

DDA & variable SWATH comparison with Plasma samples

Work from 2021-03
Composed 2022-01-31

1

Instrument Conditions

- Exion UHPLC + 5600 QToF
 - ESI - Positive mode only
 - 10, 5, and 2 μ l conditions tested
 - Variable SWATH windows (see next page for conditions)
- HPLC conditions
 - Phenomenex Luna Omega Polar C18 2.6 μ M 100 x 2.1 mm @ 50°C
 - Mobile phase A) 0.1% FA B) MeCN 0.1% FA
 - Gradient 5 – 100%
 - 10 min/injection

2

Variable Windows

- Generated using DDA MS1 density information plus SCIEX Excel Calculator
- 30 targeted windows
- 50 – 900 m/z
- 1 Da overlap
- 3 Da window width
- 15 Collision Energy Spread
- Needs refining

SWATH Variable Window Assay Controls

Target number of windows: (actual # may be less depending on min window width setting)

Lower m/z limit: (max 1250 for TripleTOF 5600+, max 2250 for TripleTOF 6600)

Upper m/z limit:

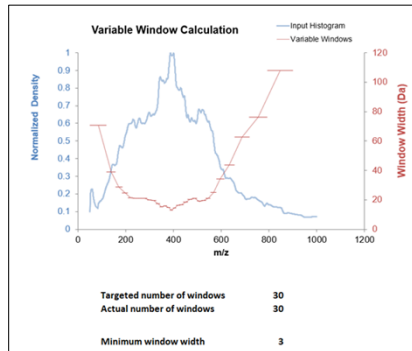
Round bin edges to x figures: (1 figure past decimal recommended)

Window overlap (Da): (1 Da overlap recommended)

Minimum window width (Da):

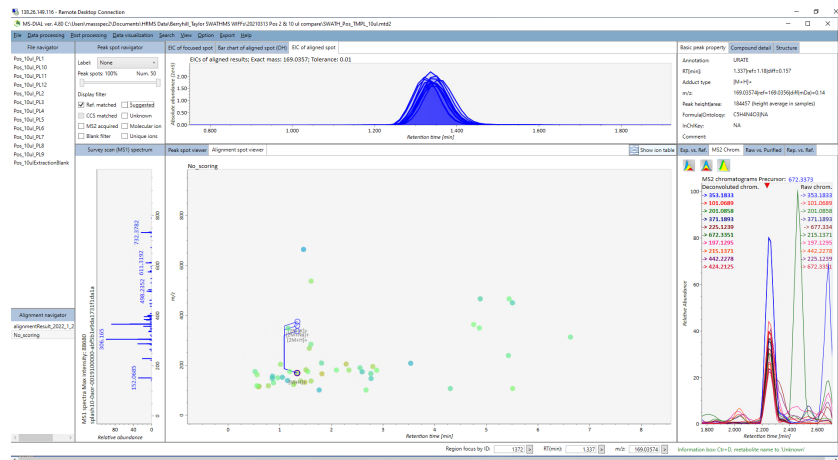
CES:

49.5	120.3
119.3	158.3
157.3	185.9
184.9	209.6
208.6	230
229	250
249	269.9
268.9	289.9
288.9	308.9
307.9	327.4
326.4	343.6
342.6	357.8
356.8	372.6
371.6	386.3
385.3	398.2
397.2	411.5
410.5	426.7
425.7	442.4
441.4	460
459	479.4
478.4	499.4
498.4	517.4
516.4	536
535	555.9
554.9	580.1
579.1	613.4
612.4	656.1
655.1	717.9
716.9	792.9
791.9	898.8



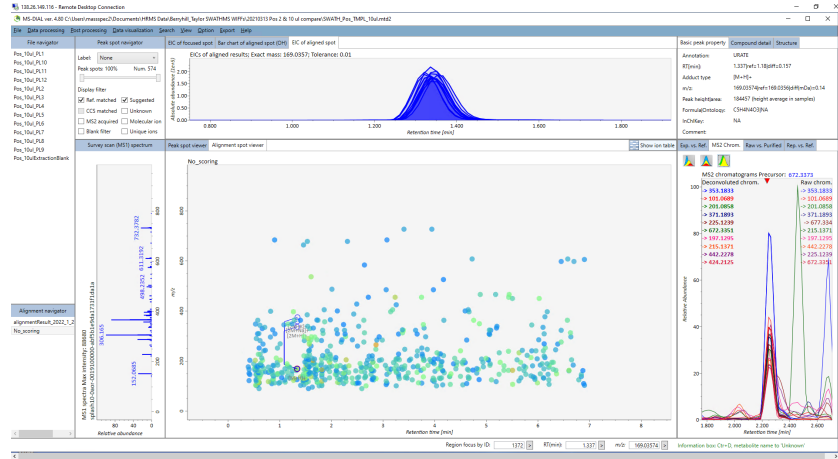
3

vSWATH – TMPL Lib – ref matched



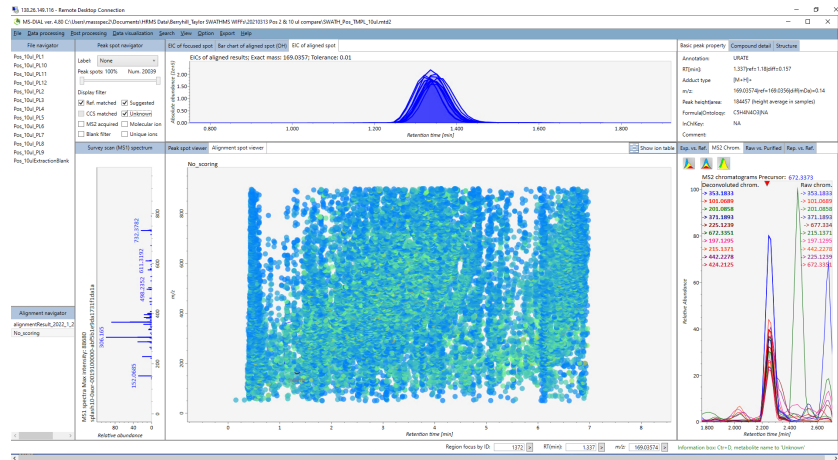
4

vSWATH – TMPL Lib – ref matched + suggested



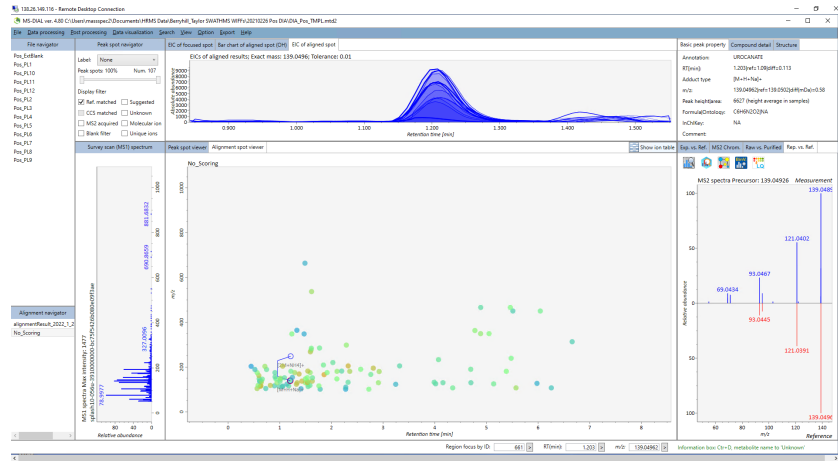
5

vSWATH – TMPL Lib – ref matched + suggested + unknown



6

DDA – TMPL Lib – Ref matched



7

DDA – TMPL Lib – Ref matched + Suggested



8

DDA – TMPL Lib – Ref matched + Suggested + Unknown

