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Supporting information for article:

Organizing a Crystallization laboratory

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StockAide setup for external users

A1. Definitions

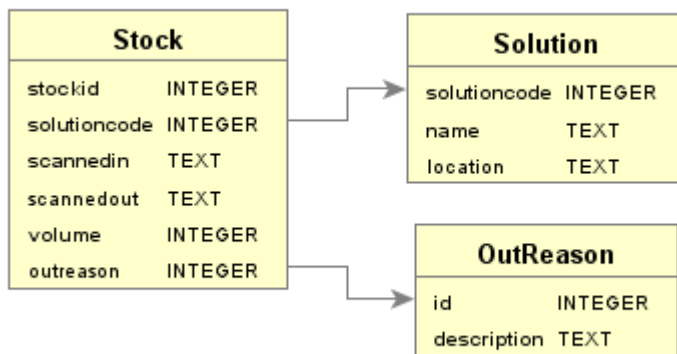
Solutions and Stocks

A *stock* refers to a physical tube which contains a *solution*. A *solution* has an associated concentration, unit, chemical name [and potentially pH] e.g. *5M sodium chloride*, *1M tris chloride pH 9*. A *stock* is identified by both the *solution* it contains and its date of creation.

Date

A date is in the form of *ddMonyy* e.g. 1Jan00.

A2. Database Setup



Run the included *database_creation.sql* file in a SQLite Database editor to create the StockAide database with the structure above. This will also automatically populate the OutReason table with the appropriate values.

Once created you will need to rename the database file to *StockKeep.db* and move it into the same directory that *StockAide.py* is in.

The Solution table will then need to be populated with the list of solutions that will be used.

Each solution needs:

- solutioncode – a unique integer assigned to that solution
- name – the name of the solution in the form *1M sodium chloride*
- location – a text string describing where the solution is stored

The values can be inserted into the data with the sql command:

```
INSERT INTO `Solution` (`solutioncode`,`name`,`location`) VALUES
  (1,'1M sodium chloride','Shelf 1'),
  (2,'2M sodium chloride','Shelf 1');
```

Replacing the red text with the list of chemicals to be used.

A3. Database Update

StockAide has been built to automatically populate and update the solutions in its database from the main C3 database each time it starts. This will not work outside of C3 so it will need to be disabled. Open *StockAide.py* in a text editor and at the top just below the import statements there is line that says

```
UPDATE_DATABASE = True
```

Change this to

```
UPDATE_DATABASE = False
```

A4. Stocks

A stock will need to be labelled with the appropriate solutioncode and the date on which it is made separated by a hyphen (Figure 1 shows this is printed on the bottom left of the C3 labels). A 1M sodium chloride solution made on the 2nd January 2012 would need to be labelled *1-2Jan12* (assuming the solutioncode '1' from the Insert statement shown above).

The combination of date-solutioncode is the key used by StockAide to keep a track of the physical stock. In C3 the date-solutioncode key is printed both as a human readable string and a barcode enabling easy upload into the StockAide forms using a USB barcode scanner. This is just for convenience and the same information can be entered by hand.