

Creating and Searching an in-house unit cell data base with Olex2

Thanks to John Warren for most of this information.

1. Create a new database.

```
Lcells.update Y:\ celldata.db
```

Where Y: is the location containing the archived X-ray data and celldata.db the name of the database. This will take a while. The program may not be able to read some CIF files, but it goes on to other files containing unit cell info. The errors during the db creation are usually not critical.

2. Search the database

The easiest way to search the database is to load a SHELX file in Olex2 or even a p4p file containing the unit cell information and then type

```
Lcells.search -d=50
```

This will search for the current unit cell volume with $d=\pm 50 \text{ \AA}^3$. This will immediately show whether the structure you are working on is a repeat!

To view all the unit cells in the database increase the value of -d.

The matching unit cells are shown on the console. Since they may have many lines of text, it's usually better to view the output in a text editor simply by clicking the text-target icon on the olex2 panel.

3. Periodically update the database by typing

```
Lcells.update
```

This will add cells to the current database from the same archive location (Y:/).