



## Report of targets per Run (Skyline)

2025-07-31

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### File Processed:

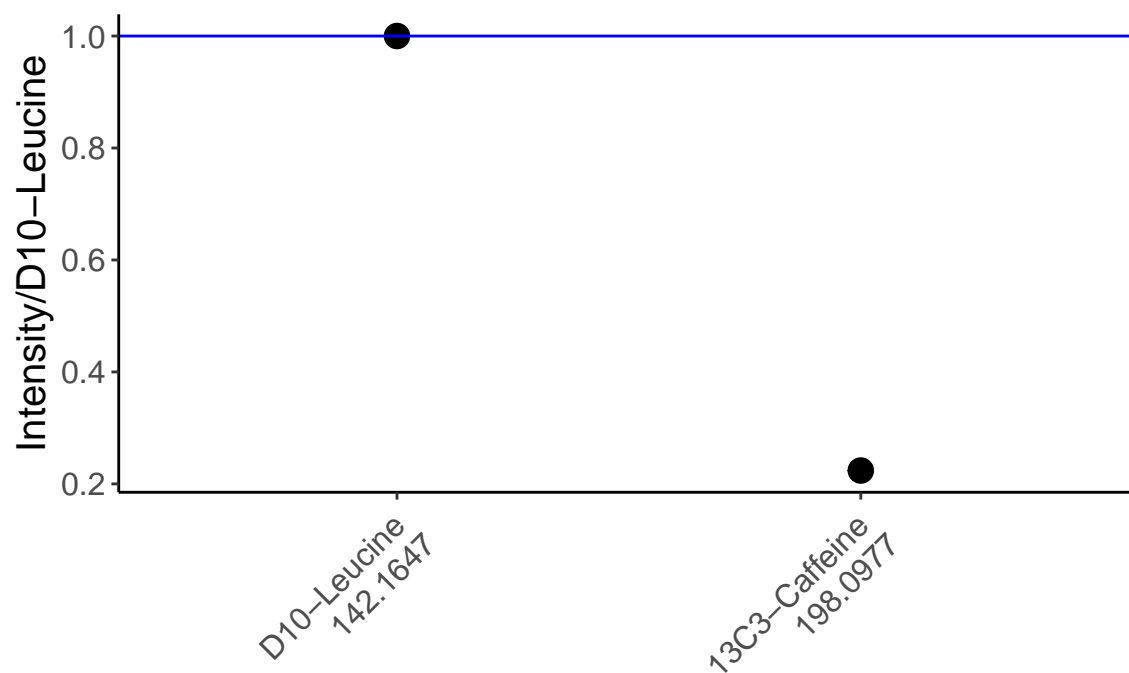
QC-2\_Blank-2\_Pos\_20241212\_A\_EC\_JM-Breath-2\_23.d

### Column Ionization:

ESI+

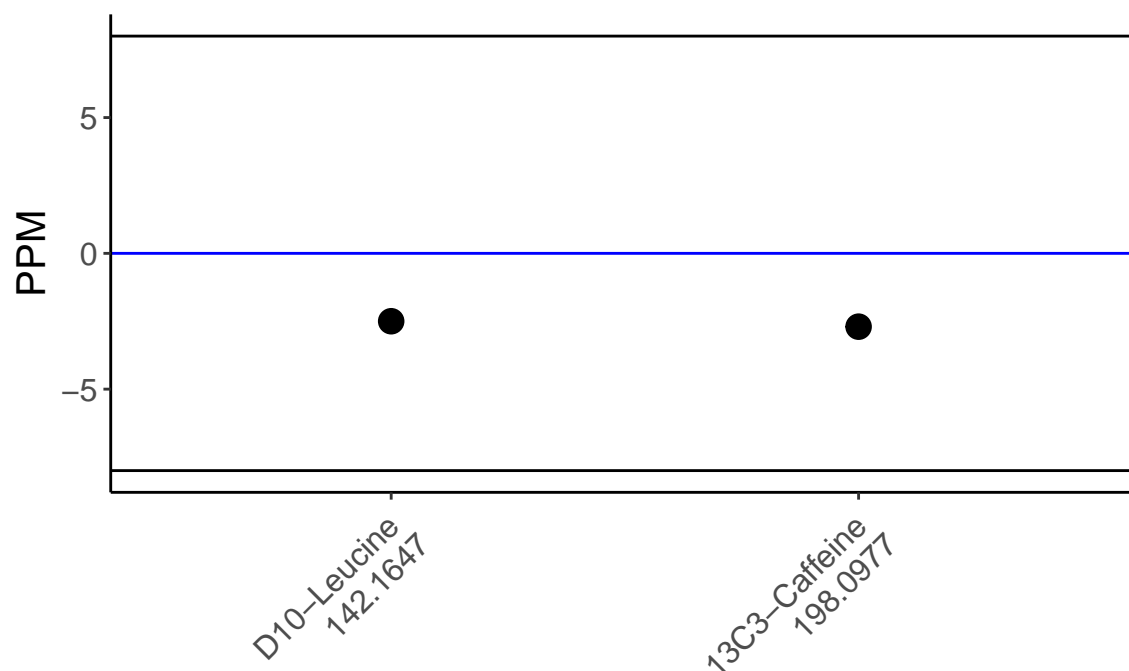
## Intensity

Individual peak Intensity normalized to D10-Leucine peak intensity.



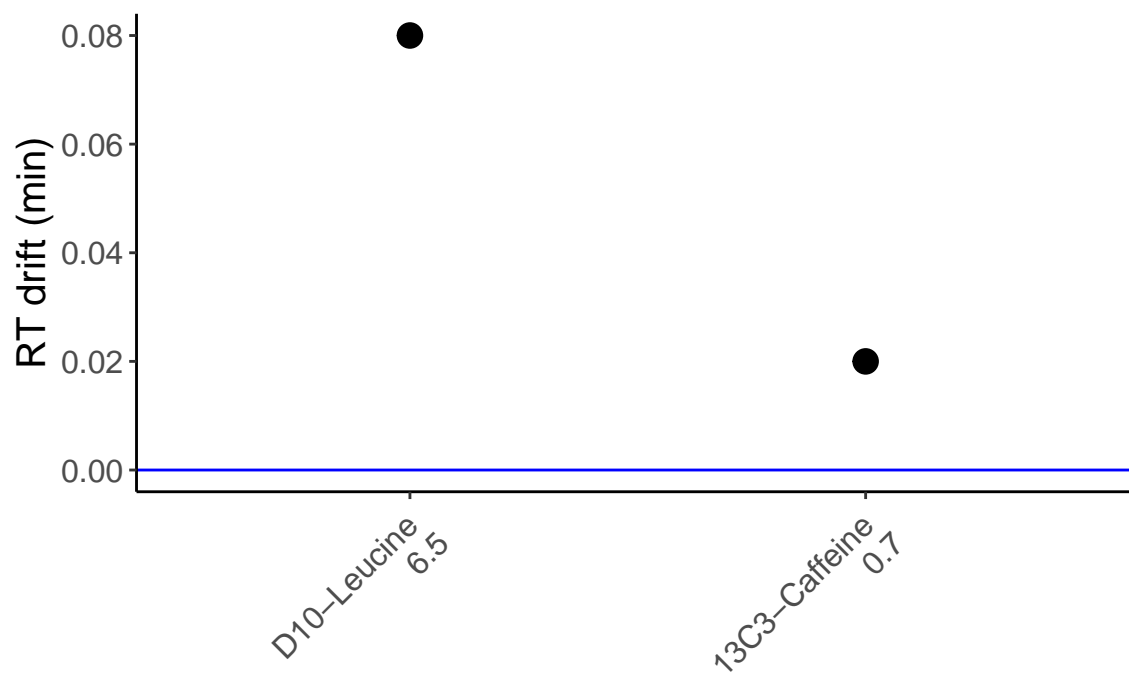
## Mass tolerance (ppm)

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)

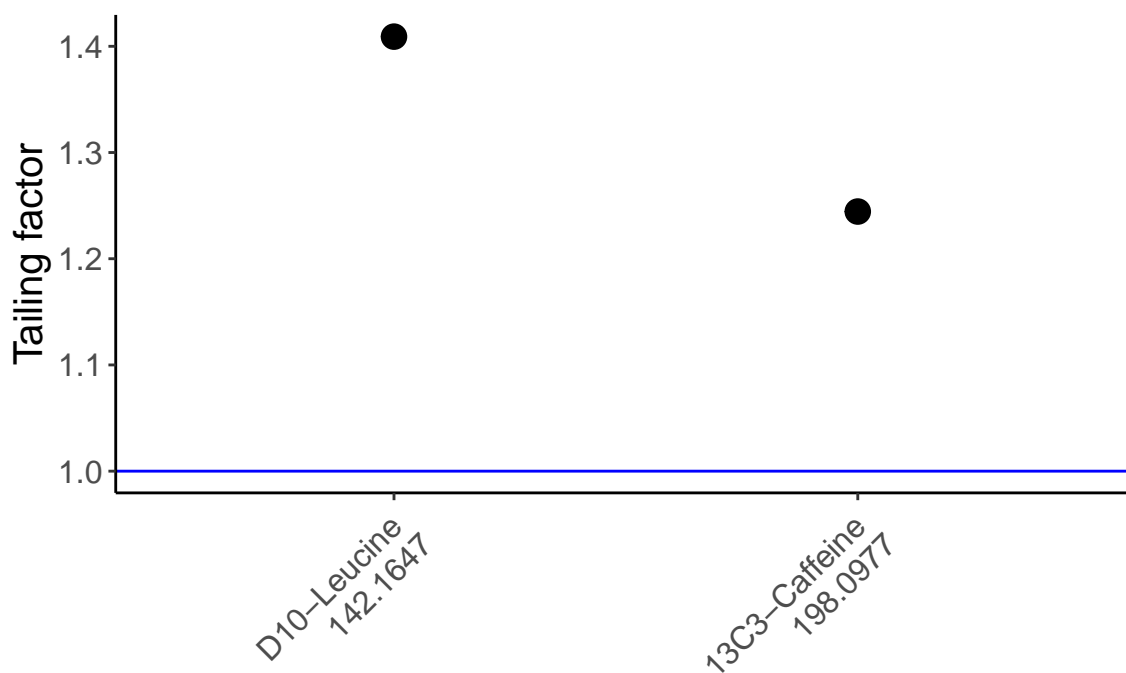
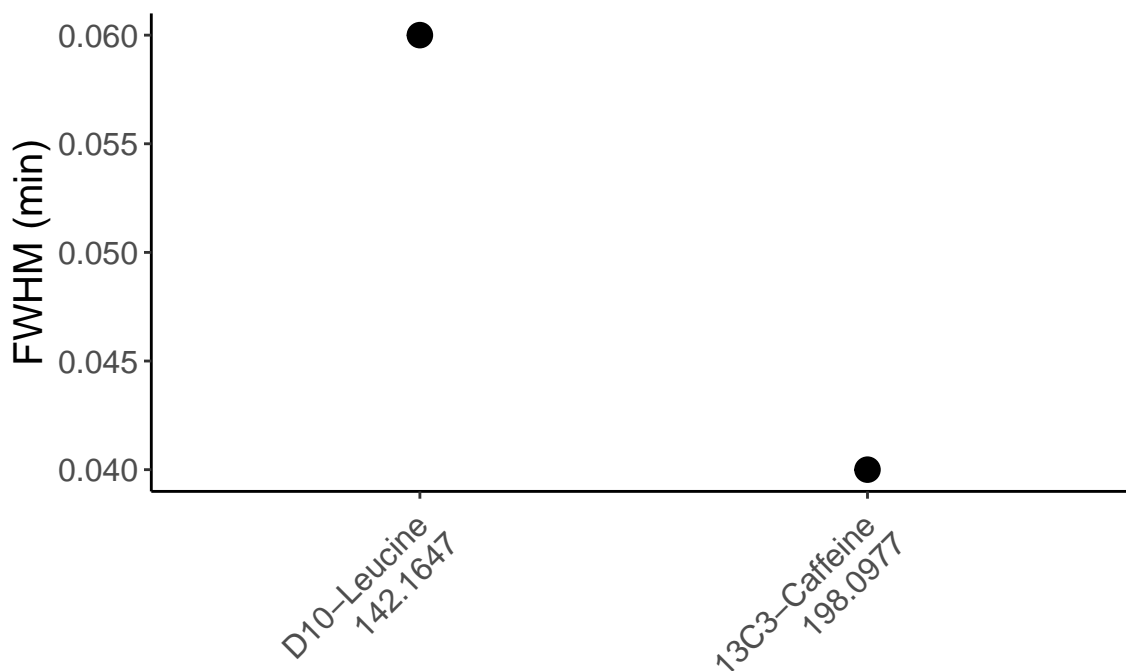


## Peak Shape Scores

**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)



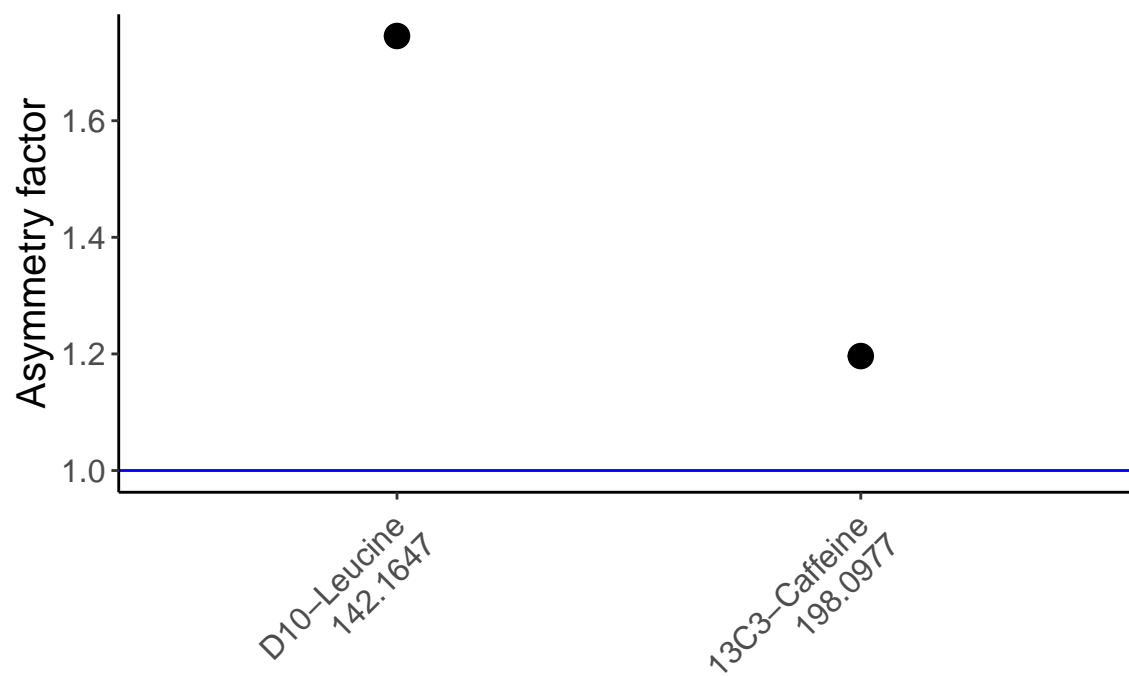


Table 1: QC Summary Table

Name	Molecular Formula	Expected RT	Expected m/z	Adduct	Ionization	Quench/Resuspension QC
13C3-Alanine	[13C]3H7NO2	5.8	93.0650	[M3C13+H]	ESI+	Quench QC
13C6-Leucine	[13C]6H13NO2	6.5	138.1220	[M6C13+H]	ESI+	Quench QC
13C6-Phenylalanine	C3[13C]6H11NO2	2.8	172.1064	[M6C13+H]	ESI+	Quench QC
13C6-Tyrosine	C3[13C]6H11NO3	4.8	188.1013	[M6C13+H]	ESI+	Quench QC
13C11-Tryptophan	[13C]11H12N2O2	3.5	216.1341	[M11C13+H]	ESI+	Quench QC
D10-Leucine	C6H3D10NO2	6.5	142.1647	[M10D+H]	ESI+	Resuspension QC
13C3-Caffeine	C5[13C]3H10N4O2	0.7	198.0977	[M3C13+H]	ESI+	Resuspension QC

## QC Summary Table

Targets that were not detected in samples.