Sample Purity and Accurate Mass Confirmation by LC-UV-MS
Report for ABC-123456

Instrumentation and parameters:

LC:	Agilent 1200 series
Colum:	Phenomenex Luna 3um C18, 100A, 50x2 mm
MS:	Agilent 6210A Time of Flight
Ionization Mode:	Dual ESI
Mass Calibration:	Both External and Internal
Aqueous Reservoir (A):	H2O, 0.1% formic acid
Organic Reservoir (B):	Acetonitrile, 0.1% formic acid
Temperature:	40 ^{o}C
Injection Volume:	5 µL
Sample Concentration:	5 ug/mL
UV Wave Length:	254 nm
Band width:	8nm

Gradient Information:

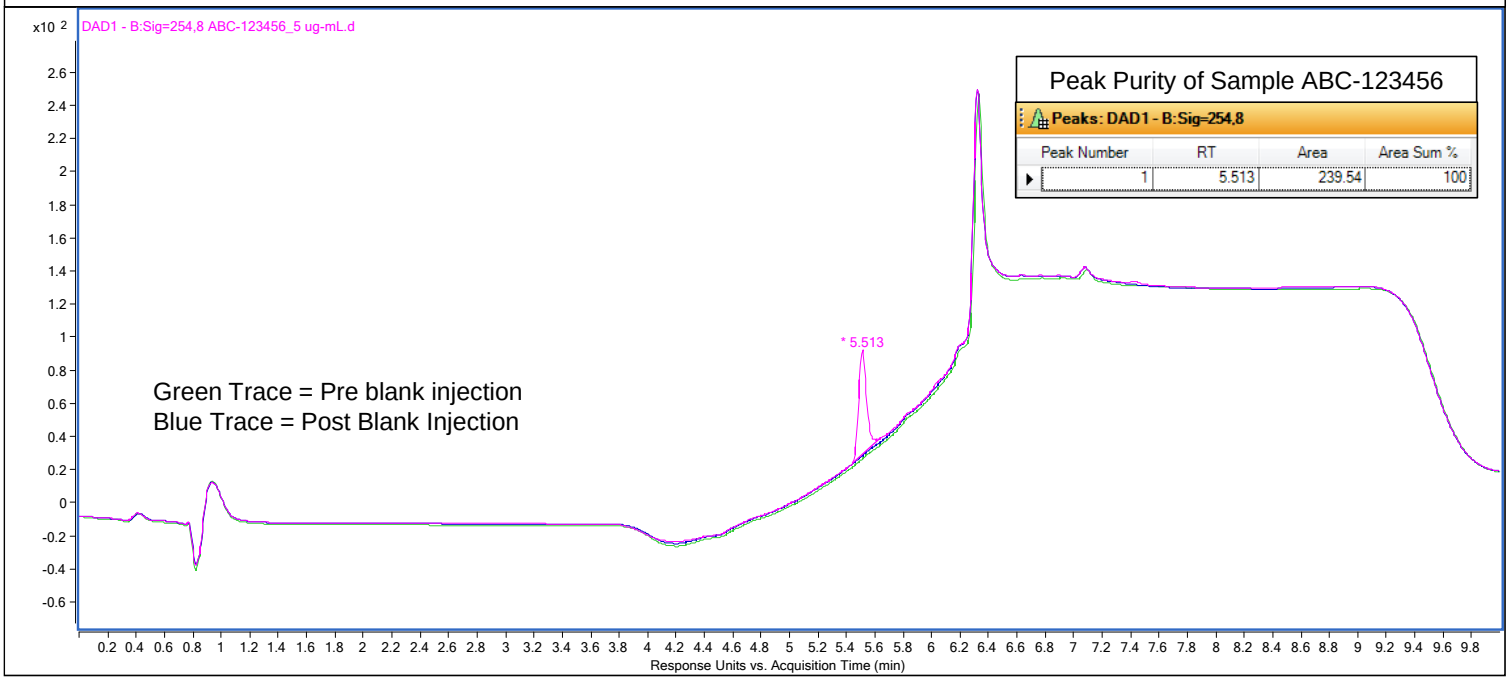
Time (min)	Flow Rate (uL/min)	%A	%B
0.0	250	100	0
1.0	250	100	0
4.0	250	10	90
7.0	250	10	90
7.1	250	100	0
9.9	250	100	0

UV Chromatogram: Sample and pre and post blank injections are in overlay mode. Integrated peaks are the unique peaks not common in blanks.

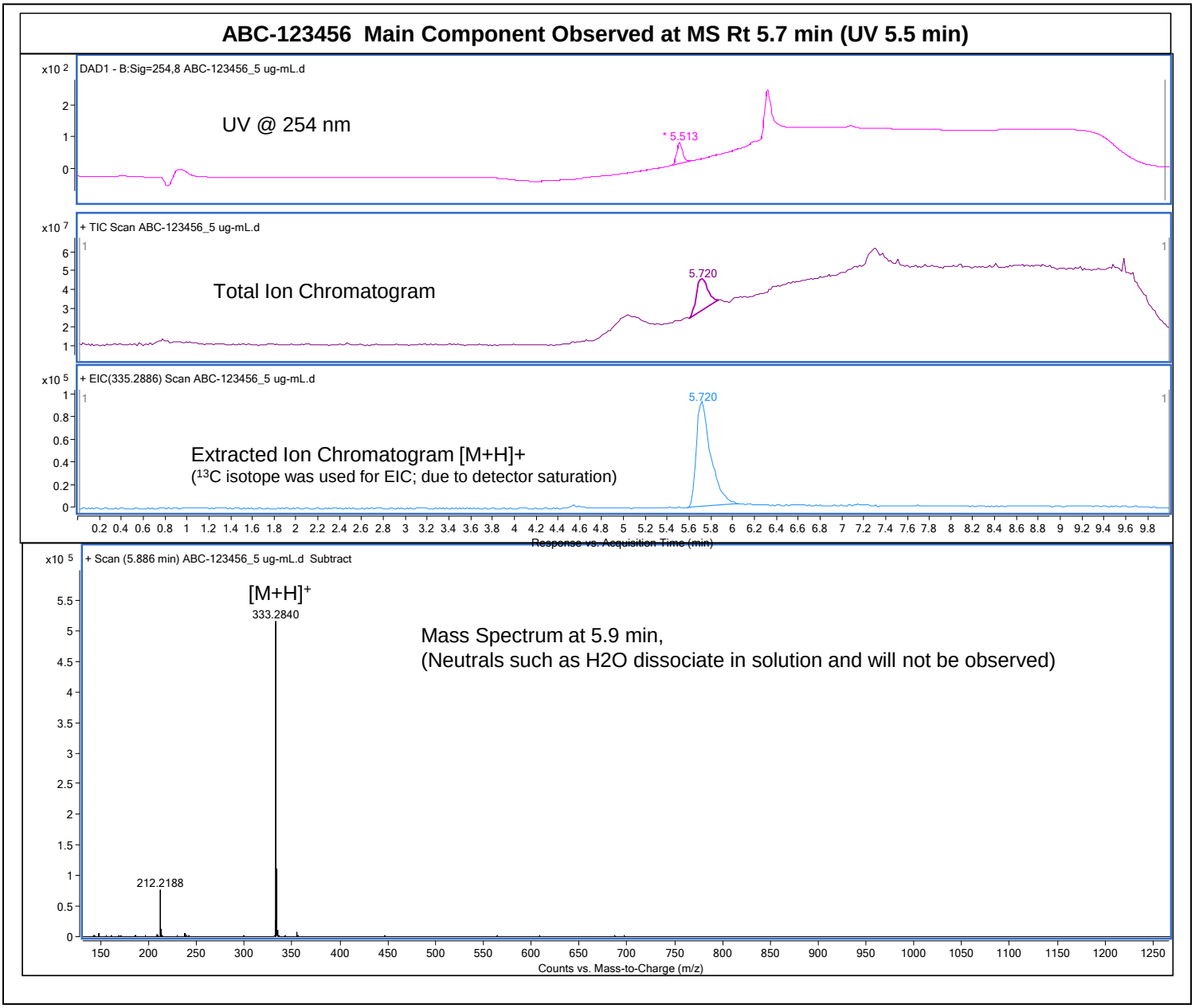
ABC-123456

Molecular Formula CxxHxxNxxOxxSxx, Expected Accurate Mass xxx.zzzz, Average Molecular Weight xxx.zzzz
(Neutral components, e.g. H2O, dissociate in solution and will not be observed in MS)

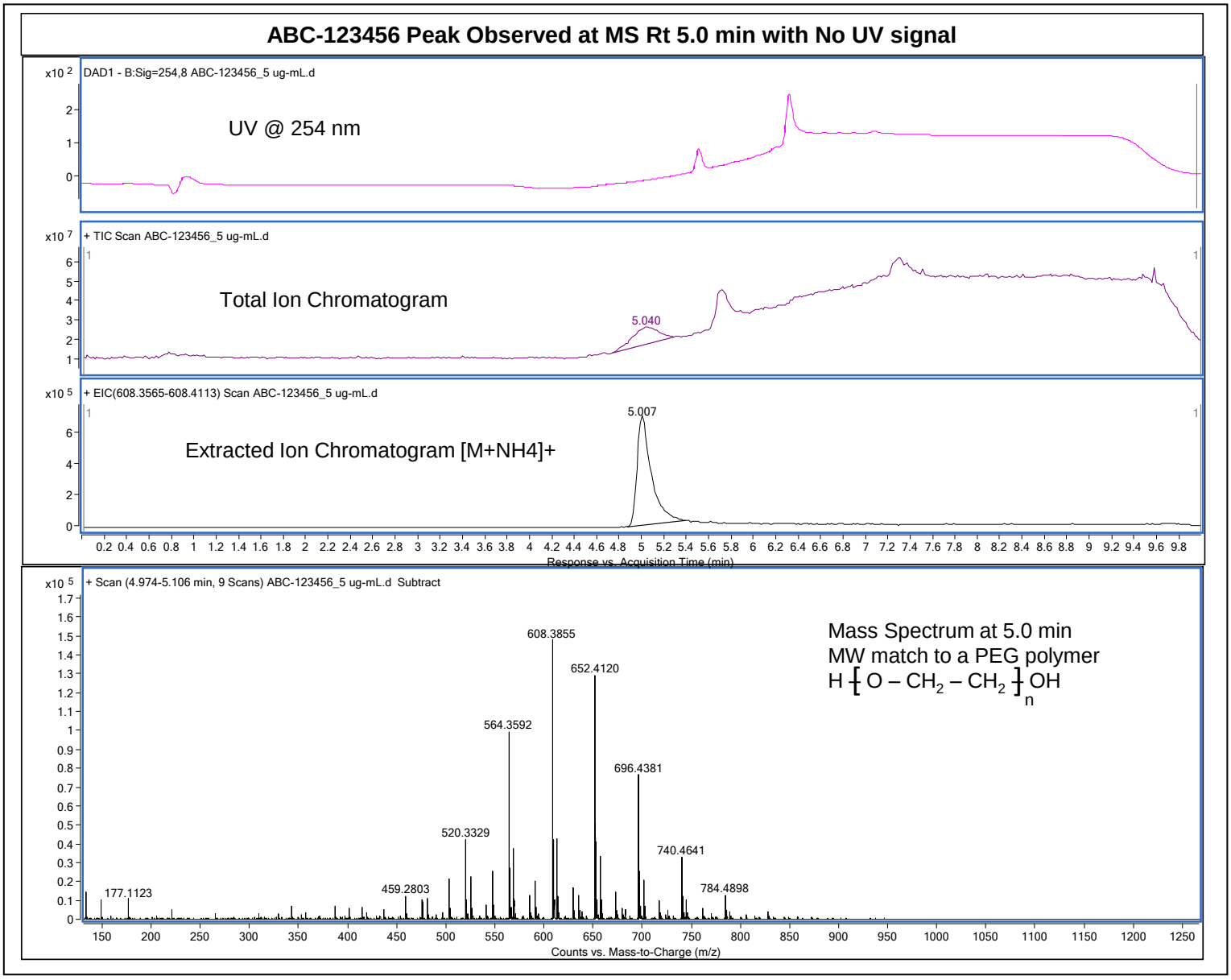
UV signal @ 254 nm overlay comparison: Test Sample, pre, and post blank injections
ABC-123456, UV retention time 5.5 min; Peaks common with blank injections are excluded.



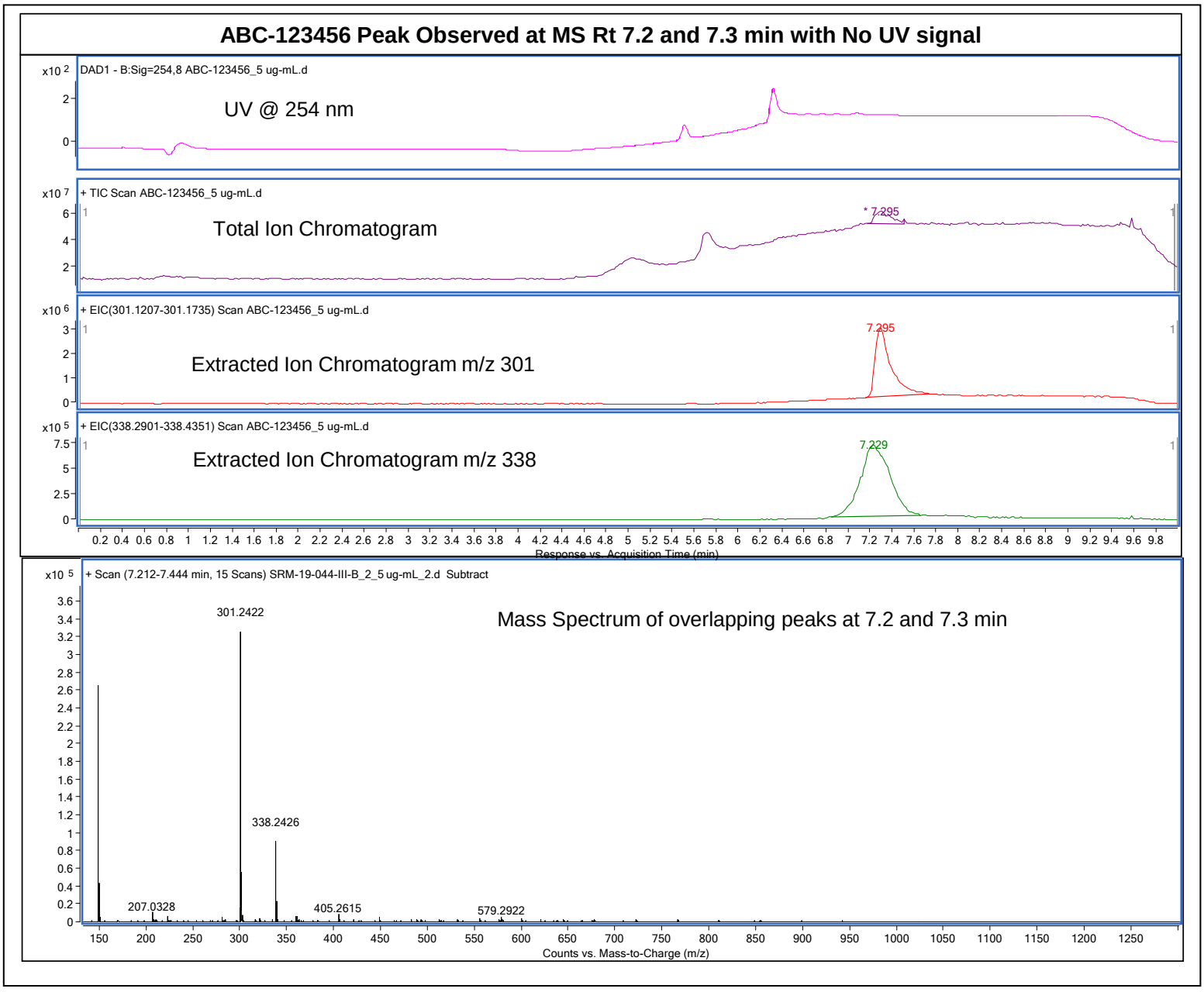
MS Ion Chromatogram and Spectra: Note retention time delay between UV and MS signal is 0.2 min



Potential Impurities: No impurity was observed by UV at 254 nm. The additional peaks observed in MS TIC, are present in the blank injections as well, but do not have a UV signature; they are reported here as an FYI.



Potential Impurities, Continued:



Results Summary and Comments: The mass analysis was performed in accurate mass mode with external calibration and constant infusion of reference ions for internal calibration. The accurate mass for [M+H]+ ion was measured at xxx.zzzz, expected value was xxx.zzzz, with an error of <0.0010 Da or 3.0 ppm. In-source fragmentation was also observed, as well as other adduct formation at high concentrations. Other peaks detected by mass spectrometry and common to blank (pre and post) and sample injections and were reported here as an FYI. The amount of compound injected on column was calculated to be 50 ng. Due to MS detector saturation, EIC and accurate mass measurements were obtained by either using a lower abundant isotope and/or a lower intense part of the chromatogram. The purity table is generated from the UV signal only and seems to be 100%.