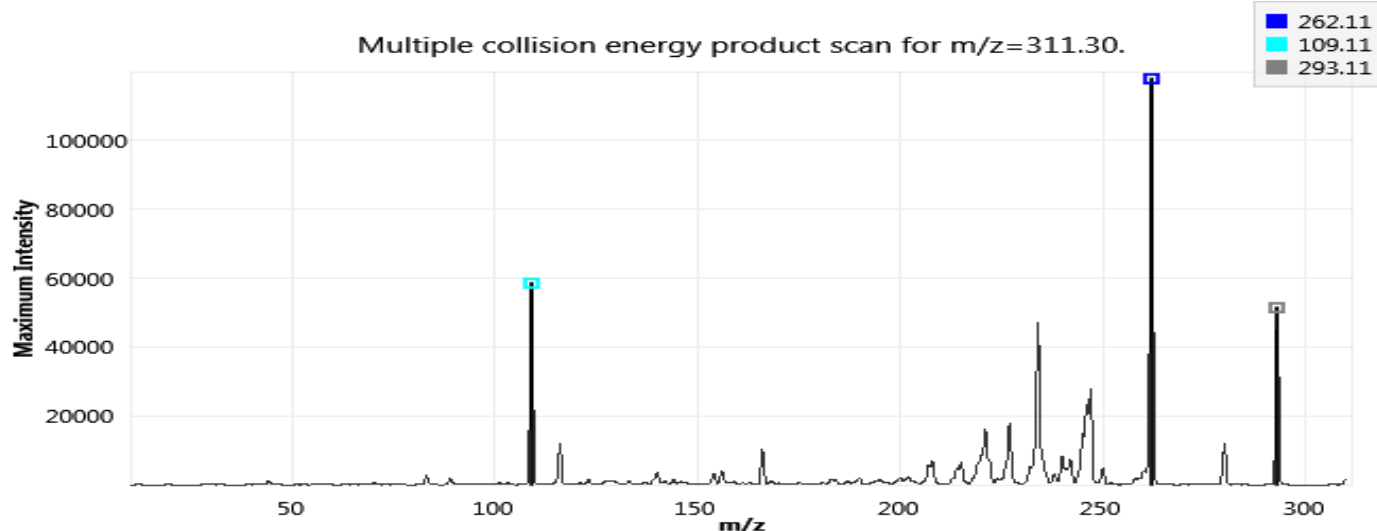


# Compound Optimization Report

Date & Time Monday, November 25, 2019 10:49 AM  
Instrument Model TSQ Quantiva  
Instrument Serial TQH-Q1-0381  
Software Version 2.0.1292.15

| Source Parameters           |       | Compound Optimization Input |         |
|-----------------------------|-------|-----------------------------|---------|
| Source Type                 | H-ESI | Source Fragmentation (V)    | 0       |
| Spray Voltage (V)           | 3500  | Step Collision Energy Value | 10      |
| Sheath Gas (Arb)            | 42    | Collision Energy Start (V)  | 5       |
| Aux Gas (Arb)               | 12    | Collision Energy End (V)    | 55      |
| Sweep Gas (Arb)             | 1     | Charge State                | 1       |
| Ion Transfer Tube Temp (°C) | 338   | Step Collision Energy       | Yes     |
| Vaporizer Temp (°C)         | 338   | Unknown/Known Products      | Unknown |
|                             |       | Exclude Loss Masses         | None    |
|                             |       | Compound Name               | desCIT  |
|                             |       | Low Mass Exclusion          | 10      |
|                             |       | Product                     | True    |
|                             |       | CID Gas (mTorr)             | 1.5     |
|                             |       | Adjust Precursor Mass       | Yes     |
|                             |       | m/z Value                   | 311.3   |
|                             |       | Q1 Resolution               | 0.7     |
|                             |       | Adjust Product Mass         | Yes     |
|                             |       | Number of Products          | 3       |
|                             |       | Top N                       | 3       |
|                             |       | Optimize RF Lens            | Yes     |

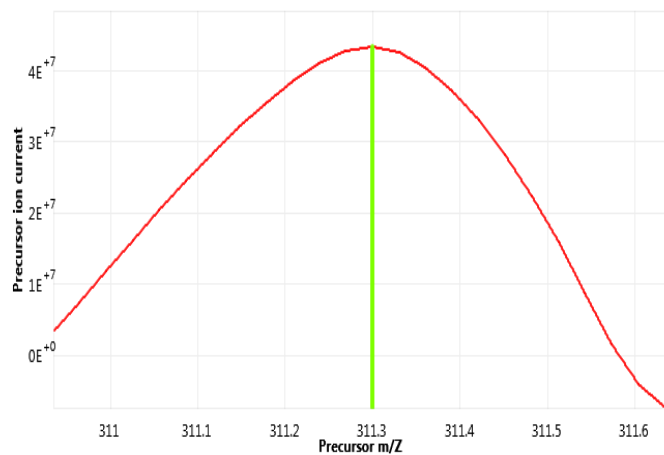
| Compound Optimization Results |               |             |                      |             |             |                          |
|-------------------------------|---------------|-------------|----------------------|-------------|-------------|--------------------------|
| Compound Name                 | Precursor m/z | Product m/z | Collision Energy (V) | RF Lens (V) | Intensity   | Source Fragmentation (V) |
| desCIT                        | 311.3         | 262.111     | 15.916               | 74.494      | 2298991.232 | 0                        |
| desCIT                        | 311.3         | 109.111     | 24.208               | 74.494      | 3878175.09  | 0                        |
| desCIT                        | 311.3         | 293.111     | 15.107               | 74.494      | 840593.096  | 0                        |



# Compound Optimization Report

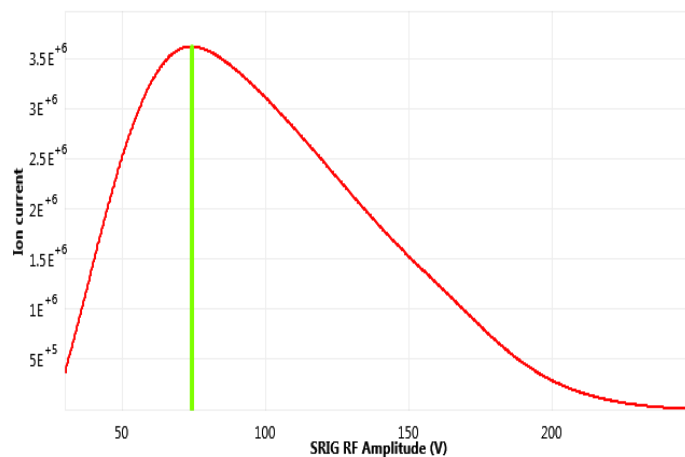
Precursor Mass Isolation for 311.30

311.30



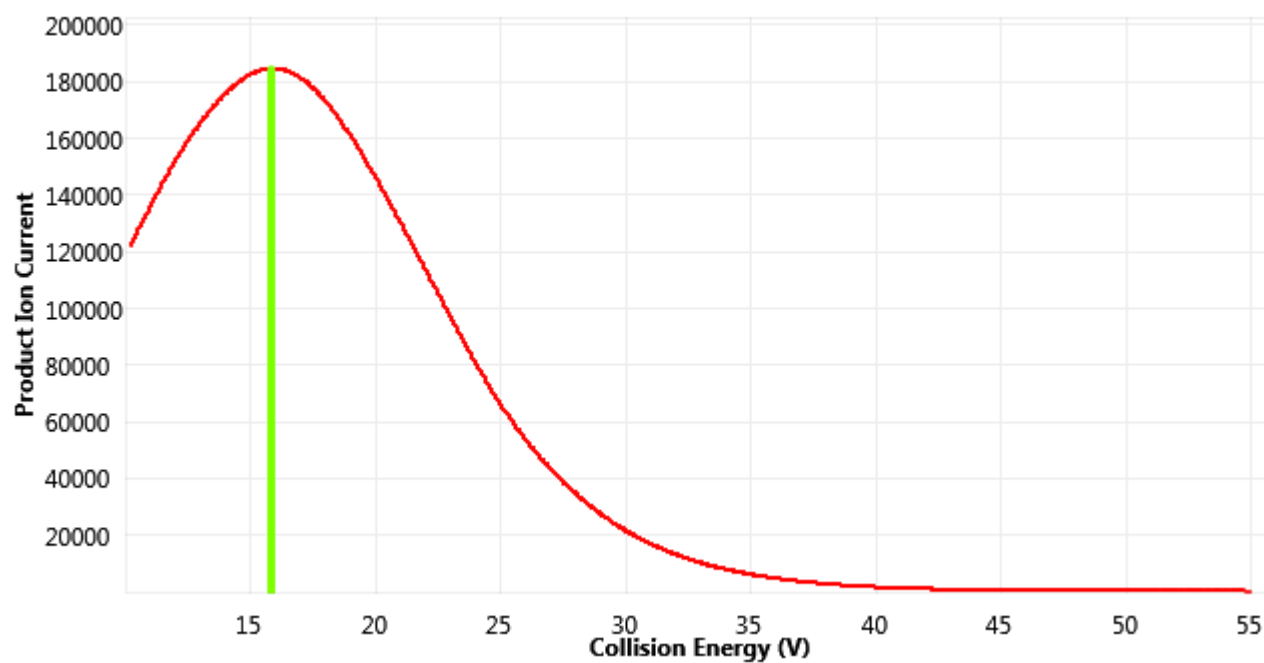
SRIG tuning for 311.30

74.49



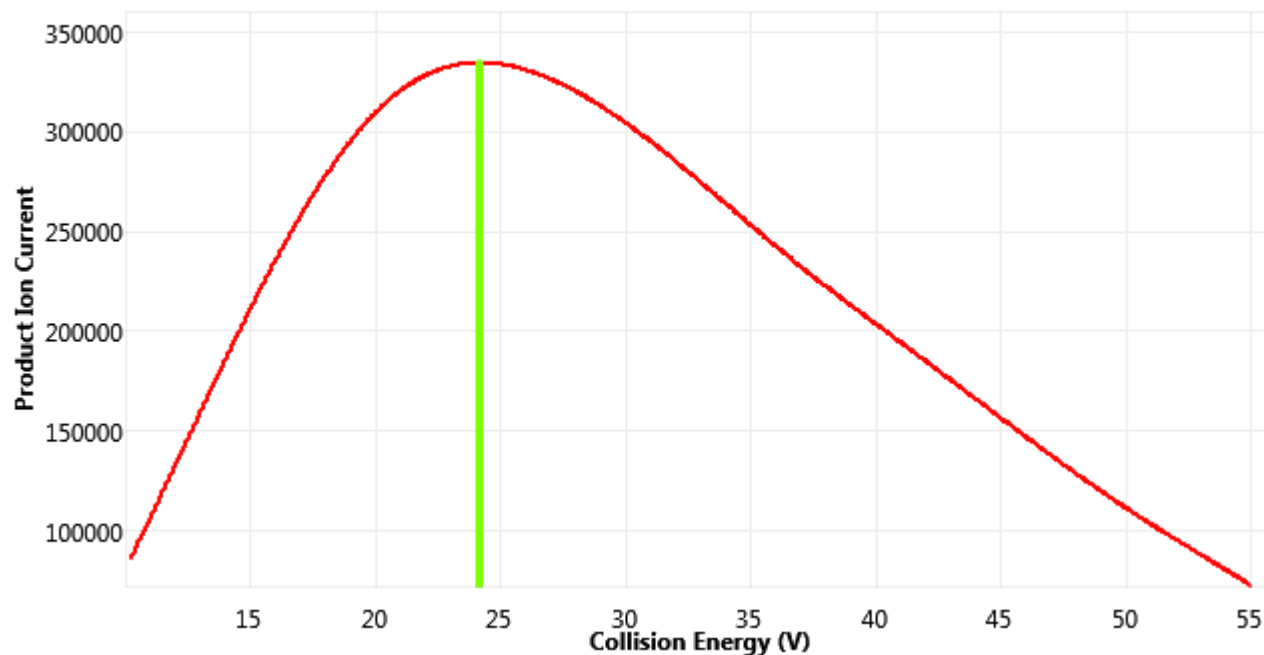
Breakdown Curve for 311.30 to 262.11 transition

15.92



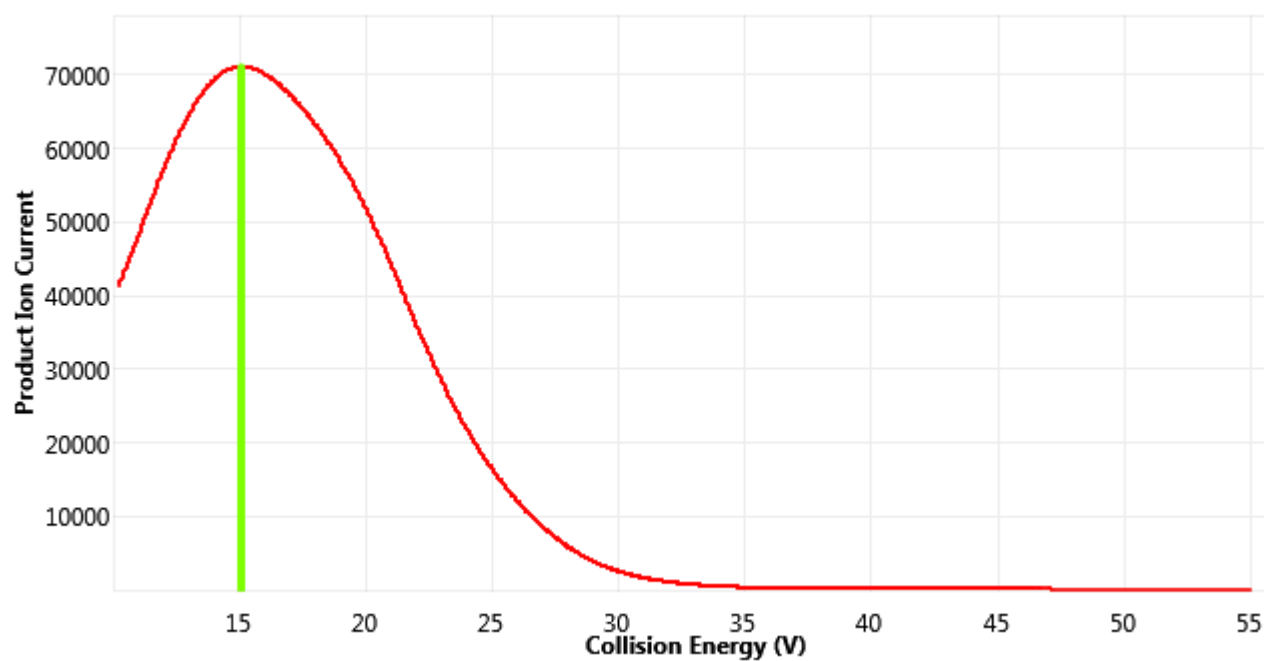
24.21

Breakdown Curve for 311.30 to 109.11 transition



15.11

Breakdown Curve for 311.30 to 293.11 transition



# Compound Optimization Report

