

Another example. Heavy Arginine (arginine\_13C6,15N4) in sample '\_10' is not picked correctly though it is marked with grey dotted lines. Slide 2 shows



Sample '\_11' (or any other samples) are ok picked

The screenshot displays the Skyline software interface with several panels and a dialog box. The 'Targets' panel on the left lists various samples, with 'MS206430QEM\_frederick\_birsoy\_11' selected. A 'Replicates' dialog box is open, showing a list of replicates and a table with columns for 'Replicate', 'Current Size', and 'Minimized Size'. The 'Retention Times - Replicate Comparison' panel shows a bar chart of retention times for two arginine samples across multiple replicates. The 'Peak Areas - Replicate Comparison' panel shows a bar chart of peak areas for the same samples. The bottom panel displays a mass spectrum plot of 'Intensity (10<sup>6</sup>)' vs 'Retention Time' with a peak at 19.2 minutes and a label '19.4 -0.1 ppm'. The Windows taskbar at the bottom shows the time as 9:27 AM on 12/18/2020.

**Replicates Table:**

| Replicate               | Current Size | Minimized Size |
|-------------------------|--------------|----------------|
| MS206430QEM_frederic... | 9.62 MB      | 30%            |
| MS206430QEM_frederic... | 9.61 MB      | 30%            |
| MS206430QEM_frederic... | 9.65 MB      | 30%            |
| MS206430QEM_frederic... | 9.66 MB      | 30%            |
| MS206430QEM_frederic... | 9.64 MB      | 30%            |
| MS206430QEM_frederic... | 9.61 MB      | 30%            |
| MS206430QEM_frederic... | 9.64 MB      | 30%            |

'User Set Peak' are ALL false

Test:

A) Did Re-score. No Difference

B) 'Minimize in place' followed by 're-score in place'. Did not change anything (still dotted grey)

I have uploaded 2 examples: #10 (problematic) and #11 (ok).