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Supporting information for article:

Organizing a Crystallization laboratory

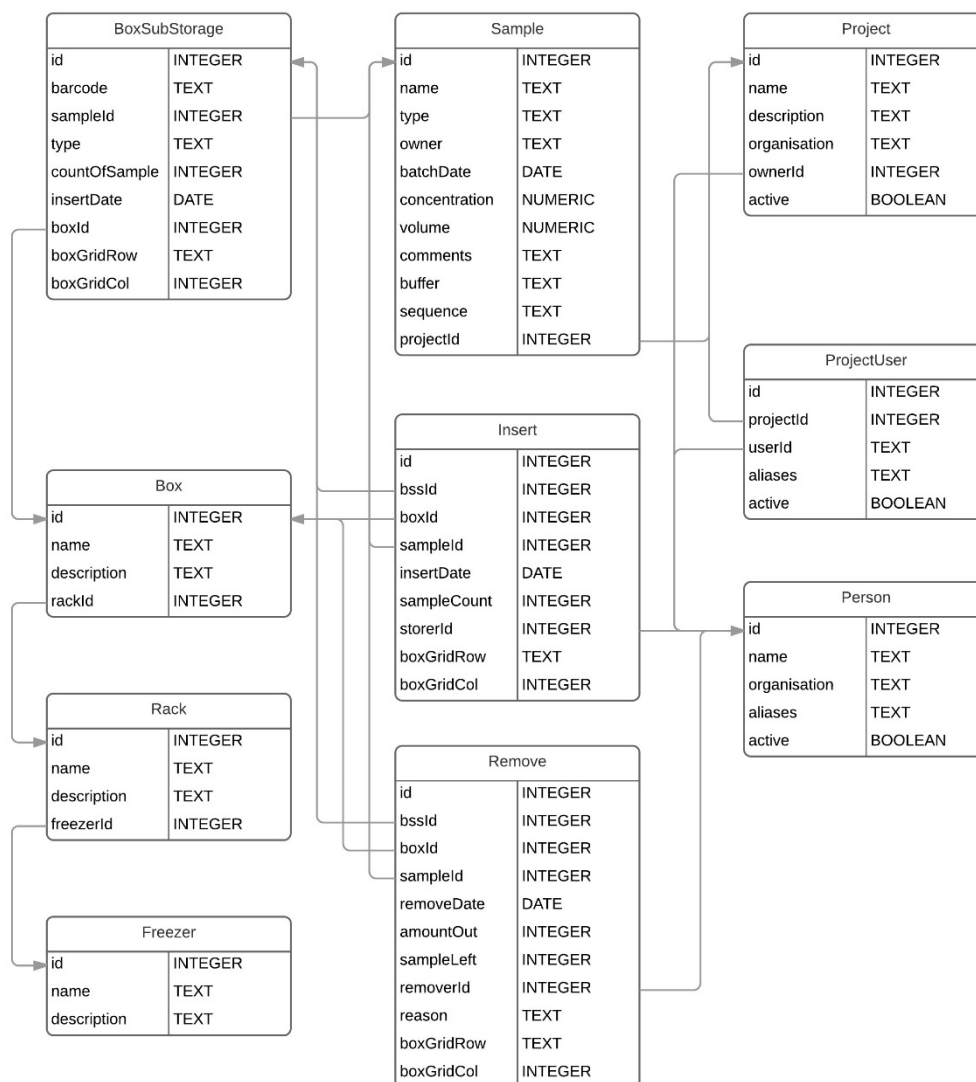
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GPSamplr setup for external users

A1. Definitions

Samples are protein solutions, buffers, cell pastes etc. In the majority of cases, these samples are stored in aliquot tubes which are in turn stored in various different "box sub storage" tubes (e.g. 50mL centrifuge tubes). These tubes are then placed in boxes, racks and freezers.

A2. Database Setup



Install PostgreSQL. Run the included *gpsDB_creation.sql* file in a PostgreSQL editor (eg. PgAdmin) to create the GPSamplr database with the structure above.

Open *settings.ini* and change the host address to the address where the PostgreSQL database is located. This address may be localhost if the database is installed locally, or the IP address of the network computer hosting the database. This creates the connection between the Python application and the database.

A3. Barcoding and Labelling

The use of a label-printing software, with the ability to connect to and pull data from a PostgreSQL database, is recommended. Alternatively, labels can also be created by hand. Each label corresponds to a specific box sub storage tube (eg. 50mL Falcon tube). It is recommended that the labels be placed inside the tube rather than being stuck on the outside, since labels may come unstuck when under freezer conditions.

A label should contain the following information:

- Sample name
- Owner name
- Batch date
- Location
- Concentration
- Volume
- Barcode

Note that each tube should contain identical aliquots.