



## Certificate of Analysis

These products were manufactured in accordance with compliance to ISO 9001:2015.

### Product Identification

**Product Name:** APCI Negative Calibration Solution**Part Number:** 4460134      **Storage:** 2 – 8 °C

### Lot Specific Information

**Lot Number:**

M312181

**Manufacture Date:**

2024-01-05

(YYYY-MM-DD)

**Expiration Date:**

2024-12-01

(YYYY-MM-DD)

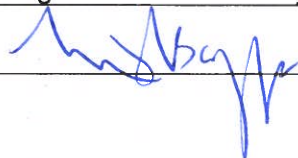
Component	Mass	Verification of Mass Accuracy and Signal Intensity (Pass/Fail)
Calibration Ion A	144.1030	Pass
Calibration Ion B	264.1453	Pass
Calibration Ion C	277.0983	Pass
Calibration Ion E	352.1977	Pass
Calibration Ion F	403.1122	Pass
Calibration Ion G	440.2501	Pass
Calibration Ion I	616.3550	Pass
Calibration Ion J	792.4598	Pass

### Quality Assurance Statement

The information on this certificate has been reviewed and accurately reflects manufacturing and analysis data for the product lot specified.

These reagents were tested and released by SCIEX Quality Control, and the results above were obtained utilizing qualified equipment.

### Quality Control

**Print Name:** Migdalia Febus-Bozzay**Signature:**

 2024-01-05
**Date:**

2024-01-05

(YYYY-MM-DD)

### Support

Technical Support call 1 800-952-4716 or 877-740-2129 or E-mail: [sciexnow@sciex.com](mailto:sciexnow@sciex.com) (Global) or [sciexnowamericas@sciex.com](mailto:sciexnowamericas@sciex.com) (US and Canada)

This certificate and product safety data sheets (SDS) may be obtained at: <https://www.sciex.com/support/tech-regulatory>



## APCI Calibration Solutions for the AB SCIEX TripleTOF™ 5600 System

	100ml	5 x 100ml
APCI Positive Calibration Solution for the AB SCIEX TripleTOF™ 5600 System	4460131	4460136
APCI Negative Calibration Solution for the AB SCIEX TripleTOF™ 5600 System	4460134	4460138

Table 1: List of TOF MS Calibration Ions:

Component	Positive Mass (Da)	Negative Mass (Da)
Calibration ion A	146.1176	144.1030
Calibration ion B	266.1598	264.1453
Calibration ion C	n/a	277.0983
Calibration ion D	315.1623	n/a
Calibration ion E	354.2122	352.1977
Calibration ion F	n/a	403.1122
Calibration ion G	442.2647	440.2501
Calibration ion H	609.2807	n/a
Calibration ion I	618.3695	616.3550
Calibration ion J	n/a	792.4598
Calibration ion K	922.0098	n/a
Calibration ion L	1521.9715	n/a

*\*Calibration ions C and F are temperature dependent*

Table 2: List of Product Ion (MS/MS) Calibration Ions, Positive Mode:

Precursor Ion (Da)	315.1623	609.2807
Declustering Potential (V)	80	80
Collision Energy (V)	27	45
Fragment Ion 1	315.1623	609.2807
Fragment Ion 2	270.1044	577.2544
Fragment Ion 3	242.0731	448.1966
Fragment Ion 4	235.1356	397.2122
Fragment Ion 5	227.0496	365.1860
Fragment Ion 6	220.1121	236.1281
Fragment Ion 7	86.0964	195.0652
Fragment Ion 8	58.0651	174.0913



Table 3: List of Product Ion (MS/MS) Calibration Ions, Negative Mode:

Precursor Ion (Da)	277.0983	403.1122
Declustering Potential (V)	-80	-80
Collision Energy (V)	-30	-30
Fragment Ion 1	277.0983	403.1122
Fragment Ion 2	249.1033	277.0983
Fragment Ion 3	217.0771	158.0611
Fragment Ion 4	200.0591	125.0067
Fragment Ion 5	158.0611	93.0344
Fragment Ion 6	130.0662	n/a
Fragment Ion 7	116.0506	n/a
Fragment Ion 8	77.0397	n/a

### To Use APCI Calibration Solution

(Store calibration solution at 4°C if calibration solution is not going to be used for an extended period of time)

1. Bring to room temperature and shake well before using.
2. Insert one of the calibration lines from the Calibration Delivery System (CDS) into the calibration solution. Note the CAL port, eg. CAL A. Refer to the DuoSpray™ Ion Source Operator's Guide for more details on setting up the CDS device.
3. In the Analyst® software, activate a hardware profile containing the CDS device.
4. In Tune and Calibrate Mode, open the Manual Tuning window.
5. From the drop-down list, select Calibrate.
6. In the calibrate window, select the appropriate Calibrant Reference Table from the drop-down List.
7. Select View to display the calibration ions and the calibrant valve position. Ensure that the correct ions for the experimental mass range, and the correct calibration valve position are selected. Refer to the Analyst® TF software Online Help for details about editing the Reference Table.
8. Select CDS Purge button to prime the CDS device with the calibration solution.
9. Set the CDS Flow rate to 200 µL/min.
10. Select MS Method from the drop-down list at the top of the pane.
11. In the Manual Tuning window, create a MS method. Set the Source/Gas and Compound parameters to values that are typical for your application.
12. Introduce LC flow into ESI probe of the ion source at the initial starting conditions of your typical LC method.
13. Once the CDS has been primed, select CDS inject to begin infusing the calibration solution into the APCI probe.
14. Select Start to begin acquiring data. The calibration ions should appear in the mass spectrum. Note: If the CDS device has not been used recently, or another calibration solution was used previously, it may take a couple of minutes for the desired calibration ions to appear. To decrease the time, temporarily increase the CDS flow rate.



15. Once the solution has been primed, the calibration system can be used to automatically calibrate the mass spectrometer in batch mode. For more information, refer to the Mass Calibration Tutorial.

Figure 1: TOF MS, APCI Positive Calibration Solution for the AB SCIEX TripleTOF™ 5600 System

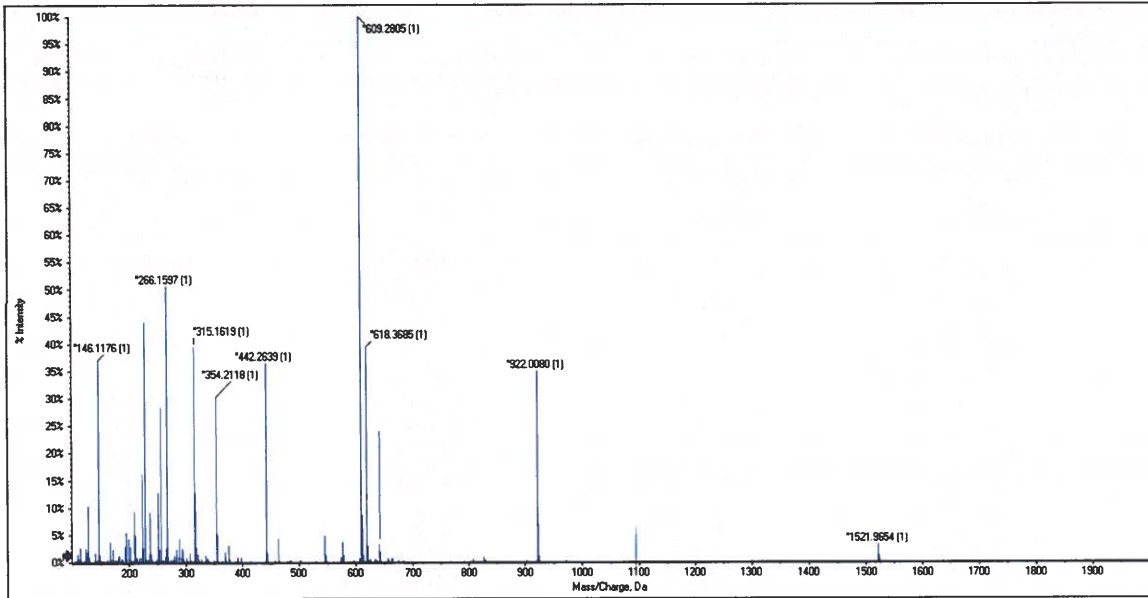


Figure 2: TOF MS, APCI Positive Calibration Solution for the AB SCIEX TripleTOF™ 5600 System (zoomed to highlight each calibration ion)

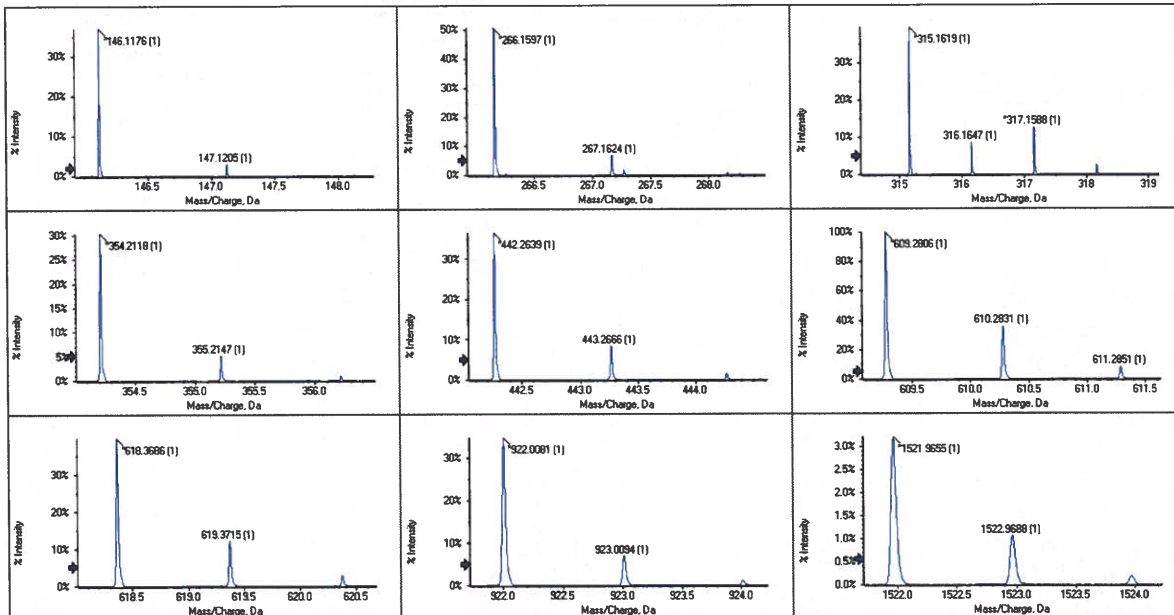


Figure 3: TOF MS, APCI Negative Calibration Solution for the AB SCIEX TripleTOF™ 5600 System

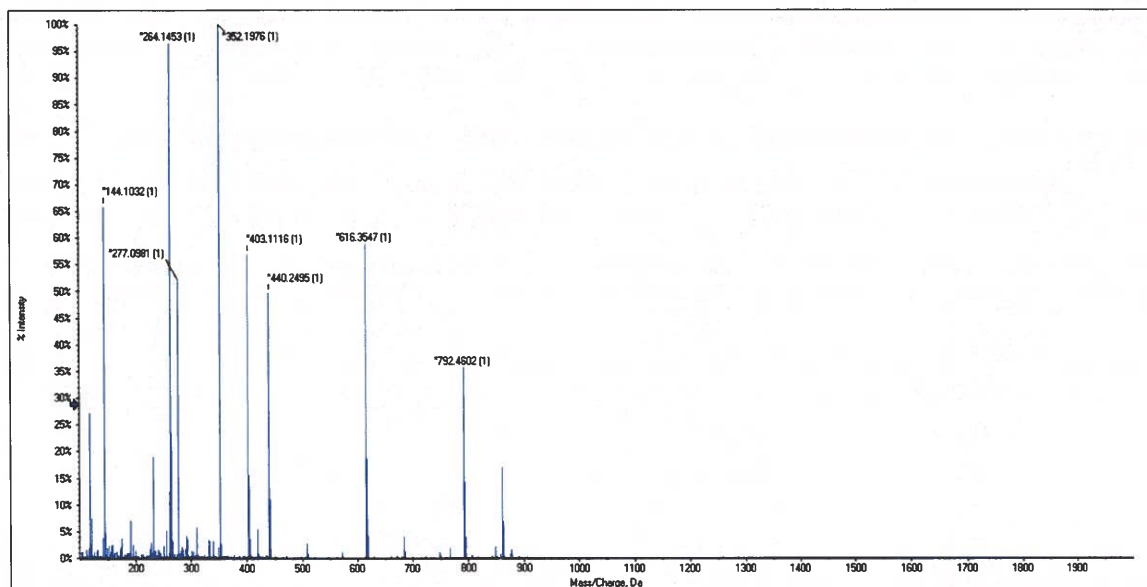
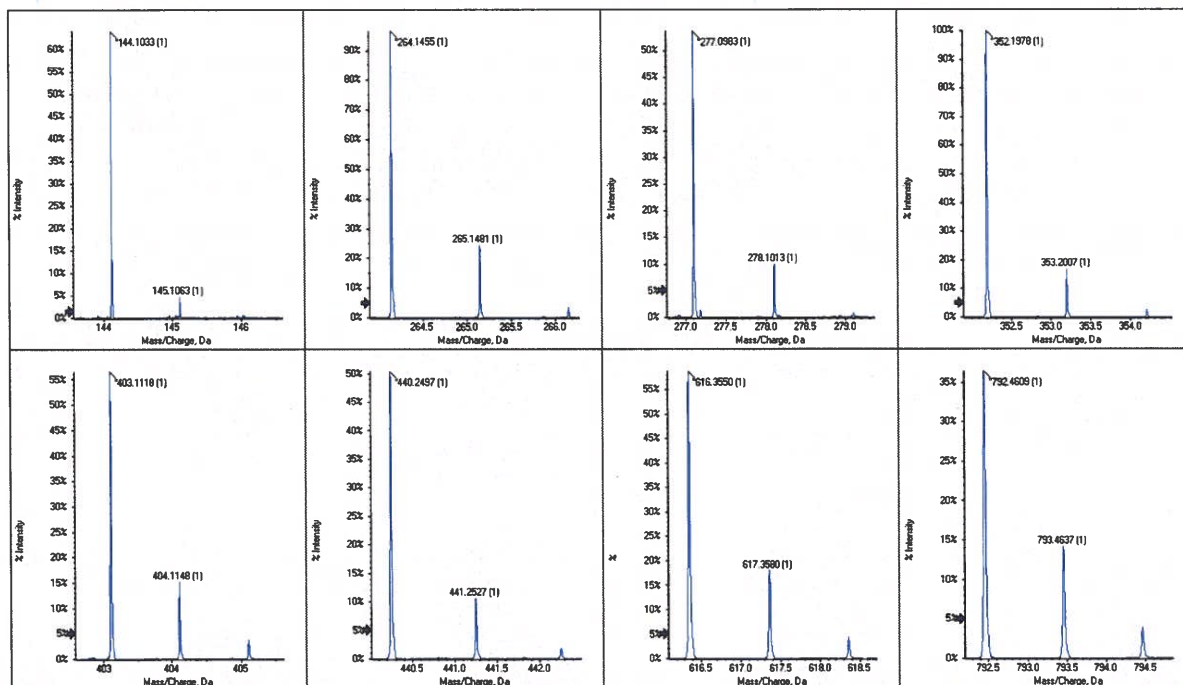


Figure 4: TOF MS, APCI Negative Calibration Solution for the AB SCIEX TripleTOF™ 5600 System (zoomed to highlight each calibration ion)





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Figure 5: MS/MS Calibration Ion D (zoomed), APCI Positive Calibration Solution for the AB SCIEX TripleTOF™ 5600 System

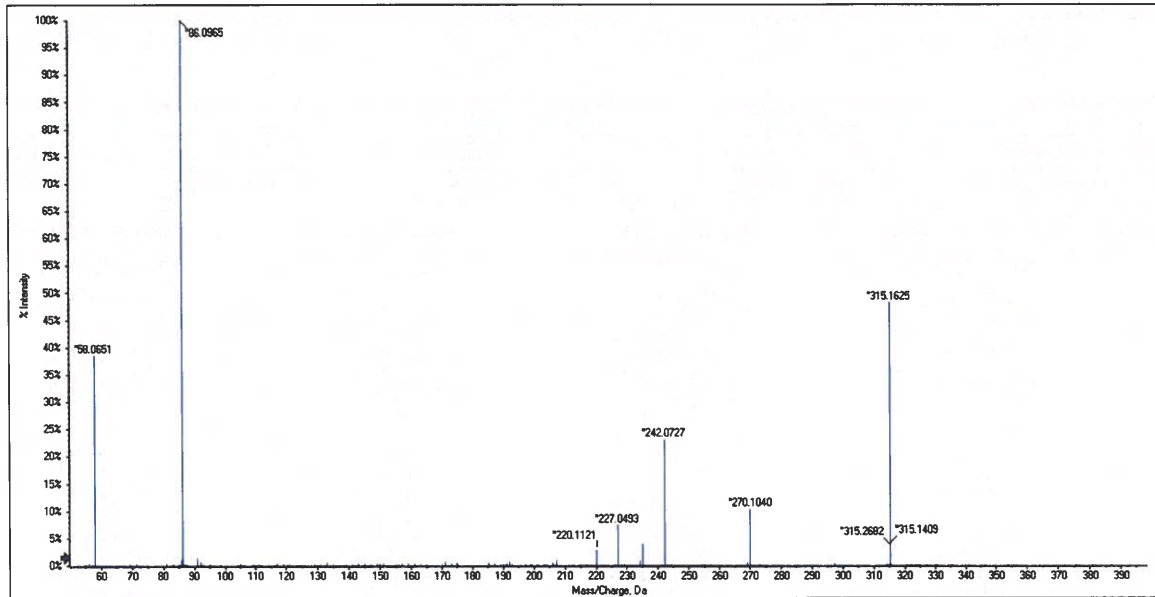


Figure 6: MS/MS Calibration Ion H (zoomed), APCI Positive Calibration Solution for the AB SCIEX TripleTOF™ 5600 System

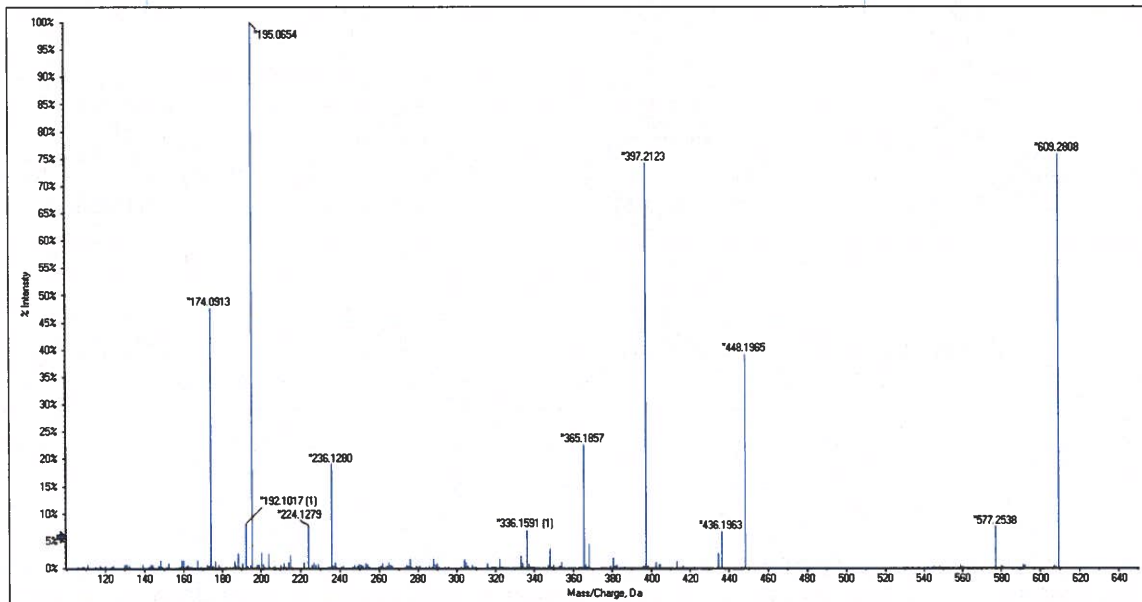


Figure 7: MS/MS Calibration Ion C (zoomed), APCI Negative Calibration Solution for the AB SCIEX TripleTOF™ 5600 System

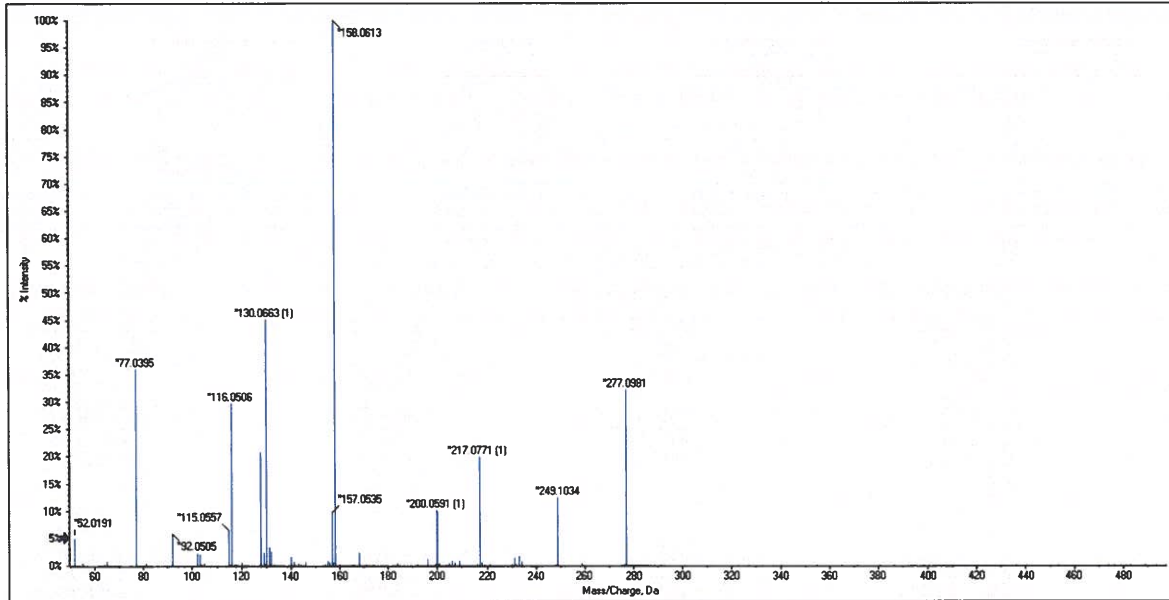


Figure 8: MS/MS Calibration Ion F (zoomed), APCI Negative Calibration Solution for the AB SCIEX 5600 TripleTOF™ System

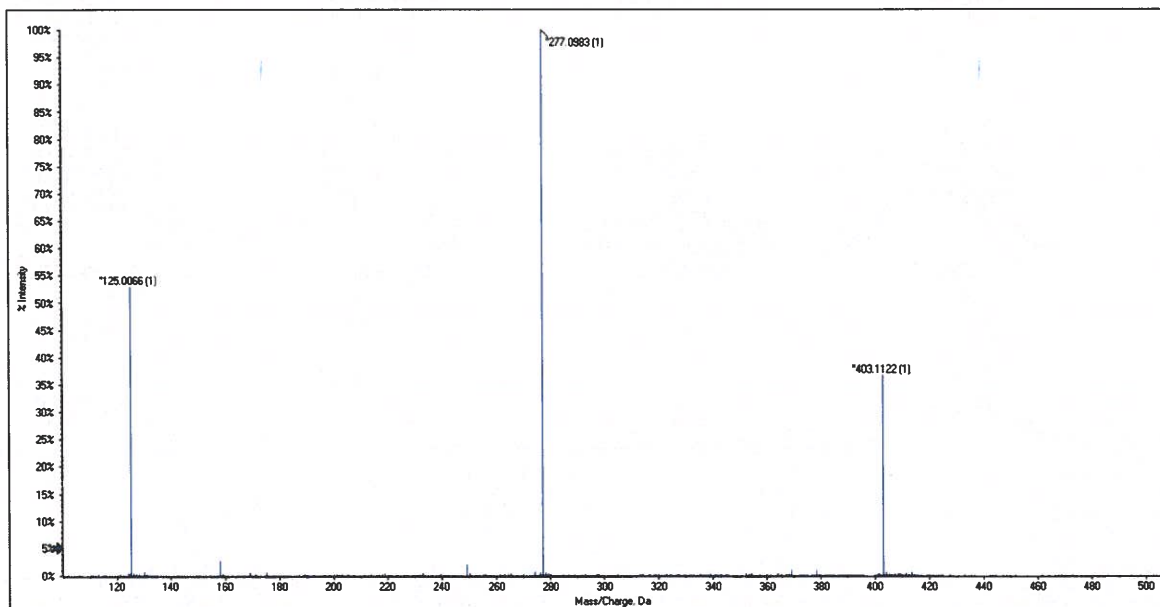
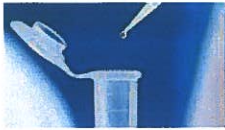




Table 4: Trouble-shooting APCI Calibration Solutions

Symptom	Possible Cause	Remedy
Calibration ions are not observed in the spectrum	CDS device has not been primed properly with calibration solution	Ensure calibrant tubing from CDS Select Valve is in the calibration solution. Purge the CDS device.
Calibration ions are not observed in the spectrum	Air bubbles in calibrant tubing after purging or refilling the solution	Ensure calibrant tubing from CDS Select Valve is in the calibration solution. Purge the CDS device. Decrease the CDS Refill/Purge Flow rate.
Calibration ions are not observed in the spectrum	Incorrect Select valve position selected for calibration solution	In the Reference Table Editor, modify the Valve Position to the correct position.
Calibration ion intensity is weak	CDS Inject Flow Rate is too slow	Increase the CDS inject Flow Rate.
Calibrant ion C or F is not observed	Calibration ions C and F are temperature dependent	At high temperatures, do not include Calibration Ion F. At lower temperatures, do not include Calibration Ion C.
Batch Calibration fails	Incorrect Calibrant Reference table selected	Choose the appropriate Calibration Reference table for the calibration solution.
Batch Calibration fails	Calibration ion intensity is too weak	Increase the CDS Inject Flow Rate
Batch Calibration fails	Initial mass calibration is greater than 200 ppm off	Manually recalibrate the instrument using the Re-Calibrate TOF feature in Tune and Calibrate mode. Ensure that <i>Set as Instrument Default</i> is selected
Batch Calibration fails in MS/MS mode	One or more fragment ions are not present, or weak in intensity	Increase the CDS Inject Flow Rate In the Reference table, uncheck the calibration ions that are low in intensity (3 or more calibration ions are recommended for achieving good calibration)
Batch fails to submit. Error message indicates one or more calibration reference ions are out of the mass range.	One or more calibration reference ions are out of the mass range in the acquisition method selected for the batch.	Edit the reference table to include only the ions that are within the mass range of the acquisition method.





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Printed in the USA, 12/2015

Part Number 4465917 Rev. C

RUO-IDV-09-3168A