

Targeted metabolite Analysis using Skyline

Nirpendra Singh, Ph.D.

[InStem]

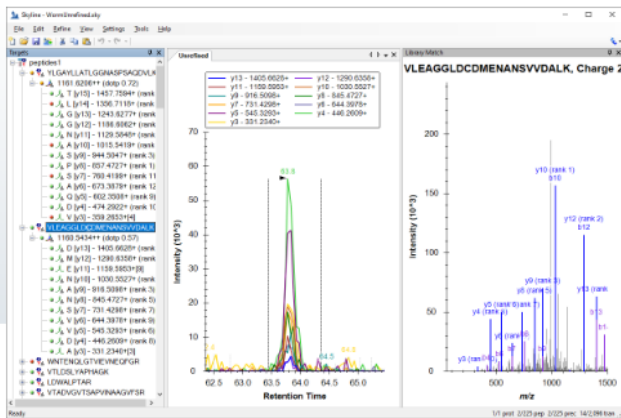


Skyline

Skyline Targeted Mass Spec Environment

[Check out the Presentations](#) from the Skyline User Group Meeting
at ASMS Anaheim, CA (June 2, 2024)

[Watch Videos](#) of the latest Skyline Tutorial Webinars
DIA to SRM, Ion Mobility, Calibrated Quant, and much more



Tutorial: Targeted Method Refinement Refine a broad set of SRM measurements, importing instrument data, and refining the document. Start with an unrefined document requiring over 2000 transitions and 39 injections to measure unscheduled on a Thermo TSQ. Learn how to import all 39 injections into a single replicate. Use the Skyline refinement dialog to remove all but the best transitions for the highest confidence peaks. (28 pages)

Download & Install:

Skyline 24.1 - 64 bit

Skyline-daily (beta)


External Tools

Skyline is a freely-available and [open source](#) Windows client application for building Selected Reaction Monitoring (SRM) / Multiple Reaction Monitoring (MRM), Parallel Reaction Monitoring (PRM), Data Independent Acquisition (DIA/SWATH) and DDA with MS1 quantitative methods and analyzing the resulting mass spectrometer data. It aims to employ cutting-edge technologies for creating and iteratively refining targeted methods for large-scale quantitative mass spectrometry studies in life sciences.

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Get Started


Webinars



- **New!** Using DIA Data To Create SRM Methods
- Analysis of diaPASEF Data With Skyline
- Using Skyline Batch for Large-Scale DIA
- Ion Mobility Spectrum Filtering with Skyline
- DIA/SWATH Data Analysis in Skyline Revisited

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Tutorials



- Grouped Study Data Processing
- Small Molecule Targets
- Data Independent Acquisition
- Creating Chromatogram Libraries with Panorama

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Skyline

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Skyline

File Edit Refine Vie



Targets

.....

Blank Document



Import Transition List

Open File

Show start page at startup

.....



File Edit Refine View

Targets

.....

- Settings
- Tools
- Help
- ✓ Default
- Save Current...
- Edit List...
- Share...
- Import...
- Molecule Settings...
- Transition Settings...
- Document Settings...
- Integrate All

Type here to search

25°C Mostly clear 21:08 24-06-2024

.....



⚙️

- Proteomics interface
- Molecule interface
- Mixed interface

Show all menus and controls

File Edit Refine View Settings Tools Help

Targets

- Undo Ctrl+Z
- Redo Ctrl+Y
- Cut Ctrl+X
- Copy Ctrl+C
- Paste Ctrl+V
- Delete Del
- Select All Ctrl+A
- Find... Ctrl+F
- Find Next F3
- Edit Note Shift+F2
- Integration
- Insert** ▶ Transition List...
- Expand All ▶
- Collapse All ▶
- Set Standard Type ▶
- Modify Molecule...
- Unique Molecules...
- Edit Spectrum Filter...
- Manage Results... Ctrl+R

Insert Transition List



Press Ctrl-V to paste here.

Cancel

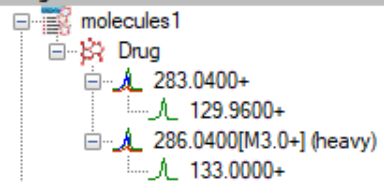


Transition setting

1	Molecule List	Molecule Name	Label Type	Precursor m/z	Precursor Charge	Product m/z	Product Charge	Cone Voltage	Explicit Collision	Explicit Retention Time
2	DrugX	Drug	light	283.04	1	129.96	1	26	16	2.7
3	DrugX	Drug	heavy	286.04	1	133	1	26	16	2.7



Targets



Import Transition List: Identify Columns

Molecule List Name	Molecule Name	Label Type	Precursor m/z	Precursor Charge	Product m/z	Product Charge	Cone Voltage	Explicit Collision Energy	Explicit Retention Time
Molecule Li... ▾	Molecule Name ▾	Label Type ▾	Precursor m/z ▾	Precursor Charge ▾	Product m/z ▾	Product Charge ▾	Cone Voltage ▾	Explicit Collisio... ▾	Explicit Retenti... ▾
DrugX	Drug	light	283.04	1	129.96	1	26	16	2.7
DrugX	Drug	heavy	286.04	1	133	1	26	16	2.7

Peptides Molecules Show unused columns



Targets

- 📄 molecules1
 - 📄 Drug
 - 📄 283.0400+
 - 📄 129.9600+
 - 📄 286.0400[M3.0+] (heavy)
 - 📄 133.0000+



File Edit Refine View

Settings Tools Help



Targets

- molecules1
 - Drug
 - 283.0400+
 - 129.9600+
 - 286.0400[M3.0+] (he
 - 133.0000+

- Default
- Save Current...
- Edit List...
- Share...
- Import...
- Molecule Settings...
- Transition Settings...**
- Document Settings...
- Integrate All



Targets

Target list showing a hierarchy of molecules and their associated peaks:

- molecules1
 - Drug
 - 283.0400+
 - 129.9600+
 - 286.0400[M3.0+] (heavy)
 - 133.0000+

Transition Settings

Prediction Filter Library Instrument Full-Scan Ion Mobility

Precursor mass: Monoisotopic
Product ion mass: Monoisotopic

Collision energy: Waters Xevo
Declustering potential: None

Optimization library: None
Compensation voltage: None

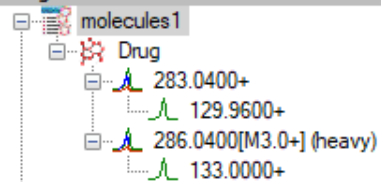
 Use optimization values when present

Optimize by:
Transition

OK Cancel



Targets



Transition Settings

Prediction Filter Library Instrument Full-Scan Ion Mobility

Molecules

Precursor adducts:

[M+H]

Fragment adducts:

[M+]

Ion types:

f

Precursor m/z exclusion window:

 m/z Auto-select all matching transitions

OK

Cancel



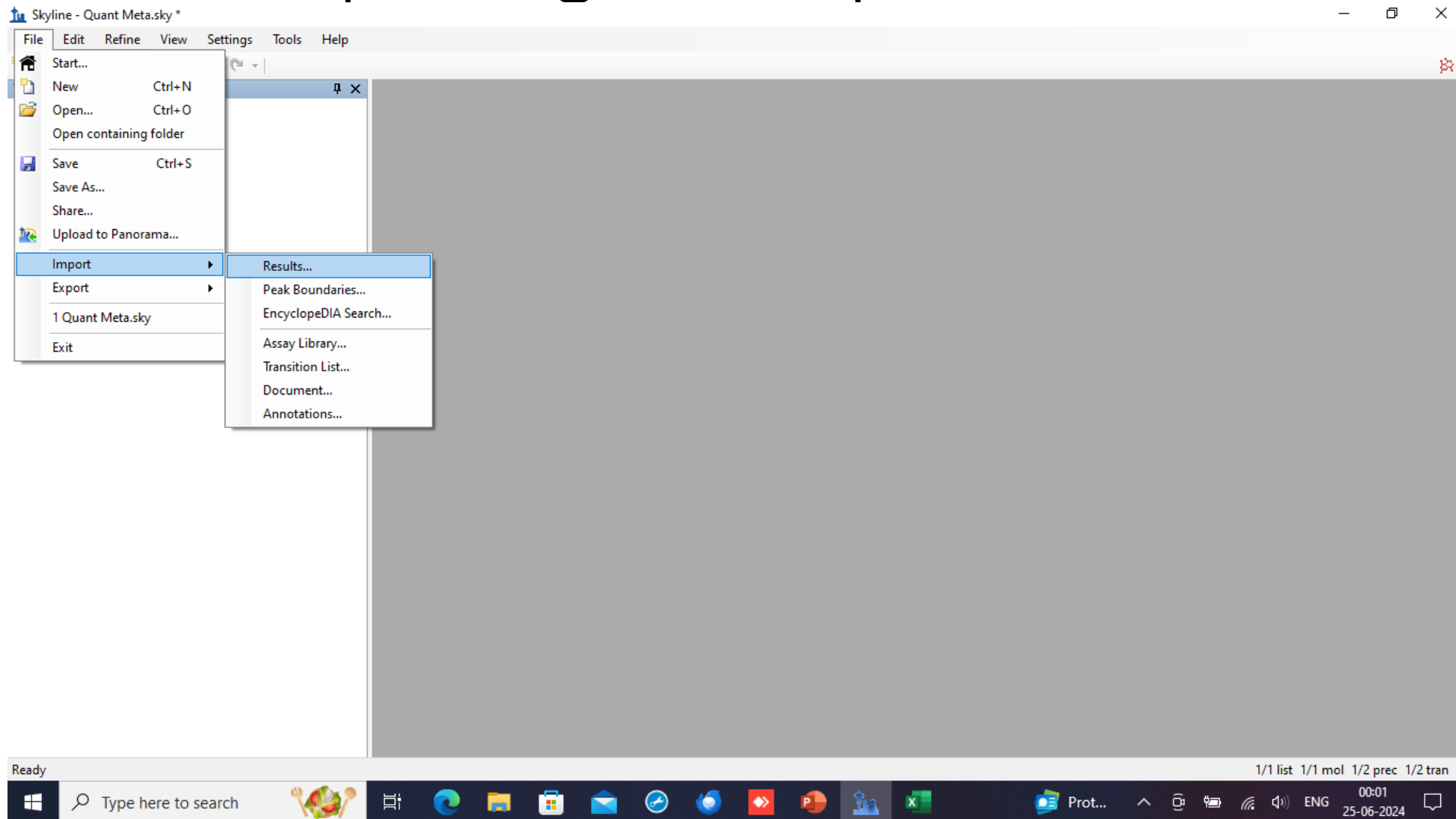
Experiment Planning

Injections were performed in this order:

- Serum Sample Injection Sequence
- double blank
 - PBS 'zero' samples
 - Calibration curve Low to High
 - Low, Mid, High QC Samples
 - Global Reference QC
 - ① 4765 Serum SPQC
 - ① NIST SRM 1950
 - Study Samples 1 to 38
 - Low, Mid, High QC Samples
 - Global Reference QC
 - ② 4765 Serum SPQC
 - Study Samples 39 to 76
 - Global Reference QC
 - ③ 4765 Serum SPQC
 - ② NIST SRM 1950
 - High, Mid, Low QC Samples
 - Calibration Curve Low to High

In all, 113 injections were used in collecting the mass spec data for these samples.

Importing mass spec runs





Targets [icon] [x]

- molecules1
 - Drug
 - 283.0400+
 - 129.9600+
 - 286.0400[M3.0+] (heavy)
 - 133.0000+

Import Results [x]

Add single-injection replicates in files OK

Optimizing:
None [v]

Add multi-injection replicates in directories

Add one new replicate
Name:
[text input]

Add files to an existing replicate
Name:
[dropdown menu]

Files to import simultaneously:
Many [v]

Show chromatograms during import

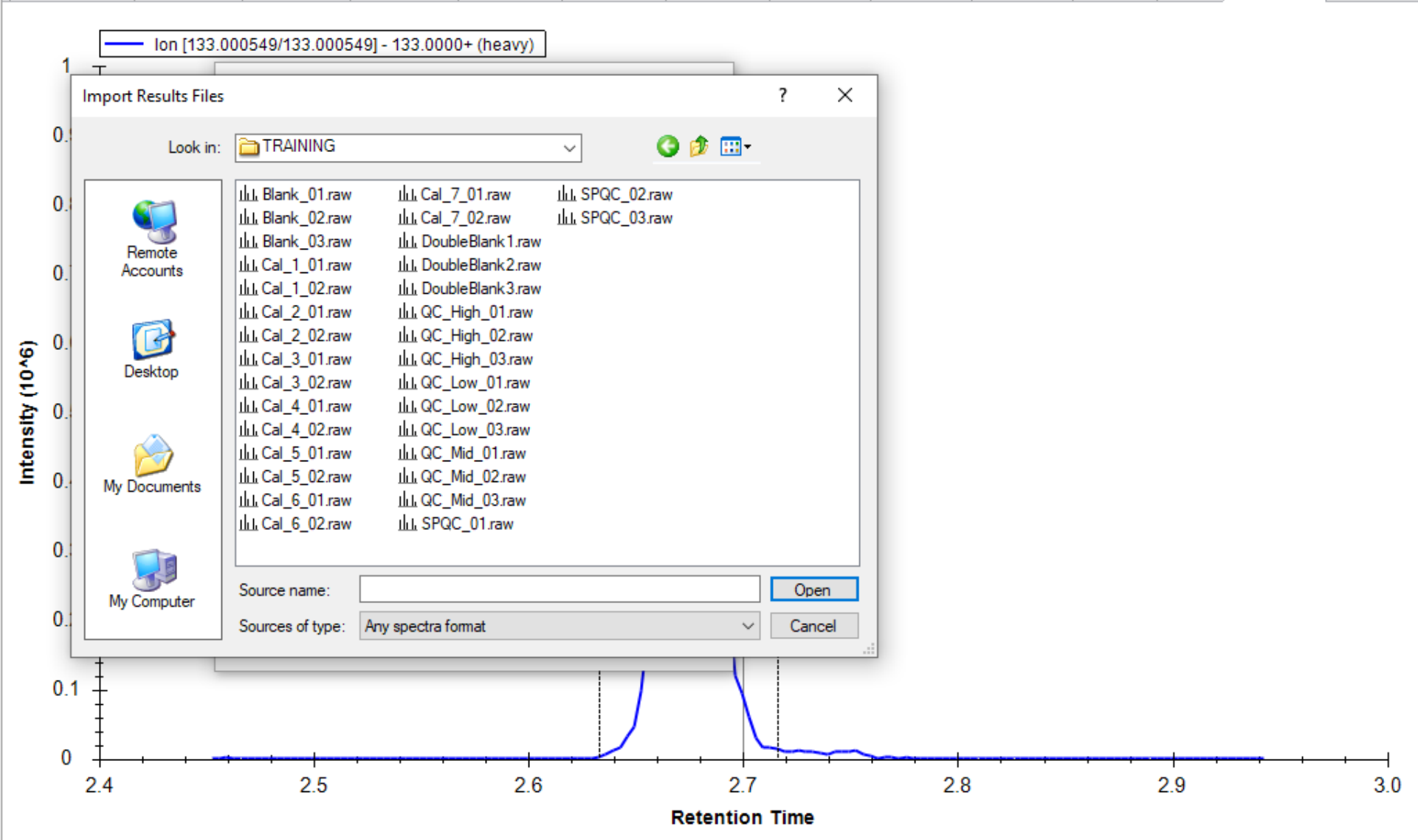
Retry after import failure

Cancel



ates: SPQC_03

- molecules1
 - Drug
 - 283.0400+ (total ratio 0.59)
 - 129.9600+[1] (ratio 0.59)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+[1]



Import Results Files

Look in: TRAINING

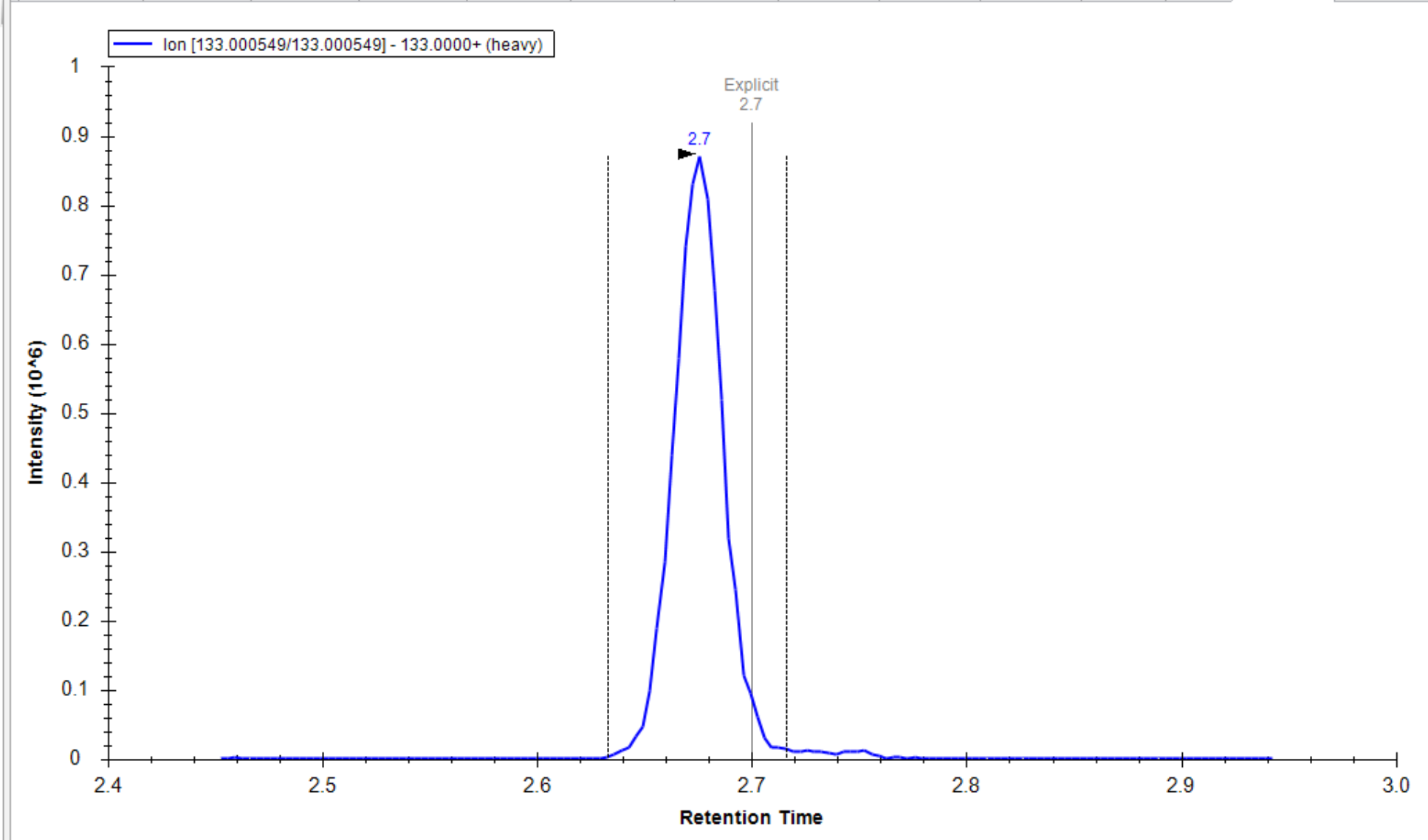
Blank_01.raw	Cal_7_01.raw	SPQC_02.raw
Blank_02.raw	Cal_7_02.raw	SPQC_03.raw
Blank_03.raw	DoubleBlank1.raw	
Cal_1_01.raw	DoubleBlank2.raw	
Cal_1_02.raw	DoubleBlank3.raw	
Cal_2_01.raw	QC_High_01.raw	
Cal_2_02.raw	QC_High_02.raw	
Cal_3_01.raw	QC_High_03.raw	
Cal_3_02.raw	QC_Low_01.raw	
Cal_4_01.raw	QC_Low_02.raw	
Cal_4_02.raw	QC_Low_03.raw	
Cal_5_01.raw	QC_Mid_01.raw	
Cal_5_02.raw	QC_Mid_02.raw	
Cal_6_01.raw	QC_Mid_03.raw	
Cal_6_02.raw	SPQC_01.raw	

Source name: Open

Sources of type: Any spectra format Cancel

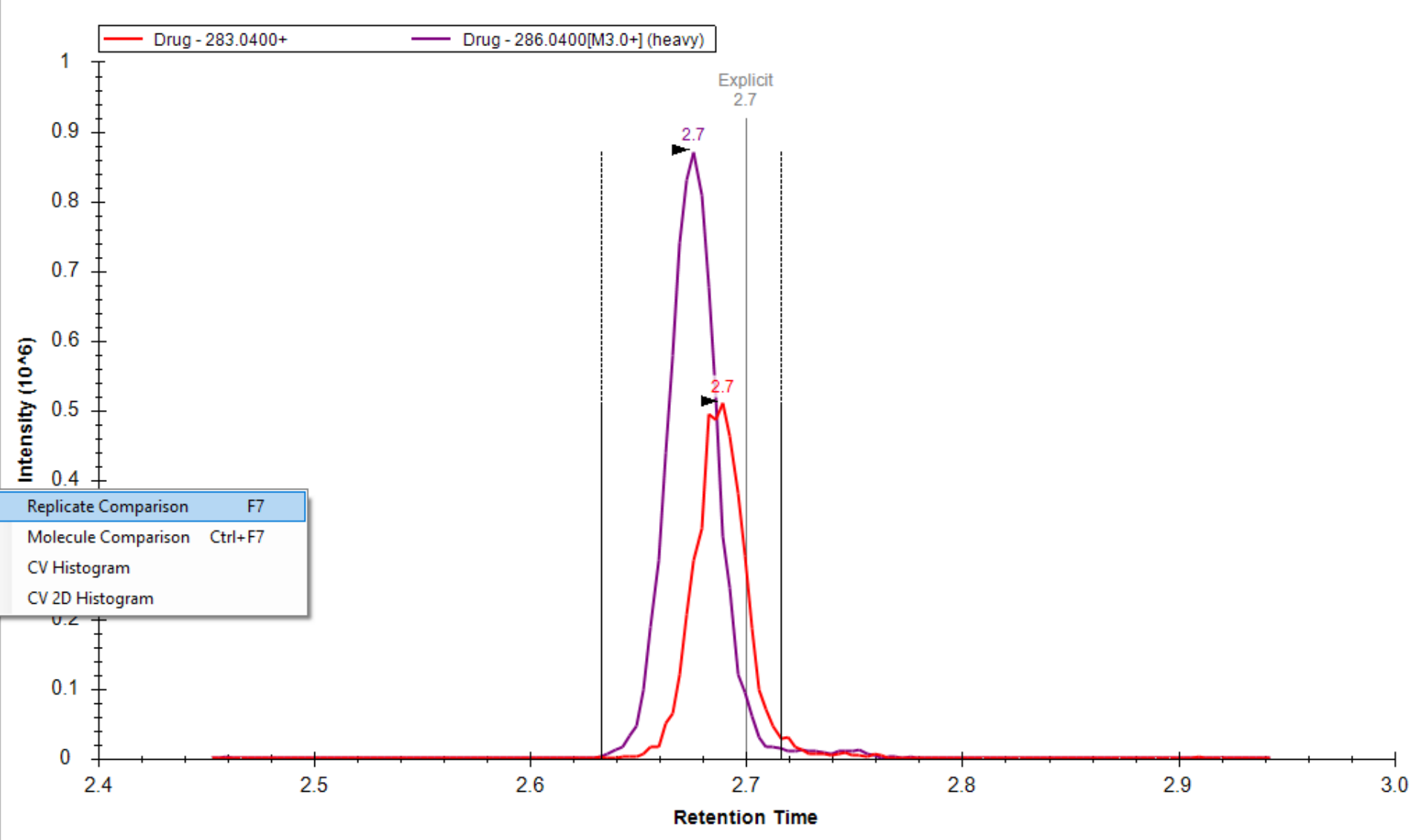
molecules1

- Drug
 - 283.0400+ (total ratio 0.59)
 - 129.9600+[1] (ratio 0.59)
 - 286.0400[M3.0+] (heavy)**
 - 133.0000+[1]



- File
 - Edit
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 - Precursor
 - Charges
 - Ranks
 - Chromatograms
 - Transitions
 - Transform
 - Auto-Zoom
 - Retention Times
 - Peak Areas
 - Replicate Comparison F7
 - Molecule Comparison Ctrl+F7
 - CV Histogram
 - CV 2D Histogram
 - Detections
 - Mass Errors
 - Calibration Curve
 - Document Grid Alt+3
 - Other Grids
- Tool Bar
 - Status Bar

DoubleBlank3 QC_High_01 QC_High_02 QC_High_03 QC_Low_01 QC_Low_02 QC_Low_03 QC_Mid_01 QC_Mid_02 QC_Mid_03 SPQC_01 SPQC_02 SPQC_03

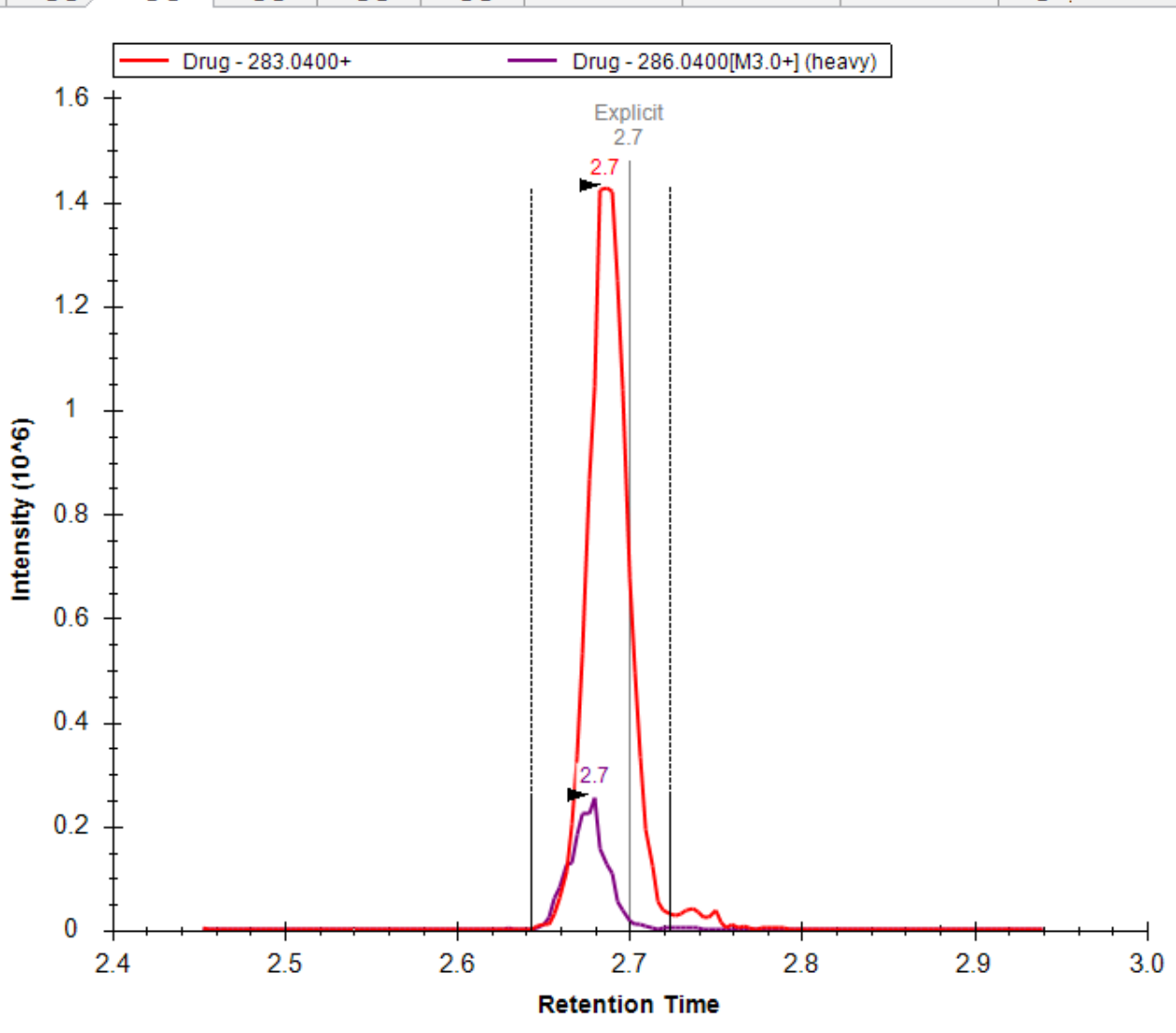


Targets

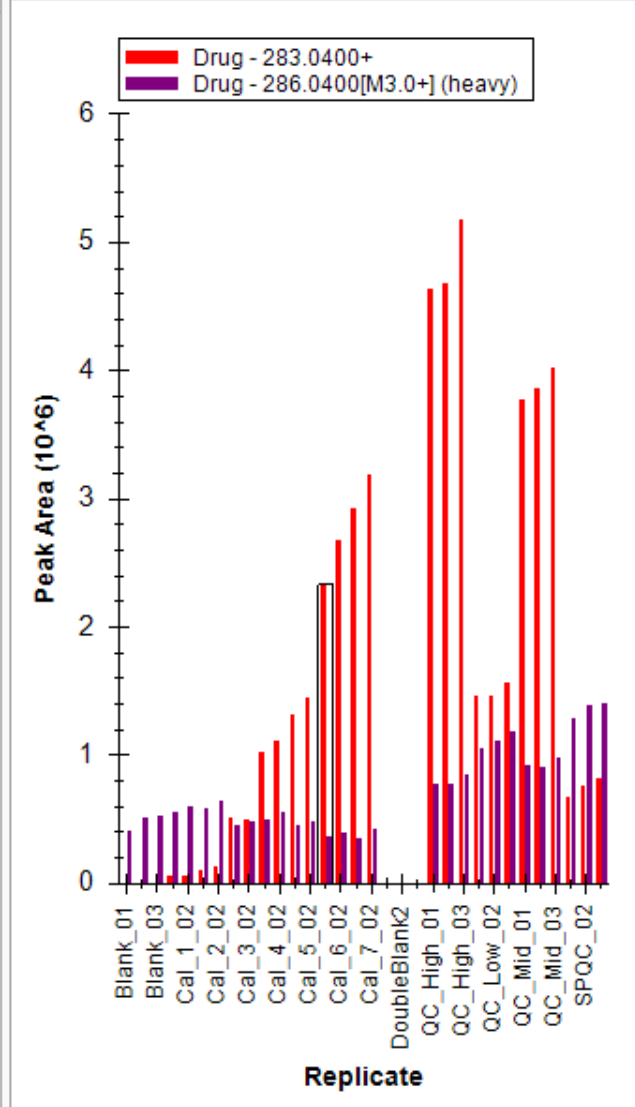
Replicates: Cal_6_01

molecules 1
Drug

Cal_5_02 Cal_6_01 Cal_6_02 Cal_7_01 Cal_7_02 DoubleBlank1 DoubleBlank2 DoubleBlank3 QC_Hi

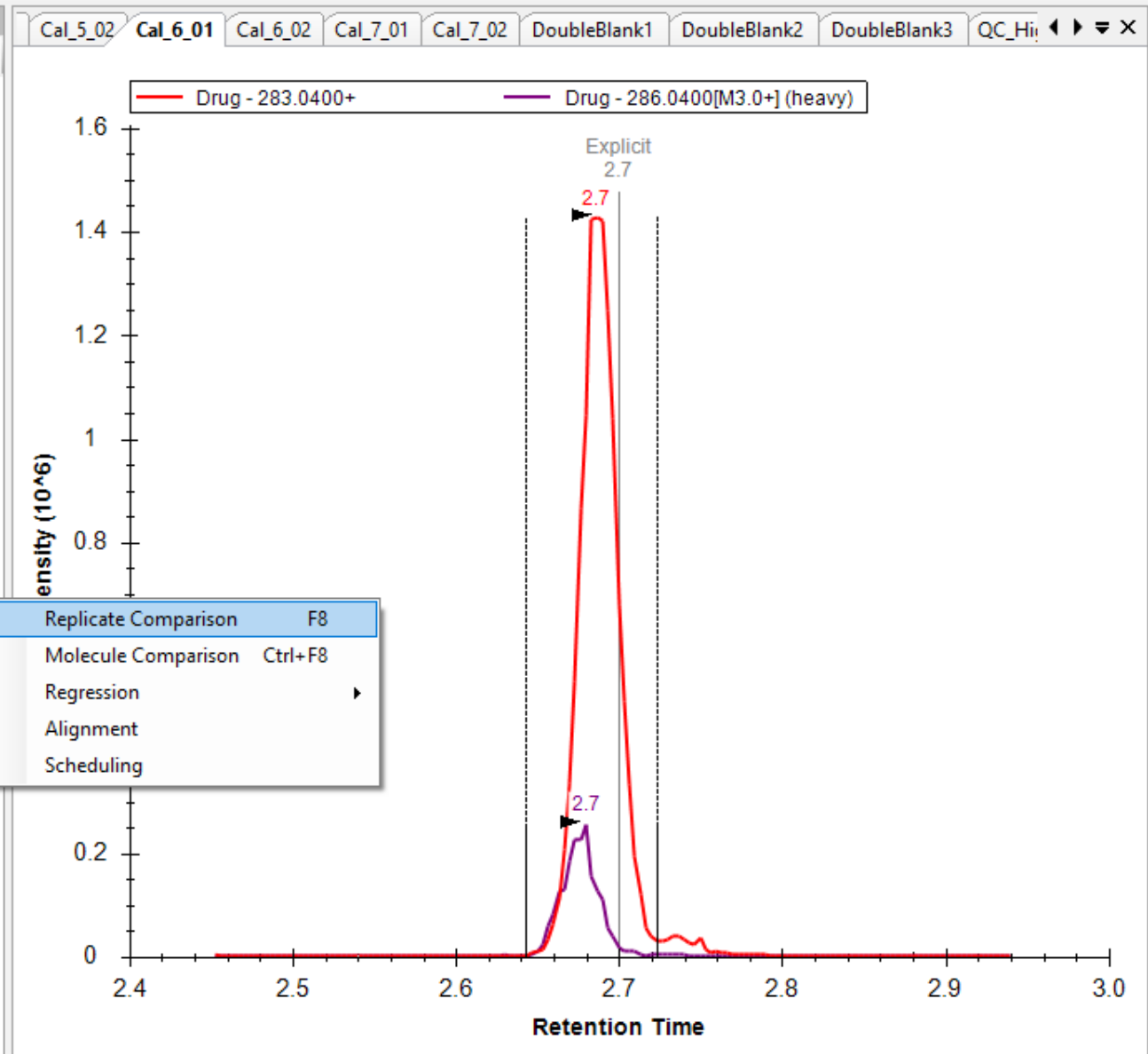


Peak Areas - Replicate Comparison

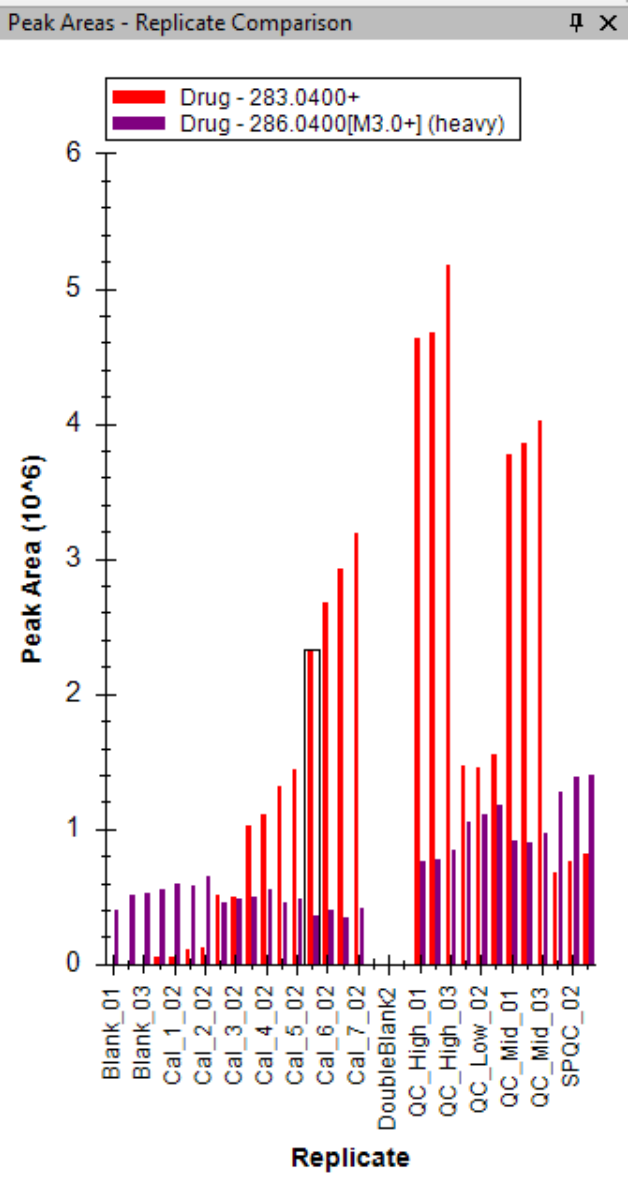


File Edit Refine View Settings Tools Help

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 - Special Ions
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 - Detections
 - Mass Errors
 - Calibration Curve
 - Document Grid Alt+3
 - Other Grids
- Tool Bar
- Status Bar



- Replicate Comparison F8
- Molecule Comparison Ctrl+F8
- Regression
- Alignment
- Scheduling

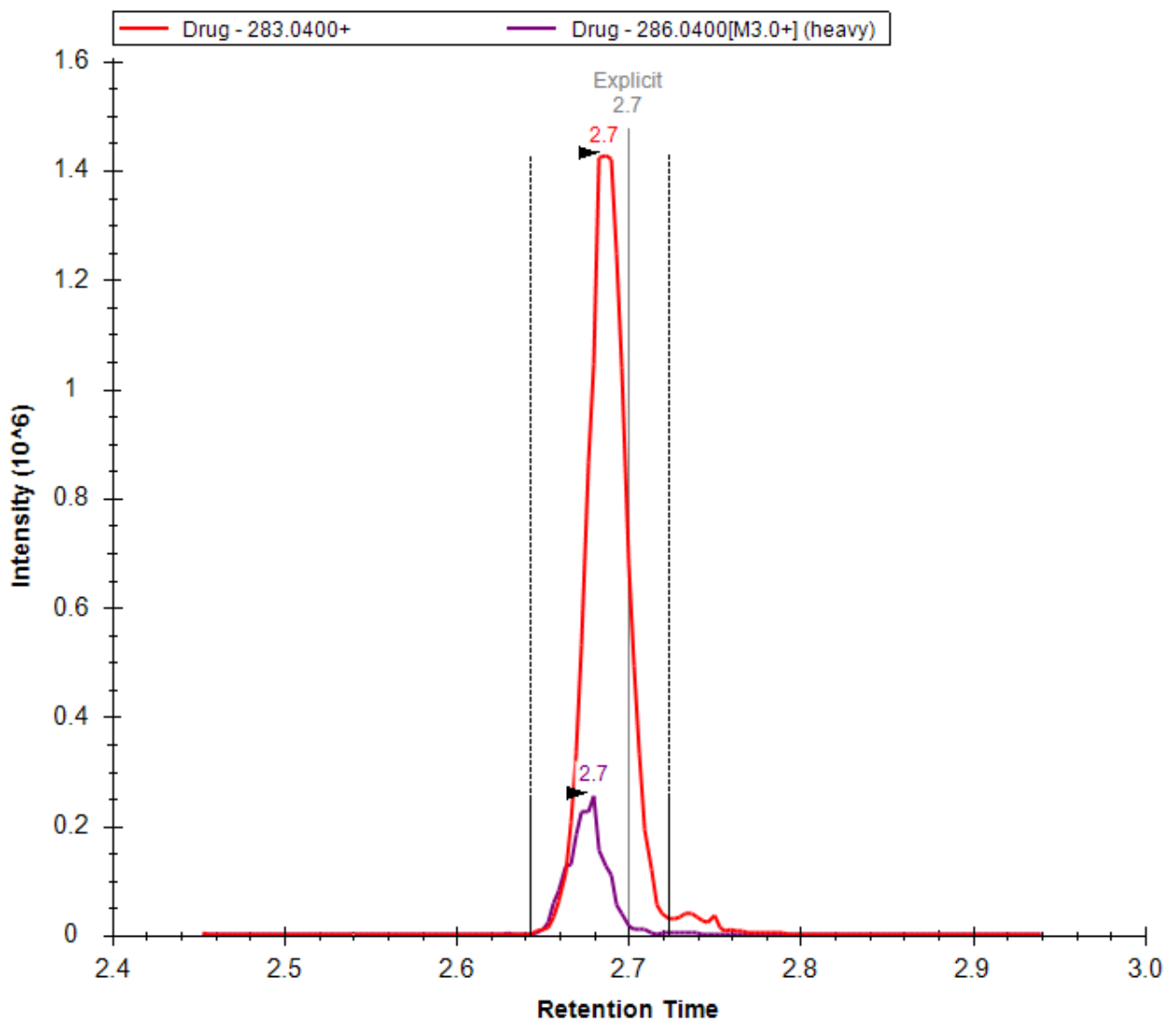
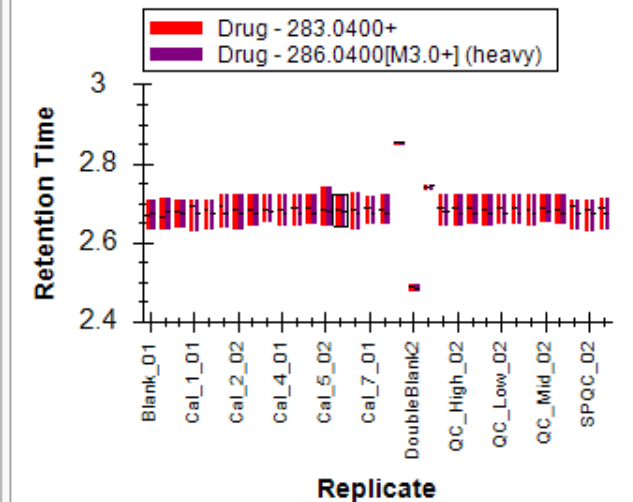
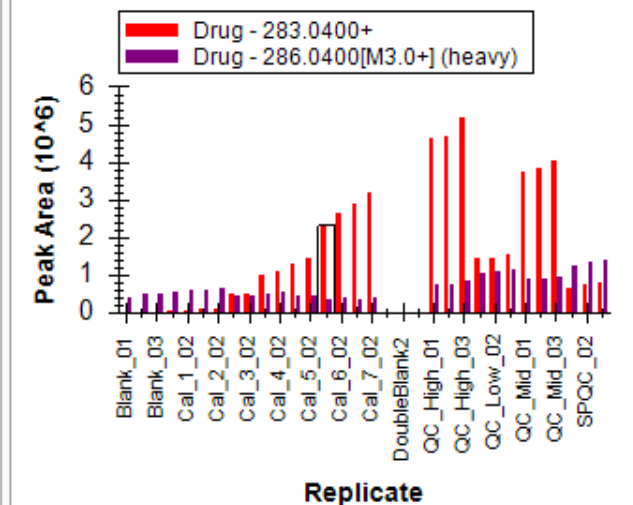


Targets ↑ ×

Replicates: Cal_6_01

molecules1

Drug

Cal_5_02 Cal_6_01 Cal_6_02 Cal_7_01 Cal_7_02 DoubleBlank1 DoubleBlank2 DoubleBlank3 QC_Hi: ◀ ▶ ×Retention Times - Replicate Comparison ↑ ×Peak Areas - Replicate Comparison ↑ ×

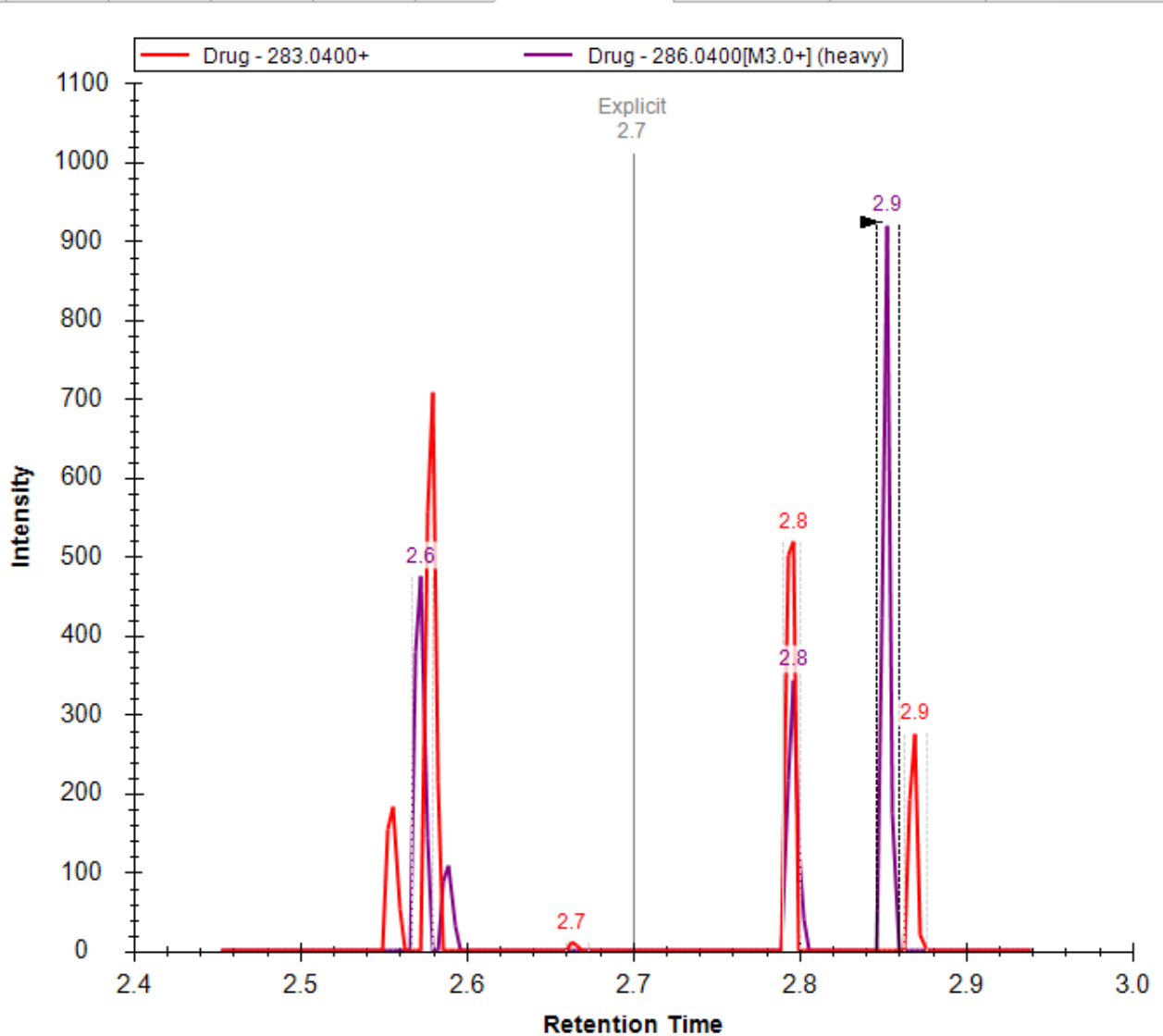


Targets

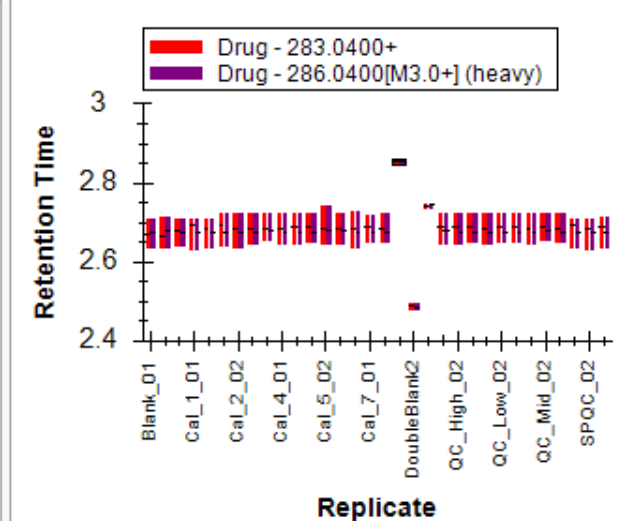
Replicates: DoubleBlank1

- molecules1
- Drug
 - 283.0400+ (total ratio 0)
 - 129.9600+ (ratio 0)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+[1]

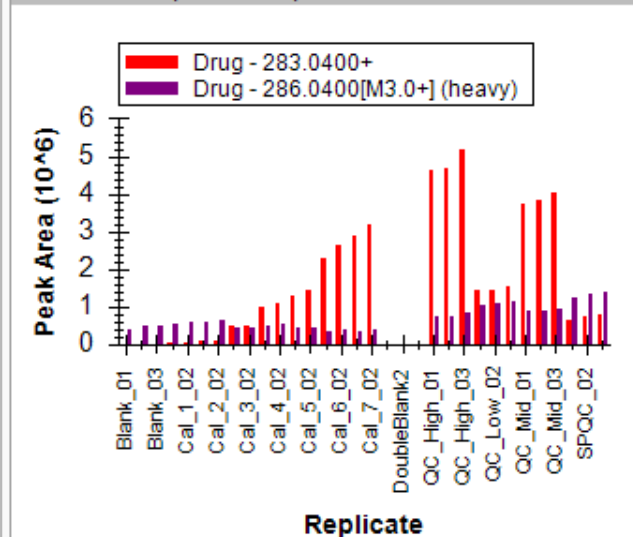
Cal_5_02 Cal_6_01 Cal_6_02 Cal_7_01 Cal_7_02 DoubleBlank1 DoubleBlank2 DoubleBlank3 QC_Hi



Retention Times - Replicate Comparison



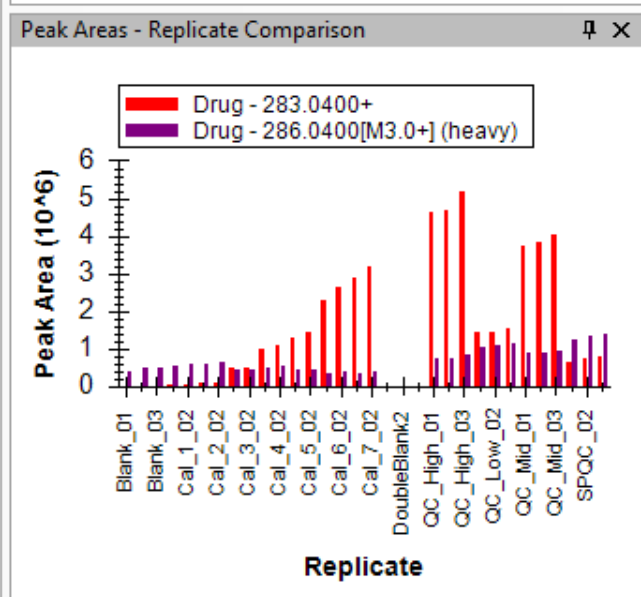
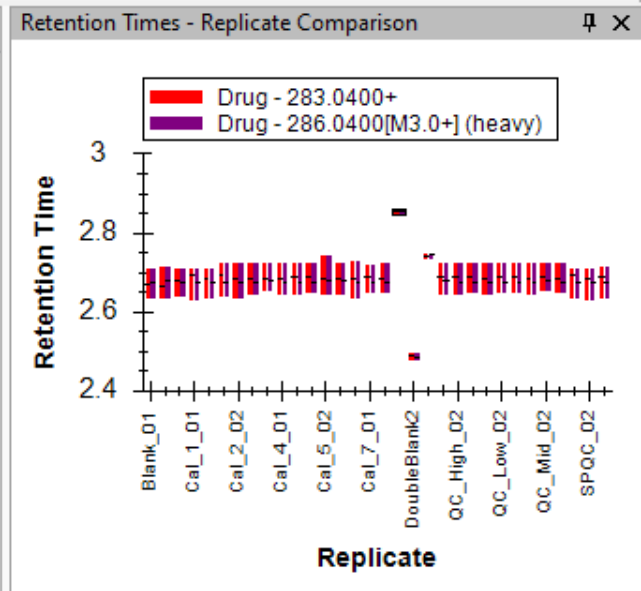
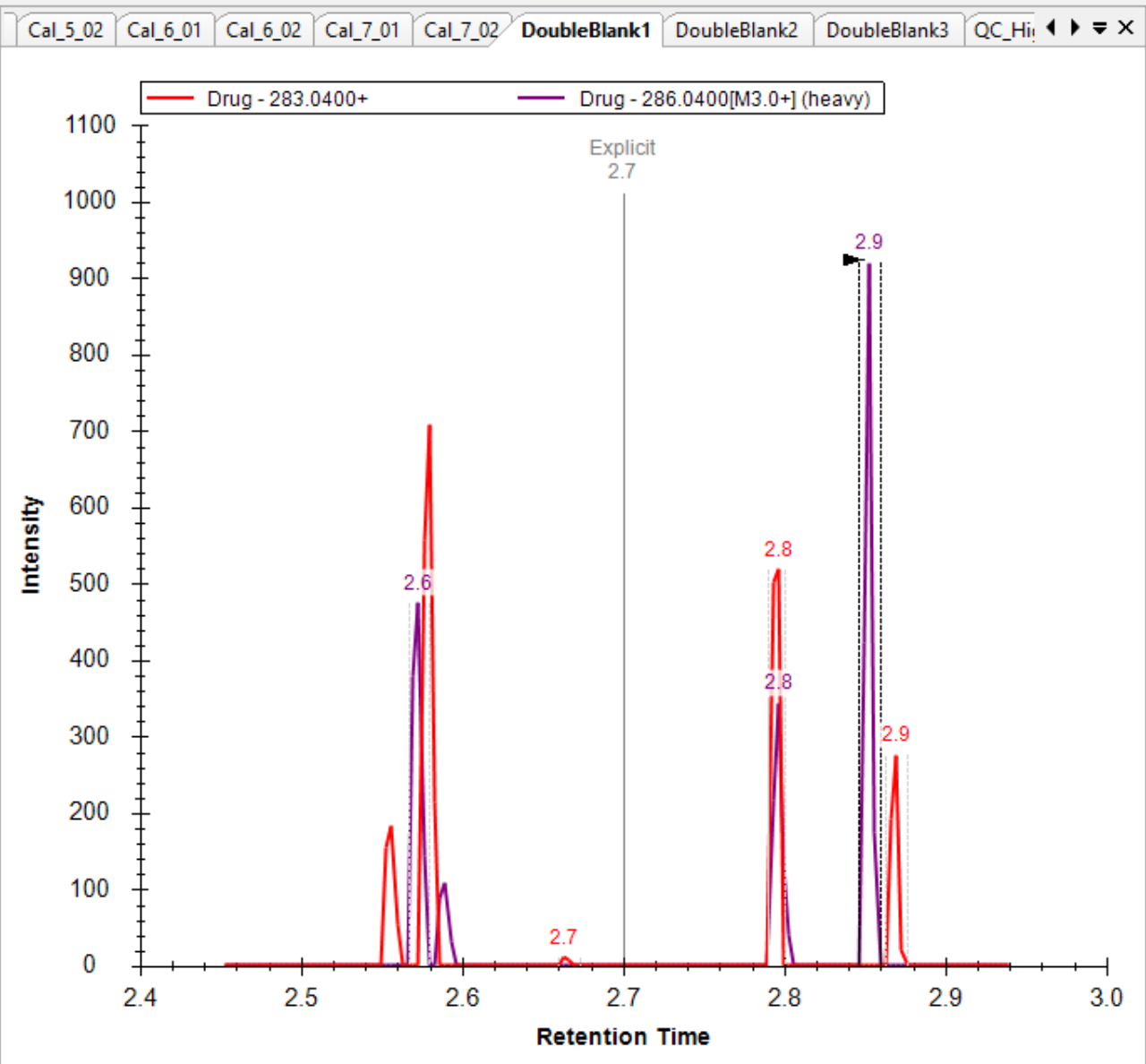
Peak Areas - Replicate Comparison



Targets

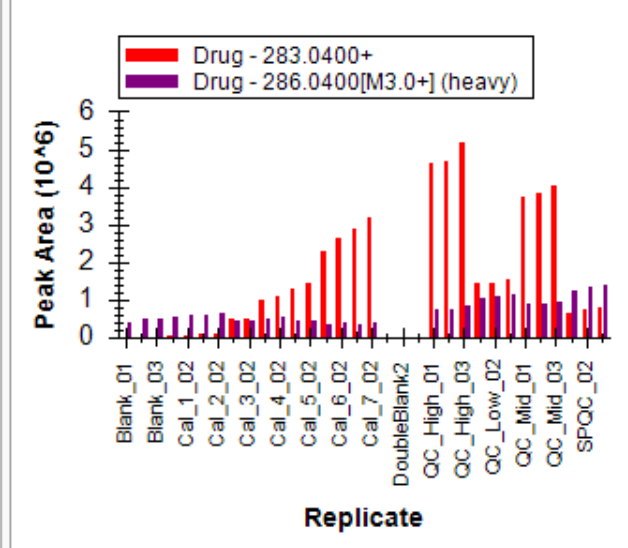
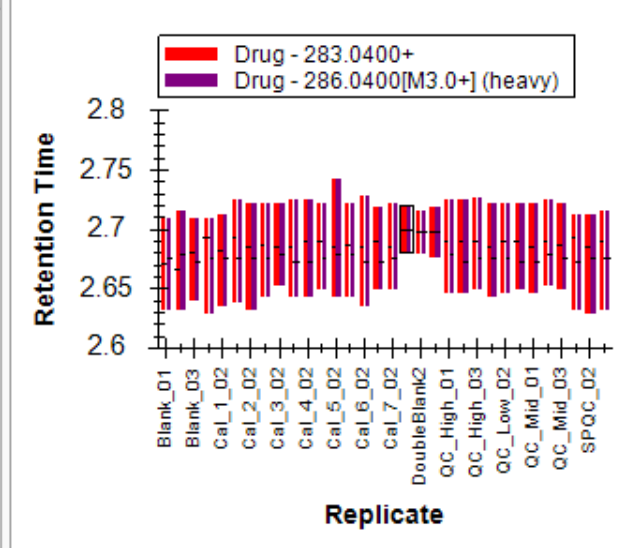
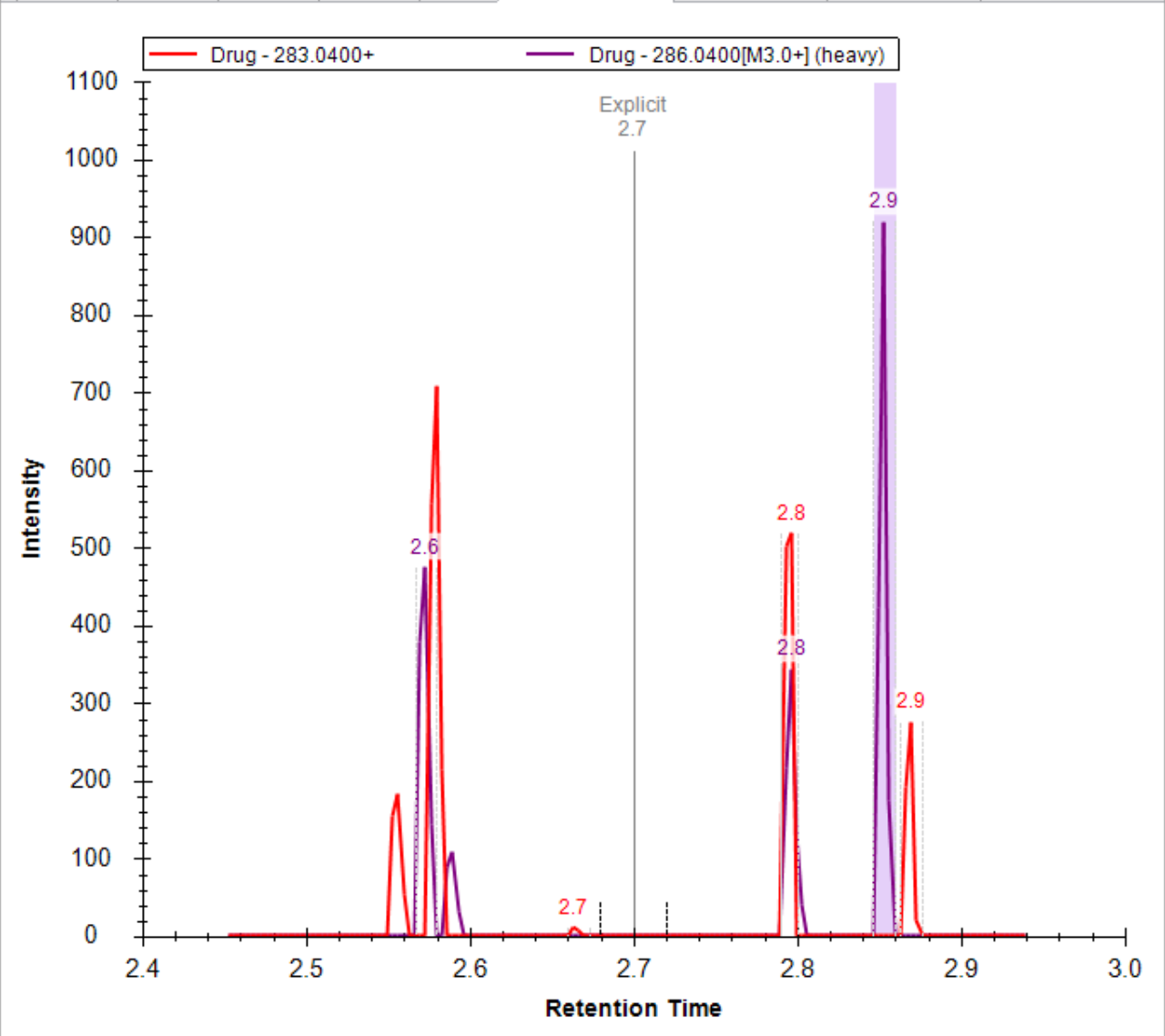
Replicates: DoubleBlank1

- Blank_03
- Cal_1_01
- Cal_1_02
- Cal_2_01
- Cal_2_02
- Cal_3_01
- Cal_3_02
- Cal_4_01
- Cal_4_02
- Cal_5_01
- Cal_5_02
- Cal_6_01
- Cal_6_02
- Cal_7_01
- Cal_7_02
- DoubleBlank1**
- DoubleBlank2
- DoubleBlank3
- QC_High_01
- QC_High_02
- QC_High_03
- QC_Low_01
- QC_Low_02
- QC_Low_03
- QC_Mid_01
- QC_Mid_02
- QC_Mid_03
- SPQC_01
- SPQC_02
- SPQC_03



📁 molecules1

- 🔥 Drug
 - 📄 283.0400+ (total ratio 0)
 - 📄 129.9600+ (ratio 0)
 - 📄 286.0400[M3.0+] (heavy)
 - 📄 133.0000+





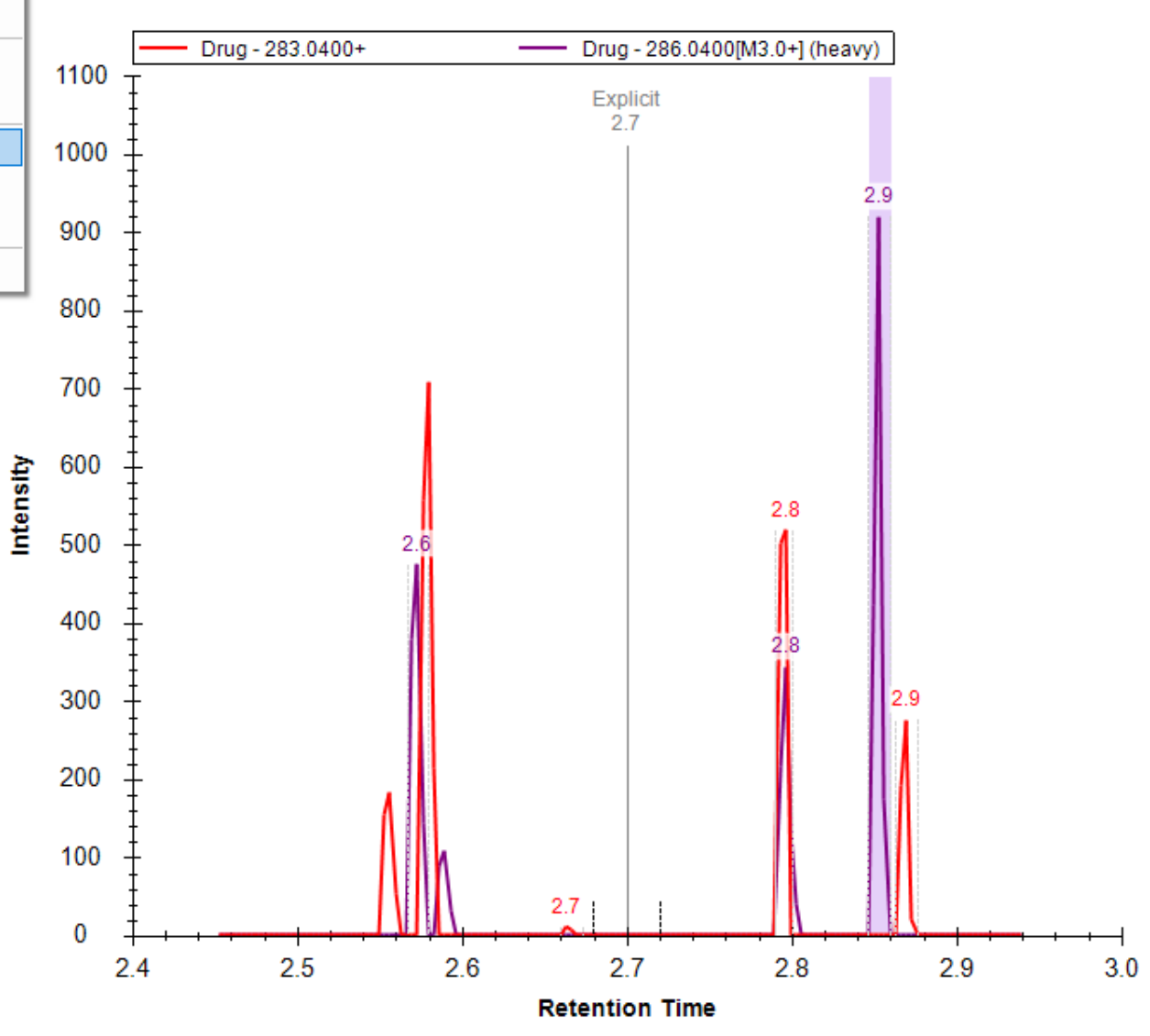
Targets

Replicates: DoubleBlank1

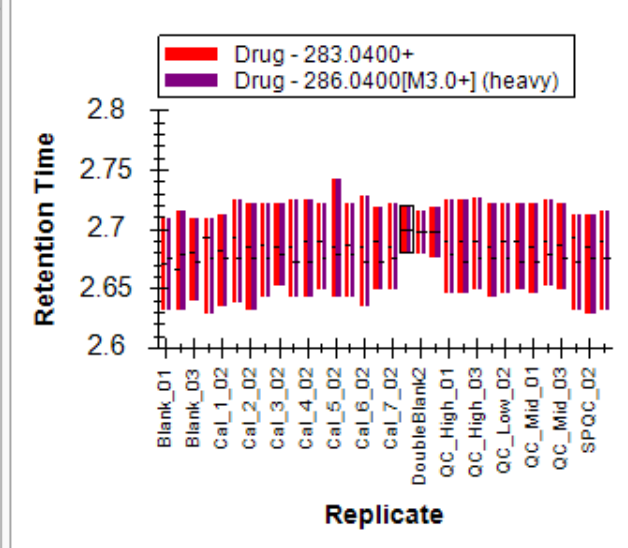
- 283.0400+ (total)
 - 129.9600+ (f)
 - 286.0400[M3.0+]
 - 133.0000+

- Default
- Save Current...
- Edit List...
- Share...
- Import...
- Molecule Settings...
- Transition Settings...
- Document Settings...
- Integrate All

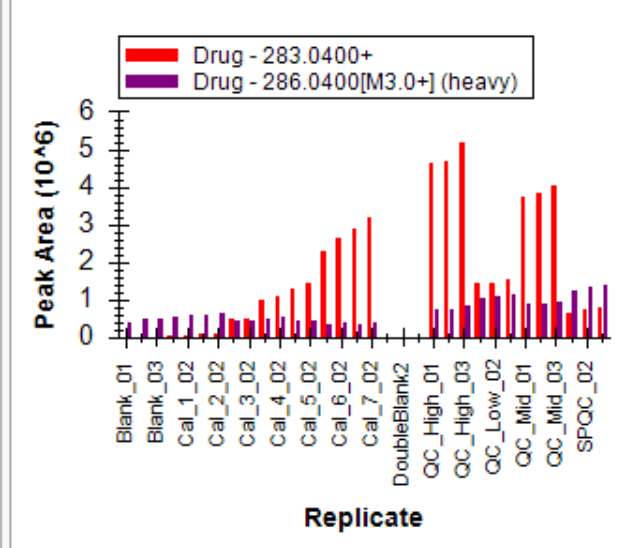
Cal_5_02 Cal_6_01 Cal_6_02 Cal_7_01 Cal_7_02 DoubleBlank1 DoubleBlank2 DoubleBlank3 QC_Hi



Retention Times - Replicate Comparison



Peak Areas - Replicate Comparison

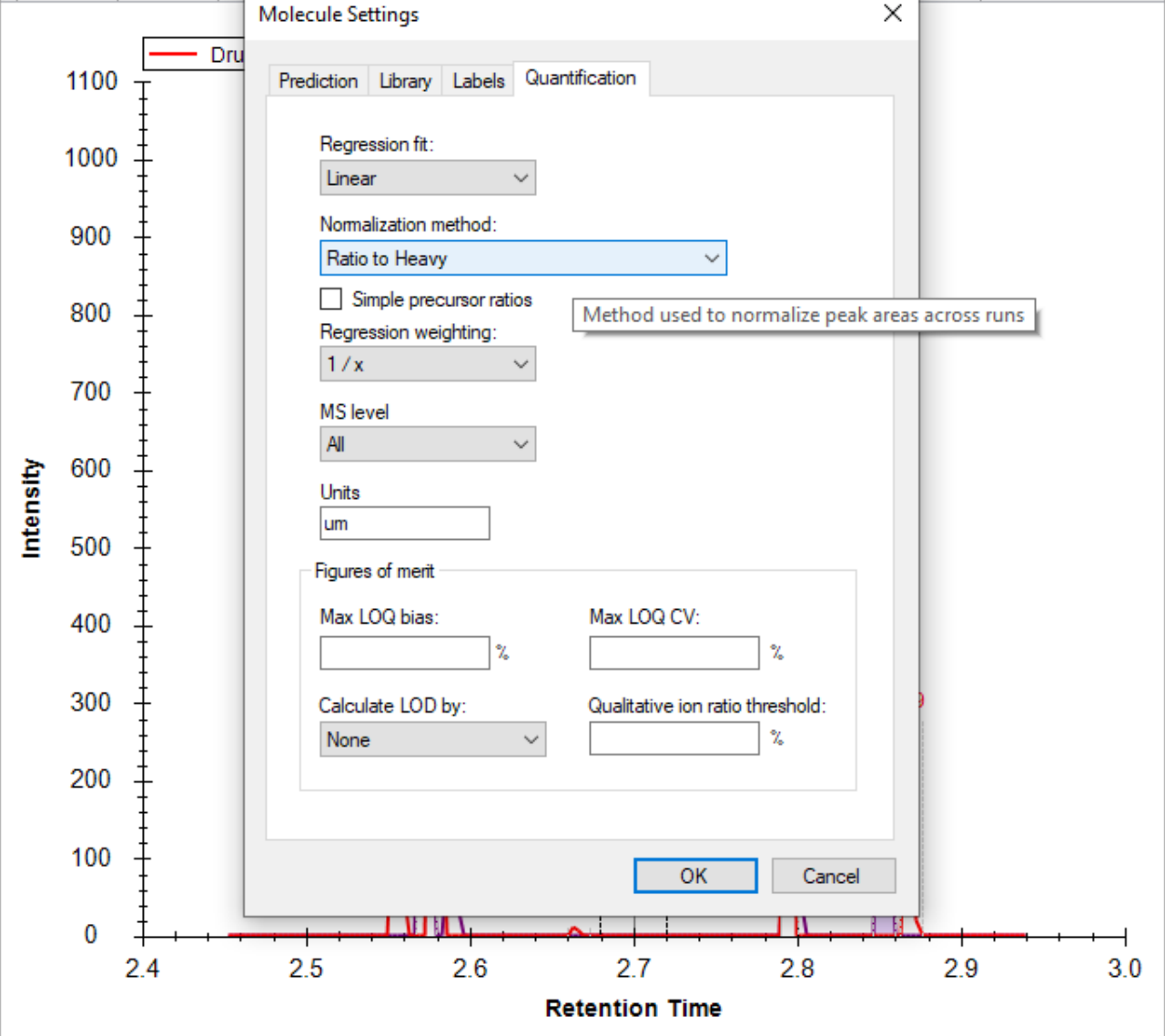


Targets

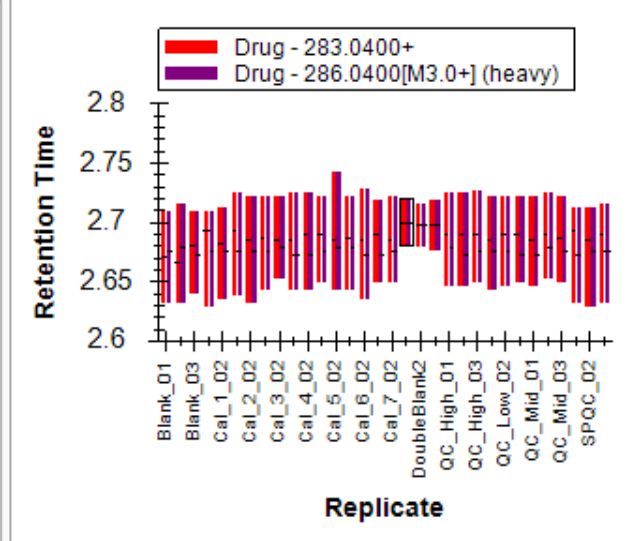
Replicates: DoubleBlank1

- molesules 1
 - Drug
 - 283.0400+ (total ratio 0)
 - 129.9600+ (ratio 0)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+

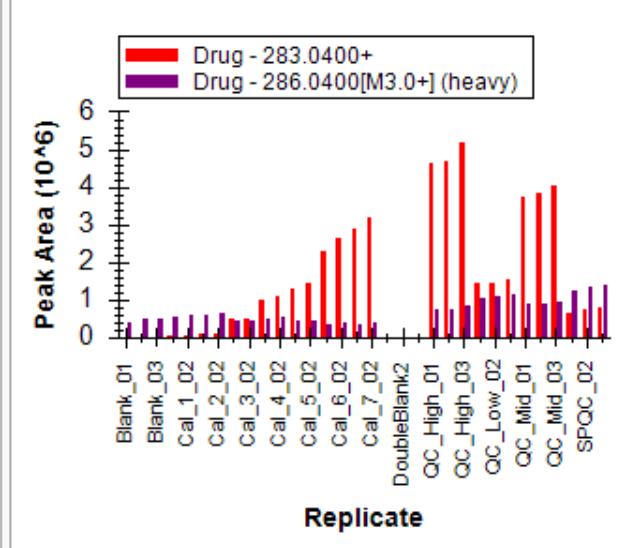
Cal_5_02 Cal_6_01 Cal_6_02 Cal_7_01 Cal_7_02 DoubleBlank1 DoubleBlank2 DoubleBlank3 QC_Hi



Retention Times - Replicate Comparison



Peak Areas - Replicate Comparison



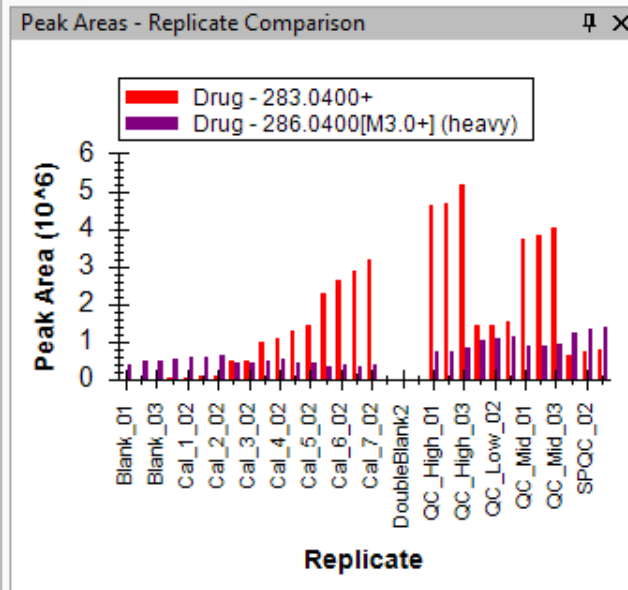
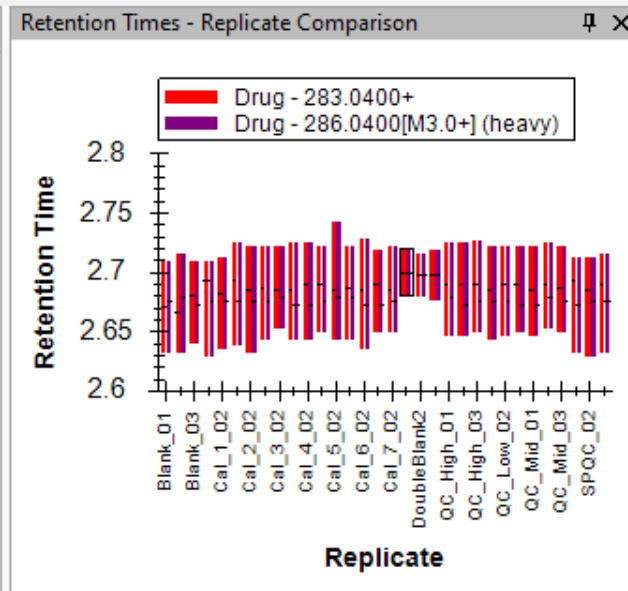
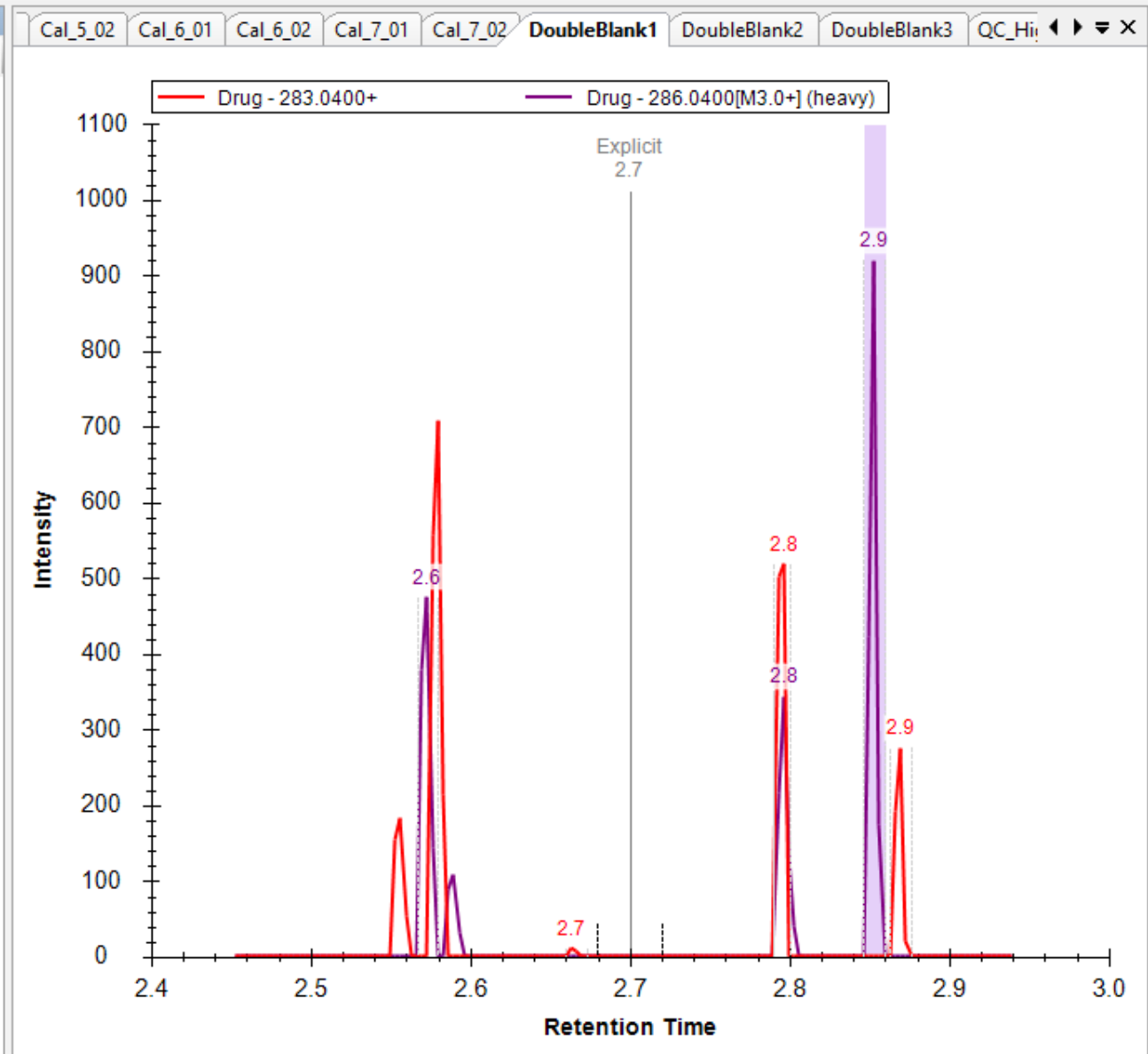
File Edit Refine View Settings Tools Help

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Replicates: DoubleBlank

molecules 1

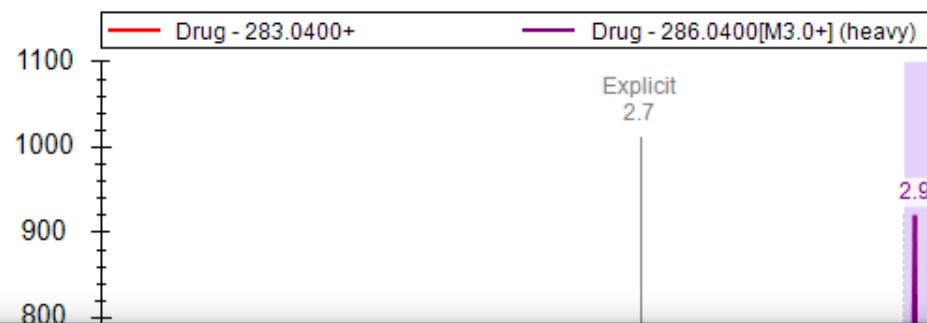
- Drug
- 283.040
- 129
- 286.040
- 133



Targets ↑ ×

Replicates: DoubleBlank1

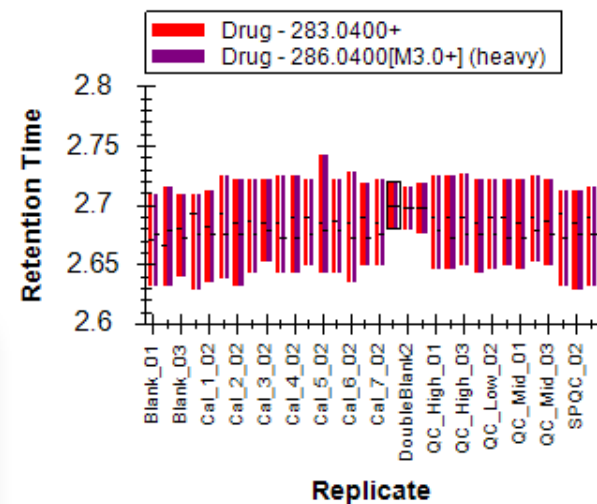
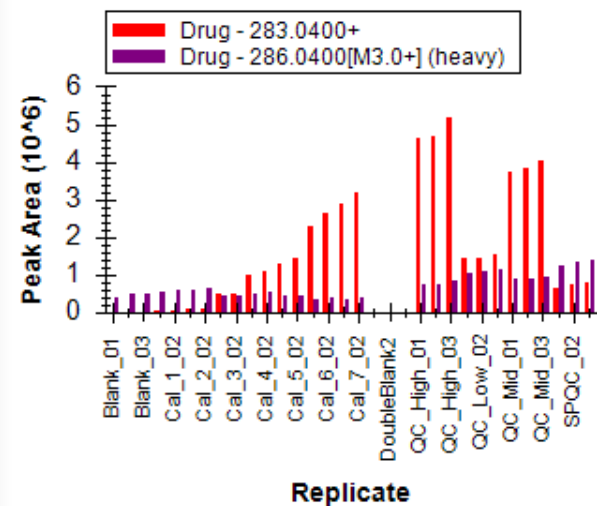
- molecules1
 ● Drug
 ● 283.0400+ (total ratio 0)
 ● 129.9600+ (ratio 0)
 ● 286.0400[M3.0+] (heavy)
 ● 133.0000+

 Cal_5_02 Cal_6_01 Cal_6_02 Cal_7_01 Cal_7_02 **DoubleBlank1** DoubleBlank2 DoubleBlank3 QC_Hi: ◀ ▶ ▾


Document Grid: Molecule Lists

 Reports ↓ ↶ ↷ 1 of 1 ↶ ↷ ✕ Export... Actions ▼ Find: A^a

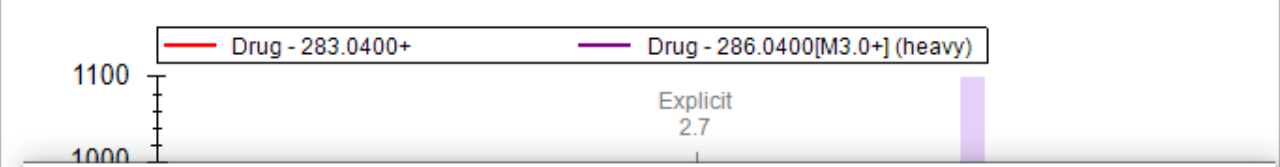
- Molecule Lists
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- Precursors
- Transitions
- Replicates
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- Molecule Quantification
- Molecule Ratio Results
- Molecule RT Results
- Molecule Transition Results
- Small Molecule Transition List
- Customize Report...
- Manage Reports...

Retention Times - Replicate Comparison ↑ ×Peak Areas - Replicate Comparison ↑ ×

Replicates: DoubleBlank1

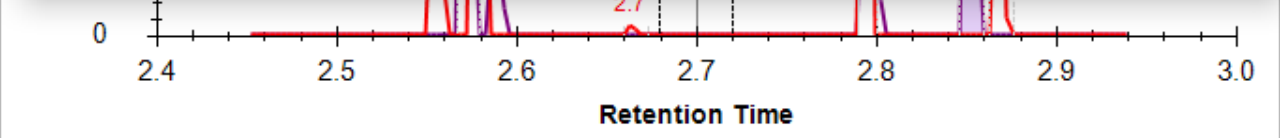
- 283.0400+ (total ratio 0)
- 129.9600+ (ratio 0)
- 286.0400[M3.0+] (heavy)
- 133.0000+

Cal_5_02 Cal_6_01 Cal_6_02 Cal_7_01 Cal_7_02 DoubleBlank1 DoubleBlank2 DoubleBlank3 QC_Hi

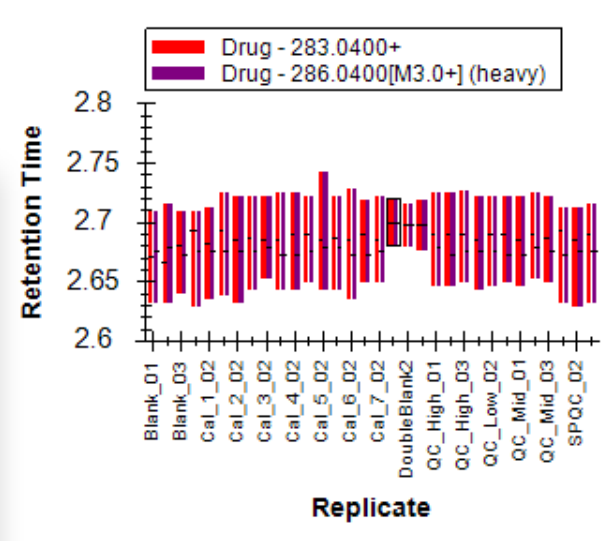


Document Grid: Replicates Reports of 32 Export... Actions Find:

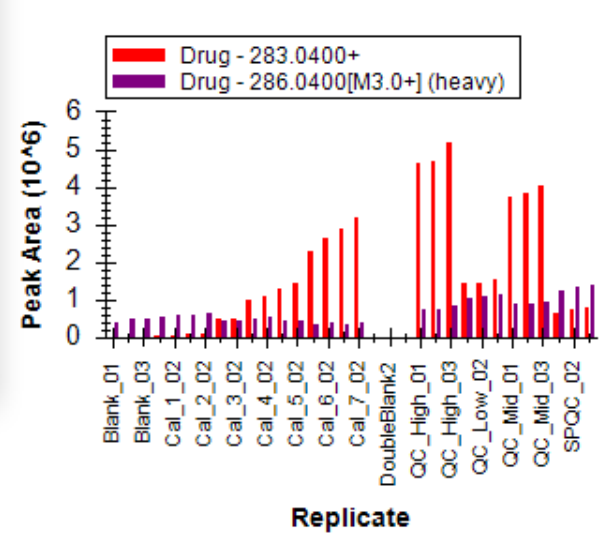
Replicate	Sample Type	Analyte Concentration
Blank_01	Unknown	
Blank_02	Unknown	
Blank_03	Standard	
Cal_1_01	Quality Control	
Cal_1_02	Solvent	
Cal_2_01	Blank	
Cal_2_02	Double Blank	
Cal_3_01	Unknown	
Cal_3_02	Unknown	
Cal_4_01	Unknown	
Cal_4_02	Unknown	
Cal_5_01	Unknown	
Cal_5_02	Unknown	
Cal_6_01	Unknown	
Cal_6_02	Unknown	
Cal_7_01	Unknown	



Retention Times - Replicate Comparison

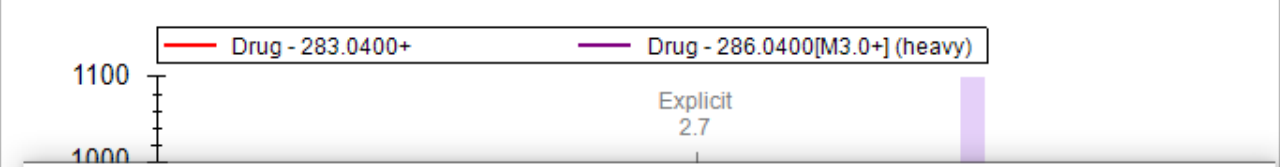


Peak Areas - Replicate Comparison

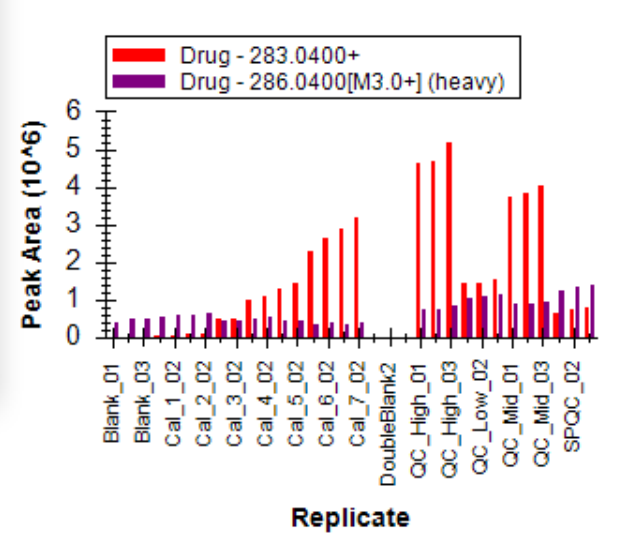
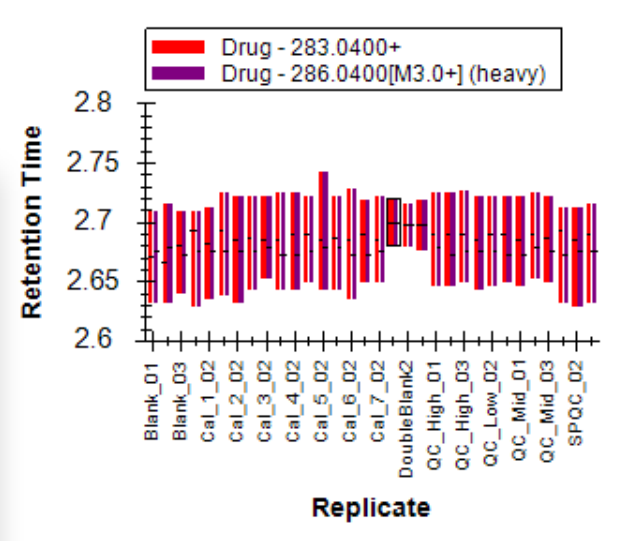
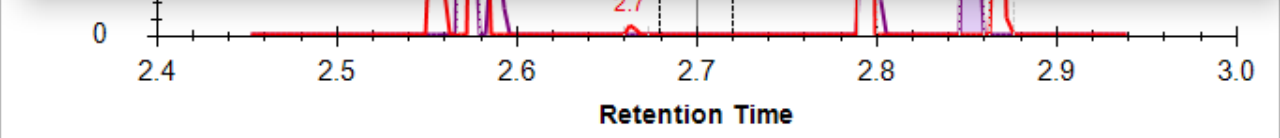


Target: Drug

- 283.0400+ (total ratio 0)
- 129.9600+ (ratio 0)
- 286.0400[M3.0+] (heavy)
- 133.0000+

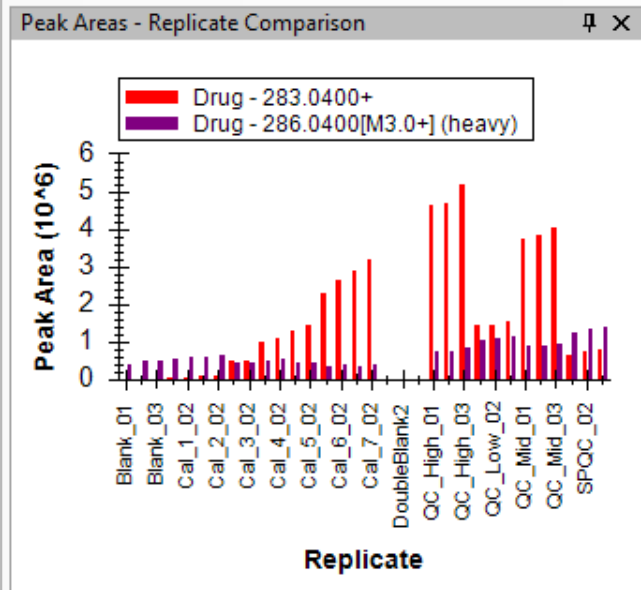
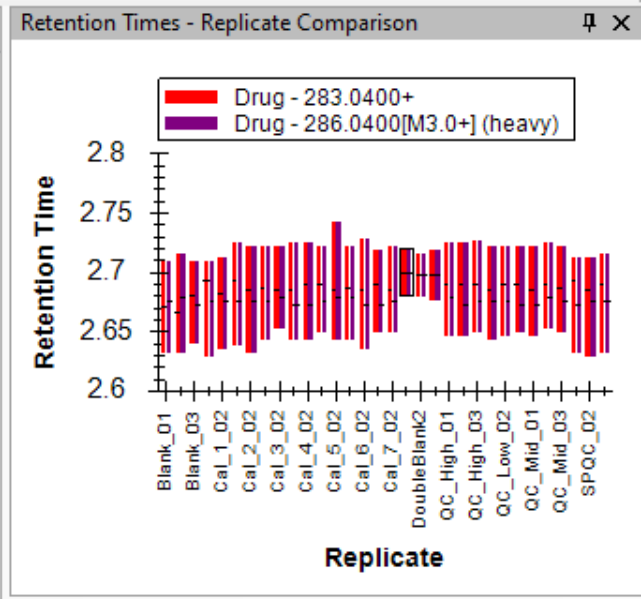
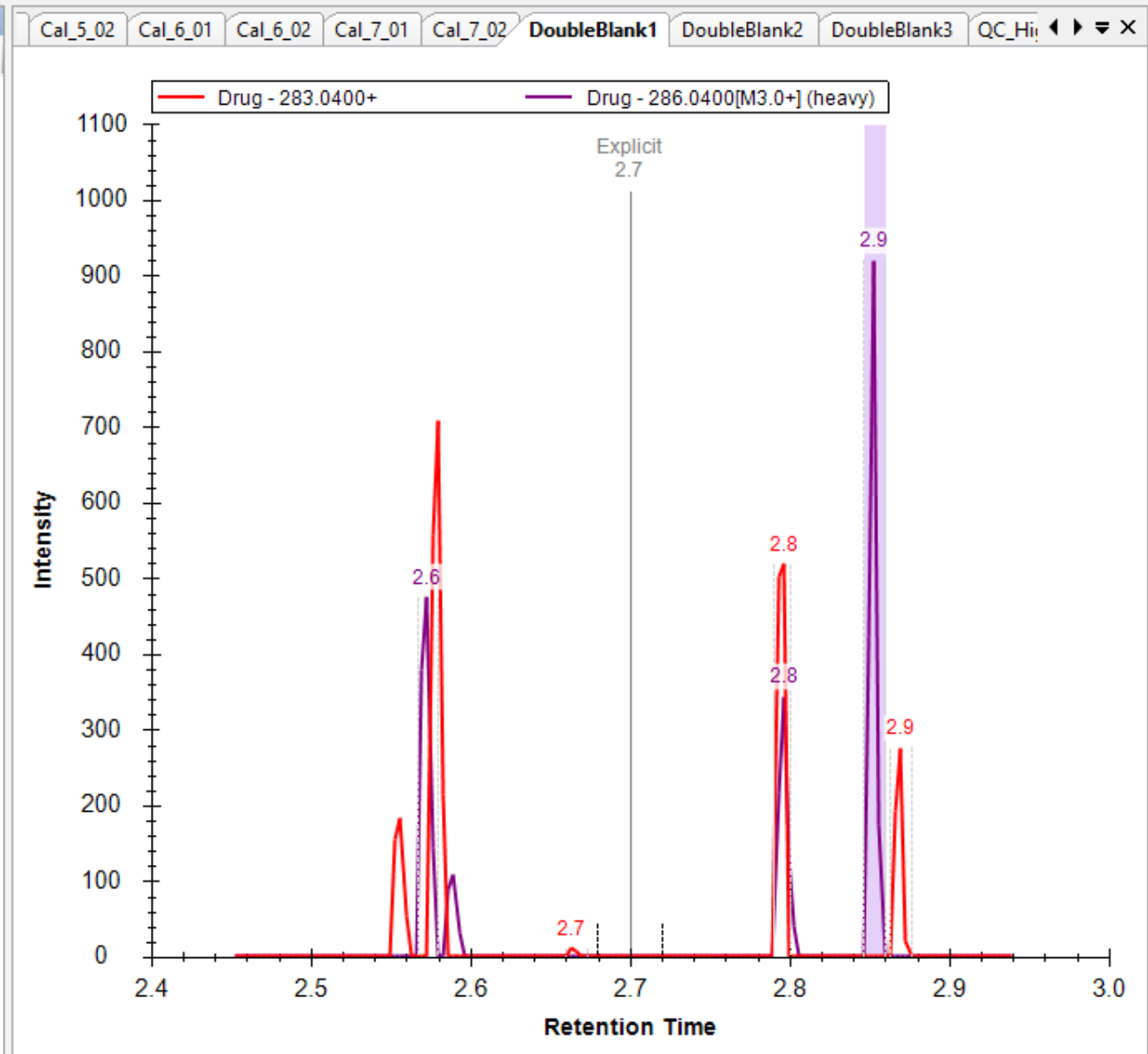


Replicate	Sample Type	Analyte Concentration
Blank_01	Blank	
Blank_02	Blank	
Blank_03	Blank	
Cal_1_01	Standard	10
Cal_1_02	Standard	10
Cal_2_01	Standard	20
Cal_2_02	Standard	20
Cal_3_01	Standard	100
Cal_3_02	Standard	100
Cal_4_01	Standard	200
Cal_4_02	Standard	200
Cal_5_01	Standard	400
Cal_5_02	Standard	400
Cal_6_01	Standard	600
Cal_6_02	Standard	600
Cal_7_01	Standard	800



File Edit Refine View Settings Tools Help

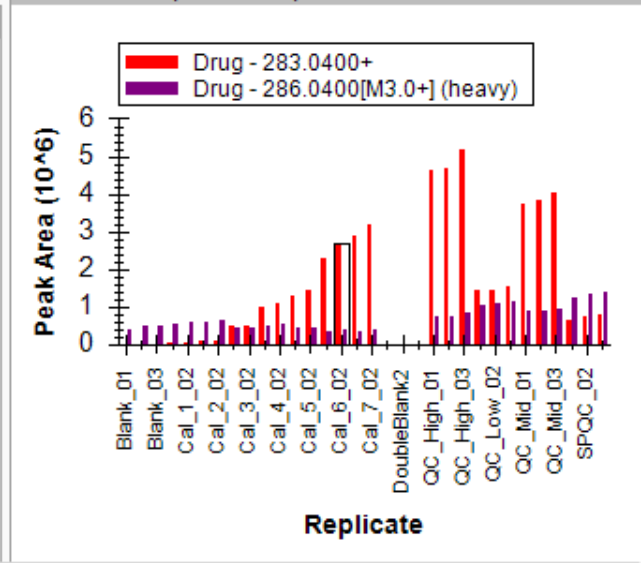
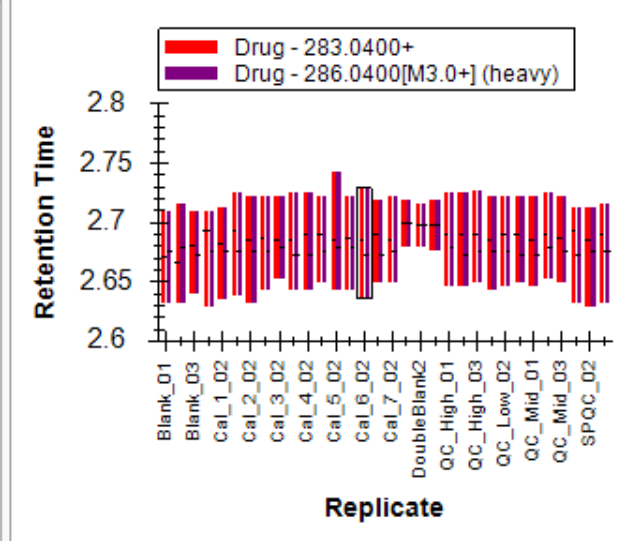
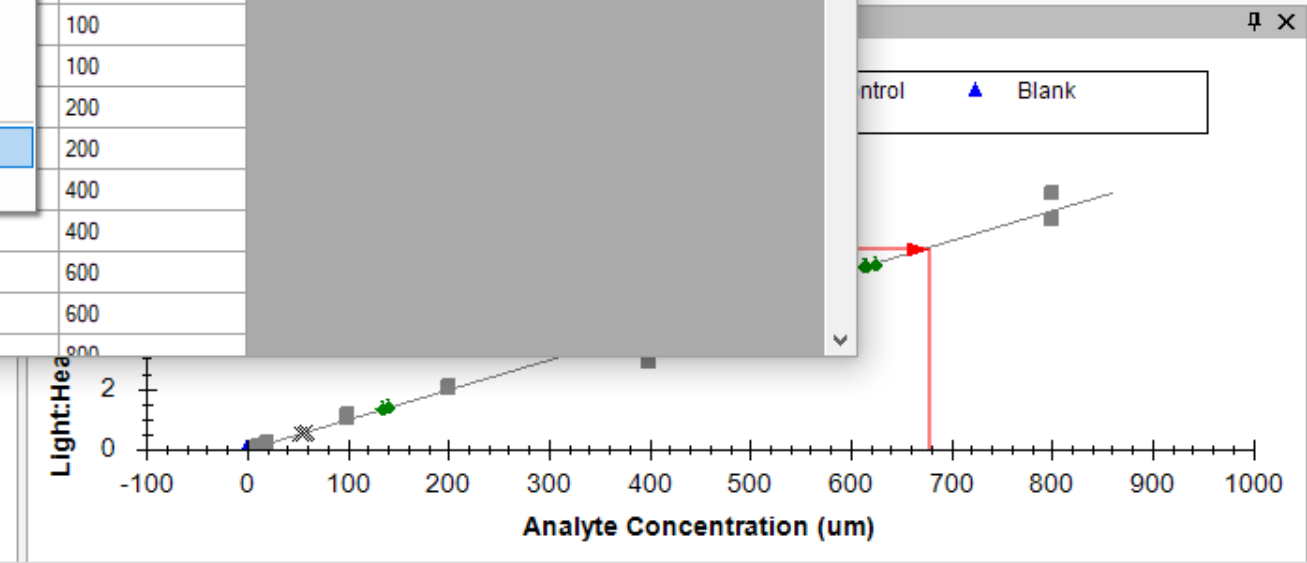
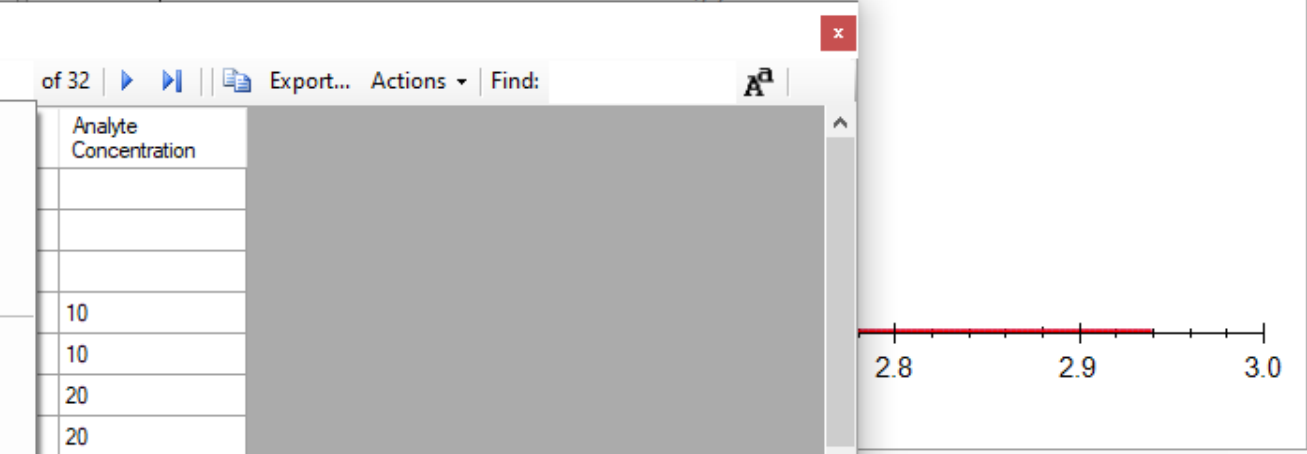
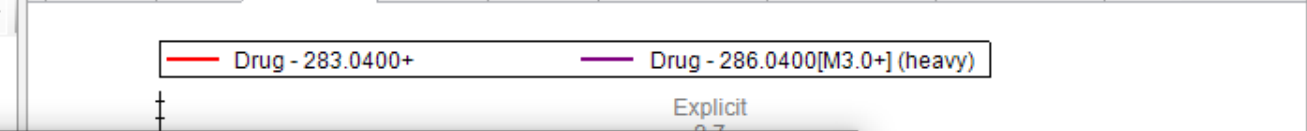
- Targets
 - Text Zoom
 - User Interface
 - Spectral Libraries
 - Arrange Graphs
 - Library Match Alt+1
 - Ion Types
 - Fragments
 - Special Ions
 - Precursor
 - Charges
 - Ranks
 - Chromatograms
 - Transitions
 - Transform
 - Auto-Zoom
 - Retention Times
 - Peak Areas
 - Detections
 - Mass Errors
 - Calibration Curve
 - Document Grid Alt+3
 - Other Grids
- Tool Bar
- Status Bar



Document Grid: Replicates

Reports

- Molecule Lists
- Molecules
- Precursors
- Transitions
- Replicates**
- Molecule Peak Boundaries
- Molecule Quantification
- Molecule Ratio Results
- Molecule RT Results
- Molecule Transition Results
- Small Molecule Transition List
- Customize Report...
- Manage Reports...



Document Grid: Replicates

Reports

Replicate	Sample Type	Area
Blank_01	Blank	
Blank_02	Blank	
Blank_03	Blank	
Cal_1_01	Standard	10
Cal_1_02	Standard	10
Cal_2_01	Standard	20
Cal_2_02	Standard	20
Cal_3_01	Standard	10
Cal_3_02	Standard	10
Cal_4_01	Standard	20
Cal_4_02	Standard	20
Cal_5_01	Standard	40
Cal_5_02	Standard	40
Cal_6_01	Standard	60
Cal_6_02	Standard	60
Cal_7_01	Standard	800

Customize Report

Report Name:

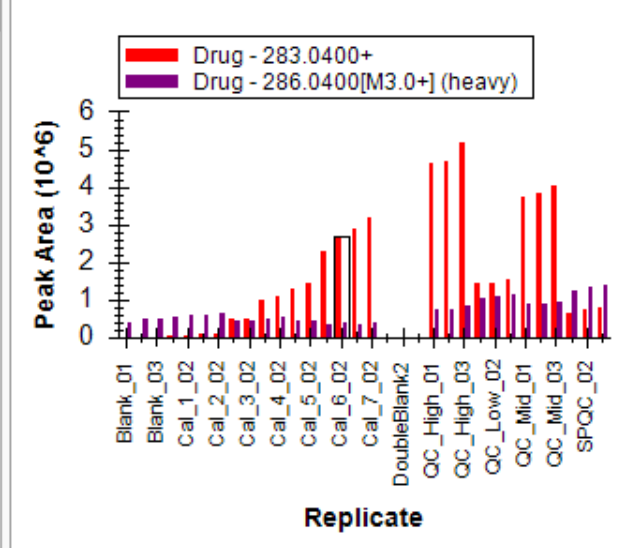
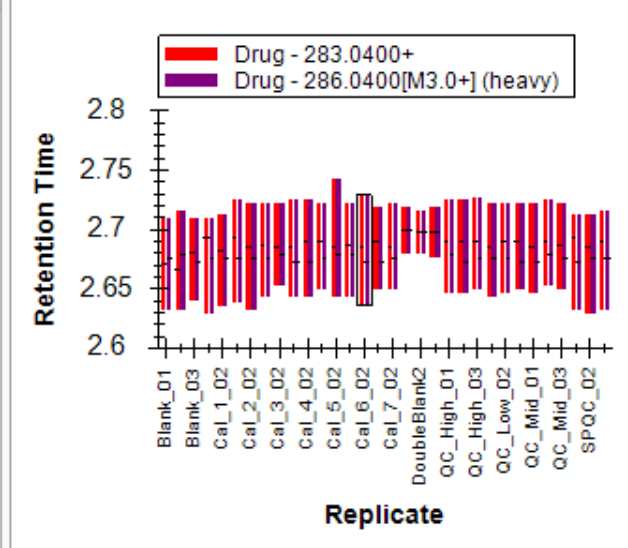
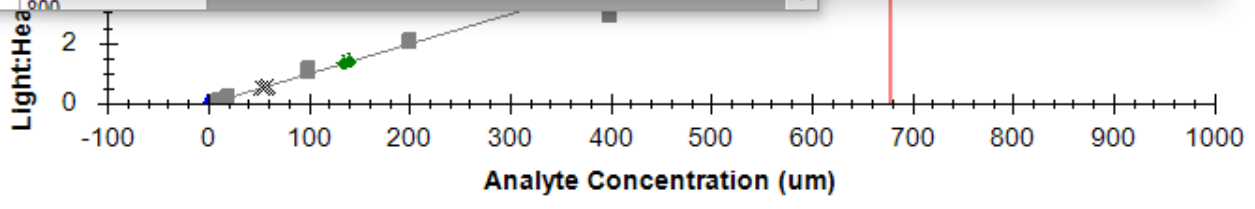
Columns Filter

- Molecule Lists
 - Molecules
 - Molecule List Results
 - Molecule List Name
 - Auto Select Molecules
 - Molecule List Note
 - Molecule List Locator
- Replicates
 - Replicate Name
 - Files
 - Sample Type
 - Analyte Concentration
 - Sample Dilution Factor
 - Batch Name
 - Replicate Locator

Replicate
Sample Type
Analyte Concentration

Pivot Replicate Name Pivot Isotope Label

OK Cancel

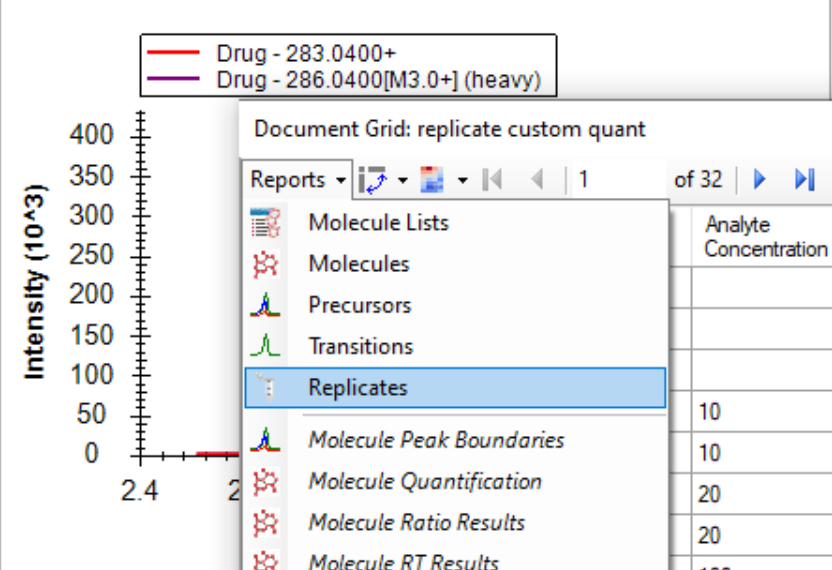


Targets Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca

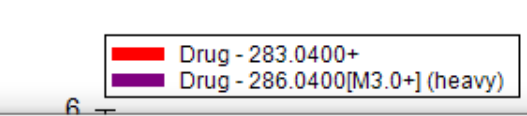
Replicates: Cal_3_01

- molecules1
 - Drug
 - 283.0400+ (total ratio 1.12)
 - 129.9600+[1] (ratio 1.12)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+[1]

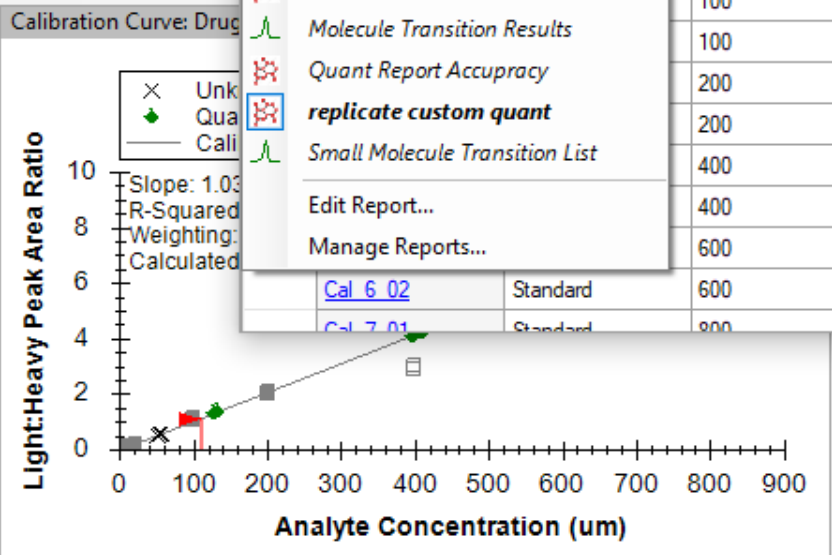
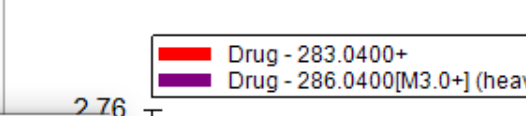
Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca



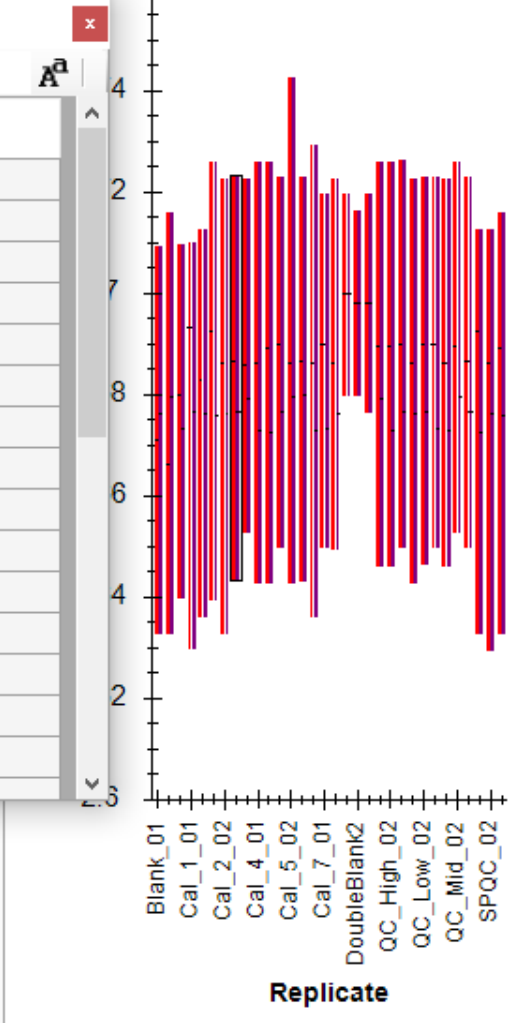
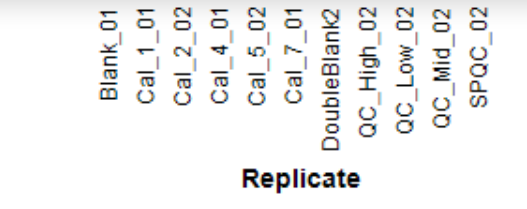
Peak Areas - Replicate Comparison



Retention Times - Replicate Comparison



Analyte Concentration	Exclude From Calibration	Quantification	Accuracy
	<input type="checkbox"/>	0.1342 um	#N/A
	<input type="checkbox"/>	0.3242 um	#N/A
	<input type="checkbox"/>	0.2408 um	#N/A
10	<input type="checkbox"/>	10.3 um	103%
10	<input type="checkbox"/>	9.7712 um	97.7%
20	<input type="checkbox"/>	18.6481 um	93.2%
20	<input type="checkbox"/>	19.5628 um	97.8%
100	<input type="checkbox"/>	108.8353 um	108.8%
100	<input type="checkbox"/>	101.0449 um	101%
200	<input type="checkbox"/>	199.111 um	99.6%
200	<input type="checkbox"/>	192.8198 um	96.4%
400	<input checked="" type="checkbox"/>	277.9943 um	69.5%
400	<input checked="" type="checkbox"/>	289.8102 um	72.5%
600	<input type="checkbox"/>	617.8728 um	103%
600	<input type="checkbox"/>	639.7133 um	106.6%
800	<input type="checkbox"/>	812.7228 um	101.6%

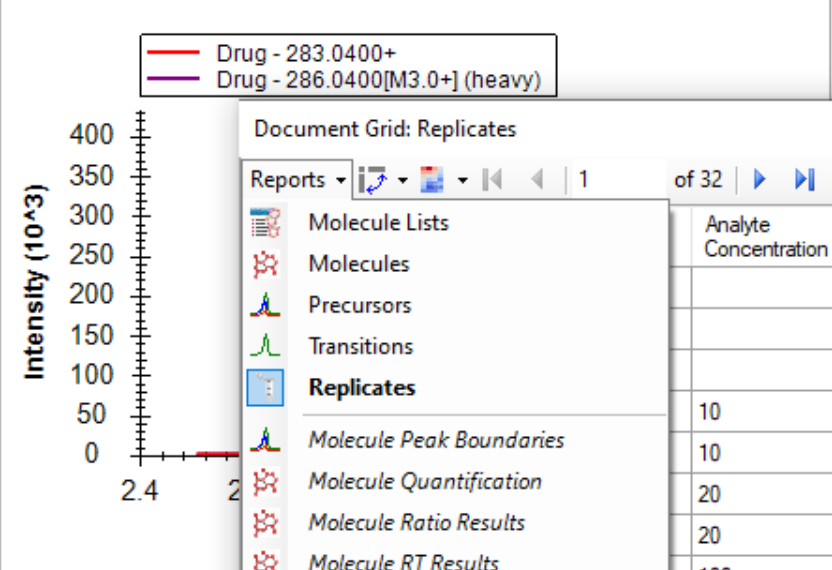


Targets Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca

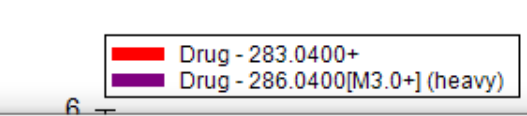
Replicates: Cal_3_01

- molesules1
 - Drug
 - 283.0400+ (total ratio 1.12)
 - 129.9600+[1] (ratio 1.12)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+[1]

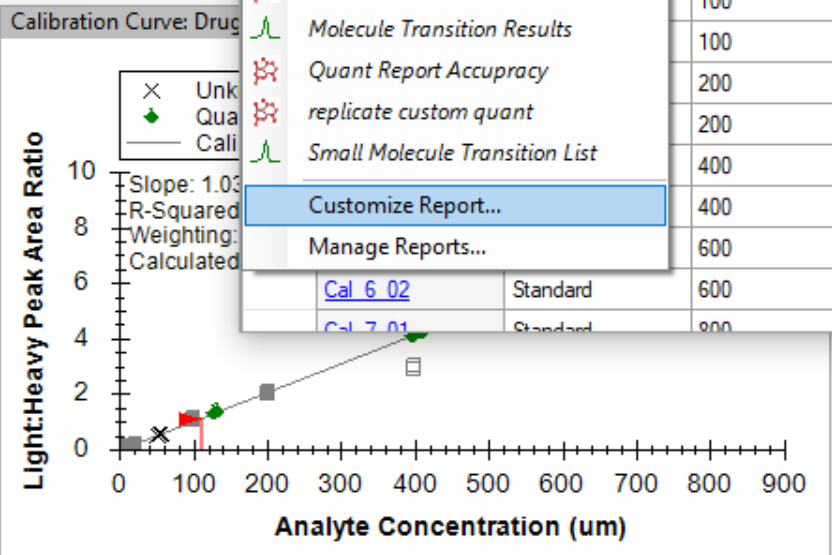
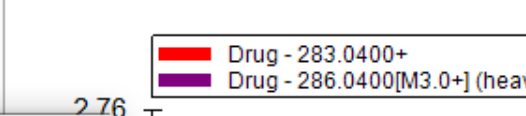
Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca



Peak Areas - Replicate Comparison



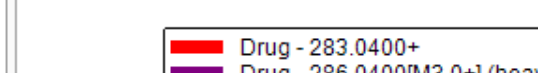
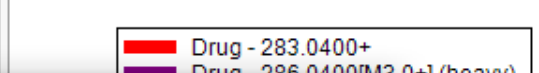
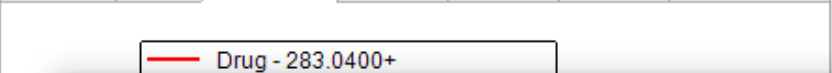
Retention Times - Replicate Comparison



Replicate	Drug - 283.0400+	Drug - 286.0400[M3.0+] (heavy)
Blank_01		
Cal_1_01		
Cal_2_02		
Cal_4_01		
Cal_5_02		
Cal_7_01		
DoubleBlank2		
QC_High_02		
QC_Low_02		
QC_Mid_02		
SPQC_02		

Target Hierarchy:

- Target 1: 283.0400+ (total ratio 1.12)
 - Peak 1: 129.9600+[1] (ratio 1.12)
 - Peak 2: 286.0400[M3.0+] (heavy)
 - Peak 3: 133.0000+[1]



Customize Report

Report Name:

Columns Filter

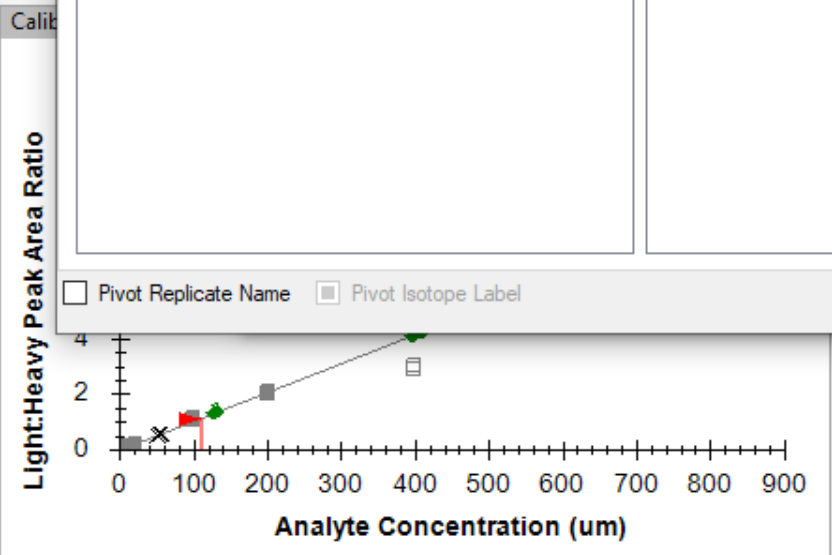
- Molecule Lists
 - Molecules
 - Molecule List Results
 - Molecule List Name
 - Auto Select Molecules
 - Molecule List Note
 - Molecule List Locator
 - Replicates

Replicate

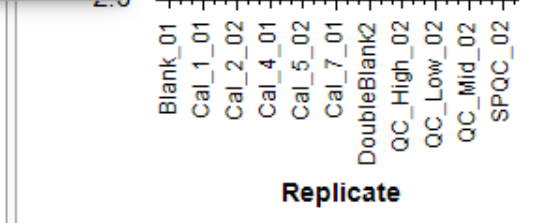
- Sample Type
- Analyte Concentration

Pivot Replicate Name Pivot Isotope Label

OK Cancel

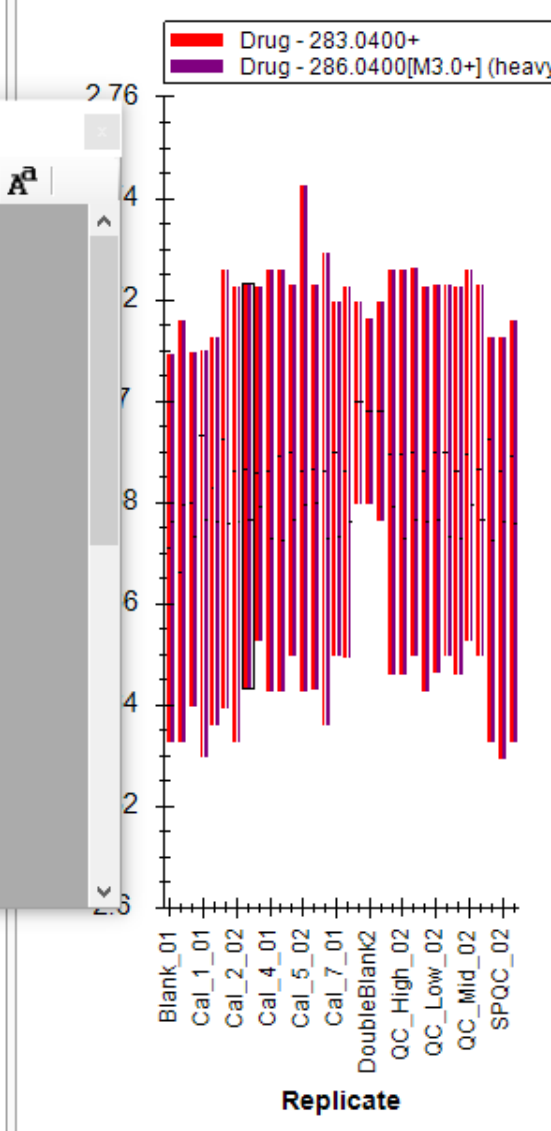
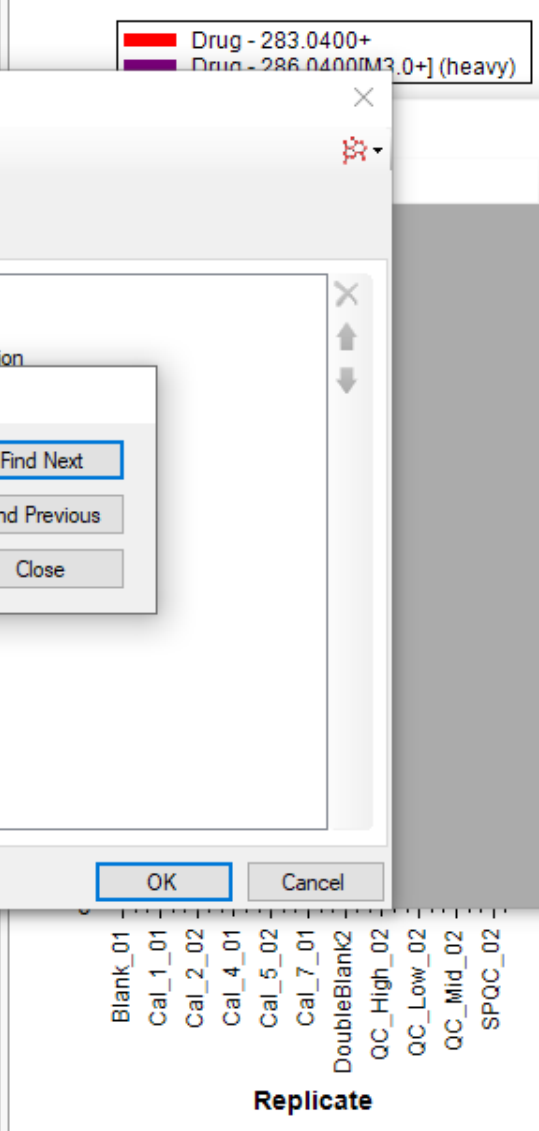
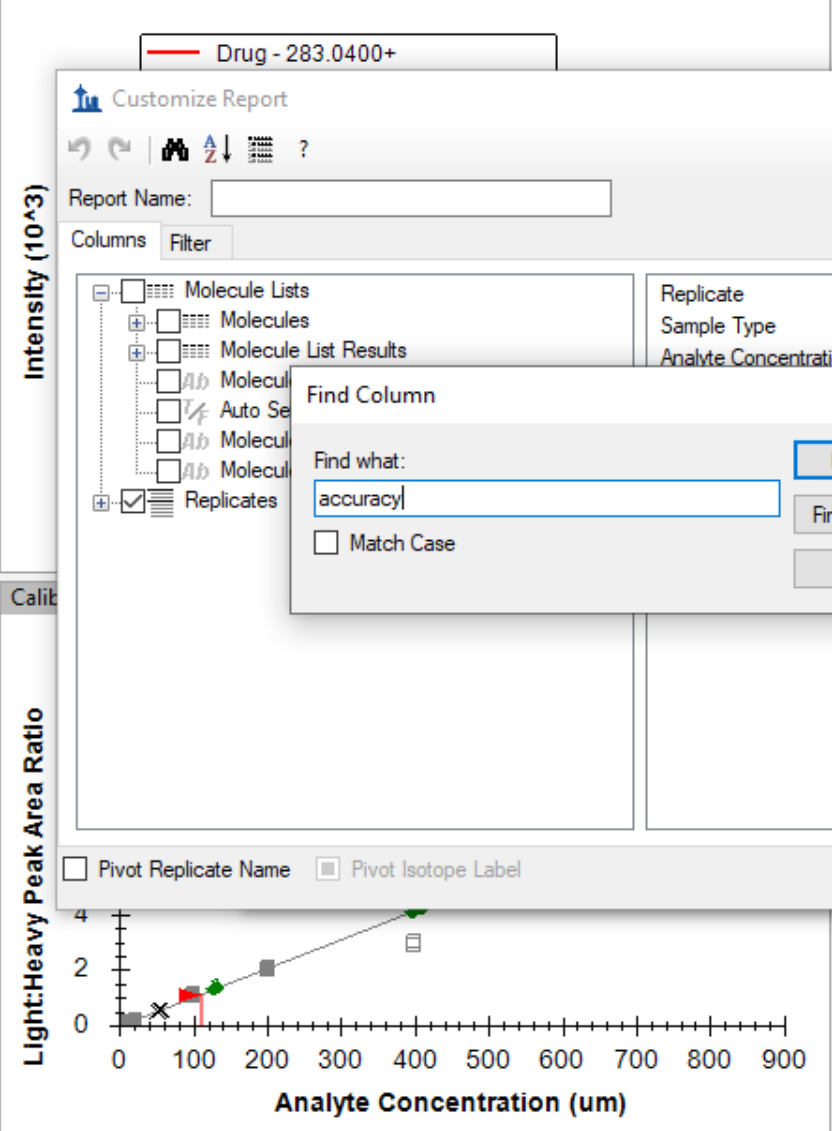


Replicate	Drug - 283.0400+ (Area)	Drug - 286.0400[M3.0+] (heavy) (Area)
Blank_01	~0	~0
Cal_1_01	~1.0	~1.0
Cal_2_02	~2.0	~2.0
Cal_4_01	~2.5	~2.5
Cal_5_02	~2.2	~2.2
Cal_7_01	~2.0	~2.0
DoubleBlank2	~0	~0
QC_High_02	~2.5	~2.5
QC_Low_02	~1.5	~1.5
QC_Mid_02	~2.0	~2.0
SPQC_02	~2.0	~2.0



Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca

- Drug
- 283.0400+ (total ratio 1.12)
- 129.9600+[1] (ratio 1.12)
- 286.0400[M3.0+] (heavy)
- 133.0000+[1]



Customize Report

Report Name: _____

Columns Filter

- Molecule Lists
- Molecules
- Molecule List Results
- Ab Molecule
- Auto Se
- Ab Molecule
- Ab Molecule
- Replicates

Replicate
Sample Type
Analyte Concentration

Find Column

Find what: accuracy

Match Case

Find Next
Find Previous
Close

Pivot Replicate Name
Pivot Isotope Label

OK Cancel



Targets Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca

Replicates: Cal_3_01

Target Hierarchy:

- Target: Drug
 - 283.0400+ (total ratio 1.12)
 - 129.9600+[1] (ratio 1.12)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+[1]

Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca

Drug - 283.0400+

Customize Report Dialog:

Report Name:

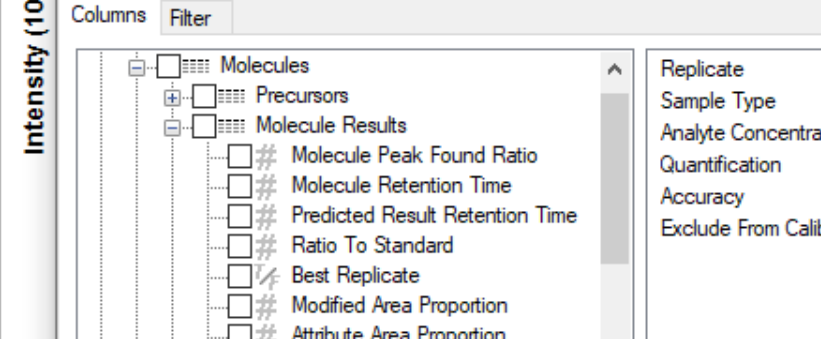
Columns Filter

- Molecules
 - Precursors
 - Molecule Results
 - Molecule Peak Found Ratio
 - Molecule Retention Time
 - Predicted Result Retention Time
 - Ratio To Standard
 - Best Replicate
 - Modified Area Proportion
 - Attribute Area Proportion
 - Exclude From Calibration**
 - Quantification
 - Normalized Area
 - Calculated Concentration
 - Accuracy
 - Replicate Calibration Curve
 - Batch Figures Of Merit
 - Explicit Analyte Concentration

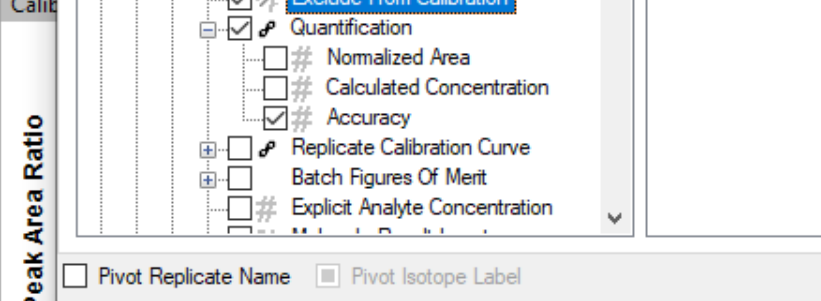
Replicate List:

- Replicate
- Sample Type
- Analyte Concentration
- Quantification
- Accuracy
- Exclude From Calibration

Buttons: OK Cancel

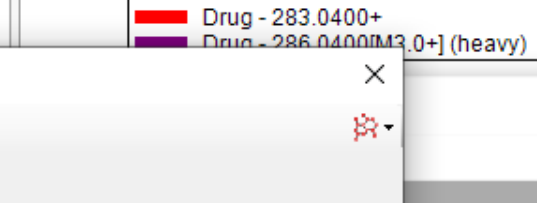


Calib



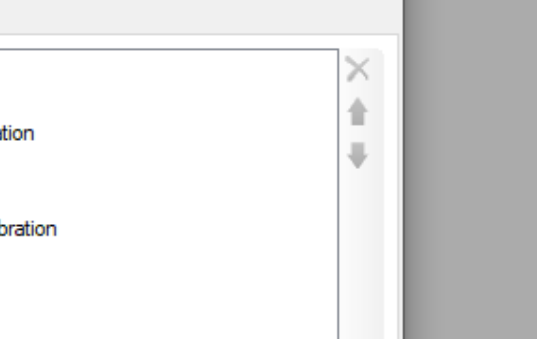
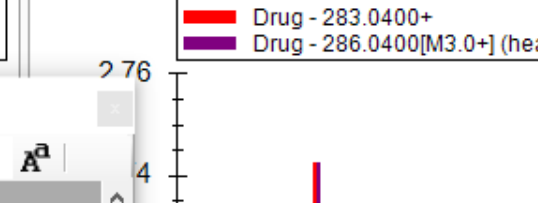
Peak Areas - Replicate Comparison

Drug - 283.0400+ Drug - 286.0400[M3.0+] (heavy)



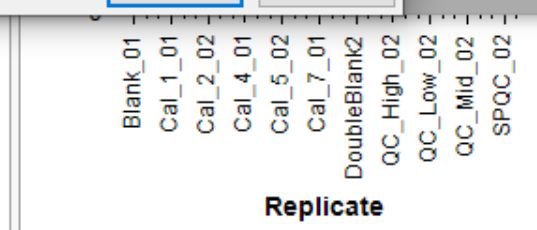
Retention Times - Replicate Comparison

Drug - 283.0400+ Drug - 286.0400[M3.0+] (heavy)

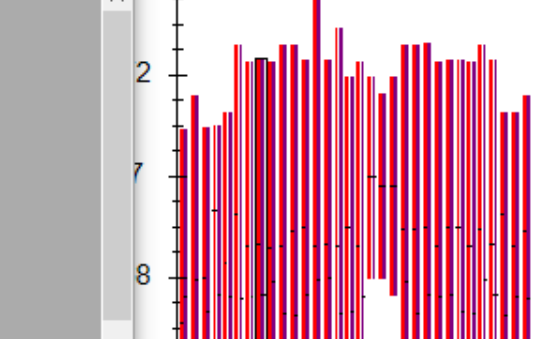


Replicate

Replicate	Drug - 283.0400+	Drug - 286.0400[M3.0+] (heavy)
Blank_01		
Cal_1_01		
Cal_2_02		
Cal_4_01		
Cal_5_02		
Cal_7_01		
DoubleBlank2		
QC_High_02		
QC_Low_02		
QC_Mid_02		
SPQC_02		

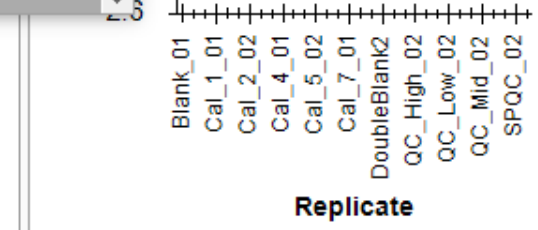


Replicate



Replicate

Replicate	Drug - 283.0400+	Drug - 286.0400[M3.0+] (heavy)
Blank_01		
Cal_1_01		
Cal_2_02		
Cal_4_01		
Cal_5_02		
Cal_7_01		
DoubleBlank2		
QC_High_02		
QC_Low_02		
QC_Mid_02		
SPQC_02		



Replicate

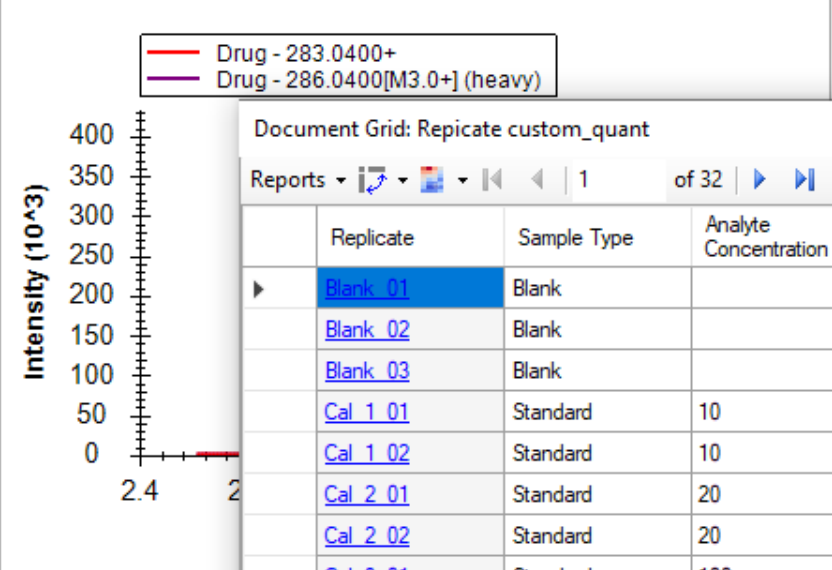
Targets Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca

Replicates: Cal_3_01

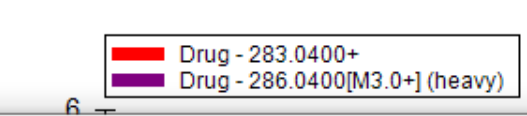
molescules 1

- Drug
 - 283.0400+ (total ratio 1.12)
 - 129.9600+[1] (ratio 1.12)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+[1]

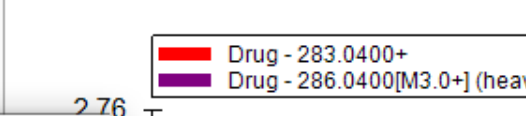
Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01 Cal_4_02 Ca



Peak Areas - Replicate Comparison



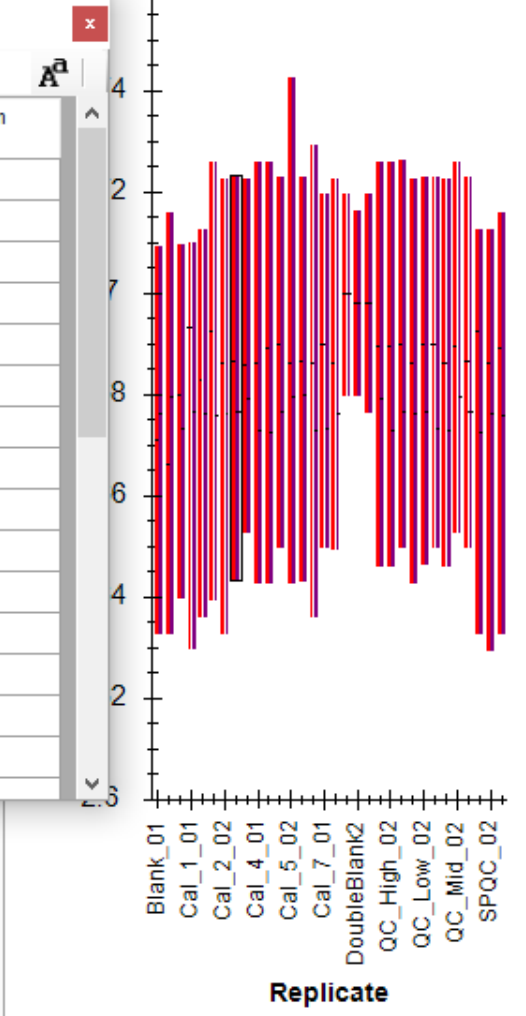
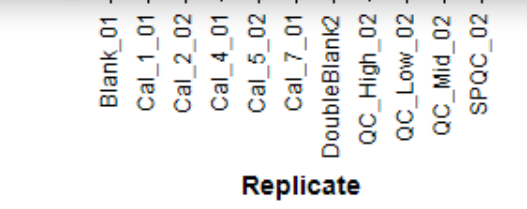
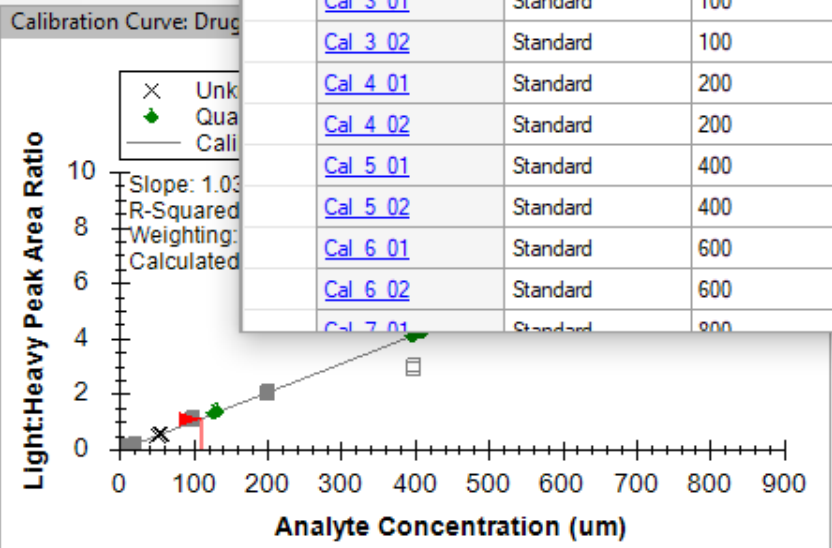
Retention Times - Replicate Comparison



Document Grid: Replicate custom_quant

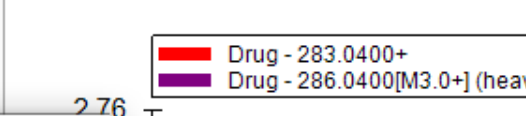
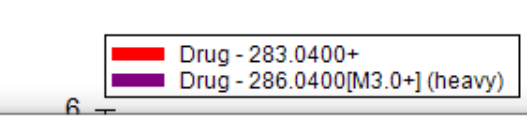
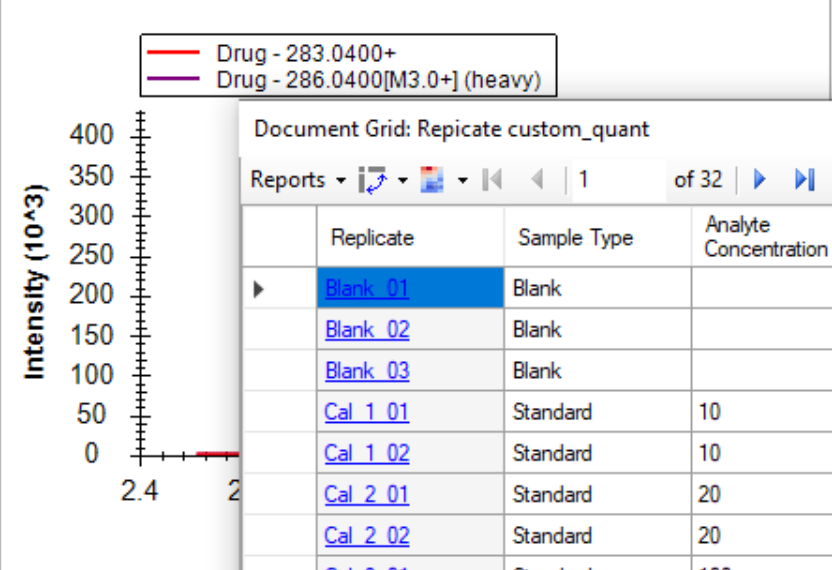
Reports 1 of 32

Replicate	Sample Type	Analyte Concentration	Quantification	Accuracy	Exclude From Calibration
Blank_01	Blank		0.1342 um	#N/A	<input type="checkbox"/>
Blank_02	Blank		0.3242 um	#N/A	<input type="checkbox"/>
Blank_03	Blank		0.2408 um	#N/A	<input type="checkbox"/>
Cal_1_01	Standard	10	10.3 um	103%	<input type="checkbox"/>
Cal_1_02	Standard	10	9.7712 um	97.7%	<input type="checkbox"/>
Cal_2_01	Standard	20	18.6481 um	93.2%	<input type="checkbox"/>
Cal_2_02	Standard	20	19.5628 um	97.8%	<input type="checkbox"/>
Cal_3_01	Standard	100	108.8353 um	108.8%	<input type="checkbox"/>
Cal_3_02	Standard	100	101.0449 um	101%	<input type="checkbox"/>
Cal_4_01	Standard	200	199.111 um	99.6%	<input type="checkbox"/>
Cal_4_02	Standard	200	192.8198 um	96.4%	<input type="checkbox"/>
Cal_5_01	Standard	400	277.9943 um	69.5%	<input checked="" type="checkbox"/>
Cal_5_02	Standard	400	289.8102 um	72.5%	<input checked="" type="checkbox"/>
Cal_6_01	Standard	600	617.8728 um	103%	<input type="checkbox"/>
Cal_6_02	Standard	600	639.7133 um	106.6%	<input type="checkbox"/>
Cal_7_01	Standard	800	813.7328 um	101.6%	<input type="checkbox"/>



molescules 1

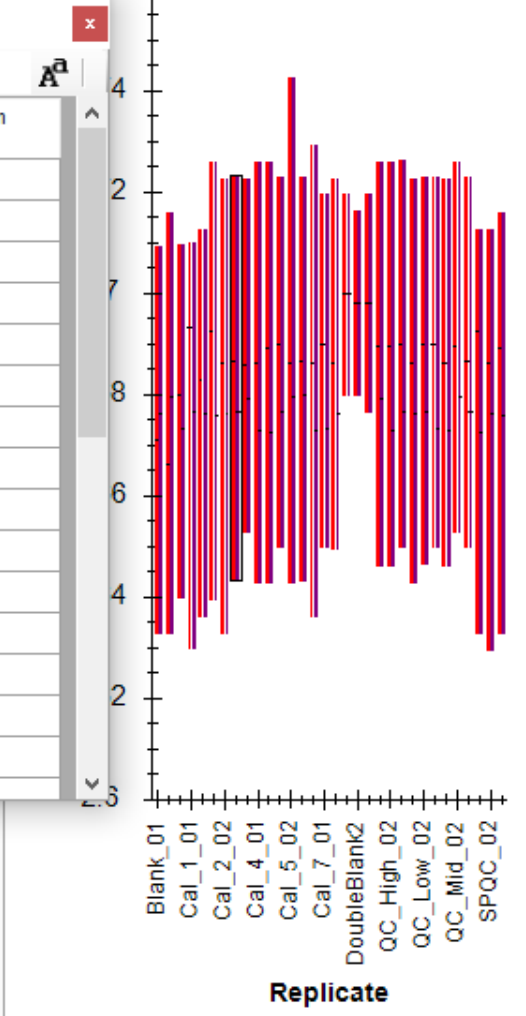
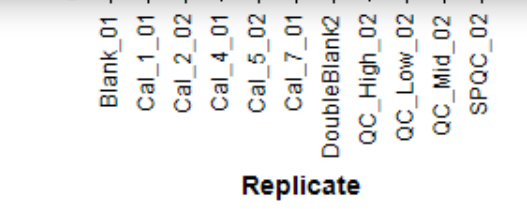
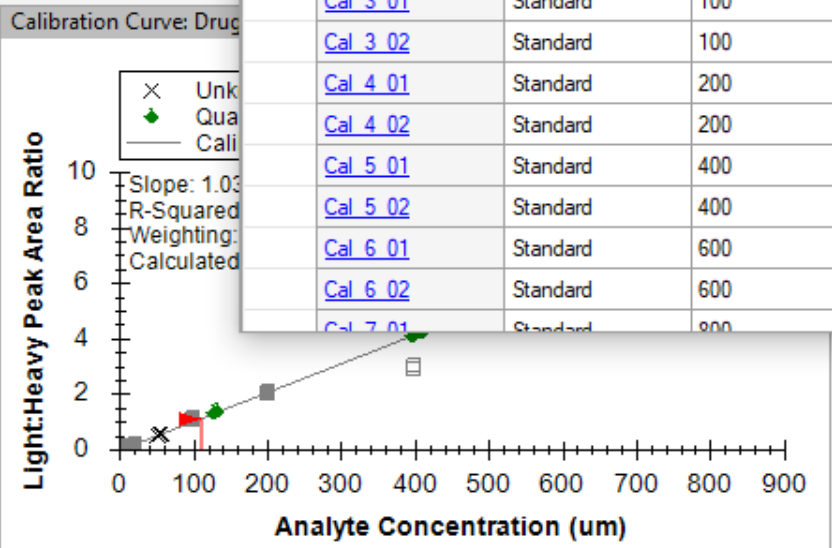
- Drug
 - 283.0400+ (total ratio 1.12)
 - 129.9600+[1] (ratio 1.12)
 - 286.0400[M3.0+] (heavy)
 - 133.0000+[1]



Document Grid: Replicate custom_quant

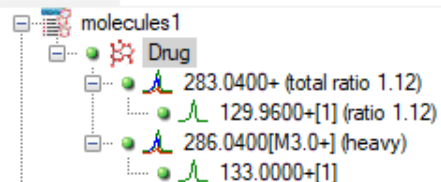
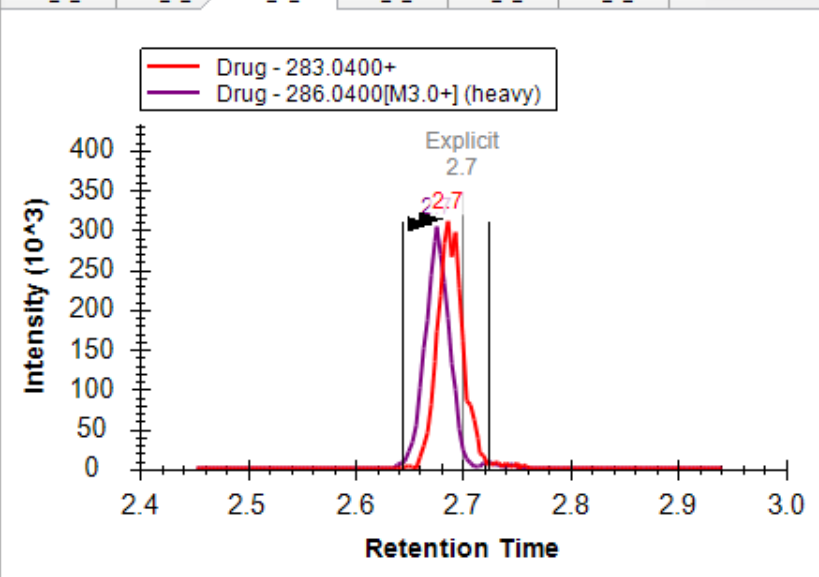
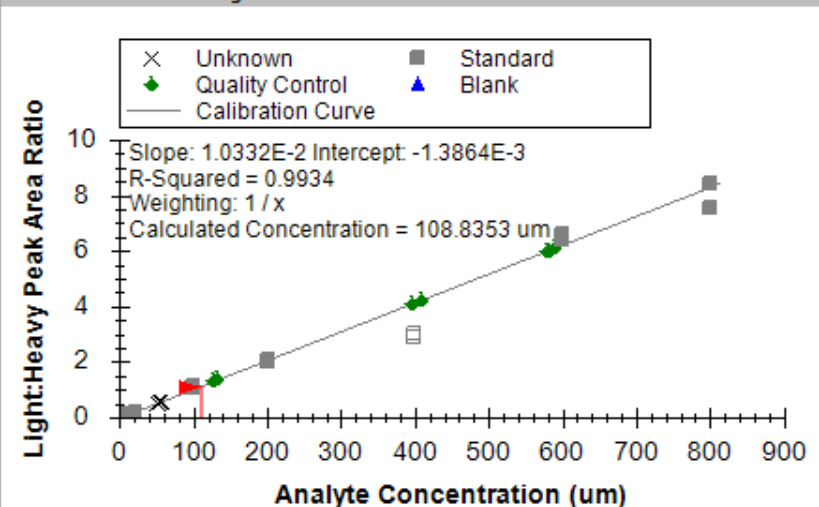
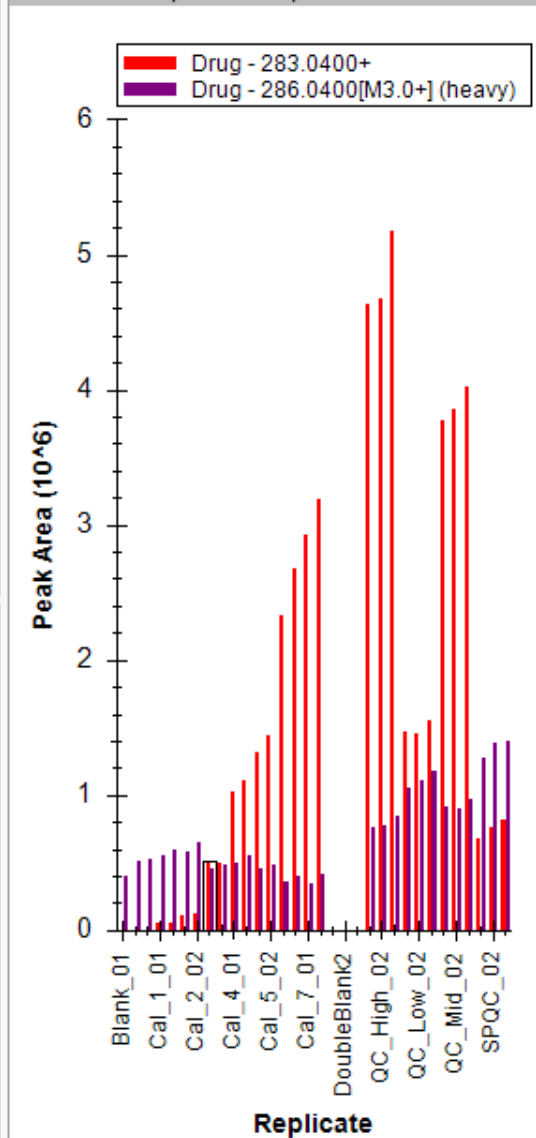
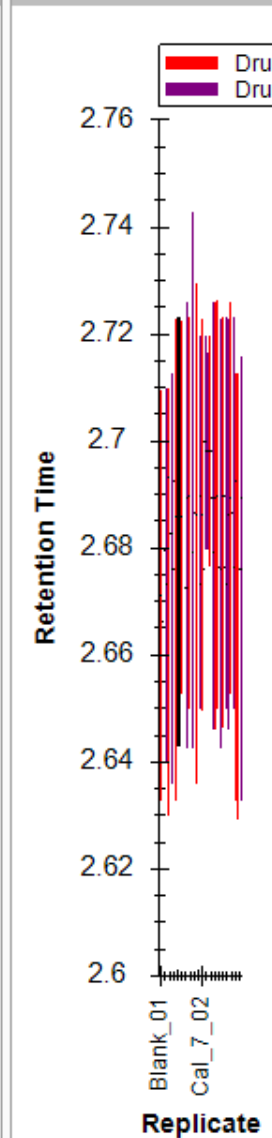
Reports 1 of 32

Replicate	Sample Type	Analyte Concentration	Quantification	Accuracy	Exclude From Calibration
Blank_01	Blank		0.1342 um	#N/A	<input type="checkbox"/>
Blank_02	Blank		0.3242 um	#N/A	<input type="checkbox"/>
Blank_03	Blank		0.2408 um	#N/A	<input type="checkbox"/>
Cal_1_01	Standard	10	10.3 um	103%	<input type="checkbox"/>
Cal_1_02	Standard	10	9.7712 um	97.7%	<input type="checkbox"/>
Cal_2_01	Standard	20	18.6481 um	93.2%	<input type="checkbox"/>
Cal_2_02	Standard	20	19.5628 um	97.8%	<input type="checkbox"/>
Cal_3_01	Standard	100	108.8353 um	108.8%	<input type="checkbox"/>
Cal_3_02	Standard	100	101.0449 um	101%	<input type="checkbox"/>
Cal_4_01	Standard	200	199.111 um	99.6%	<input type="checkbox"/>
Cal_4_02	Standard	200	192.8198 um	96.4%	<input type="checkbox"/>
Cal_5_01	Standard	400	277.9943 um	69.5%	<input checked="" type="checkbox"/>
Cal_5_02	Standard	400	289.8102 um	72.5%	<input checked="" type="checkbox"/>
Cal_6_01	Standard	600	617.8728 um	103%	<input type="checkbox"/>
Cal_6_02	Standard	600	639.7133 um	106.6%	<input type="checkbox"/>
Cal_7_01	Standard	800	813.7328 um	101.6%	<input type="checkbox"/>



Targets ↑ ×

Replicates: Cal_3_01

Cal_2_01 Cal_2_02 **Cal_3_01** Cal_3_02 Cal_4_01 Cal_4_02 Ca ← → ⌵ ⌶ ×Calibration Curve: Drug ↑ ×Peak Areas - Replicate Comparison ↑ ×Retention Time... ↑ ×Document Grid... ↑ ×

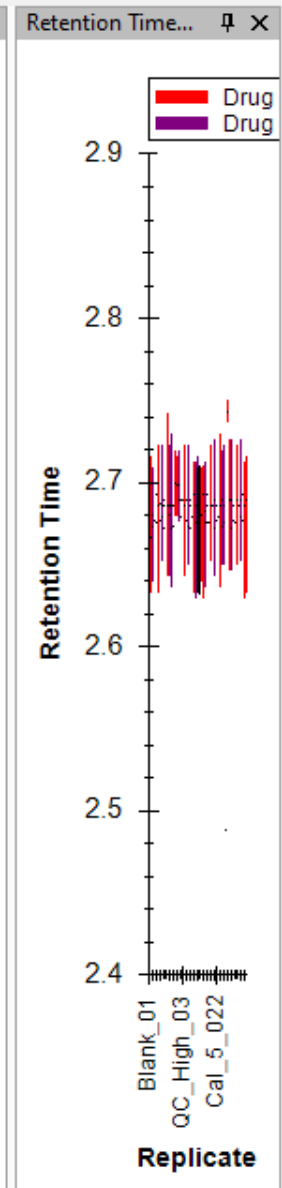
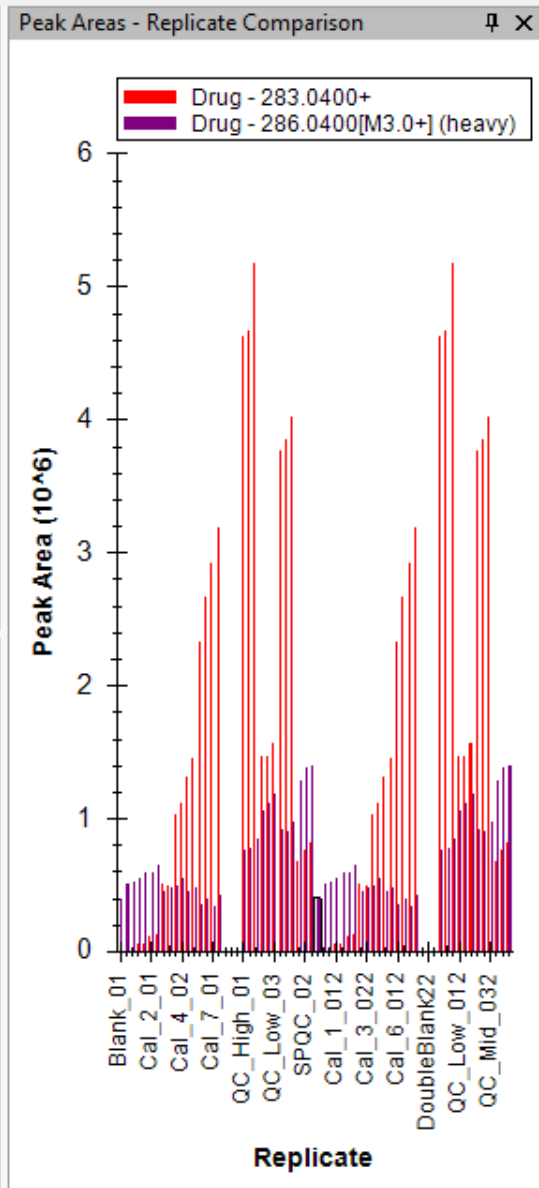
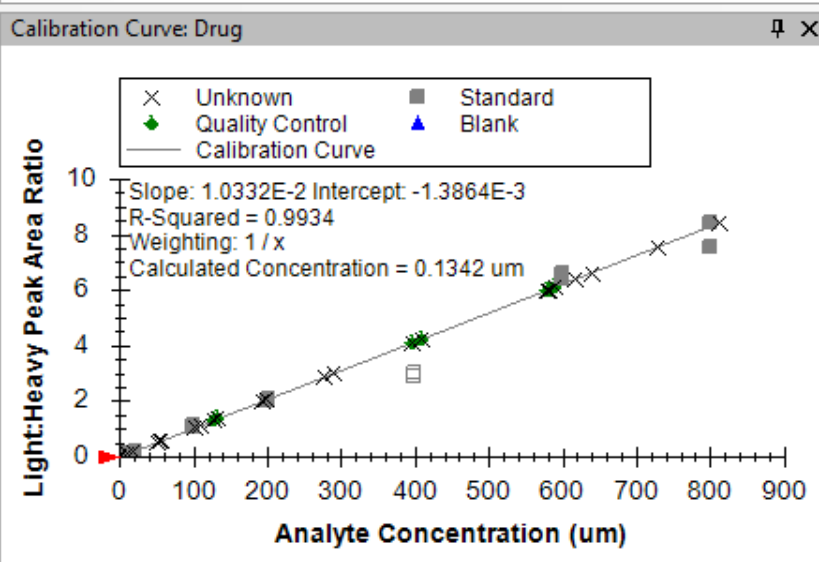
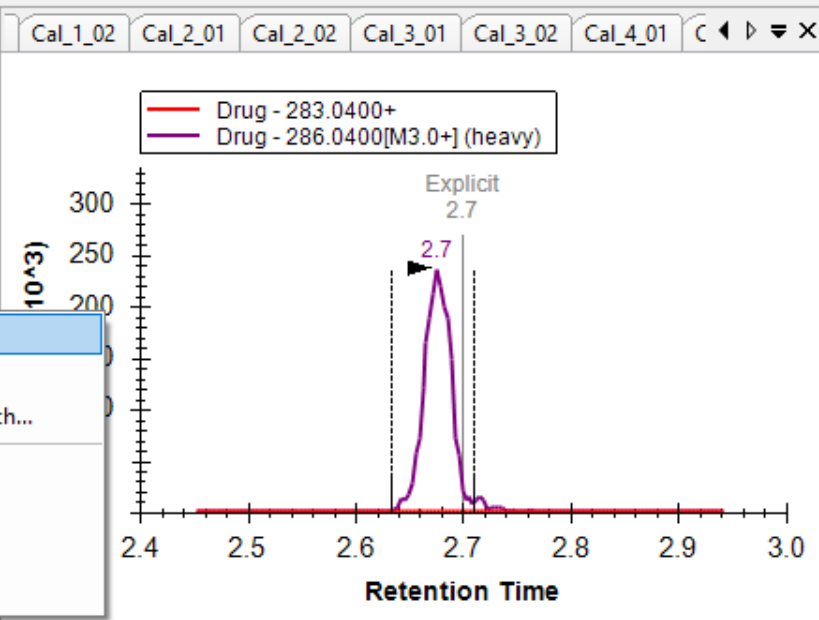
Reports ↑ ×

Replicate
Blank_01
Blank_02
Blank_03
Cal_1_01
Cal_1_02
Cal_2_01
Cal_2_02
Cal_3_01
Cal_3_02
Cal_4_01
Cal_4_02
Cal_5_01
Cal_5_02
Cal_6_01
Cal_6_02
Cal_7_01
Cal_7_02
DoubleBlank1
DoubleBlank2
DoubleBlank3
QC_High_01
QC_High_02
QC_High_03
QC_Low_01
QC_Low_02



- Start...
- New Ctrl+N
- Open... Ctrl+O
- Open containing folder
- Save Ctrl+S
- Save As...
- Share...
- Upload to Panorama...
- Import
- Export
- 1 Quant Meta.sky
- Exit

- Results...
- Peak Boundaries...
- EncyclopeDIA Search...
- Assay Library...
- Transition List...
- Document...
- Annotations...



Document Grid... Reports

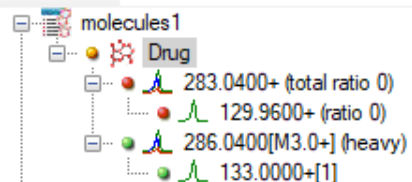
Replicate
Blank_01
Blank_02
Blank_03
Cal_1_01
Cal_1_02
Cal_2_01
Cal_2_02
Cal_3_01
Cal_3_02
Cal_4_01
Cal_4_02
Cal_5_01
Cal_5_02
Cal_6_01
Cal_6_02
Cal_7_01
Cal_7_02
DoubleBlank1
DoubleBlank2
DoubleBlank3
QC_High_01
QC_High_02
QC_High_03
QC_Low_01
QC_Low_02



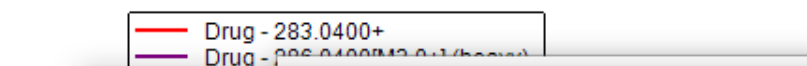


Targets

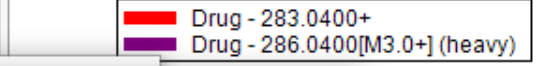
Replicates: Blank_012



Cal_1_02 Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01



Peak Areas - Replicate Comparison



Retention Time...



Document Grid...

Reports

Replicate
Blank_01
Blank_02
Blank_03
Cal_1_01
Cal_1_02
Cal_2_01
Cal_2_02
Cal_3_01
Cal_3_02
Cal_4_01
Cal_4_02
Cal_5_01
Cal_5_02
Cal_6_01
Cal_6_02
Cal_7_01
Cal_7_02
DoubleBlank1
DoubleBlank2
DoubleBlank3
QC_High_01
QC_High_02
QC_High_03
QC_Low_01
QC_Low_02

Import Results Files

Look in: TRAINING

Blank_01.raw	Cal_7_01.raw	SPQC_02.raw
Blank_02.raw	Cal_7_02.raw	SPQC_03.raw
Blank_03.raw	DoubleBlank1.raw	
Cal_1_01.raw	DoubleBlank2.raw	
Cal_1_02.raw	DoubleBlank3.raw	
Cal_2_01.raw	QC_High_01.raw	
Cal_2_02.raw	QC_High_02.raw	
Cal_3_01.raw	QC_High_03.raw	
Cal_3_02.raw	QC_Low_01.raw	
Cal_4_01.raw	QC_Low_02.raw	
Cal_4_02.raw	QC_Low_03.raw	
Cal_5_01.raw	QC_Mid_01.raw	
Cal_5_02.raw	QC_Mid_02.raw	
Cal_6_01.raw	QC_Mid_03.raw	
Cal_6_02.raw	SPQC_01.raw	

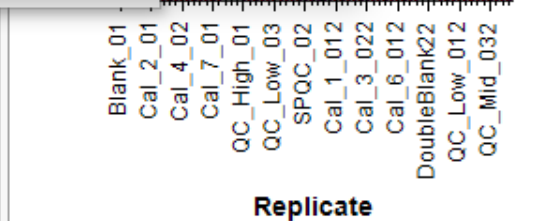
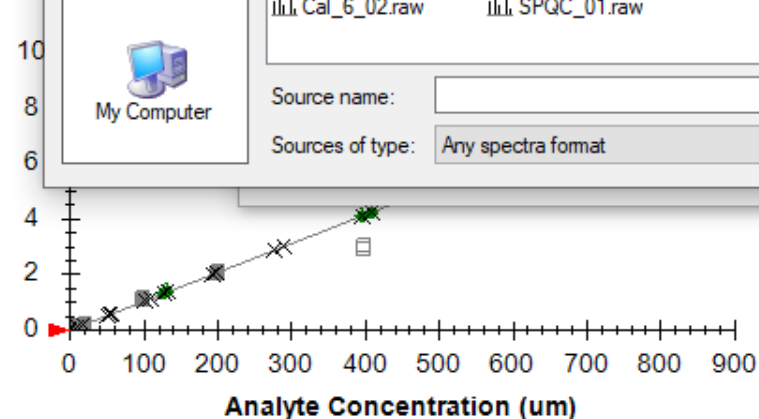
Source name:

Sources of type: Any spectra format

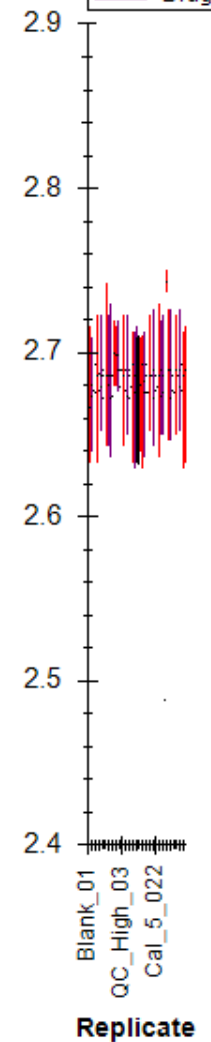
Buttons: Open, Cancel

Calibrati

Light:Heavy Peak Area Ratio



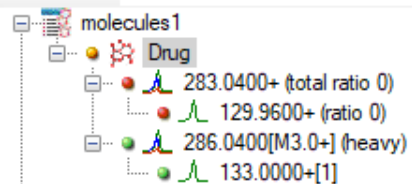
Retention Time



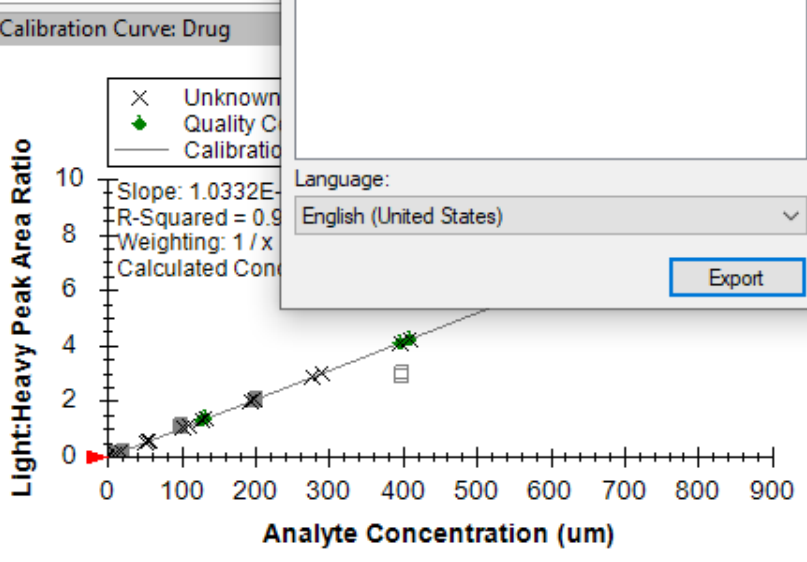
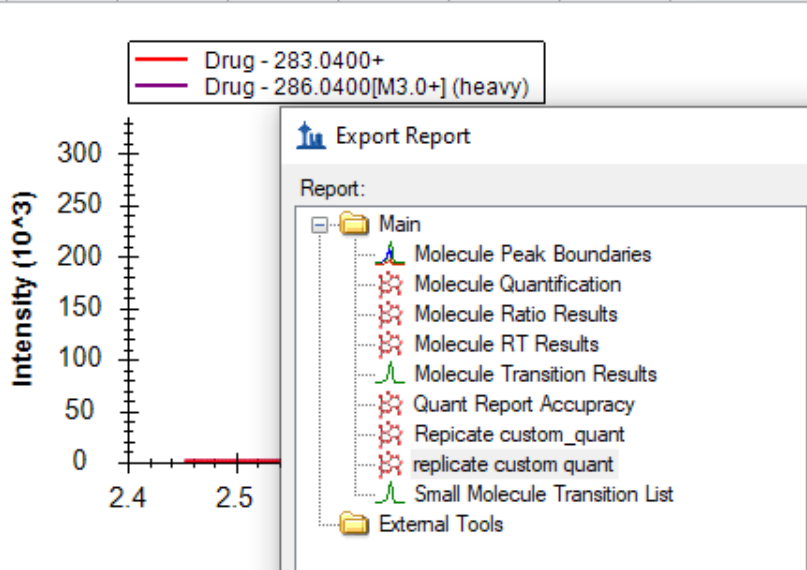


Targets

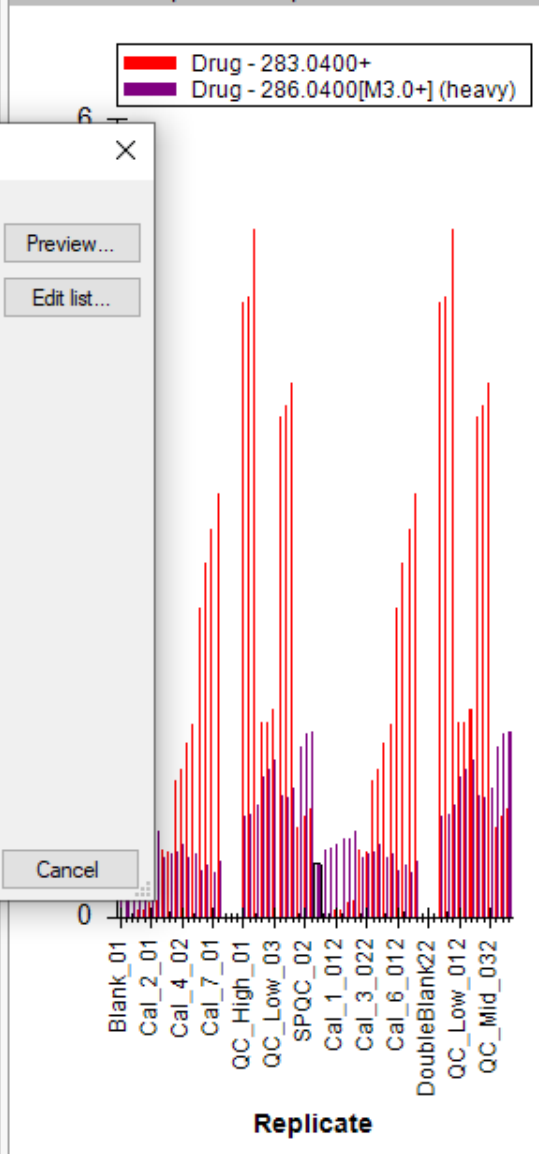
Replicates: Blank_012



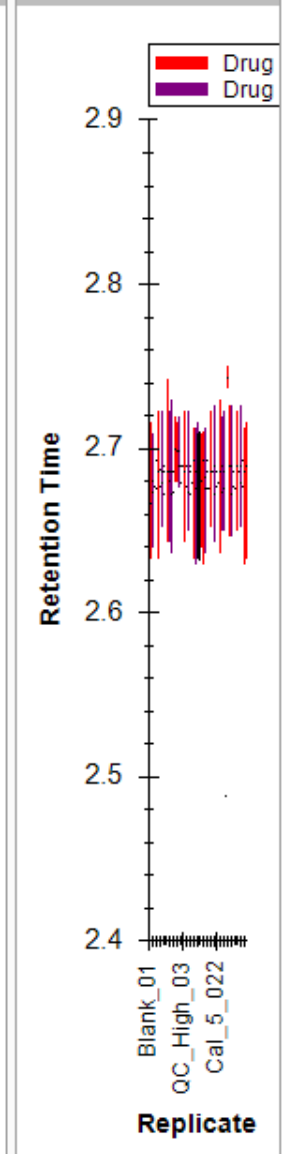
Cal_1_02 Cal_2_01 Cal_2_02 Cal_3_01 Cal_3_02 Cal_4_01



Peak Areas - Replicate Comparison



Retention Time...



Document Grid...

Reports

Replicate
Blank_01
Blank_02
Blank_03
Cal_1_01
Cal_1_02
Cal_2_01
Cal_2_02
Cal_3_01
Cal_3_02
Cal_4_01
Cal_4_02
Cal_5_01
Cal_5_02
Cal_6_01
Cal_6_02
Cal_7_01
Cal_7_02
DoubleBlank1
DoubleBlank2
DoubleBlank3
QC_High_01
QC_High_02
QC_High_03
QC_Low_01
QC_Low_02

Export Report

Report:

- Main
 - Molecule Peak Boundaries
 - Molecule Quantification
 - Molecule Ratio Results
 - Molecule RT Results
 - Molecule Transition Results
 - Quant Report Accuracy
 - Replicate custom_quant
 - replicate custom quant
 - Small Molecule Transition List
- External Tools

Language: English (United States)

Export Cancel