ChemOffice

Creating Database in ChemFinder.

I. Main steps.

Step 1. *Creating a logical structure of a database including all its elements and relationships between them.*
1. Creating a database.
2. Creating tables.
3. Creating new fields in each table and definition of the field types.
4. Establishing links between tables.

Step 2. *Creating Form(s)*
Step 3. *Alimentating a database.*

Any database in ChemFinder format contains information in minimum 4 files:
***.mst** and ***.msi** chemical structures and indexes, respectively;
***.mdb** tables of data (readable by MS ACCESS);
***.cfw** *ChemFinder* form.

II. Manipulations with ChemFinder

Variant 1: Step 2 -> Step 1.

1. Creating data boxes.
   ChemFinder->File->New. A new window appears.
2. Select *Layout tool* button.
3. Prepare Data boxes or Framed boxes by Layout tools.
   Enter in the *Label dialog* a name for Framed box.
   One box will be destined for chemical structure or reaction.
4. Select *Selection tool* for editing and resizing boxes.
5. From the *File* menu, choose *Save As*, and save new form as **.CFW*
6. Right-click in the *Structure data box* and choose *Data Source -> Create Database -> Save* new database as **.MDB -> OK*.
7. Assigning Fields:
   Right-click in the *Structure data box* and choose *Structure*.
   If a field exists (*e.g.*, the *MOL_ID, Formula, MolWeight* fields are automatically created with *Structure* field), Right-click in a box and choose existed field.
   If a field doesn't exist: Right-click in *data box* and choose *Field ->*
   Create Field -> input a *Name* and *Type* of field *-> OK*.

Table 1. Types of the data fields in *ChemFinder*.

no	*Field Type*	*Description*
1	**Text**	User can specify widths of text fields as large as 254 characters. If this is insufficient, user needs to create a Memo field instead.
2	**Integer**	Long integer: 2^{32} = 4294967296
3	**Real**	Real double-precision
4	**Picture**	a Windows metafile
5	**Memo**	Used to display text. Memo fields can be of any length.
6	**Date**	Allows you to store dates. The dates are displayed according to the settings in the Windows Regional Settings control panel.
7	**Structure**	Consists of four fields: a numeric ID stored in the relational database, plus three fields (Structure, Formula, MolWeight) that take data from the ChemFinder structure database files. User can create more than one set of structure fields in a table. Each is assigned a unique set of names, and each refers to its own ID column in the table, although all structural data is taken from the same structure database files.

Attention: Since the field type is defined, it cannot be modified anymore.

8. Adding Records.

Deselect the *Layout tool.*

Double-click in the *Structure* data box for edit or prepare structure by *ChemDraw*.

Input data in other data boxes (data for *MOL_ID*, *Formula*, *MolWeight* will automatically appear with *Structure*).

For the first record in the database: from the *Record menu*, Choose *Commit Changes*.

For input of any next record, choose *Record -> Add New Record* or click *Add Record*.

View -> Switch Views to view all records.

9. Preparing Subforms.

Creating a ***Subform***: *Layout toolbar -> Subform.*

Prepare Data boxes in ***Subform*** (see items 3-4).

Fields: Right-click in a *Subform data box* and choose *Data Source -> Create Table ->* prepare *Name* for new table and click on it -> and choose *Field -> Create Field ->* input a *Name* and *Type* of field -> *OK*.

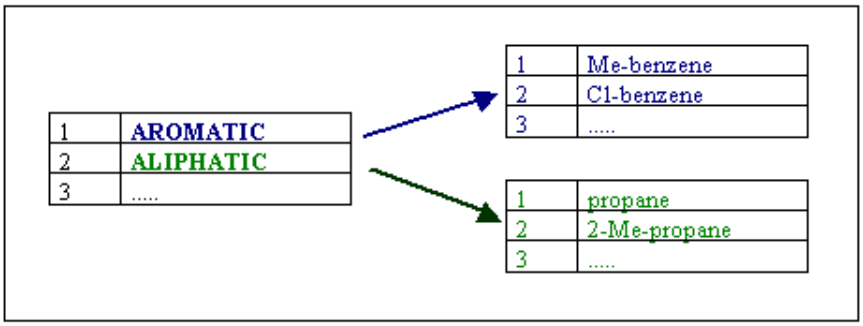
Linking the Subform: Right-click in the title area of the *Subform -> Data Source -> Subform -> Relate by* (for example, MOL_ID) -> *Relate to* (for example, ID) -> *OK*.

Variant 2: Step 1 -> Step 2.

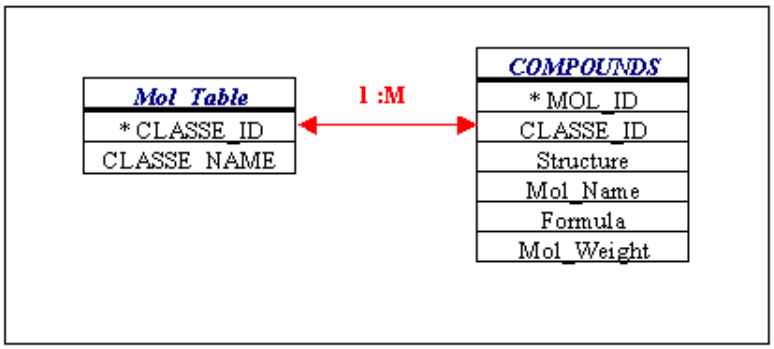
1. *ChemFinder->File->New.* A new window appears.
2. *File-> Database*

Exercice 1. Une base de données de types de composés (Class_Comp)

Modèle Conceptuel de Données



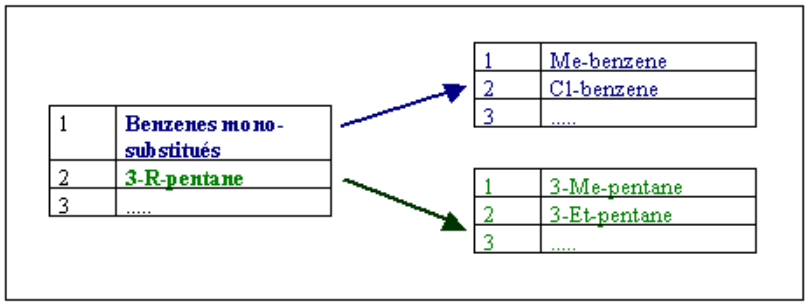
Tables relationnelles



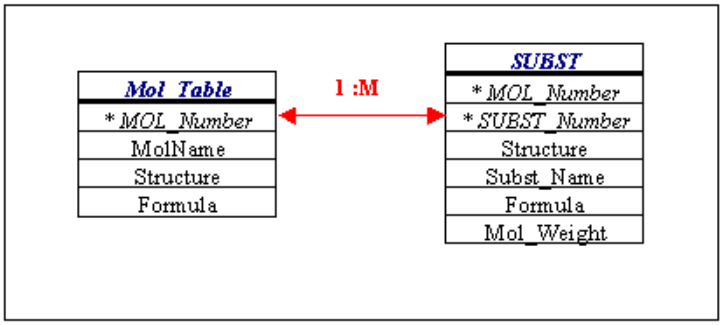
Composition par rapport aux structures chimiques

Exercice 2. Une base de données de composés substitués (Subst)

Modèle Conceptuel de Données

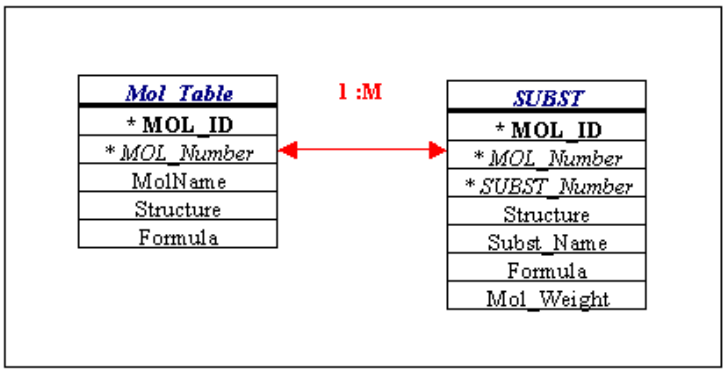


Tables relationnelles



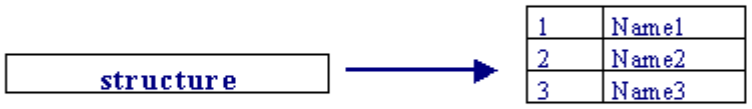
Composition par rapport aux structures chimiques

Tables relationnelles de ChemFinder

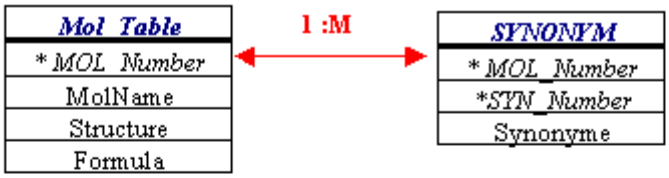


Exercice 3. Une base de données de types de synonymes (SYNONYME)

Modèle Conceptuel de Données



Tables relationnelles



Composition par rapport aux structures chimiques

Searching Database in ChemFinder.

Play with the data boxes in *Search -> Enter Query*.

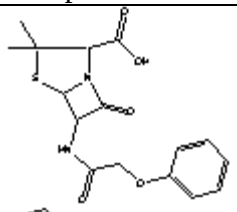
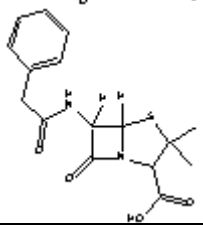
Exercise 1.

In the ***Cs-Demo*** database, perform a search on cyclopropane and pyridine molecules using *Substructure* or *Similarity* options. Compare results of these two types of search.

Exercise 2. *Combined Searching*

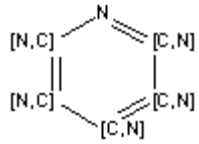
In the ***Cs-Demo*** database, perform a search on benzene  as substructure and '*penicillin' in *Molecule name* field.

Result: 2 structures

no	Compound	Molecule name
1		Penicillin V
2		Benzylpenicillin

Exercise 3.

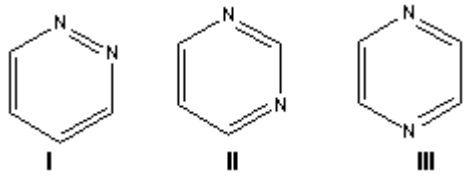
In the ***Cs-Demo*** database, perform a substructural search on cyclic aromatic fragments of 6 atoms containing two nitrogen atoms.



1. Perform search for the fragment and 'N2' in the *Formula* field.

ChemFinder founds 5 structures, two of which don't fit the target molecules.

Use *Record -> Omit from List* to withdraw useless hits.



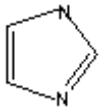
2. Perform 3 searches for fragments **I**, **II** and **III**. Use *Save List* and *Restore List* options to combine results of these 3 searches.

Exercise 4.

In the ***Cs-Demo*** database, perform a search on molecules for which MolWeight > 200 and which don't contain the benzene ring.

1. Perform substructural search on benzene and *MW* > 200. Save results in the list (*List1*).
2. Perform search on compounds with *MW* > 200. Save results in the list (*List2*).
3. Substrate *List1* from *List2*.

Exercise 5.



In the ***ISICCRsm*** database, perform a search of imidazole as a fragment of the reactant then as a fragment of the product.