

Stage 3: Data processing, analysis and reporting_Step 8

Chromeleon Console

ChimericIgG DP vs BS_SeqVariant

Imported

Save Studio Print Up Insert Row Fill Down Lock Filtering Grouping Custom Columns Find Next

#	TIC	Name	Type	Level	Position	Volume	Instrument Method	Processing Method	Status	Inject Time	Lock Status	Weight	Dilution	IntStd	Replicate ID	Comment	Re-injections	Spike G
2		iclgG1 DP_1	Unknown		0	1.0000	MAM	Proc Method_SeqVarian..	Idle			1.0000	1.0000	1.0000			0	
3		iclgG1 DP_2	Unknown			1.0000	MAM	Proc Method_SeqVarian..	Finished	8/6/2020 3:15:56 PM +..		1.0000	1.0000	1.0000			0	
4		iclgG1 DP_3	Unknown			1.0000	MAM	Proc Method_SeqVarian..	Finished	8/6/2020 7:17:44 PM +..		1.0000	1.0000	1.0000			0	
5		iclgG1 BS_1	Unknown			1.0000	MAM	Proc Method_SeqVarian..	Finished	8/6/2020 11:19:32 PM..		1.0000	1.0000	1.0000			0	
6		iclgG1 BS_2	Unknown			1.0000	MAM	Proc Method_SeqVarian..	Finished	8/7/2020 4:27:08 AM +..		1.0000	1.0000	1.0000			0	
7		iclgG1 BS_3	Unknown			1.0000	MAM	Proc Method_SeqVarian..	Finished	8/7/2020 12:31:08 PM..		1.0000	1.0000	1.0000			0	

Click here to add a new injection

Export...

Report Template & Channel

Use report template: MAM Report IgG1BS CQAs_01

With selected channel: [Dropdown]

Destination Path

Parent Folder: [Field]

Sub Folder: [Field]

Export Formats & Filenames

- Text format (Results) (*.txt)
- Text format (Raw Data) (*.txt, *.csv)
- Excel file format (*.xls)
- PDF file format (*.pdf)
- GAML file format (*.gaml)
- AnDI/NetCDF file format (*.cdf)
- Raw file format (*.raw)
- Chromeleon data file format (*.cmbx)
- Allotrope data file format (*.adf)

External Program

Call external program

Notifications

Enable Notifications

OK Cancel

Associated Items: Custom Sequence Variables (0), Custom Formulas

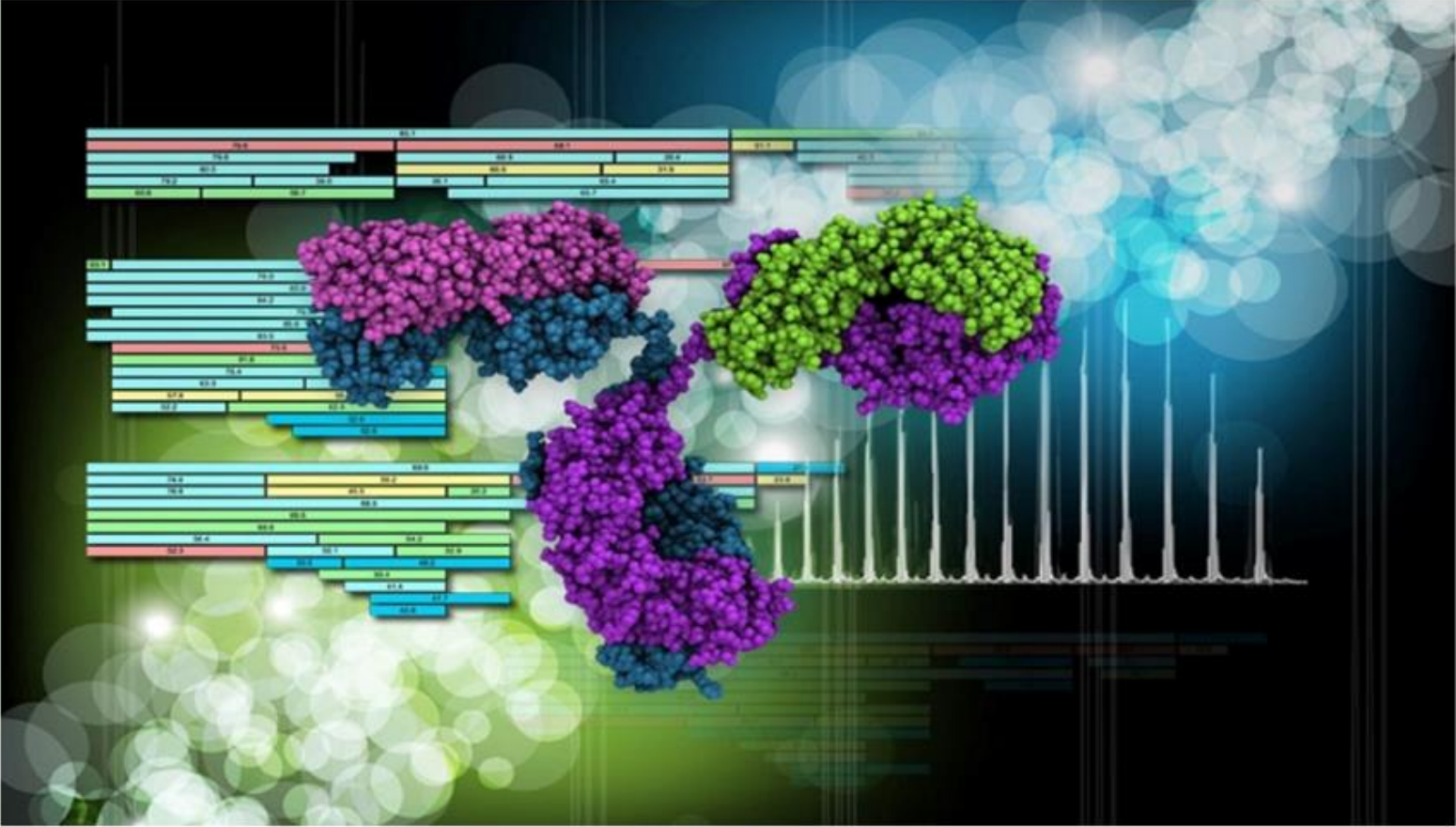
Stage 3: Data processing, analysis and reporting_Step 9

Home

Select an experiment type.

Experiment Types

- Sequence Manager >
- Peptide Mapping Analysis >
- Oligonucleotide Analysis >
- Intact Mass Analysis >
- Top Down Analysis >



Peptide Mapping Analysis Oligonucleotide Analysis Intact Mass Analysis Top Down Analysis

Stage 3: Data processing, analysis and reporting_Step 9

Protein Sequence Editor

Variable modifications selection. Import Fasta File Define Modification List Save Save As New Cancel

Protein Sequence Information

Target Protein

Name:

Description:

Category:

Monoisotopic Mass:

Average Mass:

Formula:

Chain

Chain:

Monoisotopic Mass:

Average Mass:

Manual Input Protein Sequence

Variable Modifications for Intact and Peptide Analysis

Max # Modifications: Intact Protein Peptide Mapping

Glycosylation (O Glycan supported only for peptide mapping): N, O Glycan

Modifications

Modifications Selected for Search

N Terminal

Mono. Mass:

Avg. Mass:

C Terminal

Mono. Mass:

Avg. Mass:

Side Chain

Mono. Mass:

Avg. Mass:

Residues:

2AA instead of Asn
2AB instead of Asn
Acetylation (N-term)
Arg
Asp
Carbamylation (N-term)
DOTA
DOTA_Mn
DOTA_Cu
DOTA_Zn
Glu
Lys
NEM

Amide (C-term)
Arg
Asp
b ion
Glu
Lys

Acetylation
ADP-ribosylation
Amidation
Carbamylation
Carbamidomethylation
Carboxymethylation
Cysteinylation
Cysteinylation
Deamidation (N)
Deamidation (Q)
Decarboxylation
Dimethylation
DOTA

Protein Sequence Map

Disulfide Link Definitions

Chain Number	Amino Acid Site Index	Chain Number	Amino Acid Site Index
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Site-Specific Variable Modifications for Top Down Analysis

Modification Editor

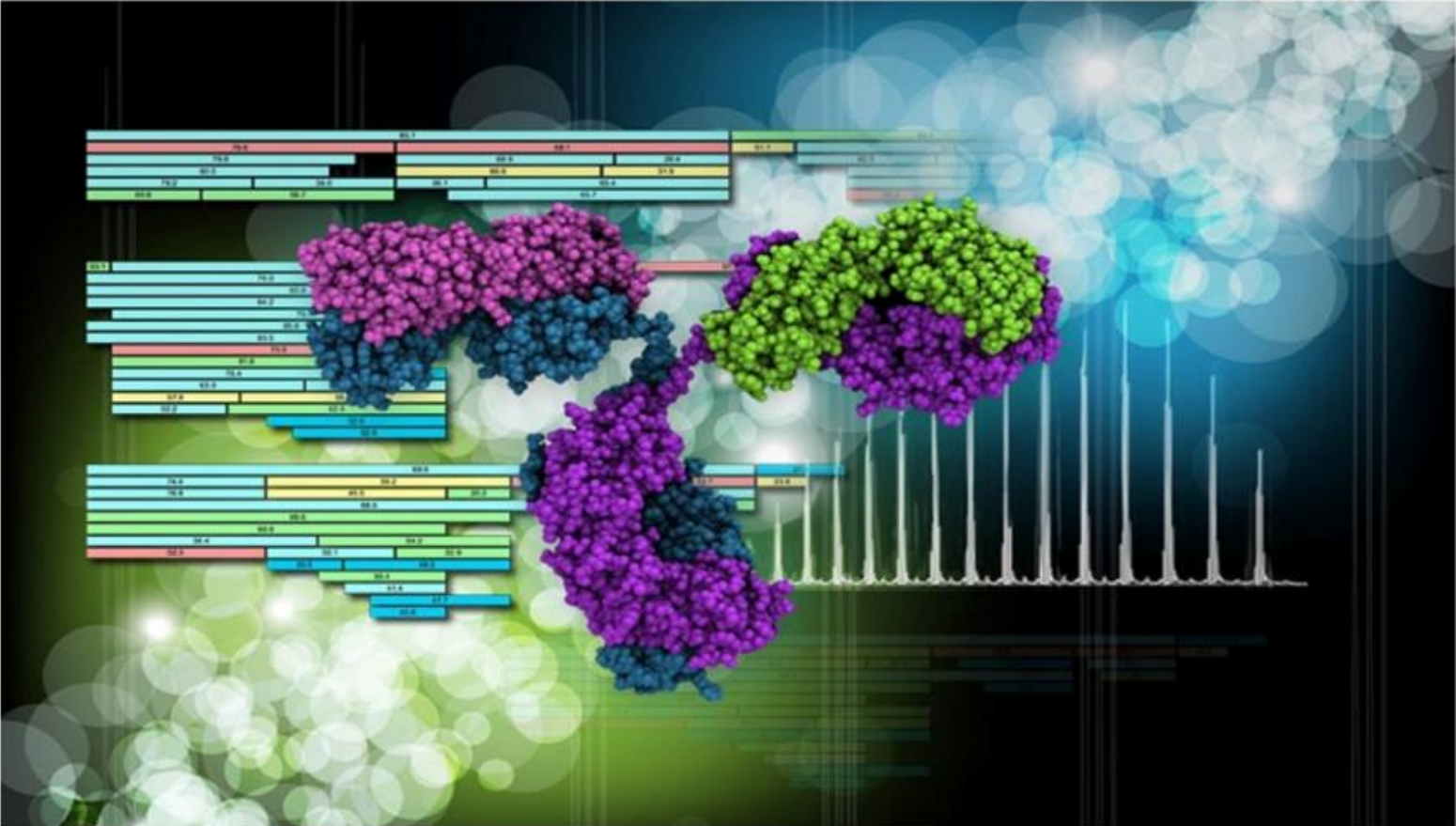
Stage 3: Data processing, analysis and reporting_Step 10

Home

Select an experiment type.

Experiment Types

- Sequence Manager >
- Peptide Mapping Analysis >
- Oligonucleotide Analysis >
- Intact Mass Analysis >
- Top Down Analysis >



Peptide Mapping Analysis Oligonucleotide Analysis Intact Mass Analysis Top Down Analysis

Stage 3: Data processing, analysis and reporting_Step 10

Peptide Mapping Analysis
 Load Results
 Queue
 Target Peptide Workbook

Import Method Export Method

Select a protein sequence.

Peptide Mapping Analysis Definition

Experiment Name:

Load Raw Data

Select Raw Data: ...

Load Raw Data Condition:

Reference Condition:

Result Format For Multiple Raw Files

Batch Processing
 Multiconsensus

Protein Sequence

Select	Name	Category	Last Modified Time	Monoisotopic Mass	Num. of Chains/ Num. of Entries	Max. Num. of Modifications	Total Number of Amino Acids
<input type="checkbox"/>		Peptide Mapping	02/01/2021 01:37 P...	73408.40	2	1	662
<input type="checkbox"/>		Peptide Mapping	02/24/2021 03:37 P...	82179.01	1	1	735
<input type="checkbox"/>		Peptide Mapping	04/12/2021 11:44...	73424.14	2	1	662
<input type="checkbox"/>		Peptide Mapping	10/26/2021 09:56...	73025.74	2	1	663
<input type="checkbox"/>	Chimeric IgG1DP...	Peptide Mapping	10/26/2021 09:57...	73025.74	2	1	663
<input type="checkbox"/>	MAM Discovery...	Targeted Peptide	11/05/2021 12:44 P...	80			

Processing Method

Enable Automatic Parameter Values

Select	Name	Method Type	Description
<input type="checkbox"/>	Basic Default Method	Non Targeted	Default Method for Basic Peptide Mappi...
<input type="checkbox"/>	Disulfide Bond Default Method	Non Targeted	Default Method for Disulfide Bond
<input type="checkbox"/>	HDX Default Method	Non Targeted	Default Method for HDX
<input type="checkbox"/>	Targeted Default Method	Targeted	Default Method for Targeted Analysis
<input type="checkbox"/>		Non Targeted	Default Host Cell Protein Method
<input type="checkbox"/>		Non Targeted	Default Host Cell Protein Method
<input type="checkbox"/>		Non Targeted	Default Host Cell Protein Method
<input type="checkbox"/>		Non Targeted	Default Host Cell Protein Method
<input type="checkbox"/>		Non Targeted	Default Method for Basic Peptide Mappi...
<input type="checkbox"/>		Non Targeted	Default Method for Basic Peptide Mappi...

Start Processing
Edit Method

Stage 3: Data processing, analysis and reporting_Step 11

The screenshot shows a software interface with a top navigation bar containing tabs: Home, Peptide Mapping Analysis, Load Results (selected), Queue, and Target Peptide Workbook. Below the tabs is a search bar with the text "Select an experiment to load its results." and buttons for Load Results, Delete, Export Results, and Import Results.

The main area displays a "Master List" table with the following columns: Experiment Name, Raw File Name, Method Name, Method Type, Method Description, Sequence Name, Completion Time, and Total Processing Time (min). The table contains 9 rows, with the 9th row selected.

Experiment Name	Raw File Name	Method Name	Method Type	Method Description	Sequence Name	Completion Time	Total Processing Time (min)
1	C:\Users\Silvia\Desktop\THERMO...		Non Targeted	Default Host Cell Protein Method		01/22/2021 03:26 PM	0.00
2	E:\BPF Datafiles\15_BPF4.1 HCP A...		Non Targeted	Default Host Cell Protein Method		01/22/2021 04:03 PM	0.00
3	C:\Users\Silvia\Desktop\THERMO...		Non Targeted	Default Host Cell Protein Method		02/24/2021 04:00 PM	16.90
4	C:\Users\Silvia\Desktop\THERMO...		Non Targeted	Default Host Cell Protein Method		04/12/2021 11:50 AM	3.82
5	C:\Users\Silvia\Desktop\BPF Data...		Non Targeted	Default Method for Basic Peptide...		04/09/2021 03:18 PM	0.00
6	C:\Users\Silvia\Desktop\BPF Data...		Non Targeted	Default Method for Basic Peptide...		05/11/2021 05:02 PM	4.12
7	C:\Users\Silvia\Desktop\THERMO...		Non Targeted	Default Method for Basic Peptide...		04/30/2021 06:10 PM	0.00
8	C:\Users\Silvia\Desktop\THERMO...		Non Targeted	Default Method for Basic Peptide...		06/04/2021 02:29 PM	0.00
9 MAM Discovery Phase Chimeric IgG1_DP	C:\Users\Silvia\Desktop\BPF Data...	Basic Default Method_NIBRT_01	Non Targeted	Default Method for Basic Peptide...	Chimeric IgG1DP_PepMap	11/05/2021 11:33 AM	6.31

On the left side of the interface, there is a vertical sidebar labeled "Experiment Management" with an orange arrow pointing to the right.

Stage 3: Data processing, analysis and reporting_Step 11



Home Peptide Mapping Analysis Load Results Queue Parameters Process and Review Mapping Target Peptide Workbook

Coverage Modification Summary

Use the check boxes in the Results table on the Process and Review page to select the components for the user-definable protein coverage map.

Chromatogram

Chromatogram 1: BPC: C:\Users\Silvia\Desktop\BPF DataFiles\25. Nature Protocols data processing\Chimeric IgG1 DP_1_MSMS.raw

Chromatogram 2: BPC: C:\Users\Silvia\Desktop\BPF DataFiles\25. Nature Protocols data processing\Chimeric IgG1 DP_2_MSMS.raw

Chromatogram 3: BPC: C:\Users\Silvia\Desktop\BPF DataFiles\25. Nature Protocols data processing\Chimeric IgG1 DP_3_MSMS.raw

Sequence Coverage Map

Created on 09/21/22 by Silvia
 Data Folder = C:\Users\Silvia\Desktop\BPF DataFiles\25. Nature Protocols data processing\
 Minimum MS Signal = 20000
 Data File = Chimeric IgG1 DP_1_MSMS.raw
 Protease = Trypsin

Proteins	Number of MS Peaks	MS Peak Area	Sequence Coverage	Abundance (mol)
Heavy Chain	1470	57.7%	98.7%	69.50%
Light Chain	691	20.5%	98.6%	30.50%
Unidentified	12904	21.7%		

Minimum Recovery = 1%
 Minimum Recovery of Overlapping Peptides = 0%
 Minimum Confidence = 0.8
 Maximum Mass = 7000

Color code for peptide recovery

>50.0%	>20.0%	>10.0%	>5.0%	>2.0%	>1.0%	>0.5%	>0.2%	>0.1%	>0.0%
good	fair	poor							

Heavy Chain

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47

Q V Q L Q Q P G A E L V K P G A S V K M S C K A S G Y T F T S Y N M H W V K Q T P G R G L E W

51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97

I Y P G N G D T S Y N Q K F K G K A T L T A D K S S S T A Y M Q L S S L T S E D S A V Y Y C A

Chromatogram

Results

Level	Flag	No.	Protein
1	Protein	1	Heavy Chain
2	Protein	2	Light Chain
3	Protein	3	Unidentified

Stage 3: Data processing, analysis and reporting_Step 12

Home
 Peptide Mapping Analysis
 Load Results
 Queue
 Parameters
 Process and Review
 Mapping
 Target Peptide Workbook

Coverage
 Modification Summary

Modification Results

Created	Data Folder	Protease	Peptide Minimum Intensity (%)	Charge State Minimum Intensity (%)	Minimum Modification Level (%)	Raw File Name
9/21/2022 by Silvia	C:\Users\Silvia\Desktop\BPF DataFiles\25. Nature Protocols data processing	Trypsin	17.00%	33.00%	0.0005%	SampleName

Protein	Residue #	Modification	Category	Comment	Normalized Time Shift	Predicted Time Shift	Peptides	Peptide Sequence
1 Heavy Chain	1	-Q1+Deamidation	+Deamidation	None	2.1%	2.8%	1:Q1-K19 = 1976.1...	QVQLQQPGAEIVK...
2 Heavy Chain	55	N55+Deamidation	+Deamidation	None	1.8%	3.2%	1:G44-K63 = 2182...	GLEWIGAIYPGNGD...
3 Heavy Chain	82	Q82+Deamidation	+Deamidation	None	0.8%	2.9%	1:S75-R98 = 2677...	SSSTAYMQLSSLTSE...
4 Heavy Chain	163	-N163+Deamidati...	+Deamidation	Retention time off?	87.8%	1.1%	1:D152-K214 = 67...	DYFPEPVTVSWNS...
5 Heavy Chain	179	-Q179+Deamidati...	+Deamidation	Retention time off?	74.9%	1.1%	1:D152-K214 = 67...	DYFPEPVTVSWNS...
6 Heavy Chain	207	-N207+Deamidati...	+Deamidation	Retention time off?	64.7%	1.1%	1:D152-K214 = 67...	DYFPEPVTVSWNS...
7 Heavy Chain	290	N290+Deamidation	+Deamidation	None	3.2%	4.7%	1:F279-K292 = 167...	FNWYVDGVEVHNAK
8 Heavy Chain	319	N319+Deamidation	+Deamidation	None	3.4%	3.9%	1:V306-K321 = 18...	VVSVLTLHQDWL...
9 Heavy Chain	329	N329+Deamidation	+Deamidation	Poor recovery	2.3%	0.0%	1:C325-K330 = 73...	CKVSNK
10 Heavy Chain	365	-N365+Deamidati...	+Deamidation	None	11.3%	7.7%	1:N365-K374 = 11...	NQVSLTCLVK; NQV...
11 Heavy Chain	393	-N393+Deamidati...	+Deamidation	None	1.6%	3.2%	1:G375-K396 = 25...	GFYPSDIAVEWESN...
12 Heavy Chain	423	Q423+Deamidation	+Deamidation	None	3.5%	3.9%	1:W421-K443 = 28...	WQQGGNVFSCVSM...
13 Light Chain	36	-Q36+Deamidation	+Deamidation	None	2.4%	4.6%	2:A25-K38 = 1666...	ASSSVYIHWFQVK

Components

Level	No.	Identification	Peptide Sequence	Modification	Site	Delta (ppm)	Confidence Score	Best Overall Average Structural Resolution	ID
1 Component	8027	1:G44-K63 = 2182.0331m	GLEWIGAIYPGNGDTSYN...	None		-0.51	100.0	1.1 MS	
2 Component	8033	1:G44-K63 = 2182.0331m	GLEWIGAIYPGNGDTSYN...	None		-0.73	100.0	1.1 MS	
3 Component	8202	1:G44-K63 = 2182.0331m(N55+Deamidati...	GLEWIGAIYPGNGDTSYN...	Deamidation	N55	-0.35	100.0	1.1 MS	
4 Component	8207	1:G44-K63 = 2182.0331m(N55+Deamidati...	GLEWIGAIYPGNGDTSYN...	Deamidation	N55	-0.23	100.0	1.2 MS	
5 Component	8413	1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.3 MS	
6 Component	8416	1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.54	100.0	1.1 MS	
7 Component	749	1:N55-K63 = 1025.4414m[nonspecific]	NGDTSYNQK	nonspecific		-76.54	0.0	0.0 Full	
8 Component	2301	1:H51-K74 = 2617.8773a[nonspecific]	IYPGNGDTSYNQKFKGKATL...	nonspecific		-351.16	0.0	0.0 Full	

Modification Plot

% Abundance: Default Custom

Legend: ● N55+Deamidation

Sample	% Abundance
R1 - Chimeric IgG1 DP_1_MSMS.raw	0.7728
R2 - Chimeric IgG1 DP_2_MSMS.raw	0.7575
R3 - Chimeric IgG1 DP_3_MSMS.raw	0.7356

Stage 3: Data processing, analysis and reporting_Step 13

Custom Filter Selection

For Field 'Modification'

+ Add Condition - Remove Condition(s) Group Selected: 'And' Group 'Or' Group Toggle

Operator	Operand
<input checked="" type="checkbox"/> Does not contain	+
<input checked="" type="checkbox"/> Does not contain	nonspecific
<input checked="" type="checkbox"/> Does not contain	gasphase
<input checked="" type="checkbox"/> Does not contain	.

Does not contain '+' AND Does not contain 'nonspecific' AND Does not contain 'gasphase' AND Does not contain '.'

'And' Group 'Or' Group OK Cancel

Custom Filter Selection

For Field 'Delta (ppm)'

+ Add Condition - Remove Condition(s) Group Selected: 'And' Group 'Or' Group

Operator	Operand
\geq Greater than or equal to	-5
\leq Less than or equal to	5

≥ -5 AND ≤ 5

'And' Group 'Or' Group OK Cancel

Custom Filter Selection

For Field 'Confidence Score'

+ Add Condition - Remove Condition(s) Group Selected: 'And' Group 'Or' Group

Operator	Operand
\geq Greater than or equal to	95

≥ 95

'And' Group 'Or' Group OK Cancel

Custom Filter Selection

For Field 'Missed Cleavages'

+ Add Condition - Remove Condition(s) Group Selected: 'And' Group 'Or' Group

Operator	Operand
= Equals	0
= Equals	1

= '0' OR = '1'

'And' Group 'Or' Group OK Cancel

Stage 3: Data processing, analysis and reporting_Steps 14 and 15

Home Peptide Mapping Analysis Load Results Queue Parameters Process and Review **Mapping** Target Peptide Workbook

Coverage Modification Summary Manual Integrate Save

Modification Summary

Modification Results

Created	Data Folder	Protease	Peptide Minimum Intensity (%)	Charge State Minimum Intensity (%)	Minimum Modification Level (%)	Raw File Name
9/21/2022 by Silvia	C:\Users\Silvia\Desktop\BPF DataFiles\25. Nature Protocols data processing	Trypsin	17.00%	33.00%	0.0005%	SampleName

Protein	Residue #	Modification	Category	Comment	Normalized Time Shift	Predicted Time Shift	Peptides	Peptide Sequence
1	Heavy Chain	1 ~Q1+Deamidation	+Deamidation	None	2.1%	2.8%	1:Q1-K19 = 1976.1...	QVQLQQPGAELVK...
2	Heavy Chain	55 N55+Deamidation	+Deamidation	None	1.8%	3.2%	1:G44-K63 = 2182...	GLEWIGAIYPGNGD...
3	Heavy Chain	82 Q82+Deamidation	+Deamidation	None	0.8%	2.9%	1:S75-R98 = 2677...	SSSTAYMQLSSLTSE...
4	Heavy Chain	163 ~N163+Deamidati...	+Deamidation	Retention time off?	87.8%	1.1%	1:D152-K214 = 67...	DYFPEPVTVSWNS...
5	Heavy Chain	179 ~Q179+Deamidati...	+Deamidation	Retention time off?	74.9%	1.1%	1:D152-K214 = 67...	DYFPEPVTVSWNS...
6	Heavy Chain	207 ~N207+Deamidati...	+Deamidation	Retention time off?	64.7%	1.1%	1:D152-K214 = 67...	DYFPEPVTVSWNS...
7	Heavy Chain	290 N290+Deamidation	+Deamidation	None	3.2%	4.7%	1:F279-K292 = 167...	FNWYVDGVEVHNAK
8	Heavy Chain	319 N319+Deamidation	+Deamidation	None	3.4%	3.9%	1:V306-K321 = 18...	VVSVLTVLHQDWL...
9	Heavy Chain	329 N329+Deamidation	+Deamidation	Poor recovery	2.3%	0.0%	1:C325-K330 = 73...	CKVSNK
10	Heavy Chain	365 ~N365+Deamidati...	+Deamidation	None	11.3%	7.7%	1:N365-K374 = 11...	NQVSLTCLVK; NQV...
11	Heavy Chain	393 ~N393+Deamidati...	+Deamidation	None	1.6%	3.2%	1:G375-K396 = 25...	GFYPSDIAVEWESN...
12	Heavy Chain	423 Q423+Deamidation	+Deamidation	None	3.5%	3.9%	1:W421-K443 = 28...	WQQGNVFCFSVM...
13	Light Chain	36 ~Q36+Deamidation	+Deamidation	None	2.4%	4.6%	2:A25-K38 = 1666...	ASSSVYIHWFQQK

Modification Results

Components

Level	No.	Identification	Peptide Sequence	Modification	Site	Delta (ppm)	Confidence Score	Best Overall Average Structural Resolution	ID
1	Component	8027 1:G44-K63 = 2182.0331m	GLEWIGAIYPGNGDTSYN...	None		-0.51	100.0	1.1	MS2
2	Component	8033 1:G44-K63 = 2182.0331m	GLEWIGAIYPGNGDTSYN...	None		-0.73	100.0	1.1	MS2
3	Component	8202 1:G44-K63 = 2182.0331m(N55+Deamidati...	GLEWIGAIYPGNGDTSYN...	Deamidation	N55	-0.35	100.0	1.1	MS2
4	Component	8207 1:G44-K63 = 2182.0331m(N55+Deamidati...	GLEWIGAIYPGNGDTSYN...	Deamidation	N55	-0.23	100.0	1.2	MS2
5	Component	8413 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.3	MS2
6	Component	8416 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.54	100.0	1.1	MS2
7	Component	8417 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
8	Component	8418 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
9	Component	8419 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
10	Component	8420 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
11	Component	8421 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
12	Component	8422 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
13	Component	8423 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
14	Component	8424 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
15	Component	8425 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
16	Component	8426 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
17	Component	8427 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
18	Component	8428 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
19	Component	8429 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
20	Component	8430 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
21	Component	8431 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
22	Component	8432 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
23	Component	8433 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
24	Component	8434 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
25	Component	8435 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
26	Component	8436 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
27	Component	8437 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
28	Component	8438 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
29	Component	8439 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
30	Component	8440 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
31	Component	8441 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
32	Component	8442 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
33	Component	8443 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
34	Component	8444 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
35	Component	8445 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
36	Component	8446 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
37	Component	8447 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
38	Component	8448 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
39	Component	8449 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
40	Component	8450 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
41	Component	8451 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
42	Component	8452 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
43	Component	8453 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
44	Component	8454 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
45	Component	8455 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
46	Component	8456 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
47	Component	8457 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
48	Component	8458 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
49	Component	8459 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
50	Component	8460 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
51	Component	8461 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
52	Component	8462 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
53	Component	8463 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
54	Component	8464 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
55	Component	8465 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
56	Component	8466 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
57	Component	8467 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
58	Component	8468 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
59	Component	8469 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
60	Component	8470 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
61	Component	8471 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
62	Component	8472 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
63	Component	8473 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
64	Component	8474 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
65	Component	8475 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
66	Component	8476 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
67	Component	8477 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
68	Component	8478 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
69	Component	8479 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
70	Component	8480 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
71	Component	8481 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
72	Component	8482 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
73	Component	8483 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
74	Component	8484 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
75	Component	8485 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
76	Component	8486 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
77	Component	8487 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
78	Component	8488 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
79	Component	8489 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
80	Component	8490 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
81	Component	8491 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
82	Component	8492 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
83	Component	8493 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
84	Component	8494 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
85	Component	8495 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
86	Component	8496 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
87	Component	8497 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
88	Component	8498 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2
89	Component	8499 1:G44-K63 = 2182.0331m(N55+NH3 loss)	GLEWIGAIYPGNGDTSYN...	NH3 loss	N55	-0.43	100.0	1.1	MS2

Stage 3: Data processing, analysis and reporting_Step 16



Save Peptide Workbook As

Enter a value between 1 and 10.

Create a New Peptide Workbook Select an Existing Workbook

Workbook Name: MAM Discovery Phase Chimeric IgG1_DP

Description:

Number of Isotopes per Peptide: 4

Save Cancel

Stage 3: Data processing, analysis and reporting_Step 17

The screenshot shows a software interface with a top navigation bar containing several menu items: Home, Peptide Mapping Analysis, Load Results, Queue, Parameters, Process and Review, Mapping, and Target Peptide Workbook. Below this is a 'Workbook Manager' section with a search bar and buttons for Edit, Export, and Import. A table lists workbooks with columns for Name, Category, Creation Date and Time, Last Modified Time, Number of Entities, Number of Groups, and Description. One workbook is listed: 'MAM Discovery Phase Chimeric IgG1_DP' under the 'Targeted Peptide' category. A 'Save As' dialog box is open in the foreground, showing the file path 'This PC > OS (C:) > Xcalibur > data'. The file name is 'MAM Discovery Phase Chimeric IgG1_DP_peptide' and the save type is 'BioPharma Workbook (.wbpf)'. The dialog box also shows a list of folders on the left and a search bar at the top.

Name	Category	Creation Date and Time	Last Modified Time	Number of Entities	Number of Groups	Description
MAM Discovery Phase Chimeric IgG1_DP	Targeted Peptide	11/05/2021 11:52 AM	11/05/2021 12:44 PM	80	14	

Stage 3: Data processing, analysis and reporting_Step 18

ChimericIg DP vs BS_SeqVariant

Name	Type	Level	Position	Volume	Instrument Method	Processing Method	Status	Inject Time	Lock Status	Weight	Dilution	IntStd	Replicate ID	Comment	Re-injections	Spike G
clgG1 DP_1	Unknown		0	1.0000	MAM	Proc Method_SeqVari...	Idle			1.0000	1.0000	1.0000			0	
clgG1 DP_2	Unknown			1.0000	MAM	Proc Method_SeqVari...	Finished	8/6/2020 3:15:56 PM +...		1.0000	1.0000	1.0000			0	
clgG1 DP_3	Unknown			1.0000	MAM	Proc Method_SeqVari...	Finished	8/6/2020 7:17:44 PM +...		1.0000	1.0000	1.0000			0	
clgG1 BS_1	Unknown			1.0000	MAM	Proc Method_SeqVari...	Finished	8/6/2020 11:19:32 PM...		1.0000	1.0000	1.0000			0	
clgG1 BS_2	Unknown			1.0000	MAM	Proc Method_SeqVari...	Finished	8/7/2020 4:27:08 AM +...		1.0000	1.0000	1.0000			0	
clgG1 BS_3	Unknown			1.0000	MAM	Proc Method_SeqVari...	Finished	8/7/2020 8:29:08 AM +...		1.0000	1.0000	1.0000			0	
clgG1 BS_3	Unknown			1.0000	MAM	Proc Method_SeqVari...	Finished	8/7/2020 12:31:08 PM...		1.0000	1.0000	1.0000			0	

Create Processing Method

Specify the layout and/or default settings of the new Processing Method by choosing a template or an existing Processing Method.

Choose a Processing Method template

Processing Method Layout Templates

- Basic Quantitative
- Quantitative
- 3D Quantitative
- MS.Quantitative...**
- Qualitative

Default Processing Method Templates

- 7-Anion Retention Time Std
- 6-Cation Retention Time Std

Choose existing Processing Method

More...

MAM Proc ...

Next >> Cancel

Stage 3: Data processing, analysis and reporting_Step 18

The screenshot displays the Proteome Discoverer interface during data processing. The left sidebar shows the workflow: Data Processing, Non-Targeted MS Processing, Intact Protein Deconvolution, and Report Designer. The main window is divided into several panels:

- Compound Data Import:** A table listing peptides and their isotopes. 63 out of 63 peptides are selected (540 isotopes).
- MS Component Table:** A table showing the results of MS detection for selected peptides.
- Chromatogram:** A plot of counts vs. time (min) showing a peak at RT=17.46 with an area of 2479079.
- Mass Spectrum:** A plot of relative intensity (%) vs. m/z for the peak at RT=17.46 min. The base peak is at m/z 987.0555.

Compound Data Import Table:

Name	RT	Charge	PrecursorMass	Isotope 1	Isotope 2	Isotope 3	Isotope 4
VSNK	1.600	1	447.25620	447.25620	448.25900	449.26130	450.26360
VSN[Deamidation]K	1.967	1	448.24020	448.24020	449.24300	450.24530	451.24760
EEM[Oxidation]TK	2.156	1	653.28110	653.28110	654.28390	655.28270	656.28400
C[Carboxymethylation]KVSNK	4.590	2	327.14420	327.14420	327.64560	328.14490	328.64560
C[Carboxymethylation]KVS[N[Deamidation]K	6.637	2	368.68650	368.68650	369.18790	369.68750	370.18800
EEMTK	8.254	1	637.28620	637.28620	638.28900	639.28770	640.28900
EEQYN[A2Ga2F]STYR	9.290	2	1641.63220	1642.13380	1642.63520	1641.63220	1643.13670
EEQYN[A3G3F]STYR	9.298	3	1108.43280	1108.76710	1109.10140	1108.43280	1109.43570
EEQYN[A2Ga1G1F]STYR	9.363	2	1560.60580	1561.10730	1561.60880	1560.60580	1562.11020
EEQYN[A2G0F]STYR	9.374	2	1040.73960	1041.07400	1041.40830	1040.73960	1041.74250
EEQYN[A2G2F]STYR	9.374	2	1317.52660	1318.02810	1317.52660	1318.52950	1319.03090
EEQYN[A3G2F]STYR	9.381	2	878.68680	879.02120	878.68680	879.35540	879.68970
EEQYN[A3G2F]STYR	9.381	2	1581.11910	1581.62060	1582.12210	1581.11910	1582.62350
EEQYN[A2G2F]STYR	9.381	2	1054.41510	1054.74950	1055.08380	1054.41510	1055.41800
EEQYN[A2G2F]STYR	9.381	2	1479.57940	1480.08090	1480.58240	1479.57940	1481.08380

MS Component Table:

#	Name	Ret.Time	Window	Ref.Mass.Spec.	Peak.Mass.Spec.Filter	Ref.Mass.Spec.Settings	Channel	Eval.Type	Stand.Meth.	Cal.Type	Conc.Unit
46	EEQYN[A1G1F]STYR	17.457	0.500 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	1.
47	(+3) EEQYN[A1G1F]STYR	17.457	0.500 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	1.
48	EEQYN[A2G2F]STYR	17.472	0.500 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	1.
49	(+2) EEQYN[A2G2F]STYR	17.472	0.500 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	1.

Stage 3: Data processing, analysis and reporting_Step 19

The screenshot displays the Chromeleon Console interface. At the top, the window title is 'ChimericG DP vs BS_SeqVariant'. Below the title bar is a menu bar with 'Create', 'File', 'Edit', 'View', 'Tools', and 'Help'. The main area shows a data table with the following columns: #, Name, Type, Date Modified, and Comment. The table contains four rows of data. Below the table, there are sections for 'Associated Items', 'Custom Sequence Variables (0)', and 'Custom Formulas'. On the left side, there is a sidebar with a tree view showing folders and files. At the bottom, there is a status bar with 'eWork' and other icons.

#	Name	Type	Date Modified	Comment
1	ChimericG DP vs BS_SeqVari...	Electronic Report	11/10/2021 10:24:43 AM +01:00	
2	Default	View Settings	10/8/2020 10:04:03 AM +01:00	
3	MAM Processing Method View	View Settings	11/6/2020 2:45:10 PM +00:00	
4	MAM Report IgG1BS CQAs_01	Report Template	11/11/2021 5:19:53 PM +01:00	

Stage 3: Data processing, analysis and reporting_Step 19

ChimericG DP vs BS_SeqVariant (Sequence) - Chromeleon Chromatography Studio

Data Processing

Injections

- ChimericG1 DP_1
- ChimericG1 DP_2
- ChimericG1 DP_3
- ChimericG1 BS_1
- ChimericG1 BS_2
- ChimericG1 BS_3

Channels

- MS Quantitation
- TIC

Components (18 of 151)

- PKDTLMISR
- (+3) PKDTLMISR
- DTLM[Oxidation]ISR
- (+2) DTLM[Oxidation]ISR
- (+1) DTLM[Oxidation]ISR
- DTLMISR
- (+2) DTLMISR
- (+1) DTLMISR
- GLEWIGAIYPGNGDTSYNQK
- (+3) GLEWIGAIYPGNGDTSYNQK
- (+4) GLEWIGAIYPGNGDTSYNQK
- (+2) GLEWIGAIYPGNGDTSYNQK
- GLEWIGAIYPGN[Deamidation]GDSYNQK
- (+2) GLEWIGAIYPGN[Deamidation]GDSYNQK
- (+3) GLEWIGAIYPGN[Deamidation]GDSYNQK
- GLEWIGAIYPGN[NH3 loss]GDSYNQK
- (+2) GLEWIGAIYPGN[NH3 loss]GDSYNQK

Chromatogram

5 - ChimericG DP vs BS_SeqVariant #1 [manually integrated] RT=59.91; Area=4477872834.

4 - ChimericG DP vs BS_SeqVariant #1 RT=59.91; Area=1448967649.

3 - ChimericG DP vs BS_SeqVariant #1 RT=59.91; Area=1237427799.

2 - ChimericG DP vs BS_SeqVariant #1 RT=59.91; Area=946862085.

1 - ChimericG DP vs BS_SeqVariant #1 RT=59.87; Area=435775970.

Mass Spectra

Apex GLEWIGAIYPGNGDTSYNQK Scan: #5626 RT: 59.91 min NL: 9.99E+007 Apex

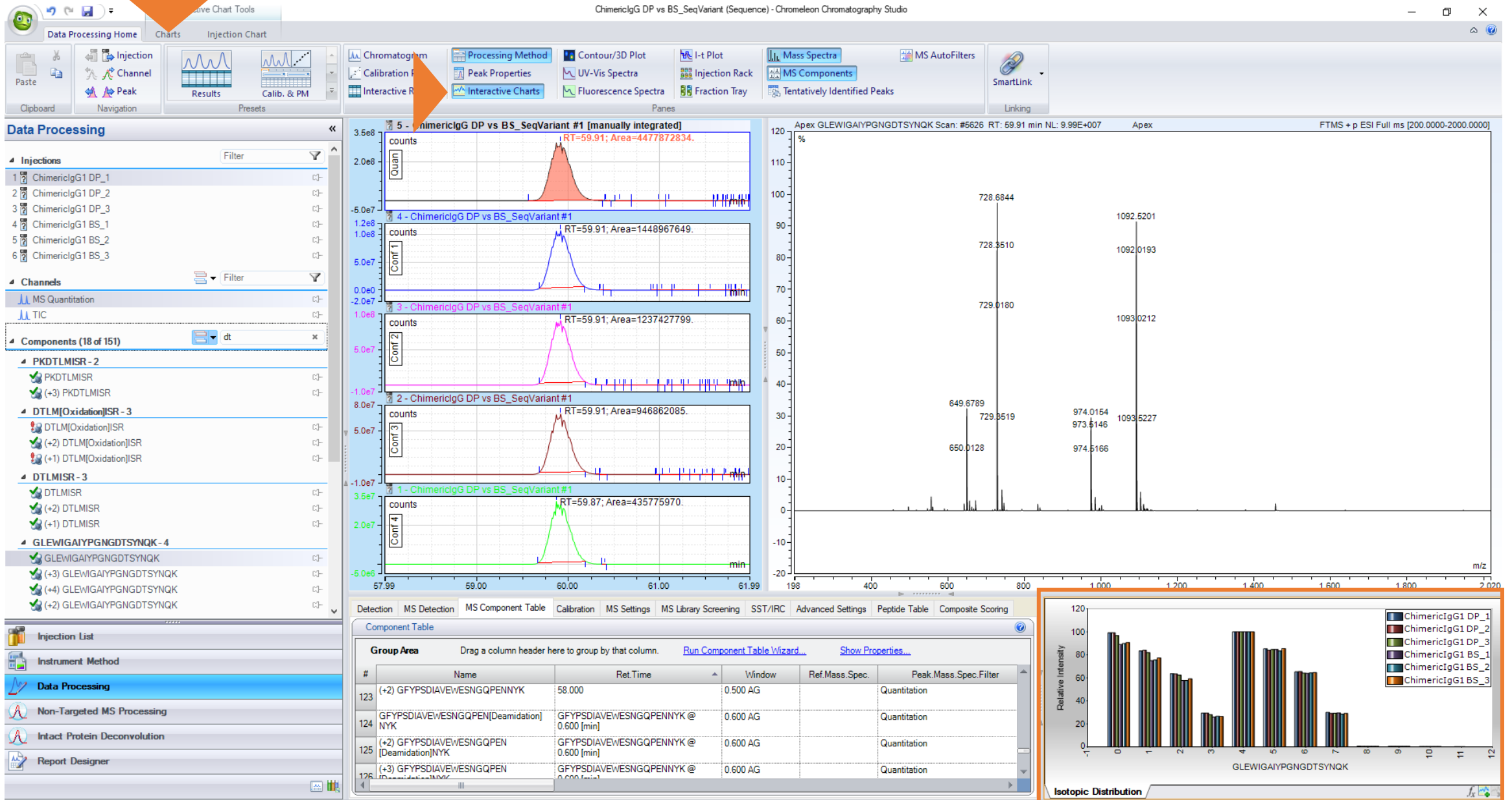
FTMS + p ESI Full ms [200.0000-2000.0000]

728.6844, 728.3510, 729.0180, 1092.5201, 1092.0193, 1093.0212, 649.6789, 650.0128, 974.0154, 974.5166, 1093.6227

Component Table

#	Name	Ret.Time	Window	Ref.Mass.Spec.	Peak.Mass.Spec.Filter	Het.Mass.Spec.Settings	Channel	Eval.Type	Stand.Meth.	Cal.Type	Conc.Unit
123	(+2) GFYPSDIAVEWESNGQPENNYK	58.000	0.500 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
124	GFYPSDIAVEWESNGQPEN[Deamidation]NYK	GFYPSDIAVEWESNGQPENNYK @ 0.600 [min]	0.600 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
125	(+2) GFYPSDIAVEWESNGQPEN[Deamidation]NYK	GFYPSDIAVEWESNGQPENNYK @ 0.600 [min]	0.600 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
126	(+3) GFYPSDIAVEWESNGQPEN[Deamidation]NYK	GFYPSDIAVEWESNGQPENNYK @ 0.600 [min]	0.600 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
127	GFYPSDIAVEWESN[NH3 loss]GQPENNYK	GFYPSDIAVEWESNGQPENNYK @ 1.600 [min]	0.600 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
128	(+2) GFYPSDIAVEWESN[NH3 loss]GQPENNYK	GFYPSDIAVEWESNGQPENNYK @ 1.600 [min]	0.600 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
129	(+3) GFYPSDIAVEWESN[NH3 loss]GQPENNYK	GFYPSDIAVEWESNGQPENNYK @ 1.600 [min]	0.600 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
130	GLEWIGAIYPGNGDTSYNQK	59.990	0.500 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	
131	(+3) GLEWIGAIYPGNGDTSYNQK	59.990	0.500 AG		Quantitation	SI:0, RSI:0	All Channels	Area	External	Lin, WithOffset	

Stage 3: Data processing, analysis and reporting_Step 20



Stage 3: Data processing, analysis and reporting_Step 21-24

ChimericG DP vs BS_SeqVariant (Sequence) - Chromeleon Chromatography Studio

Home | Processing | Chromatogram Plot | Start | Idle | Score All Injections

Clipboard | Navigation | Panes | Processing | Status | Scoring

Non-Targeted MS Processing

Injections

- ChimericG1 DP_1
- ChimericG1 DP_2
- ChimericG1 DP_3
- ChimericG1 BS_1
- ChimericG1 BS_2
- ChimericG1 BS_3

Channels

- Aligned Base Peak
- Reference Base Peak
- Unaligned Base Peak

Frames

Processing Methods

- MAM Proc Method_SeqVariant_01

Processing Method: Alignment Detection

Reference Injection: Relative 1 Fixed

Frame Parameters:

- m/z Min: 200.00
- m/z Max: 1,800.00
- m/z Width [ppm]: 10.00
- Retention Time Start [min]: 1.00
- Retention Time Stop [min]: 90.00
- Frame Time Width [min]: 1.00
- Maximum Number of Frames: 5,000
- Peak Intensity Threshold: Fixed 1,000,000 Auto-compute
- Scan Filter(s): TIC

Start

Advanced... Reset

No results found.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Frame ID	Component ID	Mass	RT	Ratio	Base Component	PR Element	PR Root	PR Size	Charge	Molecular Weight							
2			m/z	min							m/z							
5	There are no frames																	
6																		
7																		
8																		
9																		
10																		
11																		
12																		
13																		
14																		
15																		
16																		
17																		
18																		
19																		
20																		

Injection List | Instrument Method | Data Processing | **Non-Targeted MS Processing** | Intact Protein Deconvolution | Report Designer

Frame Table | Frame Filter

Stage 3: Data processing, analysis and reporting_Step 25-26

ChimericG DP vs BS_SeqVariant (Sequence) - Chromeleon Chromatography Studio

Home | Injection | Processing | Chromatogram Plot | Start | Start All | Idle | Score All Injections

Clipboard | Navigation | Panes | Processing | Status | Scoring

Non-Targeted MS Processing

Injections

- 1 ChimericG1 DP_1
- 2 ChimericG1 DP_2
- 3 ChimericG1 DP_3
- 4 ChimericG1 BS_1
- 5 ChimericG1 BS_2
- 6 ChimericG1 BS_3

Channels

- Aligned Base Peak
- Reference Base Peak
- Unaligned Base Peak

Frames

Processing Methods

- MAM Proc Method_SeqVariant_01

Reference Injection: Relative 1 Fixed

Frame Parameters:

- m/z Min: 200.00
- m/z Max: 1,800.00
- m/z Width [ppm]: 10.00
- Retention Time Start [min]: 1.00
- Retention Time Stop [min]: 90.00
- Frame Time Width [min]: 1.00
- Maximum Number of Frames: 5,000
- Peak Intensity Threshold: Fixed 1,000,000 Auto-compute TIC 0.00 %

Scan Filter(s):

Advanced... Reset

No results found.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Frame ID	Component ID	Mass	RT	Ratio	Base Component	PR Element	PR Root	PR Size	Charge	Molecular Weight							
2			m/z	min							m/z							
5	There are no frames																	

Frame Filter

Match ALL of the following rules:

- PR Element = 0
- PR Size > 1
- Charge is between 1 and 2
- Ratio > 1000.00000

and

Injection List | Instrument Method | Data Processing | **Non-Targeted MS Processing** | Intact Protein Deconvolution | Report Designer

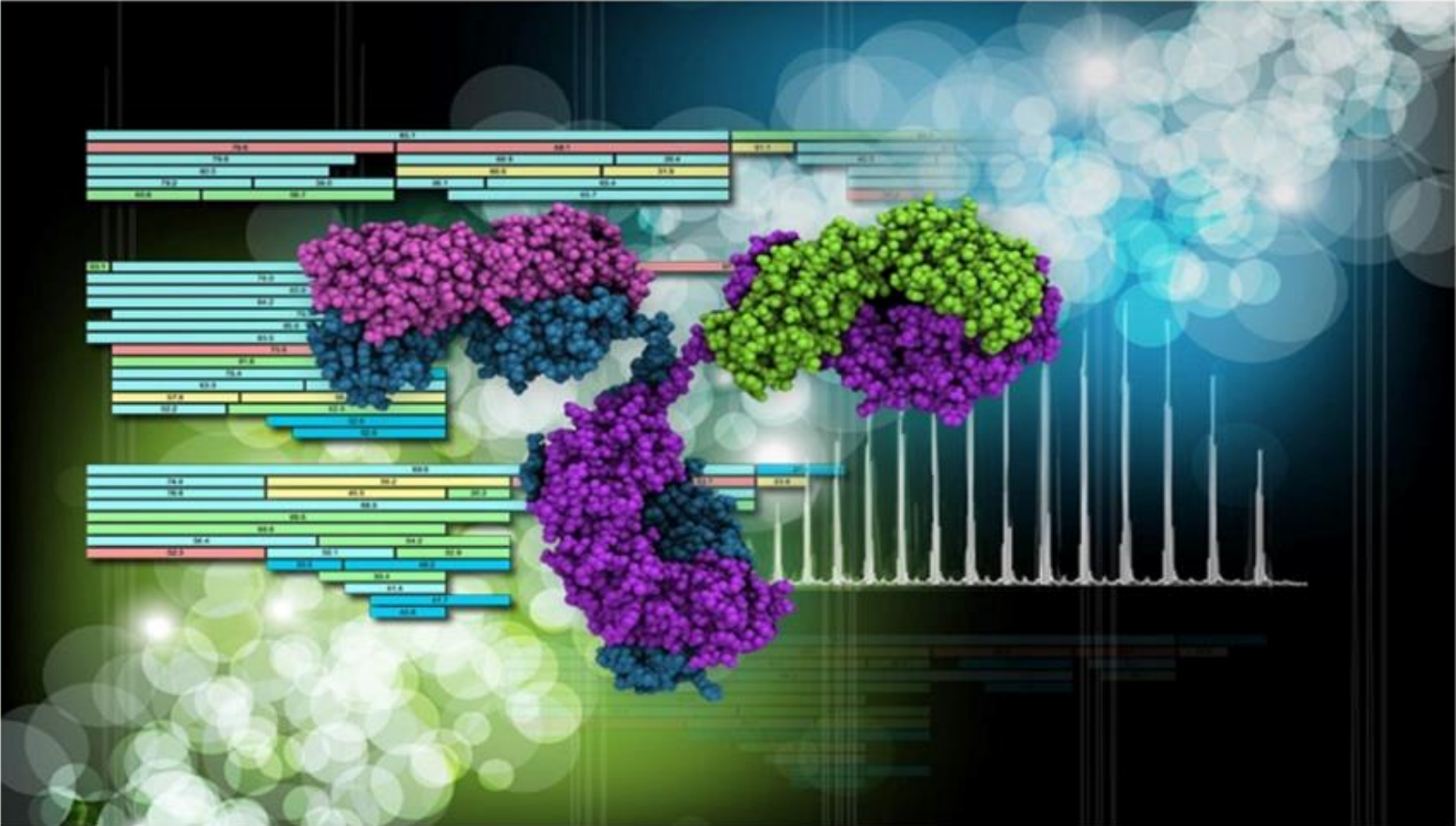
Stage 3: Data processing, analysis and reporting_Step 27

Home

Select an experiment type.

Experiment Types

- Sequence Manager >
- Peptide Mapping Analysis >
- Oligonucleotide Analysis >
- Intact Mass Analysis >
- Top Down Analysis >



Peptide Mapping Analysis Oligonucleotide Analysis Intact Mass Analysis Top Down Analysis

Stage 3: Data processing, analysis and reporting_Step 28

The screenshot shows the Chromeleon Console interface. The 'Data' menu is open, with 'Report Template...' selected. The 'New Report Template' dialog box is displayed, showing a list of default templates under 'Thermo Scientific Templates'. The 'Empty Template' option is highlighted with a blue box. An orange arrow points from the 'Report Template...' menu item to the dialog box. Another orange arrow points from the 'Empty Template' box to the right. The background shows a data table with columns: Type, Level, Position, Volume, Instrument Method, Processing Method, Status, Inject Time, Lock Status, Weight, Dilution, IntStd, Replicate ID, Comment, Re-injections, and Spike G.

Type	Level	Position	Volume	Instrument Method	Processing Method	Status	Inject Time	Lock Status	Weight	Dilution	IntStd	Replicate ID	Comment	Re-injections	Spike G
ChimericIgG DP_1	Unknown		1.0000	MAM	Proc Method_SeqVari...	Finished	8/6/2020 3:15:56 PM +...		1.0000	1.0000	1.0000			0	
ChimericIgG DP_2	Unknown		1.0000	MAM	Proc Method_SeqVari...	Finished	8/6/2020 7:17:44 PM +...		1.0000	1.0000	1.0000			0	
ChimericIgG DP_3	Unknown		1.0000	MAM	Proc Method_SeqVari...	Finished	8/6/2020 11:19:32 PM...		1.0000	1.0000	1.0000			0	
ChimericIgG BS_1	Unknown		1.0000	MAM	Proc Method_SeqVari...	Finished	8/7/2020 4:27:08 AM +...		1.0000	1.0000	1.0000			0	
ChimericIgG BS_2	Unknown		1.0000	MAM	Proc Method_SeqVari...	Finished	8/7/2020 8:22:06 AM...		1.0000	1.0000	1.0000			0	
ChimericIgG BS_3	Unknown		1.0000	MAM	Proc Method_SeqVari...	Finished	8/7/2020 8:22:06 AM...		1.0000	1.0000	1.0000			0	

Stage 3: Data processing, analysis and reporting_Step 29-32

ChimericIg DP vs BS_SeqVariant (Sequence) - Chromeleon Chromatography Studio

Home Insert Page Layout

Blank All Sheets... Integration Peak Summary All Tables... Sequence Injection Chromatogram All Variables... Chromatogram Calibration All Plots... Retention Time Column Performance All Charts... Line Column All Charts... Picture Shapes

Sheets Report Tables Report Variables Plots Result Charts General Charts Illustrations

Report Designer

- (+5) WQQGNVFSC[Carboxymethylation]SVMHEALHNHYTQKSLSPG
- SSSTAYM[Oxidation]QLSSLTSEDSAVYYC[Carboxymethylation]AR
- (+3) SSSTAYM[Oxidation]QLSSLTSEDSAVYYC[Carboxymethylation]AR
- SSSTAYM[Oxidation]QLSSLTSEDSAVYYC[Carboxymethylation]AR
- (+3) SSSTAYM[Oxidation]QLSSLTSEDSAVYYC[Carboxymethylation]AR
- SSSTAYMQLSSLTSEDSAVYYC[Carboxymethylation]AR
- (+2) SSSTAYMQLSSLTSEDSAVYYC[Carboxymethylation]AR
- (+3) SSSTAYMQLSSLTSEDSAVYYC[Carboxymethylation]AR
- (+4) SSSTAYMQLSSLTSEDSAVYYC[Carboxymethylation]AR
- GFYPSDIAVEWESNGQPENNYK
- (+3) GFYPSDIAVEWESNGQPENNYK
- (+4) GFYPSDIAVEWESNGQPENNYK
- (+2) GFYPSDIAVEWESNGQPENNYK
- GFYPSDIAVEWESNGQPEN[Deamidation]NYK
- (+2) GFYPSDIAVEWESNGQPEN[Deamidation]NYK
- (+3) GFYPSDIAVEWESNGQPEN[Deamidation]NYK
- GFYPSDIAVEWESN[NH3 loss]GQPENNYK
- (+2) GFYPSDIAVEWESN[NH3 loss]GQPENNYK
- (+3) GFYPSDIAVEWESN[NH3 loss]GQPENNYK
- GLEWIGAIYPGNGDTSYNQK
- (+3) GLEWIGAIYPGNGDTSYNQK
- (+4) GLEWIGAIYPGNGDTSYNQK
- (+2) GLEWIGAIYPGNGDTSYNQK
- GLEWIGAIYPGN[Deamidation]GDTSYNQK
- (+2) GLEWIGAIYPGN[Deamidation]GDTSYNQK
- (+3) GLEWIGAIYPGN[Deamidation]GDTSYNQK
- GLEWIGAIYPGN[NH3 loss]GDTSYNQK
- (+2) GLEWIGAIYPGN[NH3 loss]GDTSYNQK
- (+3) GLEWIGAIYPGN[NH3 loss]GDTSYNQK

Report Templates

- MAM Report IgG1BS CQAs_01
- MAM Report SeqVariant_01

Injection List

Instrument Method

Data Processing

Non-Targeted MS Processing

Intact Protein Deconvolution

Report Designer

B43

	A	B	C	D	E	F	G	H	I	J	K	
1	Sequence Overview											
2												
3	Sequence details											
4	Name:		ChimericIg DP vs BS_SeqVariant						Created on:		8/27/2020	
5	Instrument:								Updated on:			
6	Imported data:		True									
7	First Injection:											
8	Processing Method:		MAM									
9	MS Acquisition Time (min):		120.02									
10												
11	DataVault:		ChromeleonLocal						Created by:		Sivia Millán	
12	Number of Injections:		6						Updated by:			
13												
14												
15												
16												
17	No.	Injection Name	Position	Type	Instrument Method	Processing Method	Inject Time	Status				
18												
19												
20												
21	1	ChimericIgG1 DP 1		Unknown	n.a.	MAM	Proc Method SeqVariant_01 06/Aug/20 15:15:56	Finished				
22	2	ChimericIgG1 DP 2		Unknown	n.a.	MAM	Proc Method SeqVariant_01 06/Aug/20 19:17:44	Finished				
23	3	ChimericIgG1 DP 3		Unknown	n.a.	MAM	Proc Method SeqVariant_01 06/Aug/20 23:19:32	Finished				
24	4	ChimericIgG1 BS 1		Unknown	n.a.	MAM	Proc Method SeqVariant_01 07/Aug/20 04:27:08	Finished				
25	5	ChimericIgG1 BS 2		Unknown	n.a.	MAM	Proc Method SeqVariant_01 07/Aug/20 08:29:08	Finished				
26	6	ChimericIgG1 BS 3		Unknown	n.a.	MAM	Proc Method SeqVariant_01 07/Aug/20 12:31:08	Finished				
27												
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< > Sequence Overview / Oxidation / Deamidation-Succinimide formation / N-Glycosylation / Composite Scoring / NPD / <

Stage 3: Data processing, analysis and reporting_Step 33

The screenshot displays the Chromeleon Chromatography Studio interface. The main window title is "ChimericG DP vs BS_SeqVariant (Sequence) - Chromeleon Chromatography Studio". The interface includes a top toolbar with options like "Print", "Page Setup", "Navigation", "Page Setup", "Autorepeat", "Scale to Fit", "Zoom", and "Close".

The left sidebar shows the "Report Designer" section with a list of report templates. The "Report Templates" section is expanded, showing two templates: "MAM Report IgG1BS CQAs_01" and "MAM Report SeqVariant_01".

The main workspace is divided into two panes. The left pane shows a list of peptide sequences with their corresponding injection numbers and modifications. The right pane shows the "Sequence Overview" report, which includes a table with the following data:

Sequence Overview		
Name:	ChimericG DP vs BS_SeqVariant	Created on: 8/2/2020
Instrument:	True	Updated on:
Injection:	True	
Processing Method:	MAM (RuminAb Proc Method, SeqVariant_01)	
MS Acquisition Time (min):	125.02	
Default:	Chromatogram	Created by: Steve Miller
Number of Injections:	6	Updated by:

The "Print" dialog box is open, showing the "Apply to" section with "Current Injection" selected. The "Printer" is set to "Microsoft Print to PDF". The "Select sheets to be printed" section contains a table with the following data:

Sheet Name	Print
Sequence Overview	<input checked="" type="checkbox"/>
Oxidation	<input checked="" type="checkbox"/>
Deamidation-Succinimi...	<input checked="" type="checkbox"/>
N-Glycosylation	<input checked="" type="checkbox"/>
Composite Scoring	<input checked="" type="checkbox"/>
NPD	<input checked="" type="checkbox"/>

The bottom status bar shows the current report view: "Sequence Overview | Oxidation | Deamidation-Succinimide formation | N-Glycosylation | Composite Scoring | NPD".