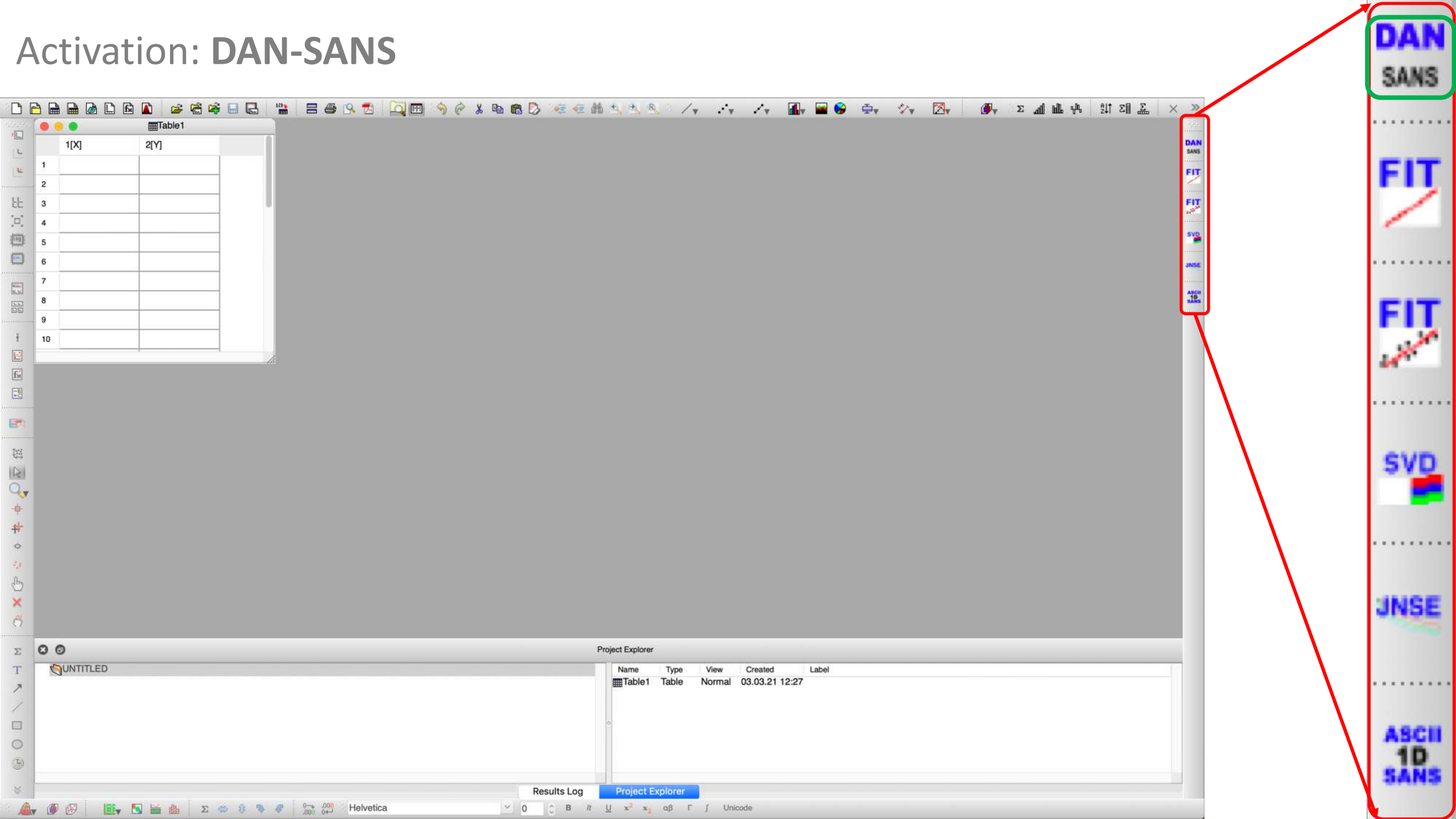
DAN-SANS. Data Reduction. Example.

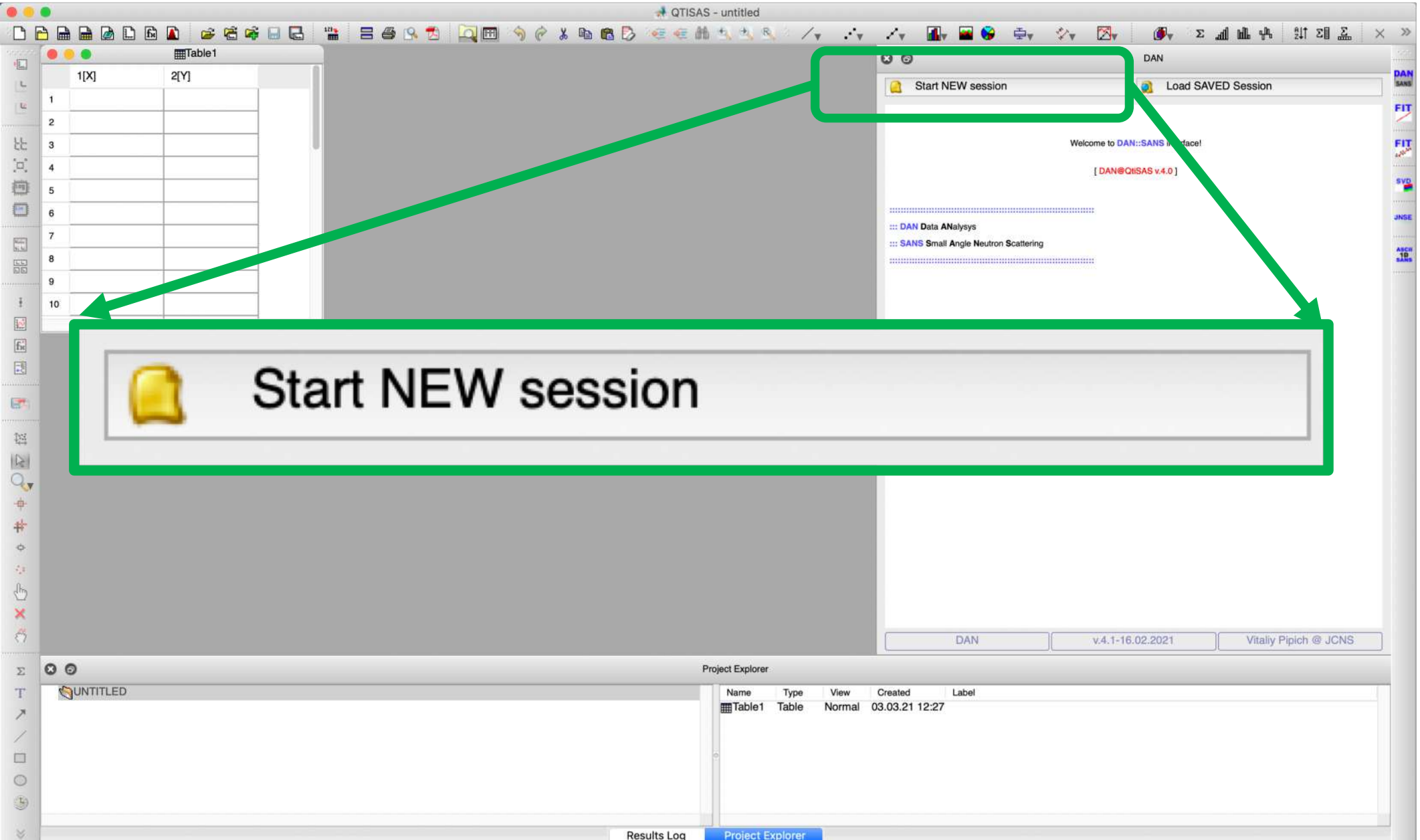
Instrument:	**KWS-3**
Date of the Experiment:	**March.2020**
QtiSAS Version:	**>01.03.2021**
DAN-SANS “Instrument”:	**KWS3-2020**

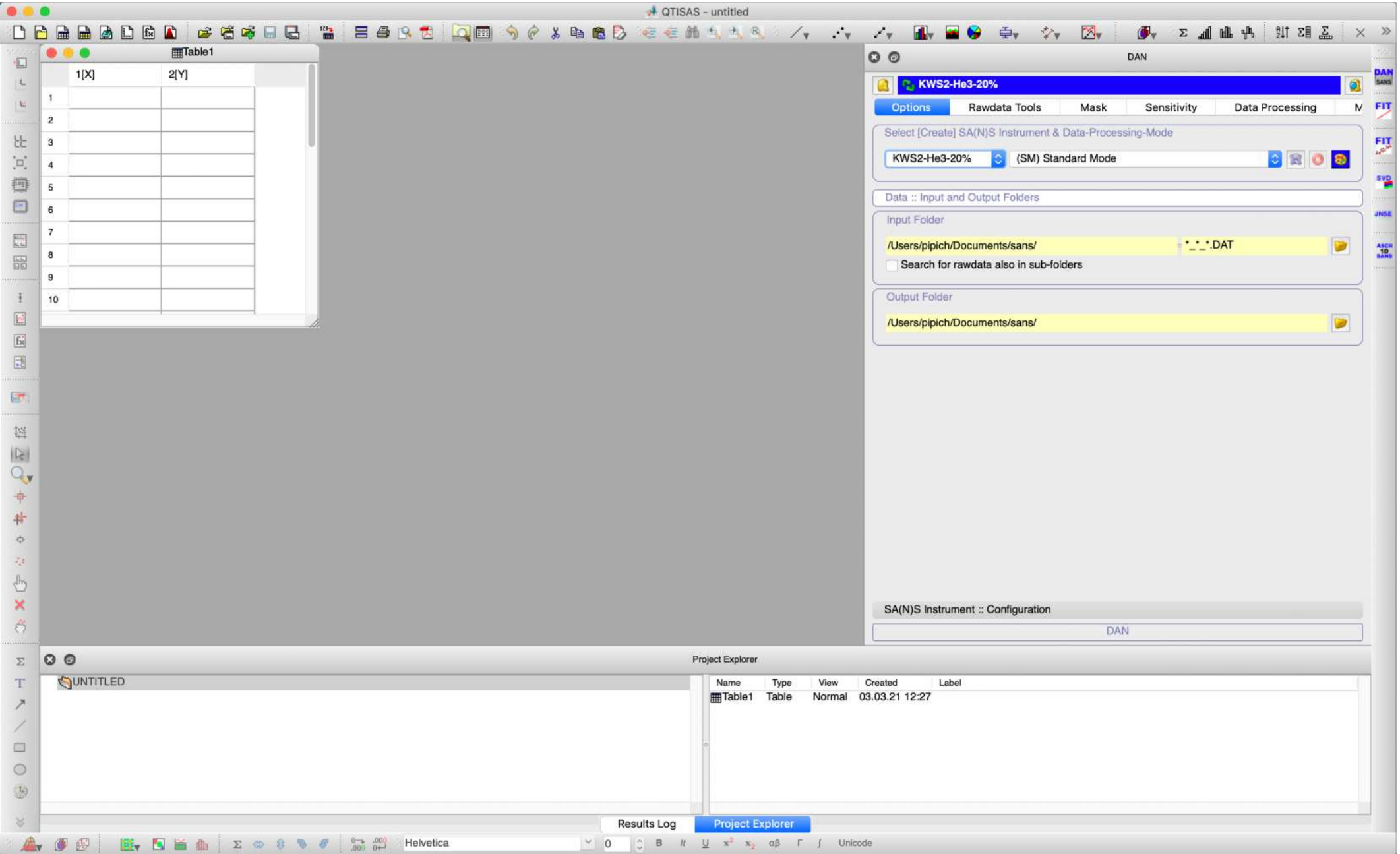
STEP 0: Preparations

Activation: **DAN-SANS**



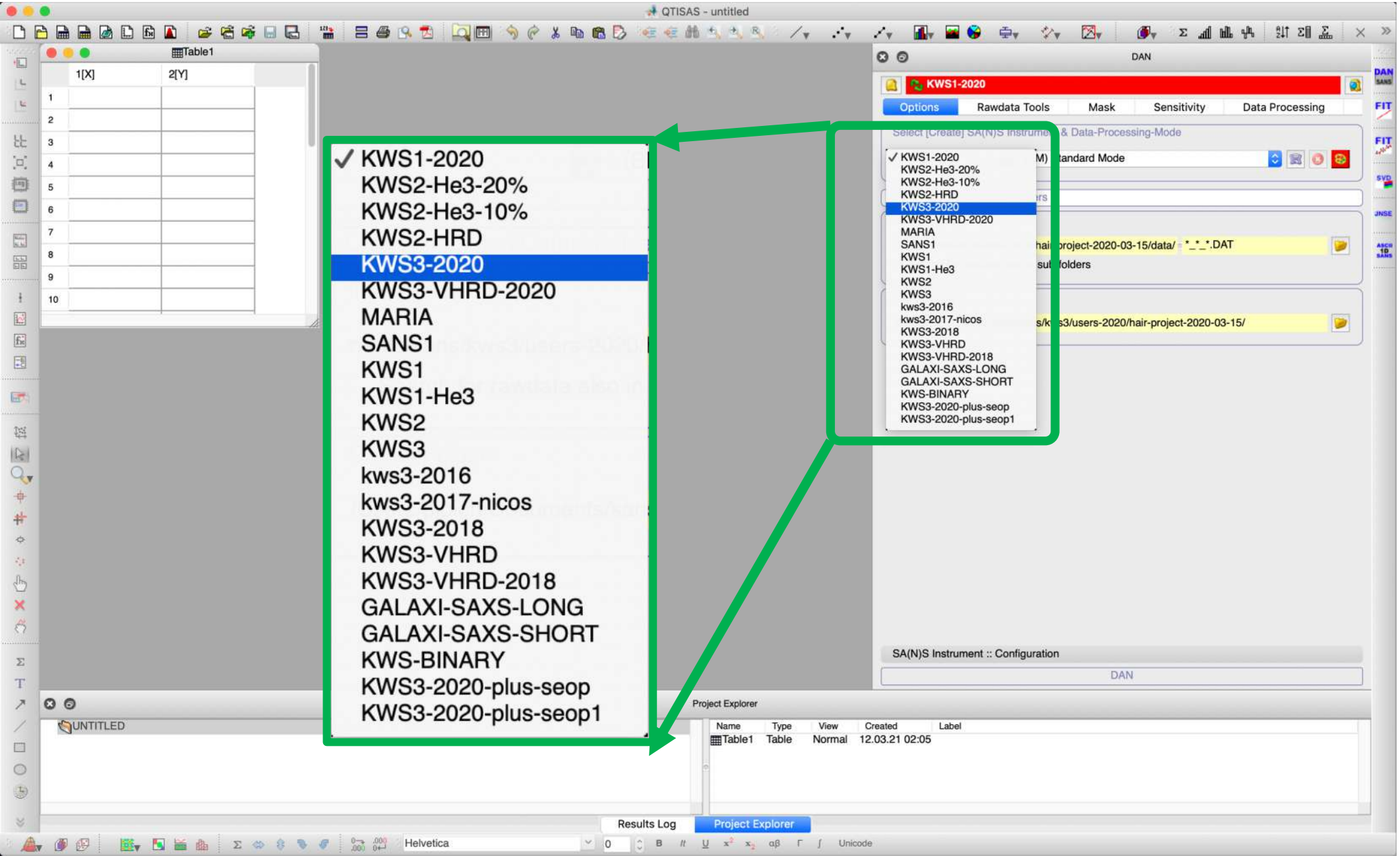
Starting of “New Session”



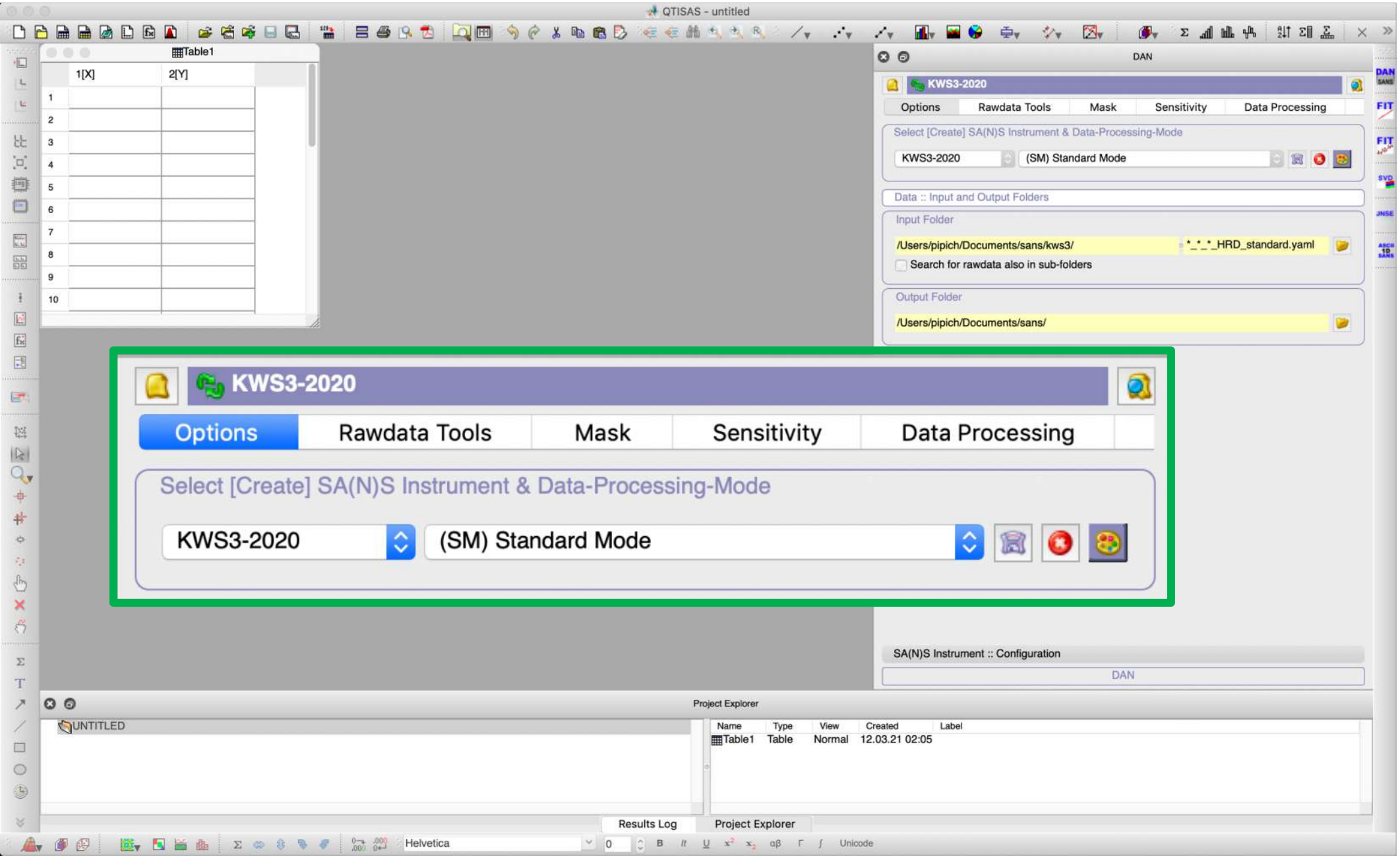

QTISAS - untitled
Table1
1[X]
2[Y]
DAN
KWS2-He3-20%
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Select [Create] SA(N)S Instrument & Data-Processing-Mode
KWS2-He3-20%
(SM) Standard Mode
Data :: Input and Output Folders
Input Folder
/Users/pipich/Documents/sans/
*_*_*.DAT
Search for rawdata 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: **KWS3-2020**

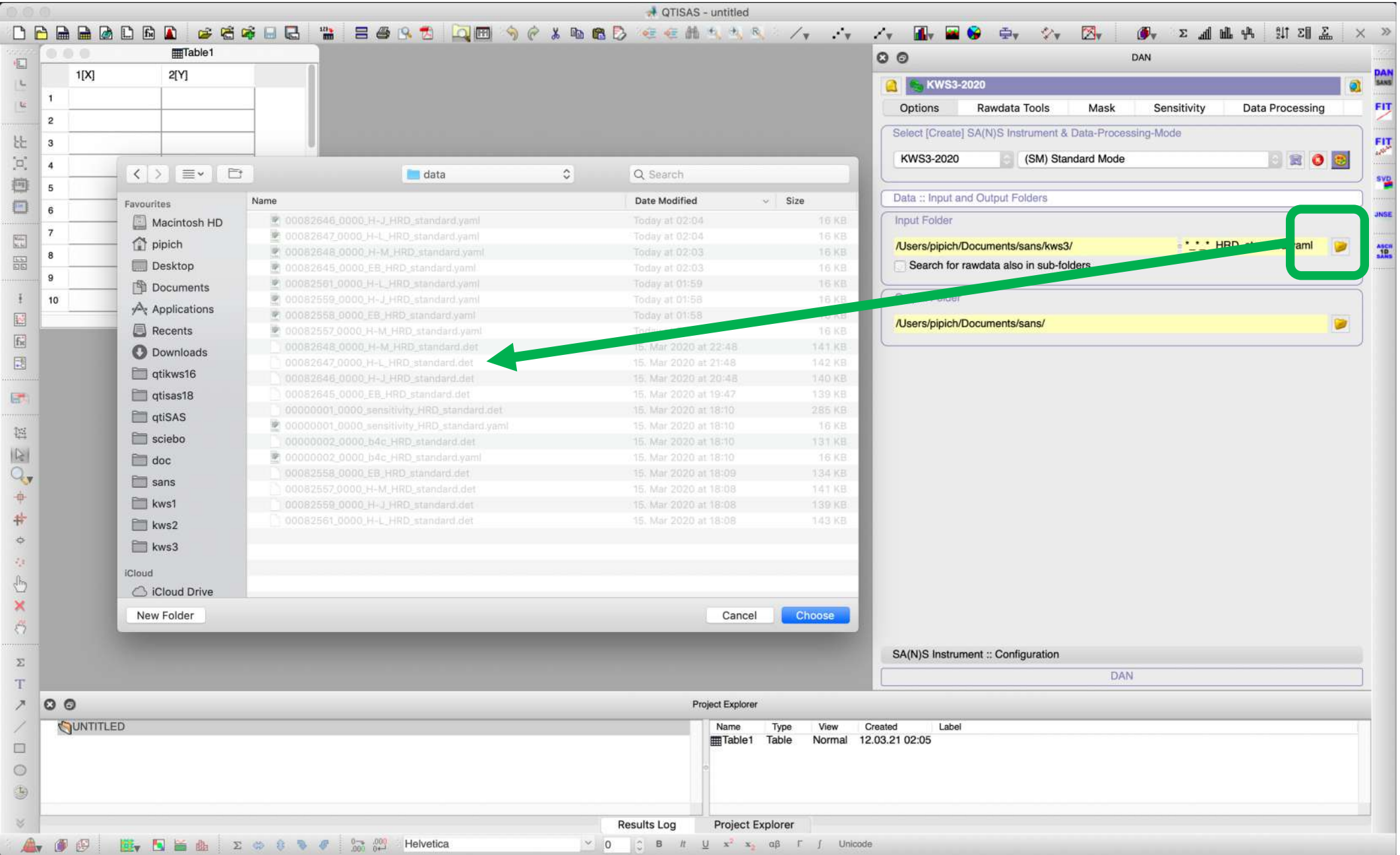


Selected: **KWS3-2020**

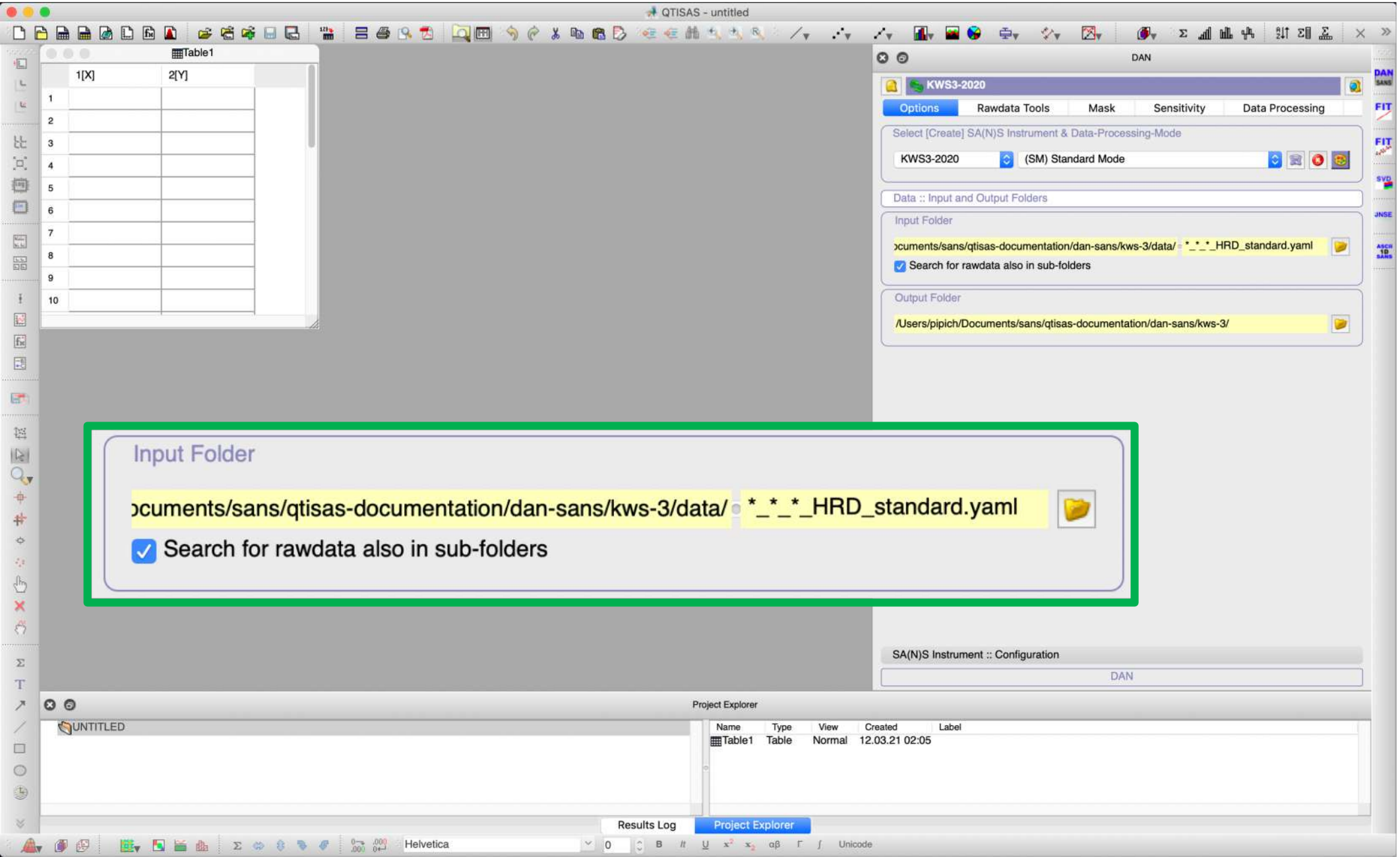


STEP 2: Raw-Data Path Selection

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

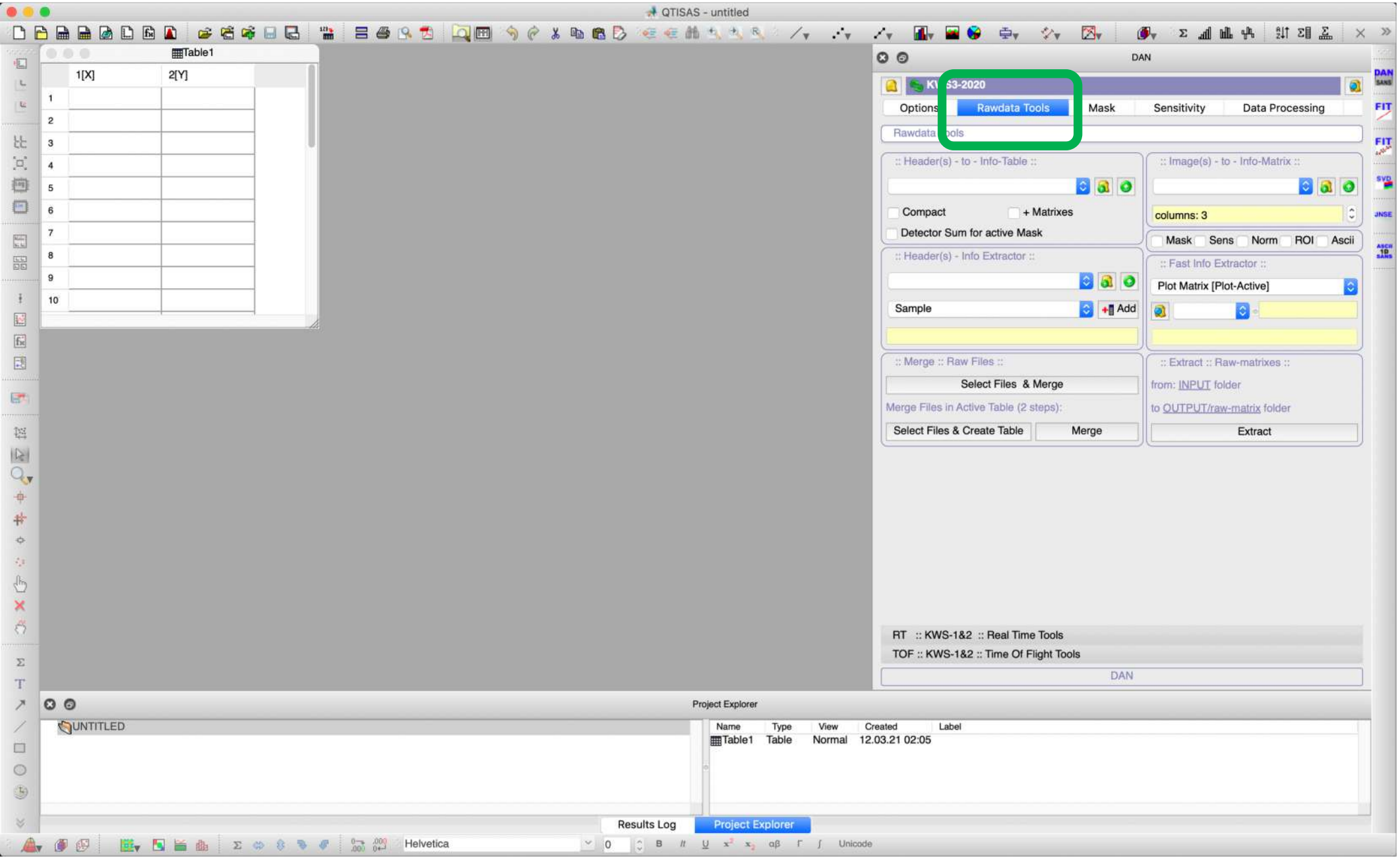


Path (Folder): selected

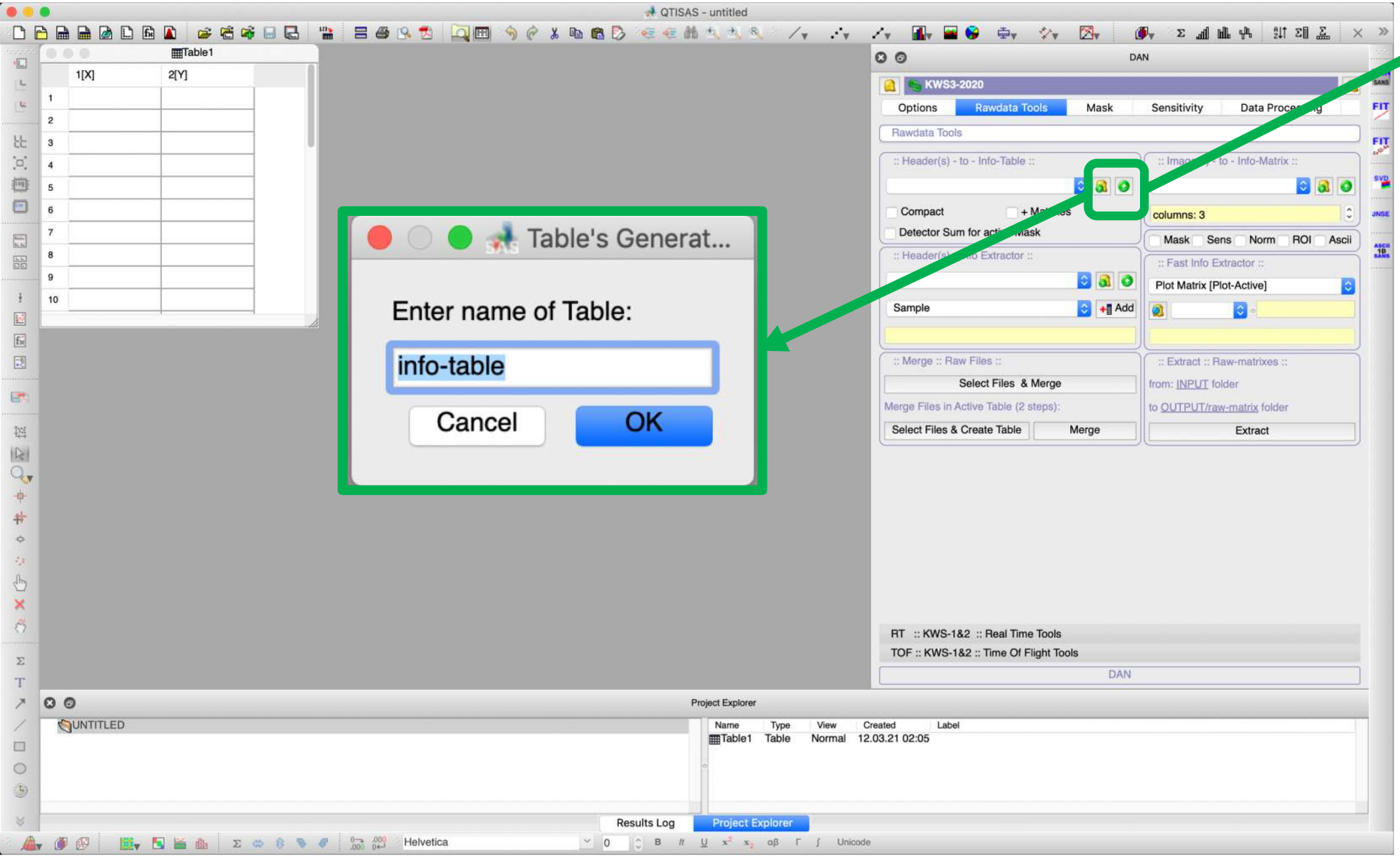


STEP 3 (optional): Data-Information-Table Generation

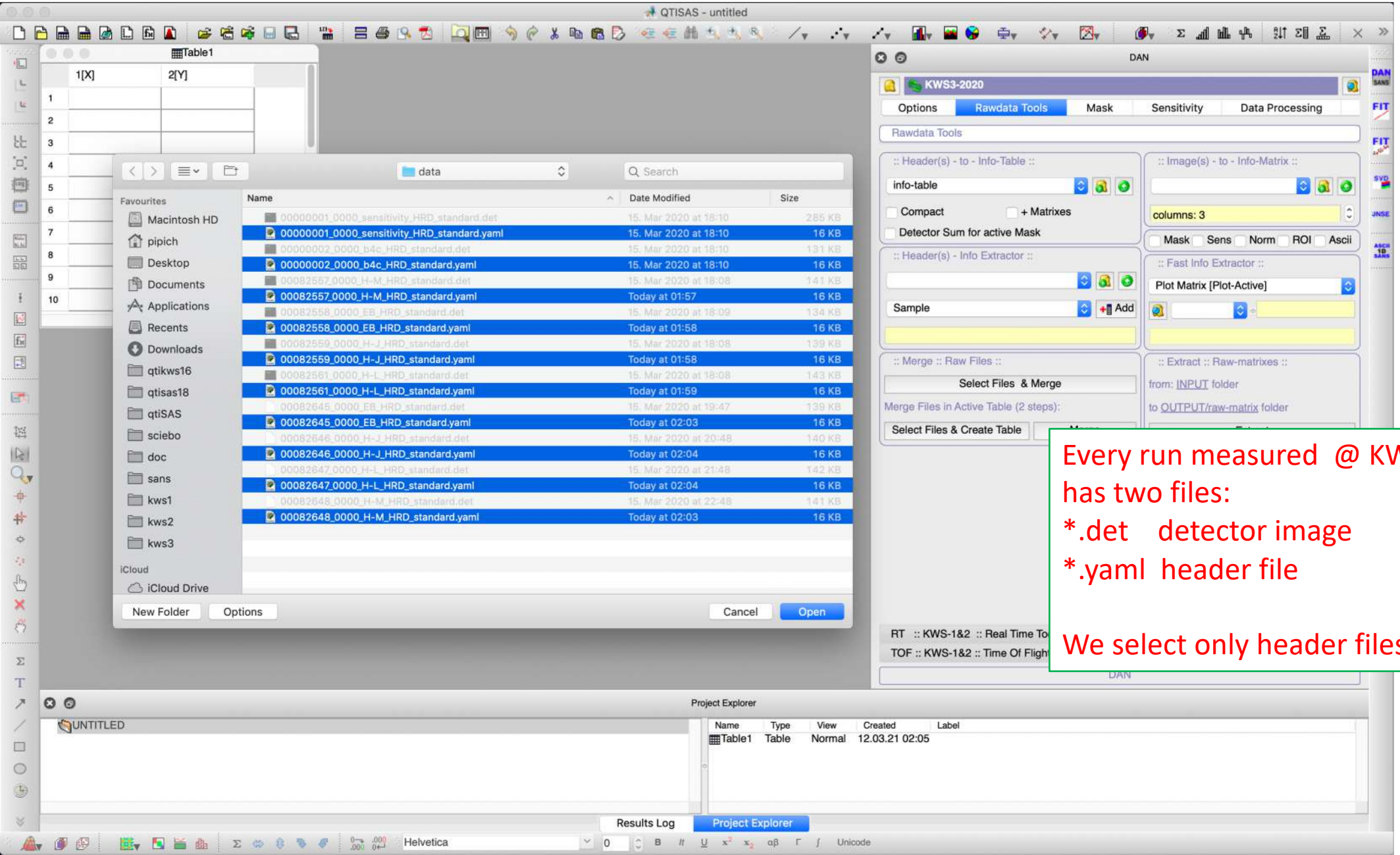
3.1 Go to **Rawdata Tools** tab



3.2 Push **“+”** Button and enter **Table Name**



3.3 Select Data to get Information



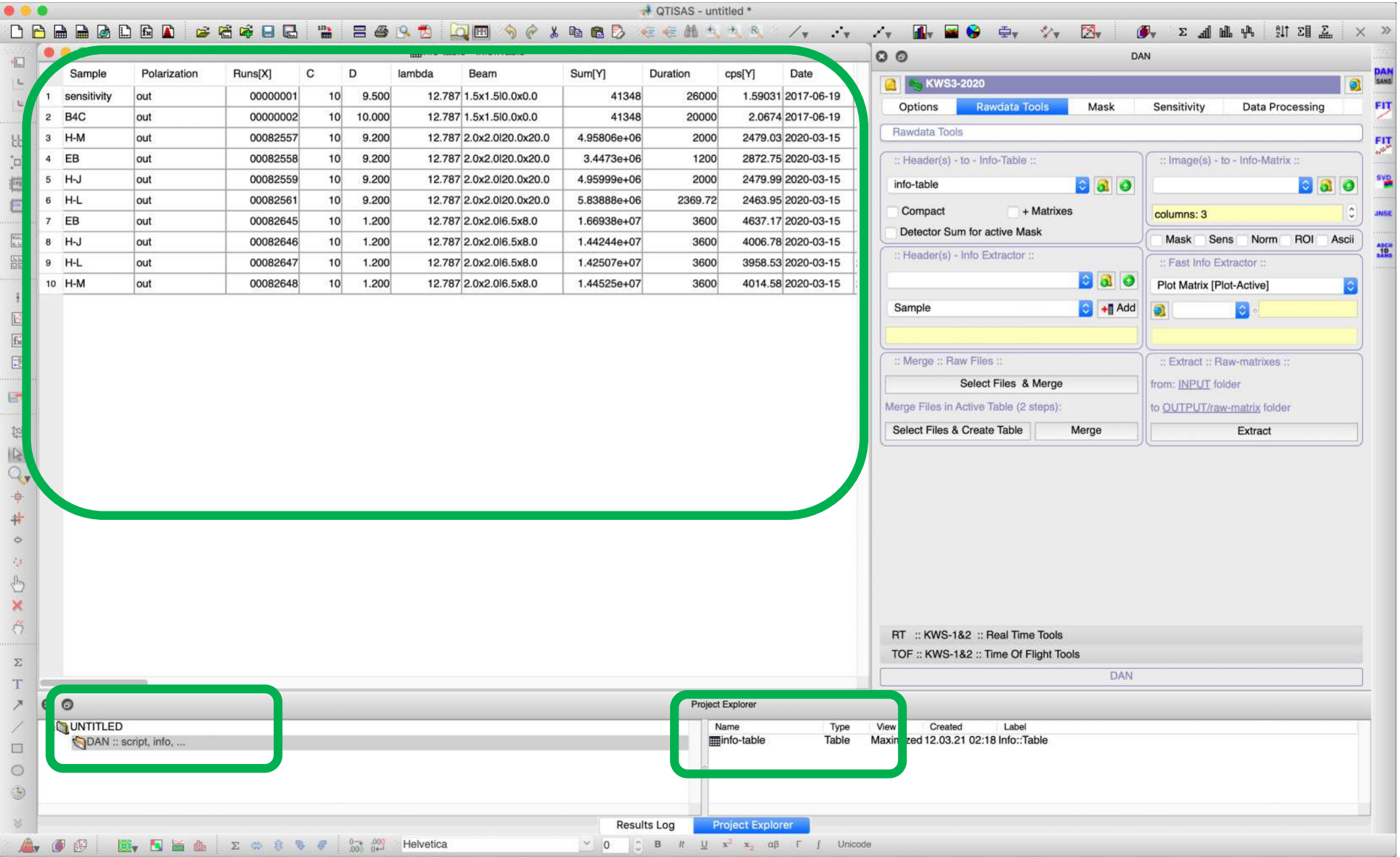
Every run measured @ KWS-3 has two files:

*.det detector image

*.yaml header file

We select only header files!

3.4 **“info-table”** is generated



	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date
1	sensitivity	out	00000001	10	9.500	12.787	1.5x1.5|0.0x0.0	41348	26000	1.59031	2017-06-19
2	B4C	out	00000002	10	10.000	12.787	1.5x1.5|0.0x0.0	41348	20000	2.0674	2017-06-19
3	H-M	out	00082557	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95806e+06	2000	2479.03	2020-03-15
4	EB	out	00082558	10	9.200	12.787	2.0x2.0|20.0x20.0	3.4473e+06	1200	2872.75	2020-03-15
5	H-J	out	00082559	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95999e+06	2000	2479.99	2020-03-15
6	H-L	out	00082561	10	9.200	12.787	2.0x2.0|20.0x20.0	5.83888e+06	2369.72	2463.95	2020-03-15
7	EB	out	00082645	10	1.200	12.787	2.0x2.0|6.5x8.0	1.66938e+07	3600	4637.17	2020-03-15
8	H-J	out	00082646	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44244e+07	3600	4006.78	2020-03-15
9	H-L	out	00082647	10	1.200	12.787	2.0x2.0|6.5x8.0	1.42507e+07	3600	3958.53	2020-03-15
10	H-M	out	00082648	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44525e+07	3600	4014.58	2020-03-15

STEP 4 (optional): Data “Understanding”

Samples

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time	F
1	sensitivity	out	00000001	10	9.500	12.787	1.5x1.5|0.0x0.0	41348	26000	1.59031	2017-06-19	11:35:01	
2	B4C	out	00000002	10	10.000	12.787	1.5x1.5|0.0x0.0	41348	20000	2.0674	2017-06-19	11:35:01	
3	H-M	out	00082557	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95806e+06	2000	2479.03	2020-03-15	14:29:50	
4	EB	out	00082558	10	9.200	12.787	2.0x2.0|20.0x20.0	3.4473e+06	1200	2872.75	2020-03-15	15:03:54	
5	H-J	out	00082559	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95999e+06	2000	2479.99	2020-03-15	15:24:45	
6	H-L	out	00082561	10	9.200	12.787	2.0x2.0|20.0x20.0	5.83888e+06	2369.72	2463.95	2020-03-15	16:39:50	
7	EB	out	00082645	10	1.200	12.787	2.0x2.0|6.5x8.0	1.66938e+07	3600	4637.17	2020-03-15	18:47:23	
8	H-J	out	00082646	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44244e+07	3600	4006.78	2020-03-15	19:48:09	
9	H-L	out	00082647	10	1.200	12.787	2.0x2.0|6.5x8.0	1.42507e+07	3600	3955.53	2020-03-15	20:48:35	
10	H-M	out	00082648	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44525e+07	3600	4014.58	2020-03-15	21:48:58	

D9.2m

D1.2m

3 samples: **H-J, H-L, H-M**;
2 configurations: **D9.2m**[s.aperture 20x20mm^2]**, D1.2m** [s.aperture 6.5x8mm^2]
(WaveLength 12.8A, c.aperture 2x2mm^2)

“Dark Current”

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time	F
1	sensitivity	out	00000001	10	9.500	12.787	1.5x1.5|0.0x0.0	41348	26000	1.59031	2017-06-19	11:35:01	
2	B4C	out	00000002	10	10.000	12.787	1.5x1.5|0.0x0.0	41348	20000	2.0674	2017-06-19	11:35:01	
3	H-M	out	00082557	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95806e+06	2000	2479.03	2020-03-15	14:29:50	
4	EB	out	00082558	10	9.200	12.787	2.0x2.0|20.0x20.0	3.4473e+06	1200	2872.75	2020-03-15	15:03:54	
5	H-J	out	00082559	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95999e+06	2000	2479.99	2020-03-15	15:24:45	
6	H-L	out	00082561	10	9.200	12.787	2.0x2.0|20.0x20.0	5.83888e+06	2369.72	2463.95	2020-03-15	16:39:50	
7	EB	out	00082645	10	1.200	12.787	2.0x2.0|6.5x8.0	1.66938e+07	3600	4637.17	2020-03-15	18:47:23	
8	H-J	out	00082646	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44244e+07	3600	4006.78	2020-03-15	19:48:09	
9	H-L	out	00082647	10	1.200	12.787	2.0x2.0|6.5x8.0	1.42507e+07	3600	3958.53	2020-03-15	20:48:35	
10	H-M	out	00082648	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44525e+07	3600	4014.58	2020-03-15	21:48:58	

Dark Current, B4C

Detector Dark Current : #00000002 (blocked beam with B4C)

Ask local contact to provide this file (single file will be used in all configurations)

Empty Beam/Cell

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time	F
1	sensitivity	out	00000001	10	9.500	12.787	1.5x1.5|0.0x0.0	41348	26000	1.59031	2017-06-19	11:35:01	
2	B4C	out	00000002	10	10.000	12.787	1.5x1.5|0.0x0.0	41348	20000	2.0674	2017-06-19	11:35:01	
3	H-M	out	00082557	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95806e+06	2000	2479.03	2020-03-15	14:29:50	
4	EB	out	00082558	10	9.200	12.787	2.0x2.0|20.0x20.0	3.4473e+06	1200	2874.75	2020-03-15	15:03:54	
5	H-J	out	00082559	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95999e+06	2000	2479.99	2020-03-15	15:24:45	
6	H-L	out	00082561	10	9.200	12.787	2.0x2.0|20.0x20.0	5.83888e+06	2369.72	2463.95	2020-03-15	16:39:50	
7	EB	out	00082645	10	1.200	12.787	2.0x2.0|6.5x8.0	1.66938e+07	3600	4637.17	2020-03-15	18:47:23	
8	H-J	out	00082646	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44244e+07	3600	4006.78	2020-03-15	19:48:09	
9	H-L	out	00082647	10	1.200	12.787	2.0x2.0|6.5x8.0	1.42507e+07	3600	3958.53	2020-03-15	20:48:35	
10	H-M	out	00082648	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44525e+07	3600	4014.58	2020-03-15	21:48:58	

D9.2m

D1.2m

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

Absolute calibration of KWS-3 data is done in direct way: we measure empty beam without beam stop and calculate number of neutrons coming to samples

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date	Time	F
1	sensitivity	out	00000001	10	9.500	12.787	1.5x1.5|0.0x0.0	41348	26000	1.59031	2017-06-19	11:35:01	
2	B4C	out	00000002	10	10.000	12.787	1.5x1.5|0.0x0.0	41348	20000	2.0674	2017-06-19	11:35:01	
3	H-M	out	00082557	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95806e+06	2000	2479.03	2020-03-15	14:29:50	
4	EB	out	00082558	10	9.200	12.787	2.0x2.0|20.0x20.0	3.4473e+06	1200	2874.75	2020-03-15	15:03:54	
5	H-J	out	00082559	10	9.200	12.787	2.0x2.0|20.0x20.0	4.95999e+06	2000	2479.99	2020-03-15	15:24:45	
6	H-L	out	00082561	10	9.200	12.787	2.0x2.0|20.0x20.0	5.83888e+06	2369.72	2463.95	2020-03-15	16:39:50	
7	EB	out	00082645	10	1.200	12.787	2.0x2.0|6.5x8.0	1.66938e+07	3600	4637.17	2020-03-15	18:47:23	
8	H-J	out	00082646	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44244e+07	3600	4006.78	2020-03-15	19:48:09	
9	H-L	out	00082647	10	1.200	12.787	2.0x2.0|6.5x8.0	1.42507e+07	3600	3958.53	2020-03-15	20:48:35	
10	H-M	out	00082648	10	1.200	12.787	2.0x2.0|6.5x8.0	1.44525e+07	3600	4014.58	2020-03-15	21:48:58	

D9.2m

D1.2m

Absolute Calibration Runs (direct beam mode):

- EB (“Empty Beam”)
- B4C (“Dark Current”)

STEP 5: Masking Matrixes

For Sensitivity, Absolute Calibration, and Detector Center calculation we need
"full" mask (only detector edge is masked): **mask**

We have two configurations: D9.2m and D1.2m.
For every configuration we need 2 masks:

- For radial averaging (detector edge and direct beam are masked): **mask-bs-9m** & **mask-bs-1m**
- For Transmission Calculation (masked everything except director beam area): **mask-tr-9m** & **mask-tr-1m**

STEP 5.1: Standard Detector “**mask**” Creation

Go to **MASK** tab

QTISAS - untitled *

info-table - Info::Table

	Sample	Polarization	Runs[X]	C	D	lambda	Beam	Sum[Y]	Duration	cps[Y]	Date
1	sensitivity	out	00000001	10	9.500	12.787	1.5x1.5l0.0x0.0	41348	26000	1.59031	2017-06-19
2	B4C	out	00000002	10	10.000	12.787	1.5x1.5l0.0x0.0	41348	20000	2.0674	2017-06-19
3	H-M	out	00082557	10	9.200	12.787	2.0x2.0l20.0x20.0	4.95806e+06	2000	2479.03	2020-03-15
4	EB	out	00082558	10	9.200	12.787	2.0x2.0l20.0x20.0	3.4473e+06	1200	2872.75	2020-03-15
5	H-J	out	00082559	10	9.200	12.787	2.0x2.0l20.0x20.0	4.95999e+06	2000	2479.99	2020-03-15
6	H-L	out	00082561	10	9.200	12.787	2.0x2.0l20.0x20.0	5.83888e+06	2369.72	2463.95	2020-03-15
7	EB	out	00082645	10	1.200	12.787	2.0x2.0l6.5x8.0	1.66938e+07	3600	4637.17	2020-03-15
8	H-J	out	00082646	10	1.200	12.787	2.0x2.0l6.5x8.0	1.44244e+07	3600	4006.78	2020-03-15
9	H-L	out	00082647	10	1.200	12.787	2.0x2.0l6.5x8.0	1.42507e+07	3600	3958.53	2020-03-15
10	H-M	out	00082648	10	1.200	12.787	2.0x2.0l6.5x8.0	1.44525e+07	3600	4014.58	2020-03-15

DAN

KWS3-2020

Options | Rawdata Tools | Mask | Sensitivity | Data Processing

Select Active Area of Detector

Active Mask-Matrix :: GenerateIOpenISelect

mask | Update | ... as Tr | New

Edge

X Y

2 3 Left-Bottom

254 255 Right-Top

Ellipse :: Shape of Edge

Beam-Stop I Direct-Beam

X Y

123 123 Left-Bottom

133 133 Right-Top

Ellipse :: Shape of Beam-Stop

"Dead" rows

"Dead" cols

Thriangular mask(s)

Mask I Tools

DAN

Project Explorer

UNTITLED

DAN :: script, info, ...

Name	Type	View	Created	Label
info-table	Table	Maximized	12.03.21 02:18	Info::Table

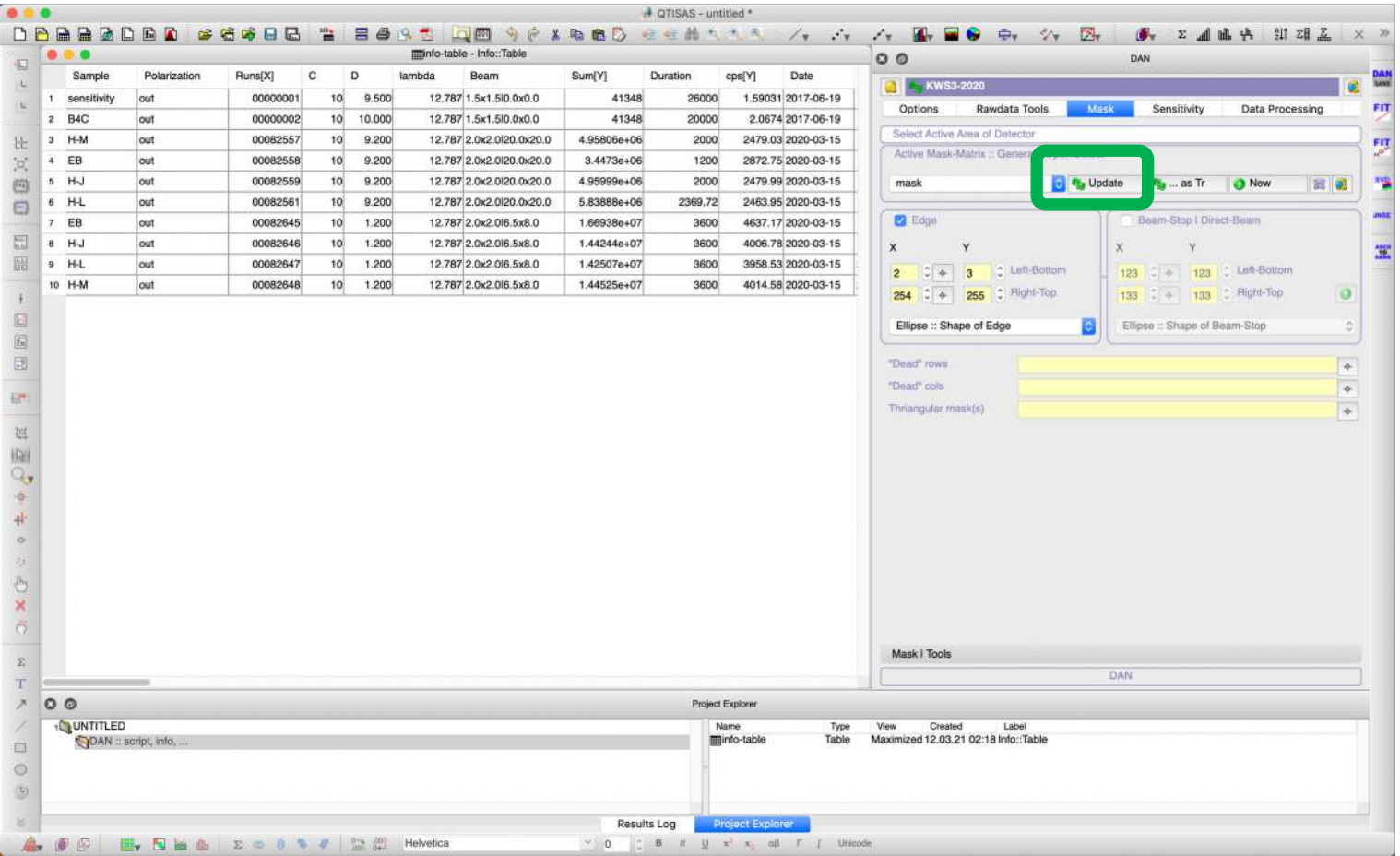
Results Log | Project Explorer

Helvetica 0 Unicode

mask

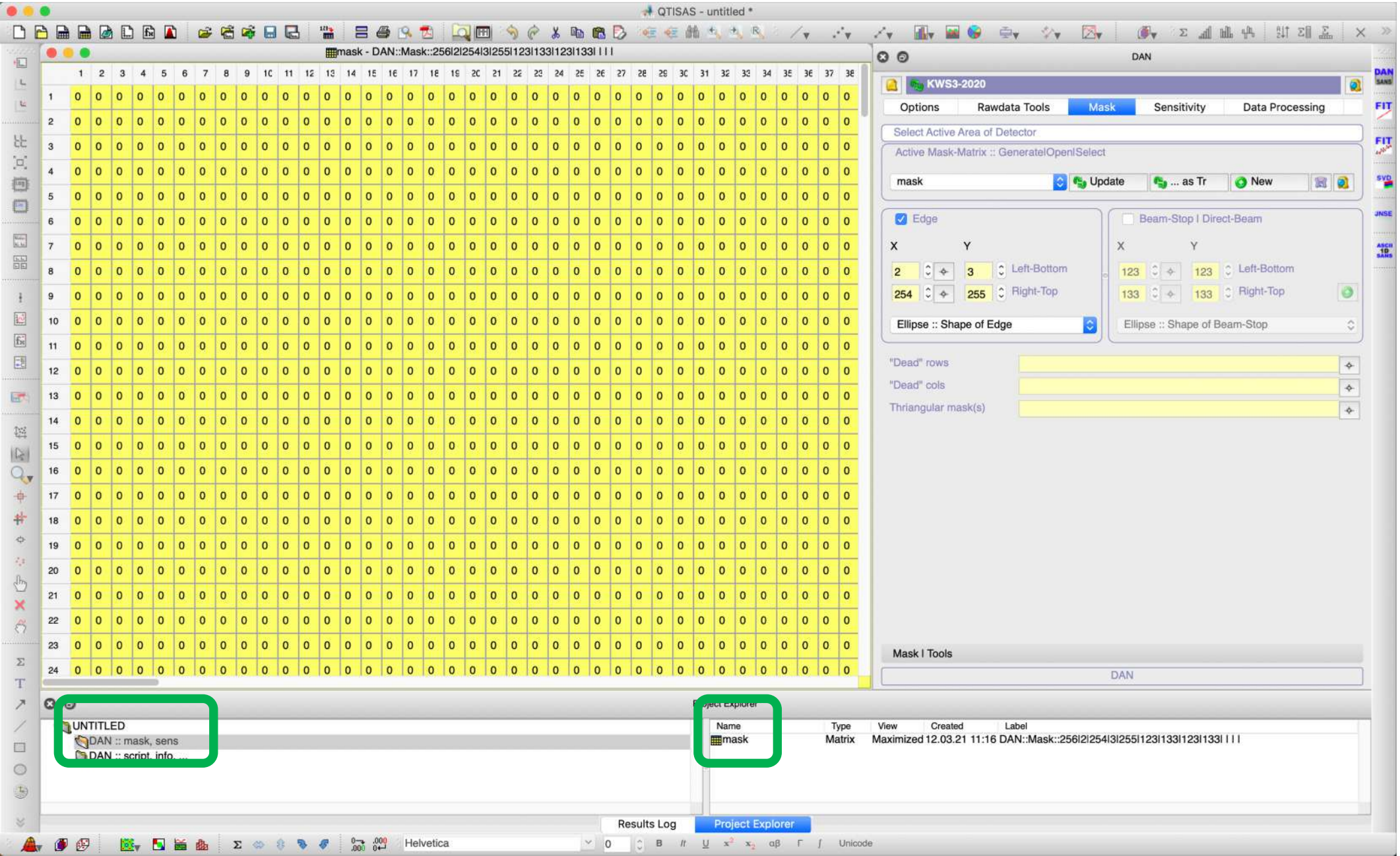
For Sensitivity, Absolute Calibration, and Detector Center calculation we need “full” mask (only detector edge is masked)

Push : 

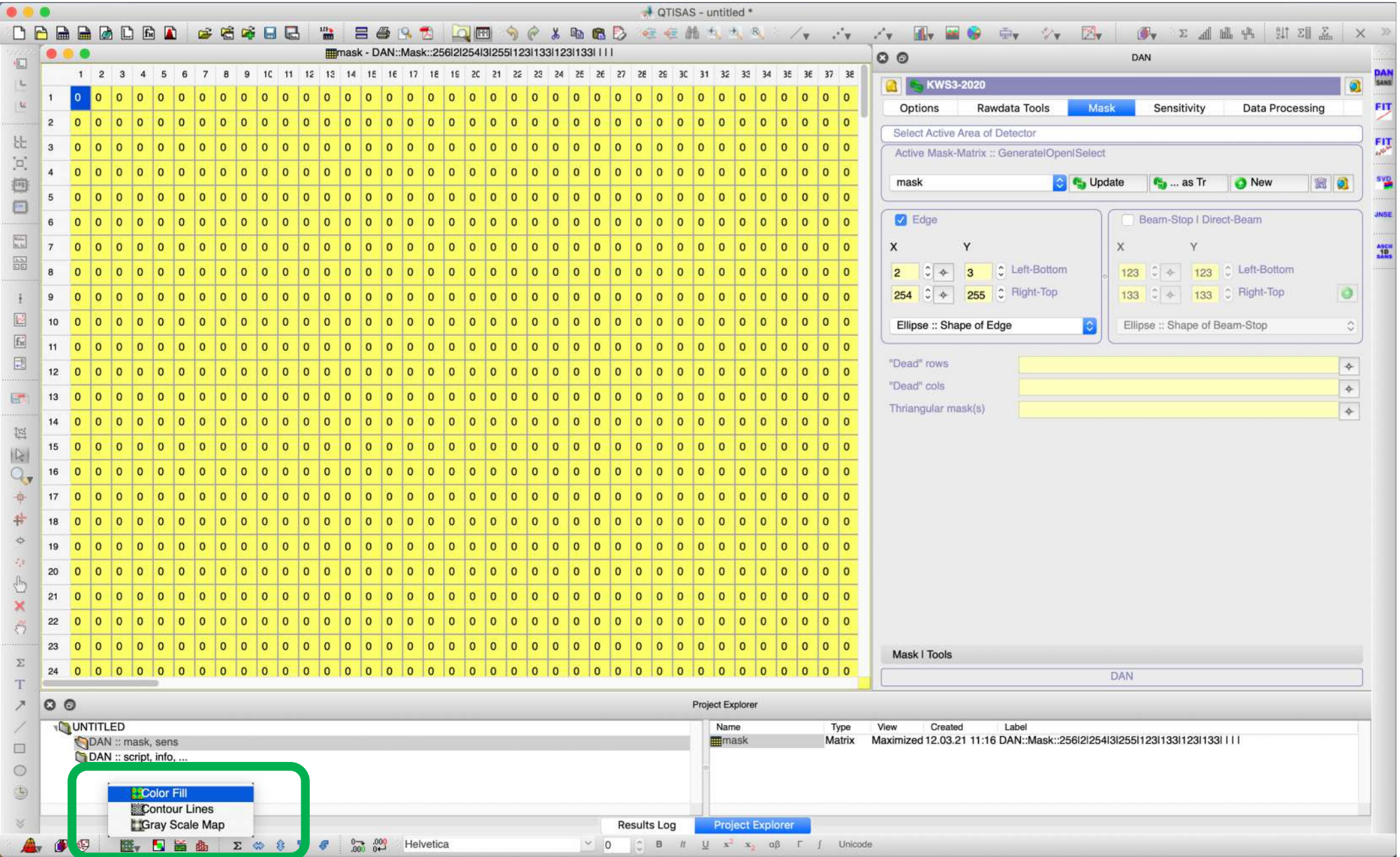


“Edge” is checked (default values)
“Beam Stop | Direct Beam” is unchecked
Active Mask Name is “mask”

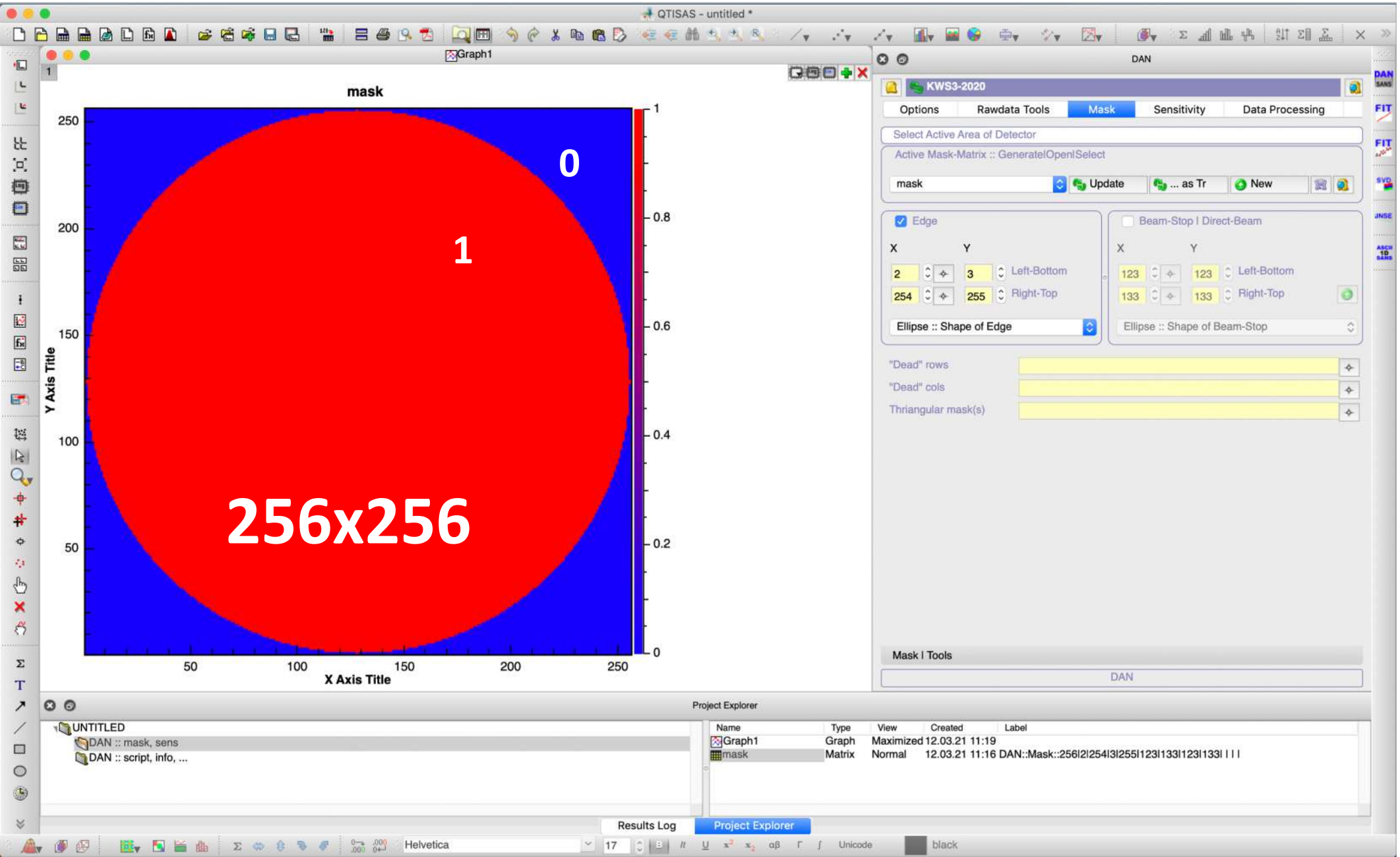
“mask” matrix is created in “DAN:: mask, sens” folder



Plotting Example: “Color Fill”



Plotting Example: “Color Fill”

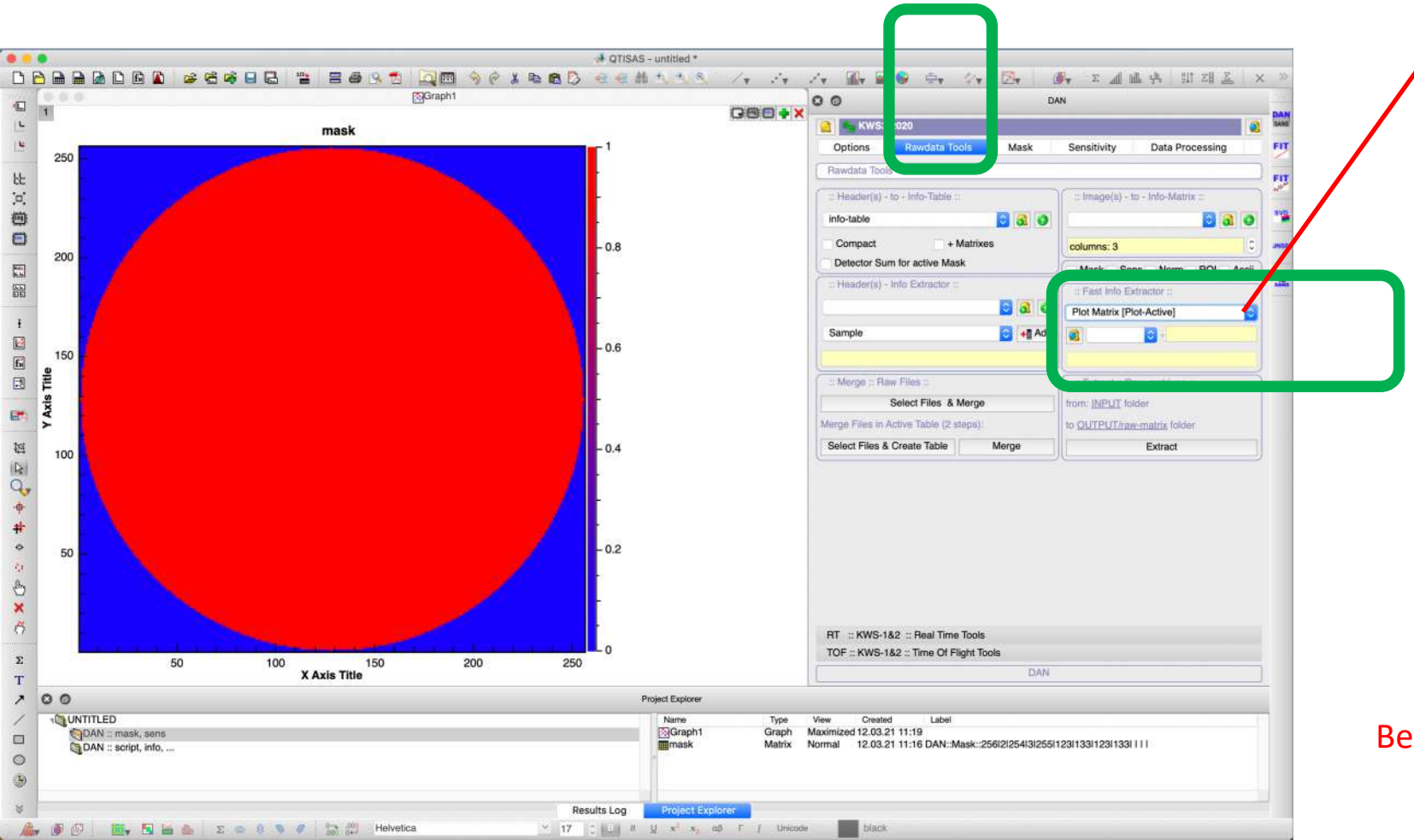


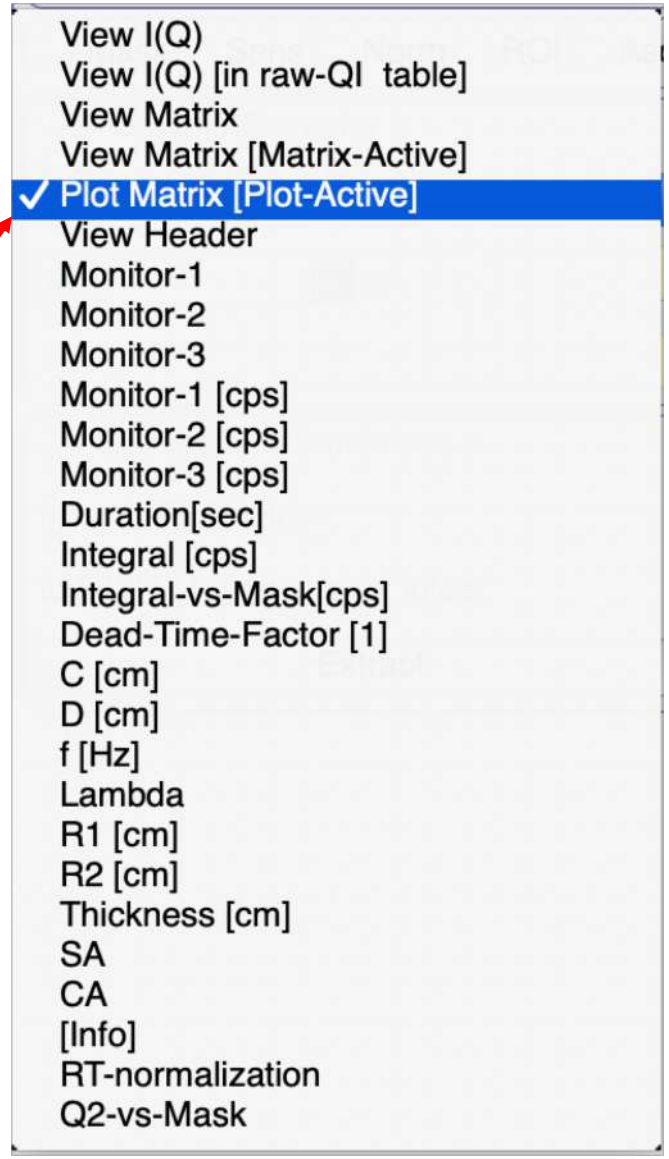
STEP 5.2: “mask-bs-9m” generation

Beam center could be located at any position of the detector, sometimes even out of the detector area. Therefore position of the direct beam is not pre-defined. Every time we should calculate position of the beam spot basing on Empty Beam run for every configuration. To make “mask-bs-9m” matrix we will open “00082558” matrix and will plot it.

4	EB	out	00082558	10	9.200	12.787	2.0x2.0|20.0x20.0	3.4473e+06	1200	2872.75	2020-03-15	15:03:54	

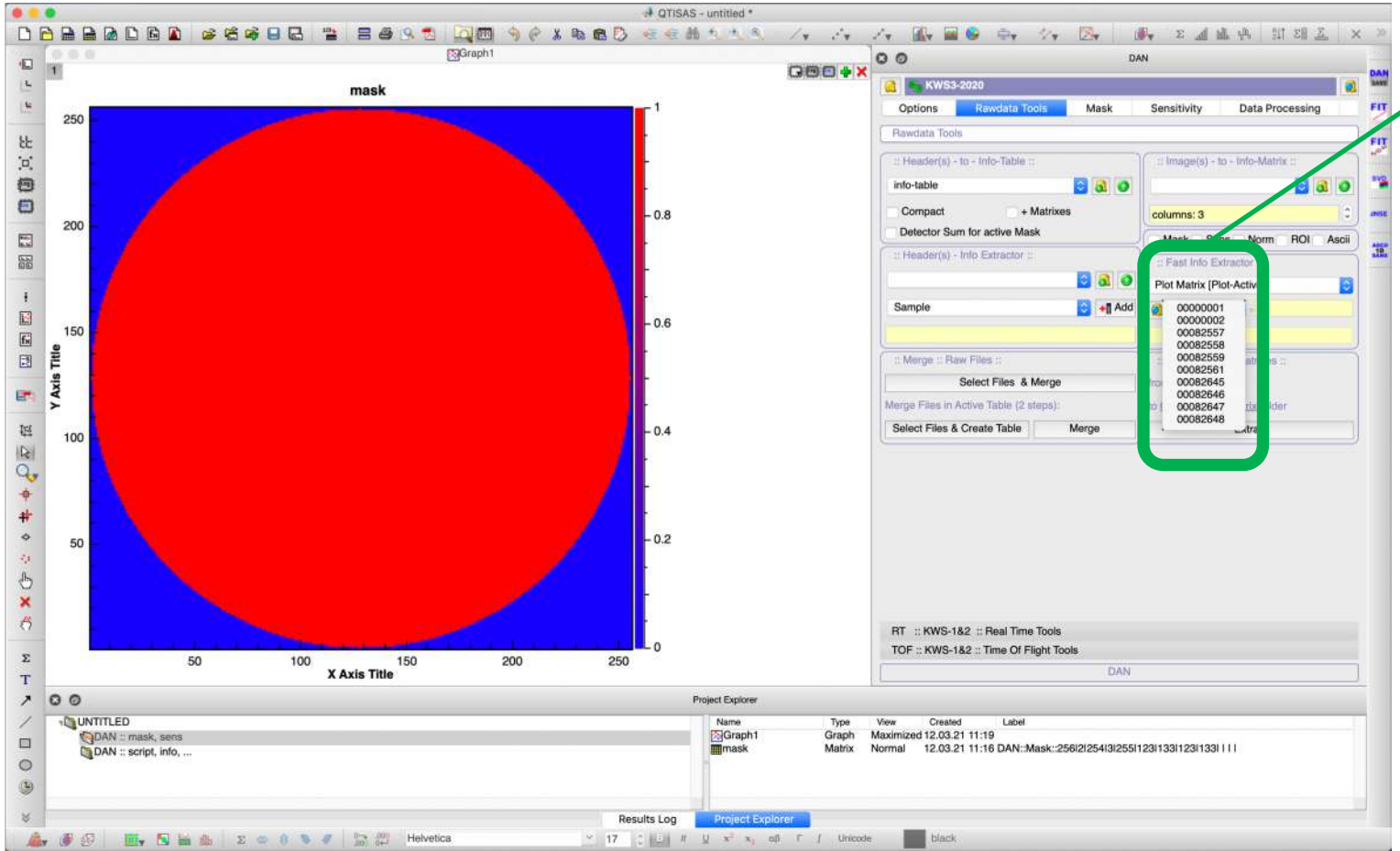
To plot rawdata-matrix of **00082558** run we will use **Fast Info Extractor** of **Rawdata Tools**

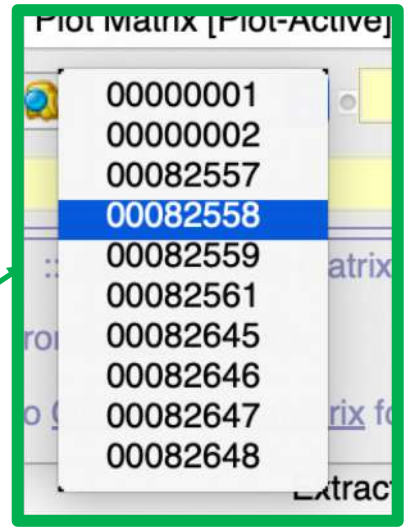


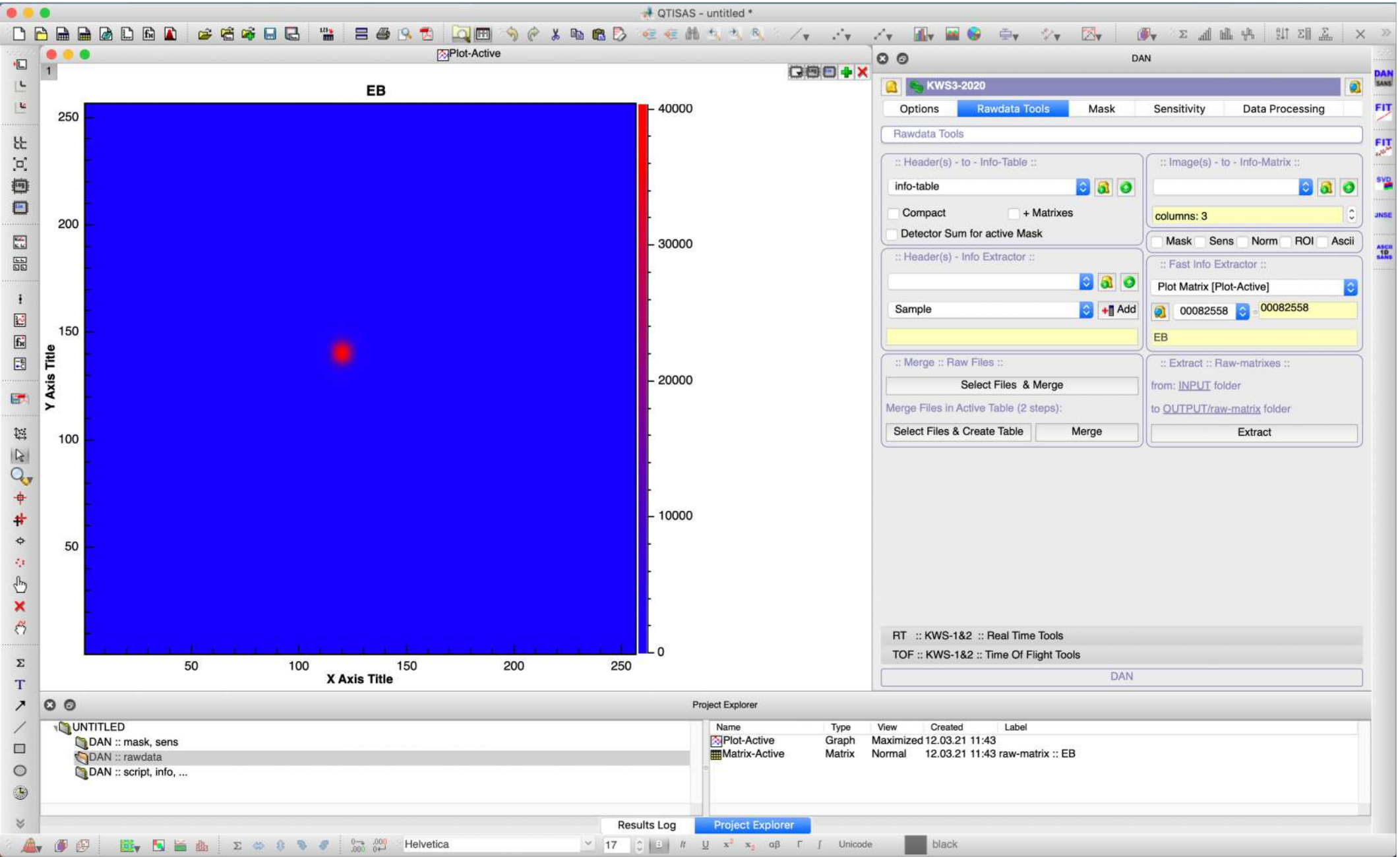


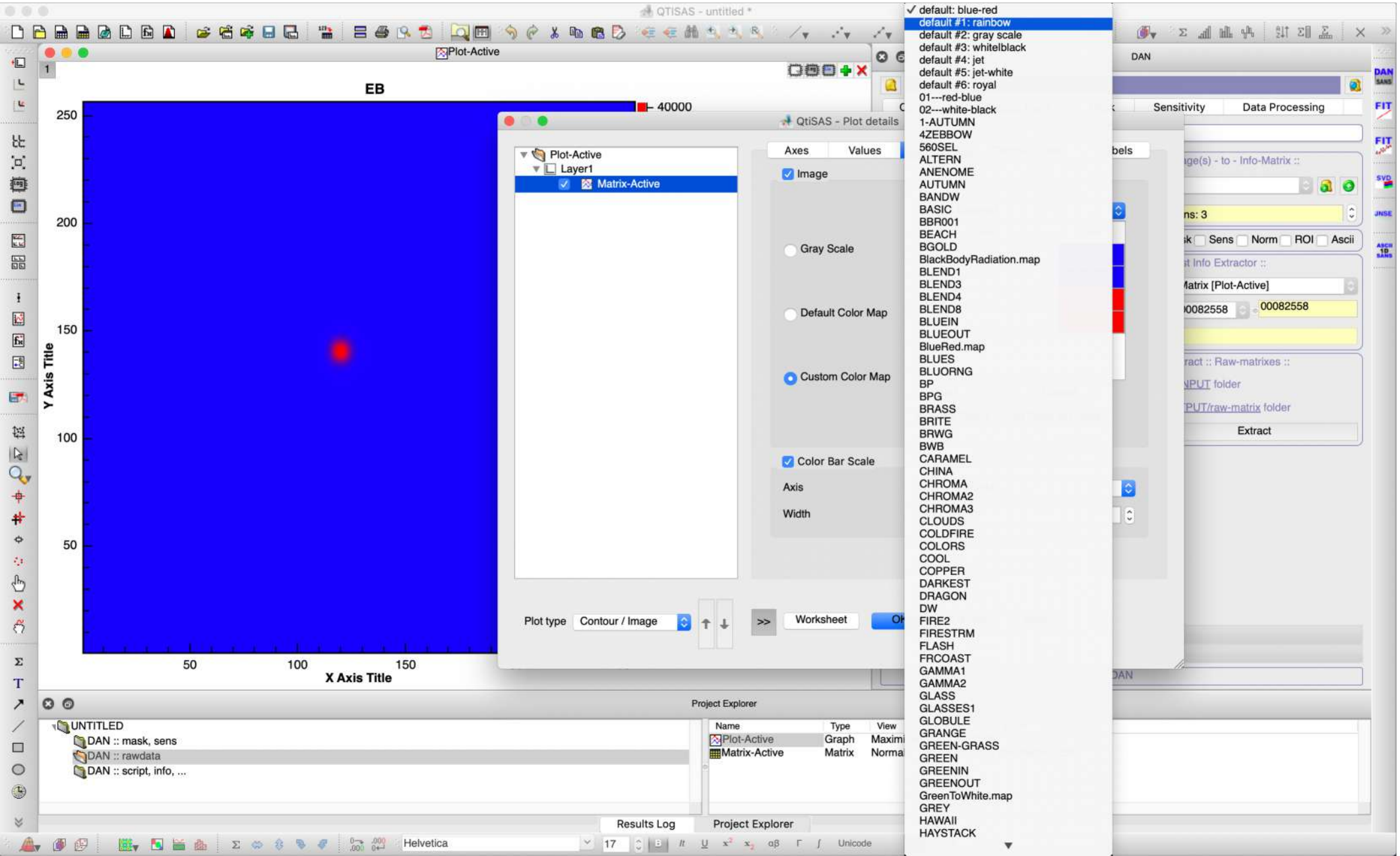
Be sure, that **Plot Matrix [Plot-Active]** is selected

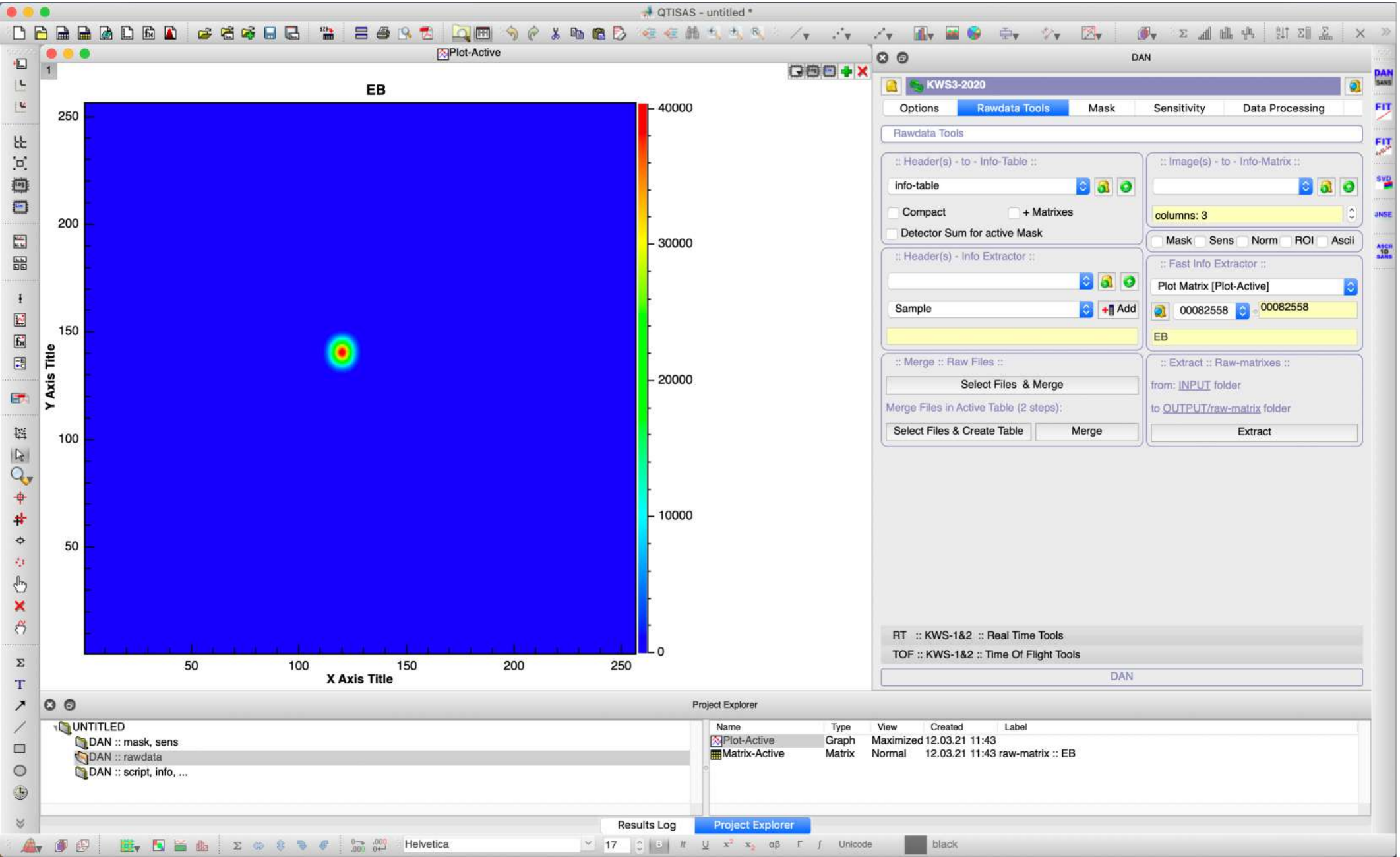
Select in the drop-down list **00082558** run

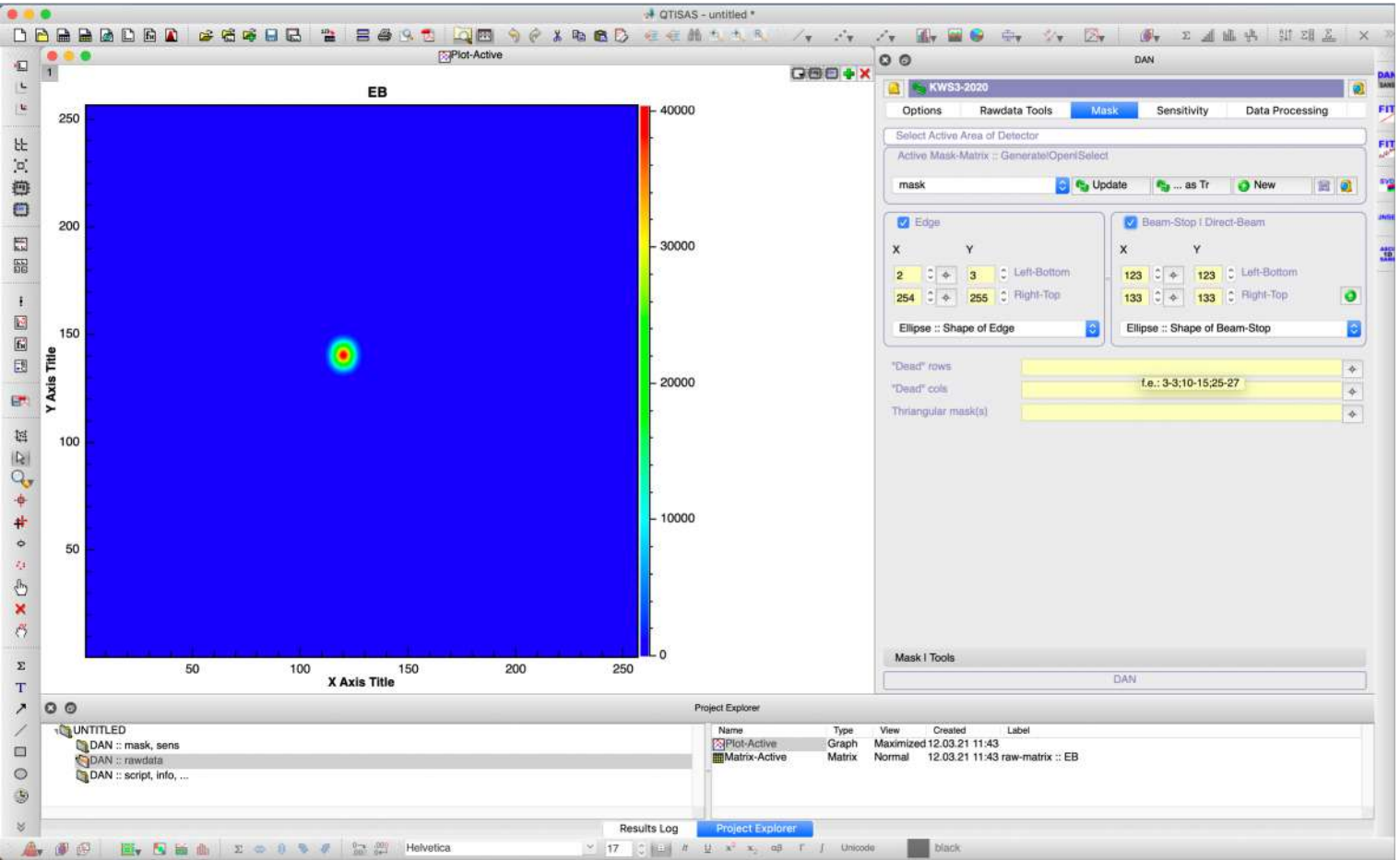


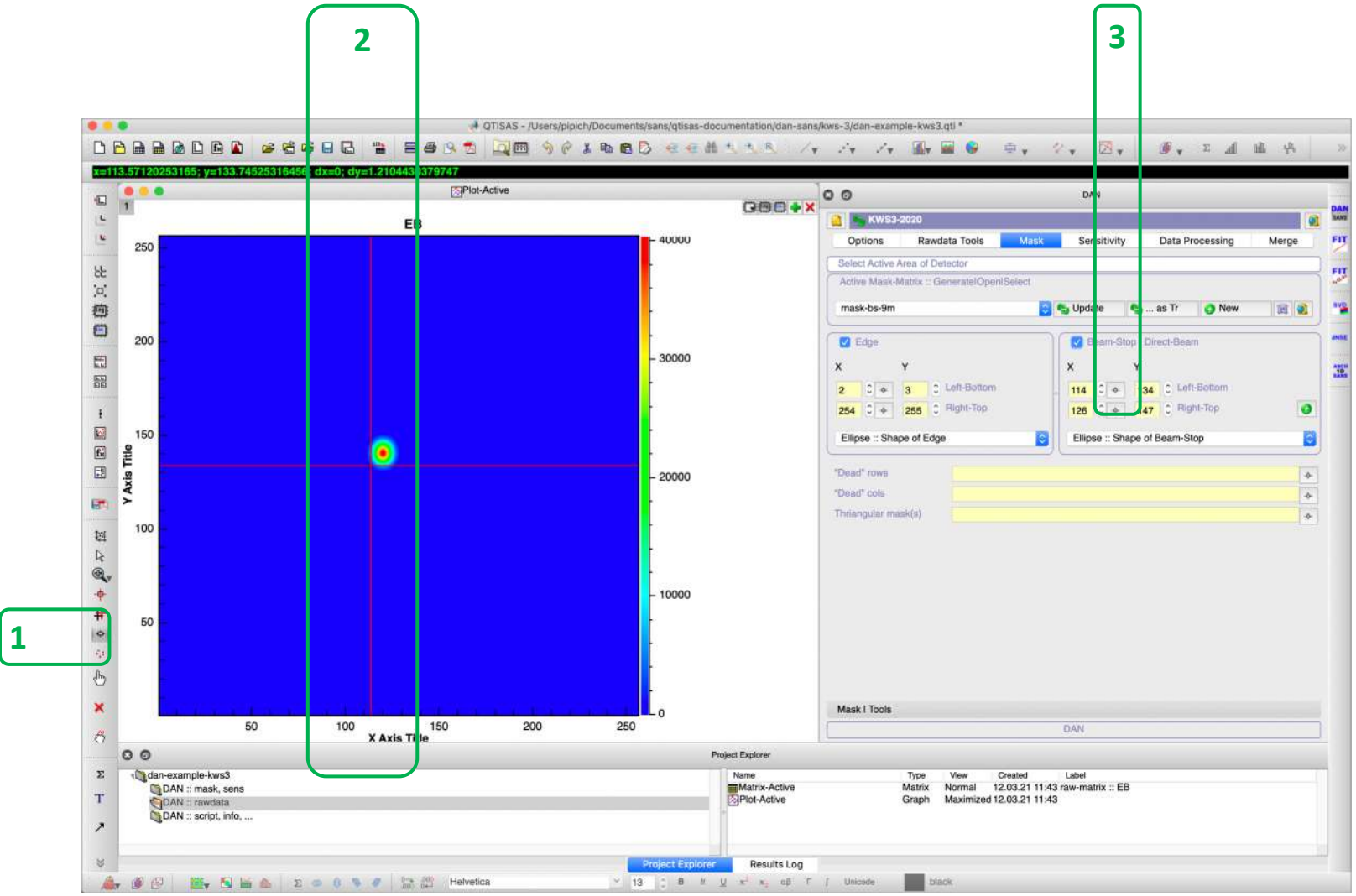


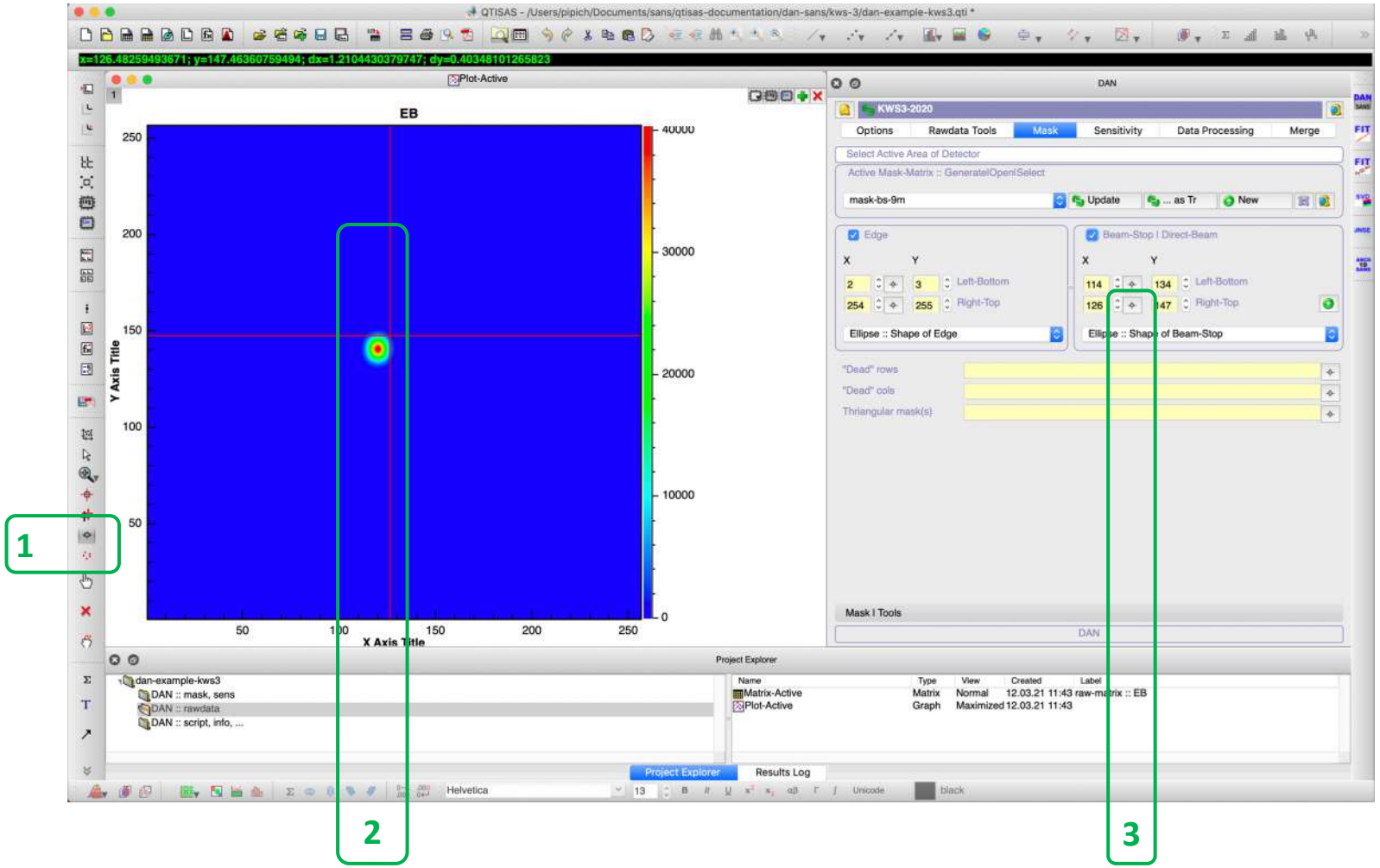

QTISAS - untitled *
Plot-Active
EB
Y Axis Title
X Axis Title
250
200
150
100
50
50
100
150
200
250
40000
30000
20000
10000
0
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Rawdata Tools
:: Header(s) - to - Info-Table ::
info-table
Compact
+ Matrixes
Detector Sum for active Mask
:: Image(s) - to - Info-Matrix ::
columns: 3
Mask
Sens
Norm
ROI
Ascii
:: Header(s) - Info Extractor ::
Sample
Add
:: Fast Info Extractor ::
Plot Matrix [Plot-Active]
00082558
00082558
EB
:: Merge :: Raw Files ::
Select Files & Merge
Merge Files in Active Table (2 steps):
Select Files & Create Table
Merge
:: Extract :: Raw-matrixes ::
from: INPUT folder
to OUTPUT/raw-matrix folder
Extract
RT :: KWS-1&2 :: Real Time Tools
TOF :: KWS-1&2 :: Time Of Flight Tools
DAN
Project Explorer
UNTITLED
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Plot-Active
Graph
Maximized
12.03.21 11:43
Matrix-Active
Matrix
Normal
12.03.21 11:43
raw-matrix :: EB
Results Log
Project Explorer
Helvetica
17
Unicode
black


QTISAS - untitled *
Plot-Active
EB
40000
250
200
150
100
50
Y Axis Title
50
100
150
X Axis Title
QtiSAS - Plot details
Plot-Active
Layer1
Matrix-Active
Axes
Values
Image
Gray Scale
Default Color Map
Custom Color Map
Color Bar Scale
Axis
Width
Plot type
Contour / Image
Worksheet
default: blue-red
default #1: rainbow
default #2: gray scale
default #3: whitelblack
default #4: jet
default #5: jet-white
default #6: royal
01---red-blue
02---white-black
1-AUTUMN
4ZEBBOW
560SEL
ALTERN
ANENOME
AUTUMN
BANDW
BASIC
BBR001
BEACH
BGOLD
BlackBodyRadiation.map
BLEND1
BLEND3
BLEND4
BLEND8
BLUEIN
BLUEOUT
BlueRed.map
BLUES
BLUORNG
BP
BPG
BRASS
BRITE
BRWG
BWB
CARAMEL
CHINA
CHROMA
CHROMA2
CHROMA3
CLOUDS
COLDFIRE
COLORS
COOL
COPPER
DARKEST
DRAGON
DW
FIRE2
FIRESTRM
FLASH
FRCOAST
GAMMA1
GAMMA2
GLASS
GLASSES1
GLOBULE
GRANGE
GREEN-GRASS
GREEN
GREENIN
GREENOUT
GreenToWhite.map
GREY
HAWAII
HAYSTACK
DAN
Sensitivity
Data Processing
Sens
Norm
ROI
Ascii
Extract
Project Explorer
UNTITLED
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Plot-Active
Graph
Matrix-Active
Matrix
Results Log
Project Explorer
Helvetica
17
Unicode


QTISAS - untitled *
Plot-Active
EB
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Rawdata Tools
:: Header(s) - to - Info-Table ::
info-table
Compact
+ Matrixes
Detector Sum for active Mask
:: Image(s) - to - Info-Matrix ::
columns: 3
Mask
Sens
Norm
ROI
Ascii
:: Header(s) - Info Extractor ::
Sample
Add
:: Fast Info Extractor ::
Plot Matrix [Plot-Active]
00082558
00082558
EB
:: Merge :: Raw Files ::
Select Files & Merge
Merge Files in Active Table (2 steps):
Select Files & Create Table
Merge
:: Extract :: Raw-matrixes ::
from: INPUT folder
to OUTPUT/raw-matrix folder
Extract
RT :: KWS-1&2 :: Real Time Tools
TOF :: KWS-1&2 :: Time Of Flight Tools
DAN
Project Explorer
UNTITLED
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Plot-Active
Graph
Maximized
12.03.21 11:43
Matrix-Active
Matrix
Normal
12.03.21 11:43
raw-matrix :: EB
Results Log
Project Explorer
Helvetica
17
Unicode
black

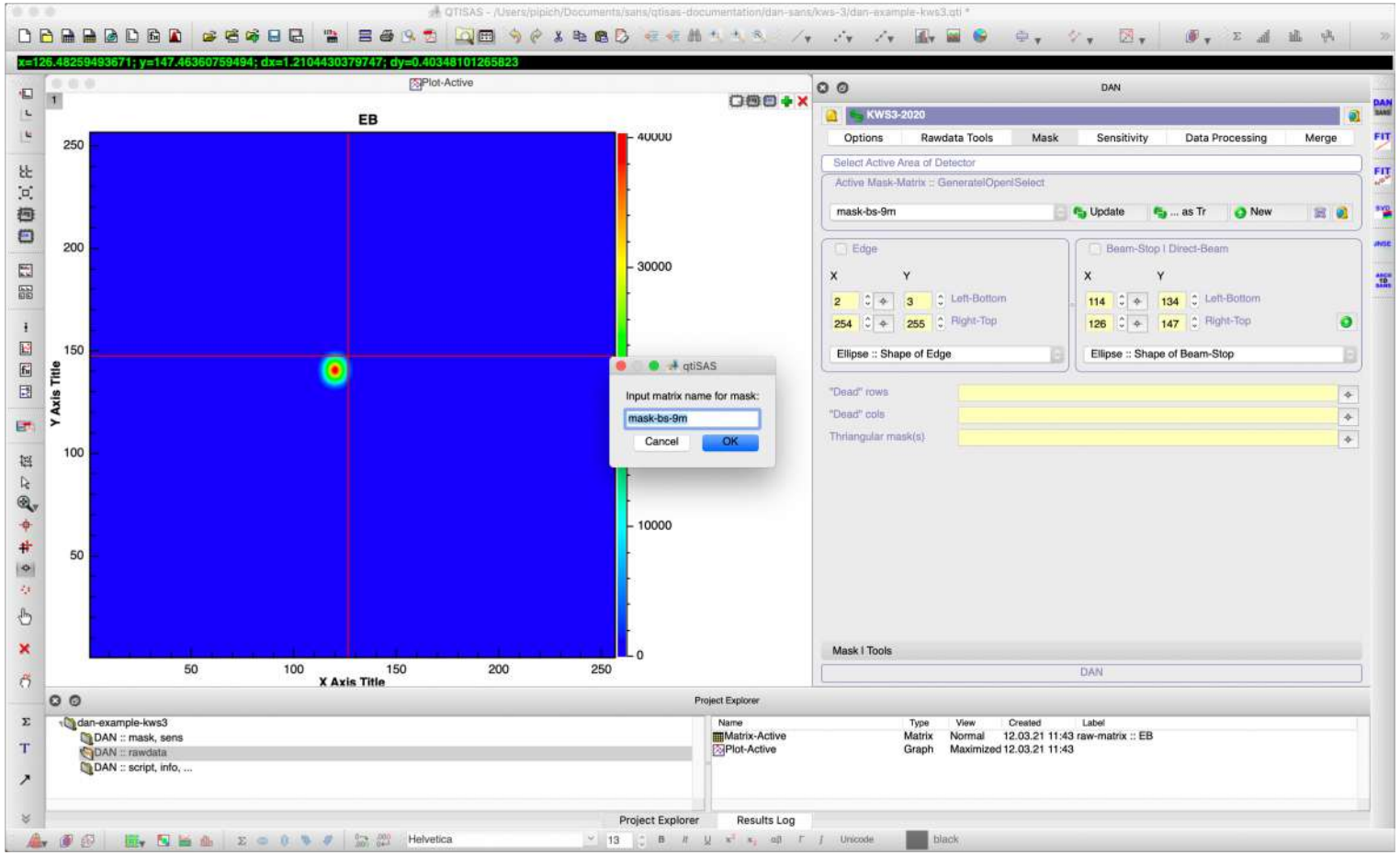

QTISAS - untitled *
Plot-Active
EB
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask
Update
... as Tr
New
Edge
Beam-Stop | Direct-Beam
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
f.e.: 3-3;10-15;25-27
Thriangular mask(s)
Mask | Tools
DAN
Project Explorer
UNTITLED
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Plot-Active
Graph
Maximized
12.03.21 11:43
Matrix-Active
Matrix
Normal
12.03.21 11:43 raw-matrix :: EB
Results Log
Project Explorer
Helvetica
Unicode
black

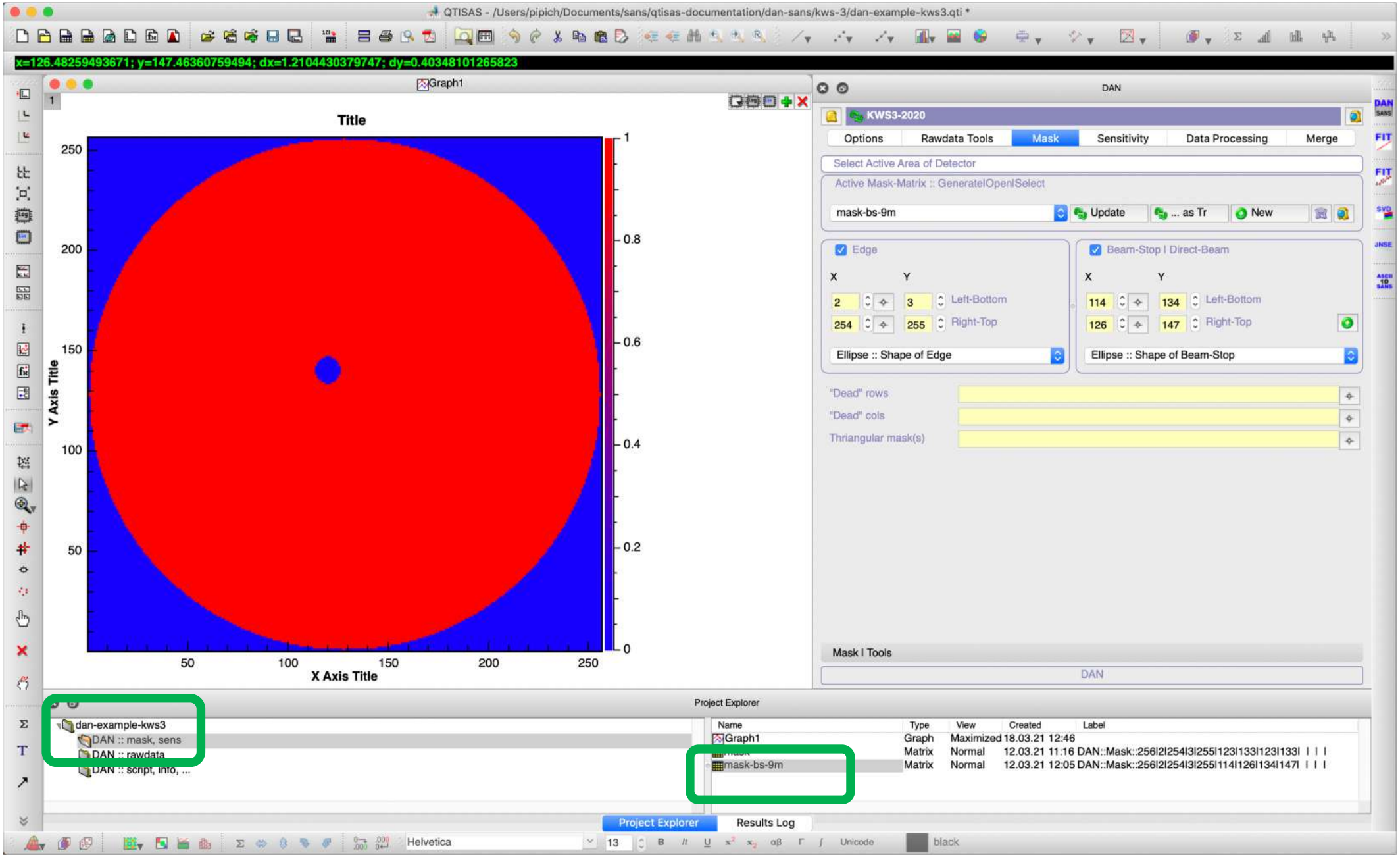

1
2
3
QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
Plot-Active
EB
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
mask-bs-9m
Edge
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask I Tools
Project Explorer
dan-example-kws3
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Matrix-Active
Plot-Active
Results Log

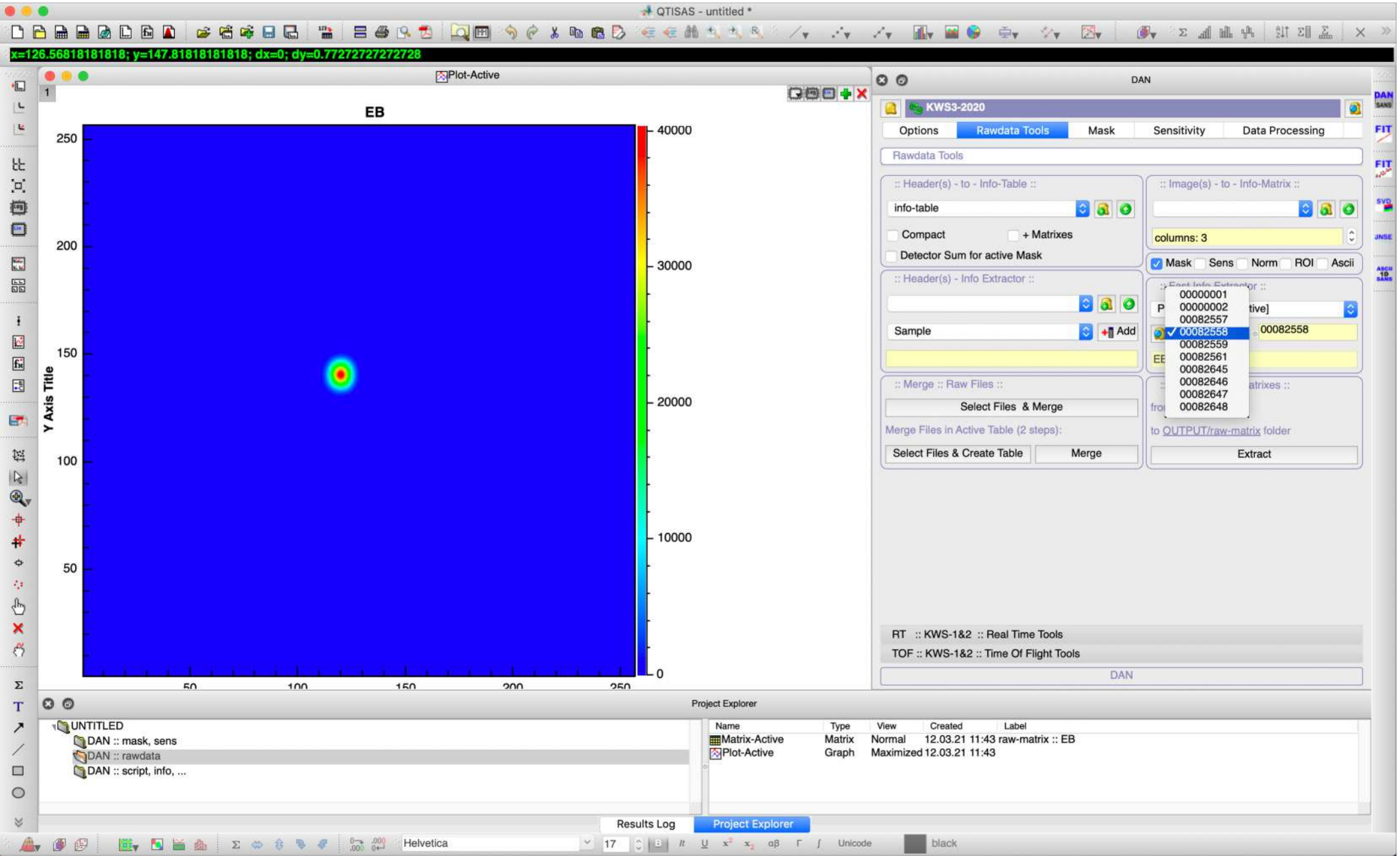

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
x=126.48259493671; y=147.46360759494; dx=1.2104430379747; dy=0.40348101265823
Plot-Active
EB
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-bs-9m
Update
... as Tr
New
Edge
Beam-Stop | Direct-Beam
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask | Tools
Project Explorer
dan-example-kws3
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Matrix-Active
Plot-Active
Results Log
1
2
3

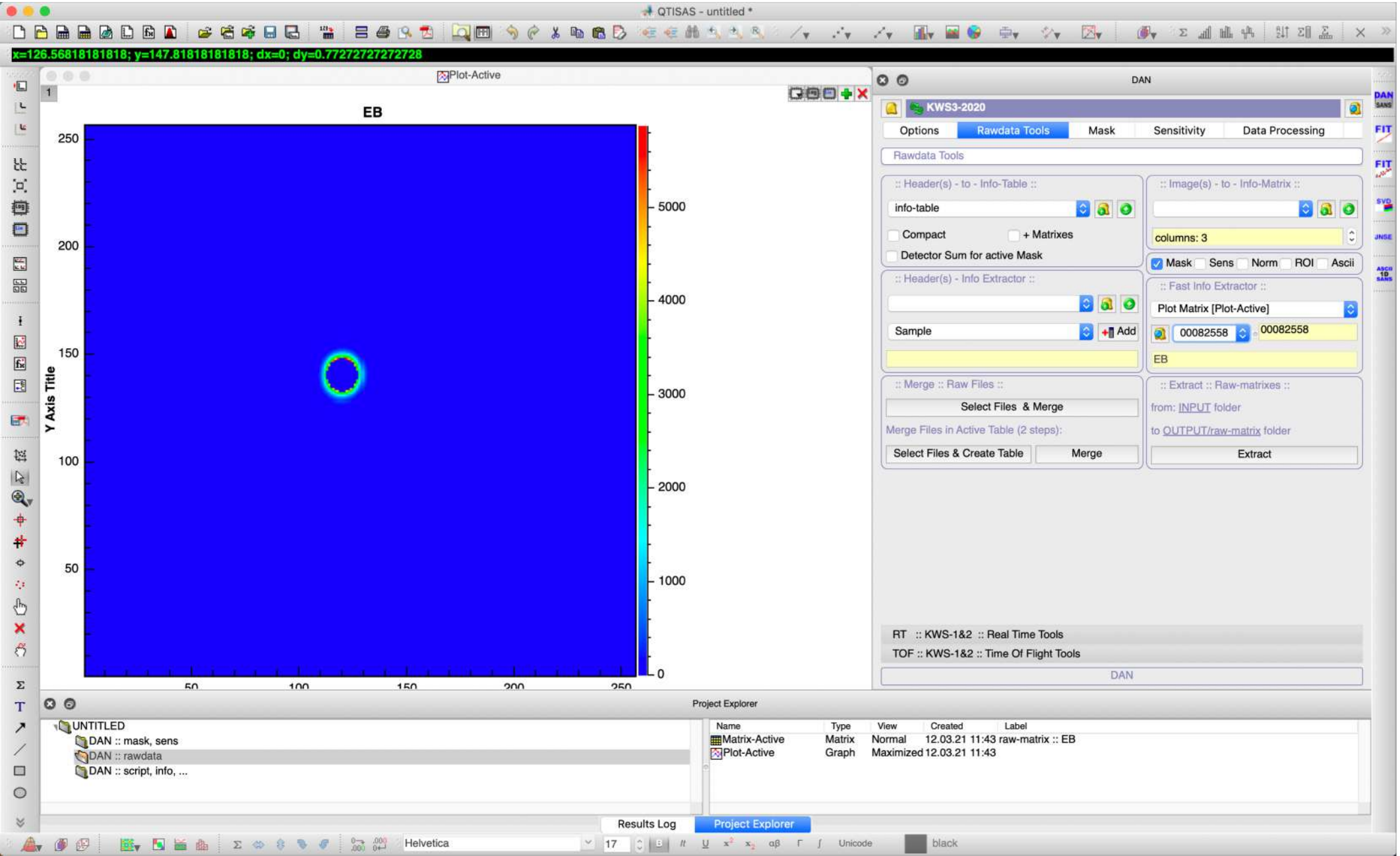

New


qtiSAS
Input matrix name for mask:
mask-bs-9m
Cancel
OK

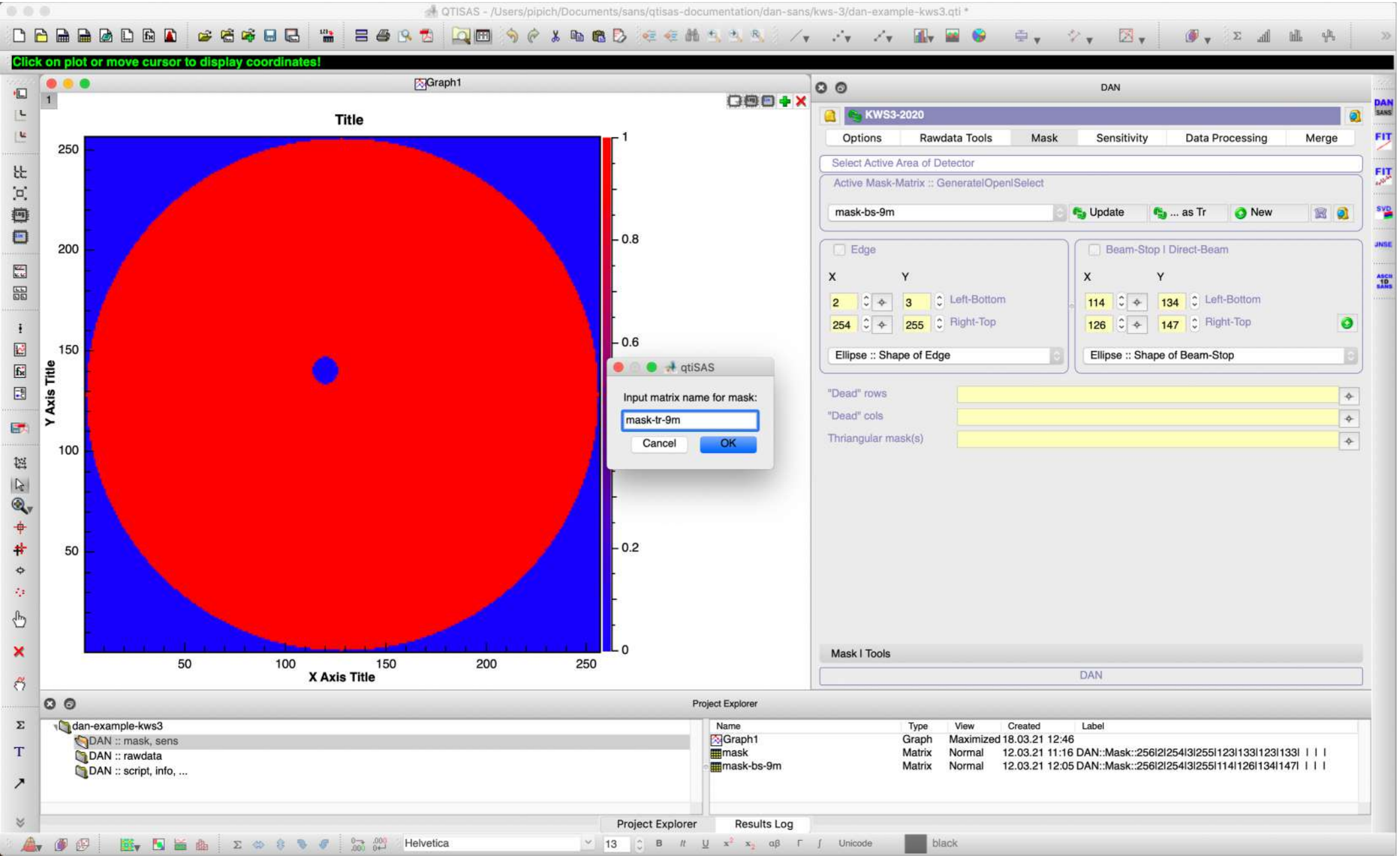

Plot-Active
EB
Y Axis Title
X Axis Title
qtiSAS
Input matrix name for mask:
mask-bs-9m
Cancel
OK
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-bs-9m
Update
New
Edge
Beam-Stop | Direct-Beam
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask | Tools
Project Explorer
dan-example-kws3
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Matrix-Active
Plot-Active
Results Log


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
x=126.48259493671; y=147.46360759494; dx=1.2104430379747; dy=0.40348101265823
Graph1
Title
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: GenerateIOpenISelect
mask-bs-9m
Update
... as Tr
New
Edge
Beam-Stop I Direct-Beam
X
Y
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask I Tools
DAN
Project Explorer
dan-example-kws3
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Graph1
Graph
Maximized
18.03.21 12:46
Matrix
Normal
12.03.21 11:16 DAN::Mask::256|2|254|3|255|123|133|123|133|
mask-bs-9m
Matrix
Normal
12.03.21 12:05 DAN::Mask::256|2|254|3|255|114|126|134|147|
Project Explorer
Results Log
Helvetica
13
Unicode
black


QTISAS - untitled *
x=126.56818181818; y=147.81818181818; dx=0; dy=0.77272727272728
Plot-Active
EB
Y Axis Title
250
200
150
100
50
50
100
150
200
250
40000
30000
20000
10000
0
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Rawdata Tools
:: Header(s) - to - Info-Table ::
info-table
Compact
+ Matrixes
Detector Sum for active Mask
:: Image(s) - to - Info-Matrix ::
columns: 3
Mask
Sens
Norm
ROI
Ascii
:: Header(s) - Info Extractor ::
Sample
Add
00000001
00000002
00082557
00082558
00082559
00082561
00082645
00082646
00082647
00082648
00082558
:: Merge :: Raw Files ::
Select Files & Merge
Merge Files in Active Table (2 steps):
Select Files & Create Table
Merge
to OUTPUT/raw-matrix folder
Extract
RT :: KWS-1&2 :: Real Time Tools
TOF :: KWS-1&2 :: Time Of Flight Tools
DAN
Project Explorer
UNTITLED
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Matrix-Active
Matrix
Normal
12.03.21 11:43
raw-matrix :: EB
Plot-Active
Graph
Maximized
12.03.21 11:43
Results Log
Project Explorer
Helvetica
17
Unicode
black

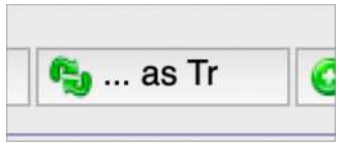

QTISAS - untitled *
x=126.56818181818; y=147.81818181818; dx=0; dy=0.77272727272728
Plot-Active
EB
Y Axis Title
250
200
150
100
50
50
100
150
200
250
5000
4000
3000
2000
1000
0
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Rawdata Tools
:: Header(s) - to - Info-Table ::
info-table
Compact
+ Matrixes
Detector Sum for active Mask
:: Image(s) - to - Info-Matrix ::
columns: 3
Mask
Sens
Norm
ROI
Ascii
:: Header(s) - Info Extractor ::
Sample
Add
:: Fast Info Extractor ::
Plot Matrix [Plot-Active]
00082558
00082558
EB
:: Merge :: Raw Files ::
Select Files & Merge
Merge Files in Active Table (2 steps):
Select Files & Create Table
Merge
:: Extract :: Raw-matrixes ::
from: INPUT folder
to OUTPUT/raw-matrix folder
Extract
RT :: KWS-1&2 :: Real Time Tools
TOF :: KWS-1&2 :: Time Of Flight Tools
DAN
Project Explorer
UNTITLED
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Matrix-Active
Matrix
Normal
12.03.21 11:43
raw-matrix :: EB
Plot-Active
Graph
Maximized
12.03.21 11:43
Results Log
Project Explorer
Helvetica
17
Unicode
black

STEP 5.3: “mask-tr-9m” generation

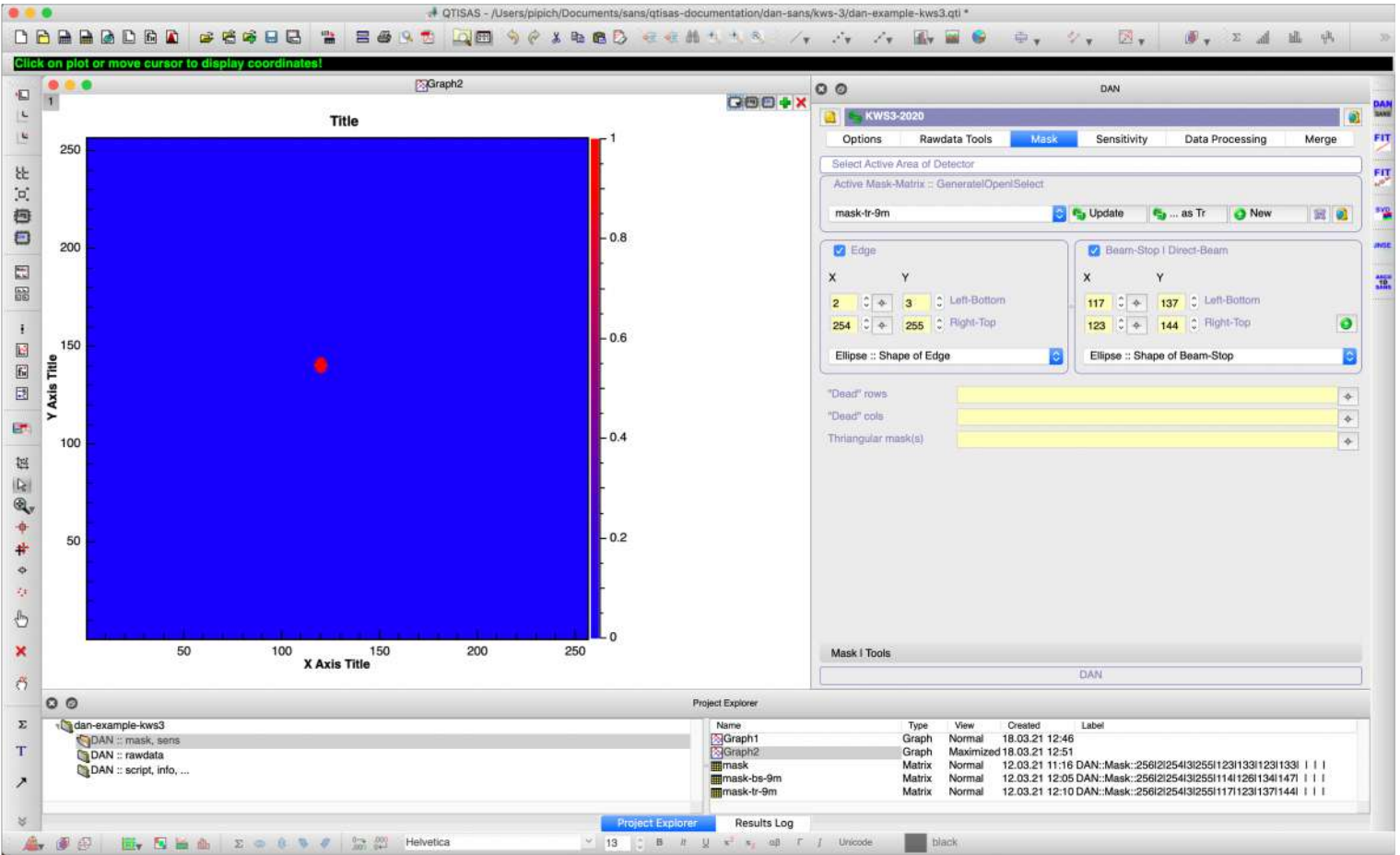

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
Click on plot or move cursor to display coordinates!
Graph1
Title
Y Axis Title
X Axis Title
qtiSAS
Input matrix name for mask:
mask-tr-9m
Cancel
OK
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-bs-9m
Update
... as Tr
New
Edge
Beam-Stop | Direct-Beam
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask | Tools
Project Explorer
dan-example-kws3
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Graph1
mask
mask-bs-9m
Results Log
Helvetica
Unicode
black

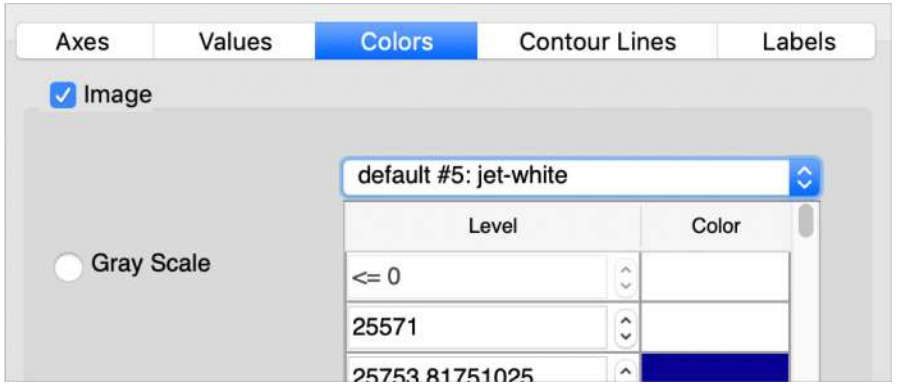

Beam-Stop I Direct-Beam
X
Y
114
134
Left-Bottom
126
147
Right-Top

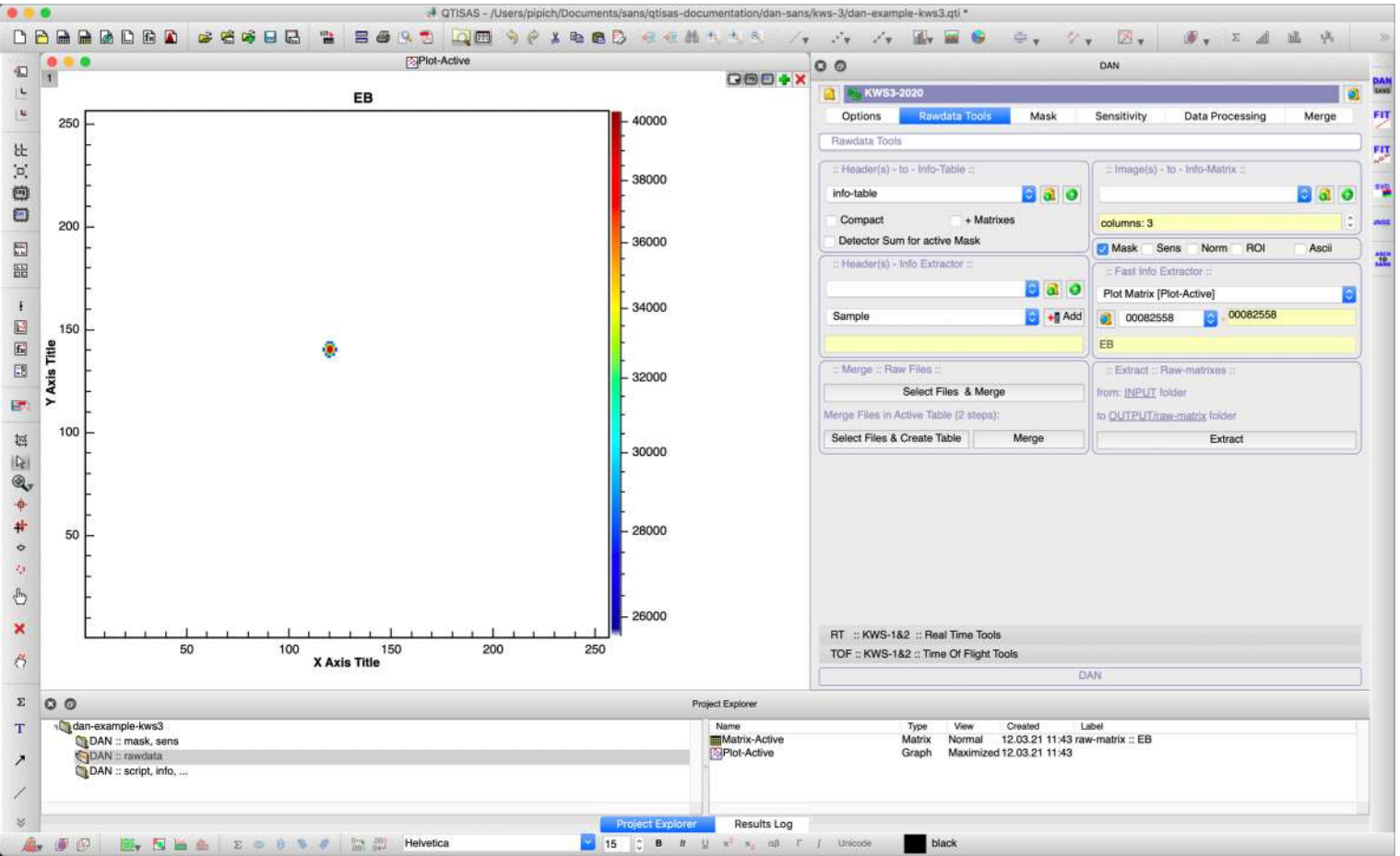

Beam-Stop I Direct-Beam
X
Y
117
137
Left-Bottom
123
144
Right-Top


... as Tr

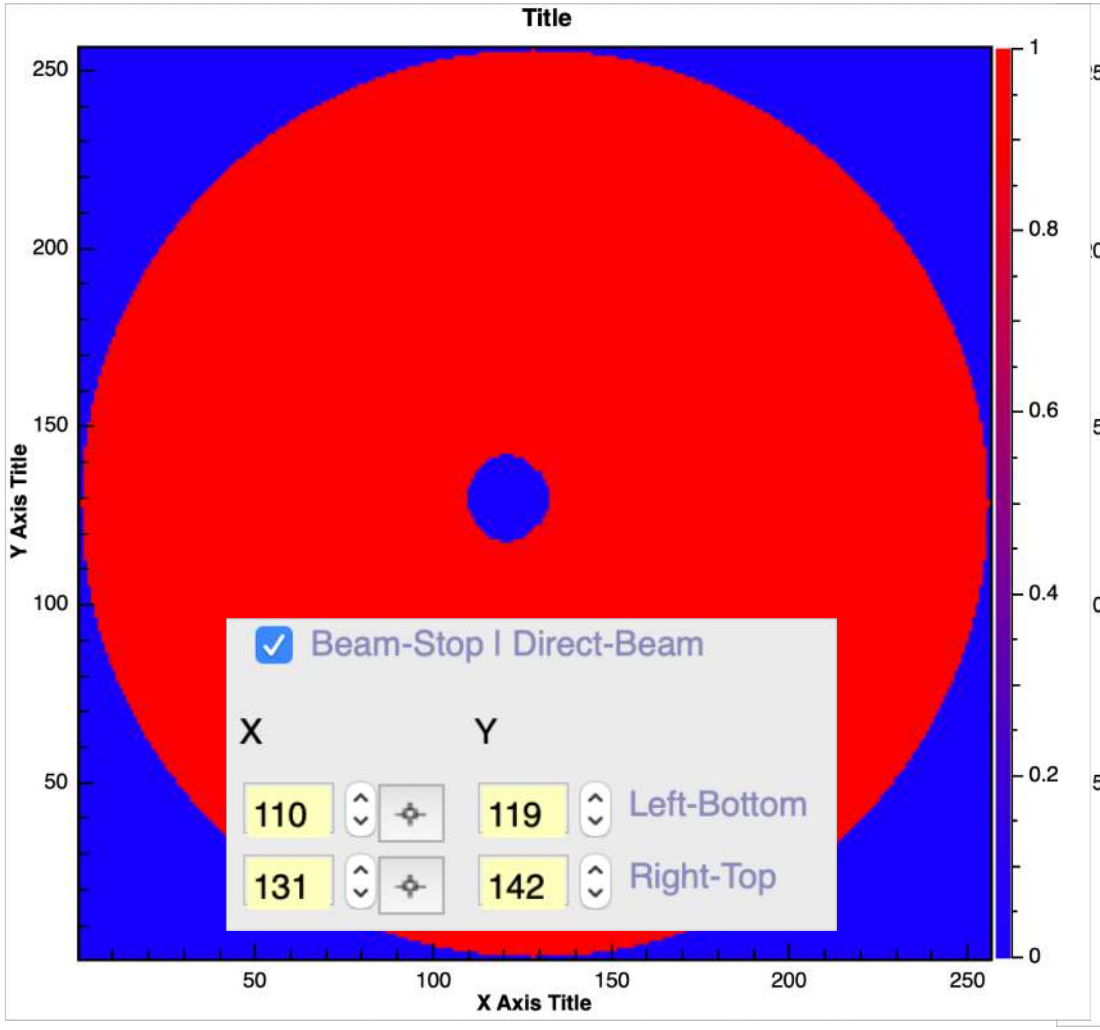

Color Fill
Contour Lines
Gray Scale Map
Σ

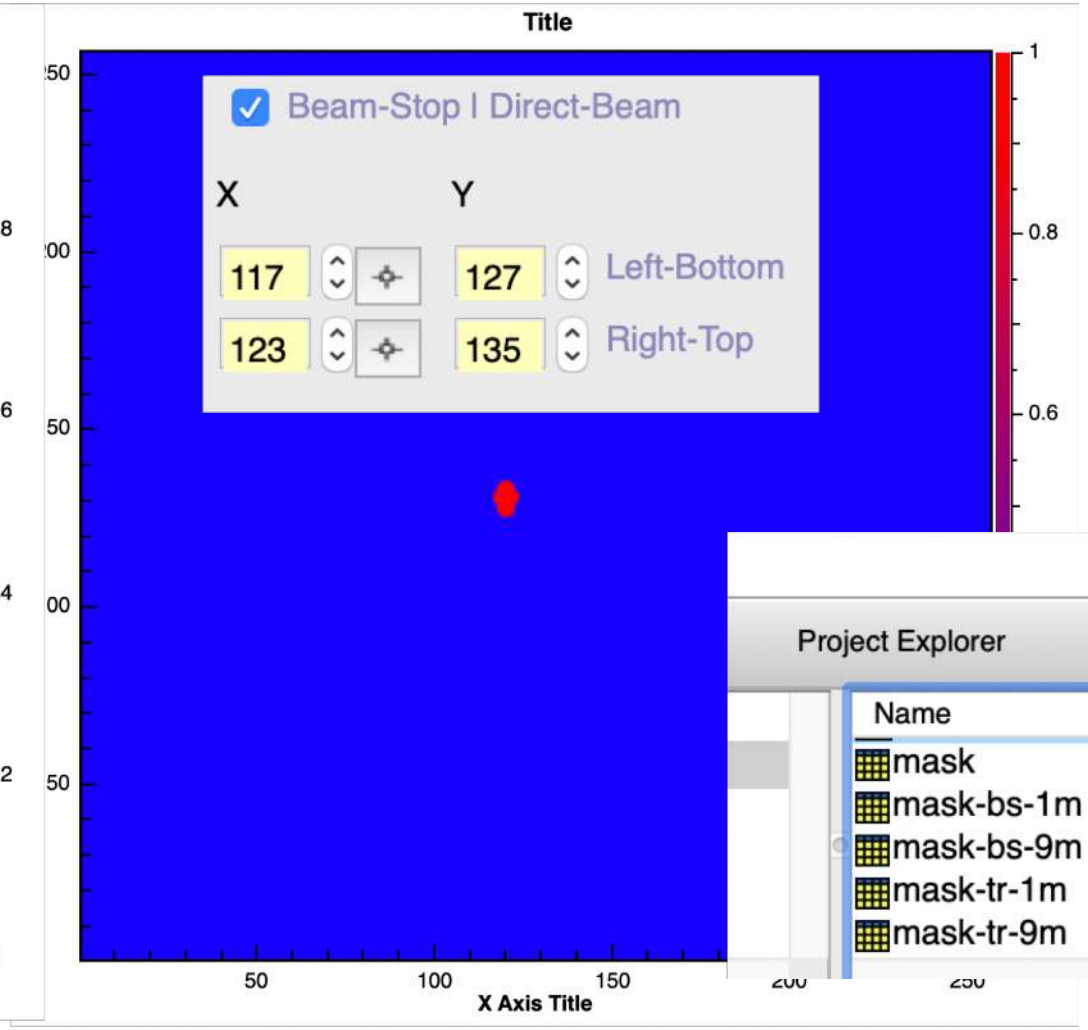

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
Click on plot or move cursor to display coordinates!
Graph2
Title
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-tr-9m
Update
... as Tr
New
Edge
Beam-Stop I Direct-Beam
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask I Tools
DAN
Project Explorer
dan-example-kws3
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Graph1
Graph2
mask
mask-bs-9m
mask-tr-9m
Project Explorer
Results Log

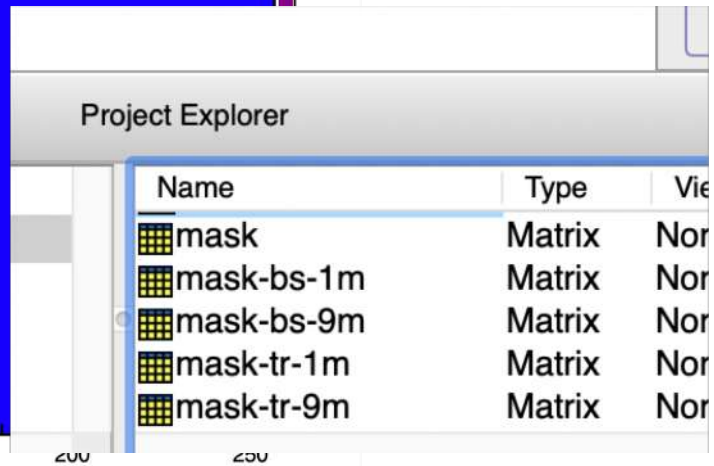

Axes
Values
Colors
Contour Lines
Labels
Image
default #5: jet-white
Gray Scale
Level
Color
<= 0
25571
25753.81751025


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
Plot-Active
EB
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Rawdata Tools
:: Header(s) - to - Info-Table ::
info-table
Compact
+ Matrixes
Detector Sum for active Mask
:: Image(s) - to - Info-Matrix ::
columns: 3
Mask
Sens
Norm
ROI
Ascii
:: Header(s) - Info Extractor ::
Sample
Add
:: Fast Info Extractor ::
Plot Matrix [Plot-Active]
00082558
00082558
EB
:: Merge :: Raw Files ::
Select Files & Merge
Merge Files in Active Table (2 steps):
Select Files & Create Table
Merge
:: Extract :: Raw-matrixes ::
from: INPUT folder
to OUTPUT/raw-matrix folder
Extract
RT :: KWS-1&2 :: Real Time Tools
TOF :: KWS-1&2 :: Time Of Flight Tools
DAN
Project Explorer
dan-example-kws3
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Matrix-Active
Matrix
Normal
12.03.21 11:43
raw-matrix :: EB
Plot-Active
Graph
Maximized
12.03.21 11:43
Project Explorer
Results Log
Helvetica
15
Unicode
black

STEP 5.4 & 5.5: “mask-tr-9m” generation





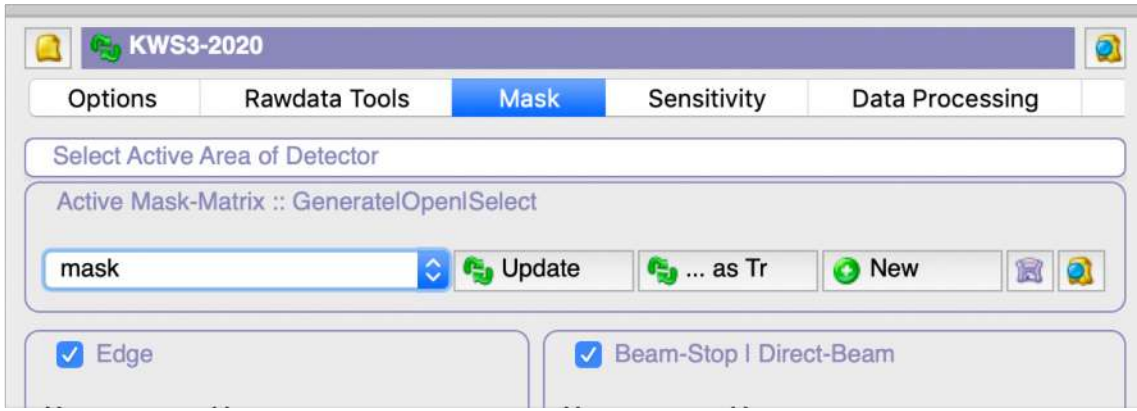


STEP 6: Detector Sensitivity (“Sens”) Reading

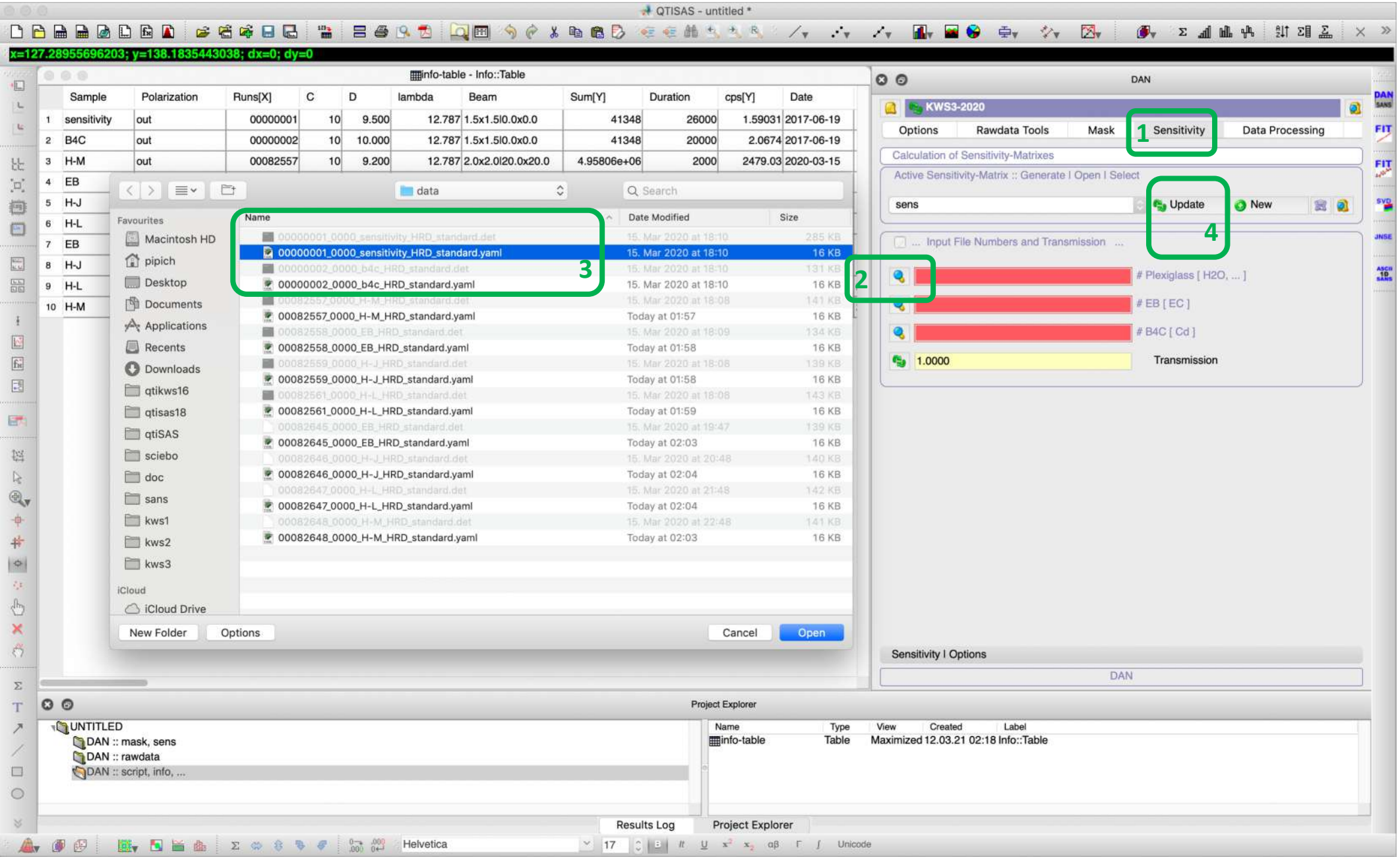
KWS-3 case: ask Local Contact to provide sensitivity files

In this example we use: **#00000001 run**

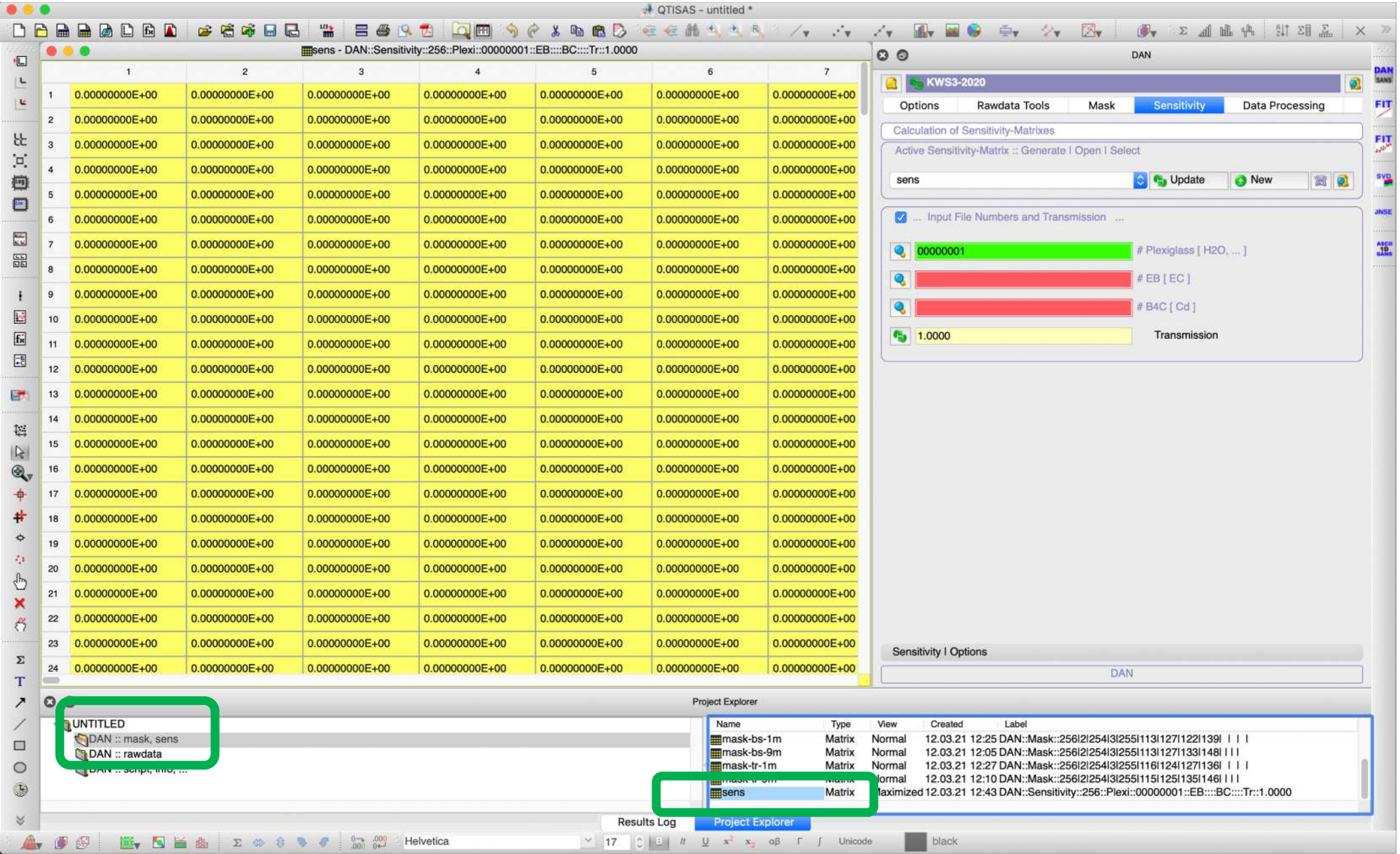
“mask” matrix should be active in Mask Tab



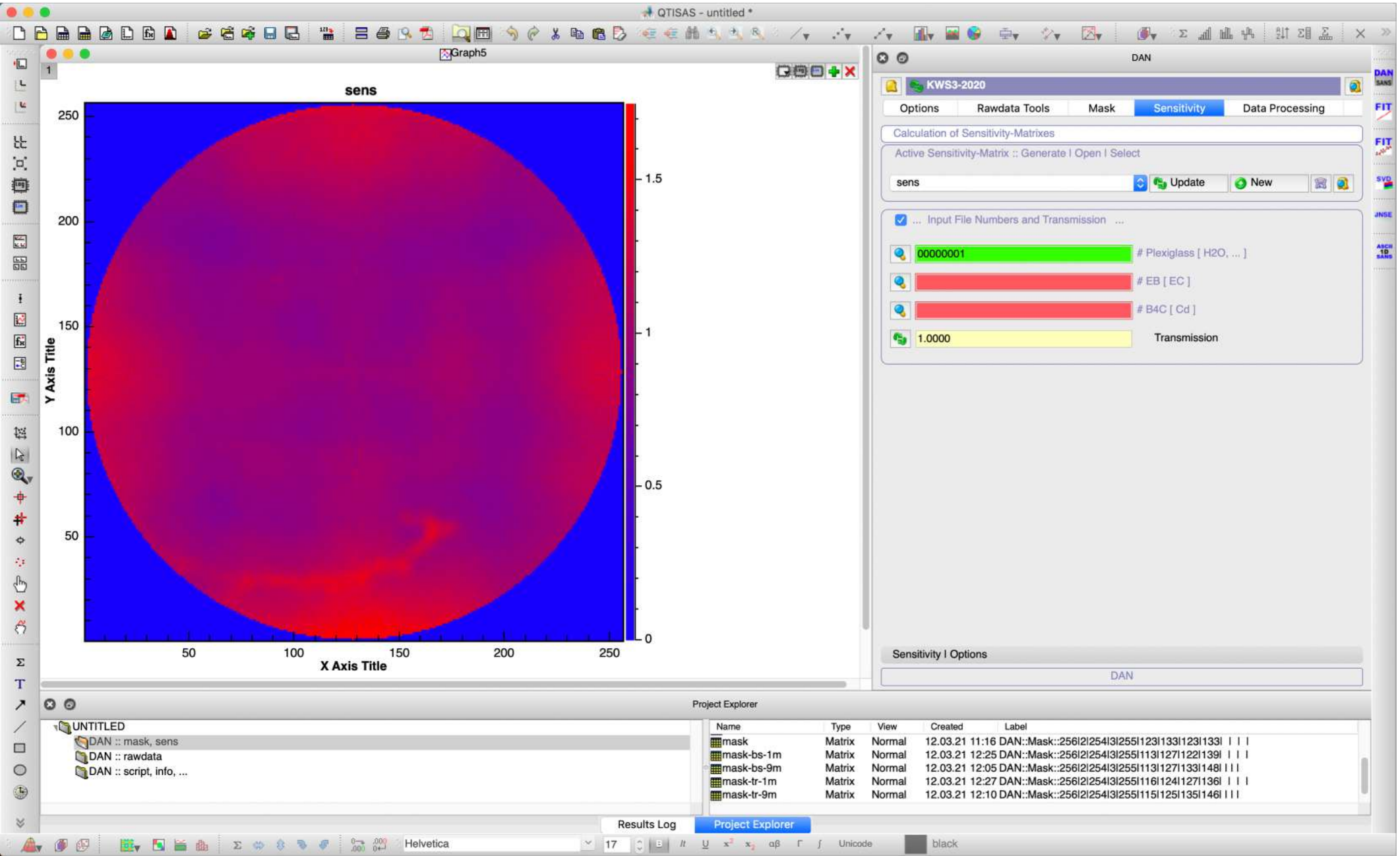
Go to **Sensitivity** tab & do 4 steps



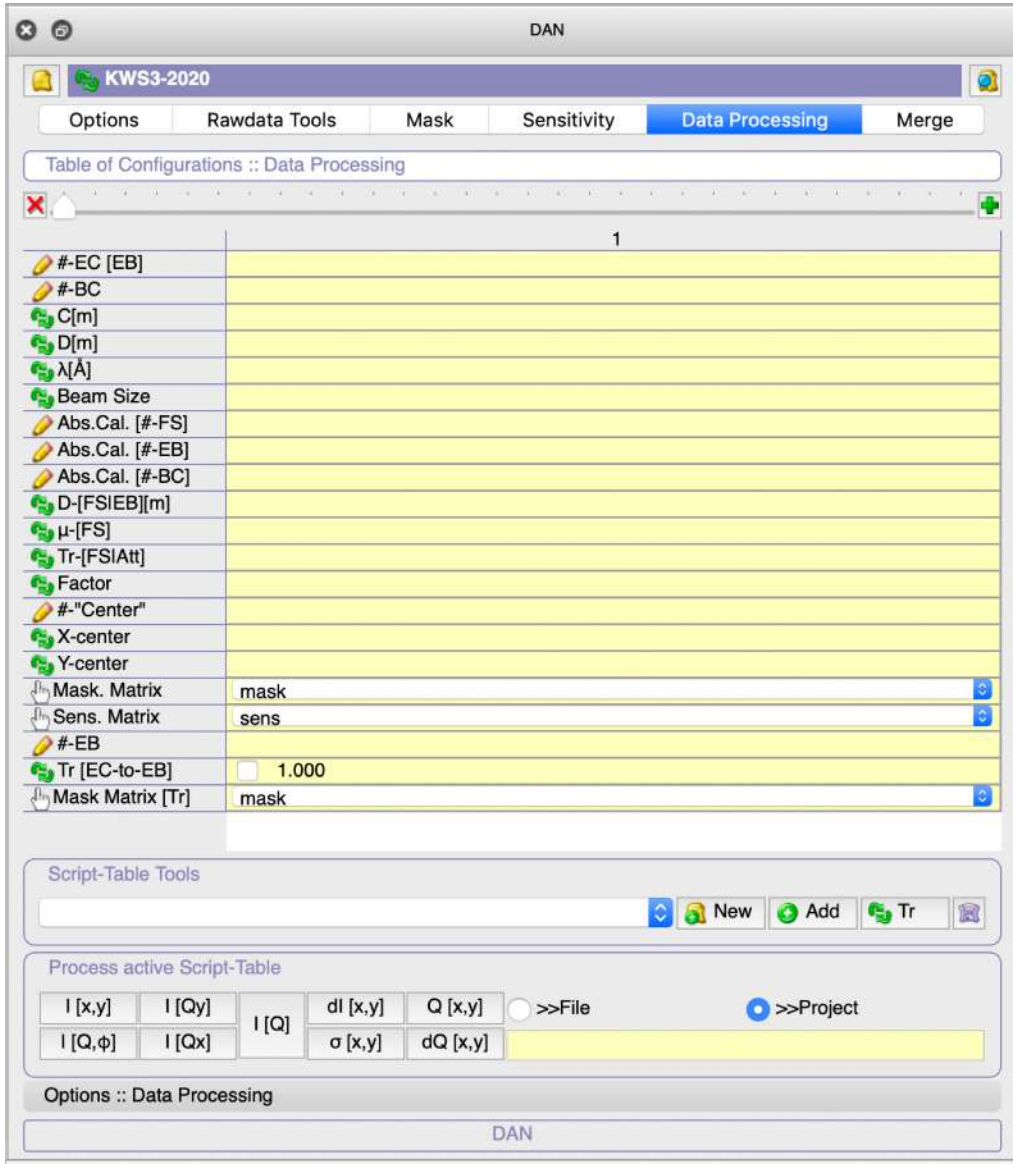
“sens” matrix is created in “DAN:: mask, sens” folder



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



STEP 7: Filling ”Table of Configurations”



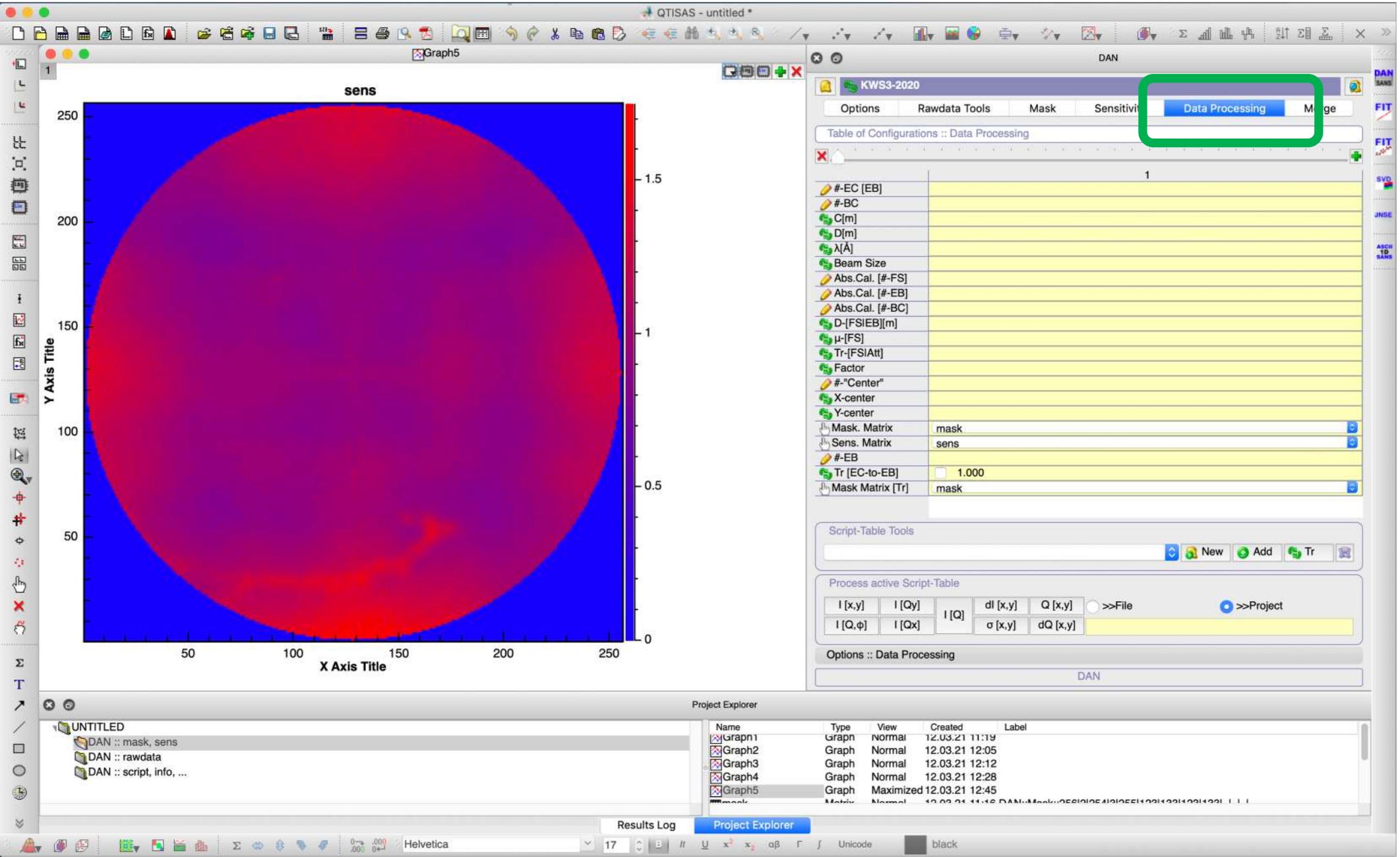
Icons meaning:

Select from list

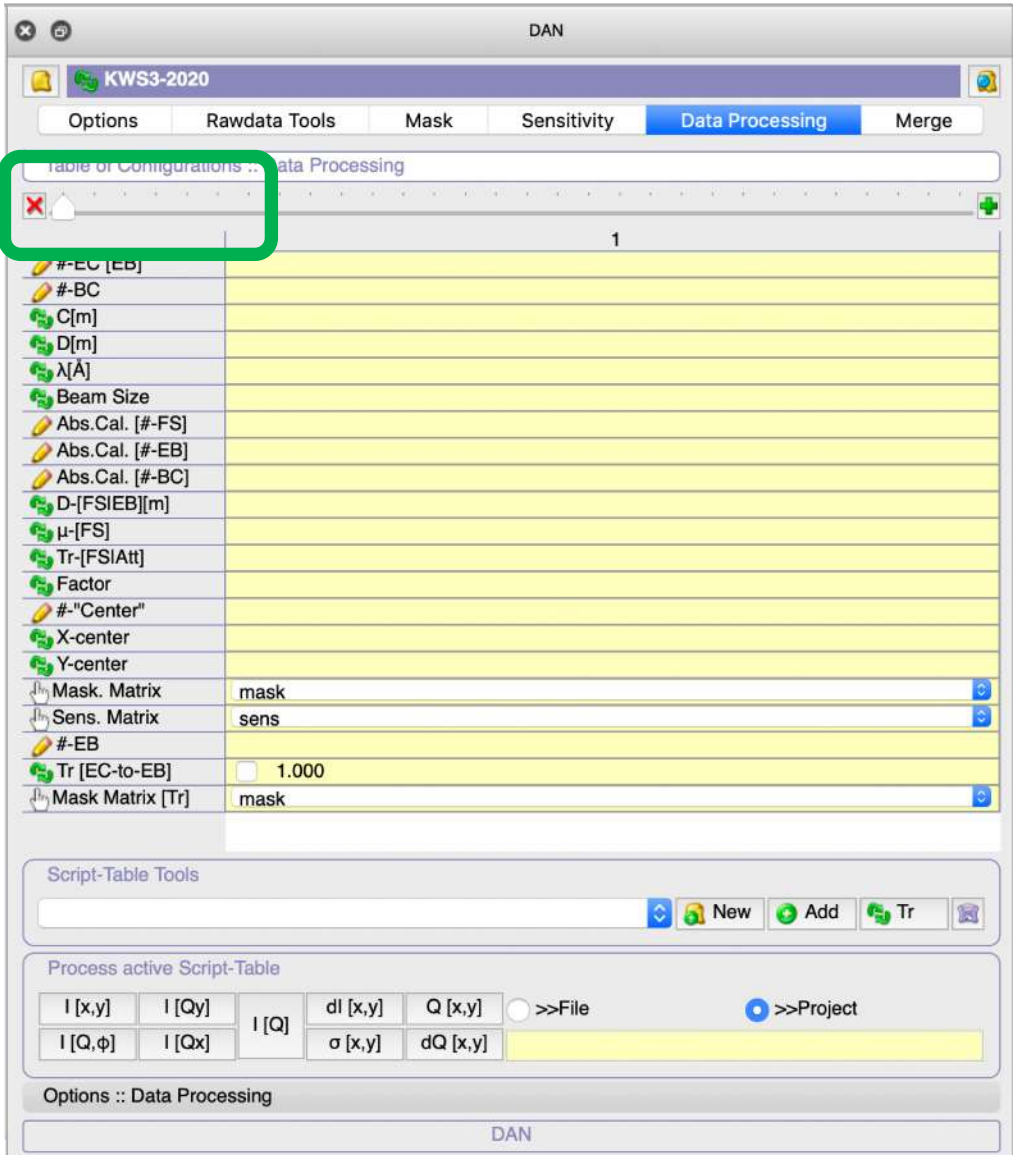
Input something (type or double click to select)

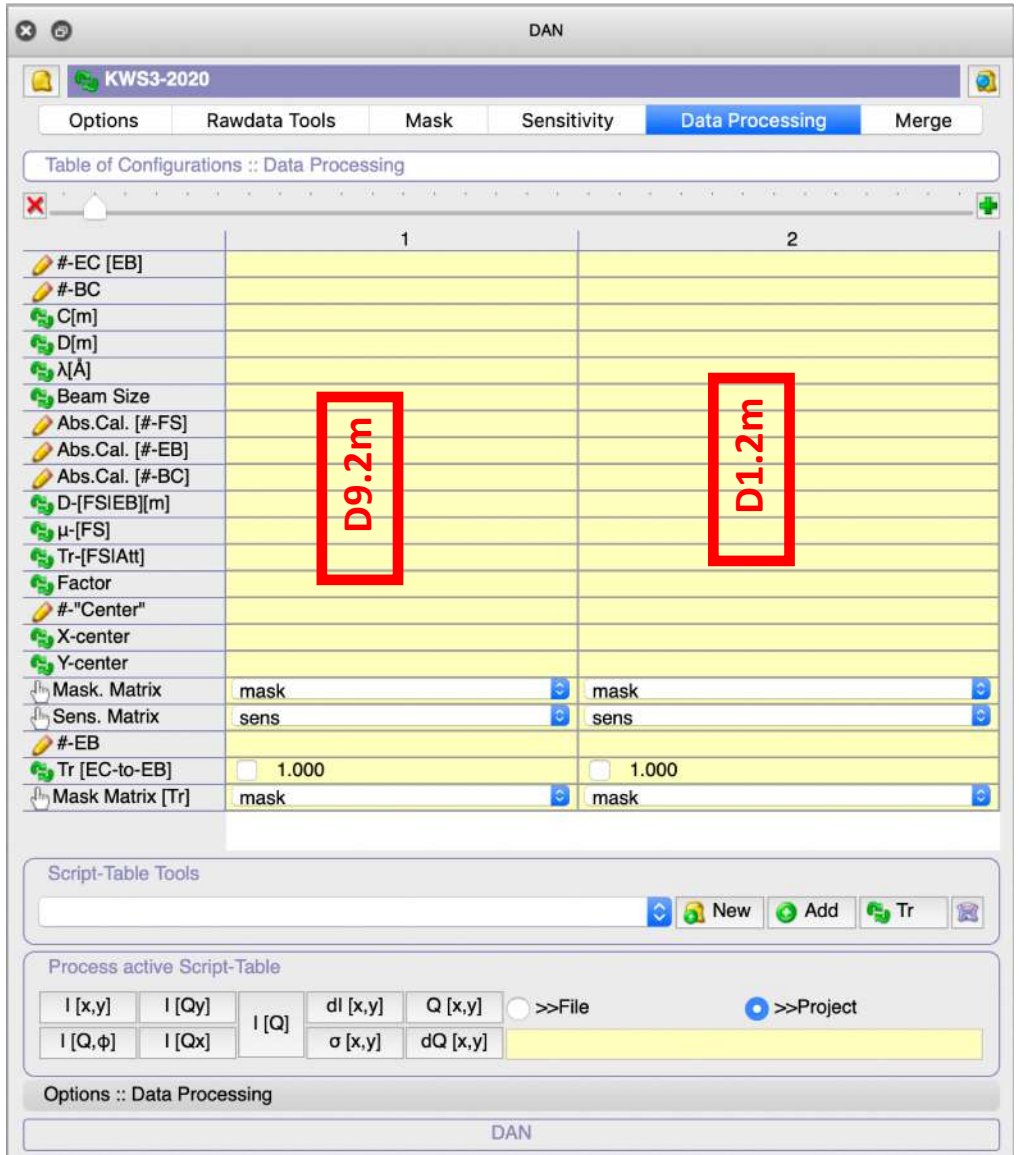
Calculate/read

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

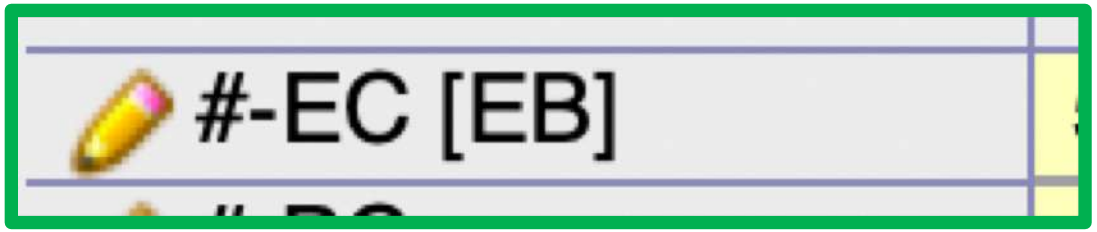


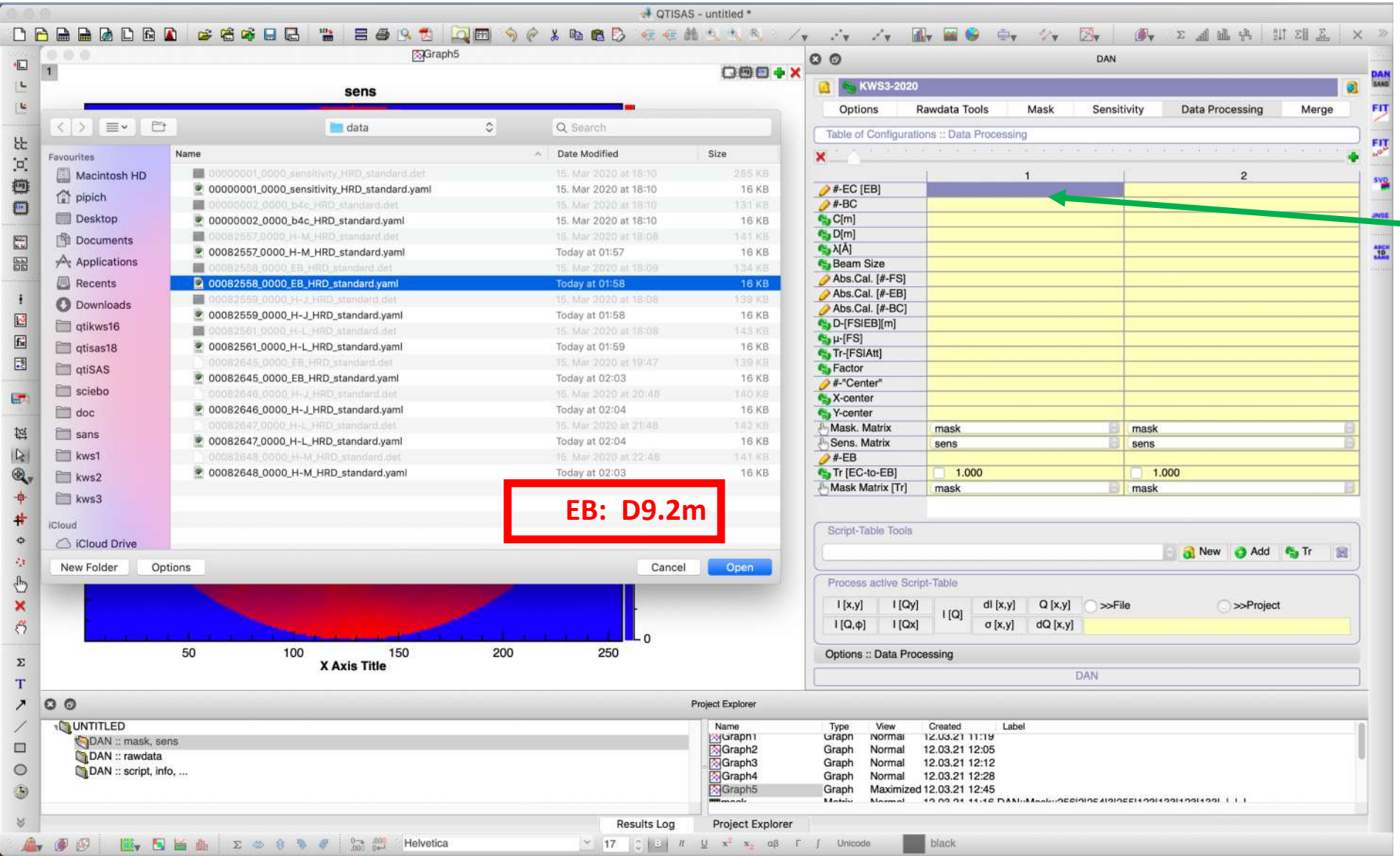
Set Number of Instrument Configuration: in this example 2





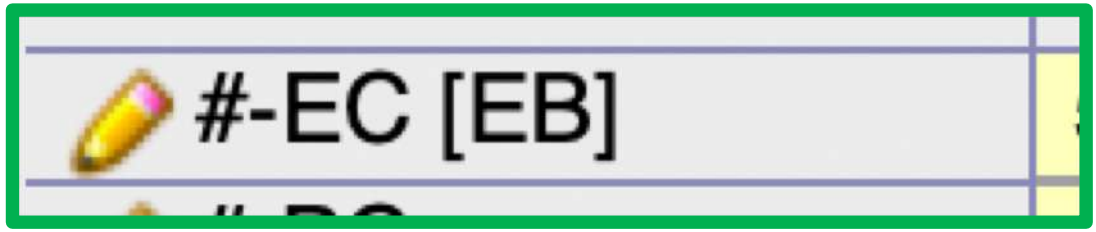
Empty Beam/Cell Runs

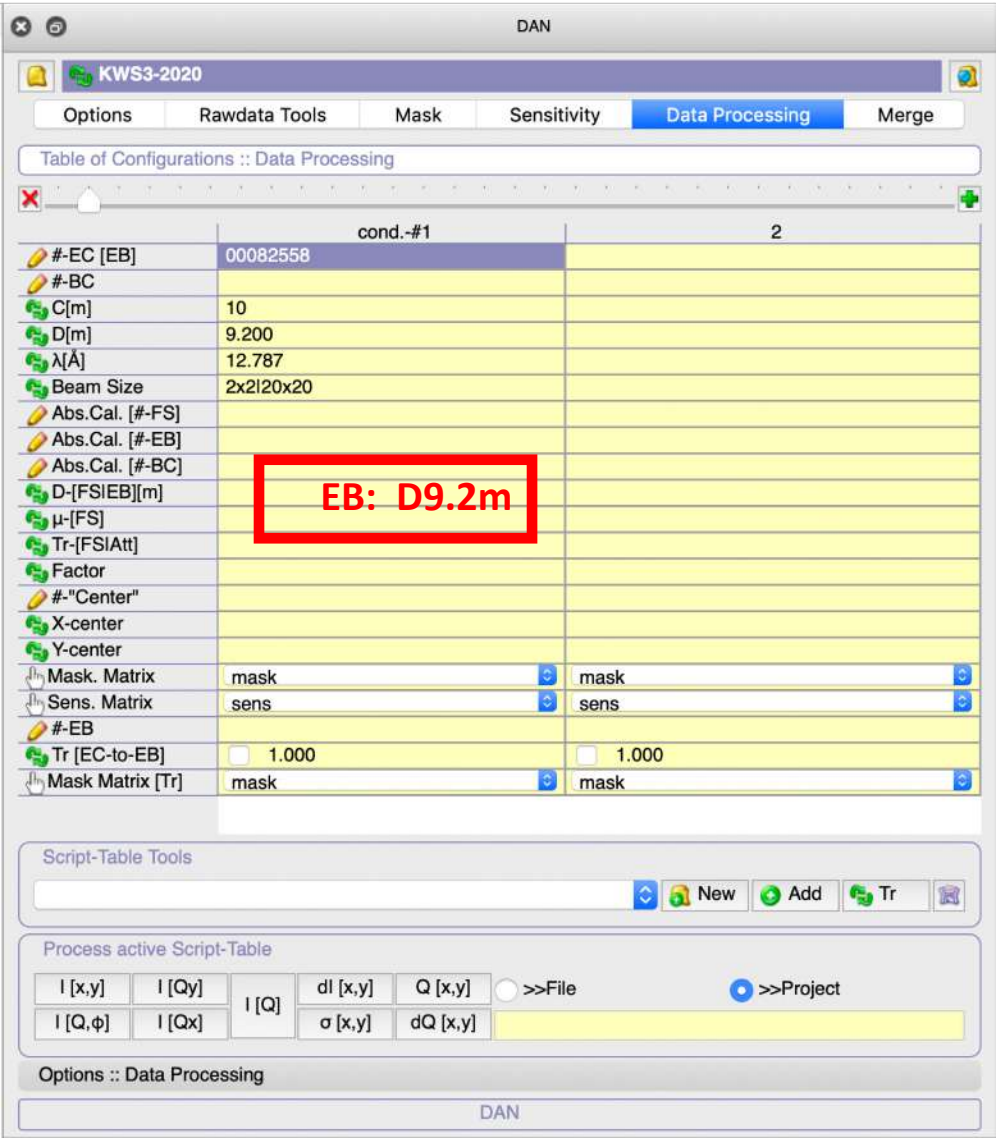


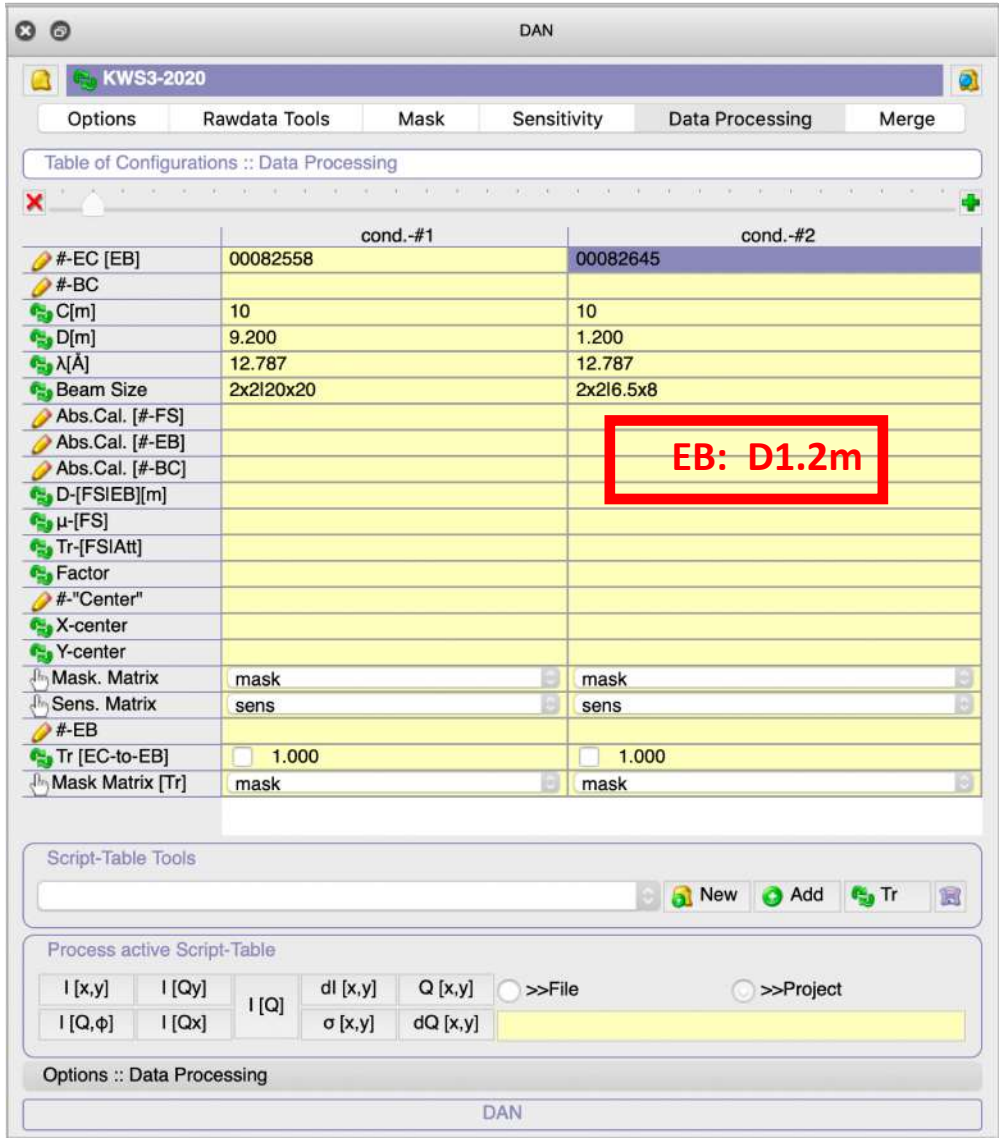


Double Click

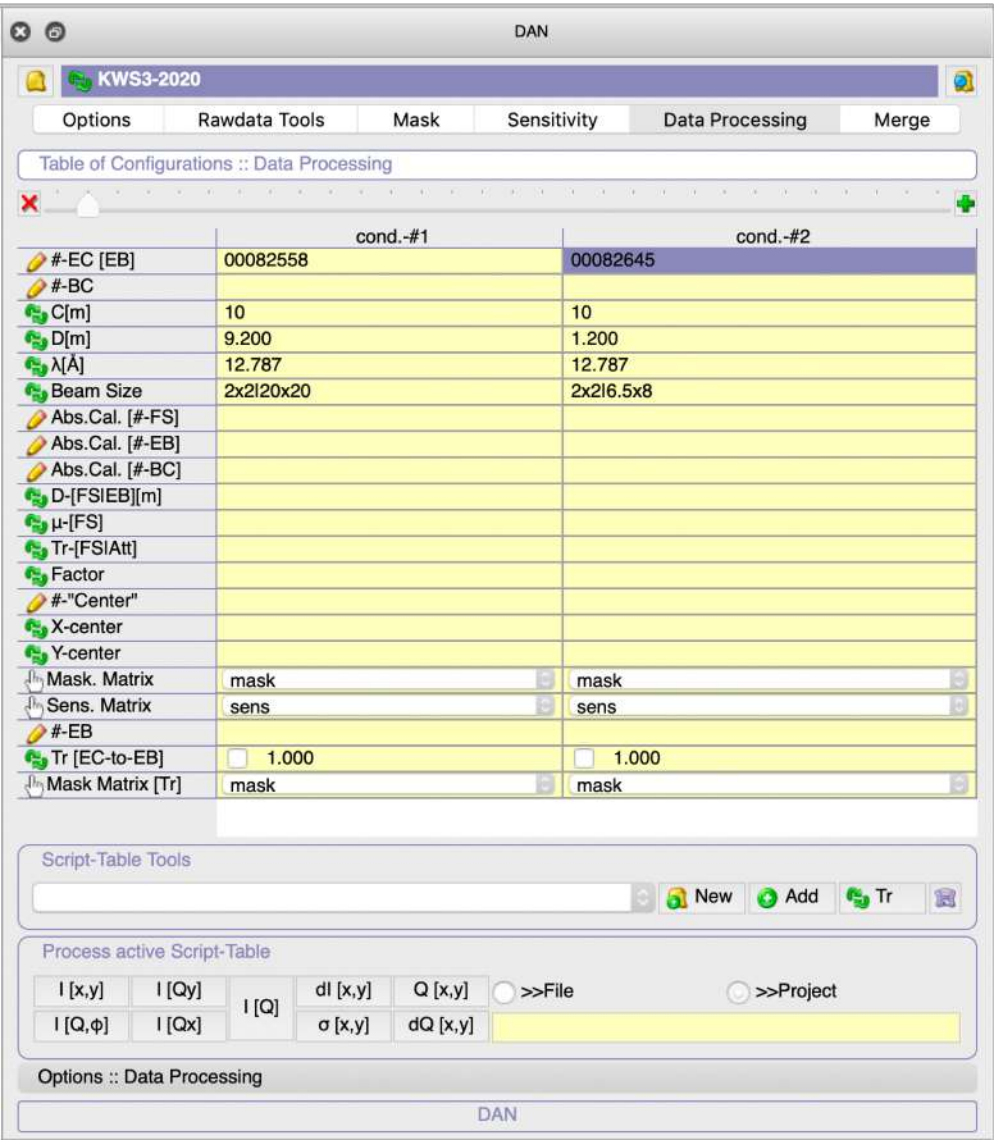
Fill: Empty Beam/Cell Runs

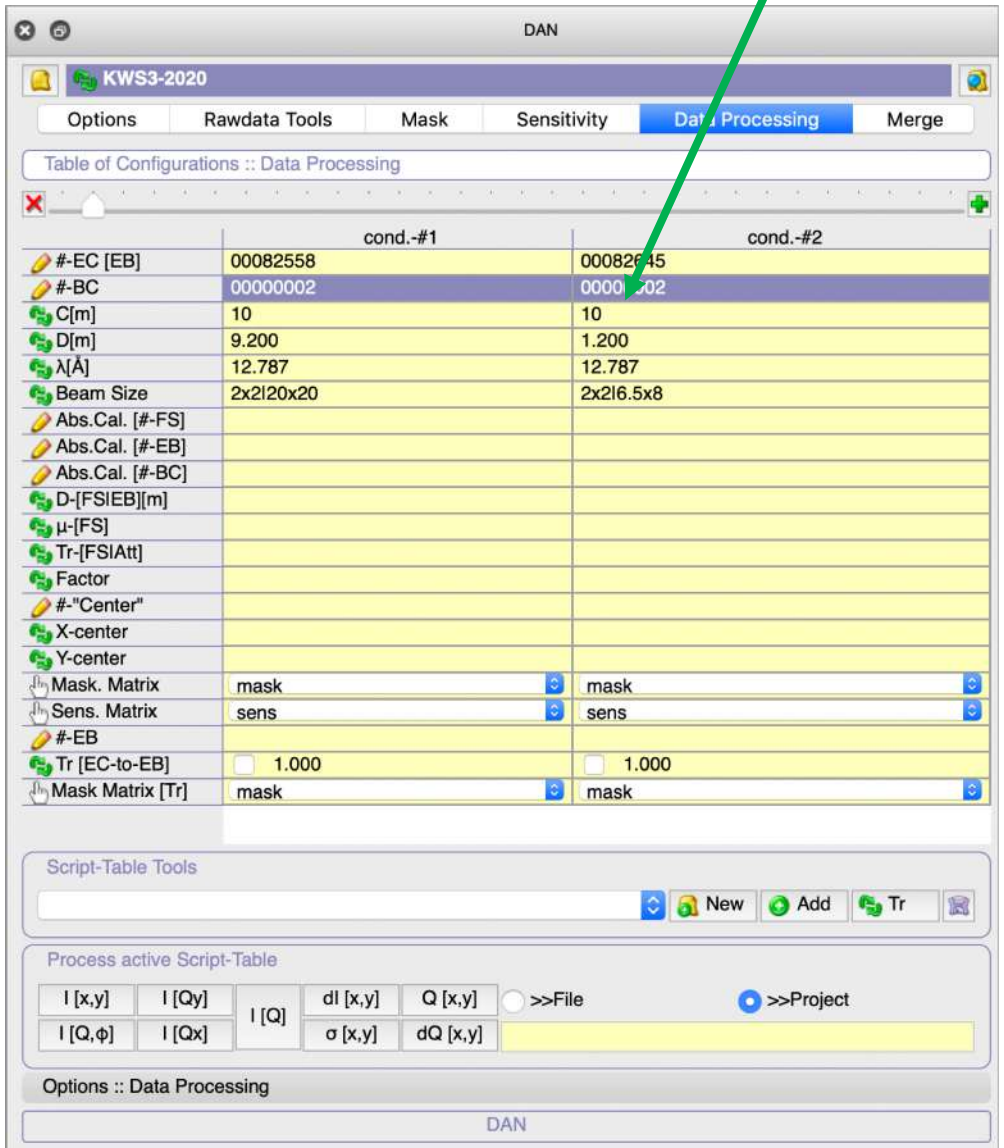




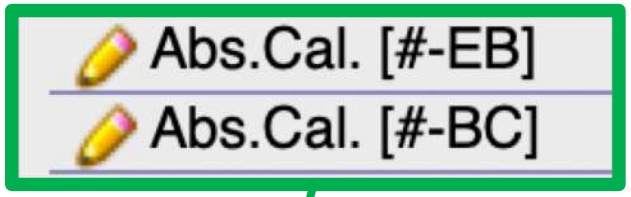


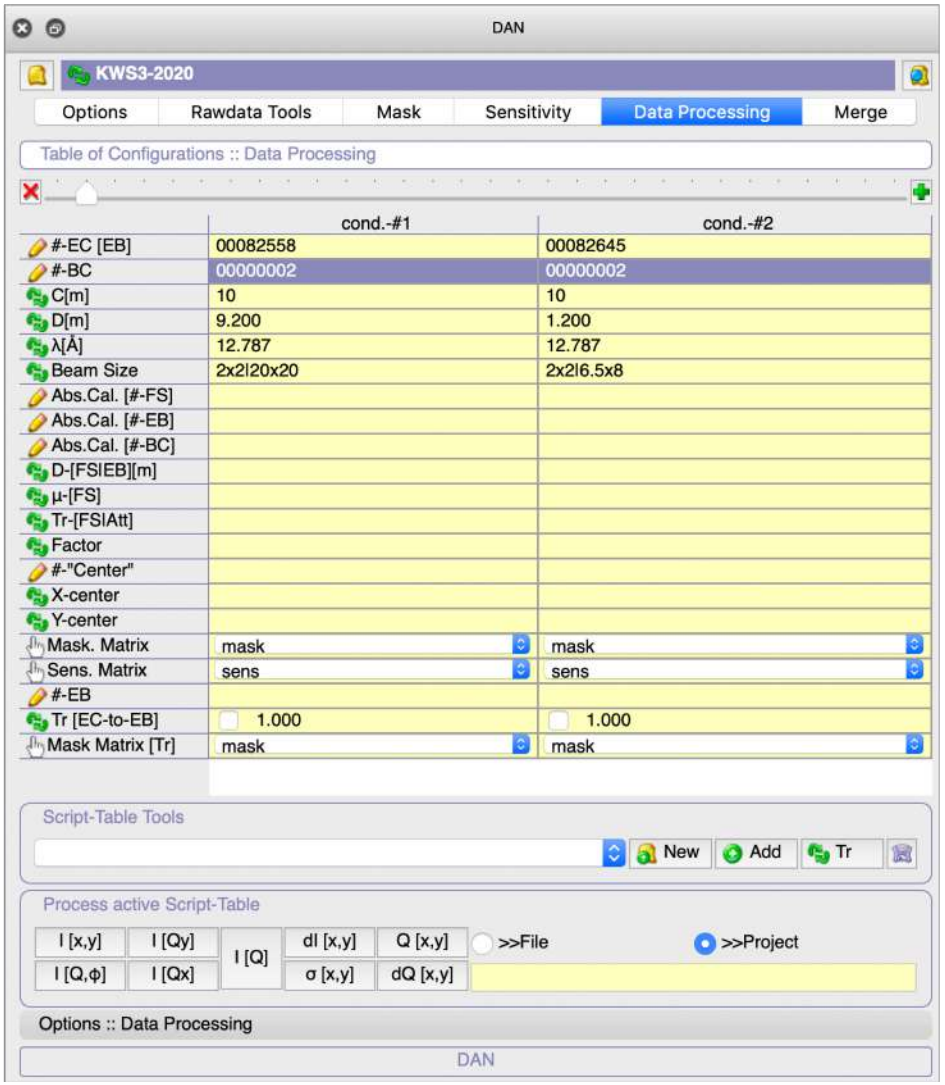
Fill: Detector Dark Current Runs

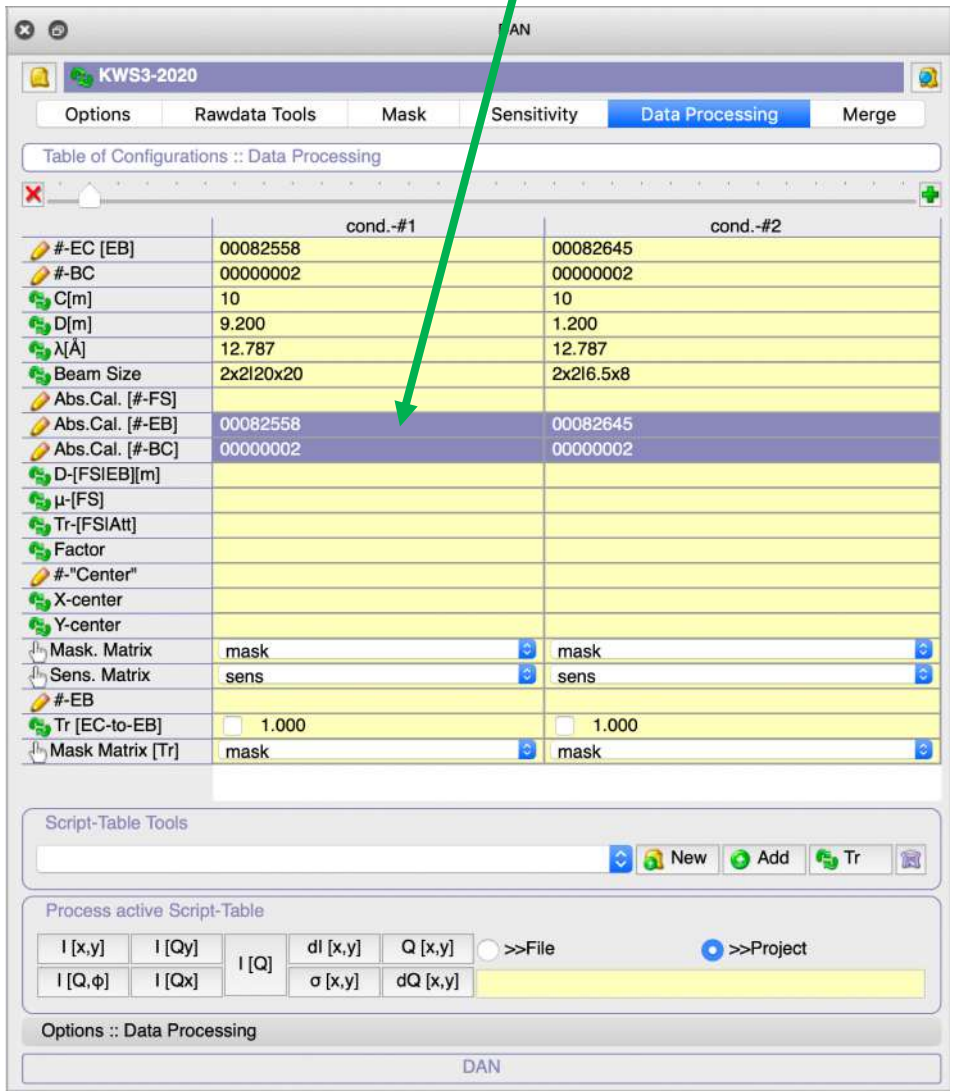


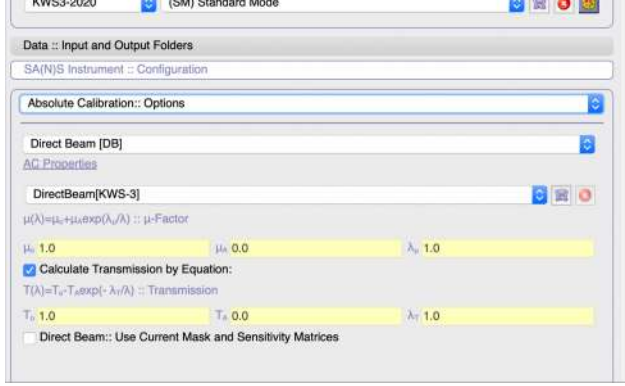


Fill: Absolute Calibration Runs (Direct Beam Mode)









Push : 

to read Sample to Detector Distances from Headers

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]		
μ-[FS]		
Tr-[FS|Att]		
Factor		
#-"Center"		
X-center		
Y-center		
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.000	1.000
Mask Matrix [Tr]	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

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]		
Tr-[FS|Att]		
Factor		
#-"Center"		
X-center		
Y-center		
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.000	1.000
Mask Matrix [Tr]	mask	mask

Script-Table Tools

New | Add | Tr

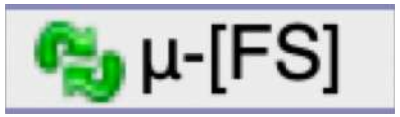
Process active Script-Table

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

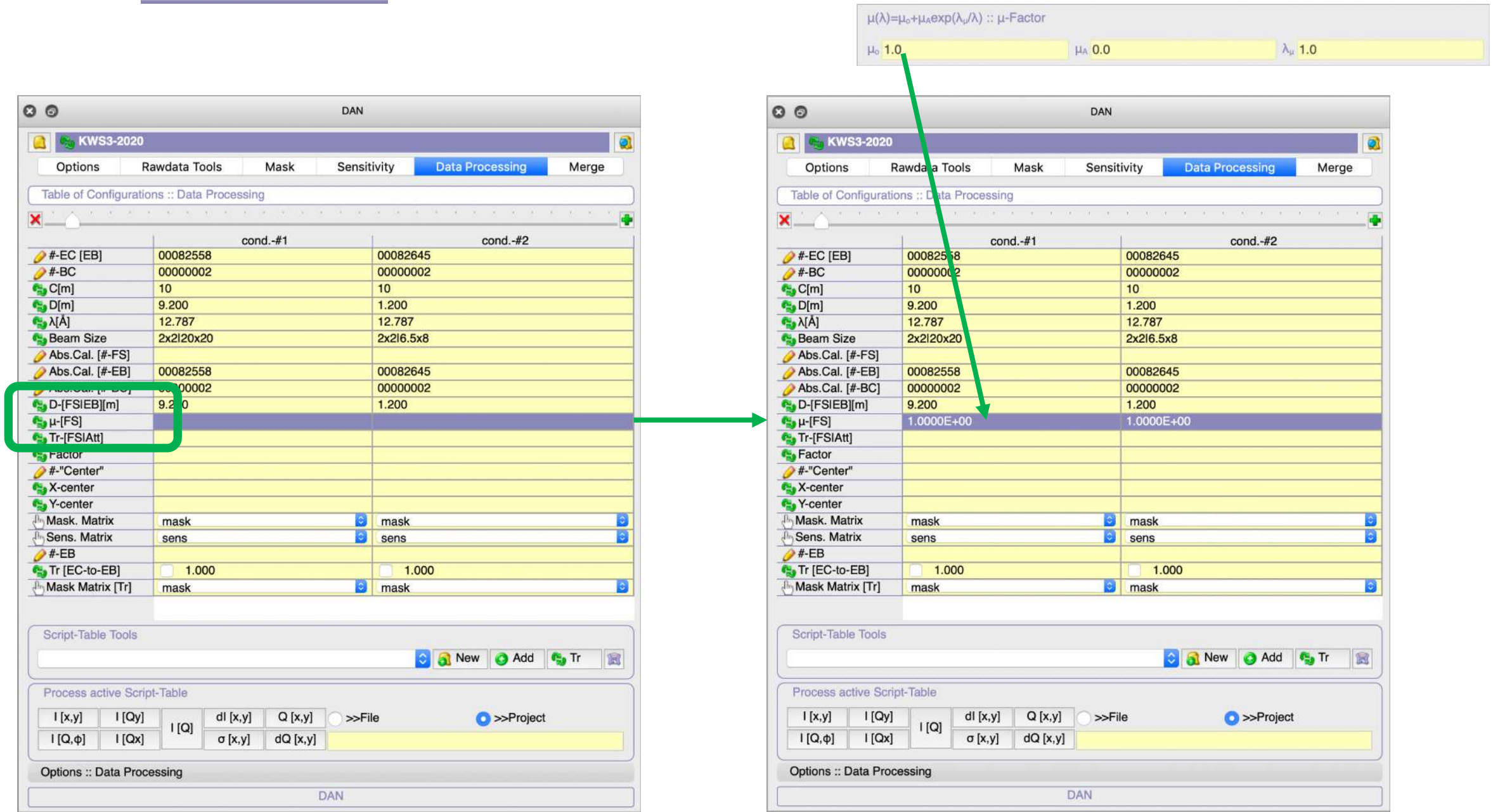
I [Q,ϕ] | I [Qx] | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

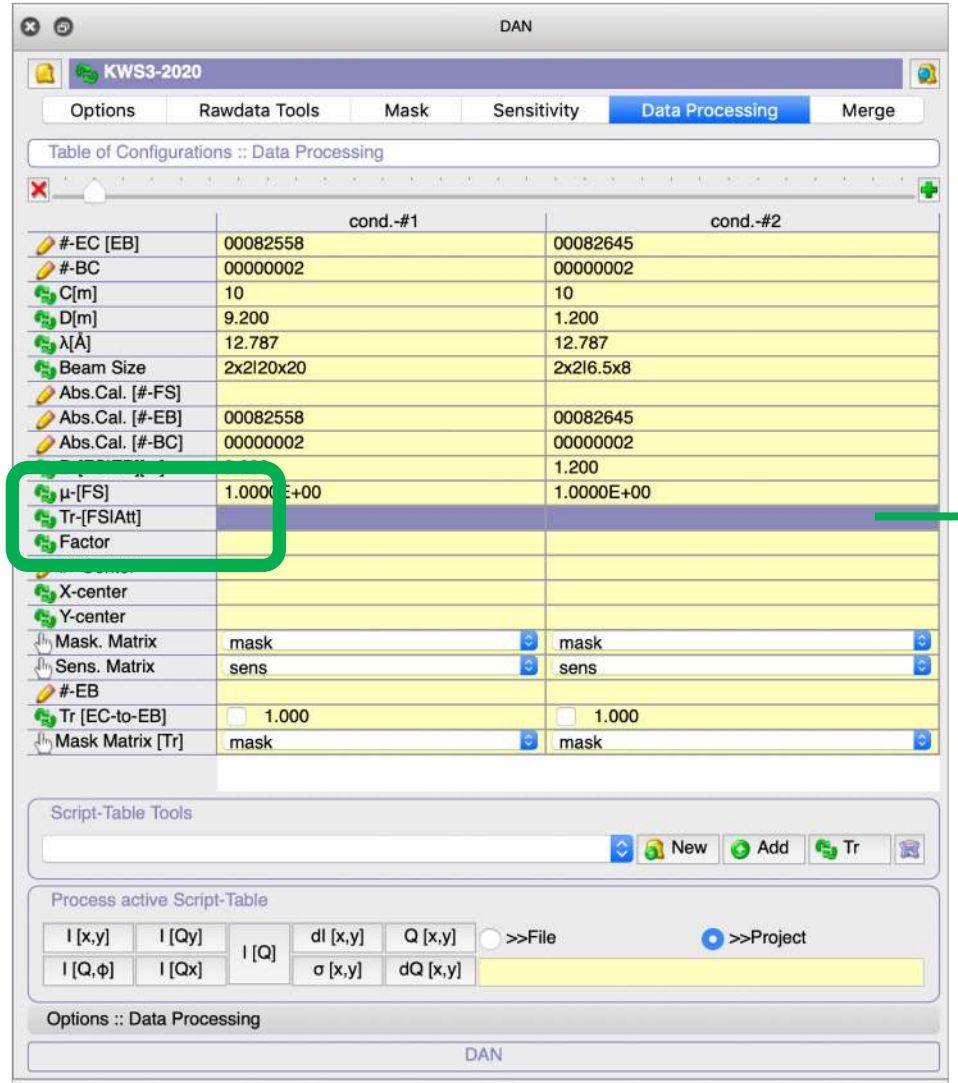
Push : 

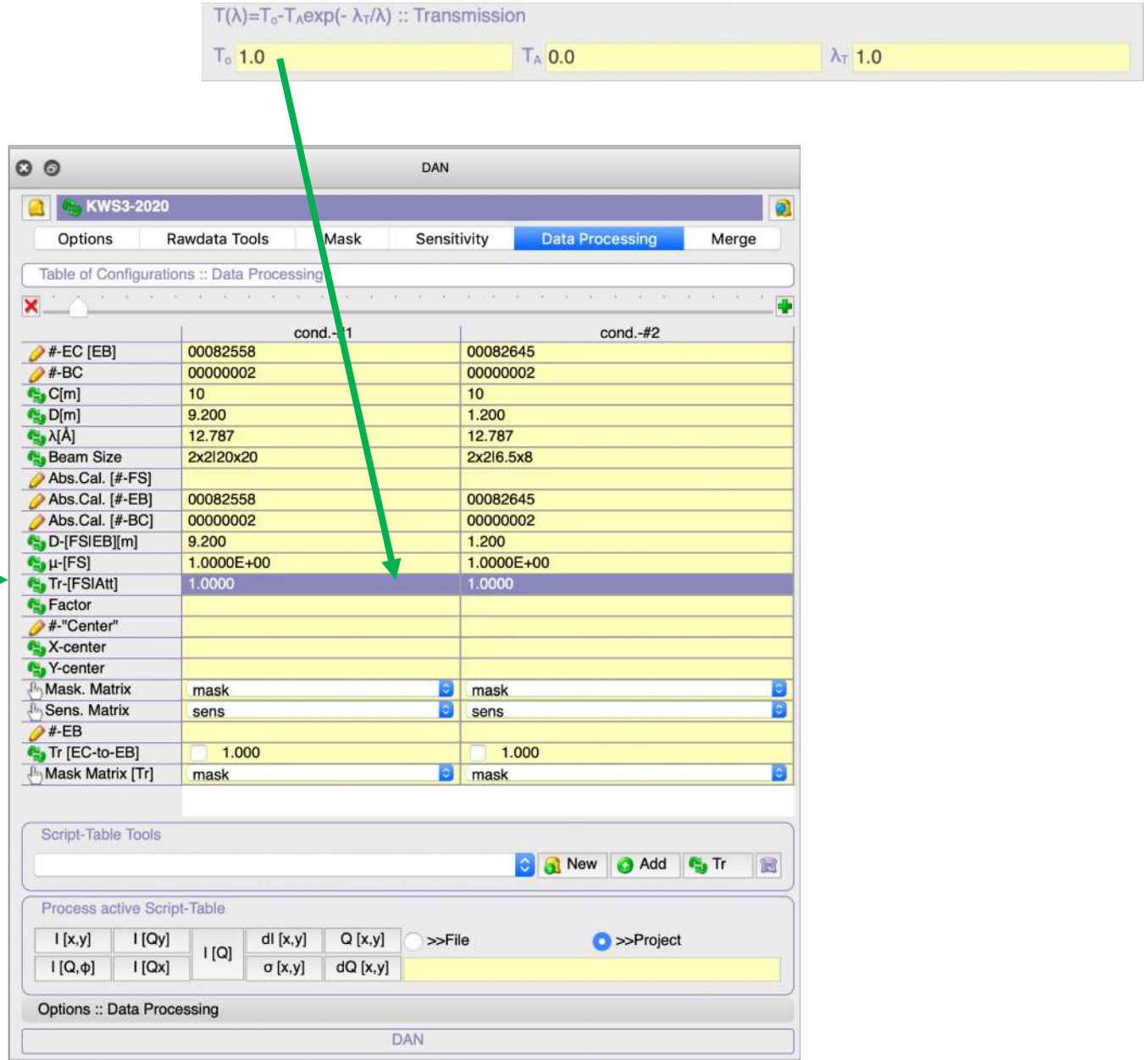
to calculate mu-factor for every configuration



Push : 

to read transmission of “EB/EB” for every configuration





Push : 

to calculate Absolute Factor for every configuration

! Important: at this step “mask” and “sens” matrixes should be active here !

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor		
#-"Center"		
X-center		
Y-center		
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.000	1.000
Mask Matrix [Tr]	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

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"		
X-center		
Y-center		
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.000	1.000
Mask Matrix [Tr]	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

Results Log

```
Sensitivity matrix: "sens".
Mask matrix: "mask".

| Plexi-run-#:: 00000001 | EB-run:: ...not used... | BC-run:: ...not used... | Tr : 1.0000
| Normalized Mean Intensity : 0.0803198 ± 0.000357002 | Normalization : Time : 26
| Dead-time correction : 1 | High Q Corrections : Yes : Center : 128.00x128.00 |

DAN :: Abs.Factor (DB) | Condition #1 | 2.8010E+05
DAN :: Abs.Factor (DB) | Condition #2 | 2.8162E+03
```

Results Log: Output

Fill: **“Center” Runs**

“Center” Runs: at KWS-3 we use Empty-Cell/Empty-beam runs to calculate center

#-"Center"

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"		
X-center		
Y-center		
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.000	1.000
Mask Matrix [Tr]	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

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center		
Y-center		
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.000	1.000
Mask Matrix [Tr]	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

We use “EB” sample also here

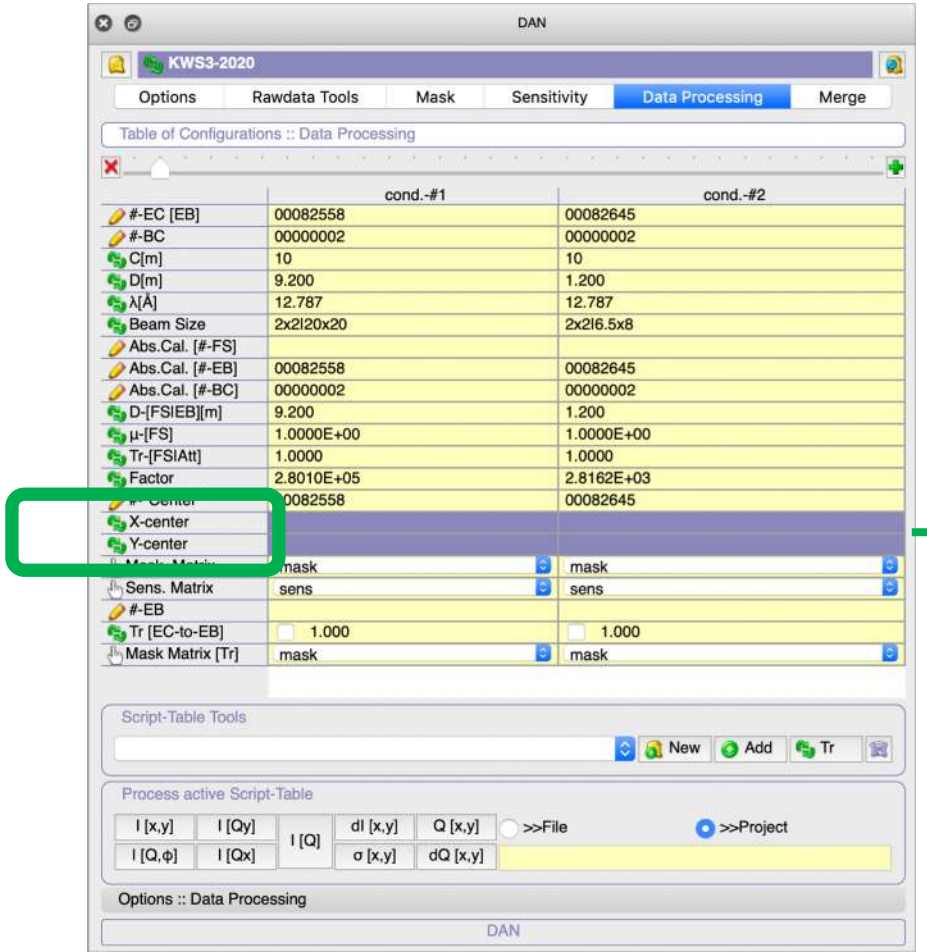
Push : 

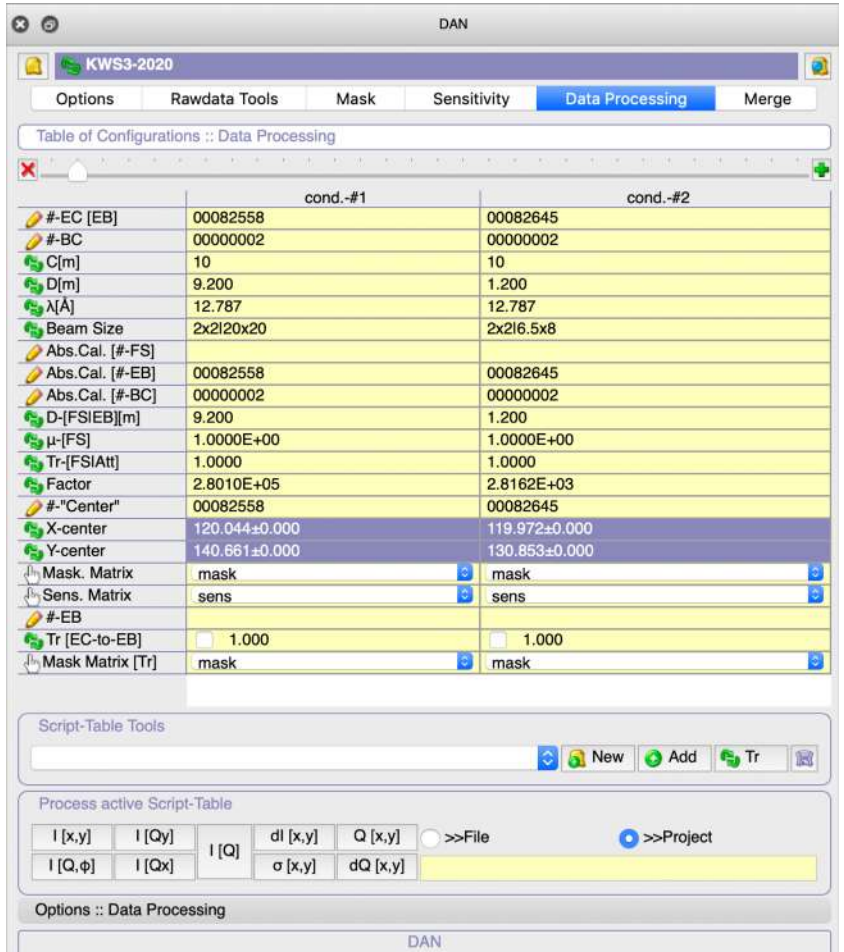
to calculate center of the beam for all configurations

or/and

120.044±0.000	119.972±0.000
140.661±0.000	130.853±0.000

! Important: at this step “mask” and “sens” matrixes should be active here !





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

- **D9.2m** and **D1.2m** configuration: transmission will be calculated separately (both checked);

Tr [EC-to-EB]	☑ 1.000	☑ 1.000

- **mask-tr-9m** and **mask-tr-1m** matrixes will be used to calculate transmission

Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	☐ 1.000	☐ 1.000
Mask Matrix [Tr]	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

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask	mask
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	☑ 1.000	☑ 1.000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

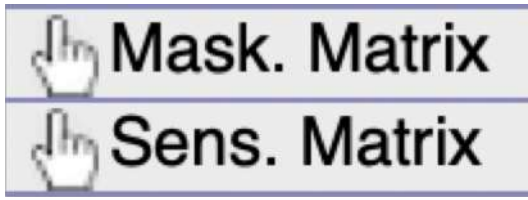
Script-Table Tools: New | Add | Tr

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]

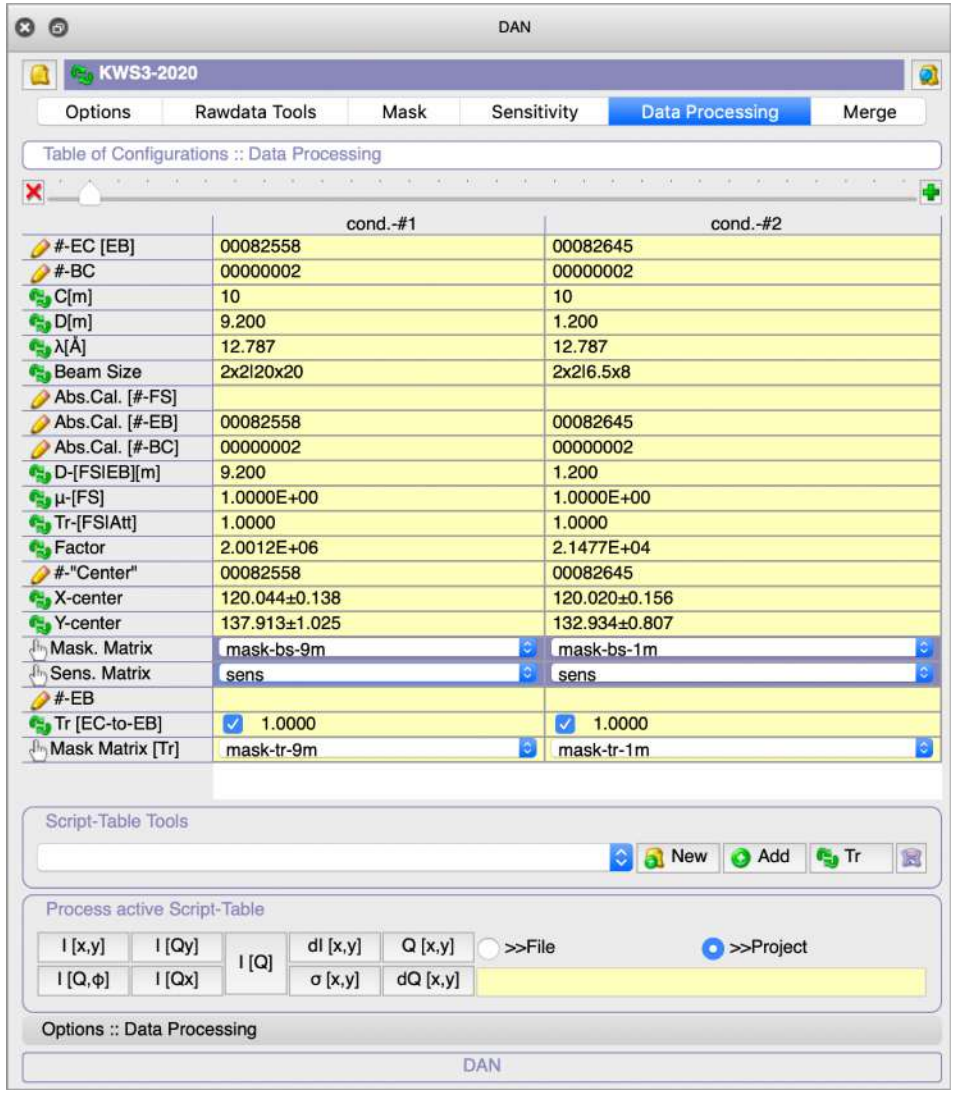
Options :: Data Processing

DAN

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



Mask. Matrix	mask-bs-9m	mask-bs-1m
Sens. Matrix	sens	sens



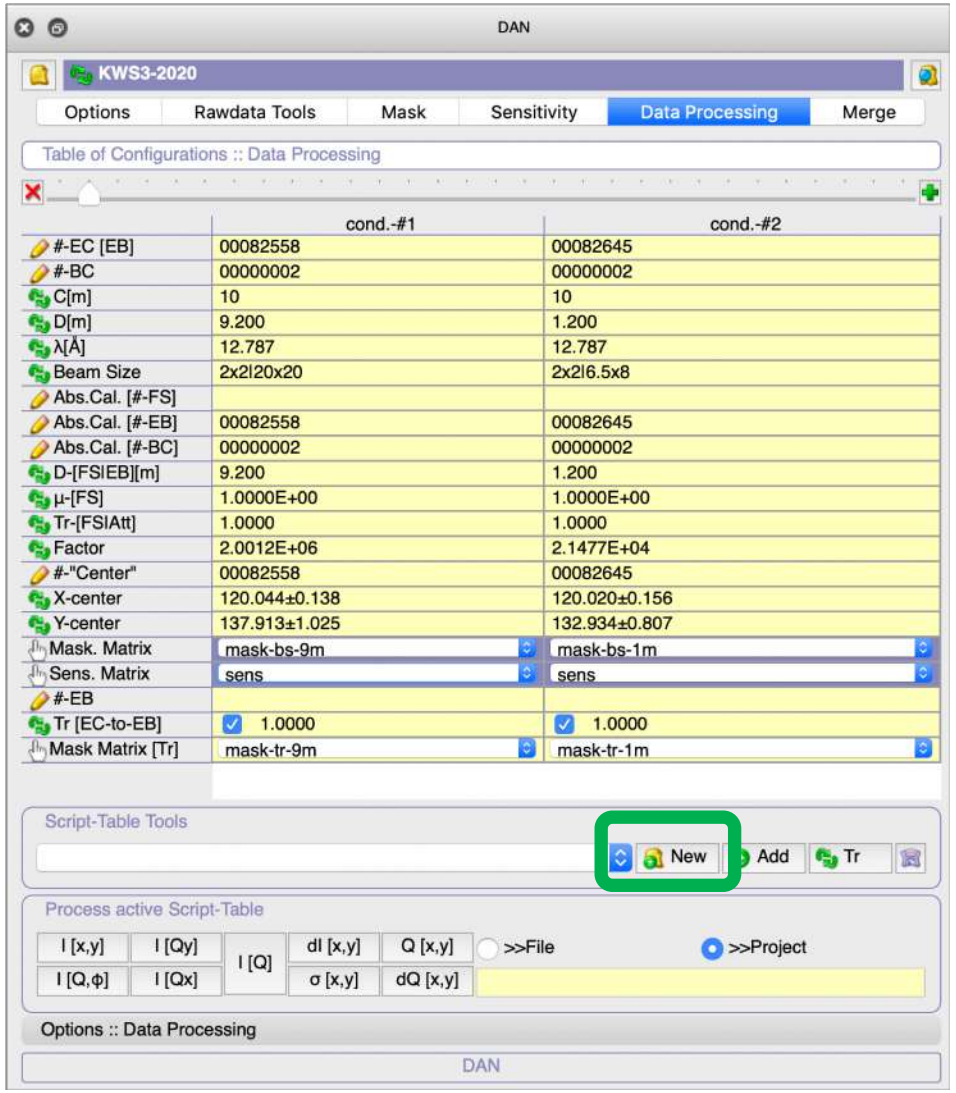
	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.0012E+06	2.1477E+04
#-"Center"	00082558	00082645
X-center	120.044±0.138	120.020±0.156
Y-center	137.913±1.025	132.934±0.807
Mask. Matrix	mask-bs-9m	mask-bs-1m
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	✓ 1.0000	✓ 1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

mask-bs-9m and **mask-bs-1m** matrixes will be used for radial averaging

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

QTISAS - untitled *

script - DAN::Script::Table

un-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m	mask-bs-1m
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.0000	1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

UNTITLED

DAN :: rawdata

DAN :: script, info, ...

	Type	View	Created	Label
info-table	Table	Normal	12.03.21 02:18	Info::Table
script	Table	Maximized	12.03.21 17:47	DAN::Script::Table
script-Settings	Table	Hidden	12.03.21 17:47	DAN::Settings::Table

Project Explorer | Results Log

Helvetica 17 Unicode

! Current parameters of !
! DAN-SANS is saved in:!
! Script-Settings table !

Push : Add to add files for “script” table

QTISAS - untitled *

script - DAN::Script::Table

Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Tra

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m	mask-bs-1m
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.0000	1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

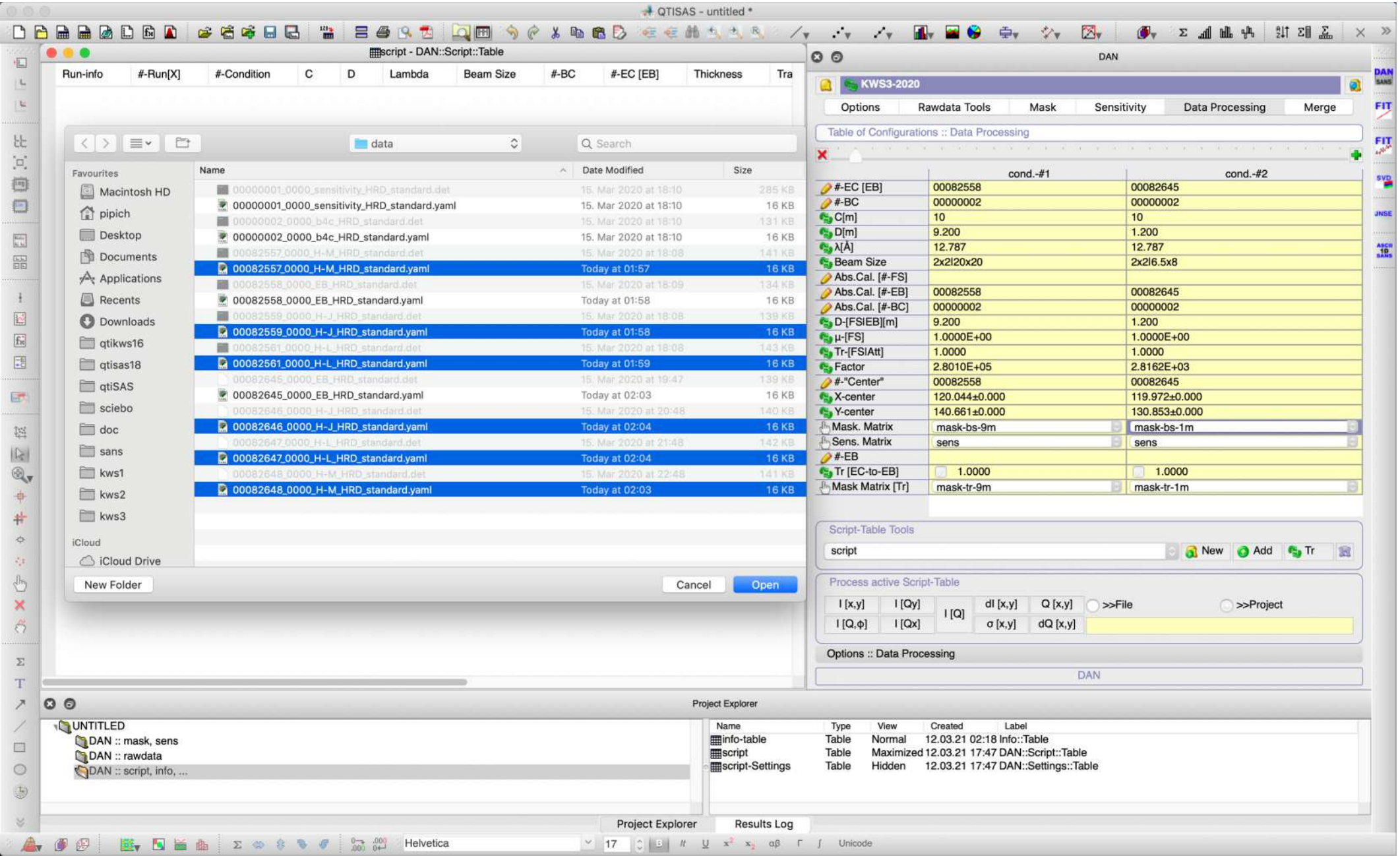
UNTITLED
- DAN :: mask, sens
- DAN :: rawdata
- DAN :: script, info, ...

Name	Type	View	Created	Label
info-table	Table	Normal	12.03.21 02:18	Info::Table
script	Table	Maximized	12.03.21 17:47	DAN::Script::Table
script-Settings	Table	Hidden	12.03.21 17:47	DAN::Settings::Table

Project Explorer | Results Log

Helvetica 17 Unicode

Selecting of files for data reduction



“Script” table contains now 3 samples measured in 2 configurations

QTISAS - untitled *

Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness
H-M	00082557	1	10	9.200	12.787	2x2l20x20	00000002	00082558	0.100
H-J	00082559	1	10	9.200	12.787	2x2l20x20	00000002	00082558	0.100
H-L	00082561	1	10	9.200	12.787	2x2l20x20	00000002	00082558	0.100
H-J	00082646	2	10	1.200	12.787	2x2l6.5x8	00000002	00082645	0.100
H-L	00082647	2	10	1.200	12.787	2x2l6.5x8	00000002	00082645	0.100
H-M	00082648	2	10	1.200	12.787	2x2l6.5x8	00000002	00082645	0.100

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2l20x20	2x2l6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m	mask-bs-1m
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.0000	1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

UNTITLED
- DAN :: mask, sens
- DAN :: rawdata
- DAN :: script, info, ...

Name	Type	View	Created	Label
info-table	Table	Normal	12.03.21 02:18	Info::Table
script	Table	Maximized	12.03.21 17:47	DAN::Script::Table
script-Settings	Table	Hidden	12.03.21 17:47	DAN::Settings::Table

Project Explorer | Results Log

Helvetica 17 Unicode

“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	Sta
1	H-M	00082557	1	10	9.200	12.787	2x2l20x20	00000002	00082558	0.100	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
2	H-J	00082559	1	10	9.200	12.787	2x2l20x20	00000002	00082558	0.100	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
3	H-L	00082561	1	10	9.200	12.787	2x2l20x20	00000002	00082558	0.100	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m	sens	
4	H-J	00082646	2	10	1.200	12.787	2x2l6.5x8	00000002	00082645	0.100	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
5	H-L	00082647	2	10	1.200	12.787	2x2l6.5x8	00000002	00082645	0.100	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
6	H-M	00082648	2	10	1.200	12.787	2x2l6.5x8	00000002	00082645	0.100	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	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	Sta
1	H-M	00082557	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
2	H-J	00082559	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
3	H-L	00082561	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m	sens	
4	H-J	00082646	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
5	H-L	00082647	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
6	H-M	00082648	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	

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

1. **Sample Name** 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 **C**arbonate): “I_{BC}”

“Script” table structure

1 | 2: I_{sample} | 3 | 4 | 5 | 6: λ | 7 | 8: I_{BC} | 9: I_{EC} | 10: d | 11: Tr | 12: AC_{factor} | 13: X_{center} | 14: Y_{center} | 15: mask | 16: sens | 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	Sta
1	H-M	00082557	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
2	H-J	00082559	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
3	H-L	00082561	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m	sens	
4	H-J	00082646	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
5	H-L	00082647	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
6	H-M	00082648	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	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”
17. **After-Processing-Status** column

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

5 | 9: I_{EC} | 11: Tr | 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	Sta
1	H-M	00082557	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
2	H-J	00082559	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
3	H-L	00082561	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m	sens	
4	H-J	00082646	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
5	H-L	00082647	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
6	H-M	00082648	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	

2: I_{sample} | 8: I_{BC} | 10: d | 12: AC_{factor} | 16: 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 HEADE !

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

5

13: X_{center}

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	Sta
1	H-M	00082557	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
2	H-J	00082559	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens	
3	H-L	00082561	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m	sens	
4	H-J	00082646	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
5	H-L	00082647	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	
6	H-M	00082648	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens	

6: λ

14: Y_{center}

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

$$pixel_{size} = 0.034cm$$

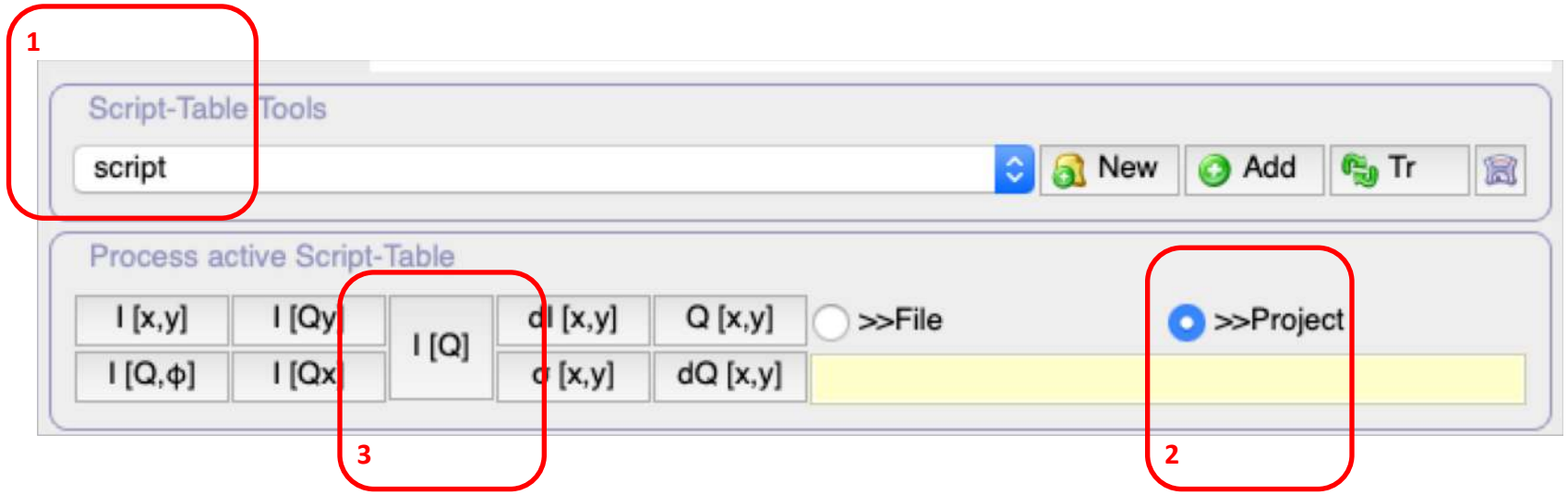
+ Wide Angle corrections

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

“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…

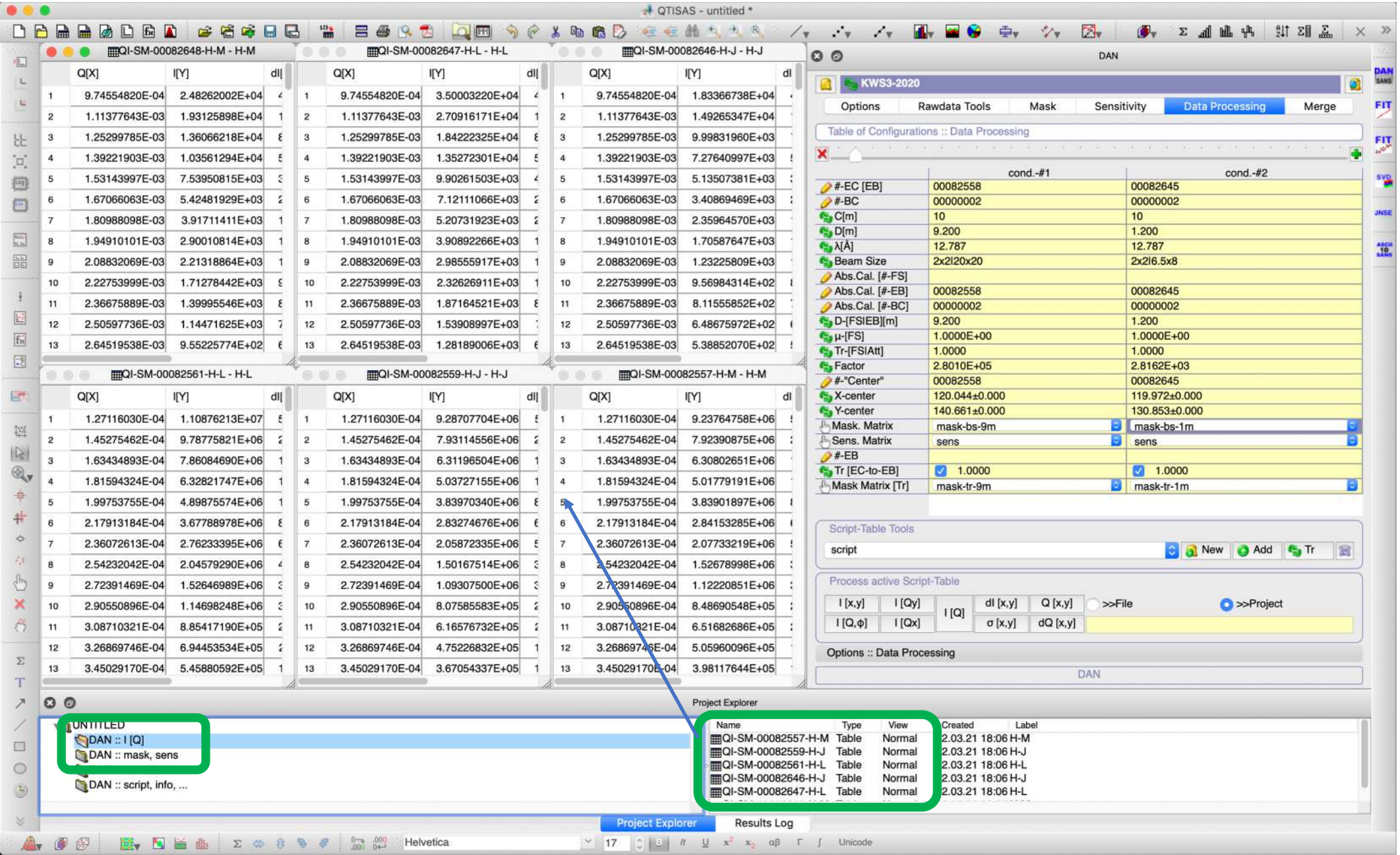
STEP 9: Radial Averaging

1. **Selected:** “script” table

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

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

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



Default **Table's name** Format

ject Explorer

Name	Type	View	Created	Label
QI-SM-00082557-H-M	Table	Normal	12.03.21 18:06	H-M
QI-SM-00082559-H-J	Table	Normal	12.03.21 18:06	H-J
QI-SM-00082561-H-L	Table	Normal	12.03.21 18:06	H-L
QI-SM-00082646-H-J	Table	Normal	12.03.21 18:06	H-J
QI-SM-00082647-H-L	Table	Normal	12.03.21 18:06	H-L
QI-SM-00082648-H-M	Table	Normal	12.03.21 18:07	H-M

QI-SM-#####-SampleName

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

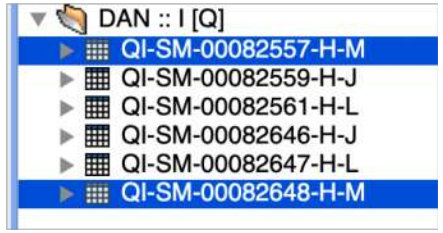
Example of Plotting of Radial Averaged Datasets

Plotting example:

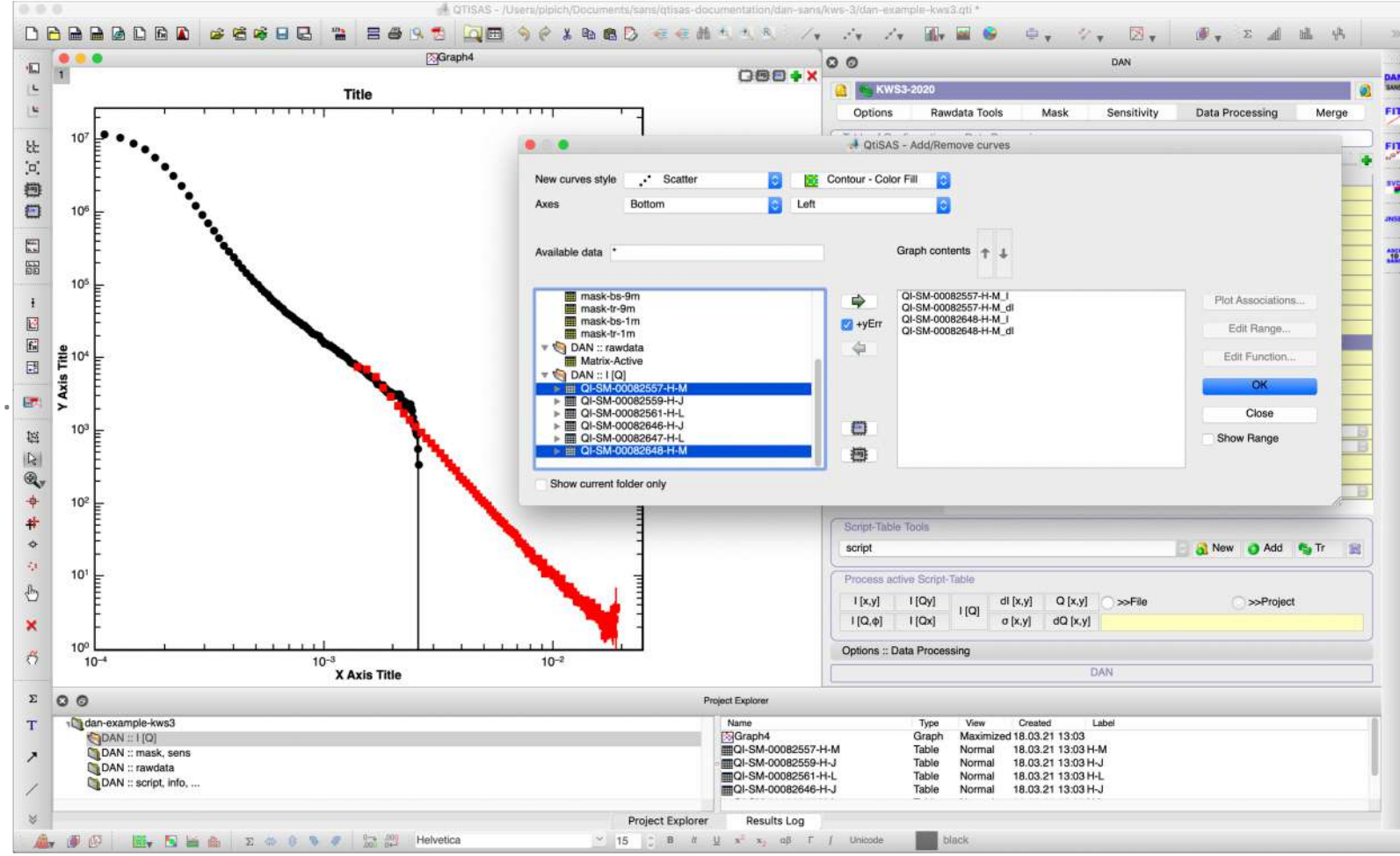
1. **Create empty 2D Plot**

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

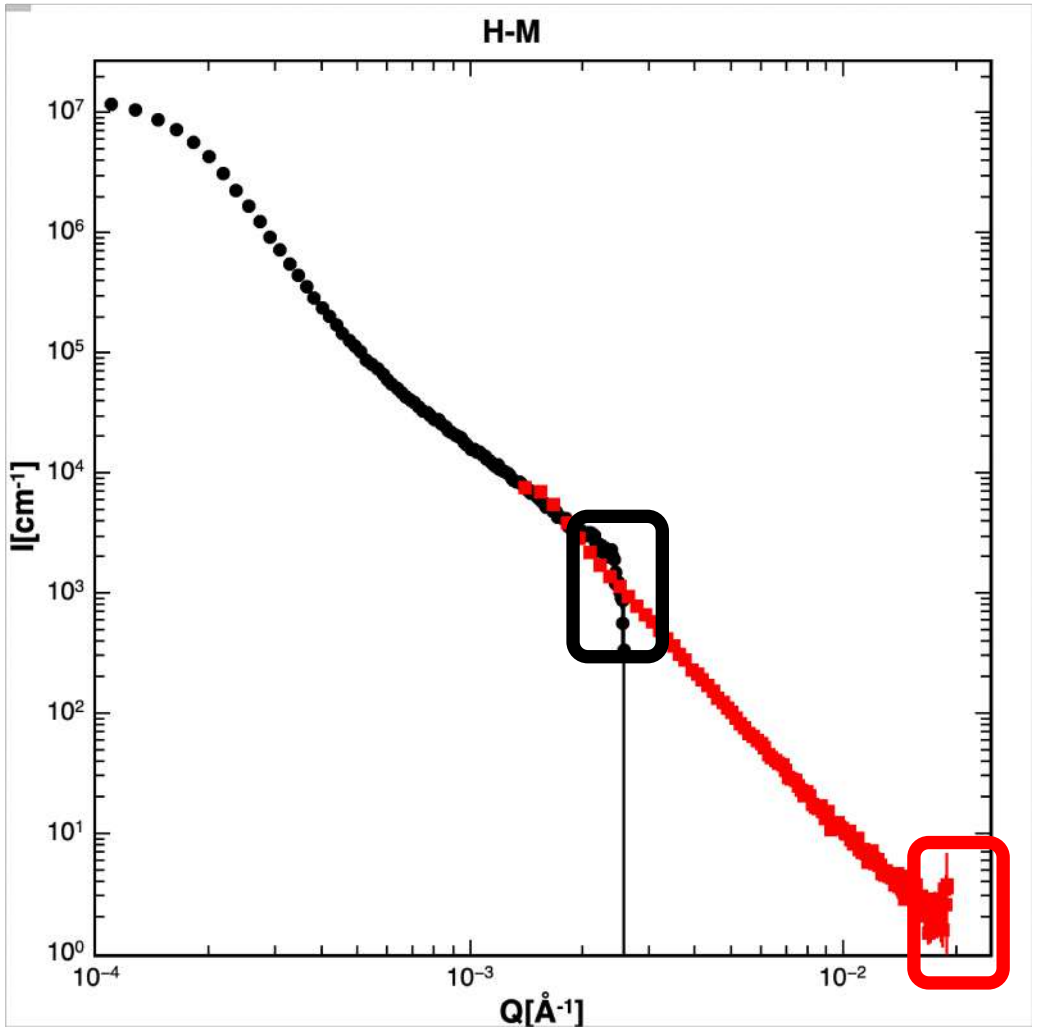


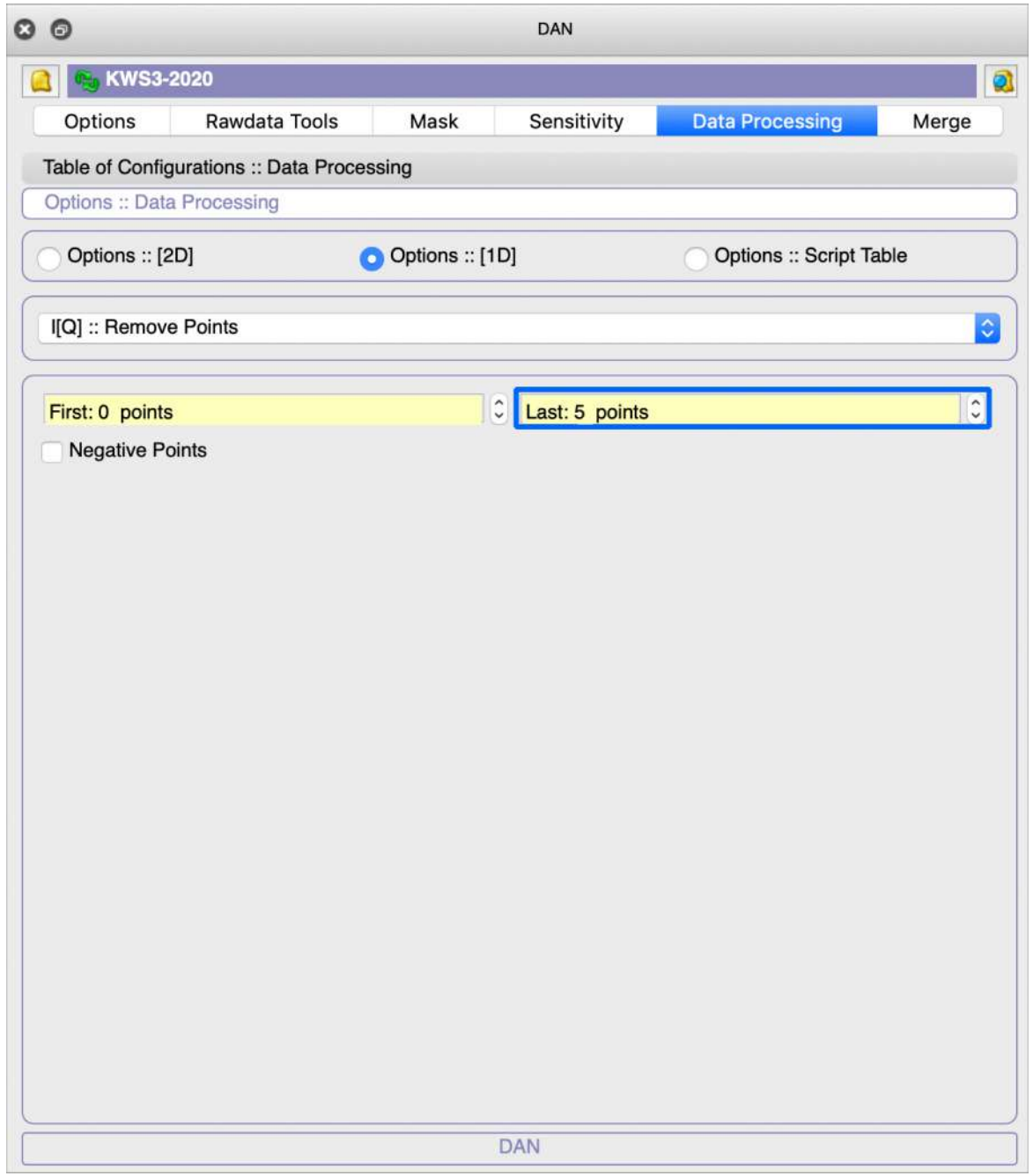
5. **Push “Add” button:**

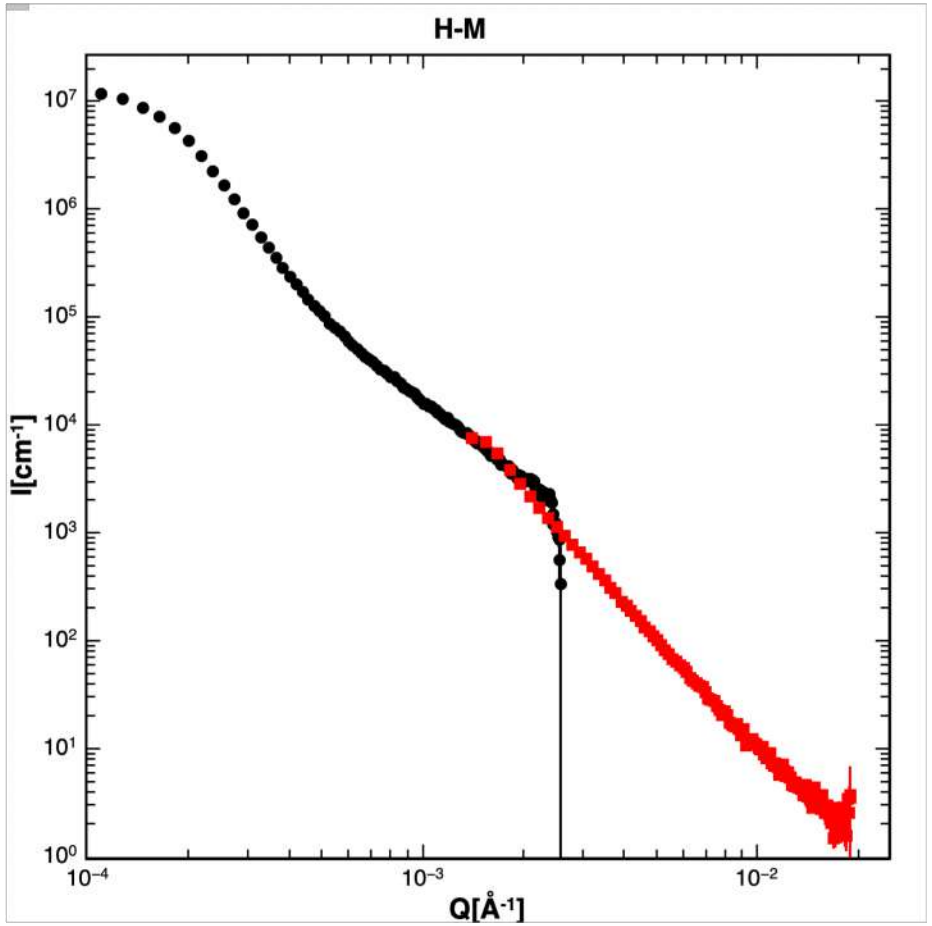
6 (optional). **Push “log” for double-logarithmic presentation**

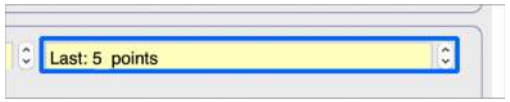
7. **Push “OK” button to close “Add/Remove” interface**

Plotting example: result

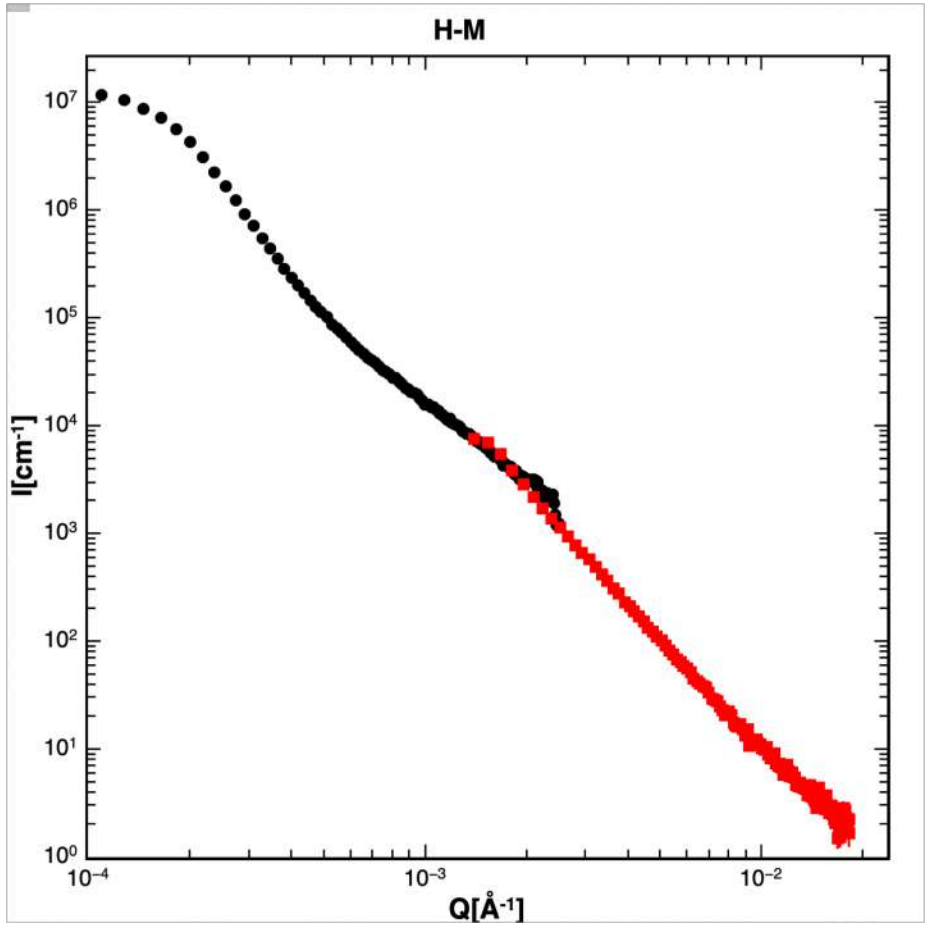





H-M
I[cm⁻¹]
Q[Å⁻¹]

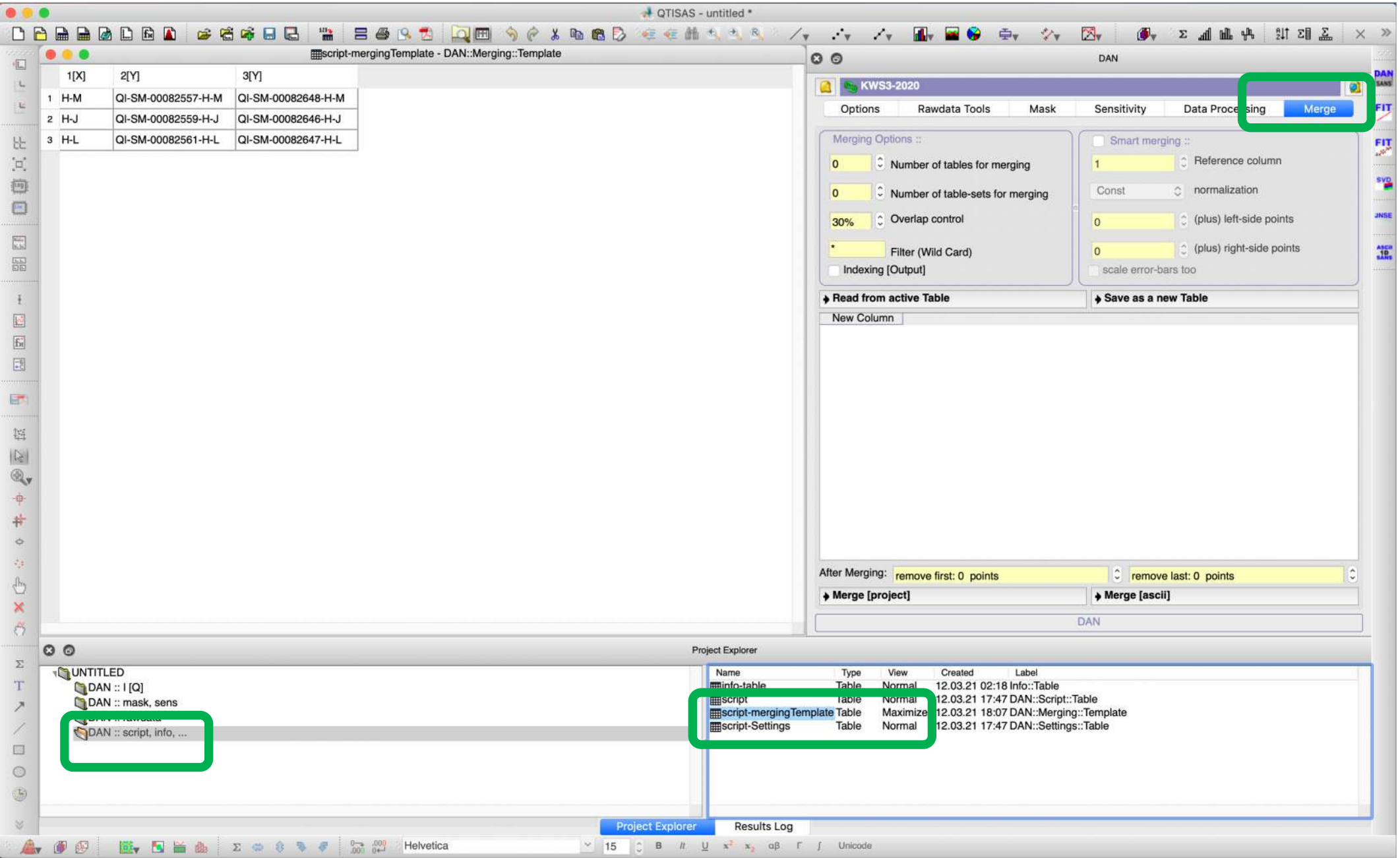

Last: 5 points


I [Q]
dI
σ

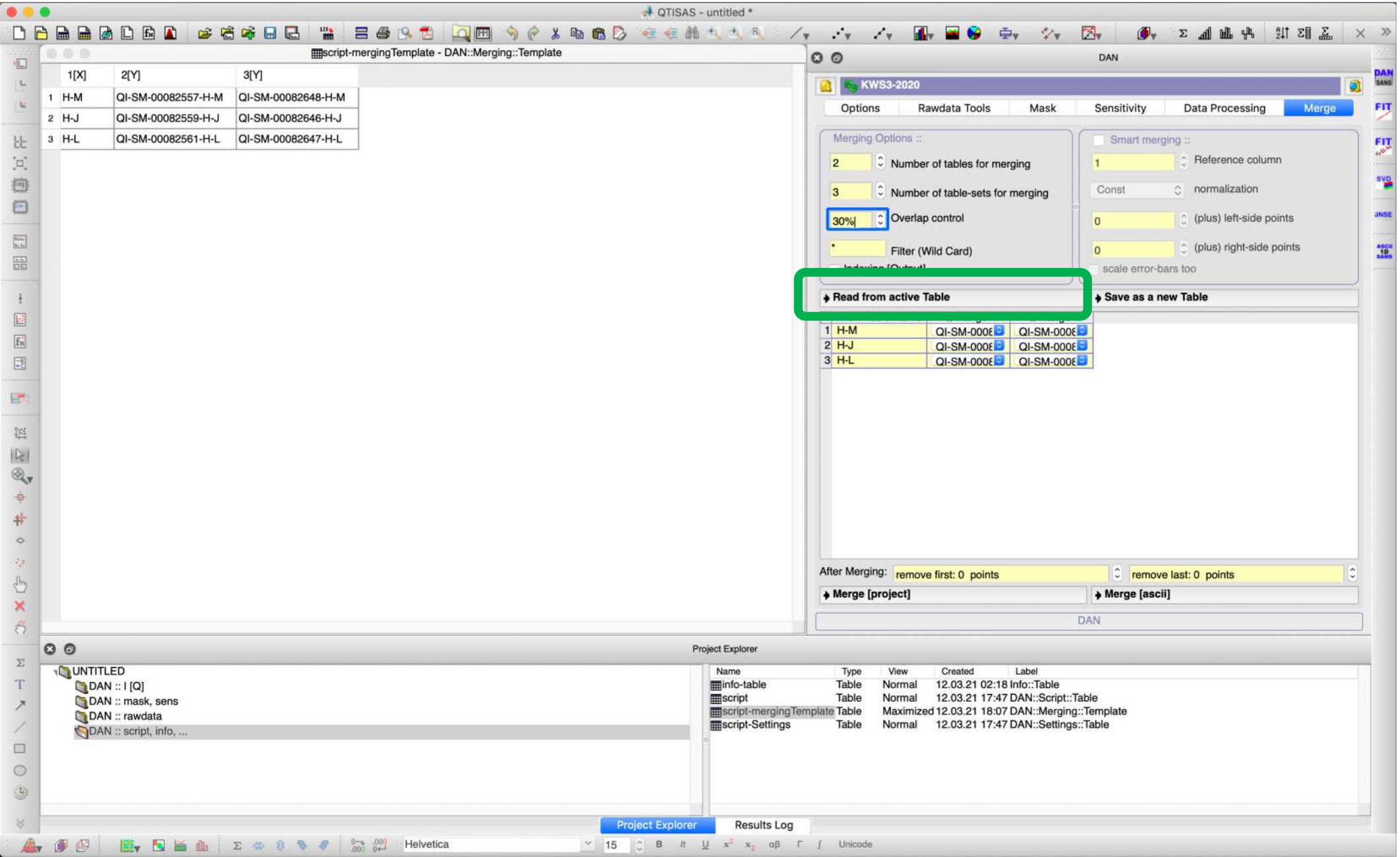

H-M
I[cm⁻¹]
Q[Å⁻¹]

STEP 10: Data Merging

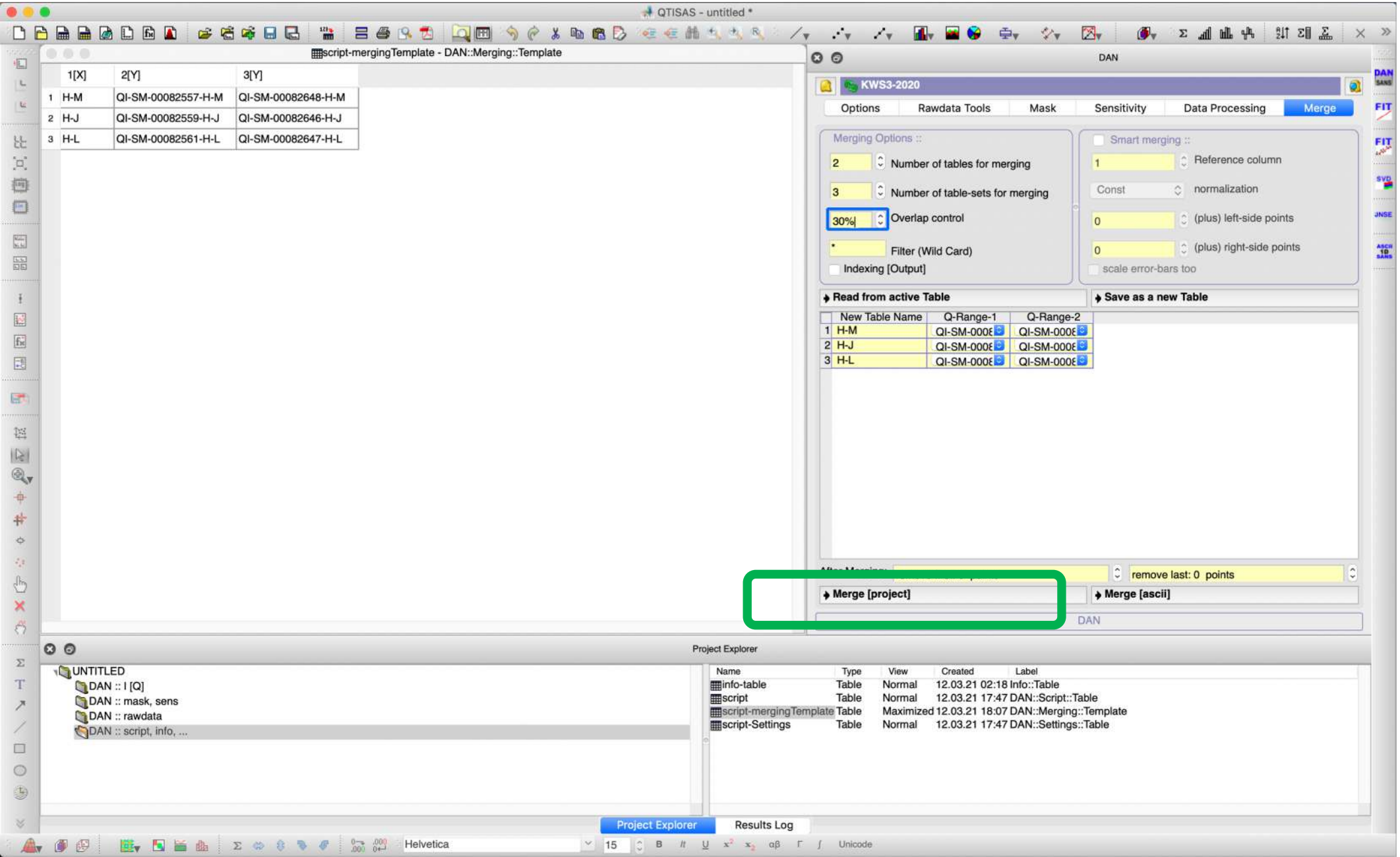
Merging Step #1: go to “Merge” tab (DAN-SANS) and activate “script-mergingTemplate”



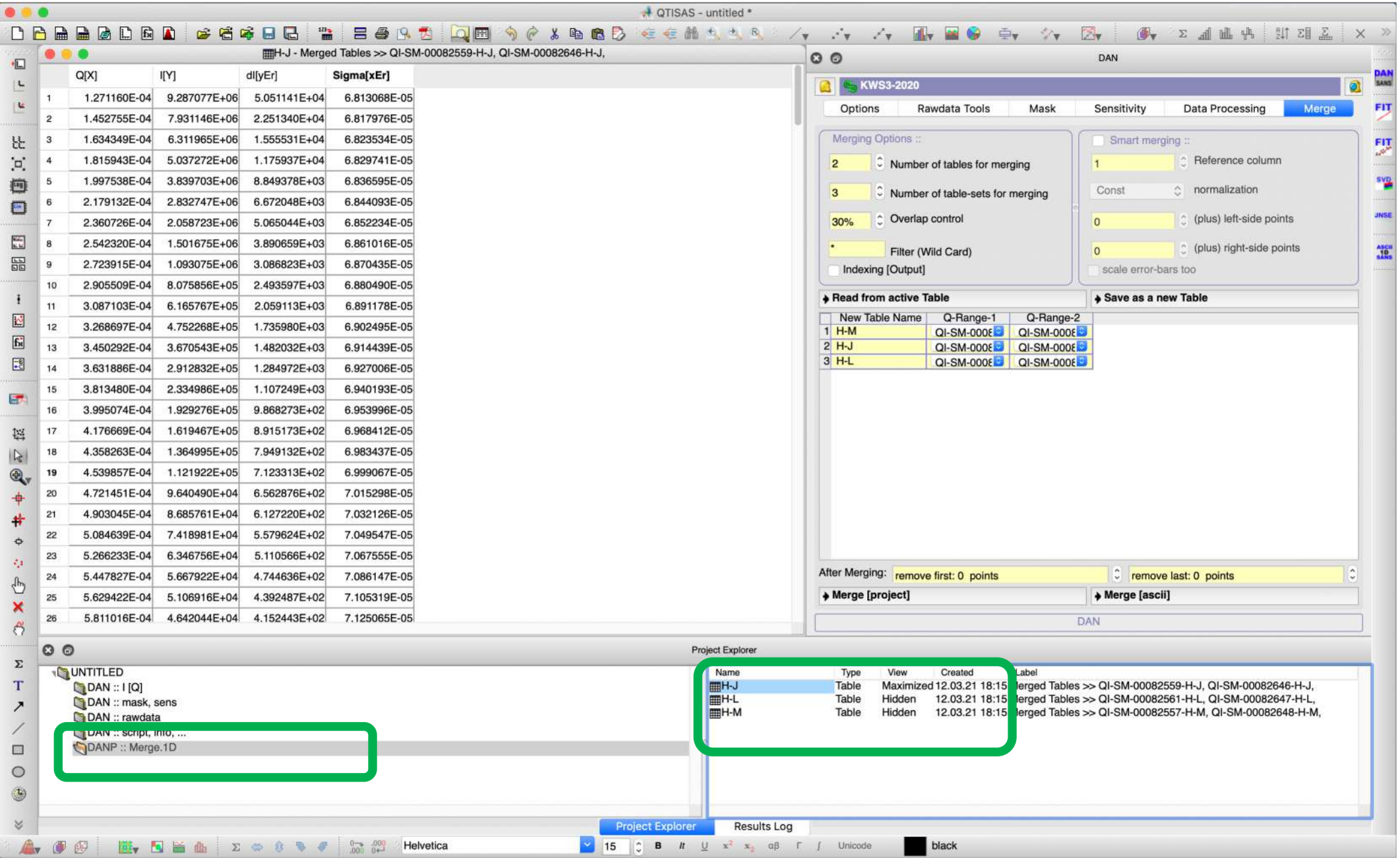
Merging Step #2: push button “Read active Table” to transfer data to Merge-interface



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-M - Merged Tables >> QI-SM-00082557-H-M, QI-SM-00082648-H-M,

	Q[X]	I[Y]	dI[yEr]	Sigma[xEr]
1	1.271160E-04	9.237648E+06	5.0	
2	1.452755E-04	7.923909E+06	2.2	
3	1.634349E-04	6.308027E+06	1.5	
4	1.815943E-04	5.017792E+06	1.1	
5	1.997538E-04	3.839019E+06	8.9	
6	2.179132E-04	2.841533E+06	6.7	
7	2.360726E-04	2.077332E+06	5.1	
8	2.542320E-04	1.526790E+06	3.9	
9	2.723915E-04	1.122209E+06	3.1	
10	2.905509E-04	8.486905E+05	2.5	
11	3.087103E-04	6.516827E+05	2.1	
12	3.268697E-04	5.059601E+05	1.8	
13	3.450292E-04	3.981176E+05	1.5	
14	3.631886E-04	3.204110E+05	1.3	
15	3.813480E-04	2.626791E+05	1.1	
16	3.995074E-04	2.188616E+05	1.0	
17	4.176669E-04	1.829712E+05	9.4	
18	4.358263E-04	1.553340E+05	8.471072E+02	6.983437E-05
19	4.539857E-04	1.317065E+05	7.686507E+02	6.999067E-05
20	4.721451E-04	1.152279E+05	7.117695E+02	7.015298E-05
21	4.903045E-04	1.027416E+05	6.587884E+02	7.032126E-05
22	5.084639E-04	9.170521E+04	6.108560E+02	7.049547E-05
23	5.266233E-04	7.995979E+04	5.623221E+02	7.067555E-05
24	5.447827E-04	7.250249E+04	5.260211E+02	7.086147E-05
25	5.629422E-04	6.761023E+04	4.941126E+02	7.105319E-05
26	5.811016E-04	6.076941E+04	4.630169E+02	7.125065E-05

Plot
- Line
- Scatter
- Line + Symbol
- Special Line/Symbol
- Columns
- Rows
- Special Bar/Column
- Area
- Vectors XYXY
- Vectors XYAM
- Statistical Graphs
- Panel
- Shared Axes Panel

Cut
Copy
Paste
Clear
Delete
Hide Selected
Show All Columns
Insert
Add Column ⌥C
Set As
Fill Columns With
Normalize
Sort Columns
Sort Table...
Statistics on Columns
Statistics on Rows
Adjust Column Width

DAN

KWS3-2020

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

Merging Options ::
- 2 Number of tables for merging
- 3 Number of table-sets for merging
- 30% Overlap control
- * Filter (Wild Card)
- Indexing [Output]

Smart merging ::
- 1 Reference column
- Const normalization
- 0 (plus) left-side points
- 0 (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
1	H-M	QI-SM-000E	QI-SM-000E
2	H-J	QI-SM-000E	QI-SM-000E
3	H-L	QI-SM-000E	QI-SM-000E

After Merging: remove first: 0 points | remove last: 0 points

Merge [project] | Merge [ascii]

DAN

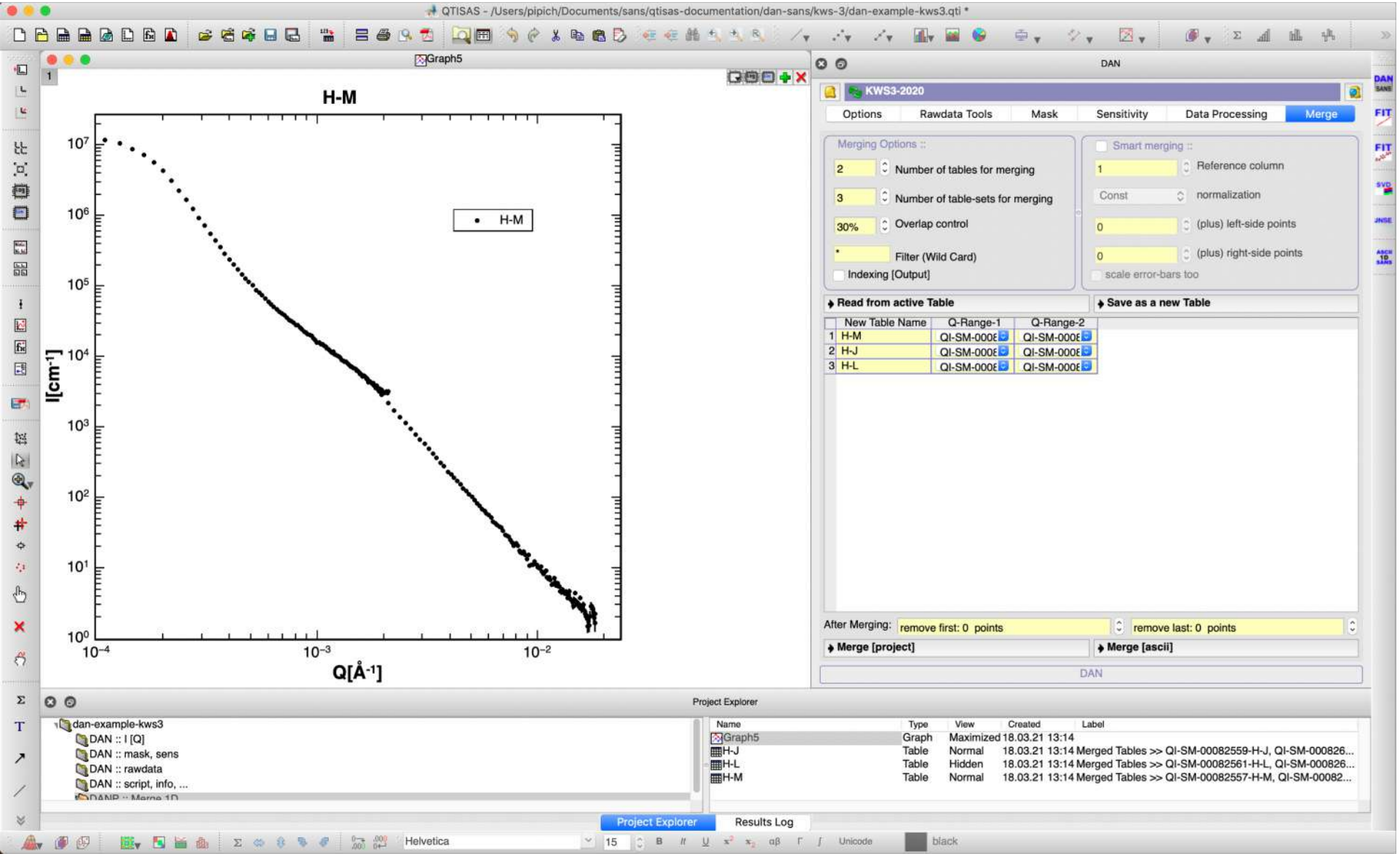
Project Explorer

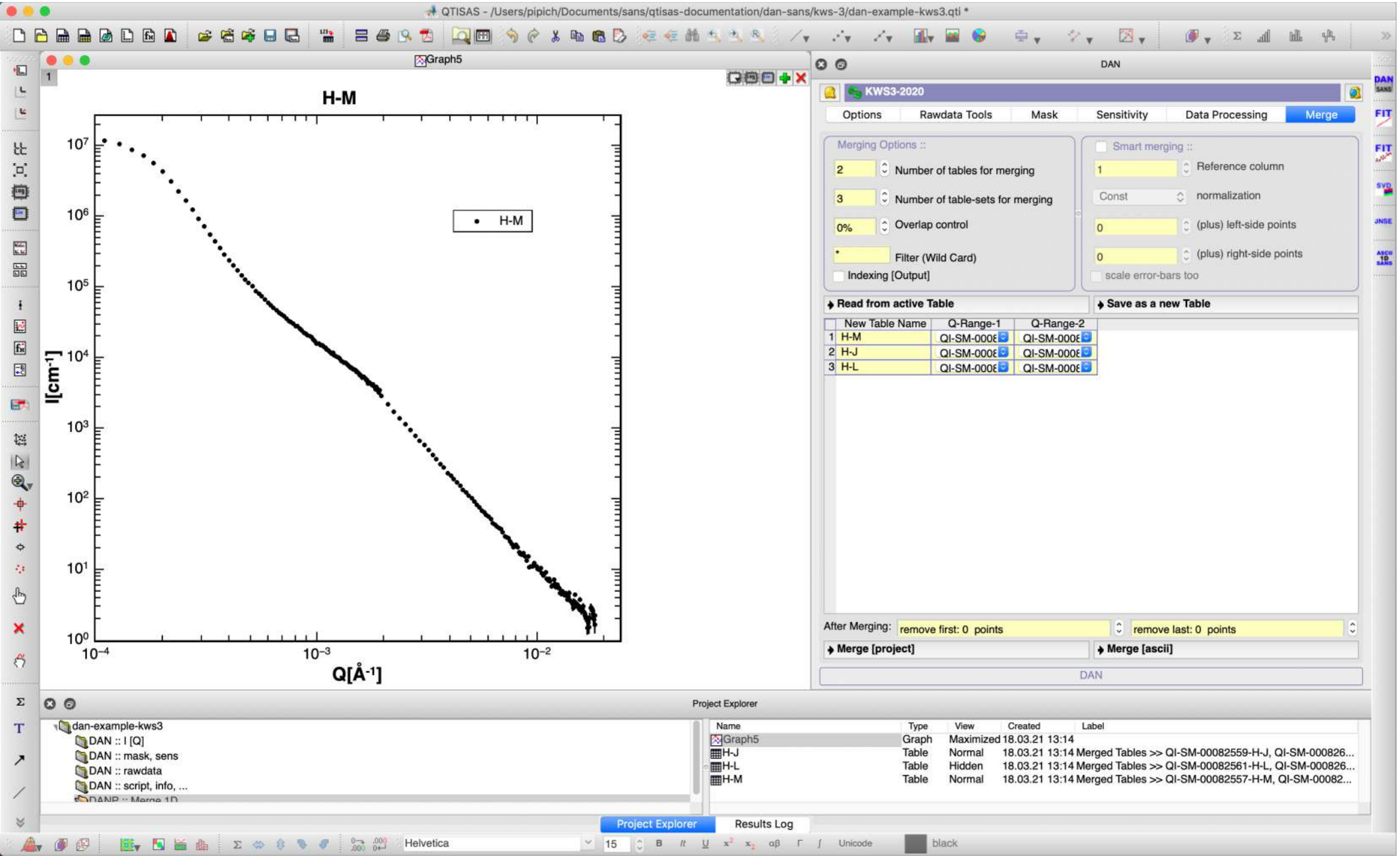
- UNTITLED
  - DAN :: I [Q]
  - DAN :: mask, sens
  - DAN :: rawdata
  - DAN :: script, info, ...
  - DANP :: Merge.1D

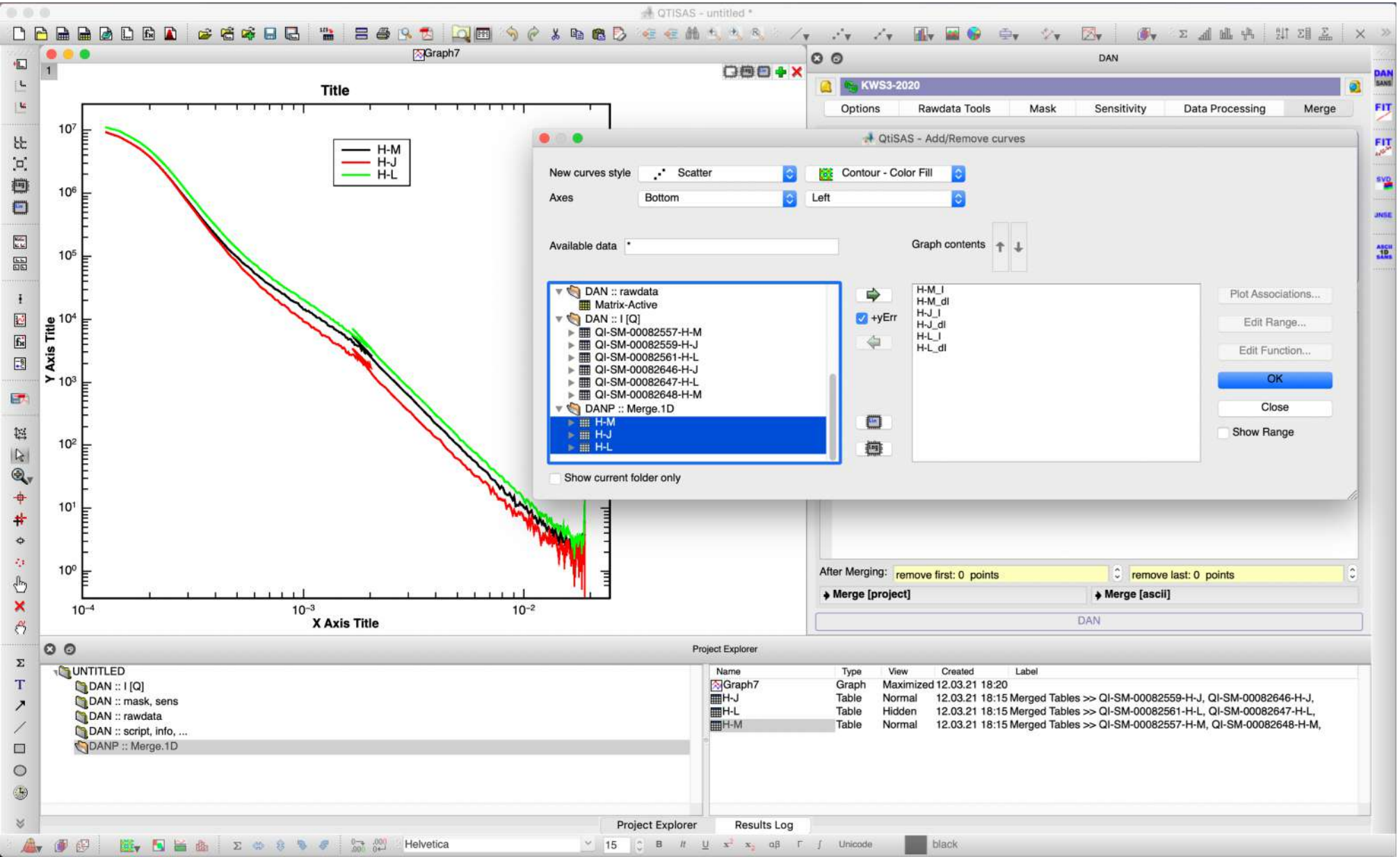
Name	Type	View	Created	Label
H-J	Table	Normal	12.03.21 18:15	Merged Tables >> QI-SM-00082559-H-J, QI-SM-00082646-H-J,
H-L	Table	Hidden	12.03.21 18:15	Merged Tables >> QI-SM-00082561-H-L, QI-SM-00082647-H-L,
H-M	Table	Maximized	12.03.21 18:15	Merged Tables >> QI-SM-00082557-H-M, QI-SM-00082648-H-M,

Project Explorer | Results Log

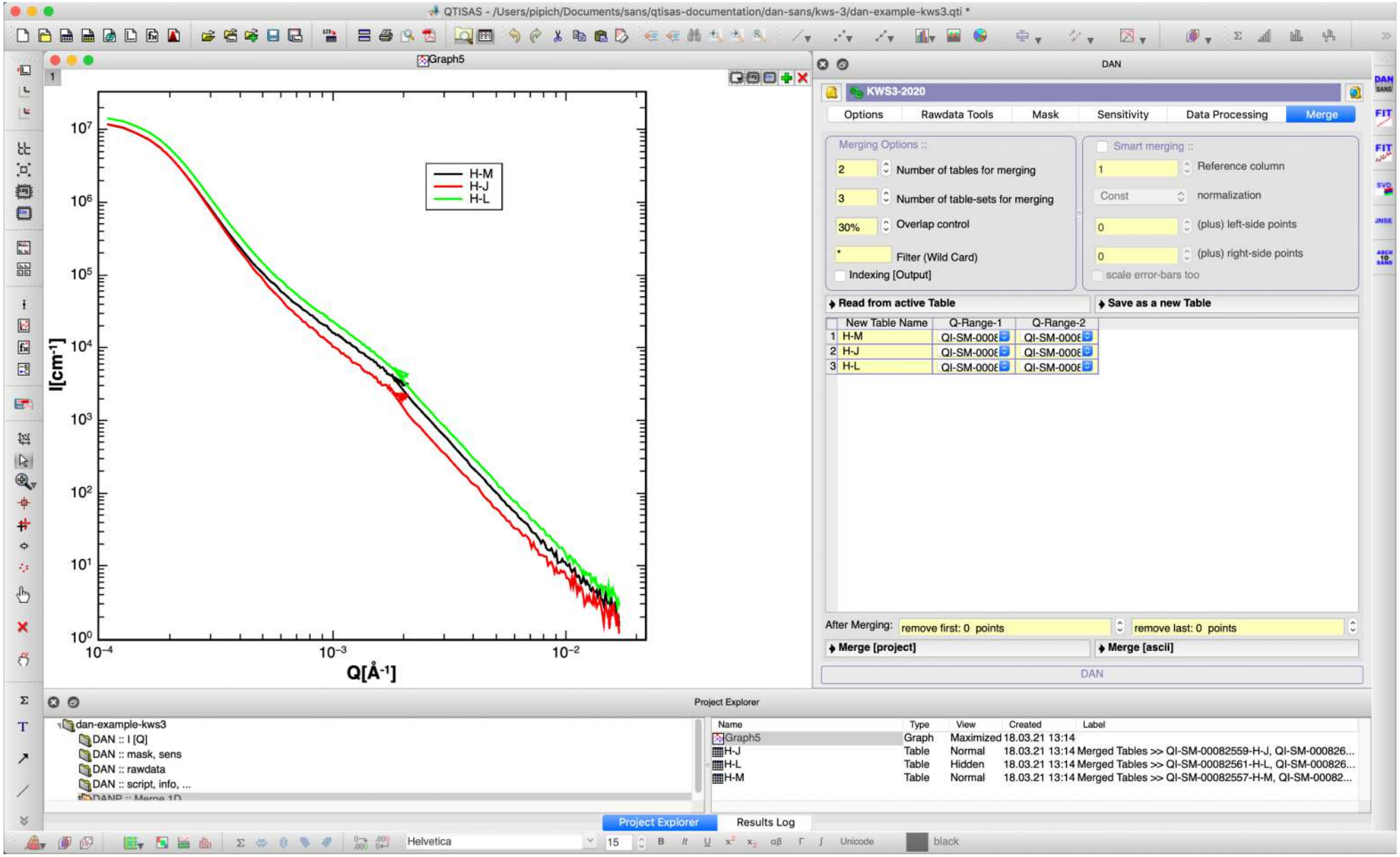
Helvetica 15 Unicode


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
Graph5
H-M
H-M
I[cm⁻¹]
Q[Å⁻¹]
DAN
KWS3-2020
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
H-M
H-J
H-L
After Merging:
remove first: 0 points
remove last: 0 points
Merge [project]
Merge [ascii]
DAN
Project Explorer
dan-example-kws3
DAN :: I [Q]
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Graph5
H-J
H-L
H-M
Project Explorer
Results Log
Helvetica
Unicode
black


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
Graph5
H-M
I[cm⁻¹]
Q[Å⁻¹]
H-M
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Merging Options ::
2 Number of tables for merging
3 Number of table-sets for merging
0% Overlap control
* Filter (Wild Card)
Indexing [Output]
Smart merging ::
1 Reference column
Const normalization
0 (plus) left-side points
0 (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
1 H-M
2 H-J
3 H-L
After Merging:
remove first: 0 points
remove last: 0 points
Merge [project]
Merge [ascii]
DAN
Project Explorer
dan-example-kws3
DAN :: I [Q]
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
Name
Type
View
Created
Label
Graph5 Graph Maximized 18.03.21 13:14
H-J Table Normal 18.03.21 13:14 Merged Tables >> QI-SM-00082559-H-J, QI-SM-000826...
H-L Table Hidden 18.03.21 13:14 Merged Tables >> QI-SM-00082561-H-L, QI-SM-000826...
H-M Table Normal 18.03.21 13:14 Merged Tables >> QI-SM-00082557-H-M, QI-SM-00082...
Project Explorer
Results Log
Helvetica
15
Unicode
black


QTISAS - untitled *
Graph7
Title
H-M
H-J
H-L
Y Axis Title
X Axis Title
DAN
KWS3-2020
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
DAN :: rawdata
Matrix-Active
DAN :: I [Q]
QI-SM-00082557-H-M
QI-SM-00082559-H-J
QI-SM-00082561-H-L
QI-SM-00082646-H-J
QI-SM-00082647-H-L
QI-SM-00082648-H-M
DANP :: Merge.1D
H-M
H-J
H-L
+yErr
H-M_I
H-M_dI
H-J_I
H-J_dI
H-L_I
H-L_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 :: rawdata
DAN :: script, info, ...
DANP :: Merge.1D
Name
Type
View
Created
Label
Graph7
Graph
Maximized
12.03.21 18:20
H-J
Table
Normal
12.03.21 18:15
Merged Tables >> QI-SM-00082559-H-J, QI-SM-00082646-H-J,
H-L
Table
Hidden
12.03.21 18:15
Merged Tables >> QI-SM-00082561-H-L, QI-SM-00082647-H-L,
H-M
Table
Normal
12.03.21 18:15
Merged Tables >> QI-SM-00082557-H-M, QI-SM-00082648-H-M,
Project Explorer
Results Log
Helvetica
15
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-3/dan-example-kws3.qti *

I-SM-00082648-H-M - H-M

	1	2
1	0.00000000E+00	0.00000000E+00
2	0.00000000E+00	0.00000000E+00
3	0.00000000E+00	0.00000000E+00
4	0.00000000E+00	0.00000000E+00
5	0.00000000E+00	0.00000000E+00
6	0.00000000E+00	0.00000000E+00
7	0.00000000E+00	0.00000000E+00
8	0.00000000E+00	0.00000000E+00
9	0.00000000E+00	0.00000000E+00
10	0.00000000E+00	0.00000000E+00
11	0.00000000E+00	0.00000000E+00

I-SM-00082647-H-L - H-L

	1	2
1	0.00000000E+00	0.00000000E+00
2	0.00000000E+00	0.00000000E+00
3	0.00000000E+00	0.00000000E+00
4	0.00000000E+00	0.00000000E+00
5	0.00000000E+00	0.00000000E+00
6	0.00000000E+00	0.00000000E+00
7	0.00000000E+00	0.00000000E+00
8	0.00000000E+00	0.00000000E+00
9	0.00000000E+00	0.00000000E+00
10	0.00000000E+00	0.00000000E+00
11	0.00000000E+00	0.00000000E+00

I-SM-00082646-H-J - H-J

	1	2
1	0.00000000E+00	0.00000000E+00
2	0.00000000E+00	0.00000000E+00
3	0.00000000E+00	0.00000000E+00
4	0.00000000E+00	0.00000000E+00
5	0.00000000E+00	0.00000000E+00
6	0.00000000E+00	0.00000000E+00
7	0.00000000E+00	0.00000000E+00
8	0.00000000E+00	0.00000000E+00
9	0.00000000E+00	0.00000000E+00
10	0.00000000E+00	0.00000000E+00
11	0.00000000E+00	0.00000000E+00

I-SM-00082561-H-L - H-L

	1	2
1	0.00000000E+00	0.00000000E+00
2	0.00000000E+00	0.00000000E+00
3	0.00000000E+00	0.00000000E+00
4	0.00000000E+00	0.00000000E+00
5	0.00000000E+00	0.00000000E+00
6	0.00000000E+00	0.00000000E+00
7	0.00000000E+00	0.00000000E+00
8	0.00000000E+00	0.00000000E+00
9	0.00000000E+00	0.00000000E+00
10	0.00000000E+00	0.00000000E+00
11	0.00000000E+00	0.00000000E+00

I-SM-00082559-H-J - H-J

	1	2
1	0.00000000E+00	0.00000000E+00
2	0.00000000E+00	0.00000000E+00
3	0.00000000E+00	0.00000000E+00
4	0.00000000E+00	0.00000000E+00
5	0.00000000E+00	0.00000000E+00
6	0.00000000E+00	0.00000000E+00
7	0.00000000E+00	0.00000000E+00
8	0.00000000E+00	0.00000000E+00
9	0.00000000E+00	0.00000000E+00
10	0.00000000E+00	0.00000000E+00
11	0.00000000E+00	0.00000000E+00

I-SM-00082557-H-M - H-M

	1	2
1	0.00000000E+00	0.00000000E+00
2	0.00000000E+00	0.00000000E+00
3	0.00000000E+00	0.00000000E+00
4	0.00000000E+00	0.00000000E+00
5	0.00000000E+00	0.00000000E+00
6	0.00000000E+00	0.00000000E+00
7	0.00000000E+00	0.00000000E+00
8	0.00000000E+00	0.00000000E+00
9	0.00000000E+00	0.00000000E+00
10	0.00000000E+00	0.00000000E+00
11	0.00000000E+00	0.00000000E+00

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m	mask-bs-1m
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	☑ 1.0000	☑ 1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

dan-example-kws3

DAN :: I [x,y]

DAN :: mask, sens

DAN :: script, info, ...

Name	Type	View	Created	Label
I-SM-00082557-H-M	Matrix	Normal	18.03.21 13:23	H-M
I-SM-00082559-H-J	Matrix	Normal	18.03.21 13:23	H-J
I-SM-00082561-H-L	Matrix	Normal	18.03.21 13:23	H-L
I-SM-00082646-H-J	Matrix	Normal	18.03.21 13:23	H-J
I-SM-00082647-H-L	Matrix	Normal	18.03.21 13:23	H-L

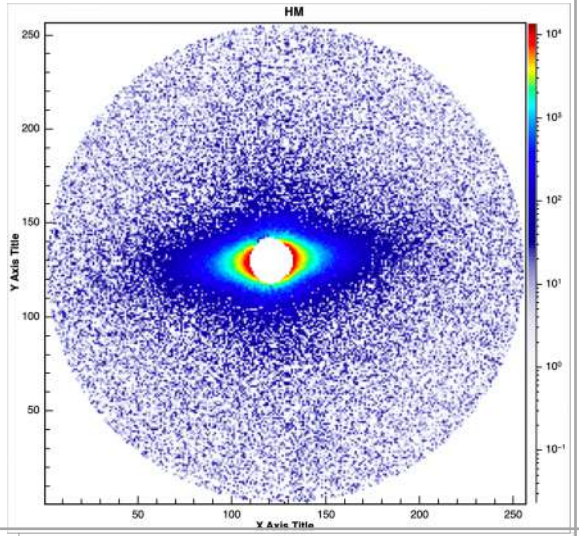
Project Explorer | Results Log

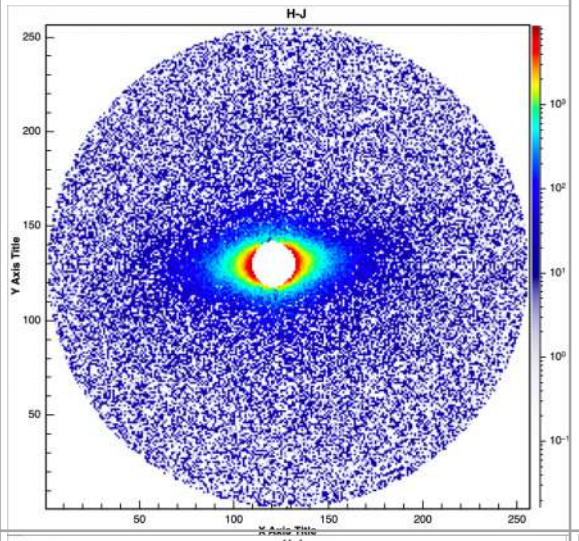
Helvetica 15 Unicode

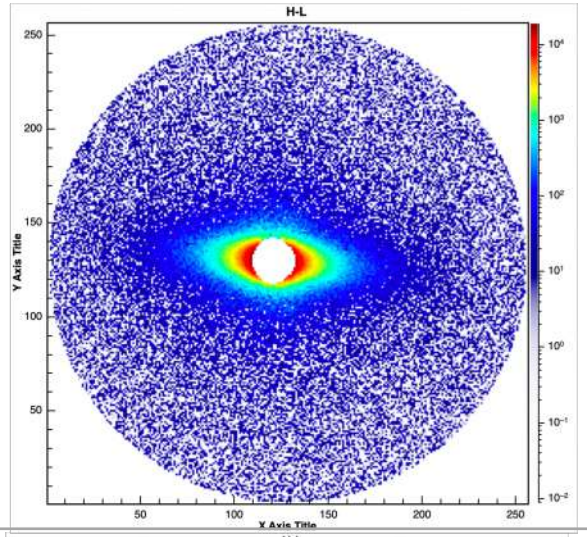
H-M

H-J

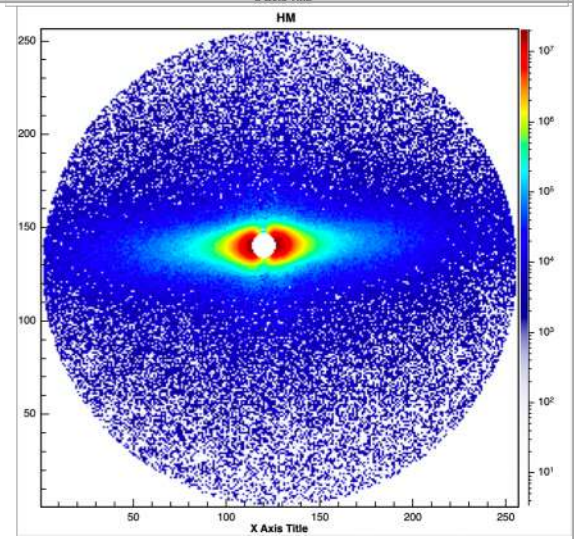
H-L

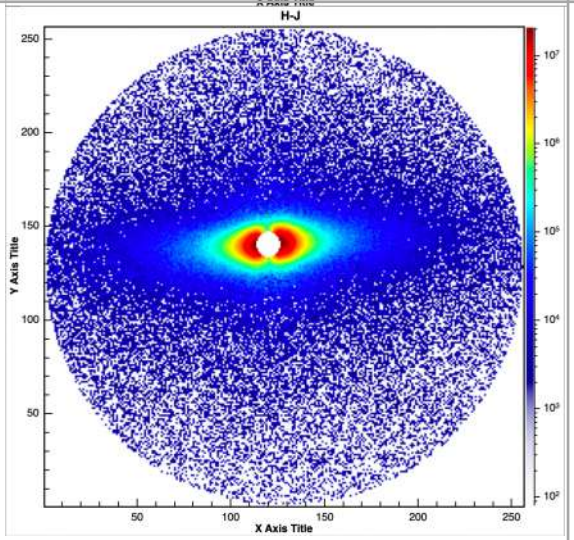


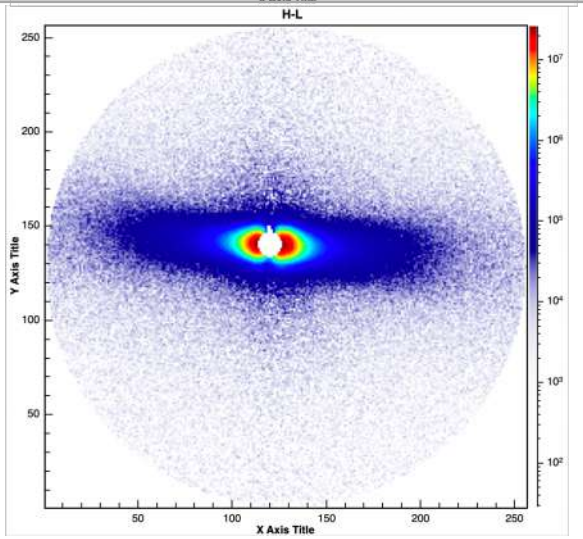




D1.2m

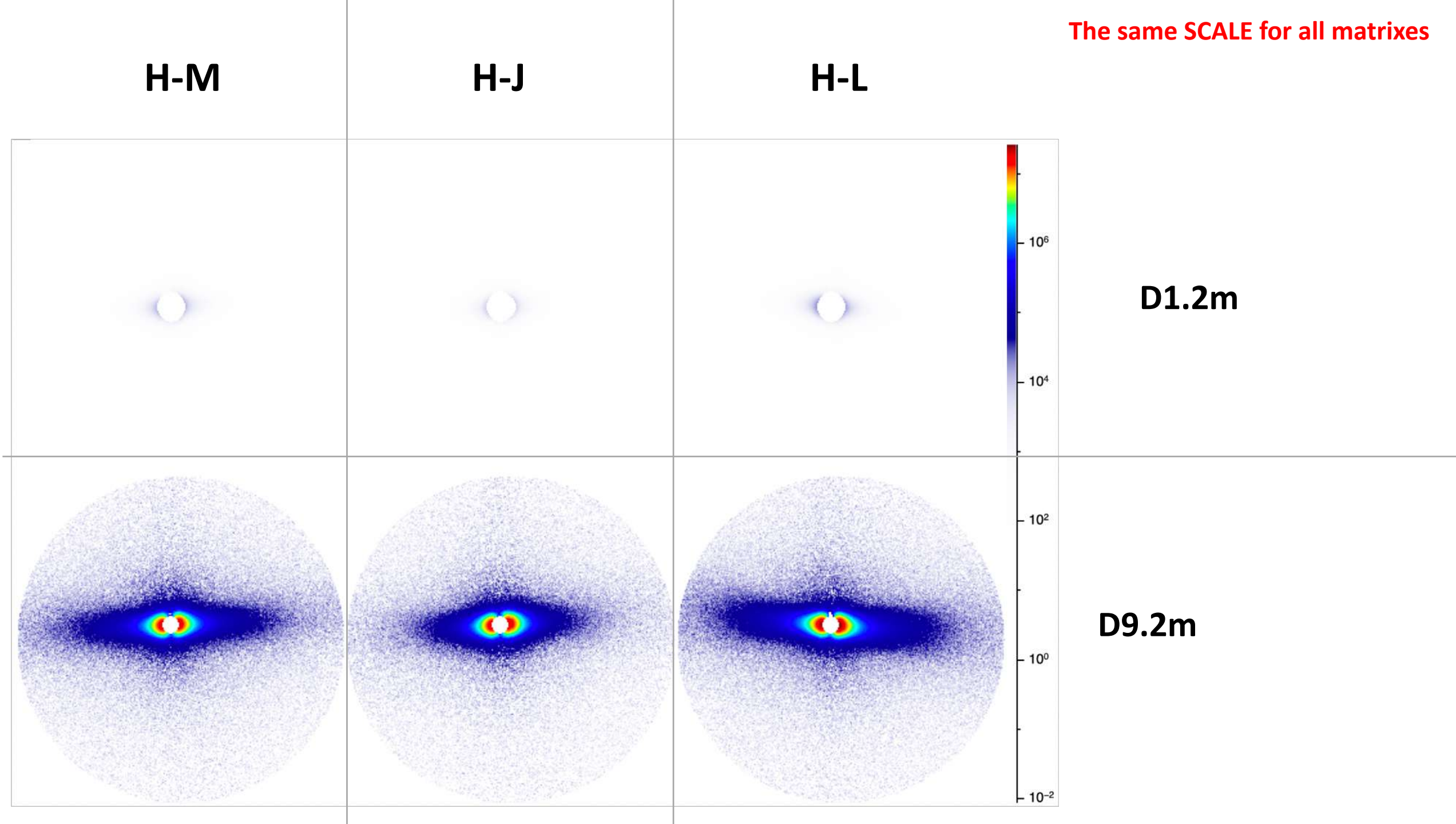






D9.2m

The same SCALE for all matrixes



DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2|20x20	2x2|6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m	mask-bs-1m
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	☑ 1.0000	☑ 1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | New | Add | Tr

Process active Script-Table

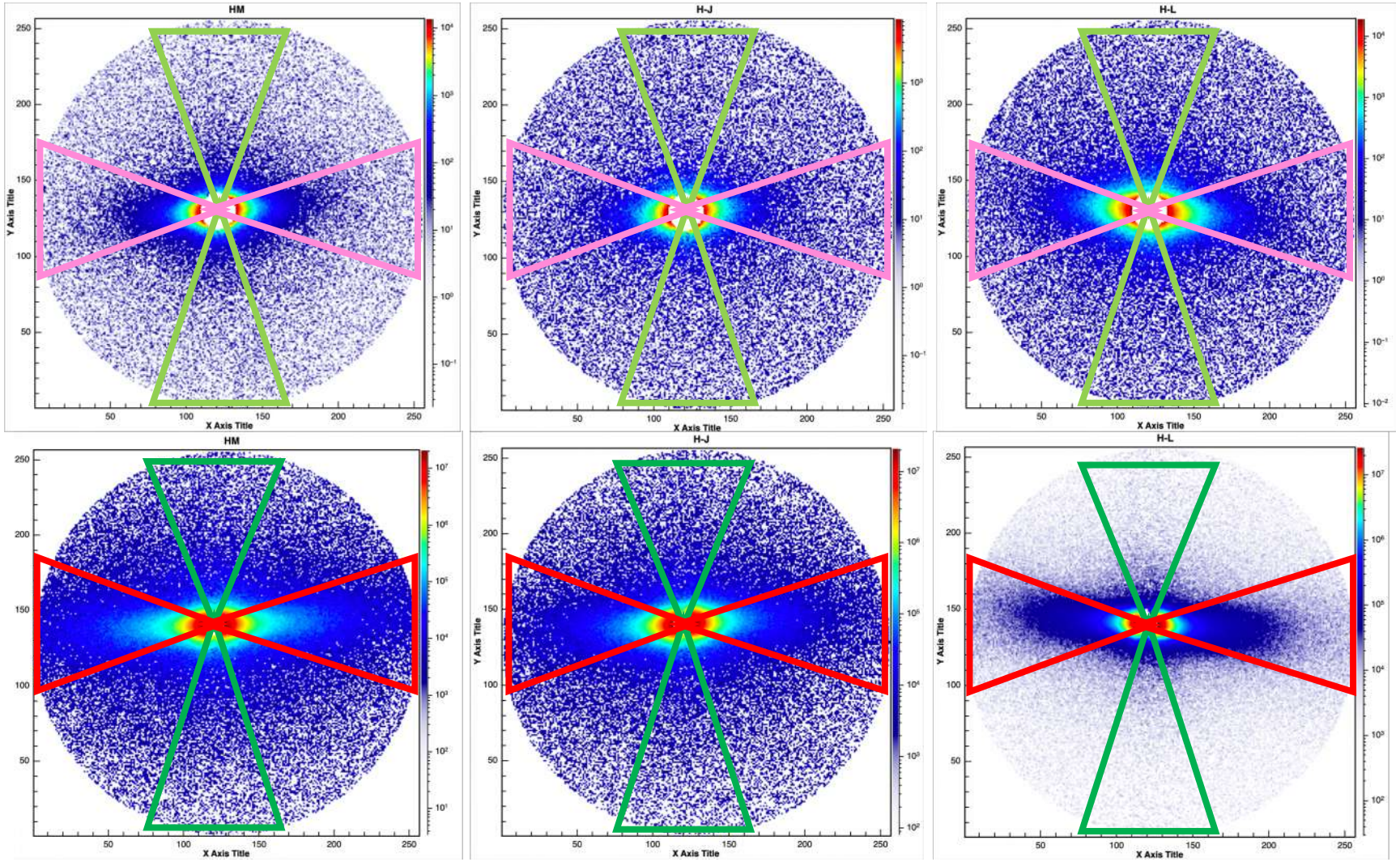
I [x,y] | I [Qy] | I [Q] | dI [x,y] | Q [x,y] | >>File | >>Project

I [Q,ϕ] | I [Qx] | σ [x,y] | dQ [x,y]

Options :: Data Processing

DAN

Problem: scattering is not ISOTROPIC



mask-bs-1m-vertical

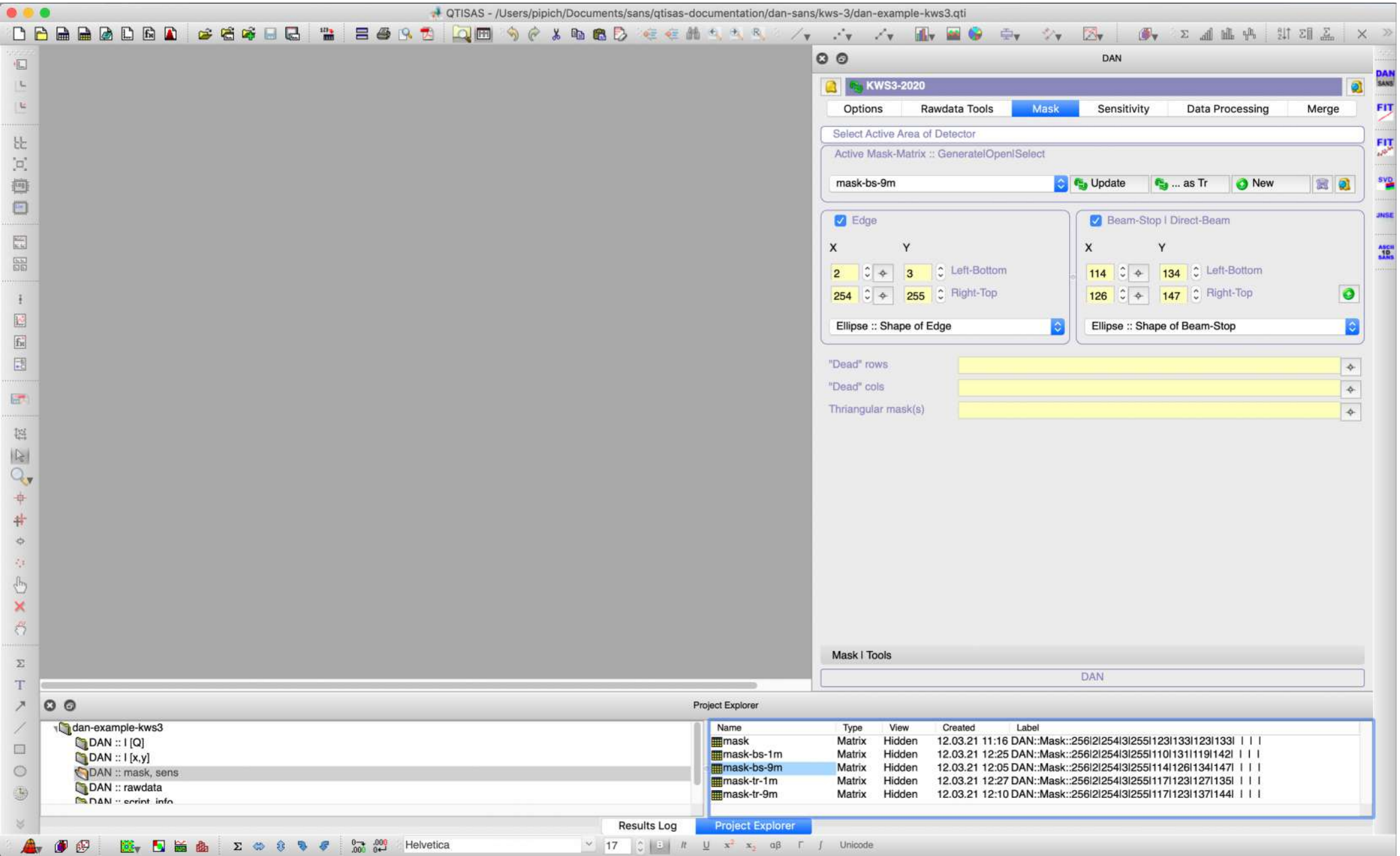
mask-bs-1m-horizontal

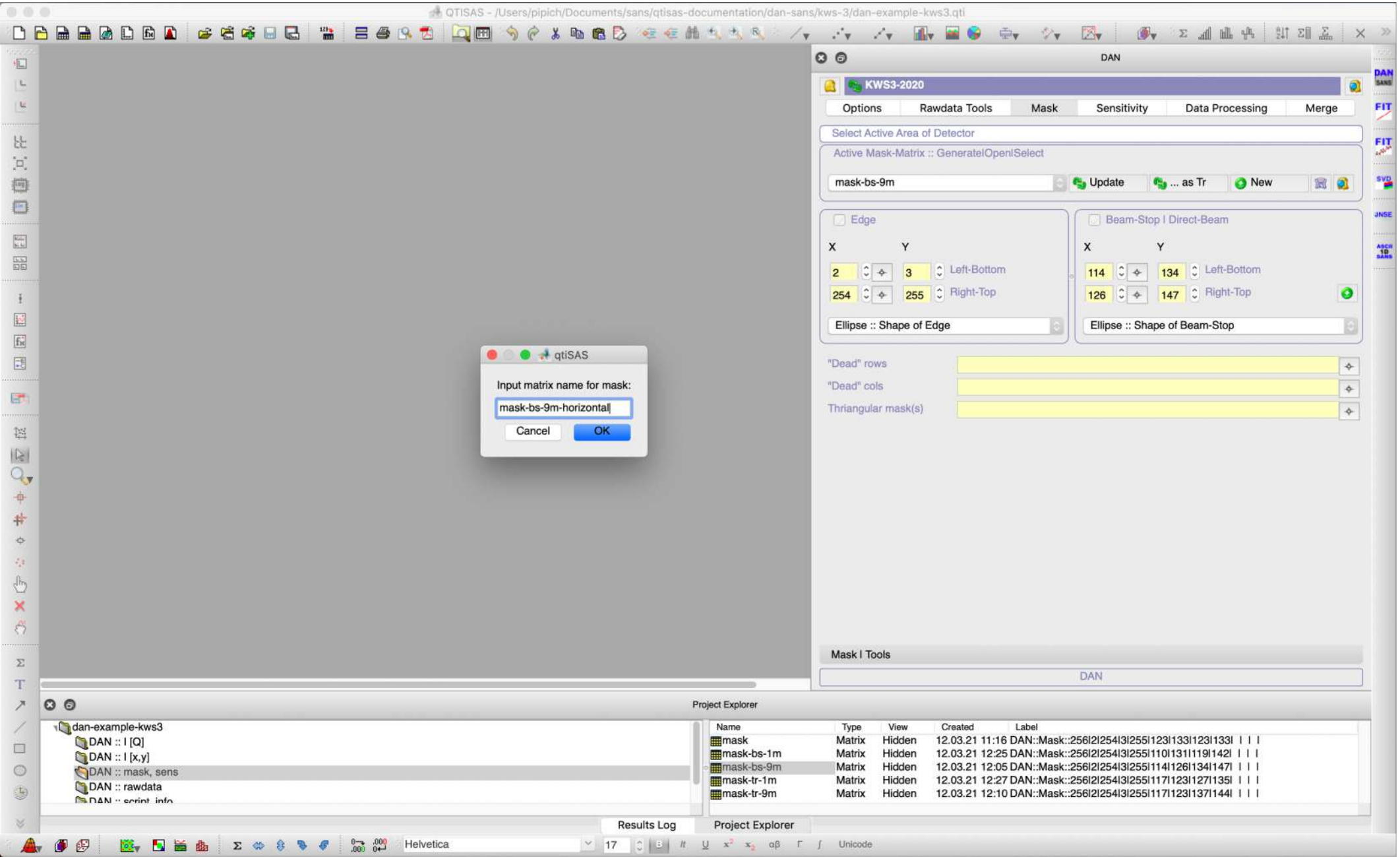
mask-bs-9m-vertical

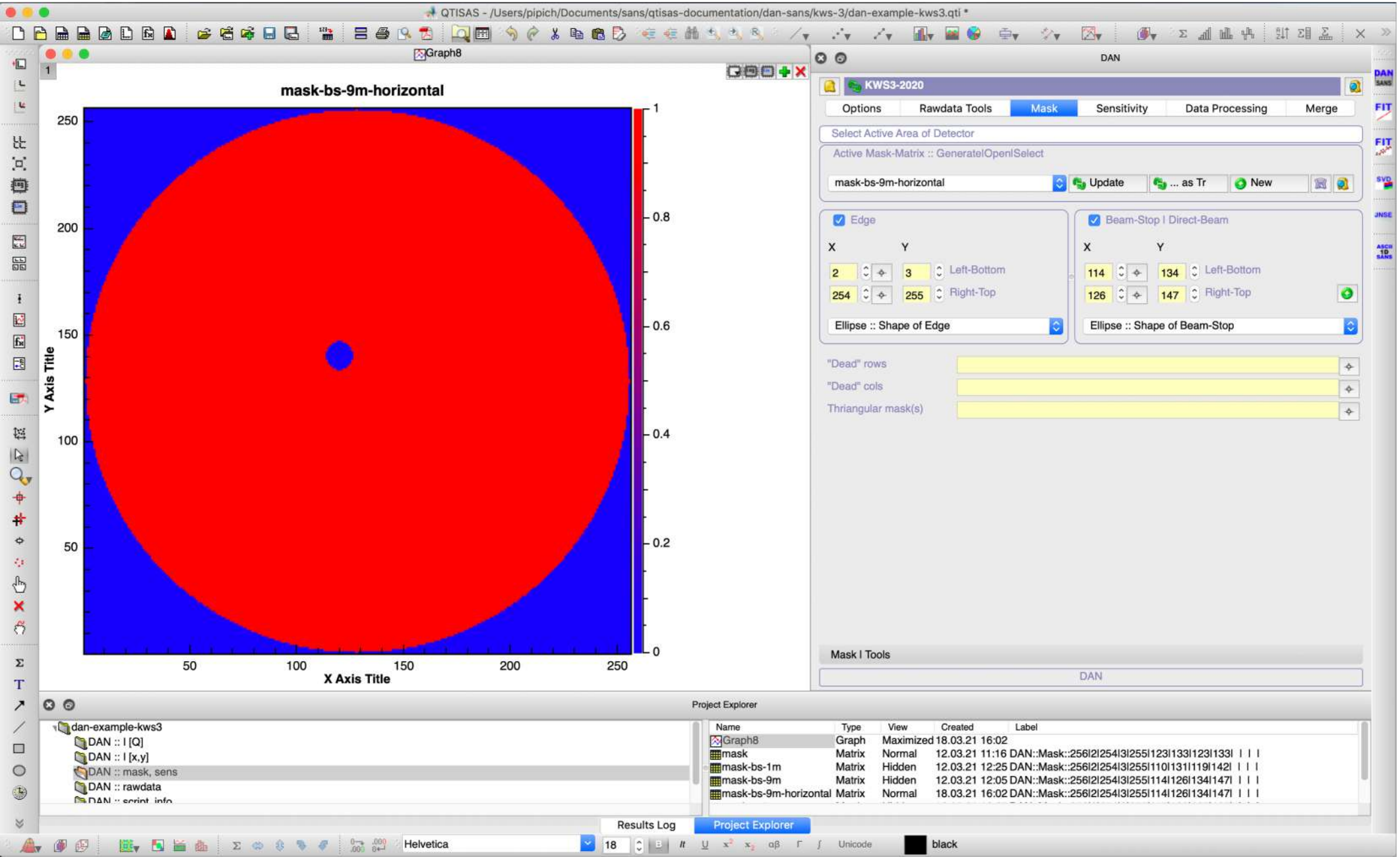
mask-bs-9m-horizontal

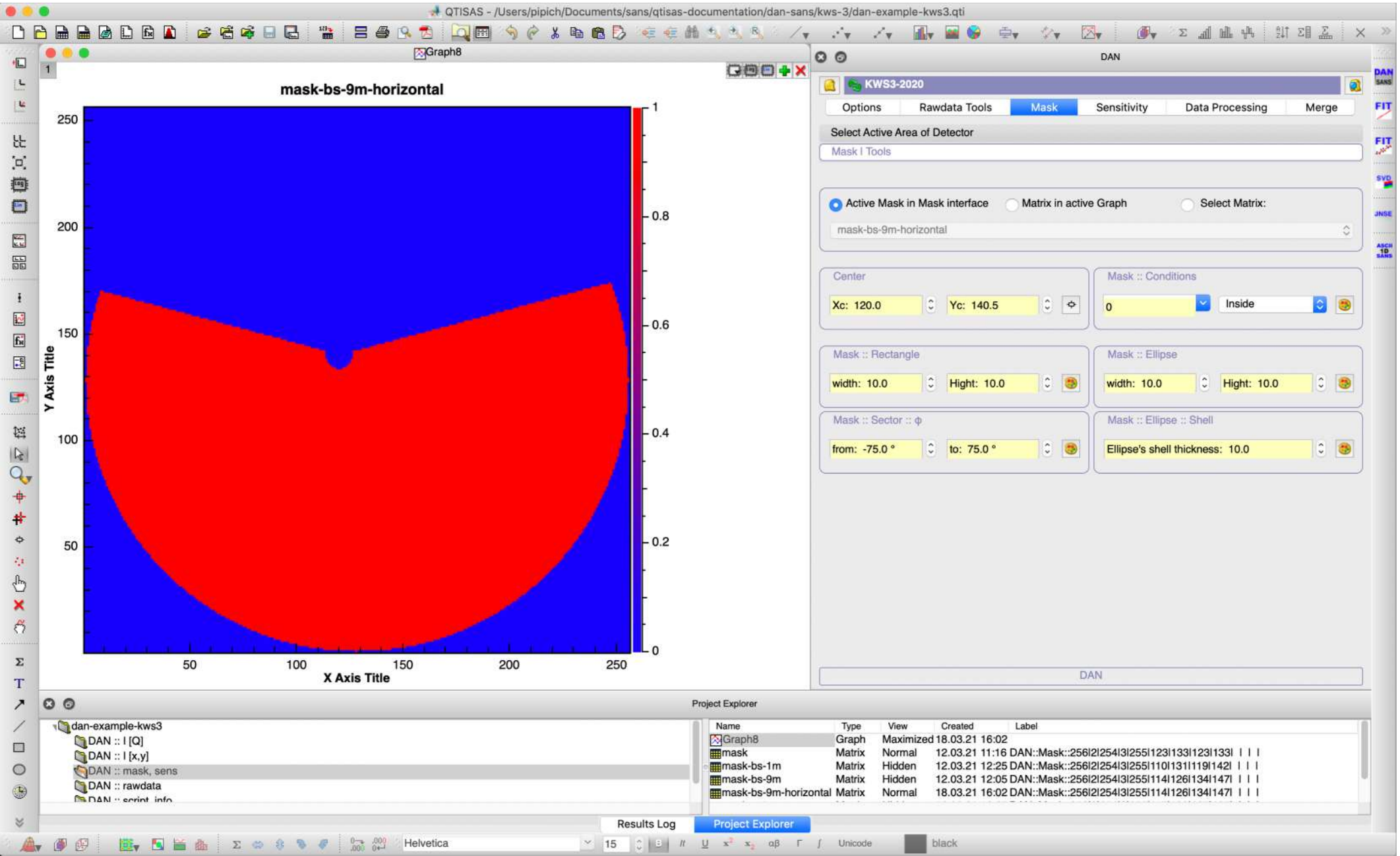
We need **Vertical** & **Horizontal** Masks for 2 configurations (9.2m and 1.2m) !

mask-bs-9m-horizontal

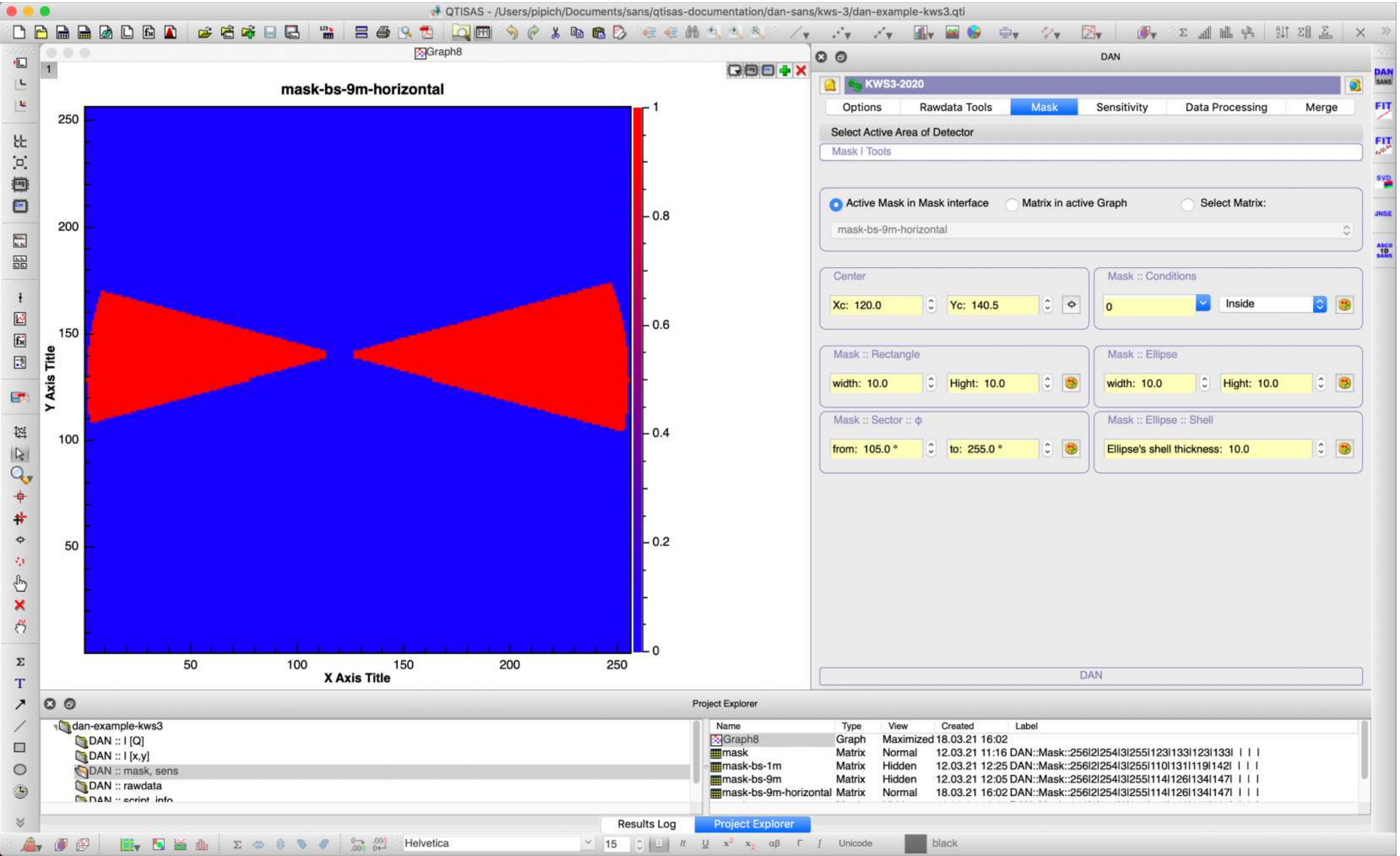

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-bs-9m
Update
... as Tr
New
Edge
X
Y
2
3
Left-Bottom
254
255
Right-Top
Ellipse :: Shape of Edge
Beam-Stop | Direct-Beam
X
Y
114
134
Left-Bottom
126
147
Right-Top
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask | Tools
DAN
Project Explorer
dan-example-kws3
DAN :: I [Q]
DAN :: I [x,y]
DAN :: mask, sens
DAN :: rawdata
Name
Type
View
Created
Label
mask
Matrix
Hidden
12.03.21 11:16
mask-bs-1m
Matrix
Hidden
12.03.21 12:25
mask-bs-9m
Matrix
Hidden
12.03.21 12:05
mask-tr-1m
Matrix
Hidden
12.03.21 12:27
mask-tr-9m
Matrix
Hidden
12.03.21 12:10
Results Log
Project Explorer
Helvetica
17
Unicode


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-bs-9m
Update
... as Tr
New
Edge
X
Y
2
3
Left-Bottom
254
255
Right-Top
Ellipse :: Shape of Edge
Beam-Stop | Direct-Beam
X
Y
114
134
Left-Bottom
126
147
Right-Top
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask | Tools
DAN
qtiSAS
Input matrix name for mask:
mask-bs-9m-horizontal
Cancel
OK
Project Explorer
dan-example-kws3
DAN :: I [Q]
DAN :: I [x,y]
DAN :: mask, sens
DAN :: rawdata
Name
Type
View
Created
Label
mask
Matrix
Hidden
12.03.21 11:16
mask-bs-1m
Matrix
Hidden
12.03.21 12:25
mask-bs-9m
Matrix
Hidden
12.03.21 12:05
mask-tr-1m
Matrix
Hidden
12.03.21 12:27
mask-tr-9m
Matrix
Hidden
12.03.21 12:10
Results Log
Project Explorer
Helvetica
17
Unicode

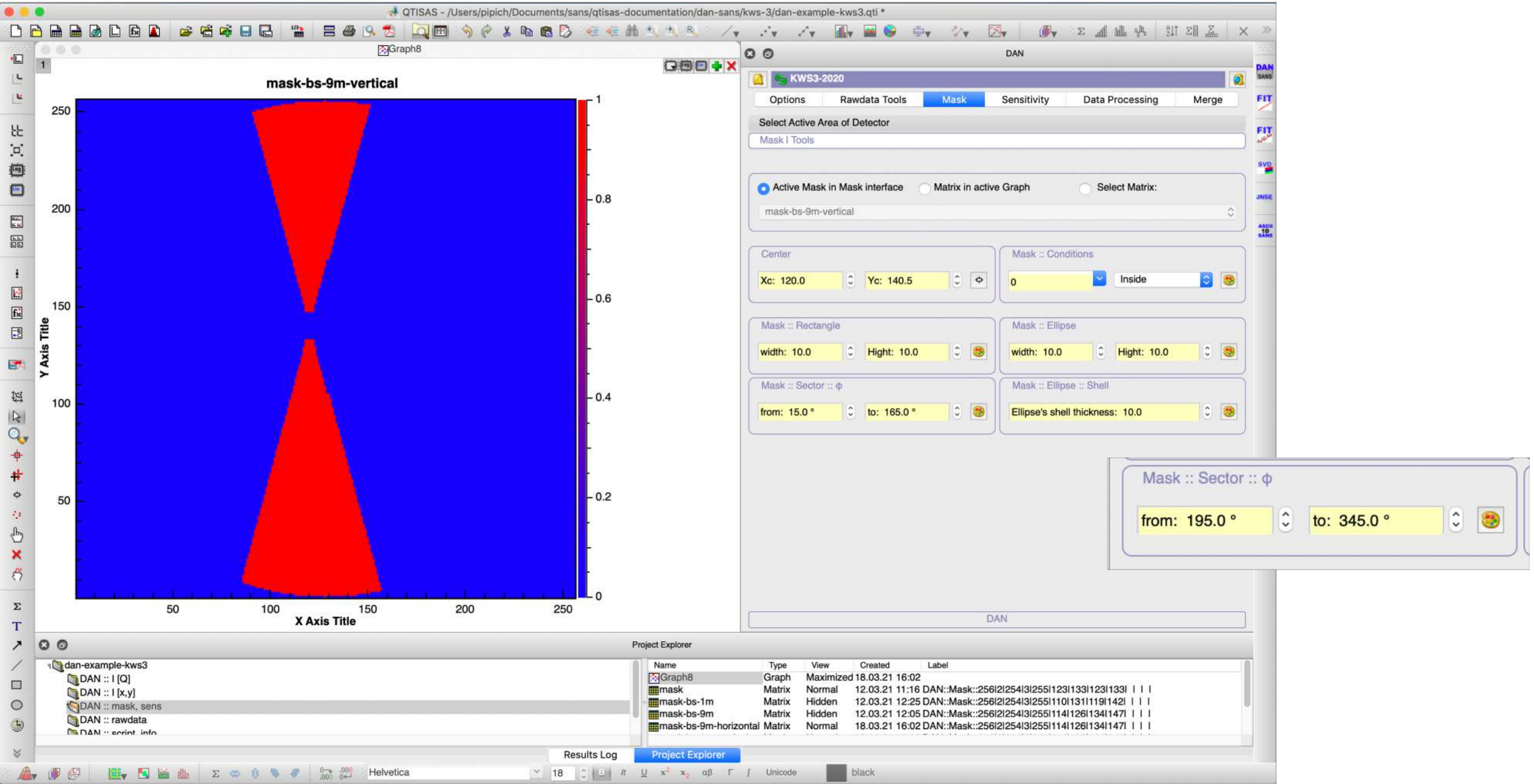

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *
Graph8
mask-bs-9m-horizontal
Y Axis Title
X Axis Title
DAN
KWS3-2020
Options
Rawdata Tools
Mask
Sensitivity
Data Processing
Merge
Select Active Area of Detector
Active Mask-Matrix :: Generate|Open|Select
mask-bs-9m-horizontal
Update
... as Tr
New
Edge
Beam-Stop | Direct-Beam
X
Y
Left-Bottom
Right-Top
Ellipse :: Shape of Edge
Ellipse :: Shape of Beam-Stop
"Dead" rows
"Dead" cols
Thriangular mask(s)
Mask | Tools
DAN
Project Explorer
dan-example-kws3
DAN :: I [Q]
DAN :: I [x,y]
DAN :: mask, sens
DAN :: rawdata
Name
Type
View
Created
Label
Graph8 Graph Maximized 18.03.21 16:02
mask Matrix Normal 12.03.21 11:16 DAN::Mask::256|2|254|3|255|123|133|123|133|
mask-bs-1m Matrix Hidden 12.03.21 12:25 DAN::Mask::256|2|254|3|255|110|131|119|142|
mask-bs-9m Matrix Hidden 12.03.21 12:05 DAN::Mask::256|2|254|3|255|114|126|134|147|
mask-bs-9m-horizontal Matrix Normal 18.03.21 16:02 DAN::Mask::256|2|254|3|255|114|126|134|147|
Results Log
Project Explorer
Helvetica
18
Unicode
black


QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti
Graph8
mask-bs-9m-horizontal
Y Axis Title
X Axis Title
DAN
KWS3-2020
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-bs-9m-horizontal
Center
Xc: 120.0
Yc: 140.5
Mask :: Conditions
0
Inside
Mask :: Rectangle
width: 10.0
Hight: 10.0
Mask :: Ellipse
width: 10.0
Hight: 10.0
Mask :: Sector :: ϕ
from: -75.0 °
to: 75.0 °
Mask :: Ellipse :: Shell
Ellipse's shell thickness: 10.0
DAN
Project Explorer
dan-example-kws3
DAN :: I [Q]
DAN :: I [x,y]
DAN :: mask, sens
DAN :: rawdata
Name
Type
View
Created
Label
Graph8 Graph Maximized 18.03.21 16:02
mask Matrix Normal 12.03.21 11:16 DAN::Mask::256|2|254|3|255|123|133|123|133| | | |
mask-bs-1m Matrix Hidden 12.03.21 12:25 DAN::Mask::256|2|254|3|255|110|131|119|142| | | |
mask-bs-9m Matrix Hidden 12.03.21 12:05 DAN::Mask::256|2|254|3|255|114|126|134|147| | | |
mask-bs-9m-horizontal Matrix Normal 18.03.21 16:02 DAN::Mask::256|2|254|3|255|114|126|134|147| | | |
Results Log
Project Explorer
Helvetica
15
Unicode
black

mask-bs-9m-horizontal

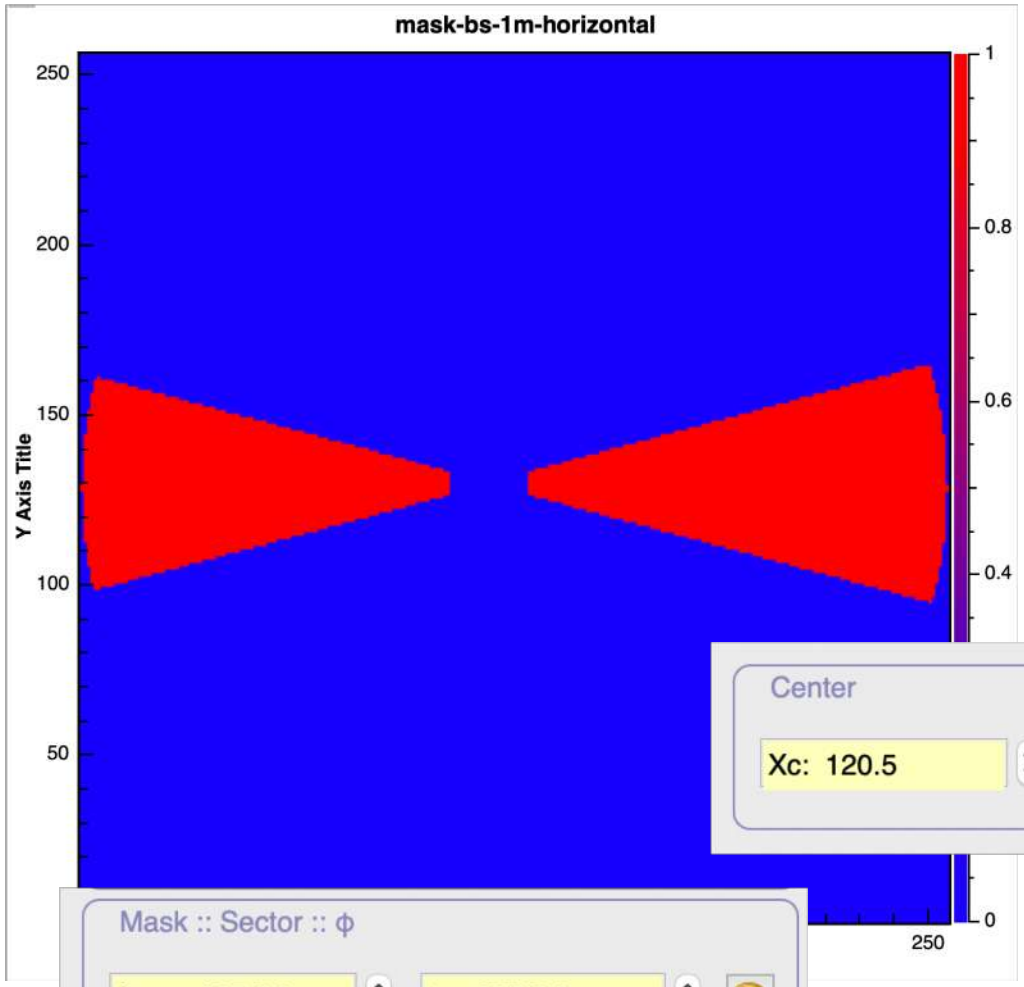


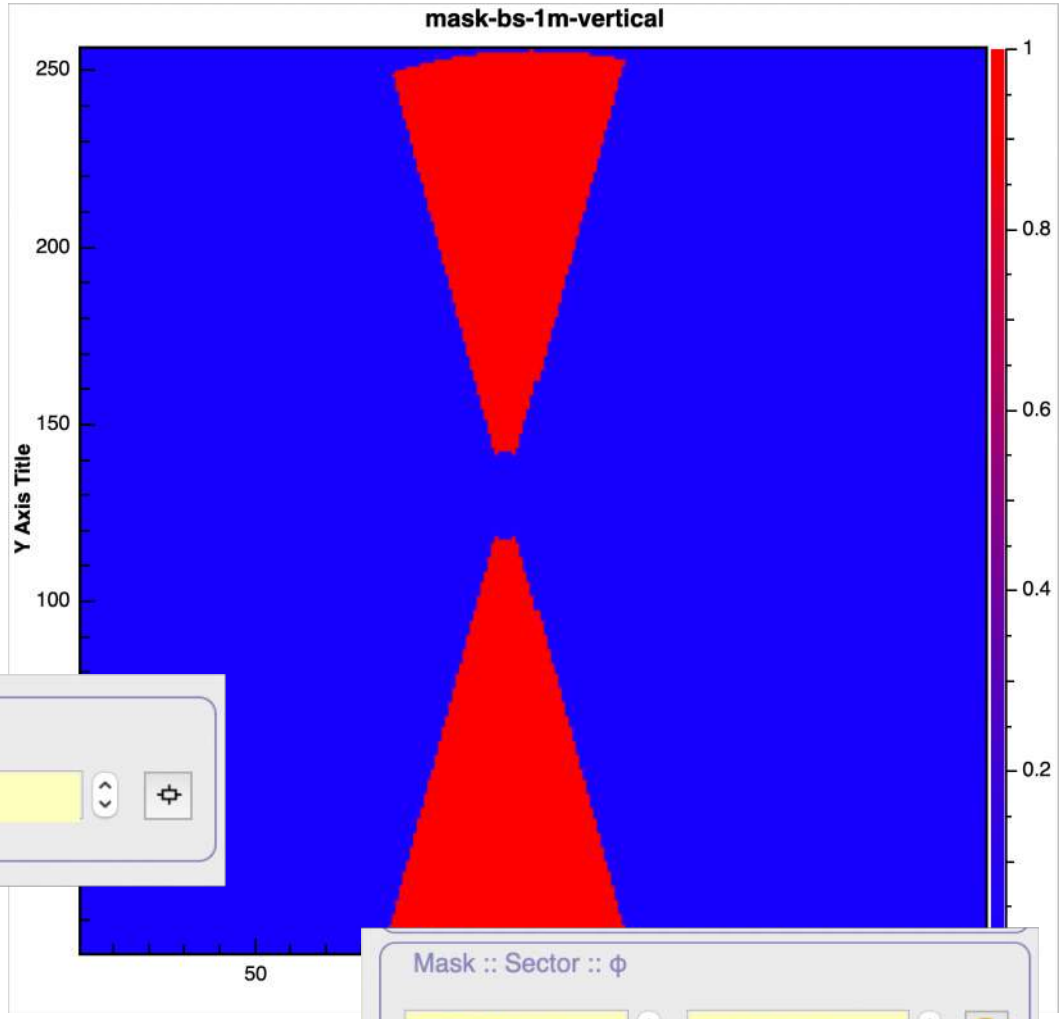
mask-bs-9m-vertical



mask-bs-1m-horizontal

mask-bs-1m-vertical





Center

Xc: 120.5 Yc: 130.5

Mask :: Sector :: ϕ

from: 105.0 ° to: 255.0 °

Mask :: Sector :: ϕ

from: -75.0 ° to: 75.0 °

Mask :: Sector :: ϕ

from: 15.0 ° to: 165.0 °

Mask :: Sector :: ϕ

from: 195.0 ° to: 345.0 °

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

Mask. Matrix	mask-bs-9m-horizontal	mask-bs-1m-horizontal
Sens. Matrix	sens	sens

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	Transmission-Sa
1	H-M	00082557	1	10	9.2	12.787	2x2l20x20	00000002	00082558	0.1	0.5380 [±0.0007
2	H-J	00082559	1	10	9.2	12.787	2x2l20x20	00000002	00082558	0.1	0.5471 [±0.0007
3	H-L	00082561	1	10	9.2	12.787	2x2l20x20	00000002	00082558	0.1	0.4829 [±0.0006

data

Search

Favourites: Macintosh HD, pipich, Desktop, Documents, Applications, Recent, Downloads, qtikws6, qtisas, qtiSAS, sciebo, doc, sans, kws1, kws2, kws3

iCloud: iCloud Drive

Name	Date Modified	Size
00000001_0000_sensitivity_HRD_standard.yaml	15. Mar 2020 at 18:10	16 KB
00000002_0000_b4c_HRD_standard.det	15. Mar 2020 at 18:10	131 KB
00000002_0000_b4c_HRD_standard.yaml	15. Mar 2020 at 18:10	16 KB
00082557_0000_H-M_HRD_standard.det	15. Mar 2020 at 18:08	141 KB
00082557_0000_H-M_HRD_standard.yaml	12. Mar 2021 at 01:57	16 KB
00082558_0000_EB_HRD_standard.det	15. Mar 2020 at 18:09	134 KB
00082558_0000_EB_HRD_standard.yaml	12. Mar 2021 at 01:58	16 KB
00082559_0000_H-J_HRD_standard.det	15. Mar 2020 at 18:08	139 KB
00082559_0000_H-J_HRD_standard.yaml	12. Mar 2021 at 01:58	16 KB
00082561_0000_H-L_HRD_standard.det	15. Mar 2020 at 18:08	143 KB
00082561_0000_H-L_HRD_standard.yaml	12. Mar 2021 at 01:59	16 KB
00082645_0000_EB_HRD_standard.det	15. Mar 2020 at 19:47	139 KB
00082645_0000_EB_HRD_standard.yaml	12. Mar 2021 at 02:03	16 KB
00082646_0000_H-J_HRD_standard.det	15. Mar 2020 at 20:48	140 KB
00082646_0000_H-J_HRD_standard.yaml	12. Mar 2021 at 02:04	16 KB
00082647_0000_H-L_HRD_standard.det	15. Mar 2020 at 21:48	142 KB
00082647_0000_H-L_HRD_standard.yaml	12. Mar 2021 at 02:04	16 KB
00082648_0000_H-M_HRD_standard.det	15. Mar 2020 at 22:48	141 KB
00082648_0000_H-M_HRD_standard.yaml	12. Mar 2021 at 02:03	16 KB

New Folder | Cancel | Open

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2l20x20	2x2l6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FSlEB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FSlAtt]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m-horizontal	mask-bs-1m-horizontal
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.0000	1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

DAN :: I [x,y]
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
DANP :: Merge.1D

Name	Type	View	Created	Label
info-table	Table	Normal	12.03.21 02:18	Info::Table
script	Table	Maximized	12.03.21 17:47	DAN::Script::Table
script-mergingTemplate	Table	Normal	18.03.21 13:23	DAN::Merging::Template
script-Settings	Table	Normal	12.03.21 17:47	DAN::Settings::Table

Results Log | Project Explorer

Helvetica 18 Unicode

Sample Names: added suffix “-horizontal”

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	T
1	H-M	00082557	1	10	9.2	12.787	2x2I20x20	00000002	00082558	0.1	
2	H-J	00082559	1	10	9.2	12.787	2x2I20x20	00000002	00082558	0.1	
3	H-L	00082561	1	10	9.2	12.787	2x2I20x20	00000002	00082558	0.1	
4	H-J	00082646	2	10	1.2	12.787	2x2I6.5x8	00000002	00082645	0.1	
5	H-L	00082647	2	10	1.2	12.787	2x2I6.5x8	00000002	00082645	0.1	
6	[illegible]	[illegible]2648	2	10	1.2	12.787	2x2I6.5x8	00000002	00082645	0.1	
	H-M-horizontal	0008[illegible]57	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100	
	H-J-horizontal	0008[illegible]59	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100	
0	H-L-horizontal	0008[illegible]61	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100	
1	H-J-horizontal	0008[illegible]46	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100	
2	H-L-horizontal	0008[illegible]47	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100	
3	H-M-horizontal	0008[illegible]48	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100	

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2I20x20	2x2I6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FS|EB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FS|Att]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m-horizontal	mask-bs-1m-horizontal
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	1.0000	1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

DAN :: I [x,y]
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
DANP :: Merge.1D

Name	Type	View	Created	Label
info-table	Table	Normal	12.03.21 02:18	Info::Table
script	Table	Maximized	12.03.21 17:47	DAN::Script::Table
script-mergingTemplate	Table	Normal	18.03.21 13:23	DAN::Merging::Template
script-Settings	Table	Normal	12.03.21 17:47	DAN::Settings::Table

Results Log | Project Explorer

Helvetica 18 Unicode

Sample Names: added suffix “-vertical”

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *

script - DAN::Script::Table

	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness
1	H-M	00082557	1	10	9.2	12.787	2x2I20x20	00000002	00082558	0.1
2	H-J	00082559	1	10	9.2	12.787	2x2I20x20	00000002	00082558	0.1
3	H-L	00082561	1	10	9.2	12.787	2x2I20x20	00000002	00082558	0.1
4	H-J	00082646	2	10	1.2	12.787	2x2I6.5x8	00000002	00082645	0.1
5	H-L	00082647	2	10	1.2	12.787	2x2I6.5x8	00000002	00082645	0.1
6	H-M	00082648	2	10	1.2	12.787	2x2I6.5x8	00000002	00082645	0.1
7										
8	H-M-horizontal	00082557	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100
9	H-J-horizontal	00082559	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100
10	H-L-horizontal	00082561	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100
11	H-J-horizontal	00082646	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100
12	H-L-horizontal	00082647	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100
13	H-M-horizontal	00082648	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100
14										
15	H-M-vertical	00082557	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100
16	H-J-vertical	00082559	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100
17	H-L-vertical	00082561	1	10	9.200	12.787	2x2I20x20	00000002	00082558	0.100
18	H-J-vertical	00082646	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100
19	H-L-vertical	00082647	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100
20	H-M-vertical	00082648	2	10	1.200	12.787	2x2I6.5x8	00000002	00082645	0.100

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2I20x20	2x2I6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FSIEB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FSIAtt]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Mask. Matrix	mask-bs-9m-vertical	mask-bs-1m-vertical
#-EB		
Tr [EC-to-EB]	1.0000	1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

DAN :: I [x,y]
DAN :: mask, sens
DAN :: rawdata
DAN :: script, info, ...
DANP :: Merge.1D

Name	Type	View	Created	Label
info-table	Table	Normal	12.03.21 02:18	Info::Table
script	Table	Maximized	12.03.21 17:47	DAN::Script::Table
script-mergingTemplate	Table	Normal	18.03.21 13:23	DAN::Merging::Template
script-Settings	Table	Normal	12.03.21 17:47	DAN::Settings::Table

Results Log | Project Explorer

Helvetica 18 Unicode

Modified ”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-M	00082557	1	10	9.2	12.787	2x2|20x20	00000002	00082558	0.1	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens
2	H-J	00082559	1	10	9.2	12.787	2x2|20x20	00000002	00082558	0.1	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m	sens
3	H-L	00082561	1	10	9.2	12.787	2x2|20x20	00000002	00082558	0.1	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m	sens
4	H-J	00082646	2	10	1.2	12.787	2x2|6.5x8	00000002	00082645	0.1	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens
5	H-L	00082647	2	10	1.2	12.787	2x2|6.5x8	00000002	00082645	0.1	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens
6	H-M	00082648	2	10	1.2	12.787	2x2|6.5x8	00000002	00082645	0.1	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m	sens
7																
8	H-M-horizontal	00082557	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m-horizontal	sens
9	H-J-horizontal	00082559	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m-horizontal	sens
10	H-L-horizontal	00082561	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m-horizontal	sens
11	H-J-horizontal	00082646	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m-horizontal	sens
12	H-L-horizontal	00082647	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m-horizontal	sens
13	H-M-horizontal	00082648	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m-horizontal	sens
14																
15	H-M-vertical	00082557	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5380 [±0.0007]	280100	120.04	140.66	mask-bs-9m-vertical	sens
16	H-J-vertical	00082559	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.5471 [±0.0007]	280100	120.04	140.66	mask-bs-9m-vertical	sens
17	H-L-vertical	00082561	1	10	9.200	12.787	2x2|20x20	00000002	00082558	0.100	0.4829 [±0.0006]	280100	120.04	140.66	mask-bs-9m-vertical	sens
18	H-J-vertical	00082646	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8232 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m-vertical	sens
19	H-L-vertical	00082647	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.7811 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m-vertical	sens
20	H-M-vertical	00082648	2	10	1.200	12.787	2x2|6.5x8	00000002	00082645	0.100	0.8088 [±0.0005]	2816.2	119.97	130.85	mask-bs-1m-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

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *

QI-SM-00082557-H-M - H-M

	Q[X]	I[Y]	dI[yEr]	Sigma[xEr]
1	1.08956598E-04	1.17169340E+07	7.32425696E+04	6.80881135E-05
2	1.27116030E-04	1.05110122E+07	3.14837196E+04	6.81306789E-05
3	1.45275462E-04	8.76786379E+06	2.23664452E+04	6.81797598E-05
4	1.63434893E-04	7.25730993E+06	1.71959791E+04	6.82353422E-05
5	1.81594324E-04	5.66264311E+06	1.29498742E+04	6.82974101E-05
6	1.99753755E-04	4.28102757E+06	9.76231390E+03	6.83659459E-05
7	2.17913184E-04	3.14632986E+06	7.36244658E+03	6.84409302E-05
8	2.36072613E-04	2.29117220E+06	5.62388530E+03	6.85223417E-05
9	2.54232042E-04	1.68073980E+06	4.33791373E+03	6.86101577E-05
10	2.72391469E-04	1.23502164E+06	3.45765263E+03	6.87043536E-05
11	2.90550896E-04	9.33938100E+05	2.82750482E+03	6.88049031E-05
12	3.08710321E-04	7.17420205E+05	2.33399663E+03	6.89117784E-05
13	3.26869746E-04	5.57421772E+05	1.97007886E+03	6.90249502E-05
14	3.45029170E-04	4.38985610E+05	1.69081590E+03	6.91443876E-05
15	3.63188593E-04	3.53539475E+05	1.47238389E+03	6.92700581E-05
16	3.81348014E-04	2.89993832E+05	1.28031914E+03	6.94019278E-05
17	3.99507435E-04	2.41802131E+05	1.14205168E+03	6.95399615E-05
18	4.17666854E-04	2.02273163E+05	1.02678871E+03	6.96841226E-05
19	4.35826272E-04	1.71826655E+05	9.17337757E+02	6.98343731E-05
20	4.53985689E-04	1.45859180E+05	8.31840898E+02	6.99906739E-05
21	4.72145104E-04	1.27660762E+05	7.70072844E+02	7.01529843E-05
22	4.90304518E-04	1.13828702E+05	7.12632452E+02	7.03212630E-05
23	5.08463930E-04	1.01675512E+05	6.60356734E+02	7.04954670E-05
24	5.26623341E-04	8.87047466E+04	6.07655502E+02	7.06755526E-05
25	5.44782750E-04	8.04169195E+04	5.68641896E+02	7.08614749E-05
26	5.62942157E-04	7.49666344E+04	5.34214455E+02	7.10531882E-05
27	5.81101563E-04	6.74113556E+04	5.00403344E+02	7.12506456E-05

DAN

KWS3-2020

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

Table of Configurations :: Data Processing

	cond.-#1	cond.-#2
#-EC [EB]	00082558	00082645
#-BC	00000002	00000002
C[m]	10	10
D[m]	9.200	1.200
λ[Å]	12.787	12.787
Beam Size	2x2I20x20	2x2I6.5x8
Abs.Cal. [#-FS]		
Abs.Cal. [#-EB]	00082558	00082645
Abs.Cal. [#-BC]	00000002	00000002
D-[FSIEB][m]	9.200	1.200
μ-[FS]	1.0000E+00	1.0000E+00
Tr-[FSIAtt]	1.0000	1.0000
Factor	2.8010E+05	2.8162E+03
#-"Center"	00082558	00082645
X-center	120.044±0.000	119.972±0.000
Y-center	140.661±0.000	130.853±0.000
Mask. Matrix	mask-bs-9m-vertical	mask-bs-1m-vertical
Sens. Matrix	sens	sens
#-EB		
Tr [EC-to-EB]	☑ 1.0000	☑ 1.0000
Mask Matrix [Tr]	mask-tr-9m	mask-tr-1m

Script-Table Tools

script | 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

Project Explorer

- dan-example-kws3
  - DAN :: I [Q]
  - DAN :: I [x,y]
  - DAN :: mask, sens
  - DAN :: rawdata
  - DAN :: script, info, ...
  - DANP :: Merge.1D

Name	Type	Vi	Created	Label
QI-SM-00082557-H-M	Table	Ma mized	18.03.21 13:03	H-M
QI-SM-00082557-H-M-horizontal	Table	No al	18.03.21 18:50	H-M-horizontal
QI-SM-00082557-H-M-vertical	Table	No al	18.03.21 18:50	H-M-vertical
QI-SM-00082559-H-J	Table	No al	18.03.21 13:03	H-J
QI-SM-00082559-H-J-horizontal	Table	No al	18.03.21 18:50	H-J-horizontal
QI-SM-00082559-H-J-vertical	Table	Normal	18.03.21 18:50	H-J-vertical
QI-SM-00082561-H-L	Table	Normal	18.03.21 13:03	H-L

Results Log | Project Explorer

Helvetica 18 Unicode

Merging Data

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *

script-mergingTemplate - DAN::Merging::Template

	1[X]	2[Y]	3[Y]
1	H-M	QI-SM-00082557-H-M	QI-SM-00082648-H-M
2	H-J	QI-SM-00082559-H-J	QI-SM-00082646-H-J
3	H-L	QI-SM-00082561-H-L	QI-SM-00082647-H-L
4	H-M-horizontal	QI-SM-00082557-H-M-horizontal	QI-SM-00082648-H-M-horizontal
5	H-J-horizontal	QI-SM-00082559-H-J-horizontal	QI-SM-00082646-H-J-horizontal
6	H-L-horizontal	QI-SM-00082561-H-L-horizontal	QI-SM-00082647-H-L-horizontal
7	H-M-vertical	QI-SM-00082557-H-M-vertical	QI-SM-00082648-H-M-vertical
8	H-J-vertical	QI-SM-00082559-H-J-vertical	QI-SM-00082646-H-J-vertical
9	H-L-vertical	QI-SM-00082561-H-L-vertical	QI-SM-00082647-H-L-vertical

DAN

KWS3-2020

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

Merging Options ::

2 Number of tables for merging

9 Number of table-sets for merging

30% Overlap control

* Filter (Wild Card)

Indexing [Output]

Smart merging ::

1 Reference column

Const normalization

0 (plus) left-side points

0 (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
1	H-M	QI-SM-00082557-H-M	QI-SM-00082648-H-M
2	H-J	QI-SM-00082559-H-J	QI-SM-00082646-H-J
3	H-L	QI-SM-00082561-H-L	QI-SM-00082647-H-L
4	H-M-horizontal	QI-SM-00082557-H-M-horizontal	QI-SM-00082648-H-M-horizontal
5	H-J-horizontal	QI-SM-00082559-H-J-horizontal	QI-SM-00082646-H-J-horizontal
6	H-L-horizontal	QI-SM-00082561-H-L-horizontal	QI-SM-00082647-H-L-horizontal
7	H-M-vertical	QI-SM-00082557-H-M-vertical	QI-SM-00082648-H-M-vertical
8	H-J-vertical	QI-SM-00082559-H-J-vertical	QI-SM-00082646-H-J-vertical
9	H-L-vertical	QI-SM-00082561-H-L-vertical	QI-SM-00082647-H-L-vertical

After Merging: remove first: 0 points | remove last: 0 points

Merge [project] | Merge [ascii]

DAN

Project Explorer

- dan-example-kws3
  - DAN :: I [Q]
  - DAN :: I [x,y]
  - DAN :: mask, sens
  - DAN :: rawdata
  - DAN :: script, info, ...
  - DANP :: Merge.1D

Name	Type	View	Created	Label
info-table	Table	Normal	12.03.21 02:18	Info::Table
script	Table	Normal	12.03.21 17:47	DAN::Script::Table
script-mergingTemplate	Table	Maximized	18.03.21 18:50	DAN::Merging::Template
script-Settings	Table	Normal	12.03.21 17:47	DAN::Settings::Table

Results Log | Project Explorer

Helvetica 18 Unicode

Tables are ready

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/dan-sans/kws-3/dan-example-kws3.qti *

H-J - Merged Tables >> QI-SM-00082559-H-J, QI-SM-00082646-H-J,

	Q[X]	I[Y]	dI[yEr]	Sigma[xEr]
1	1.089566E-04	1.179794E+07	7.293790E+04	6.808811E-05
2	1.271160E-04	1.061157E+07	3.147259E+04	6.813068E-05
3	1.452755E-04	8.792229E+06	2.220430E+04	6.817976E-05
4	1.634349E-04	7.266609E+06	1.703185E+04	6.823534E-05
5	1.815943E-04	5.687315E+06	1.283828E+04	6.829741E-05
6	1.997538E-04	4.284102E+06	9.646464E+03	6.836595E-05
7	2.179132E-04	3.138337E+06	7.268970E+03	6.844093E-05
8	2.360726E-04	2.271971E+06	5.517267E+03	6.852234E-05
9	2.542320E-04	1.654117E+06	4.237377E+03	6.861016E-05
10	2.723915E-04	1.203793E+06	3.360038E+03	6.870435E-05
11	2.905509E-04	8.894877E+05	2.713162E+03	6.880490E-05
12	3.087103E-04	6.794198E+05	2.238870E+03	6.891178E-05
13	3.268697E-04	5.241226E+05	1.885942E+03	6.902495E-05
14	3.450292E-04	4.052701E+05	1.608585E+03	6.914439E-05
15	3.631886E-04	3.218974E+05	1.393743E+03	6.927006E-05
16	3.813480E-04	2.582635E+05	1.199954E+03	6.940193E-05
17	3.995074E-04	2.135951E+05	1.068675E+03	6.953996E-05
18	4.176669E-04	1.794096E+05	9.652391E+02	6.968412E-05
19	4.358263E-04	1.513404E+05	8.601429E+02	6.983437E-05
20	4.539857E-04	1.246181E+05	7.700088E+02	6.999067E-05
21	4.721451E-04	1.071658E+05	7.091223E+02	7.015298E-05
22	4.903045E-04	9.653691E+04	6.620528E+02	7.032126E-05
23	5.084639E-04	8.259584E+04	6.021654E+02	7.049547E-05
24	5.266233E-04	7.073623E+04	5.512187E+02	7.067555E-05
25	5.447827E-04	6.317474E+04	5.118898E+02	7.086147E-05
26	5.629422E-04	5.693747E+04	4.737998E+02	7.105319E-05
27	5.811016E-04	5.177286E+04	4.477911E+02	7.125065E-05

DAN

KWS3-2020

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

Merging Options ::

2 Number of tables for merging

9 Number of table-sets for merging

30% Overlap control

* Filter (Wild Card)

Indexing [Output]

Smart merging ::

1 Reference column

Const normalization

0 (plus) left-side points

0 (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
1	H-M	QI-SM-00082557-H-M	QI-SM-00082648-H-M
2	H-J	QI-SM-00082559-H-J	QI-SM-00082646-H-J
3	H-L	QI-SM-00082561-H-L	QI-SM-00082647-H-L
4	H-M-horizontal	QI-SM-00082557-H-M-horizontal	QI-SM-00082648-H-M-horizontal
5	H-J-horizontal	QI-SM-00082559-H-J-horizontal	QI-SM-00082646-H-J-horizontal
6	H-L-horizontal	QI-SM-00082561-H-L-horizontal	QI-SM-00082647-H-L-horizontal
7	H-M-vertical	QI-SM-00082557-H-M-vertical	QI-SM-00082648-H-M-vertical
8	H-J-vertical	QI-SM-00082559-H-J-vertical	QI-SM-00082646-H-J-vertical
9	H-L-vertical	QI-SM-00082561-H-L-vertical	QI-SM-00082647-H-L-vertical

After Merging: remove first: 0 points | remove last: 0 points

Merge [project] | Merge [ascii]

DAN

Project Explorer

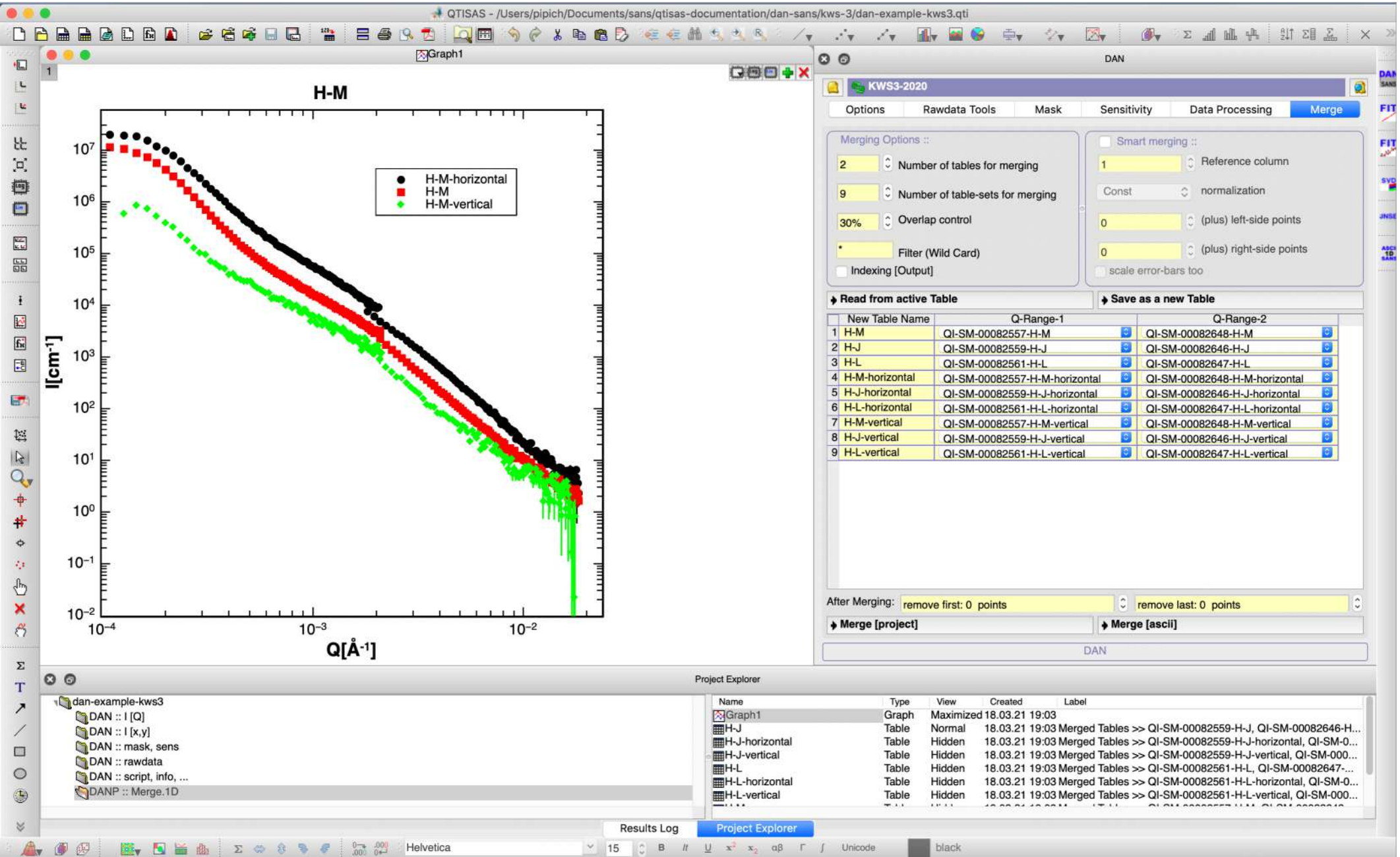
dan-example-kws3
- DAN :: I [Q]
- DAN :: I [x,y]
- DAN :: mask, sens
- DAN :: rawdata
- DAN :: script, info, ...
- DANP :: Merge.1D

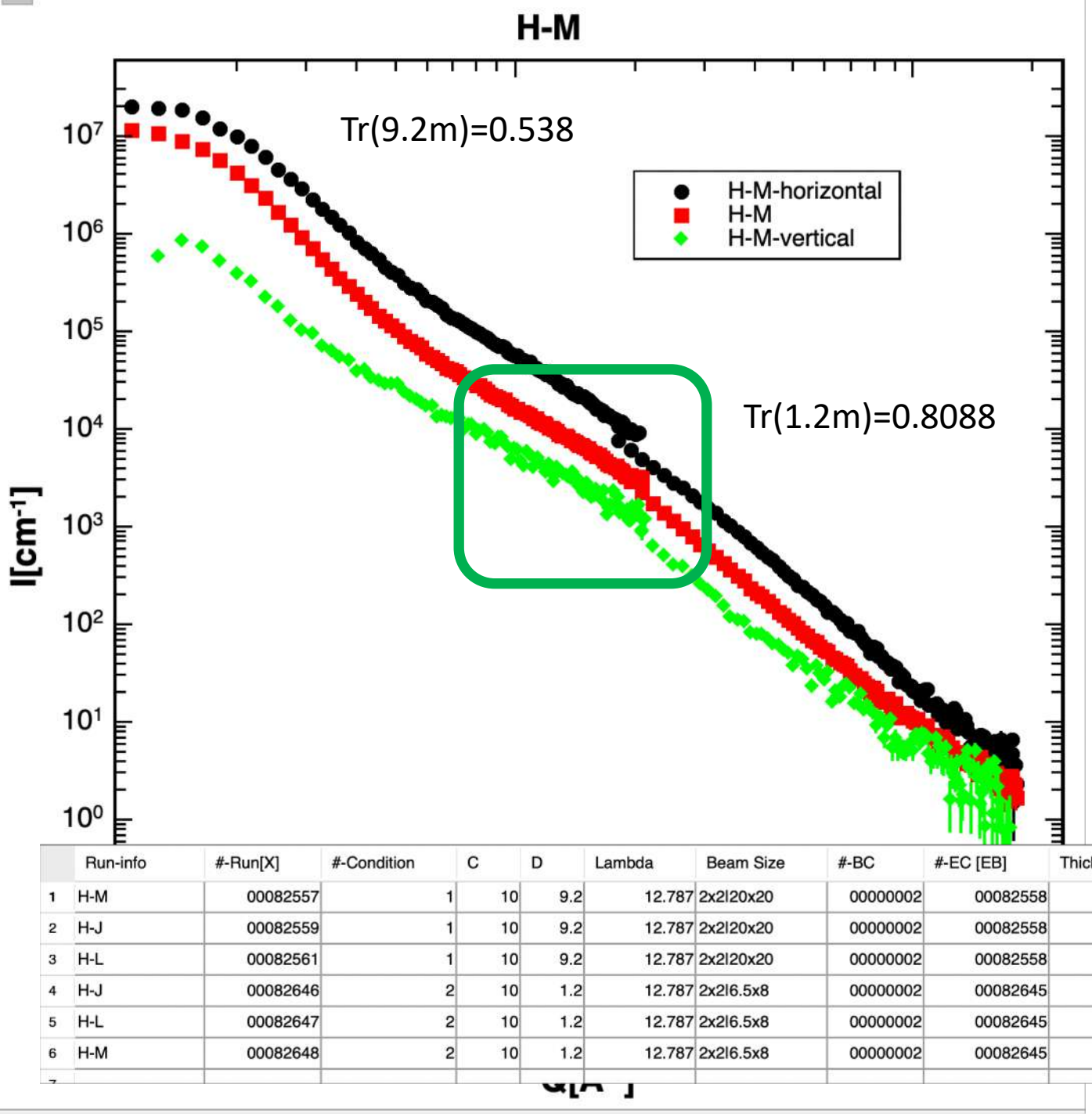
Name	Type	View	Created	Label
H-J	Table	Maximized	18.03.21 19:03	Merged Tables >> QI-SM-00082559-H-J, QI-SM-00082646-H...
H-J-horizontal	Table	Hidden	18.03.21 19:03	Merged Tables >> QI-SM-00082559-H-J-horizontal, QI-SM-0...
H-J-vertical	Table	Hidden	18.03.21 19:03	Merged Tables >> QI-SM-00082559-H-J-vertical, QI-SM-000...
H-L	Table	Hidden	18.03.21 19:03	Merged Tables >> QI-SM-00082561-H-L, QI-SM-00082647-...
H-L-horizontal	Table	Hidden	18.03.21 19:03	Merged Tables >> QI-SM-00082561-H-L-horizontal, QI-SM-0...
H-L-vertical	Table	Hidden	18.03.21 19:03	Merged Tables >> QI-SM-00082561-H-L-vertical, QI-SM-000...
H-M	Table	Hidden	18.03.21 19:03	Merged Tables >> QI-SM-00082557-H-M, QI-SM-00082648-...

Results Log | Project Explorer

Helvetica 18 Unicode

Plotting “H-M” sample averaged with 3 masks

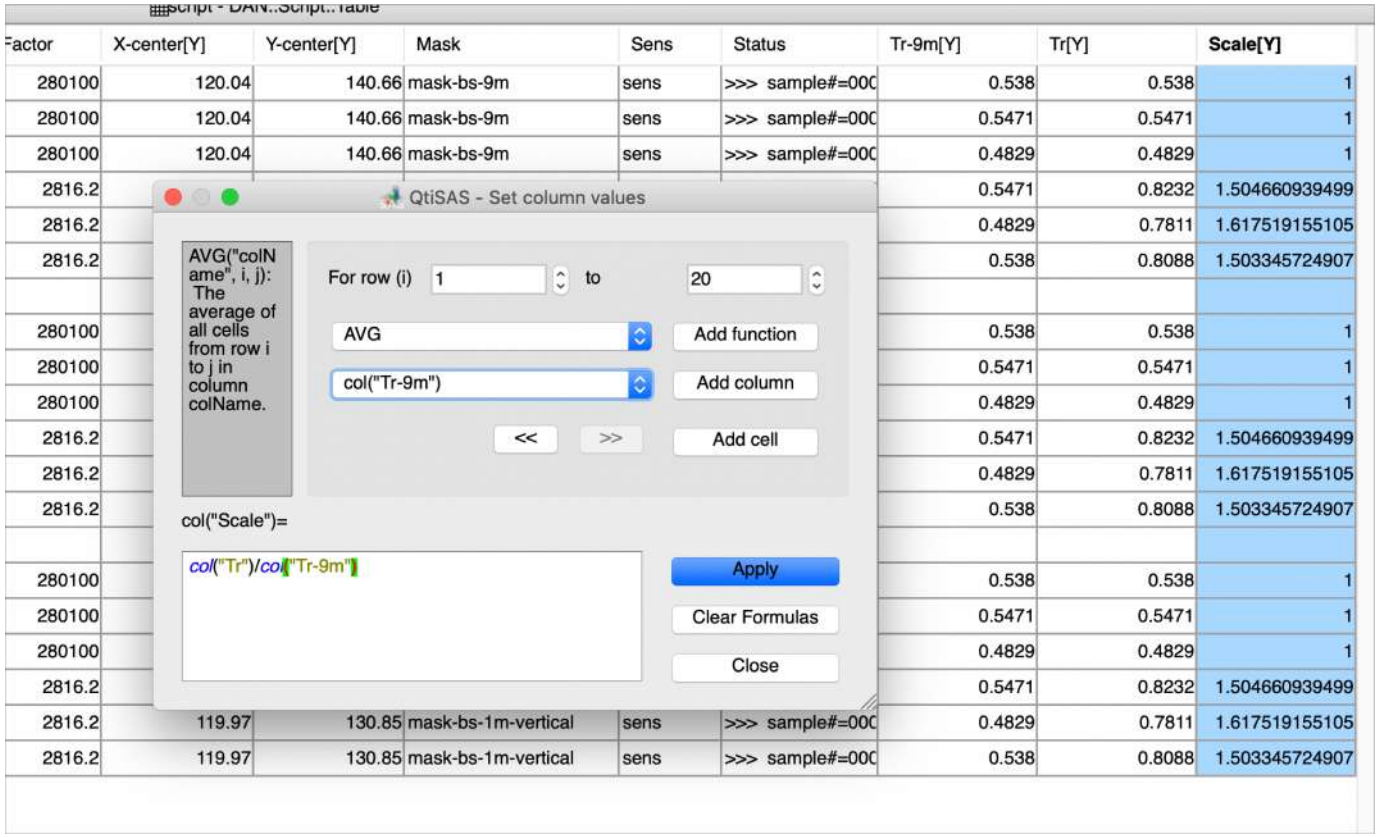


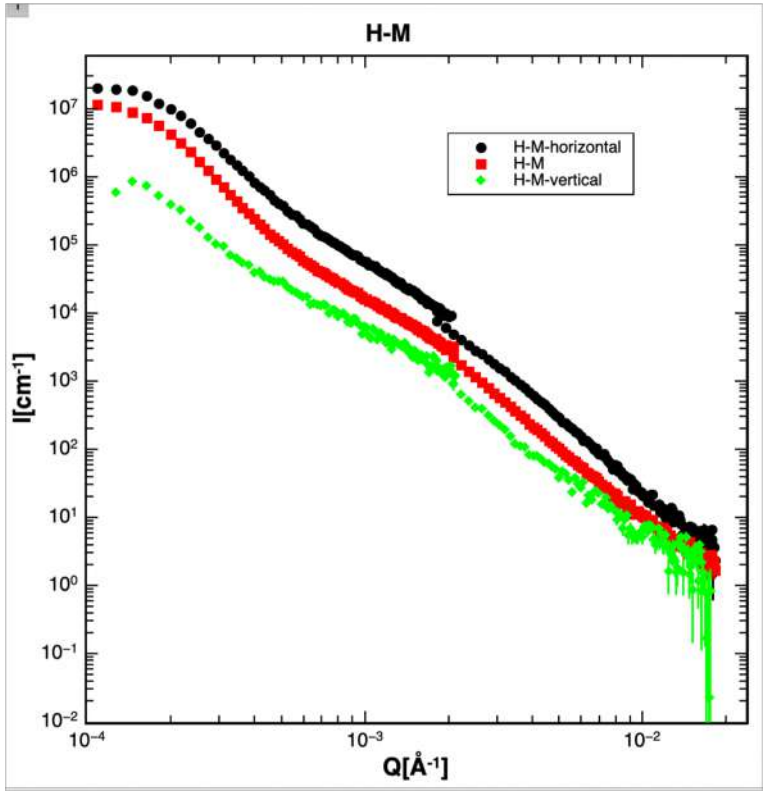


	Run-info	#-Run[X]	#-Condition	C	D	Lambda	Beam Size	#-BC	#-EC [EB]	Thickness	**Transmission-Sample**	Fac
1	H-M	00082557	1	10	9.2	12.787	2x2l20x20	00000002	00082558	0.1	0.5380 [±0.0007]	
2	H-J	00082559	1	10	9.2	12.787	2x2l20x20	00000002	00082558	0.1	0.5471 [±0.0007]	
3	H-L	00082561	1	10	9.2	12.787	2x2l20x20	00000002	00082558	0.1	0.4829 [±0.0006]	
4	H-J	00082646	2	10	1.2	12.787	2x2l6.5x8	00000002	00082645	0.1	0.8232 [±0.0005]	
5	H-L	00082647	2	10	1.2	12.787	2x2l6.5x8	00000002	00082645	0.1	0.7811 [±0.0005]	
6	H-M	00082648	2	10	1.2	12.787	2x2l6.5x8	00000002	00082645	0.1	0.8088 [±0.0005]	

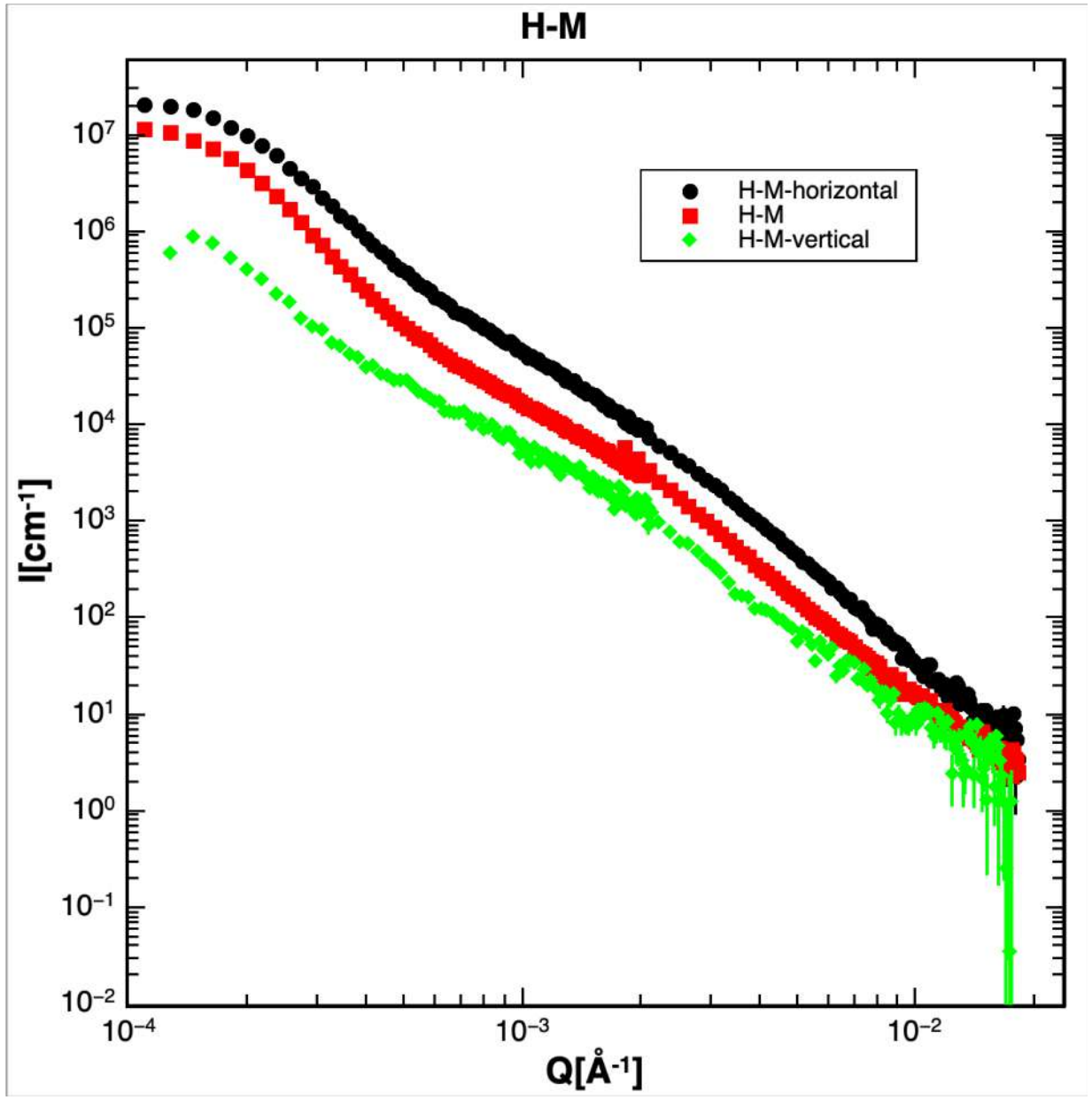
! We should scale 1.2m data to

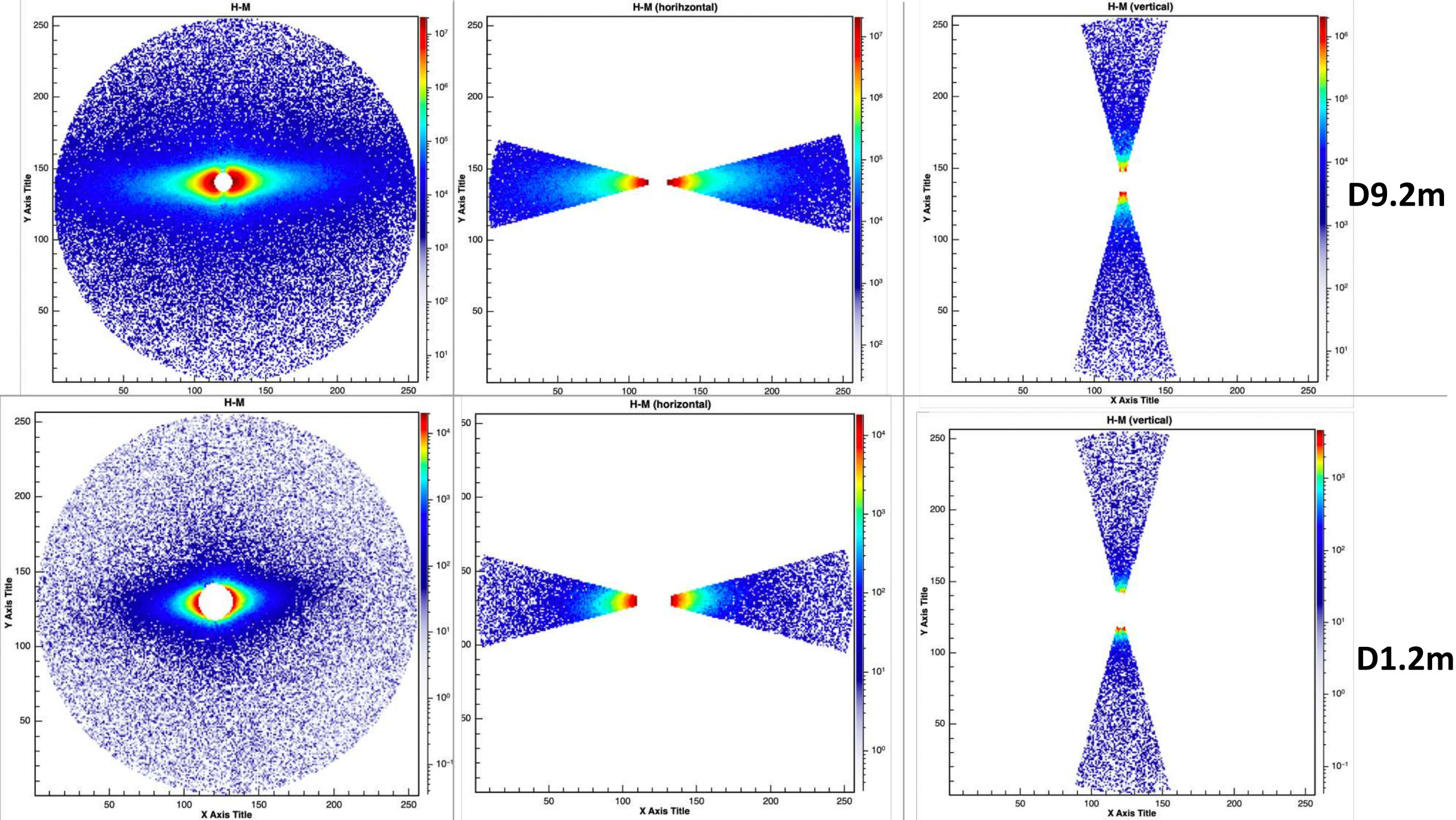
Factor = Tr(1.2m)/Tr(9.2m) !

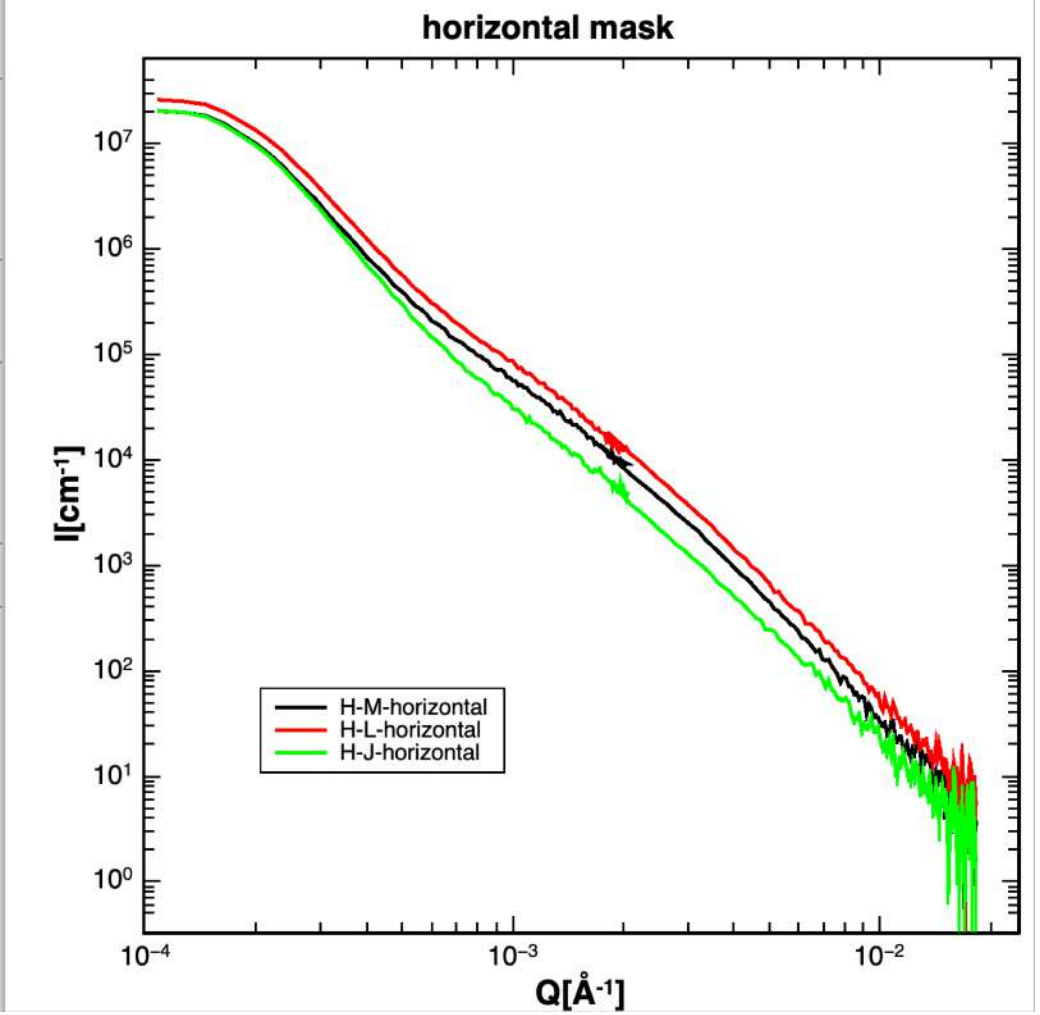

QtiSAS - Set column values
AVG("colName", i, j): The average of all cells from row i to j in column colName.
For row (i) 1 to 20
AVG
Add function
col("Tr-9m")
Add column
<<
>>
Add cell
col("Scale")=
col("Tr")/col("Tr-9m")
Apply
Clear Formulas
Close

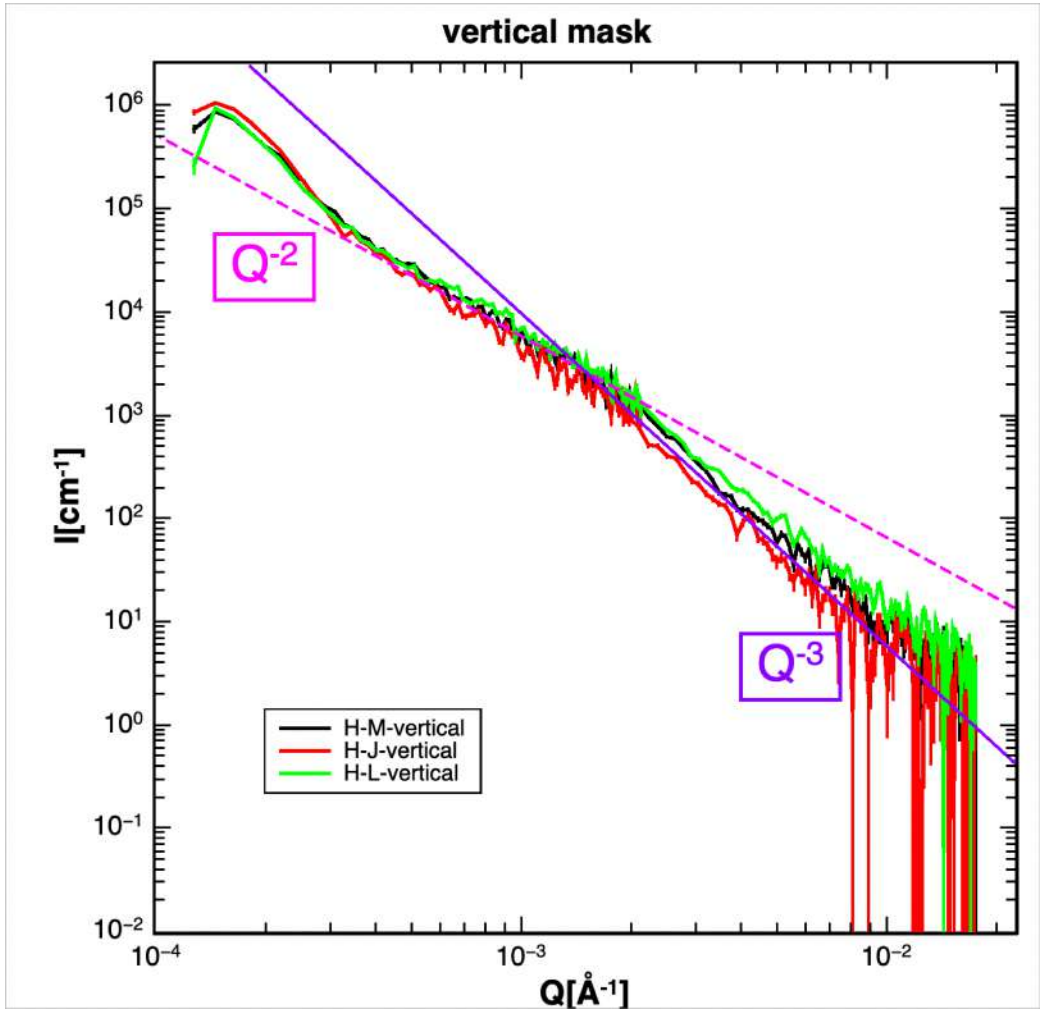


	Scale[Y]
0.538	1
0.5471	1
0.4829	1
0.8232	1.504660939499
0.7811	1.617519155105
0.8088	1.503345724907
0.538	1
0.5471	1
0.4829	1
0.8232	1.504660939499
0.7811	1.617519155105
0.8088	1.503345724907
0.538	1
0.5471	1
0.4829	1
0.8232	1.504660939499
0.7811	1.617519155105
0.8088	1.503345724907




H-M
H-M (horihzontal)
H-M (vertical)
Y Axis Title
X Axis Title
D9.2m
H-M
H-M (horizontal)
H-M (vertical)
Y Axis Title
X Axis Title
D1.2m


horizontal mask
I[cm-1]
Q[Å-1]
H-M-horizontal
H-L-horizontal
H-J-horizontal


vertical mask
I[cm-1]
Q[Å-1]
Q-2
Q-3
H-M-vertical
H-J-vertical
H-L-vertical