

Untargeted C18 with ESI+



Thermo Scientific SII for

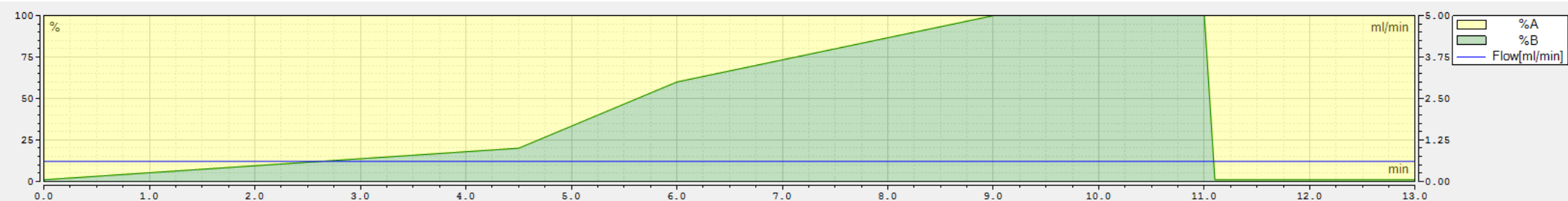


Orbitrap ID-X

✓ Check Method Insert Stage Insert Time Insert Command Insert Delete

- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup Shutdown
- Script Editor

General Settings Flow Gradient

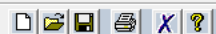


No	Time	Flow [ml/min]	%B	Curve
1	0.000			Run
2	0.000	0.600	1.0	5
3	4.500	0.600	20.0	5
4	6.000	0.600	60.0	5
5	9.000	0.600	100.0	5
6	11.000	0.600	100.0	5
7	11.100	0.600	1.0	5
8	13.000	0.600	1.0	5
9	New Row			
10	13.000			Stop Run

Add Equilibration Stage

Insert

Delete

Thermo
Scientific SII for

Orbitrap ID-X

Method Editor

Global Parameters

Scan Parameters

Summary

Document View

Tree View



Method Summary

Method Settings

Application Mode: **Small Molecule**
Method Duration (min): **13**

Global Parameters

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **60**
Aux Gas (Arb): **15**
Sweep Gas (Arb): **2**
Ion Transfer Tube Temp (°C): **350**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

MS Global Settings

Default Charge State: **1**
Enable Xcalibur AcquireX method modifications:
False
Internal Mass Calibration: **EASY-IC**

Divert Valve A

Time (min)	Position
	1-6
0.25	
11	

Experiment#1 [MS]

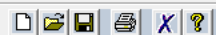
Start Time (min): **0.25**
End Time (min): **11**

Master Scan:

MS OT

Detector Type: **Orbitrap**
Orbitrap Resolution: **120000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **55-1000**
RF Lens (%): **35**
AGC Target: **2.0e5**
Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Positive**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**
Scan Description:

Untargeted C18 with ESI+
ddMS2



Thermo Scientific SII for



Orbitrap ID-X

✓ Check Method Insert Stage Insert Time Insert Command Insert Delete

- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup Shutdown
- Script Editor

General Settings Flow Gradient



No	Time	Flow [ml/min]	%B	Curve
1	0.000		Run	
2	0.000	0.600	1.0	5
3	4.500	0.600	20.0	5
4	6.000	0.600	60.0	5
5	9.000	0.600	100.0	5
6	11.000	0.600	100.0	5
7	11.100	0.600	1.0	5
8	13.000	0.600	1.0	5
9	New Row			
10	13.000		Stop Run	

Insert

Delete

Add Equilibration Stage



Thermo Scientific SII for



Orbitrap ID-X

Method Editor

Global Parameters

Scan Parameters

Summary

Document View

Tree View



Method Summary

Method Settings

Application Mode: **Small Molecule**
Method Duration (min): **13**

Global Parameters

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **60**
Aux Gas (Arb): **15**
Sweep Gas (Arb): **2**
Ion Transfer Tube Temp (°C): **350**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

MS Global Settings

Default Charge State: **1**
Enable Xcalibur AcquireX method modifications: **False**
Internal Mass Calibration: **EASY-IC**

Divert Valve A

Time (min)	Position
	1-6
0.25	
11	

Experiment#1 [Identification - MS2]

Start Time (min): **0**
End Time (min): **13**
Cycle Time (sec): **0.6**

Master Scan:

MS OT

Detector Type: **Orbitrap**
Orbitrap Resolution: **60000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **55-1000**
RF Lens (%): **35**
AGC Target: **1.0e5**
Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Positive**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**
Scan Description:

Filters:

Intensity

Filter Type: **Intensity Threshold**
Intensity Threshold: **2.0e4**

Dynamic Exclusion

Exclude after n times: **1**
Exclusion duration (s): **2.5**
Mass Tolerance: **ppm**
Low: **5**
High: **5**
Exclude Isotopes: **True**

Data Dependent

Data Dependent Mode: **Cycle Time**Time between Master Scans (sec): **0.6**

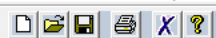
Scan Event Type 1:

Scan:

ddMS² OT HCD

Isolation Mode: **Quadrupole**
Isolation Window (m/z): **1.5**
Isolation Offset: **Off**
Activation Type: **HCD**
Collision Energy Mode: **Stepped**
HCD Collision Energies (%): **20,35,50**
Detector Type: **Orbitrap**
Scan Range Mode: **Auto: m/z Normal**
Orbitrap Resolution: **15000**
First Mass (m/z): **55**
AGC Target: **2.0e4**
Inject Ions for All Available Parallelizable Time: **False**
Maximum Injection Time (ms): **22**
Microscans: **1**
Data Type: **Profile**
Use EASY-IC™: **False**
Scan Description:

Untargeted C18 with ESI-



Thermo Scientific SII for



Orbitrap ID-X

✓ Check Method Insert Stage Insert Time Insert Command Insert Delete

- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup Shutdown
- Script Editor

General Settings Flow Gradient

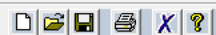


No	Time	Flow [ml/min]	%B	Curve
1	0.000		Run	
2	0.000	0.600	1.0	5
3	4.500	0.600	20.0	5
4	6.000	0.600	60.0	5
5	9.000	0.600	100.0	5
6	11.000	0.600	100.0	5
7	11.100	0.600	1.0	5
8	13.000	0.600	1.0	5
9	New Row			
10	13.000		Stop Run	

Insert

Delete

Add Equilibration Stage

Thermo
Scientific SII for

Orbitrap ID-X

Method Editor

Global Parameters

Scan Parameters

Summary

Document View

Tree View



Method Summary

Experiment#1 [MS]

Method Settings

Application Mode: **Small Molecule**
Method Duration (min): **13**

Start Time (min): **0.25**
End Time (min): **11**

Master Scan:

MS OT

Global Parameters

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **60**
Aux Gas (Arb): **15**
Sweep Gas (Arb): **2**
Ion Transfer Tube Temp (°C): **350**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

Detector Type: **Orbitrap**
Orbitrap Resolution: **120000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **55-1000**
RF Lens (%): **35**
AGC Target: **2.0e5**
Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Negative**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**
Scan Description:

MS Global Settings

Default Charge State: **1**
Enable Xcalibur AcquireX method modifications:
False
Internal Mass Calibration: **EASY-IC**

Divert Valve A

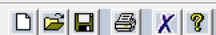
Time (min)	Position
	1-6
0.25	
11	



◀ 1 of 1 ▶



Untargeted C18 with ESI-,
ddMS2



Thermo Scientific SII for



Orbitrap ID-X

✓ Check Method Insert Stage Insert Time Insert Command Insert Delete

- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup Shutdown
- Script Editor

General Settings Flow Gradient

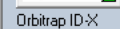


No	Time	Flow [ml/min]	%B	Curve
1	0.000		Run	
2	0.000	0.600	1.0	5
3	4.500	0.600	20.0	5
4	6.000	0.600	60.0	5
5	9.000	0.600	100.0	5
6	11.000	0.600	100.0	5
7	11.100	0.600	1.0	5
8	13.000	0.600	1.0	5
9	New Row			
10	13.000		Stop Run	

Add Equilibration Stage

Insert

Delete



Summary

Tree View

Method Settings

Global Parameters

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **60**
Aux Gas (Arb): **15**
Sweep Gas (Arb): **2**
Ion Transfer Tube Temp (°C): **350**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

Default Charge State: 1
Enable Xcalibur AcquireX method modifications: **False**
Internal Mass Calibration: **EASY-IC**

Time (min)	Position
	1-6
0.25	
11	

Start Time (min): 0
End Time (min): 13
Cycle Time (sec): 0.6

MS OT

Detector Type: Orbitrap
Orbitrap Resolution: 60000
Use Quadrupole Isolation: True
Scan Range (m/z): 55-1000
RF Lens (%): 35
AGC Target: 1.0e5
Maximum Injection Time (ms): 50
Microscans: 1
Data Type: Profile
Polarity: Negative
Source Fragmentation: Disabled
Use EASY-IC™: True
Scan Description:

Filters:

Intensity

Filter Type: **Intensity Threshold**
Intensity Threshold: **2.0e4**

Dynamic Exclusion

Exclude after n times: 1
Exclusion duration (s): 2.5
Mass Tolerance: ppm
Low: 5
High: 5
Exclude Isotopes: True

Data Dependent

Data Dependent Mode: **Cycle Time**

Time between Master Scans (sec): 0.6

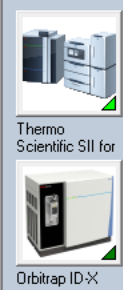
Scan Event Type 1:

Scan:

ddMS² OT HCD

Isolation Mode: **Quadrupole**
Isolation Window (m/z): **1.5**
Isolation Offset: **Off**
Activation Type: **HCD**
Collision Energy Mode: **Stepped**
HCD Collision Energies (%): **20,35,50**
Detector Type: **Orbitrap**
Scan Range Mode: **Auto: m/z Normal**
Orbitrap Resolution: **15000**
First Mass (m/z): **55**
AGC Target: **2.0e4**
Inject Ions for All Available Parallelizable Time: **False**
Maximum Injection Time (ms): **22**
Microscans: **1**
Data Type: **Profile**
Use EASY-IC™: **False**
Scan Description:

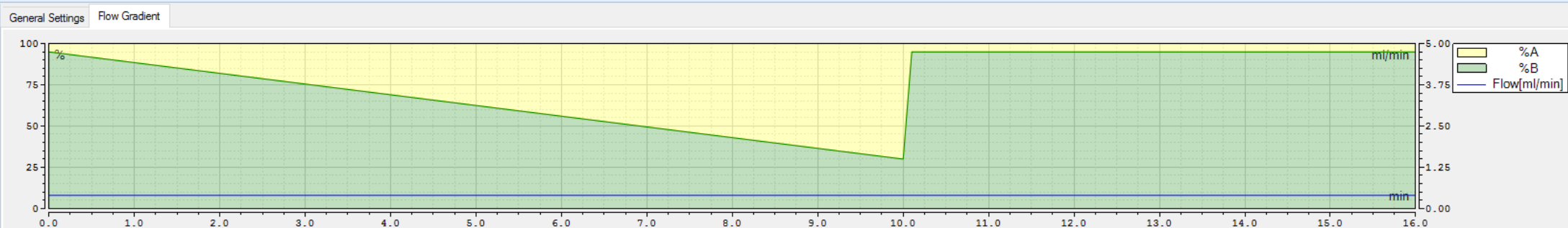
Untargeted HILIC with ESI+



Orbitrap ID-X

✓ Check Method Insert Stage Insert Time Insert Command Insert Delete

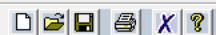
- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup
- Shutdown
- Script Editor



No	Time	Flow [ml/min]	%B	Curve
1	0.000		Run	
2	0.000	0.400	95.0	5
3	10.000	0.400	30.0	5
4	10.100	0.400	95.0	5
5	16.000	0.400	95.0	5
6	New Row			
7	16.000		Stop Run	

Insert
Delete

Add Equilibration Stage

Thermo
Scientific SII for

Orbitrap ID-X

Method Editor

Global Parameters

Scan Parameters

Summary

Document View

Tree View



Method Summary

Method Settings

Application Mode: **Small Molecule**
Method Duration (min): **16**

Global Parameters

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **50**
Aux Gas (Arb): **10**
Sweep Gas (Arb): **1**
Ion Transfer Tube Temp (°C): **325**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

MS Global Settings

Default Charge State: **1**
Enable Xcalibur AcquireX method modifications:
False
Internal Mass Calibration: **EASY-IC**

Divert Valve A

Time (min)	Position
	1-6
0.25	
10	

Experiment#1 [MS]

Start Time (min): **0.25**
End Time (min): **10**

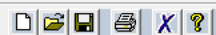
Master Scan:

MS OT

Detector Type: **Orbitrap**
Orbitrap Resolution: **120000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **55-1000**
RF Lens (%): **35**
AGC Target: **2.0e5**

Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Positive**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**
Scan Description:

Untargeted HILIC with ESI+,
ddMS2



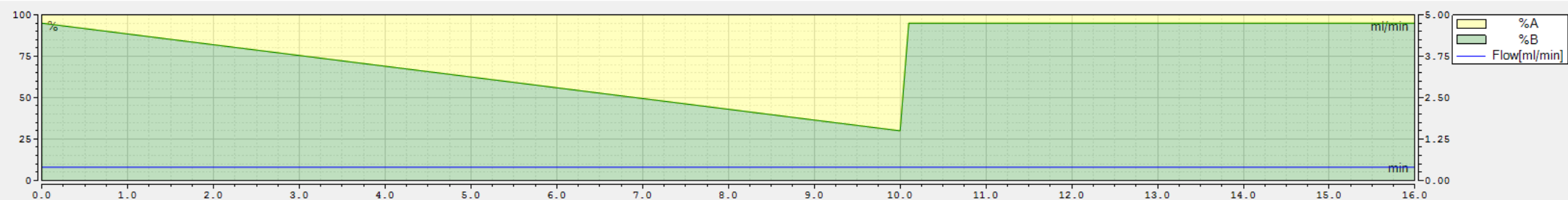
Orbitrap ID-X

✓ Check Method Insert Stage Insert Time Insert Command Insert Delete

- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup Shutdown
- Script Editor

General Settings

Flow Gradient

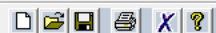


No	Time	Flow [ml/min]	%B	Curve
1	0.000		Run	
2	0.000	0.400	95.0	5
3	10.000	0.400	30.0	5
4	10.100	0.400	95.0	5
5	16.000	0.400	95.0	5
6	New Row			
7	16.000		Stop Run	

Insert

Delete

Add Equilibration Stage

Thermo
Scientific SII for

Orbitrap ID-X

Method Editor

Global Parameters

Scan Parameters

Summary

Document View

Tree View



Method Summary

Method Settings

Application Mode: **Small Molecule**
Method Duration (min): **16**

Global Parameters

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **50**
Aux Gas (Arb): **10**
Sweep Gas (Arb): **1**
Ion Transfer Tube Temp (°C): **325**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

MS Global Settings

Default Charge State: **1**
Enable Xcalibur AcquireX method modifications: **False**
Internal Mass Calibration: **EASY-IC**

Divert Valve A

Time (min)	Position
	1-6
0.25	
10	

Experiment#1 [MS]

Start Time (min): **0.25**
End Time (min): **10**
Cycle Time (sec): **0.6**

Master Scan:

MS OT

Detector Type: **Orbitrap**
Orbitrap Resolution: **60000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **55-1000**
RF Lens (%): **35**
AGC Target: **1.0e5**
Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Positive**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**
Scan Description:

Filters:

Intensity

Filter Type: **Intensity Threshold**
Intensity Threshold: **2.0e4**

Dynamic Exclusion

Exclude after n times: **1**
Exclusion duration (s): **2.5**
Mass Tolerance: **ppm**
Low: **5**
High: **5**
Exclude Isotopes: **True**

Data Dependent

Data Dependent Mode: **Cycle Time**Time between Master Scans (sec): **0.6**

Scan Event Type 1:

Scan:

ddMS² OT HCD

Isolation Mode: **Quadrupole**
Isolation Window (m/z): **1.5**
Isolation Offset: **Off**
Activation Type: **HCD**
Collision Energy Mode: **Stepped**
HCD Collision Energies (%): **20,35,50**
Detector Type: **Orbitrap**
Scan Range Mode: **Auto: m/z Normal**
Orbitrap Resolution: **15000**
First Mass (m/z): **55**
AGC Target: **2.0e4**
Inject Ions for All Available Parallelizable Time: **False**
Maximum Injection Time (ms): **22**
Microscans: **1**
Data Type: **Centroid**
Use EASY-IC™: **False**
Scan Description:

Untargeted HILIC with ESI-



Thermo Scientific SII for

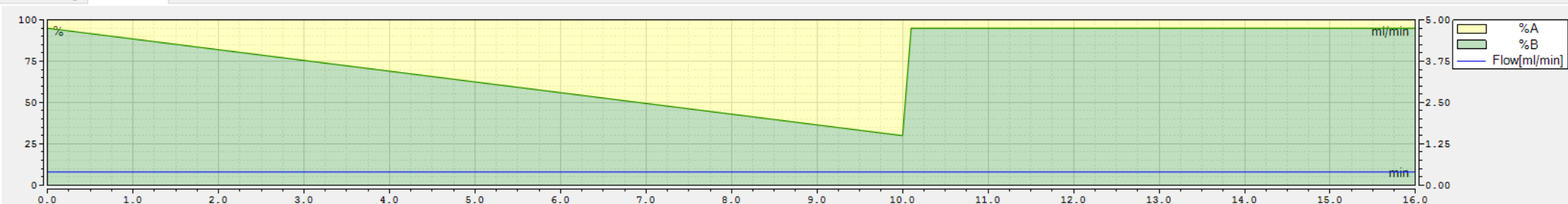


Orbitrap ID-X

Check Method Insert Stage Insert Time Insert Command Insert Delete

- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup Shutdown
- Script Editor

General Settings Flow Gradient

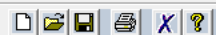


No	Time	Flow [ml/min]	%B	Curve
1	0.000		Run	
2	0.000	0.400	95.0	5
3	10.000	0.400	30.0	5
4	10.100	0.400	95.0	5
5	16.000	0.400	95.0	5
6	New Row			
7	16.000		Stop Run	

Add Equilibration Stage

Insert

Delete

Thermo
Scientific SII for

Orbitrap ID-X

Method Editor

Global Parameters

Scan Parameters

Summary

Document View

Tree View



Method Summary

Method Settings

Application Mode: **Small Molecule**
Method Duration (min): **16**

Global Parameters

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **50**
Aux Gas (Arb): **10**
Sweep Gas (Arb): **1**
Ion Transfer Tube Temp (°C): **325**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

MS Global Settings

Default Charge State: **1**
Enable Xcalibur AcquireX method modifications:
False
Internal Mass Calibration: **EASY-IC**

Divert Valve A

Time (min)	Position
	1-6
0.25	
10	

Experiment#1 [MS]

Start Time (min): **0.25**
End Time (min): **10**

Master Scan:

MS OT

Detector Type: **Orbitrap**
Orbitrap Resolution: **120000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **55-1000**
RF Lens (%): **35**
AGC Target: **2.0e5**
Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Negative**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**
Scan Description:

Untargeted HILIC with ESI-,
ddMS2



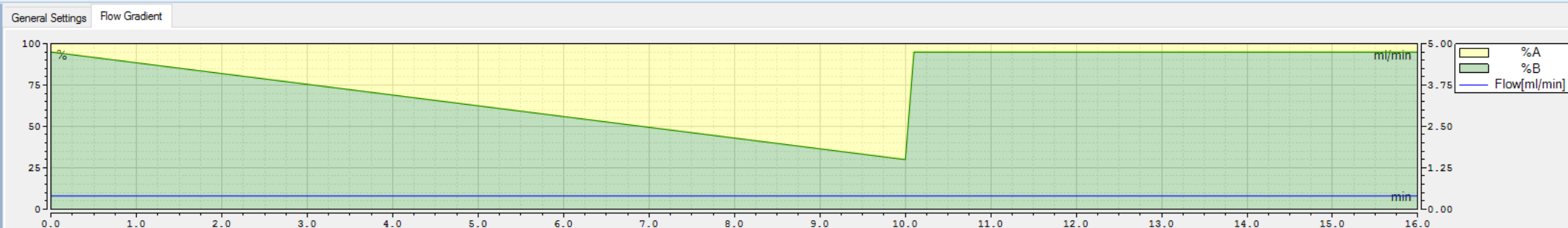
Thermo Scientific SII for



Orbitrap ID-X

✓ Check Method Insert Stage Insert Time Insert Command Insert Delete

- Pump (VH-P10-A)
- SamplerModule (VH-A10-A)
- ColumnComp (VH-C10-A)
- System
- Startup Shutdown
- Script Editor

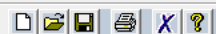


No	Time	Flow [ml/min]	%B	Curve
1	0.000		Run	
2	0.000	0.400	95.0	5
3	10.000	0.400	30.0	5
4	10.100	0.400	95.0	5
5	16.000	0.400	95.0	5
6	New Row			
7	16.000		Stop Run	

Insert

Delete

Add Equilibration Stage

Thermo
Scientific SII for

Orbitrap ID-X

Method Editor

Global Parameters

Scan Parameters

Summary

Document View

Tree View



Method Summary

Method Settings

Application Mode: **Small Molecule**
Method Duration (min): **16**

Global Parameters

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **50**
Aux Gas (Arb): **10**
Sweep Gas (Arb): **1**
Ion Transfer Tube Temp (°C): **325**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**
FAIMS Mode: **Not Installed**

MS Global Settings

Default Charge State: **1**
Enable Xcalibur AcquireX method modifications: **False**
Internal Mass Calibration: **EASY-IC**

Divert Valve A

Time (min)	Position
	1-6
0.25	
10	

Experiment#1 [MS]

Start Time (min): **0.25**
End Time (min): **10**
Cycle Time (sec): **0.6**

Master Scan:

MS OT

Detector Type: **Orbitrap**
Orbitrap Resolution: **60000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **55-1000**
RF Lens (%): **35**
AGC Target: **1.0e5**
Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Negative**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**
Scan Description:

Filters:

Intensity

Filter Type: **Intensity Threshold**
Intensity Threshold: **2.0e4**

Dynamic Exclusion

Exclude after n times: **1**
Exclusion duration (s): **2.5**
Mass Tolerance: **ppm**
Low: **5**
High: **5**
Exclude Isotopes: **True**

Data Dependent

Data Dependent Mode: **Cycle Time**Time between Master Scans (sec): **0.6**

Scan Event Type 1:

Scan:

ddMS² OT HCD

Isolation Mode: **Quadrupole**
Isolation Window (m/z): **1.5**
Isolation Offset: **Off**
Activation Type: **HCD**
Collision Energy Mode: **Stepped**
HCD Collision Energies (%): **20,35,50**
Detector Type: **Orbitrap**
Scan Range Mode: **Auto: m/z Normal**
Orbitrap Resolution: **15000**
First Mass (m/z): **55**
AGC Target: **2.0e4**
Inject Ions for All Available Parallelizable Time: **False**
Maximum Injection Time (ms): **22**
Microscans: **1**
Data Type: **Centroid**
Use EASY-IC™: **False**
Scan Description: