



Report of targets per Run (Skyline)

2025-07-31

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File Processed:

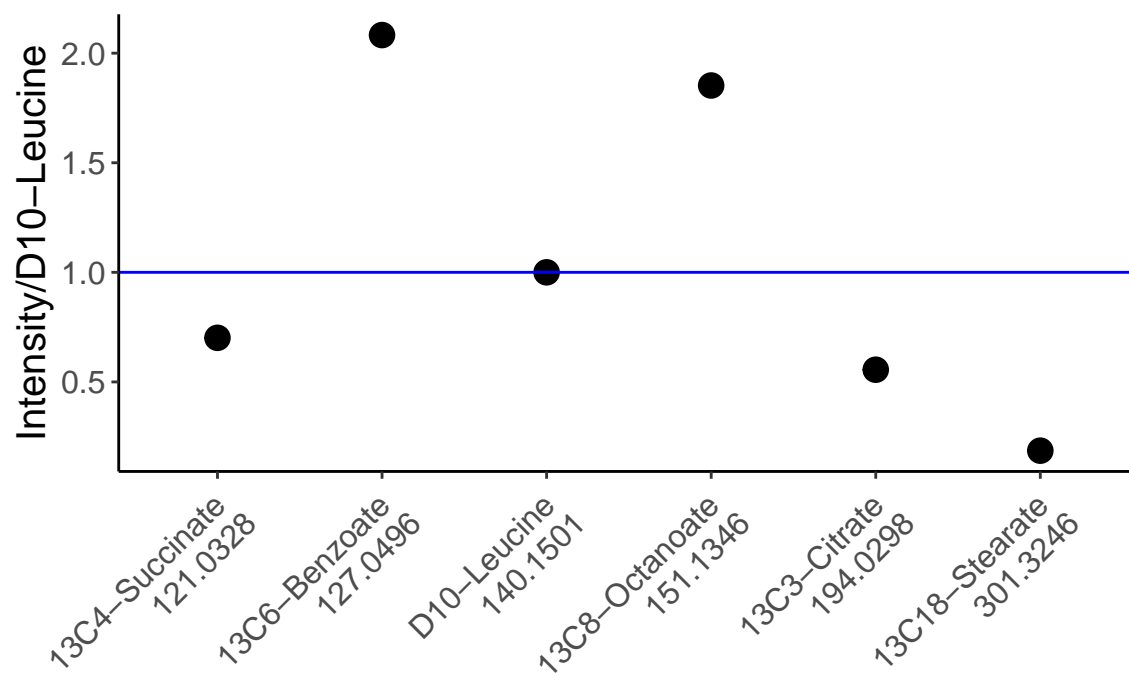
QC-2_Blank-1_20241212_A_EC_JM-Breath-2_02.d

Column Ionization:

ESI-

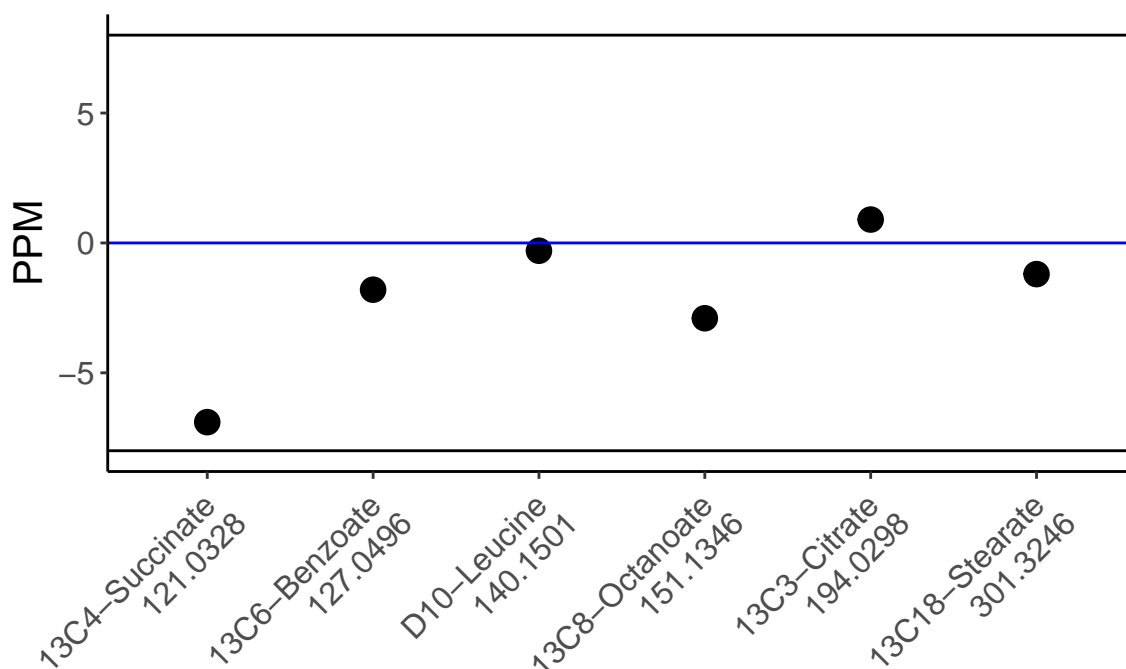
Intensity

Individual peak Intensity normalized to D10-Leucine peak intensity.



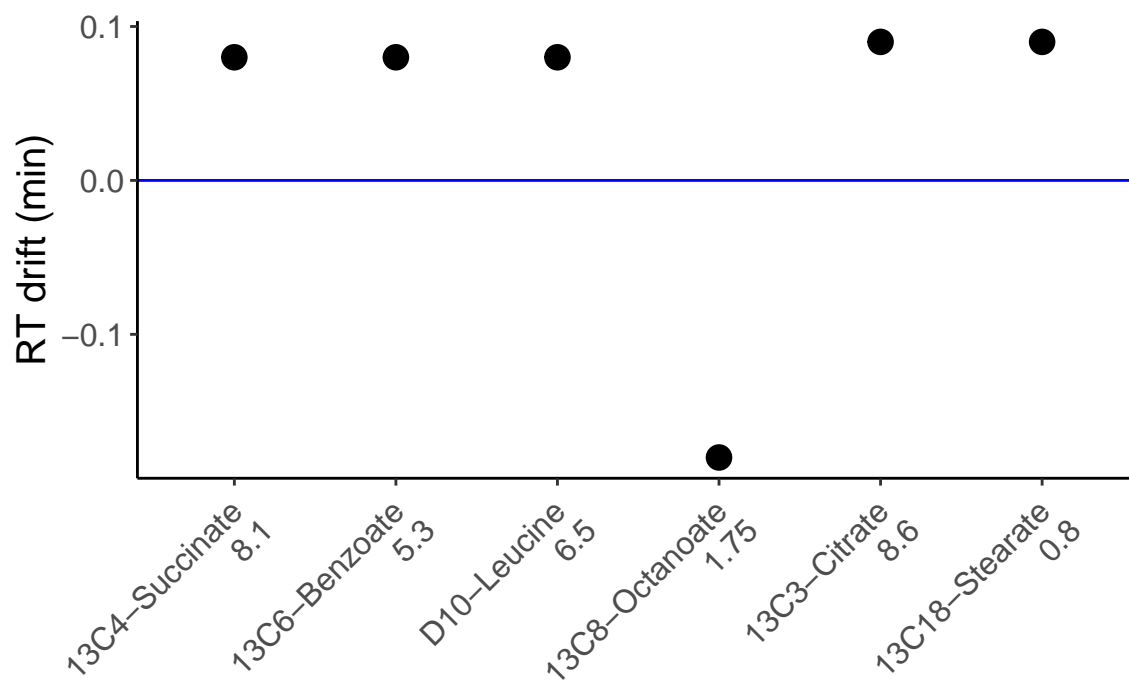
Mass tolerance (ppm)

Mass tolerance (ppm) = ((Theoretical m/z - Observed m/z)/Theoretical m/z)*1E+6



RT drift

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

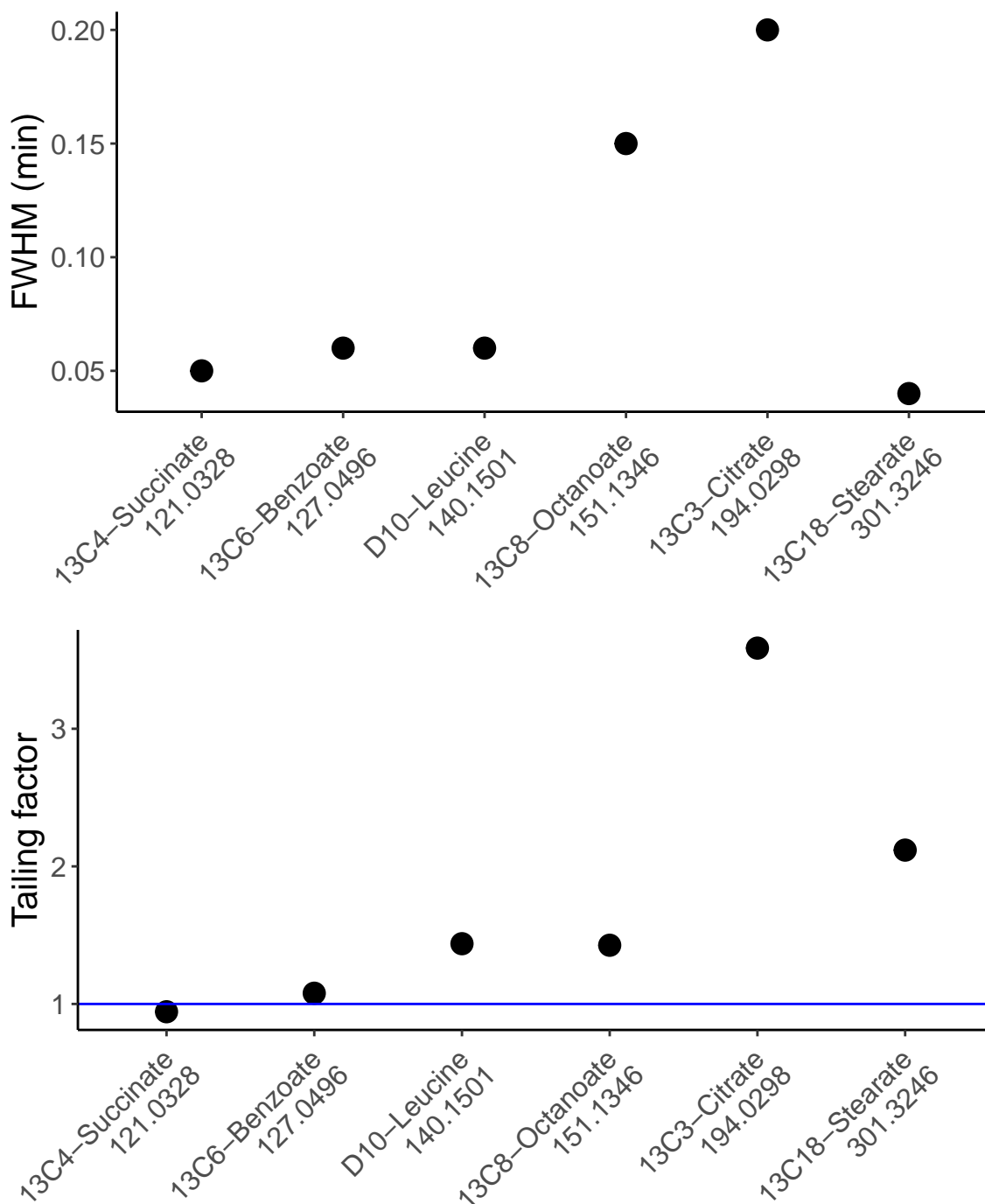


Peak Shape Scores

FWHM = width of peak in retention time space at 50% peak height

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

Asymmetry factor = B/A (ideal = 1)



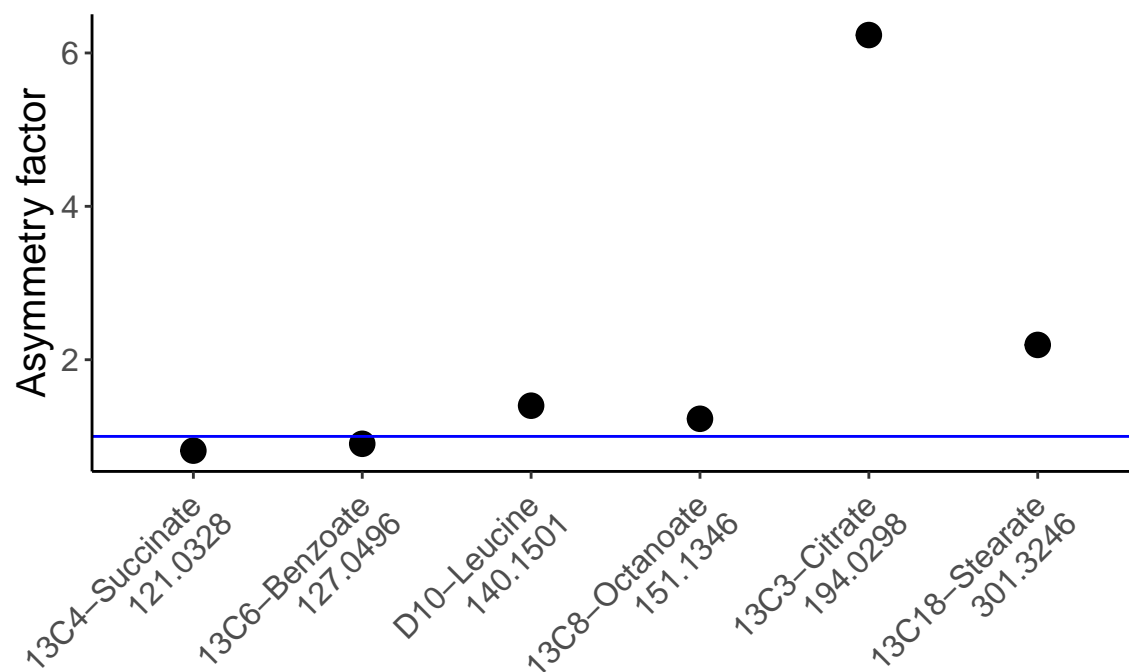


Table 1: QC Summary Table

| 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 |

QC Summary Table

Targets that were not detected in samples.