



Report of targets per Run (Skyline)

2025-08-11

Contents

Intensity	2
Mass tolerance (ppm)	2
RT drift	3
Peak Shape Scores	4
QC Summary Table	6

File Processed:

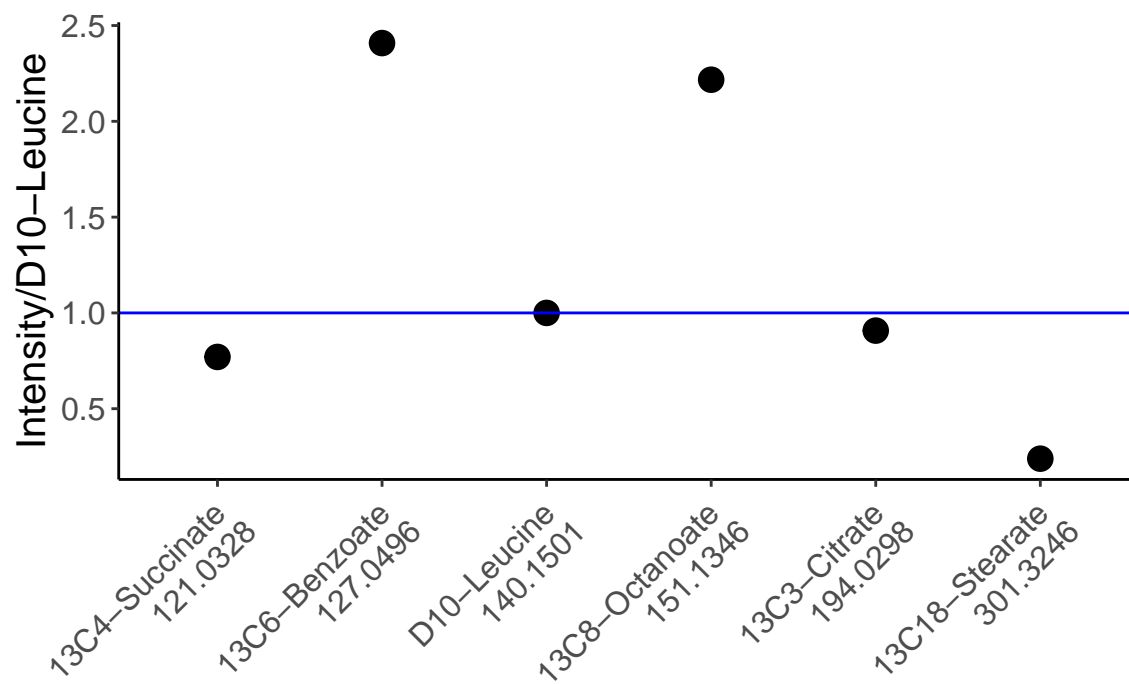
QC-2_Blank-3_20241212_A_EC_JM-Breath-2_04.d

Column Ionization:

ESI-

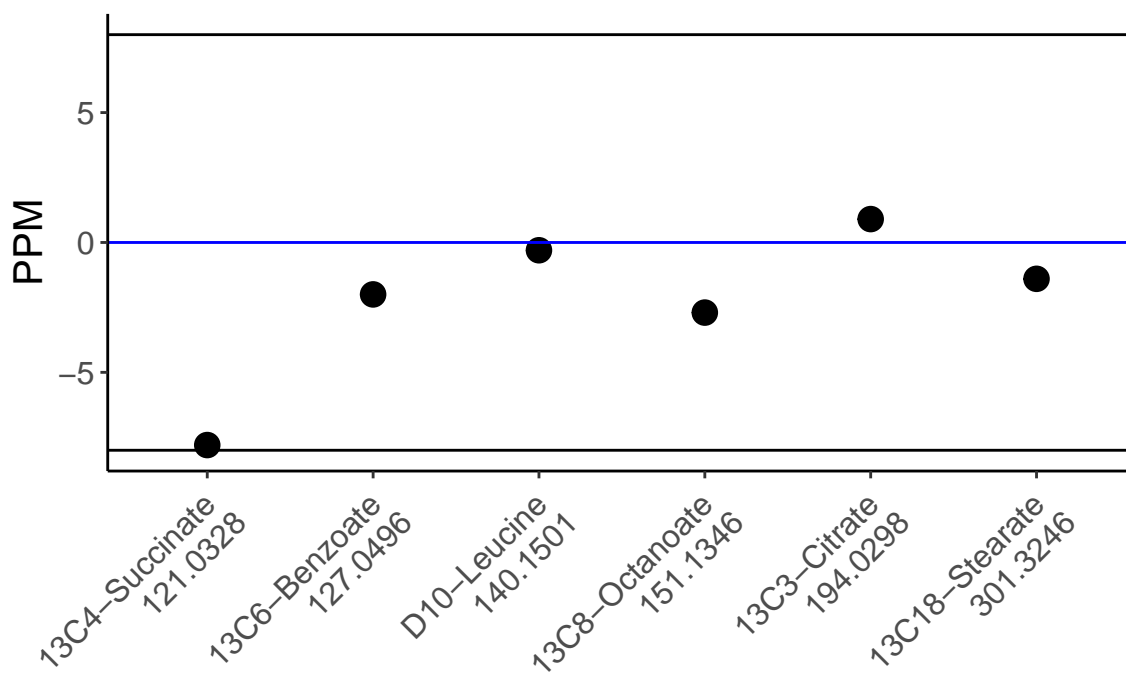
Intensity

Individual peak Intensity normalized to D10-Leucine peak intensity if D10-Leucine peak was measured.



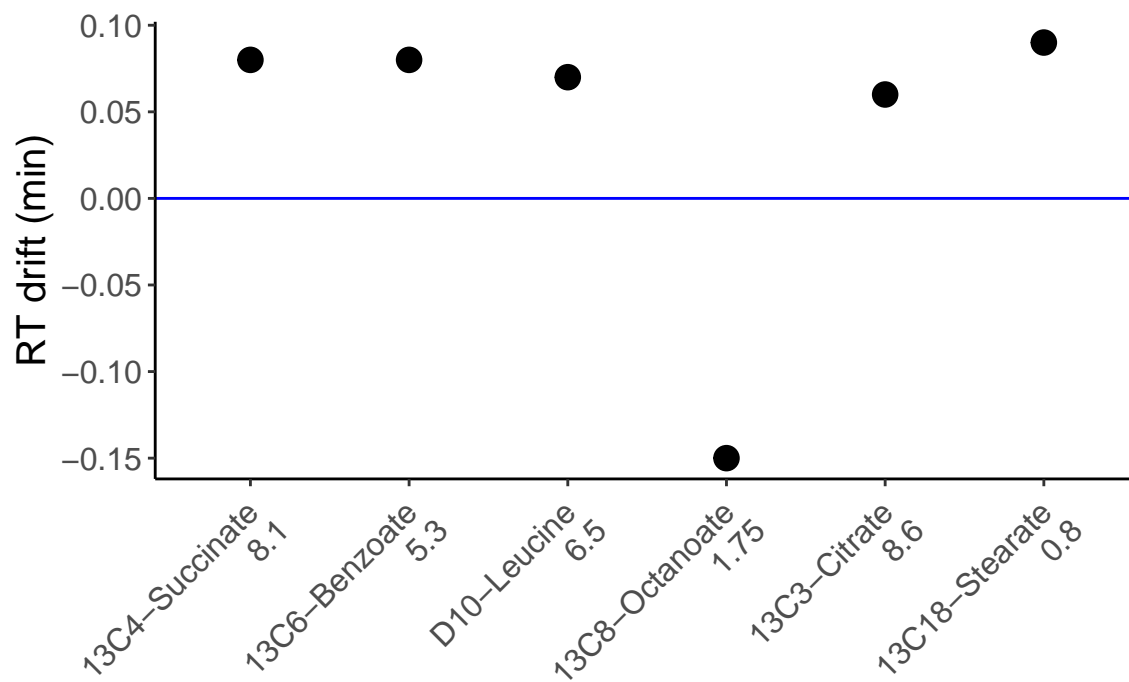
Mass tolerance (ppm)

Output provided as part of Skyline report.



RT drift

Peak Retention Time Drift calculated as (observed retention time - Expected retention time of compound)

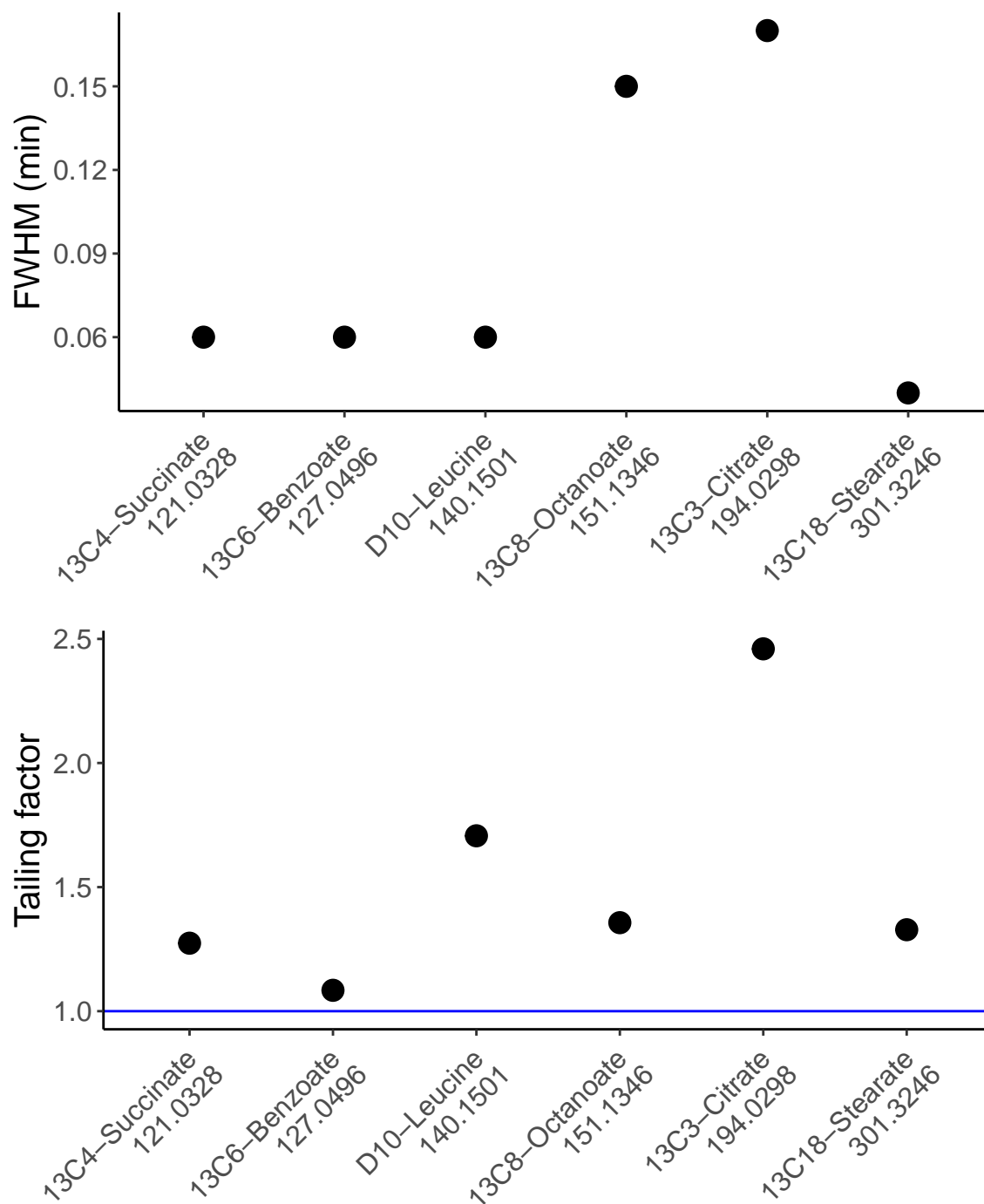


Peak Shape Scores

FWHM = width of peak in retention time space at 50% peak height (Output provided as part of Skyline report.)

Tailing factor = $(C+D)/2C$ (ideal = 1)

Asymmetry factor = B/A (ideal = 1)



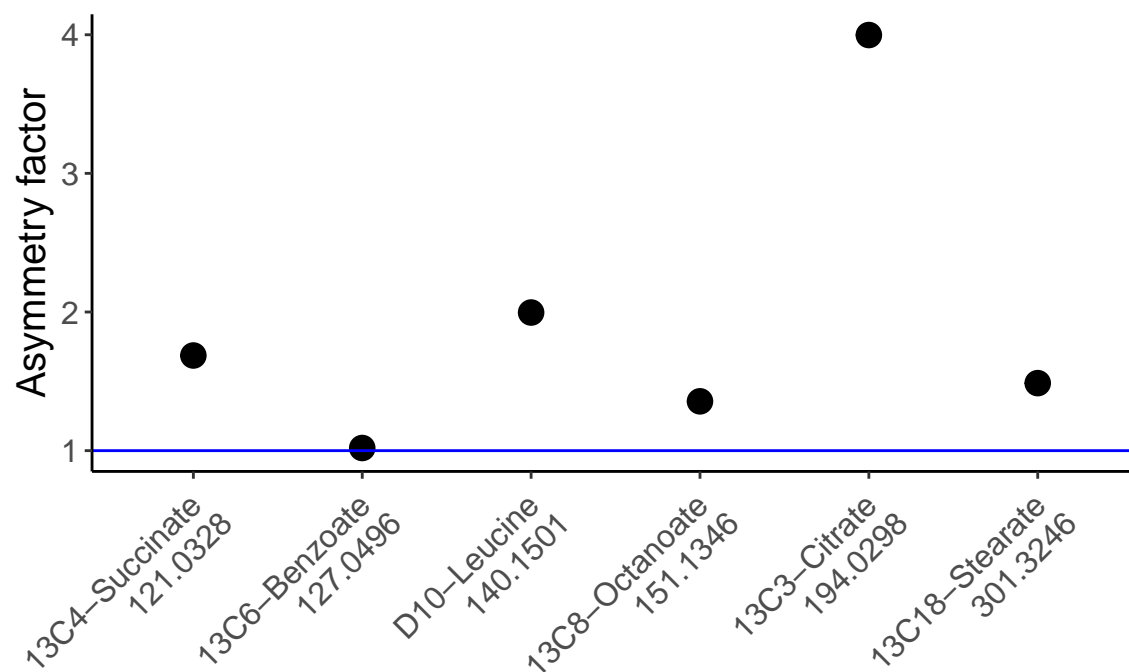


Table 1: QC Summary Table

Name	Molecular Formula	Expected RT	Expected m/z	Adduct	Ionization	Quench/Resuspension QC
13C3-Alanine	[13C]3H7NO2	5.80	91.0505	[M3C13-H]	ESI-	Quench QC
13C6-Leucine	[13C]6H13NO2	6.50	136.1075	[M6C13-H]	ESI-	Quench QC
13C6-Phenylalanine	C3[13C]6H11NO2	2.80	170.0918	[M6C13-H]	ESI-	Quench QC
13C6-Tyrosine	C3[13C]6H11NO3	4.80	186.0867	[M6C13-H]	ESI-	Quench QC
13C11-Tryptophan	[13C]11H12N2O2	3.50	214.1195	[M11C13-H]	ESI-	Quench QC
13C4-Succinate	[13C]4H6O4	8.10	121.0328	[M4C13-H]	ESI-	Resuspension QC
13C6-Benzoate	C[13C]6H6O2	5.30	127.0496	[M6C13-H]	ESI-	Resuspension QC
D10-Leucine	C6H3D10NO2	6.50	140.1501	[M10D-H]	ESI-	Resuspension QC
13C8-Octanoate	[13C]8H16O2	1.75	151.1346	[M8C13-H]	ESI-	Resuspension QC
13C3-Citrate	C3[13C]3H8O7	8.60	194.0298	[M3C13-H]	ESI-	Resuspension QC
13C18-Stearate	[13C]18H36O2	0.80	301.3246	[M18C13-H]	ESI-	Resuspension QC
13C6-Sucrose	C6[13C]6H22O11	7.40	347.1291	[M6C13-H]	ESI-	Resuspension QC

QC Summary Table

Targets that were not detected in samples.