



XChem training: TexRank & SoakDB

May 2022

TexRank

TexRank

- Use 'tserver' to go on Windows machine
 - TexRank shortcut on desktop
- 1 Select plate
 - 2 Select (toggle!!) Formulatrix (RC)
 - 3 Select 1 Subwell
 - 4 Target dispensing location (right click)
 - 5 Save list before moving to next plate (ECHO – 1 Target)

Save to here:

Y:\data\proposal\visit\processing\lab36\crystal-targets

Repeat steps 1, 2, 4, and 5 (yes, step 2 also, bug!!) for another plate

Arrow keys on keyboard to move previous/next

Check the crystal target output csv files X and Y should be within +/- 1300 (for swissCI-3drops)

The screenshot displays the TexRank software interface. On the left, a list of targets is shown, with 'Formulatrix (RC)' selected and marked with a red circle '2'. Below the list, the 'ECHO - 1 Target' button is highlighted with a red circle '5'. The main window shows a microscope view of a subwell with a red circle '4' indicating a target location. A red circle '3' is next to the '3 Subwells' button. The bottom right shows a graph with 'Drop Qual.: 9' and 'Precip. Score: 10'.

SoakDB

SoakDB

soakDB [Read-Only] - Excel

Douangamath, Alice (DLSLtd,

File Home Insert Page Layout Formulas Data Review View Help Tell me what you want to do

Undo/Redo in case of major errors

UNDO REDO

Do NOT save this file

1 Click: Load Data File

The red bar at the top means that the datafile and soakDB are not in sync, that the datafile is currently updating, or there is another error.

Do NOT keep working with a red bar! Try the error reset button (to the right).

Datafile activity is indicated in the bottom left corner

Load Data File (first thing to click) 1

Lab Visit:

or enter a full path here:

Source (Library/Solvent)

Slpoised_001_Set1

Update Library values

| Library Name (or solvent) | SMILES | Code |
|---------------------------|--------|------|
| | | |

XLSQLite: Placing values in array...

5

Protein:

Step 2

Crystals

Load Crystal Plate(s)

Crystals:

Plates:

Drop volume:

SwissCI-3drop

Get image links

| Plate | Well | X | Y | Drop Volume (nL) | Protein |
|-------|------|---|---|------------------|---------|
| | | | | | |

soakDB.xlsm [Read-Only] - Excel

OUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

| | AV | AW | AX | AY | AZ | BA | BB |
|----|------------------------|--------------------------|----------|-----------------------------------|-----------------|----------|---------|
| | Error Reset | | | | | | |
| 5 | Data Collection | | | | | | |
| 6 | | | | | | | |
| 7 | beamline visit: | Space Group | A | B | C | α | β |
| 8 | lb13385-2 | P212121 | 40 | 50 | 60 | 90 | 90 |
| 9 | | | | | | | |
| 10 | update ISPyB status | Export pending for ISPyB | Recipe | Resolution | Centring Method | | |
| 11 | ISPyB Status | Beamline Visit | Comments | ---- not saved to datafile! ----> | | | |
| 12 | | | | | | | |
| 13 | | | | | | | |
| 14 | | | | | | | |
| 15 | | | | | | | |
| 16 | | | | | | | |
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| 19 | | | | | | | |
| 20 | | | | | | | |
| 21 | | | | | | | |
| 22 | | | | | | | |
| 23 | | | | | | | |
| 24 | | | | | | | |

Lookup protein

Before doing anything else, protein acronym (**must match your ERA!**), beamline visit, crystal details and data collection strategy need to be entered (far right of sheet)

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 80%

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FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

E4

1 0.678

2 **Do NOT save this file**

3 data is written to an external datafile

4

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Load Data File

Lab Visit: lb13385-70

or enter a full path here: Y:\data\2016\lb13385-70\pro

Source (Library/Solvent)

2 Select Library: DSPLfull D1_R1
(or manually enter below)

Update Library values

Fragments: 756

| ID | Lab Visit | Library Plate | Source Well | Library Name (or solvent) | SMILES | Code |
|----|------------|----------------|-------------|---------------------------|-----------------------------|--------------|
| 1 | lb13385-70 | DSPLfull_D1_R1 | A1 | DSPLfull | COc1cc(ccc1N)N2CCOCC2 | FMOPL000065a |
| 2 | lb13385-70 | DSPLfull_D1_R1 | A2 | DSPLfull | CC[NH+]1CCCCC1 | FMOPL000001a |
| 3 | lb13385-70 | DSPLfull_D1_R1 | A3 | DSPLfull | CC(=O)Nc1nnc(s1)COC | FMOPL000154a |
| 4 | lb13385-70 | DSPLfull_D1_R1 | A4 | DSPLfull | CCNC(=O)Nc1cc(on1)C | FMOPL000207a |
| 5 | lb13385-70 | DSPLfull_D1_R1 | A5 | DSPLfull | CC(C)(C)OC(=O)N1CC[NH+](CC1 | FMOPL000067a |
| 6 | lb13385-70 | DSPLfull_D1_R1 | A6 | DSPLfull | CN(C)c1cc[nH+]cc1 | XST00000847b |
| 7 | lb13385-70 | DSPLfull_D1_R1 | A7 | | | |
| 8 | lb13385-70 | DSPLfull_D1_R1 | A8 | | | |
| 9 | lb13385-70 | DSPLfull_D1_R1 | A9 | | | |
| 10 | lb13385-70 | DSPLfull_D1_R1 | A10 | | | |
| 11 | lb13385-70 | DSPLfull_D1_R1 | A11 | | | |
| 12 | lb13385-70 | DSPLfull_D1_R1 | A12 | | | |
| 13 | lb13385-70 | DSPLfull_D1_R1 | A13 | | | |

Setup Pucks Overview Library ChangeLog

READY

After loading datafile, the red bar will be gone, lab visit will be identified

2 Select a library from the dropdown; compound information will be populated

↓ Alternatively, for solvent characterisation or custom library, enter manually in green columns

soakDB.xlsm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

E16 :

1 0.678

2 **Do NOT save this file**

3 data is written to an external datafile

4

5 **Lab Visit: lb13385-70**

6 or enter a full path here: Y:\data\2016\lb13385-70\pro

7 **Source (Library/Solvent)**

8 Select Library:

9 (or manually enter below)

10

11 Fragments:

| ID | Lab Visit | Library Plate | Source Well | Library Name (or solvent) | SMILES | Code |
|----|------------|---------------|-------------|---------------------------|--------|------|
| 1 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 2 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 3 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 4 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 5 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 6 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 7 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 8 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 9 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 10 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 11 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 12 | lb13385-70 | solvent | A1 | DMSO | | DMSO |
| 13 | lb13385-70 | solvent | A1 | DMSO | | DMSO |

↓ Alternatively, for solvent characterisation or custom library, enter manually in green columns

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 80%

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FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

DropVolu... :

Lab Visit: **lb13385-70** Protein: **JMJD2DA** Error Reset

or enter a full path here: Y:\data\2016\lb13385-70\processing\

Library/Solvent)

Update Library values

Crystals

Import Plates

Get image links

Crystals: 131
Plates: 2
Drop volume: **200**

| Plate | Well | X | Y | Drop Volume (nL) | Protein |
|------------------|------|-----|------|------------------|---------|
| JMJD2DA-CI054837 | E01a | 336 | -455 | 200 | JMJD2DA |
| JMJD2DA-CI054837 | G01c | 510 | -366 | 200 | JMJD2DA |
| JMJD2DA-CI054837 | H01a | 602 | 240 | 200 | JMJD2DA |
| JMJD2DA-CI054837 | H01c | | | | |
| JMJD2DA-CI054837 | H01d | | | | |
| JMJD2DA-CI054837 | E02a | | | | |
| JMJD2DA-CI054837 | E02c | | | | |
| JMJD2DA-CI054837 | H02a | | | | |
| JMJD2DA-CI054837 | H02c | | | | |
| JMJD2DA-CI054837 | H02d | | | | |
| JMJD2DA-CI054837 | H03c | | | | |
| JMJD2DA-CI054837 | H03d | 587 | -412 | 200 | JMJD2DA |
| JMJD2DA-CI054837 | F04c | 345 | 200 | 200 | JMJD2DA |

Batch

crystals/batch:

or

1 batch per plate:

Create Batches

Batch Number

| SMILES | Code | Plate | Well | X | Y | Drop Volume (nL) | Protein | Batch Number |
|-------------------------------|--------------|------------------|------|-----|------|------------------|---------|--------------|
| COc1cc(ccc1N)N2CCOCC2 | FMOPL000065a | JMJD2DA-CI054837 | E01a | 336 | -455 | 200 | JMJD2DA | |
| CC[NH+]1CCCCC1 | FMOPL000001a | JMJD2DA-CI054837 | G01c | 510 | -366 | 200 | JMJD2DA | |
| CC(=O)Nc1nnc(s1)COC | FMOPL000154a | JMJD2DA-CI054837 | H01a | 602 | 240 | 200 | JMJD2DA | |
| CCNC(=O)Nc1cc(on1)C | FMOPL000207a | JMJD2DA-CI054837 | H01c | | | | | |
| CC(C)(C)OC(=O)N1CC[NH+](CC1 | FMOPL000067a | JMJD2DA-CI054837 | H01d | | | | | |
| CN(C)c1cc[nH+]cc1 | XST00000847b | JMJD2DA-CI054837 | E02a | | | | | |
| Cc1c([nH]c2c1cc(cc2)F)C | FMOPL000155a | JMJD2DA-CI054837 | E02c | | | | | |
| c1cc(ccc1NC(=O)C2CCC2)n3cnn | FMOPL000208a | JMJD2DA-CI054837 | H02a | | | | | |
| c1ccc(c(c1)C[NH3+])N2CCC(CC2 | FMOPL000066a | JMJD2DA-CI054837 | H02c | | | | | |
| COc1ccc(cc1)Cl | FMOPL000002a | JMJD2DA-CI054837 | H02d | | | | | |
| C[NH+](C)Cc1ccc(o1)C(=O)[O-] | FMOPL000156a | JMJD2DA-CI054837 | H03c | | | | | |
| c1ccc(cc1)COc2ccc(cc2)C(=O)NN | FMOPL000209a | JMJD2DA-CI054837 | H03d | 587 | -412 | 200 | JMJD2DA | |

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

3 Enter the crystallisation drop volume

4 Import plates. Select crystal target lists from TeXRANK targeting (csv files)

soakDB.xlsm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

DropVolu... : *fx* 200

P Q R S T U V W X Y Z

1

2 2DA Error Reset Error Reset

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8 2

9 200 **5**

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12 Protein Batch Number PlateBatch Name

13 JMJD2DA 1 JMJD2DA-CI054837_B1

14 JMJD2DA 1 JMJD2DA-CI054837_B1

15 JMJD2DA 1 JMJD2DA-CI054837_B1

16 JMJD2DA 1 JMJD2DA-CI054837_B1

17 JMJD2DA 1 JMJD2DA-CI054837_B1

18 JMJD2DA 1 JMJD2DA-CI054837_B1

19 JMJD2DA 1 JMJD2DA-CI054837_B1

20 JMJD2DA 1 JMJD2DA-CI054837_B1

21 JMJD2DA 1 JMJD2DA-CI054837_B1

22 JMJD2DA 1 JMJD2DA-CI054837_B1

23 JMJD2DA 1 JMJD2DA-CI054837_B1

24 JMJD2DA 1 JMJD2DA-CI054837_B1

Batches

crystals/batch:

or

1 batch per plate:

Create Batches Refresh Names

Soak

Compound [stock] mM:

Desired Solvent %:

Export pending

(re)calculate and add to pending

done

Compound [compound] Transfer

[stock] mM

5 Click Create Batches. If 1 batch per plate is selected, each crystal plate will be assigned a batch.

Alternatively, uncheck 1 batch per plate, and enter the desired number of crystals/batch

↓ or manually assign batch numbers

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 80%

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FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

SolventFr... :

T U V **W** X Y Z AA AB AC AD AE AF

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Soak

Compound [stock] mM:

Desired Solvent %:

6

Cryo (optional)

Cryo [stock] %:

Desired Cryo %:

Cryo location:

| | Compound [stock] mM | [compound] mM | Solvent % | Transfer Vol | Soak Status | Soak Transfer Date/Time | | Cryo [stock] % | Desired Cryo % | Cryo location | Cryo Transfer Vol | Cryo Status |
|----|---------------------|---------------|-----------|--------------|-------------|-------------------------|--|----------------|----------------|---------------|-------------------|-------------|
| 12 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 13 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 14 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 15 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 16 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 17 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 18 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 19 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 20 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 21 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 22 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 23 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |
| 24 | 500 | 100 | 20 | 50.0 | pending | | | | | | | |

6 Enter the library/compound concentration, and the desired final solvent concentration. Click (re)calculate and add to pending

↓ Alternatively, manually enter desired values in the green columns, and then click (re)calculate and add to pending

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 80%

soakDB.xlsm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

W23 : X 40

S T U V W X Y Z AA AB AC AD

1

2 Error Reset Error Reset

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5 ches

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9 Refresh Names

10

11 PlateBatch Name

12 JMJD2DA-CI054837_B1

13 JMJD2DA-CI054837_B1

14 JMJD2DA-CI054837_B1

15 JMJD2DA-CI054837_B1

16 JMJD2DA-CI054837_B1

17 JMJD2DA-CI054837_B1

18 JMJD2DA-CI054837_B1

19 JMJD2DA-CI054837_B1

20 JMJD2DA-CI054837_B1

21 JMJD2DA-CI054837_B1

22 JMJD2DA-CI054837_B1

23 JMJD2DA-CI054837_B1

24 JMJD2DA-CI054837_B1

Soak

Compound [stock] mM: 500

Desired Solvent %: 20

(re)calculate and add to pending

Export pending

done

Cryo

Cryo [stock] %: 100

Desired Cryo %: 15

Cryo location: A1

(re)calculate and add to pen

| Compound [stock] mM | [compound] mM | Solvent % | Transfer Vol | Soak Status | Soak Transfer Date/Time | Cryo [stock] % | Desired Cryo % | Cryo location |
|---------------------|---------------|-----------|--------------|-------------|-------------------------|----------------|----------------|---------------|
| 100 | | 0 | | | | | | |
| 100 | | 0 | | | | | | |
| 100 | | 5 | | | | | | |
| 100 | | 5 | | | | | | |
| 100 | | 10 | | | | | | |
| 100 | | 10 | | | | | | |
| 100 | | 20 | | | | | | |
| 100 | | 20 | | | | | | |
| 100 | | 30 | | | | | | |
| 100 | | 30 | | | | | | |
| 100 | | 40 | | | | | | |
| 100 | | 40 | | | | | | |

↓ Example for solvent characterisation: Manually entered 6 concentrations of DMSO, in duplicate.

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 80%

soakDB.xlsm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

W23 : *fx* 40

S T U V **W** X Y Z AA AB AC AD

1

2 Error Reset Error Reset

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5 **ches**

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9 Refresh Names

10

11 **Soak**

Compound [stock] mM: 500

Desired Solvent %: 20

Export pending

(re)calculate and add to pending

done

12 **Cryo**

Cryo [stock] %: 100

Desired Cryo %: 15

Cryo location: A1

(re)calculate and add to pen

| PlateBatch Name | Compound [stock] mM | [compound] mM | Solvent % | Transfer Vol | Soak Status | Soak Transfer Date/Time | Cryo [stock] % | Desired Cryo % | Cryo location |
|---------------------|---------------------|---------------|-----------|--------------|-------------|-------------------------|----------------|----------------|---------------|
| JMJD2DA-CI054837_B1 | 100 | 0 | 0 | 0.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 0 | 0 | 0.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 4.8 | 5 | 10.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 4.8 | 5 | 10.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 10.1 | 10 | 22.5 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 10.1 | 10 | 22.5 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 20 | 20 | 50.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 20 | 20 | 50.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 29.8 | 30 | 85.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 29.8 | 30 | 85.0 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 39.8 | 40 | 132.5 | pending | | | | |
| JMJD2DA-CI054837_B1 | 100 | 39.8 | 40 | 132.5 | pending | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | pending | | | | |

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 80%

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FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

BC8

S T U V W X Y Z AA AB AC AD

1

2 Error Reset Error Reset

3

4

5 ches

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9 Refresh Names

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Soak

Compound [stock] mM: 500
Desired Solvent %: 20

(re)calculate and add to pending

7 Export pending

done

Cryo

Cryo [stock] %:
Desired Cryo %:
Cryo location:

(re)calculate and add to pen

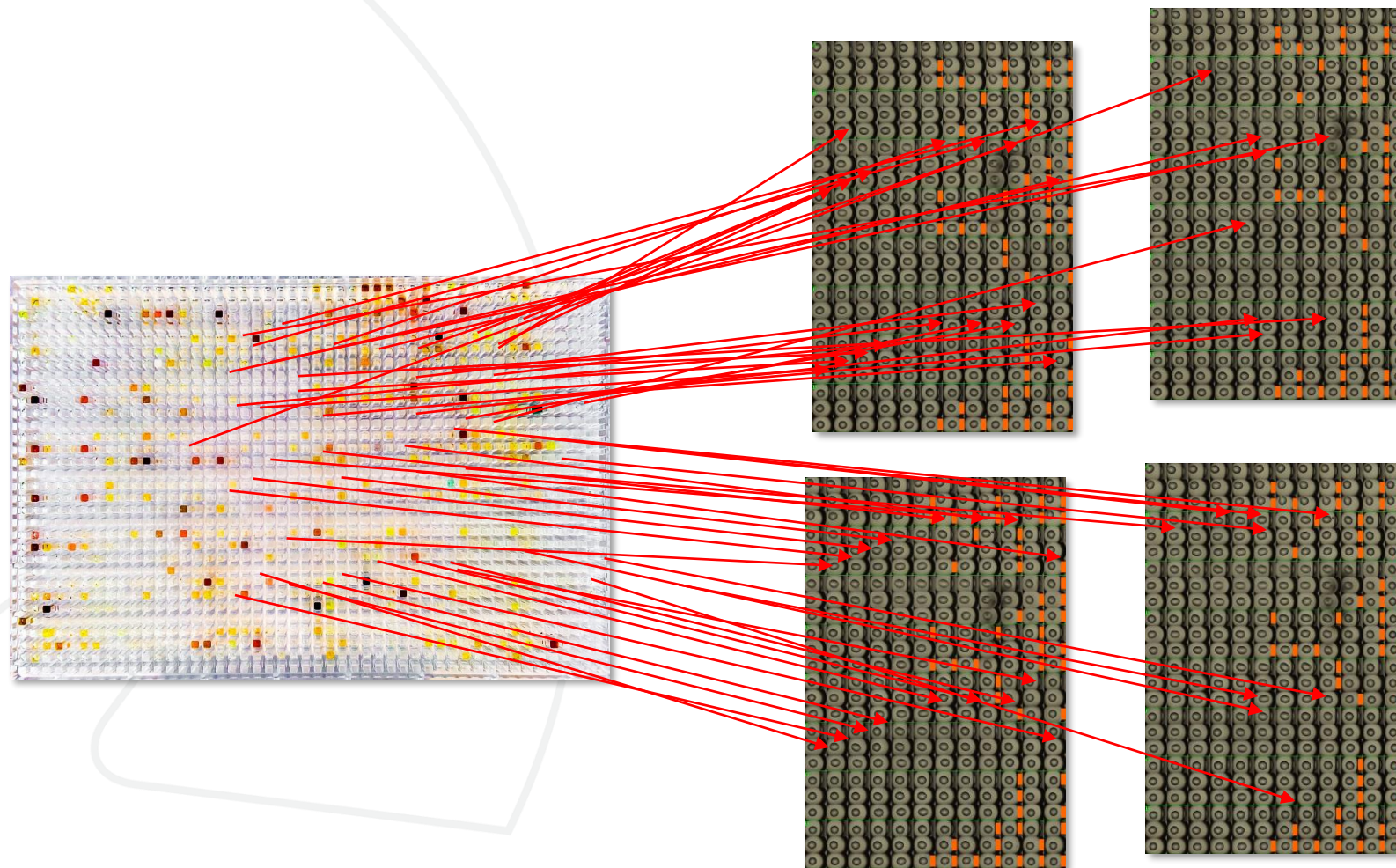
| PlateBatch Name | Compound [stock] mM | [compound] mM | Solvent % | Transfer Vol | Soak Status | Soak Transfer Date/Time | Cryo [stock] % | Desired Cryo % | Cryo location |
|---------------------|---------------------|---------------|-----------|--------------|-------------|-------------------------|----------------|----------------|---------------|
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | exported | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | exported | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | exported | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | exported | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | exported | | | | |
| JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | exported | | | | |

7 Click Export Pending. This will place csv files for the Echo into the lab36/echo folder.
One csv file is created for each batch

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 80%

Soak crystals!



soakDB.xlsm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

BC8

S T U V W X Y Z AA AB AC AD

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2 Error Reset Error Reset

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5 ches Soak Cryo

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8 Compound [stock] mM: 500

9 Desired Solvent %: 20

10 Refresh Names (re)calculate and add to pending Export pending

11 PlateBatch Name

| | Compound [stock] mM | [compound] mM | Solvent % | Transfer Vol | Soak Status | Soak Transfer Date/Time | Cryo [stock] % | Desired Cryo % | Cryo location |
|----|---------------------|---------------|-----------|--------------|-------------|-------------------------|---------------------|----------------|---------------|
| 12 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | done | 16/01/2017 11:18:19 | | |
| 13 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | done | 16/01/2017 11:18:19 | | |
| 14 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | done | 16/01/2017 11:18:19 | | |
| 15 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | |
| 16 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | |
| 17 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | |
| 18 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | |
| 19 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | |
| 20 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | |
| 21 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | | | | |
| 22 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | done | 16/01/2017 11:18:19 | | |
| 23 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | done | 16/01/2017 11:18:19 | | |
| 24 | JMJD2DA-CI054837_B1 | 500 | 100 | 20 | 50.0 | done | 16/01/2017 11:18:19 | | |

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8 After Echo transfer of each batch, click "done". This will assign a timestamp to batches that have been soaked

8

8

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY

80%

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FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

A18 : (yellow = mount!)

Z AA AB AC AD AE AF AG AH AI AJ

1

2 Error Reset Error Reset

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8 Export pending

9

10 done

11

12

13

14

15

16

17

18

19

20

21

Cryo (optional)

Cryo [stock] %: 100

Desired Cryo %: 15

Cryo location: A1

Desired soak time: 1 hours

(yellow = mount!)

(re)calculate and add to pending

Export pending

done

Refresh time

Export pending

| Soak Transfer Date/Time | Cryo [stock] % | Desired Cryo % | Cryo location | Cryo Transfer Vol | Cryo Status | Cryo Transfer Date/Time | Soaking time | Mounting Sta |
|-------------------------|----------------|----------------|---------------|-------------------|-------------|-------------------------|--------------|--------------|
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | done | 16/01/2017 11:22:16 | 0d 00:04:12 | pending |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | done | 16/01/2017 11:22:16 | 0d 00:04:12 | pending |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | done | 16/01/2017 11:22:16 | 0d 00:04:12 | pending |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |
| 16/01/2017 11:18:19 | 100 | 15 | A1 | 35.0 | | | | ing |

Repeat for cryo, if necessary

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 85%

soakDB.xlsxm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

W12 : 0

AH AI AJ AK AL AM AN AO AP

1

2 Error Reset Error Reset

3

4

5 **Harvesting**

6 Desired soak time 3 hours

7 (yellow = mount!) 44 starting at crystal number (only applies for the first import)

8 use old shifter?

9 Refresh time Export pending Load mounting manual load barcodes Generate crystal names

10

11 Soaking time Mounting Status Crystal Name Puck Position Pin Barcode Mounting Result Arrival Time Mo

12 0d 00:07:36 exported

13 0d 00:07:36 exported

14 0d 00:07:36 exported

15 0d 00:07:36 exported

16 0d 00:07:36 exported

17 0d 00:07:36 exported

18 0d 00:07:36 exported

19 0d 00:07:36 exported

20 0d 00:07:36 exported

21 0d 00:07:36 exported

22 0d 00:07:36 exported

23 0d 00:07:36 exported

24 0d 00:07:36 exported

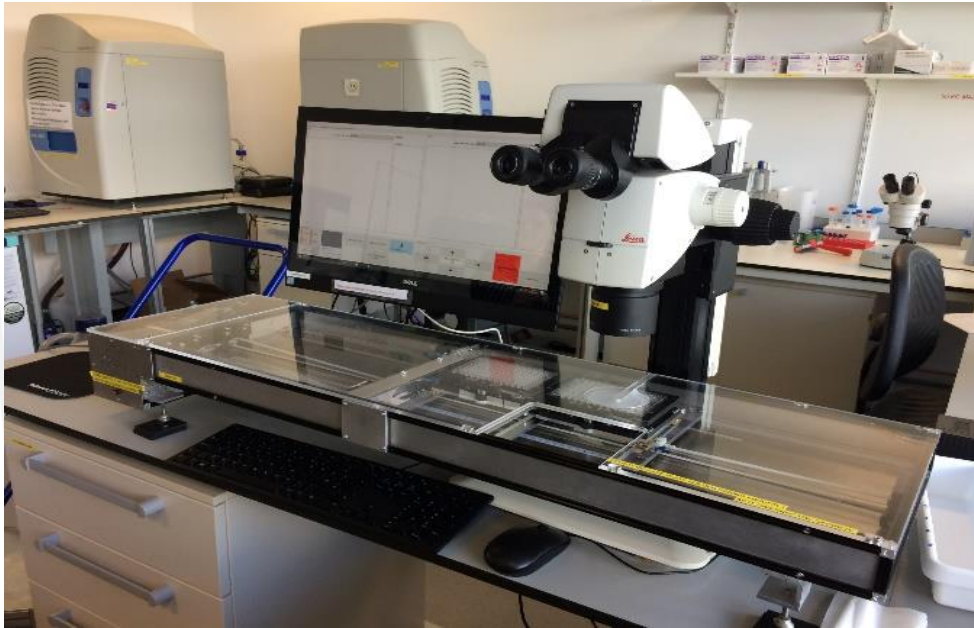
9 Click Export pending to generate csv files for shifter mounting. One csv file per batch is created.

➡ Tick this box if you are going to use the old shifter

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY AVERAGE: 17.5 COUNT: 12 SUM: 210 80%

Mount Crystals!



soakDB.xlsm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

A18 : (yellow = mount!)

AH AI AJ AK AL AM AN AO AP

1 Error Reset Error Reset

2

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5 **Harvesting**

6 Desired soak time 3 hours

7 (yellow = mount!) 44 starting at crystal number (only applies for the first import)

8 use old shifter?

9 Refresh time Export pending Load mounting 10 manual load barcodes Generate crystal names

10

| Soaking time | Mounting Status | Crystal Name | Puck | Position | Pin Barcode | Mounting Result | Arrival Time |
|--------------|-----------------|---------------|---------|----------|-------------|-----------------|------------------|
| 0d 04:43:48 | done | JMJD2DA-x0002 | DLS0166 | 9 | DF035B0154 | Mounted_Clear | 16/01/2017 16:02 |
| 0d 04:48:49 | done | JMJD2DA-x0003 | DLS350 | 2 | DF035B0059 | Mounted_Clear | 16/01/2017 16:02 |
| 0d 04:53:49 | done | JMJD2DA-x0004 | DLS350 | 11 | | | |
| 0d 04:54:26 | done | JMJD2DA-x0005 | DLS350 | 12 | | | |
| 0d 04:55:26 | done | JMJD2DA-x0006 | DLS350 | 13 | | | |
| 0d 04:44:17 | done | JMJD2DA-x0007 | DLS0166 | 10 | | | |
| 0d 04:44:43 | done | JMJD2DA-x0008 | DLS0166 | 11 | | | |
| 0d 04:55:55 | done | JMJD2DA-x0009 | DLS350 | 14 | | | |
| 0d 04:56:25 | done | JMJD2DA-x0010 | DLS350 | 15 | DF075C1083 | Mounted_Clear | 16/01/2017 16:14 |
| 0d 04:57:00 | done | JMJD2DA-x0011 | DLS350 | 16 | DF075C0512 | Mounted_Clear | 16/01/2017 16:15 |

11

12

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19

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21

10 Click Load mounting to load results of crystal mounting

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 85%

soakDB.xlsm [Read-Only] - Excel

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...

A18 : (yellow = mount!)

AS AT AU AV AW AX AY AZ BA

1 Error Reset Error Reset

2

3

4

5 **Data Collection** Lookup protein

6 EUBOpen iNEXT COVID-19 ILO Xchem
 FALSE FALSE FALSE FALSE

7 beamline visit: Space Group A B C α β

8 lb13385-2 P212121 40 50 60 90 90

9

10 update ISPyB status **12** Export pending for ISPyB **13** Recipe Resolution Centring Method **11**
 High Dose 1.7 diffraction

11 ISPyB Status Beamline Visit Comments |---- not saved to datafile! ----->

12 pyb\lb13385-2_2017-01 lb13385-2

13 pyb\lb13385-2_2017-01 lb13385-2

14 pyb\lb13385-2_2017-01 lb13385-2

15 pyb\lb13385-2_2017-01 lb13385-2

16 pyb\lb13385-2_2017-01 lb13385-2

17 pyb\lb13385-2_2017-01 lb13385-2

18 pyb\lb13385-2_2017-01 lb13385-2

19 pyb\lb13385-2_2017-01 lb13385-2

20 pyb\lb13385-2_2017-01 lb13385-2

21 pyb\lb13385-2_2017-01 lb13385-2

Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB ...

READY 85%

- 11** Ensure data collection strategy is entered
- 12** Click update ISPyB status
- 13** Click Export pending for ISPyB. A single csv file is created for all pending crystals.

Puck Management

Puck Management **15** Update/Save Changes **18** click this again if you make any edits!

14

Pucks: 8
Crystals: 115

| Puck | Robot position | Instructions | Storage shelf | Done? | Data collection | Shipment | What/Who | Priority/comments | Date Mounted | Pins |
|---------|----------------|--------------|---------------|-------|-----------------|----------|-----------------|-------------------------|--------------|------|
| | | collect | | no | standard | | JMJD2DA/patrick | high priority - solvent | | |
| DLS0166 | | collect | 1 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |
| DLS350 | | collect | 1 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |
| CPS0365 | | collect | 1 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |
| CPS0269 | | collect | 1 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |
| DLS567 | | collect | 3 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |
| DF002 | | collect | 3 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |
| DF020 | | collect | 3 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |
| DLS566 | | collect | 3 | no | standard | | JMJD2DA/patrick | high priority - solvent | 20170116 | 16 |

16

17

On the "Pucks" tab:

- 14** Enter information in green boxes
- 15** Click Update/Save Changes. Click on YES for the pop up on overwriting the list
- 16** Puck details will be brought in
- 17** Manually enter the storage dewar shelf number for each puck in this column
- 18** Click Update/Save Changes again

CSV2ISPyB



- Run script
 - Open PuTTY and connect to `ssh.diamond.ac.uk`
 - Navigate to the visit directory
(`/dls/labxchem/data/PROPOSAL/VISIT/processing/lab36/ispyb`)
 - Execute `'csv2ispyb PROPOSAL_TIMESTAMP.csv'`
 - Wait until the upload is finished, and check that no error messages occur
- Check ISPyB for newly created 'shipment'
- Add pucks to [XChemQueue](#)