Report of targets per Run (Skyline)

2025-07-08

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File Processed:

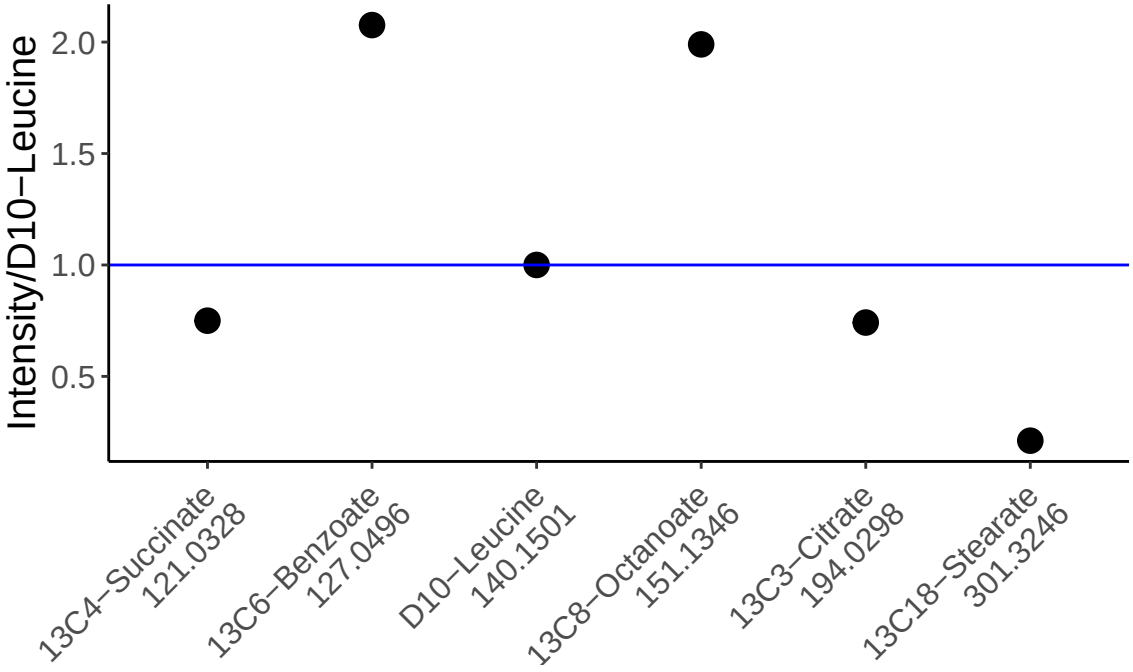
QC-2_Blank-2_20241212_A_EC_JM-Breath-2_03.d

Column Ionization:

Hilic -ESI

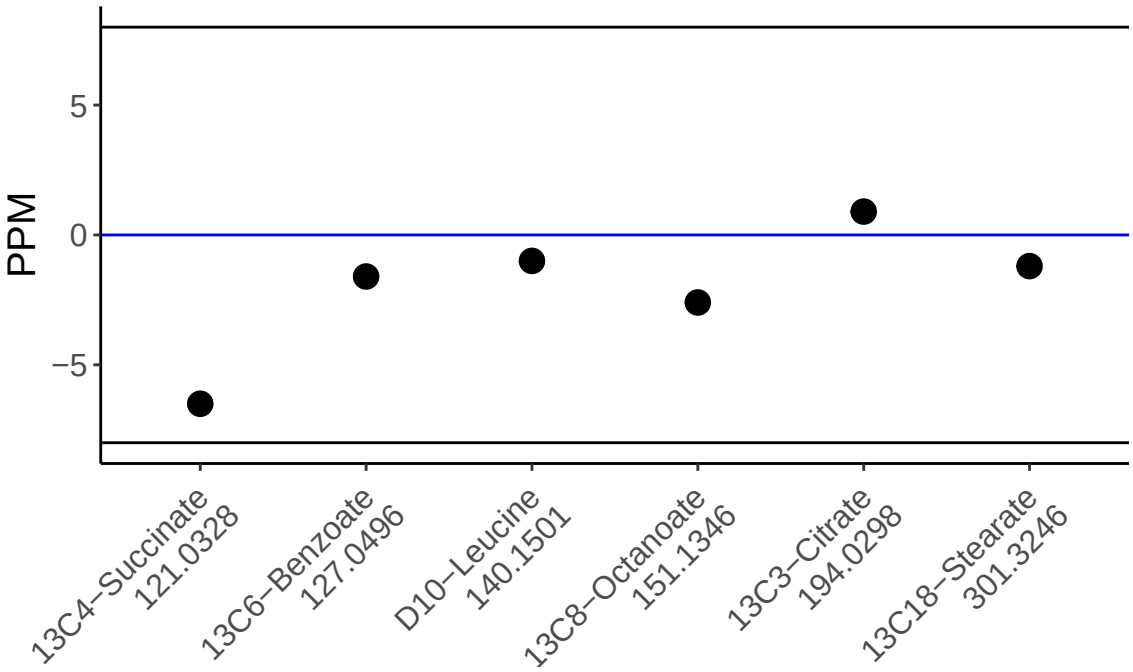
Intensity

Individual peak Intensity normalized to D10-Leucine peak intensity.



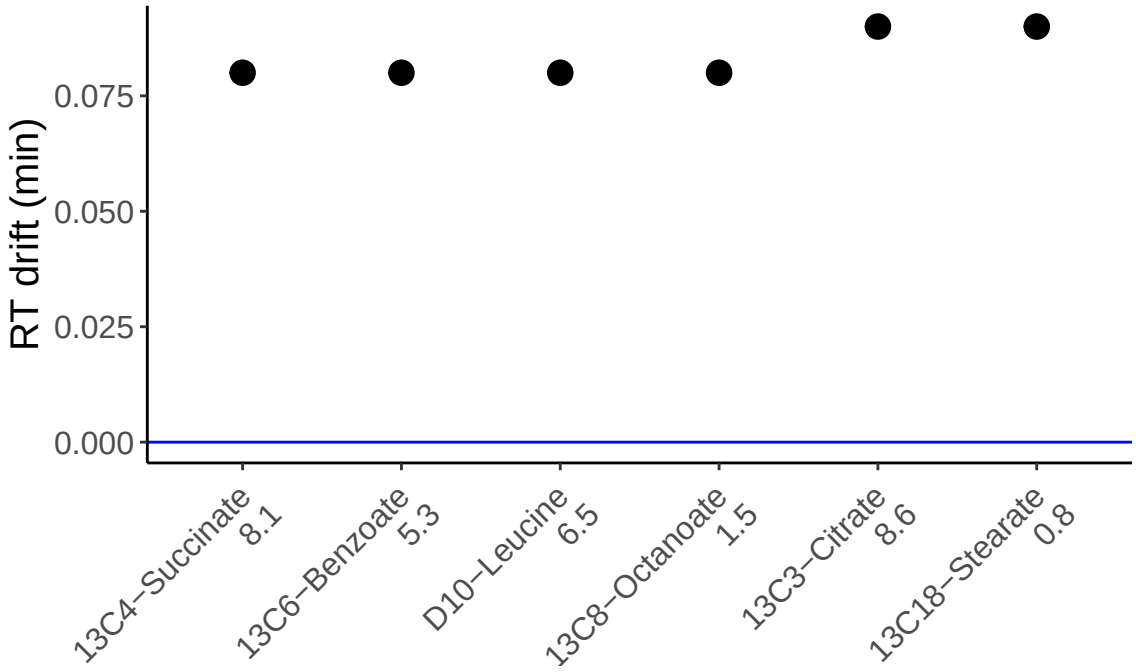
Mass tolerance (ppm)

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)

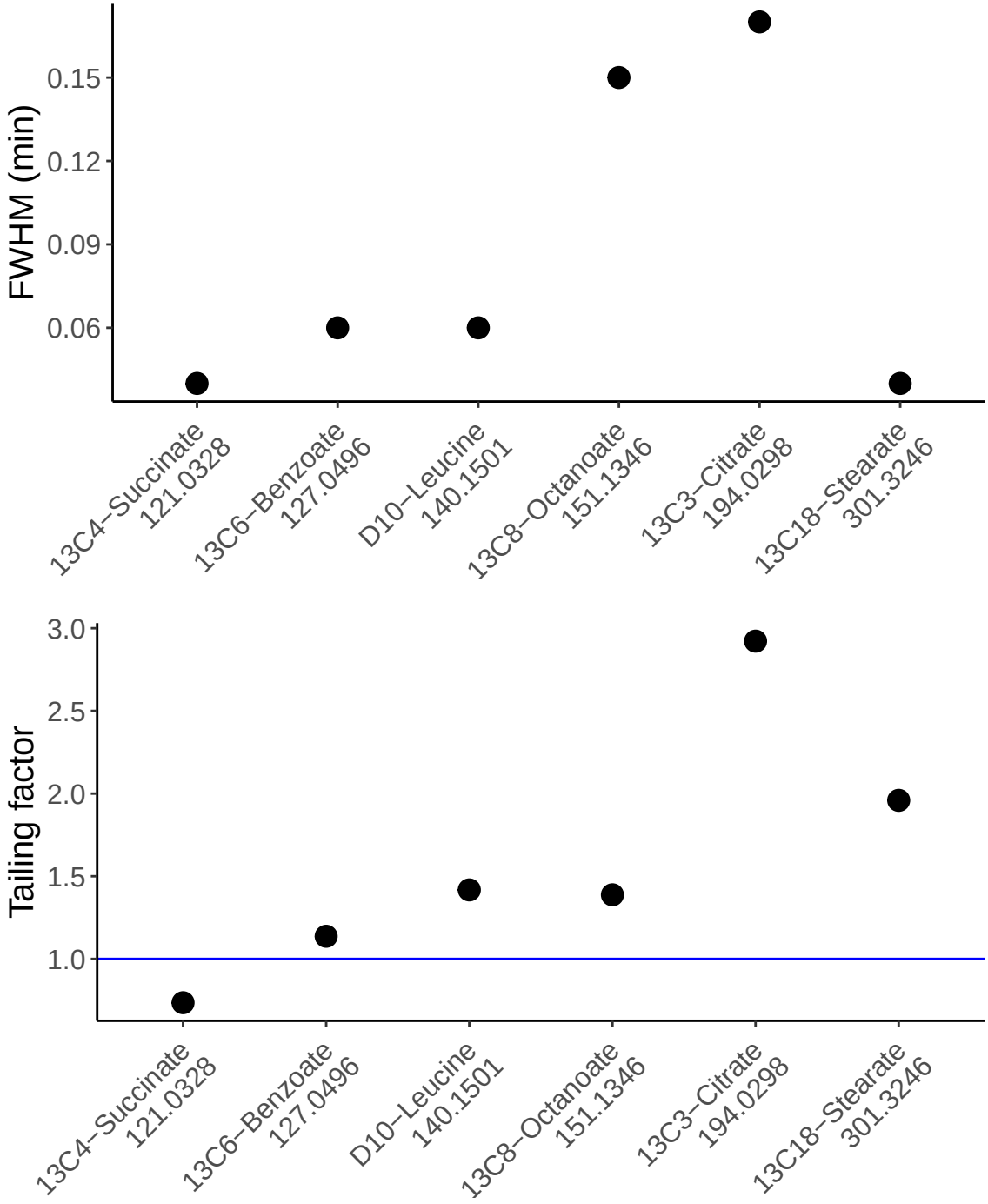


Peak Shape Scores

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)



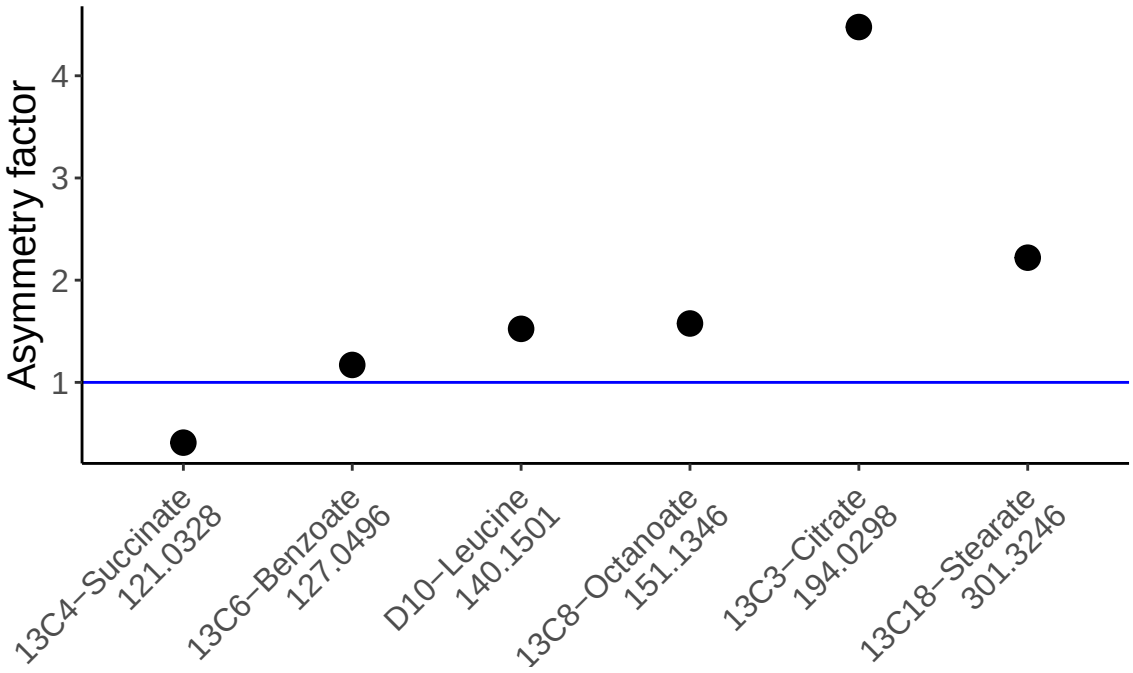

Asymmetry factor
4
3
2
1
13C4−Succinate 121.0328
13C6−Benzoate 127.0496
D10−Leucine 140.1501
13C8−Octanoate 151.1346
13C3−Citrate 194.0298
13C18−Stearate 301.3246

Table 1: QC Summary Table

Name	Formula	Expected RT	Expected m/z	Adduct	LC	Quench/Resuspension QC
13C3-Alanine	C3H7NO2	5.8	91.0505	[M3C13-H]	Hilic -ESI	Quench QC
13C6-Leucine	C6H13NO2	6.5	136.1075	[M6C13-H]	Hilic -ESI	Quench QC
13C6-Phenylalanine	C9H11NO2	2.8	170.0918	[M6C13-H]	Hilic -ESI	Quench QC
13C6-Tyrosine	C9H11NO3	4.8	186.0867	[M6C13-H]	Hilic -ESI	Quench QC
13C11-Tryptophan	C11H12N2O2	3.5	214.1195	[M11C13-H]	Hilic -ESI	Quench QC
13C4-Succinate	C4H6O4	8.1	121.0328	[M4C13-H]	Hilic -ESI	Resuspension QC
13C6-Benzoate	C7H6O2	5.3	127.0496	[M6C13-H]	Hilic -ESI	Resuspension QC
D10-Leucine	C6H13NO2	6.5	140.1501	[M10D-H]	Hilic -ESI	Resuspension QC
13C8-Octanoate	C8H16O2	1.5	151.1346	[M8C13-H]	Hilic -ESI	Resuspension QC
13C3-Citrate	C6H8O7	8.6	194.0298	[M3C13-H]	Hilic -ESI	Resuspension QC
13C18-Stearate	C18H36O2	0.8	301.3246	[M18C13-H]	Hilic -ESI	Resuspension QC
13C6-Sucrose	C12H22O11	5.8	347.1291	[M6C13-H]	Hilic -ESI	Resuspension QC

QC Summary Table

Targets that were not detected in samples.