Method Sheet 44

Mapping experimental data to library plate maps

Overview

This method sheet explains how to align and map experimental data to the information contained within library plate maps. This process is necessary to identify which compounds or extracts are “hits” from your screening experiments. You should progress to this step only after you have completed the data background correction and normalisation tasks from the previous method sheet. In this method, the first step will be to convert the plate-based orientation of the data values to a column format. The second step will be to align those values with the extract or compound ID and information from the respective plate map and plant or compound information tables. These processes will work equally well for data from screens of the *Phytotitre* 800 extract collection, the *Phytotitre* 400 extract collection (student project version) and the *Puretitre* 200 compound collection, by choosing to use the relevant plate map for each screen.

Converting data from plate location format to column format

1) At this stage, your background corrected and normalised data from each plate should look like a table of 12 x 8 values in percentage format.
2) You should calculate the Z’ factor in a cell just below this table of normalised values to gauge the quality and reproducibility of the assay (see Method sheet 22).
3) Then below this, give the following titles to two columns below your Z’ factor: ‘Extract ID’ and ‘% Max’.
4) In the cell directly below ‘Extract ID’, type the ID number of the first extract or compound present in the library plate used for that screen (i.e. in well A2 of the plate), which you can find in the plate map file, or in the table below:

Plate number →	1	2	3	4	5	6	7	8	9	10
Phytotitre 400	1	81	161	241	321	-	-	-	-	-
Phytotitre 800	1	81	161	241	321	401	481	561	641	721
Puretitre 200	1	81	161	-	-	-	-	-	-	-

5) Just below this cell, type the equals symbol, then the cell reference for the cell containing the starting number for the plate and then ‘`+1`’ - for example, if the starting number is in cell `A16`, type: `=A16+1`
6) The cells just below your normalised data table should now look like this:

	A	B	C	D	E	F	G	H	I	J	K	L	M
1													
2	**Experiment # 1**		Time = 21 h										
3		1	2	3	4	5	6	7	8	9	10	11	12
4	A	91%	100%	84%	84%	103%	115%	113%	115%	112%	99%	96%	0%
5	B	102%	103%	127%	123%	128%	109%	121%	107%	100%	108%	126%	0%
6	C	97%	120%	123%	124%	126%	125%	110%	124%	114%	92%	87%	0%
7	D	104%	123%	116%	124%	126%	124%	121%	109%	113%	96%	82%	0%
8	E	104%	129%	125%	130%	131%	74%	115%	109%	100%	102%	81%	0%
9	F	104%	107%	118%	132%	119%	121%	118%	92%	103%	93%	105%	0%
10	G	111%	88%	125%	123%	120%	115%	98%	91%	91%	76%	87%	0%
11	H	88%	90%	103%	104%	102%	90%	88%	93%	90%	84%	78%	0%
12													
13	Z' factor		0.77										
14													
15	Extract	% Max											
16	1												
17	=A16+1												

7) Now drag the green square at the bottom right of the cell containing that formula, and drag down to copy and fill the formula into a further 79 cells in the same column, so that you now have 80 values, incrementing by 1 each time - you have now created a list of the extract IDs for that particular plate in column format, it should look like this near the top:

13	Z' factor		0.77
14			
15	Extract	% Max	
16	1		
17	2		
18	3		
19	4		
20	5		

8) In the cell just below the '% Max' heading, type a formula to point to well A2 of the plate just above your column - note that we do NOT point to well A1, since the negative controls are in column 1, and no extracts or compounds were present there.

9) For example, if well A2 of your plate layout corresponds to cell `C4`, then type `=C4`

10) Now drag to fill downwards a further 7 cells, so this formula is copied into a column of 8 cells just below the '% Max' heading, and let go of the mouse button.

11) Next, highlight the same column of 8 cells with your mouse, then click and hold the green square at the bottom right of the lowest cell in the column and drag the column rightwards a further 9 columns, then let go of the mouse button again.

12) You should now have a table of 10 x 8 cells that looks something like this:

13	Z' factor		0.77								
14											
15	Extract	% Max									
16	1	100%	84%	84%	103%	115%	113%	115%	112%	99%	96%
17	2	103%	127%	123%	128%	109%	121%	107%	100%	108%	126%
18	3	120%	123%	124%	126%	125%	110%	124%	114%	92%	87%
19	4	123%	116%	124%	126%	124%	121%	109%	113%	96%	82%
20	5	129%	125%	130%	131%	74%	115%	109%	100%	102%	81%
21	6	107%	118%	132%	119%	121%	118%	92%	103%	93%	105%
22	7	88%	125%	123%	120%	115%	98%	91%	91%	76%	87%
23	8	90%	103%	104%	102%	90%	88%	93%	90%	84%	78%
24	9										
25	10										

13) Note that you do not have to copy references to the final (12th) column of the plate, since this contains the positive controls and no data from extracts or compounds.

14) Now highlight the second column of this new table with your mouse, and either Cut (Ctrl & X), then paste the formulas just below the end of column 1.

15) Or alternatively you can highlight the second column, then click carefully on the green outer border, then move the group of 8 cells into the new position with the mouse.

16) Both of these methods preserve the original cell references without converting them to a new relative position - this is why we CANNOT use a simple copy and paste for this step, as the formulas would then point to relative cell references in the wrong places - you must use either cut and paste, or drag the outer border, for this step.

17) Now repeat this process for all the other columns of the table, ensuring you progress from left to right, and aligning them just below the lowest cell of the previous column.

18) You should now have a column of 80 cell references that collectively point to each position in the extract or compound challenged wells of the plate.

19) Double click on several cells in your column to check that they point to the correct position in your plate layout arrangement of values above the columns.

20) This will highlight in blue which cell you are referring to from the column reference, as in the example below:

	A	B	C	D	E	F	G	H	I	J	K	L	M
1													
2	**Experiment # 1**		Time = 21 h										
3		1	2	3	4	5	6	7	8	9	10	11	12
4	A	91%	100%	84%	84%	103%	115%	113%	115%	112%	99%	96%	0%
5	B	102%	103%	127%	123%	128%	109%	121%	107%	100%	108%	126%	0%
6	C	97%	120%	123%	124%	126%	125%	110%	124%	114%	92%	87%	0%
7	D	104%	123%	116%	124%	126%	124%	121%	109%	113%	96%	82%	0%
8	E	104%	129%	125%	130%	131%	74%	115%	109%	100%	102%	81%	0%
9	F	104%	107%	118%	132%	119%	121%	118%	92%	103%	93%	105%	0%
10	G	111%	88%	125%	123%	120%	115%	98%	91%	91%	76%	87%	0%
11	H	88%	90%	103%	104%	102%	90%	88%	93%	90%	84%	78%	0%
12													
13	Z' factor		0.77										
14													
15	Extract	% Max											
16	1	100%											
17	2	103%											
18	3	120%											
19	4	=C7											
20	5	129%											
21	6	107%											

How to save a lot of time and effort in your data analysis

1) You only have to do the method described above once in your data analysis workflow.
2) After you have checked that the cell references are all correct in your column, you now have an automated way of converting the plate layout data into column layout data.
3) You can now copy and paste this whole block of two columns, including the headings, into any other worksheet containing data in 96-well format.
4) So long as you ensure the block is copied into exactly the same position relative to the table of data values (e.g. first cell four rows down from table, and first column aligned with plate row headings), then it will do the conversion automatically in the new worksheet.
5) Straight after you complete the copy and paste, click on the cell containing the first cell reference number (i.e. the cell just below 'Extract ID'), and type in the correct first value for that plate by checking the plate map or the table given above in this method sheet - the other extract ID values should automatically populate below this one.
6) As an extra timesaver, you can include the cell containing the Z' factor calculation in the block of formulas you copy into other worksheets, again being careful to ensure the block is pasted in the same location relative to the bottom of the plate data.

Combining data from multiple, separate plate reads

1) Now that you have a column of 80 normalised values aligned with the correct extract or compound ID for one particular plate, you should repeat that process for your other plates and experiments.
2) After this process is complete, you will have to combine the data from all of the plates in the screening programme into one large table.
3) Create a new worksheet in your analysis file by double clicking the '+' tab icon at the bottom of the page in Excel, and call it '`Combined data`' or similar.
4) Create the following headings in a row in this new worksheet:
   '`Extract ID`', '`Exp 1`', '`Exp 2`', '`Exp 3`', '`Exp 4`'
5) Just below the Extract ID heading, prepare a single column containing a list of numbers ranging from 1 to 200 (for *Puretitre* screening data), 1 to 400 (for *Phytotitre* student wet lab projects) or 1-800 (for *Phytotitre* student dry projects).

6) Now open the Excel file and tab containing the column of 80 values for experiment 1 of plate 1, and copy the percentages only (i.e. the values below '%Max') from that tab.
7) Select your analysis tab and **paste as values** into the correct location (i.e. just below the 'Exp 1' heading in this example) - do not paste as normal, since this will paste cell references which will not work here and will simply give `#REF1` errors.
8) You will notice the format of the numbers changes from a percentage to a long decimal - switch it back to percentage by highlighting the whole column then clicking on the percentage icon in the Home ribbon.
9) Transfer 80 normalised values from every plate and every experiment you have been working on, one plate at a time, into the new summary table, being sure to copy only the percentage values and not the extract IDs, using paste values each time.
10) Remember to also paste your column of 80 values in the correct starting position in the new table, for example the column of 80 values from Plate 3 of the screen would begin from extract or compound 161, so you should select the cell opposite extract ID 161 in your table and paste the whole column from that starting point - see the table above for the correct starting Extract ID locations for the other plates.
11) You should now have a table of normalised screening values organised by Extract ID across all the plates from your experiments, which should look something like this:

	A	B	C	D	E
1					
2	Combined data from multiple plates and experiments				
3					
4	**Extract ID**	**Exp 1**	**Exp 2**	**Exp 3**	**Exp 4**
5	1	100%	103%	96%	Exp 4
6	2	103%	107%	99%	Exp 5
7	3	120%	124%	116%	Exp 6
8	4	123%	127%	118%	Exp 7
9	5	129%	133%	124%	Exp 8
10	6	107%	110%	102%	Exp 9
11	7	88%	91%	84%	Exp 10
12	8	90%	93%	87%	Exp 11
13	9	84%	87%	81%	Exp 12
14	10	127%	131%	122%	Exp 13
15	11	123%	127%	118%	Exp 14
16	12	116%	119%	111%	Exp 15
17	13	125%	129%	120%	Exp 16
18	14	118%	122%	114%	Exp 17
19	15	125%	129%	120%	Exp 18
20	16	103%	106%	99%	Exp 19
21	17	84%	87%	81%	Exp 20

12) Note that if you have done only 3 experiments and not 4, simply remove the Exp 4 column.
13) Make sure there are no gaps in your table, this suggests an error in the alignment of your data from the multiple plates.

Calculating the mean and SD of your screening experiments

1) You should now calculate the mean and SD of the results from your multiple separate experiments for each well on every plate.
2) To the right of your new table, prepare headings for three new columns: '`Extract ID`', '`Mean`' and '`SD`'
3) Copy and paste the extract IDs so the sheet should now look something like this:

	A	B	C	D	E	F	G	H	I
1									
2	Combined data from multiple plates and experiments								
3									
4	Extract ID	Exp 1	Exp 2	Exp 3	Exp 4		Extract ID	Mean	SD
5	1	100%	103%	96%	Exp 4		1		
6	2	103%	107%	99%	Exp 5		2		
7	3	120%	124%	116%	Exp 6		3		
8	4	123%	127%	118%	Exp 7		4		

4) In the first cell below the 'Mean' heading, type the following formula:

```
=AVERAGE(B5:E5)
```

5) In the cell to the right of that one, type the following formula:

```
=STDEV(B5:E5)
```

6) Note that this example assumes the first data points for Extract ID number 1, for each of four separate experiments, are located in cells B5 to E5, check where they are in your own worksheet as they may be in different locations.
7) Select both of these new cells with the mouse, then click the small green square at the bottom right of the right-hand cell and drag to copy all the way down to the bottom of the table.
8) You should now have calculations of mean and SD for every extract you have studied, and the table should look something like this:

	A	B	C	D	E	F	G	H	I
1									
2	Combined data from multiple plates and experiments								
3									
4	Extract ID	Exp 1	Exp 2	Exp 3	Exp 4		Extract ID	Mean	SD
5	1	100%	103%	96%	Exp 4		1	99%	3%
6	2	103%	107%	99%	Exp 5		2	103%	4%
7	3	120%	124%	116%	Exp 6		3	120%	4%
8	4	123%	127%	118%	Exp 7		4	123%	4%
9	5	129%	133%	124%	Exp 8		5	129%	5%

Aligning screening data with extract or compound ID

1) Now that you have a list of the results of the screen for every extract, averaged over three or four experiments, you can align the IDs with the plant or compound names to find out which extracts or compounds elicit the most potent effects in your screen.
2) Open the 'Plant info' worksheet (select correct tab at bottom of page) of the phytotitre_layout or dry project *Phytotitre* screen Excel files available from the website Downloads page (or the equivalent file for *Puretitre* compound screens).
3) Highlight the whole table of plant or compound information, except for the extract ID column, and copy it.
4) Then paste it directly (as normal or as values, either is fine here) from the first available column in your results table.
5) Note: make sure that the rows of the plant or compound information match up correctly with the corresponding ID number at this stage, or the wrong compounds or extracts will be identified as hits.
6) You should now have a table of results and extract / compound information that may look something like this:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1																		
2	Combined data from multiple plates and experiments																	
3																		
4	**Extract ID**	**Exp 1**	**Exp 2**	**Exp 3**	**Exp 4**		**Extract ID**	**Mean**	**SD**	**Common name**	**Latin**	**Part for e:**	**Descriptic**	**Rationale**	**Notes**			
5	1	100%	103%	96%	Exp 4		1	99%	3%	Acacia Gum	Acacia senegal	Resin	A small, tl	Traditiona	Contains hentriacontane, a solid, long-c			
6	2	103%	107%	99%	Exp 5		2	103%	4%	Yarrow	Achillea millefolium	Leaves	A small flc	Traditiona	Reported to reduce disease severity in a			
7	3	120%	124%	116%	Exp 6		3	120%	4%	Calamus Root	Acorus calamus	Root	A tall pere	Used in Cl	Contains alpha-asarone, beta-asarone a			
8	4	123%	127%	118%	Exp 7		4	123%	4%	Kiwi fruit	Actinidia deliciosa	Fruit	The kiwifr	Dietary in	Ethanol extract of peel protected neural			
9	5	129%	133%	124%	Exp 8		5	129%	5%	Horse Chestnut	Aesculus hippocastan	Seed	A large de	A Cochran	Horse chestnut seed is classified by the			

7) Congratulations! You can now progress to identifying the hits from your screen.

Notes

- Be very careful with every step of this part of the analysis - any errors in alignment or copying / pasting here will impact on all further stages of the analysis, and could result in incorrect identification of hits and a requirement to repeat lots of data analysis.
- If you see any `#REF1` errors in your analysis file, it is because you have copied and pasted incorrectly so that the cell references are now pointing to the wrong place - go back to the methods above and ensure you either cut then paste or paste as values, as necessary for the specific step in the analysis.

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