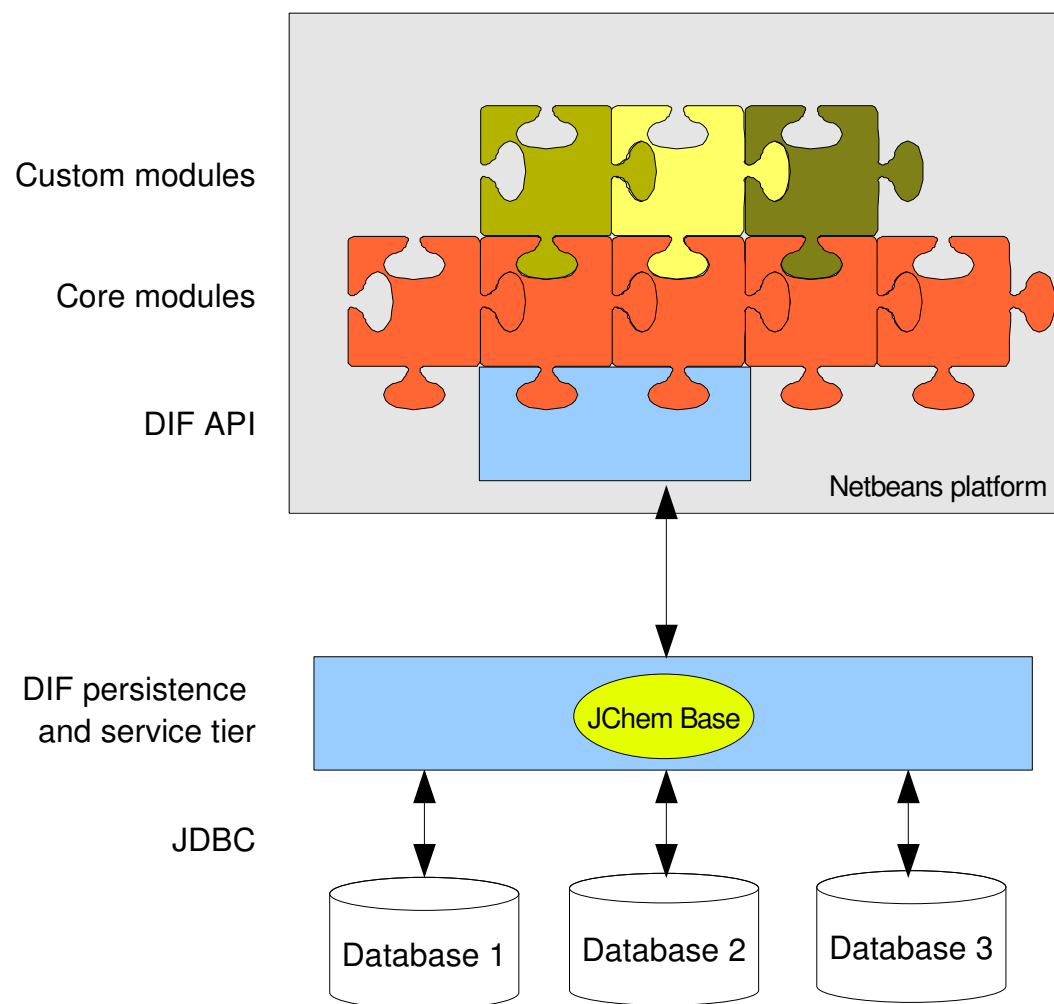
Background

- **JChem provides a great set of tools and API, but some customers require end user apps**
- **Instant JChem provides**
 - an “out of the box” desktop application that utilises Marvin and JChem
 - a modular platform for developing future chemistry applications

Aims

- **Simple to use end user application**
- **To provide a desktop alternative to current applications such as ISIS, Accord etc.**
- **Shop window to Marvin/JChem functionality**
- **Modular architecture and API allowing extensibility by us, customers and VARS**
- **Easy to install, manage and update**
- **Quality documentation and support**
- **Localizable**

Architecture summary

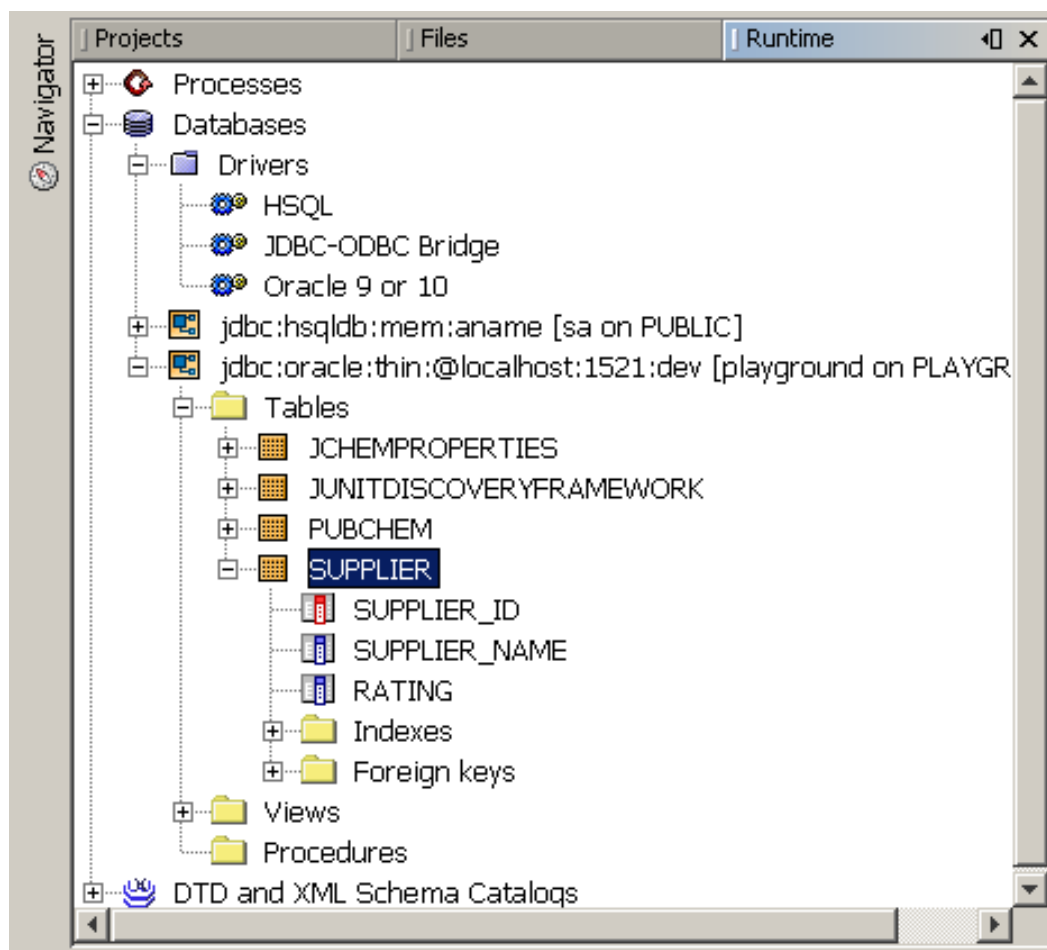


Current status

- **Initial version provides ability to create, manage, query and view JChem databases**
 - HSQL and Oracle databases supported
 - Supports most Marvin and JChem Base features
- **“Out of the box” experience**
 - No developers, no database administrators, minimal training
- **Beta version available for download**
- **Embedded database version foc to commercial and academic users.**

Demo

IJC in action – database explorer



Database Explorer, showing the different JDBC drivers and some database connections that have been defined.

The database explorer lets an advanced user work directly with the database tables.

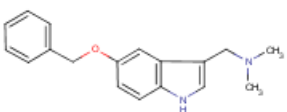
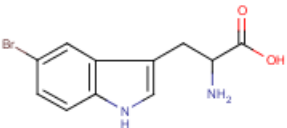
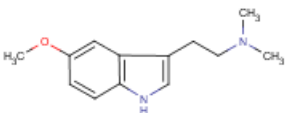
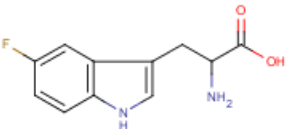
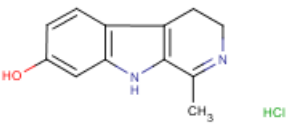
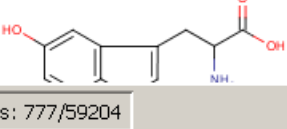
IJC in action – query tool

The screenshot displays the JChem query tool interface. On the left, a search criteria panel includes fields for 'cd_id', 'Structure' (set to 'Substructure'), 'Formula', 'MolWeight', 'HBA', 'HBD', 'CLogP', 'Code', 'Name', 'ROTB', and 'ALogP'. A 'Similarity options' dialog box is open, showing a 'Threshold' of 0.3, 'Stereochemistry' set to 'On', and 'Atom matching' options for 'Charges', 'Isotopes', and 'Radicals'. 'Display options' include 'Align hits to query' and 'Highlight substructure', both checked. The main window shows a table of results with four rows, each containing a chemical structure. The structures are: 1. A benzene ring with a methoxy group and a vinyl group; 2. A benzene ring with a bromine atom and an indole ring; 3. A benzene ring with a methoxy group and an indole ring; 4. A benzene ring with a fluorine atom and an indole ring. The bottom right corner of the window shows 'Rows: 777/59204'.

Query tool, showing the ability to enter query terms for each field. The advanced structure query options are shown. Part of the results is shown in the table on the right.

IJC in action – spreadsheet tool

Table view for new maybridge hts

	Structure	cd_id	Formula	MolWeight	HBA	HBD	CLogP	ROTB	Code	Name
1		4	C18H20N2O	280.36	2.00	1.00	3.23	5.00	AC 10608	3-(benzyloxy)indole-5-carboxamide, N,N-dimethyl
2		6	C11H11BrN2O2	283.12	3.00	3.00	1.72	3.00	AC 10751	3-(5-bromo-1H-indol-3-yl)propanoic acid
3		10	C13H18N2O	218.29	2.00	1.00	1.71	4.00	AC 11641	3-(3-methoxyphenyl)indole-5-carboxamide, N,N-dimethyl
4		11	C11H11FN2O2	222.22	3.00	3.00	1.07	3.00	AC 11968	3-(5-fluoro-1H-indol-3-yl)propanoic acid
5		12	C12H13ClN2O	236.70	2.00	2.00	1.32	3.00	AC 12028	7-hydroxy-1-methyl-1H-pyrido[2,3-b]indole hydrochloride
6		14	C11H12N2O3	220.22	4.00	4.00	0.64	3.00	AC 12199	3-(5-hydroxy-1H-indol-3-yl)propanoic acid

Rows: 777/59204

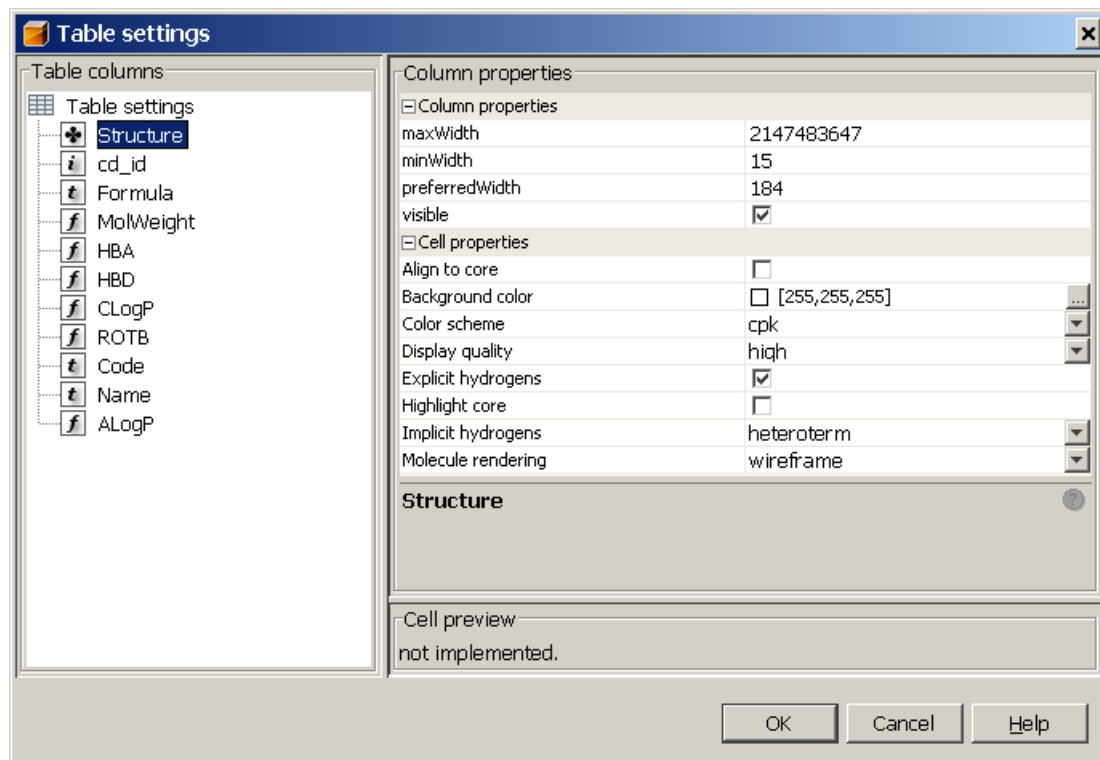
A chemically aware table.

Multiple views can be open and visible at any one time.

Views from the same dataset are coordinated.

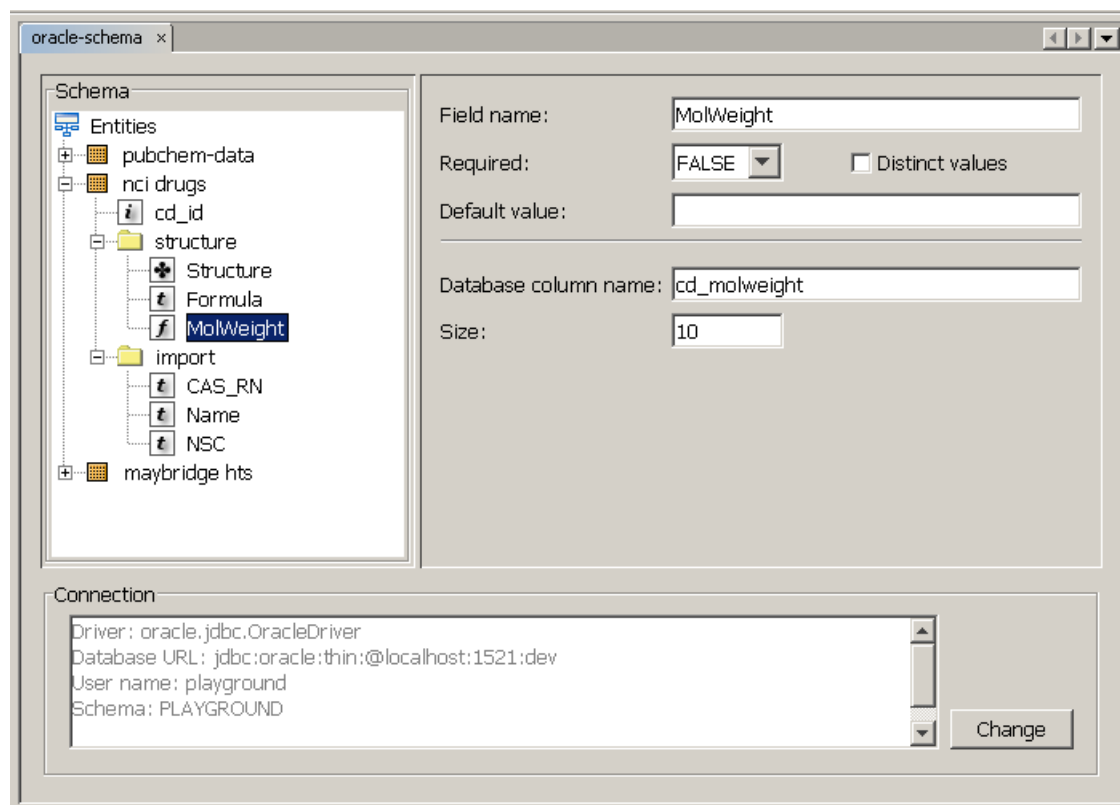
Data in the table can be sorted and formatted.

IJC in action – table configuration



The table can be configured to display data according to users needs.

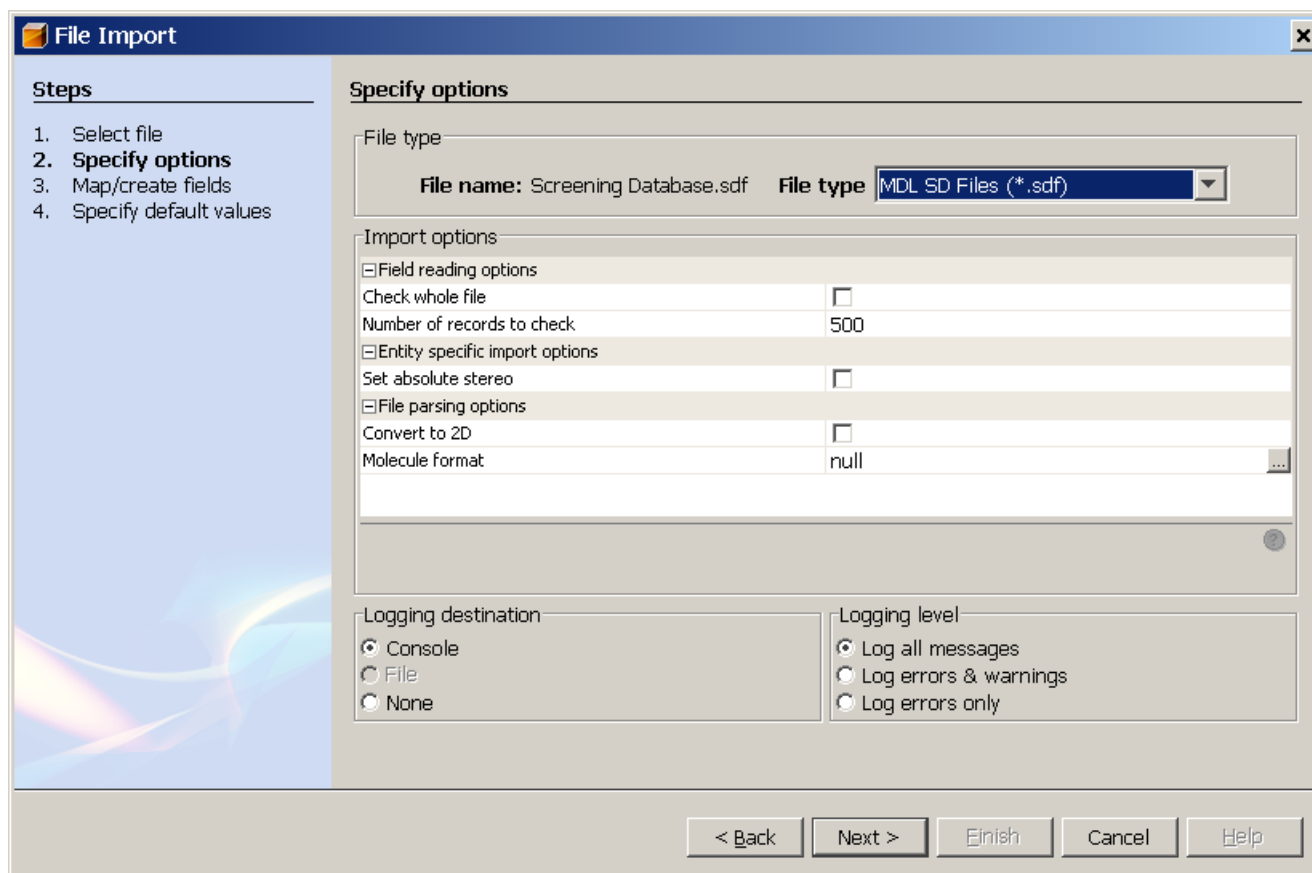
IJC in action – schema editor



The schema editor lets you create new databases and edit the contents of each database,

for instance adding or editing fields.

IJC in action – import wizard (1)



The file import wizard lets you import data from a file, such as an SD file.

This shows one step of the wizard where the import options are being set.

IJC in action – import wizard (2)

The screenshot shows the 'File Import' wizard window. On the left, a 'Steps' panel lists: 1. Select file, 2. Specify options, 3. **Map/create fields**, 4. Specify default values. The main area is titled 'Map/create fields' and contains the instruction: 'Specify the mapping between the fields in the file and the database by making sections from the second column'. Below this is a table with three columns: 'Field from file', 'Mapping', and 'New Field Name'. The table contains the following rows:

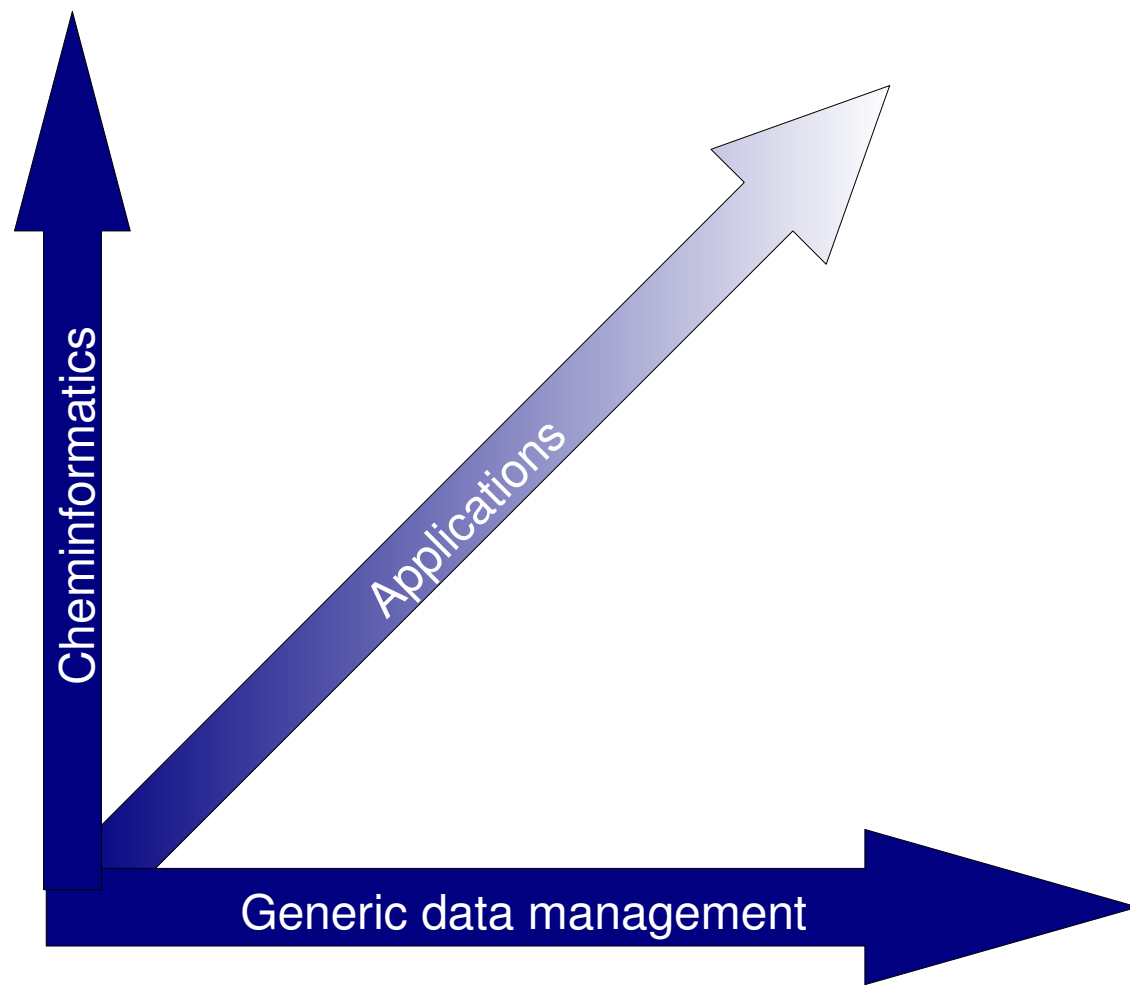
Field from file	Mapping	New Field Name
Structure	Structure	
ID	Create new field	ID
list	Do not import	
melting_point	Create new field	melting_point
Bionet_Name	Create new field	Bionet_Name
Number of Heteroatoms	Do not import	
Number of Halogen Atoms	Do not import	
ADME Rotatable Bonds	Create new field	ADME Rotatable Bonds
ADME H-bond Acceptors	Create new field	ADME H-bond Acceptors
ADME H-bond Donors	Create new field	ADME H-bond Donors

At the bottom of the window are buttons for '< Back', 'Next >', 'Finish', 'Cancel', and 'Help'.

The next step of the wizard allows you to specify how the fields in the file map to fields in the database.

Options are to map to an existing field, create a new field, or to ignore the field

Future – multiple complimentary paths



Future – next steps

- **Relational data (one-to-one, one-to-many...) displayed as master-detail tables**
- **Calculations, Chemical Terms**
- **List management**
- **Conditional formatting**

Future – planned functionality

- **Form builder**
- **Charting & visualisation**
- **Enterprise features**
 - Multi-tier architectures + security
 - Applications
 - Chemical registration
 - Sample management
 - Assay data management

Future – does it involve you?

- **We need your help in the development of enterprise capabilities**
 - Prioritise features
 - Define functionality
 - Become IJC users and testers!
- **Become part of the “IJC partners program”**
- **Q & A session tomorrow**
 - Hacker room 1.30 - 2.00
 - Aimed at organisations and developers who might want to use IJC for enterprise applications
 - Either as developers or pre-built modules