# Acquisition Method Report

Agilent | Trusted Answers

## Acquisition Method Info

**Method Name** NH415_1-18-21_H.m

**Method Path** D:\MassHunter\methods\Thomas\NH415_1-18-21_H.m

**Method Description** Default Method

**Device List**

Sampler
Binary Pump
Column Oven
QQQ

**MS QQQ Mass Spectrometer**

| | | | |
|---|---|---|---|
| **Ion Source** | AJS ESI | **Tune File** | D:\MassHunter\Tune\QQQ\G6470A \atunes.TUNE.XML |
| **Stop Mode** | By StopTime | **Stop Time (min)** | 40 |
| **Time Filter** | On | **Time Filter Width (min)** | 0.1 |

**Time Segments**

| Index | Start Time (min) | Scan Type | Ion Mode | Div Valve | Delta EMV (+) | Delta EMV (-) | Store |
|---|---|---|---|---|---|---|---|
| 1 | 0 | MRM | ESI+Agilent Jet Stream | To MS | 300 | 300 | Yes |

**Time Segment 1**

**Scan Segments**

| Cpd Group | Cpd Name | ISTD? | Prec Ion | MS1 Res | Prod Ion | MS2 Res | Dwell | Frag (V) | CE (V) | Cell Acc (V) | Polarity |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | GMP | No | 364 | Unit/Enh (6490) | 152 | Unit/Enh (6490) | 10 | 40 | 18 | 5 | Positive |
| | IMP | No | 349 | Unit/Enh (6490) | 137 | Unit/Enh (6490) | 10 | 40 | 19 | 5 | Positive |
| | AMP | No | 348 | Unit/Enh (6490) | 136 | Unit/Enh (6490) | 10 | 40 | 21 | 5 | Positive |
| | UMP M+1 | No | 326 | Unit/Enh (6490) | 97 | Unit/Enh (6490) | 10 | 30 | 14 | 5 | Positive |
| | UMP | No | 325 | Unit/Enh (6490) | 97 | Unit/Enh (6490) | 10 | 30 | 14 | 5 | Positive |
| | Guanosine | No | 284 | Unit/Enh (6490) | 152 | Unit/Enh (6490) | 10 | 30 | 20 | 5 | Positive |
| | Inosine | No | 269 | Unit/Enh (6490) | 137 | Unit/Enh (6490) | 10 | 35 | 20 | 5 | Positive |
| | deoxyguanosine | No | 268.1 | Unit/Enh (6490) | 152 | Unit/Enh (6490) | 10 | 30 | 14 | 5 | Positive |
| | Adenosine | No | 268 | Unit/Enh (6490) | 136 | Unit/Enh (6490) | 10 | 40 | 18 | 5 | Positive |
| | deoxyadenosine | No | 252 | Unit/Enh (6490) | 136 | Unit/Enh (6490) | 10 | 35 | 20 | 5 | Positive |
| | Uridine Standard | No | 249.2 | Unit/Enh (6490) | 112.96 | Unit/Enh (6490) | 10 | 30 | 14 | 5 | Positive |
| | Uridine M+1 | No | 246.2 | Unit/Enh (6490) | 115.96 | Unit/Enh (6490) | 10 | 30 | 14 | 5 | Positive |
| | Cytidine M+1 | No | 245.22 | Unit/Enh (6490) | 111.92 | Unit/Enh (6490) | 10 | 28 | 10 | 5 | Positive |
| | Uridine | No | 245.2 | Unit/Enh (6490) | 112.96 | Unit/Enh (6490) | 10 | 30 | 14 | 5 | Positive |
| | Cytidine | No | 244.22 | Unit/Enh (6490) | 111.92 | Unit/Enh (6490) | 10 | 28 | 10 | 5 | Positive |
| | deoxyuridine | No | 229.1 | Unit/Enh (6490) | 113 | Unit/Enh (6490) | 10 | 28 | 20 | 5 | Positive |
| | deoxycytidine | No | 228.1 | Unit/Enh (6490) | 112 | Unit/Enh (6490) | 10 | 28 | 20 | 5 | Positive |
| | Arginine Standard | No | 185.2 | Unit/Enh (6490) | 64 | Unit/Enh (6490) | 10 | 40 | 14 | 5 | Positive |

| Cpd Group | Cpd Name | ISTD? | Prec Ion | MS1 Res | Prod Ion | MS2 Res | Dwell | Frag (V) | CE (V) | Cell Acc (V) | Polarity |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | Citrulline | No | 176.1 | Unit/Enh (6490) | 70 | Unit/Enh (6490) | 10 | 35 | 13 | 5 | Positive |
| | Arginine | No | 175.2 | Unit/Enh (6490) | 60 | Unit/Enh (6490) | 10 | 40 | 14 | 5 | Positive |
| | Xanthene | No | 153 | Unit/Enh (6490) | 110 | Unit/Enh (6490) | 10 | 30 | 20 | 5 | Positive |
| | Hypoxanthine | No | 137.1 | Unit/Enh (6490) | 109.9 | Unit/Enh (6490) | 10 | 44 | 20 | 5 | Positive |
| | Aspartate | No | 134 | Unit/Enh (6490) | 74 | Unit/Enh (6490) | 10 | 40 | 15 | 5 | Positive |
| | Ornithine | No | 133 | Unit/Enh (6490) | 70 | Unit/Enh (6490) | 10 | 35 | 12 | 5 | Positive |
| | Leucine | No | 132 | Unit/Enh (6490) | 86.1 | Unit/Enh (6490) | 10 | 40 | 15 | 5 | Positive |
| | d2_ND | No | 127 | Unit/Enh (6490) | 84 | Unit/Enh (6490) | 10 | 100 | 20 | 5 | Positive |
| | Proline M+5 | No | 121 | Unit/Enh (6490) | 74.1 | Unit/Enh (6490) | 10 | 80 | 20 | 5 | Positive |
| | Proline | No | 116 | Unit/Enh (6490) | 70 | Unit/Enh (6490) | 10 | 80 | 20 | 5 | Positive |
| | Serine Standard | No | 109 | Unit/Enh (6490) | 63 | Unit/Enh (6490) | 10 | 40 | 13 | 5 | Positive |
| | Serine | No | 106 | Unit/Enh (6490) | 60 | Unit/Enh (6490) | 10 | 40 | 13 | 5 | Positive |
| | Beta-Aminolsobutyrate M+3 | No | 105 | Unit/Enh (6490) | 39 | Unit/Enh (6490) | 10 | 40 | 30 | 5 | Positive |
| | Beta-Aminolsobutyrate | No | 104 | Unit/Enh (6490) | 39 | Unit/Enh (6490) | 10 | 40 | 30 | 5 | Positive |
| | Alanine M+1 | No | 91 | Unit/Enh (6490) | 45 | Unit/Enh (6490) | 10 | 40 | 17 | 5 | Positive |
| | Alanine | No | 90 | Unit/Enh (6490) | 44 | Unit/Enh (6490) | 10 | 40 | 17 | 5 | Positive |
| | Glycine | No | 76 | Unit/Enh (6490) | 30 | Unit/Enh (6490) | 10 | 40 | 20 | 5 | Positive |
| | ATP Standard | No | 542.9 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 80 | 50 | 5 | Negative |
| | dATP Standard | No | 527 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 35 | 32 | 5 | Negative |
| | GTP | No | 522.2 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 32 | 5 | Negative |
| | dGTP | No | 506 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 32 | 5 | Negative |
| | ATP | No | 506 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 35 | 40 | 5 | Negative |
| | dATP | No | 490.1 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 35 | 32 | 5 | Negative |
| | UTP M+1 | No | 484 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | CTP M+1 | No | 483.16 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 34 | 36 | 5 | Negative |
| | UTP | No | 483 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | CTP | No | 482.16 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 34 | 36 | 5 | Negative |
| | dTTP M+1 | No | 482 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | dTTP | No | 481 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 46 | 5 | Negative |
| | dUTP M+1 | No | 468 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 46 | 5 | Negative |
| | dCTP M+1 | No | 467 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 34 | 35 | 5 | Negative |
| | dUTP | No | 467 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | dCTP | No | 466 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 34 | 35 | 5 | Negative |

| Cpd Group | Cpd Name | ISTD? | Prec Ion | MS1 Res | Prod Ion | MS2 Res | Dwell | Frag (V) | CE (V) | Cell Acc (V) | Polarity |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | GDP | No | 442 | Unit/Enh (6490) | 150 | Unit/Enh (6490) | 10 | 35 | 24 | 5 | Negative |
| | ADP | No | 426 | Unit/Enh (6490) | 134 | Unit/Enh (6490) | 10 | 135 | 20 | 5 | Negative |
| | UDP M+1 | No | 404.16 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | CDP M+1 | No | 403.18 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | UDP | No | 403.16 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | CDP | No | 402.18 | Unit/Enh (6490) | 159 | Unit/Enh (6490) | 10 | 30 | 26 | 5 | Negative |
| | dTDP M+1 | No | 402 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 36 | 44 | 5 | Negative |
| | dTDP | No | 401 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 36 | 44 | 5 | Negative |
| | AMP Neg | No | 346 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 40 | 21 | 5 | Negative |
| | UMP Neg M +1 | No | 324 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 40 | 30 | 5 | Negative |
| | CMP M+1 | No | 323 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 35 | 30 | 5 | Negative |
| | UMP Neg | No | 323 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 40 | 30 | 5 | Negative |
| | dTMP M+1 | No | 322.2 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 30 | 30 | 5 | Negative |
| | CMP | No | 322 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 35 | 30 | 5 | Negative |
| | dTMP | No | 321 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 30 | 30 | 5 | Negative |
| | dUMP M+1 | No | 308 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 40 | 30 | 5 | Negative |
| | dUMP | No | 307 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 40 | 30 | 5 | Negative |
| | Thymidine M +1 | No | 242 | Unit/Enh (6490) | 44 | Unit/Enh (6490) | 10 | 35 | 10 | 5 | Negative |
| | Thymidine | No | 241 | Unit/Enh (6490) | 42 | Unit/Enh (6490) | 10 | 35 | 10 | 5 | Negative |
| | Dihydroorotate | No | 157 | Unit/Enh (6490) | 113 | Unit/Enh (6490) | 10 | 35 | 12 | 5 | Negative |
| | Carbamoyl-phosphate | No | 140 | Unit/Enh (6490) | 79 | Unit/Enh (6490) | 10 | 70 | 20 | 5 | Negative |
| | Fumaric acid d2 Std | No | 117 | Unit/Enh (6490) | 72.8 | Unit/Enh (6490) | 10 | 50 | 20 | 5 | Negative |
| | Uracil M+1 | No | 112 | Unit/Enh (6490) | 44 | Unit/Enh (6490) | 10 | 30 | 20 | 5 | Negative |
| | Uracil | No | 111 | Unit/Enh (6490) | 42 | Unit/Enh (6490) | 10 | 30 | 20 | 5 | Negative |
| | Lactate | No | 89 | Unit/Enh (6490) | 43 | Unit/Enh (6490) | 10 | 40 | 16 | 5 | Negative |

### Source Parameters

| Parameter | Value (+) | Value (-) |
|---|---|---|
| Gas Temp (°C) | 350 | 350 |
| Gas Flow (l/min) | 9 | 9 |
| Nebulizer (psi) | 50 | 50 |
| SheathGasHeater | 375 | 375 |
| SheathGasFlow | 12 | 12 |
| Capillary (V) | 3500 | 3500 |
| VCharging | 1000 | 1000 |

### Scan Parameters

| Data Stg | Threshold |
|---|---|
| Centroid | 0 |

### Chromatograms

| Chrom Type | Label | Offset | Y-Range |
|---|---|---|---|
| TIC | TIC | 0 | 10000000 |

### Instrument Curves

**Actual**

## Name: Sampler — Module: G7129B

**Auxiliary**

| | |
|---|---|
| Draw Speed | 100 µL/min |
| Eject Speed | 400 µL/min |
| Wait Time After Draw | 1.2 s |
| Needle Height Offset | 0.0 mm |

**Injection**

| | |
|---|---|
| Injection Mode | Standard injection |
| Injection Volume | 10.00 µL |

**High throughput**

| | |
|---|---|
| Sample Flush-Out Factor | 5.0 |
| Injection Valve to Bypass for Delay Volume Reduction | No |
| Overlapped Injection | |
| Overlapped Injection Mode | Off |

**Stop Time**

| | |
|---|---|
| Stoptime Mode | As pump/No limit |

**Post Time**

| | |
|---|---|
| Posttime Mode | Off |

## Name: Binary Pump — Module: G7120A

| | |
|---|---|
| Flow | 0.350 mL/min |
| Use Solvent Types | Yes |
| Stroke Mode | Synchronized |
| Low Pressure Limit | 0.00 bar |
| High Pressure Limit | 700.00 bar |
| Max. Flow Ramp Up | 100.000 mL/min² |
| Max. Flow Ramp Down | 100.000 mL/min² |
| Expected Mixer | No check |
| Stroke A | |
| Automatic Stroke Calculation A | Yes |
| Stop Time | |
| Stoptime Mode | Time set |
| Stoptime | 40.00 min |
| Post Time | |
| Posttime Mode | Off |

**Solvent Composition**

| | Channel | Ch. 1 Solv. | Name 1 | Ch2 Solv. | Name 2 | Selected | Used | Percent (%) |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 100.0 % Water V.02 | | 100.0 % Water V.02 | | Ch. 1 | Yes | 15.00 % |
| 2 | B | 100.0 % Acetonitrile V.02 | | 100.0 % Acetonitrile V.02 | | Ch. 1 | Yes | 85.00 % |

**Timetable**

| | Time (min) | A (%) | B (%) | Flow (mL/min) |
|---|---|---|---|---|
| 1 | 5.00 min | 70.00 % | 30.00 % | 0.350 mL/min |
| 2 | 30.00 min | 98.00 % | 2.00 % | 0.350 mL/min |
| 3 | 35.00 min | 98.00 % | 2.00 % | 0.350 mL/min |
| 4 | 40.00 min | 15.00 % | 85.00 % | 0.350 mL/min |

| | Pressure (bar) |
|---|---|
| 1 | 700.00 bar |
| 2 | 700.00 bar |
| 3 | 700.00 bar |
| 4 | 700.00 bar |

| | Time (min) | A (%) | B (%) | Flow (mL/min) |
|---|---|---|---|---|
| 5 | 45.00 min | 15.00 % | 85.00 % | 0.350 mL/min |

**Name:** Column Oven **Module:** G7130A

**Temperature Control**

| | |
|---|---|
| Temperature Control Mode | Not Controlled |
| **Temperature Not Ready Limit** | |
| Temperature Not Ready Limit On | Yes |
| Temperature Not Ready Limit Value | 0.8 °C |
| Temperature Equilibration Time | 0.0 min |

**Enforce column for run**

| | |
|---|---|
| Enforce column for run enabled | No |

**Stop Time**

| | |
|---|---|
| Stoptime Mode | As pump/injector |

**Post Time**

| | |
|---|---|
| Posttime Mode | Off |

**Timetable**

| | Pressure (bar) |
|---|---|
| **5** | 700.00 bar |