

The background of the slide features a vibrant red color scheme. On the left, there is a faint, artistic depiction of a molecular structure. On the right, a stylized globe is shown with white orbital lines and dots, suggesting a scientific or technological theme.

ASMS 2019

June 2 - 6 | Atlanta, GA, USA

ThermoFisher
SCIENTIFIC

Instrument API and XML Method Modification Interface

A brief introduction

Tony Zhao and Jesse Canterbury

The world leader in serving science

1. Instrument Application Programming Interface (I-API)

- Introduction
- Architecture
- Example

2. XML Method Modification Interface (XMMI)

- Architecture
- Example

1. Instrument Application Programming Interface (I-API)

- Introduction
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2. XML Method Modification Interface (XMMI)

- Architecture
- Example

Why an API?

“I wish I could do ...”

“Can I do this in method editor?”

“I only want to select peaks that have odd masses ...”

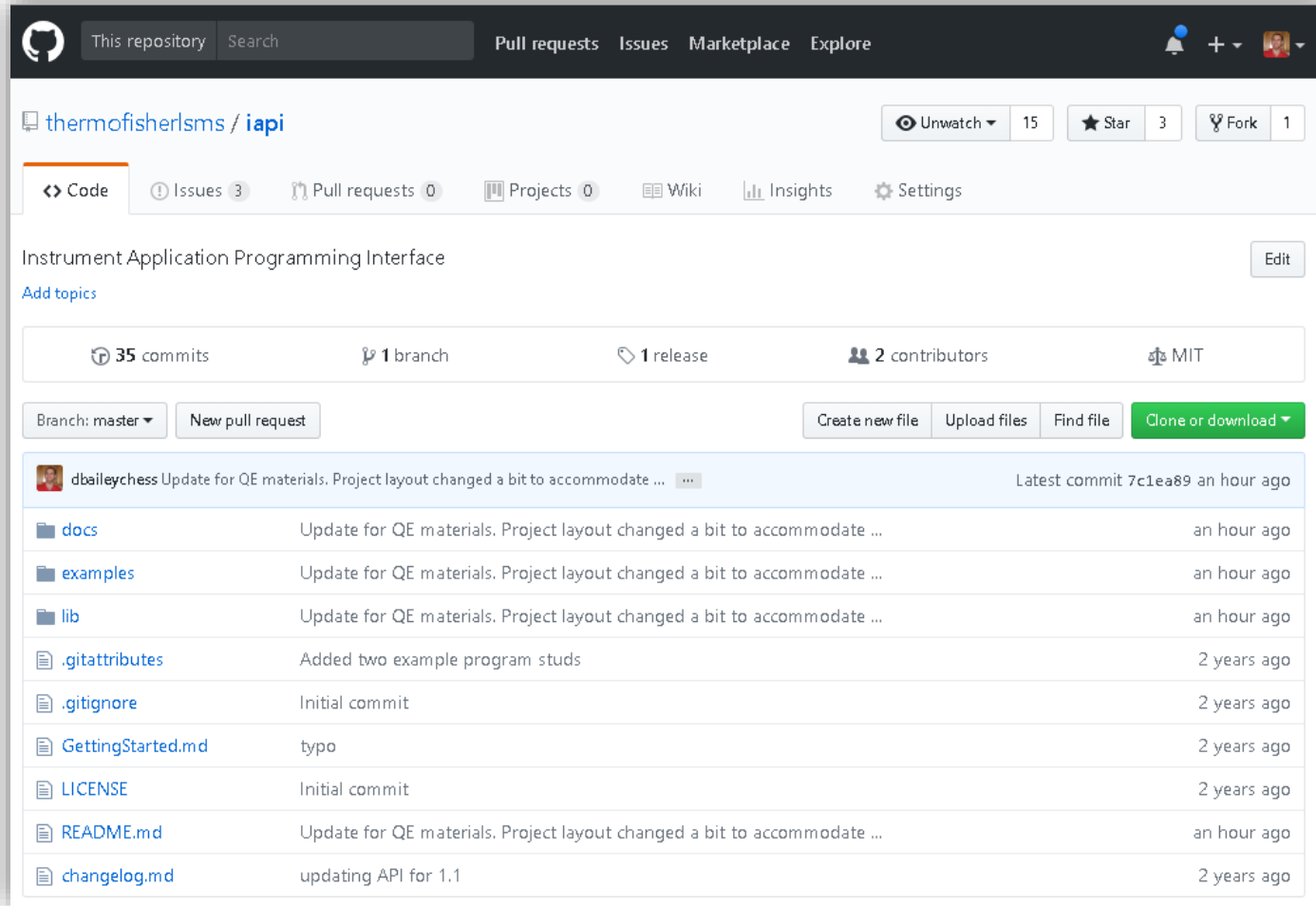
“I have this awesome new experiment ...”

“I only want to select peaks that have odd masses ...”

The screenshot displays the Thermo Scientific Orbitrap Fusion MS software interface. The main window is titled "Orbitrap Fusion MS Tune Application 3.1.2140 - DEV MODE". The interface is divided into several sections:

- Top Bar:** Contains the Thermo Scientific logo, application name, and various control buttons (Play, Pause, Stop, Record, etc.).
- Left Panel:** A sidebar with tabs for "KIN SOURCE", "DEFINE SCAN", and "CALIBRATION". Under "DEFINE SCAN", there are settings for Scan Type (MS Scan), Detector Type (Orbitrap), Orbitrap Resolution (120k), Mass Range (Non), Use Quadrupole Isolation (checked), Scan Range (m/z) (150), RF Lens (%) (60), AGC Target (40k), Maximum Injection Time (ms) (100), Microscans (1), and Source Fragmentation (unchecked).
- Main Display Area:**
 - Top:** A diagram showing the MS/MS workflow: "MS OT" (Orbitrap) leading to "MIPS" (Microscans).
 - Bottom:** A section titled "Experiments" with a list of experiments. The "Full MS / dd-MS2 (TopN)" experiment is selected. Below the list is a diagram showing the workflow: "Full MS" leading to "dd-MS2".
- Right Panel:** A "Properties" section showing the settings for the selected experiment. It includes:
 - Global Settings:** User Role (Standard), Use lock masses (best), Chrom. peak w. (15 s), Time (Method duration 90.00 min).
 - General:** Runtime (0 to 90 min), Polarity (positive), Default charge (2), Inclusion (checked), Exclusion (unchecked), Tags (unchecked).
 - Full MS:** Resolution (60,000), AGC target (3e5), Maximum IT (30 ms), Scan range (380 to 2000 m/z).
 - dd-MS2 / dd-SIM:** Resolution (15,000), AGC target (5e4), Maximum IT (60 ms), Loop count (15), TopN (15), Isolation window (1.5 m/z), Fixed first mass (checked), NCE / stepped (1-27).
 - dd Settings:** Underfill ratio (1.0 %), Intensity threshold (6.3e3), Apex trigger (checked), Change exclusion (unassigned), Peptide match (preferred), Exclude isotopes on (checked), and a checkbox for "Exclude isotopes on" (unchecked).

<https://github.com/thermofisherlisms/iapi>



- Public interfaces for
 - Thermo Scientific Tribrid MS
 - Thermo Scientific Exactive MS
- Documentation
 - Previous ASMS Posters
 - Help files
- VS Solution of Example Applications

External Requirements

- Tune Installation
- .NET 4.6.2+
- License Agreement in place
- IAPI License Key Activated

Thermo Scientific Exactive Series



I-API Version

 API-1.0.dll

 API-1.1.dll

Instrument Extensions

 ESAPI-1.0.dll

 ESAPI-1.1.dll


Misc.

 VI-1.0.dll


Thermo Scientific Tribid Series



 API-2.0.dll

 Spectrum-1.0.dll

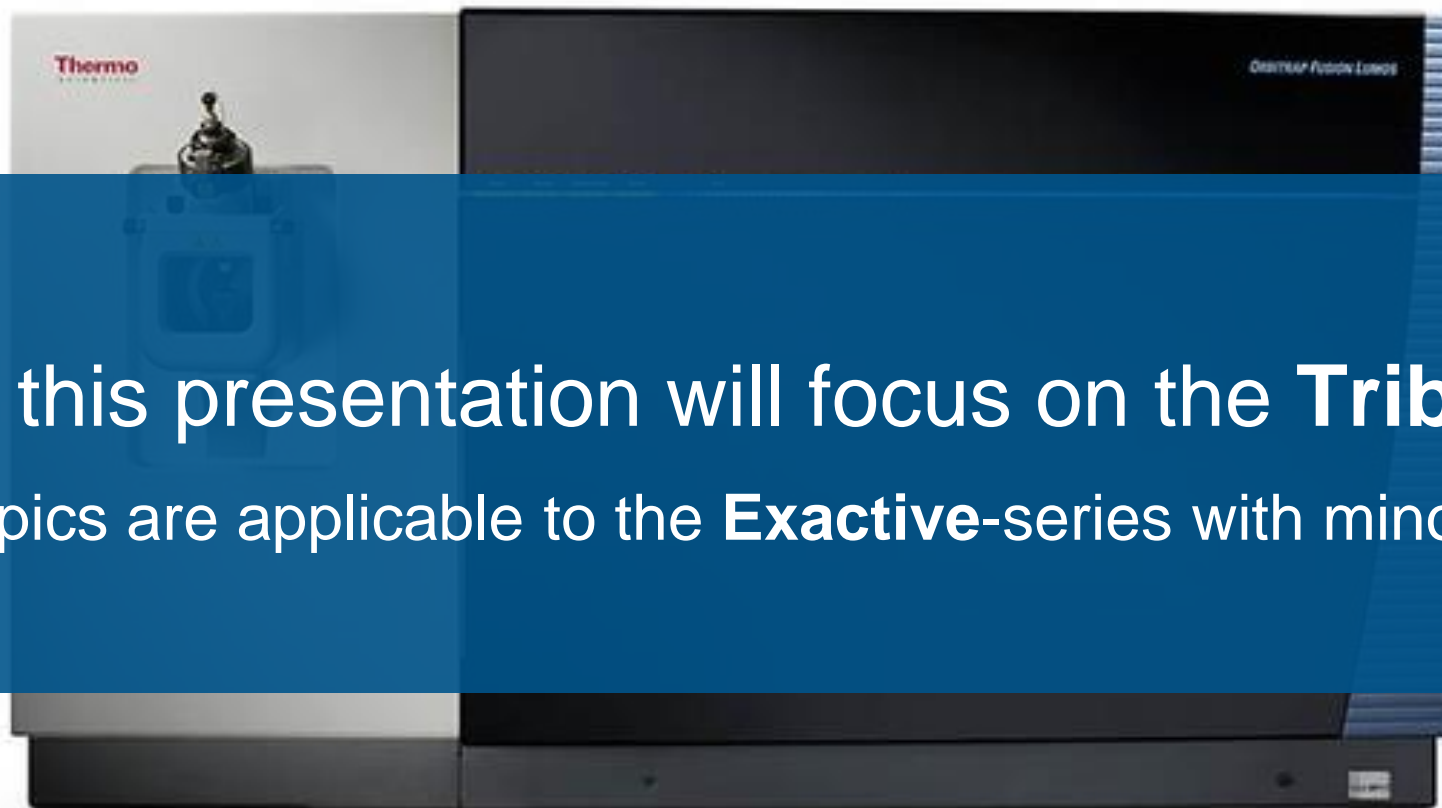
 Fusion.API-1.0.dll

 Thermo.TNG.Factory.dll

Differences and Similarities between Exactive and Tribrid Series IAPI

- Although IAPI 1.X (supports Exactives) is **not binary compatible** with IAPI 2.X (supports Tribrids), they share considerable amount of structure
 - Namespaces and hierarchies are virtually unchanged
 - A few name changes or minor reorganization
 - Removal of some interfaces
 - Spectrum-related interfaces moved into own assembly
- The logical flow for both receiving scan data and sending scans definitions to the instrument is **identical**
- Different methods for instantiating the IAPIs
 - Tribrid-series uses a **Factory** method model with Microsoft's Managed Extensibility Framework (MEF)
 - Exactive-series uses the **System.Reflection.Assembly** API





The rest of this presentation will focus on the **Tribrid-series** IAPI.

Most topics are applicable to the **Exactive**-series with minor differences.

1. IAPI Architecture

- Interfaces
- Data and Control Flow

2. Receiving Data from the MS

- Interfaces
- Scan Data Stream Subscription

3. Controlling the MS

- Sending Scan Definitions
- Changing other MS parameters

4. Getting Started

Mass Spectrometer



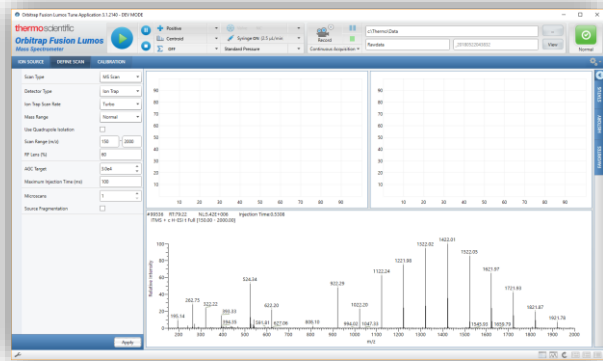
Local Switch



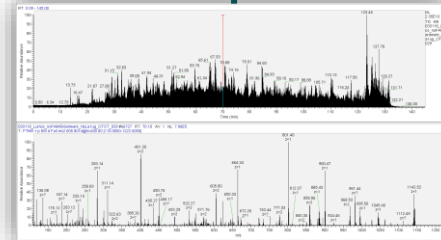
Data System



Tune Application



Instrument Service



Rawfile

IAP1 Architecture

Mass Spectrometer



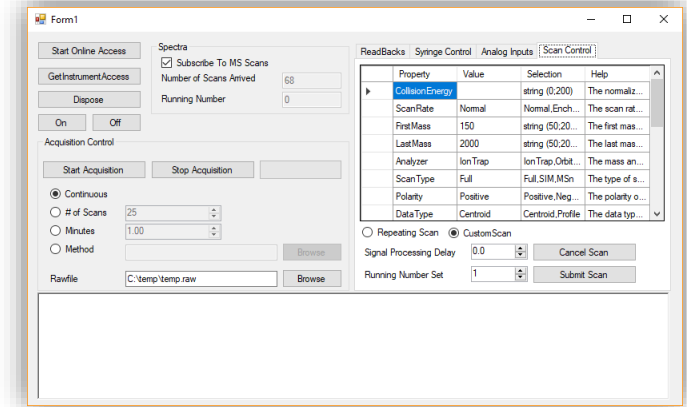
Local Switch



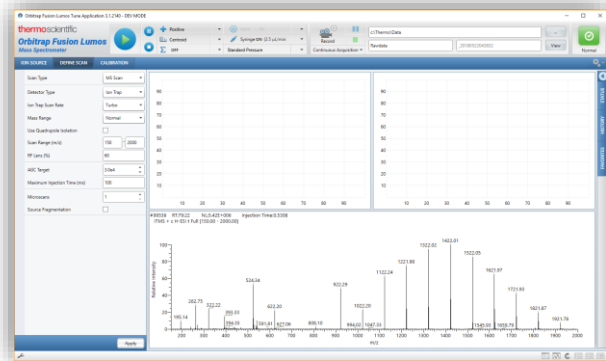
Data System



IAPI-Enabled App

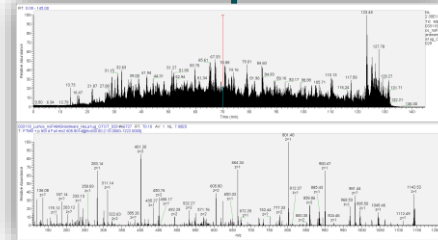


Tune Application



Instrument Service

3rd Party Application

 API-2.0.dll

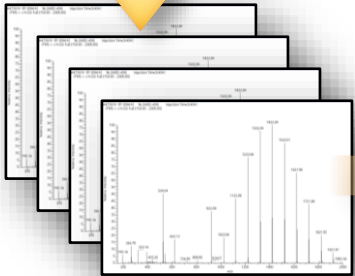
Rawfile

I-API Data and Control Flow

Mass Spectrometer



Scan Data
Stream



Data System



API-2.0.dll



3rd Party
Application

- Displays scan in Tune
- Writes to Rawfile
- Forwards data to API

- Converts data into I-API format
- Raises **Event** to any subscribers

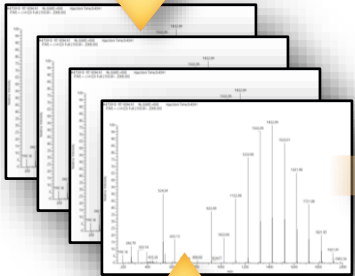
- Handles scan **Event**
- Processes the data
- Do whatever you want!

I-API Data and Control Flow

Mass Spectrometer



Scan Data Stream



Scan Definition

Scan Type	MS Scan
Detector Type	Ion Trap
Ion Trap Scan Rate	Normal
Mass Range	Normal
Use Quadrupole Isolation	<input checked="" type="checkbox"/>
Scan Range (m/z)	150 - 2000
RF Lens (%)	80
AGC Target	3.0e4
Maximum Injection Time (ms)	100
Microscans	1
Source Fragmentation	<input type="checkbox"/>

Data System

 Instrument Service

 API-2.0.dll

 3rd Party Application

- Displays scan in Tune
- Writes to Rawfile
- Forwards data to API

- Converts data into I-API format
- Raises **Event** to any subscribers

- Handles scan **Event**
- Processes the data
- Do whatever you want!

- Logs event
- Downloads scan definition to instrument

- Validates scan definition
- Forwards scan to Instrument Service

- Calls I-API to create **IScanDefinition** object
- Changes definition as sees fit

1. IAPI Architecture

- Interfaces
- Data and Control Flow

2. Receiving Data from the MS

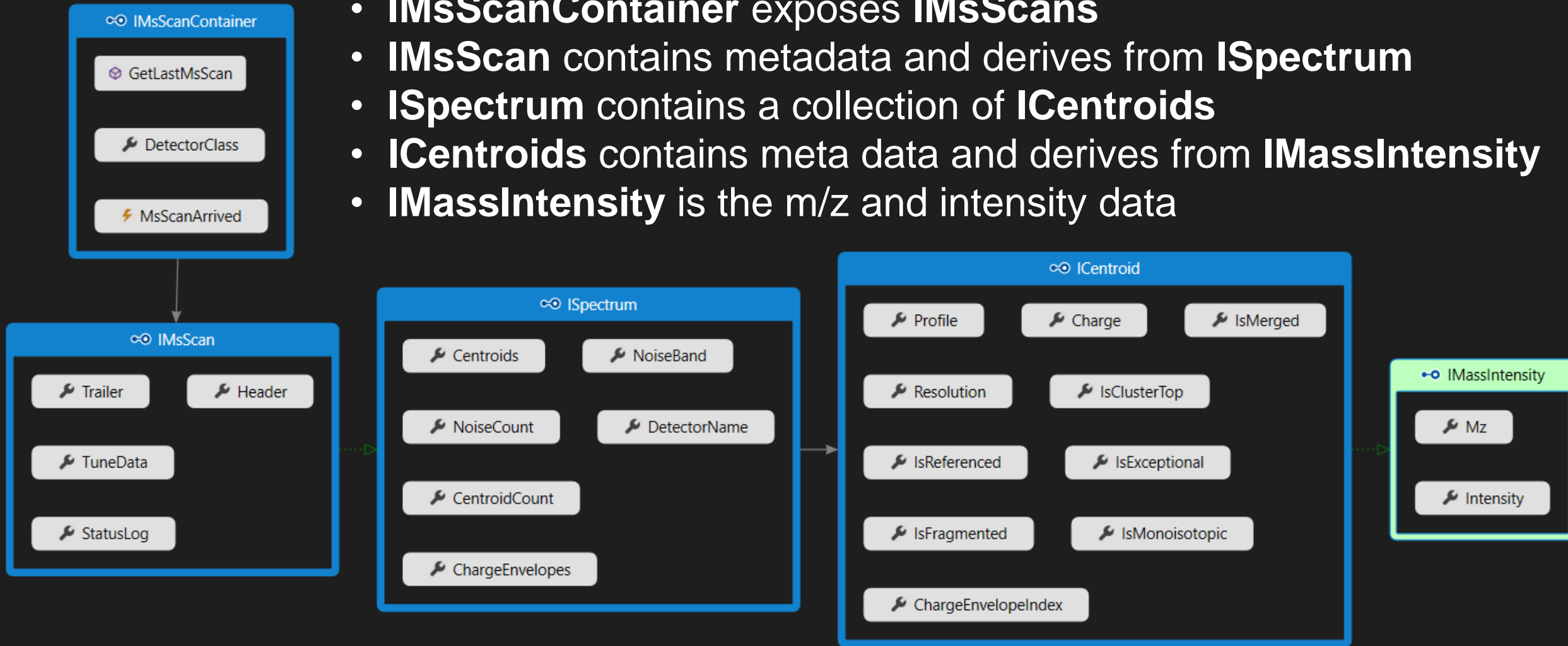
- Interfaces
- Scan Data Stream Subscription

3. Controlling the MS

- Sending Scan Definitions
- Changing other MS parameters

4. Getting Started

- **IMsScanContainer** exposes **IMsScans**
- **IMsScan** contains metadata and derives from **ISpectrum**
- **ISpectrum** contains a collection of **ICentroids**
- **ICentroids** contains meta data and derives from **IMassIntensity**
- **IMassIntensity** is the m/z and intensity data



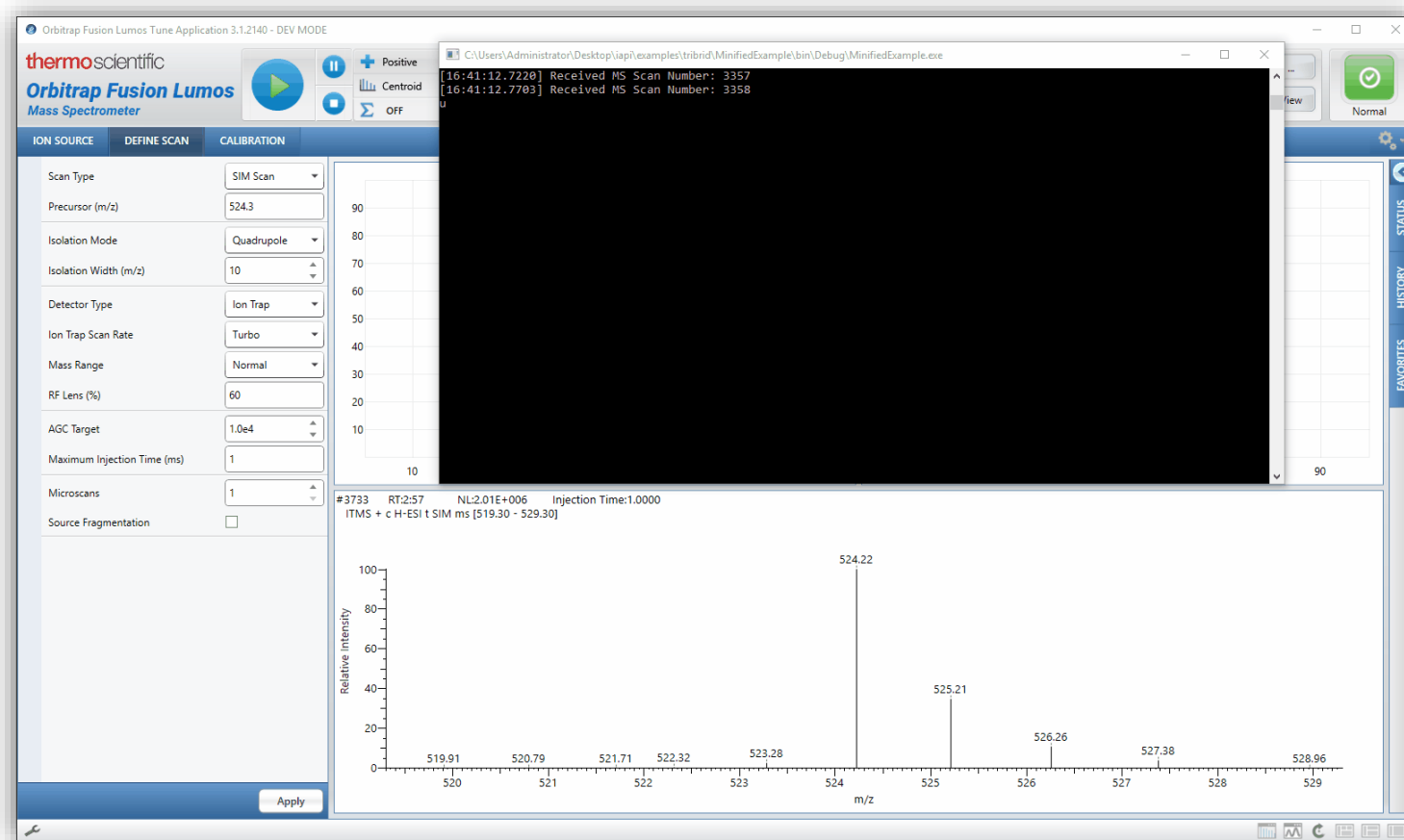
Scan Data Stream

- Receiving the scan data is through the **Event Driven** programming model
- Scans are sent via the .NET **Event** and **EventHandler** mechanism
 - Multiple handlers per scan can be registered
 - Minimal overhead and latency
- Receives Scans from both Tune and Method acquisitions

```
26 .....//Get the MS Scan Container from the fusion
27 .....IFusionMsScanContainer fusionScanContainer = fusionAccess.GetMsScanContainer(0);
28
29 .....//Run forever until the user Escapes
30 .....ConsoleKeyInfo cki;
31 .....while ((cki = Console.ReadKey()).Key != ConsoleKey.Escape)
32 .....{
33 .....    switch(cki.Key)
34 .....    {
35 .....        case ConsoleKey.S:
36 .....            //Subscribe to whenever a new MS scan arrives
37 .....            fusionScanContainer.MsScanArrived += FusionScanContainer_MsScanArrived;
38 .....            break;
39 .....        case ConsoleKey.U:
40 .....            //Unsubscribe
41 .....            fusionScanContainer.MsScanArrived -= FusionScanContainer_MsScanArrived;
42 .....            break;
43 .....        default:
44 .....            Console.WriteLine("Unsupported Key: {0}", cki.Key);
45 .....            break;
46 .....    }
47 .....}
48 .....}
49
50 .....2 references | Thermo Scientific, 1 hour ago | 2 authors, 2 changes
51 .....private static void FusionScanContainer_MsScanArrived(object sender, MsScanEventArgs e)
52 .....{
53 .....    //Print out the scan number of the scan received to console
54 .....    Console.WriteLine("[{0:HH:mm:ss.ffff}] Received MS Scan Number: {1}",
55 .....        DateTime.Now,
56 .....        e.GetScan().Header["Scan"]);
57 .....}
58 }
```

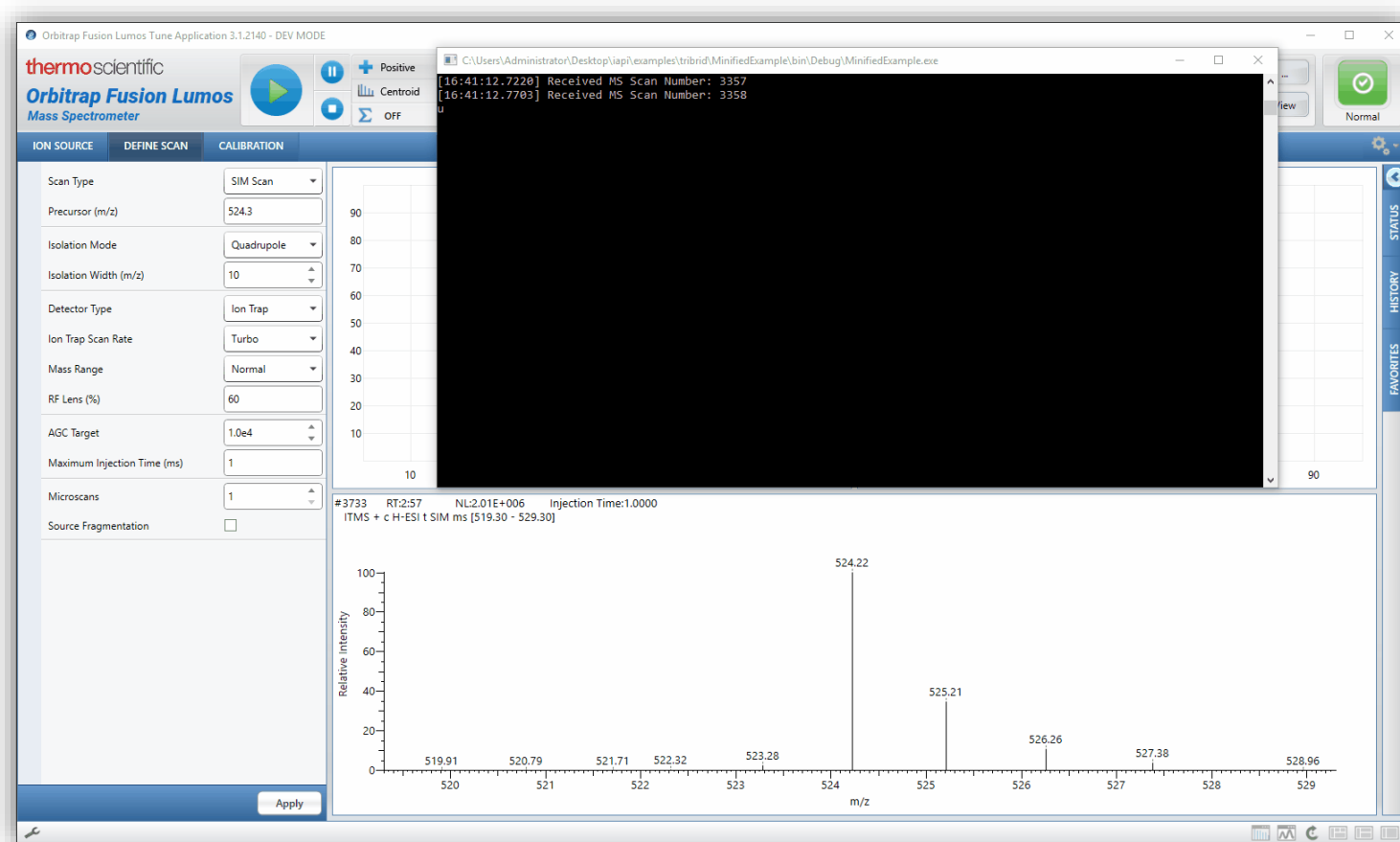
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- tSIM running ~21 Hz (**47.5 ms**) from Tune.
 - Average time of **48.4 ms** between scans received (n = 200)



Scan Data Stream

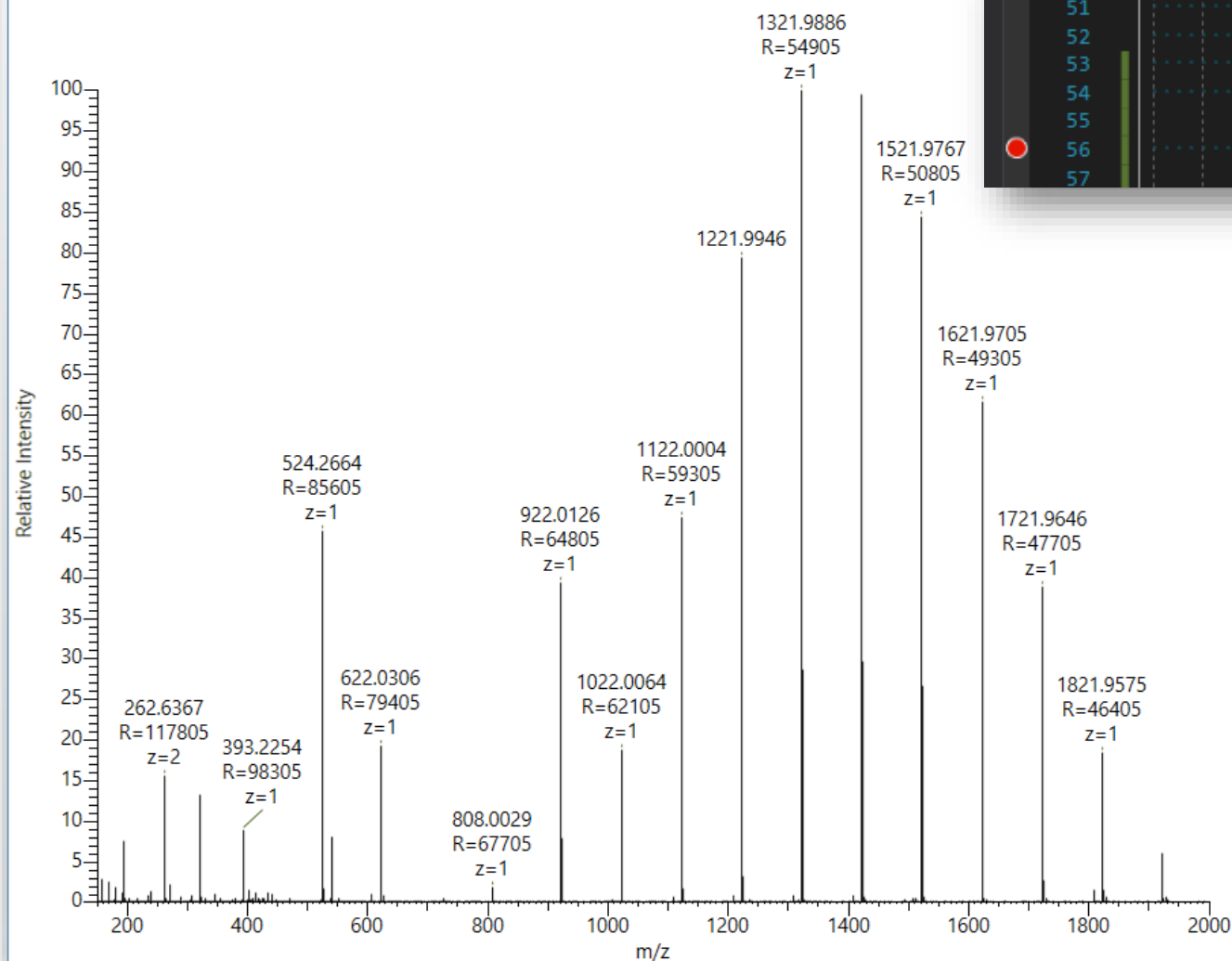
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 - Average time of **48.4 ms** between scans received (n = 200)



The IAPI is responsive and has no impact on the MS acquisition

Scan Data Contents

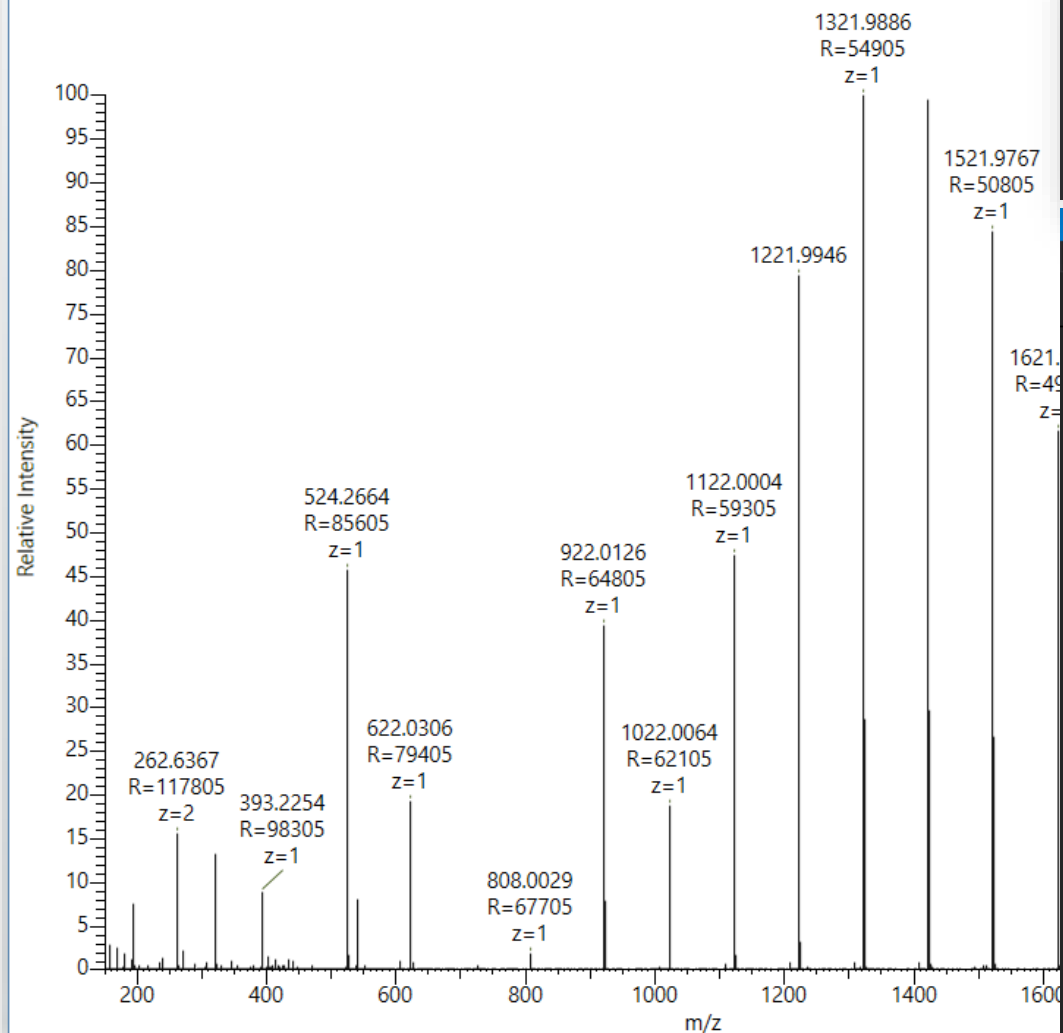
#518053 RT:1234:11 NL:5.89E+007 Injection Time:6.3361
FTMS + c H-ESI Full [150.00 - 2000.00]



```
50 .....private static void FusionScanContainer_MsScanArrived(object sender, MsScanEventArgs e)
51 .....{
52 .....    //Print out the scan number of the scan received to console
53 .....    Console.WriteLine("[{0:HH:mm:ss.ffff}] Received MS Scan Number: {1}",
54 .....        DateTime.Now, e.GetScan().Header["Scan"]);
55 .....
56 .....    var scan = e.GetScan();
57 }
```

Scan Data Contents

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55 .....
56 .....    var scan = e.GetScan();
57 }
```

Watch 1		
Name	Value	Type
scan	{Thermo.TNG.Client.API.MsScanContainer.MsScan}	Thermo.

1. IAPI Architecture

- Interfaces
- Data and Control Flow

2. Receiving Data from the MS

- Interfaces
- Scan Data Stream Subscription

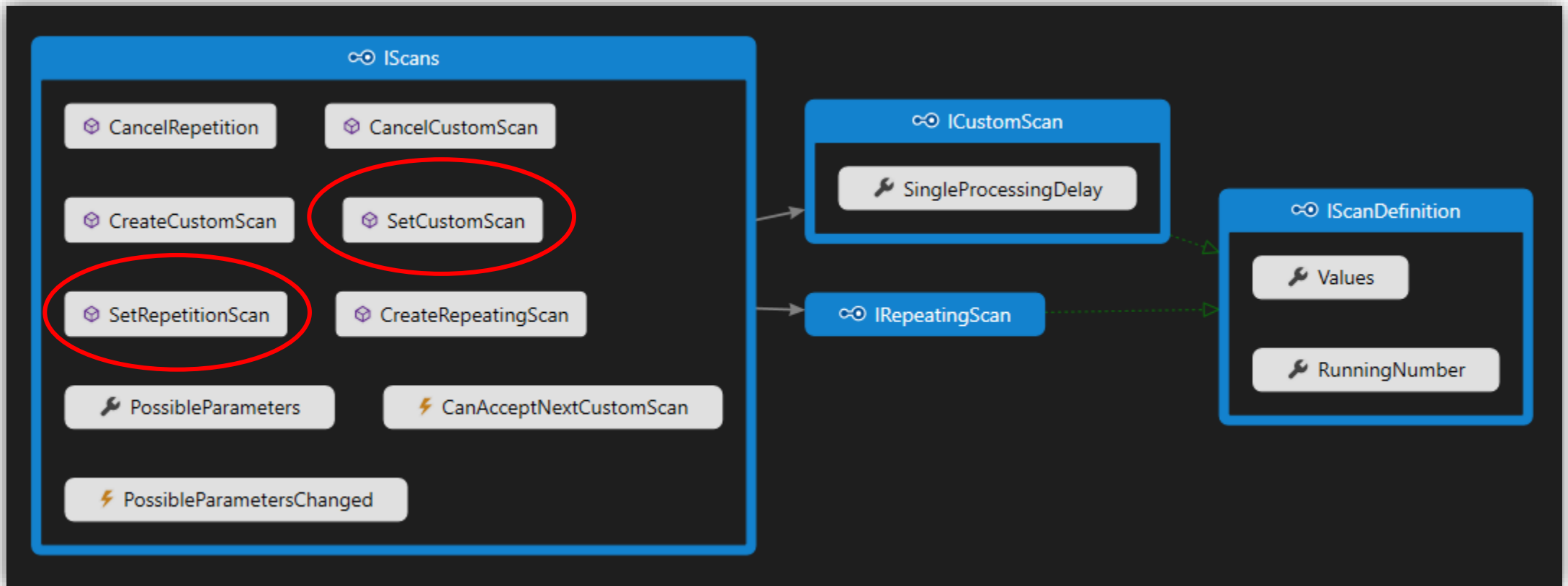
3. Controlling the MS

- Sending Scan Definitions
- Changing other MS parameters

4. Getting Started

IScans Interface

- Sending scans to the instrument is through the **IScans** interface
 - Provides methods for creating different types of **IScanDefinitions**
 - Provides methods for setting and cancelling scans.

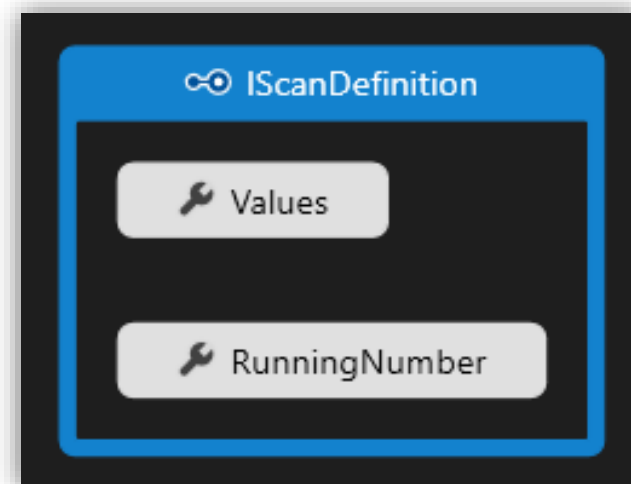


- Scans are defined in the **IScanDefinition** interface
- The **RunningNumber** property is for general purpose use
 - It shows up in the Scan Trailer as the '**Access ID**' field

Scan Header 557 - Rawdata_20180522033041

Name	Value
Dependency Type:	0
Access ID:	1

- The **Values** property is a Dictionary<string,string>
 - Keys are the scan parameters
 - Values are their associated values
 - Values can take different formats based on the parameter
 - Invalid, or nonsense values, are ignored



Example of MS³ of 524@35 191@25
Scan 150 – 550 m/z

```
scan.RunningNumber := "123456789";  
scan.Values["FirstMass"] := "150";  
scan.Values["LastMass"] := "550";  
scan.Values["ScanType"] := "MSn";  
scan.Values["PrecursorMass"] := "524.3;191.2";  
scan.Values["CollisionEnergy"] := "35;25";
```


	Property	Value	Selection	Help
►	ChargeStates		string (0;25)	Charge states for HCD(default 0 is unknown) It is expressed as a string of values, with eac...
	IsolationMode	Quadrupole	None,Quadrupole,Ion Trap	Isolate using the quadrupole or ion trap
	SourceCIDEnergy	0	0-100	Source CID Energy (0 = off).
	ActivationQ	0.25	string (0.05;0.8)	The Activation Q value (0.05-0.8). It is expressed as a string of values, with each value se...
	ActivationType	CID	string (CID;HCD)	The activation type to use at a given MS stage. The available types are (CID,HCD). It is e...
	AGCTarget	3000	3000-100000	The Automatic Gain Control (AGC) target value.
	Data Type	Centroid	Centroid,Profile	The data type to collect the scan in.
	FirstMass	150	string (50;2000)	The first mass of the scan range. It is expressed as a string of values, with each value sep...
	IsolationWidth	0.7	string (0.4;2000)	The isolation width (full-width) for a given MS stage It is expressed as a string of values, wit...
	LastMass	2000	string (50;2000)	The last mass of the scan range. It is expressed as a string of values, with each value sep...
	Analyzer	Ion Trap	Ion Trap,Orbitrap	The mass analyzer.
	MaxIT	100	0.001-8000	The maximum injection time (ms)
	CollisionEnergy		string (0;200)	The normalized collision energy (NCE) It is expressed as a string of values, with each value...
	Microscans	1	1-6000	The number of microscans to collect (1 = don't use microscans)
	OrbitrapResolution	120000	7500,15000,30000,50000,60000,120000,240000,500000	The Orbitrap Resolution
	Polarity	Positive	Positive,Negative	The polarity of the scan.
	PrecursorMass		string (50;2000)	The precursor m/z to isolate at a given MS stage. The first value will be the MS1->MS2 tra...
	ReactionTime	10	string (0.001;100)	The reaction/activation time (ms) for CID activations. It is expressed as a string of values, ...
	SrcRFLens	60	string (0;150)	The RF Lens (%) for the source. It is expressed as a string of values, with each value sepe...
	ScanRate	Normal	Normal,Enhanced,Zoom,Rapid,Turbo	The scan rate of the ion trap
	ScanType	Full	Full,SIM,MSn	The type of scan to perform.

Scan Management

Mass Spectrometer



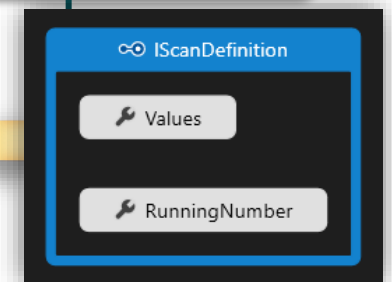
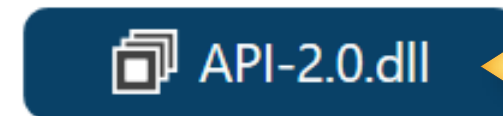
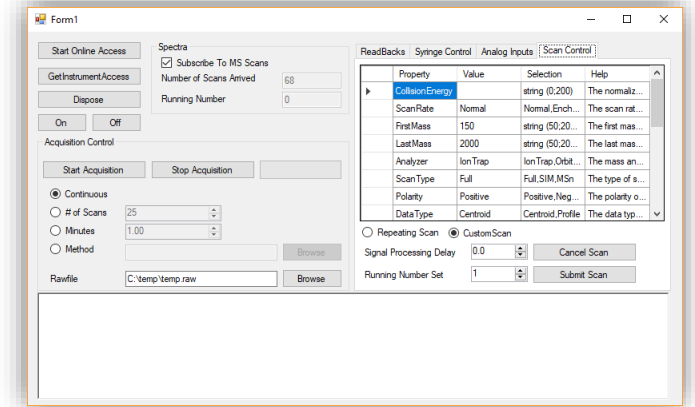
Local Switch



Data System



I-API-Enabled App



Sending Scan to MS

Scan Management

Mass Spectrometer



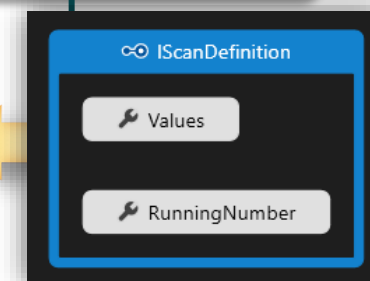
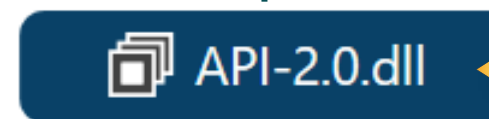
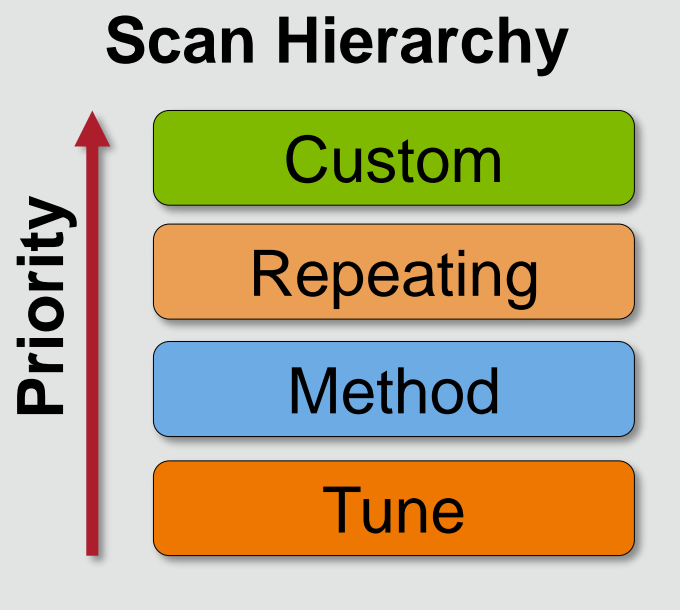
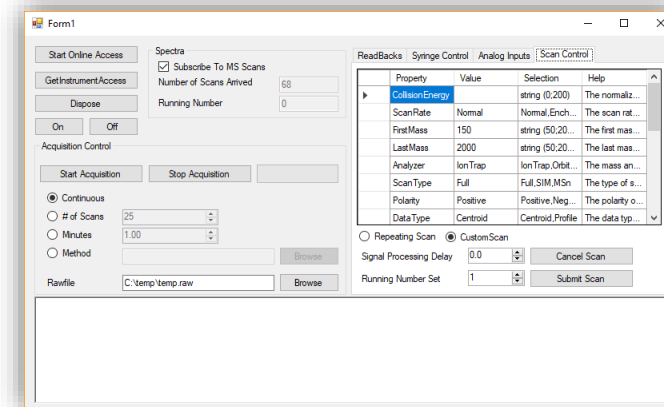
Local Switch



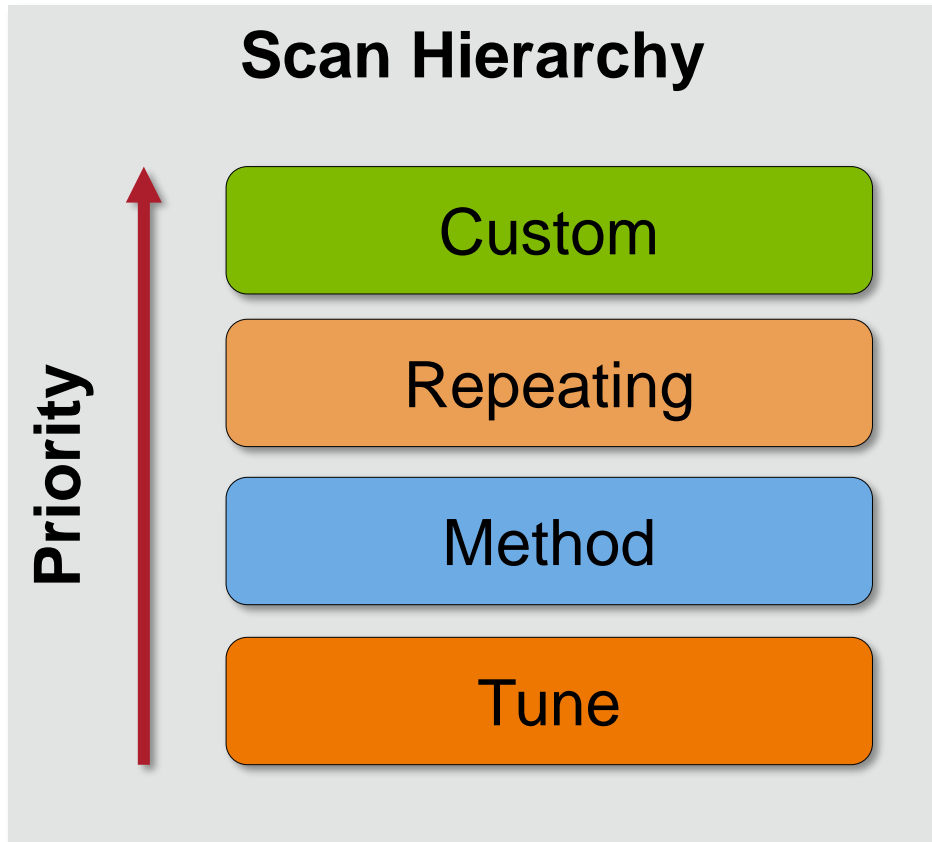
Data System

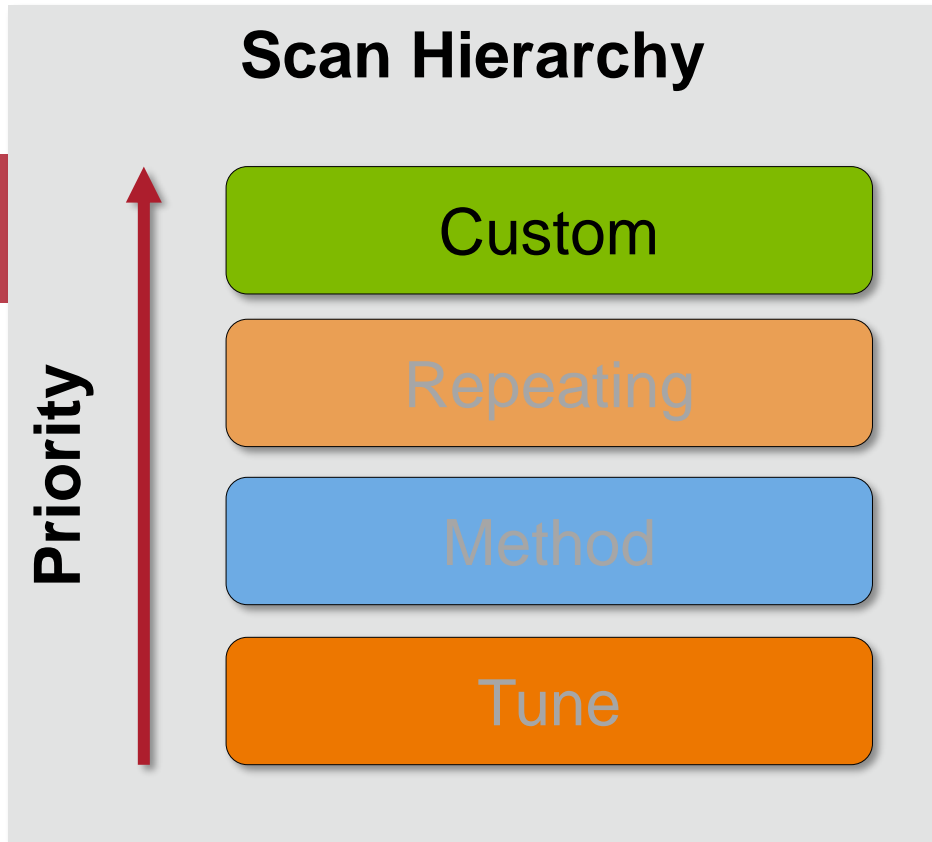


I-API-Enabled App

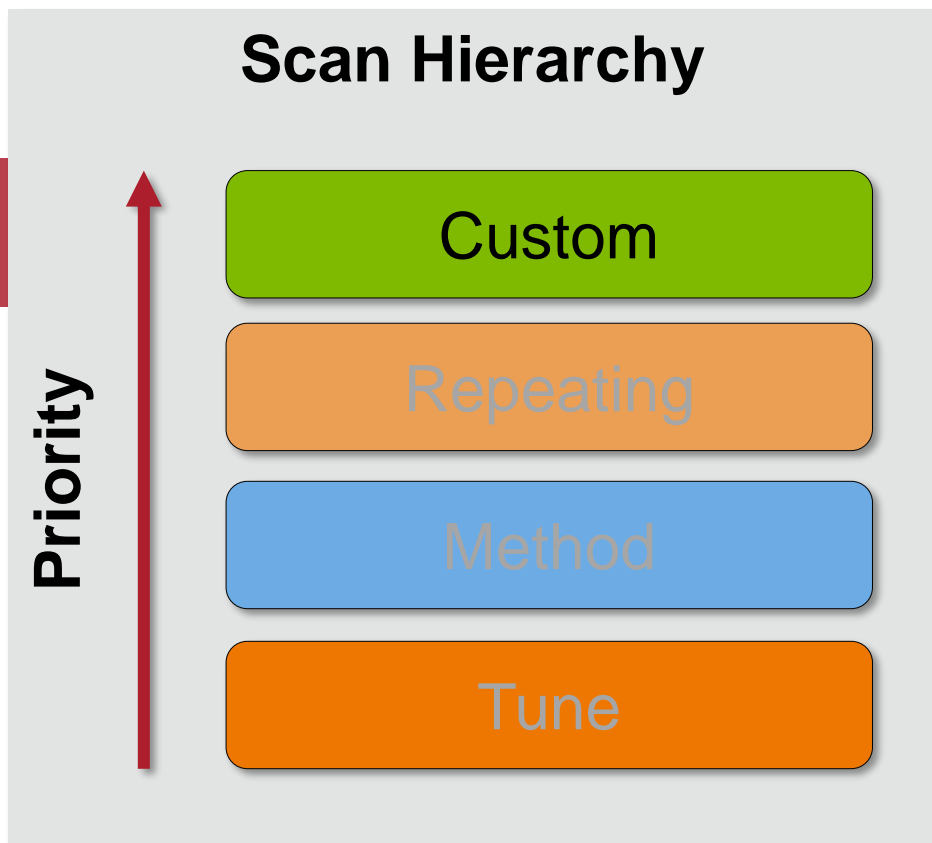


Sending Scan to MS



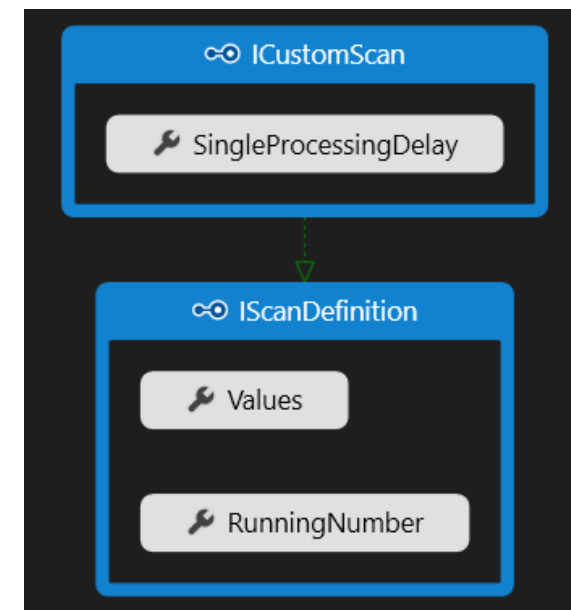


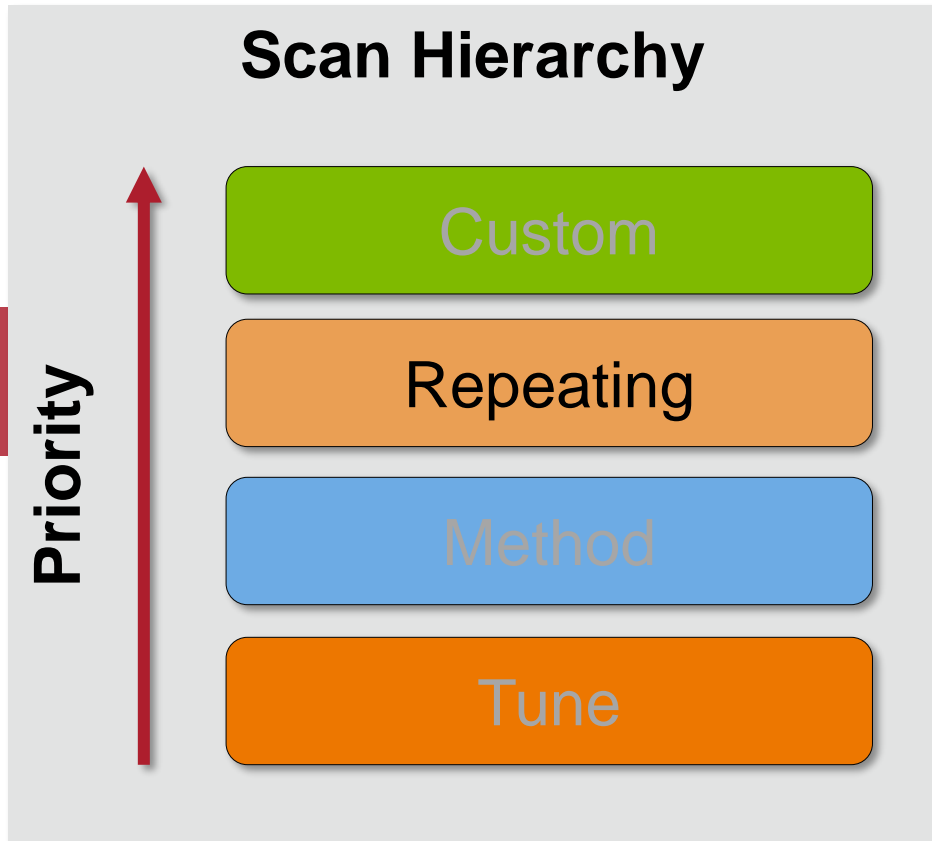
Single scan, drops to lower level after completion



Single scan, drops to lower level after completion

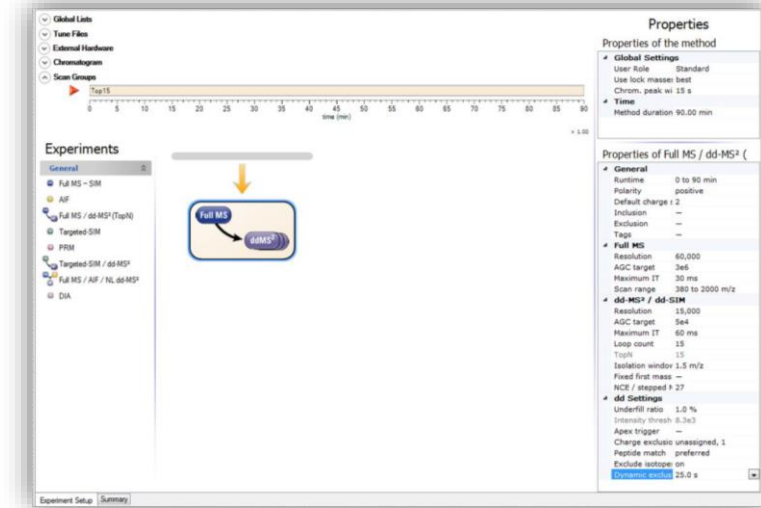
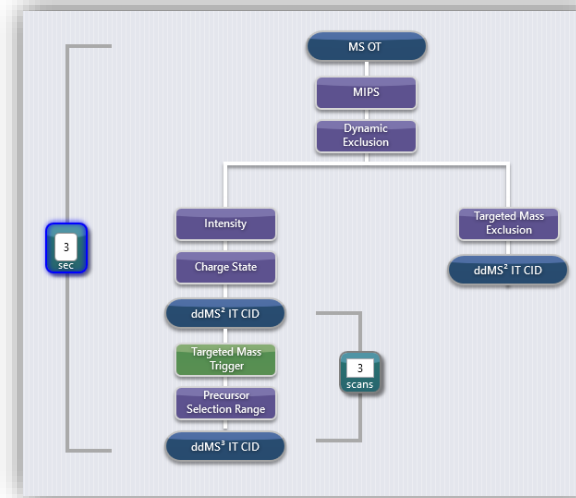
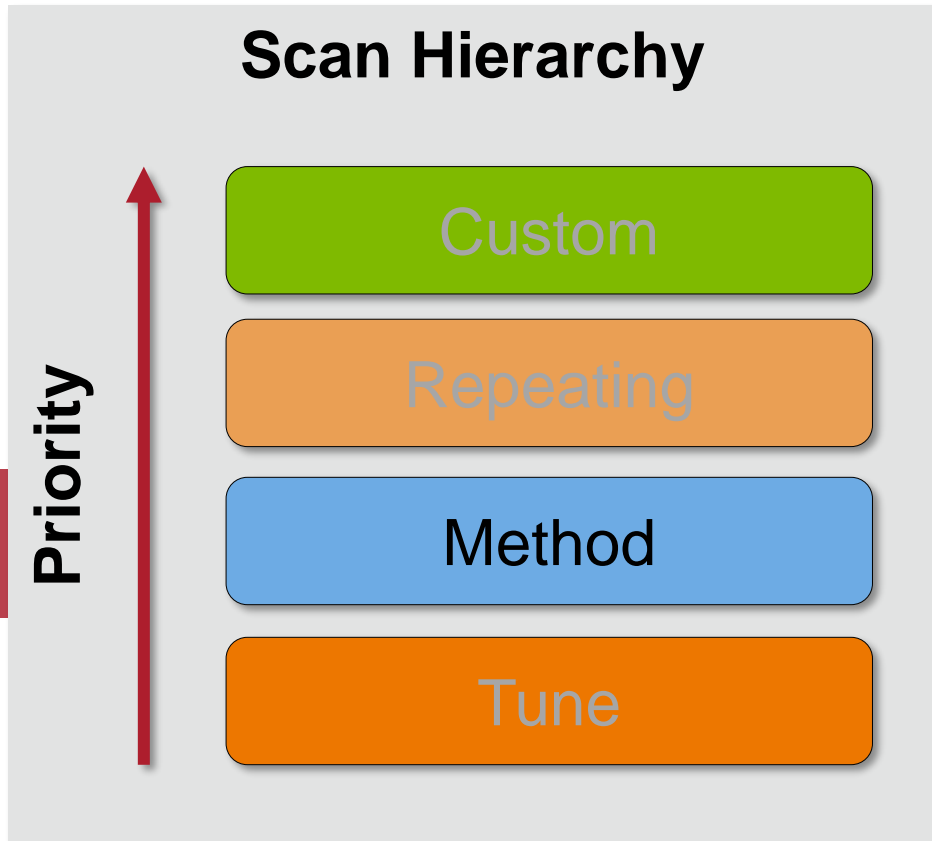
- Once executed, waits the **Single Processing Delay** (s) for a new **Custom** scan to arrive*
- Default delay is 0 seconds (no waiting)
- Immediately ends the wait if a new **Custom** scan arrives or there are pending ones
 - The Tribrid uses a circular buffer (40-capacity) to store them





Repeats scan until explicitly canceled by user

- Continually runs the same scan until:
 1. Cancelled by the user
 2. Replaced by a new Repeating Scan
 3. Preempted by a Custom Scan



Runs Scans and logic defined in the method

- Runs the normal method logic until completion or new IAPI scan arrives

Scan Hierarchy

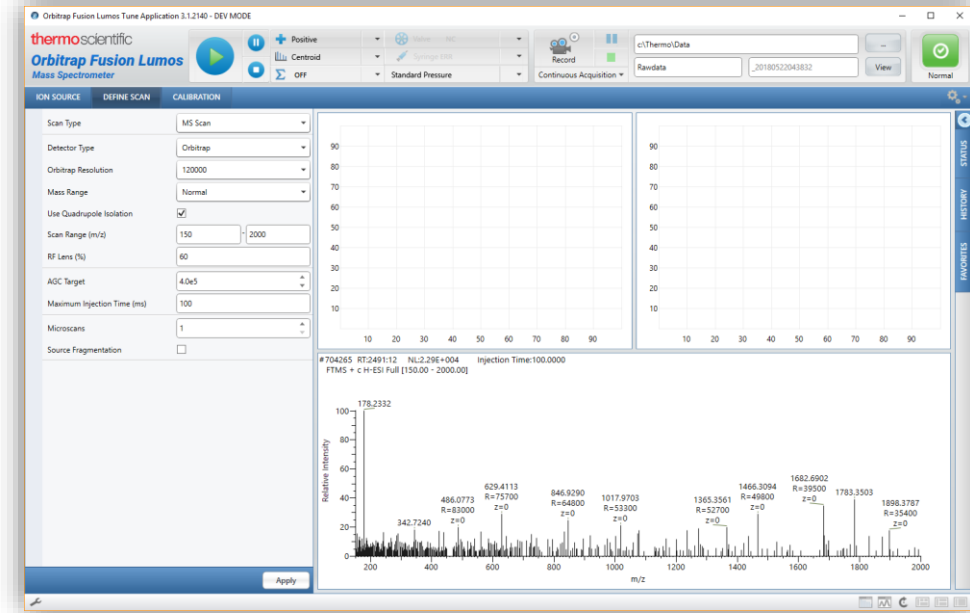
Priority

Custom

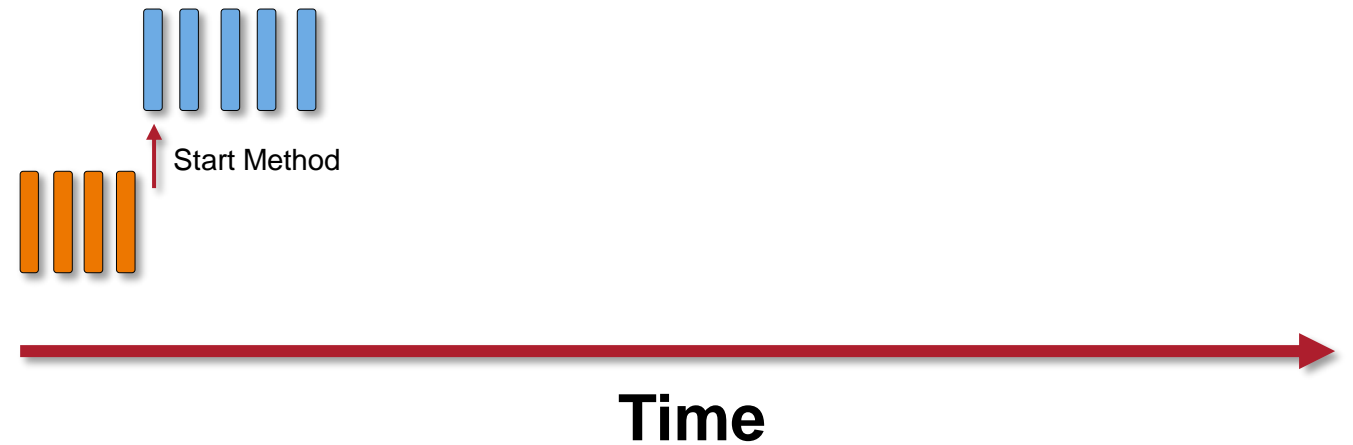
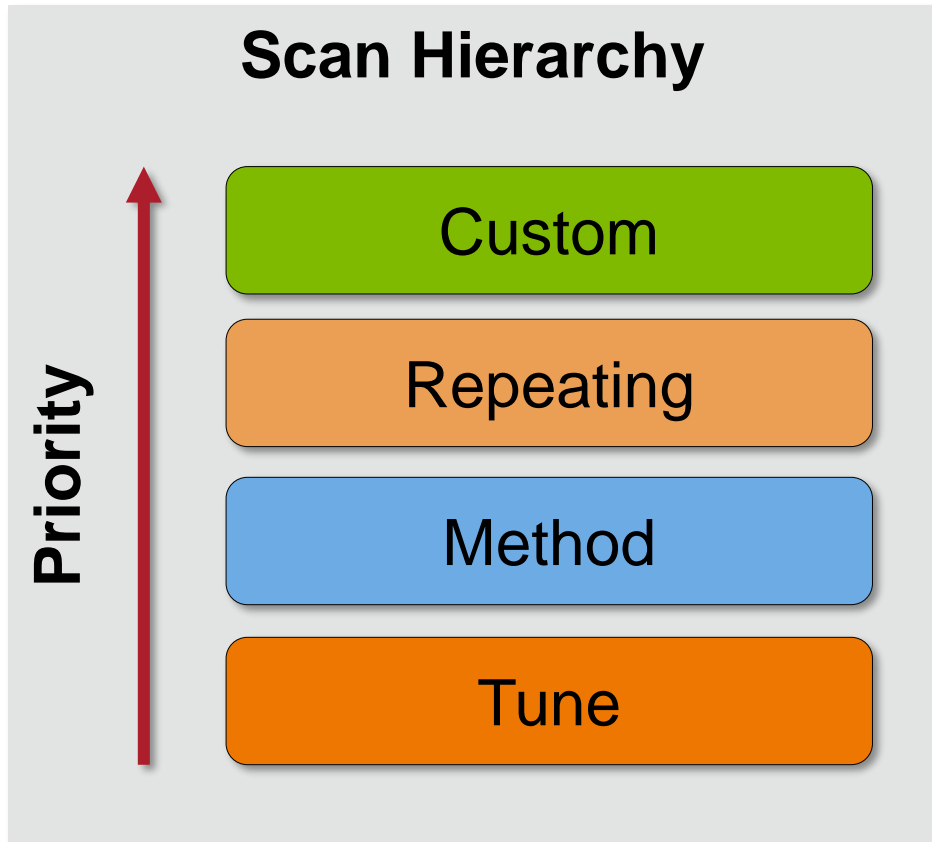
Repeating

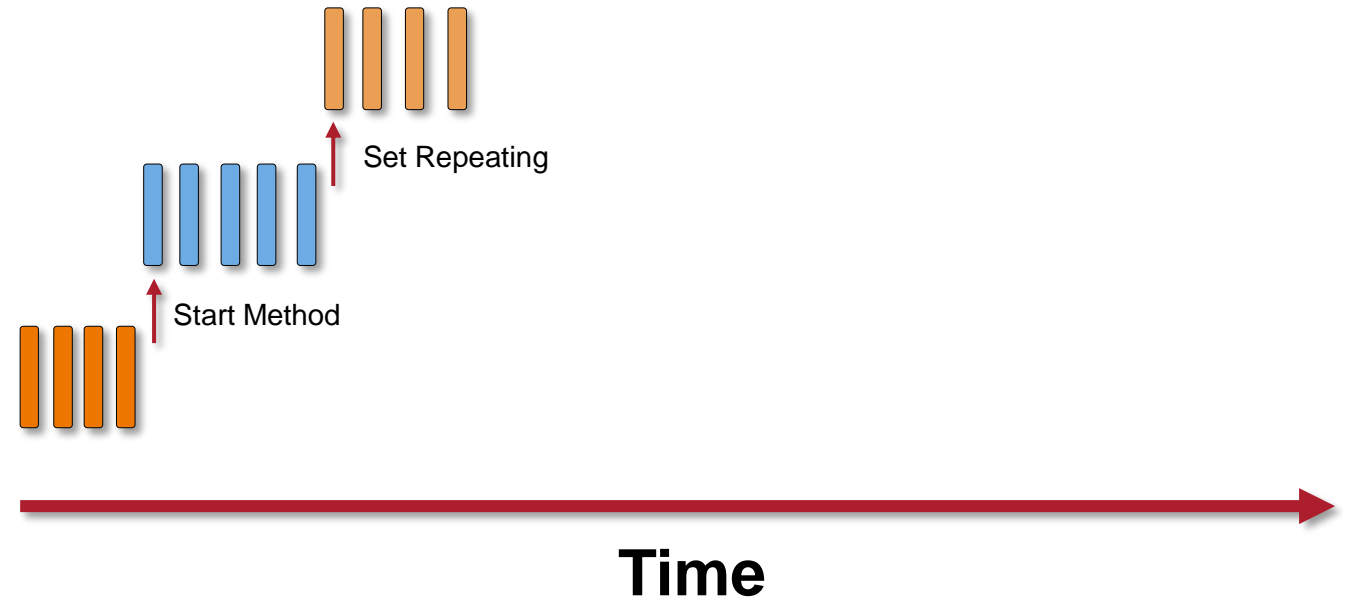
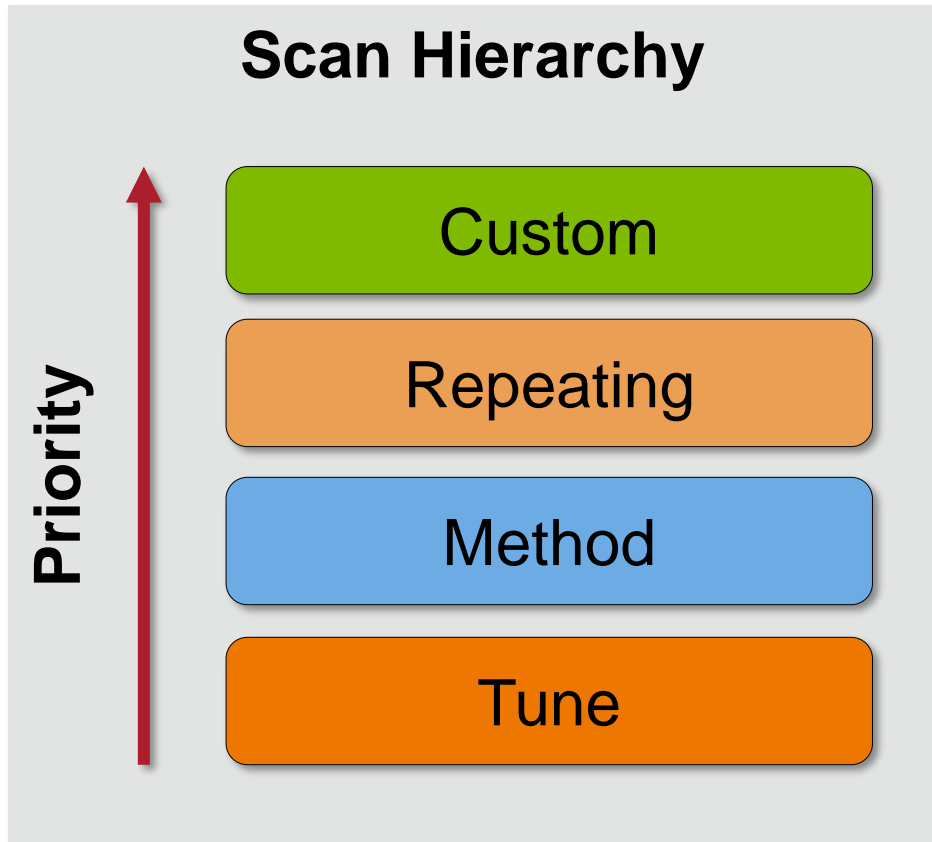
Method

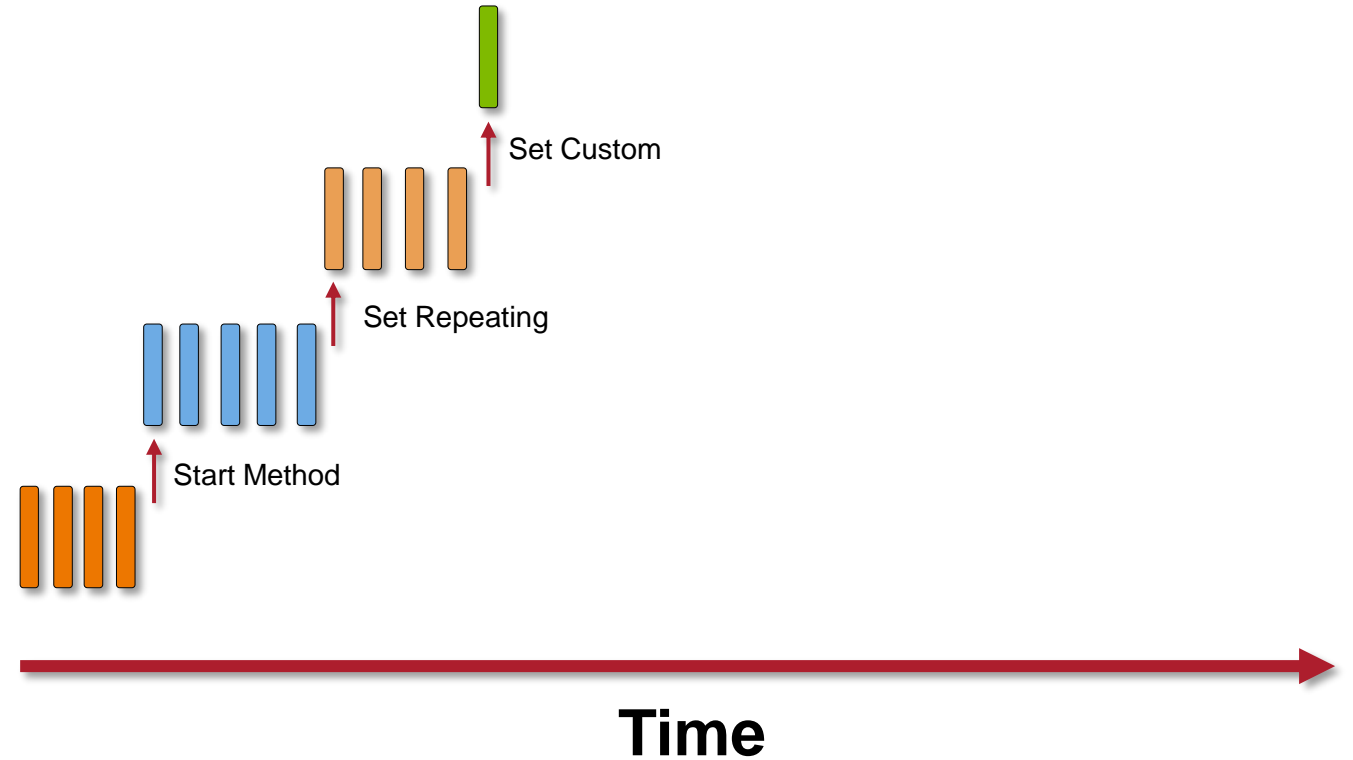
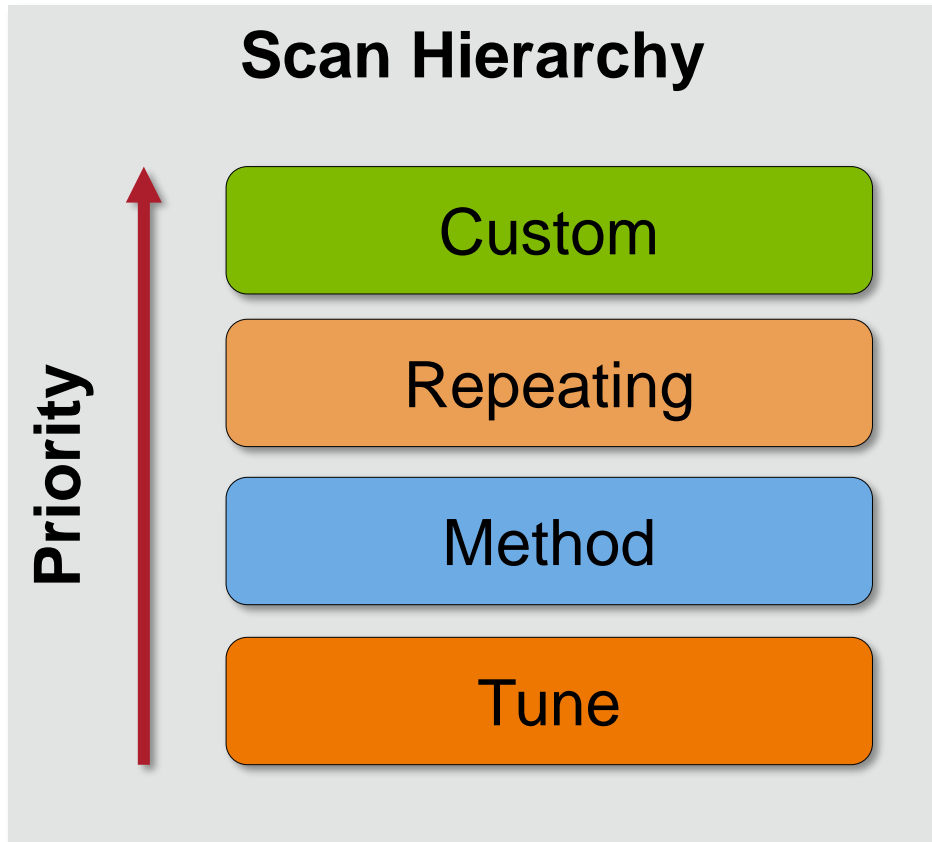
Tune

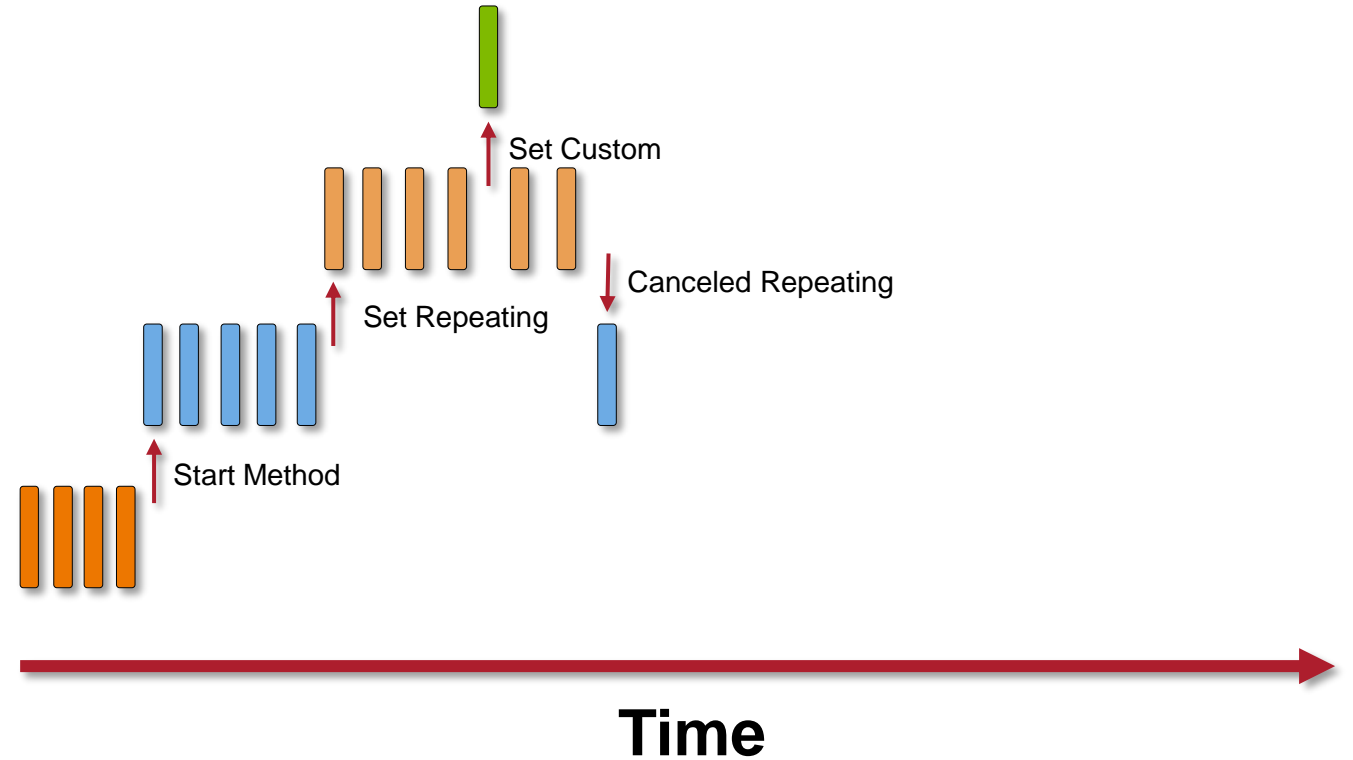
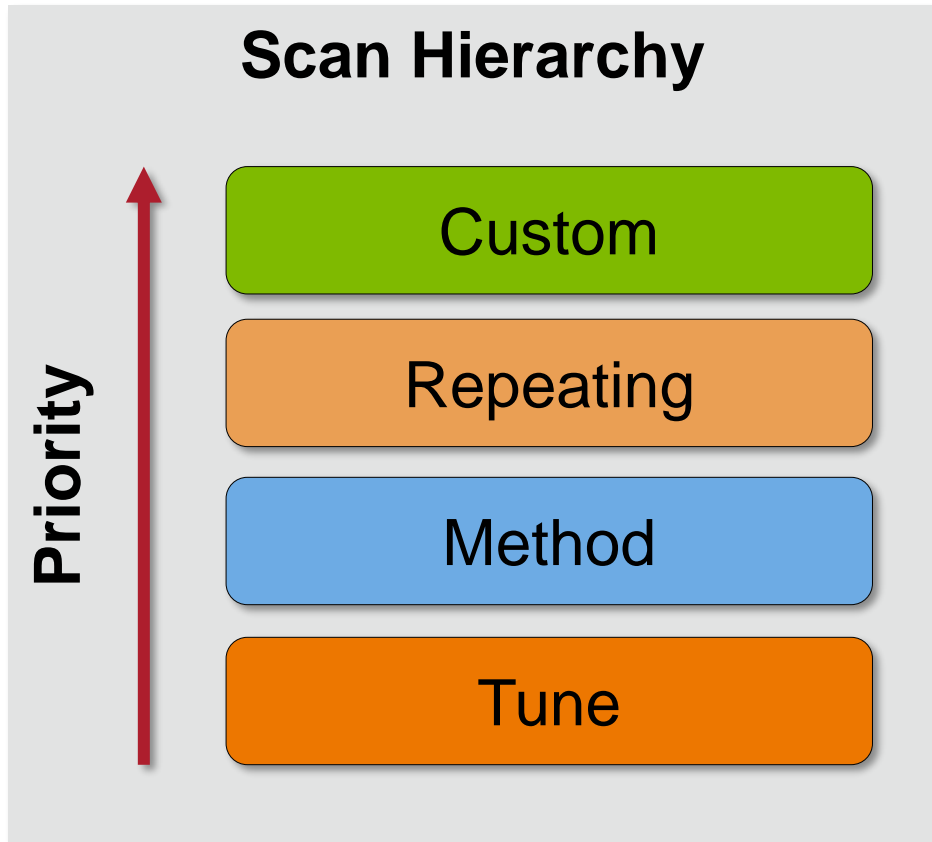


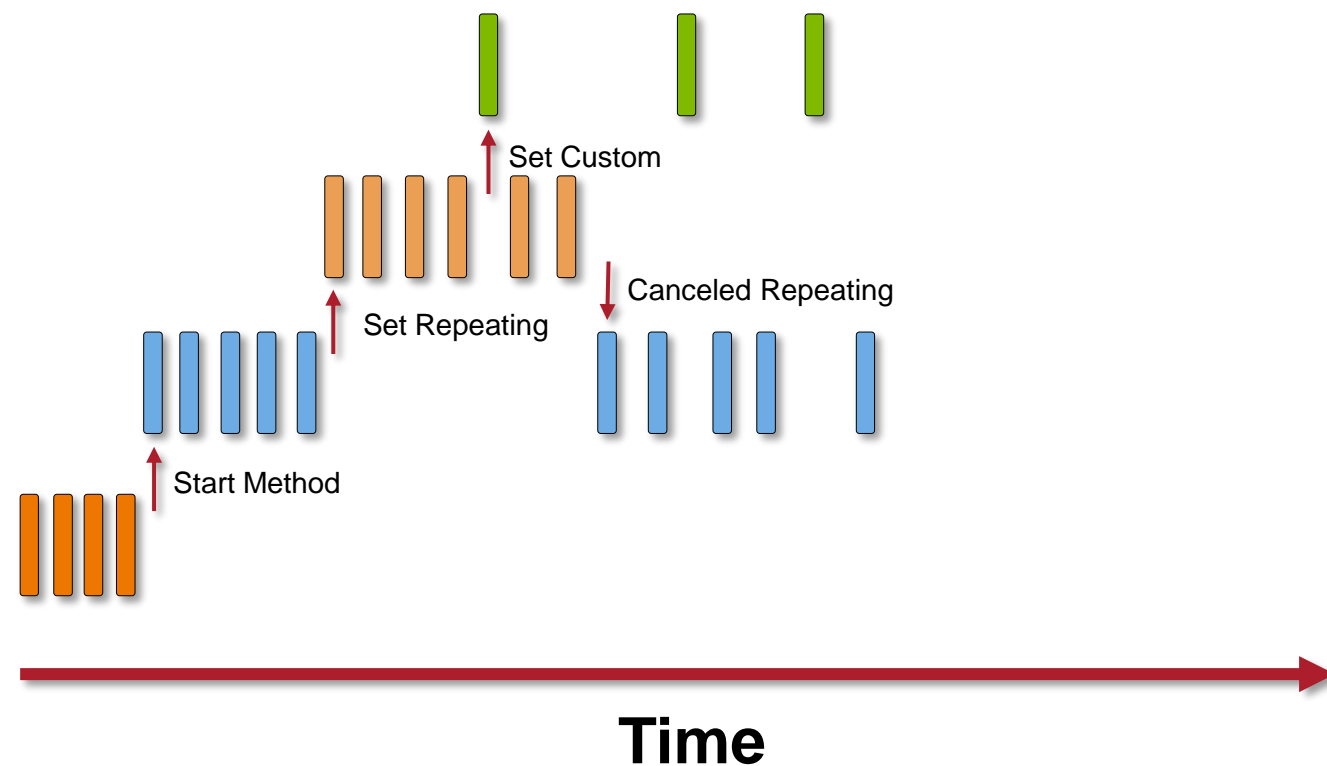
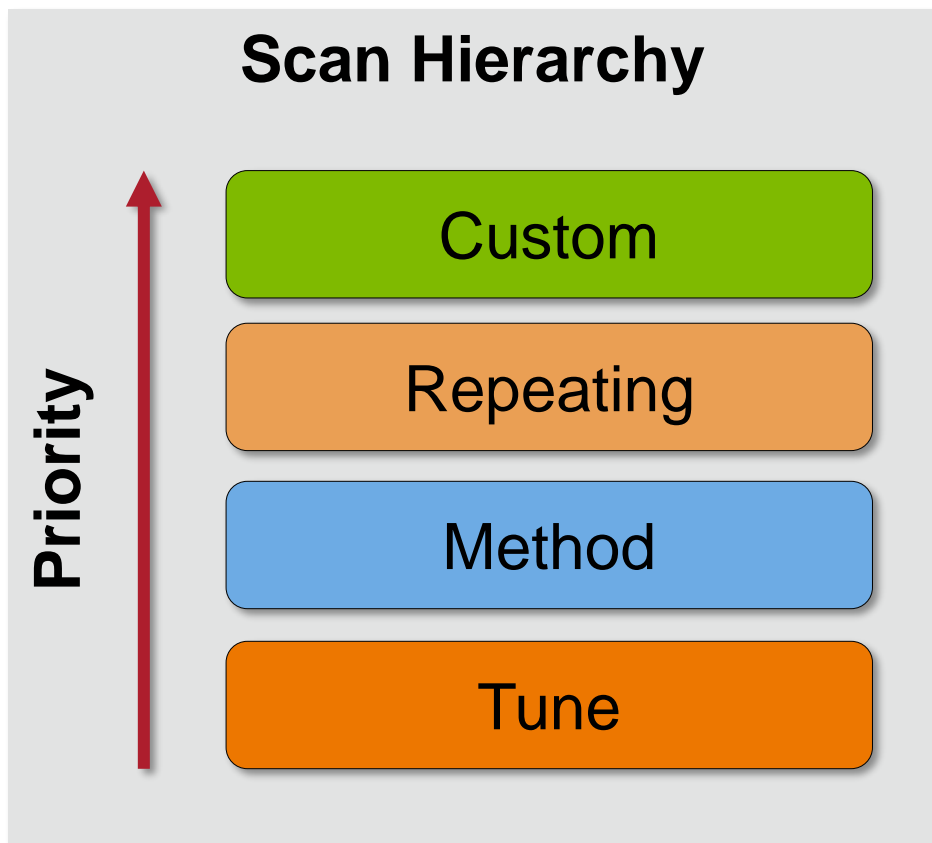
Runs the Scan defined in Tune

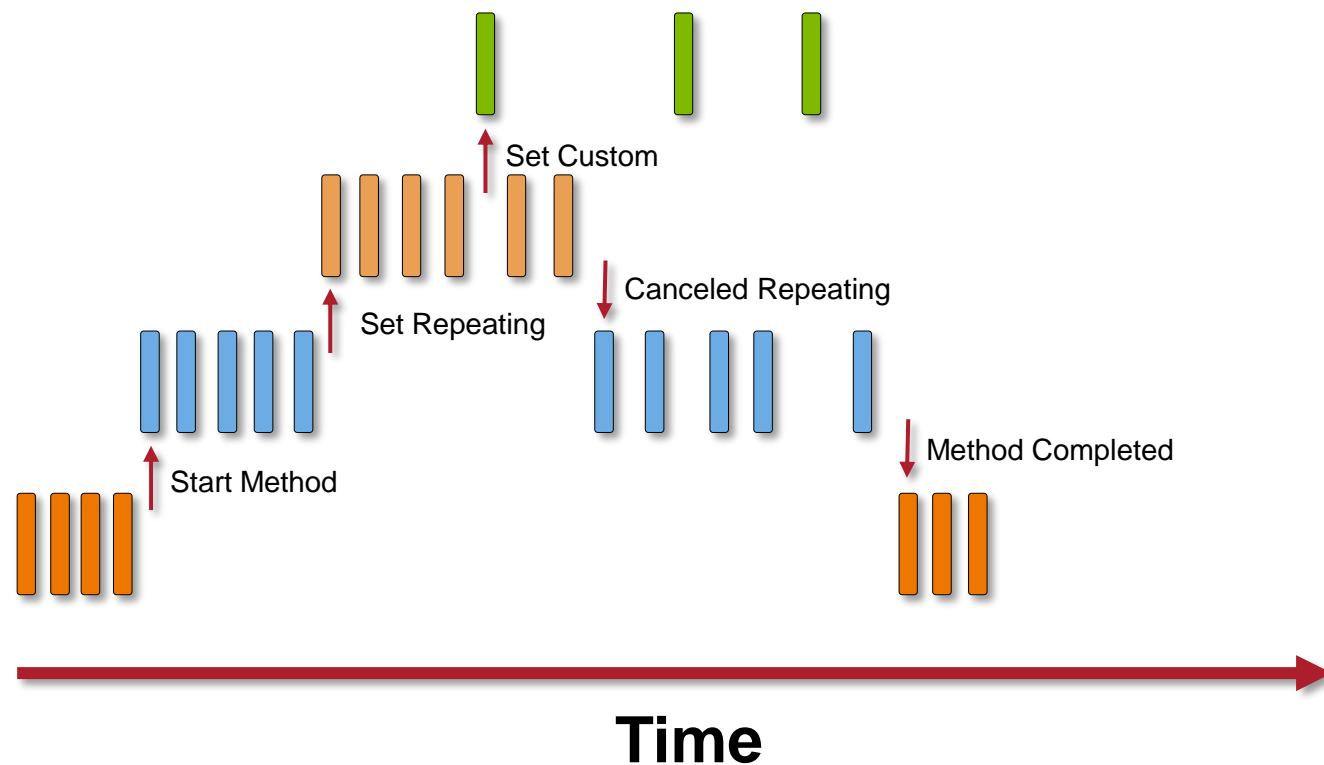
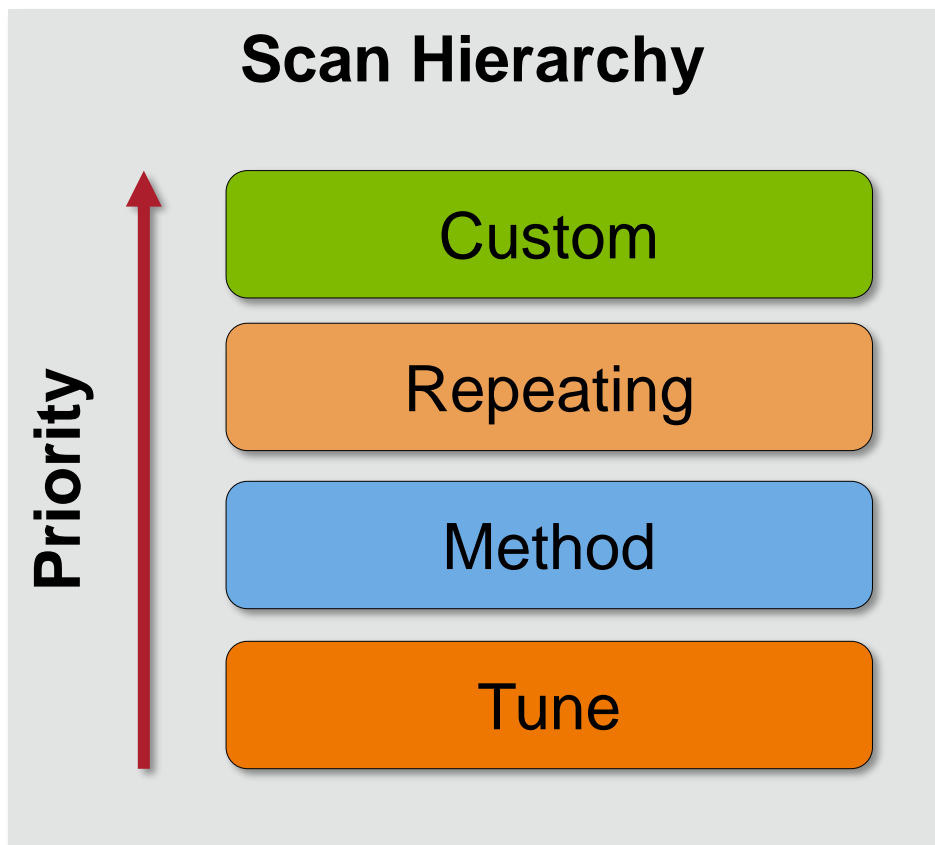


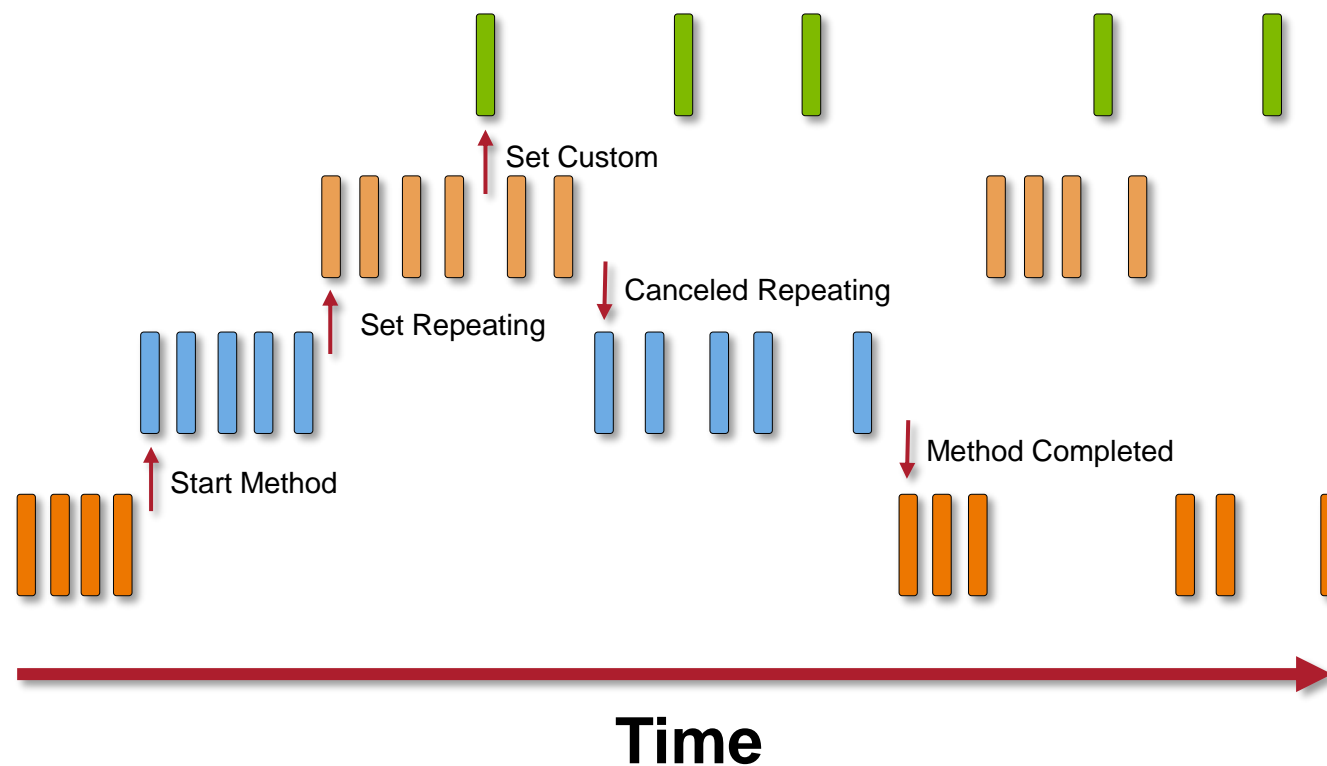
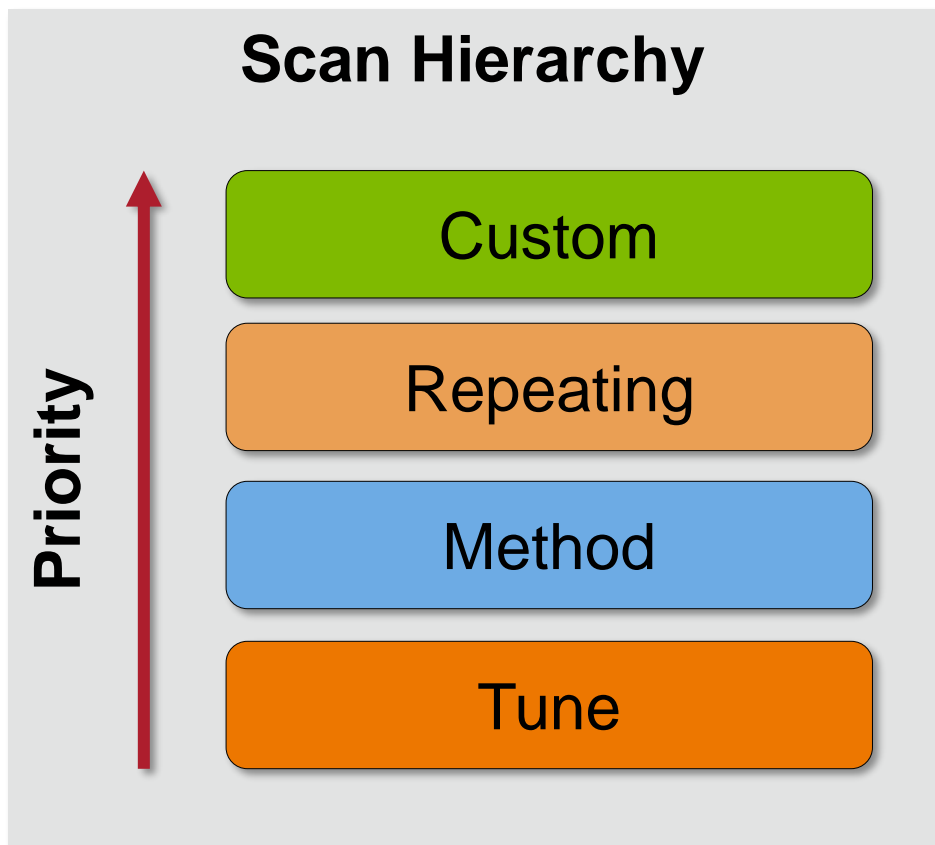












Scan Hierarchy

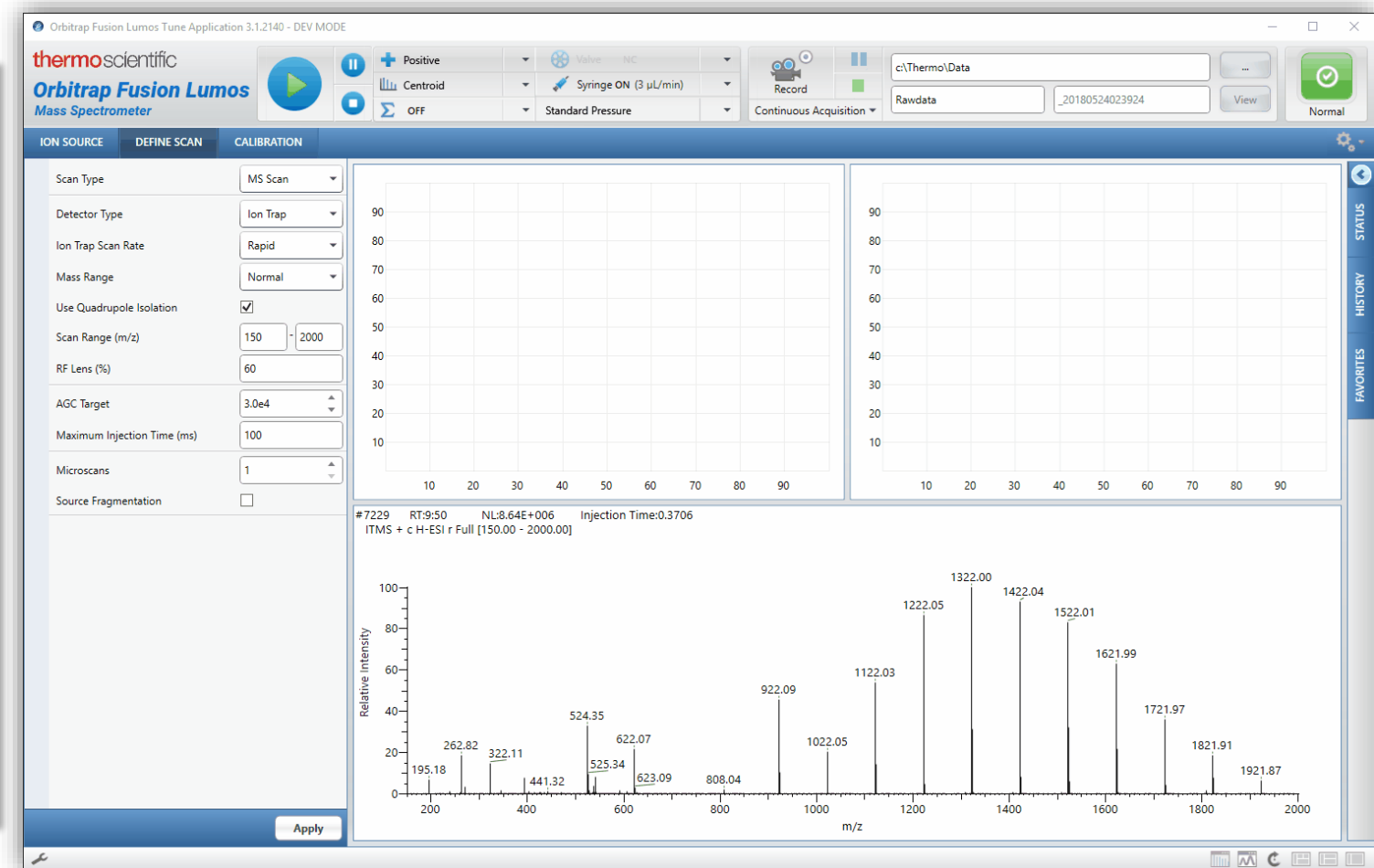
Priority

Custom

Repeating

Method

Tune



Scan Hierarchy

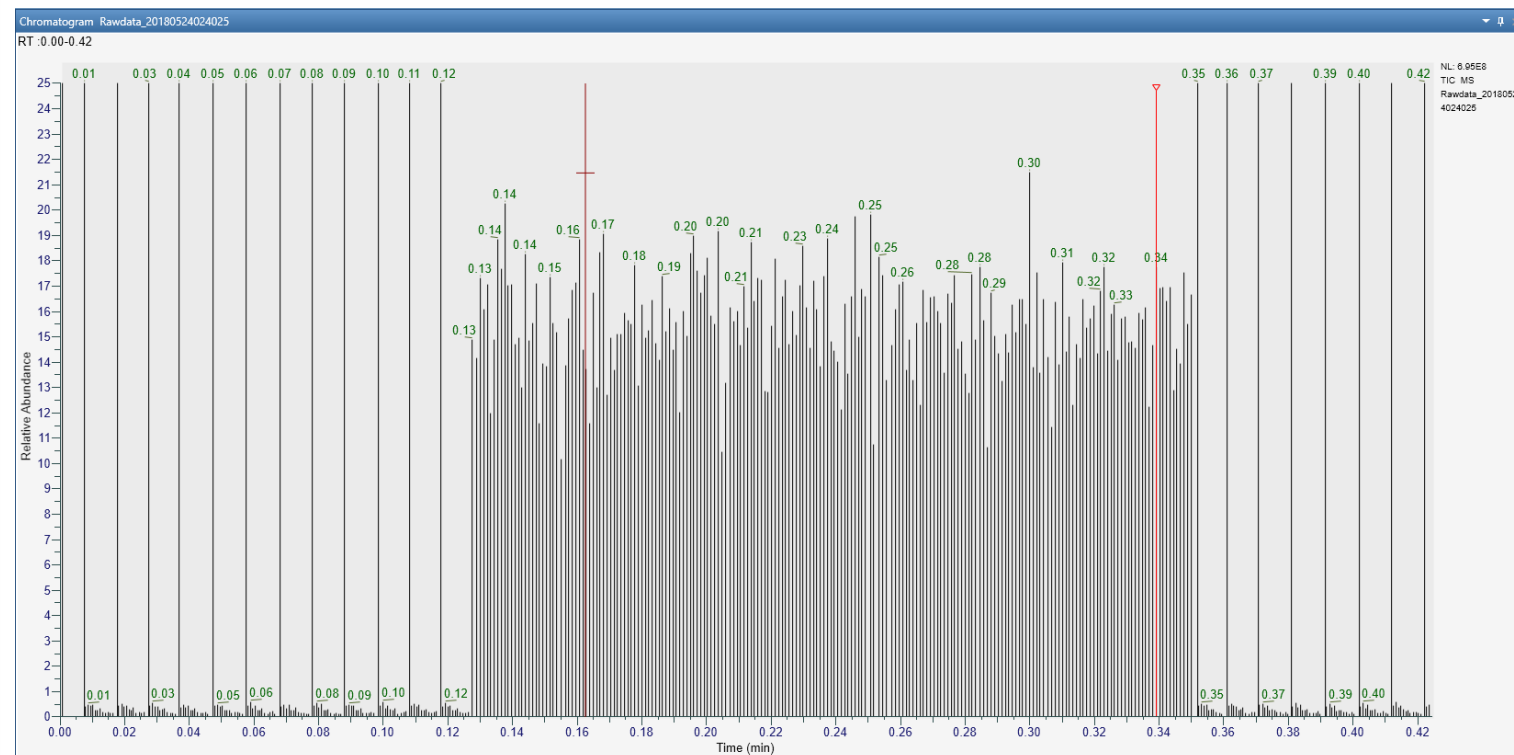
Priority

Custom

Repeating

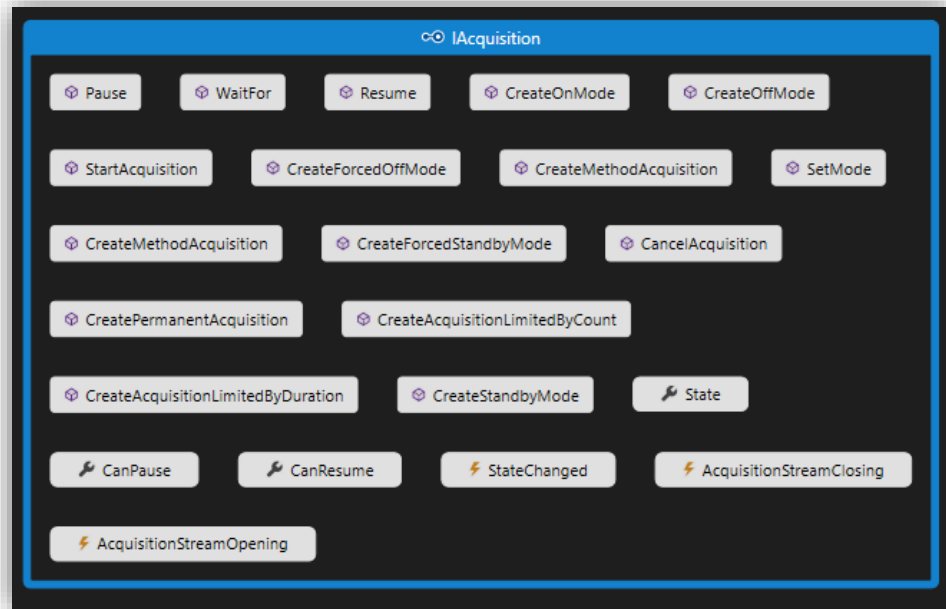
Method

Tune



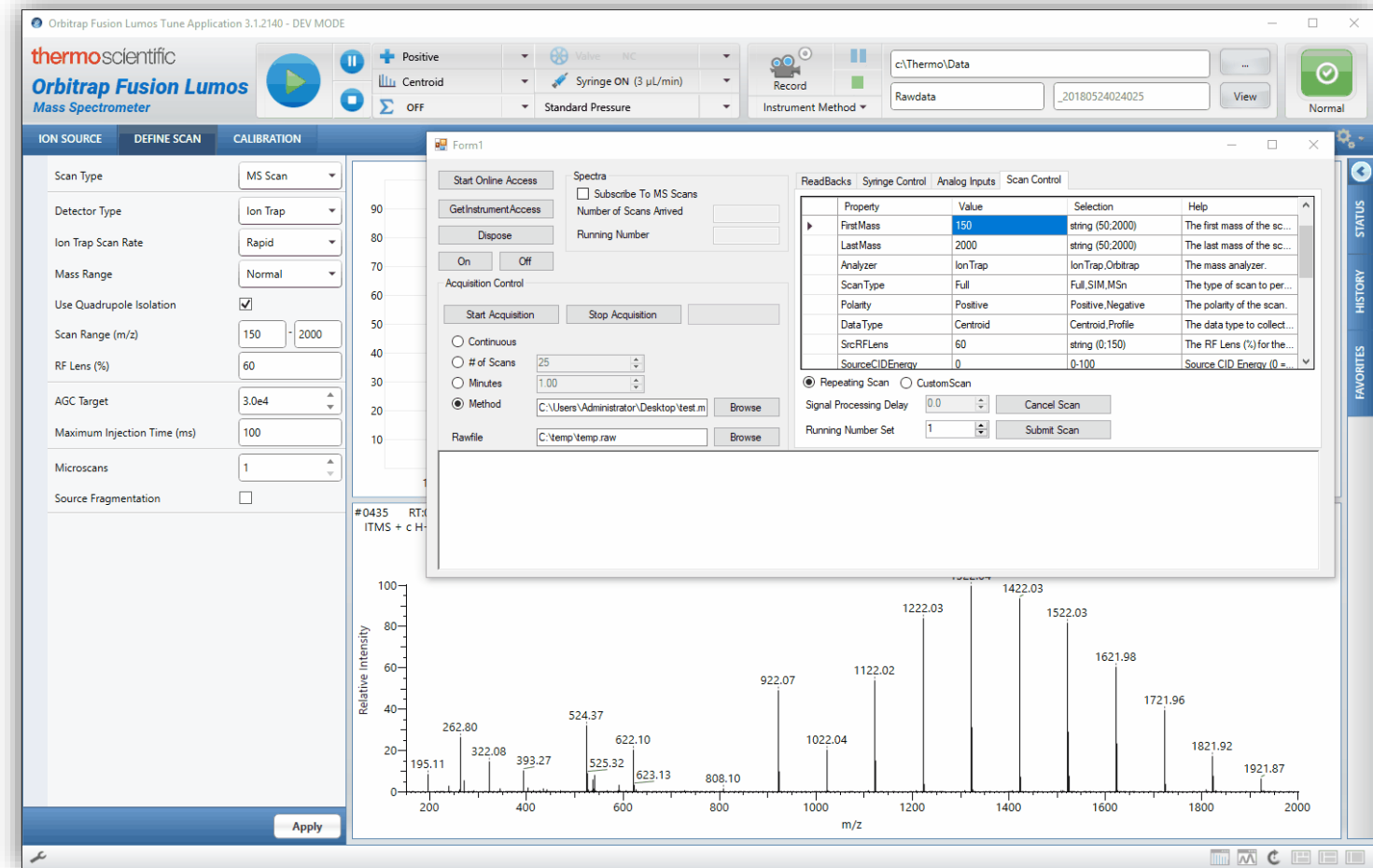
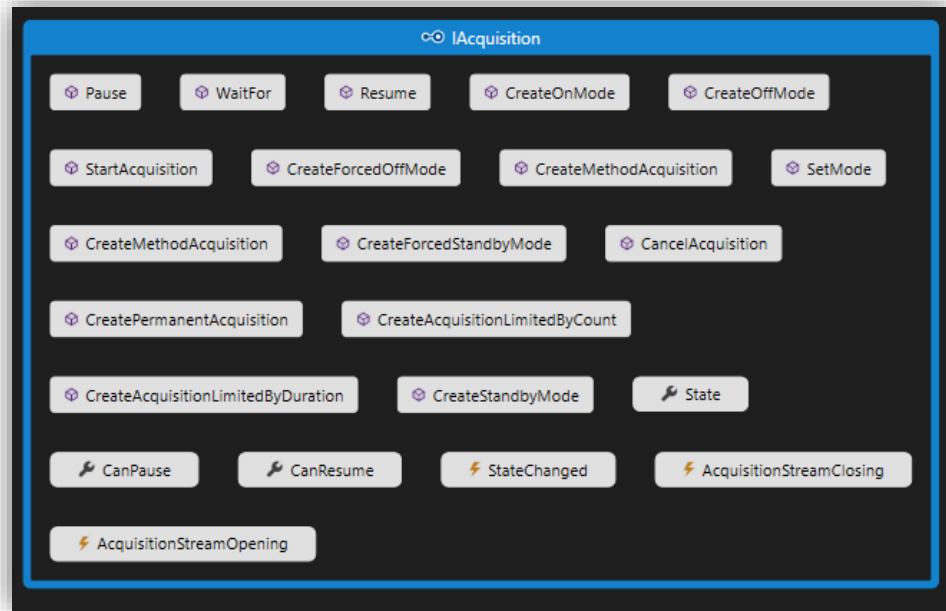
Starting Acquisitions from the IAPI

- The **IAcquisition** interface enables the IAPI to start/stop acquisitions
- It also has **Events** for listening to when an acquisition starts and stops



Starting Acquisitions from the IAPI

- The **IAcquisition** interface enables the IAPI to start/stop acquisitions
- It also has **Events** for listening to when an acquisition starts and stops



1. IAPI Architecture

- Interfaces
- Data and Control Flow

2. Receiving Data from the MS

- Interfaces
- Scan Data Stream Subscription

3. Controlling the MS

- Sending Scan Definitions
- Changing other MS parameters

4. Getting Started

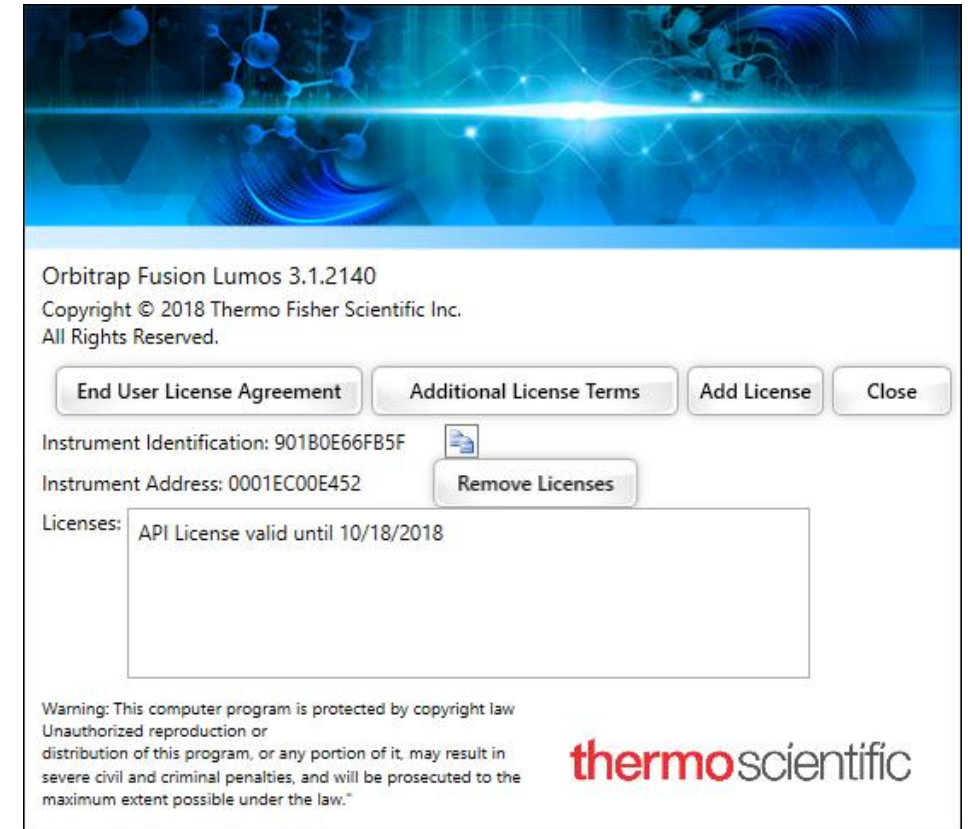
- Access to the IAPI is given after a fully executed IAPI License is in force.
- Contact info.IAPI@thermofisher.com to get started
 - <https://github.com/thermofisher/lsms>
 - Please include which IAPI (**Tribrid** or **Exactive**) you would like access to in your initial correspondence

License Activation

- Access to the IAPI is given after a fully executed IAPI License is in force.
- Contact info.IAPI@thermofisher.com to get started
 - Please include which IAPI (**Tribrid** or **Exactive**) you would like access to in your initial correspondence

Activating the License on the Tribrids

- A license key will be provided to you and is entered in Tune's "About Tune" dialog
- Restart both the Instrument and Data system computer and the API will be enabled



1. Instrument Application Programming Interface (I-API)

- Introduction
- Architecture
- Example

2. XML Method Modification Interface (XMMI)

- Architecture
- Example

Method Editor | Global Parameters | Scan Parameters | Summary

METHOD TIMELINE | EXPERIMENT | ACTIONS | SETTINGS

Application Mode: Peptide
Method Duration (min): 60

Experiment # 1 | Time Range (min): 0-60 | CLEAR

Scans

- MS
- MSⁿ

Filters

- Precursor Selection Range
- MIPS
- Intensity
- Purity
- Charge State
- Dynamic Exclusion
- Targeted Inclusion
- Targeted Exclusion
- Apex Detection

Triggers

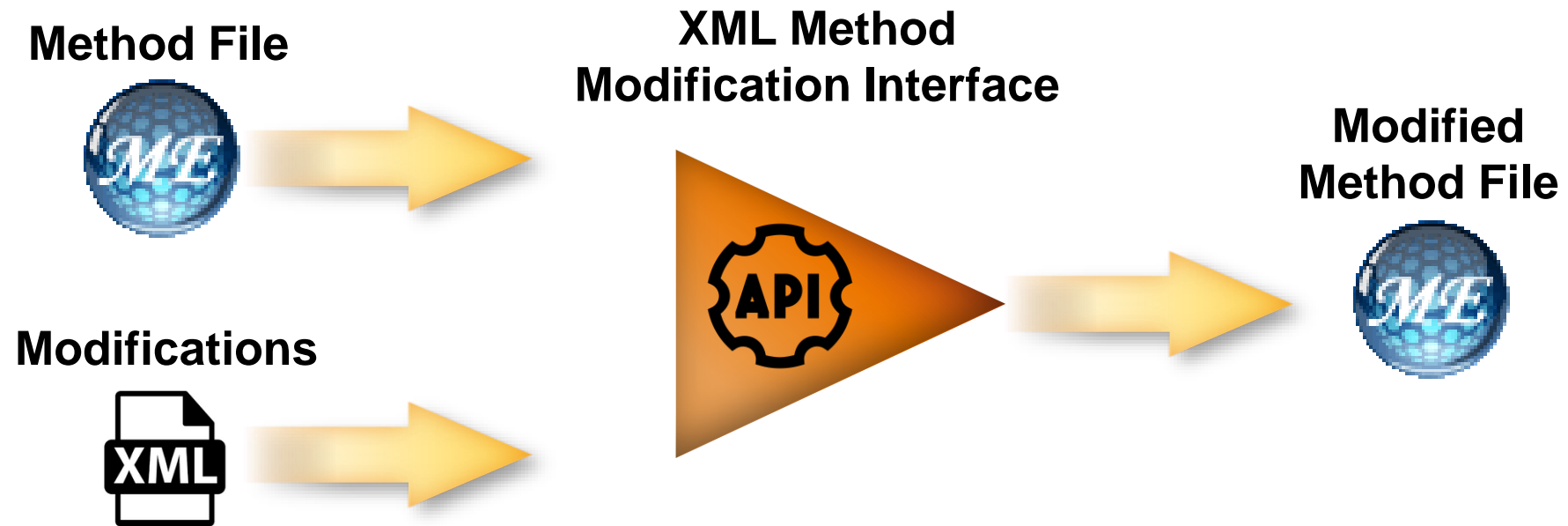
- Targeted Mass Trigger
- Targeted Loss Trigger

MS Scan Properties | Show All

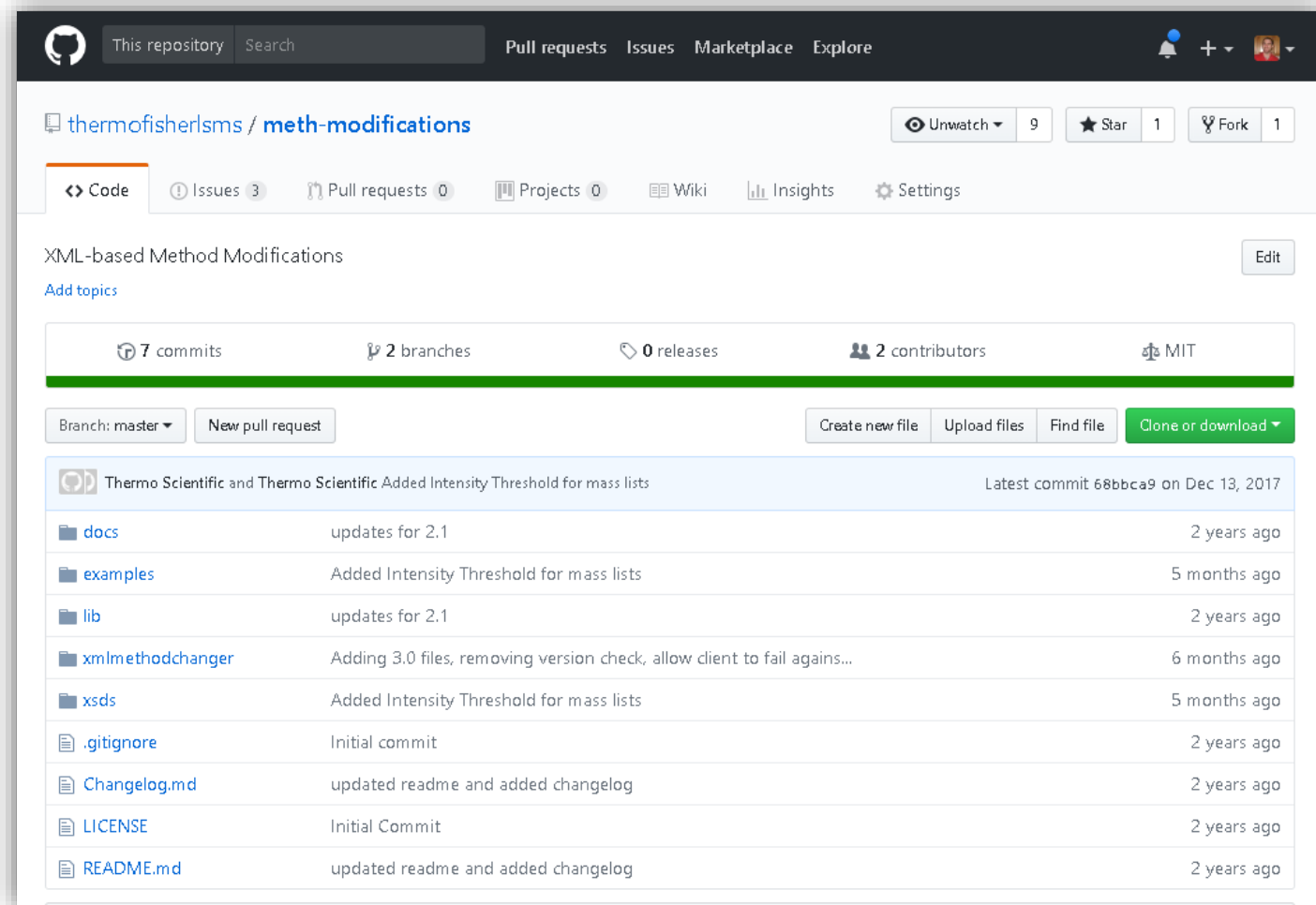
- Orbitrap Resolution: 60000
- Scan Range (m/z): 450-750
- RF Lens (%): 30
- AGC Target: 1.0e6
- Maximum Injection Time (ms): 50

The Method Editor offers tremendous **flexibility** in method creation; sometimes manually editing complex methods is laborious.

Programmatically Modify Fusion Methods



<https://github.com/thermofisherlms/meth-modifications>

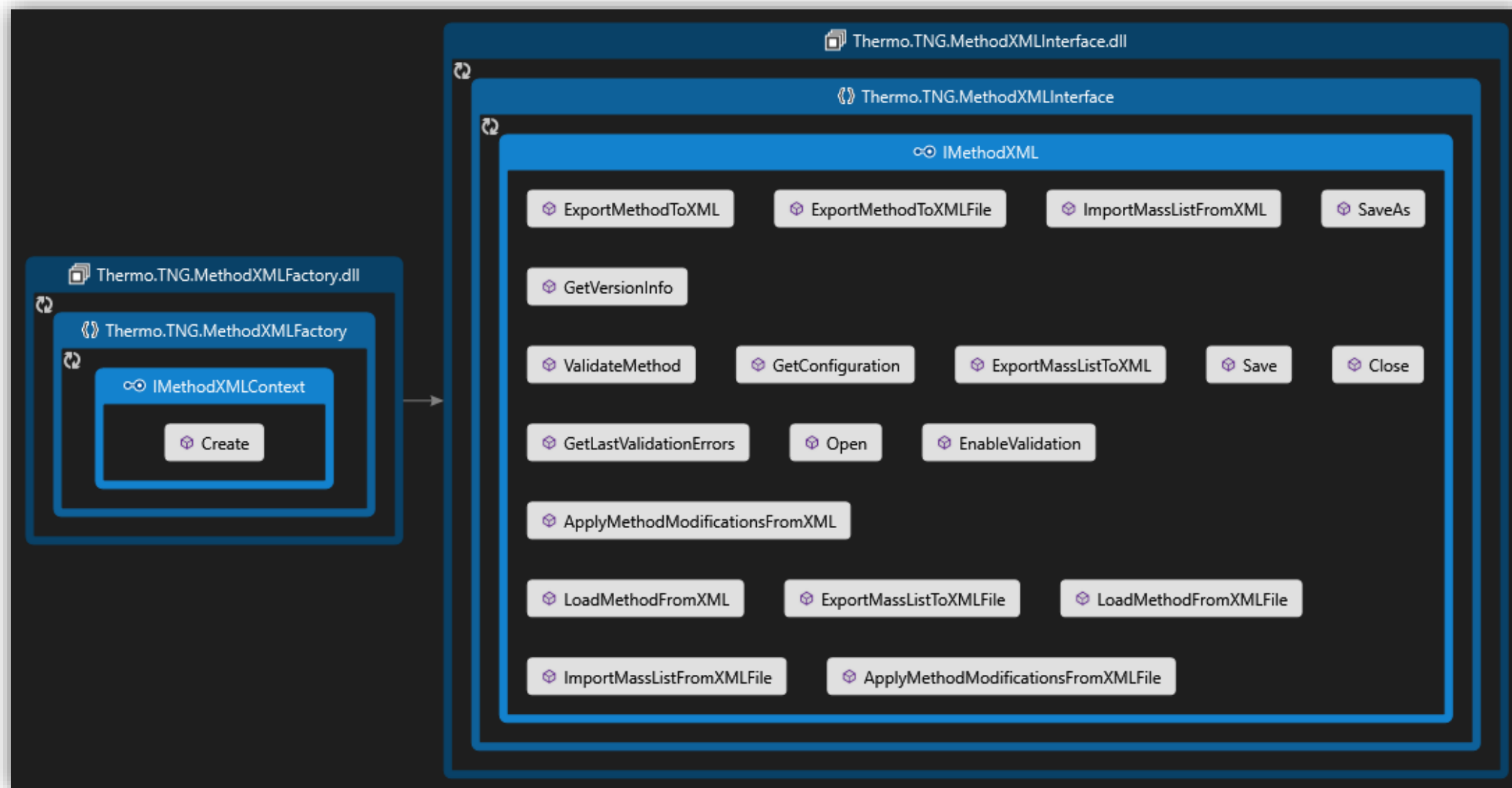


- Supports Fusion and Triple-Quad Methods
 - Versions **1.2, 2.0, 2.1, 3.0, 3.1, 3.3**
- Documentation
- Complete Examples
- VS Solution
 - Command Line Program
 - Heavily commented code
- Schemas

External Requirements

- Tune Installation
 - Full or Workstation
- .NET 4.6.2+

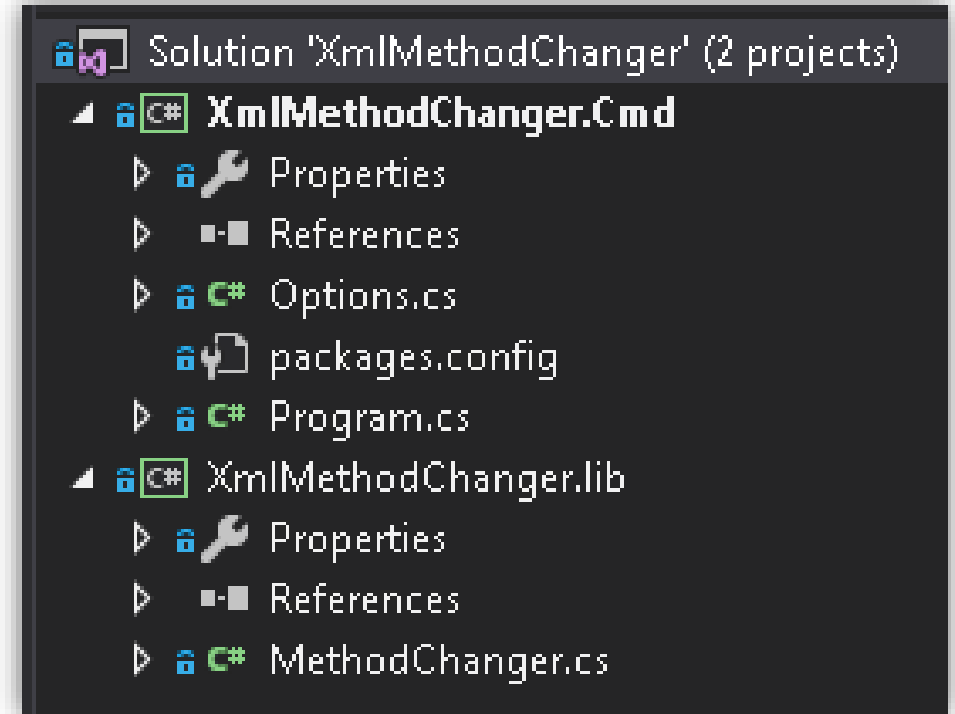
XML Modification Interfaces



Complete Code Example

```
1  using Thermo.TNG.MethodXMLFactory;
2  using Thermo.TNG.MethodXMLInterface;
3
4  string templateMethod = @"Files/Fusion/DIA/DIA_Template.meth";
5  string modificationXML = @"Files/Fusion/DIA/DIA.xml";
6  string outputMethod = @"Files/Fusion/DIA/DIA_output.meth";
7
8  string instrumentModel = "OrbitrapFusion"; // alternatively "TSQEndura" or "TSQQuantiva"
9  string instrumentVersion = "1.2"; // just the version number as a string
10
11  using(IMethodXMLContext mxc = MethodXMLFactory.CreateContext(instrumentModel, instrumentVersion))
12  using(IMethodXML mx = mxc.Create()) {
13
14      mx.Open(templateMethod); // Open the template method file
15
16      mx.ApplyMethodModificationsFromXMLFile(modificationXML); // Apply the xml modifications
17
18      mx.SaveAs(outputMethod); // Save the method in memory to disk
19  }
20
```

- The **XmlMethodChanger** Solution contains two projects
 1. XmlMethodChanger.lib
 - A public, static class library (**MethodChanger**)
 - Wraps the two Thermo.TNG.*.dll assemblies
 - Provides public methods for common tasks
 - Serves as an example of the API Usage
 2. XmlMethodChanger.cmd
 - Command-line program that uses XmlMethodChanger.lib
 - Uses third-party NuGet package (Command Line Parser Library)
 - Can be used as a standalone tool for modifying methods



Demonstration

- The “template” method contains the structure of the experiment

The diagram on the left illustrates a 3-second experiment sequence. It features a vertical stack of four components: a green box labeled '3 sec' on the left, and a sequence of four rounded rectangular boxes on the right: 'MS OT' (blue), 'Targeted Mass' (purple), 'Targeted Mass Exclusion' (purple), and 'ddMS² IT CID' (blue). Arrows indicate the flow from 'MS OT' to 'Targeted Mass', then to 'Targeted Mass Exclusion', and finally to 'ddMS² IT CID'. A bracket on the left groups the '3 sec' box with the sequence of components.

The screenshot on the right shows the 'Targeted Mass Exclusion Properties' dialog. It has a 'MASS LIST' section with the following options:

- Include Start/End Times: ☐
- Include Intensity Threshold: ☐
- Mass List Type:

Below these options is a table with columns 'Compound' and 'm/z'. The table contains one row with the value '1' in the 'Compound' column and '500' in the 'm/z' column. The table has buttons for 'ADD', 'DELETE', 'IMPORT', and 'EXPORT' above it.

Demonstration

- The “template” method contains the structure of the experiment

The diagram on the left shows a 3-second experiment sequence with the following steps: MS OT, Targeted Mass, Targeted Mass Exclusion, and ddMS² IT CID. The screenshot on the right shows the 'Targeted Mass Exclusion Properties' dialog. It includes a 'MASS LIST' section with checkboxes for 'Include Start/End Times' and 'Include Intensity Threshold', and a 'Mass List Type' dropdown set to 'm/z'. Below this is a table with one row containing '1' in the 'Compound' column and '500' in the 'm/z' column.

Compound	m/z
1	500

- The modification XML specifies a list of transformations to perform on the “template” method file

```
1 <?xml version="1.0" encoding="utf-8" ?>
2 <MethodModifications Version="2" Model="OrbitrapFusionLumos" Family="Calcium" Type="SL">
3   <Modification Order="1">
4     <Experiment ExperimentIndex="0">
5       <MassListFilter MassListType="TargetedMassExclusion">
6         <MassList IntensityThreshold="true">
7           <MassListRecord>
8             <MOverZ>195.12</MOverZ>
9             <Z>1</Z>
10            <IntensityThreshold>5e6</IntensityThreshold>
11          </MassListRecord>
12          <MassListRecord>
13            <MOverZ>262.3</MOverZ>
14            <Z>2</Z>
15            <IntensityThreshold>1e4</IntensityThreshold>
16          </MassListRecord>
17        </MassList>
18      </MassListFilter>
19    </Experiment>
20  </Modification>
21  <Modification Order="2">
22    <Experiment ExperimentIndex="0">
23      <MassListFilter MassListType="TargetedMassInclusion">
24        <MassList IntensityThreshold="true">
25          <MassListRecord>
26            <MOverZ>195.12</MOverZ>
27            <Z>1</Z>
28            <IntensityThreshold>5e7</IntensityThreshold>
29          </MassListRecord>
30          <MassListRecord>
31            <MOverZ>262.3</MOverZ>
32            <Z>2</Z>
33            <IntensityThreshold>1e2</IntensityThreshold>
34          </MassListRecord>
35        </MassList>
36      </MassListFilter>
37    </Experiment>
38  </Modification>
39 </MethodModifications>
```


Demonstration

- The “template” method contains the structure of the experiment

The diagram on the left shows a 3-second experiment setup with the following components: MS OT, Targeted Mass, Targeted Mass Exclusion, and ddMS² IT CID. The screenshot on the right shows the 'Targeted Mass Exclusion Properties' dialog. It includes a 'MASS LIST' section with checkboxes for 'Include Start/End Times' and 'Include Intensity Threshold', and a 'Mass List Type' dropdown set to 'm/z'. Below this is a table with columns 'Compound', 'm/z', and an empty column. The table contains one row with '1' in the 'Compound' column and '500' in the 'm/z' column.

- The modification XML specifies a list of transformations to perform on the “template” method file
- The transformed method can then be saved to a separate .meth file

```
1 <?xml version="1.0" encoding="utf-8" ?>
2 <MethodModifications Version="2" Model="OrbitrapFusionLumos" Family="Calcium" Type="SL">
3   <Modification Order="1">
4     <Experiment ExperimentIndex="0">
5       <MassListFilter MassListType="TargetedMassExclusion">
6         <MassList IntensityThreshold="true">
7           <MassListRecord>
8             <MOverZ>195.12</MOverZ>
9             <Z>1</Z>
10            <IntensityThreshold>5e6</IntensityThreshold>
11          </MassListRecord>
12          <MassListRecord>
13            <MOverZ>262.3</MOverZ>
14            <Z>2</Z>
15            <IntensityThreshold>1e4</IntensityThreshold>
16          </MassListRecord>
17        </MassList>
18      </MassListFilter>
19    </Experiment>
20  </Modification>
21  <Modification Order="2">
22    <Experiment ExperimentIndex="0">
23      <MassListFilter MassListType="TargetedMassInclusion">
24        <MassList IntensityThreshold="true">
25          <MassListRecord>
26            <MOverZ>195.12</MOverZ>
27            <Z>1</Z>
28            <IntensityThreshold>5e7</IntensityThreshold>
29          </MassListRecord>
30          <MassListRecord>
31            <MOverZ>262.3</MOverZ>
32            <Z>2</Z>
33            <IntensityThreshold>1e2</IntensityThreshold>
34          </MassListRecord>
35        </MassList>
36      </MassListFilter>
37    </Experiment>
38  </Modification>
39 </MethodModifications>
```

Demonstration

New Volume (J:) > meth-modifications > examples > Fusion > IntensityThreshold

Name	Date modified	Type	Size
Convert.bat	5/16/2018 10:19 AM	Windows Batch File	1 KB
IntensityThreshold.xml	5/16/2018 10:19 AM	XML File	2 KB
Template.meth	5/17/2018 1:58 PM	Xcalibur Instrume...	42 KB

Orbitrap Fusion Lumos Method Editor 3.1.2140 - DEV MODE

File Orbitrap Fusion Lumos

Method Editor

Global Parameters | **Scan Parameters** | Summary

Method Timeline Experiment ACTIONS

Application Mode: Peptide
Method Duration (min): 60

Default Charge State: 1
Internal Mass Calibration: Off

Experiment # 1 Time Range (min) 0-60

Scans: MS, MSⁿ

Filters: Precursor Selection Range, MIPS, Intensity

Place Scan Here

Properties

An abstract graphic featuring a globe with a dotted map of the world, surrounded by several white orbital lines with small dots, set against a red background.

ASMS 2019

June 2 - 6 | Atlanta, GA, USA

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THANK YOU!

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