TELL Sample Spreadsheet User Instructions

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Table of contents

Current file: V6_TELLSampleSpreadsheetTemplate.xls

Download from: https://www.psi.ch/en/sls/pxi/sample-changer

Validation

Login to https://rp.psi.ch with your PSI ext-account and select mx-webapps to access the spreadsheet validator application. The spreadsheet validator checks the uploaded spreadsheet for compatibility with TELL sample changer, DA+ server and ADP.

Note: the spreadsheet validator does not check if your data collection or processing parameters make sense - so if you supply incorrect information it will be used for collection and processing.

Rows, one per sample

- Leave all rows up to, and including, the header rows **untouched**.
- Include one row per sample.
- If a puck is missing samples, *i.e.* not fully loaded, then **do not include** rows for these samples.

Mandatory Columns

DewarName: This name is displayed in the GUI and helps the operator to identify which shipping dewar each puck belongs to.

PuckName: This name should correspond to the datamatrix engraved onto the puck which will be scanned during loading/unloading operations. Only letters [a-z] and digits [0-9] are considered when matching the PuckName with the resulting scanned datamatrix.

The following strings would match a datamatrix scanned as "PSIMX-100":

- "PSIMX100"
- "psimx:100"
- "PSI:MX-100"
- "PSIMX 100"

The PuckName is made available in the ***sgPuck*** macro (see section **On the use of Macros** below).

CrystalName: by default the text in this column will be transferred to the Prefix field in the DA+GUI. The text is also made available as the macro ***sgPrefix*** in the DA+GUI. Valid characters: a-z 0-9 minus period plus underscore. Spaces will be replaced by underscores.

PositionInPuck: An integer number indicating the position within the puck. For unipucks this number must be within 1-16. Available in the ***sgPosition*** macro.

Optional but Highly Recommended Columns

Optional means that the content of the cells may be omitted but the column itself must be present.

Priority: This should be an integer number. The operator will see this number in the TELL-GUI. This number may be used to sort the samples within the TELL-GUI. This number is made available as the macro "sgPriority".

Comments: This text is available to the operator and may be used to sort samples within the TELL-GUI.

Directory: by default the text in this column will be transferred to the Folder field in the DA+GUI. The text is also made available as the macro "sgFolder" in the DA+GUI. Macros may be used in this field to compose folder locations using other macros corresponding to fields from the spreadsheet or dynamic macros corresponding to parameters from the DA+GUI. Spaces in the Directory field will be replaced by underscores.

Sample Information									
DewarName*	PuckName*	PuckType*	PuckLocationInDewar*	CrystalName*	PositionInPuck*	Priority	Comments	PinBarcode	Directory
Dewar-1	889911	Unipuck	1	lyso_1	1	1	small crystals		{date}/{prefix}
Dewar-1	889911	Unipuck	1	lyso_2	2	1	long needles		{date}/{prefix}
Dewar-1	889911	Unipuck	1	lyso_3	3	1	backup-1		{date}/{prefix}
Dewar-1	**889911**	**Unipuck**	**1**	**lyso_4**	**4**	**2**	**backup-2**		**{date}/{prefix}**
Dewar-1	**889911**	**Unipuck**	**1**	**lyso_5**	**5**	**2**	**backup-3**		**{date}/{prefix}**
Dewar-1	**889911**	**Unipuck**	**1**	**lyso_6**	**6**	**2**	**backup-4**		**{date}/{prefix}**
Dewar-1	**889911**	**Unipuck**	**1**	**lyso_7**	**7**	**2**	**backup-5**		**{date}/{prefix}**
Dewar-1	**889911**	**Unipuck**	**1**	**Thau 2**	**8**	**3**	**porcupine**		**{date}/{prefix}**
Dewar-1	**889911**	**Unipuck**	**1**	**Thau 3**	**9**	**3**	**backup-1**		**{date}/{prefix}**
Dewar-1	**889911**	**Unipuck**	**1**	**Thau 4**	**10**	**3**	**backup-2**		**{date}/{prefix}**
Dewar-1	**889911**	**Unipuck**	**1**	**Thau 5**	**11**	**88**	**backup-3**		**{date}/{prefix}**
Dewar-1	889911	Unipuck	1	Thau 6	12	88	backup-4		{date}/{prefix}
Dewar-1	889911	Unipuck	1	Insu_1	13	999	test crystal		{date}/{prefix}
Dewar-1	889911	Unipuck	1	Insu_2	14	999	test crystal		{date}/{prefix}
Dewar-1	889911	Unipuck	1	Insu_3	15	999	test crystal		{date}/{prefix}
Dewar-1	889911	Unipuck	1	Insu_4	16	999	test crystal		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	3234567	8	3	aaa- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	2344766	9	4	aaa- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	3457698	10	4	bbb- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	8775643	11	4	bbb- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	4573478	12	5	ccc- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	4568734	13	5	ccc- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	KinA-1	1	1	ccc- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	KinA-2	2	1	bbb- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	KinA-3	3	1	bbb- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	KinA-4	4	2	aaa- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	2302765	5	2	ccc- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	4785622	6	2	vvv- we can sort on comments too		{date}/{prefix}
Dewar-2	PSIMX-042	Unipuck	2	4564889	7	3	zzz- we can sort on comments too		{date}/{prefix}

Columns in blue background are **mandatory**, i.e. they must contain **valid text** in them. Columns in yellow background are optional but **highly** recommended.

On the use of MACROS

Spreadsheet Macros:

- **sgPrefix**: text in the column CrystalName
- **sgFolder**: text in the column Directory
- **sgPuck**: text in the column PuckName
- **sgPriority**: text in the column Priority
- **sgPosition**: text in the column PositionInPuck

Dynamic Beamline Macros:

- **date**: the current date as YYYYMMDD; date will not change after midnight unless DA+GUI is restarted
- **run**: the run number
- **beamline**: the official beamline name: X06SA, X10SA, or X06DA
- **prefix**: the contents of the GUI field "Prefix"; may differ from the macro sgPrefix
- **dtz:** the detector to sample distance rounded to the mm.
- **dty**: the detector height offset rounded to the mm.
- **ev**: the beam energy in electron volts, rounded.
- **method**: either the string "screen" or "dataset" depending on the experiment
- **phi**: the phi angle, rounded.
- **chi**: the chi angle, rounded.

Optional Columns

Sample Information Column

Protein Name [str]: Name of protein and/or project.

Data Collection Columns

All Data collection columns are optional if you are performing manual collections but are recommended if you are performing automated collections. In manual data collection mode data collection parameters are automatically transferred to DA+ GUI.

Oscillation [deg]: Data collection oscillation angle. DEFAULT: 0.2 / 0.1 (X06DA)

Exposure [s]: Data collection exposure time. DEFAULT: 0.01 / 0.2 (X06DA)

Total Range [deg]: Total angular range for data collection. DEFAULT: 220

Transmission [%]: Transmission used during data collection. DEFAULT: 60 / 100 (X06DA)

Target Resolution [A]: Target resolution will be used to calculate detector distance. DEFAULT: 200

Aperture [int]: PXII/X10SA specific. Allowed are 1 (30um) and 2 (150um). DEFAULT: 2.

Chi Phi Angles [str]: List of chi phi angles for multi-orientation SDU data collection type. Accepted format is as shown in example: (0.0,0.0), (10,0.0), (0.0,10.0). DEFAULT: (0.0,0.0), (30.0, 0.0)

Automation Column

Data Collection Type [str]: Currently standard and multi-orientation (X06SA only) data collection is supported for automated data collection (ADC). DEFAULT: standard

Sample Information	Data Collection					Automation
Protein Name [str]	Oscillation [deg]	Exposure [s]	Total Range [deg]	Transmission [%]	Target Resolution [A]	Data Collection Type [str]
myfavoritelyso	0.1	0.02	270	20	1.5	standard
myfavoritelyso	0.1	0.02	270	20	1.5	standard
myfavoritelyso	0.1	0.02	270	20	1.5	standard
myfavoritelyso	0.1	0.02	270	20	1.5	standard
lyso11	0.1	0.02	270	20	1.5	standard
lyso11	0.1	0.02	270	20	1.5	standard
lyso11	0.1	0.02	270	20	1.5	standard
Mathaumatin	0.1	0.02	360	20	1.5	standard
Mathaumatin	0.1	0.02	360	20	1.5	standard
Mathaumatin	0.1	0.02	360	20	1.5	standard
Mathaumatin	0.1	0.02	360	20	1.5	standard
Mathaumatin	0.1	0.02	360	10	2.0	standard
	0.1	0.02	360	10	2.0	standard
	0.1	0.02	360	10	2.0	standard
	0.1	0.02	360	10	2.0	standard
	0.1	0.02	360	10	2.0	standard
project078	0.1	0.02	180	20	1.5	standard
project078	0.1	0.02	180	20	1.5	standard
project078	0.1	0.02	180	20	1.5	standard
project078	0.1	0.02	180	20	1.5	standard
project078	0.1	0.02	180	20	1.5	standard
project078	0.1	0.02	180	20	2.5	standard
project078	0.1	0.02	180	20	2.5	standard
project078	0.1	0.02	180	20	2.5	standard
project078	0.1	0.02	180	20	2.5	standard

Data Processing Columns

All columns from Processing Pipeline are optional and can be applied to both manual and automated data collections.

1. Processing Pipeline [str]: Available options are: gopy, autoproc or xia2dials. DEFAULT: gopy

2. Space Group Number [1x int]: Available for Processing Pipeline gopy, autoproc and xia2dials. DEFAULT: None

3. Cell Parameters [6x real number]: Available for Processing Pipeline gopy, autoproc and xia2dials. DEFAULT: None

4. Res Cut Key [str]: Resolution cutoff type used during data processing. Allowed values are is or cchalf. DEFAULT: is

5. Res Cut Value [float] : Resolution cutoff value used during data processing. DEFAULT: 1.0 (is), 30 (cchalf)

6. User Resolution [A]: Alternative to Res Cut Key and Value (used only in gopy and serial-xtal data collection type). DEFAULT: None

7. PDB Model [str] : Name of PDB model file used for automated dimple run. PDB should be uploaded to ~/Data10/data_exchange/processing_input/PDB_models/. DEFAULT: None

8. Autoproc Full [bool]: Allows processing with full version of autoPROC without use of fast.macro. DEFAULT: False

9. Proc Full [bool]: Option to disable the last step of adp (full dataset processing with gopy, autoPROC or xia2dials). By default it is set to True. To disable full processing, set it to False. DEFAULT: True

10. Adp Enabled [bool]: Option to disable all automatic processing. DEFAULT: True

11. No Ano [bool]: Defines whether Friedel pairs are False or True during xds processing. Used by adp for gopy, autoPROC and serial crystallography. DEFAULT: False

12. Trusted High [float]: Defines trusted region of detector for xds processing, used by all types of data collection apart from serial crystallography. DEFAULT: 1.21

13. Ffcs Campaign [bool]: Enables creation of linked mtz files in the FFCS campaign folder. DEFAULT: False

14. Autoproc Extra Params [str]: Additional autoPROC parameters that will be appended to the processing command. Example: -M LowResOrTricky autoPROC_ReRunIdxrefAtEnd=yes. DEFAULT: None

Data Processing											
Processing Pipeline [str]	Space Group Number [1x int]	Cell Parameters [6x real number]	Res Cut Key [str]	Res Cut Value [float]	PDB Model [str]	Autoproc Full [bool]	Autoproc Extra Params [str]	Proc Full [bool]	No Ano [bool]	Trusted High [floatl]	FFCS campaign [bool]
autoproc	89	78 78 60 90 90 90	cchalf	60	my_lysozyme_model	True	-M LowResOrTricky	False	True	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	30	my_lysozyme_model	True	-M LowResOrTricky		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True	-M LowResOrTricky		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True	-M LowResOrTricky		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True			False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True			False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True			False	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True			False	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True			False	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True			True	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True			True	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True			True	1.1	True
autoproc	89	78 78 60 90 90 90	is	1.5		True			True	1.1	True
autoproc	89	78 78 60 90 90 90	is	1.5		True			True	1.1	True
autoproc	89	78 78 60 90 90 90	is	2.0		True			True	1.1	True
autoproc	89	78 78 60 90 90 90	is	2.0		True			True	1.1	True
autoproc	89	78 78 60 90 90 90	is	1.5	4y39_MOD.pdb					1.1	
autoproc	89	78 78 60 90 90 90	is	1.5	4y39_MOD.pdb			False		1.1	
autoproc	89	78 78 60 90 90 90	is	2.0	4y39_MOD.pdb			False		1.1	
autoproc	89	78 78 60 90 90 90	is	2.0	4y39_MOD.pdb			False		1.1	
gopy			is	2.0	4y39_MOD.pdb			False		1.1	
gopy			is	2.0	4y39_MOD.pdb					1.1	
gopy			is	2.0						1.1	
gopy			is	2.0						1.1	
gopy			is	2.0						1.1	
gopy			is	2.0						1.1	
gopy			is	2.0						1.1	
gopy			cchalf	20	4y39_MOD.pdb					1.1	
gopy			cchalf	20	4y39_MOD.pdb					1.1	