XChem training: TexRank & SoakDB

May 2022

TexRank

TexRank

- Use ‘tserver’ to go on Windows machine
- TexRank shortcut on desktop

❶ Select plate

❷ Select (toggle!!) Formulatrix (RC)

❸ Select 1 Subwell

❹ Target dispensing location (right click)

❺ Save list before moving to next plate (ECHO – 1 Target)

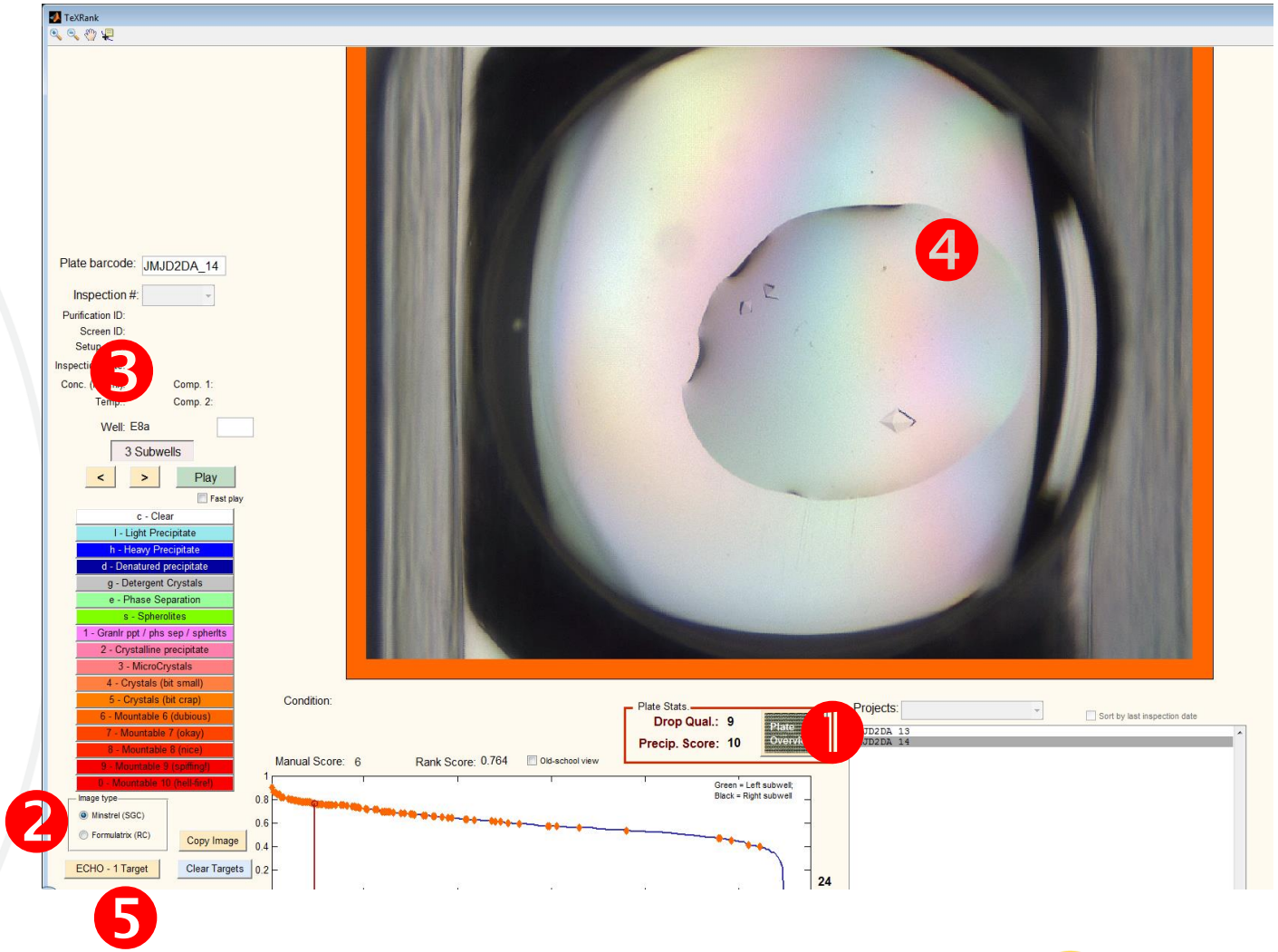
Save to here:

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

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

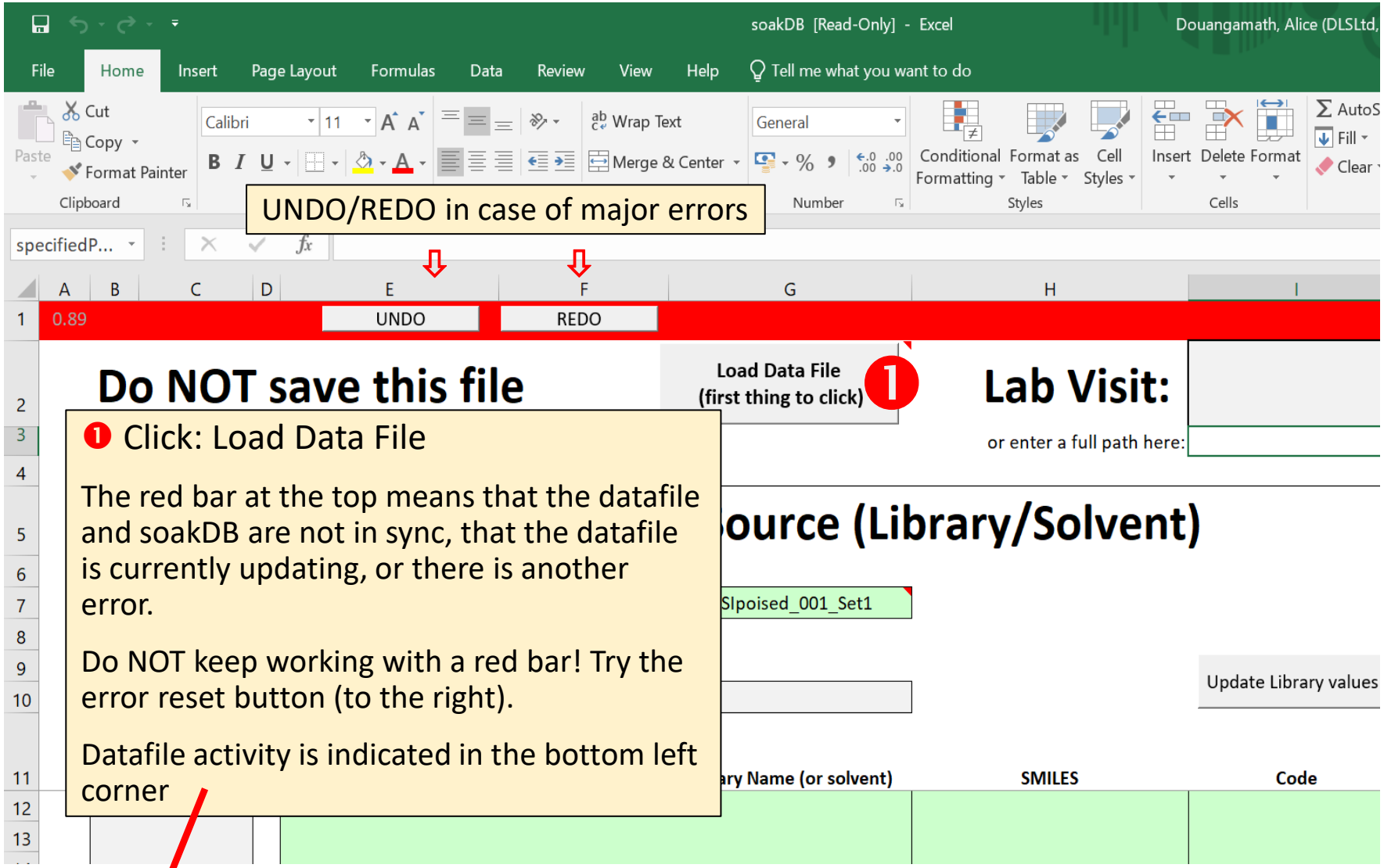
Arrow keys on keyboard to move previous/next

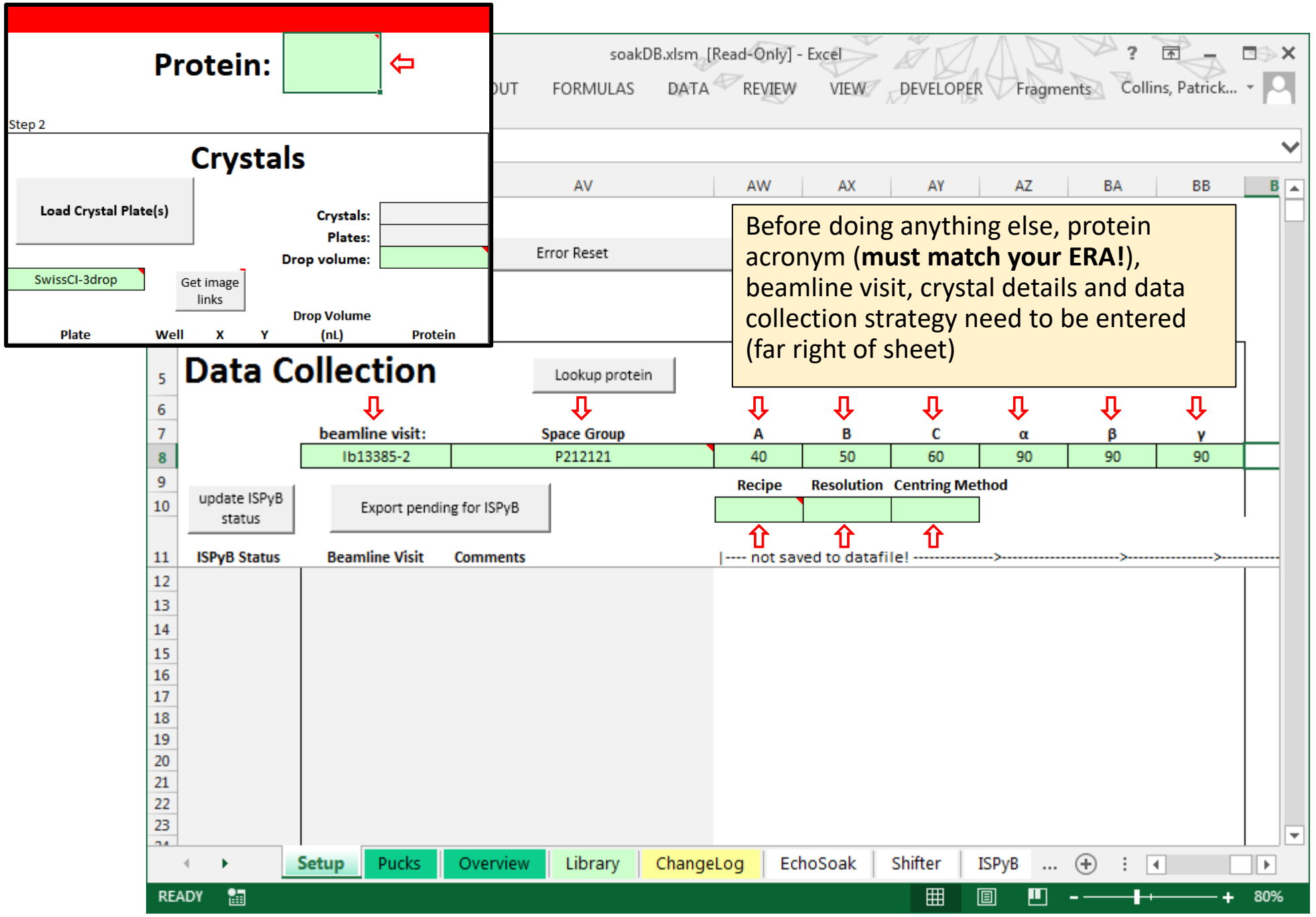
Check the crystal target output csv files X and Y should be within +/- 1300 (for swissCI-3drops)

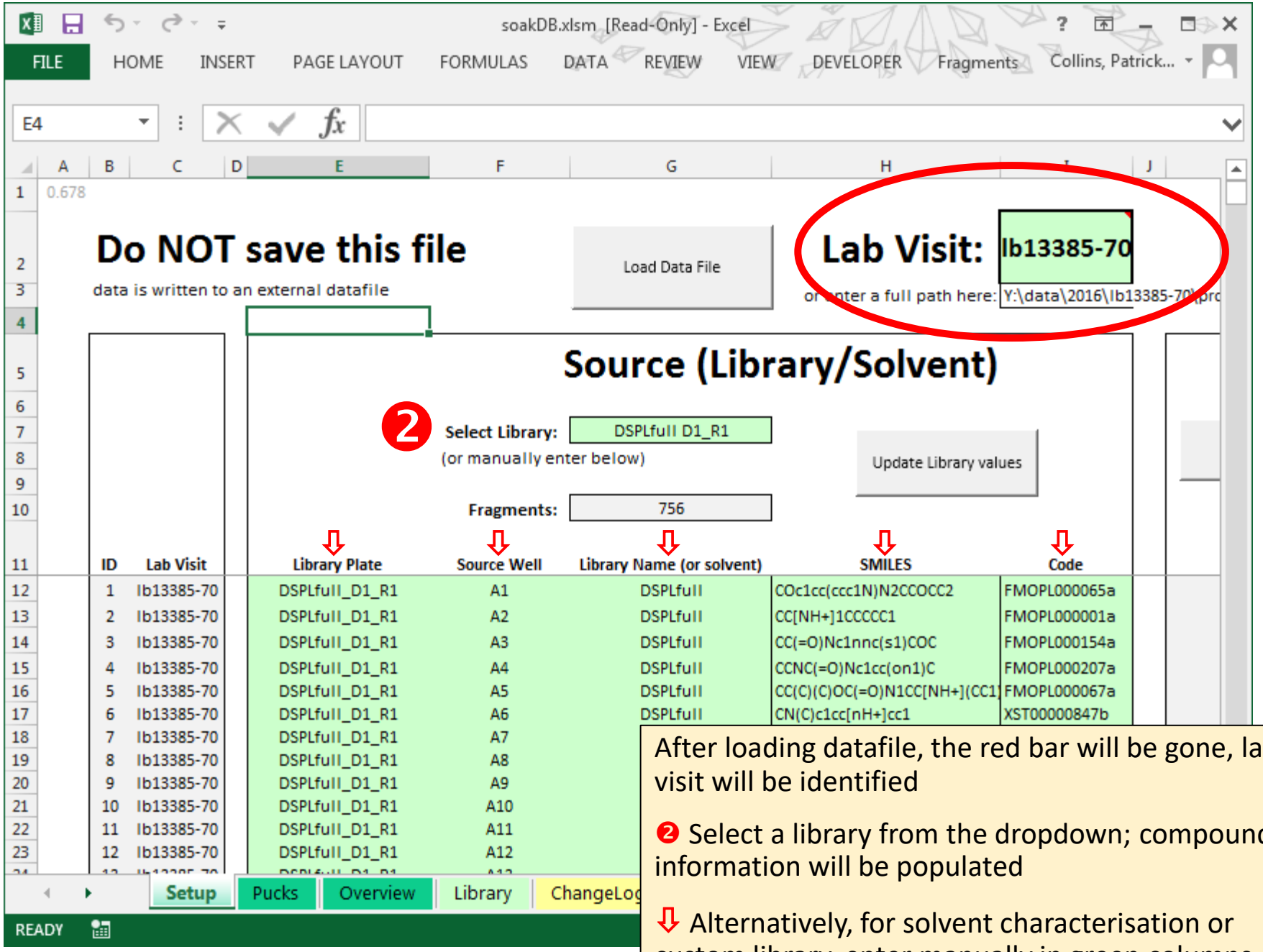


SoakDB

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
Cut
Copy
Format Painter
Paste
Clipboard
Calibri
11
Wrap Text
Merge & Center
General
Number
Conditional Formatting
Format as Table
Cell Styles
Styles
Insert
Delete
Format
Cells
AutoS
Fill
Clear
UNDO/REDO in case of major errors
specifiedP...
A
B
C
D
E
F
G
H
I
1
0.89
UNDO
REDO
Do NOT save this file
Load Data File
(first thing to click)
1
Lab Visit:
or enter a full path here:
ource (Library/Solvent)
SIpoised_001_Set1
Update Library values
ary Name (or solvent)
SMILES
Code
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
XLSQLite: Placing values in array...

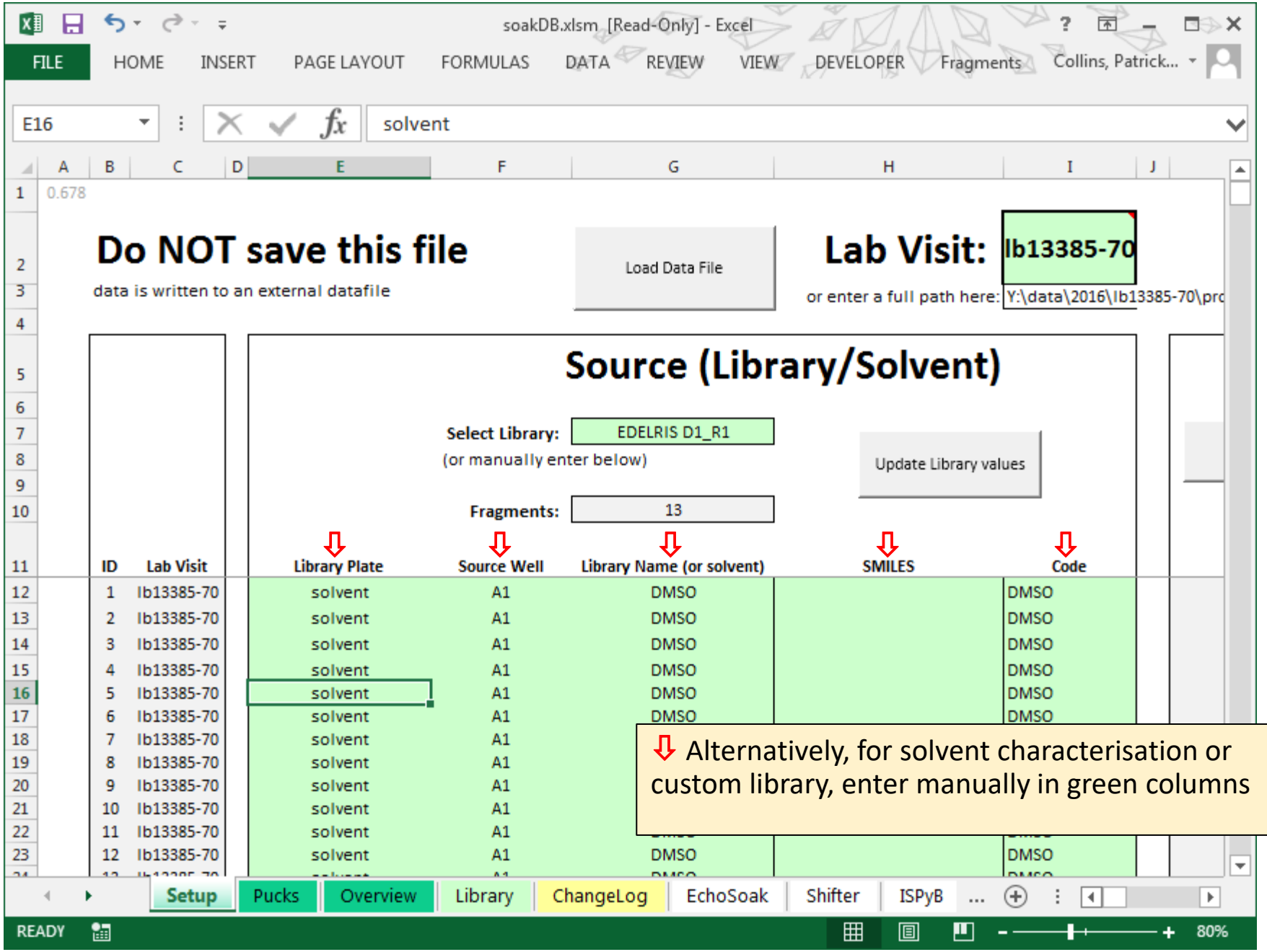

Protein:
Step 2
Crystals
Load Crystal Plate(s)
Crystals:
Plates:
Drop volume:
SwissCI-3drop
Get image links
Drop Volume
Plate
Well
X
Y
(nL)
Protein
soakDB.xlsm [Read-Only] - Excel
FORMULAS
DATA
REVIEW
VIEW
DEVELOPER
Fragments
Collins, Patrick...
AV
AW
AX
AY
AZ
BA
BB
Error Reset
Before doing anything else, protein acronym (must match your ERA!), beamline visit, crystal details and data collection strategy need to be entered (far right of sheet)
Data Collection
Lookup protein
beamline visit:
Space Group
A
B
C
α
β
γ
Ib13385-2
P212121
40
50
60
90
90
90
Recipe
Resolution
Centring Method
update ISPyB status
Export pending for ISPyB
ISPyB Status
Beamline Visit
Comments
not saved to datafile!
Setup
Pucks
Overview
Library
ChangeLog
EchoSoak
Shifter
ISPyB
READY
80%

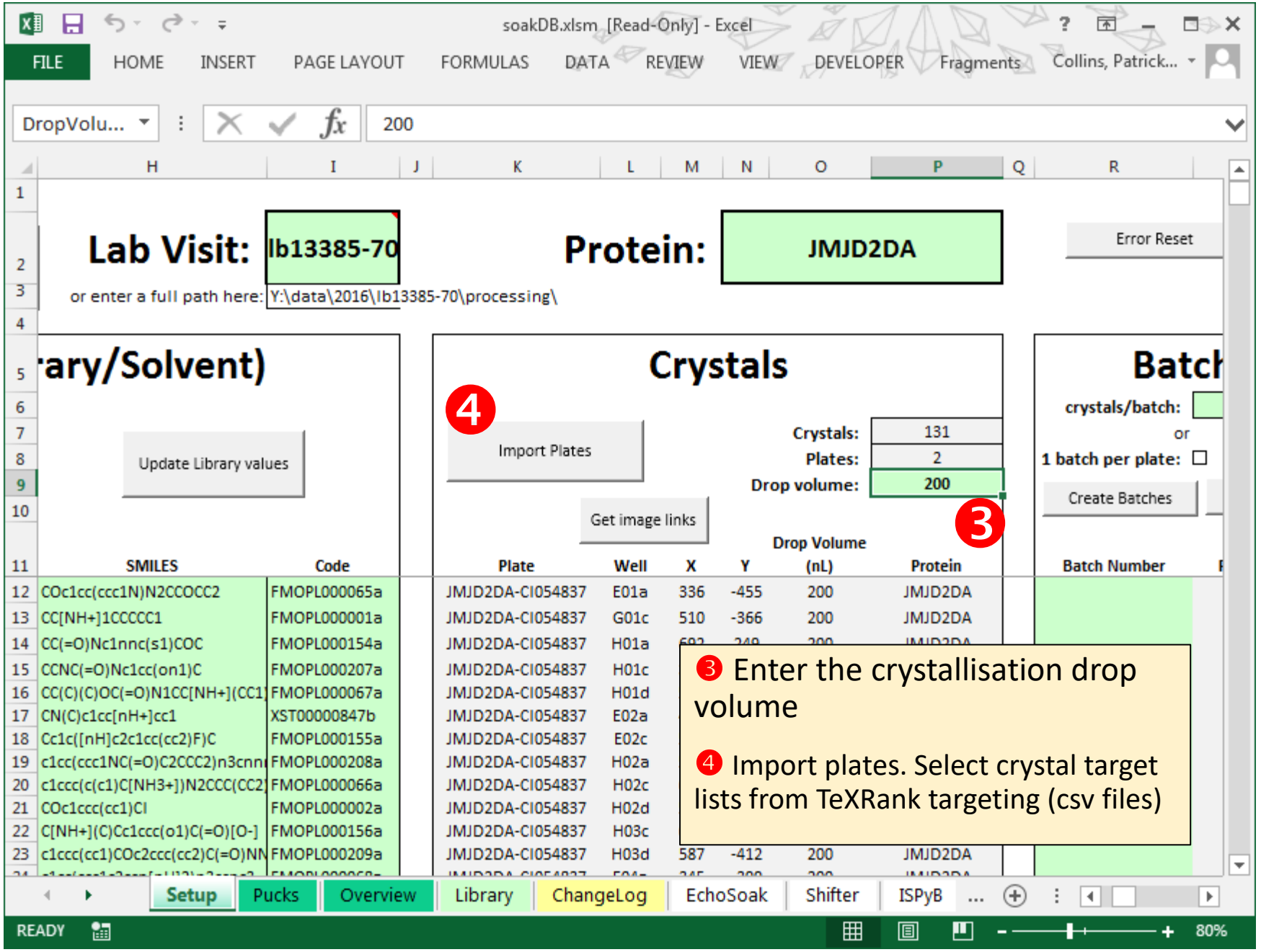


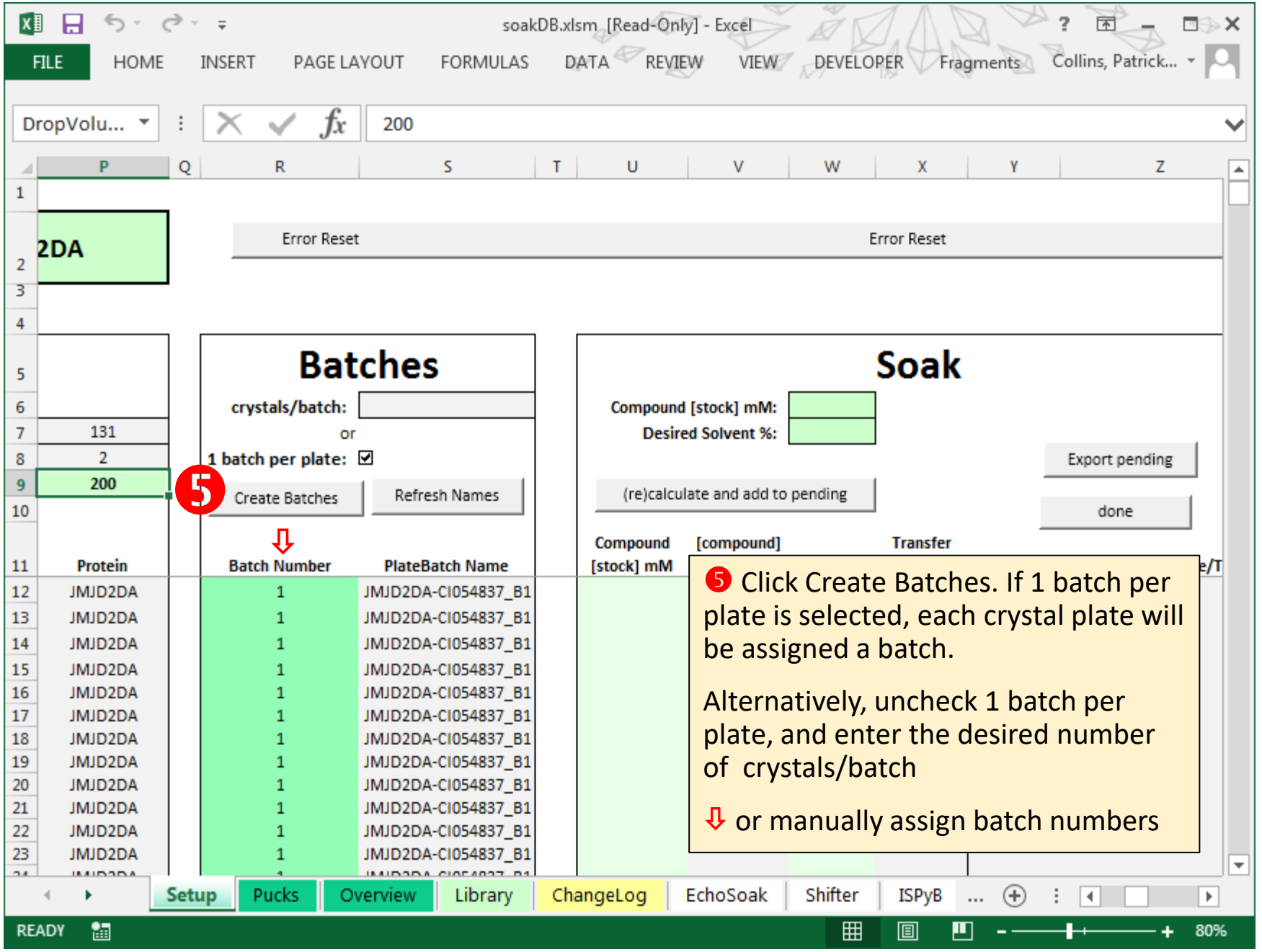
After loading datafile, the red bar will be gone, lab visit will be identified

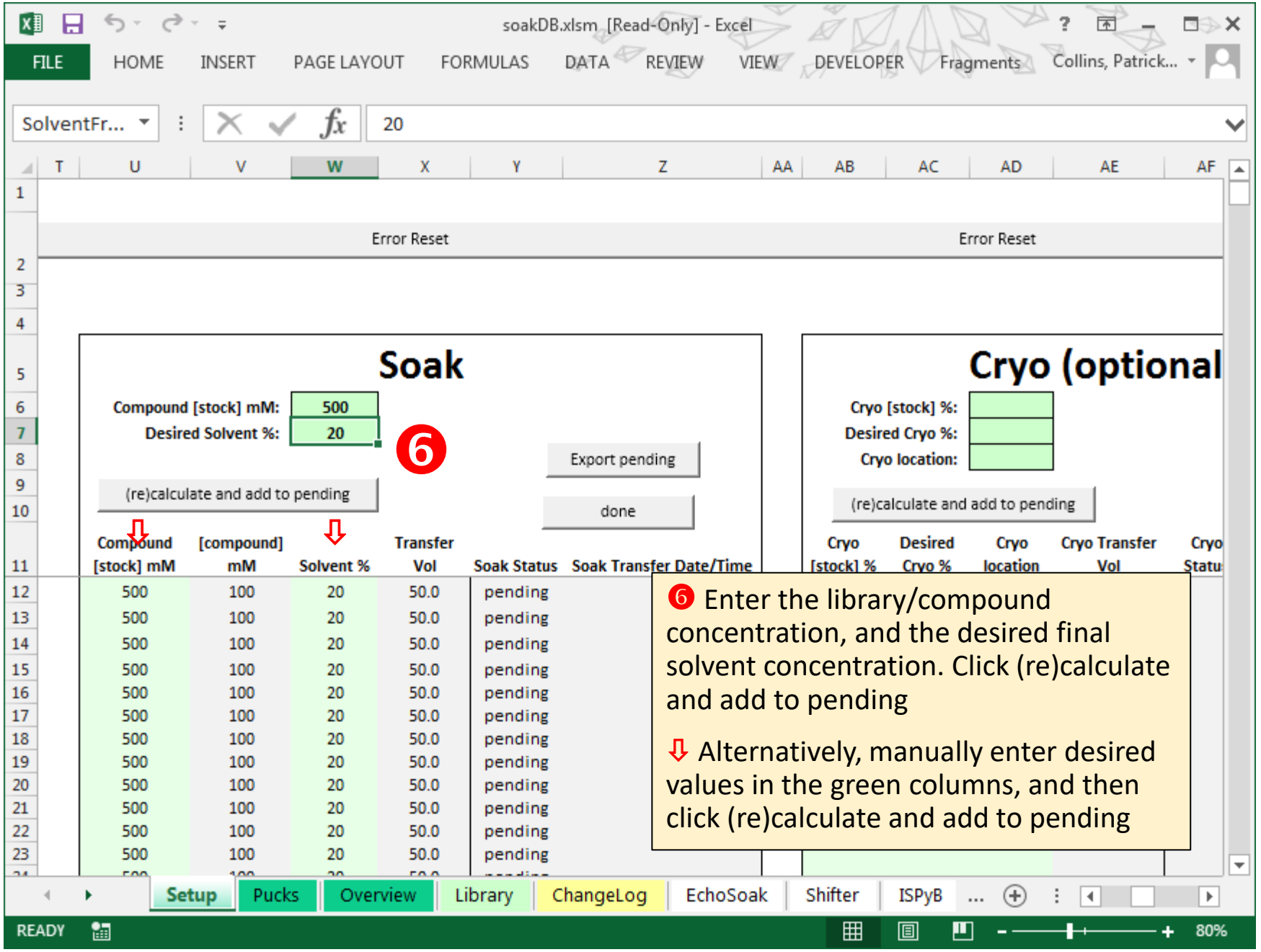
❷ Select a library from the dropdown; compound information will be populated

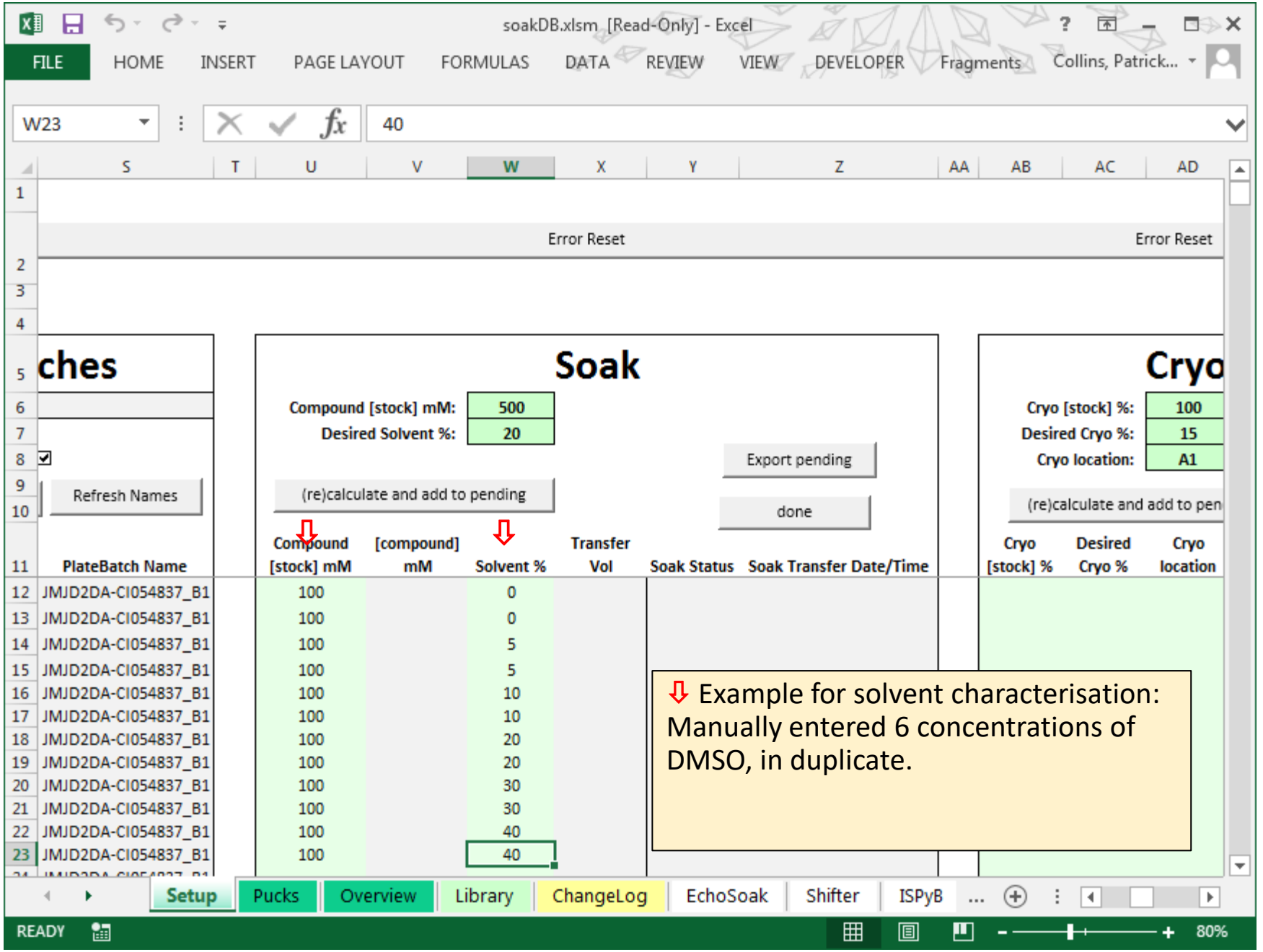
⇩ Alternatively, for solvent characterisation or custom library, enter manually in green columns

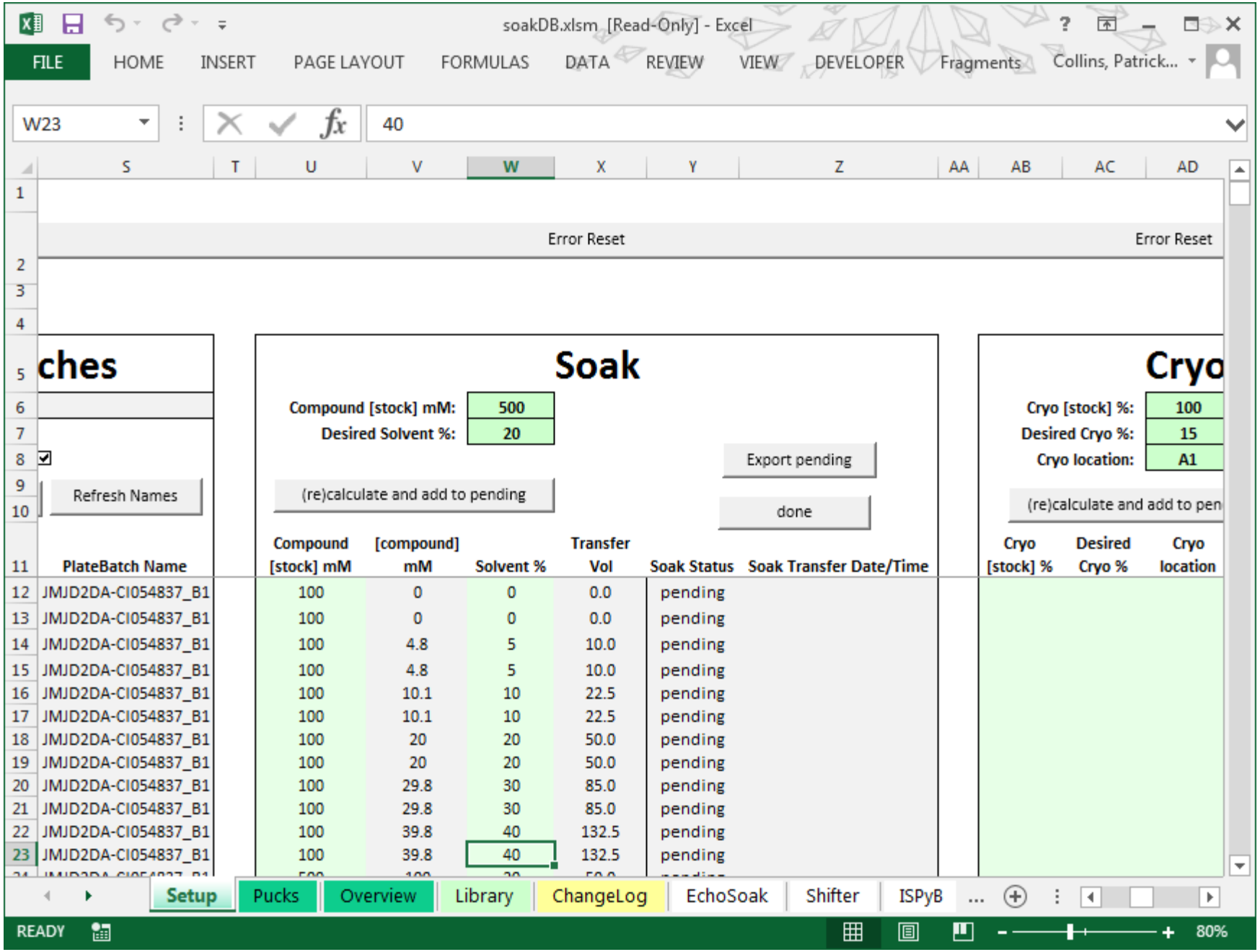

soakDB.xlsm [Read-Only] - Excel
FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...
E16
solvent
0.678
Do NOT save this file
data is written to an external datafile
Load Data File
Lab Visit:
lb13385-70
or enter a full path here: Y:\data\2016\lb13385-70\pro
Source (Library/Solvent)
Select Library:
EDELRIS D1_R1
(or manually enter below)
Update Library values
Fragments:
13
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
8 lb13385-70 solvent A1
9 lb13385-70 solvent A1
10 lb13385-70 solvent A1
11 lb13385-70 solvent A1
12 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%

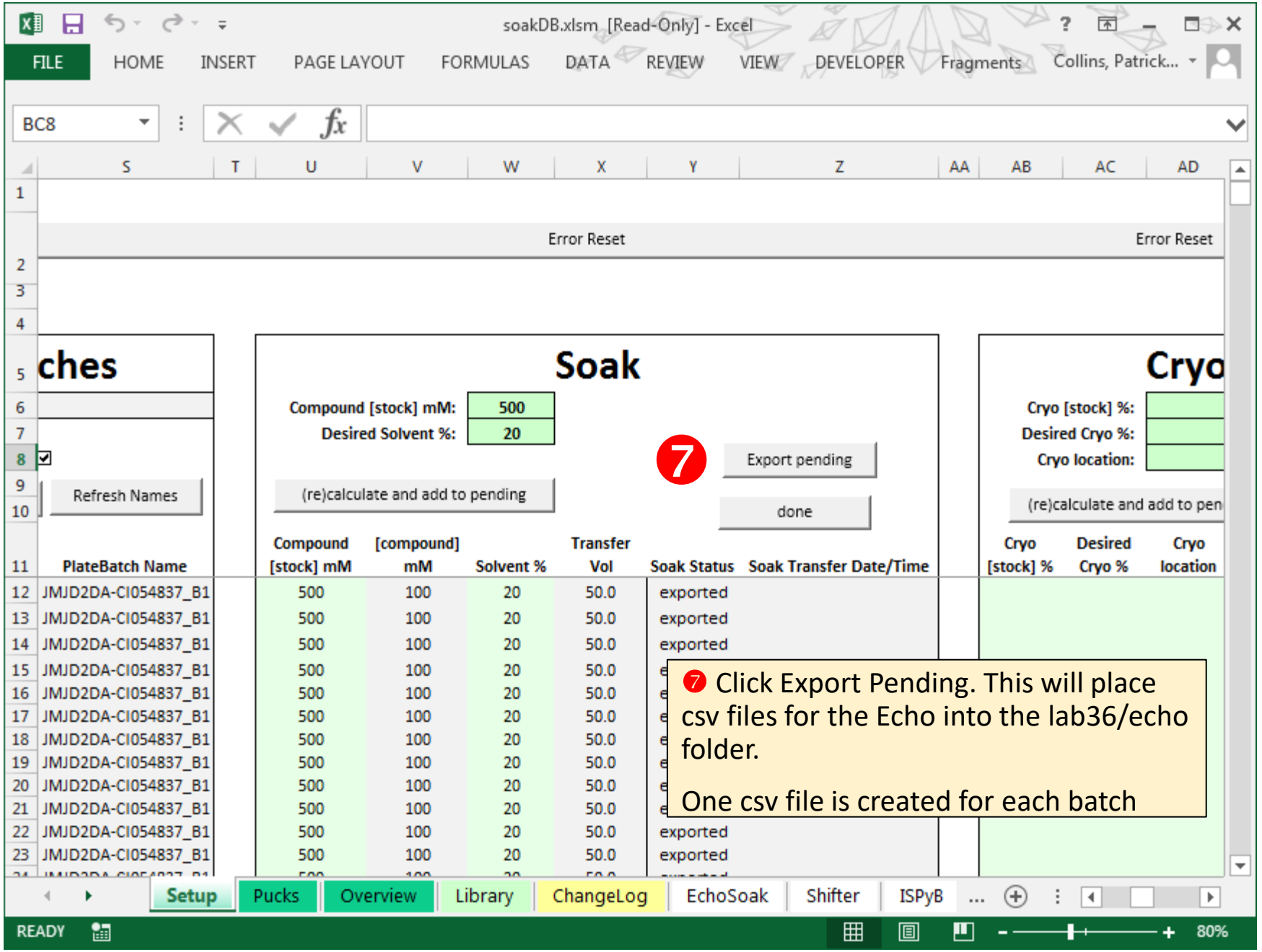

soakDB.xlsm [Read-Only] - Excel
FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...
DropVolu...
200
Lab Visit:
lb13385-70
Protein:
JMJD2DA
Error Reset
or enter a full path here:
Y:\data\2016\lb13385-70\processing\
rary/Solvent)
Update Library values
Crystals
4
Import Plates
Get image links
Crystals:
131
Plates:
2
Drop volume:
200
3
Batch
crystals/batch:
or
1 batch per plate:
Create Batches
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
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
❸ Enter the crystallisation drop volume
❹ Import plates. Select crystal target lists from TeXRank targeting (csv files)
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...
DropVolu...
200
2DA
Error Reset
Error Reset
Batches
crystals/batch:
or
1 batch per plate:
5
Create Batches
Refresh Names
Soak
Compound [stock] mM:
Desired Solvent %:
Export pending
(re)calculate and add to pending
done
131
2
200
Protein
Batch Number
PlateBatch Name
Compound [stock] mM
[compound]
Transfer
JMJD2DA
1
JMJD2DA-CI054837_B1
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%

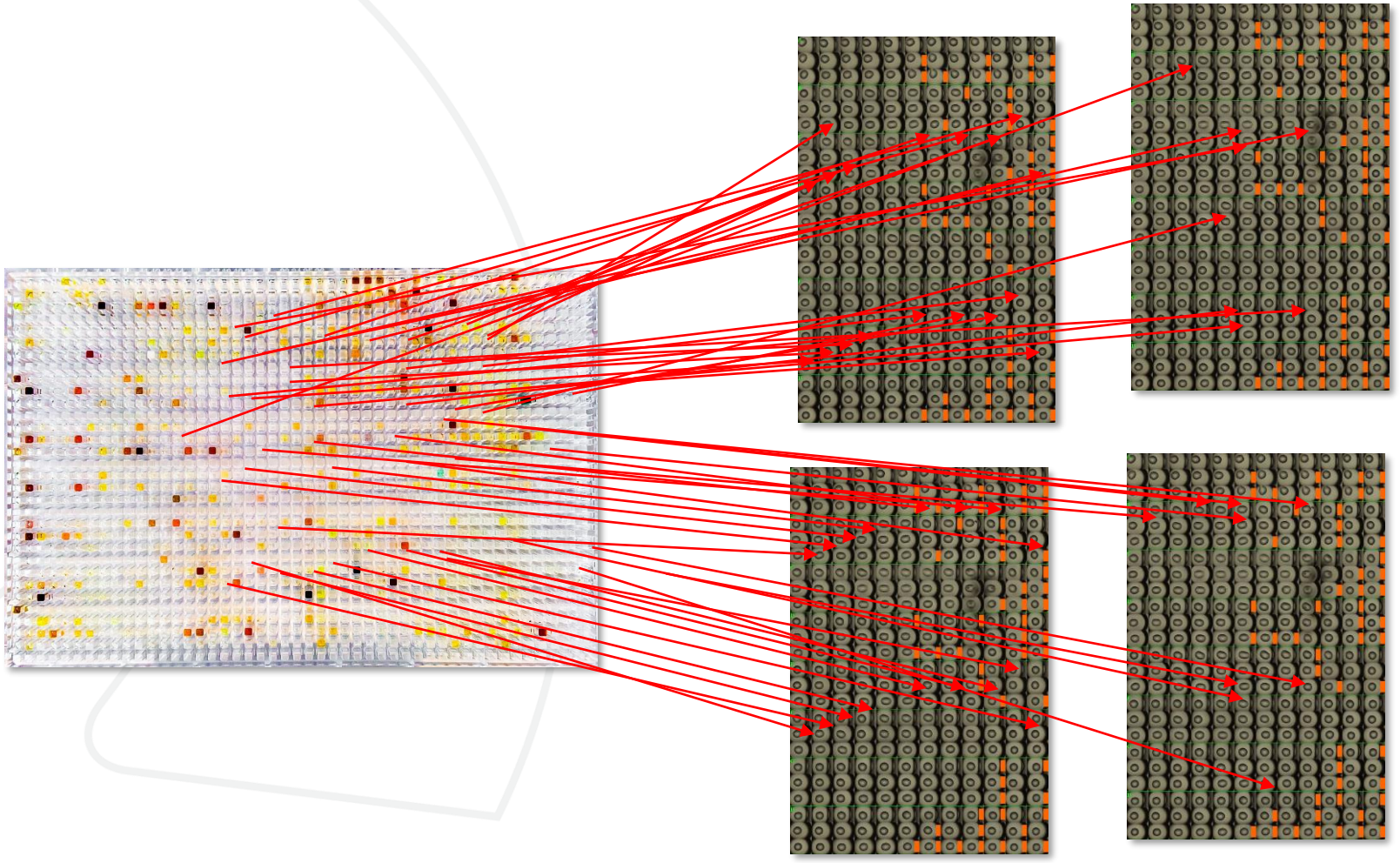

soakDB.xlsm [Read-Only] - Excel
FILE
HOME
INSERT
PAGE LAYOUT
FORMULAS
DATA
REVIEW
VIEW
DEVELOPER
Fragments
Collins, Patrick...
SolventFr...
20
Error Reset
Error Reset
Soak
Compound [stock] mM:
500
Desired Solvent %:
20
6
Export pending
(re)calculate and add to pending
done
Compound [stock] mM
[compound] mM
Solvent %
Transfer Vol
Soak Status
Soak Transfer Date/Time
500 100 20 50.0 pending
Cryo (optional
Cryo [stock] %:
Desired Cryo %:
Cryo location:
(re)calculate and add to pending
Cryo [stock] %
Desired Cryo %
Cryo location
Cryo Transfer Vol
Cryo Statu
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%

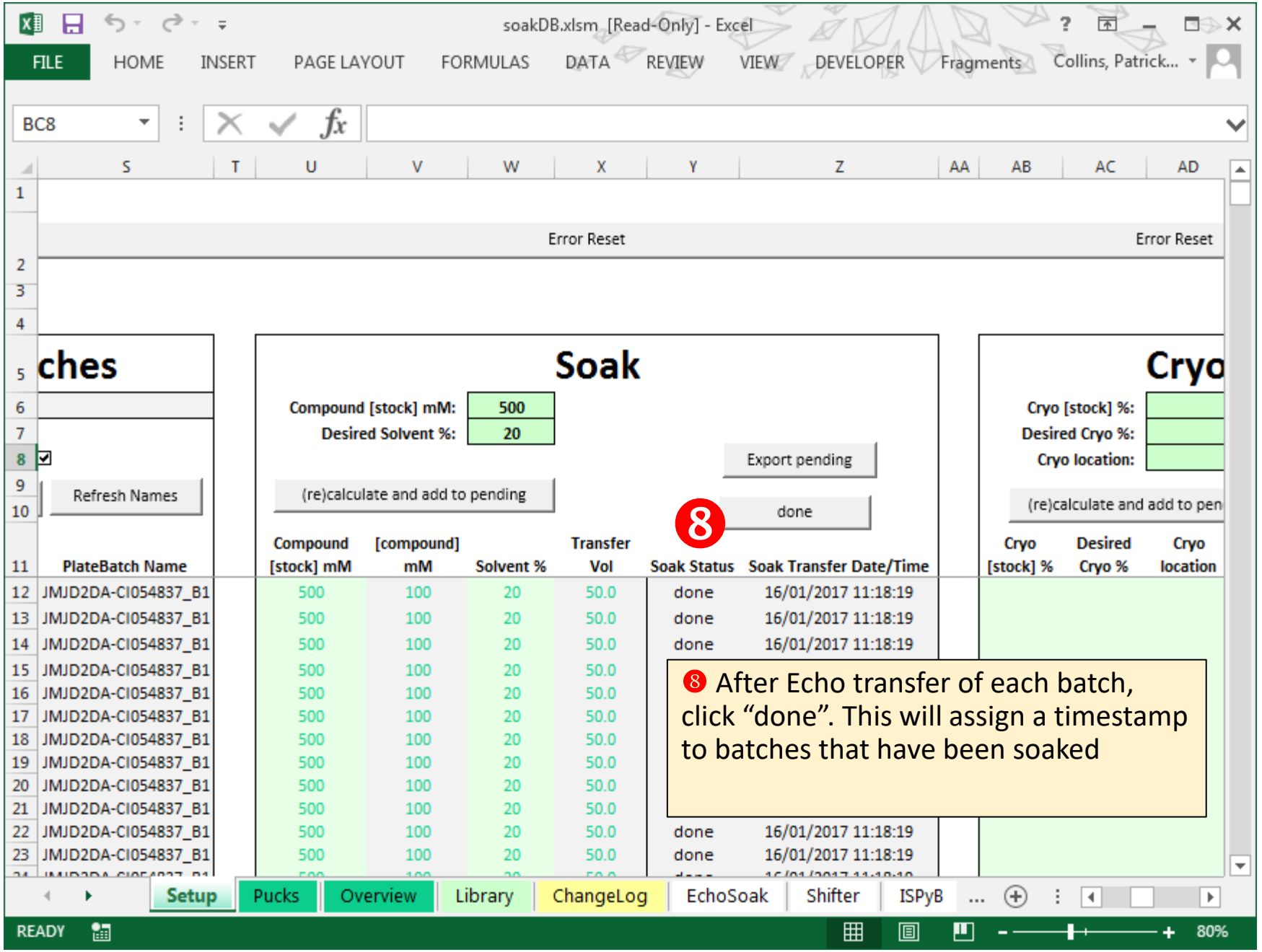

soakDB.xlsm [Read-Only] - Excel
FILE
HOME
INSERT
PAGE LAYOUT
FORMULAS
DATA
REVIEW
VIEW
DEVELOPER
Fragments
Collins, Patrick...
W23
40
Error Reset
Error Reset
ches
Soak
Cryo
Compound [stock] mM: 500
Desired Solvent %: 20
Refresh Names
(re)calculate and add to pending
Export pending
done
Cryo [stock] %: 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
JMJD2DA-CI054837_B1 100 0
JMJD2DA-CI054837_B1 100 5
JMJD2DA-CI054837_B1 100 5
JMJD2DA-CI054837_B1 100 10
JMJD2DA-CI054837_B1 100 10
JMJD2DA-CI054837_B1 100 20
JMJD2DA-CI054837_B1 100 20
JMJD2DA-CI054837_B1 100 30
JMJD2DA-CI054837_B1 100 30
JMJD2DA-CI054837_B1 100 40
JMJD2DA-CI054837_B1 100 40
⇩ Example for solvent characterisation: Manually entered 6 concentrations of DMSO, in duplicate.
Setup
Pucks
Overview
Library
ChangeLog
EchoSoak
Shifter
ISPyB
READY
80%

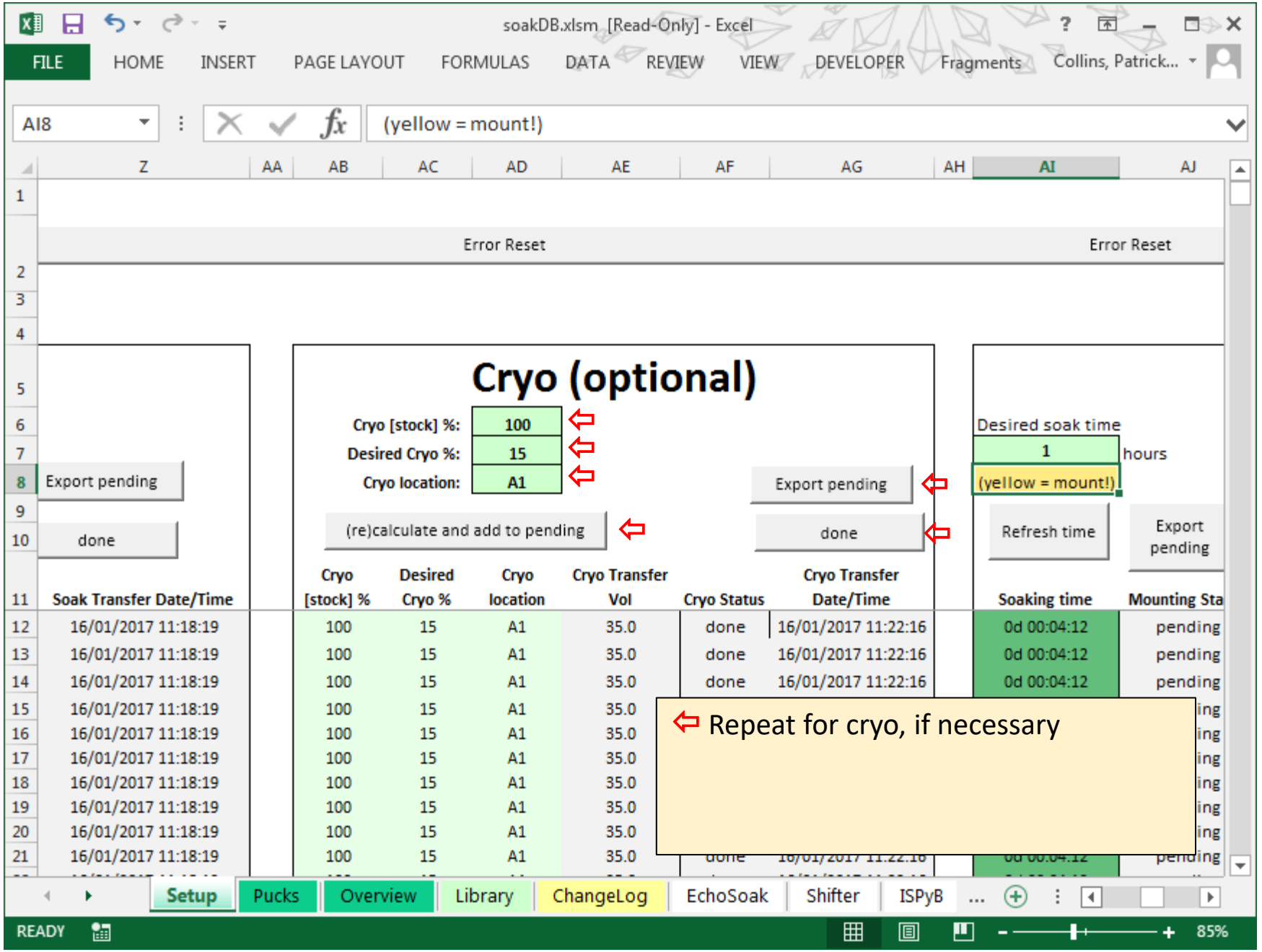

soakDB.xlsm [Read-Only] - Excel
FILE
HOME
INSERT
PAGE LAYOUT
FORMULAS
DATA
REVIEW
VIEW
DEVELOPER
Fragments
Collins, Patrick...
W23
40
Error Reset
Error Reset
ches
Soak
Cryo
Compound [stock] mM: 500
Desired Solvent %: 20
Cryo [stock] %: 100
Desired Cryo %: 15
Cryo location: A1
Refresh Names
(re)calculate and add to pending
Export pending
done
(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
Setup
Pucks
Overview
Library
ChangeLog
EchoSoak
Shifter
ISPyB
READY
80%

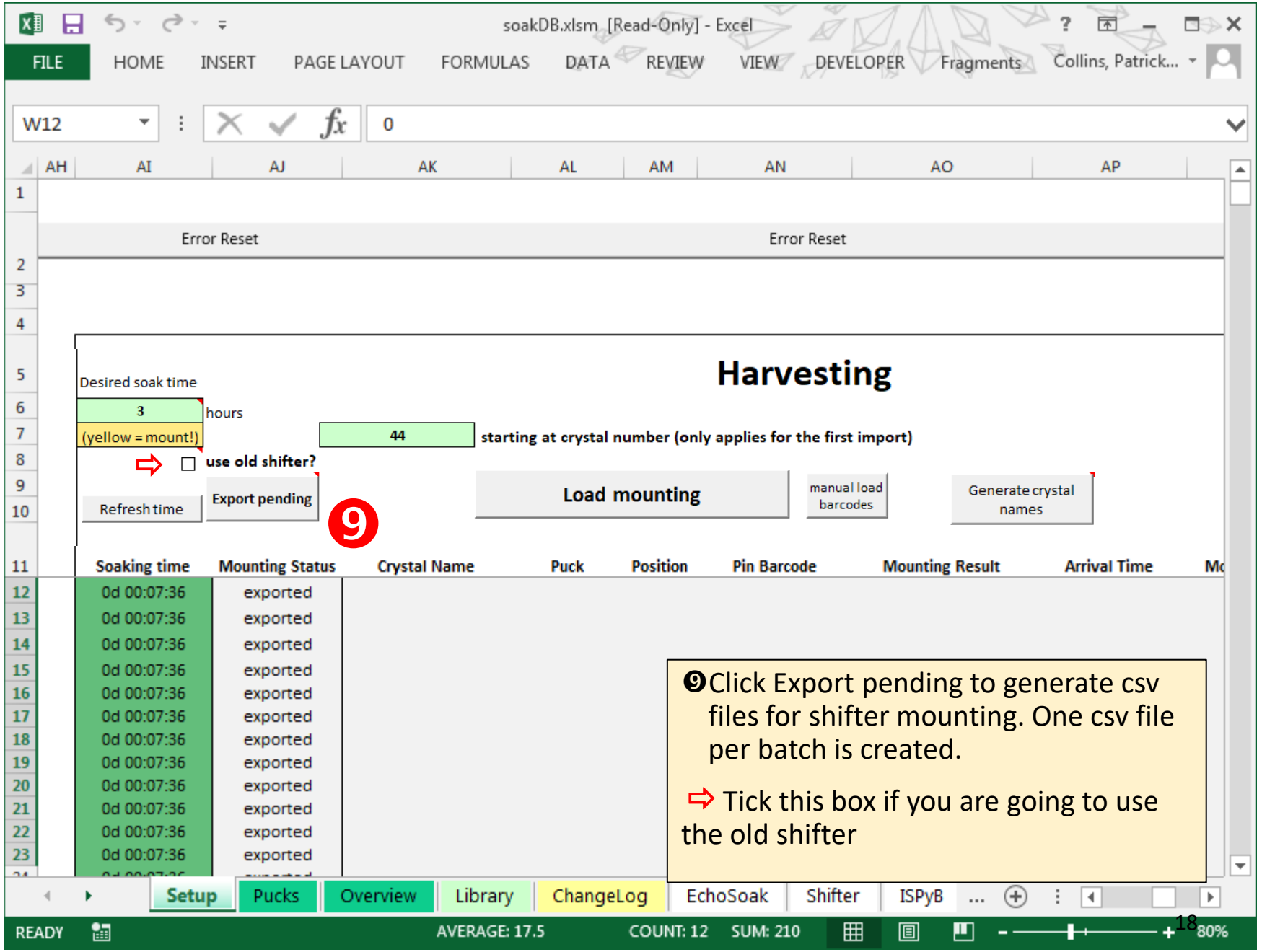

soakDB.xlsm [Read-Only] - Excel
FILE
HOME
INSERT
PAGE LAYOUT
FORMULAS
DATA
REVIEW
VIEW
DEVELOPER
Fragments
Collins, Patrick...
BC8
Error Reset
Error Reset
ches
Refresh Names
Soak
Compound [stock] mM: 500
Desired Solvent %: 20
(re)calculate and add to pending
7
Export pending
done
Cryo
Cryo [stock] %:
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
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
Error Reset
Error Reset
ches
Refresh Names
Soak
Compound [stock] mM: 500
Desired Solvent %: 20
(re)calculate and add to pending
Export pending
done
8
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 done 16/01/2017 11:18:19
8 After Echo transfer of each batch, click “done”. This will assign a timestamp to batches that have been soaked
Setup
Pucks
Overview
Library
ChangeLog
EchoSoak
Shifter
ISPyB
READY
80%

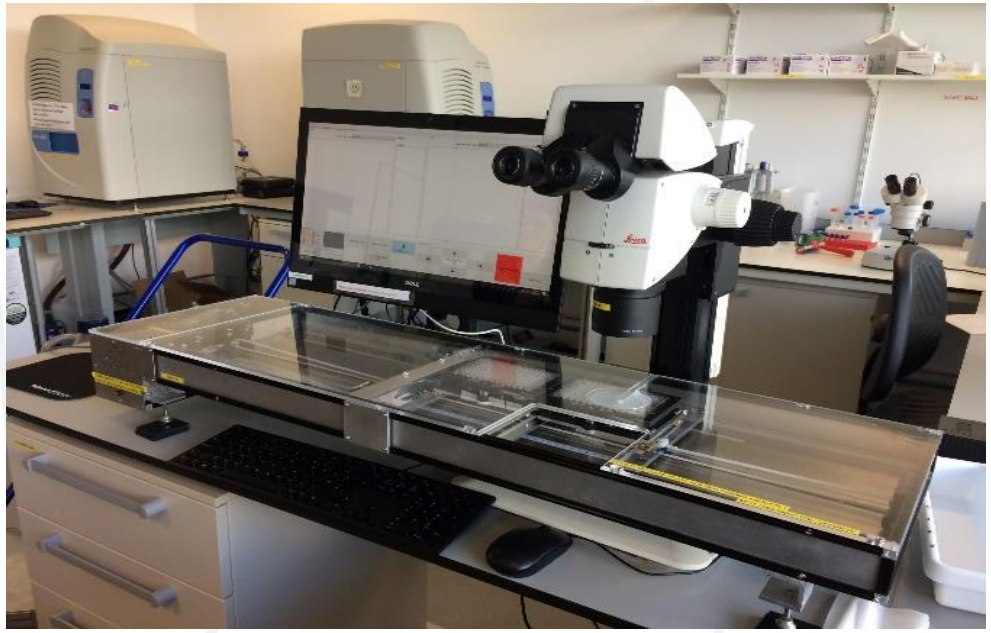

soakDB.xlsm [Read-Only] - Excel
FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW DEVELOPER Fragments Collins, Patrick...
AI8
(yellow = mount!)
Error Reset
Error Reset
Cryo (optional)
Cryo [stock] %: 100
Desired Cryo %: 15
Cryo location: A1
Export pending
done
(re)calculate and add to pending
Export pending
done
Desired soak time
1 hours
(yellow = mount!)
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
Repeat for cryo, if necessary
Setup Pucks Overview Library ChangeLog EchoSoak Shifter ISPyB
READY
85%

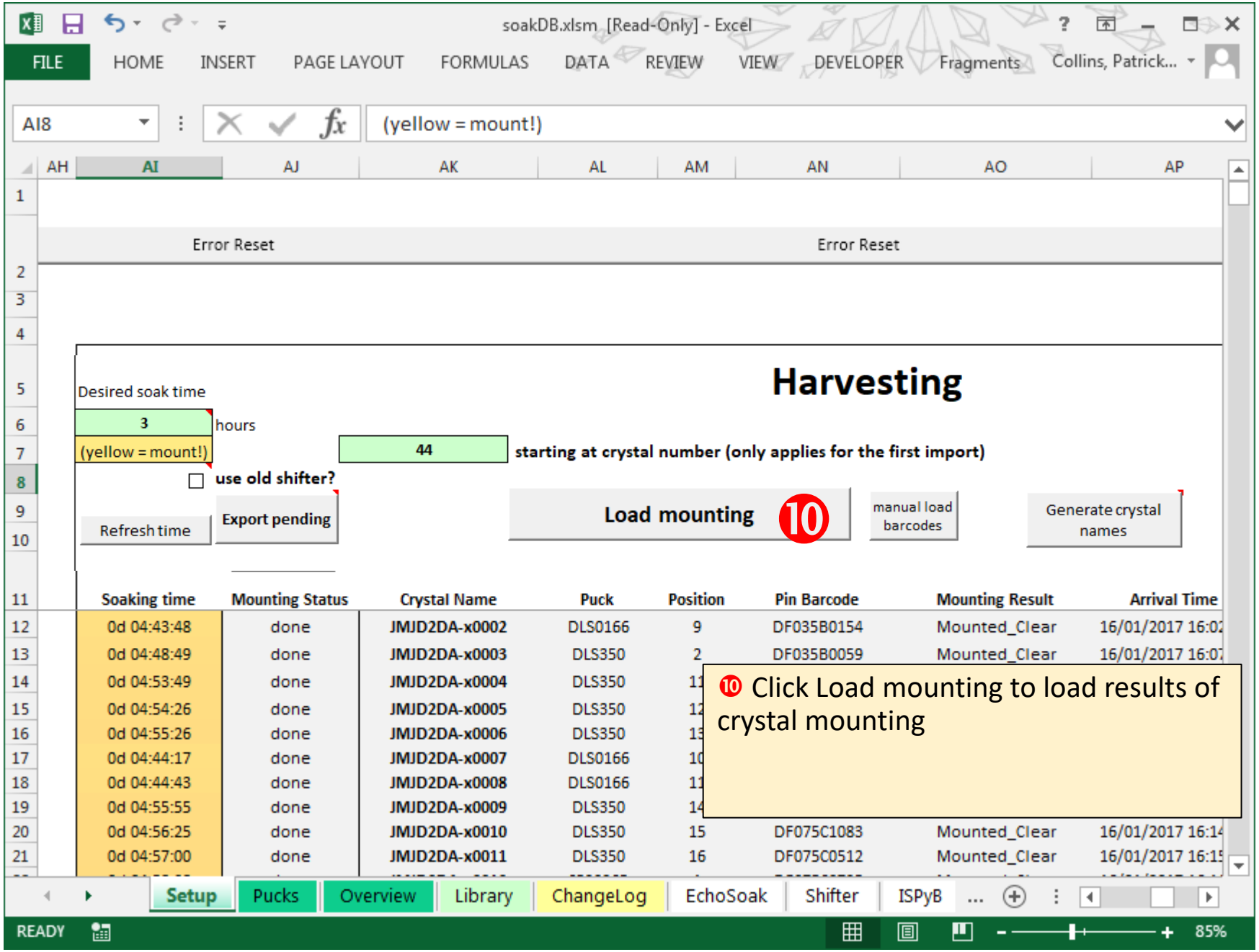


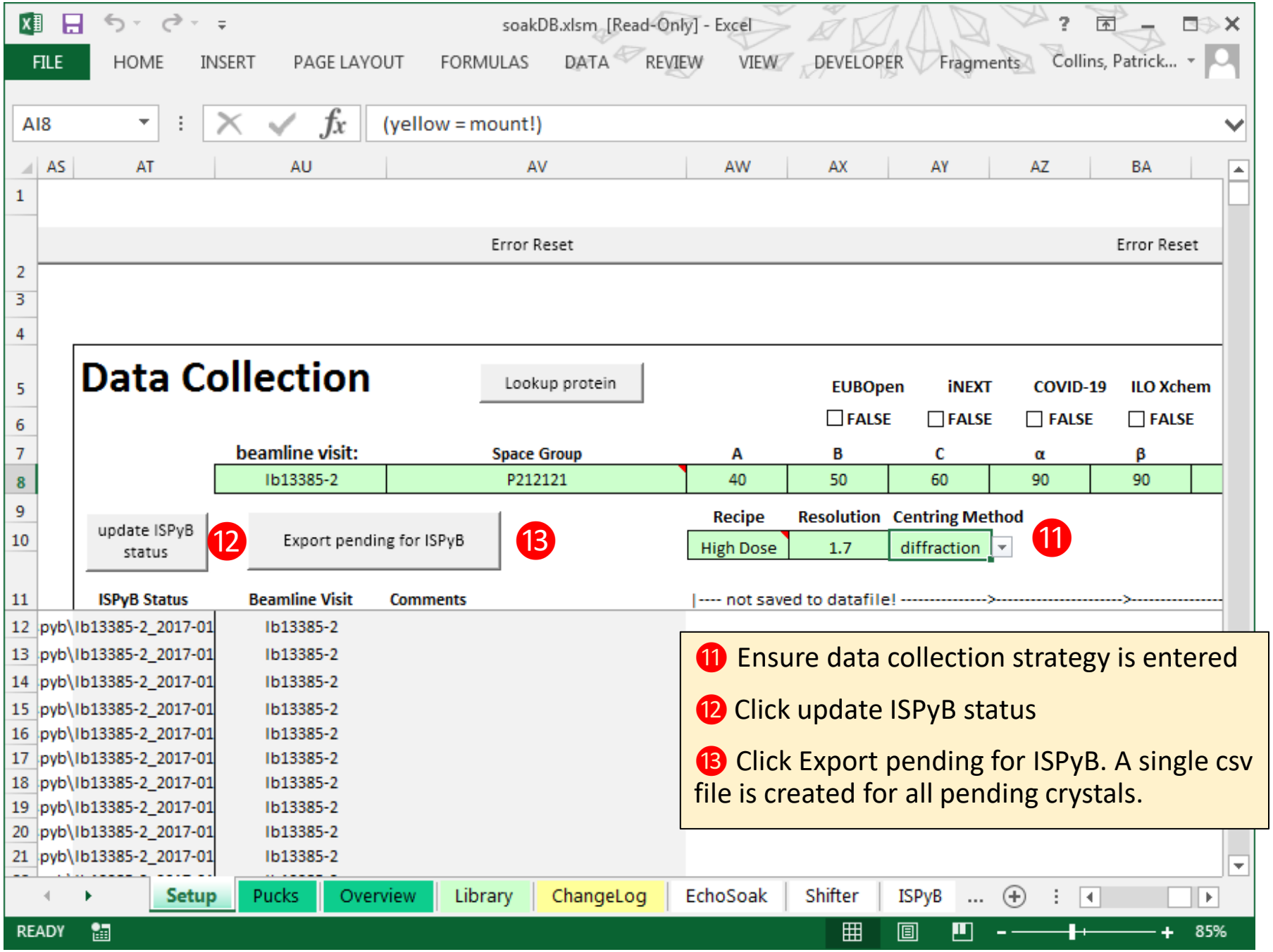
❾Click Export pending to generate csv files for shifter mounting. One csv file per batch is created.

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

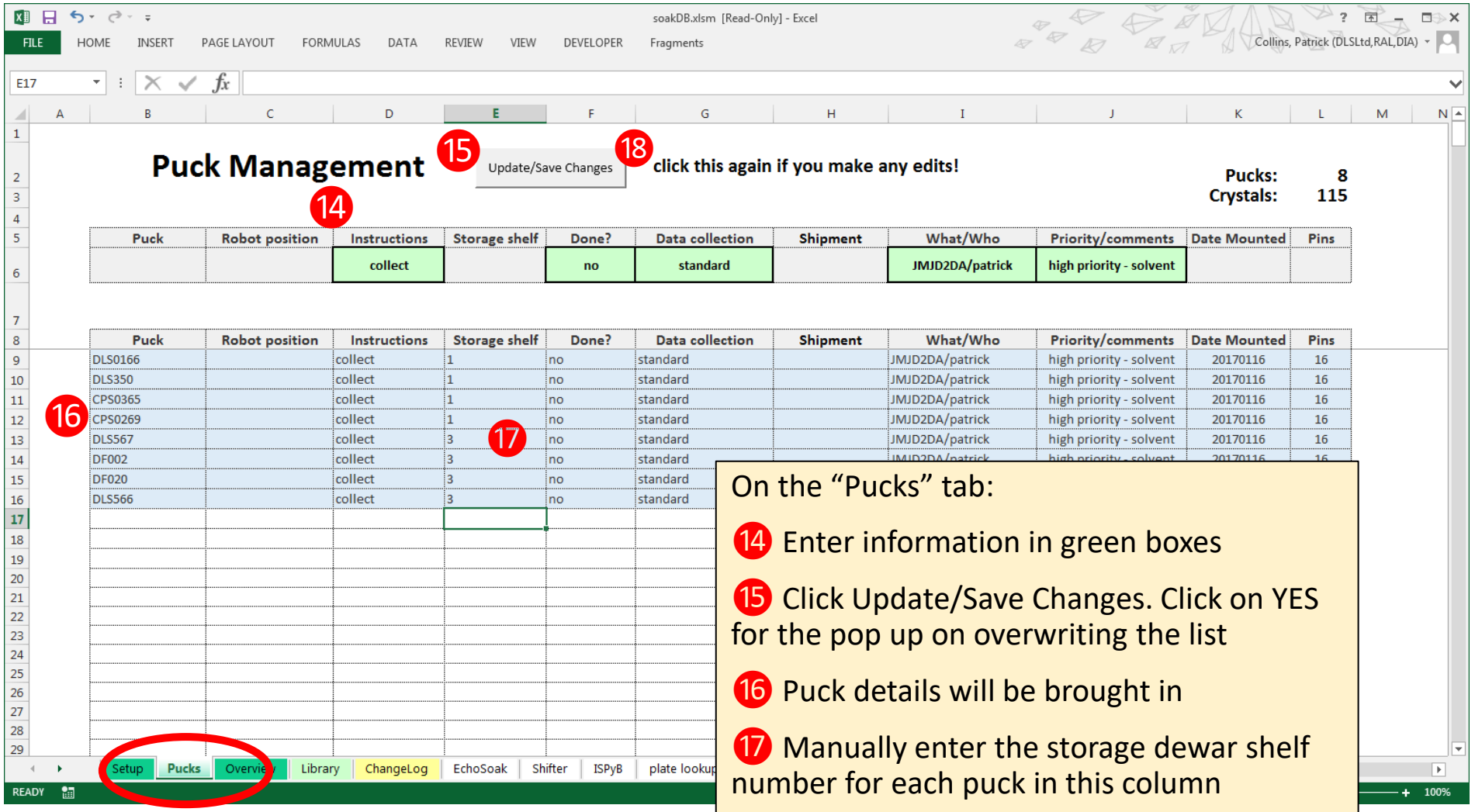
Mount Crystals!




soakDB.xlsm [Read-Only] - Excel
FILE
HOME
INSERT
PAGE LAYOUT
FORMULAS
DATA
REVIEW
VIEW
DEVELOPER
Fragments
Collins, Patrick...
AI8
(yellow = mount!)
Error Reset
Error Reset
Harvesting
Desired soak time
3
hours
(yellow = mount!)
44
starting at crystal number (only applies for the first import)
use old shifter?
Refresh time
Export pending
Load mounting
10
manual load barcodes
Generate crystal names
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 16:07
0d 04:53:49 done JMJD2DA-x0004 DLS350
0d 04:54:26 done JMJD2DA-x0005 DLS350
0d 04:55:26 done JMJD2DA-x0006 DLS350
0d 04:44:17 done JMJD2DA-x0007 DLS0166
0d 04:44:43 done JMJD2DA-x0008 DLS0166
0d 04:55:55 done JMJD2DA-x0009 DLS350
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
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...
AI8
(yellow = mount!)
Error Reset
Error Reset
Data Collection
Lookup protein
EUBOpen
iNEXT
COVID-19
ILO Xchem
FALSE
FALSE
FALSE
FALSE
beamline visit:
Space Group
A
B
C
α
β
Ib13385-2
P212121
40
50
60
90
90
update ISPyB status
12
Export pending for ISPyB
13
Recipe
Resolution
Centring Method
11
High Dose
1.7
diffraction
ISPyB Status
Beamline Visit
Comments
|---- not saved to datafile! ---------->---------->----------
pyb\Ib13385-2_2017-01
Ib13385-2
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.
Setup
Pucks
Overview
Library
ChangeLog
EchoSoak
Shifter
ISPyB
READY
85%

Puck Management



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		

Puck	Robot position	Instructions	Storage shelf	Done?	Data collection	Shipment	What/Who	Priority/comments	Date Mounted	Pins
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					
DLS566		collect	3	no	standard					

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