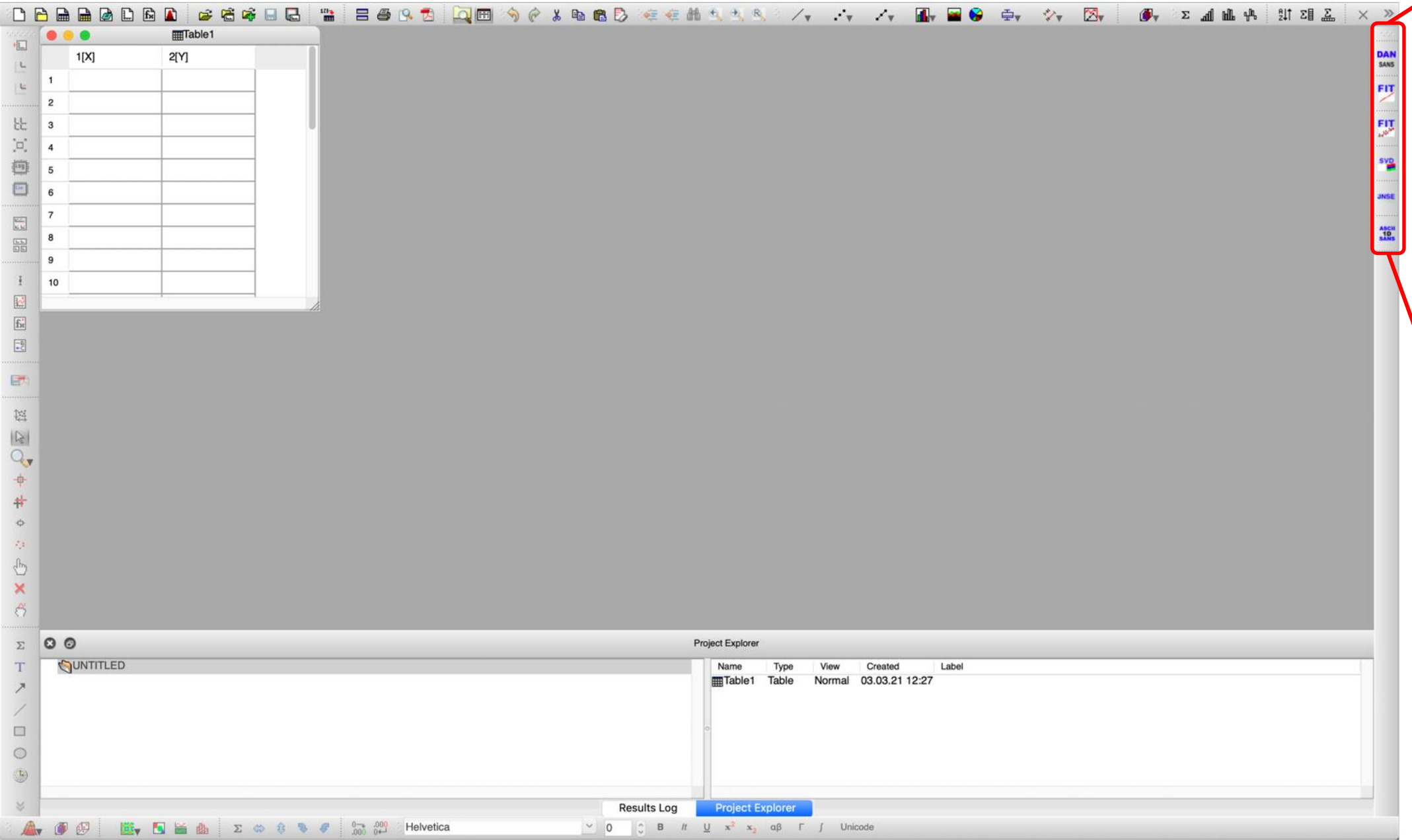
QtiSAS| DAN-SANS | Screenshots
2021-03-24
V. Pipich and M.-S. Appavou

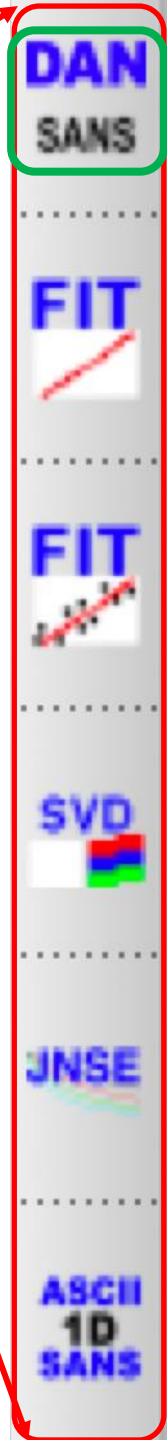
DAN-SANS. Data Reduction. Example.

Instrument:	**KWS-1**
Date of the Experiment:	**March.2020**
QtiSAS Version:	**>01.03.2021**
DAN-SANS “Instrument”:	**KWS1-2020**

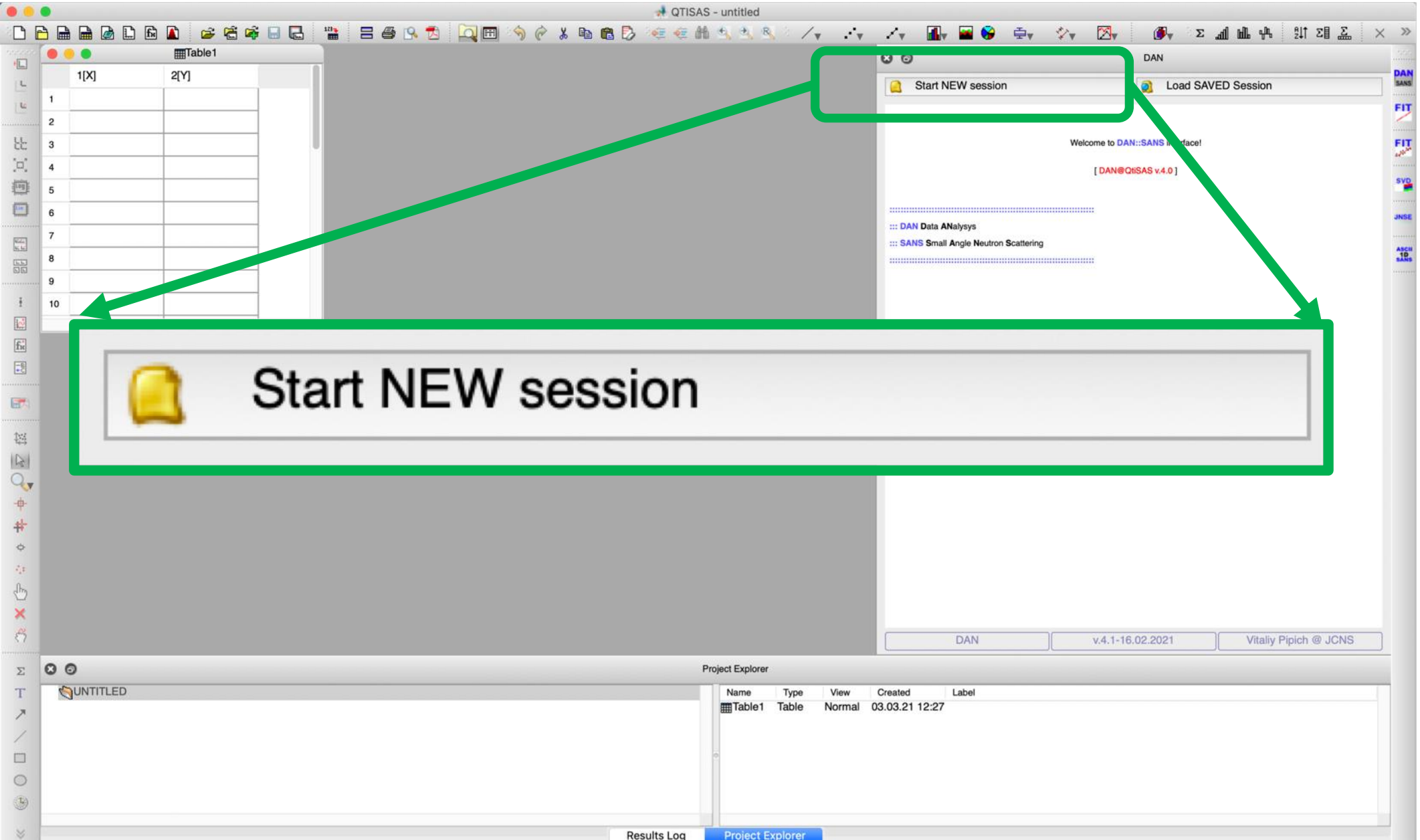
STEP 0: Preparations

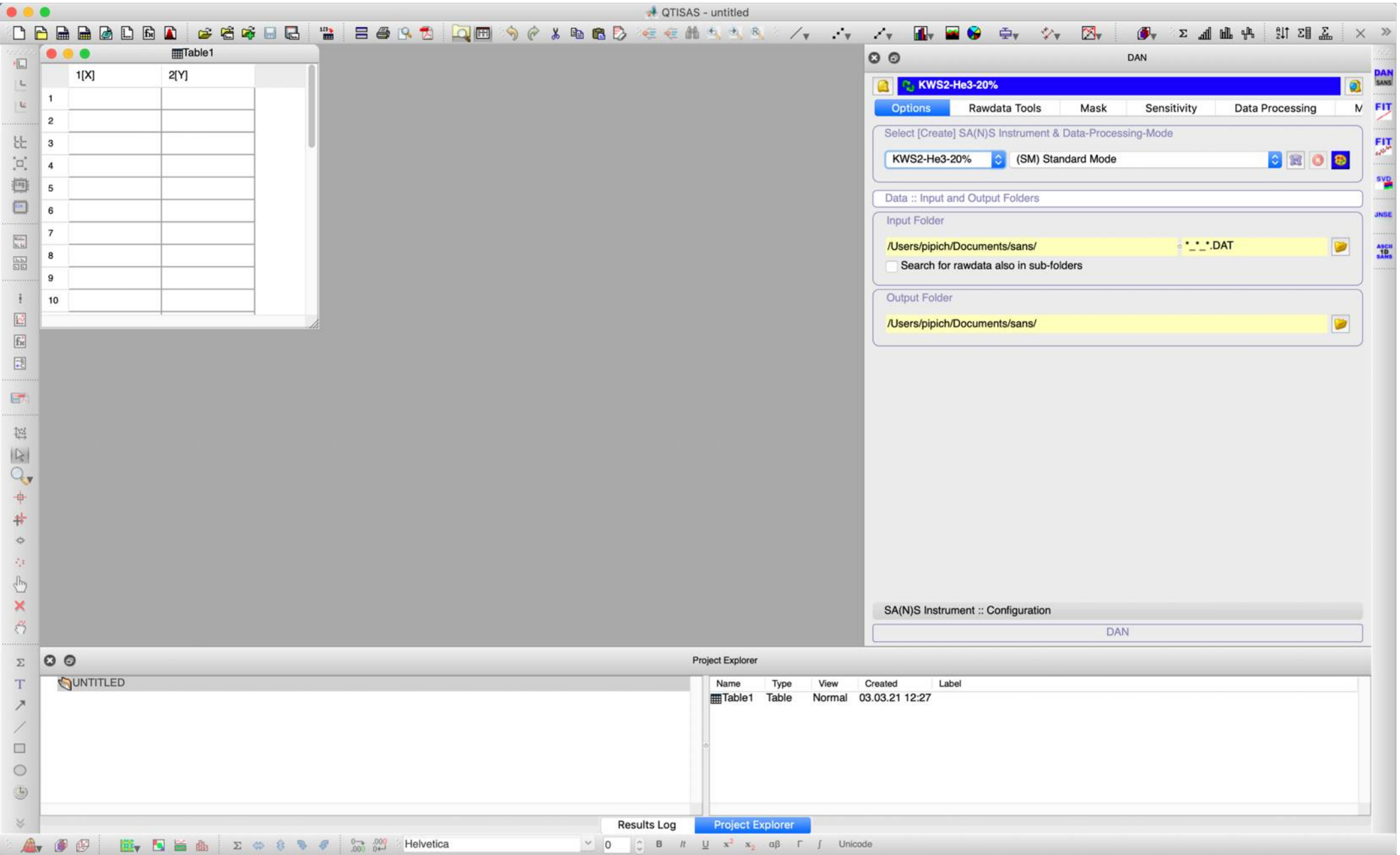
Activation: **DAN-SANS**





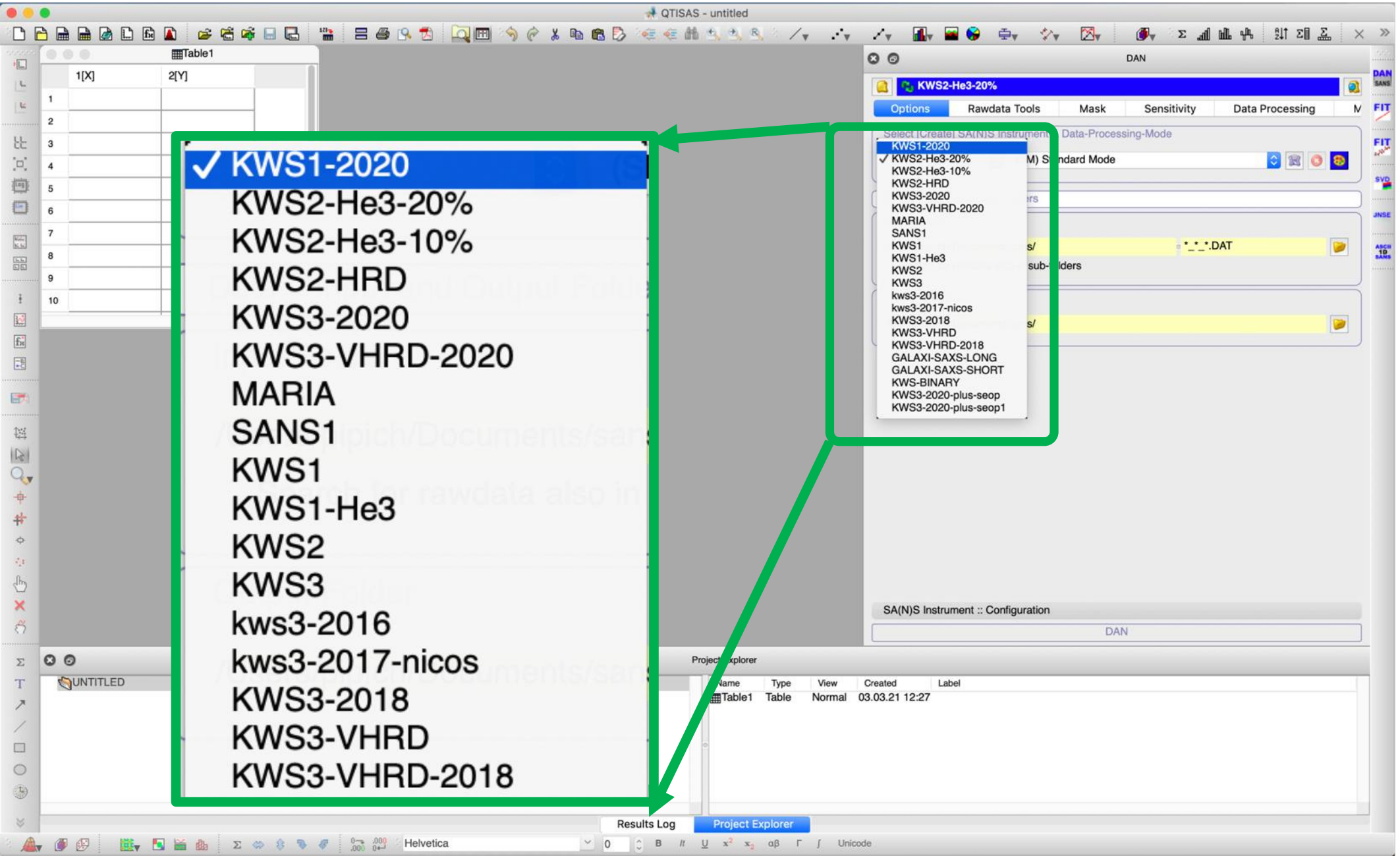
Starting of “New Session”



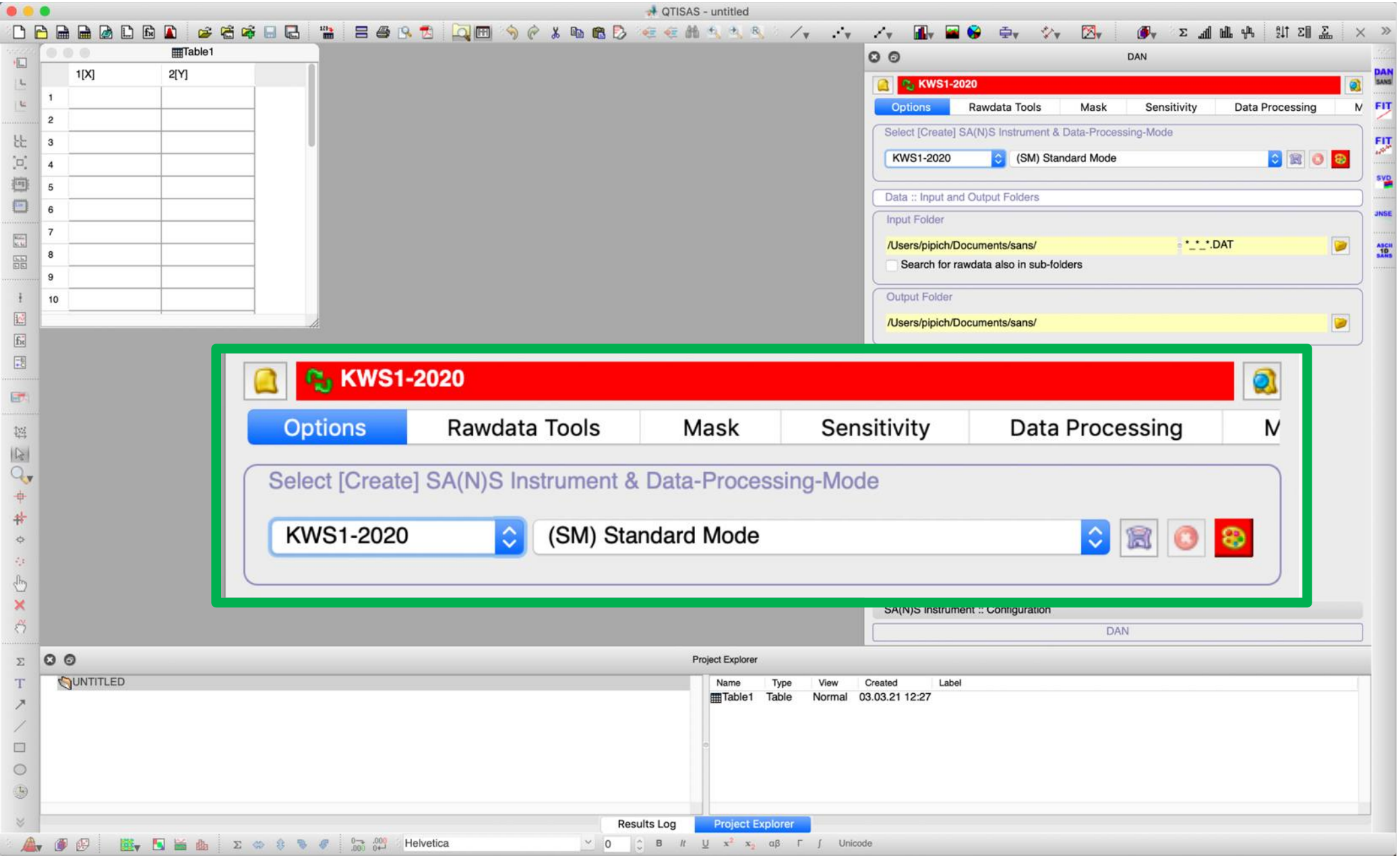

QTISAS - untitled
Table1
1[X]
2[Y]
DAN
KWS2-He3-20%
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Select [Create] SA(N)S Instrument & Data-Processing-Mode
KWS2-He3-20%
(SM) Standard Mode
Data :: Input and Output Folders
Input Folder
/Users/pipich/Documents/sans/
*_*_*.DAT
Search for rawdata also in sub-folders
Output Folder
/Users/pipich/Documents/sans/
SA(N)S Instrument :: Configuration
DAN
Project Explorer
UNTITLED
Name
Type
View
Created
Label
Table1
Table
Normal
03.03.21 12:27
Results Log
Project Explorer
Helvetica
Unicode

STEP 1: Instrument Selection

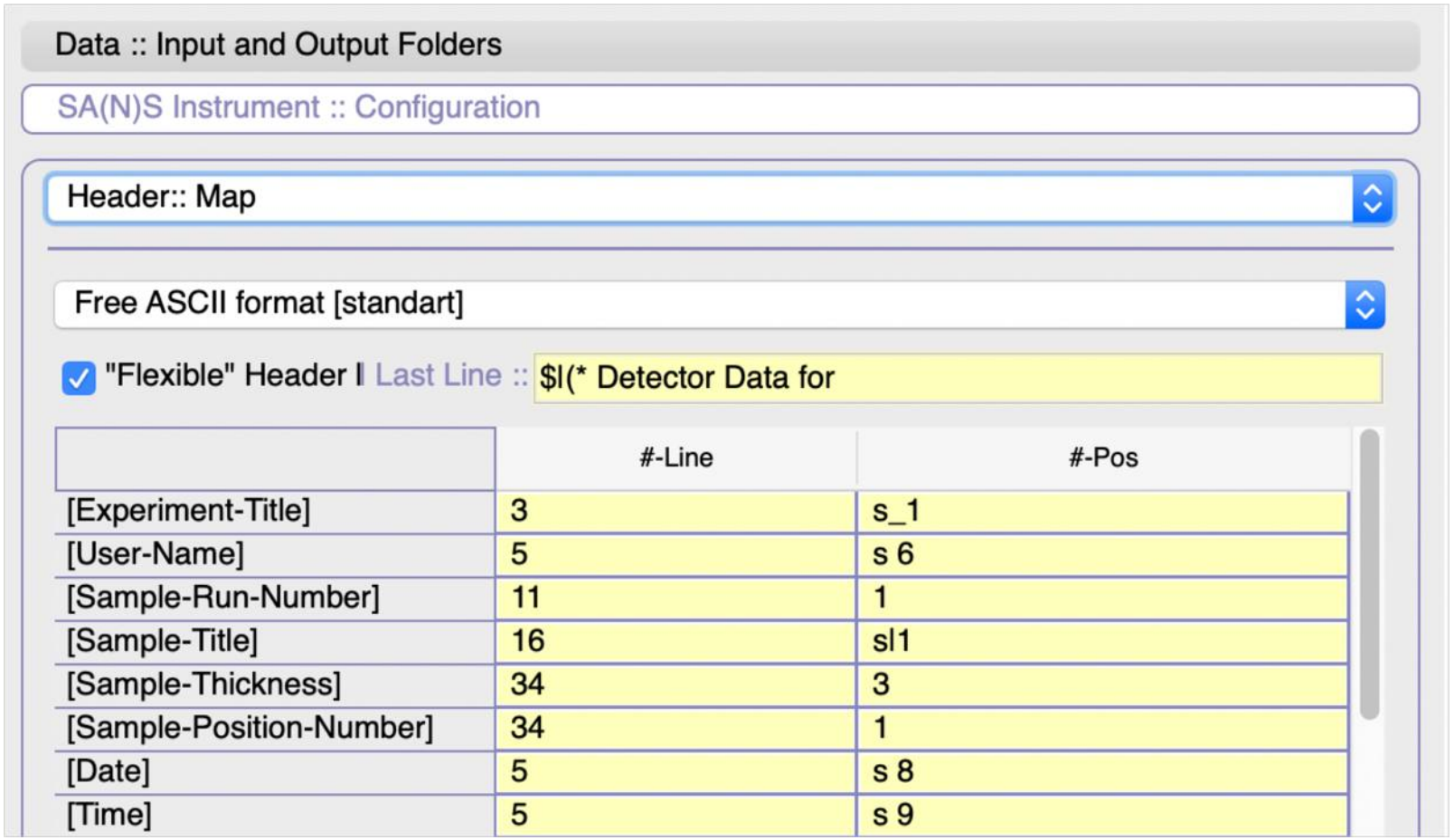
Select Data-Reduction-Instrument: **KWS1-2020**



Selected: **KWS1-2020**



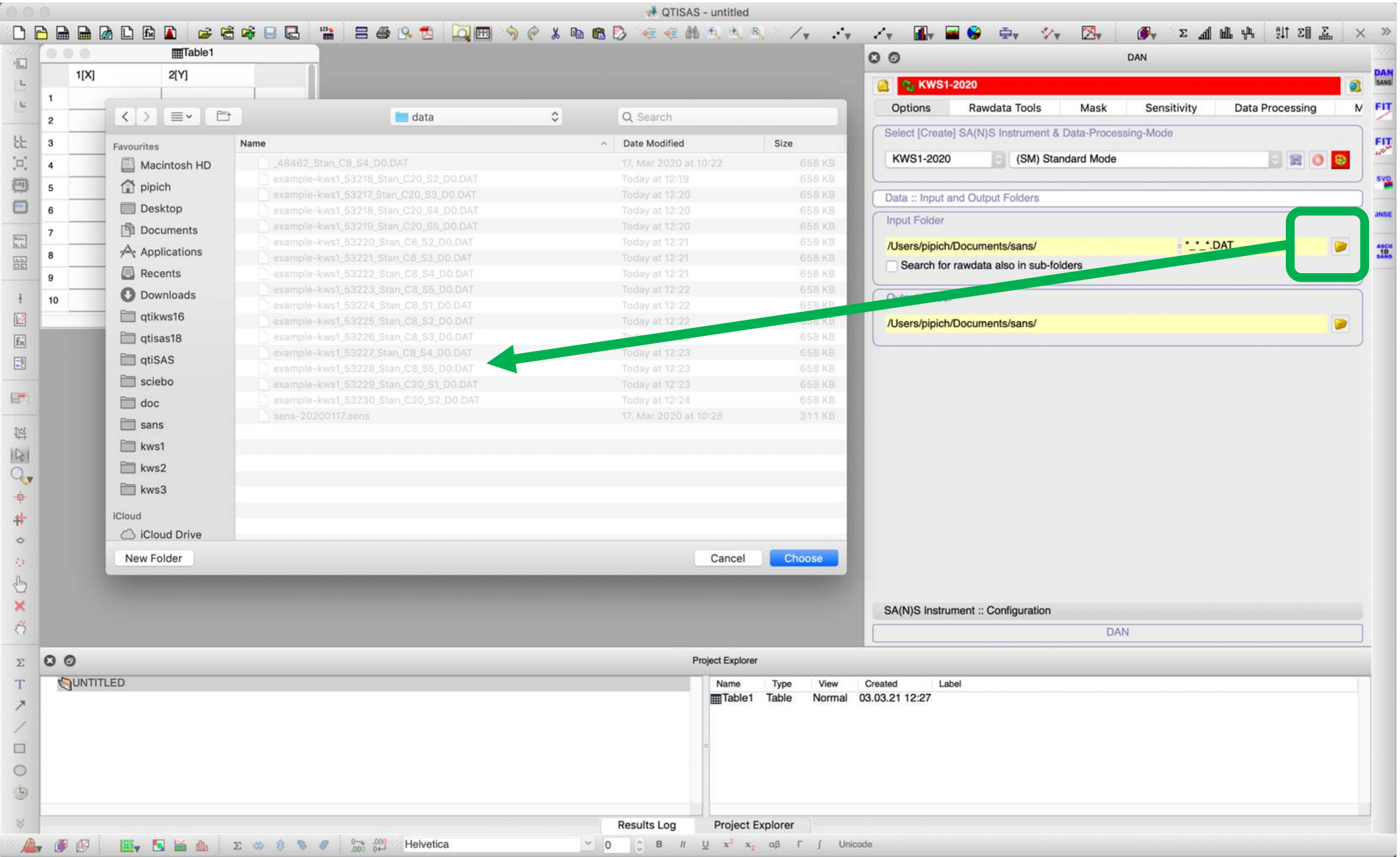
Instrument related parameters are “hidden” in “SA(N)S Instrument :: configuration” tab (**not explained in this file**)



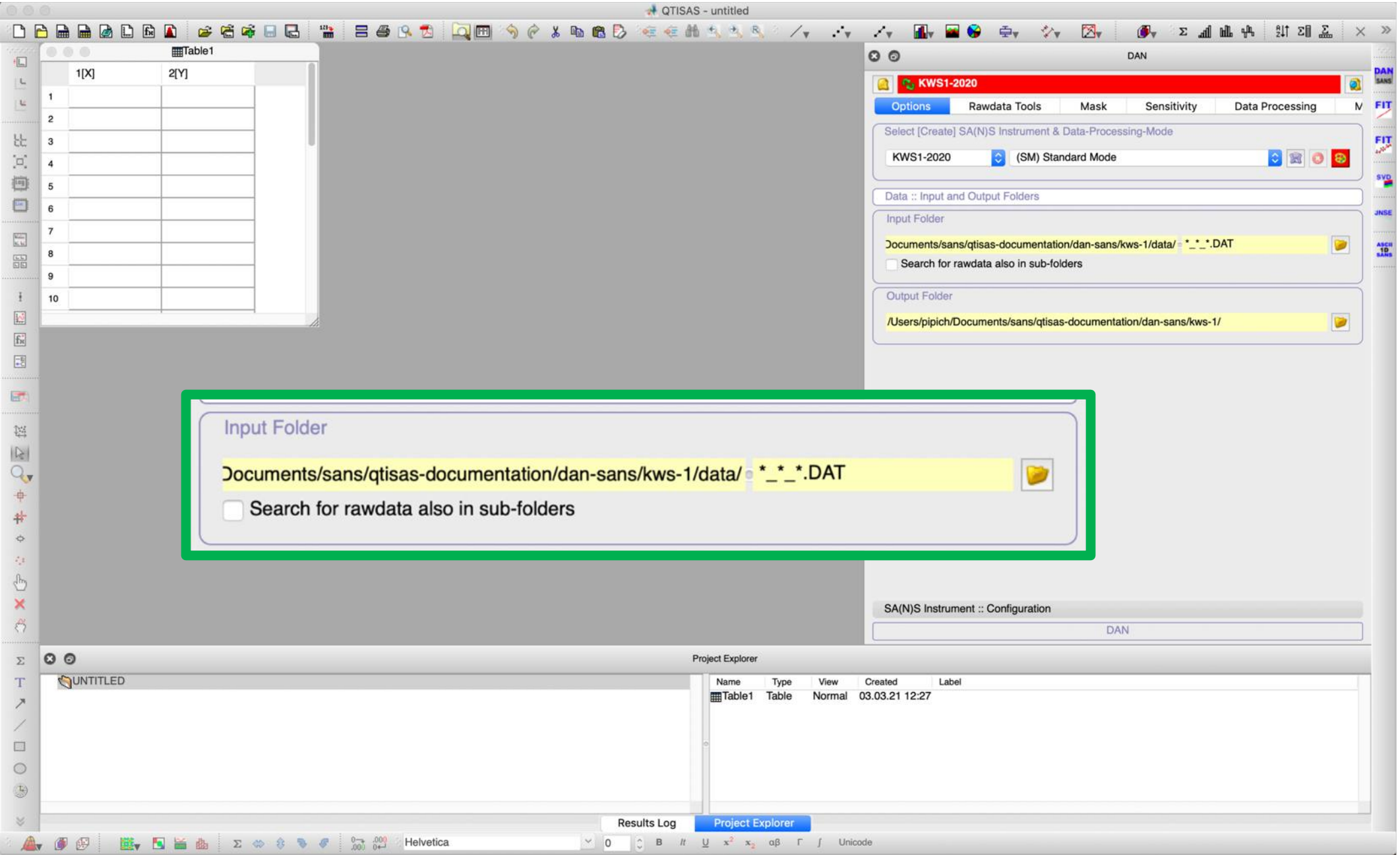
	#-Line	#-Pos
[Experiment-Title]	3	s_1
[User-Name]	5	s 6
[Sample-Run-Number]	11	1
[Sample-Title]	16	sl1
[Sample-Thickness]	34	3
[Sample-Position-Number]	34	1
[Date]	5	s 8
[Time]	5	s 9

STEP 2: Raw-Data Path Selection

Select **Path (Folder)** where your data is located



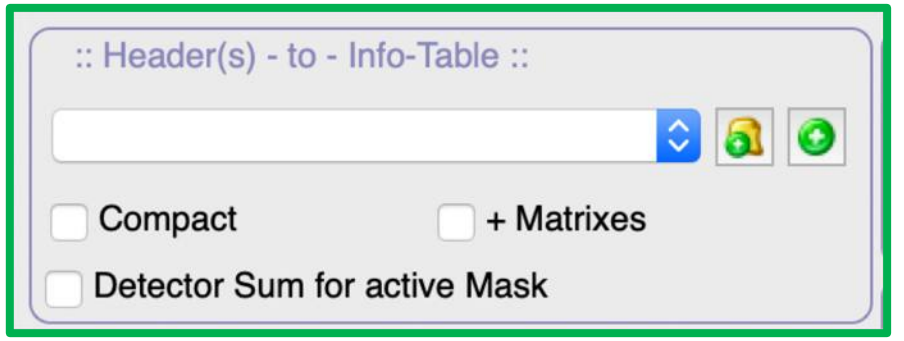
Path (Folder): selected



Input Folder

Documents/sans/qtisas-documentation/dan-sans/kws-1/data/ *_*_*.DAT

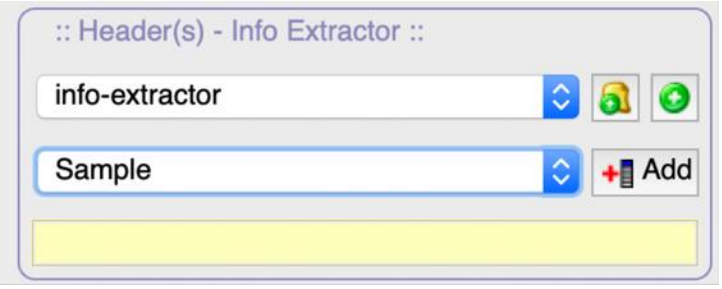
Search for rawdata also in sub-folders



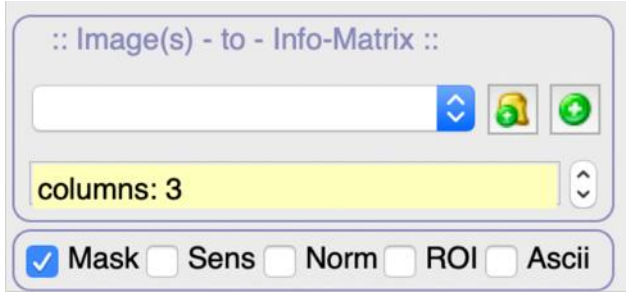
Experiment „logbook“ generation: “Header(s) - to – Info-Table” interface

STEP 3 (optional): Data-Information-Table Generation

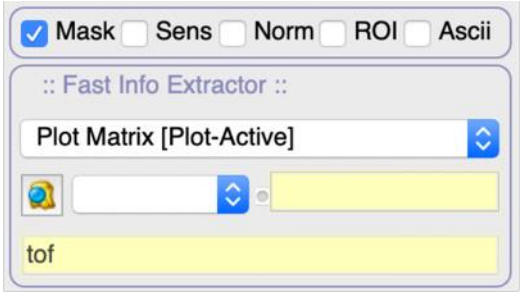
More tools below (**not explained in this file**)



Header(s) - to – Info Extractor
Step-by-step adding of
parameters to your „logbook“

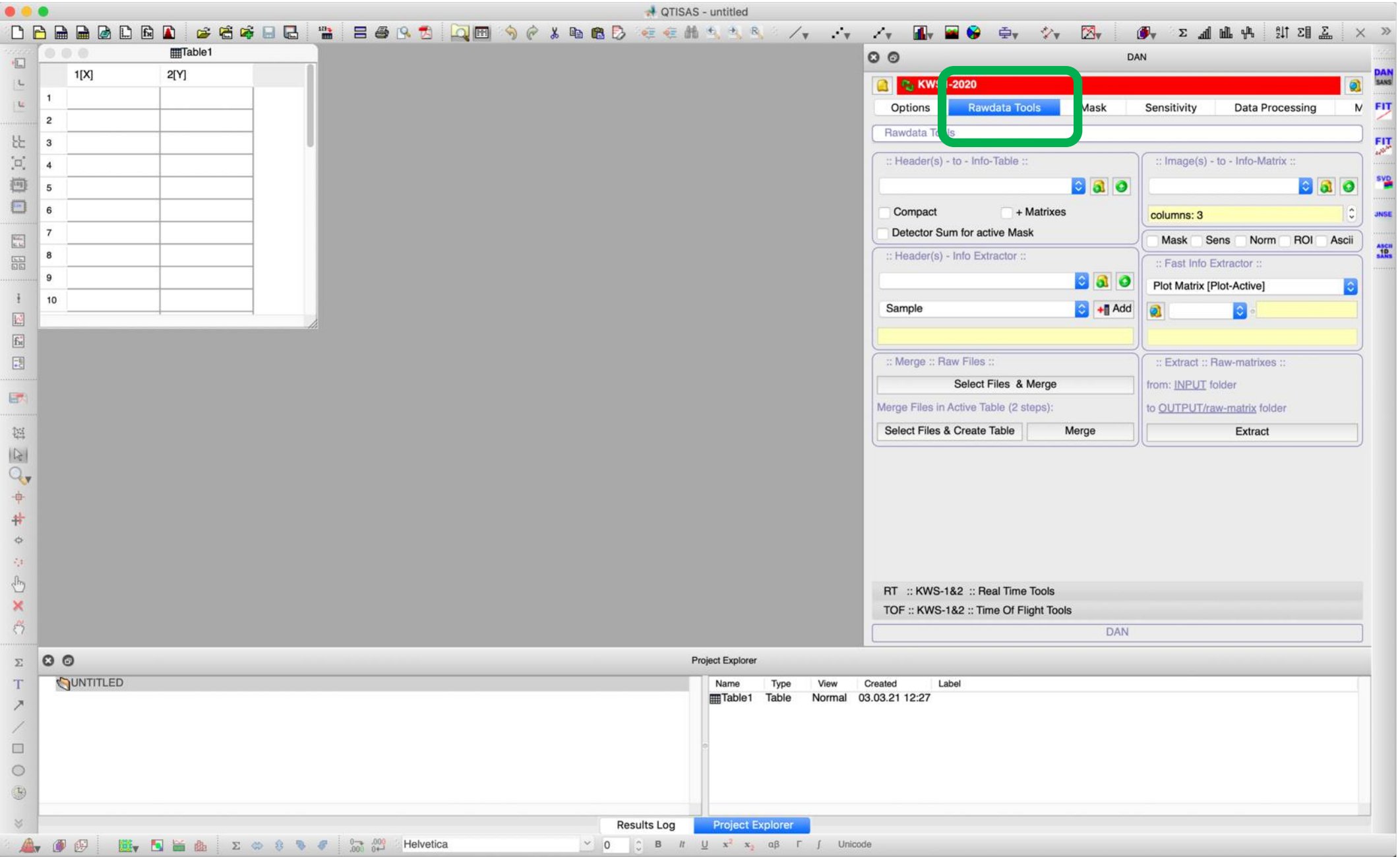


Image(s) - to - Info Matrix
Step-by-step adding of
Raw-matrixes to single matrix

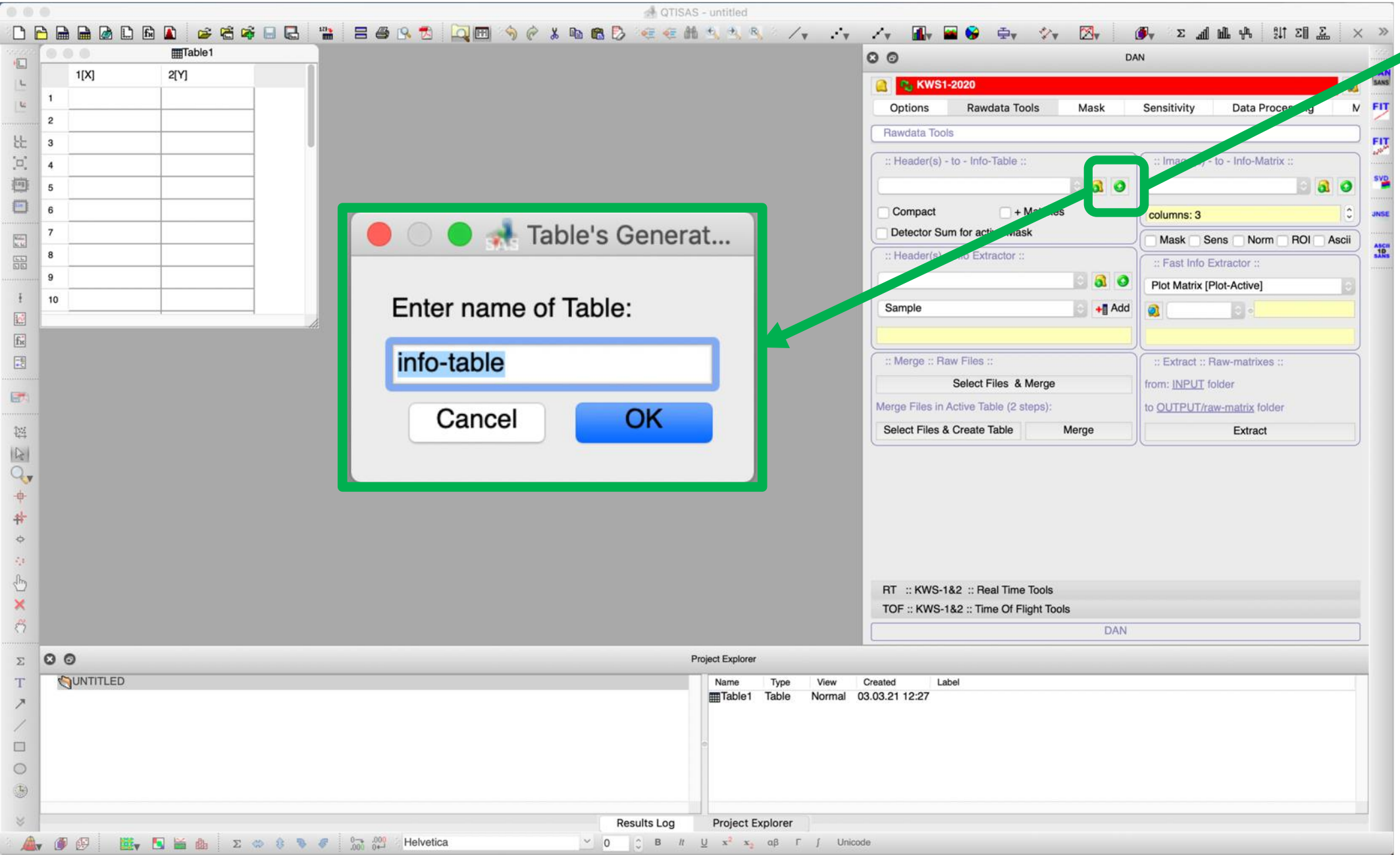


Fast Info Extractor
Every raw-file could be investigated
Here in details

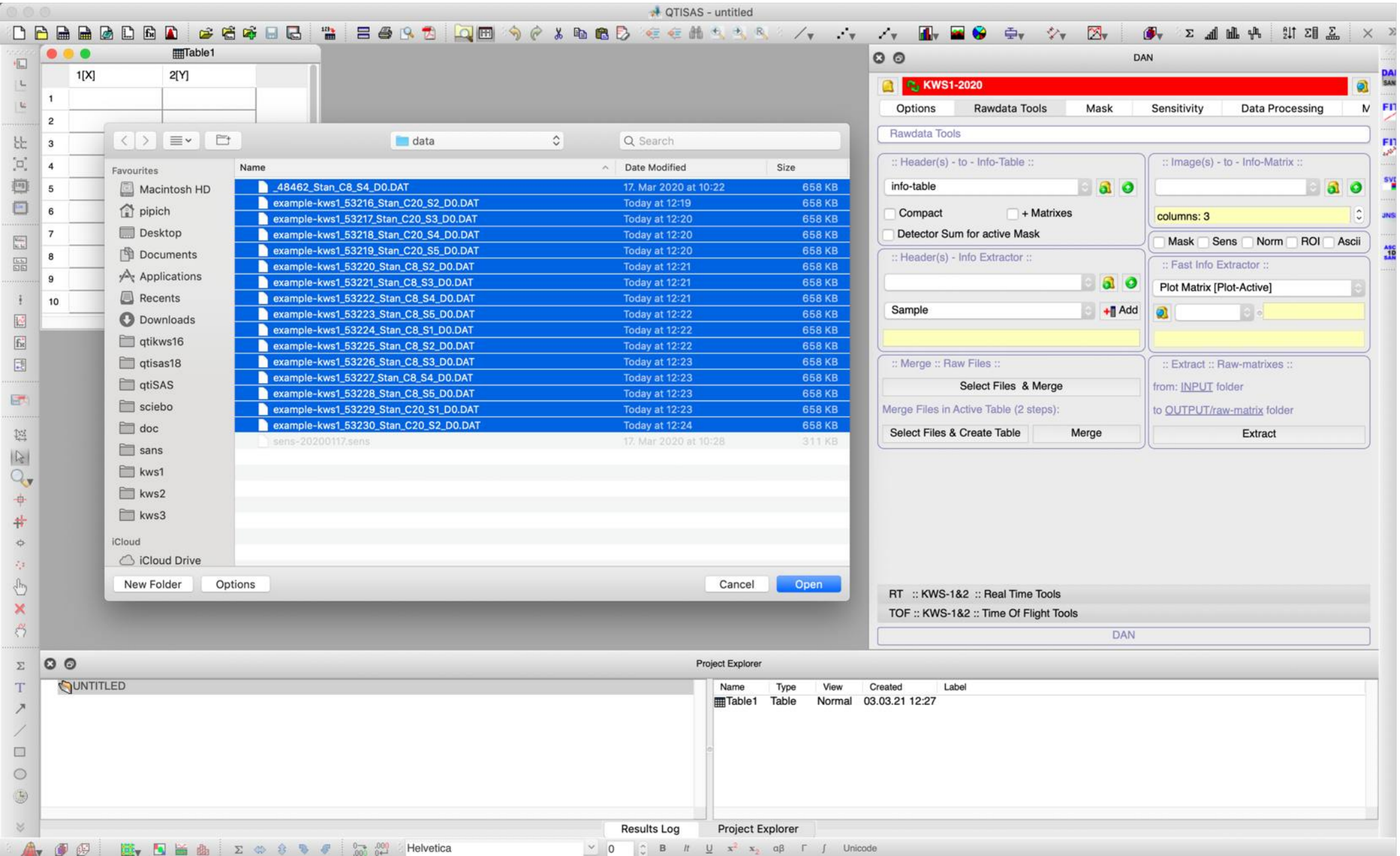
3.1 Go to **Rawdata Tools** tab



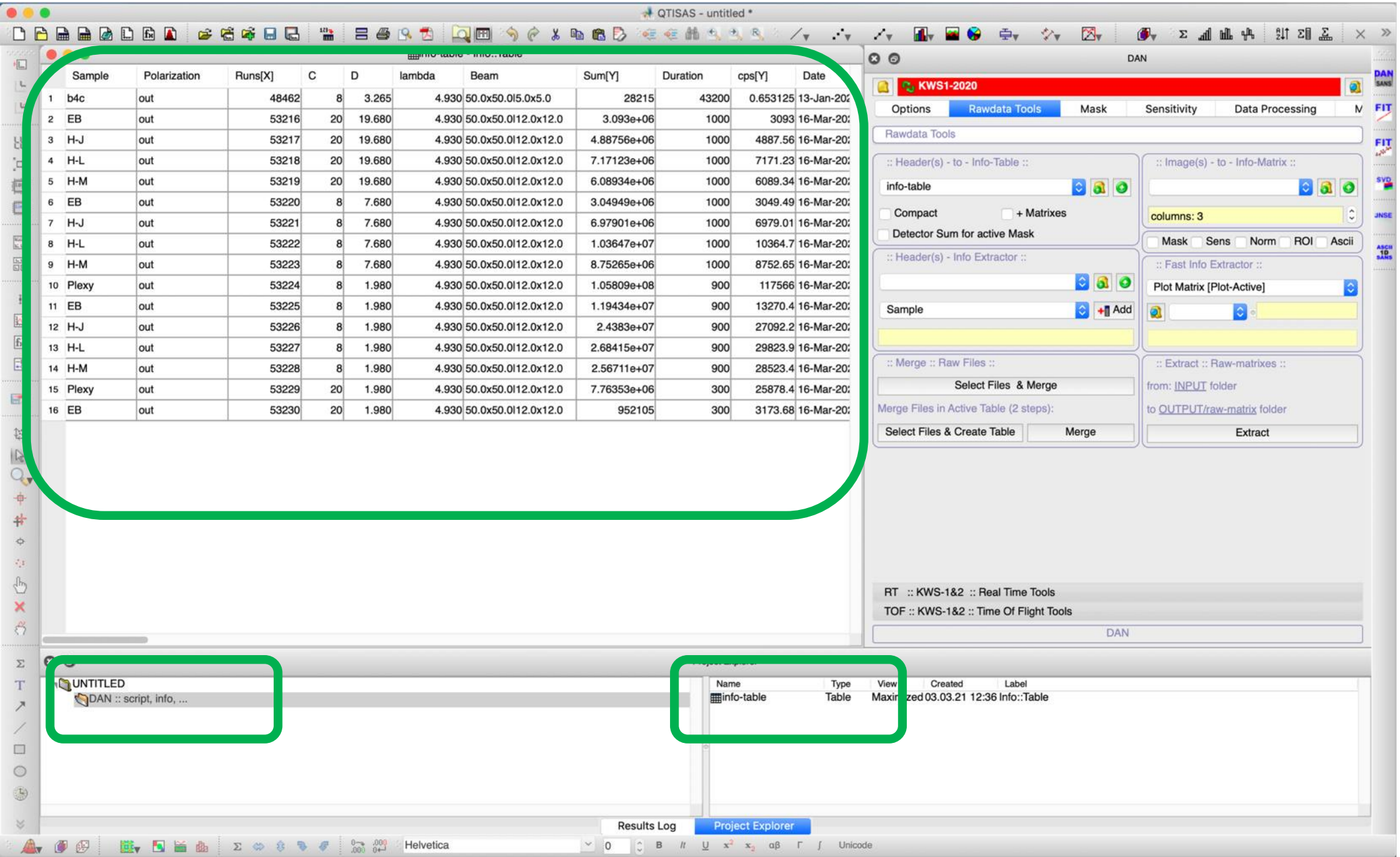
3.2 Push Button and enter **Table Name**



3.3 Select Data to get Information



3.4 “**info-table**” is generated



	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date
1	b4c	out	48462	8	3.265	4.930	50.0x50.0l5.0x5.0	28215	43200	0.653125	13-Jan-202
2	EB	out	53216	20	19.680	4.930	50.0x50.0l12.0x12.0	3.093e+06	1000	3093	16-Mar-202
3	H-J	out	53217	20	19.680	4.930	50.0x50.0l12.0x12.0	4.88756e+06	1000	4887.56	16-Mar-202
4	H-L	out	53218	20	19.680	4.930	50.0x50.0l12.0x12.0	7.17123e+06	1000	7171.23	16-Mar-202
5	H-M	out	53219	20	19.680	4.930	50.0x50.0l12.0x12.0	6.08934e+06	1000	6089.34	16-Mar-202
6	EB	out	53220	8	7.680	4.930	50.0x50.0l12.0x12.0	3.04949e+06	1000	3049.49	16-Mar-202
7	H-J	out	53221	8	7.680	4.930	50.0x50.0l12.0x12.0	6.97901e+06	1000	6979.01	16-Mar-202
8	H-L	out	53222	8	7.680	4.930	50.0x50.0l12.0x12.0	1.03647e+07	1000	10364.7	16-Mar-202
9	H-M	out	53223	8	7.680	4.930	50.0x50.0l12.0x12.0	8.75265e+06	1000	8752.65	16-Mar-202
10	Plexy	out	53224	8	1.980	4.930	50.0x50.0l12.0x12.0	1.05809e+08	900	117566	16-Mar-202
11	EB	out	53225	8	1.980	4.930	50.0x50.0l12.0x12.0	1.19434e+07	900	13270.4	16-Mar-202
12	H-J	out	53226	8	1.980	4.930	50.0x50.0l12.0x12.0	2.4383e+07	900	27092.2	16-Mar-202
13	H-L	out	53227	8	1.980	4.930	50.0x50.0l12.0x12.0	2.68415e+07	900	29823.9	16-Mar-202
14	H-M	out	53228	8	1.980	4.930	50.0x50.0l12.0x12.0	2.56711e+07	900	28523.4	16-Mar-202
15	Plexy	out	53229	20	1.980	4.930	50.0x50.0l12.0x12.0	7.76353e+06	300	25878.4	16-Mar-202
16	EB	out	53230	20	1.980	4.930	50.0x50.0l12.0x12.0	952105	300	3173.68	16-Mar-202

STEP 4 (optional): Data “Understanding”

Samples

info-table - Info::Table

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time
1	b4c	out	48462	8	3.265	4.930	50.0x50.0l5.0x5.0	28215	43200	0.653125	13-Jan-2020	19:18:02.00
2	EB	out	53216	20	19.680	4.930	50.0x50.0l12.0x12.0	3.093e+06	1000	3093	16-Mar-2020	17:00:32.00
3	H-J	out	53217	20	19.680	4.930	50.0x50.0l12.0x12.0	4.88756e+06	1000	4887.56	16-Mar-2020	17:17:27.00
4	H-L	out	53218	20	19.680	4.930	50.0x50.0l12.0x12.0	7.17123e+06	1000	7171.23	16-Mar-2020	17:34:17.00
5	H-M	out	53219	20	19.680	4.930	50.0x50.0l12.0x12.0	6.08934e+06	1000	6089.34	16-Mar-2020	17:51:07.00
6	EB	out	53220	8	7.680	4.930	50.0x50.0l12.0x12.0	3.04949e+06	1000	3049.49	16-Mar-2020	18:22:04.00
7	H-J	out	53221	8	7.680	4.930	50.0x50.0l12.0x12.0	6.97901e+06	1000	6979.01	16-Mar-2020	18:38:59.00
8	H-L	out	53222	8	7.680	4.930	50.0x50.0l12.0x12.0	1.03647e+07	1000	10364.7	16-Mar-2020	18:55:49.00
9	H-M	out	53223	8	7.680	4.930	50.0x50.0l12.0x12.0	8.75265e+06	1000	8752.65	16-Mar-2020	19:12:39.00
10	Plexy	out	53224	8	1.980	4.930	50.0x50.0l12.0x12.0	1.05809e+08	900	117566	16-Mar-2020	19:38:28.00
11	EB	out	53225	8	1.980	4.930	50.0x50.0l12.0x12.0	1.19434e+07	900	13270.4	16-Mar-2020	19:53:41.00
12	H-J	out	53226	8	1.980	4.930	50.0x50.0l12.0x12.0	2.4383e+07	900	27092.2	16-Mar-2020	20:08:56.00
13	H-L	out	53227	8	1.980	4.930	50.0x50.0l12.0x12.0	2.68415e+07	900	29823.9	16-Mar-2020	20:24:06.00
14	H-M	out	53228	8	1.980	4.930	50.0x50.0l12.0x12.0	2.56711e+07	900	28523.4	16-Mar-2020	20:39:17.00
15	Plexy	out	53229	20	1.980	4.930	50.0x50.0l12.0x12.0	7.76353e+06	300	25878.4	16-Mar-2020	20:54:46.00
16	EB	out	53230	20	1.980	4.930	50.0x50.0l12.0x12.0	952105	300	3173.68	16-Mar-2020	20:59:59.00

C20D20

C8D8

C8C2

3 samples: **H-J, H-L, H-M**;

3 configurations: **C20D20, C8D8, C8C2** (WaveLength 4.93A, s.aperture 12x12mm^2, c.aperture 50x50mm^2)

“Dark Current”

info-table - Info::Table

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time
1	b4c	out	48462	8	3.265	4.930	50.0x50.0|5.0x5.0	28215	43200	0.653125	13-Jan-2020	19:18:02.00
2	EB	out	53216	20	19.680	4.930	50.0x50.0|12.0x12.0	3.093e+06	1000	3093	16-Mar-2020	17:00:32.00
3	H-J	out	53217	20	19.680	4.930	50.0x50.0|12.0x12.0	4.88756e+06	1000	4887.56	16-Mar-2020	17:17:27.00
4	H-L	out	53218	20	19.680	4.930	50.0x50.0|12.0x12.0	7.17123e+06	1000	7171.23	16-Mar-2020	17:34:17.00
5	H-M	out	53219	20	19.680	4.930	50.0x50.0|12.0x12.0	6.08934e+06	1000	6089.34	16-Mar-2020	17:51:07.00
6	EB	out	53220	8	7.680	4.930	50.0x50.0|12.0x12.0	3.04949e+06	1000	3049.49	16-Mar-2020	18:22:04.00
7	H-J	out	53221	8	7.680	4.930	50.0x50.0|12.0x12.0	6.97901e+06	1000	6979.01	16-Mar-2020	18:38:59.00
8	H-L	out	53222	8	7.680	4.930	50.0x50.0|12.0x12.0	1.03647e+07	1000	10364.7	16-Mar-2020	18:55:49.00
9	H-M	out	53223	8	7.680	4.930	50.0x50.0|12.0x12.0	8.75265e+06	1000	8752.65	16-Mar-2020	19:12:39.00
10	Plexy	out	53224	8	1.980	4.930	50.0x50.0|12.0x12.0	1.05809e+08	900	117566	16-Mar-2020	19:38:28.00
11	EB	out	53225	8	1.980	4.930	50.0x50.0|12.0x12.0	1.19434e+07	900	13270.4	16-Mar-2020	19:53:41.00
12	H-J	out	53226	8	1.980	4.930	50.0x50.0|12.0x12.0	2.4383e+07	900	27092.2	16-Mar-2020	20:08:56.00
13	H-L	out	53227	8	1.980	4.930	50.0x50.0|12.0x12.0	2.68415e+07	900	29823.9	16-Mar-2020	20:24:06.00
14	H-M	out	53228	8	1.980	4.930	50.0x50.0|12.0x12.0	2.56711e+07	900	28523.4	16-Mar-2020	20:39:17.00
15	Plexy	out	53229	20	1.980	4.930	50.0x50.0|12.0x12.0	7.76353e+06	300	25878.4	16-Mar-2020	20:54:46.00
16	EB	out	53230	20	1.980	4.930	50.0x50.0|12.0x12.0	952105	300	3173.68	16-Mar-2020	20:59:59.00

Dark Current, B4C

Detector Dark Current : **#48462 (blocked beam with B4C**;
Ask local contact to provide this file (single file will be used in all configurations)

Empty Beam/Cell

info-table - Info::Table

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time
1	b4c	out	48462	8	3.265	4.930	50.0x50.0\5.0x5.0	28215	43200	0.653125	13-Jan-2020	19:18:02.00
2	EB	out	53216	20	19.680	4.930	50.0x50.0\12.0x12.0	3.39364e+06	1000	3093	16-Mar-2020	17:00:32.00
3	H-J	out	53217	20	19.680	4.930	50.0x50.0\12.0x12.0	4.88756e+06	1000	4887.56	16-Mar-2020	17:17:27.00
4	H-L	out	53218	20	19.680	4.930	50.0x50.0\12.0x12.0	7.17123e+06	1000	7171.23	16-Mar-2020	17:34:17.00
5	H-M	out	53219	20	19.680	4.930	50.0x50.0\12.0x12.0	6.08534e+06	1000	6089.34	16-Mar-2020	17:51:07.00
6	EB	out	53220	8	7.680	4.930	50.0x50.0\12.0x12.0	3.04949e+06	1000	3049.49	16-Mar-2020	18:22:04.00
7	H-J	out	53221	8	7.680	4.930	50.0x50.0\12.0x12.0	6.97901e+06	1000	6979.01	16-Mar-2020	18:38:59.00
8	H-L	out	53222	8	7.680	4.930	50.0x50.0\12.0x12.0	1.03647e+07	1000	10364.7	16-Mar-2020	18:55:49.00
9	H-M	out	53223	8	7.680	4.930	50.0x50.0\12.0x12.0	8.75265e+06	1000	8752.65	16-Mar-2020	19:12:39.00
10	Plexy	out	53224	8	1.980	4.930	50.0x50.0\12.0x12.0	1.05809e+08	900	117566	16-Mar-2020	19:38:28.00
11	EB	out	53225	8	1.980	4.930	50.0x50.0\12.0x12.0	1.19424e+07	900	13270.4	16-Mar-2020	19:53:41.00
12	H-J	out	53226	8	1.980	4.930	50.0x50.0\12.0x12.0	2.4383e+07	900	27092.2	16-Mar-2020	20:08:56.00
13	H-L	out	53227	8	1.980	4.930	50.0x50.0\12.0x12.0	2.68415e+07	900	29823.9	16-Mar-2020	20:24:06.00
14	H-M	out	53228	8	1.980	4.930	50.0x50.0\12.0x12.0	2.56711e+07	900	28523.4	16-Mar-2020	20:39:17.00
15	Plexy	out	53229	20	1.980	4.930	50.0x50.0\12.0x12.0	7.76353e+06	300	25878.4	16-Mar-2020	20:54:46.00
16	EB	out	53230	20	1.980	4.930	50.0x50.0\12.0x12.0	952105	300	3173.68	16-Mar-2020	20:59:59.00

EB: C20D20

EB: C8D8

EB: C8D2

EC (Empty cell/beam) to subtract from sample's runs

info-table - Info::Table

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time
1	b4c	out	48462	8	3.265	4.930	50.0x50.0|12.0x12.0	26315	43200	0.653125	13-Jan-2020	19:18:02.00
2	EB	out	53216	20	19.680	4.930	50.0x50.0|12.0x12.0	3.093e+06	1000	3093	16-Mar-2020	17:00:32.00
3	H-J	out	53217	20	19.680	4.930	50.0x50.0|12.0x12.0	4.88756e+06	1000	4887.56	16-Mar-2020	17:17:27.00
4	H-L	out	53218	20	19.680	4.930	50.0x50.0|12.0x12.0	7.17123e+06	1000	7171.23	16-Mar-2020	17:34:17.00
5	H-M	out	53219	20	19.680	4.930	50.0x50.0|12.0x12.0	6.08934e+06	1000	6089.34	16-Mar-2020	17:51:07.00
6	EB	out	53220	8	7.680	4.930	50.0x50.0|12.0x12.0	3.04949e+06	1000	3049.49	16-Mar-2020	18:22:04.00
7	H-J	out	53221	8	7.680	4.930	50.0x50.0|12.0x12.0	6.97901e+06	1000	6979.01	16-Mar-2020	18:38:59.00
8	H-L	out	53222	8	7.680	4.930	50.0x50.0|12.0x12.0	1.03647e+07	1000	10364.7	16-Mar-2020	18:55:49.00
9	H-M	out	53223	8	7.680	4.930	50.0x50.0|12.0x12.0	8.75265e+06	1000	8752.65	16-Mar-2020	19:12:39.00
10	Plexy	out	53224	8	1.980	4.930	50.0x50.0|12.0x12.0	1.05809e+08	900	117566	16-Mar-2020	19:38:28.00
11	EB	out	53225	8	1.980	4.930	50.0x50.0|12.0x12.0	1.19434e+07	900	13270.4	16-Mar-2020	19:53:41.00
12	H-J	out	53226	8	1.980	4.930	50.0x50.0|12.0x12.0	2.43833e+07	900	27092.2	16-Mar-2020	20:08:56.00
13	H-L	out	53227	8	1.980	4.930	50.0x50.0|12.0x12.0	2.68415e+07	900	29823.9	16-Mar-2020	20:24:06.00
14	H-M	out	53228	8	1.980	4.930	50.0x50.0|12.0x12.0	2.56711e+07	900	28523.4	16-Mar-2020	20:39:17.00
15	Plexy	out	53229	20	1.980	4.930	50.0x50.0|12.0x12.0	5.76353e+06	300	25878.4	16-Mar-2020	20:54:46.00
16	EB	out	53230	20	1.980	4.930	50.0x50.0|12.0x12.0	952105	300	3173.68	16-Mar-2020	20:59:59.00

AC: Dark Current C20D20, C8D8, C8D2

AC: Plexy, EB C8D8 C8D2

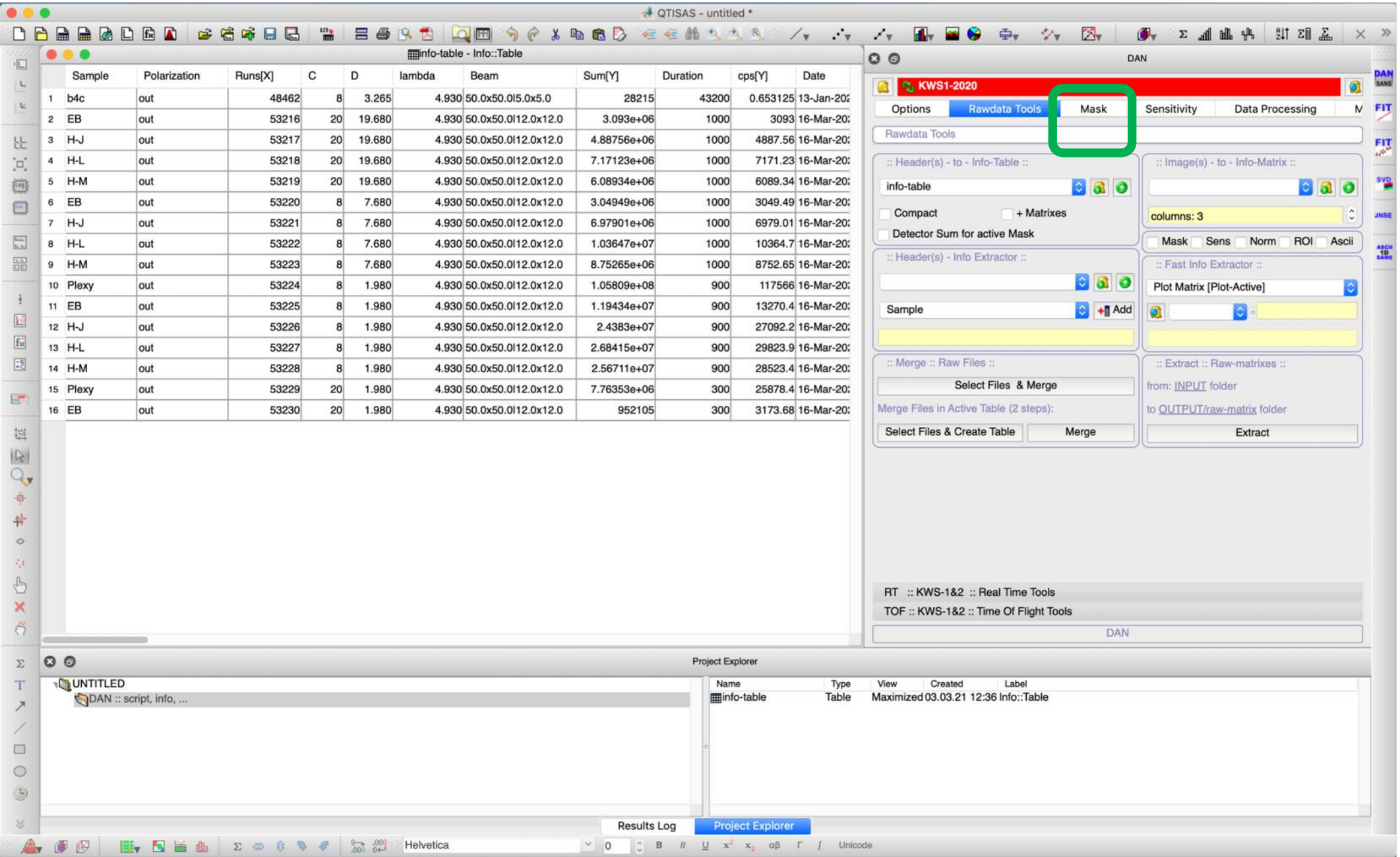
AC : Plexy, EB C20D20

Absolute Calibration Runs:

- Plexy (“flat scattering sample”, like Plexiglas or H2O)
- EB (“Empty Beam”)
- B4C (“Dark Current”)

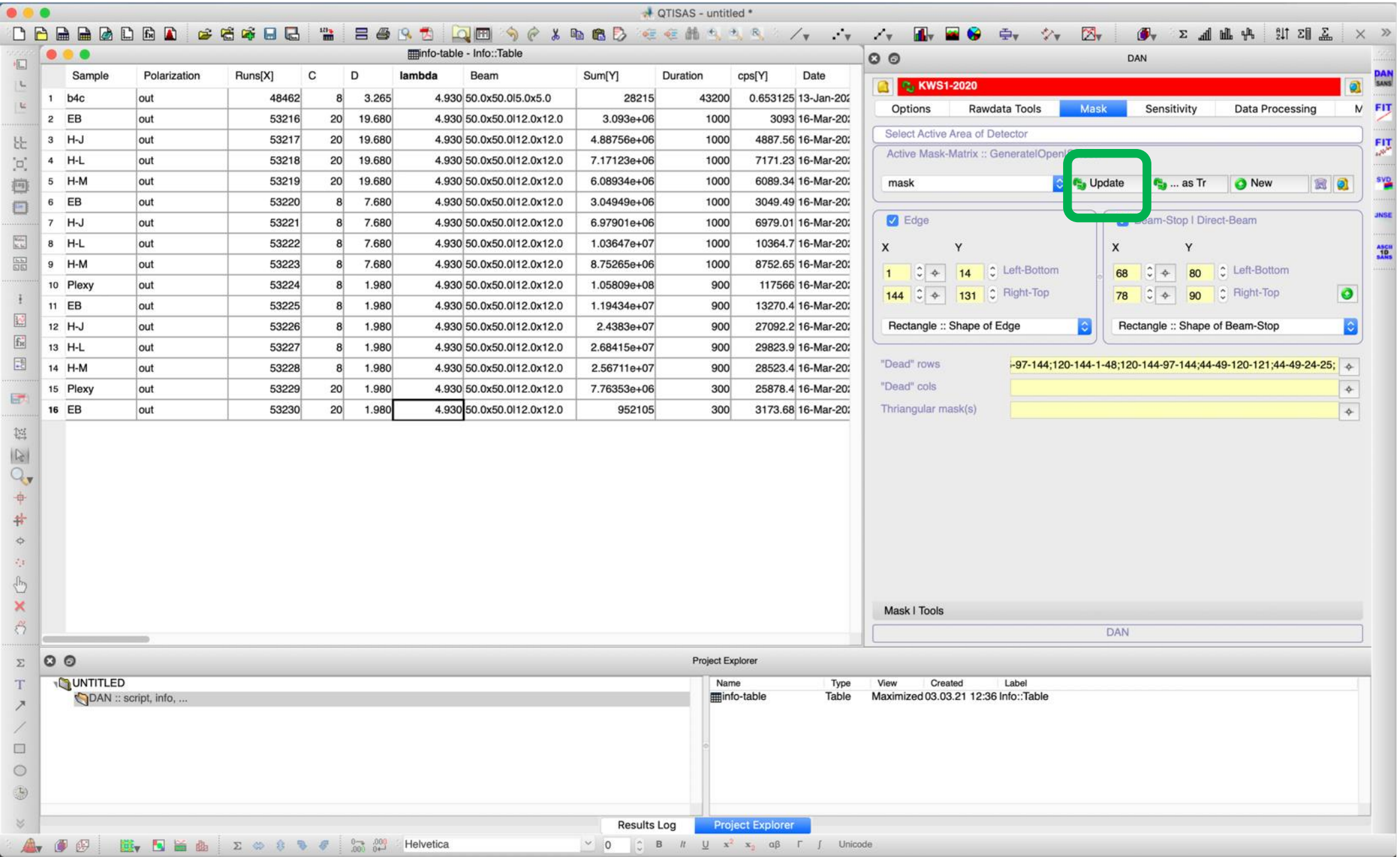
STEP 5: Standard Detector “Mask” Creation

Go to **MASK** tab



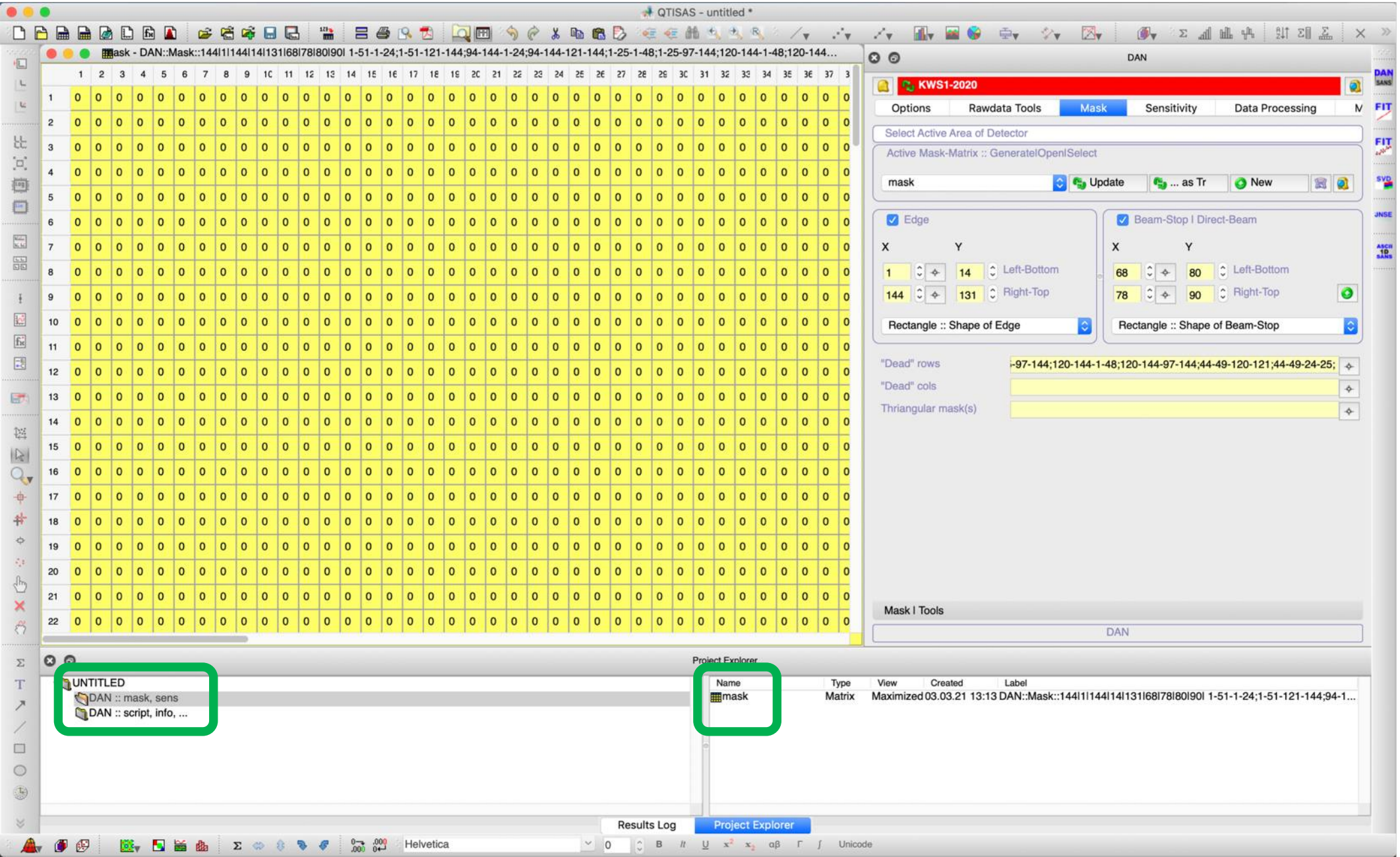
	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date
1	b4c	out	48462	8	3.265	4.930	50.0x50.0l5.0x5.0	28215	43200	0.653125	13-Jan-202
2	EB	out	53216	20	19.680	4.930	50.0x50.0l12.0x12.0	3.093e+06	1000	3093	16-Mar-202
3	H-J	out	53217	20	19.680	4.930	50.0x50.0l12.0x12.0	4.88756e+06	1000	4887.56	16-Mar-202
4	H-L	out	53218	20	19.680	4.930	50.0x50.0l12.0x12.0	7.17123e+06	1000	7171.23	16-Mar-202
5	H-M	out	53219	20	19.680	4.930	50.0x50.0l12.0x12.0	6.08934e+06	1000	6089.34	16-Mar-202
6	EB	out	53220	8	7.680	4.930	50.0x50.0l12.0x12.0	3.04949e+06	1000	3049.49	16-Mar-202
7	H-J	out	53221	8	7.680	4.930	50.0x50.0l12.0x12.0	6.97901e+06	1000	6979.01	16-Mar-202
8	H-L	out	53222	8	7.680	4.930	50.0x50.0l12.0x12.0	1.03647e+07	1000	10364.7	16-Mar-202
9	H-M	out	53223	8	7.680	4.930	50.0x50.0l12.0x12.0	8.75265e+06	1000	8752.65	16-Mar-202
10	Plexy	out	53224	8	1.980	4.930	50.0x50.0l12.0x12.0	1.05809e+08	900	117566	16-Mar-202
11	EB	out	53225	8	1.980	4.930	50.0x50.0l12.0x12.0	1.19434e+07	900	13270.4	16-Mar-202
12	H-J	out	53226	8	1.980	4.930	50.0x50.0l12.0x12.0	2.4383e+07	900	27092.2	16-Mar-202
13	H-L	out	53227	8	1.980	4.930	50.0x50.0l12.0x12.0	2.68415e+07	900	29823.9	16-Mar-202
14	H-M	out	53228	8	1.980	4.930	50.0x50.0l12.0x12.0	2.56711e+07	900	28523.4	16-Mar-202
15	Plexy	out	53229	20	1.980	4.930	50.0x50.0l12.0x12.0	7.76353e+06	300	25878.4	16-Mar-202
16	EB	out	53230	20	1.980	4.930	50.0x50.0l12.0x12.0	952105	300	3173.68	16-Mar-202

Push button **“Update”:** matrix “mask” will be created (updated)

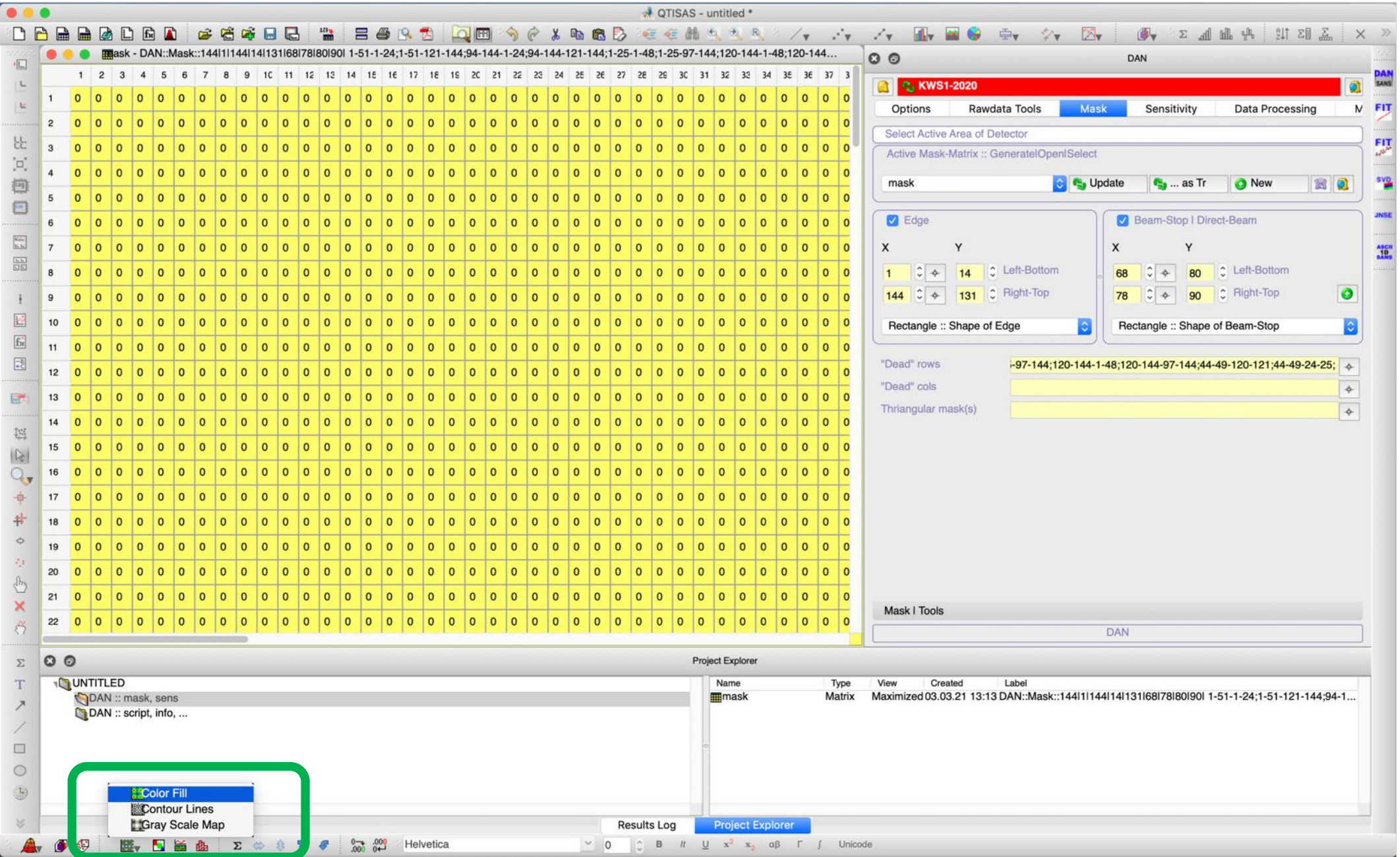


	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date
1	b4c	out	48462	8	3.265	4.930	50.0x50.0l5.0x5.0	28215	43200	0.653125	13-Jan-202
2	EB	out	53216	20	19.680	4.930	50.0x50.0l12.0x12.0	3.093e+06	1000	3093	16-Mar-202
3	H-J	out	53217	20	19.680	4.930	50.0x50.0l12.0x12.0	4.88756e+06	1000	4887.56	16-Mar-202
4	H-L	out	53218	20	19.680	4.930	50.0x50.0l12.0x12.0	7.17123e+06	1000	7171.23	16-Mar-202
5	H-M	out	53219	20	19.680	4.930	50.0x50.0l12.0x12.0	6.08934e+06	1000	6089.34	16-Mar-202
6	EB	out	53220	8	7.680	4.930	50.0x50.0l12.0x12.0	3.04949e+06	1000	3049.49	16-Mar-202
7	H-J	out	53221	8	7.680	4.930	50.0x50.0l12.0x12.0	6.97901e+06	1000	6979.01	16-Mar-202
8	H-L	out	53222	8	7.680	4.930	50.0x50.0l12.0x12.0	1.03647e+07	1000	10364.7	16-Mar-202
9	H-M	out	53223	8	7.680	4.930	50.0x50.0l12.0x12.0	8.75265e+06	1000	8752.65	16-Mar-202
10	Plexy	out	53224	8	1.980	4.930	50.0x50.0l12.0x12.0	1.05809e+08	900	117566	16-Mar-202
11	EB	out	53225	8	1.980	4.930	50.0x50.0l12.0x12.0	1.19434e+07	900	13270.4	16-Mar-202
12	H-J	out	53226	8	1.980	4.930	50.0x50.0l12.0x12.0	2.4383e+07	900	27092.2	16-Mar-202
13	H-L	out	53227	8	1.980	4.930	50.0x50.0l12.0x12.0	2.68415e+07	900	29823.9	16-Mar-202
14	H-M	out	53228	8	1.980	4.930	50.0x50.0l12.0x12.0	2.56711e+07	900	28523.4	16-Mar-202
15	Plexy	out	53229	20	1.980	4.930	50.0x50.0l12.0x12.0	7.76353e+06	300	25878.4	16-Mar-202
16	EB	out	53230	20	1.980	4.930	50.0x50.0l12.0x12.0	952105	300	3173.68	16-Mar-202

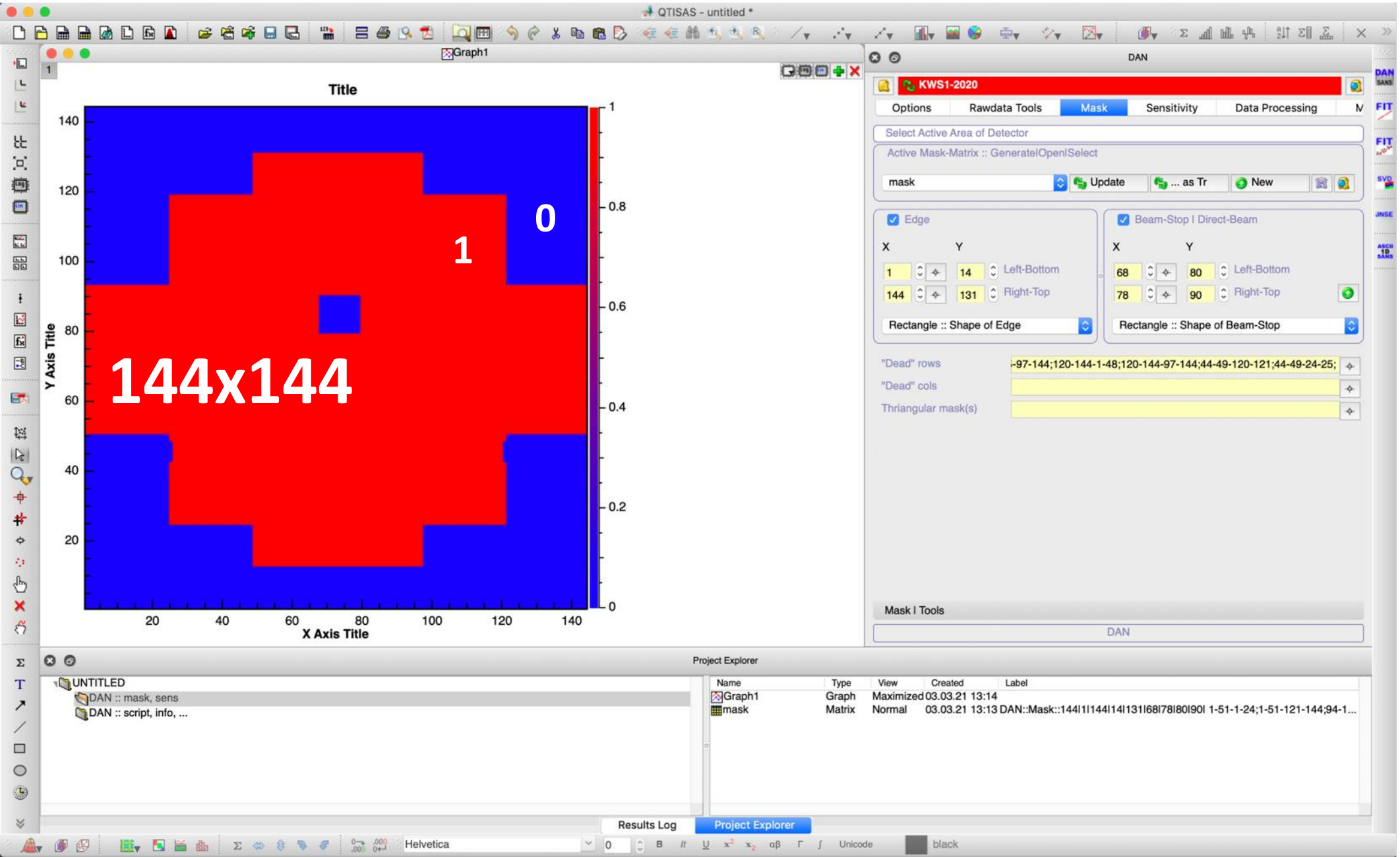
“mask” matrix is created in “DAN:: mask, sens” folder



Plotting Example: “Color Fill”



Plotting Example: “Color Fill”

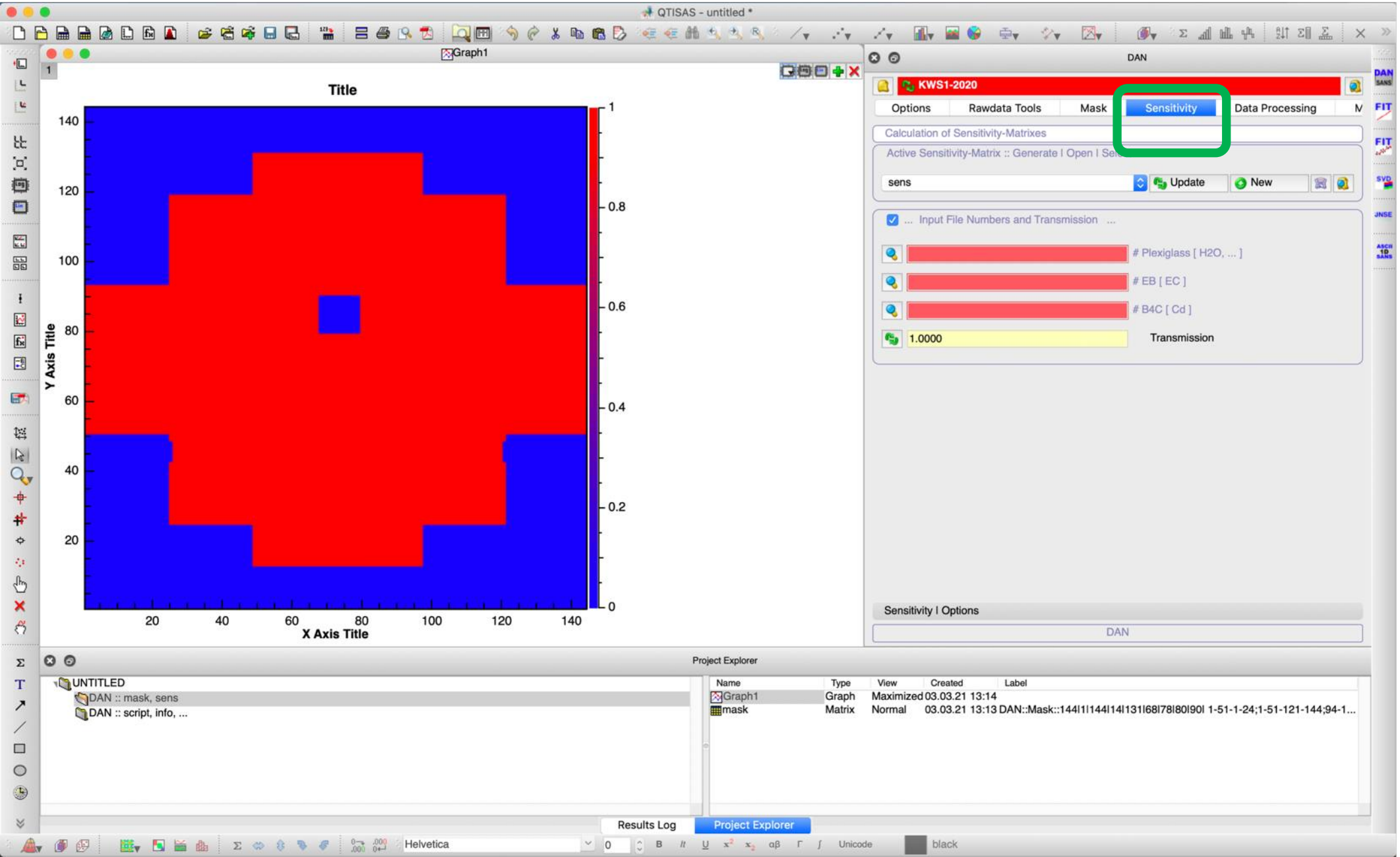


STEP 6: Detector Sensitivity (“Sens”) Reading

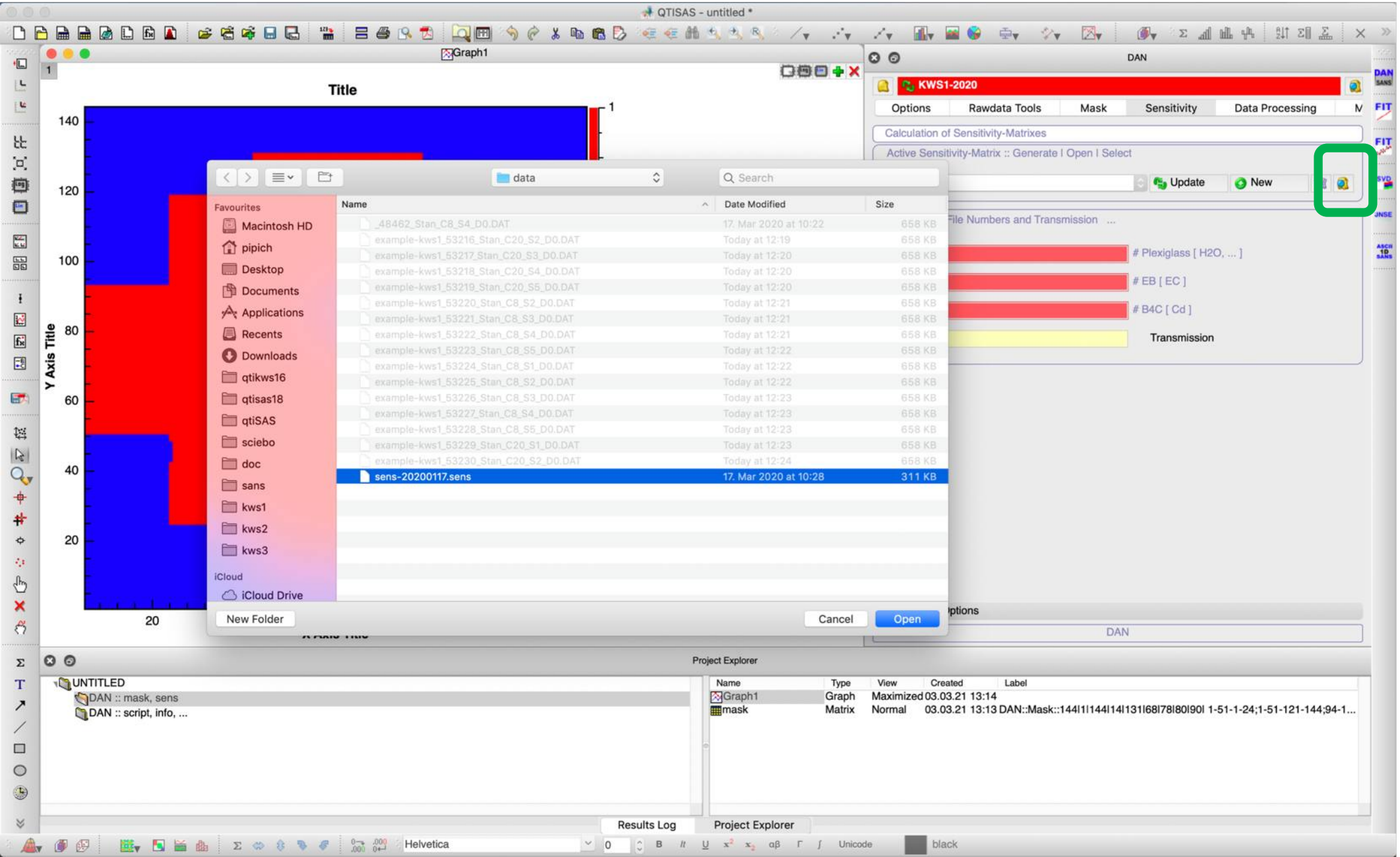
KWS-1 case: ask Local Contact to provide ***.sens** file

In this example we use: **sens-20200117.sens**

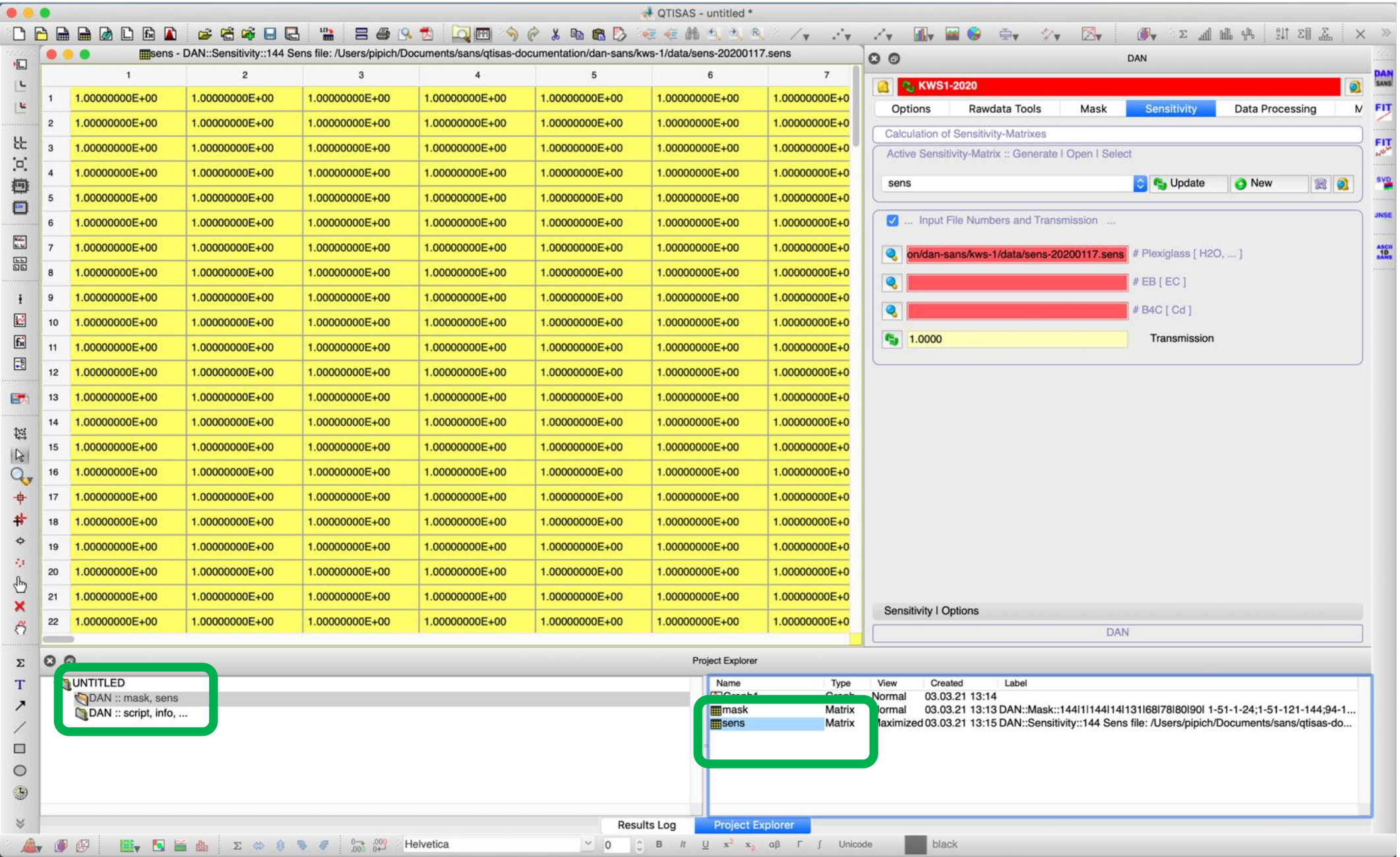
Go to **Sensitivity** tab

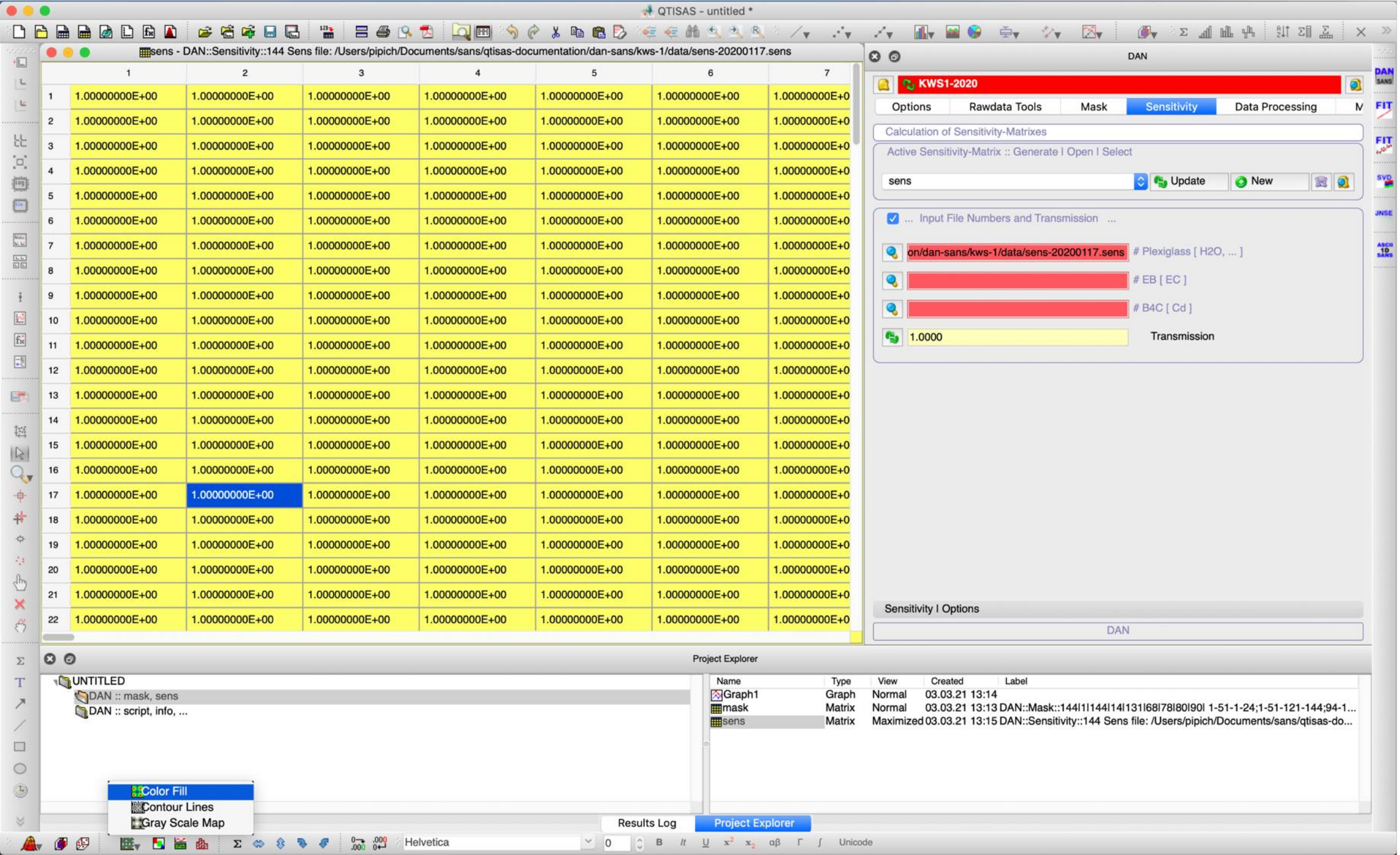


Push (open) button and select ***.sens** file

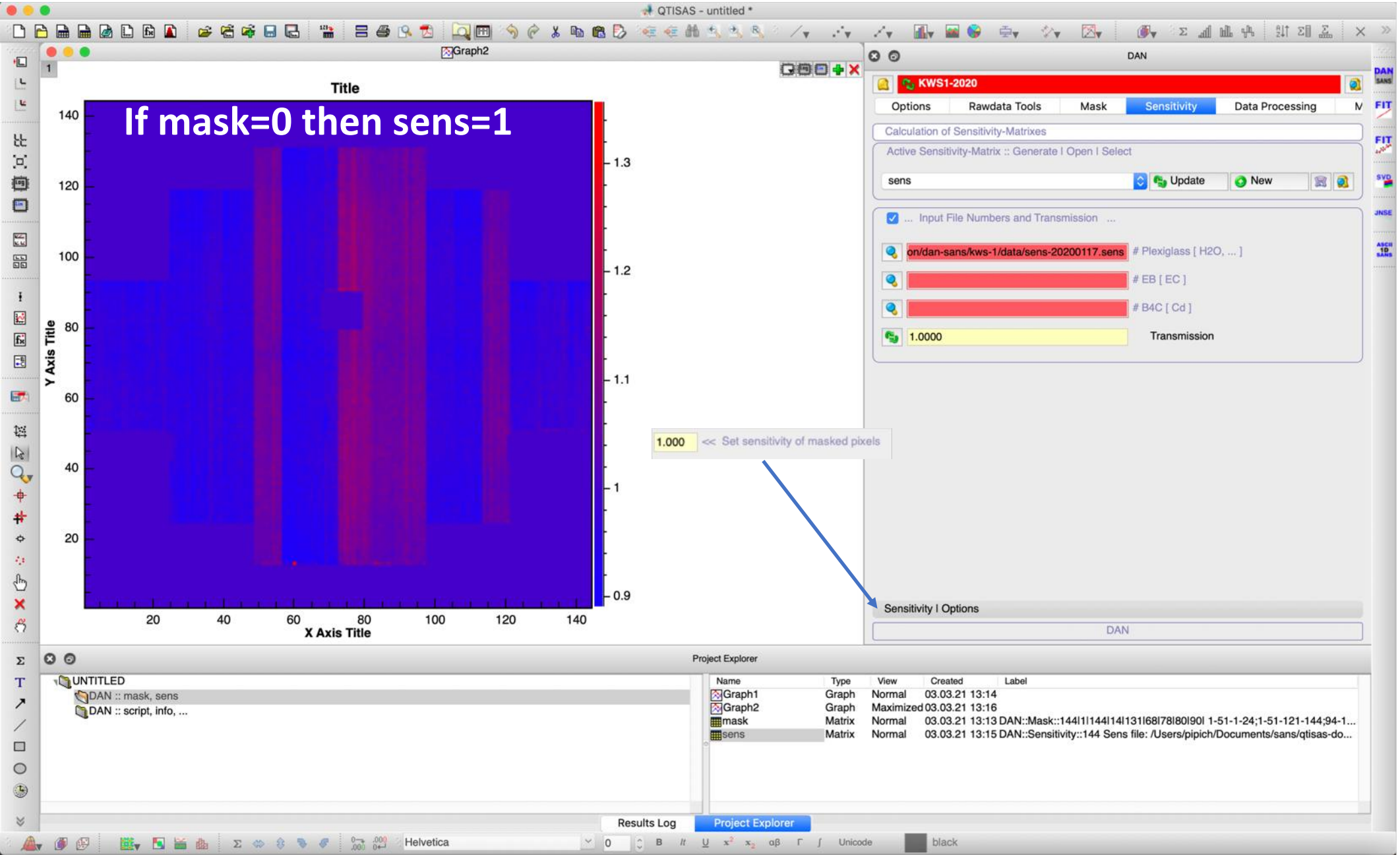


“sens” matrix is created in “DAN:: mask, sens” folder



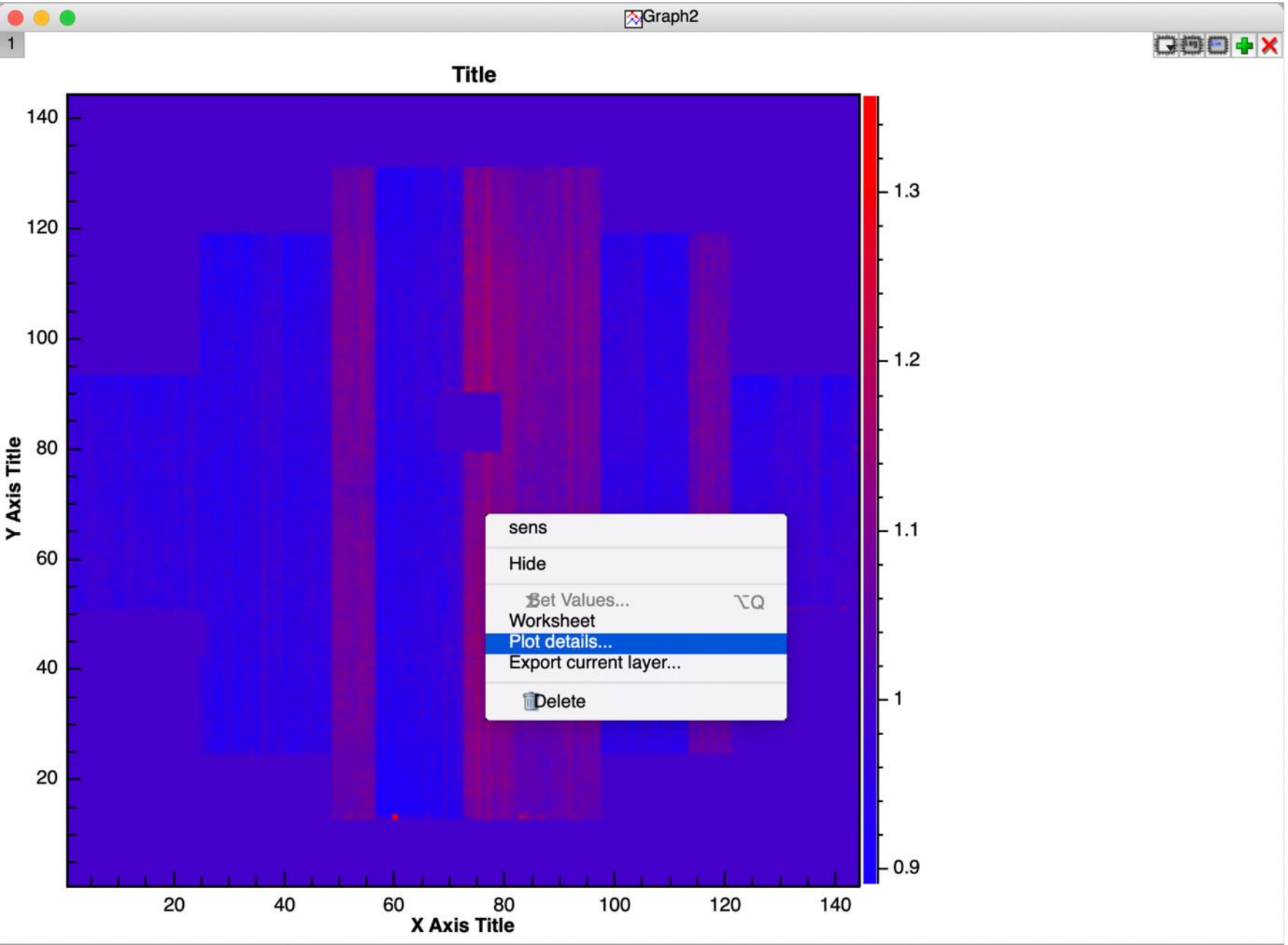

QTISAS - untitled *
sens - DAN::Sensitivity::144 Sens file: /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-1/data/sens-20200117.sens
1.00000000E+00
DAN
KWS1-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Calculation of Sensitivity-Matrixes
Active Sensitivity-Matrix :: Generate I Open I Select
sens
Update
New
... Input File Numbers and Transmission ...
on/dan-sans/kws-1/data/sens-20200117.sens
Plexiglass [H2O, ...]
EB [EC]
B4C [Cd]
1.0000
Transmission
Sensitivity I Options
DAN
Project Explorer
UNTITLED
DAN :: mask, sens
DAN :: script, info, ...
Name
Type
View
Created
Label
Graph1
Graph
Normal
03.03.21 13:14
mask
Matrix
Normal
03.03.21 13:13 DAN::Mask::144I1I144I14I131I68I78I80I90I 1-51-1-24;1-51-121-144;94-1...
sens
Matrix
Maximized
03.03.21 13:15 DAN::Sensitivity::144 Sens file: /Users/pipich/Documents/sans/qtisas-do...
Color Fill
Contour Lines
Gray Scale Map
Results Log
Project Explorer
Helvetica
Unicode

Plotting Example of “sens” matrix: “Color Fill”

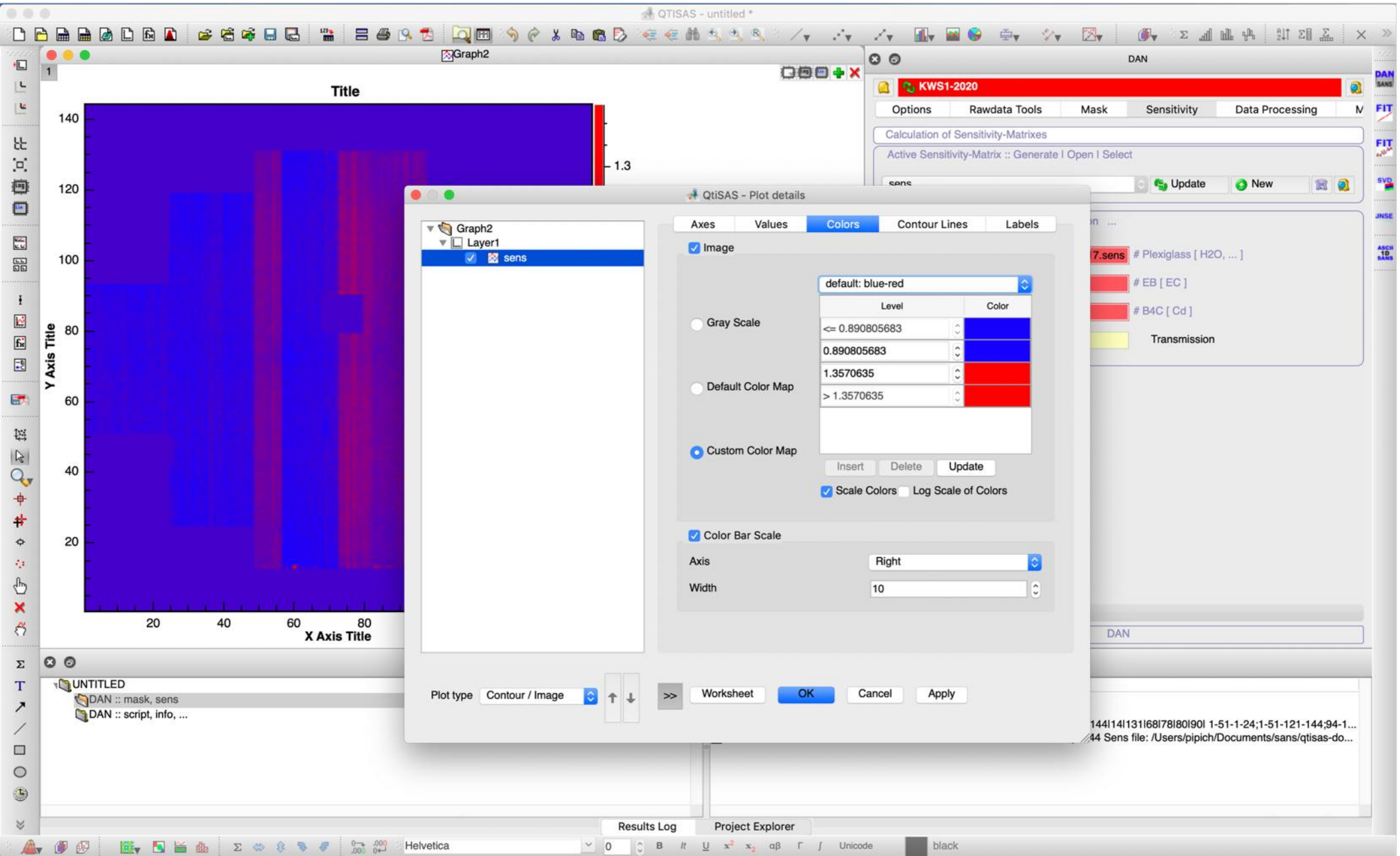


STEP 6a (optional): Change of the Color Map

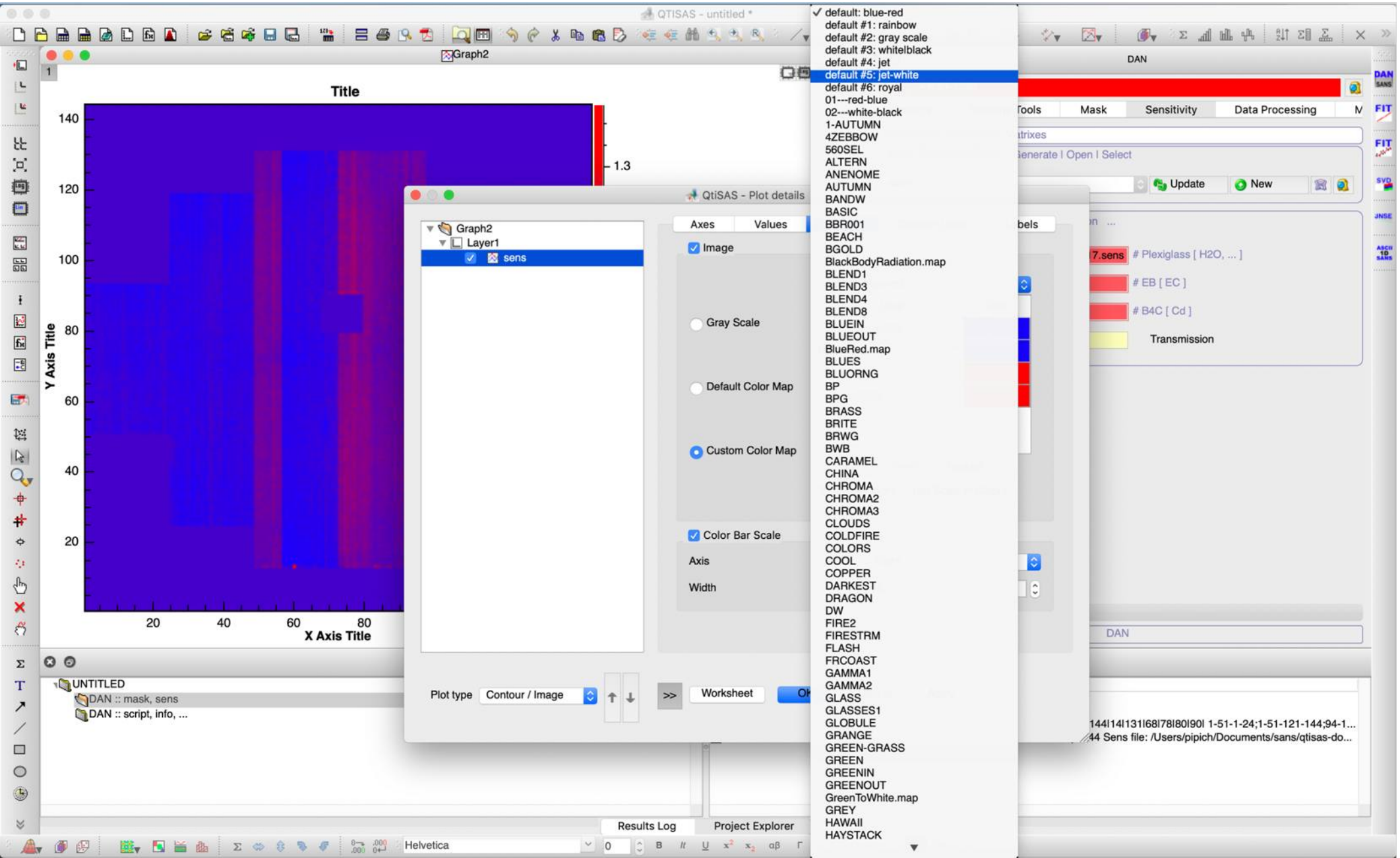
Select “Plot details…”



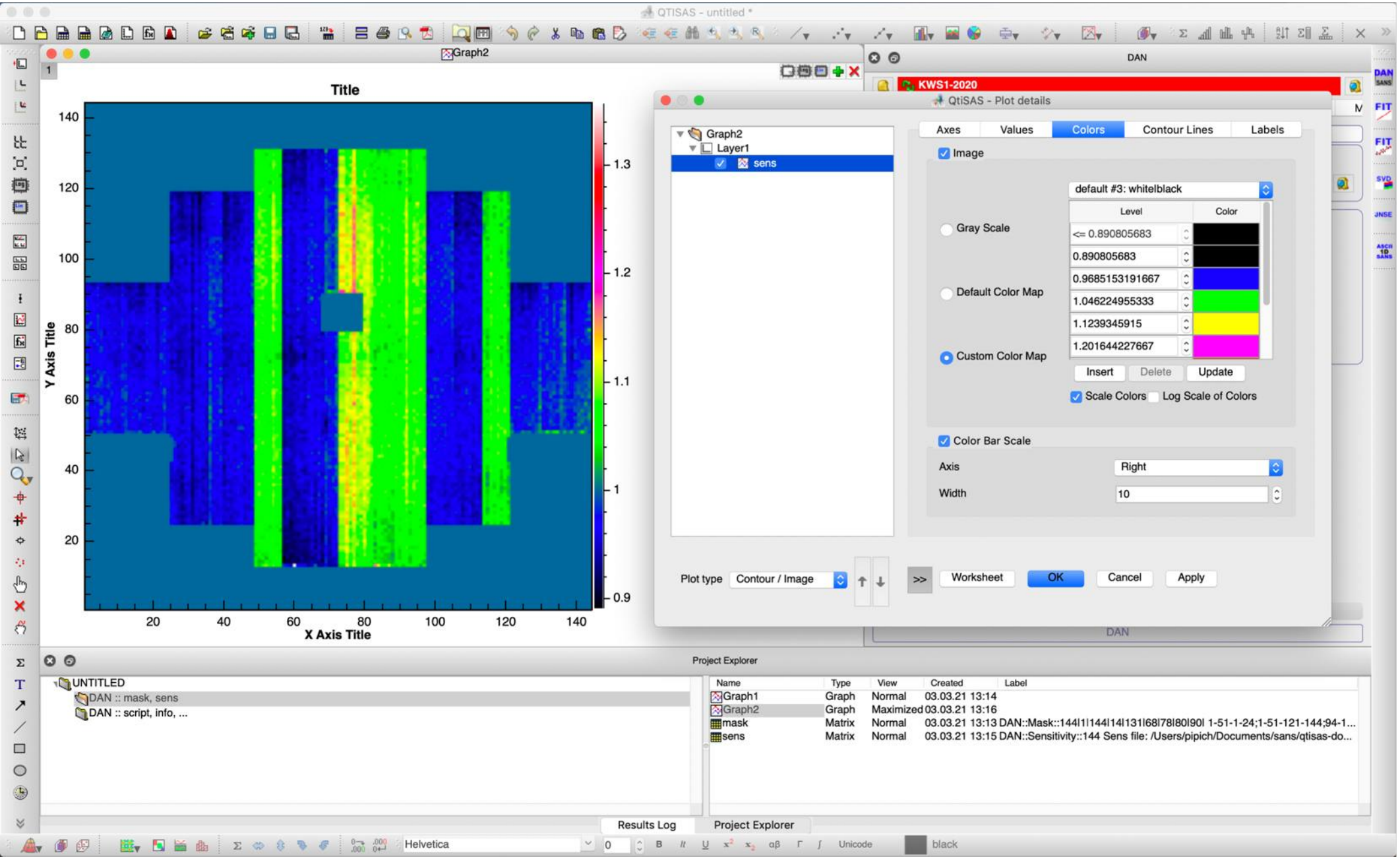
Select “Colors” tab



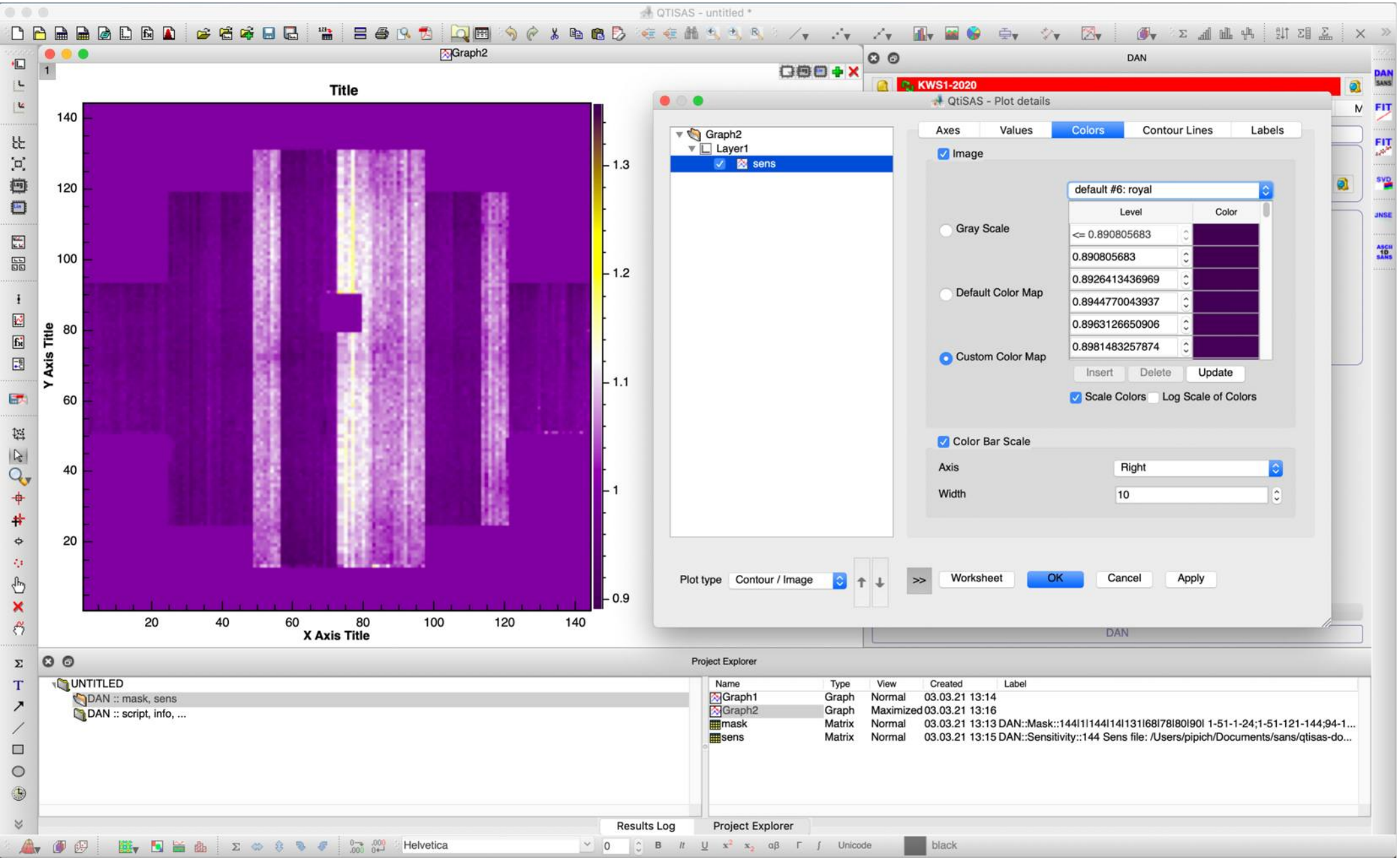
Select “Color Map”



Example: selected “default #3: whiteblack”



Example: selected “default #8: royal”

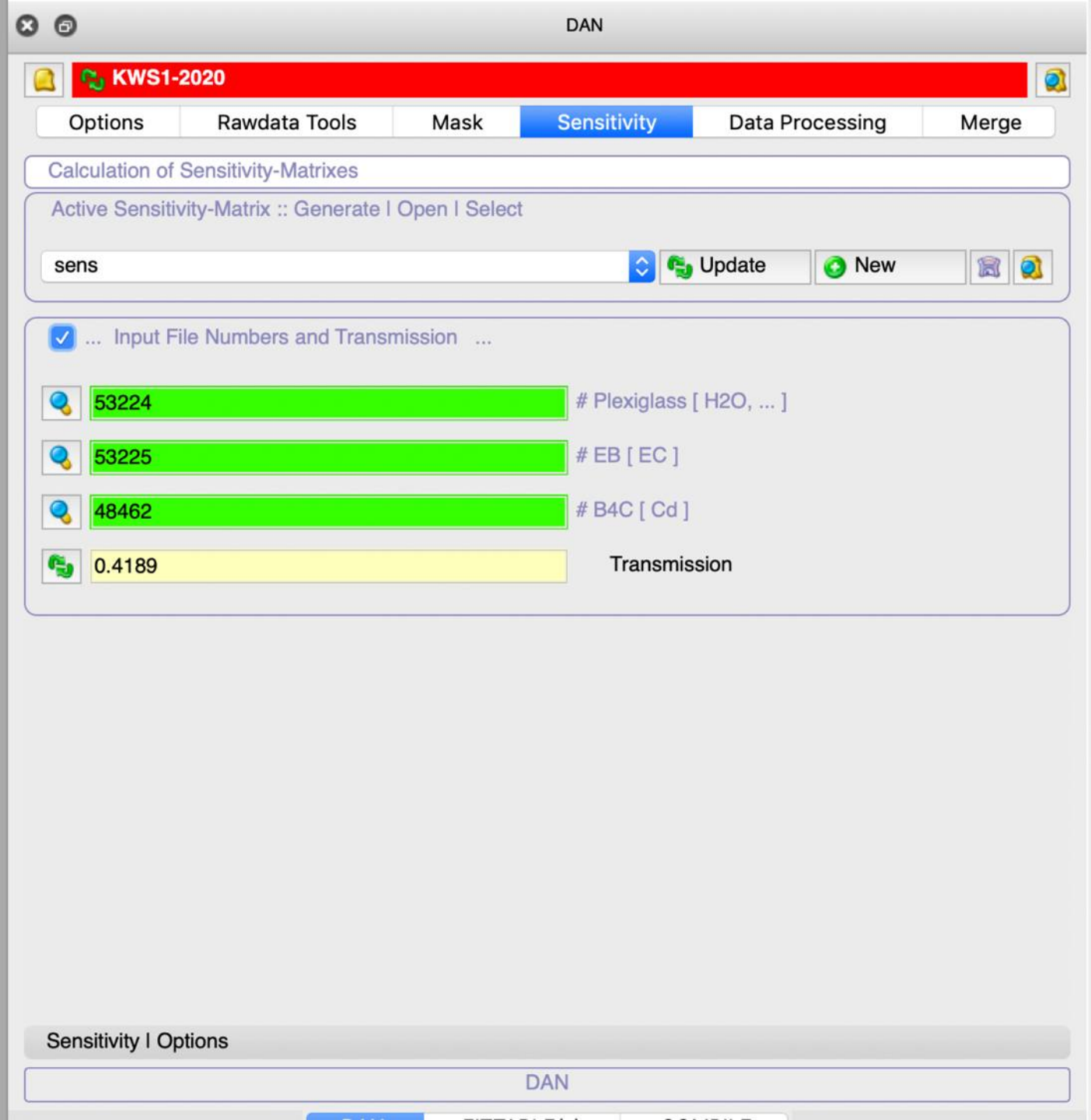


STEP 6b (alternative): Alternative Detector Sensitivity Calculation

Other way to calculate sensitivity:
we could use a Plexiglass (Water) run with good statistics (>20000000 counts).

10	Plexy	out	53224	8	1.980	4.930	50.0x50.0l12.0x12.0	1.05809e+08	900	117566
11	EB	out	53225	8	1.980	4.930	50.0x50.0l12.0x12.0	1.19434e+07	900	13270.4

1	b4c	out	48462	8	3.265	4.930	50.0x50.0l5.0x5.0	28215	43200	0.653125



1. Push & Select “Plexiglass” run

2. Push & Select “Empty Beam” run

3. Push & Select “Dark Current” run

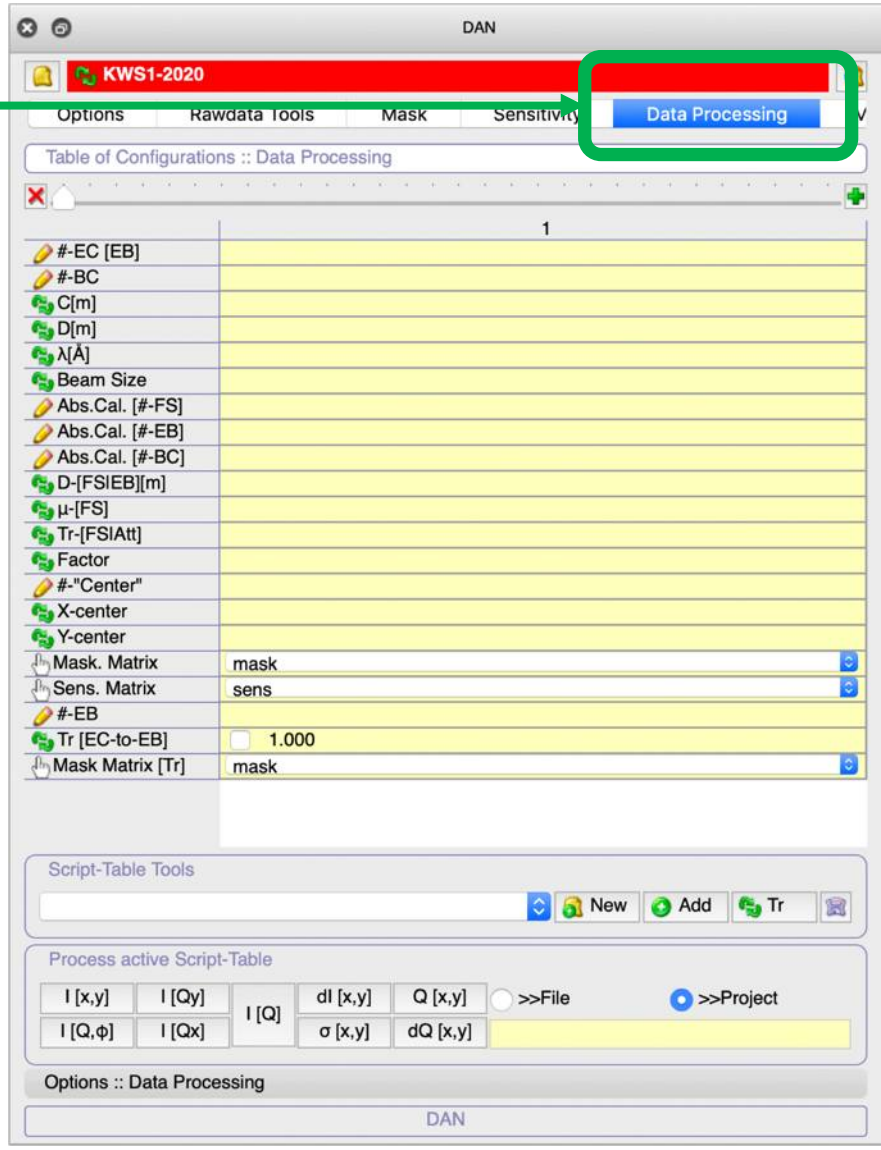
4. Push to calculate transmission

5. Push to calculate sensitivity

This is “Alternative Detector Sensitivity Calculation”
In this example we use **STEP 6** method

STEP 7: Filling ”Table of Configurations”

DAN-SANS: go to next tab “Data Processing”



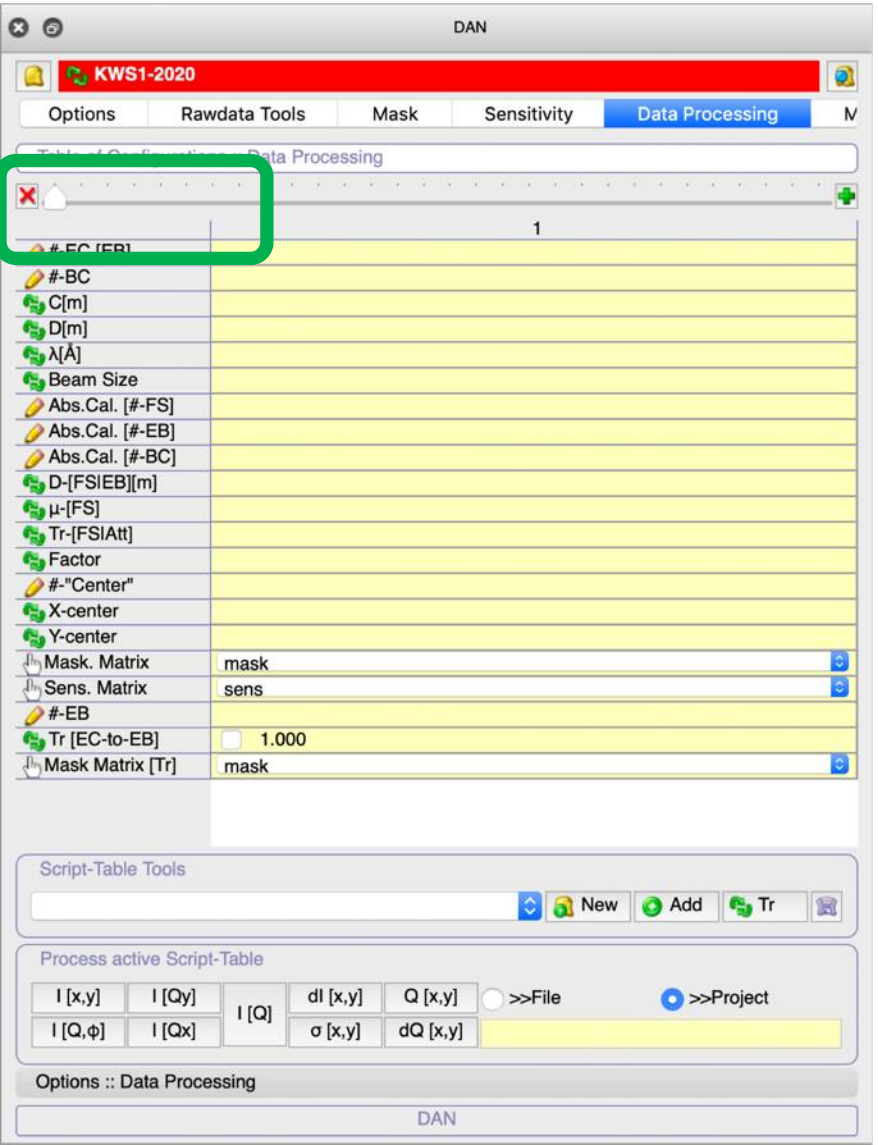
Icons meaning:

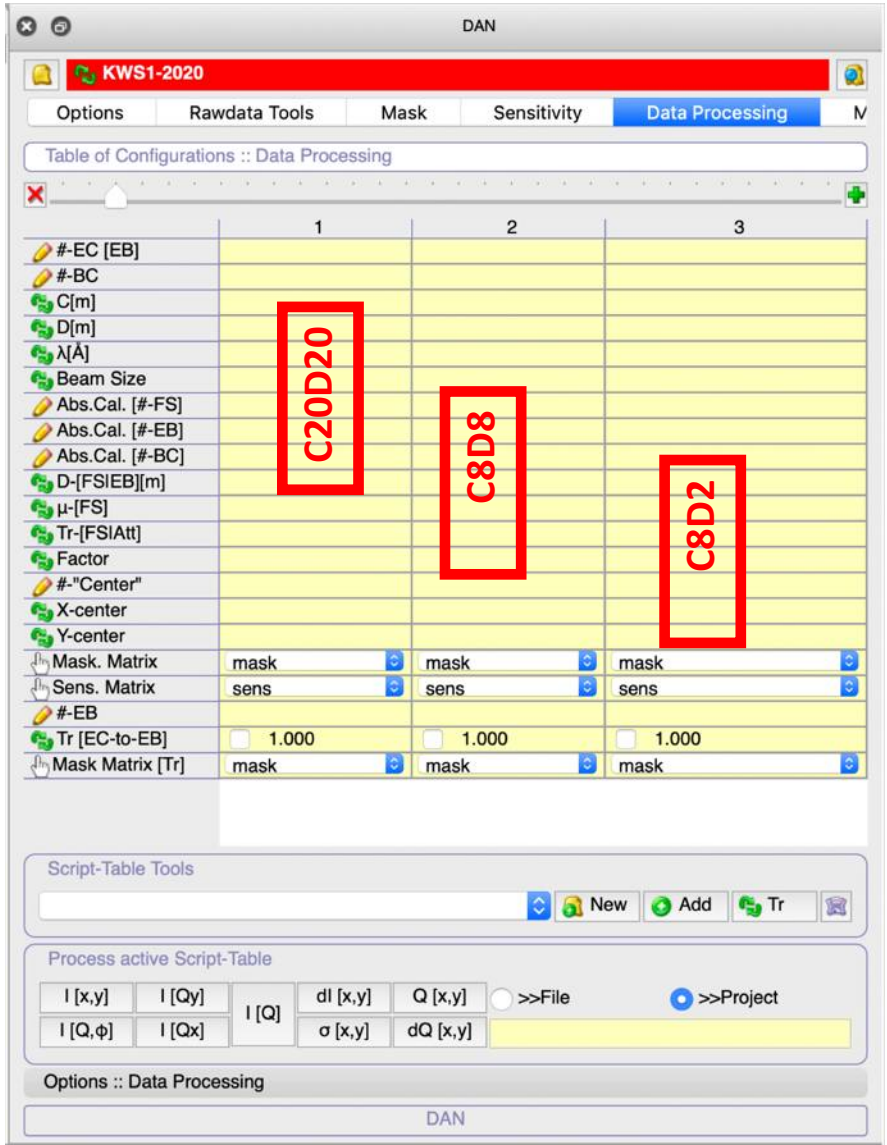
Select from list

Input something (type or double click to select)

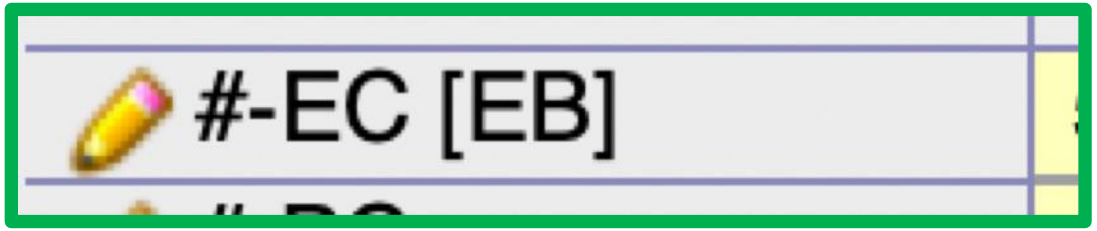
Calculate/read

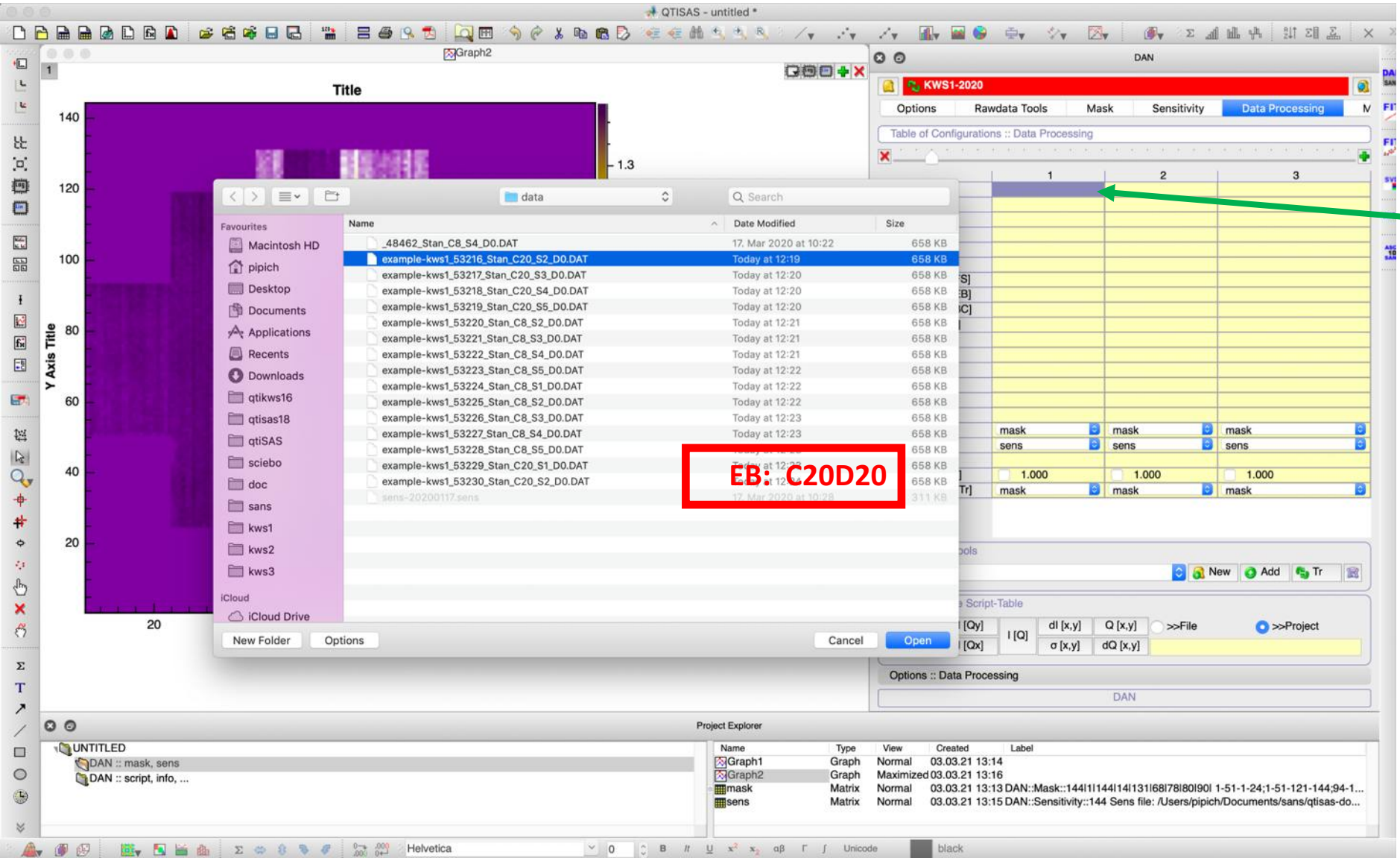
Set Number of Instrument Configuration: in this example 3





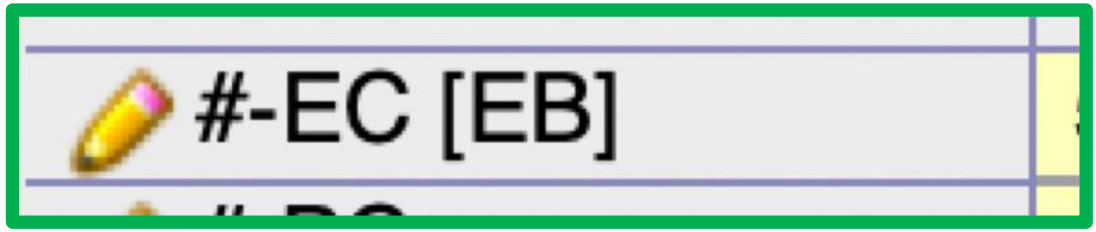
Empty Beam/Cell Runs





Double Click

Fill: Empty Beam/Cell Runs



DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | M

Table of Configurations :: Data Processing

	cond.-#1	2	3
#-EC [EB]	53216		
#-BC			
C[m]	20		
D[m]	19.680		
λ[Å]	4.930		
Beam Size	50x50|12x12		
Abs.Cal. [#-FS]			
Abs.Cal. [#-EB]			
Abs.Cal. [#-BC]			
D-[FS|EB][m]			
μ-[FS]			
Tr-[FS|Att]			
Factor			
#-"Center"			
X-center			
Y-center			
Mask. Matrix	mask	mask	mask
Sens. Matrix	sens	sens	sens
#-EB			
Tr [EC-to-EB]	1.000	1.000	1.000
Mask Matrix [Tr]	mask	mask	mask

EB: C20D20

Script-Table Tools

New | Add | Tr

Process active Script-Table

I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

I [Q,ϕ] | I [Qx] | | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | M

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2	3
#-EC [EB]	53216	53220	
#-BC			
C[m]	20	8	
D[m]	19.680	7.680	
λ[Å]	4.930	4.930	
Beam Size	50x50|12x12	50x50|12x12	
Abs.Cal. [#-FS]			
Abs.Cal. [#-EB]			
Abs.Cal. [#-BC]			
D-[FS|EB][m]			
μ-[FS]			
Tr-[FS|Att]			
Factor			
#-"Center"			
X-center			
Y-center			
Mask. Matrix	mask	mask	mask
Sens. Matrix	sens	sens	sens
#-EB			
Tr [EC-to-EB]	1.000	1.000	1.000
Mask Matrix [Tr]	mask	mask	mask

EB: C8D8

Script-Table Tools

New | Add | Tr

Process active Script-Table

I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

I [Q,ϕ] | I [Qx] | | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | M

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2	cond.-#3
#-EC [EB]	53216	53220	53225
#-BC			
C[m]	20	8	8
D[m]	19.680	7.680	1.980
λ[Å]	4.930	4.930	4.930
Beam Size	50x50|12x12	50x50|12x12	50x50|12x12
Abs.Cal. [#-FS]			
Abs.Cal. [#-EB]			
Abs.Cal. [#-BC]			
D-[FS|EB][m]			
μ-[FS]			
Tr-[FS|Att]			
Factor			
#-"Center"			
X-center			
Y-center			
Mask. Matrix	mask	mask	mask
Sens. Matrix	sens	sens	sens
#-EB			
Tr [EC-to-EB]	1.000	1.000	1.000
Mask Matrix [Tr]	mask	mask	mask

EB: C8D2

Script-Table Tools

New | Add | Tr

Process active Script-Table

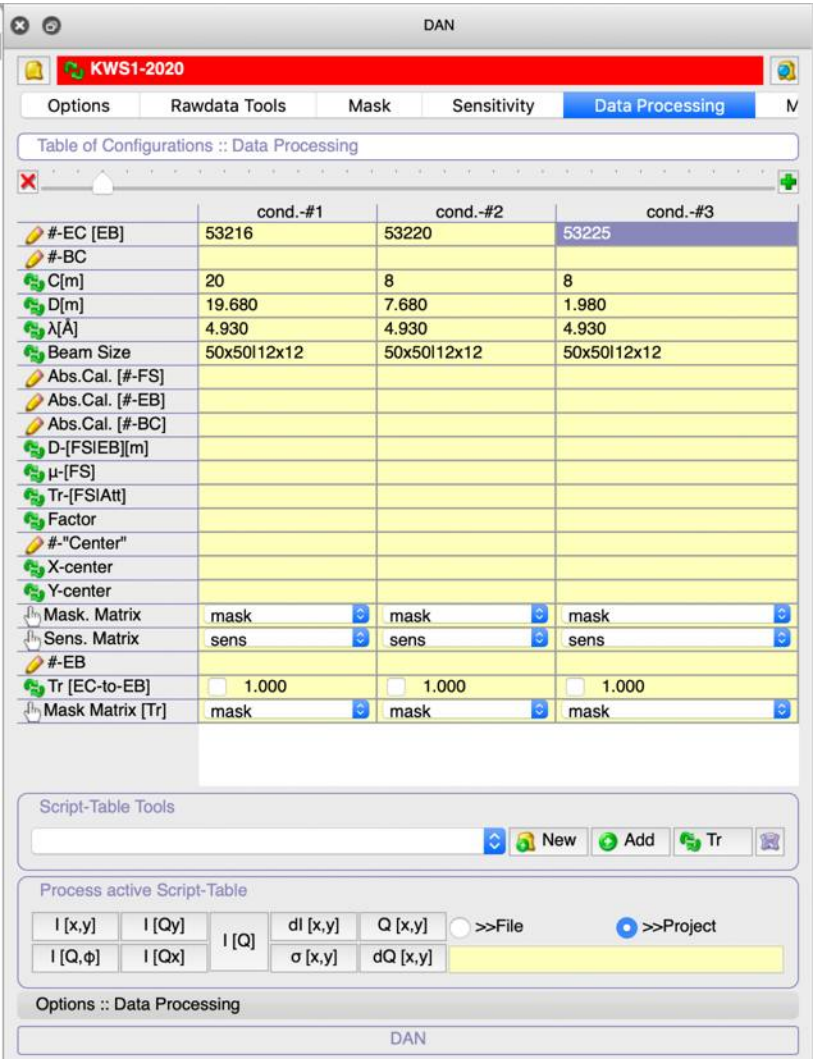
I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

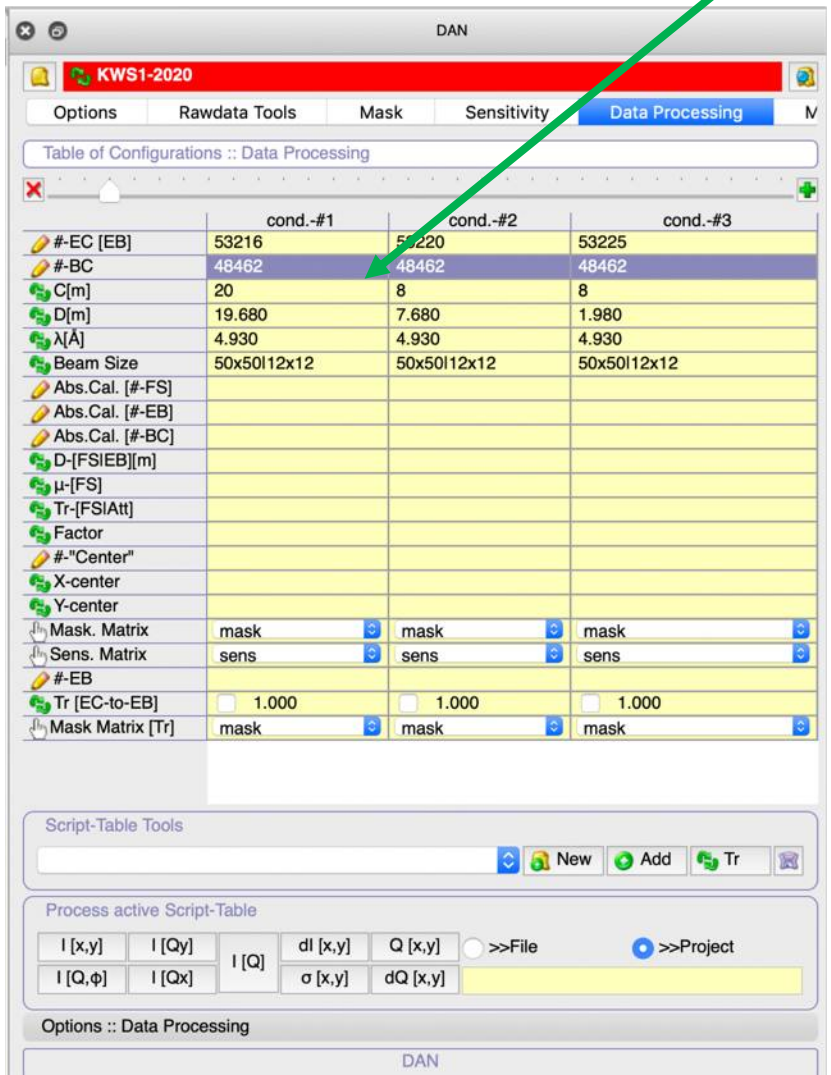
I [Q,ϕ] | I [Qx] | | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

Fill: Detector Dark Current Runs





Fill: Absolute Calibration Runs

Abs.Cal. [#-FS]
Abs.Cal. [#-EB]
Abs.Cal. [#-BC]

DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | M

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2	cond.-#3
#-EC [EB]	53216	53220	53225
#-BC	48462	48462	48462
C[m]	20	8	8
D[m]	19.680	7.680	1.980
λ[Å]	4.930	4.930	4.930
Beam Size	50x50l12x12	50x50l12x12	50x50l12x12
Abs.Cal. [#-FS]			
Abs.Cal. [#-EB]			
Abs.Cal. [#-BC]			
D-[FSlEB][m]			
μ-[FS]			
Tr-[FSlAtt]			
Factor			
#-"Center"			
X-center			
Y-center			
Mask. Matrix	mask	mask	mask
Sens. Matrix	sens	sens	sens
#-EB			
Tr [EC-to-EB]	1.000	1.000	1.000
Mask Matrix [Tr]	mask	mask	mask

Script-Table Tools

New | Add | Tr

Process active Script-Table

I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

I [Q,ϕ] | I [Qx] | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | M

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2	cond.-#3
#-EC [EB]	53216	53220	53225
#-BC	48462	48462	48462
C[m]	20	8	8
D[m]	19.680	7.680	1.980
λ[Å]	4.930	4.930	4.930
Beam Size	50x50l12x12	50x50l12x12	50x50l12x12
Abs.Cal. [#-FS]	53229	53224	53224
Abs.Cal. [#-EB]	53230	53225	53225
Abs.Cal. [#-BC]	48462	48462	48462
D-[FSlEB][m]			
μ-[FS]			
Tr-[FSlAtt]			
Factor			
#-"Center"			
X-center			
Y-center			
Mask. Matrix	mask	mask	mask
Sens. Matrix	sens	sens	sens
#-EB			
Tr [EC-to-EB]	1.000	1.000	1.000
Mask Matrix [Tr]	mask	mask	mask

Script-Table Tools

New | Add | Tr

Process active Script-Table

I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

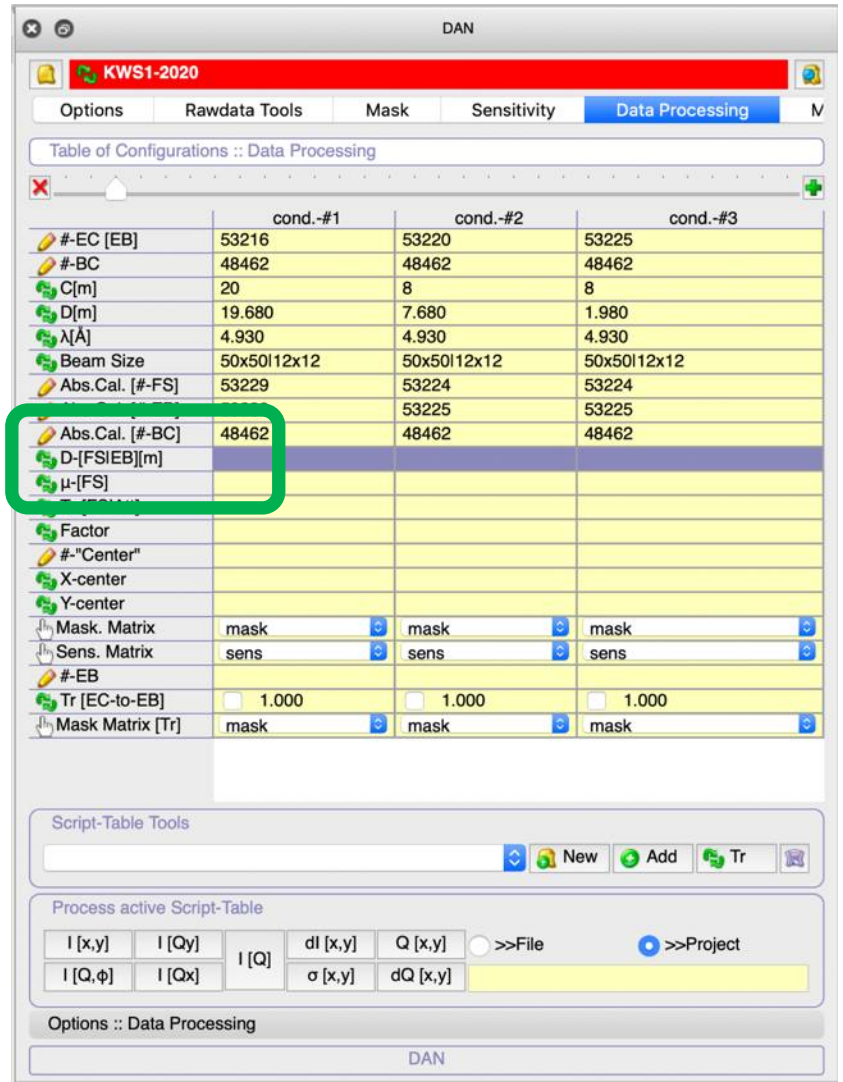
I [Q,ϕ] | I [Qx] | σ [x,y] | dQ [x,y]

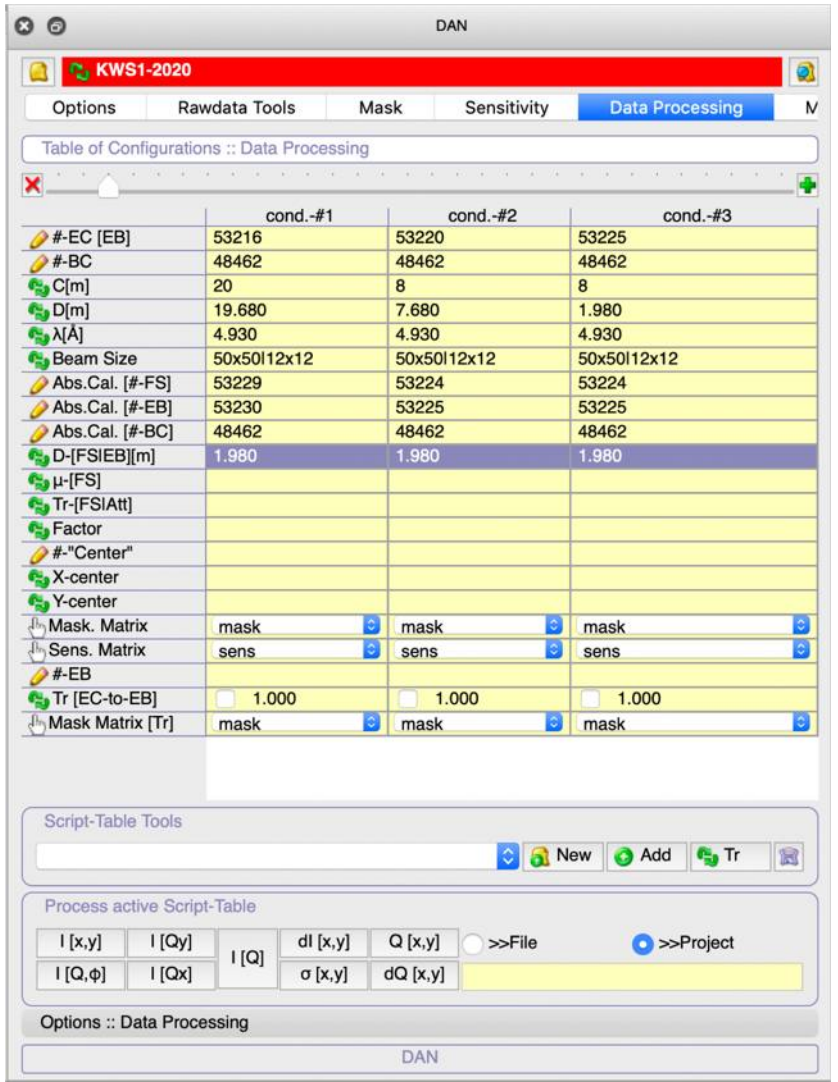
Options :: Data Processing

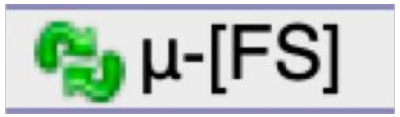
DAN

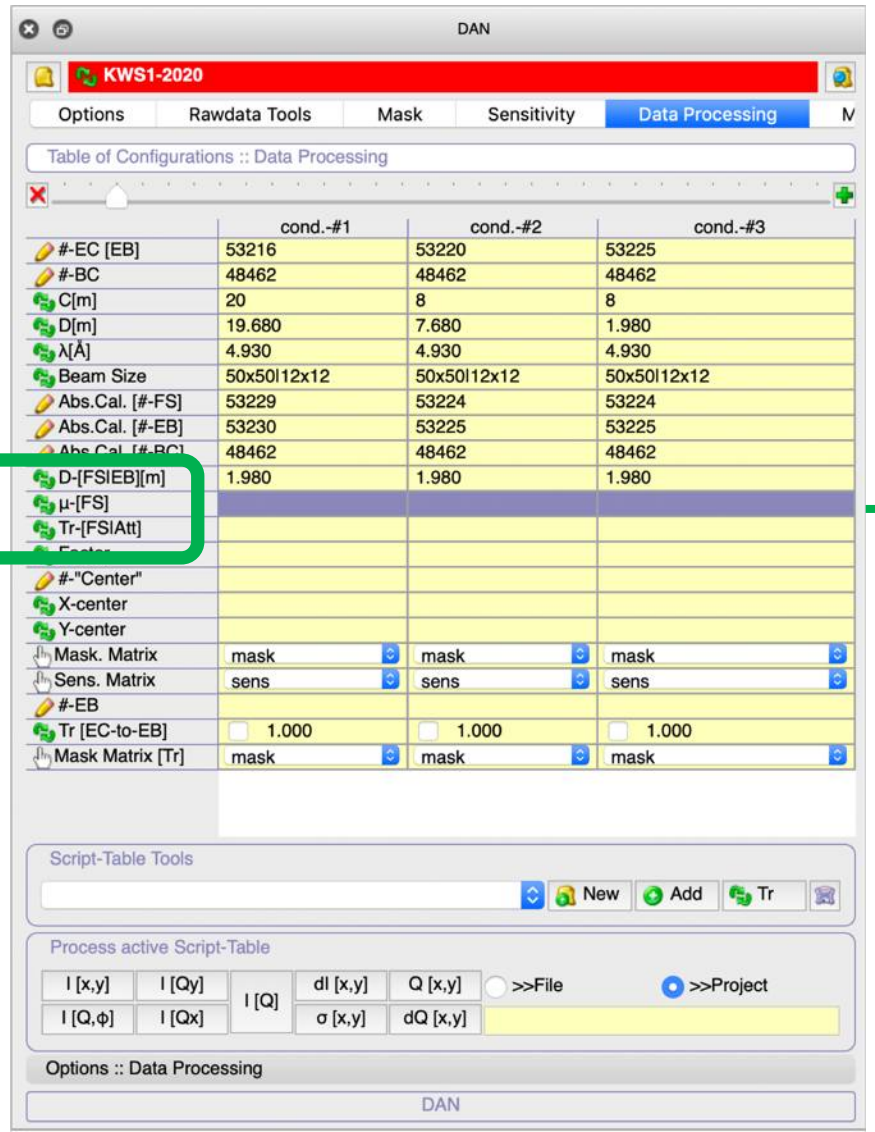
Push :

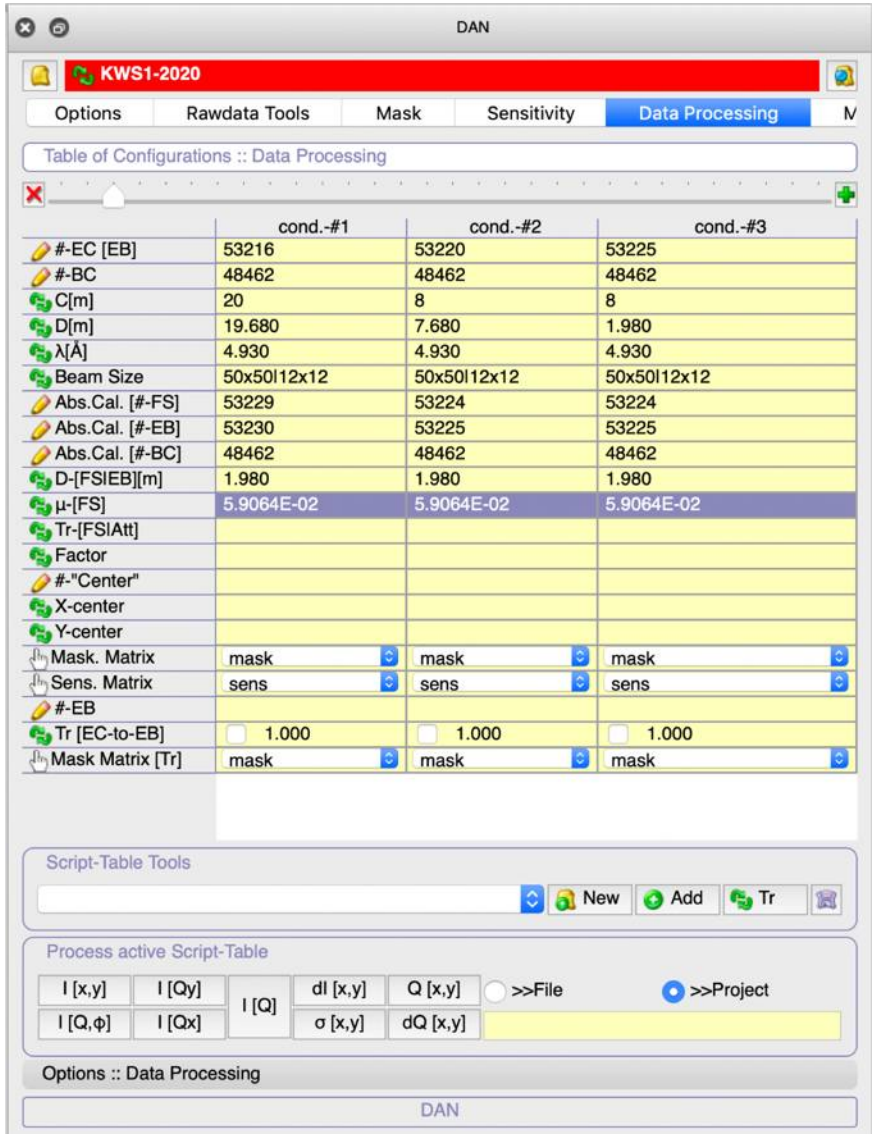
to read “Plexi” to Detector Distances from Headers





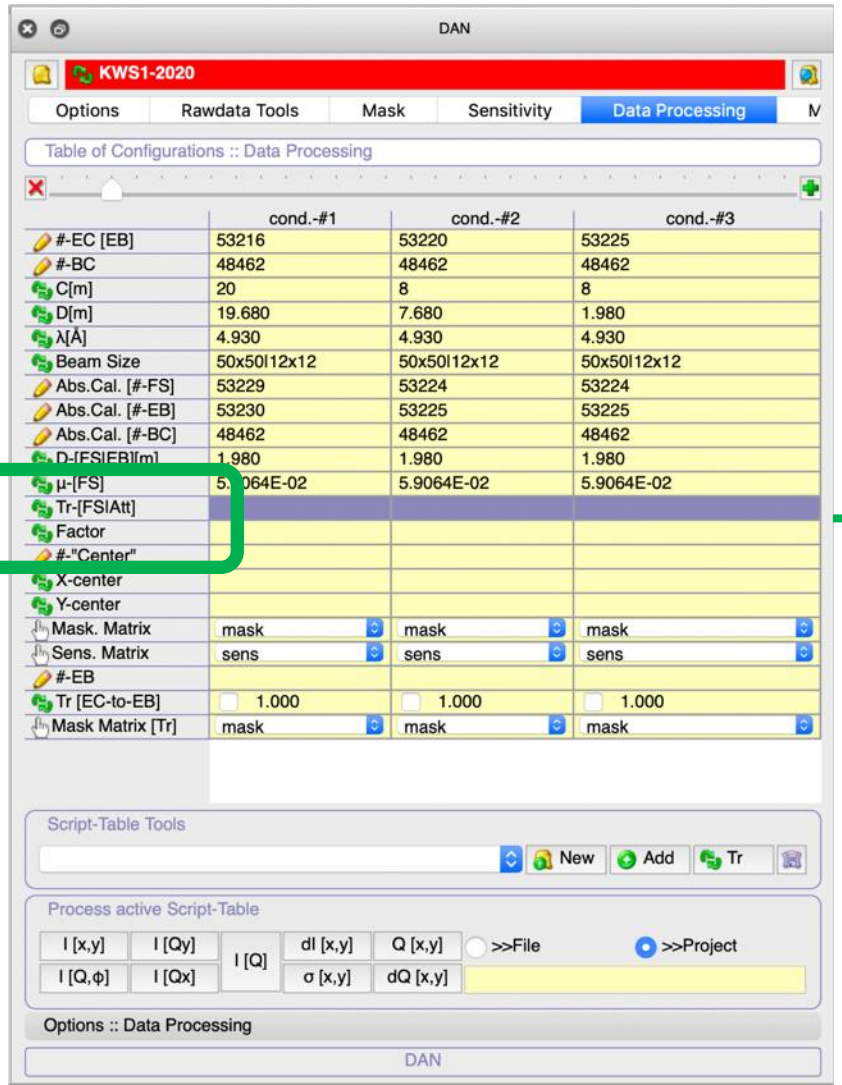
Push :  to calculate mu-factor of “Plexi” for every configuration

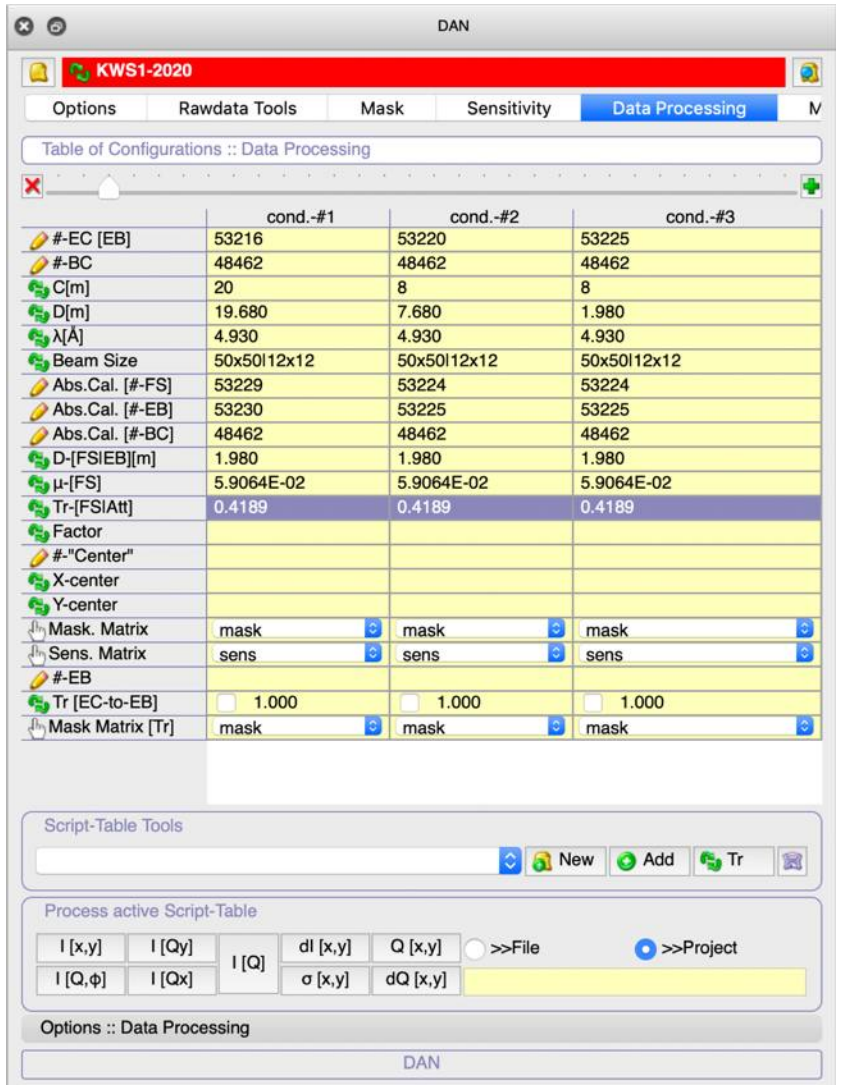




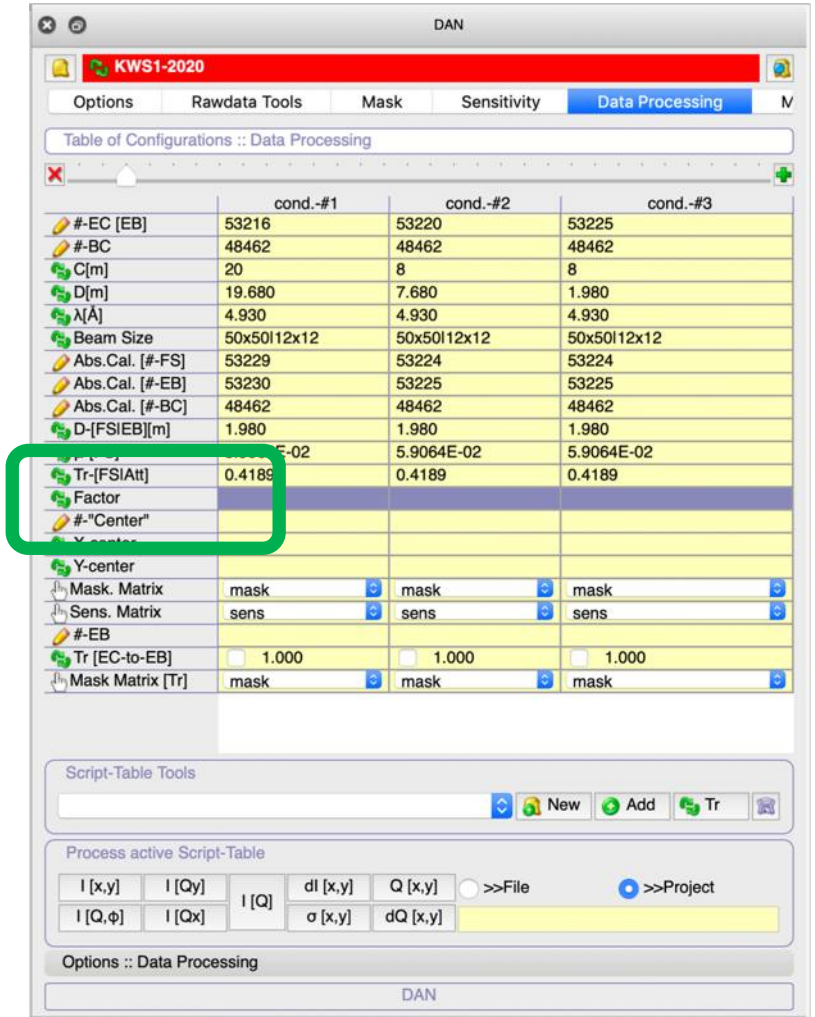
Push :

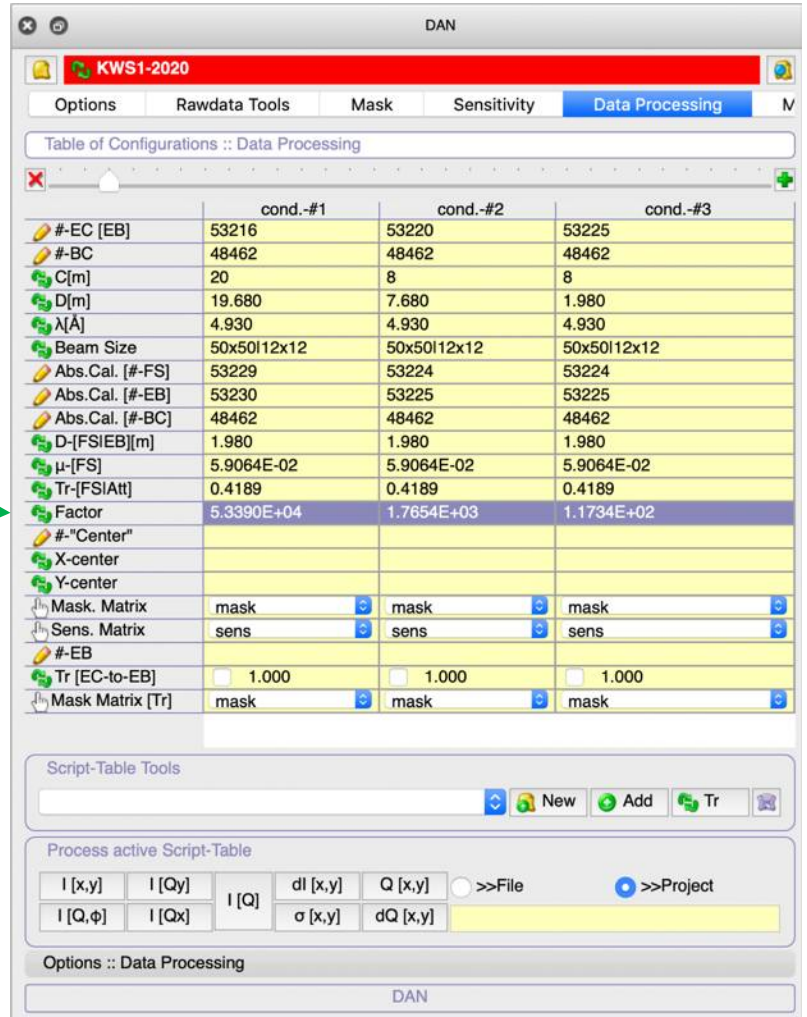
to read transmission of “Plexi” for every configuration

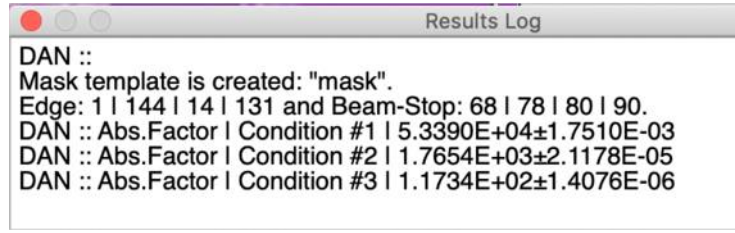




Push : Factor to calculate Absolute Factor for every configuration



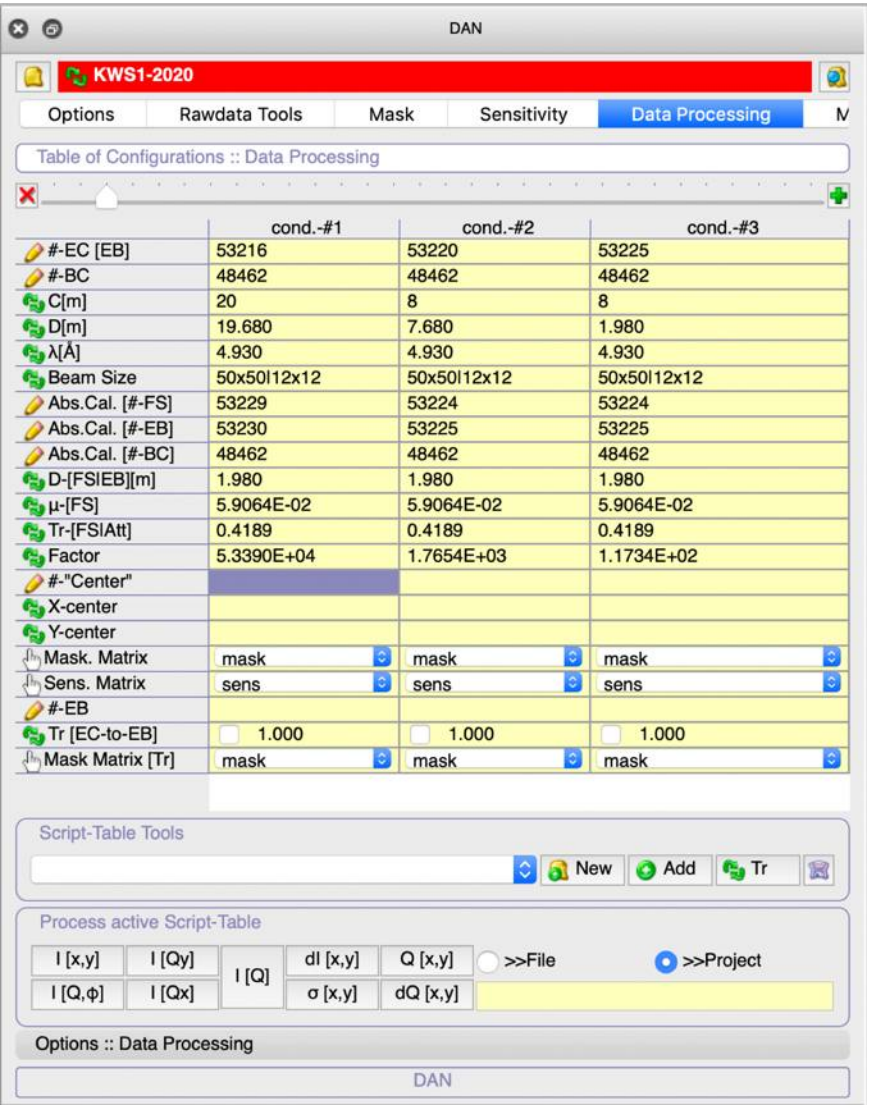


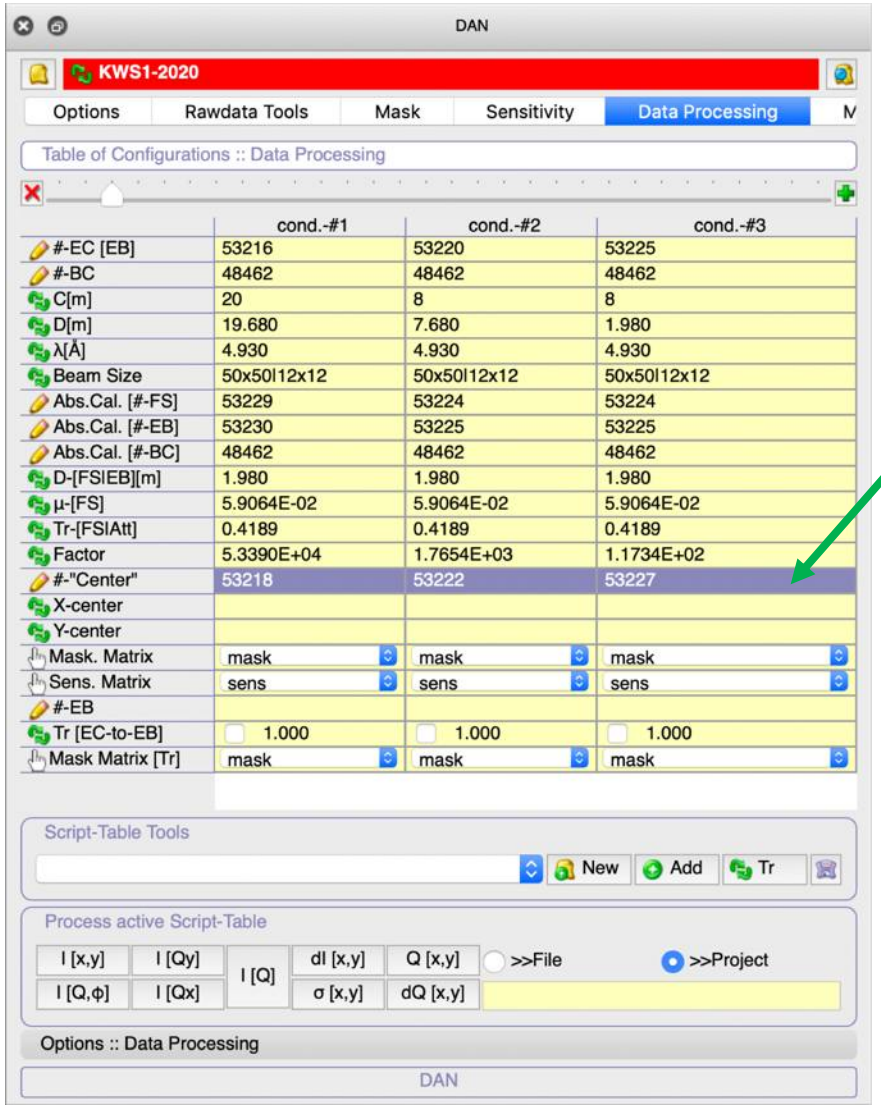


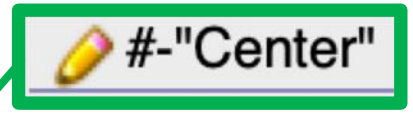
Results Log: Output

Fill: **“Center ”Runs**

“Center ”Runs: strongly scattering samples (near beam-stop) to calculate beam center positions.
Often we use our standard sample “**Corundum**” as sample to calculate beam center positions.



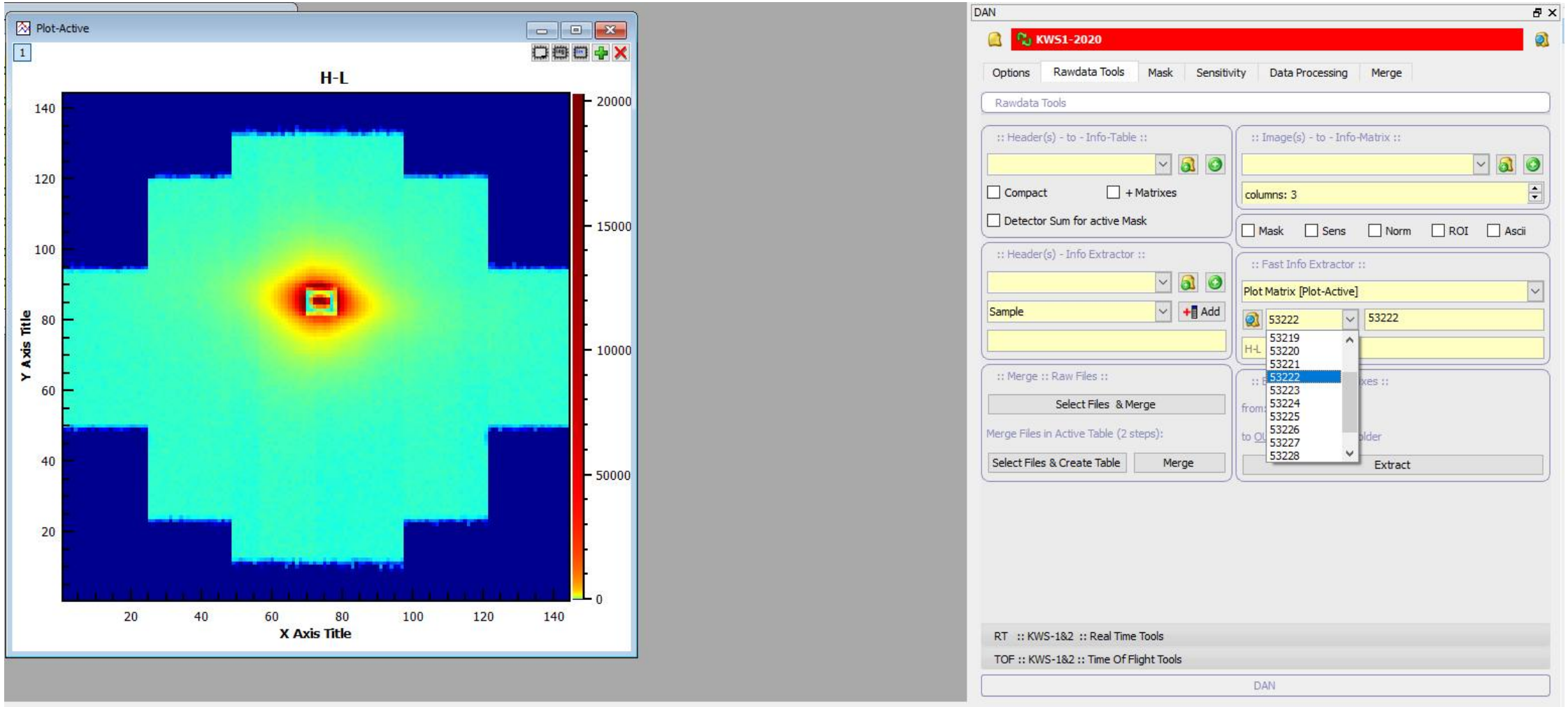




We use
“H-L” sample
as “Center” runs

Fill: **“Center ”Runs**

“Center ”Runs: strongly scattering samples (near beam-stop) to calculate beam center positions. One can use a typical user sample which scatters sufficiently around the beam stop. This can be checked in Rawdata Tools tab/Fast Info Extractor/Plot Matrix [Plot Active].

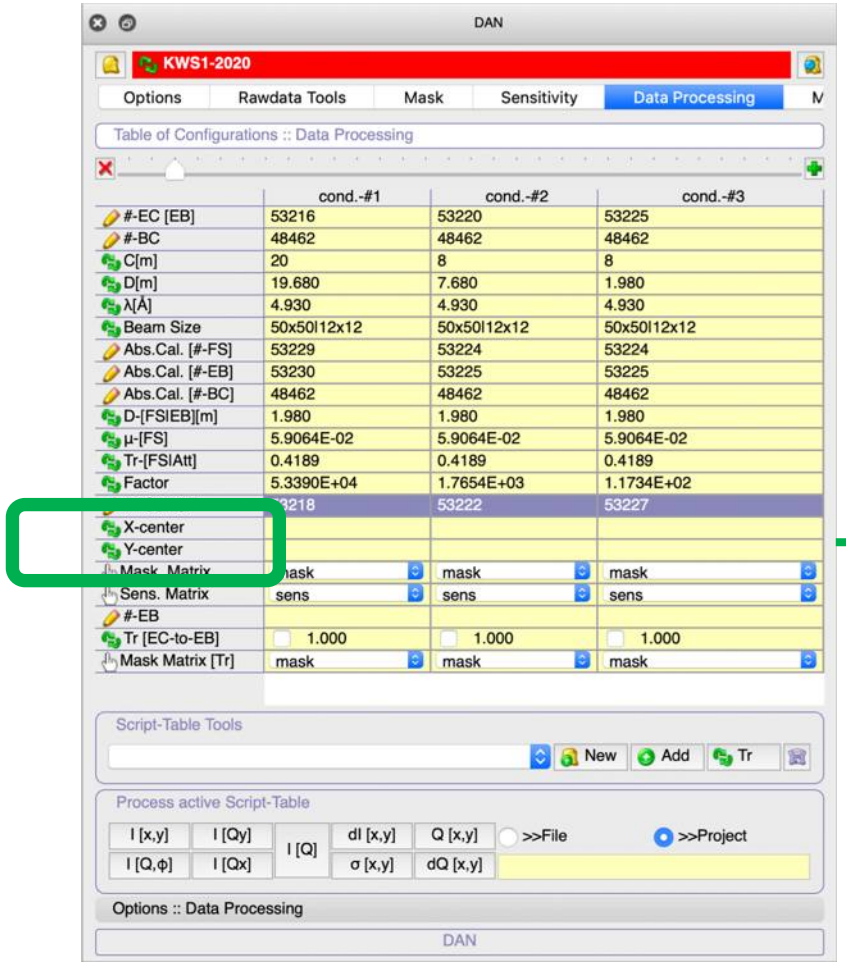


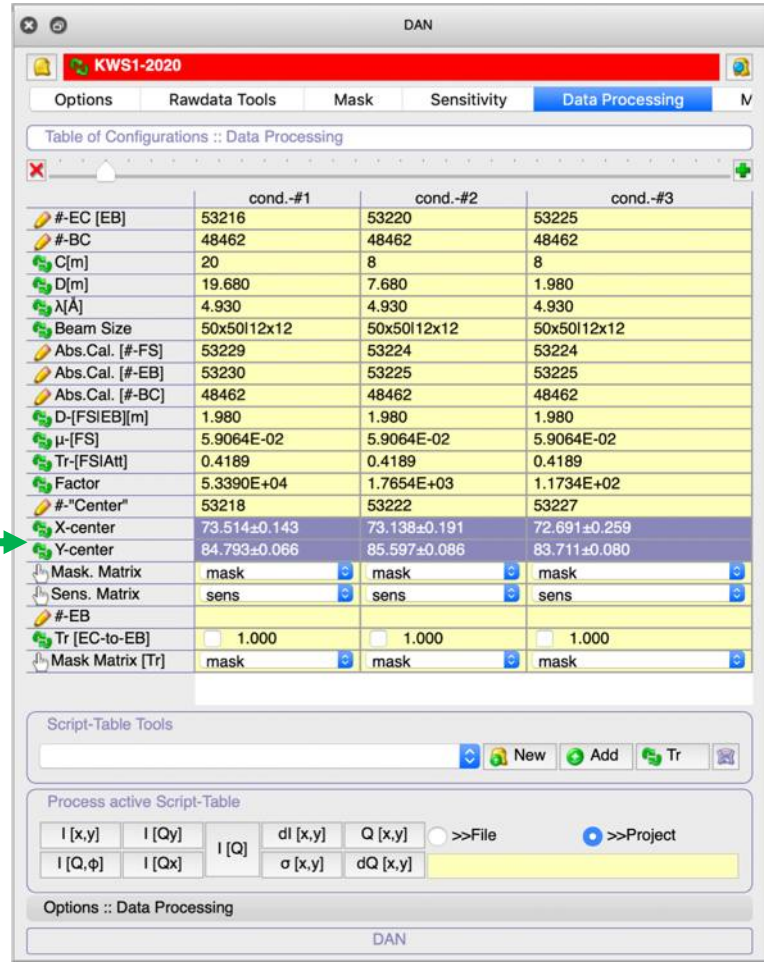
Push : X-center to calculate center of the beam for all configurations

or/and

Y-center

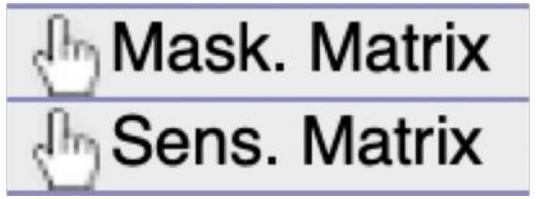
73.514±0.143	73.138±0.191	72.691±0.259
84.793±0.066	85.597±0.086	83.711±0.080

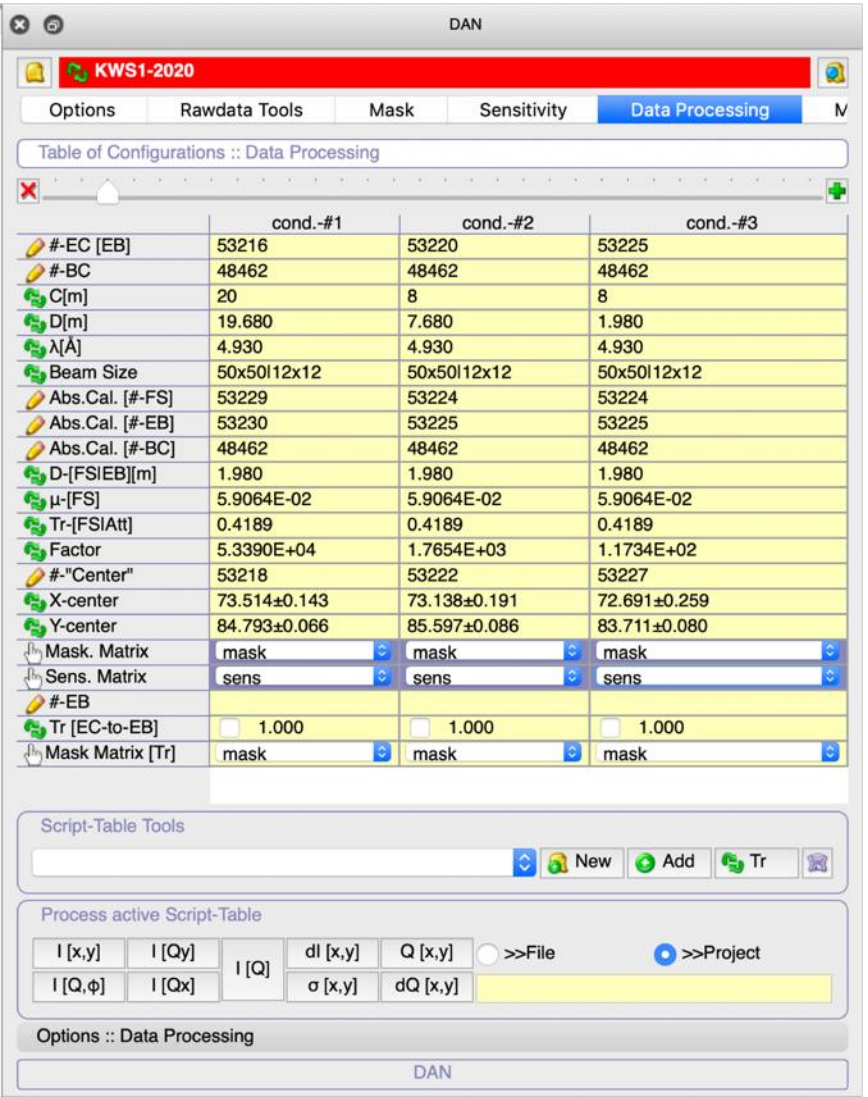


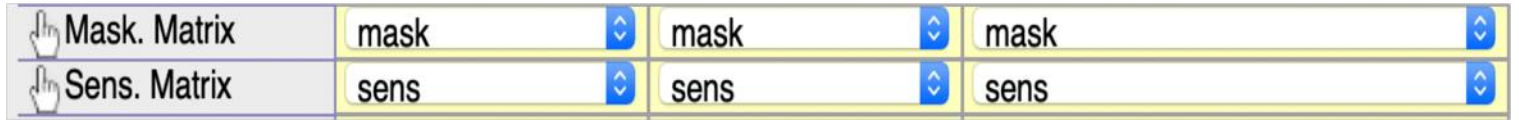


! Check errors to be sure about correctness of center determination !

Select correct **“Sensitivity”** and **“Mask”** Matrixes





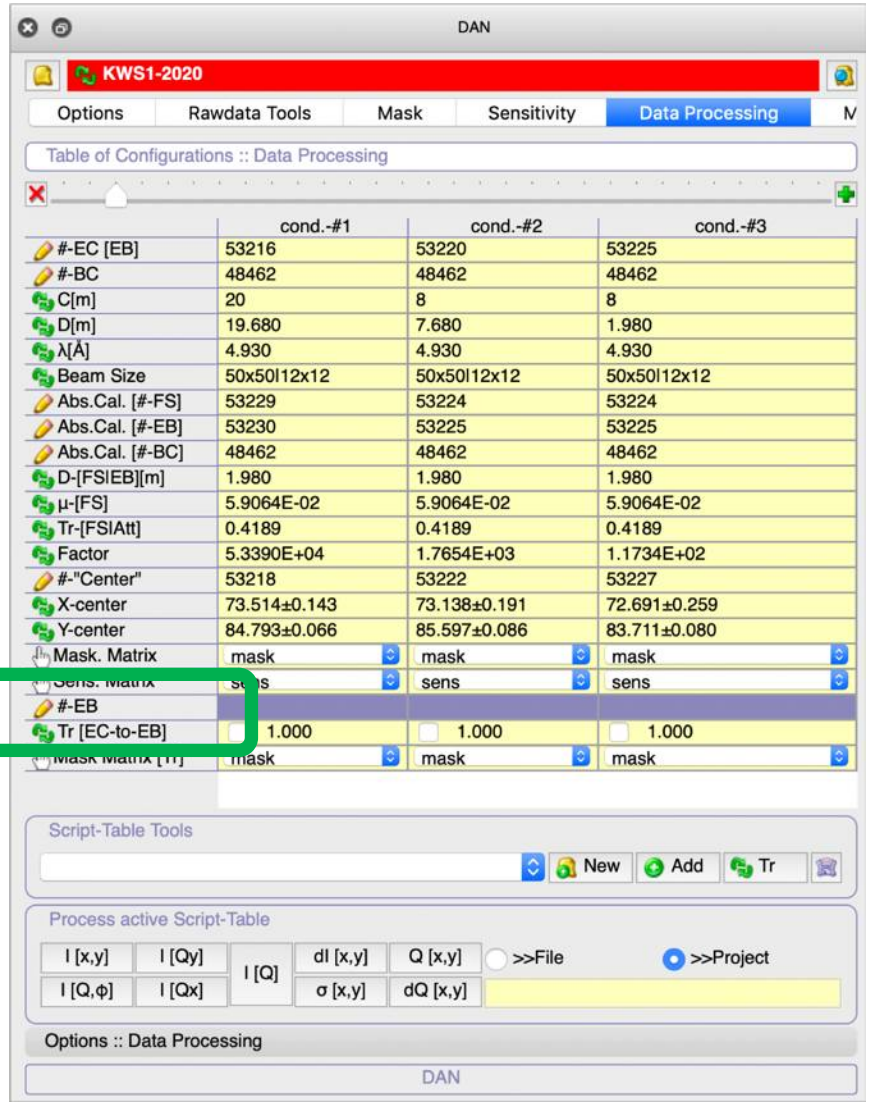


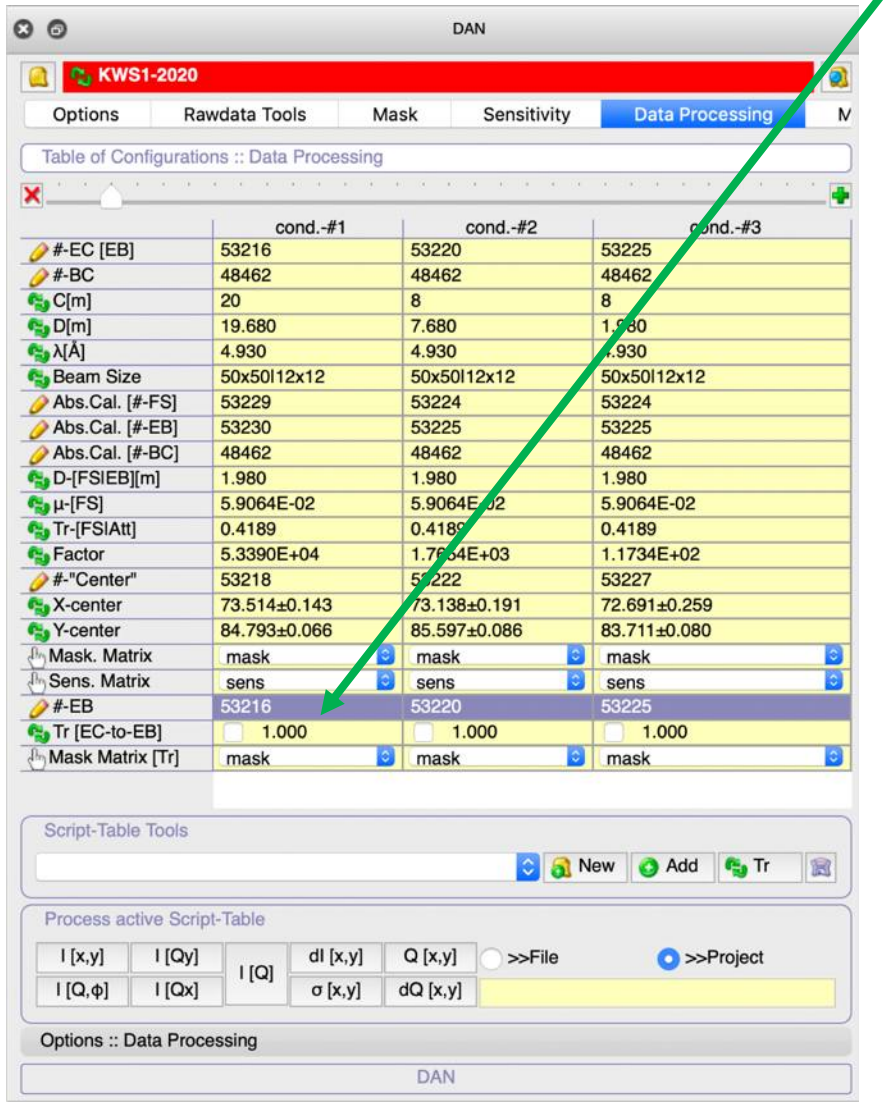
“Mask” and “Sens” matrixes could be different for different configurations

Fill: **Empty beam** runs.

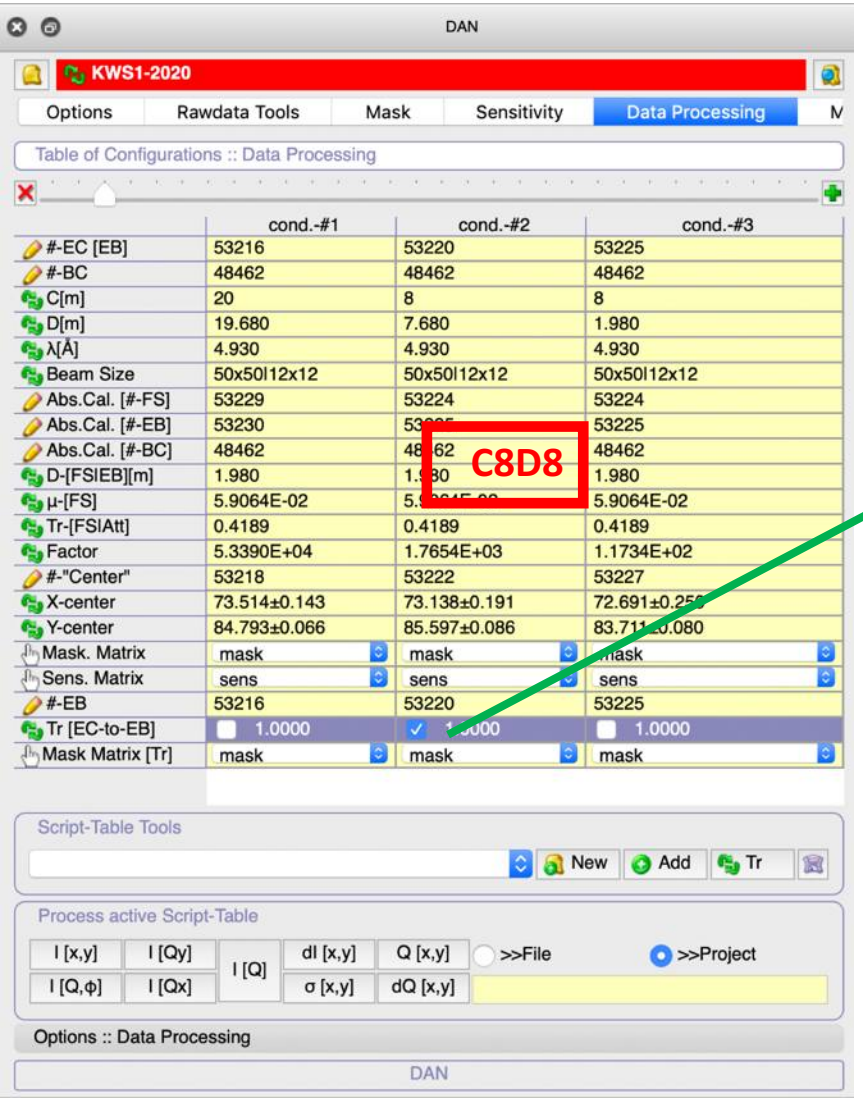
To calculate Transmission of Empty Cell

In this example: EC=EB, **Tr(EC)=1**



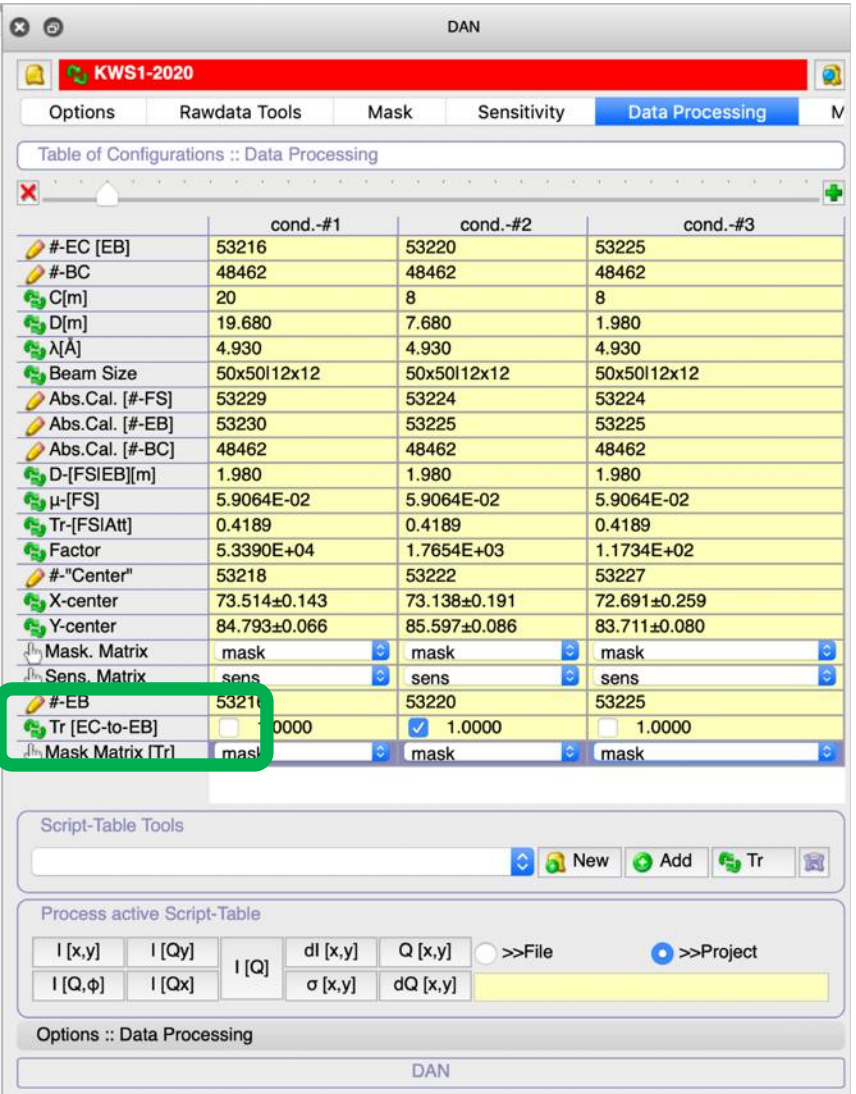


Select configuration will be used for transmission calculations.
At KWS-1 normally we use C8D8 configuration for transmission calculations



Push :

to calculate transmission of Empty Cell (to Empty beam)

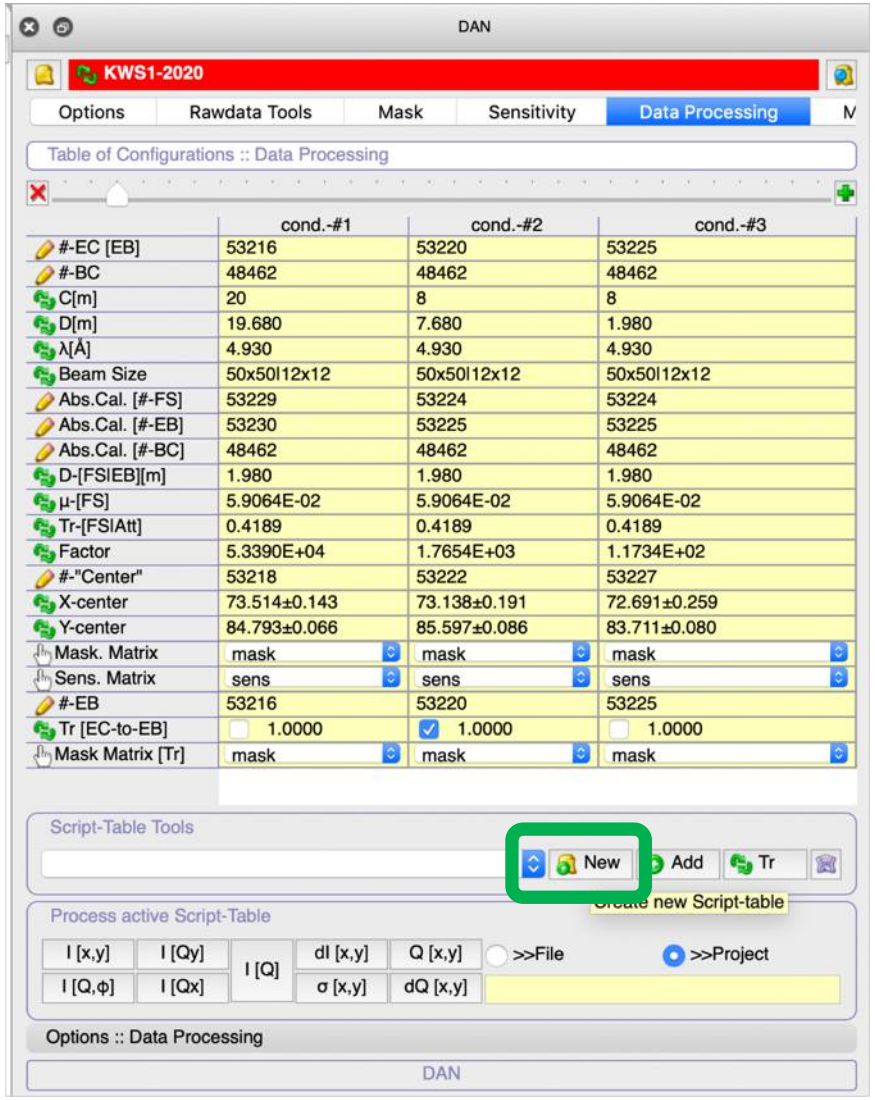


! In this example EC=EB & Tr(EC-to-EB)=1 !

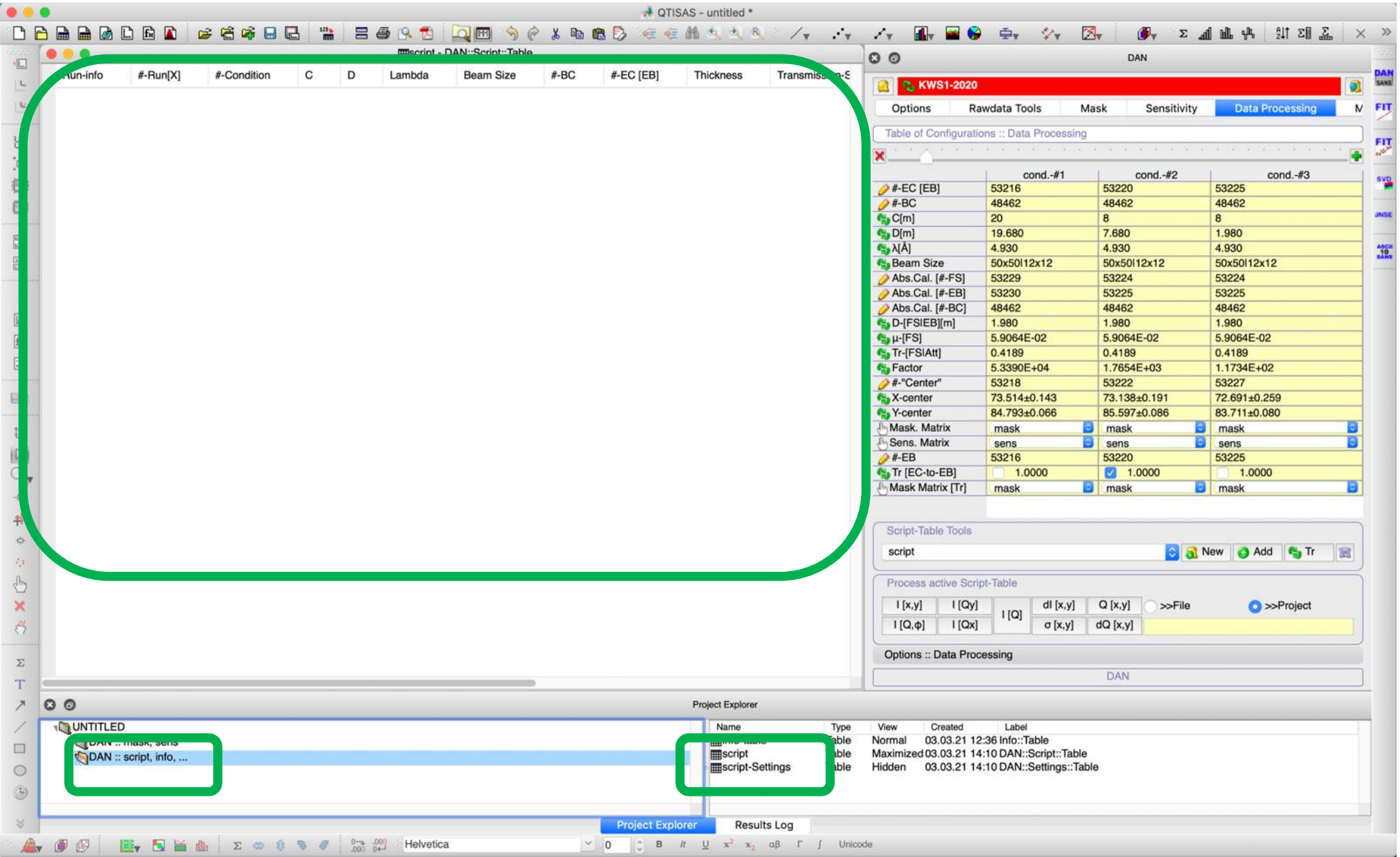
STEP 8: Creation of “Table of Samples”

Push :

to create empty script-table and than give name to it.

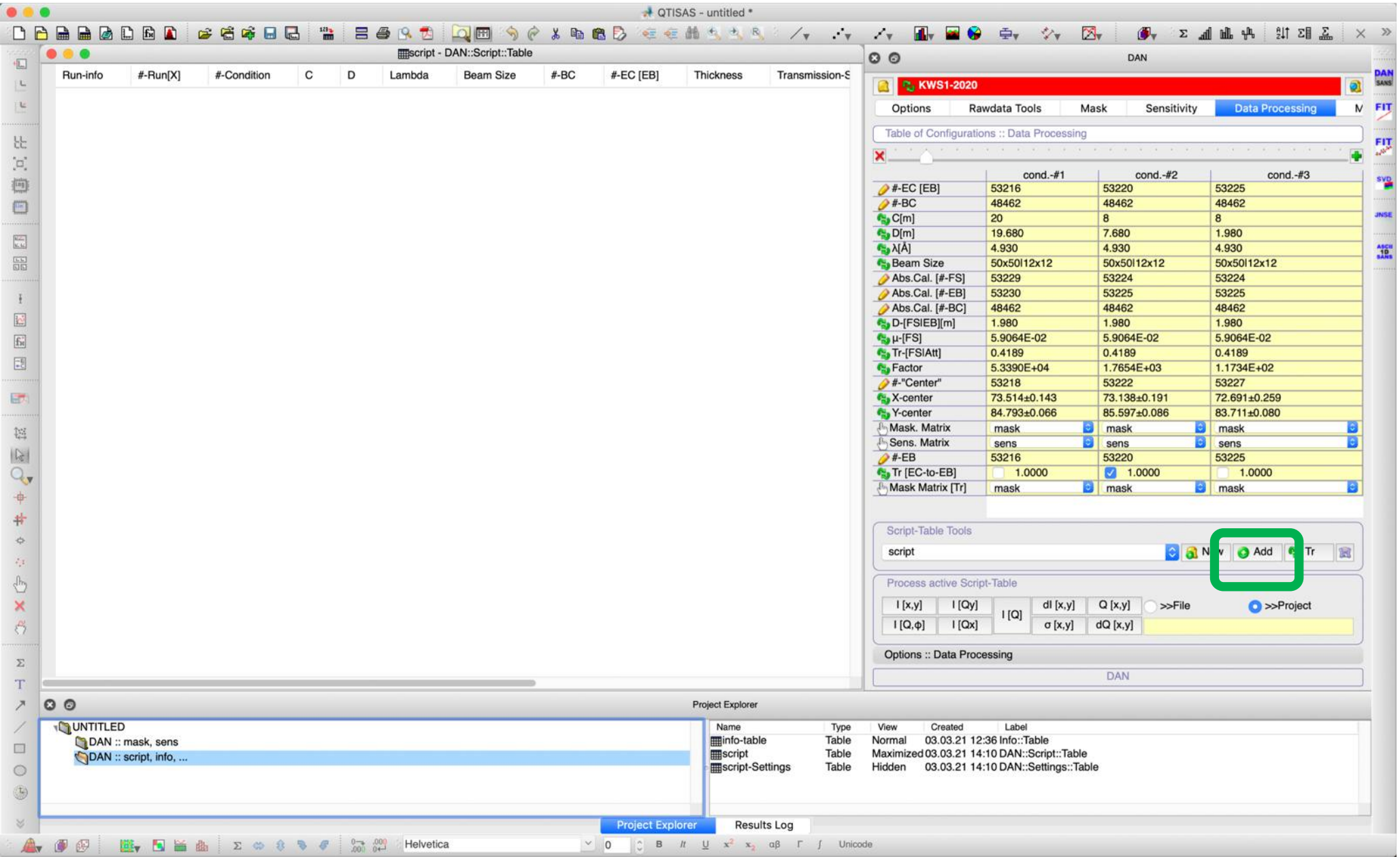


Empty “**script**” table is generated in “DAN :: script, info, ...” folder

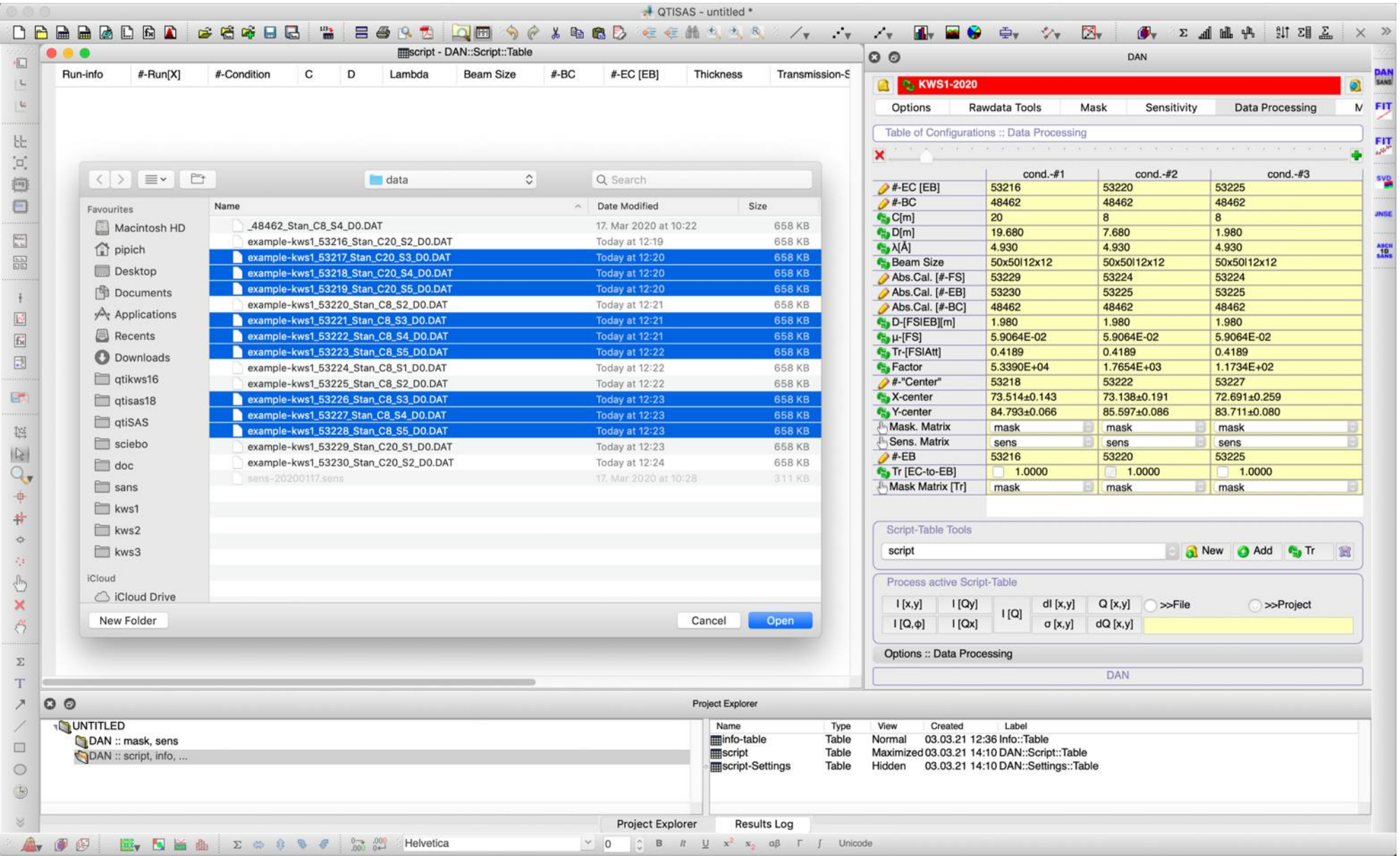


Current parameters of DAN-SANS are saved in: **Script-Settings** table

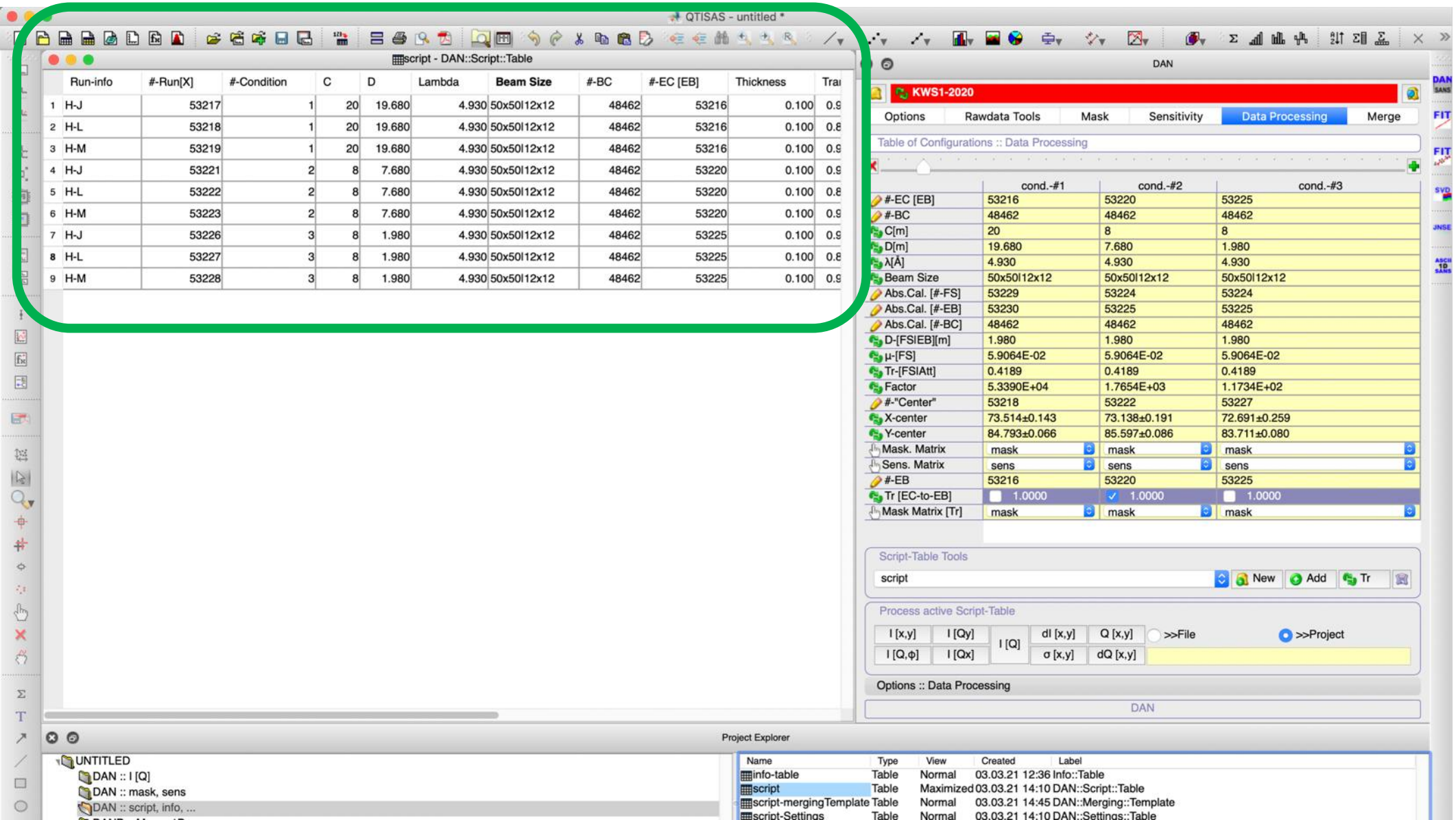
Push : Add To add files for data reduction



Selecting of files for data reduction



“Script” table contains now 3 samples measured in 3 configurations



“Script” table structure

“Script” table structure

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmission-Sample	Factor	X-center[Y]	Y-center[Y]	Mask	**Sens**	Status
1	H-J	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9061 [±0.0012]	53390	73.514	84.793	mask	sens	
2	H-L	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.8981 [±0.0012]	53390	73.514	84.793	mask	sens	
3	H-M	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9019 [±0.0012]	53390	73.514	84.793	mask	sens	
4	H-J	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9061 [±0.0012]	1765.4	73.138	85.597	mask	sens	
5	H-L	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.8981 [±0.0012]	1765.4	73.138	85.597	mask	sens	
6	H-M	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9019 [±0.0012]	1765.4	73.138	85.597	mask	sens	
7	H-J	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9061 [±0.0012]	117.34	72.691	83.711	mask	sens	
8	H-L	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.8981 [±0.0012]	117.34	72.691	83.711	mask	sens	
9	H-M	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9019 [±0.0012]	117.34	72.691	83.711	mask	sens	

“Script” table structure

1 3 5 7 9: I_{EC} 11: Tr 13: X_{center} 15: mask 17

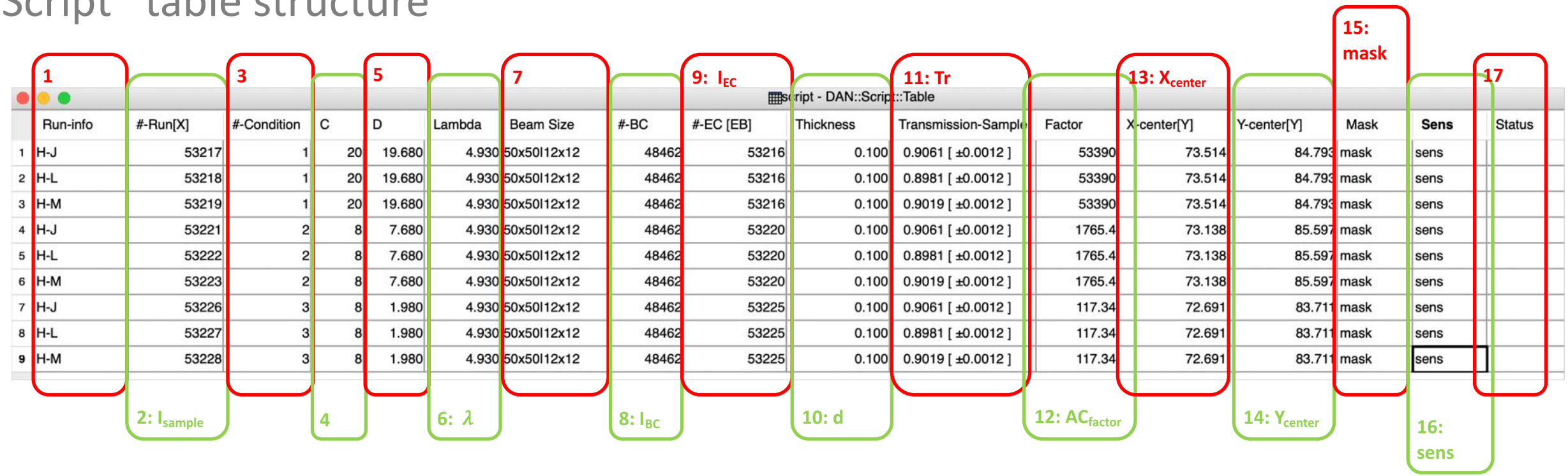
Script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmission-Sample	Factor	X-center[Y]	Y-center[Y]	Mask	Sens	Status
1	H-J	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9061 [±0.0012]	53390	73.514	84.793	mask	sens	
2	H-L	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.8981 [±0.0012]	53390	73.514	84.793	mask	sens	
3	H-M	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9019 [±0.0012]	53390	73.514	84.793	mask	sens	
4	H-J	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9061 [±0.0012]	1765.4	73.138	85.597	mask	sens	
5	H-L	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.8981 [±0.0012]	1765.4	73.138	85.597	mask	sens	
6	H-M	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9019 [±0.0012]	1765.4	73.138	85.597	mask	sens	
7	H-J	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9061 [±0.0012]	117.34	72.691	83.711	mask	sens	
8	H-L	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.8981 [±0.0012]	117.34	72.691	83.711	mask	sens	
9	H-M	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9019 [±0.0012]	117.34	72.691	83.711	mask	sens	

2: I_{sample} 4 6: λ 8: I_{BC} 10: d 12: AC_{factor} 14: Y_{center} 16: sens

1. **Sample Name** column: for smooth merging and correct transmission calculations the name of a sample should be the same in all instrument configurations. Example: “H-J” name is the same for #53217, #53221, #53226 runs… Sample name could be edited in this column
2. **Run Number** column: “I_{sample}”
3. **Condition Number** , it corresponds to column number in the table of configurations in DAN-SANS
4. **Collimation Distance** column
5. **Sample-To-detector Distance** column: “D”
6. **Wave Length** column: “λ”
7. Column **Collimation and Sample Apertures** “Beam Size”
8. **Dark Current** column with run numbers corresponding to the blocked beam measurements (Boron Carbonate): “I_{BC}”

“Script” table structure

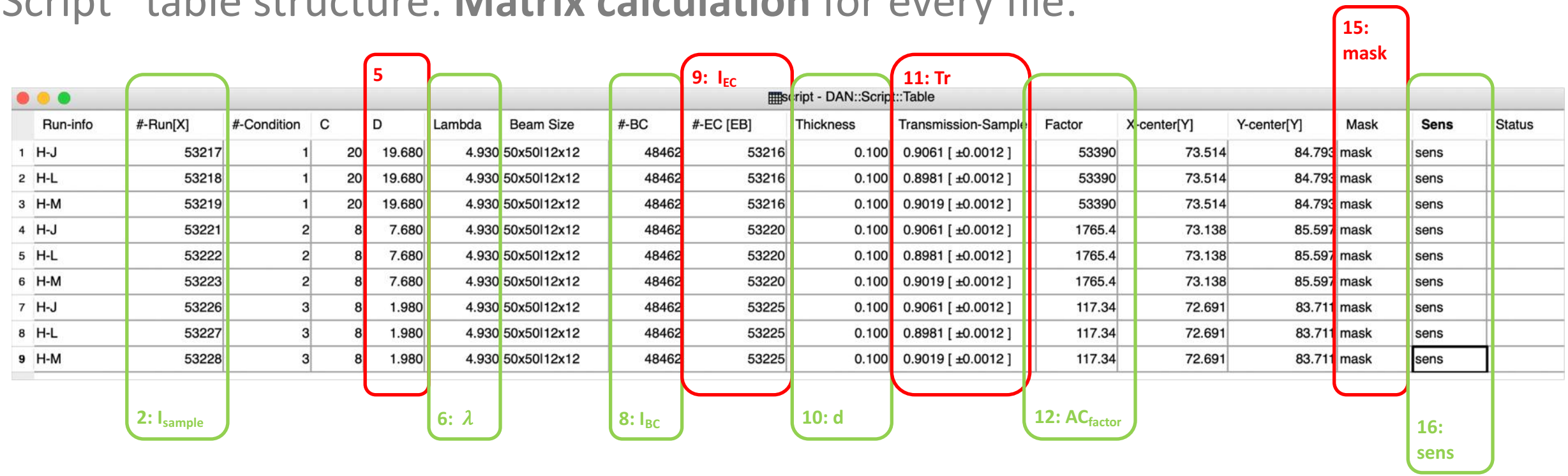


cript - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmission-Sample	Factor	X-center[Y]	Y-center[Y]	Mask	Sens	Status
1	H-J	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9061 [±0.0012]	53390	73.514	84.793	mask	sens	
2	H-L	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.8981 [±0.0012]	53390	73.514	84.793	mask	sens	
3	H-M	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9019 [±0.0012]	53390	73.514	84.793	mask	sens	
4	H-J	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9061 [±0.0012]	1765.4	73.138	85.597	mask	sens	
5	H-L	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.8981 [±0.0012]	1765.4	73.138	85.597	mask	sens	
6	H-M	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9019 [±0.0012]	1765.4	73.138	85.597	mask	sens	
7	H-J	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9061 [±0.0012]	117.34	72.691	83.711	mask	sens	
8	H-L	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.8981 [±0.0012]	117.34	72.691	83.711	mask	sens	
9	H-M	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9019 [±0.0012]	117.34	72.691	83.711	mask	sens	

9. **Empty Cell** column: run numbers will be subtracted as EC (EB) from the sample: “I_{EC}”
10. **Sample Thickness** column: “d”
11. **Sample Transmission** column: “Tr”
12. **Absolute Calibration Factor** column “AC_{factor}”
13. **X-center** column “X_{center}”
14. **Y-center** column “Y_{center}”
15. **Mask Matrix** column: “mask”
16. **Sensitivity Matrix** column: “sens”
15. **After-Processing-Status** column

“Script” table structure: **Matrix calculation** for every file:



script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmission-Sample	Factor	X-center[Y]	Y-center[Y]	Mask	Sens	Status
1	H-J	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9061 [±0.0012]	53390	73.514	84.793	mask	sens	
2	H-L	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.8981 [±0.0012]	53390	73.514	84.793	mask	sens	
3	H-M	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9019 [±0.0012]	53390	73.514	84.793	mask	sens	
4	H-J	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9061 [±0.0012]	1765.4	73.138	85.597	mask	sens	
5	H-L	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.8981 [±0.0012]	1765.4	73.138	85.597	mask	sens	
6	H-M	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9019 [±0.0012]	1765.4	73.138	85.597	mask	sens	
7	H-J	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9061 [±0.0012]	117.34	72.691	83.711	mask	sens	
8	H-L	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.8981 [±0.0012]	117.34	72.691	83.711	mask	sens	
9	H-M	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9019 [±0.0012]	117.34	72.691	83.711	mask	sens	

$$\frac{d\Sigma}{d\Omega}[i,j] = mask[i,j] \cdot sens[i,j] \cdot \frac{AC_{factor}}{d \cdot Tr} \cdot \left(I_{sample} - I_{BC} - Tr \cdot (I_{EC} - I_{BC}) \right)$$

I: means normalized intensity
+ Dead-Time correction
+ Wide Angle corrections

In “processing” only parameters in the Script-Table is used – **NOT FROM HEADERS**

“Script” table structure: **Wave Vector Q calculation** for every file, every pixel:

5: D

13: X_{center}

15: mask

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmission-Sample	Factor	X-center[Y]	Y-center[Y]	Mask	Sens	Status
1	H-J	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9061 [±0.0012]	53390	73.514	84.793	mask	sens	
2	H-L	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.8981 [±0.0012]	53390	73.514	84.793	mask	sens	
3	H-M	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9019 [±0.0012]	53390	73.514	84.793	mask	sens	
4	H-J	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9061 [±0.0012]	1765.4	73.138	85.597	mask	sens	
5	H-L	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.8981 [±0.0012]	1765.4	73.138	85.597	mask	sens	
6	H-M	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9019 [±0.0012]	1765.4	73.138	85.597	mask	sens	
7	H-J	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9061 [±0.0012]	117.34	72.691	83.711	mask	sens	
8	H-L	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.8981 [±0.0012]	117.34	72.691	83.711	mask	sens	
9	H-M	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9019 [±0.0012]	117.34	72.691	83.711	mask	sens	

6: λ

14: Y_{center}

$$Q[i,j] = \frac{4\pi}{\lambda} \cdot sin\left(tan^{-1}\left(\frac{pixel_{size} \cdot \sqrt{(i - X_{center})^2 + (j - Y_{center})^2}}{2D}\right)\right)$$

+ Wide Angle corrections

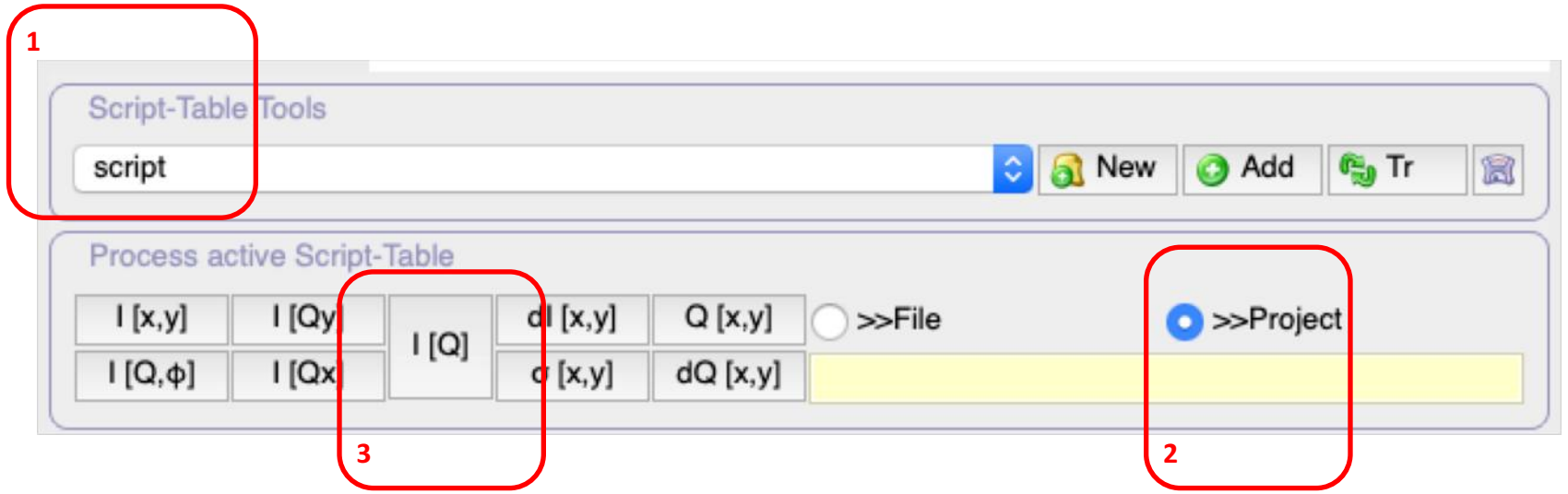
$pixel_{size} = 0.836cm$

[Options | SA(N)S Instrument::Configuration | Detector Image]

In “processing” only parameters in the Script-Table is used – **NOT FROM HEADERS**

“Processing” tools/options

Data “Processing”
in 3 steps:



1. **Select(Create)** script table

2. **Select way how data will be saved after processing**:
- as tables/matrixes in the current project (“**>>Project**”)
- or as ASCII files in “Output Folder” (“**>>File**”)

3. **Push one of Processing Buttons:**
- **I[Q]** for radial averaging;
- **I[x,y]** for matrix generation in Cartesian coordinates;
- **I[Q,ϕ]** for matrix generation in Polar coordinates;
- **I[Qx]** or **I[Qz]** for horizontal or vertical slices;
- d**I[x,y]**, **Q[x,y]**, **dQ[x,y]**, **σ[x,y]** for error-bar matrix, wave-vector matrix, error-bar matrix of wave-vector, resolution matrix…

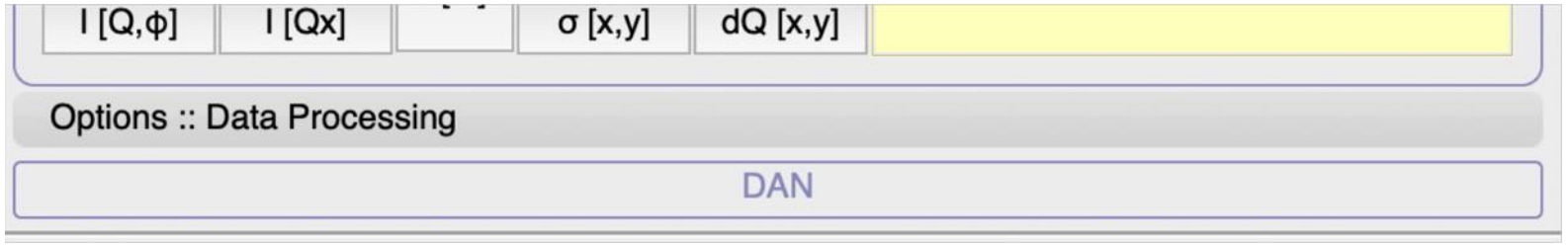
STEP 9: Radial Averaging

1. **Selected:** “script” table

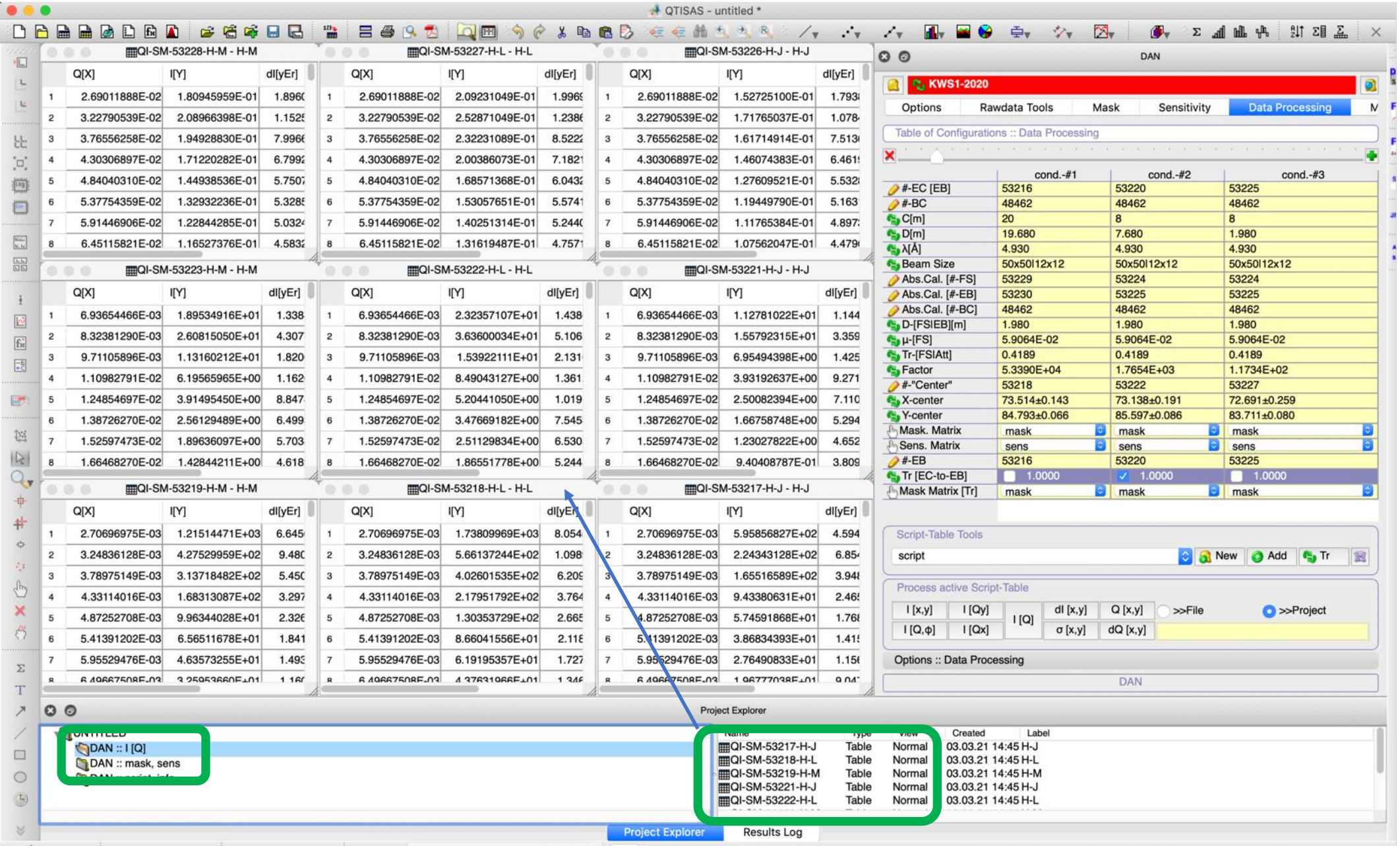
2. **Selected:** as tables/matrixes in the current project (“**>>Project**”)

3. **Pushed:** **I[Q]** for radial averaging;

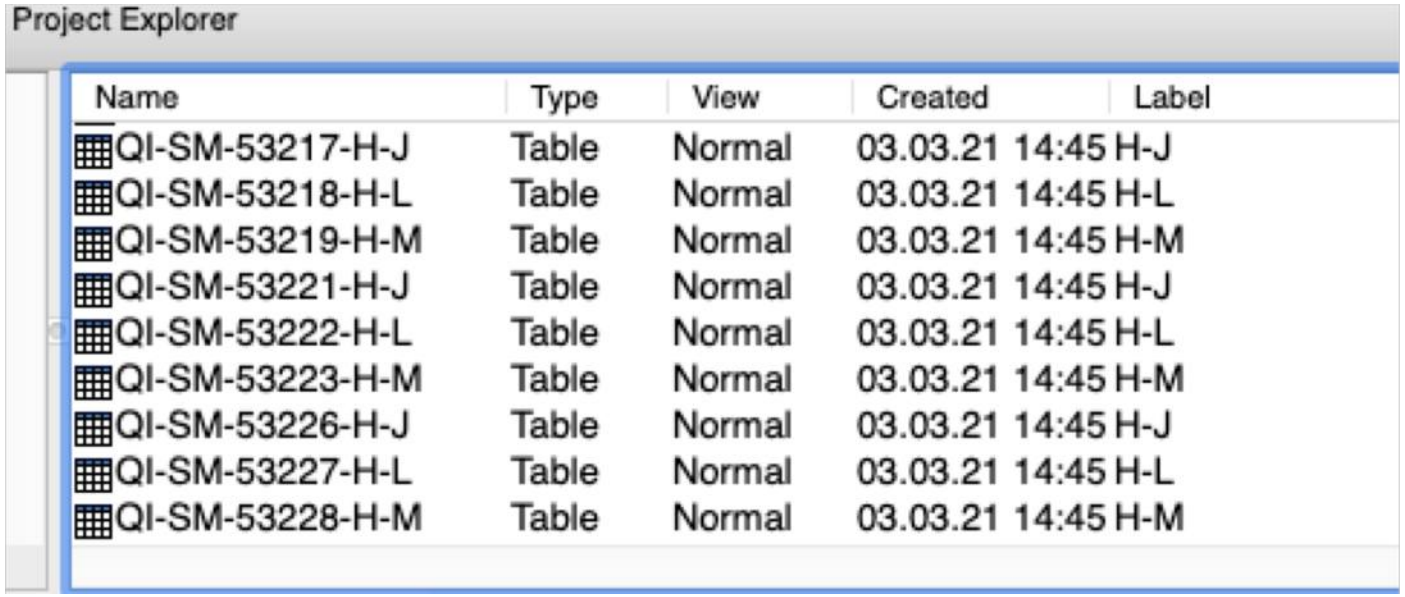
Many options of the data processing are „hidden“ in “Options :: Data Processing” tab (not explained here):



In “DAN:: I[Q]” folder 9 tables are created



Default **Table's name** Format



QI-SM-#####-SampleName

QI: radial av. Mode
SM: "Standard" Mode
#####: run number
SampleName: Sample Name ☺

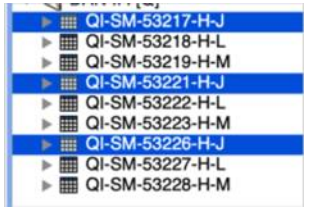
Example of Plotting of Radial Averaged Datasets

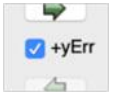
Plotting example:

1. **Create empty 2D Plot**

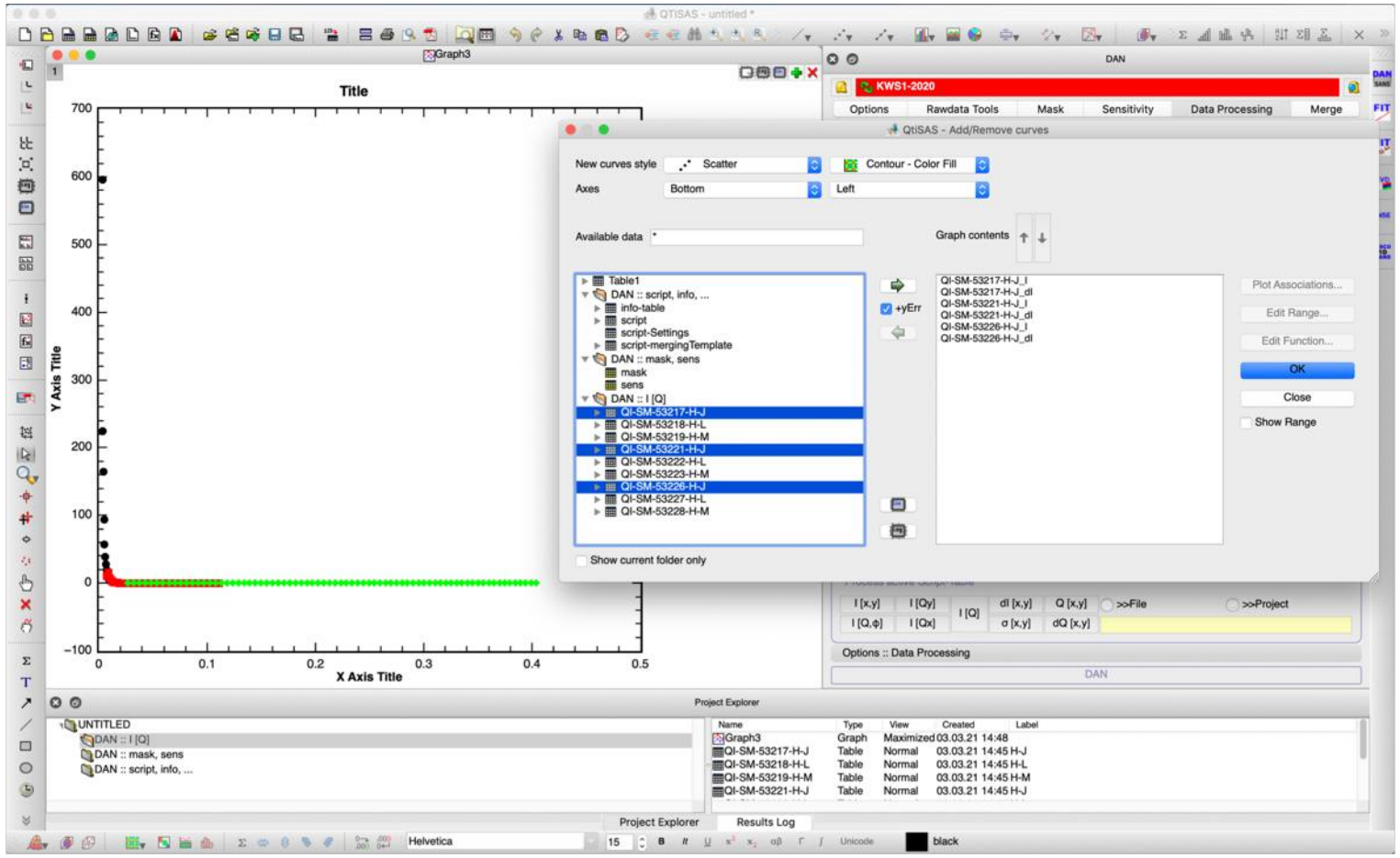
2. **Menu Graph:**
select “Add/Remove Curve …”

3. **Select Data to Plot:**
(H-J sample here)



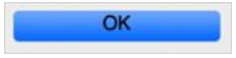


4(optional). **Check “+yErr”:**
Automatically to add also error-bars



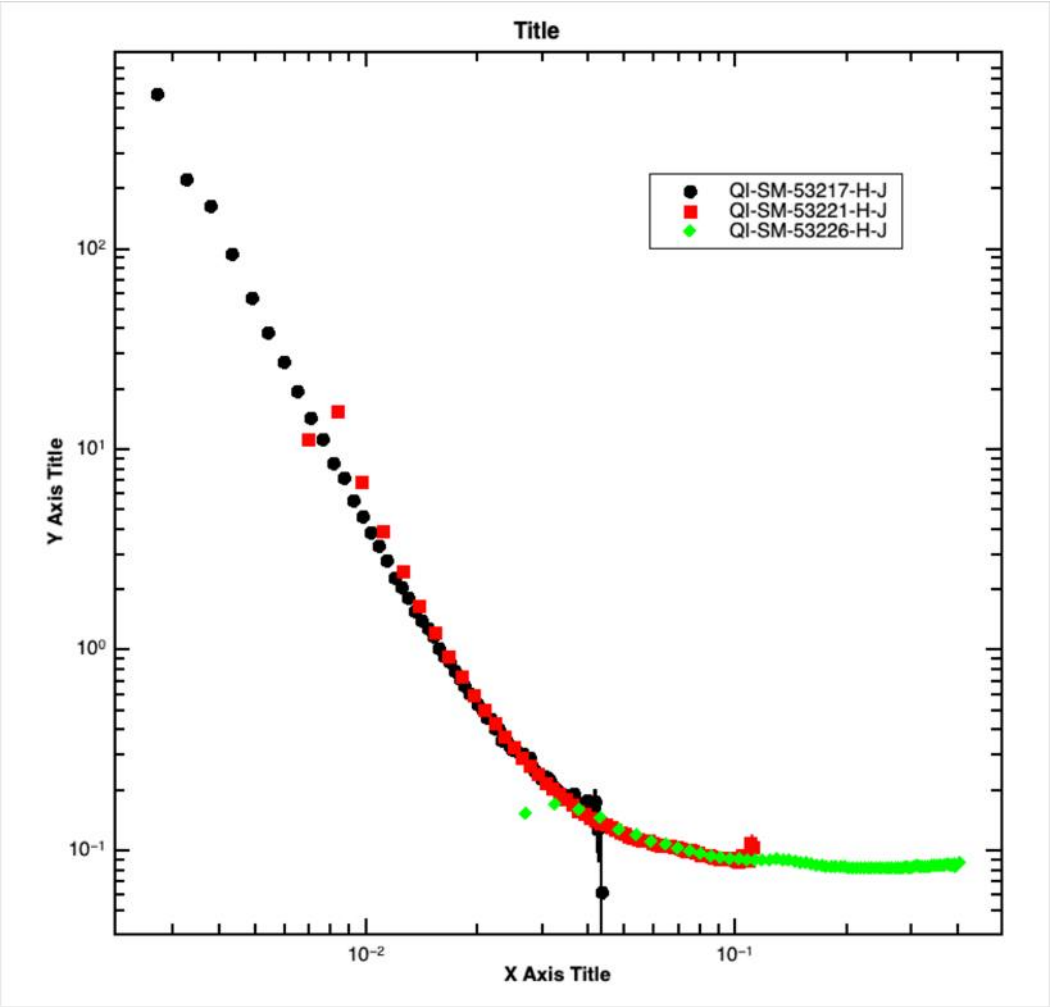
5. **Push “Add” button:**

6 (optional). **Push “log” for double-logarithmic presentation**



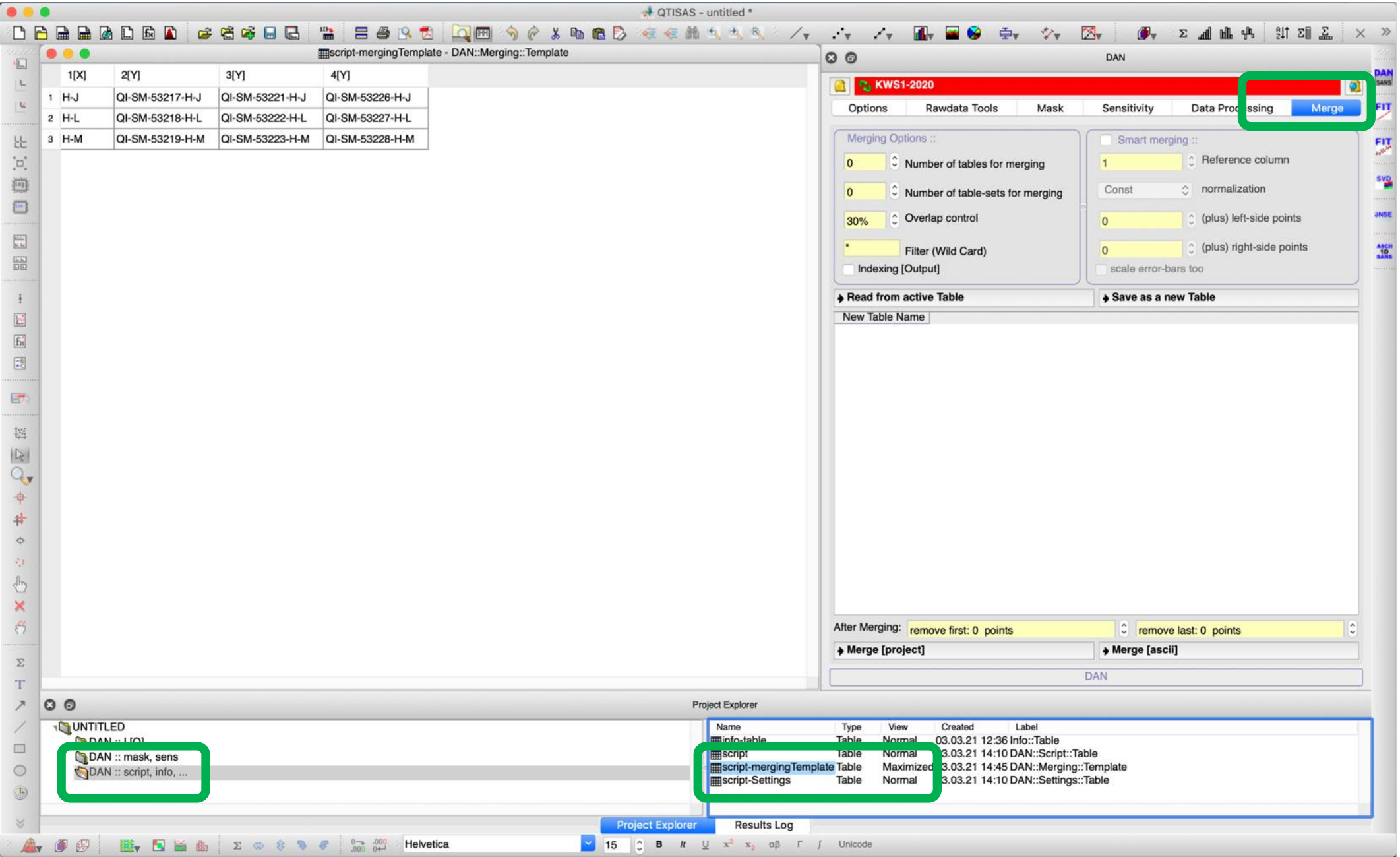
7. **Push “OK” button to close “Add/Remove” interface**

Plotting example: result

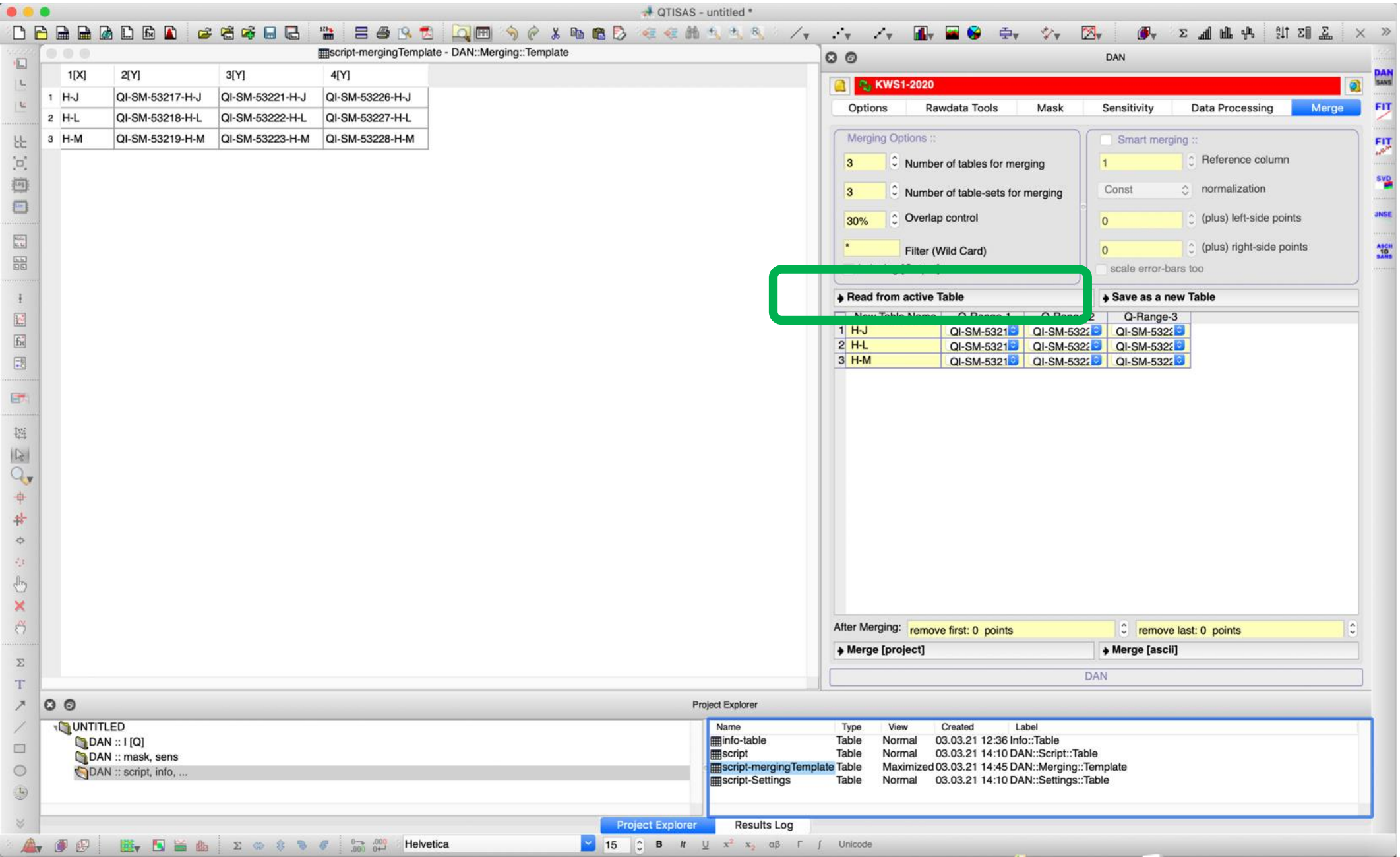


STEP 10: Data Merging

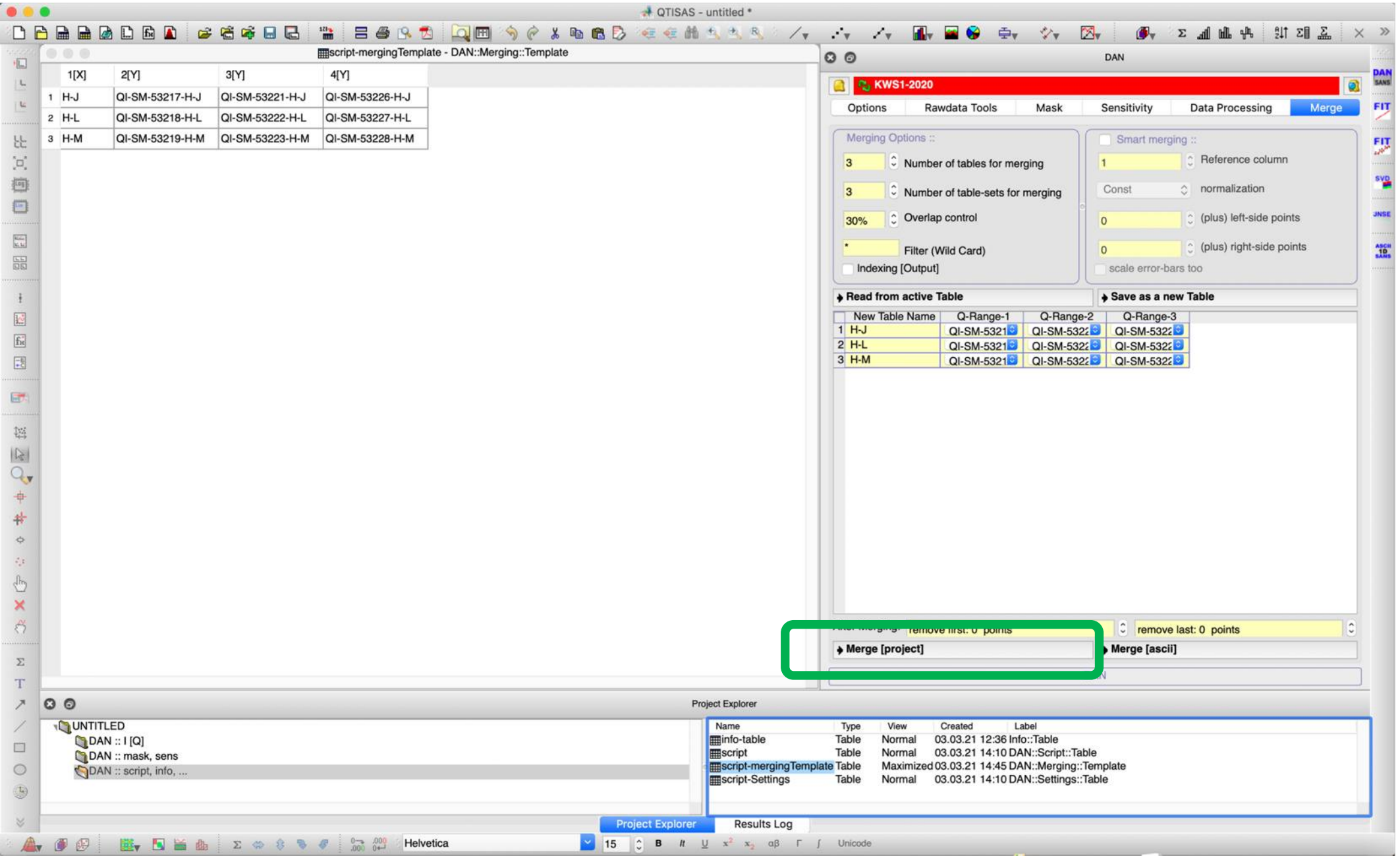
Merging Step #1: go to “Merge” tab (DAN-SANS) and activate “script-mergingTemplate”



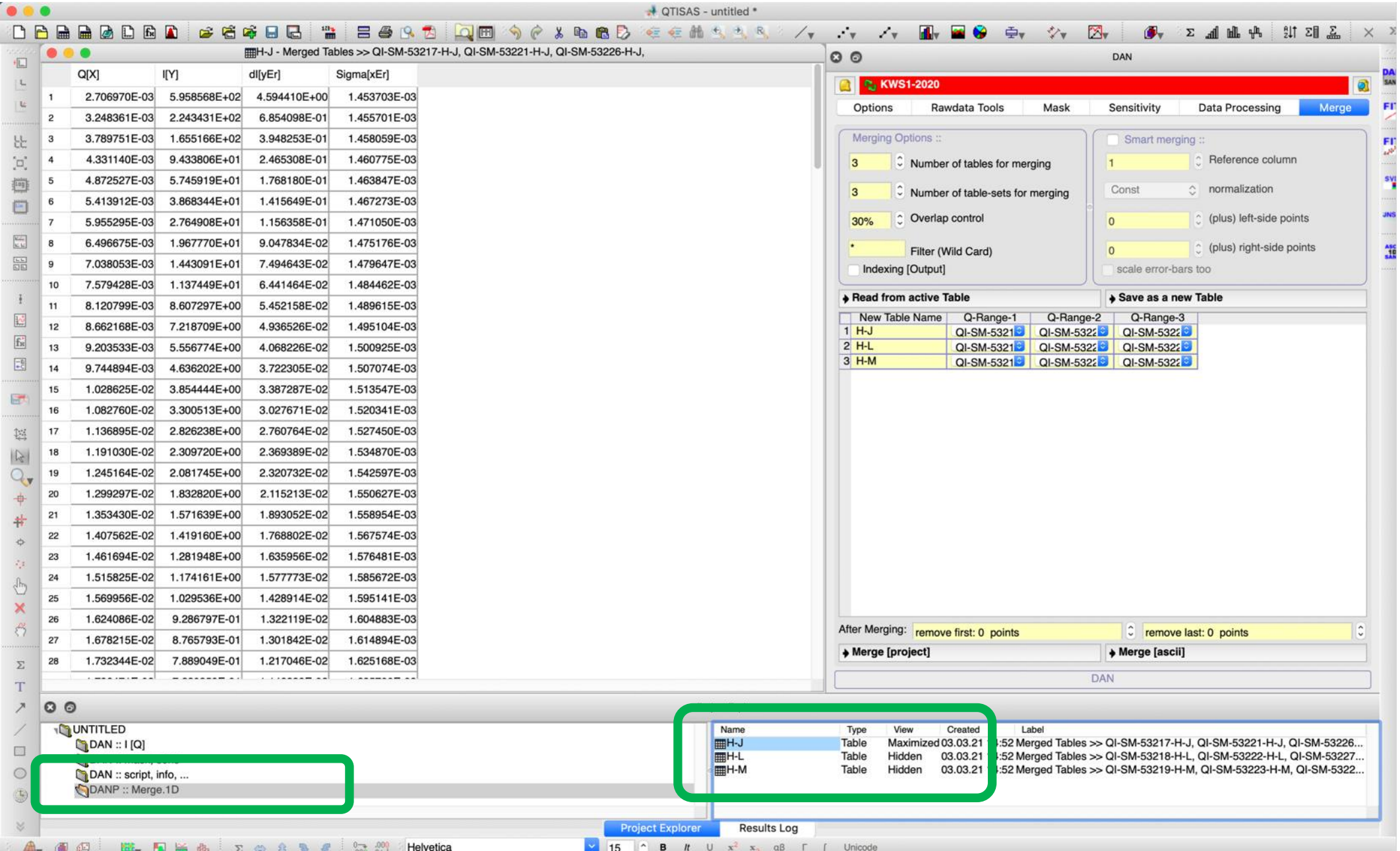
Merging Step #2: push button “Read active Table” to transfer data to Merge-interface



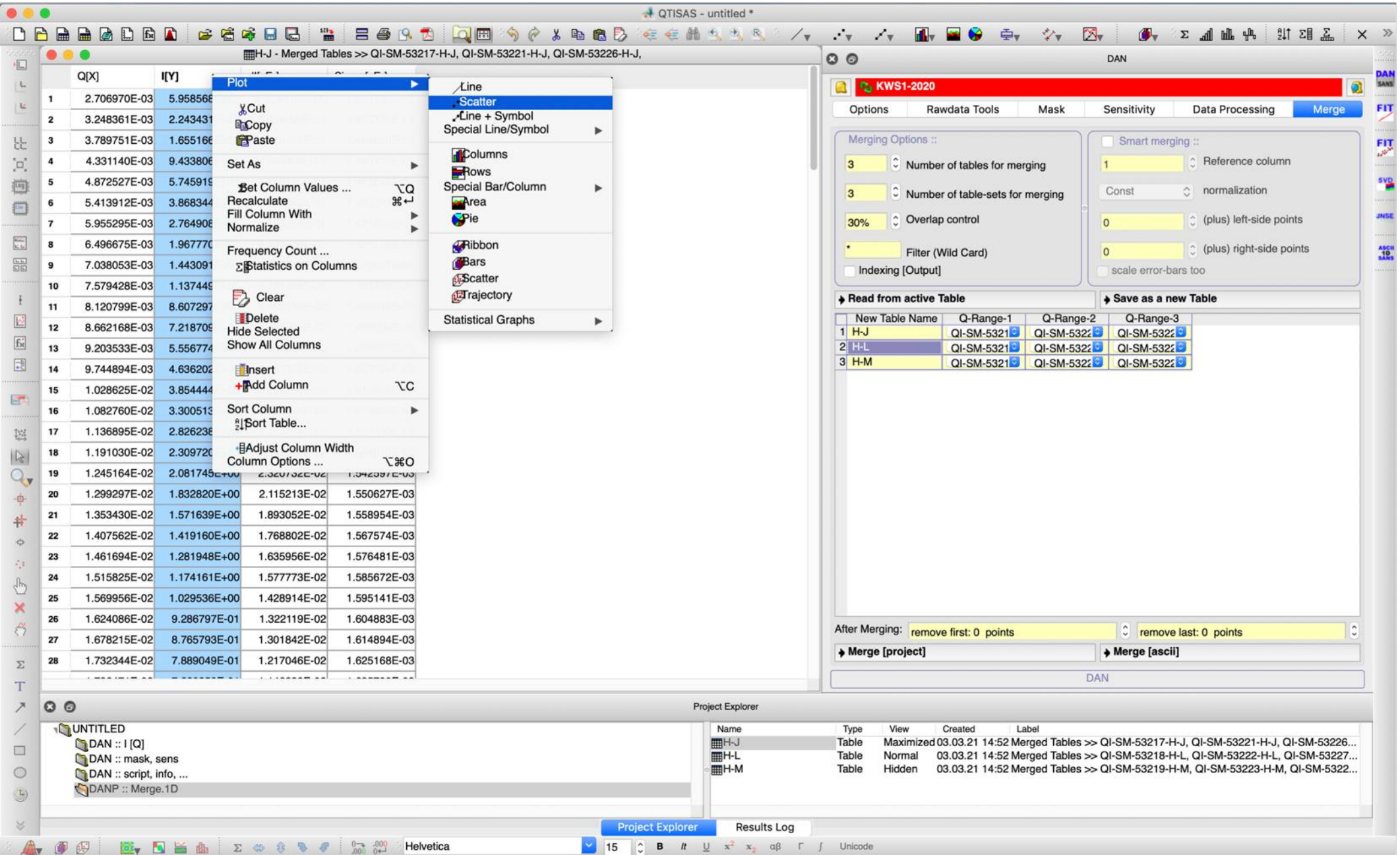
Merging Step #3: push button “Merge [Project]” or “Merge[ascii]”

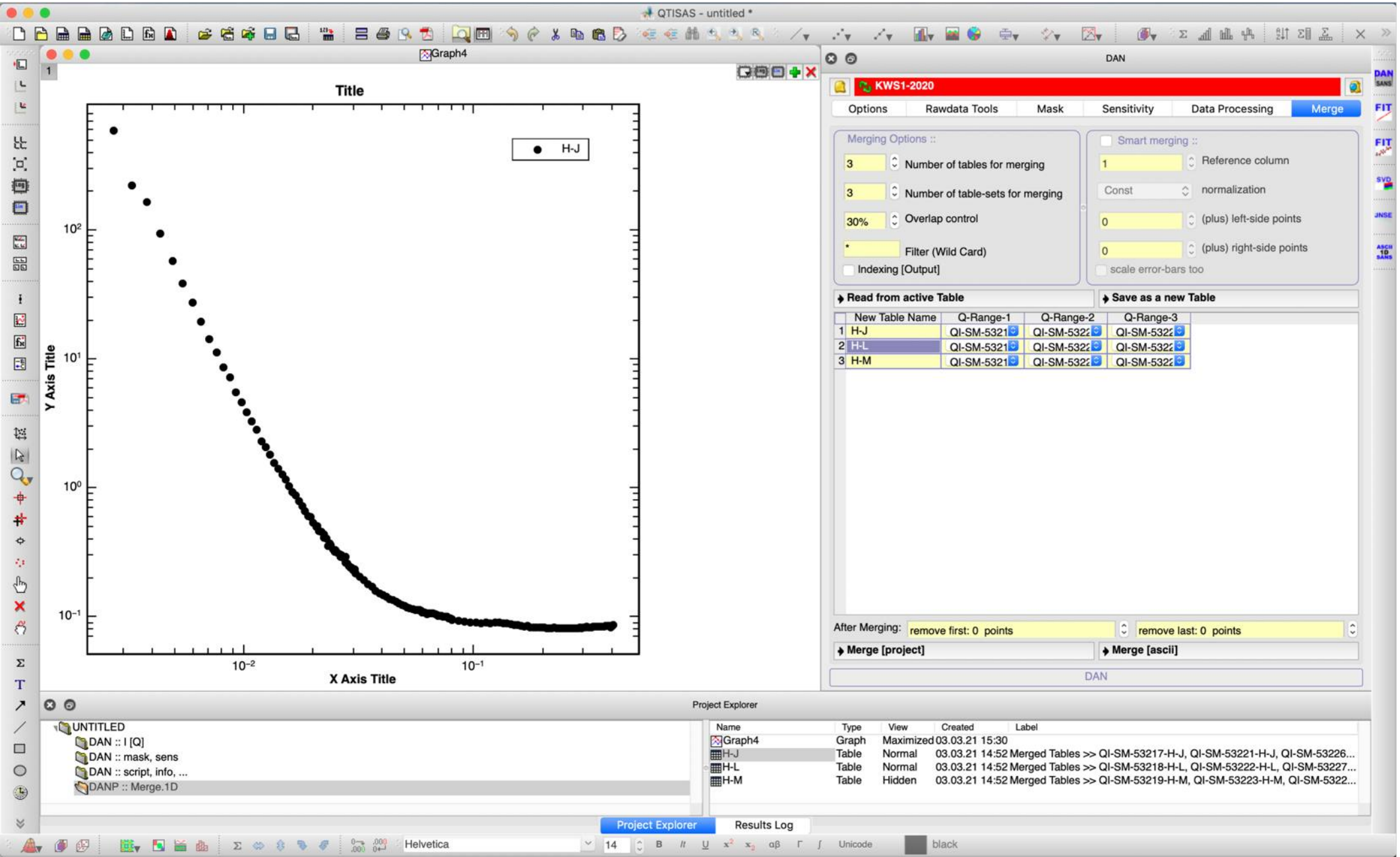


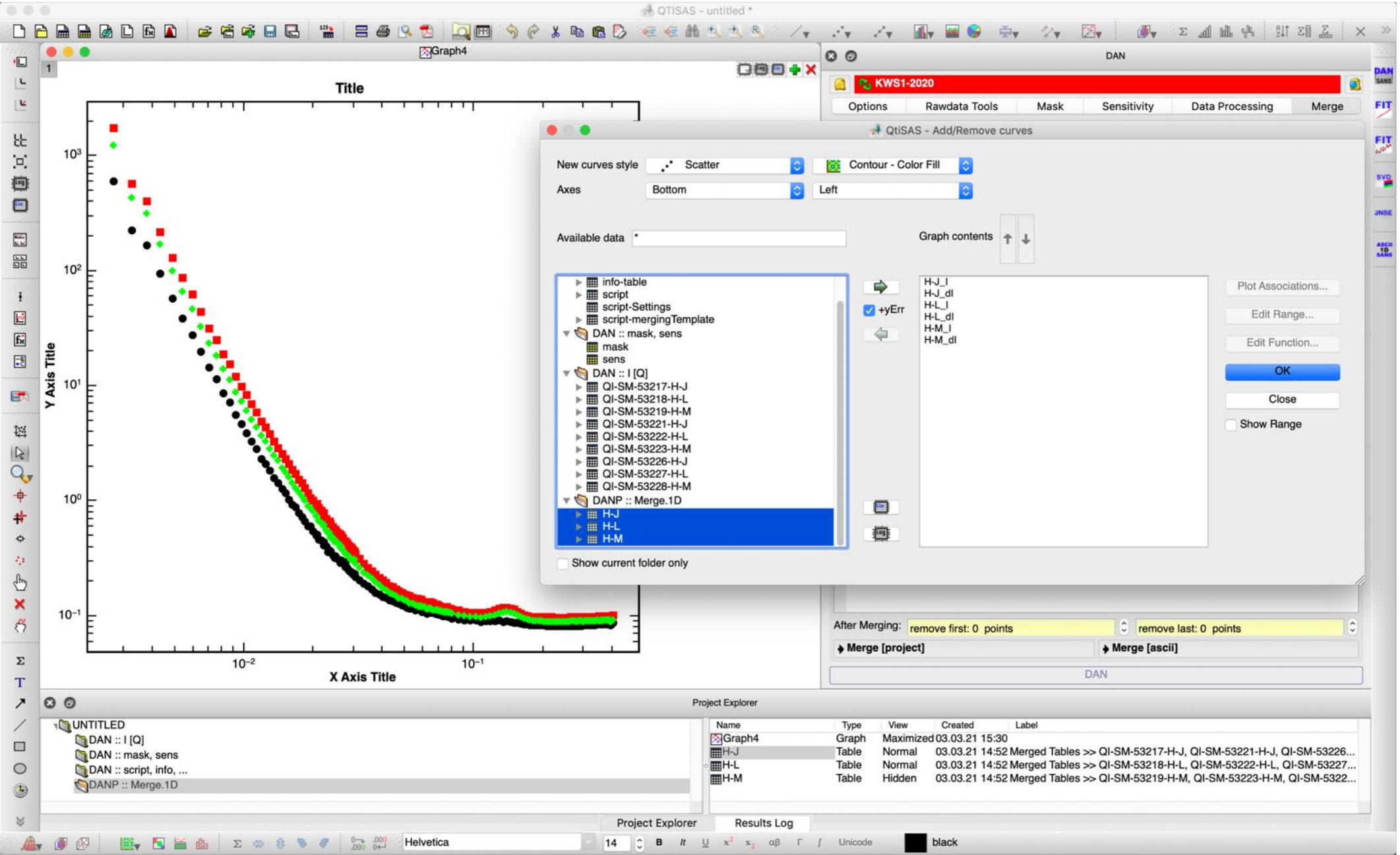
Merging Result: merged tables are located in “DANP:: Merge.1D”



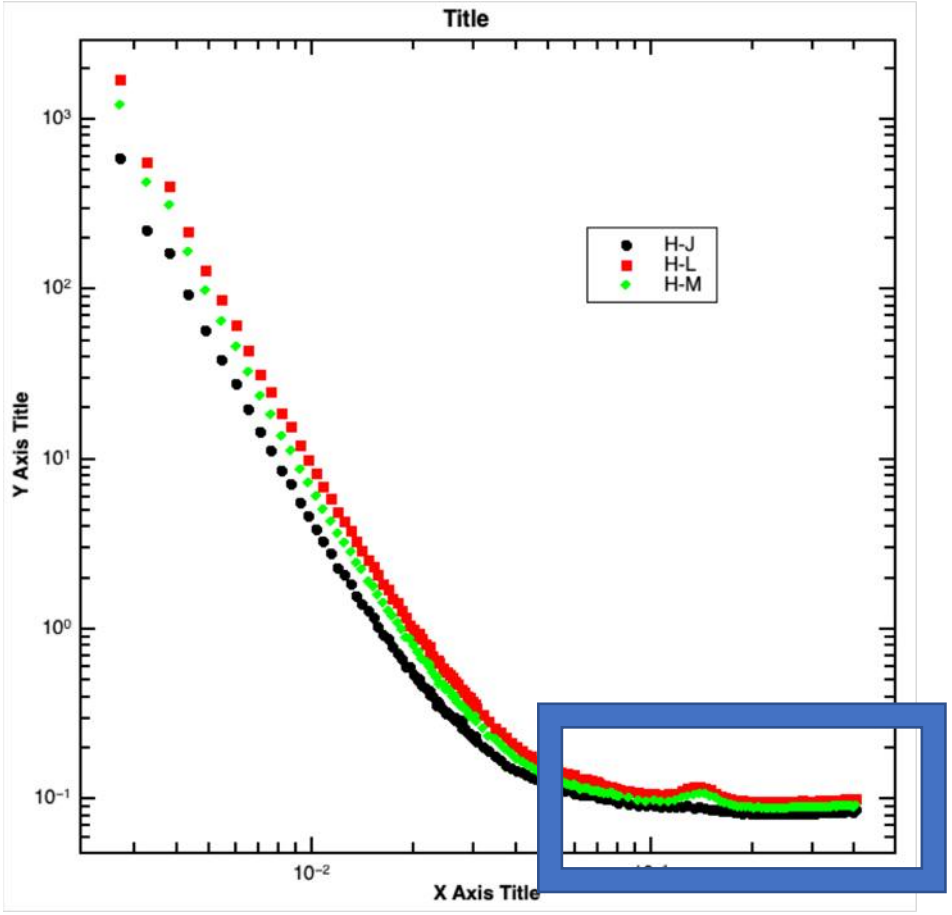
Plotting Example of Merged Data

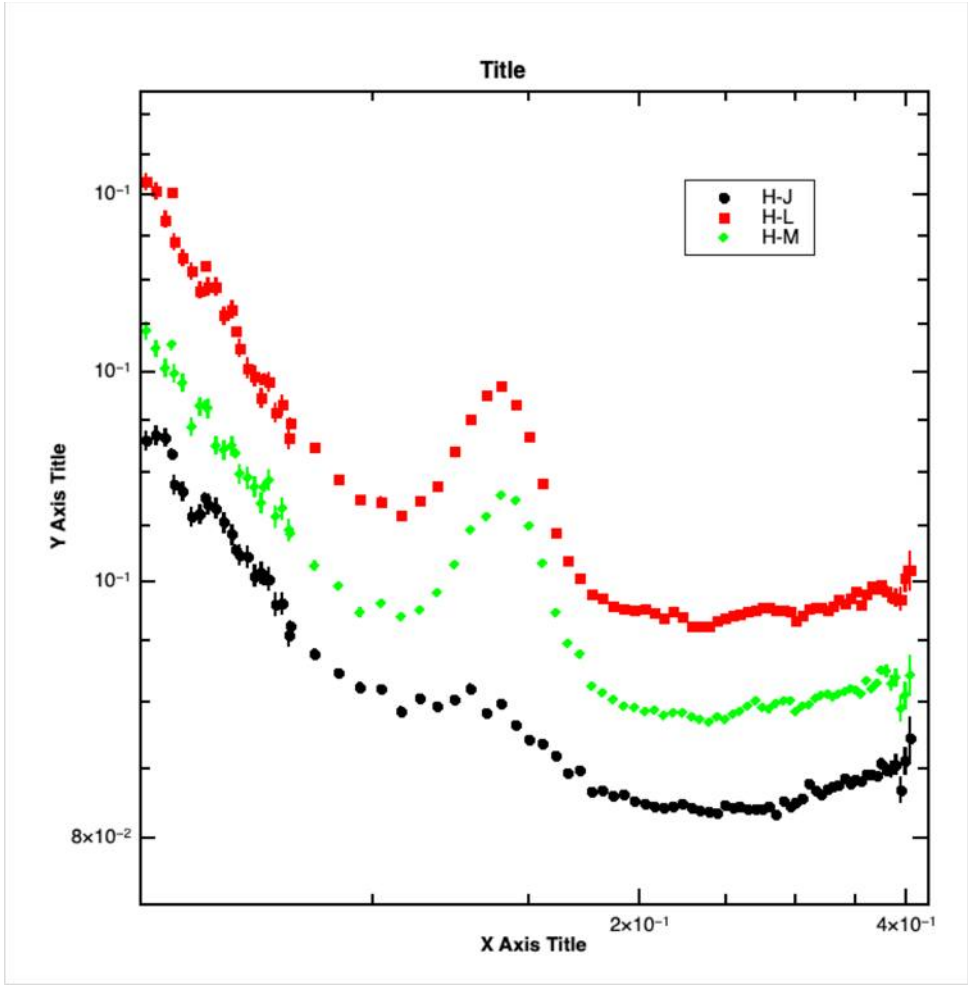

QTISAS - untitled *
H-J - Merged Tables >> QI-SM-53217-H-J, QI-SM-53221-H-J, QI-SM-53226-H-J,
Q[X]
I[Y]
Plot
Cut
Copy
Paste
Set As
Set Column Values ... ⌥Q
Recalculate ⌘↵
Fill Column With
Normalize
Frequency Count ...
Statistics on Columns
Clear
Delete
Hide Selected
Show All Columns
Insert
Add Column ⌥C
Sort Column
Sort Table...
Adjust Column Width
Column Options ... ⌥⌘O
Line
Scatter
Line + Symbol
Special Line/Symbol
Columns
Rows
Special Bar/Column
Area
Pie
Ribbon
Bars
Scatter
Trajectory
Statistical Graphs
DAN
KWS1-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Merging Options ::
Number of tables for merging
Number of table-sets for merging
Overlap control
Filter (Wild Card)
Indexing [Output]
Smart merging ::
Reference column
normalization
(plus) left-side points
(plus) right-side points
scale error-bars too
Read from active Table
Save as a new Table
New Table Name
Q-Range-1
Q-Range-2
Q-Range-3
H-J
H-L
H-M
After Merging:
remove first: 0 points
remove last: 0 points
Merge [project]
Merge [ascii]
DAN
Project Explorer
UNTITLED
DAN :: I [Q]
DAN :: mask, sens
DAN :: script, info, ...
DANP :: Merge.1D
Name
Type
View
Created
Label
Project Explorer
Results Log
Helvetica
15
Unicode


QTISAS - untitled *
Graph4
Title
H-J
Y Axis Title
X Axis Title
DAN
KWS1-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Merging Options ::
Number of tables for merging
Number of table-sets for merging
Overlap control
Filter (Wild Card)
Indexing [Output]
Smart merging ::
Reference column
normalization
(plus) left-side points
(plus) right-side points
scale error-bars too
Read from active Table
Save as a new Table
New Table Name
Q-Range-1
Q-Range-2
Q-Range-3
H-J
H-L
H-M
After Merging:
remove first: 0 points
remove last: 0 points
Merge [project]
Merge [ascii]
DAN
Project Explorer
UNTITLED
DAN :: I [Q]
DAN :: mask, sens
DAN :: script, info, ...
DANP :: Merge.1D
Name
Type
View
Created
Label
Graph4 Graph Maximized 03.03.21 15:30
H-J Table Normal 03.03.21 14:52 Merged Tables >> QI-SM-53217-H-J, QI-SM-53221-H-J, QI-SM-53226...
H-L Table Normal 03.03.21 14:52 Merged Tables >> QI-SM-53218-H-L, QI-SM-53222-H-L, QI-SM-53227...
H-M Table Hidden 03.03.21 14:52 Merged Tables >> QI-SM-53219-H-M, QI-SM-53223-H-M, QI-SM-5322...
Project Explorer
Results Log
Helvetica
14
Unicode
black


QTISAS - untitled *
Graph4
Title
Y Axis Title
X Axis Title
DAN
KWS1-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
QtiSAS - Add/Remove curves
New curves style
Scatter
Contour - Color Fill
Axes
Bottom
Left
Available data
Graph contents
info-table
script
script-Settings
script-mergingTemplate
DAN :: mask, sens
mask
sens
DAN :: I [Q]
QI-SM-53217-H-J
QI-SM-53218-H-L
QI-SM-53219-H-M
QI-SM-53221-H-J
QI-SM-53222-H-L
QI-SM-53223-H-M
QI-SM-53226-H-J
QI-SM-53227-H-L
QI-SM-53228-H-M
DANP :: Merge.1D
H-J
H-L
H-M
+yErr
H-J_I
H-J_dI
H-L_I
H-L_dI
H-M_I
H-M_dI
Plot Associations...
Edit Range...
Edit Function...
OK
Close
Show Range
Show current folder only
After Merging:
remove first: 0 points
remove last: 0 points
Merge [project]
Merge [ascii]
DAN
Project Explorer
UNTITLED
DAN :: I [Q]
DAN :: mask, sens
DAN :: script, info, ...
DANP :: Merge.1D
Name Type View Created Label
Graph4 Graph Maximized 03.03.21 15:30
H-J Table Normal 03.03.21 14:52 Merged Tables >> QI-SM-53217-H-J, QI-SM-53221-H-J, QI-SM-53226...
H-L Table Normal 03.03.21 14:52 Merged Tables >> QI-SM-53218-H-L, QI-SM-53222-H-L, QI-SM-53227...
H-M Table Hidden 03.03.21 14:52 Merged Tables >> QI-SM-53219-H-M, QI-SM-53223-H-M, QI-SM-5322...
Project Explorer
Results Log
Helvetica
14
Unicode
black

Plotting example: result



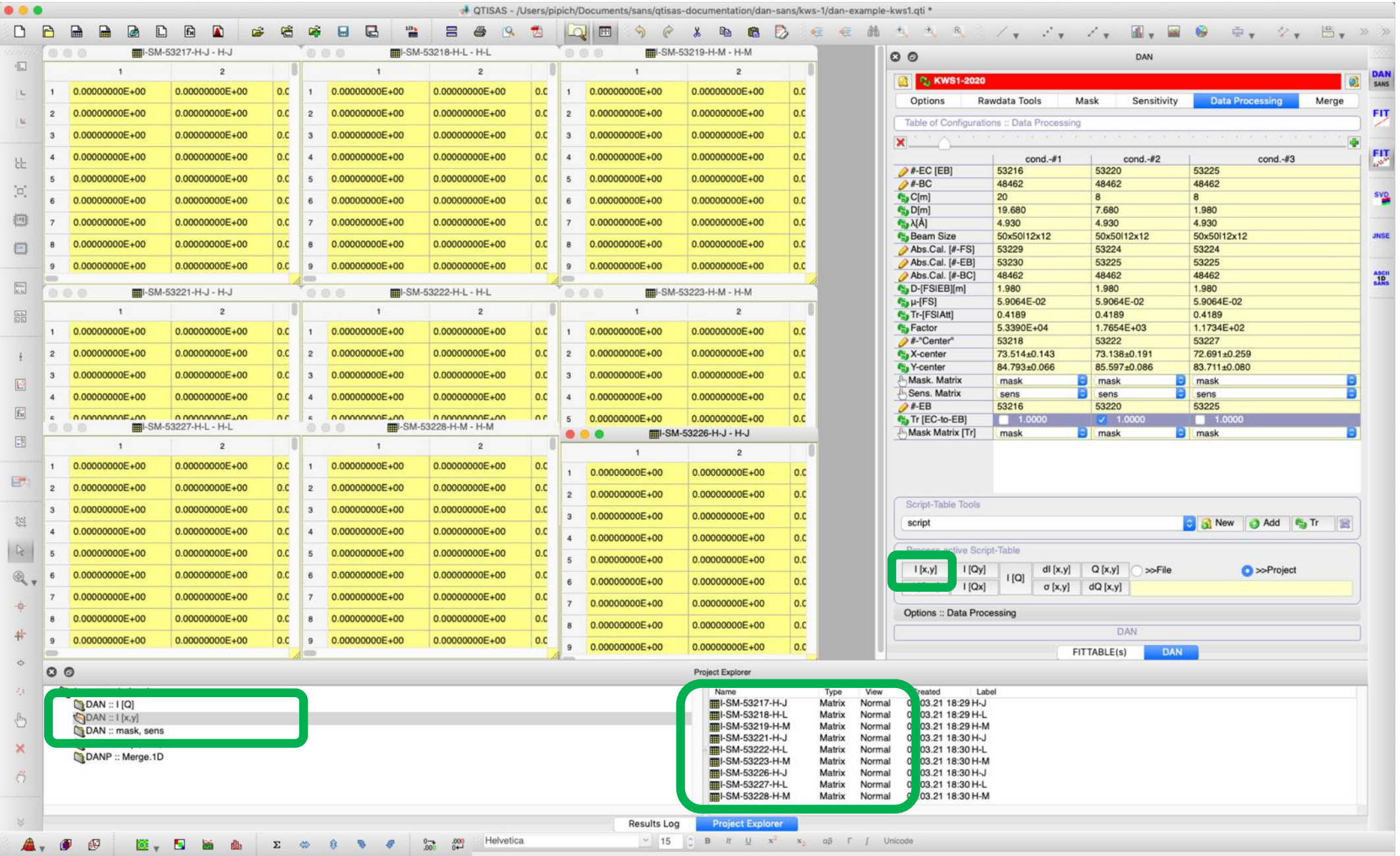


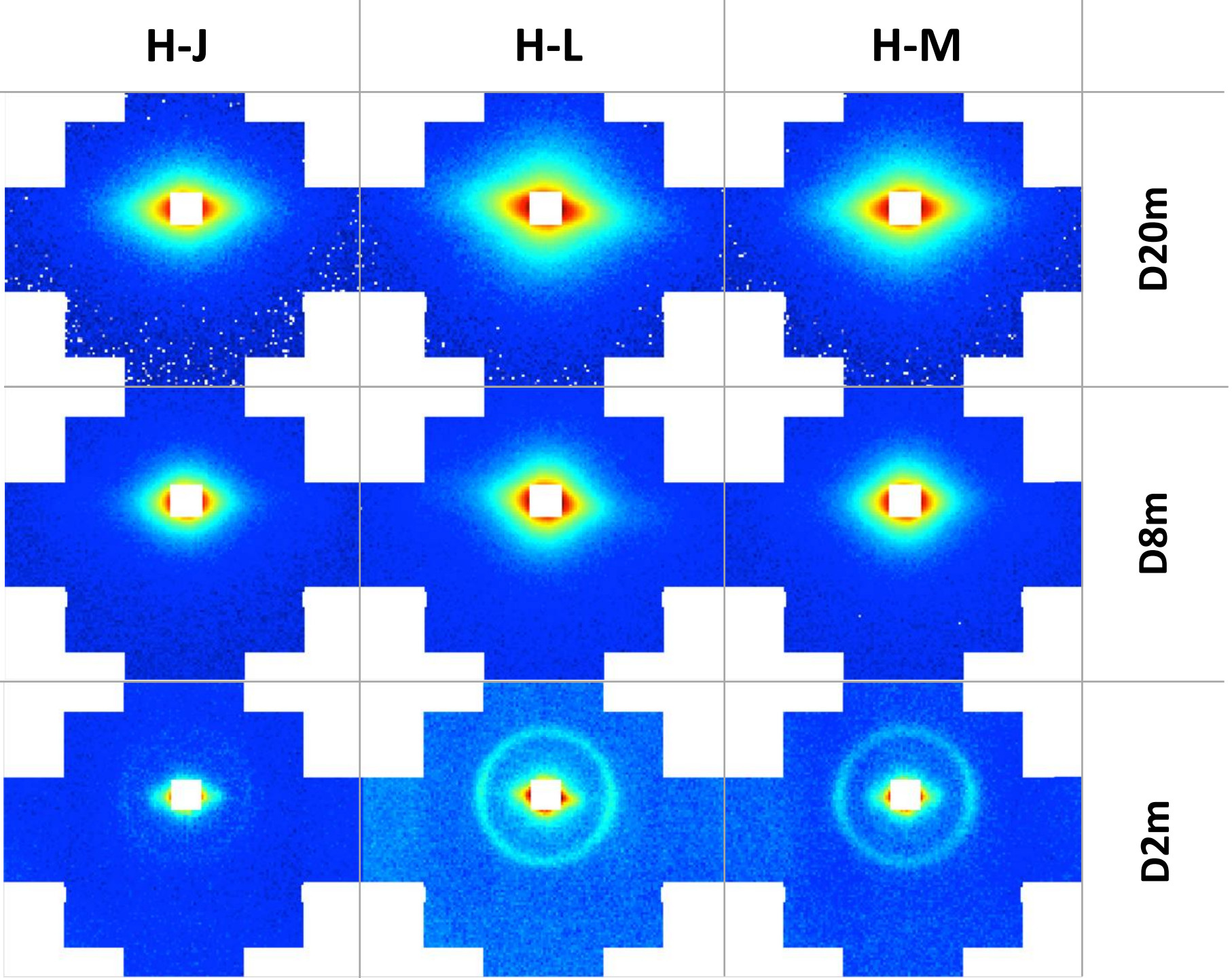
STEP 11: Reduced Detector Images

1. **Selected:** “script” table

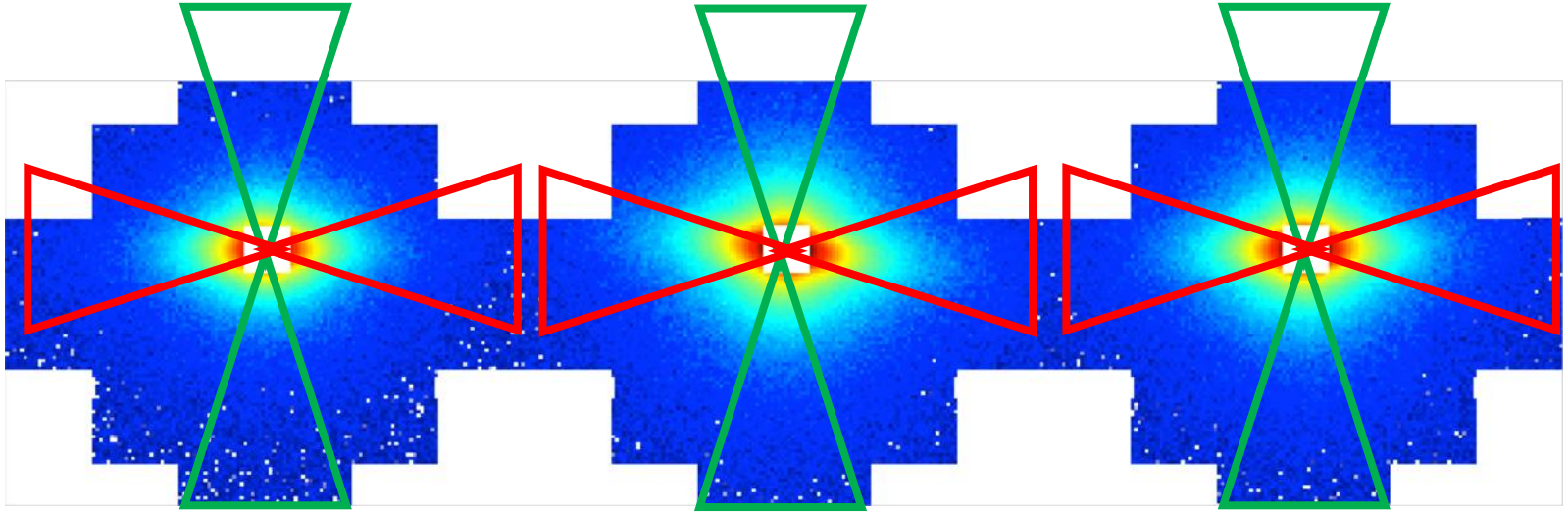
2. **Selected:** as tables/matrixes in the current project (“**>>Project**”)

3. **Pushed:** **I[x,y]** for radial averaging;


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-1/dan-example-kws1.qti *
I-SM-53217-H-J - H-J
I-SM-53218-H-L - H-L
I-SM-53219-H-M - H-M
I-SM-53221-H-J - H-J
I-SM-53222-H-L - H-L
I-SM-53223-H-M - H-M
I-SM-53227-H-L - H-L
I-SM-53228-H-M - H-M
I-SM-53226-H-J - H-J
DAN
KWS1-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Table of Configurations :: Data Processing
cond.-#1
cond.-#2
cond.-#3
#-EC [EB]
#-BC
C[m]
D[m]
λ[Å]
Beam Size
Abs.Cal. [#-FS]
Abs.Cal. [#-EB]
Abs.Cal. [#-BC]
D-[FSiEB][m]
μ-[FS]
Tr-[FSiAtt]
Factor
#-"Center"
X-center
Y-center
Mask. Matrix
Sens. Matrix
#-EB
Tr [EC-to-EB]
Mask Matrix [Tr]
Script-Table Tools
script
New
Add
Tr
I [x,y]
I [Qy]
I [Qx]
I [Q]
dI [x,y]
σ [x,y]
Q [x,y]
dQ [x,y]
>>File
>>Project
Options :: Data Processing
DAN
FITTABLE(s)
DAN
Project Explorer
DAN :: I [Q]
DAN :: I [x,y]
DAN :: mask, sens
DANP :: Merge.1D
Name
Type
View
Created
Label
Results Log
Project Explorer
Helvetica

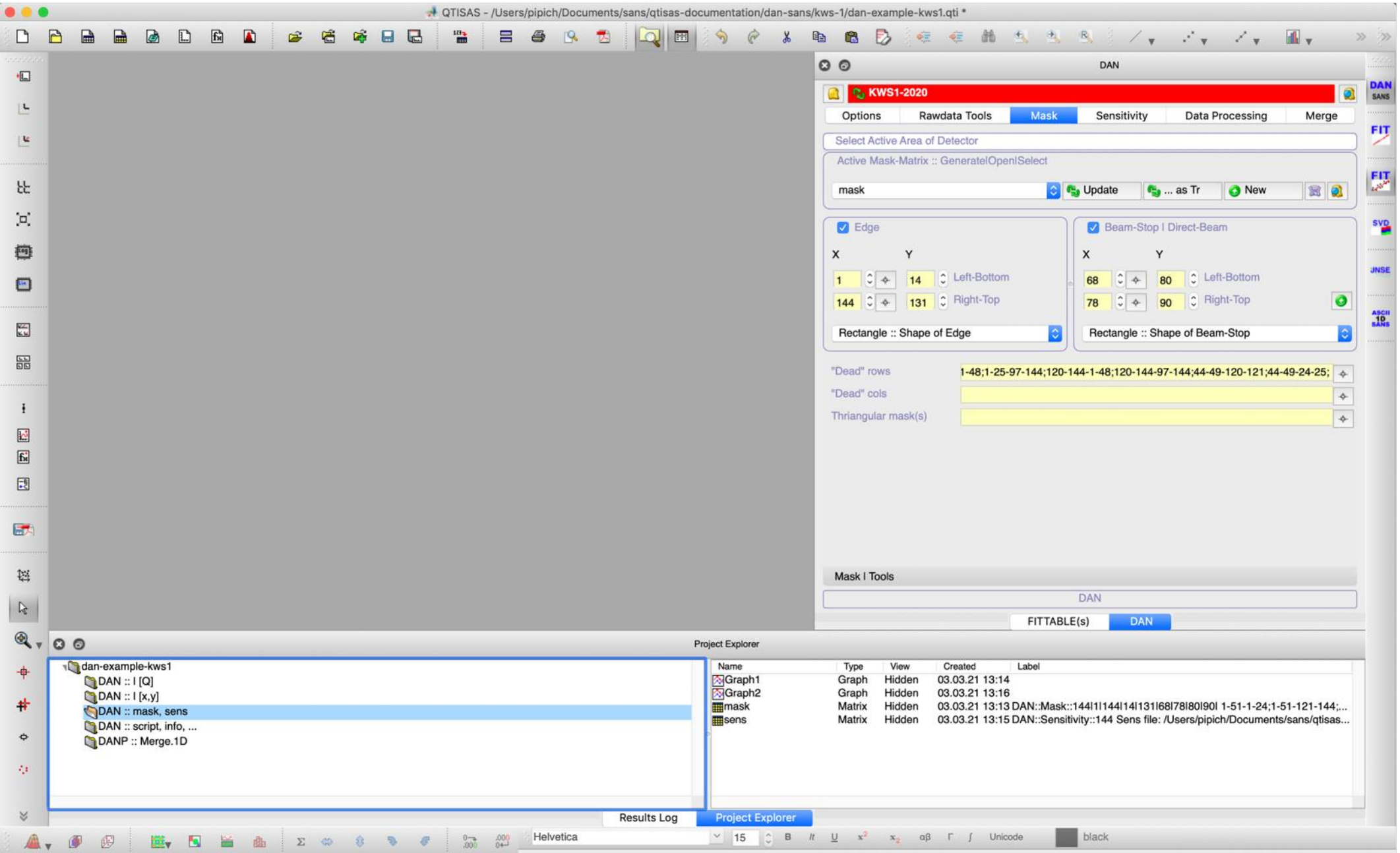

H-J
H-L
H-M
D20m
D8m
D2m

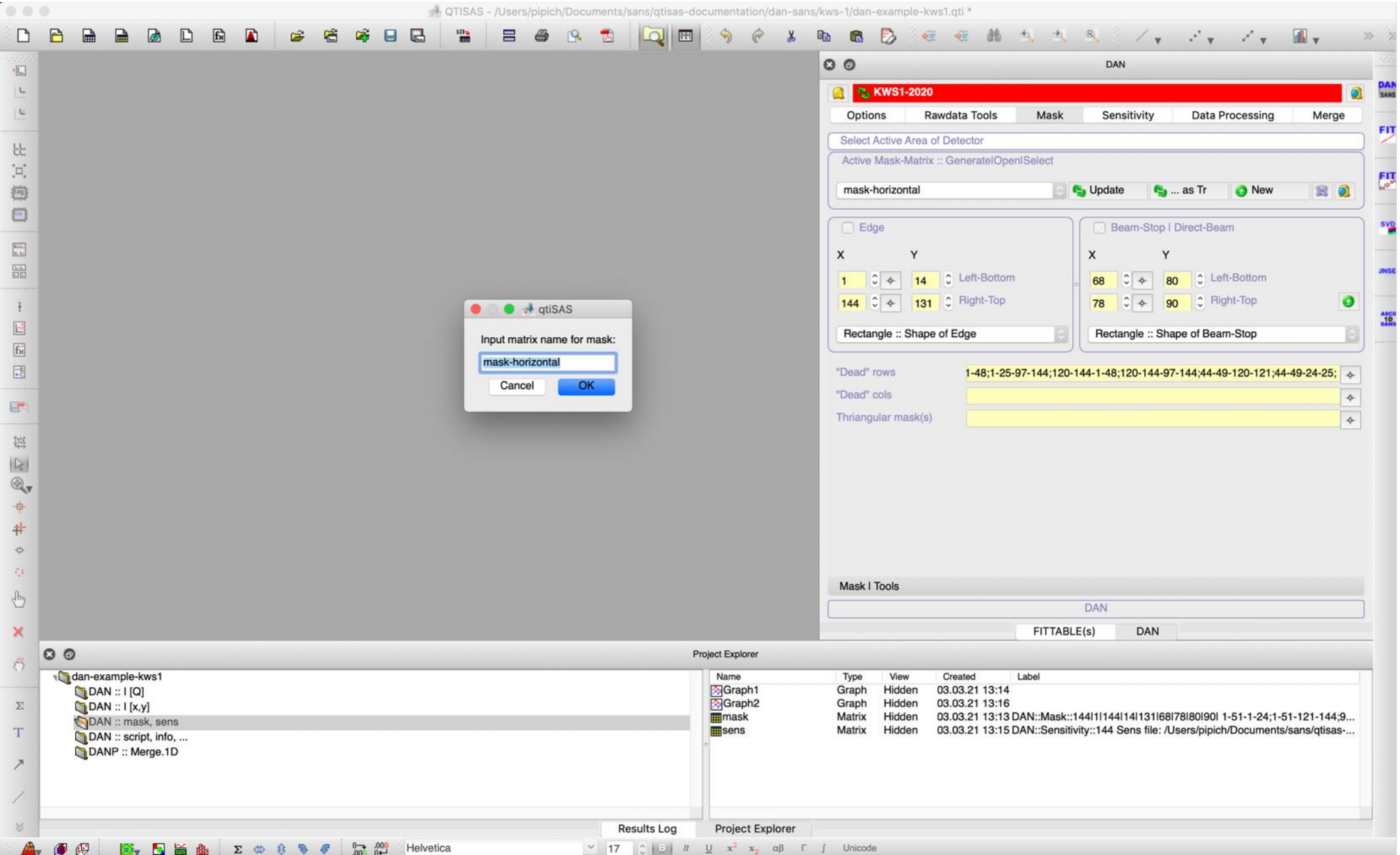
Problem: scattering is not ISOTROPIC



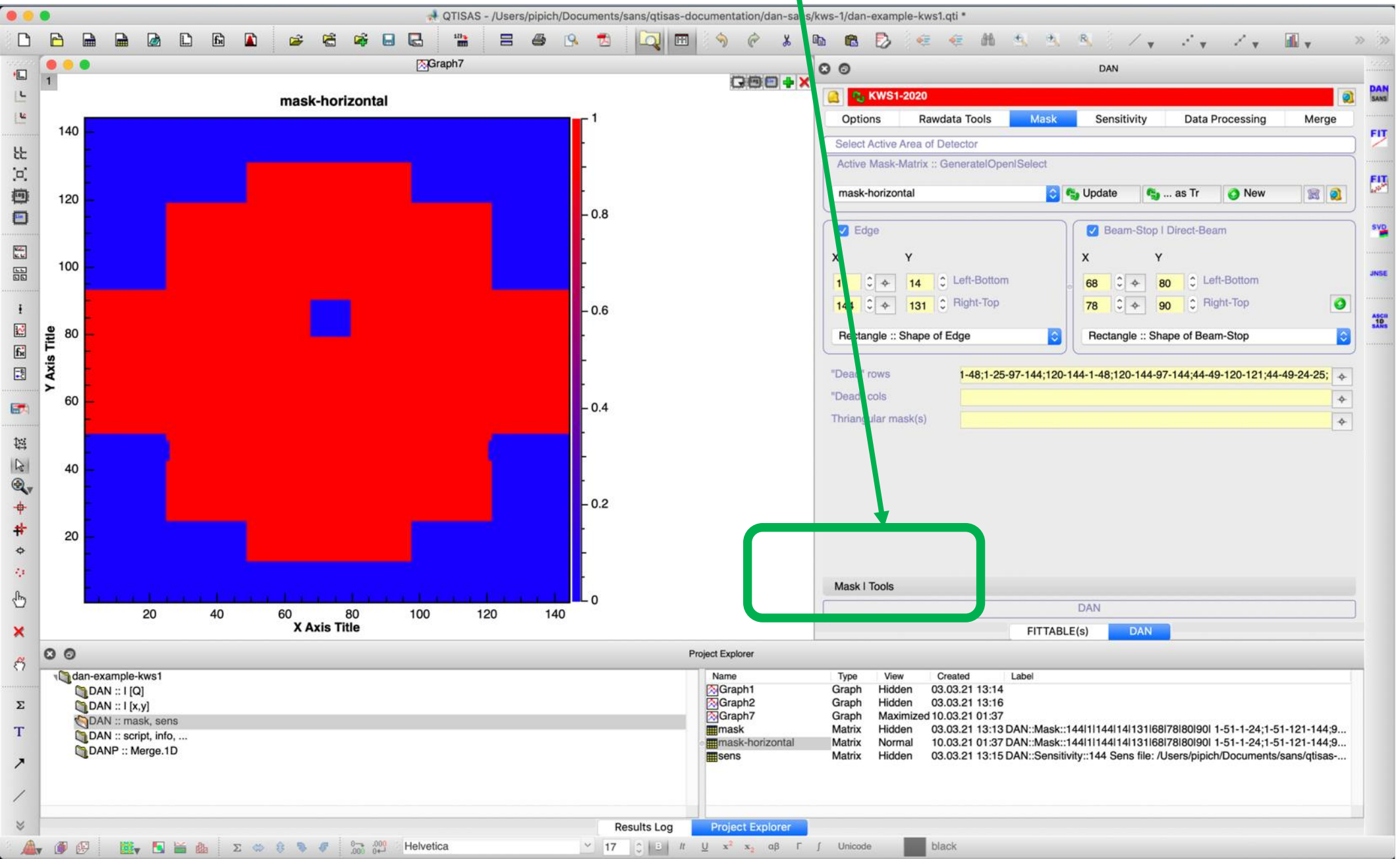
! Vertical & Horizontal Masks!

mask-horizontal


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-1/dan-example-kws1.qti *
DAN
KWS1-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask
Update
... as Tr
New
Edge
X
Y
1
14
Left-Bottom
144
131
Right-Top
Rectangle :: Shape of Edge
Beam-Stop | Direct-Beam
X
Y
68
80
Left-Bottom
78
90
Right-Top
Rectangle :: Shape of Beam-Stop
"Dead" rows
1-48;1-25-97-144;120-144-1-48;120-144-97-144;44-49-120-121;44-49-24-25;
"Dead" cols
Thriangular mask(s)
Mask | Tools
DAN
FITTABLE(s)
DAN
Project Explorer
dan-example-kws1
DAN :: I [Q]
DAN :: I [x,y]
DAN :: mask, sens
DAN :: script, info, ...
DANP :: Merge.1D
Name
Type
View
Created
Label
Graph1
Graph
Hidden
03.03.21 13:14
Graph2
Graph
Hidden
03.03.21 13:16
mask
Matrix
Hidden
03.03.21 13:13 DAN::Mask::144|1|144|14|131|68|78|80|90| 1-51-1-24;1-51-121-144;...
sens
Matrix
Hidden
03.03.21 13:15 DAN::Sensitivity::144 Sens file: /Users/pipich/Documents/sans/qtisas...
Results Log
Project Explorer
Helvetica
15
Unicode
black


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-1/dan-example-kws1.qti *
DAN
KWS1-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-horizontal
Update
... as Tr
New
Edge
X
Y
1
14
Left-Bottom
144
131
Right-Top
Rectangle :: Shape of Edge
Beam-Stop | Direct-Beam
X
Y
68
80
Left-Bottom
78
90
Right-Top
Rectangle :: Shape of Beam-Stop
"Dead" rows
1-48;1-25-97-144;120-144-1-48;120-144-97-144;44-49-120-121;44-49-24-25;
"Dead" cols
Thriangular mask(s)
Mask | Tools
DAN
FITTABLE(s)
DAN
qtiSAS
Input matrix name for mask:
mask-horizontal
Cancel
OK
Project Explorer
dan-example-kws1
DAN :: I [Q]
DAN :: I [x,y]
DAN :: mask, sens
DAN :: script, info, ...
DANP :: Merge.1D
Name
Type
View
Created
Label
Graph1
Graph
Hidden
03.03.21 13:14
Graph2
Graph
Hidden
03.03.21 13:16
mask
Matrix
Hidden
03.03.21 13:13 DAN::Mask::144|1|144|14|131|68|78|80|90| 1-51-1-24;1-51-121-144;9...
sens
Matrix
Hidden
03.03.21 13:15 DAN::Sensitivity::144 Sens file: /Users/pipich/Documents/sans/qtisas-...
Results Log
Project Explorer
Helvetica
17
Unicode

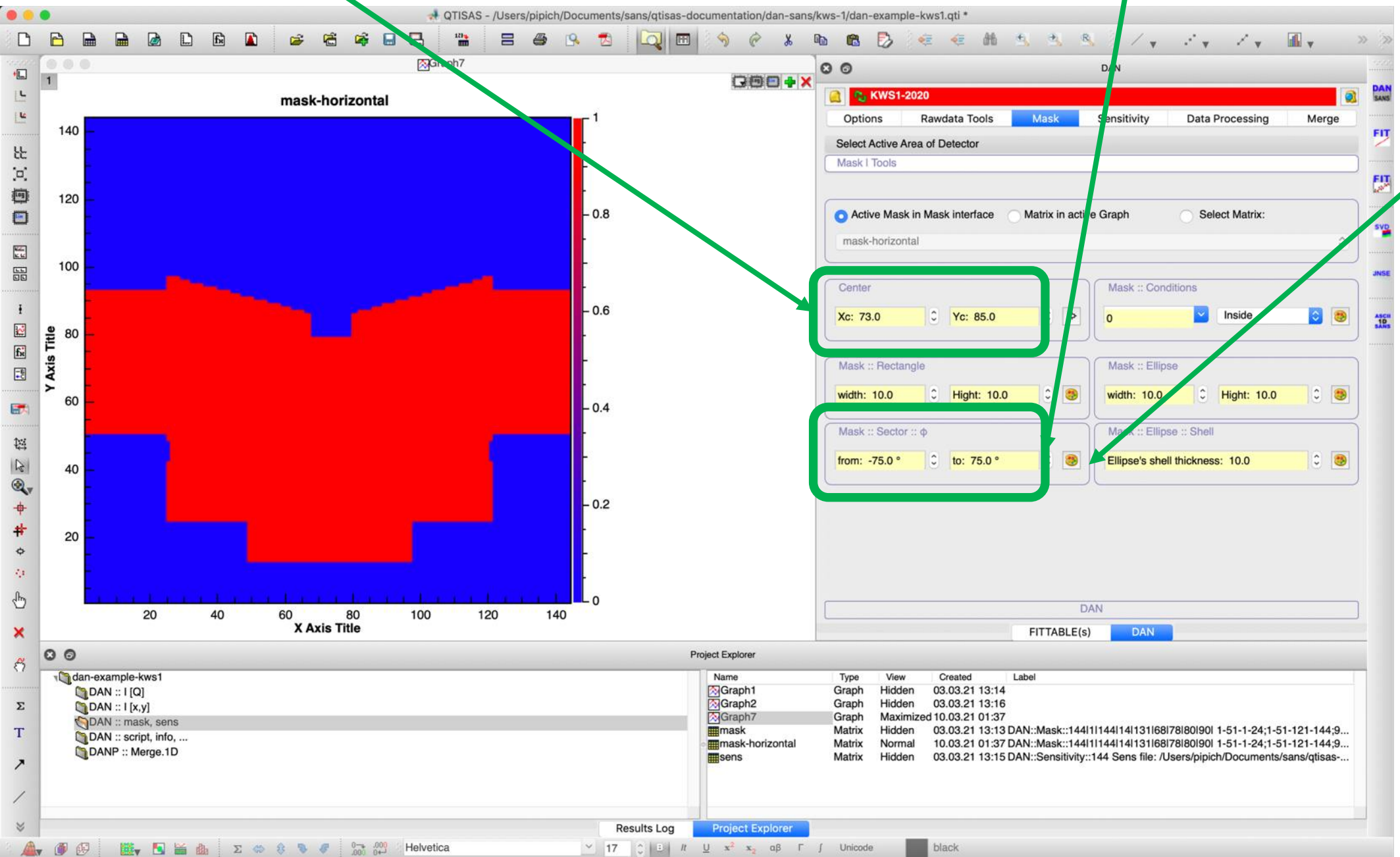
go to **Mask|Tools**



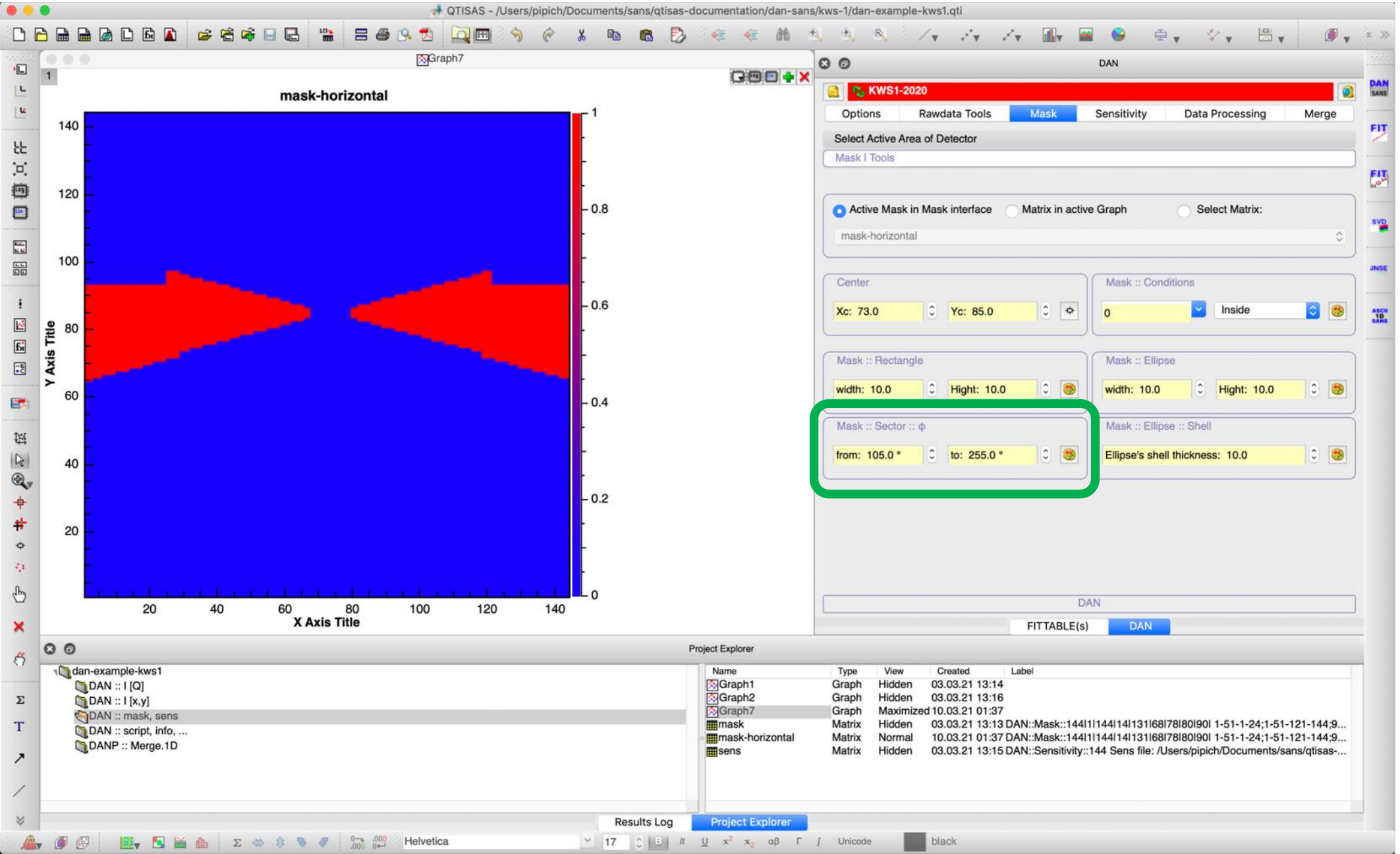
1. Set **Center** of the beam-stop

2. Set **Sector** range.

3. Push



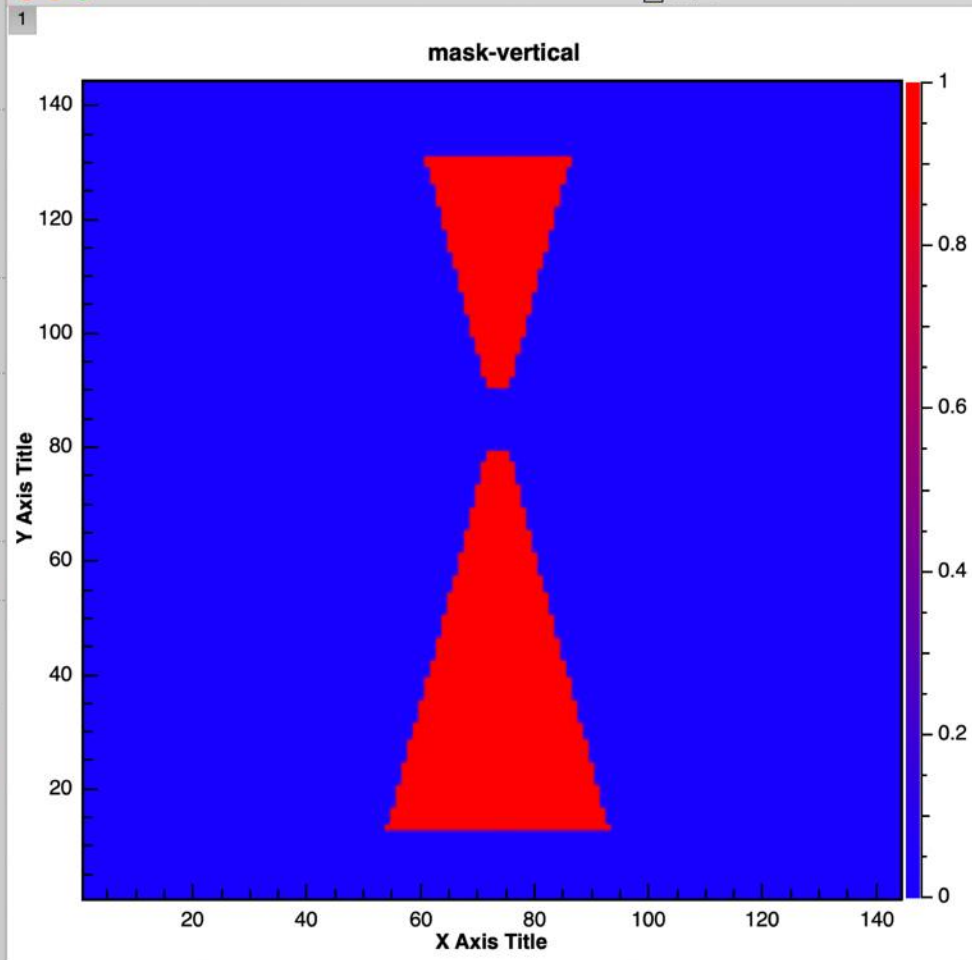
Mask also lower sector



mask-vertical

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-1/dan-example-kws1.qti *

Graph8



DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | Merge

Select Active Area of Detector

Mask I Tools

Active Mask in Mask interface | Matrix in active Graph | Select Matrix:

mask-vertical

Center

Xc: 73.0 | Yc: 85.0

Mask :: Conditions

0 | Inside

Mask :: Rectangle

width: 10.0 | Hight: 10.0

Mask :: Ellipse

width: 10.0 | Hight: 10.0

Mask :: Sector :: ϕ

from: 195.0 ° | to: 345.0 °

Mask :: Ellipse :: Shell

Ellipse's shell thickness: 10.0

DAN

FITTABLE(s) | DAN

Project Explorer

- dan-example-kws1
  - DAN :: I [Q]
  - DAN :: I [x,y]
  - DAN :: mask, sens
  - DAN :: script, info, ...
  - DANP :: Merge.1D

Name	Type	View	Created	Label
Graph1	Graph	Hidden	03.03.21 13:14	
Graph2	Graph	Hidden	03.03.21 13:16	
Graph7	Graph	Normal	10.03.21 01:37	
Graph8	Graph	Maximized	10.03.21 01:48	
mask	Matrix	Hidden	03.03.21 13:13	DAN::Mask::144|1|144|14|131|68|78|80|90| 1-51-1-24;1-51-121-144;9...
mask-horizontal	Matrix	Normal	10.03.21 01:37	DAN::Mask::144|1|144|14|131|68|78|80|90| 1-51-1-24;1-51-121-144;9...
mask-vertical	Matrix	Normal	10.03.21 01:48	DAN::Mask::144|1|144|14|131|68|78|80|90| 1-51-1-24;1-51-121-144;9...
sens	Matrix	Hidden	03.03.21 13:15	DAN::Sensitivity::144 Sens file: /Users/pipich/Documents/sans/qtisas-...

Results Log | Project Explorer

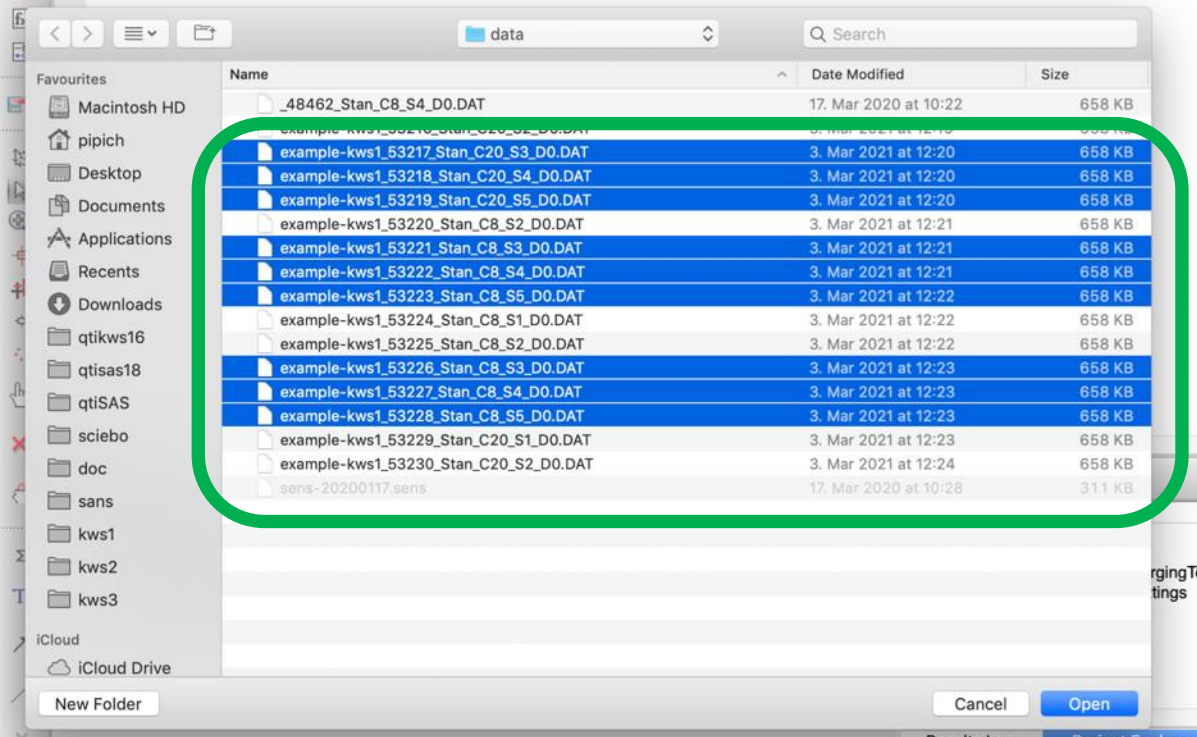
Helvetica | 17 | Unicode | black

Script-Table Modification: adding the same datasets with horizontal and vertical masks

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-1/dan-example-kws1.qti *

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmis
1	H-J	53217	1	20	19.68	4.930	50x50l12x12	48462	53216	0.1	0.9061
2	H-L	53218	1	20	19.68	4.930	50x50l12x12	48462	53216	0.1	0.8981
3	H-M	53219	1	20	19.68	4.930	50x50l12x12	48462	53216	0.1	0.9019
4	H-J	53221	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1	0.9061
5	H-L	53222	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1	0.8981
6	H-M	53223	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1	0.9019
7	H-J	53226	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1	0.9061
8	H-L	53227	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1	0.8981
9	H-M	53228	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1	0.9019



DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | Merge

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2	cond.-#3
λ[Å]	4.930	4.930	4.930
Beam Size	50x50l12x12	50x50l12x12	50x50l12x12
Abs.Cal. [#-FS]	53229	53224	53224
Abs.Cal. [#-EB]	53230	53225	53225
Abs.Cal. [#-BC]	48462	48462	48462
D-[FSlEB][m]	1.980	1.980	1.980
μ-[FS]	5.9064E-02	5.9064E-02	5.9064E-02
Tr-[FSlAtt]	0.4189	0.4189	0.4189
Factor	5.3390E+04	1.7654E+03	1.1734E+02
#-"Center"	53218	53222	53227
X-center	73.514±0.143	73.138±0.191	72.691±0.259
Y-center	84.793±0.066	85.597±0.086	83.711±0.080
Mask. Matrix	mask-horizontal	mask-horizontal	mask-horizontal
Sens. Matrix	sens	sens	sens
#-EB	53216	53220	53225
Tr [EC-to-EB]	1.0000	1.0000	1.0000
Mask Matrix [Tr]	mask	mask	mask

Script-Table Tools

script | New | Add | Tr

Script-Table

I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

I [Q,ϕ] | I [Qx] | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

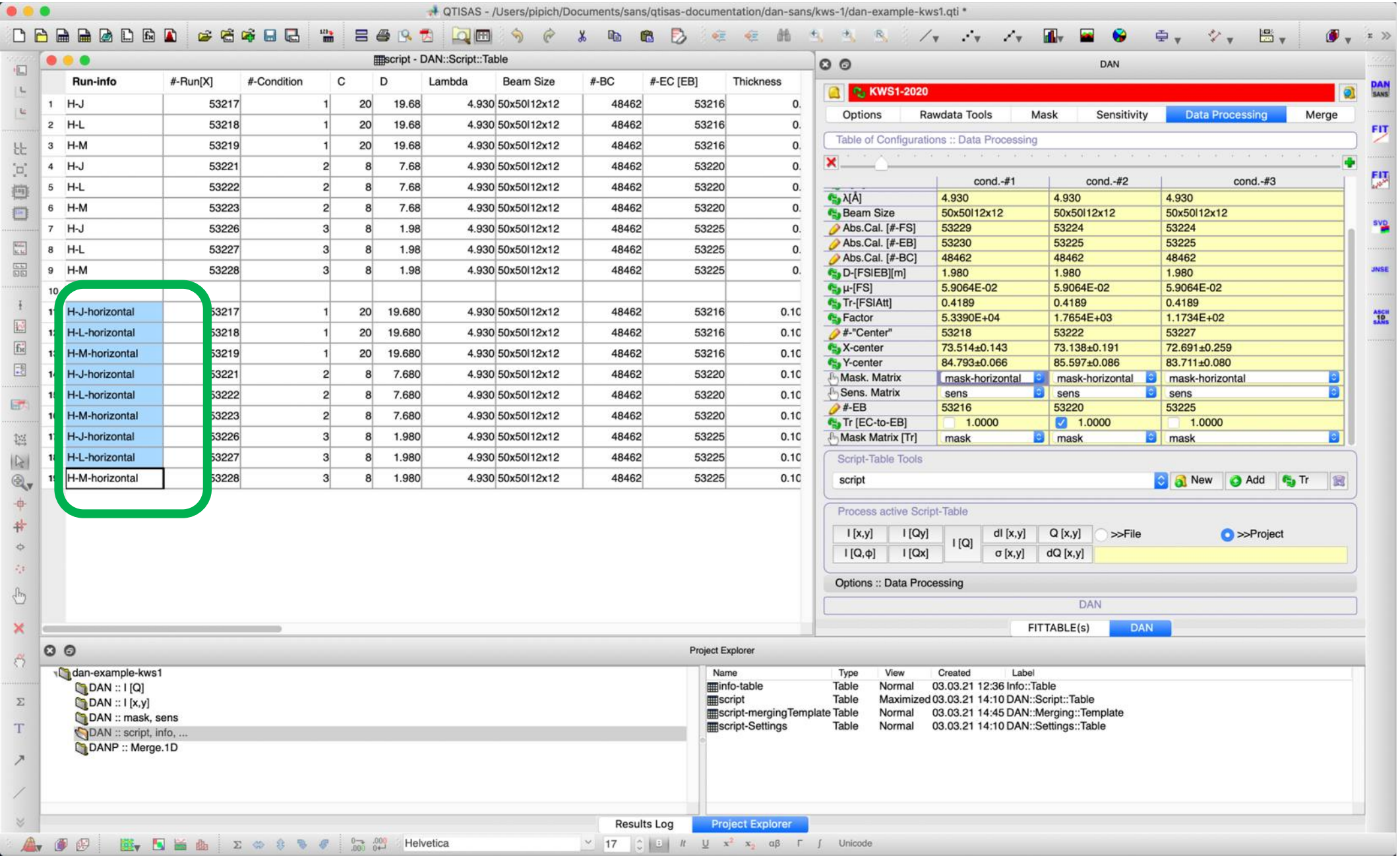
FITTABLE(s) | DAN

	Type	View	Created	Label
	Table	Normal	03.03.21 12:36	Info::Table
	Table	Maximized	03.03.21 14:10	DAN::Script::Table
rgingTemplate	Table	Normal	03.03.21 14:45	DAN::Merging::Template
tings	Table	Normal	03.03.21 14:10	DAN::Settings::Table

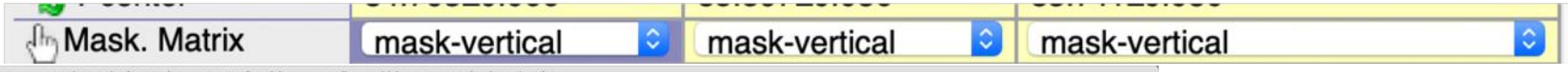
Results Log | Project Explorer

Helvetica 17 Unicode

Sample Names: added suffix “-horizontal”



Sample Names: added suffix “-vertical”



QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-1/dan-example-kws1.qti *

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness
5	H-L	53222	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1
6	H-M	53223	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1
7	H-J	53226	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1
8	H-L	53227	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1
9	H-M	53228	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1
10										
11	H-J-horizontal	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100
12	H-L-horizontal	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100
13	H-M-horizontal	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100
14	H-J-horizontal	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100
15	H-L-horizontal	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100
16	H-M-horizontal	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100
17	H-J-horizontal	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100
18	H-L-horizontal	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100
19	H-M-horizontal	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100
20										
21	H-J-vertical	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100
22	H-L-vertical	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100
23	H-M-vertical	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100
24	H-J-vertical	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100
25	H-L-vertical	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100
26	H-M-vertical	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100
27	H-J-vertical	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100
28	H-L-vertical	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100
29	H-M-vertical	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100

DAN

KWS1-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing | Merge

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2	cond.-#3
D[m]	19.680	7.680	1.980
λ[Å]	4.930	4.930	4.930
Beam Size	50x50l12x12	50x50l12x12	50x50l12x12
Abs.Cal. [#-FS]	53229	53224	53224
Abs.Cal. [#-EB]	53230	53225	53225
Abs.Cal. [#-BC]	48462	48462	48462
D-[FSIEB][m]	1.980	1.980	1.980
μ-[FS]	5.9064E-02	5.9064E-02	5.9064E-02
Tr-[FSIAtt]	0.4189	0.4189	0.4189
Factor	5.3390E+04	1.7654E+03	1.1734E+02
#-"Center"	53218	53222	53227
X-center	73.514±0.143	73.138±0.191	72.691±0.259
Mask. Matrix	mask-vertical	mask-vertical	mask-vertical
#-EB	53216	53220	53225
Tr [EC-to-EB]	1.0000	1.0000	1.0000
Mask Matrix [Tr]	mask	mask	mask

Script-Table Tools

script | New | Add

Process active Script-Table

I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

I [Q,φ] | I [Qx] | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

Project Explorer

dan-example-kws1
- DAN :: I [Q]
- DAN :: I [x,y]
- DAN :: mask, sens
- DAN :: script, info, ...
- DANP :: Merge.1D

Name	Type	View	Created	Label
info-table	Table	Normal	03.03.21 12:36	Info::Table
script	Table	Maximized	03.03.21 14:10	DAN::Script::Table
script-mergingTemplate	Table	Normal	03.03.21 14:45	DAN::Merging::Template
script-Settings	Table	Normal	03.03.21 14:10	DAN::Settings::Table

Results Log | Project Explorer

Helvetica 17 Unicode

New ”script” table

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmission-Sample	Factor	X-center[Y]	Y-center[Y]	**Mask**	Sens
1	H-J	53217	1	20	19.68	4.930	50x50l12x12	48462	53216	0.1	0.9061 [±0.0012]	5.3390E+04	73.514	84.793	mask	sens
2	H-L	53218	1	20	19.68	4.930	50x50l12x12	48462	53216	0.1	0.8981 [±0.0012]	5.3390E+04	73.514	84.793	mask	sens
3	H-M	53219	1	20	19.68	4.930	50x50l12x12	48462	53216	0.1	0.9019 [±0.0012]	5.3390E+04	73.514	84.793	mask	sens
4	H-J	53221	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1	0.9061 [±0.0012]	1.7654E+03	73.138	85.597	mask	sens
5	H-L	53222	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1	0.8981 [±0.0012]	1.7654E+03	73.138	85.597	mask	sens
6	H-M	53223	2	8	7.68	4.930	50x50l12x12	48462	53220	0.1	0.9019 [±0.0012]	1.7654E+03	73.138	85.597	mask	sens
7	H-J	53226	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1	0.9061 [±0.0012]	1.1734E+02	72.691	83.711	mask	sens
8	H-L	53227	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1	0.8981 [±0.0012]	1.1734E+02	72.691	83.711	mask	sens
9	H-M	53228	3	8	1.98	4.930	50x50l12x12	48462	53225	0.1	0.9019 [±0.0012]	1.1734E+02	72.691	83.711	mask	sens
10																
11	H-J-horizontal	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9061 [±0.0012]	53390	73.514	84.793	mask-horizontal	sens
12	H-L-horizontal	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.8981 [±0.0012]	53390	73.514	84.793	mask-horizontal	sens
13	H-M-horizontal	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9019 [±0.0012]	53390	73.514	84.793	mask-horizontal	sens
14	H-J-horizontal	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9061 [±0.0012]	1765.4	73.138	85.597	mask-horizontal	sens
15	H-L-horizontal	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.8981 [±0.0012]	1765.4	73.138	85.597	mask-horizontal	sens
16	H-M-horizontal	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9019 [±0.0012]	1765.4	73.138	85.597	mask-horizontal	sens
17	H-J-horizontal	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9061 [±0.0012]	117.34	72.691	83.711	mask-horizontal	sens
18	H-L-horizontal	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.8981 [±0.0012]	117.34	72.691	83.711	mask-horizontal	sens
19	H-M-horizontal	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9019 [±0.0012]	117.34	72.691	83.711	mask-horizontal	sens
20																
21	H-J-vertical	53217	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9061 [±0.0012]	53390	73.514	84.793	mask-vertical	sens
22	H-L-vertical	53218	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.8981 [±0.0012]	53390	73.514	84.793	mask-vertical	sens
23	H-M-vertical	53219	1	20	19.680	4.930	50x50l12x12	48462	53216	0.100	0.9019 [±0.0012]	53390	73.514	84.793	mask-vertical	sens
24	H-J-vertical	53221	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9061 [±0.0012]	1765.4	73.138	85.597	mask-vertical	sens
25	H-L-vertical	53222	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.8981 [±0.0012]	1765.4	73.138	85.597	mask-vertical	sens
26	H-M-vertical	53223	2	8	7.680	4.930	50x50l12x12	48462	53220	0.100	0.9019 [±0.0012]	1765.4	73.138	85.597	mask-vertical	sens
27	H-J-vertical	53226	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9061 [±0.0012]	117.34	72.691	83.711	mask-vertical	sens
28	H-L-vertical	53227	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.8981 [±0.0012]	117.34	72.691	83.711	mask-vertical	sens
29	H-M-vertical	53228	3	8	1.980	4.930	50x50l12x12	48462	53225	0.100	0.9019 [±0.0012]	117.34	72.691	83.711	mask-vertical	sens

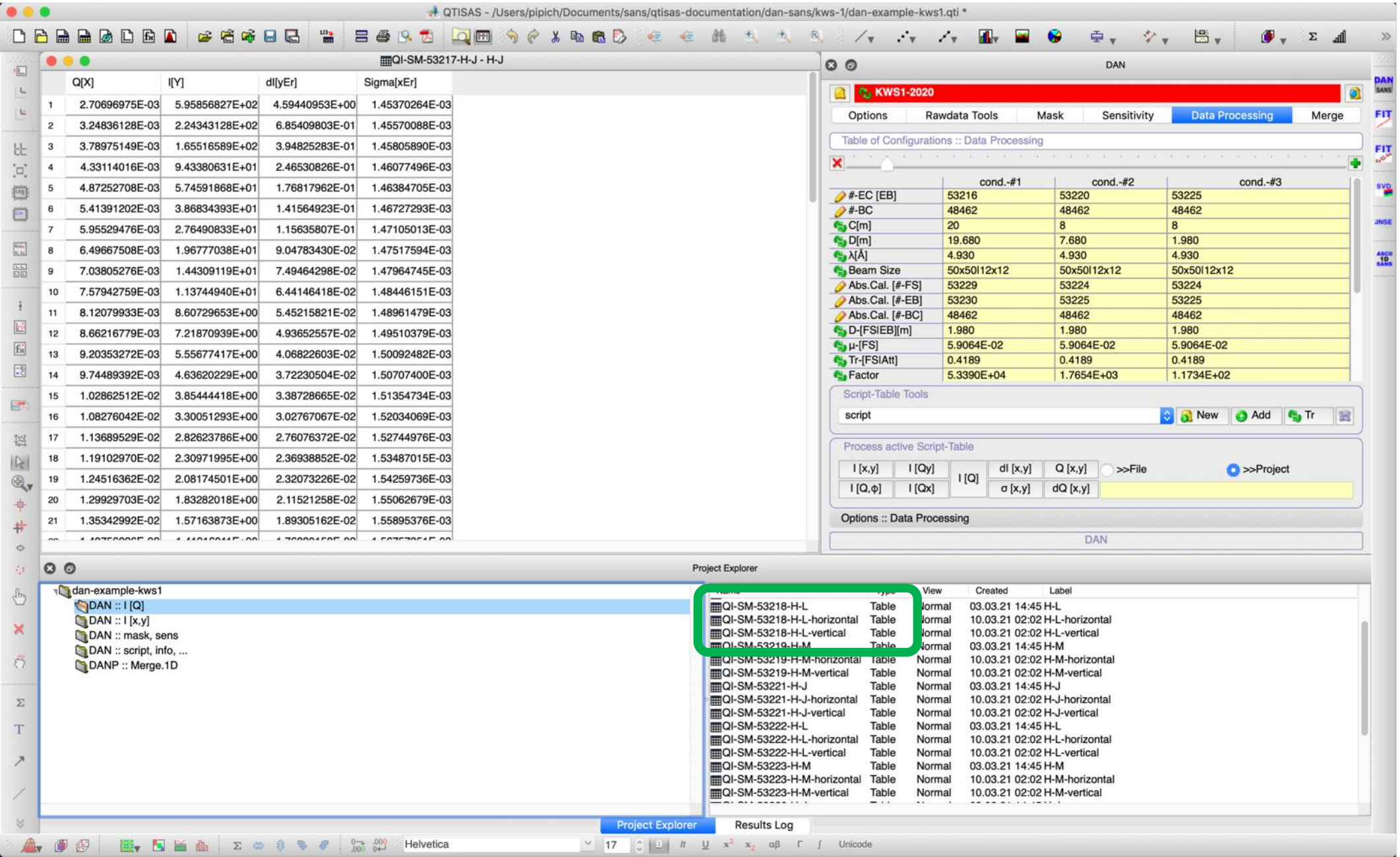
STEP 9-again: Radial Averaging

1. **Selected:** “script” table

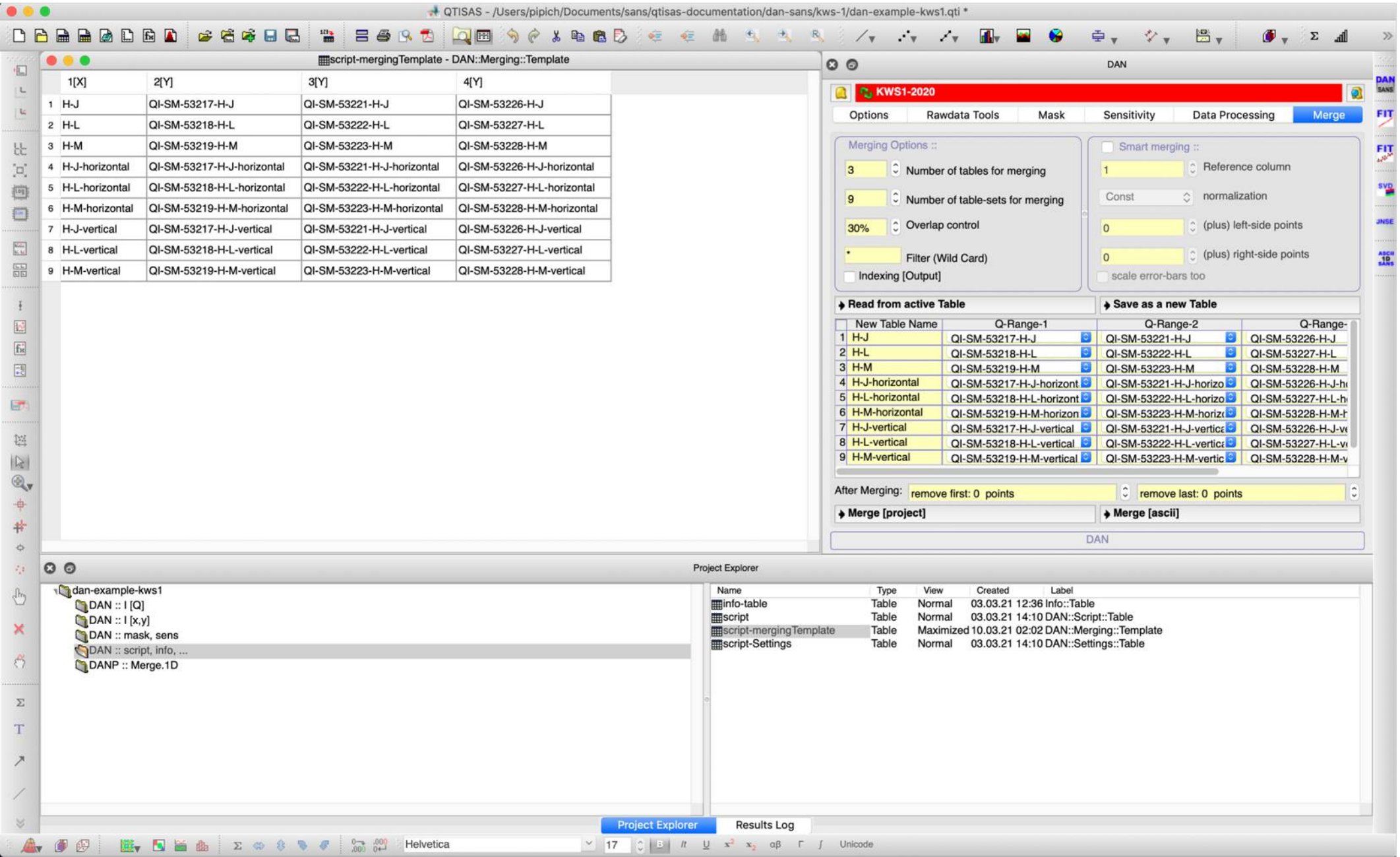
2. **Selected:** as tables/matrixes in the current project (“**>>Project**”)

3. **Pushed:** **I[Q]** for radial averaging;

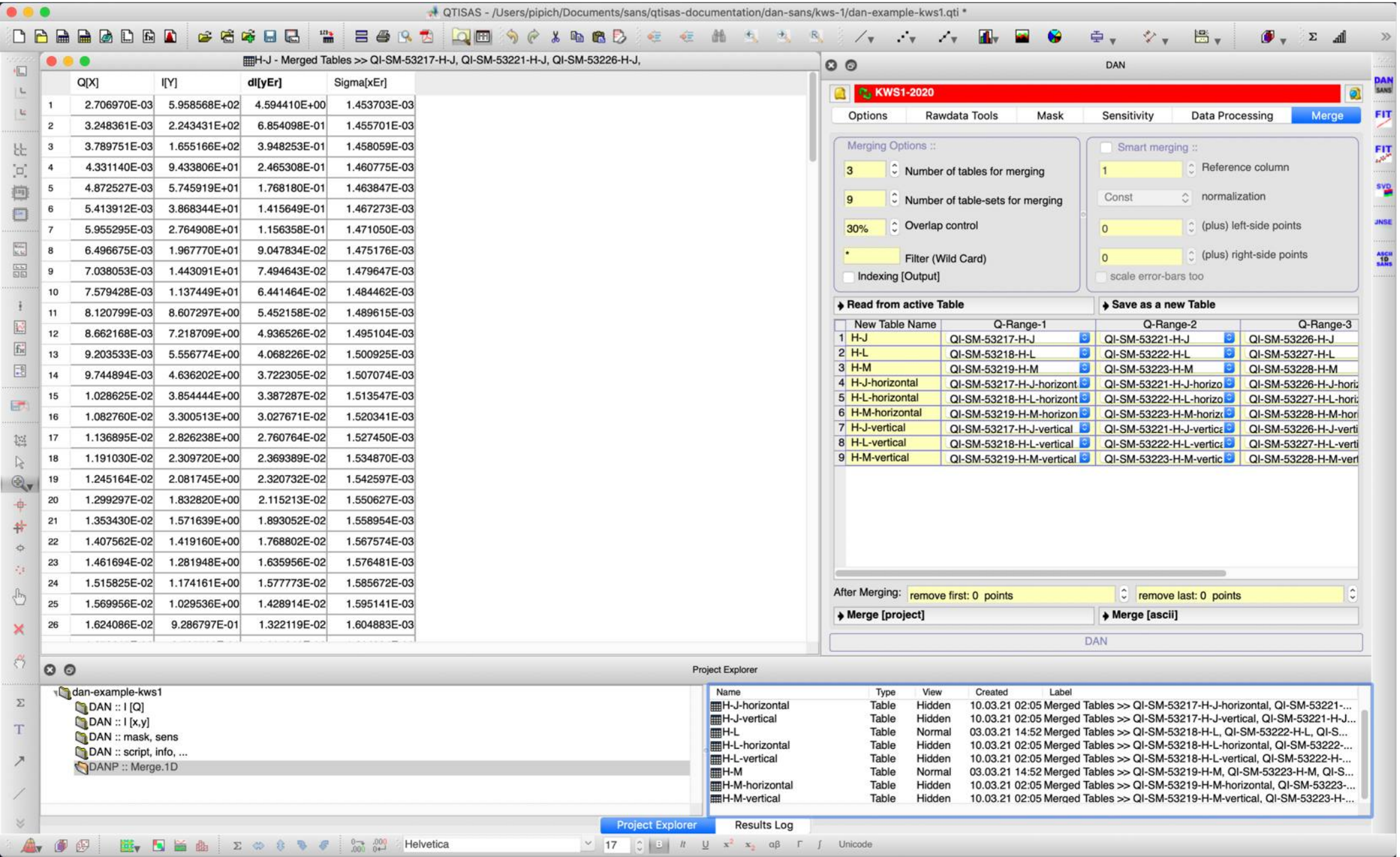
Every run has 3 tables



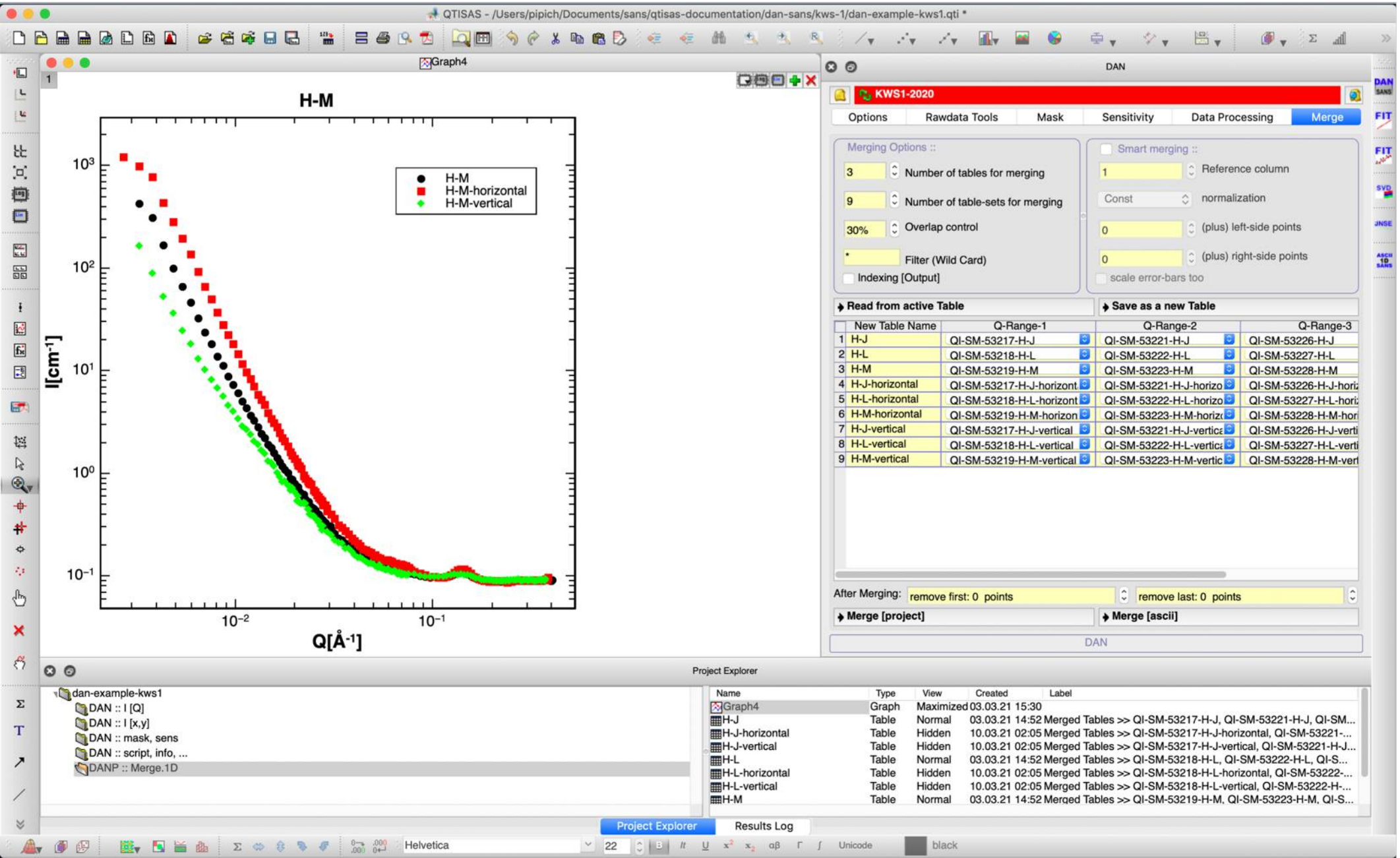
Merging Data

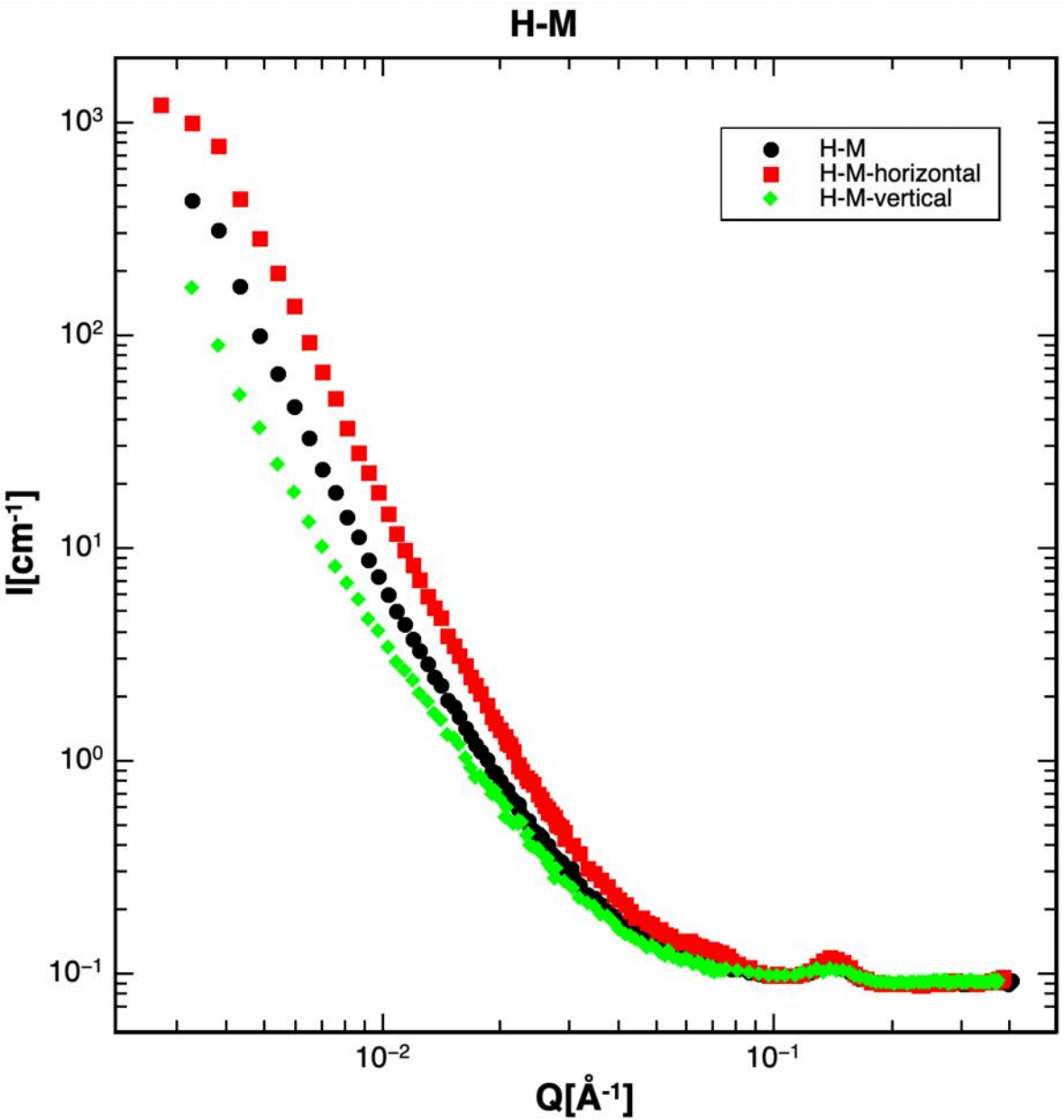


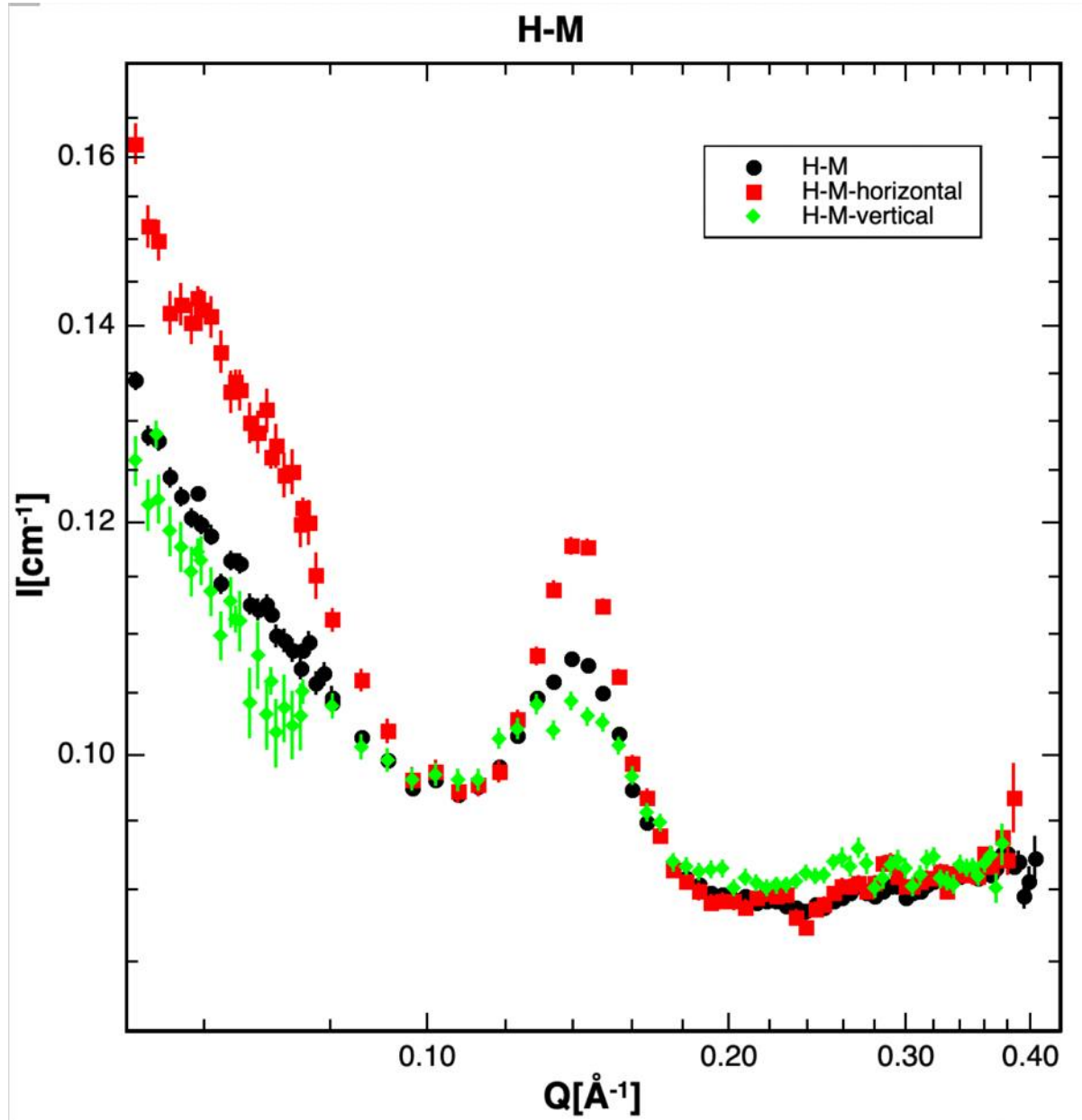
Tables are ready

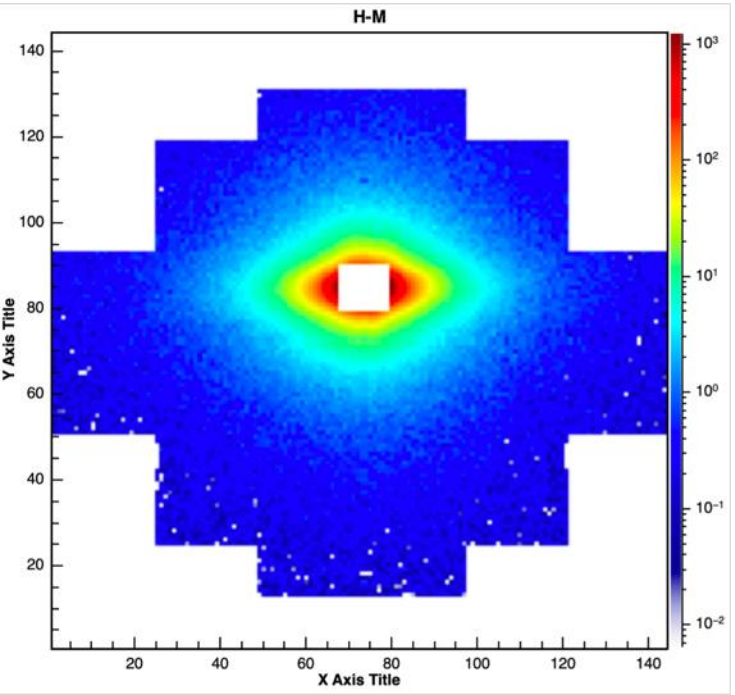


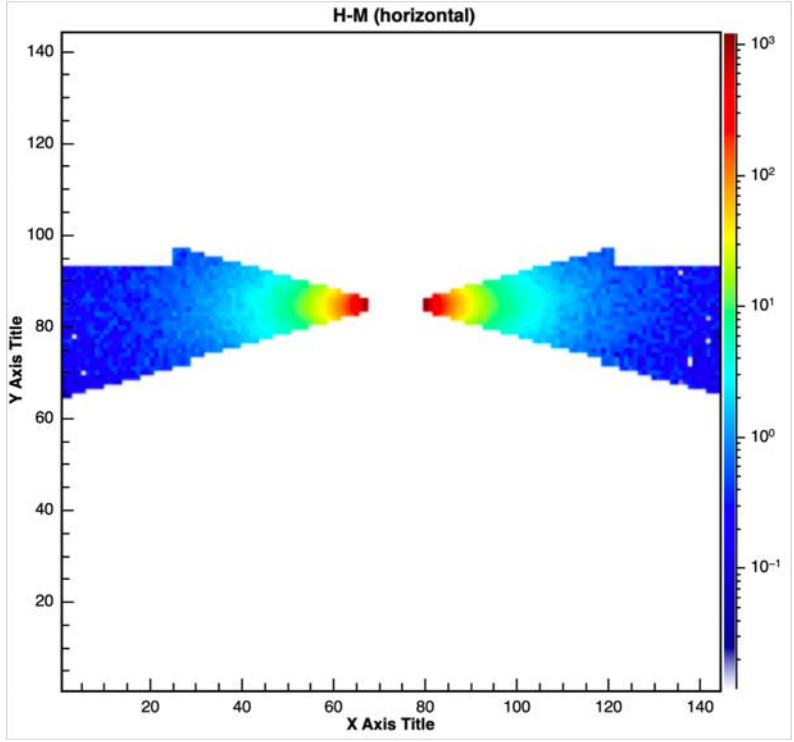
Plotting “H-M” sample averaged with 3 masks

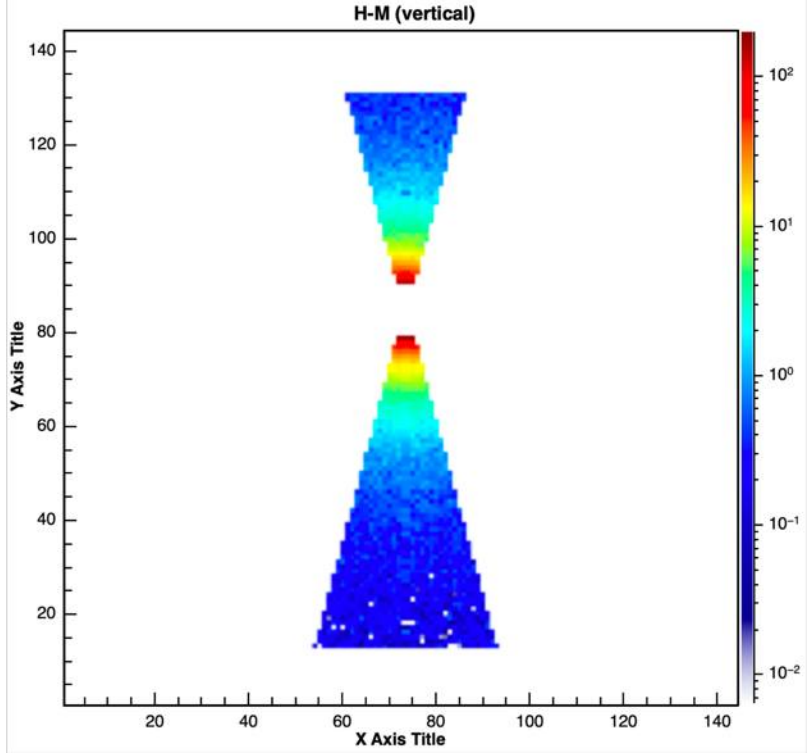



H-M
H-M
H-M-horizontal
H-M-vertical
I[cm-1]
Q[Å-1]
10³
10²
10¹
10⁰
10⁻¹
10⁻²
10⁻¹


H-M
H-M
H-M-horizontal
H-M-vertical
I[cm-1]
Q[Å-1]
0.16
0.14
0.12
0.10
0.10
0.20
0.30
0.40


H-M
Y Axis Title
X Axis Title


H-M (horizontal)
Y Axis Title
X Axis Title


H-M (vertical)
Y Axis Title
X Axis Title