

BIONUMERICS Tutorial: Setting up a BIONUMERICS database with levels

1 Aims

The database levels in BIONUMERICS form a powerful concept that allows users to structure information in a hierarchical way. Each database level reflects the physical entity from which information is collected, thereby avoiding information duplication that would occur in a "flat" table. It also provides a convenient framework to deal with replicate experiments.

This tutorial starts from following situation: A culture collection is responsible of maintaining a large number of microbial strains. Each strain is assigned a strain number and stored as a freeze-dried culture in air-tight vials. Whenever a batch of such vials is running out or when a certain amount time has passed, a single vial is resuscitated and a subculture started to prepare a new batch of vials. For the curators of the culture collection, it is very important to confirm the integrity of their strains. Therefore, they perform a high resolution DNA fingerprint on each batch of vials as a quality check. The patterns are then compared with the original DNA fingerprints from the strains and should of course match 100%.

In this use scenario, setting up a database with three levels (respectively "Strain", "Batch" and "Profile") allows the users to:

- Assign specific information fields to the corresponding database level, avoiding unnecessary duplication of information.
- Deal with replicate measurements.
 - Summarize experiments from the "Profile" to the "Batch" and "Strain" level.
 - Provides an easy way to approve experiments, without the need to actually delete suboptimal fingerprints from the database.

In this tutorial, we discuss the necessary steps to set up levels in a new, empty database.

2 Creating a new BIONUMERICS database

1. Double-click on the BIONUMERICS icon (Left) on the desktop.

2. In the *BIONUMERICS Startup* window, press the 🗟 button to enter the *New database* wizard.

- 3. Enter a database name, e.g. "Culture collection".
- 4. Click <*Next*>.

A new dialog box pops up, asking whether to create a new relational database for data storage or to use an existing one.

5. Leave the default option *Create new* enabled and press < *Next*>.

The next dialog asks which database engine should be used for storing data.

6. Select the default option and press < *Finish*>.

The Main window opens with an empty database.

3 Configuring the Main window

When working with levels in a BIONUMERICS database, the *Database design* panel is frequently needed. Therefore, we will change the layout of the *Main* window so that this panel is always in view.

1. Click on the header of the *Database design* panel (tabbed with the *Entry fields* panel of the *Main* window in default configuration) to make the panel visible. While keeping the mouse button pressed, drag the mouse over the *Database entries* panel and release it over the top part of the docking guide (see Figure 1).

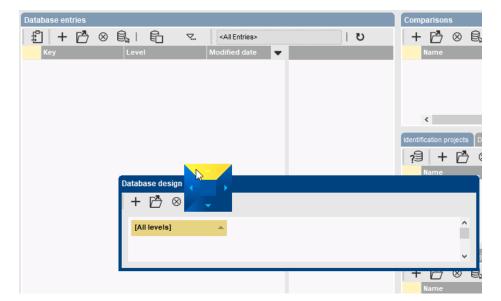


Figure 1: Docking guide.

This results in a window configuration as displayed in Figure 2, allowing easy access to the *Database design* panel.

4 Creating database levels

By default, the *Database design* panel shows only [All levels]. We will create three hierarchical levels in this example database:

Culture collection - BioNumerics		– – ×
File Edit Database Analysis Scripts Window Help		
@ =		
Experiment types	Database design	Comparisons
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Entry fields		
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Database: Culture collection (_DefaultUser_) Entries: Load	ed=0, View=0, Selected=0 0 experiments C:\Users\Public\Documents\BioNumerics\Data BN8\Culture collection This is a time limited pa	ackage valid until 2020-12-30

Figure 2: The *Main* window with the *Database design* panel shown.

- 1. **Strain:** A level that will contain all strains (sometimes also referred to as "accessions") available from the culture collection. Each strain has a unique strain number and additional descriptive information (e.g. Genus and Species).
- 2. **Batch:** This level holds information about the batches of preservation vials. A batch is always prepared from a single strain. From any given strain in the database, multiple batches can be prepared.
- 3. **Profile:** This level corresponds to individual DNA fingerprint profiles. A profile originates from a single batch. Typically, one profile would be prepared per batch, but replicates are needed when the generated profile does not meet the quality criteria.

Proceed as follows to create the Strain level:

1. Highlight [All levels] in the *Database design* panel and select *Database* > *Levels* > *Add new level...* (+).

Level informa	tion		?	\times
Name:				
Description:				
		ОК	Cano	cel

Figure 3: Adding new levels.

2. Enter "Strain" as *Name* for the level and optionally a *Description*, e.g. "Contains strains available from our culture collection". Press < *OK* >.

The level Strain is created as a child level from [All levels]. We will now create the Batch level:

- 3. With the Strain level highlighted, select *Database* > *Levels* > *Add new level...* (+) again.
- 4. This time, enter "Batch" as *Name* for the level and optionally a *Description*, e.g. "Contains preservation batches for a given strain". Press < *OK* >.

The level **Batch** is created as a child level from **Strain**. Finally, we will create the **Profile** level:

5. With the **Batch** level highlighted, select **Database** > **Levels** > **Add new level...** (+) once more.

Enter "Profile" as *Name* for the level and optionally a *Description*, e.g. "Contains Profile profiles". Press < OK >.

The Database design panel should now look like in Figure 4.



Although in theory an unlimited number of levels can be created, it is advisable to limit the number of levels to the minimum necessary.

Database design				
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[All levels]	strain	A Batch	▲ Profile	-

Figure 4: The Database design panel with three levels defined.

5 Level-specific information fields

As soon as levels are present in a database, creating entry information fields is specific for the active level, i.e. the level that is highlighted in orange in the *Database design* panel.

Proceed as follows to create the Strain-specific entry field Strain number:

- 1. Click on Strain in the Database design panel to make Strain the active database level.
- 2. In the *Entry fields* panel, select *Edit* > *Create new object...* (+).
- Enter "Strain number" as *Name* for the new information field, check *Calculate field content* from other fields and press <*Edit*>. Press *Add information field*, select *Key* and press
 OK> twice.

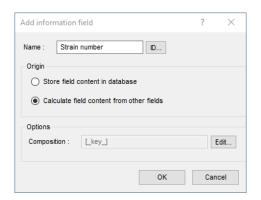


Figure 5: Strain number.

Using these settings, BIONUMERICS will create a text field in the database that is specific for the **Strain**. The content of the field will be derived from the *Key* field.

Proceed as follows to create a new field, specific to the **Batch** level:

- 4. Click on **Batch** in the *Database design* panel to make **Batch** the active level.
- 5. In the *Entry fields* panel, select *Edit* > *Create new object...* (+).

6. Enter "Preservation date" as *Name* for the new information field and press < *OK* >.

Similarly, we can create a new field in the **Profile** level:

7. Highlight the Profile level in the Database design panel, select Edit > Create new object...
 (+) in the Entry fields panel, and enter "Run number" as field name. Press < OK >.

Finally, we will create a field in the **Profile** level that will hold the information whether or not a curator has approved the DNA fingerprint profile:

- 8. Make sure **Profile** is still the active level, in the *Entry fields* panel, select *Edit* > *Create new object...* (+).
- 9. Enter "DNA fingerprint approved" as *Name* for the new information field and press < OK >.

The *Database design* panel should now look like in Figure 6.

Database desig	<u>jn</u>						
+ 🖻 🛛) ⊠↔						
[All levels]		Strain	A	Batch	Profile		^
		ABC Strain number		ARC Preservation date	All Run number		
					ARC DNA fingerprint approved	1	
							۷

Figure 6: Level-specific information fields.

10. In the *Entry fields* panel, double-click on *DNA fingerprint approved* to open the *Database field properties* dialog box.

Since the profile is either approved or not, we will add two field states (i.e. **Yes** and **No**) with color coding and will prevent the input of any other text than specified in the field states:

- 11. Press the *Add*> button, enter "Yes" and press *Add*>.
- 12. Repeat the previous step to add a second field state "No".
- 13. Check *Restrict content to states* and *Use colors*. Optionally, enter "No" as *Default content* (see Figure 7).
- 14. Press < OK > to save the information field settings.



When information fields are created in a database without levels or with [All levels] highlighted, by default a fixed entry information field will be created that occurs on all levels. If the information is level-specific, a new flexible field should be created and the information copied over for the selected entries via *Edit* > *Information fields* > *Edit field in selection...* (Ctrl+M). The original fixed field can then be deleted.

Information that is defined at a certain level will be displayed when this levels is the active one, and can be edited there if needed. Some information needs to displayed at other levels than the level at which it is defined. The information will simply be replicated there and cannot be edited.

In this example, the *Strain number* is a good example of information that needs to be shown at all three levels.

- 15. Click on Strain in the Database design panel to make Strain the active database level.
- In the *Entry fields* panel, click on *Strain number* and select *Edit* > *Open highlighted object...* ([™]), Enter). Alternatively, simply double-click on *Strain number*.

Properties for fie	Id 'DNA_FINGERPRI	NT_APPROVED		? ×
Name: DNA fi	ingerprint approved		Changes:	Allow ~
Field storage ty	pe: Optimized for s	space	Restrict conter	it to states
Content type:	Text	~	Use colors	
Field states			Opacity:	
Yes		Add	Default content:	
No		Add all	No	
		Remove	Content validation	n (regular expr.):
		Remove all		
		Edit		Level assignment
		Sort		Summary settings
				Calculation
				Ok
				Cancel

Figure 7: DNA fingerprint approved: settings.

17. In the *Database field properties* dialog box, press the <*Level assignment...*> button to display the *Level assignment* dialog box (see Figure 8).

Level assignment		? ×	
Assignment type Specified for each indiv Defined at all levels Defined at root level an	ridual level d replicated + stored on all level	3	
Level	Assignment		
Strain	Defined	\sim	
Batch	Not used	~	
Profile	Not used	\sim	
	ОК	Cancel	

Figure 8: Initial level assignment for the *Strain number* entry field: defined at the **Strain** level and not used at the other levels.

- 18. Change the **Assignment** from "Not used" to "Replicated" for the **Batch** and **Profile** level (see Figure 9).
- 19. Press < OK > to accept the level assignment settings and < OK > once more to close the *Database field properties* dialog box.

Now the strain number will be displayed in each level. It will be shown in grey at the **Batch** and **Profile** levels to indicate that it is not defined there and that it cannot be modified there.

Similarly, it might be useful to display the profile *Run number* of a profile at the **Batch** level.

20. Click on **Profile** in the *Database design* panel to make **Profile** the active database level.

Assignment type	evel assignment				?	\times
Defined at all levels Defined at root level and replicated + stored on all levels Level Assignment Strain Defined	Assignment type					
Defined at root level and replicated + stored on all levels Level Assignment Strain Defined	Specified for each	ach individual lev	el			
Level Assignment Strain Defined Y	 Defined at all le 	vels				
Strain Defined	 Defined at root 	level and replica	ted + stored on all I	evels		
Strain Defined						
	Level		Assignment			
Batch Deplicated V	Strain		Defined		>	-
Replicated	Batch		Replicated		×	1
Profile Replicated	Profile		Replicated		~	-
OK Cancel					Canc	al

Figure 9: Updated level assignments for the Strain number.

- 21. In the *Entry fields* panel, click on *Run number* and select *Edit* > *Open highlighted object...* (2), Enter). Alternatively, simply double-click on *Run number*.
- 22. Press the < Level assignment...> button to display the Level assignment dialog box.
- 23. Change the **Assignment** from "Not used" to "Replicated" for the **Batch** level and press <**OK**> (see Figure 10).

Specified for each individual level Defined at all levels Defined at root level and replicated + stored on all levels Level Assignment Strain Not used Y Batch Replicated Y	evel assignment		?	\times
Defined at all levels Defined at root level and replicated + stored on all levels Level Assignment Strain Not used Assignment Y Batch Replicated Y	Assignment type			
Defined at root level and replicated + stored on all levels Level Assignment Strain Not used Batch Replicated	Specified for ea	ch individual level		
Level Assignment Strain Not used ¥ Batch Replicated ¥	O Defined at all lev	els		
Strain Not used \checkmark Batch Replicated \checkmark	O Defined at root l	evel and replicated + stored on all levels		
Batch Replicated ~	Level	Assignment		
Paton Population	Strain	Not used		\sim
Defined Defined	Batch	Replicated		
Profile Defined Y	Profile	Defined		\sim
		ОК	Car	ncel

Figure 10: Level assignment for the Run number.

Since we are now replicating information from a child level to a parent level, we need to define how the information is summarized:

24. Press the <*Summary settings...*> button to show the *Field summary method* dialog box (see Figure 11).

The default method Combine and count will work fine for our purposes, so we will leave this

Field summary method			?	\times
Fi	ter			
combine and count				
	formation field:	<not used=""></not>		\sim
Most frequent state				
Ca	ontent:			
	aturas all the disi	tinct states of the field in th		last
		is the occurrences.	e depend	ent
	Separator: ,			
		ОК	Cano	el
			- Call	

Figure 11: Summary settings for *Run number*.

enabled.

25. Press <*OK*> to accept the summary settings and <*OK*> once more to close the *Database field properties* dialog box.

6 Level-specific experiment types

Similar to information fields (see 5), experiment types can also be defined at a specific database levels and replicated over other levels if desired. Below the steps are listed to define a new experiment type and to replicate the data over different levels. In the tutorial "Importing information in a database with levels" these steps are illustrated using a fingerprint type experiment, created during import of the data.

- Before launching the Create a new experiment type dialog box (in the Experiment types panel, select Edit > Create new object... (+), make sure the correct level is selected in the Database design panel. The created experiment type will be defined at the selected level. Alternatively, the experiment type can be created during import of the data.
- The experiment type can be replicated to other levels with the level assignment options present in the *Level assignment* dialog box. This dialog can be called from every experiment type window with the command *Settings* > *Level assignment...*.
- The method used to replicate the experimental information can be specified in the *Experiment summary method* dialog box. This dialog can be called from very experiment type window with the command *Settings* > *Summary replication settings...*.

7 Importing information in a database with levels

When importing data (descriptive information and/or experimental data) in a database with levels, it is important to highlight the corresponding level first. Typically, information will most often be imported at the deepest child level (i.e. **Profile**). In such case, all entries will be correctly linked if the **Batch** key and **Strain** key are specified during during import. For more instructions, see our separate tutorial on "Importing information in a database with levels".