

Glycoinformatics Consortium  
(GLIC) seminar series

- Glycan Arrays -



# **CarbArrayART** for glycan microarray data storage, presentation and reporting

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# Glycosciences Laboratory: glycan probe library

## Mammalian-type sequences

### N-Glycans

- high mannose
- paucimannose
- complex
- hybrid

### O-Glycans

- mucin type
- O-Fucosyl
- O-Mannosyl

### Glycolipids

- neutral
- sialylated (e.g. gangliosides)
- sulfated

### Glycosaminoglycan oligosaccharides

- hyaluronic acid
- chondroitin sulfates A & C
- dermatan sulfate
- heparin & heparan sulfate

### Other oligosaccharides

- A, B & H blood group-related
- Lewis antigens a, b, x, y
- other neutral
- sialylated and/or sulfated
- other acidic

Exogenous sequences from fungal, bacterial and plant polysaccharides

### Oligosaccharides derived from fungal, bacterial and plant polysaccharides

- glucan
- chitin and chitosan
- polysialic acids
- mannan, xylan and arabinan

**Over 900** Lipid-linked glycan probes derived from natural sources or chemically synthesized

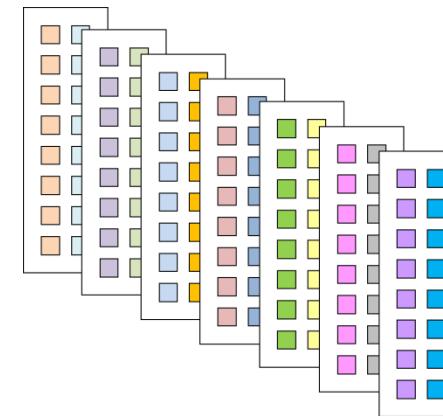
<https://glycosciences.med.ic.ac.uk/glycanLibraryIndex.html>

- Tang PW, Gooi HC, Hardy M, Lee YC, Feizi T. *Biochem Biophys Res Commun* 1985, 132: 474-480.
- Fukui S, Feizi T, Galustian C, Lawson AM, Chai W. *Nat Biotechnol* 2002, 20: 1011-1017.

- Feizi T, Chai W. *Nat Rev Mol Cell Biol* 2004, 5: 582-588.
- Liu Y, Palma AS, Feizi T. *Biol Chem* 2009, 390: 647-656.

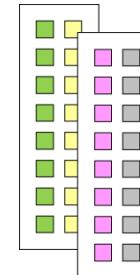
# Glycan microarray slides generated in the Glycosciences Laboratory

## Comprehensive screening oligosaccharide microarrays

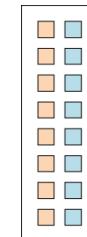


Each coloured box contains  
< 64 glycan probes arrayed

## Focused arrays for specific projects



**Glucan oligosaccharides**  
*glucan-binding receptors*  
*antibodies*  
*carbohydrate binding modules (CBMs)*



**Sialyl oligosaccharides**  
*influenza viruses and other sialic acid-binding proteins*



**Ganglioside-related polyomaviruses**  
**Glycosaminoglycan chains**  
*GAG-binding proteins and viruses*  
**N-glycans**  
*broadly neutralizing anti-HIV antibodies*

**Mucins**  
*Human microbiota*

From their earliest stages glycan microarrays signalled  
the need for a processing software



BEILSTEIN INSTITUT

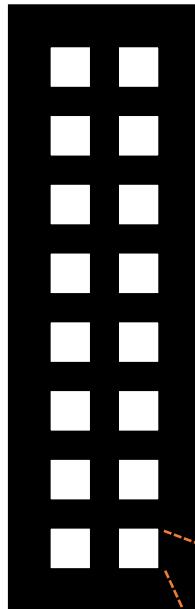
## **Software Tools for Storing, Processing and Displaying Carbohydrate Microarray Data**

Mark Stoll and Ten Feizi

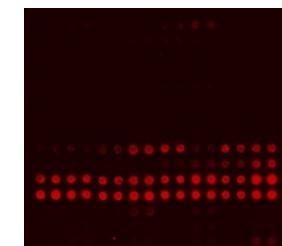
[Proceeding of the Beilstein Symposium on Glyco-Bioinformatics, 123-140 \(2009\)](#)

# Glycan microarray data

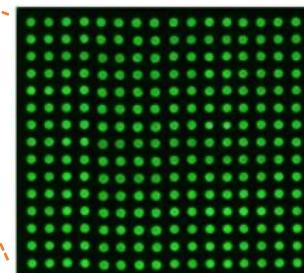
## 16-pad nitrocellulose-coated glass slide



## Overlaying with glycan binding samples (proteins, viruses, serum samples, etc)



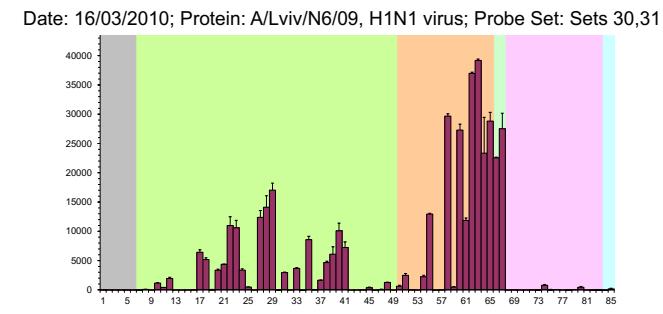
# Detection of binding Alexa Fluor 647-labelled streptavidin



# Cy3 marker for array quality control and spot location

64 glyco-probes per subarray  
2 levels of concentration per  
glyco-probe in duplicate

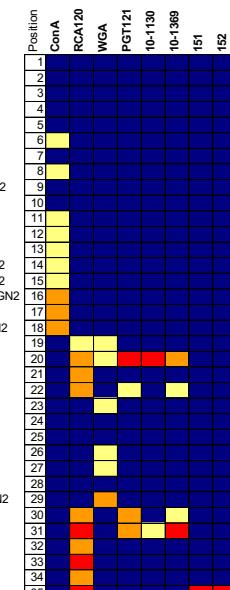
# Data processing, storage and presentation



## Chart

Position	Probe	Structure
1	Curd-12-AD	Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-AD*
2	Curd-8-AD	Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-AD*
3	GSC-270	$  \begin{array}{c}  \text{SU-6} \quad \text{SU-6} \\    \qquad \quad   \\  \text{NanA} \text{---} \text{Gal-}4\text{GlcNAc-}3\text{Gal-}3\text{Gal-}4\text{GlcNAc-}Oxer36 \\    \\  \text{Fuc-}3  \end{array}  $
4	Curd-11-AD	Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-3Glc-β-AD*
5	NA2	$  \begin{array}{c}  \text{Gal-}3\text{GlcNAc-}2\text{Man-}6 \\    \\  \text{Man-}6\text{---}4\text{GlcNAc-}8\text{GlcNAc} \\    \\  \text{Gal-}3\text{GlcNAc-}2\text{Man-}3  \end{array}  $
6	NGA2	$  \begin{array}{c}  \text{GlcNAc-}2\text{Man-}6 \\    \\  \text{Man-}6\text{---}4\text{GlcNAc-}8\text{GlcNAc} \\    \\  \text{GlcNAc-}2\text{Man-}3  \end{array}  $
7	NGA2B	$  \begin{array}{c}  \text{GlcNAc-}2\text{Man-}6 \\    \\  \text{GlcNAc-}2\text{Man-}6\text{---}4\text{GlcNAc-}8\text{GlcNAc-}4\text{GlcNAc} \\    \\  \text{GlcNAc-}2\text{Man-}3  \end{array}  $

# Tabulation



## Heat map

# Software tools are based on Microsoft Office and Visual Basic

Limited extensibility

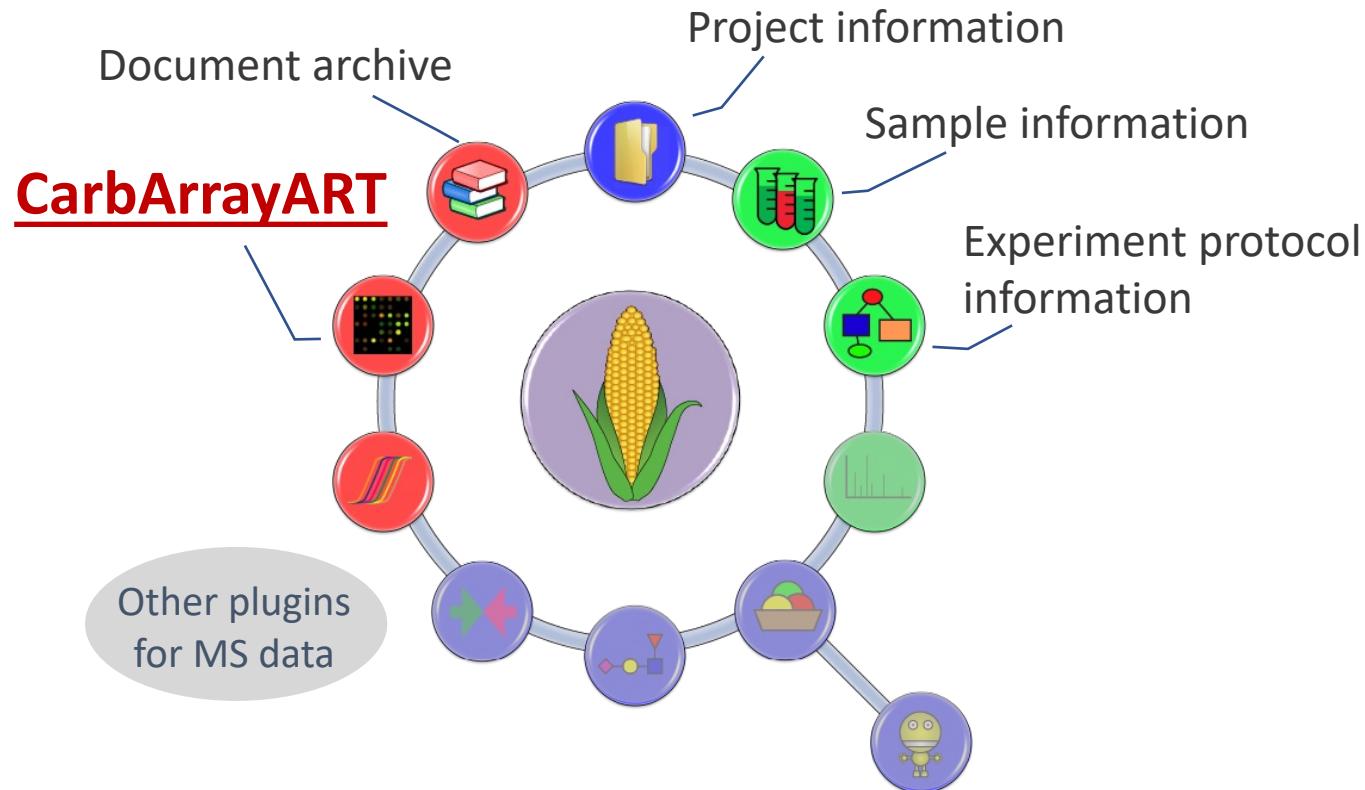
Hence, the need to develop a **robust** and **distributable** glycan array software,

Carbohydrate micro-Array Analysis and Reporting Tool



# Plugin of GRITS Toolbox

Collaboration with René Ranzinger and Sena Arpinar at Complex Carbohydrate Research Center  
Stand-alone Java application / Available in multiple platforms / Plugins and modules



# CarbArrayART webpage

<http://carbarrayart.org>



Welcome to CarbArrayART

Carbohydrate microArray Analysis and Reporting Tool (CarbArrayART) is a software tool for glycan microarray experimental design, data storage, processing, presentation and reporting. CarbArrayART capitalizes on [GRITS Toolbox](#) which was originally developed for processing, interpreting and archiving glycomic mass spectrometry data. CarbArrayART utilizes the functionalities provided by [GRITS Toolbox](#) for storing glycan microarray realated information including glycan structures and metadata such as project information, sample description and experimental details.

The main features of CarbArrayART are:

1. Storage of carbohydrate microarray related data including glycan probe lists, array geometry, information on glycan-binding samples and experimental protocols and scan data.
2. Presentation of data as tables, charts and matrices (heatmaps) with filtering and sorting of glycans as needed.
3. Reporting of microarray data in Word, PDF and Excel formats, together with metadata that are compliant with [MIRAGE \(Minimum Information Required for a Glycomics Experiment\)](#).

You will be referred to [Manual and Support](#) page for the installation and step-by-step operation.

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About 

Highlights  Firefox

Manual and Support 

Download 

# Minimum information to have in hand

## Glycan probe

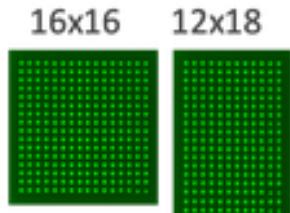
Glycan library (the list of glyco-probes) included in the array

Glycan sequence information would be required in order to use the sequence-based filtering and sorting functions in Tabulation View. [GlycoCT{condensed}](#), [2D TEXT](#), [CFG-IUPAC](#), [Glyco Workbench Sequence \(GWS\)](#) and [WURCS formats](#) can be used for entering glycan sequences.

## Subarray layout

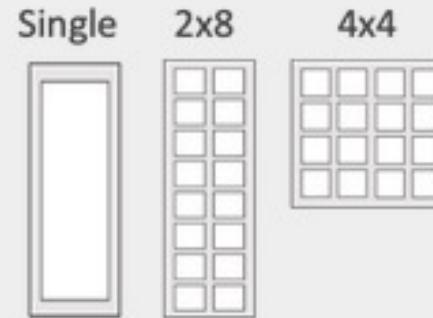
Layout of printed spots associated with glyco-probe IDs and concentrations (or doses) and the number of replicates in each Subarray (block or pad).

Examples illustrated are of 16x16 spots/subarray of 64 glyco-probes at 2 doses (2 and 5 fmol) printed in duplicate or 12x18 spots/subarray of 36 probes printed at a single dose or concentration and 6 replicates.



## Slide layout

Examples illustrated are of the layout of array(s) on a microarray slide: single array/slide or 2x8 subarrays/slide or 4x4 subarray/slide)



## Project

User-defined name for the project

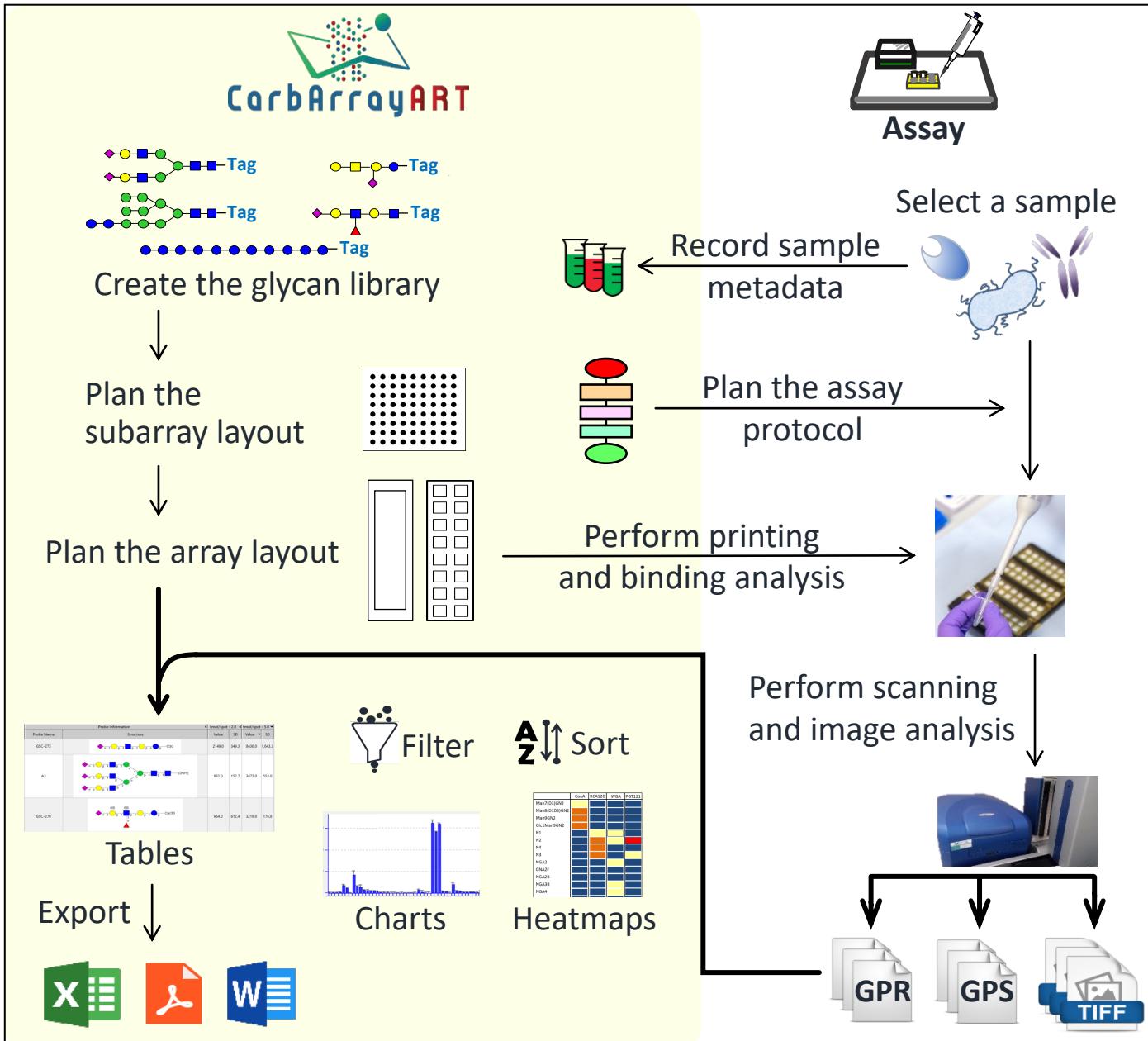
## Analyte

Name of the carbohydrate-binding sample

## Glycan array data

Quantified array data in the form of a gpr file (GenePix scanner) or an Excel file (Proscan)

# The data management workflow of a microarray analysis



The data management workflow in CarbArrayART (left, yellow background)

The experiment workflow (right)

Highlights are:

- MIRAGE\* compliant with respect to data input and output
- Data storage and management
- Data presentation
- Data sharing and publication



\* Liu, Yan, et al. Glycobiology 27.4 (2017): 280-284.

# Tools in CarbArrayART

1. Glycan probe entry tool

2. Subarray layout entry tool

3. Slide layout entry tool

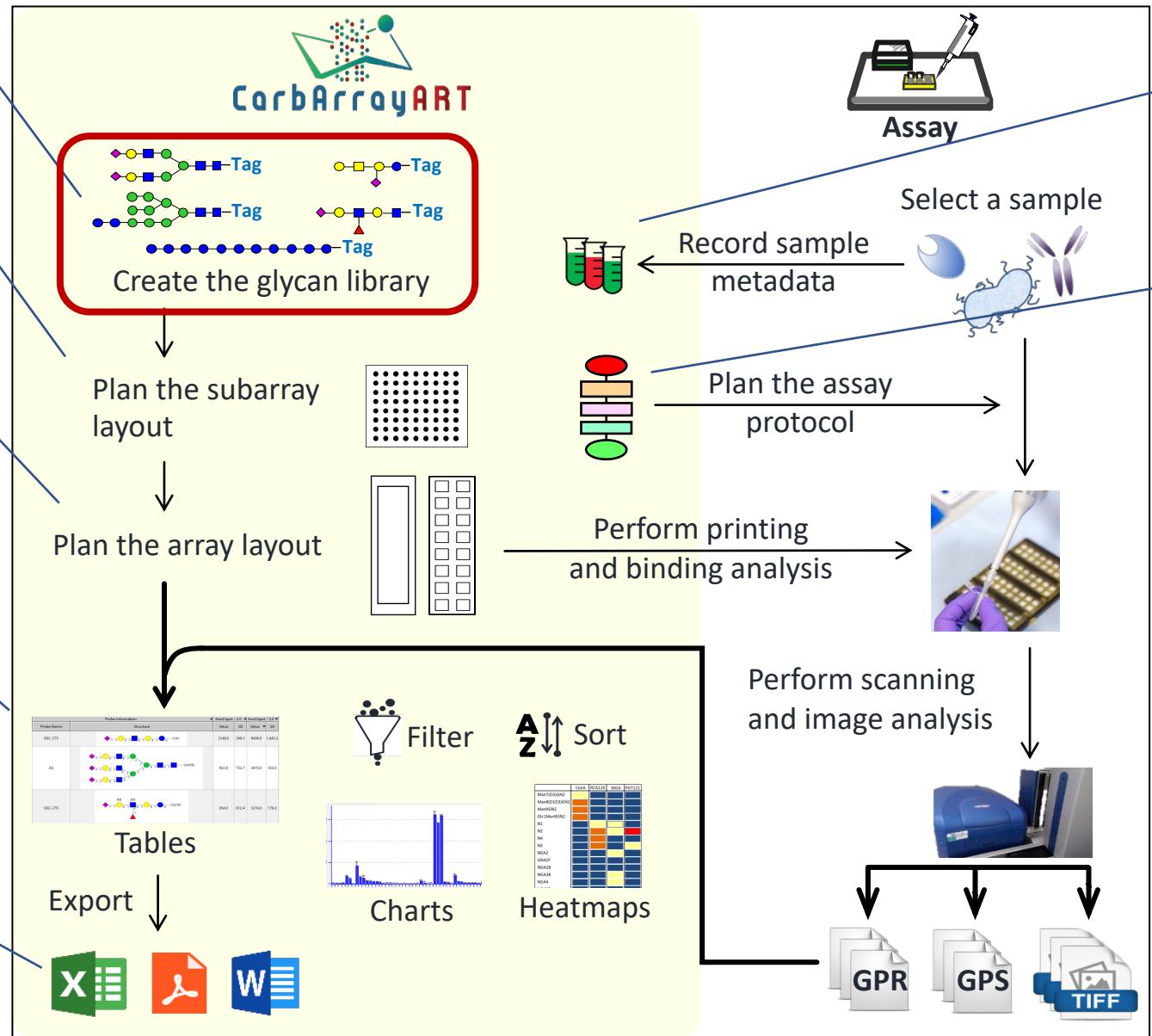
6. Data presentation

7. Data sharing

4. Sample metadata entry tool

5. Experiment design tool

User's manual:  
<http://carbarrayart.org>



Left, yellow background:  
The data management  
workflow in CarbArrayART

Right: The experiment  
workflow

# 1. Glycan Glyco-probe entry tool

## Glycan probe section

- Name (mandatory)
- Comments
- Backbone type

Texts highlighted in blue:  
MIRAGE compliant

Glyco-probe

Select from library  Search

Glyco-probe ID

Glyco-probe Name\*

Comment on purity

Other comment

Backbone type

Backbone type

Group A: Gal, Glc, Lac, LacNAc  
Group B: LNnT, LNT  
Group C: Polylactosamine (linear,branched)  
Group D: N-glycan  
Group E: Ganglioside related  
Group F: O-glycan  
Group G: Polysialyl  
Group H: GAG  
Group I: Other homo-oligomers  
Group J: Miscellaneous  
Blood group and Lewis type  
Sialylated and sulphated milk-related and Lewis type



## Tag section

- Name
- Sequence (text)
- Nature (natural, synthesized or unknown)

Tag Name

Structure if known

Tag Nature

Comment

# 1. Glycan Glyco-probe entry tool

## Glycan section

- Name
- Sequence

## Sequence formats:

- GlyTouCan ID
- GlycoCT{condensed}
- 2D TEXT
- CFG-IUPAC
- Glyco Workbench Sequence (GWS)
- WURCS

**Glycan moiety**

- Please fill below if glycan moiety information are required -

Enter another glycan moiety information

Select from library

Or enter new glycan

Glycan name

Sequence

Get sequence from GlyTouCan ID

Or upload file



Create glycan probe library

# Tools in CarbArrayART

1. Glycan probe entry tool

2. Subarray layout entry tool

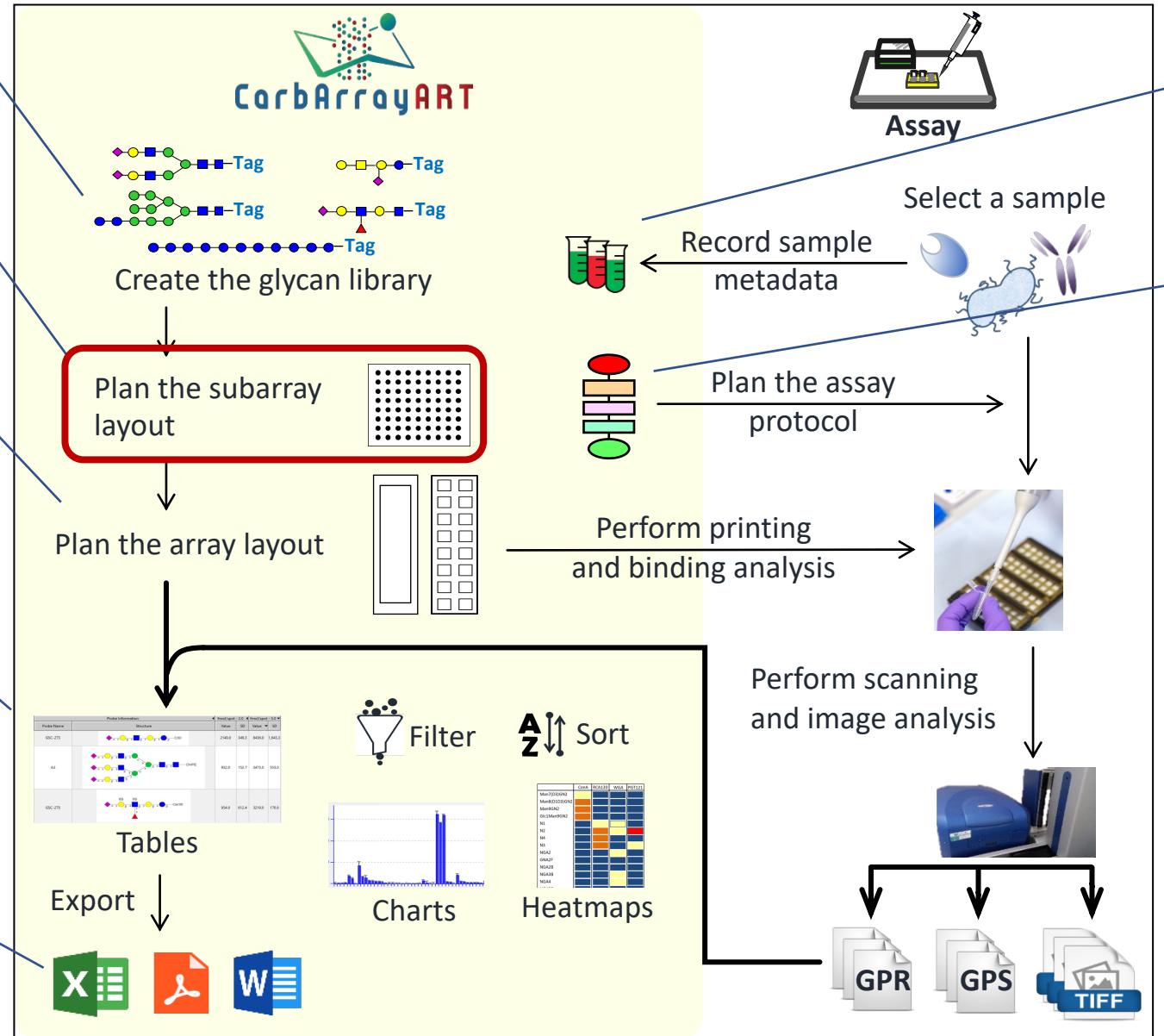
3. Slide layout entry tool

6. Data presentation

7. Data sharing

4. Sample metadata entry tool

5. Experiment design tool



Left, yellow background:  
The data management  
workflow in CarbArrayART

Right: The experiment  
workflow

## 2. Block layout entry tool: example layout

### Ganglioside dose response set

The set has 28 glycan probes with:

- 4 levels (0.3, 0.8, 1.7 and 5 fmol)
- Duplicate spots

● 0.3 fmol/spot

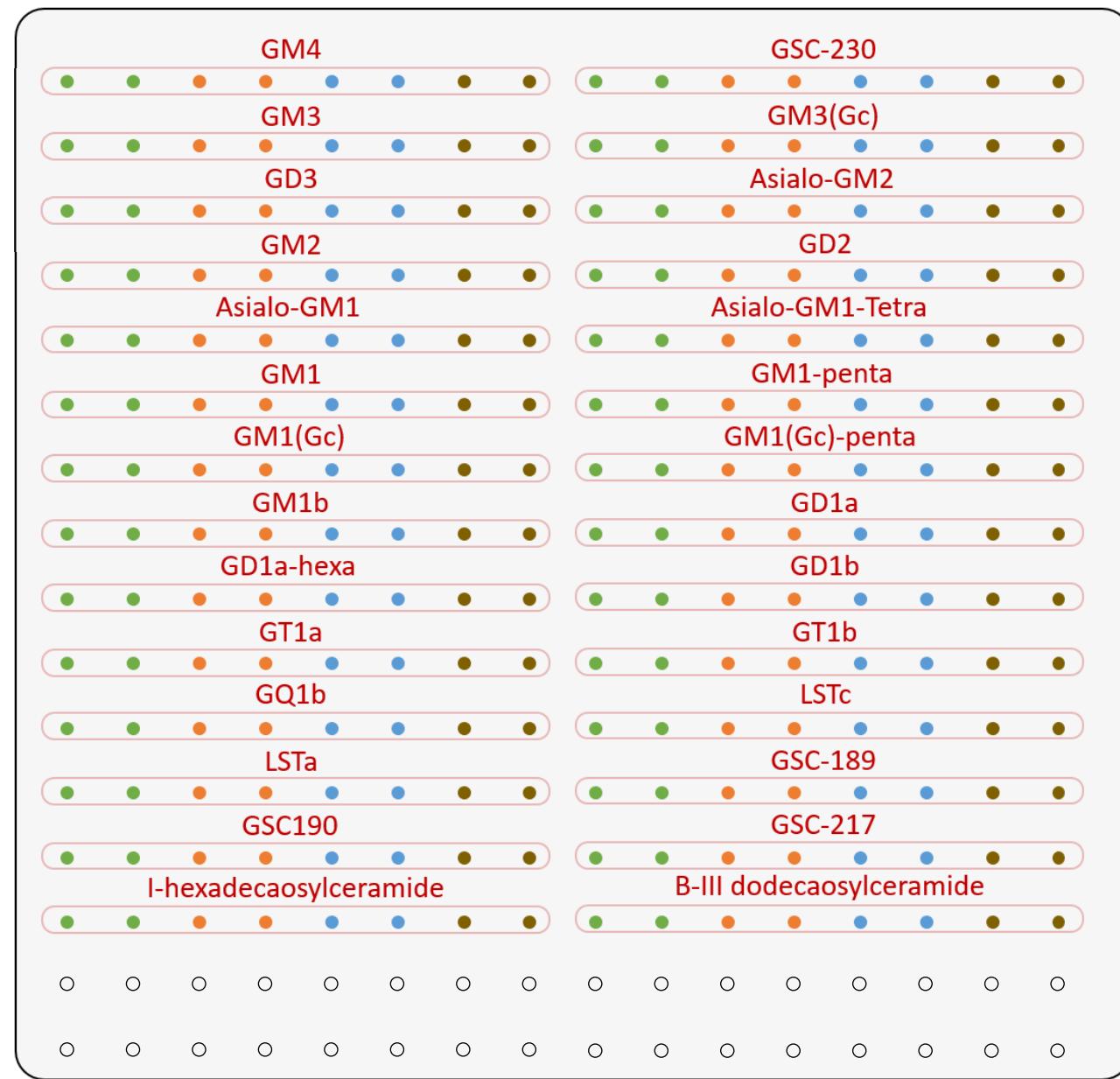
● 0.8 fmol/spot

● 1.7 fmol/spot

● 5 fmol/spot

○ Empty

- Number of Spot Columns = 16
- Number of Spot Row = 16



## 2. Block layout entry tool: entry page 1

### Ganglioside dose response set

The set has **28** glycan probes with:

- **4** levels (0.3, 0.8, 1.7 and 5 fmol)
- **Duplicate spots**

- 0.3 fmol/spot
- 0.8 fmol/spot
- 1.7 fmol/spot
- 5 fmol/spot
- Empty

- Number of Spot Columns = **16**
- Number of Spot Row = **16**

Subarray Layout Tool

Enter information about a glycan microarray subarray layout

Subarray Layout ID

Name\*

Comment

Number of replicates (option)

Number of levels (arrayed glyco-probe)\*

Number of glyco-probes\*

Subarray geometry (the number of spots)\*

Column

Row

< Back

## 2. Block layout entry tool: entry page 2

Arrayed glyco-probe levels

	Value	Unit
1	0.0	fmol/spot
2	0.0	fmol/spot
3	0.0	fmol/spot
4	0.0	fmol/spot

Glyco-probe list

Search by:  Name  ID  Search

Subarray/Block layout

ID	Glyco-probe
1	GM4-Cer
2	GSC-230-Cer36
3	GM3-Cer
4	GM3(Gc)-Cer
5	GD3-Cer
6	Asialo-GM2-Cer
7	GM2-Cer
8	GD2-Cer

Row	Col...n	Glyco-probe	Level	Ident...array
1	1		1	1
1	2		1	1
1	3		2	1
1	4		2	1
1	5		3	1
1	6		3	1
1	7		4	1
1	8		4	1

< Back Next > Finish Cancel

## 2. Block layout entry tool: entry page 2

To define the concentration or dose of glycan probes arrayed

Select the unit of the level(s)

- Units of levels:
- (a) fmol/spot
  - (b) ul/spot
  - (c) mM
  - (d) uM
  - (e) mg/ml
  - (f) pmol/ul

	Value	Unit
1	0.0	fmol/spot
2	0.0	fmol/spot
3	0.0	fmol/spot
4	0.0	fmol/spot

Glyco-probe list

Search by:   Name  ID

ID	Glyco-probe
1	GM4-Cer
2	GSC-230-Cer36
3	GM3-Cer
4	GM3(Gc)-Cer
5	GD3-Cer
6	Asialo-GM2-Cer
7	GM2-Cer
8	GD2-Cer

Subarray/Block layout

Row	Col...n	Glyco-probe
1	1	
1	2	
1	3	
1	4	
1	5	
1	6	
1	7	
1	8	

< Back  18

## 2. Block layout entry tool: entry page 2

Library of pre-saved glycan probes  
using Glycan Probe Entry Tool

	Value	Unit
1	0.0	fmol/spot
2	0.0	fmol/spot
3	0.0	fmol/spot
4	0.0	fmol/spot

Glyco-probe list

Search by:  Name  ID

ID	Glyco-probe
1	GM4-Cer
2	GSC-230-Cer36
3	GM3-Cer
4	GM3(Gc)-Cer
5	GD3-Cer
6	Asialo-GM2-Cer
7	GM2-Cer
8	GD2-Cer

Subarray/Block layout

Row	Col...n	Glyco-probe
1	1	
1	2	
1	3	
1	4	
1	5	
1	6	
1	7	
1	8	

< Back  Next >

## 2. Block layout entry tool: entry page 2

	Value	Unit
1	0.0	fmol/spot
2	0.0	fmol/spot
3	0.0	fmol/spot
4	0.0	fmol/spot

Glyco-probe list

Search by:  Name  ID

ID	Glyco-probe
1	GM4-Cer
2	GSC-230-Cer36
3	GM3-Cer
4	GM3(Gc)-Cer
5	GD3-Cer
6	Asialo-GM2-Cer
7	GM2-Cer
8	GD2-Cer

Subarray/Block layout

Row	Col...n	Glyco-probe	Level	Ident...array
1	1		1	1
1	2		1	1
1	3		2	1
1	4		2	1
1	5		3	1
1	6		3	1
1	7		4	1
1	8		4	1

## 2. Block layout entry tool: entry page 2

	Value	Unit
1	0.0	fmol/spot
2	0.0	fmol/spot
3	0.0	fmol/spot
4	0.0	fmol/spot

**Block layout table:**

- To define the printing location of each glyco-probe
- The number of rows and columns of spots (counting from the top-left corner)
- Glyco-probe arrayed
- Levels of glyco-probe arrayed
- Identification number of glyco-probes in this subarray:  
The number indicates a group of glyco-probes.

Subarray/Block layout

Row	Col...n	Glyco-probe	Level	Ident...array
1	1		1	1
1	2		1	1
1	3		2	1
1	4		2	1
1	5		3	1
1	6		3	1
1	7		4	1
1	8		4	1

< Back Next > Finish Cancel

## 2. Block layout entry tool: entry page 2

Subarray Layout Tool

Fill the tables for subarray layout.

Arrayed glyco-probe levels

	Value	Unit
1	0.3	fmol/spot
2	0.8	fmol/spot
3	1.7	fmol/spot
4	5.0	fmol/spot

Glyco-probe list

Search by:   Name  ID

Block layout

Drag and drop

Row	Column	Glyco-probe	Level	Identification number in this subarray
1	1		1	1
1	2		1	1
1	3		2	1
1	4		2	1
1	5		3	1
1	6		3	1
1	7		4	1
1	8		4	1
1	9		1	2
1	10		1	2
1	11		2	2
1	12		2	2
1	13		3	2

Processed data (average intensity values) are calculated if the glycan probes in one block are ...

- (1) The same probe ID  
and
- (2) The same group number (identification number)  
and
- (3) the same level

# Tools in CarbArrayART

1. Glycan probe entry tool

2. Subarray layout entry tool

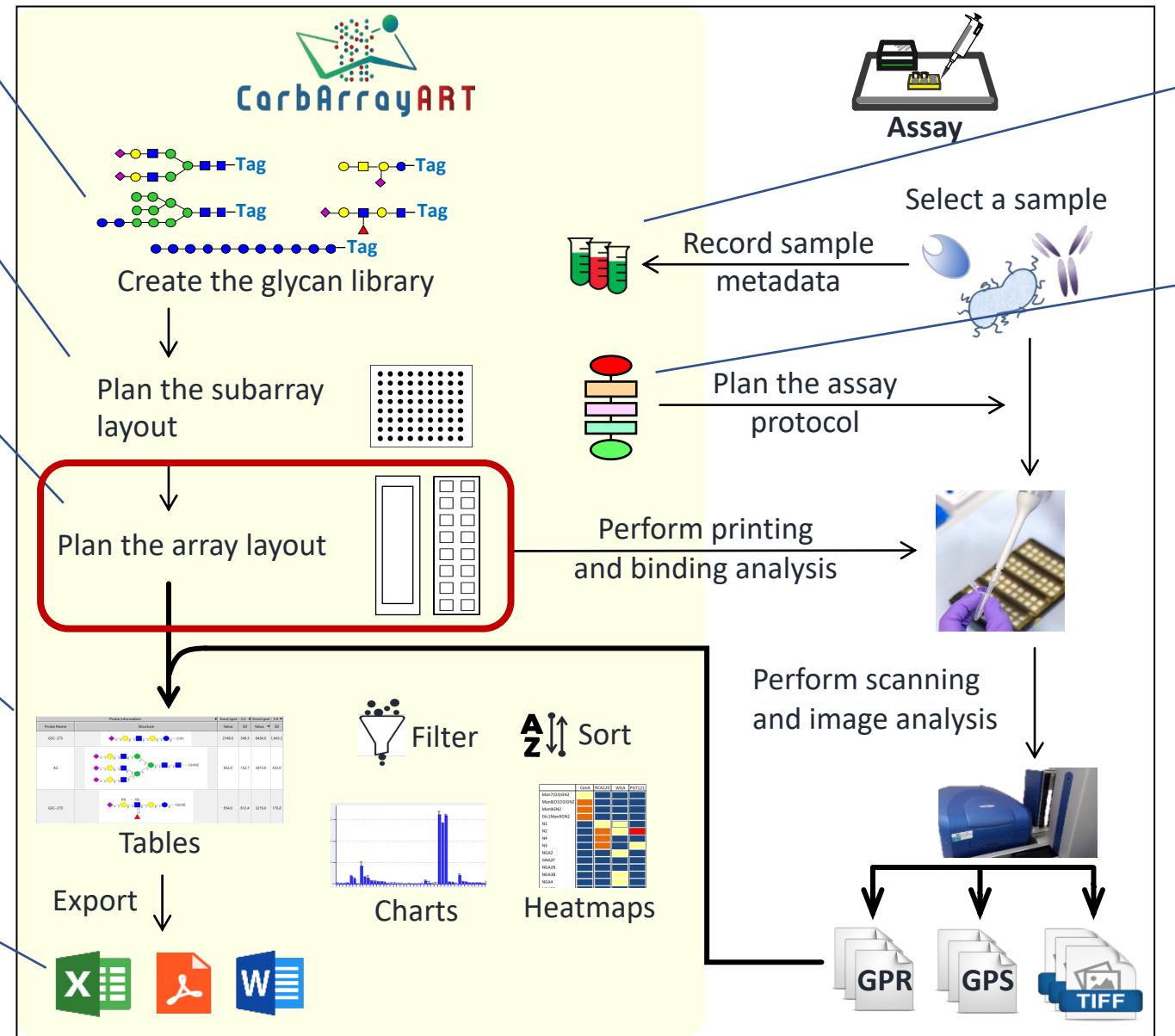
3. Slide layout entry tool

6. Data presentation

7. Data sharing

4. Sample metadata entry tool

5. Experiment design tool



Left, yellow background:  
The data management  
workflow in CarbArrayART

Right: The experiment  
workflow

### 3. Slide layout entry tool: entry page 1

Array Layout Tool

Enter information about the microarray layout

Name\* |Ganglioside dose response set

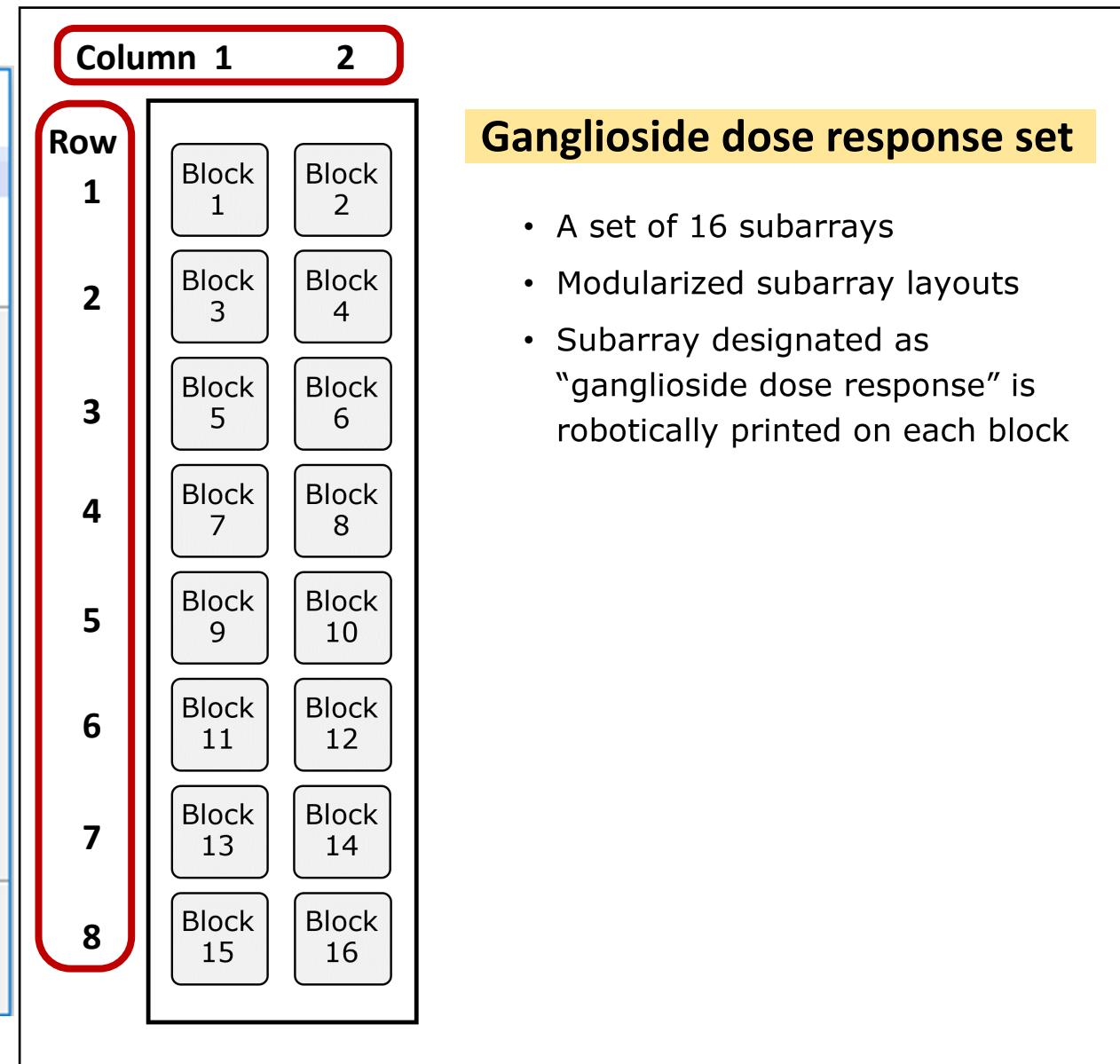
Comments

Array geometry (the number of subarrays/blocks)

column\* 2

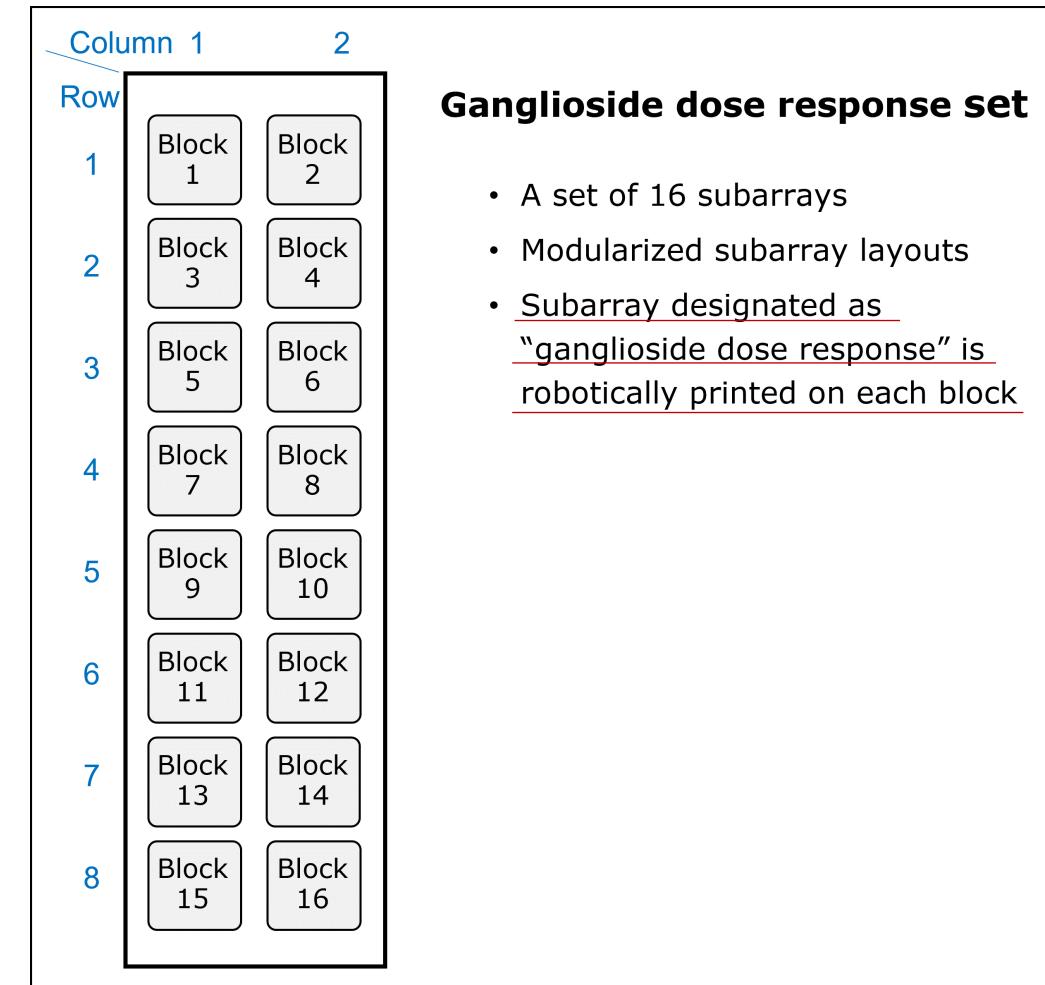
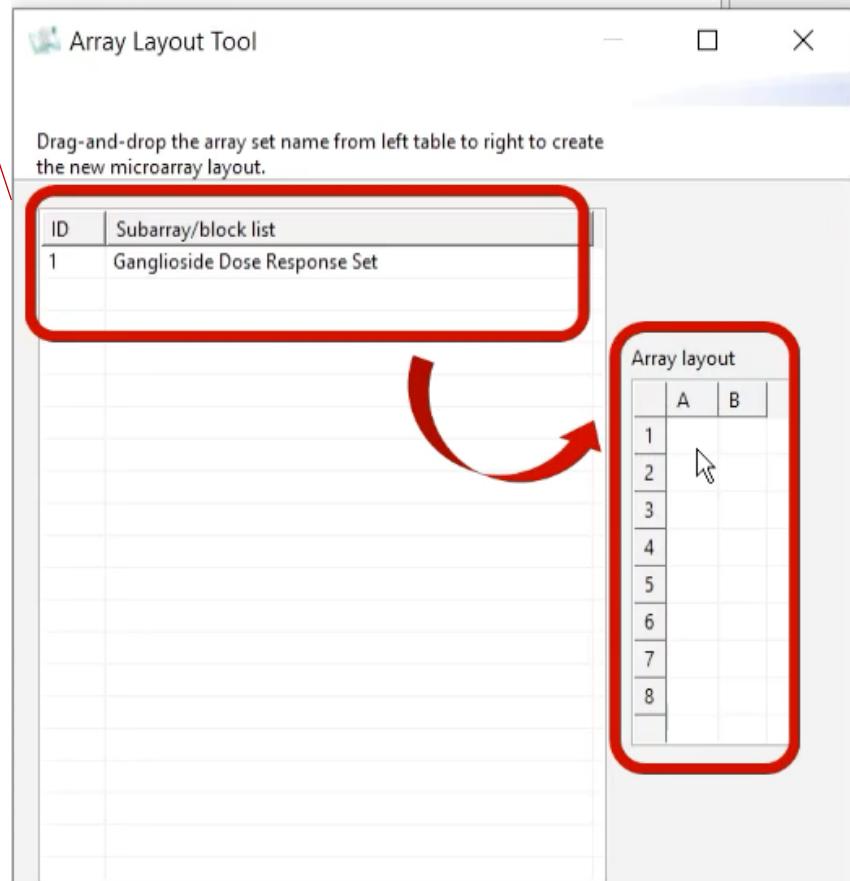
row\* 8

< Back Next > Finish Cancel



### 3. Slide layout entry tool: entry page 2

#### Library of pre-saved subarray layouts



# Data Entry - Slide layout entry from an Excel file

## GenePix Array List (GAL) like file

An Excel file contains:

- Block numbers in a slide
- Spot numbers (row and columns) in a block
- Glycan probe information arrayed in the spot

ArrayGeometry\_GALextended.xlsx - Excel

	Block	Spot column number in Block	Spot row number in Block	Glycan probe ID if the glycan is recorded in CarbArrayART (Numbers)	Printed glycan probe name (*if the spot is not empty)	Glycan probe printing concentration or dose value (Numbers) (*if the spot is not empty)	Glycan probe concentration or dose unit (Selection) (*if the spot is not empty)	Comments on purity of printed glycan probe	Other comments on printed glycan probe
1									
2	1	1	1	1	GM2	0.3	fmol/spot		
3	1	2	1	1	GM2	0.3	fmol/spot		
4	1	3	1	1	GM2	0.8	fmol/spot		
5	1	4	1	1	GM2	0.8	fmol/spot		
6	1	5	1	1	GM2	1.7	fmol/spot		
7	1	6	1	1	GM2	1.7	fmol/spot		
8	1	7	1	1	GM2	5	fmol/spot		

# Tools in CarbArrayART

1. Glycan probe entry tool

2. Subarray layout entry tool

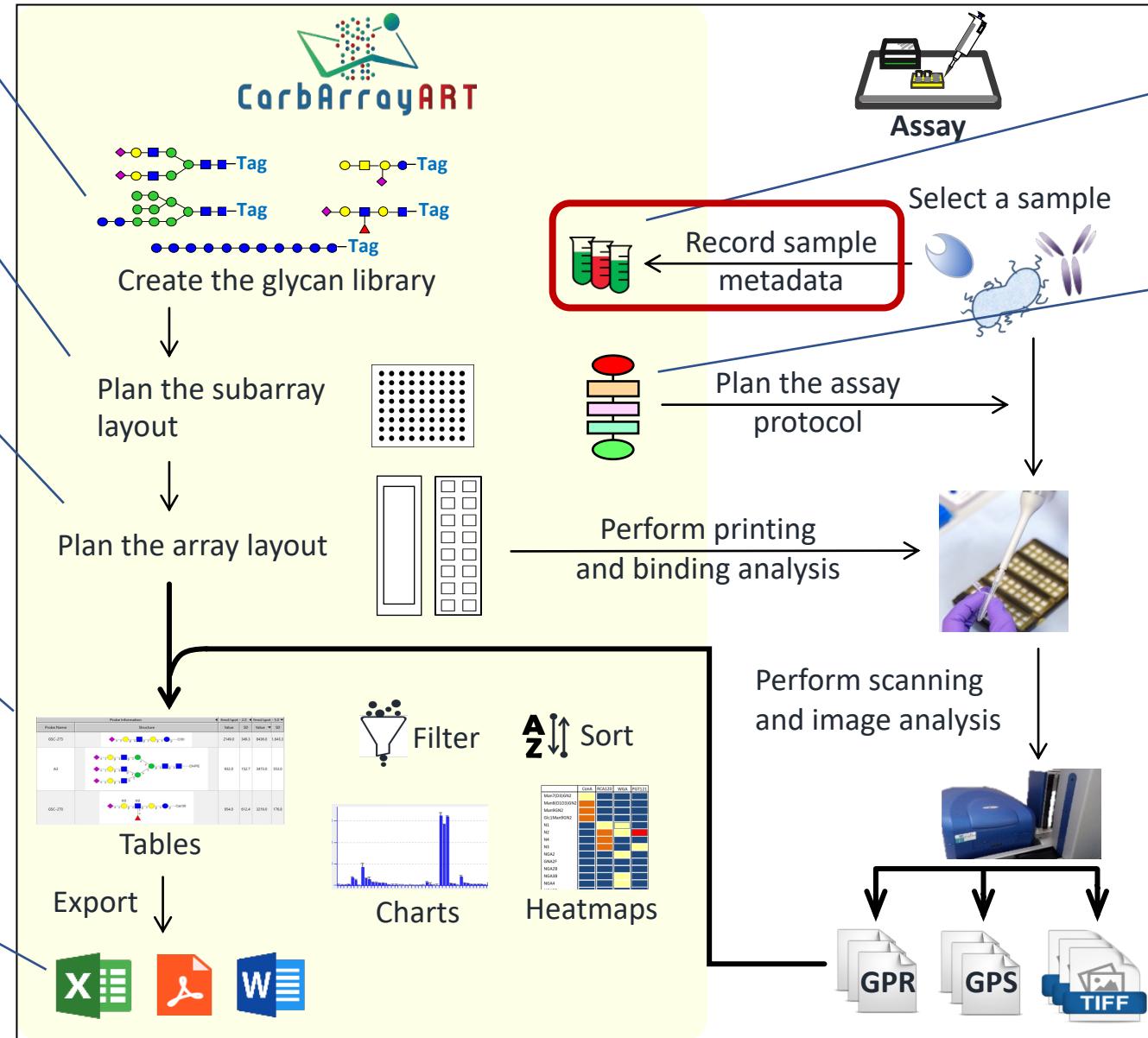
3. Slide layout entry tool

6. Data presentation

7. Data sharing

4. Sample metadata entry tool

5. Experiment design tool



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The data management  
workflow in CarbArrayART

Right: The experiment  
workflow

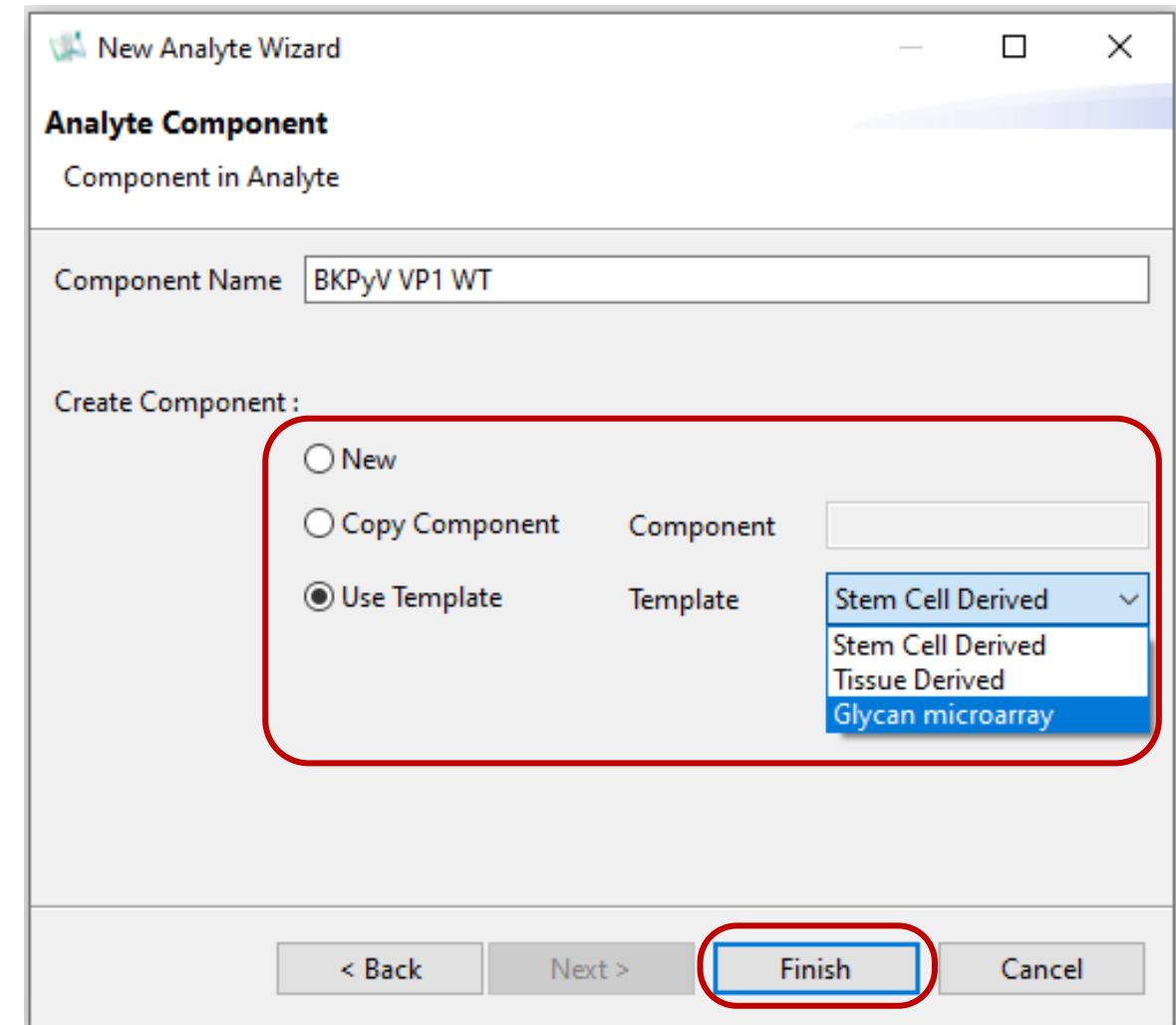
## 4. Glycan binding sample metadata entry

**New:** Create a new sample metadata from scratch

**Copy component:** Copy from the saved sample metadata (parameter values are also copied)

**Use Template:** Create a new sample metadata using the template (parameter values are empty)

Users can create a new entry using the pre-stored template from pull-down menu.



## 4. Glycan binding sample metadata entry

Component Info				Tracking			
Descriptor Group / Descriptor	Value	Unit	Guidelines	Descriptor Group / Descriptor	Value	Unit	Guidelines
Sample type			MIRAGE Glycan Microarray	Source			
Species				► Commercial			
Subtype				► Collaborator			
Strain				Delivery Date			
► Database Entry			MIRAGE Glycan Microarray	Dispatch date			
Molecular weight							
► Antibody							
► Tag			MIRAGE Glycan Microarray				
► Label			MIRAGE Glycan Microarray				
Hazardous							
► Infectious							
► Toxic							
► Treated non-hazardous							
► Preservative							
► Storage condition							
Reference for the sample preparation							
► Recombinant							
► Natural							
► Synthetic							
Amount				Purity Q.C.			
Descriptor Group / Descriptor	Value	Unit	Guidelines	Descriptor Group / Descriptor	Value	Unit	Guidelines
Sample form				► Purity, Quantitative			MIRAGE Glycan Microarray
► Solid				► Qualitative			MIRAGE Glycan Microarray
► Solution							
► Aliquot							

\* Liu, Yan, et al. "The minimum information required for a glycomics experiment (MIRAGE) project: improving the standards for reporting glycan microarray-based data." Glycobiology 27.4 (2017): 280-284.

## 4. Glycan binding sample metadata entry

The screenshot shows the CarbArrayART software interface with four main sections:

- Component Info:** A table with columns for Descriptor Group / Descriptor, Value, Unit, and Guidelines. It includes a sidebar with expandable categories like Database Entry, Antibody, Tag, Label, Hazardous, Infectious, Toxic, Treated non-hazardous, Preservative, Storage condition, Recombinant, Natural, and Synthetic.
- Tracking:** A table with columns for Descriptor Group / Descriptor, Value, Unit, and Guidelines. It includes a sidebar with Source, Commercial, Collaborator, and Delivery Date.
- Amount:** A table with columns for Descriptor Group / Descriptor, Value, Unit, and Guidelines. It includes a sidebar with Sample form, Solid, Solution, and Aliquot.
- Purity/Quality control:** A table with columns for Descriptor Group / Descriptor, Value, Unit, and Guidelines. It includes a sidebar with Purity, Quantitative, and Qualitative.

A red box highlights the 'Component Info' section, and a bulleted list describes its features:

- A default template exists in CarbArrayART designed based on MIRAGE Glycan Microarray Guidelines
- Four sections: (1) Component information, (2) Tracking, (3) Amount and (4) Purity and Quality control information
- The parameters compliant with MIRAGE guidelines are labelled in the 'Guidelines' column
- The item highlighted in red is a unique parameter which can be entered once

\* Liu, Yan, et al. "The minimum information required for a glycomics experiment (MIRAGE) project: improving the standards for reporting glycan microarray-based data." Glycobiology 27.4 (2017): 280-284.

## 4. Glycan binding sample metadata entry: example entry

Descriptor Group / Descriptor	Value	Unit	Guideli...
Sample type	Recombinant		MIRAGE ...
Species	Homo sapiens		
▼ Database Entry			MIRAGE...
Database name	Protein Data Bank		MIRAGE ...
Database URI	<a href="https://www.rcsb.org">https://www.rcsb.org</a>		
ID	4MJ1		MIRAGE ...
ID URI	<a href="https://www.rcsb.org/structure/4...">https://www.rcsb.org/structure/4...</a>		
Molecular weight	151.94	kDa	
▼ Tag			MIRAGE...
Name	His-tag (polyhistidine or His6)		MIRAGE ...
Position	N-terminal		

# Tools in CarbArrayART

1. Glycan probe entry tool

2. Subarray layout entry tool

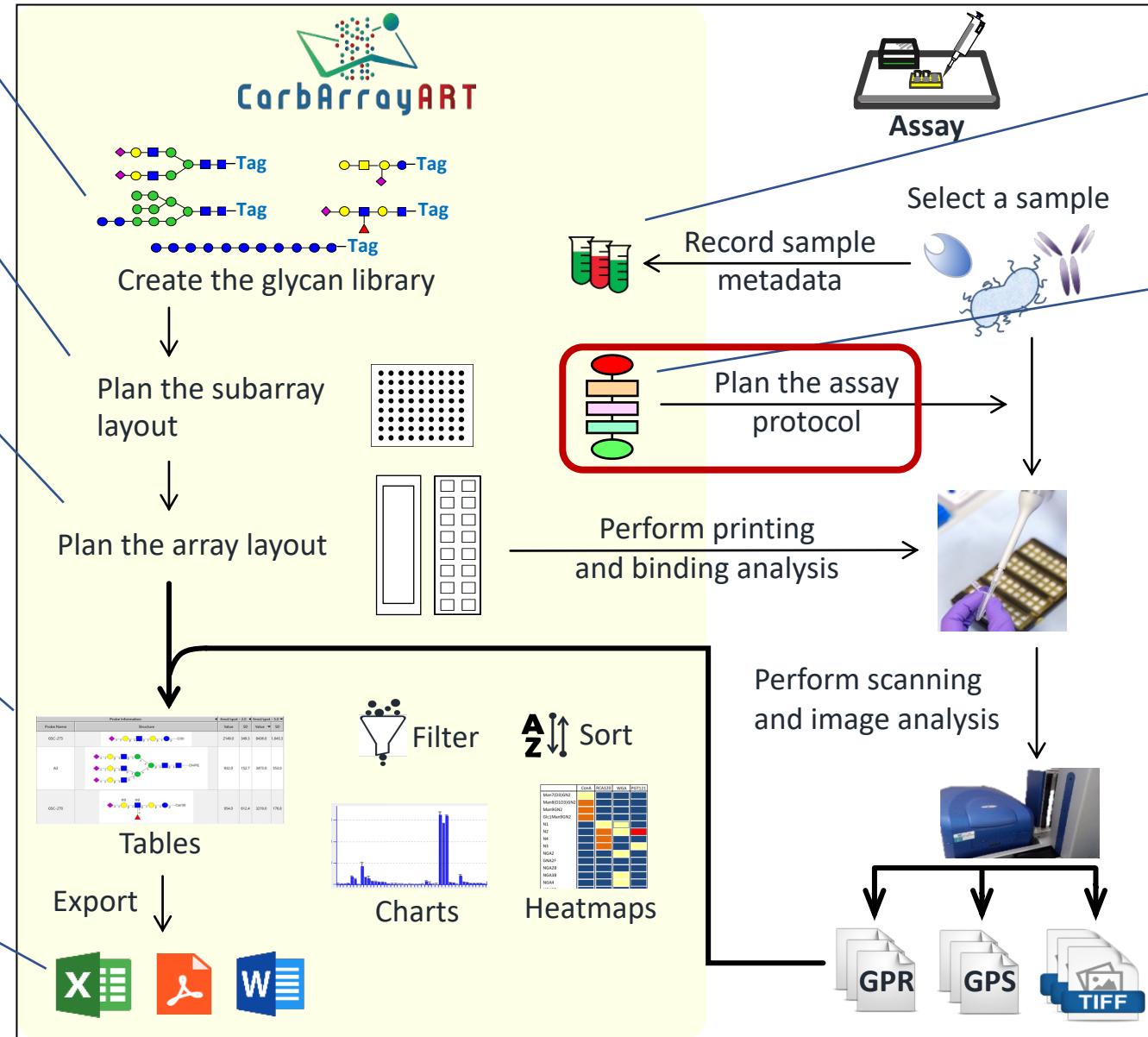
3. Slide layout entry tool

6. Data presentation

7. Data sharing

4. Sample metadata entry tool

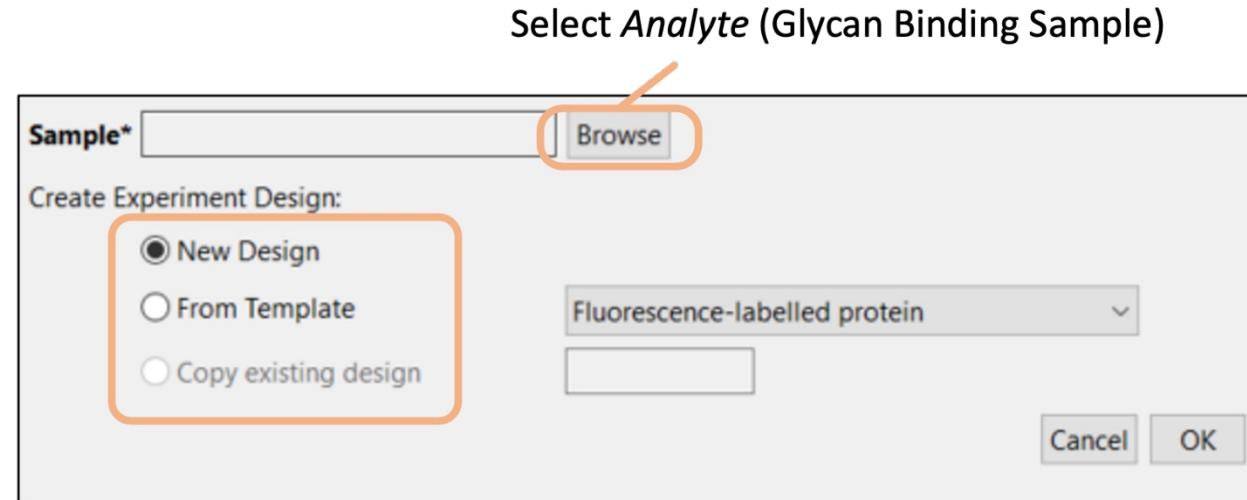
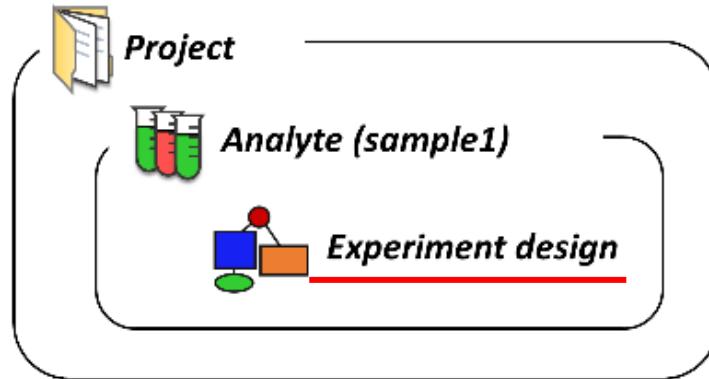
5. Experiment design tool



Left, yellow background:  
The data management workflow in CarbArrayART

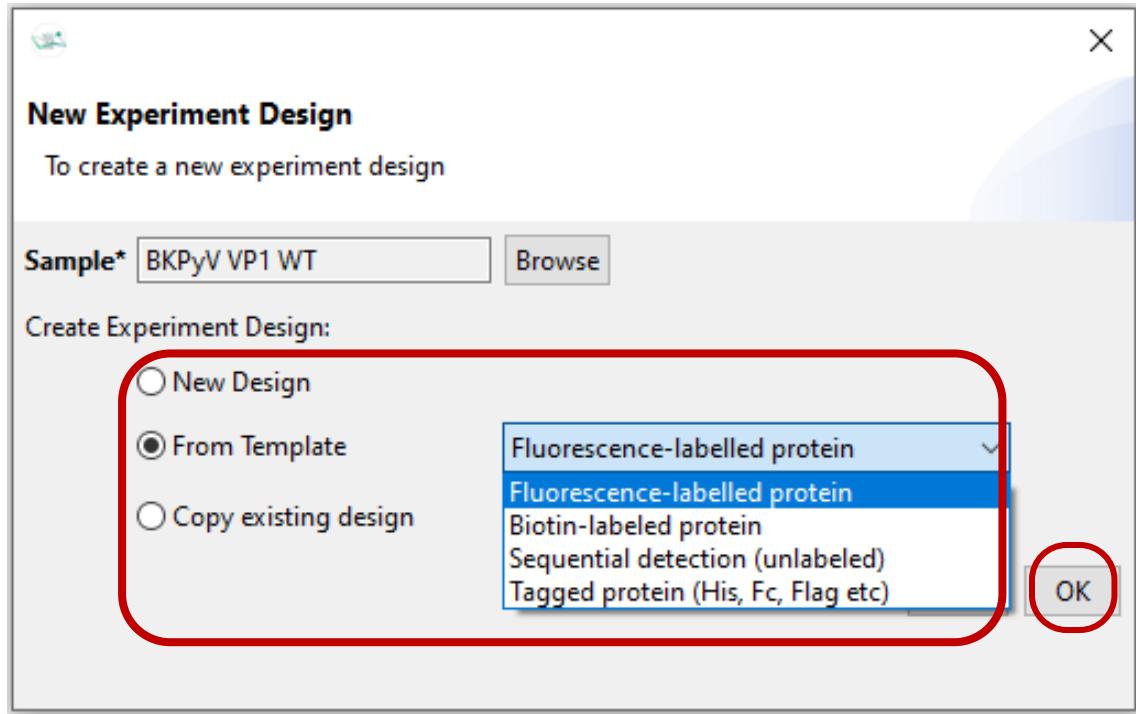
Right: The experiment workflow

## 5. Experimental protocol designing tool



Protocol and metadata used for a glycan microarray experiment is linked to the *Analyte* (glycan binding sample) information.

## 5. Experimental protocol designing tool

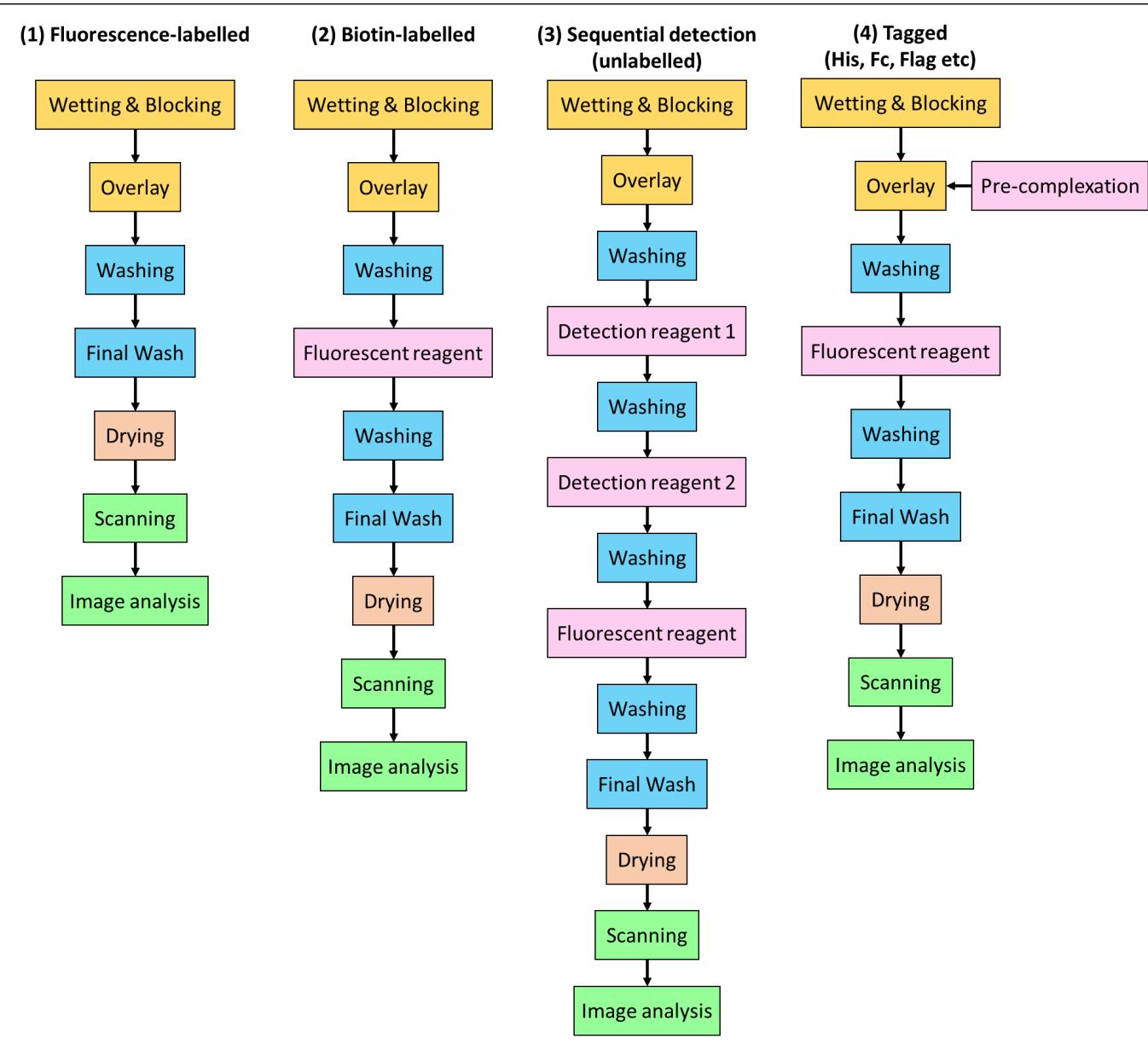


Users can create a new protocol using the template.

There are four pre-stored templates in CarbArrayART as default:

- Fluorescence-labelled sample
- Biotin-labelled sample
- Sequential detection (unlabelled)
- Tagged sample (His, Fc, Flag etc)

# 5. Experimental protocol designing tool

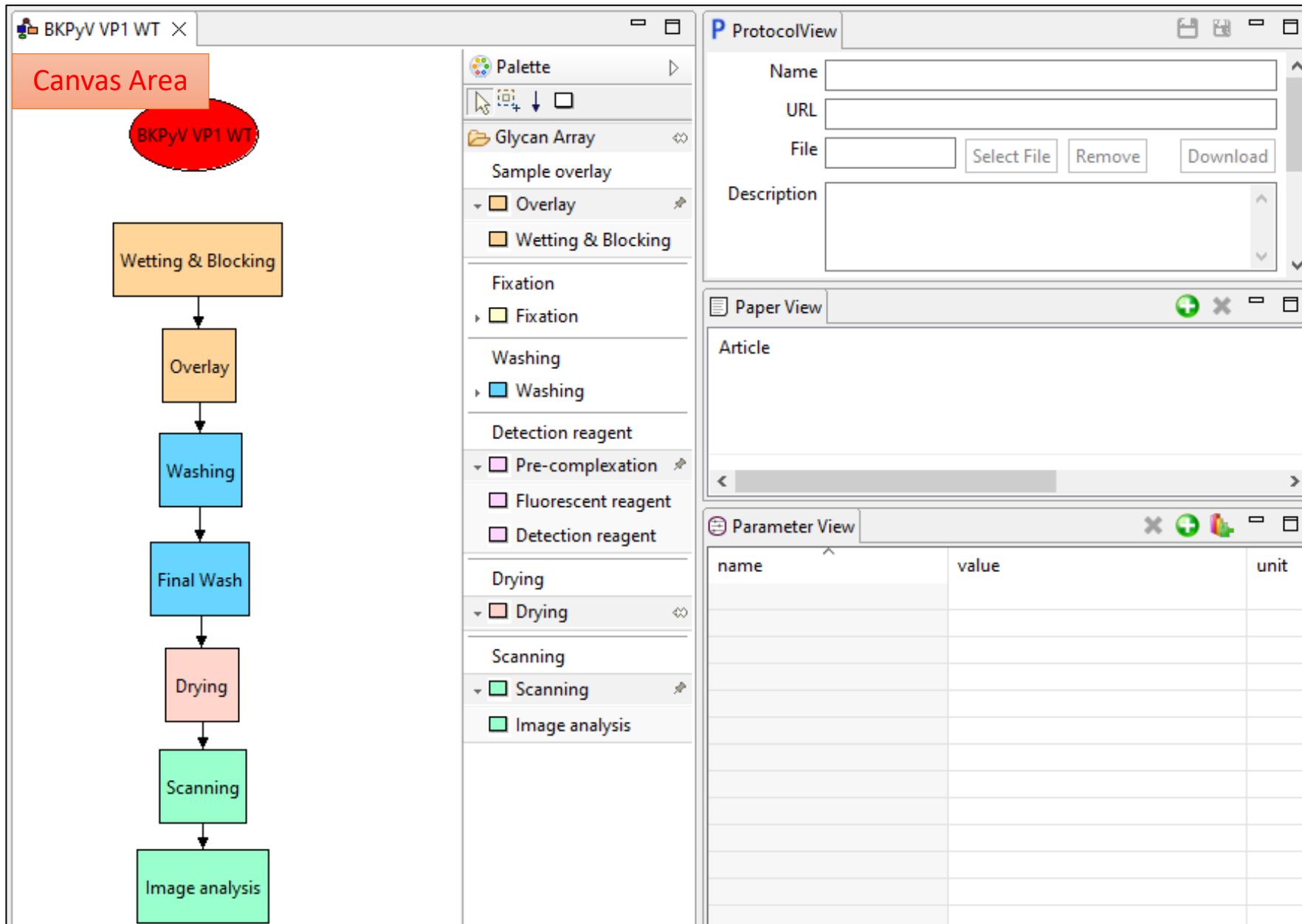


Users can create a new protocol using the template.

There are four pre-stored templates in CarbArrayART as default:

- Fluorescence-labelled sample
- Biotin-labelled sample
- Sequential detection (unlabelled)
- Tagged sample (His, Fc, Flag etc)

# 5. Experimental protocol designing tool



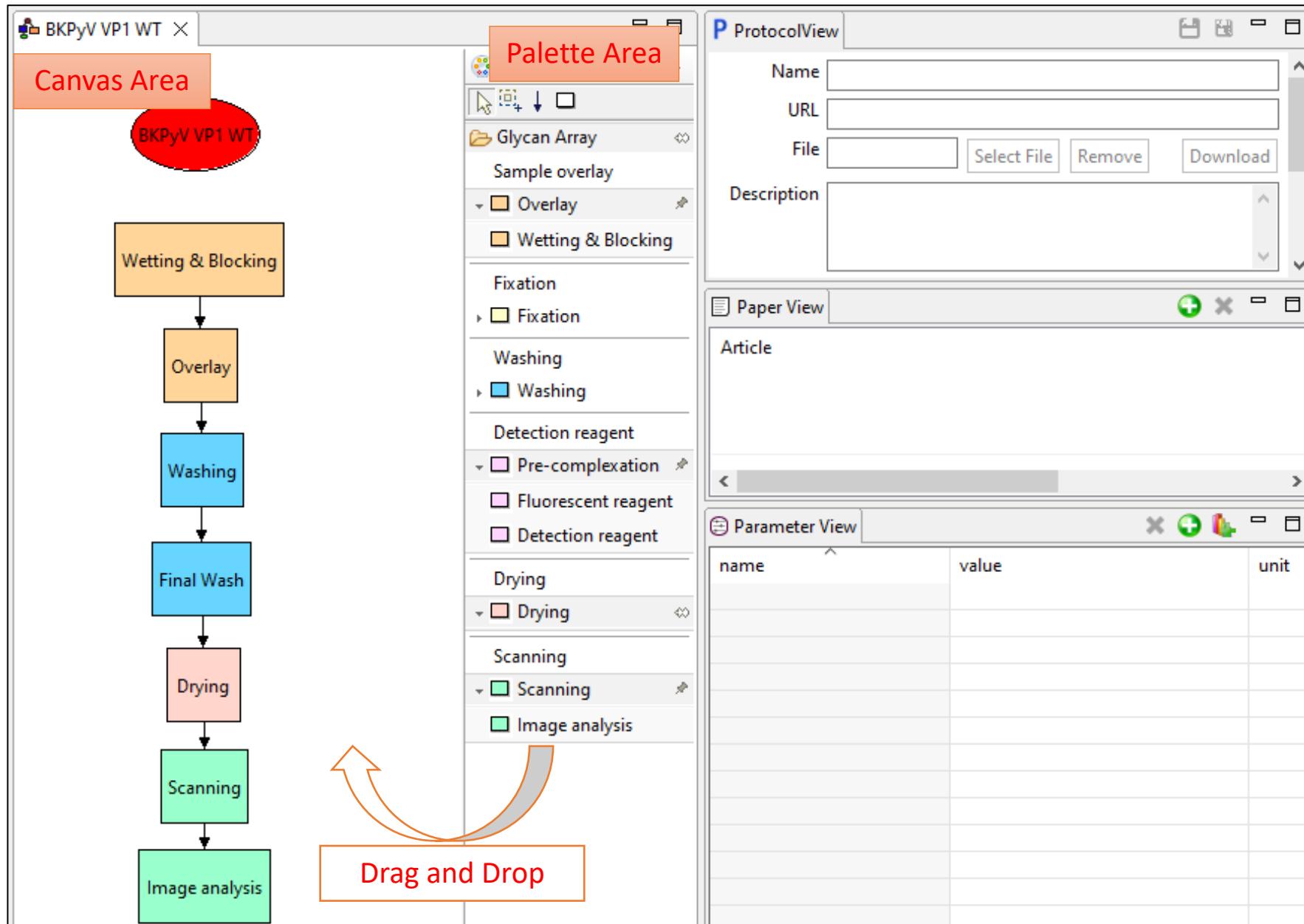
## <Canvas>

Design an experiment workflow by locating boxes and arrows.

A box in the canvas indicates each step (protocol) such as 'Overlay' and 'Washing'.

An arrow indicates the flow of the steps.

# 5. Experimental protocol designing tool



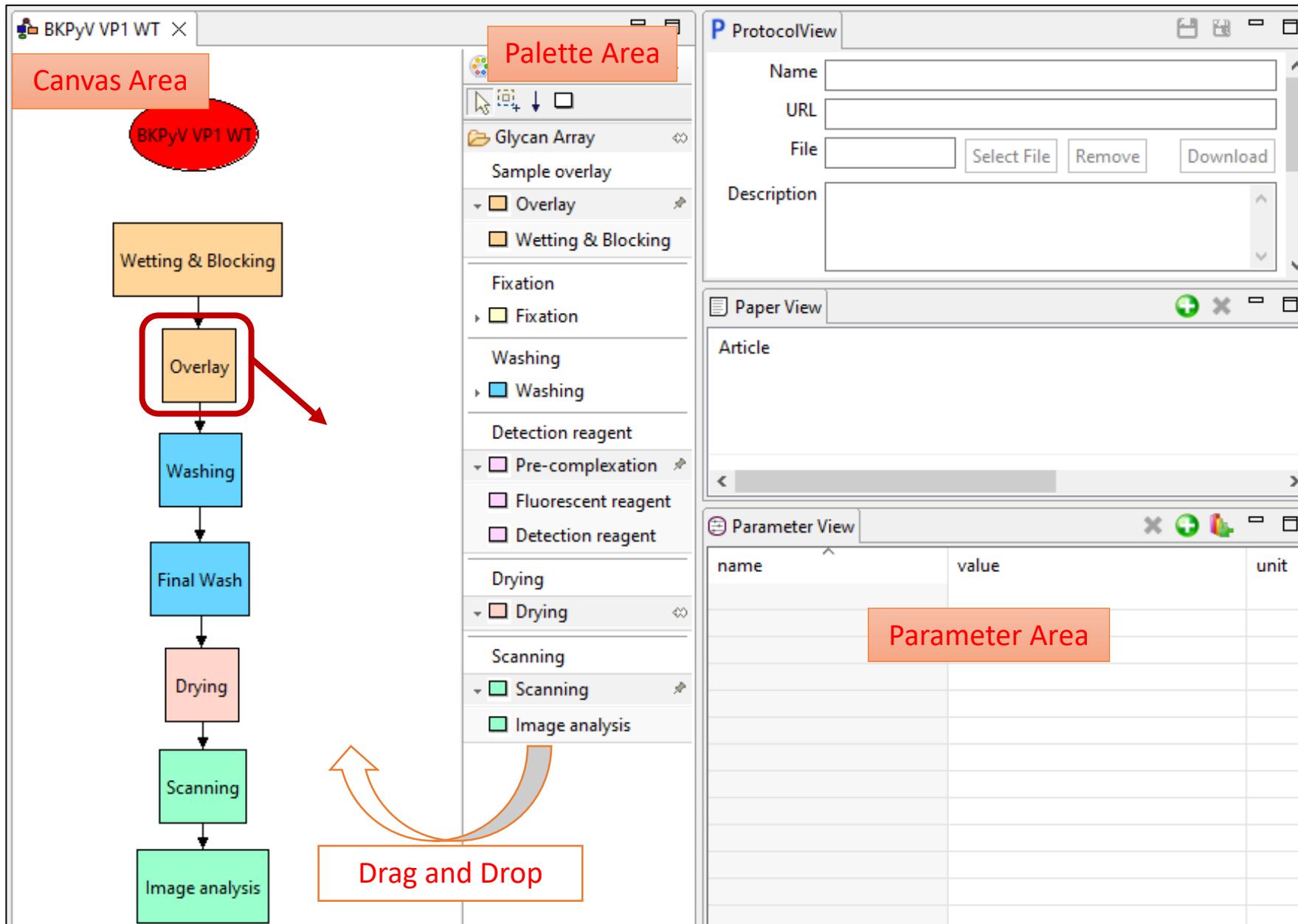
## <Palette area>

Each box indicates the pre-stored protocols:

- (1) Sample overlay
- (2) Fixation
- (3) Washing
- (4) Detection reagent
- (5) Drying
- (6) Scanning

Users can create a new protocol from scratch by drag-and-drop boxes from the Palette Area and connect them with arrows.

# 5. Experimental protocol designing tool



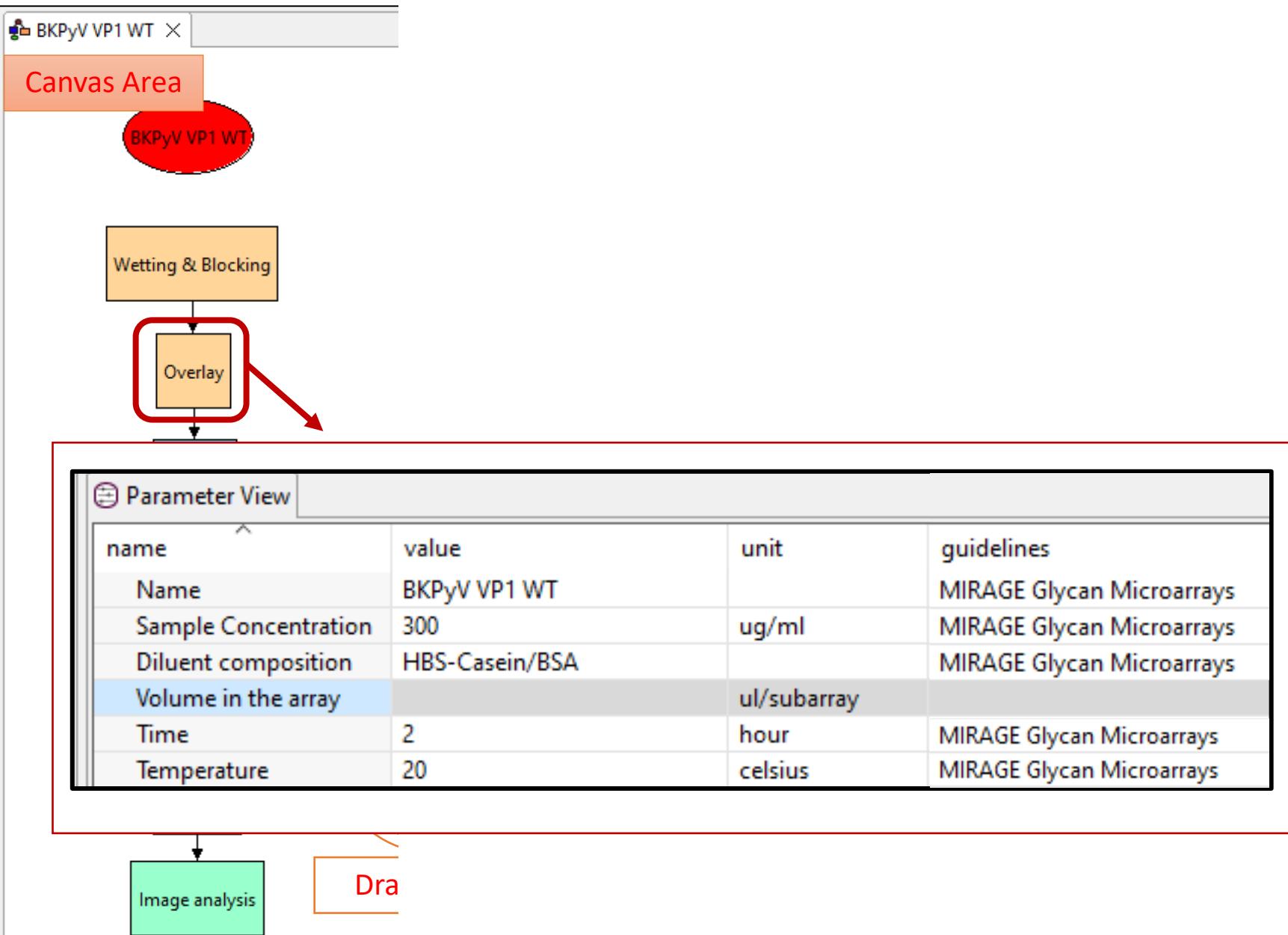
## <Parameter area>

The metadata corresponding to the protocol are stored in this section.

Each protocol has a pre-stored metadata list in CarbArrayART based on the MIRAGE Glycan Microarray Guidelines.

The parameters compliant with MIRAGE guidelines are labelled in the 'Guidelines' column.

## 5. Experimental protocol designing tool



### <Parameter area>

The metadata corresponding to the protocol are stored in this section.

Each protocol has a pre-stored metadata list in CarbArrayART based on the MIRAGE Glycan Microarray Guidelines.

The parameters compliant with MIRAGE guidelines are labelled in the 'Guidelines' column.

# Tools in CarbArrayART

1. Glycan probe entry tool

2. Subarray layout entry tool

3. Slide layout entry tool

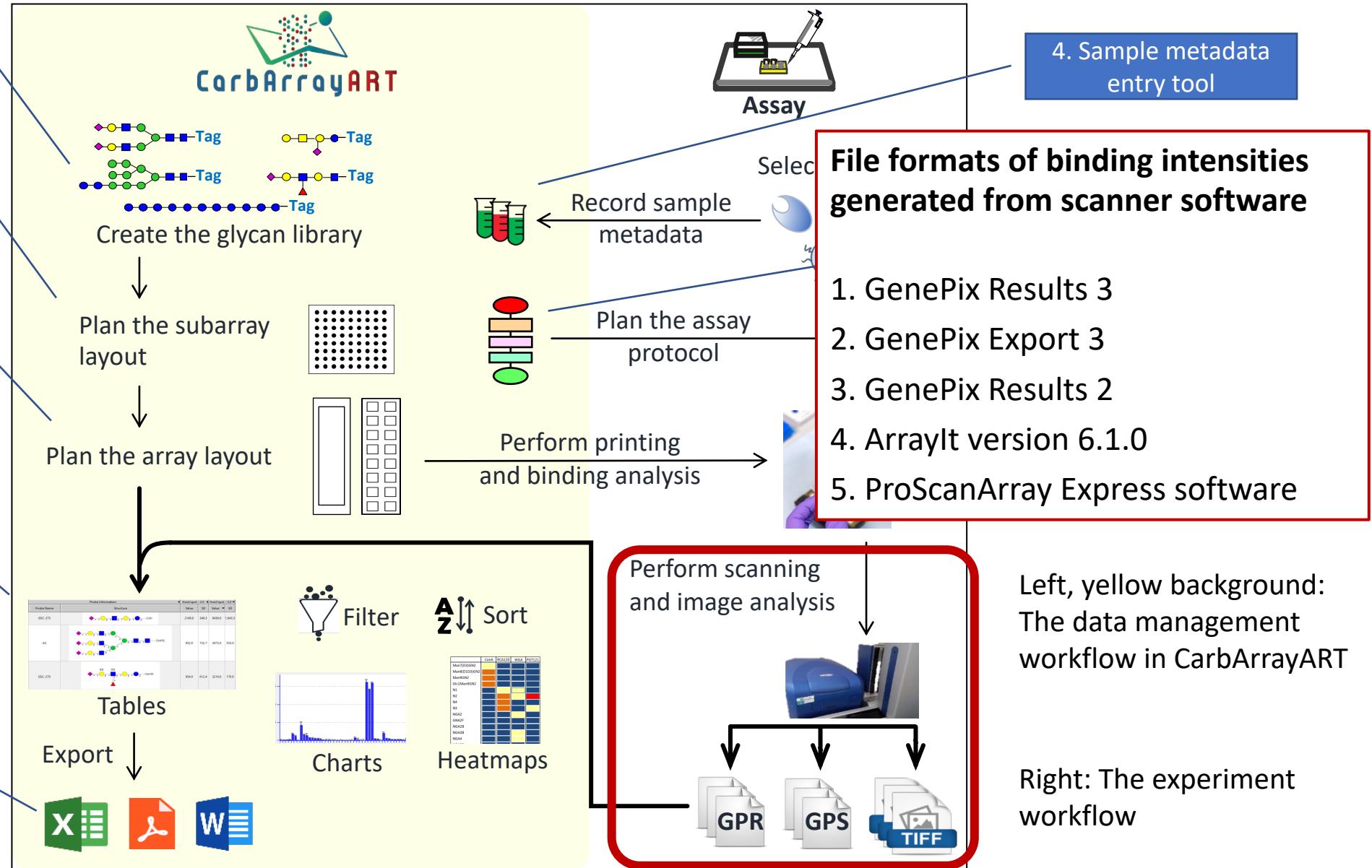
6. Data presentation

7. Data sharing

4. Sample metadata entry tool

**File formats of binding intensities generated from scanner software**

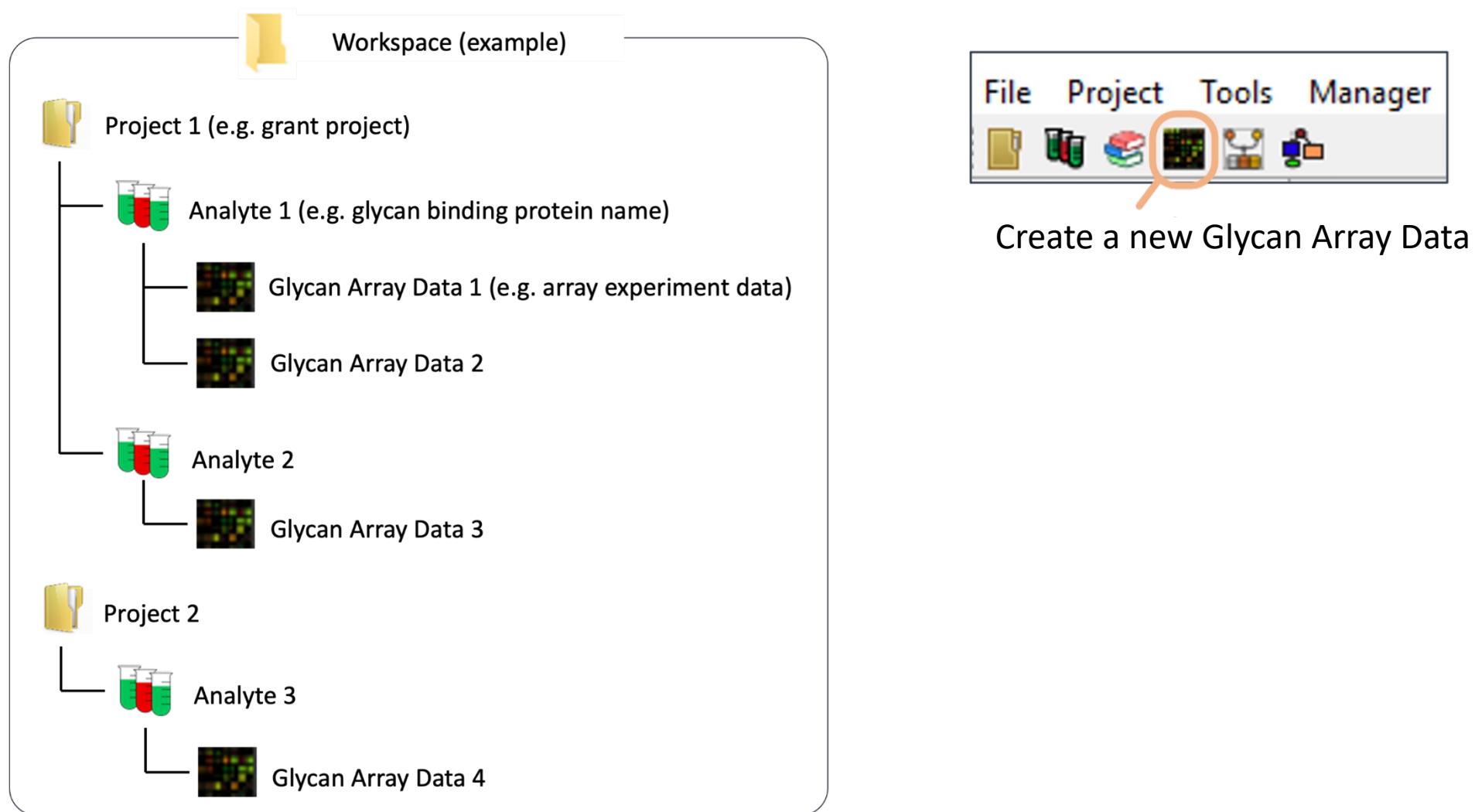
1. GenePix Results 3
2. GenePix Export 3
3. GenePix Results 2
4. ArrayIt version 6.1.0
5. ProScanArray Express software



Left, yellow background:  
The data management workflow in CarbArrayART

Right: The experiment workflow

## 6. Data presentation: Create a new *Project*, *Analyte* and *Glycan Array Data*



## 6. Data presentation: Glycan Array Data – parameter entry

The screenshot displays a software window with five input fields, each labeled with a number from 1 to 5:

- 1** Name:
- 2** File Type:
- 3** Number of Slides:
- 4** Statistical Method:
- 5** Signal to Use:

- 1. Name** – A name of scan data
- 2. File Type** – GenePix (gpr) or ProScan (Excel)
- 3. Number of Slides** – The number of slides used per experiment (in many cases 1 slide per experiment)
- 4. Statistical Method** – Select one from: Average or Elimination
  - \* Elimination method calculates an average value after removing the maximum and the minimum values per glyco-probe
- 5. Signal to Use** – Select one from: Median-B, Mean-B, Median or Mean (\*'B' stands for Background)

## 6. Data presentation: Glycan Array Data – scan file upload

After selecting the pre-saved array layout and glycan binding sample tested, users can upload the scan file(s).

Select the fluorophore used if it is recorded in the scanned file

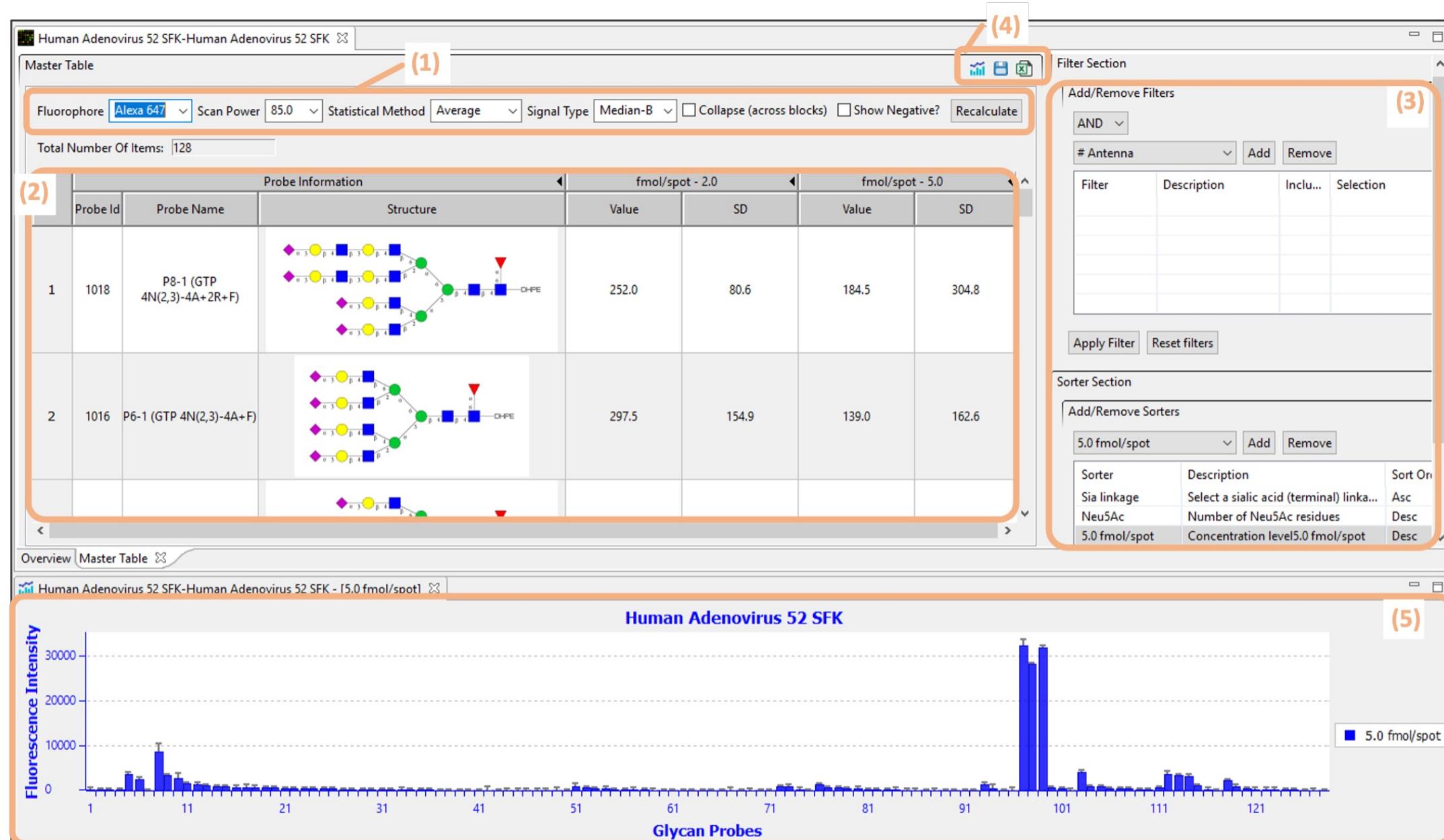
Slide	File Name	File Type	Scan Power(s)	Fluorophore (select one)
▼ Slide 1	Alexa slide 1 set...	GenePix	85.0	Alexa 647
	Alexa slide 1 set...	GenePix	90.0	Alexa 647
	Alexa slide 1 set...	GenePix	100.0	Alexa 647
	Cy3 slide 1 sets ...	GenePix	100.0	Cyanine 3

**Upload Files**

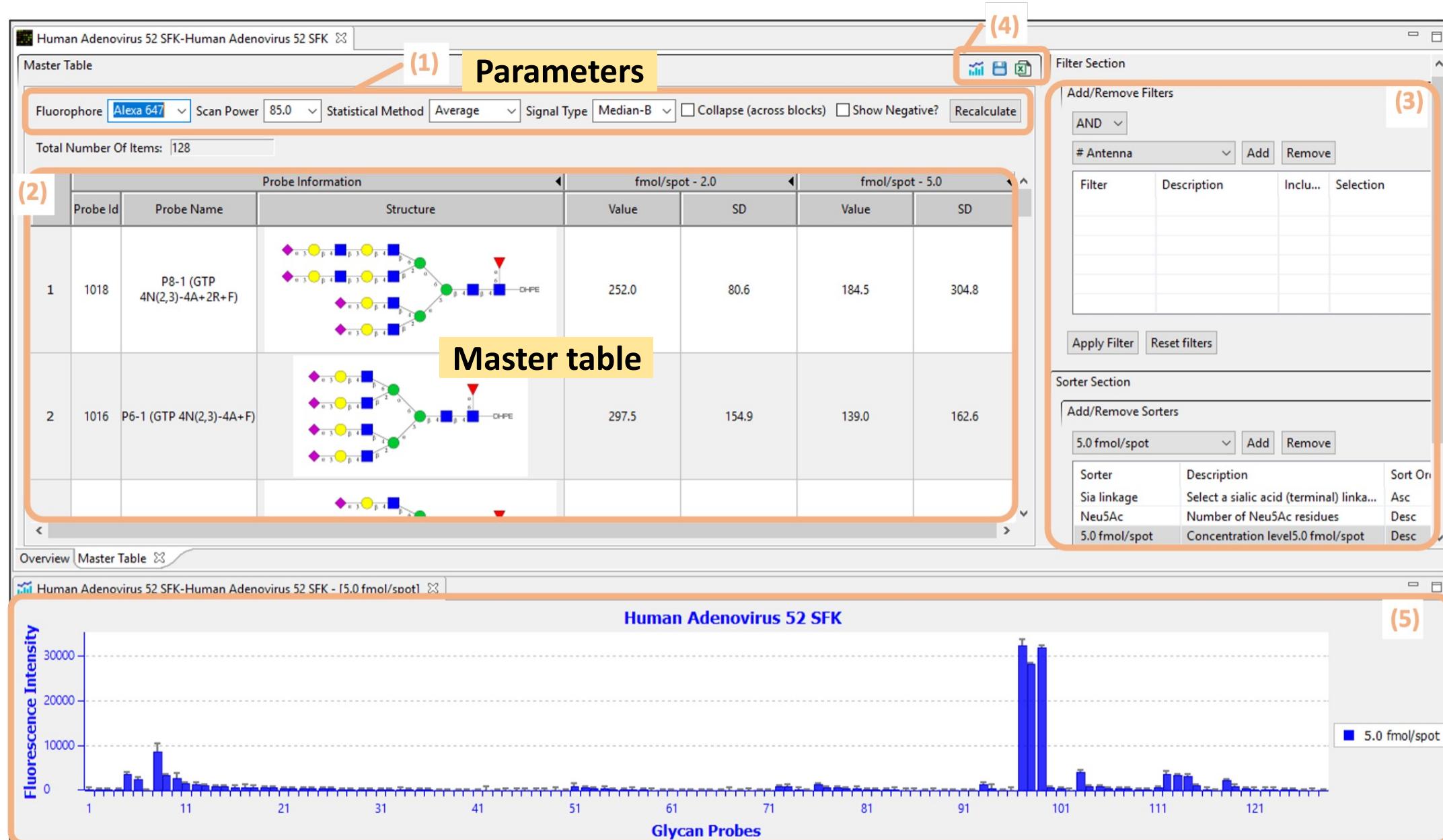
Alexa 647  
Cyanine 3  
Cyanine 5

< Back    Next >    **Finish**    Cancel

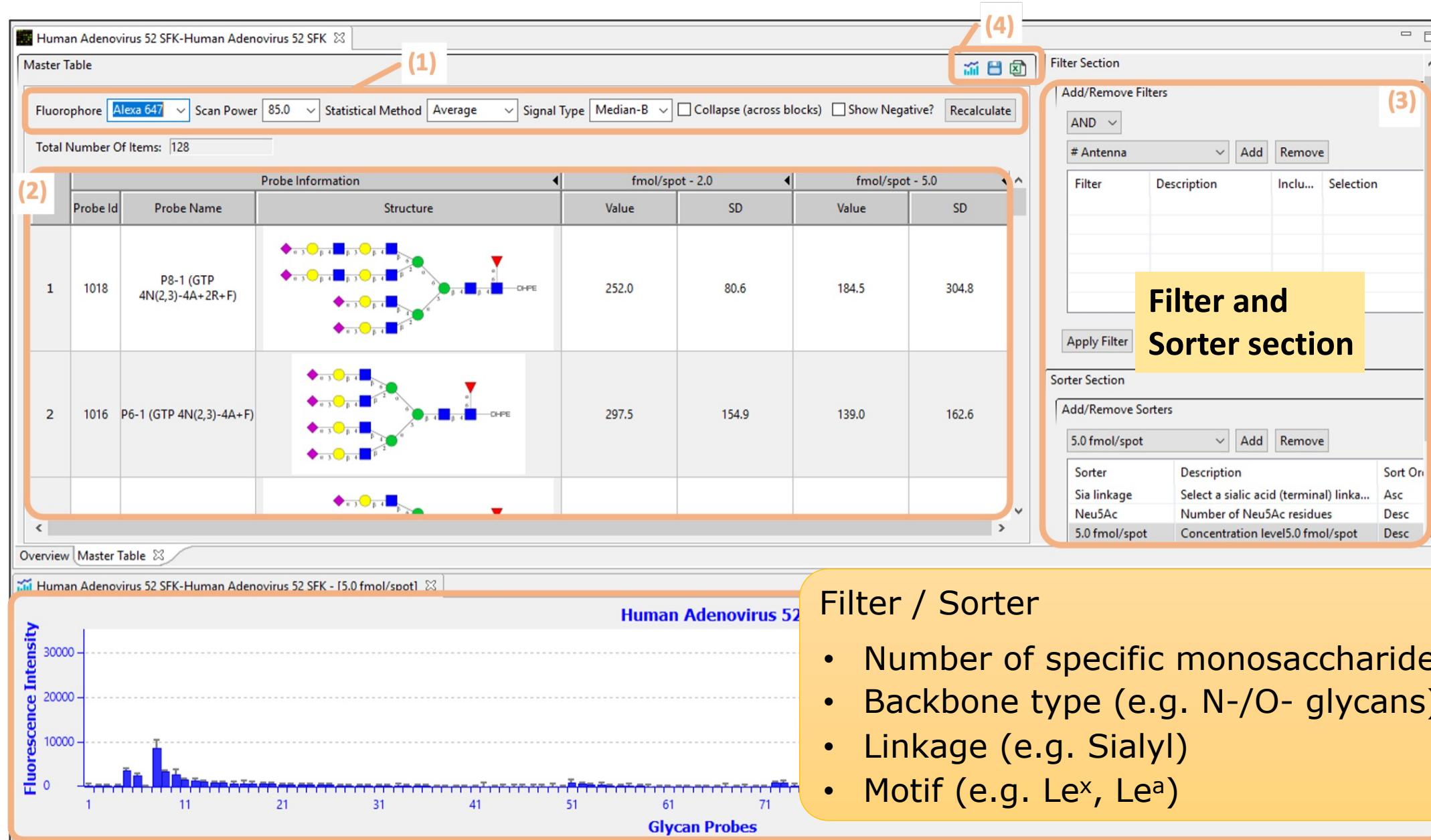
## 6. Data presentation: Tabulation view



# 6. Data presentation: Tabulation view



# 6. Data presentation: Tabulation view



# 6. Data presentation: Tabulation view

**Tool buttons** (4)

**Filter Section** (3)

**Histogram view** (5)

**Master Table**

**Probe Information**

**Chemical Structures**

**Fluorescence Intensity**

**Glycan Probes**

**Human Adenovirus 52 SFK**

**5.0 fmol/spot**

**Fluorophore: Alexa 647**, **Scan Power: 85.0**, **Statistical Method: Average**, **Signal Type: Median-B**, **Collapse (across blocks):**  **Show Negative:**  **Recalculate**

Total Number Of Items: 128

Probe Id	Probe Name	Structure	fmol/spot - 2.0		fmol/spot - 5.0	
			Value	SD	Value	SD
1	P8-1 (GTP 4N(2,3)-4A+2R+F)		252.0	80.6	184.5	304.8
2	P6-1 (GTP 4N(2,3)-4A+F)		297.5	154.9	139.0	162.6

**Filter** **Description** **Incl...** **Selection**

**Sorter** **Description** **Sort Order**

**Apply Filter** **Reset filters**

**Add/Remove Sorters**

**5.0 fmol/spot** **Add** **Remove**

**Sia linkage** Select a sialic acid (terminal) linkage... **Asc**

**Neu5Ac** Number of Neu5Ac residues **Desc**

**5.0 fmol/spot** Concentration level 5.0 fmol/spot **Desc**

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# Monosaccharides and Motifs for filtering and sorting

- 78 types of monosaccharides
- 72 motifs
- Acidic
- Number of branch
- Number of monosaccharides
- Terminal linkage (e.g. Neu5Ac α2,3 terminal)

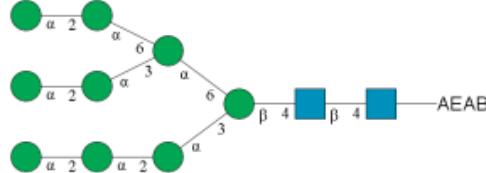
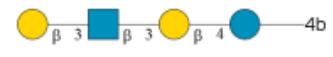
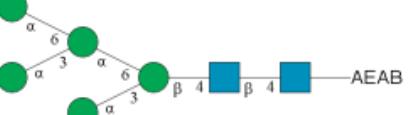
Name	Acidic
Fuc (Fucose)	▲
Gal (Galactose)	●
GalNAc (N-acetyl-galactosamine)	■
Glc (Glucose)	●
GlcA (Glucuronic acid)	◇ ✓
GlcNAc (N-acetyl-glucosamine)	■
IdoA (Iduronic acid)	◆ ✓
Kdo (3-deoxy-manno-oculosonic acid)	○ ✓
Man (Mannose)	●
Neu5Ac (N-acetylneurameric acid)	◆ ✓
Neu5Gc (N-glycolylneurameric acid)	◇ ✓
Kdn (3-deoxy-glycerol-galacto-nonulosonic acid)	◆ ✓
Ara (Arabinose)	★
Rha (Rhamnose)	▲
Xyl (Xylose)	★
Phosphate	✓
Sulphate	✓

## 6. Data presentation: Create heatmaps using the comparing tool

Data Compare Example X

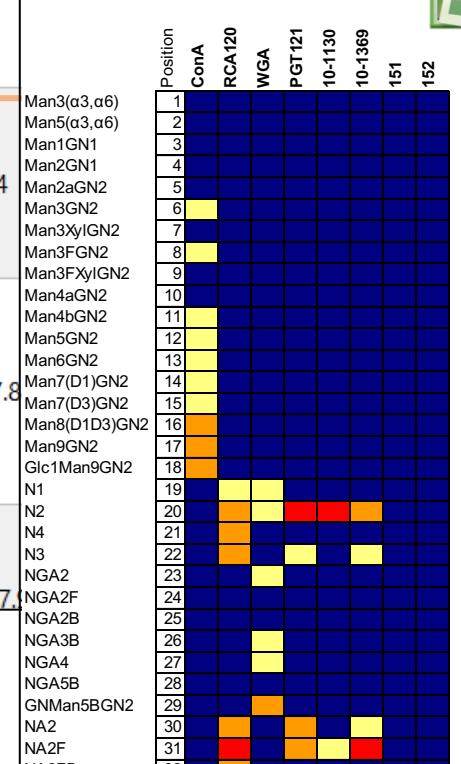
Master Table

Total Number Of Items: 66

Probe Id	Probe Name	Probe Information		GlyTouCan ID	AAL:100.0 uM		WGA:100.0 uM	
		Structure	Glycan ID		Value	SD	Value	SD
1	Man9-GN2-AEAB (NG015)		G56202TA	271.5	98.0	11734.0	1,816.2	
2	LNT-4b		G45827GY	19.25	34.6	7.5	4.4	
3	Man5-GN2-AEAB (NG016)		G03652TR	99.5	149.1	205.25	327.8	
4	Lex-Tri		G01187XC	11.75	14.2	4218.25	2,817.1	

An Excel file for creating heatmaps is included in the CarbArrayART software package.





Legend for heatmap colors:

- <10% (Light Yellow)
- 10-30% (Yellow)
- 30-70% (Orange)
- 70-100% (Red)

# Tools in CarbArrayART

1. Glycan probe entry tool

2. Subarray layout entry tool

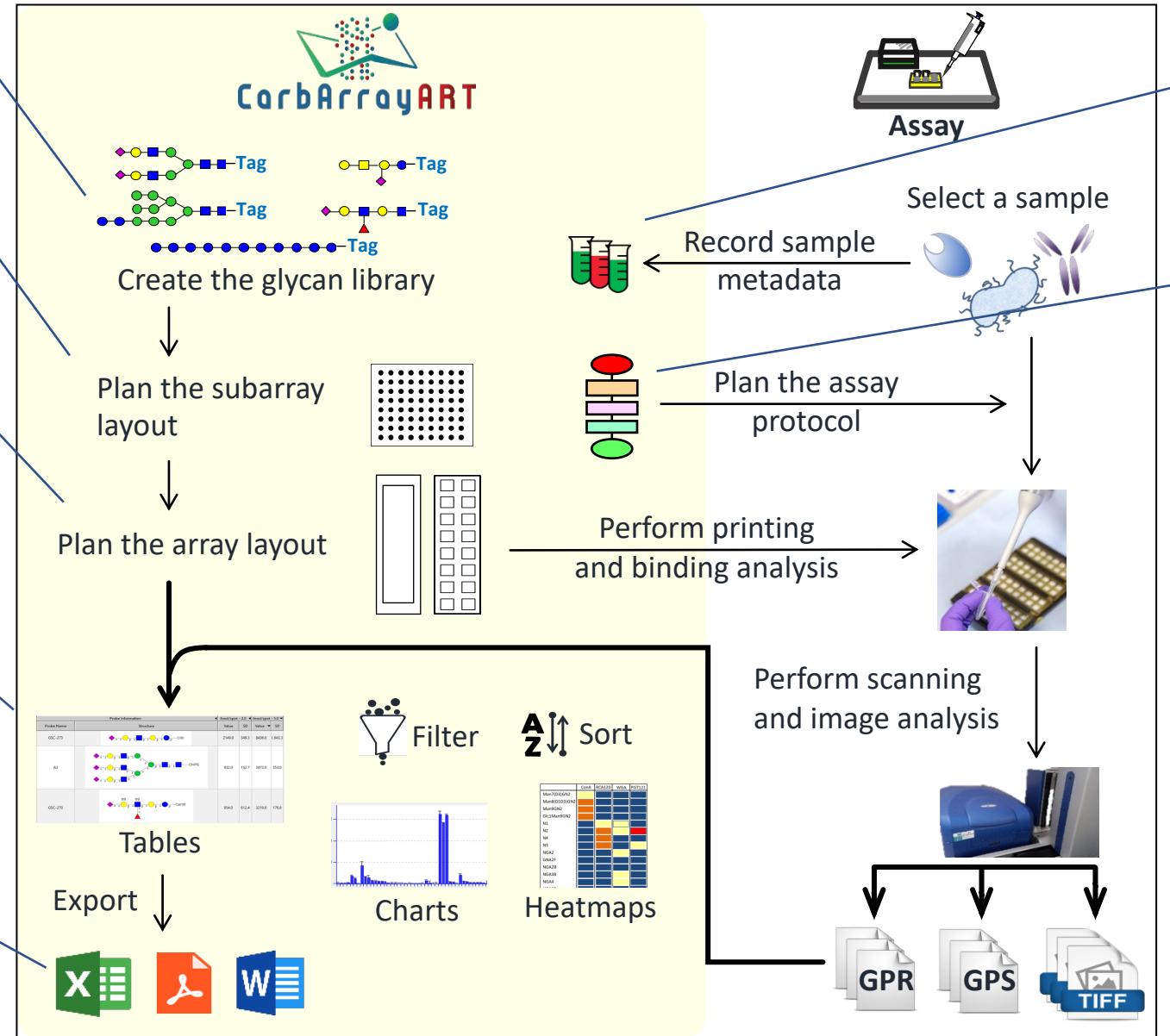
3. Slide layout entry tool

6. Data presentation

7. Data sharing

4. Sample metadata entry tool

5. Experiment design tool

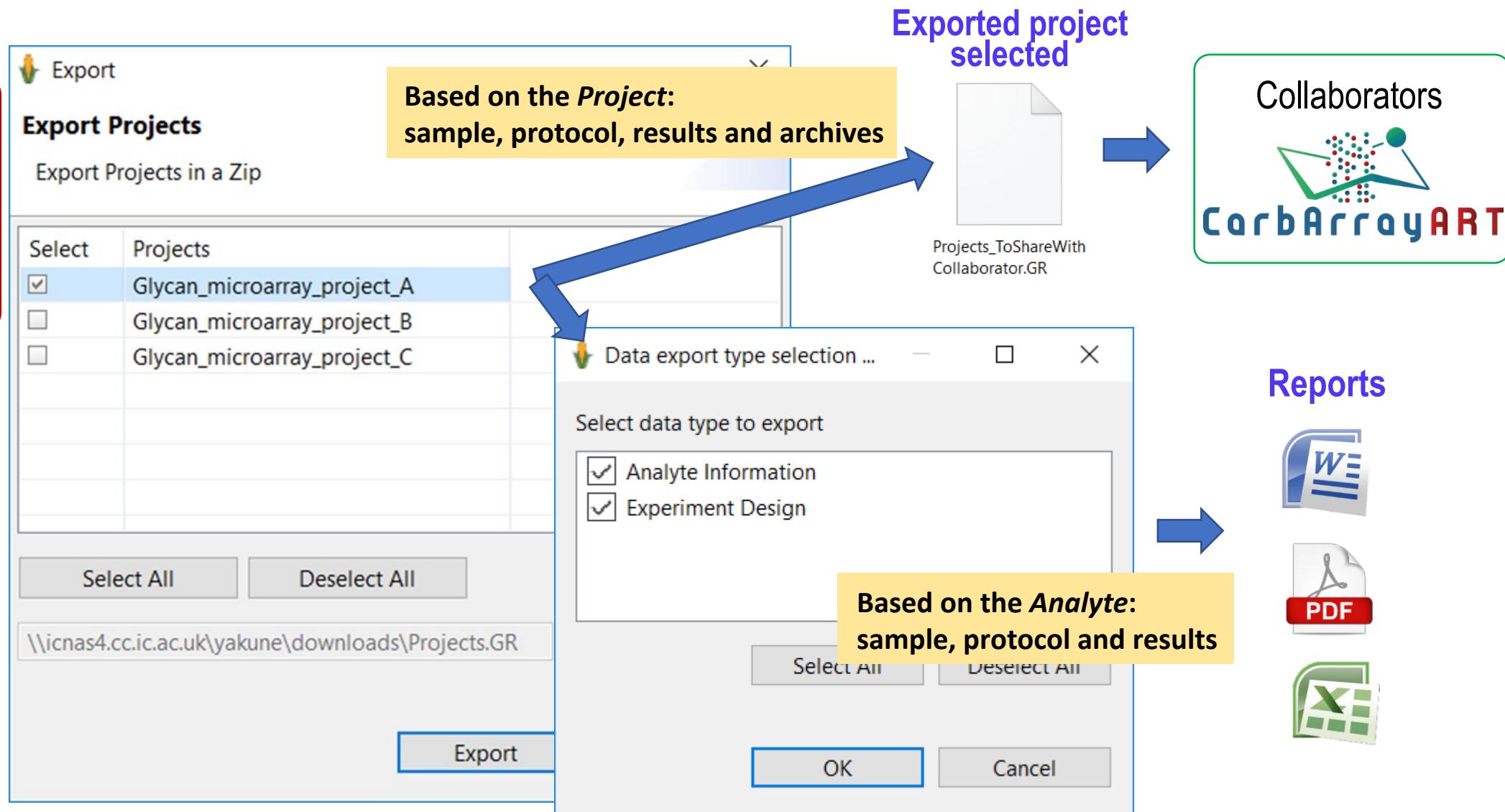
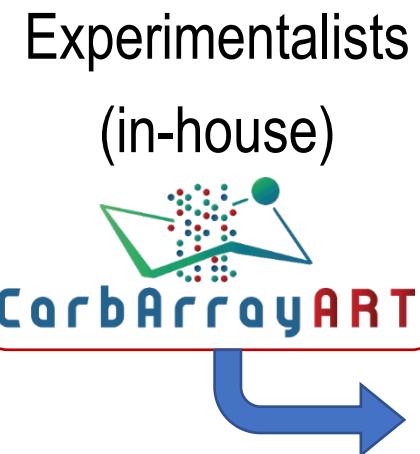


Left, yellow background:  
The data management  
workflow in CarbArrayART

Right: The experiment  
workflow

# Data sharing / publication

Data sharing with collaborators: Data export as Project(s) and Reports



# Data export: Word file

# User's manual and video tutorials

<http://carbarrayart.org>

## Manual and Support

 Home



### Manual

- Manual for sections
  - 1. [Introduction](#)
  - 2. [Software architecture](#)
  - 3. [How to download and open the software](#)
    - 1. CarbArrayART download
    - 2. [Installation and starting CarbArrayART](#)
      - [Windows](#)
      - [Mac](#)
    - 3. [Select workspace](#)
  - 4. [Glosarray of terms used in the software](#)
    - [Key terminologies](#)
  - 5. [Minimum information required for glycan microarray data presentation](#)
  - 6. [CarbArrayART: Front page](#)

### Video tutorials

- [How to start CarbArrayART \(Windows\)](#)
- [Glycan probe entry tool](#)
- [Subarray layout entry tool](#)
- [Array \(slide\) layout entry tool](#)
- [How to record Sample \(Analyte\) metadata](#)
- [Filtering function using glycan probe levels](#)

More videos coming soon...

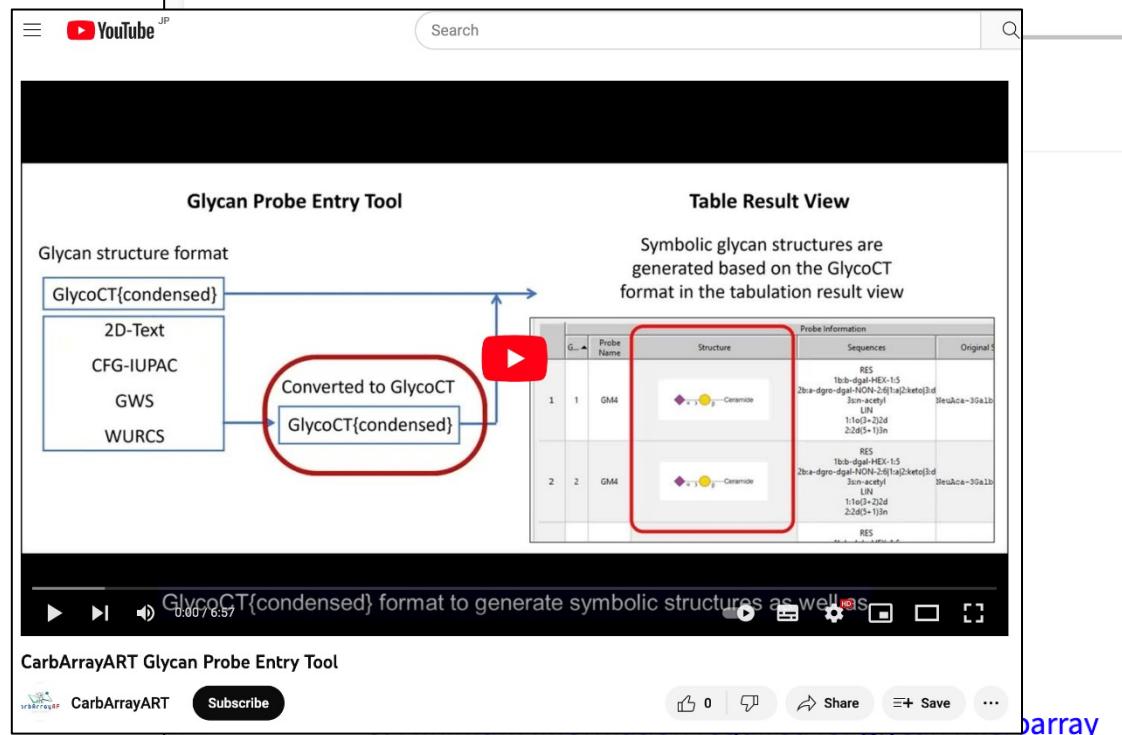
# User's manual and video tutorials

<http://carbarrayart.org>

## Manual and Support

[Home](#)





The screenshot shows the Glycan Probe Entry Tool interface. On the left, there is a legend for Glycan structure formats: GlycoCT{condensed}, 2D-Text, CFG-IUPAC, GWS, and WURCS. A red oval highlights the "Converted to GlycoCT" section, which shows "GlycoCT{condensed}" being converted from other formats. To the right, a "Table Result View" shows symbolic glycan structures generated based on the GlycoCT format. The table has columns for Probe Name, Structure, Sequences, and Original S. It lists two entries: one for GM1 and one for GM2, both labeled "Ceramide". Below the table, a video player shows a video titled "GlycoCT{condensed} format to generate symbolic structures as well".

## Video tutorials

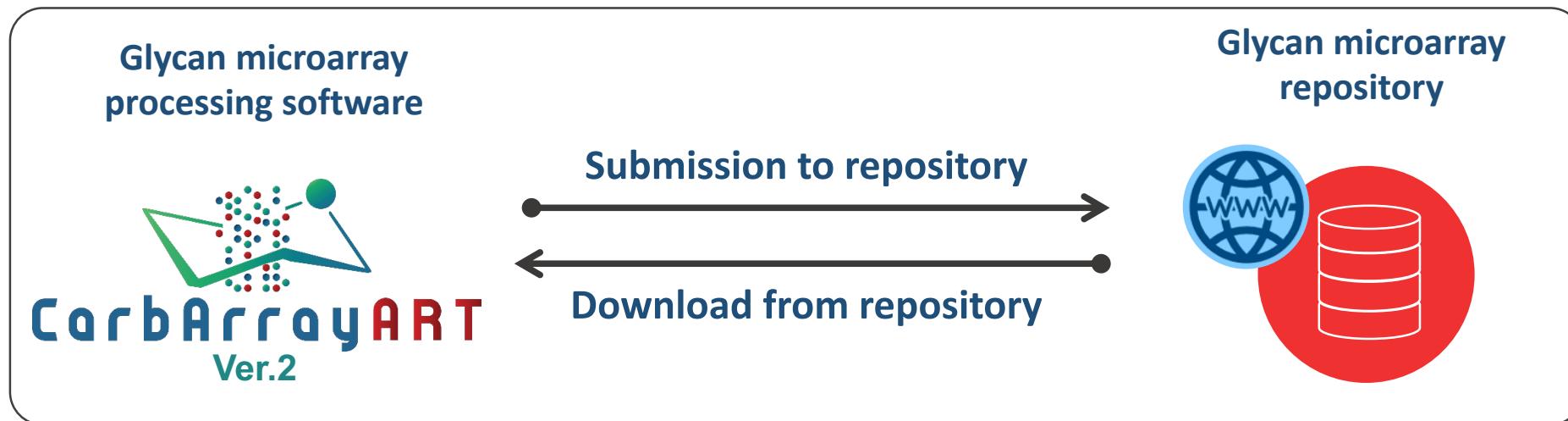
- How to start CarbArrayART (Windows)
- Glycan probe entry tool
- Subarray layout entry tool
- Array (slide) layout entry tool
- How to record Sample (Analyte) metadata
- Filtering function using glycan probe levels

## More videos coming soon...

data presentation  
6. CarbArrayART: Front page

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## Future direction: CarbArrayART as a vehicle for transfer of the data to and from the repository



# Acknowledgements

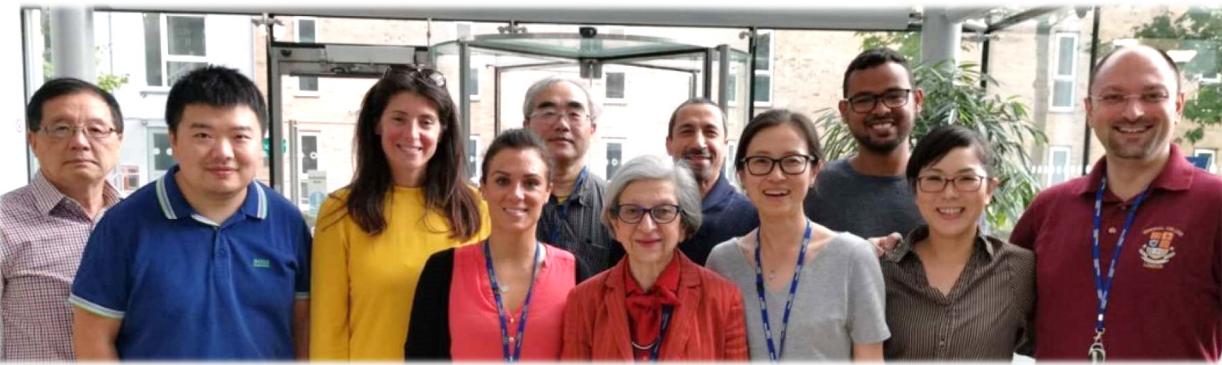
Our research in the Glycosciences Lab has been supported by Wellcome Trust, NIH Common Fund 1U01GM125267 - 01, March of Dimes and Medical Research Council

Imperial College London



## ICL – Glycosciences Laboratory

- Ten Feizi
- Yan Liu
- Wengang Chai
- Virginia Tajadura-Ortega
- Antonio Di Maio
- Jin Yu
- Jodie Abrahams



Supported by  
**wellcome** trust



The Common Fund



## Complex Carbohydrate Research Center



- René Ranzinger
- Sena Arpinar



Kiyoko F. Aoki-Kinoshita

- Angelina Palma (NOVA University of Lisbon / ICL)
- Lisete M. Silva (University of Aveiro / ICL)



# Thank you very much!

<http://carbarrayart.org>

For any query: [y.akune@imperial.ac.uk](mailto:y.akune@imperial.ac.uk)

The next talk will be...

27<sup>th</sup> February 2023 10AM (EST)



Dr. Akul Y Mehta

National Center for Functional Glycomics

Title: Using GLAD for exploratory glycan microarray  
data analysis and visualization