Instant JChem

INFORMATICS MATTERS

Informatics solutions for drug discovery

ChemAxon

Topics

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- Future

Background

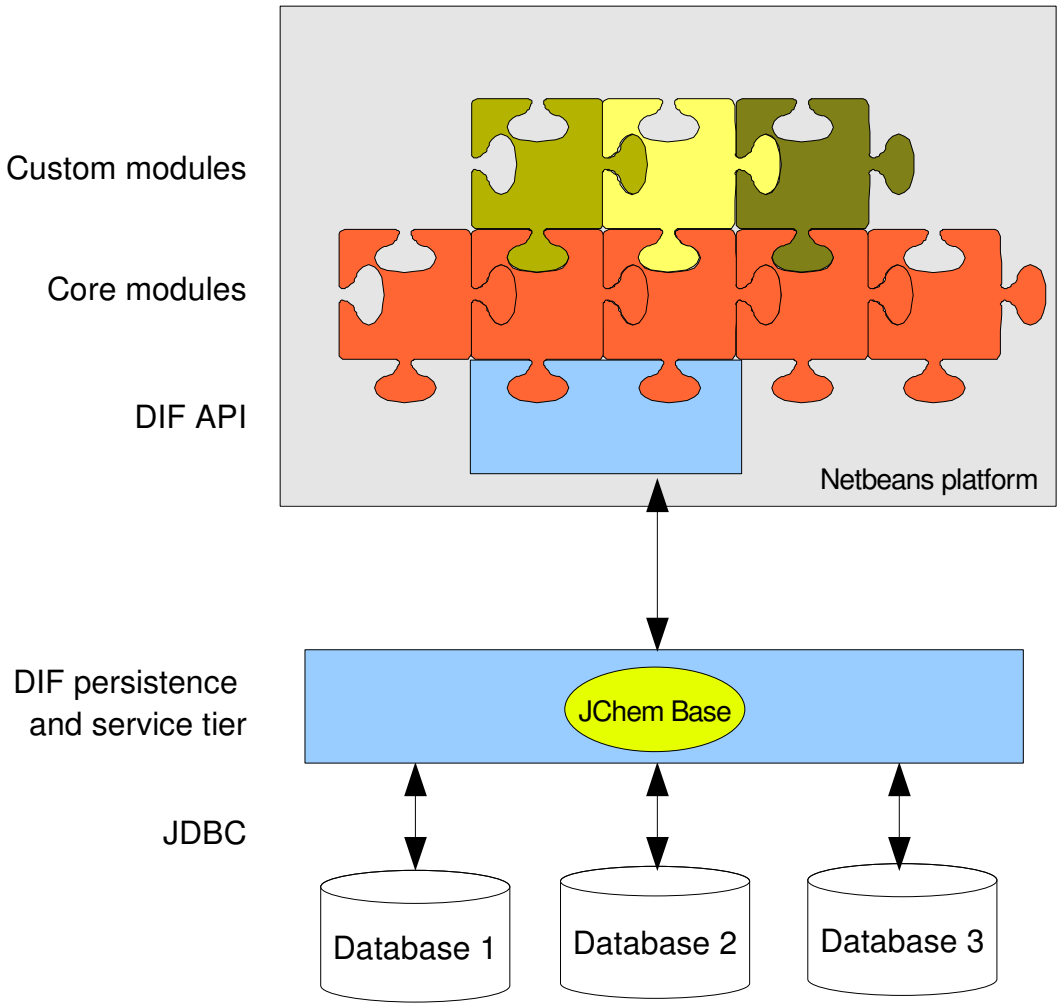
- **JChem provides a great set of tools and API, but some customers require end user apps**

- **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

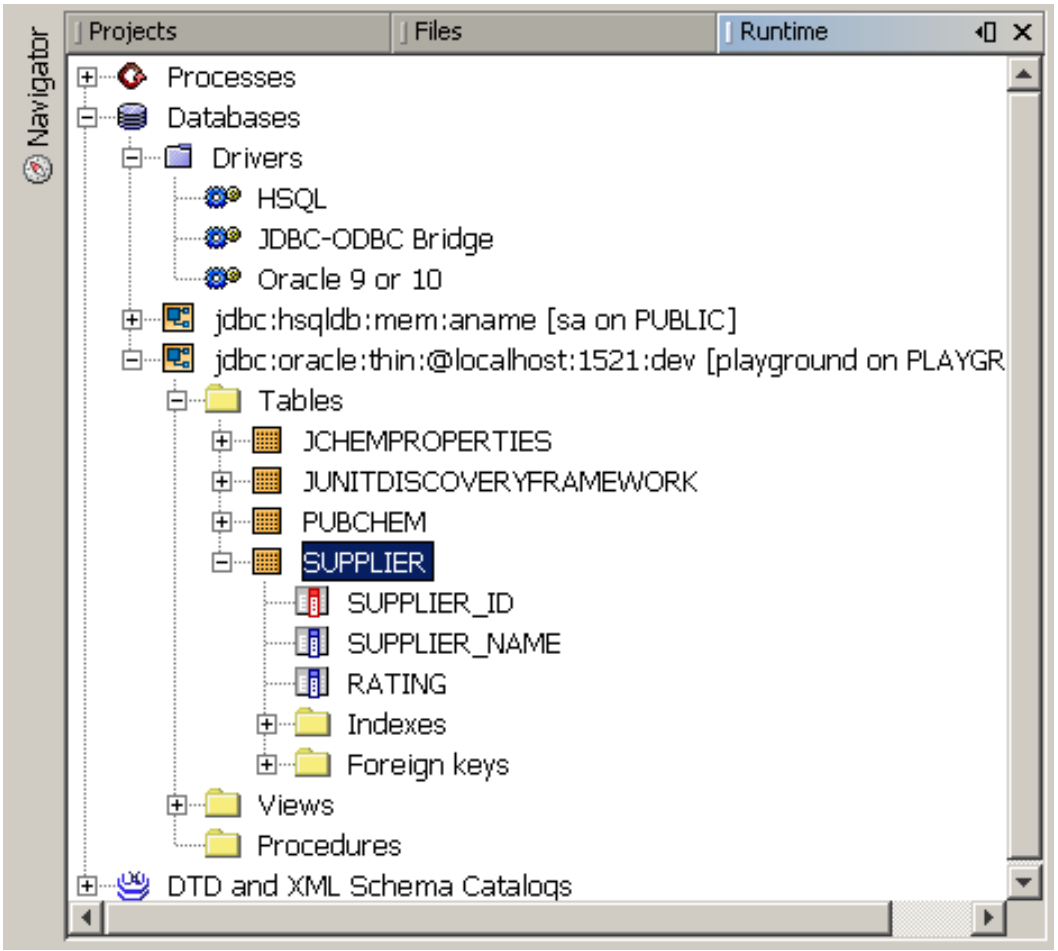


Current status

- **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

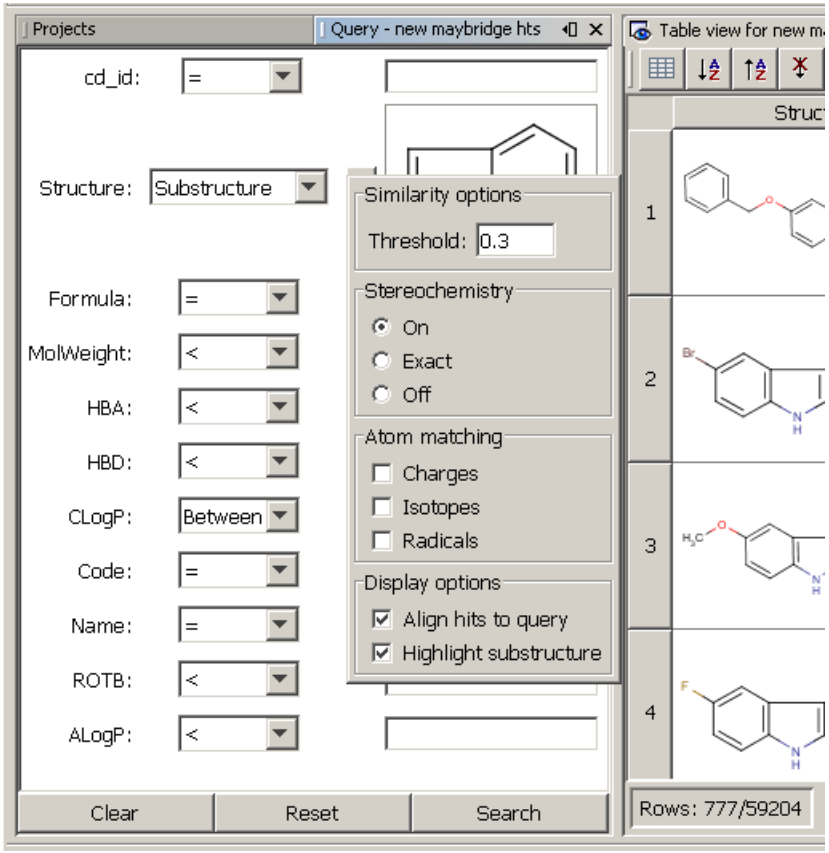
IJC in action – database explorer



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

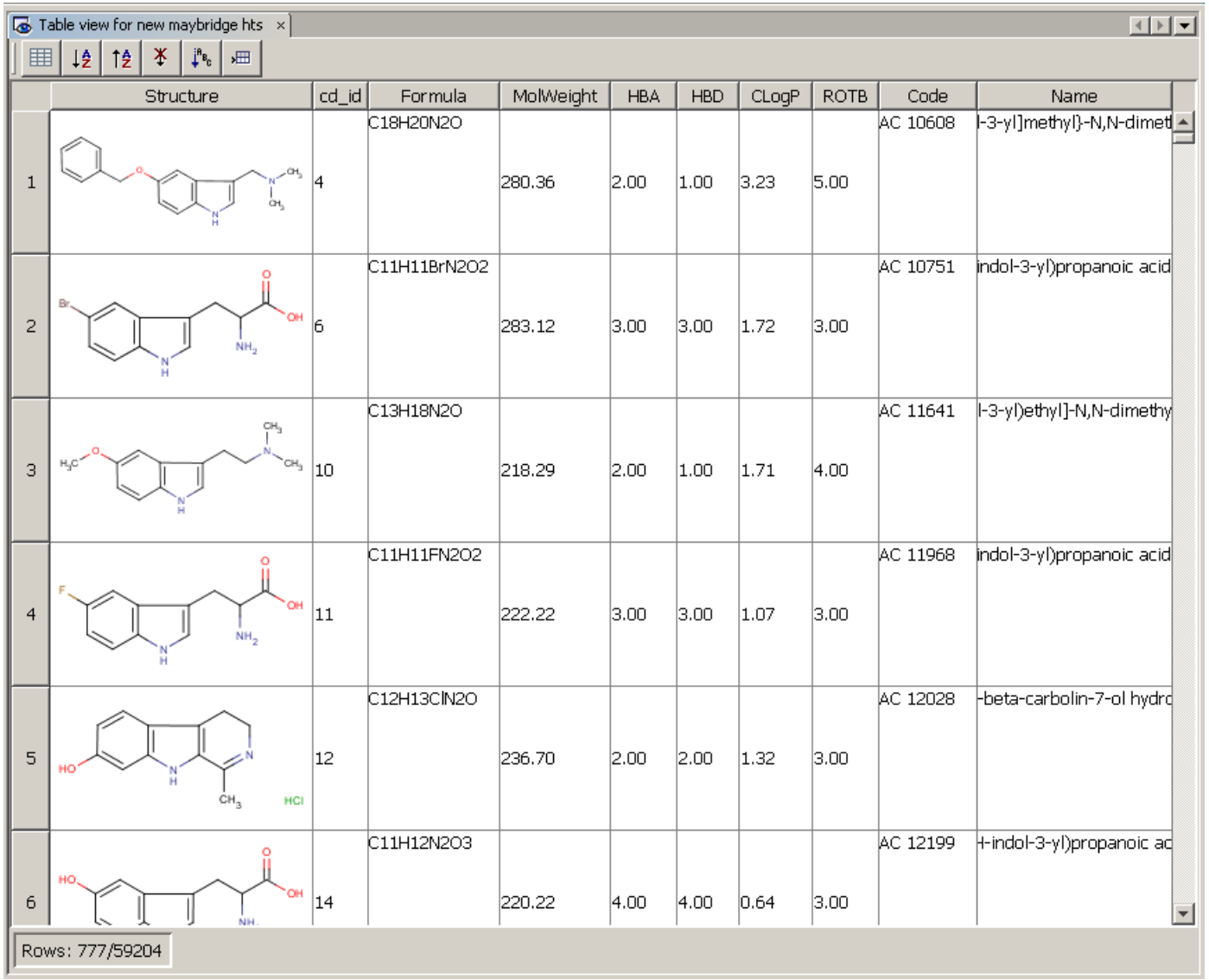
The database explorer lets an advanced user work directly with the database tables.

IJC in action – query tool



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



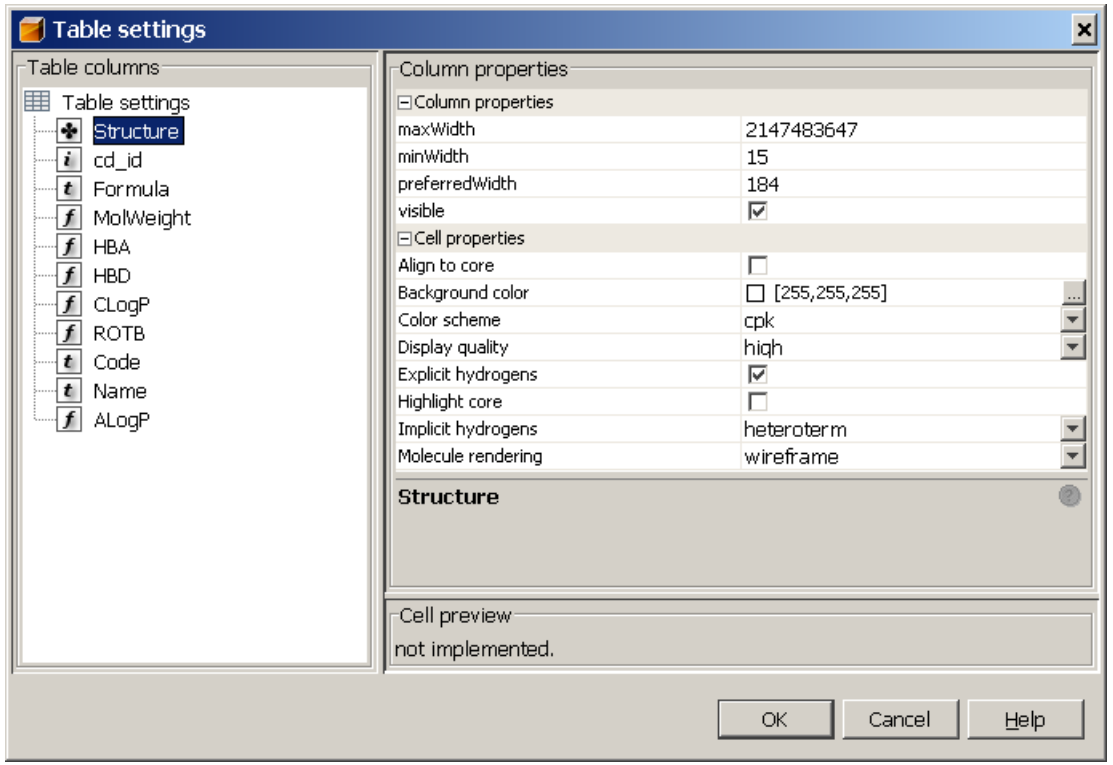
A chemically aware table.

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

Views from the same dataset are coordinated.

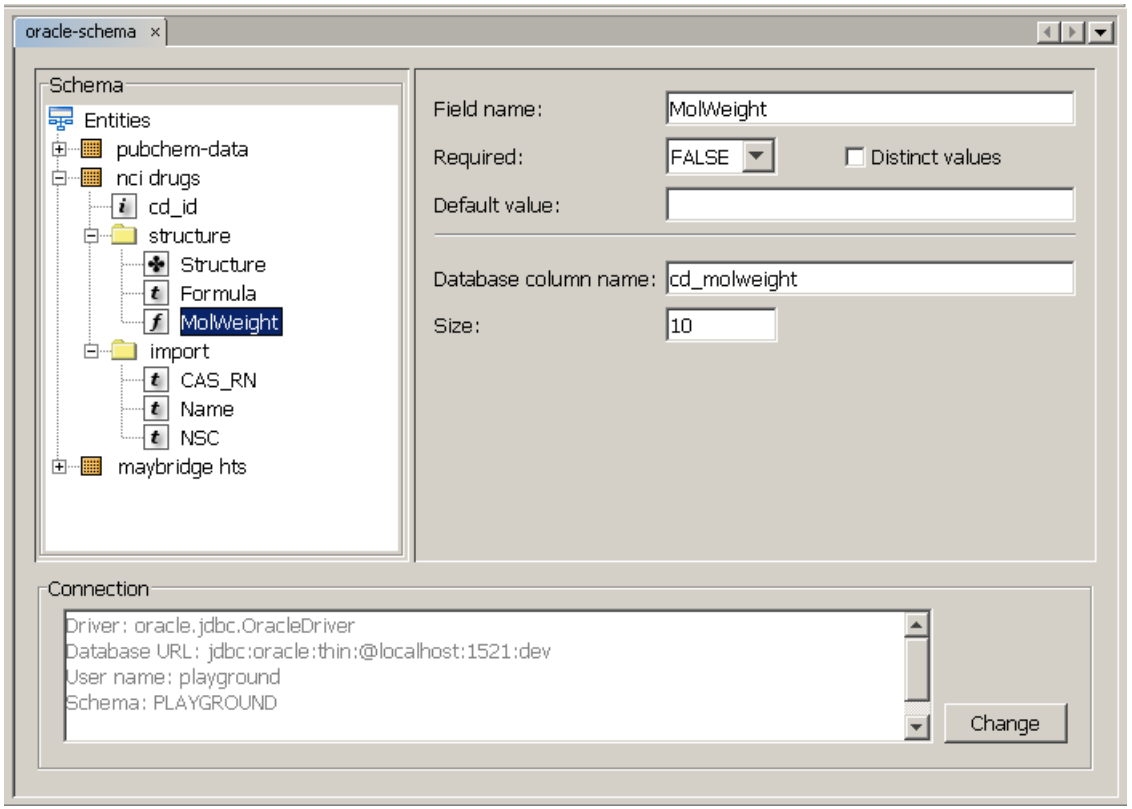
Data in the table can be sorted and formatted.

IJC in action – table configuration



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

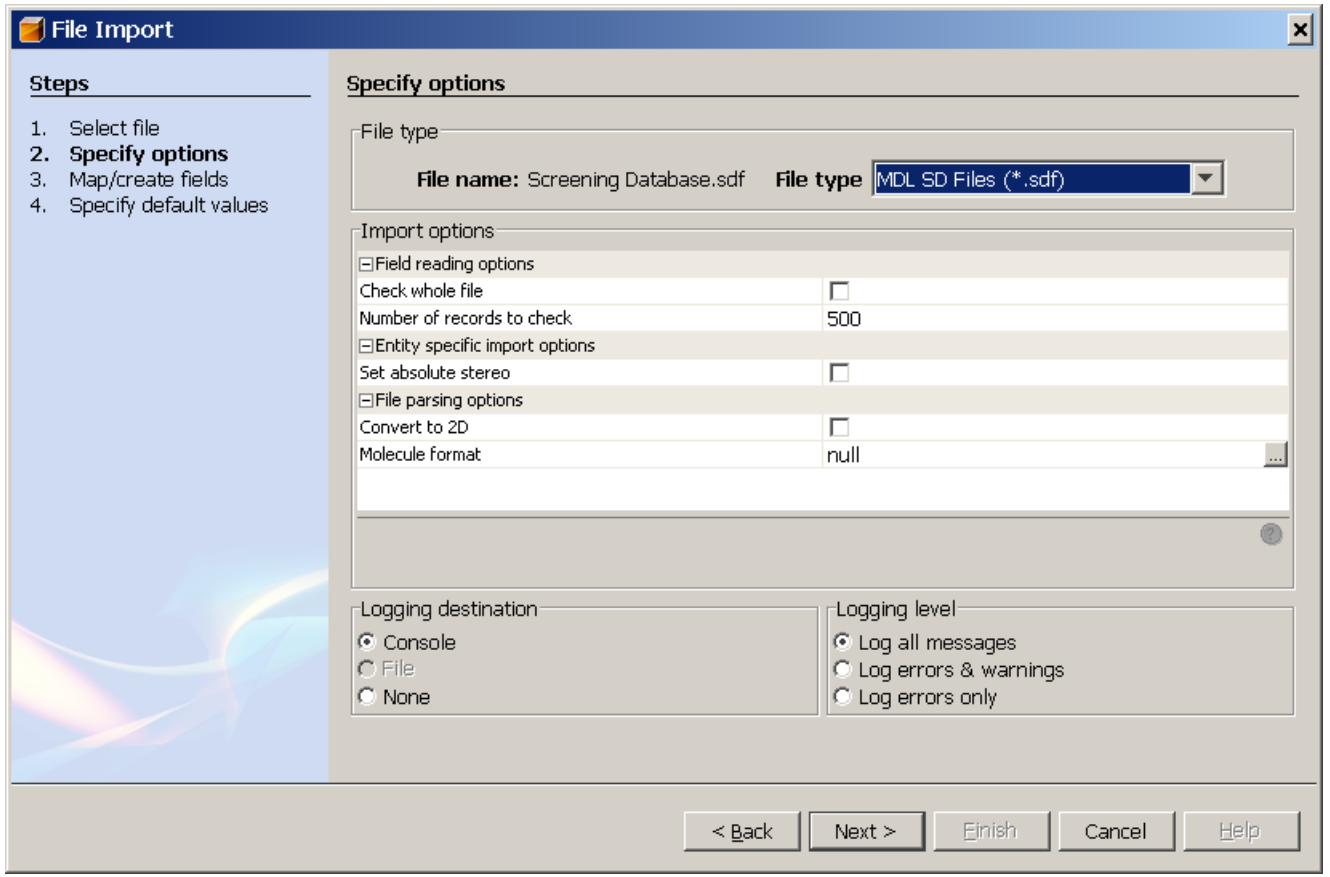
IJC in action – schema editor



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

for instance adding or editing fields.

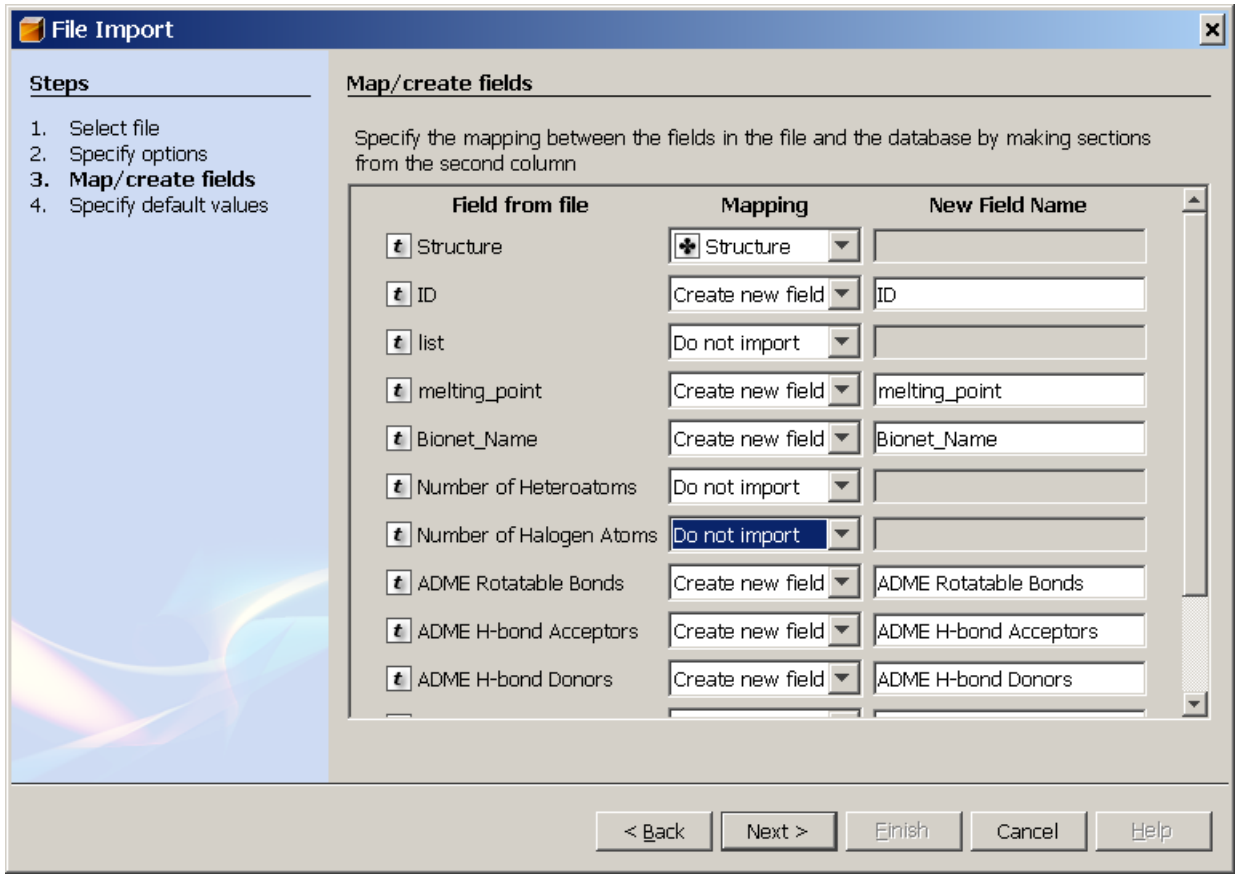
IJC in action – import wizard (1)



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.

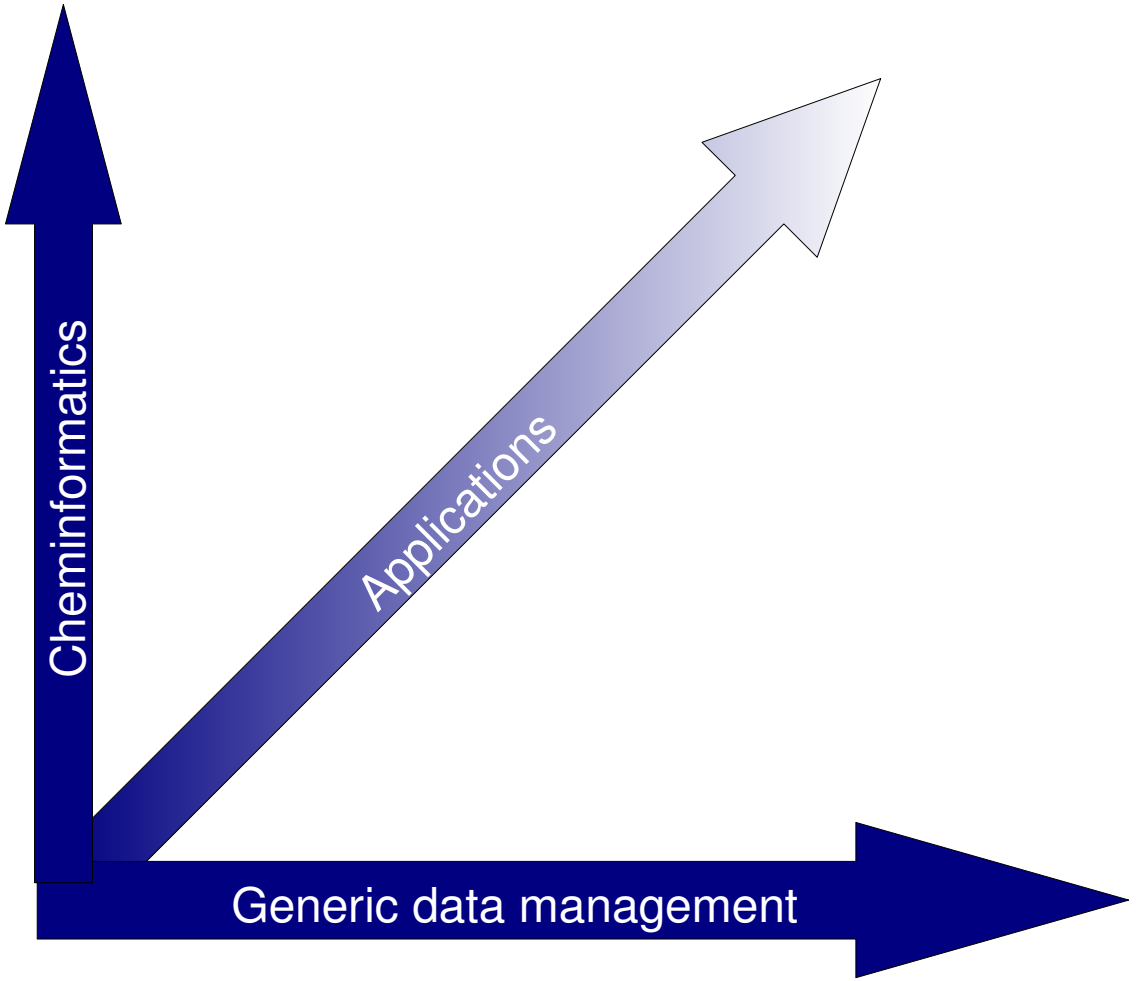
IJC in action – import wizard (2)



The 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