



**CEPLAS**

Cluster of Excellence on Plant Sciences

# Start Your ARC Workshop Series

Session 03 - Annotate your data

June 14th, 2023

Dominik Brilhaus - CEPLAS Data Science



# Goals

- Get familiar with ISA metadata and Swate
- Annotate data in your ARC

# Legend

 = Locally (on your machine)

 = Remote (in the DataHUB)

Info in `<brackets>` are placeholders - please replace with proper info

# Part 0: Check-in

# Open the online notepad

<https://pad.hhu.de/u44vMavDQLa2e4hvjx1Oyg>

## Screen-sharing during the workshop

<https://hhu.webex.com/hhu-en/j.php?MTID=me5501c7ea1607b9ee3e1edfe401598f3>

# Check Swate installation

 Make sure [Swate is installed](#):

1. Open Excel (online or Desktop)
2. Go to the [Insert](#) tab: Click the arrow next to "My Add-ins". There you should be able to select Swate.
3. Go to the [Data](#) tab: you should see the Swate (Core) add-in.

 Alternatively, you can use [Swate standalone](#)

(⚠️ this is however *work in progress* and likely to change)

## Have a simple text editor ready

- Windows Notepad
- MacOS TextEdit

Recommended text editors with code highlighting:

- Visual Studio Code <https://code.visualstudio.com/>
- BBEdit <https://www.barebones.com/products/bbedit/>
- Sublime <https://www.sublimetext.com/>

## Download the demo data

```
git clone "https://demo-user:5ehDYeHcqP2MqVXsNNPu@git.nfdi4plants.org/teaching/demo-arc_level1.git"
```

# Where we left off last time

👤 Initiated an ARC

📁 Structured and ...

🌐 Shared with collaborators

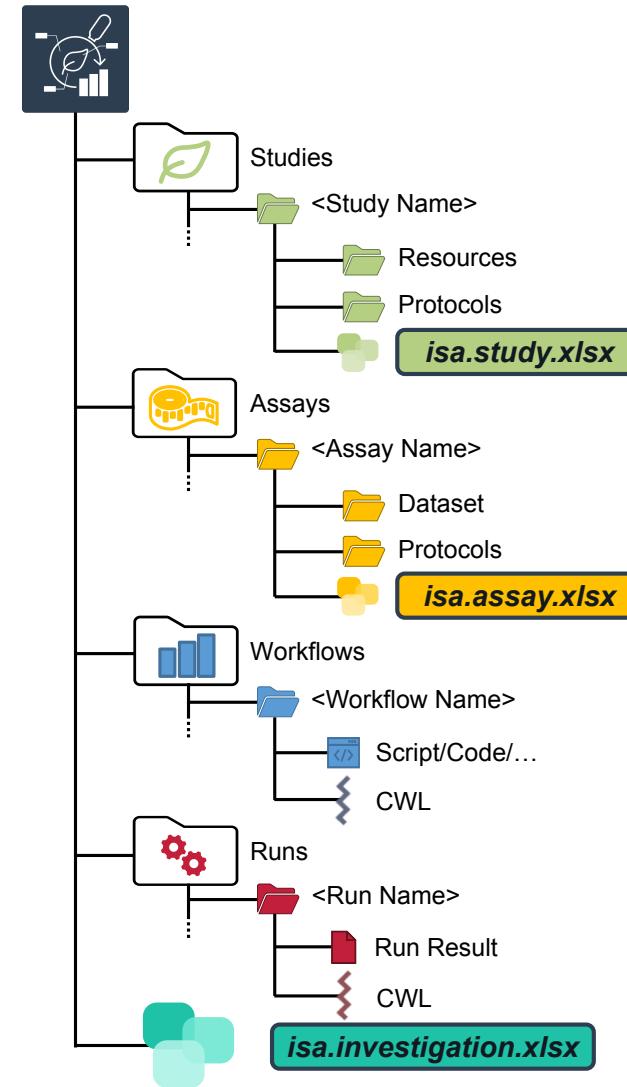
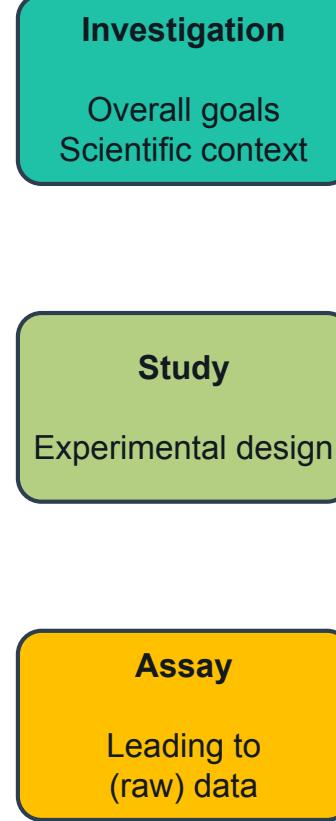
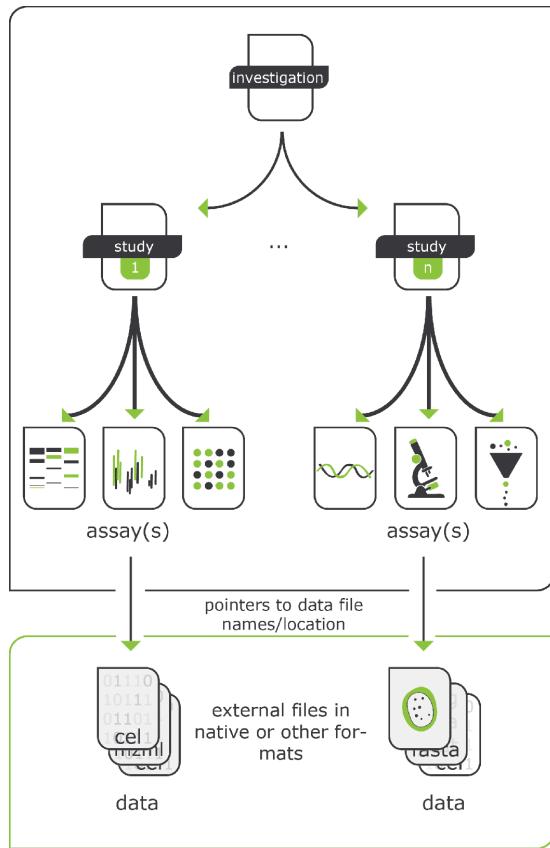
Today we want to

S+ ... annotate the experimental data



# Part 1: Intro ISA

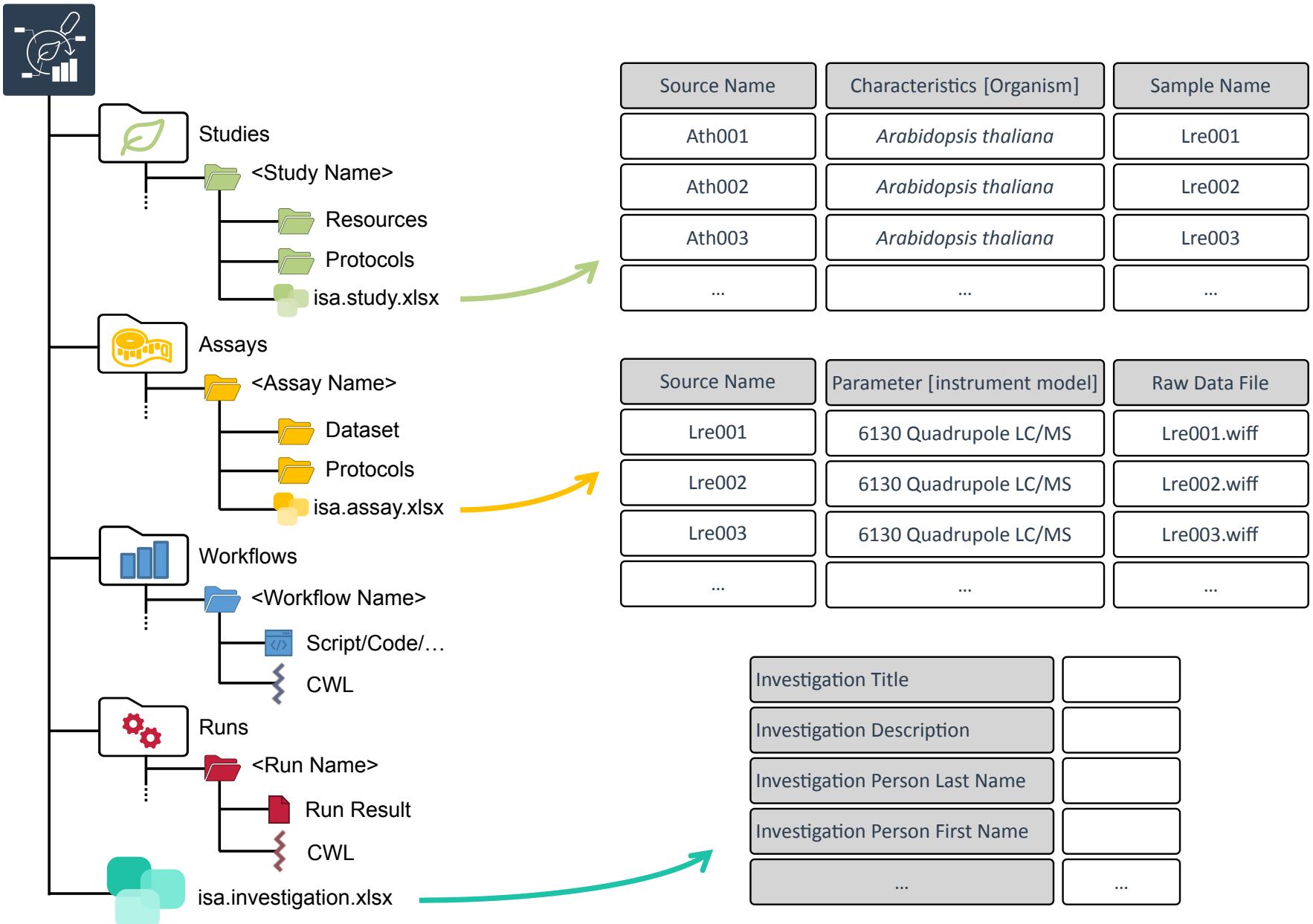
# ARC builds on ISA



<https://isa-tools.org/format/specification.html>

# ARC builds on ISA

Metadata Annotations



# isa.<>.xlsx files within ARCs

isa.investigation.xlsx						
A	B	C	D	E	F	G
1 ONTOLOGY SOURCE REFERENCE	OB: BTO NEWT LO CHEBI PATO EFO					
2 Term Source Name	http://biportal.bioArrayExpress Experimental Factor Ontology					
3 Term Source File	4793_v1.26 v1.26 v1.26 v1.26 v1.26					
4 Term Source Version	v1.26 v1.26 v1.26 v1.26 v1.26					
5 Term Source Description	Ontology for Biomed BRENDA tissue / NEWT UniProt Taxa Unit OntoLex Chemical Ent PhenoTyper c ArrayExpress Experimental factor Ontology					
6 INVESTIGATION						
7 Investigation Identifier	EII-1					
8 Investigation Title	Growth control of the eukaryote cell: a systems biology study in yeast					
9 Investigation Description	Background Cell growth underlies many key cellular and developmental processes, yet a limited number of studies have been carried out on cell growth.					
10 Investigation Submitter Date	30.04.07					
11 Investigation Public Release Date	10.03.09					
12 Comment[Created With Configuration]						
13 Comment[Last Opened With Configuration]	isaconfig default _v2013_02_13					
14 INVESTIGATION PUBLICATIONS						
15 Investigation PubMed ID	17439566					
16 Investigation Publication DOI	doi:10.1186/jbb54					
17 Investigation Publication Author List	Castroli J, Zeef LA, Hoyle DC, Zhang N, Hayes A, Gardner DC, Cornell M, Petty J, Hakes L, Wardleworth L, Rash B, Brown M, Dunn WB, Broadhurst C, Oliver SJ					
18 Investigation Publication Title	Growth control of the eukaryote cell: a systems biology study in yeast					
19 Investigation Publication Status	published					
20 Investigation Publication Status Term Accession Number	published					
21 Investigation Publication Status Term Source REF						
22 INVESTIGATION CONTACTS						
23 Investigation Person Last Name	Stephen	Castroli	Zeef			
24 Investigation Person First Name	Oliver	Juan	Lao			
25 Investigation Person Mid Initials	G		A			
26 Investigation Person Email						
27 Investigation Person Phone						
28 Investigation Person Fax						
29 Investigation Person Address	Oxford Road, Manch Oxford Road, Ms Oxford Road, Manchester M13 9PT, UK					
30 Investigation Person Affiliation	Faculty of Life Sci: Faculty of Life Sci: Faculty of Life Sciences, Michael Smith Building, University of Manchester					
31 Investigation Person Roles	corresponding auth: author					
32 Investigation Person Roles Term Accession Number						
33 Investigation Person Roles Term Source REF						
34 Comment[Investigation Person Id]						
35 STUDY						
36 Study Identifier	EII-S-1					
37 Study Title	Study of the impact of changes in flux on the transcriptome, proteome, endometabolome and exometabolome of the yeast <i>Saccharomyces cerevisiae</i> , independent of growth rate					
38 Study Description	We wished to study the impact of growth rate on the total complement of mRNA molecules, proteins, and metabolites in <i>S. cerevisiae</i> , independent of growth rate					
39 Comment[Study Grant Number]						
40 Comment[Study Funding Agency]						
41 Study Submission Date	30.04.07					
42 Study Public Release Date	10.03.09					
43 Study File	5_EII-S-1.txt					
44 STUDY DESIGN DESCRIPTORS						
45 Study Design Type	Intervention design					
46 Study Design Type Term Accession Number	http://purl.obolibrary.org/obo/OBI_0000115					
47 Study Design Type Term Source REF	OB: BTO					
48 STUDY TECHNOLOGIES						
49 Study PubMed ID	17439566					
50 Study Publication DOI	doi:10.1186/jbb54					
51 Study Publication Author List	Castroli J, Zeef LA, Hoyle DC, Zhang N, Hayes A, Gardner DC, Cornell M, Petty J, Hakes L, Wardleworth L, Rash B, Brown M, Dunn WB, Broadhurst C, Oliver SJ					
52 Study Publication Title	Growth control of the eukaryote cell: a systems biology study in yeast					
53 Study Publication Status	published					
54 Study Publication Status Term Accession Number	published					
55 Study Publication Status Term Source REF						
56 STUDY FACTORS						
57 Study Factor Name	limiting nutrient: rate					
58 Study Factor Type	chemical compound: rate					
59 Study Factor Type Term Accession Number	http://purl.obolibrary.org/obo/PATO_0000161					
60 Study Factor Type Term Source REF	PATO					
61 STUDY ASSAYS						
62 Study Assay Measurement Type	protein expression profile: metabolic profile: transcription profiling					
63 Study Assay Measurement Type Term Accession Number	http://purl.obolibrary.org/obo/OBI_0424					
64 Study Assay Measurement Type Term Source REF	OB: BTO					
65 Study Assay Technology Type	mass spectrometry					
66 Study Assay Technology Type Term Accession Number	http://purl.obolibrary.org/obo/OBI_0400148					
67 Study Assay Technology Type Term Source REF	OB: BTO					
68 Study Assay Technology Platform	iTRAQ					
69 Study Assay File Name	a_proteome.txt a_metabolome.txt a_transcriptome.txt					
70 STUDY PROTOCOLS						
71 Study Protocol Name	growth protocol	mRNA extraction	protein extraction	biotin labeling	iTRAQ labeling	EuKGE-WS4
72 Study Protocol Type	growth	mRNA extraction	protein extraction	labeling	loading	metabolite extraction
73 Study Protocol Type Term Accession Number						
74 Study Protocol Type Term Source REF						
75 Study Protocol Description	1. Biomass samples (1. Biomass samples (45 ml) were taken. This was done using Enzol! For each target, a hybridisation cocktail was made using the					
76 Study Protocol URI	OSI					

isa.study.xlsx						
A	B	C	D	E	F	G
1 Source Name	Characteristics [soluble protein content]	Parameter [Quantification method#2]	Parameter [15N Photosynthesis QconCAT mass#4]	Sample Name		
2 G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,75 microgram	WCGr2_U1	
3 G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,15 microgram	WCGr2_U2	
4 G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,03 microgram	WCGr2_U3	
5 G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,01 microgram	WCGr2_U4	
6 G2_532_15mL	50,00 microgram	absolute quantitation analysis		0,75 microgram	WCGr2_5_1	
7 G2_532_15mL	50,00 microgram	absolute quantitation analysis		0,15 microgram	WCGr2_5_2	
8 G2_532_15mL	50,00 microgram	absolute quantitation analysis		0,03 microgram	WCGr2_5_3	
9 G2_532_15mL	50,00 microgram	absolute quantitation analysis		0,01 microgram	WCGr2_5_4	
10 G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis		0,75 microgram	WCGr2_UF_1	
11 G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis		0,15 microgram	WCGr2_UF_2	
12 G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis		0,03 microgram	WCGr2_UF_3	
13 G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis		0,01 microgram	WCGr2_UF_4	
14 G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis		0,75 microgram	WCGr2_5F_1	
15 G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis		0,15 microgram	WCGr2_5F_2	
16 G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis		0,03 microgram	WCGr2_5F_3	
17 G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis		0,01 microgram	WCGr2_5F_4	
18 G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,75 microgram	WGr1_U1	
19 G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,15 microgram	WGr1_U2	
20 G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,03 microgram	WGr1_U3	
21 G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis		0,01 microgram	WGr1_U4	
22 G1_532_15mL	50,00 microgram	absolute quantitation analysis		0,75 microgram	WGr1_5_1	
23 G1_532_15mL	50,00 microgram	absolute quantitation analysis		0,15 microgram	WGr1_5_2	
24 G1_532_15mL	50,00 microgram	absolute quantitation analysis		0,03 microgram	WGr1_5_3	

isa.assay.xlsx						
A	B	C	D	E	F	G
1 Source Name	Parameter [sample volume]	Parameter [injection vol]				
2 WCGr2_U1	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_U1.wiff
3 WCGr2_U2	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_U2.wiff
4 WCGr2_U3	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_U3.wiff
5 WCGr2_U4	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_U4.wiff
6 WCGr2_S_1	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_S_1.wiff
7 WCGr2_S_2	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_S_2.wiff
8 WCGr2_S_3	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_S_3.wiff
9 WCGr2_S_4	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_S_4.wiff
10 WCGr2_UF_1	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_UF_1.wiff
11 WCGr2_UF_2	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_UF_2.wiff
12 WCGr2_UF_3	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_UF_3.wiff
13 WCGr2_UF_4	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_UF_4.wiff
14 WCGr2_SF_1	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_SF_1.wiff
15 WCGr2_SF_2	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_SF_2.wiff
16 WCGr2_SF_3	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_SF_3.wiff
17 WCGr2_SF_4	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WCGr2_SF_4.wiff
18 WGr1_U1	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_U1.wiff
19 WGr1_U2	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_U2.wiff
20 WGr1_U3	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_U3.wiff
21 WGr1_U4	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_U4.wiff
22 WGr1_S_1	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_S_1.wiff
23 WGr1_S_2	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_S_2.wiff
24 WGr1_S_3	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_S_3.wiff
25 WGr1_S_4	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_S_4.wiff
26 WGr1_UF_1	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_UF_1.wiff
27 WGr1_UF_2	100,00 microliter	2,50 microliter	1 TripleTOF 6000		87,00 minute	WGr1_UF_2.wiff

# Study and assay files are registered in the investigation file

**isa.investigation.xlsx**

A	B	C	D	E	F	G	H	I	J
1	ONTOLOGY SOURCE REFERENCE								
2	Term Source Name	OB	BIO	NEWT	UO	CHEBI	PATO	EFO	
3	Term Source URI	http://biopaxbio2rdf.org/experiment_factor.owl#			v_1.26	v_1.26	v_1.26	v_1.26	
4	Term Source Version	4793	v_1.26						
5	Term Source Description	Ontology for Biomed BIRDIA tissue / NEWT UniProt Tax Unit Ontology Chemical Ent_Phenotypic & ArrayExpress Experimental Factor							
6	INVESTIGATION								
7	Investigation Identifier	BII-1							
8	Investigation Title	Growth control of the eukaryote cell: a systems biology study in yeast							
9	Investigation Description	Background Cell growth underlies many key cellular and developmental processes, yet a limited number of studies have been carried out on cell growth.							
10	Investigation Publication Date	30.04.07							
11	Investigation Public Release Date	10.03.09							
12	Comment [Created With Configuration]								
13	Comment [Last Opened With Configuration]	isaconfig default_v2013 02_13							
14	INVESTIGATION PUBLICATIONS								
15	Investigation PubMed ID	17439666							
16	Investigation Publication DOI	doi:10.1186/jinbio54							
17	Investigation Publication Author List	Castrolo J, Zeeb LA, Hoyle DC, Zhang N, Hayes A, Gardner DC, Cornell M, Petty J, Hakes L, Wardleworth L, Rash B, Brown M, Dunn WB, Broadhurst							
18	Investigation Publication Title	Growth control of the eukaryote cell: a systems biology study in yeast.							
19	Investigation Publication Status	published							
20	Investigation Publication Status Term Accession Number								
21	Investigation Publication Status Term Source REF								
22	INVESTIGATION CONTACTS								
23	Investigation Person Last Name	Stephen							
24	Investigation Person First Name	Oliver							
25	Investigation Person Middle Initials	Juan							
26	Investigation Person Email	Castrolo.J@man.ac.uk							
27	Investigation Person Phone								
28	Investigation Person Fax								
29	Investigation Person Address	Oxford Road, Manchester M13 9PL, UK							
30	Investigation Person Affiliation	Faculty of Life Sciences Faculty of Life Sciences, Michael Smith Building, University of Manchester							
31	Investigation Person Roles	corresponding author							
32	Investigation Person Roles Term Accession Number								
33	Investigation Person Roles Term Source REF								
34	Comment [Investigation Person RfId]								
35	STUDY								
36	Study Identifier								
37	Study Title								
38	Study Description								
39	Comment [Study Grant Number]								
40	Comment [Study Funding Agency]								
41	Study Submission Date								
42	Study Public Release Date								
43	Study File Name								
44	STUDY DESIGN DESCRIPTIONS								
45	Study Design Type								
46	Study Design Type Term Accession Number								
47	Study Design Type Term Source REF								
48	STUDY PUBLICATIONS								
49	Study PubMed ID	17439666							
50	Study Publication DOI	doi:10.1186/jinbio54							
51	Study Publication Author List	Castrolo J, Zeeb LA, Hoyle DC, Zhang N, Hayes A, Gardner DC, Cornell M, Petty J, Hakes L, Wardleworth L, Rash B, Brown M, Dunn WB, Broadhurst							
52	Study Publication Title	Growth control of the eukaryote cell: a systems biology study in yeast.							
53	Study Publication Status	published							
54	Study Publication Status Term Accession Number								
55	Study Publication Status Term Source REF								
56	STUDY FACTORS								
57	Study Factor Name	limiting nutrient	rate						
58	Study Factor Type	chemical compound	rate						
59	Study Factor Type Term Accession Number								
60	Study Factor Type Term Source REF								
61	STUDY ASSAYS								
62	Study Assay Type	protein expression	p mediate profile	transcription profiling					
63	Study Assay Measurement Type Term Accession Number								
64	Study Assay Measurement Type Term Source REF								
65	Study Assay Technology Type	OB							
66	Study Assay Technology Type Term Accession Number								
67	Study Assay Technology Type Term Source REF								
68	Study Assay Technology Platform	OB							
69	Study Assay Technology Platform Term Accession Number								
70	Study Assay Technology Platform Term Source REF								
71	STUDY PROTOCOLS								
72	Study Protocol Name	growth protocol							
73	Study Protocol Type	labeling							
74	Study Protocol Type Term Accession Number								
75	Study Protocol Type Term Source REF								
76	Study Protocol Description								
77	Study Protocol URI								

**Study file**

**Assay file**

**isa.study.xlsx**

A	B	C	D	E	F	G	H	I	M
1	Sample Name	Characteristics [soluble protein content]	Parameter [Quantification method#2]	Parameter [15N Photosynthesis QconCAT mass#4]	Sample Name				
2	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_U1				
3	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_U2				
4	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_U3				
5	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_U4				
6	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_S_1				
7	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_S_2				
8	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_S_3				
9	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_S_4				
10	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_UF_1				
11	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_UF_2				
12	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_UF_3				
13	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_UF_4				
14	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_SF_1				
15	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_SF_2				
16	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_SF_3				
17	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_SF_4				
18	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr1_U1				
19	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr1_U2				
20	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr1_U3				
21	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr1_U4				
22	G1_532_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr1_S_1				
23	G1_532_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr1_S_2				
24	G1_532_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr1_S_3				

**isa.assay.xlsx**

A	B	C	D	E	F	G	H	P	T
1	Source Name	Parameter [sample volume]	Parameter [injection volume]	Parameter [sample volume]	Parameter [injection volume]	Parameter [sample volume]	Parameter [injection volume]	Raw Data File	
2	WCGr2_U1	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_U1.wiff	
3	WCGr2_U2	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_U2.wiff	
4	WCGr2_U3	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_U3.wiff	
5	WCGr2_U4	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_U4.wiff	
6	WCGr2_S_1	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_S_1.wiff	
7	WCGr2_S_2	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_S_2.wiff	
8	WCGr2_S_3	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_S_3.wiff	
9	WCGr2_S_4	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_S_4.wiff	
10	WCGr2_UF_1	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_UF_1.wiff	
11	WCGr2_UF_2	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_UF_2.wiff	
12	WCGr2_UF_3	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_UF_3.wiff	
13	WCGr2_UF_4	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_UF_4.wiff	
14	WCGr2_SF_1	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_SF_1.wiff	
15	WCGr2_SF_2	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_SF_2.wiff	
16	WCGr2_SF_3	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_SF_3.wiff	
17	WCGr2_SF_4	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr2_SF_4.wiff	
18	WCGr1_U1	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_U1.wiff	
19	WCGr1_U2	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_U2.wiff	
20	WCGr1_U3	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_U3.wiff	
21	WCGr1_U4	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_U4.wiff	
22	WCGr1_S_1	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_S_1.wiff	
23	WCGr1_S_2	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_S_2.wiff	
24	WCGr1_S_3	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_S_3.wiff	
25	WCGr1_S_4	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_S_4.wiff	
26	WCGr1_UF_1	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_UF_1.wiff	
27	WCGr1_UF_2	100,00 microliter	2,50 microliter	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	1 TripleTOF 6600	87,00 minute WCGr1_UF_2.wiff	

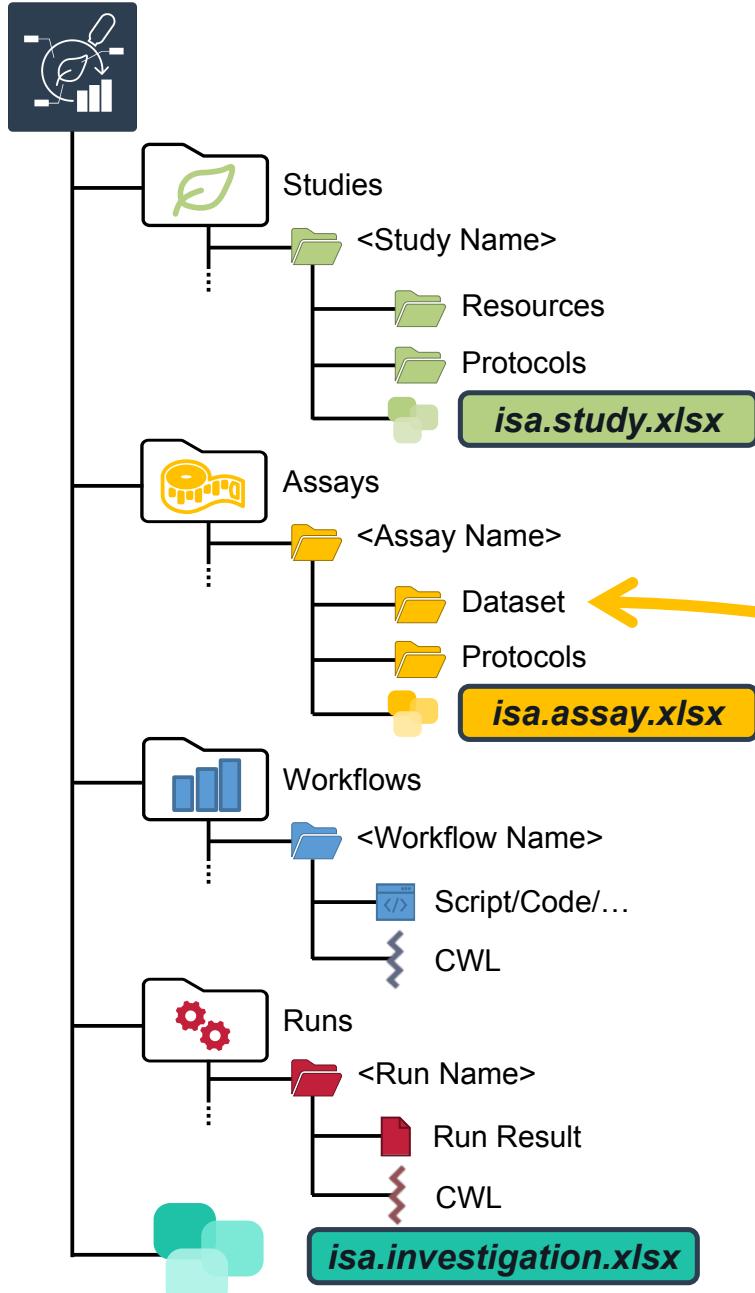
# The output of a study or assay file can function as input for a new isa.assay.xlsx

Output building blocks:

- Sample Name
- Raw Data File
- Derived Data File

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Source Name	Characteristics [soluble protein content]	Parameter [Quantification method#2]	Parameter [15N Photosynthesis QconCAT mass#4]	Sample Name								
2	G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,75 microgram WCGr2_U1
3	G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,15 microgram WCGr2_U2
4	G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,03 microgram WCGr2_U3
5	G2_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,01 microgram WCGr2_U4
6	G2_532_15mL	50,00 microgram	absolute quantitation analysis										0,75 microgram WCGr2_5_1
7	G2_532_15mL	50,00 microgram	absolute quantitation analysis										0,15 microgram WCGr2_5_2
8	G2_532_15mL	50,00 microgram	absolute quantitation analysis										0,03 microgram WCGr2_5_3
9	G2_532_15mL	50,00 microgram	absolute quantitation analysis										0,01 microgram WCGr2_5_4
10	G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis										0,75 microgram WCGr2_UF_1
11	G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis										0,15 microgram WCGr2_UF_2
12	G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis										0,03 microgram WCGr2_UF_3
13	G2_UVM4_F3_15mL	50,00 microgram	absolute quantitation analysis										0,01 microgram WCGr2_UF_4
14	G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis										0,75 microgram WCGr2_SF_1
15	G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis										0,15 microgram WCGr2_SF_2
16	G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis										0,03 microgram WCGr2_SF_3
17	G2_532_F3_15mL	50,00 microgram	absolute quantitation analysis										0,01 microgram WCGr2_SF_4
18	G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,75 microgram WCGr1_U1
19	G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,15 microgram WCGr1_U2
20	G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,03 microgram WCGr1_U3
21	G1_UVM4_15mL	50,00 microgram	absolute quantitation analysis										0,01 microgram WCGr1_U4
22	G1_532_15mL	50,00 microgram	absolute quantitation analysis										0,75 microgram WCGr1_5_1
23	G1_532_15mL	50,00 microgram	absolute quantitation analysis										0,15 microgram WCGr1_5_2
24	G1_532_15mL	50,00 microgram	absolute quantitation analysis										0,03 microgram WCGr1_5_3

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Source Name	Parameter [sample volume]	Parameter [injection volu										
2	WCGr2_U1	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_U1.wiff
3	WCGr2_U2	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_U2.wiff
4	WCGr2_U3	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_U3.wiff
5	WCGr2_U4	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_U4.wiff
6	WCGr2_5_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_5_1.wiff
7	WCGr2_5_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_5_2.wiff
8	WCGr2_5_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_5_3.wiff
9	WCGr2_5_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_5_4.wiff
10	WCGr2_UF_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_UF_1.wiff
11	WCGr2_UF_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_UF_2.wiff
12	WCGr2_UF_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_UF_3.wiff
13	WCGr2_UF_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_UF_4.wiff
14	WCGr2_SF_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_SF_1.wiff
15	WCGr2_SF_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_SF_2.wiff
16	WCGr2_SF_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_SF_3.wiff
17	WCGr2_SF_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr2_SF_4.wiff
18	WCGr1_U1	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_U1.wiff
19	WCGr1_U2	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_U2.wiff
20	WCGr1_U3	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_U3.wiff
21	WCGr1_U4	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_U4.wiff
22	WCGr1_5_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_5_1.wiff
23	WCGr1_5_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_5_2.wiff
24	WCGr1_5_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_5_3.wiff
25	WCGr1_5_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_5_4.wiff
26	WCGr1_UF_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_UF_1.wiff
27	WCGr1_UF_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600								87,00 minute WCGr1_UF_2.wiff



**isa.study.xlsx**

A	B	C	D	E	F	G	H	I	J	K	L	M
1	Source Name	Characteristics [soluble protein content]	Parameter [Quantification method#2]	Parameter [15N Photosynthesis QconCAT mass#4]	Sample Name							
2	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_U1							
3	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_U2							
4	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_U3							
5	G2_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_U4							
6	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_5_1							
7	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_5_2							
8	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_5_3							
9	G2_532_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_5_4							
10	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_UF_1							
11	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_UF_2							
12	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_UF_3							
13	G2_UVM4_F3_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_UF_4							
14	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr2_5F_1							
15	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr2_5F_2							
16	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr2_5F_3							
17	G2_532_F3_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr2_5F_4							
18	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr1_U1							
19	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr1_U2							
20	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr1_U3							
21	G1_UVM4_15mL	50,00 microgram absolute quantitation analysis			0,01 microgram WCGr1_U4							
22	G1_532_15mL	50,00 microgram absolute quantitation analysis			0,75 microgram WCGr1_5_1							
23	G1_532_15mL	50,00 microgram absolute quantitation analysis			0,15 microgram WCGr1_5_2							
24	G1_532_15mL	50,00 microgram absolute quantitation analysis			0,03 microgram WCGr1_5_3							

**isa.assay.xlsx**

A	B	C	D	E	F	G	H	I	J	K	L	M
1	Source Name	Parameter [sample volume]	Parameter [injection vol.									
2	WCGr2_U1	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
3	WCGr2_U2	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
4	WCGr2_U3	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
5	WCGr2_U4	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
6	WCGr2_5_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
7	WCGr2_5_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
8	WCGr2_5_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
9	WCGr2_5_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
10	WCGr2_UF_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
11	WCGr2_UF_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
12	WCGr2_UF_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
13	WCGr2_UF_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
14	WCGr2_5F_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
15	WCGr2_5F_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
16	WCGr2_5F_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
17	WCGr2_5F_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
18	WCGr1_U1	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
19	WCGr1_U2	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
20	WCGr1_U3	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
21	WCGr1_U4	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
22	WCGr1_5_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
23	WCGr1_5_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
24	WCGr1_5_3	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
25	WCGr1_5_4	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
26	WCGr1_UF_1	100,00 microliter	2,50 microliter	1	TripleTOF 6600							
27	WCGr1_UF_2	100,00 microliter	2,50 microliter	1	TripleTOF 6600							

**Raw data**

The raw data consists of WIFF files for each run, corresponding to the entries in the assay table. The files are named WCGr2\_5\_1.wiff, WCGr2\_5\_2.wiff, WCGr2\_5\_3.wiff, WCGr2\_5\_4.wiff, WCGr1\_U1.wiff, WCGr1\_U2.wiff, WCGr1\_U3.wiff, WCGr1\_U4.wiff, WCGr1\_5\_1.wiff, WCGr1\_5\_2.wiff, WCGr1\_5\_3.wiff, WCGr1\_5\_4.wiff, WCGr2\_UF\_1.wiff, WCGr2\_UF\_2.wiff, WCGr2\_UF\_3.wiff, WCGr2\_UF\_4.wiff, WCGr2\_5F\_1.wiff, WCGr2\_5F\_2.wiff, WCGr2\_5F\_3.wiff, and WCGr2\_5F\_4.wiff.

# Annotation Building Block types

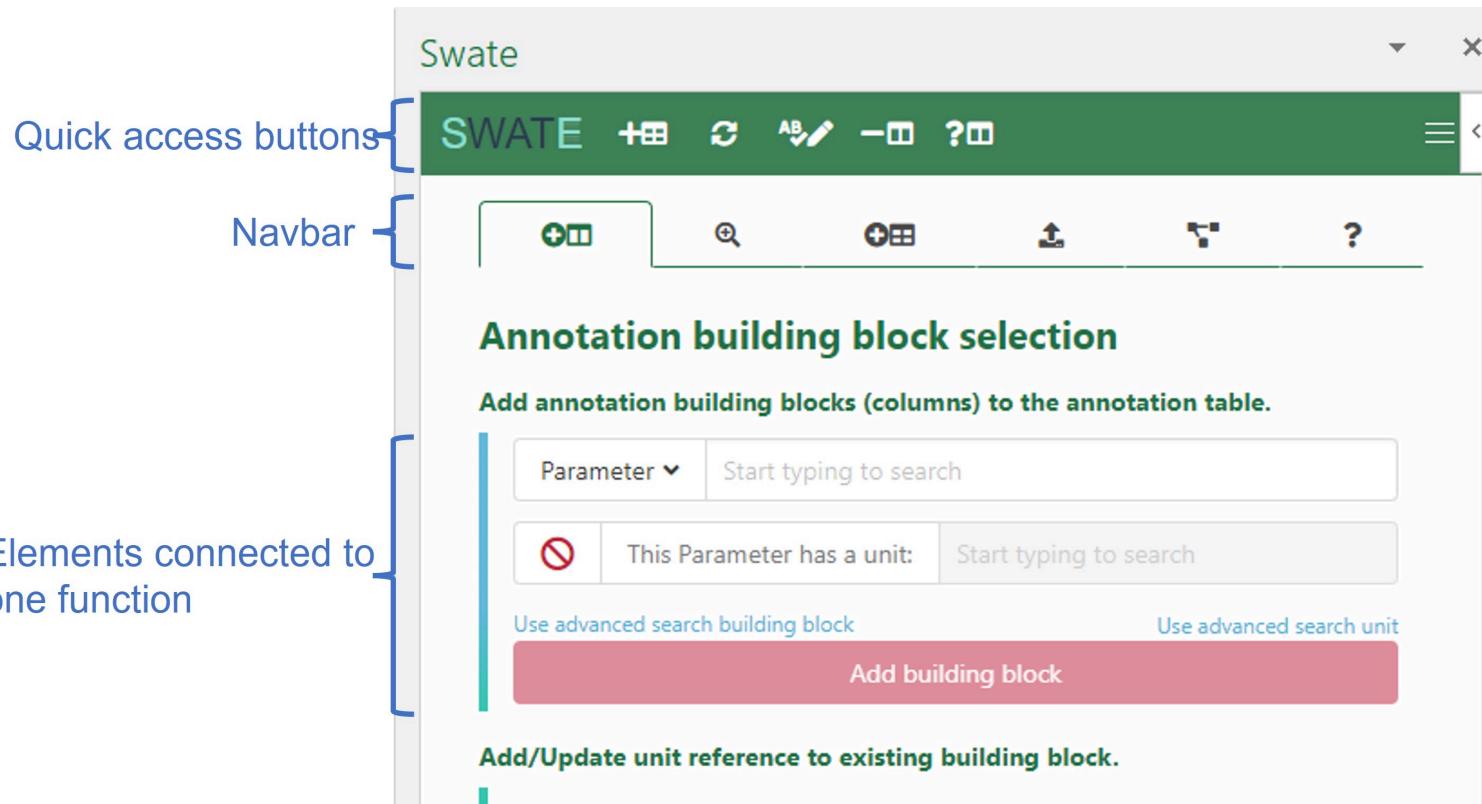
- Source Name (Input)
- Protocol Columns
  - Protocol Type, Protocol Ref
- Characteristic
- Parameter
- Factor
- Component
- Output Columns
  - Sample Name, Raw Data File, Derived Data File

Source	Characteristic	Protocol Type/ Protocol REF	Component	Factor	Sample Name/ Raw Data File Derived Data File
1 G2_UVMA_15ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_1_UP_1
2 G2_UVMA_25ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_2_UP_1
3 G2_UVMA_35ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_3_UP_1
4 G2_UVMA_15ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_4_UP_1
5 G2_UVMA_25ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_5_UP_1
6 G2_UVMA_35ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_6_UP_1
7 G2_S21_15ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_7_UP_1
8 G2_S21_25ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_8_UP_1
9 G2_S21_35ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_9_UP_1
10 G4_F3_15ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_10_UP_1
11 G4_F3_25ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_11_UP_1
12 G4_F3_35ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_12_UP_1
13 G4_UVMA_F3_15ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_13_UP_1
14 G4_UVMA_F3_25ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_14_UP_1
15 G4_UVMA_F3_35ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_15_UP_1
16 G4_S21_F3_15ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_16_UP_1
17 G4_S21_F3_25ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_17_UP_1
18 G4_UVMA_F7_15ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_18_UP_1
19 G4_UVMA_F7_25ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_19_UP_1
20 G4_UVMA_F7_35ml	data extraction protocol	15N	30,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_20_UP_1
21 G5_S21_F2_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_21_UP_1
22 G5_S21_F2_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_22_UP_1
23 G5_S21_F2_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_23_UP_1
24 G5_UVMA_F2_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_24_UP_1
25 G5_UVMA_F2_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_25_UP_1
26 G5_UVMA_F2_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_26_UP_1
27 G5_UVMA_F7_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_27_UP_1
28 G5_UVMA_F7_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_28_UP_1
29 G5_UVMA_F7_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_29_UP_1
30 G5_S21_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_30_UP_1
31 G5_S21_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_31_UP_1
32 G5_S21_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_32_UP_1
33 G5_UVMA_F1_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_33_UP_1
34 G5_UVMA_F1_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_34_UP_1
35 G5_UVMA_F1_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_35_UP_1
36 G5_UVMA_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_36_UP_1
37 G5_S21_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_37_UP_1
38 G5_S21_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_38_UP_1
39 G5_S21_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_39_UP_1
40 G5_UVMA_F1_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_40_UP_1
41 G5_S21_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_41_UP_1
42 G5_UVMA_F1_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_42_UP_1
43 G5_UVMA_F1_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_43_UP_1
44 G5_UVMA_F1_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_44_UP_1
45 G5_UVMA_F1_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_45_UP_1
46 G5_S21_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_46_UP_1
47 G5_S21_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_47_UP_1
48 G5_S21_35ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_48_UP_1
49 G5_S21_F1_15ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_49_UP_1
50 G5_S21_F1_25ml	data extraction protocol	15N	4,00 degree Celsius 6130 Quadrupole LC/MS	Analyst	WGCG_50_UP_1
51					

 For details, check out the [Annotation Principles](#).

## Part 2: Swate hands-on with demo data

# Swate Overview



Major areas of the Swate user interface.

## Let's annotate the plant samples first

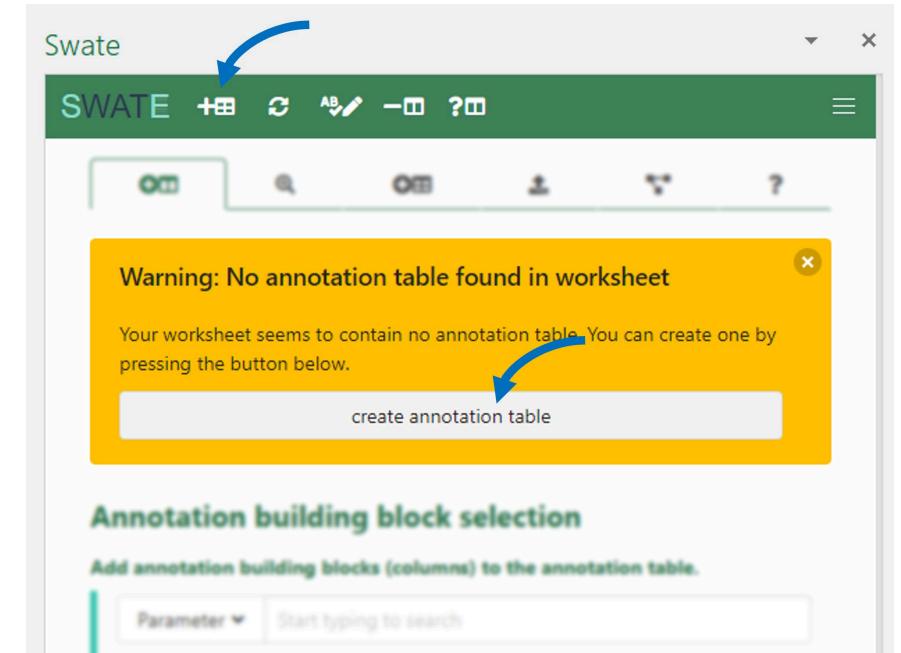
1. Navigate to the demo ARC.
2. Open the lab notes `studies/talinum_drought/protocols/plant_material.txt` in a text editor.
3. Open the empty `studies/talinum_drought/isa.study.xlsx` workbook in Excel.

# Create an annotation table

Create a Swate annotation table via the  
create annotation table button in the yellow pop-up box  
*OR* click the Create Annotation Table quick access  
button.

💡 Each table is by default created with one input ( Source Name ) and one output ( Sample Name ) column

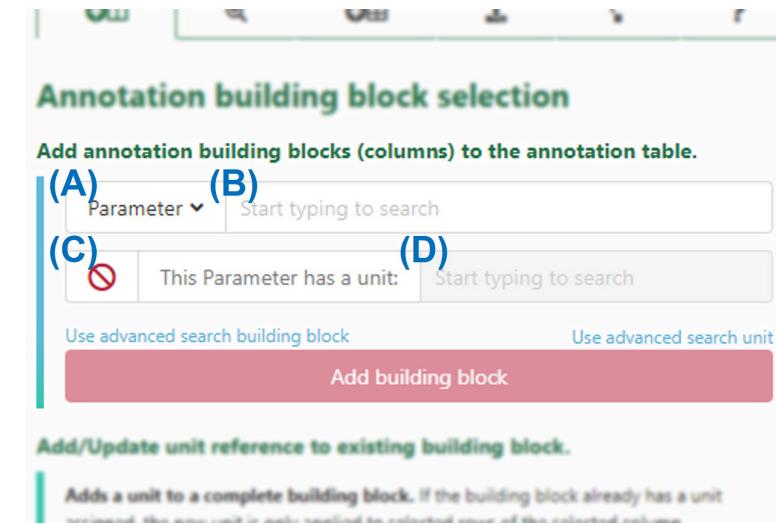
💡 Only one annotation table can be added per Excel sheet



# Add a building block

1. Navigate to the *Building Blocks* tab via the navbar. Here you can add *Building Blocks* to the table.
2. Instead of *Parameter* select *Characteristic* from the drop-down menu (A)
3. Search for **organism** in the search bar (B). This search looks for suitable *Terms* in our *Ontology* database.
4. Select the Term with the id **OBI:0100026** and,
5. Click **Add building block**.

 This adds three columns to your table, one visible and two hidden.



## Insert values to annotate your data

1. Navigate to the *Terms* tab in the Navbar
2. In the annotation table, select any number of cells below **Characteristic**  
**[organism]**

3. Click into the search field in Swate.

|  You should see **organism** showing in a field in front of the search field  
 The search will now yield results related to **organism**

4. In the search field, search for "Talinum fruticosum"

5. Select the first hit and click **Fill selected cells with this term**

## Add a building block with a unit

1. In the *Building Blocks* tab, select *Parameter*, search for `light intensity exposure` and select the term with id `PEC0:0007224`.
2. Check the box for *This Parameter has a unit* and search for `microeinsteins per square meter per second` in the adjacent search bar.
3. Select `U0:0000160`.
4. Click `Add building block`.



This adds four columns to your table, one visible and **three** hidden.

## Insert unit-values to annotate your data

In the annotation table, select any cell below Parameter [light intensity exposure] and add "425" as light intensity.

 You can see the numbers being complemented with the chosen unit, e.g. 425.00 microeinstein per square meter per second

## Showing ontology reference columns

Hold **Ctrl** and click the *Autoformat Table* quick access button to adjust column widths and un-hide all hidden columns.

 You can see that your organism of choice was added with id and source Ontology in the reference (hidden) columns.

 This feature is currently not supported on MacOS

## Update ontology reference columns

Click the **Update Ontology Terms** quick access buttons.

 This updates all reference columns according to the main column. In this case the reference columns for **Parameter [light intensity exposure]** are updated with the id and source ontology of the **microeinsteин per square meter per second** unit.

# Your ISA table is growing

At this point. Your table should look similar to this:

Input [Source Name]	Characteristic [organism]	Parameter [light intensity exposure]	Output [Sample Name]
1	Talinum fruticosum	425 microeinsteins per square meter per second	
2	Talinum fruticosum	425 microeinsteins per square meter per second	
3	Talinum fruticosum	425 microeinsteins per square meter per second	
4	Talinum fruticosum	425 microeinsteins per square meter per second	
5	Talinum fruticosum	425 microeinsteins per square meter per second	
6	Talinum fruticosum	425 microeinsteins per square meter per second	

1

## Hiding ontology reference columns

Click the  quick access button without holding  to hide all reference columns.

## Exercise



Try to add suitable *building blocks* for other pieces of metadata from the plant growth protocol ( `studies/talinum_drought/protocols/plant_material.txt` ).

## Let's annotate the RNA Seq data

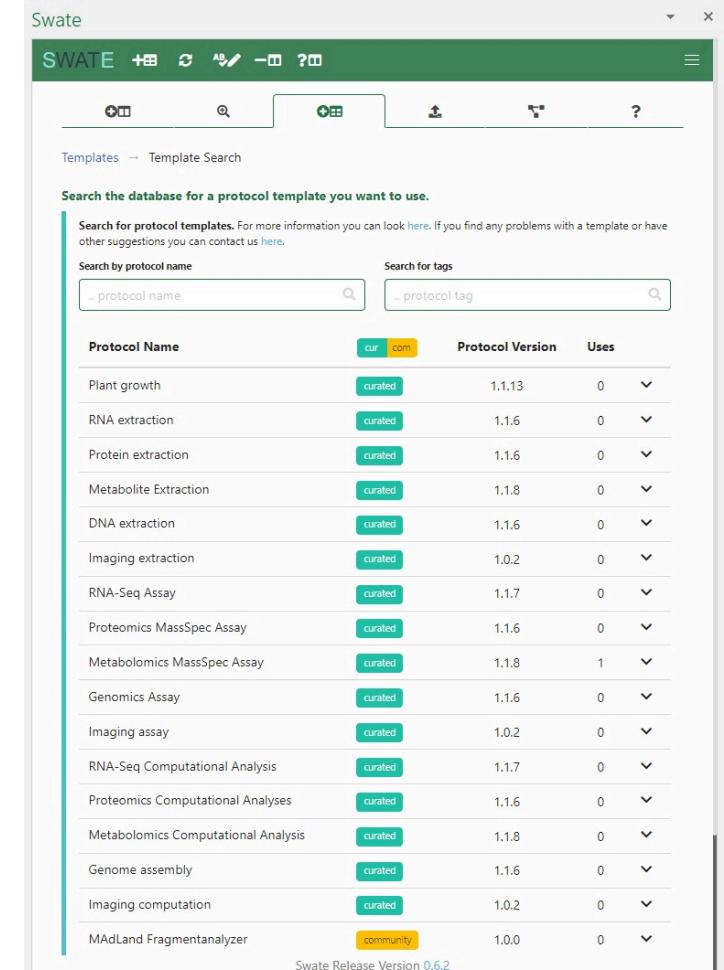
1. Navigate to the demo ARC.
2. Open the lab notes `assays/rnaseq/protocols/RNA_extraction.txt` in a text editor.
3. Open the empty `assays/rnaseq/isa.assay.xlsx` workbook in Excel.

# Use a template

1. Navigate to *Templates* in the Navbar and click *Browse database* in the first function block.

 Here you can find community created workflow annotation templates

1. Search for **RNA extraction** and click **select**
  - You will see a preview of all building blocks which are part of this template.
2. Click **Add template** to add all Building Blocks from the template to your table, which do not exist yet.



The screenshot shows the 'Template Search' page in the Swate software. The top navigation bar includes 'SWATE' and various icons. Below the header, there are search fields for 'Search by protocol name' and 'Search for tags'. A main table lists 'Protocol Name', 'Protocol Version', and 'Uses' for various templates. Most templates are marked as 'curated', while 'MADLand Fragmentanalyzer' is marked as 'community'. The table includes entries for Plant growth, RNA extraction, Protein extraction, Metabolite Extraction, DNA extraction, Imaging extraction, RNA-Seq Assay, Proteomics MassSpec Assay, Metabolomics MassSpec Assay, Genomics Assay, Imaging assay, RNA-Seq Computational Analysis, Proteomics Computational Analyses, Metabolomics Computational Analysis, Genome assembly, Imaging computation, and MADLand Fragmentanalyzer.

Protocol Name	Protocol Version	Uses
Plant growth	1.1.13	0
RNA extraction	1.1.6	0
Protein extraction	1.1.6	0
Metabolite Extraction	1.1.8	0
DNA extraction	1.1.6	0
Imaging extraction	1.0.2	0
RNA-Seq Assay	1.1.7	0
Proteomics MassSpec Assay	1.1.6	0
Metabolomics MassSpec Assay	1.1.8	1
Genomics Assay	1.1.6	0
Imaging assay	1.0.2	0
RNA-Seq Computational Analysis	1.1.7	0
Proteomics Computational Analyses	1.1.6	0
Metabolomics Computational Analysis	1.1.8	0
Genome assembly	1.1.6	0
Imaging computation	1.0.2	0
MADLand Fragmentanalyzer	1.0.0	0

# Adding / Updating unit references

Sometimes you need to add or update the unit of an existing building block.

1. Select any number of rows of the **Parameter [biosource amount]** building block to mark it for the next steps.
2. Open the *Building Blocks* tab
3. In the bottom panel "Add/Update unit reference to existing building block", search for the unit "milligram". Select the unit term and click **Update unit for cells**.  
 If you already had values in the main column they will be updated automatically.
4. Click the *Update Ontology Terms* quick access button, to update the reference columns.

## Remove building blocks

If there are any Building Blocks which do not fit your experiment you can use the  quick access button to remove it including all related (hidden) reference columns.

 Due to the hidden reference columns, we recommend not to delete table columns via usual Excel functions.

## New process, new worksheet

1. Add a new sheet to the `assays/rnaseq/isa.assay.xlsx` workbook.
2. Add the template "RNASeq Assay"

## Exercise



Try to fill the two sheets with the protocol details:

- assays/rnaseq/protocols/RNA\_extraction.txt and
- assays/rnaseq/protocols/Illumina\_libraries.txt

**Your ISA table is ready** 

Go ahead, adjust the Building Blocks you want to use to describe your experiment as you see fit.

Insert values using Swate Term search and add input and output.

# A small detour on "Excel Tables"

Swate uses Excel's "table" feature to annotate workflows. Each table represents one *process* from input (e.g. plant leaf material) to output (e.g. leaf extract).

Example workflows with three *processes* each:

- Plant growth → sampling → extraction
- Measured data files → statistical analysis → result files

 Excel tables allow to group data that belongs together inside one sheet. This is not to be confused with a (work)sheet or workbook.

```
workbook          (e.g. "isa.assay.xlsx")
  └── worksheet    (e.g. "plant_growth")
    └── table      (e.g. "annotationTable")
```

# Contributors

Slides presented here include contributions by

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