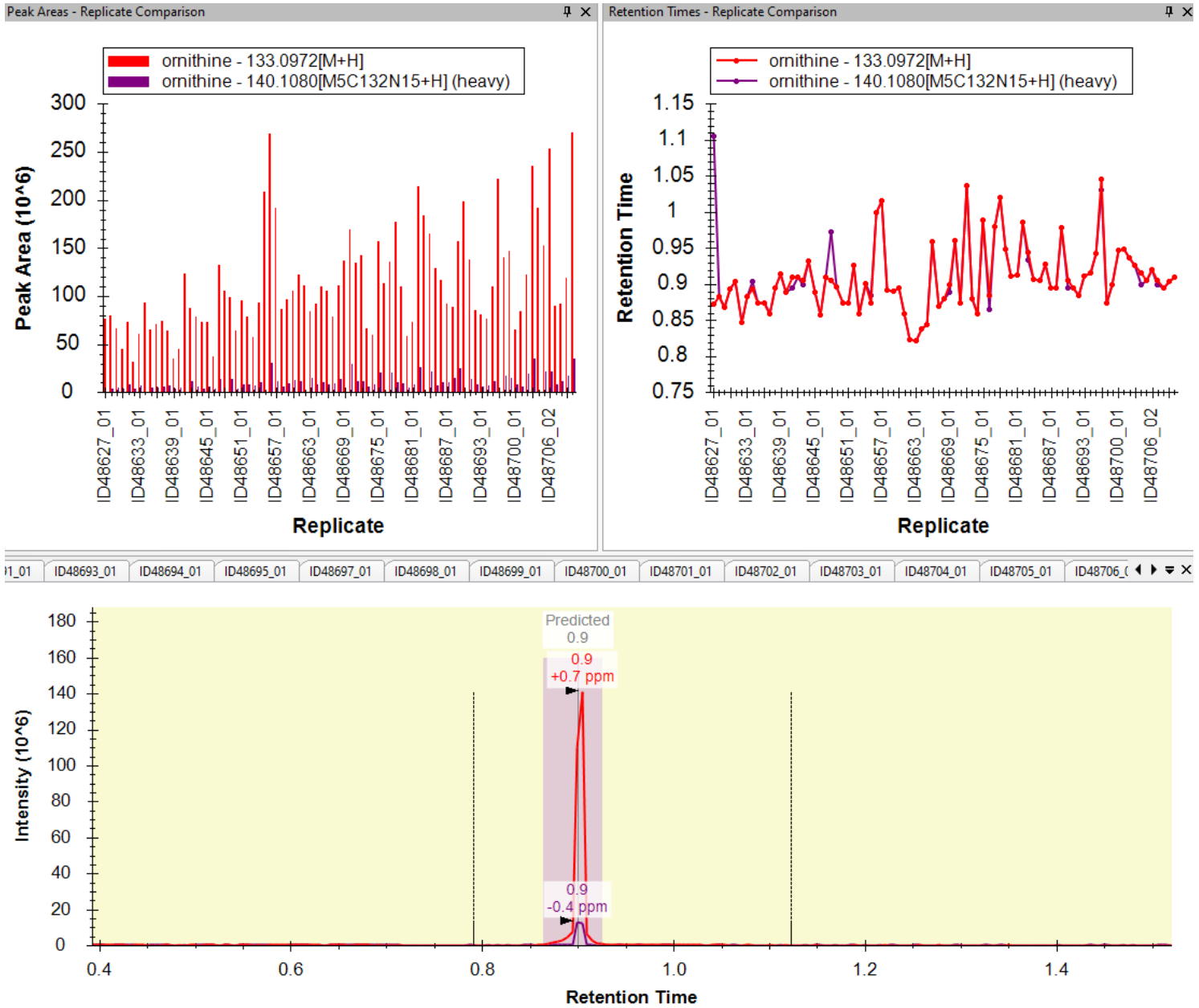
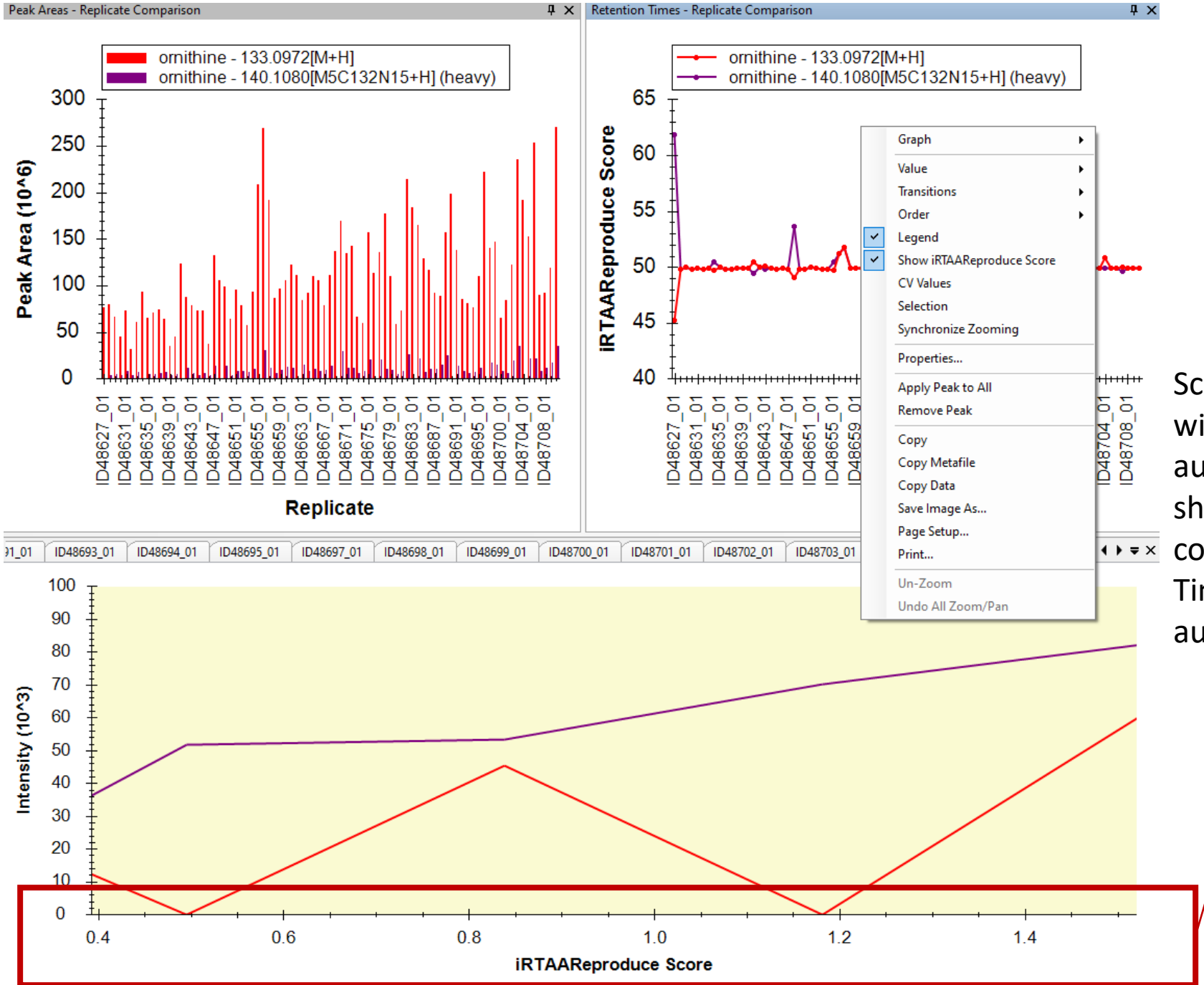
iRT calculator set up in background



Problem 1 – automatic window readjustment only works for one of the windows

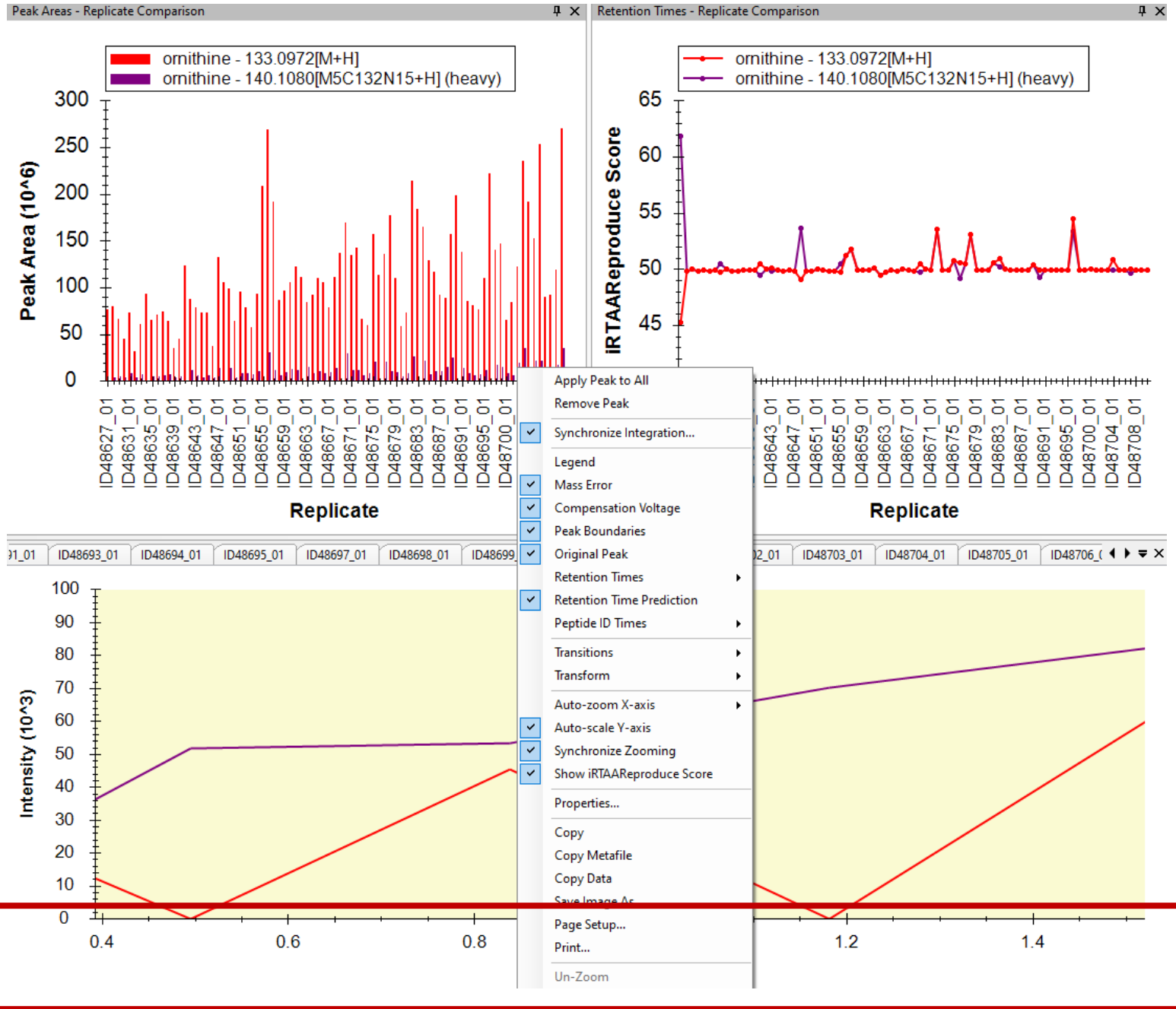
- Ideally, there would be consistent behavior between the windows shown on the next two slides

Immediate result after changing to iRT score in the Retention Times – Replicate Comparison window



Score X-axis values match previous RT window (e.g. 0.4 to 1.4 instead of automatically switching to the values shown in the “Retention times – Replicate comparison” window). The Retention Times – Replicate Comparison window automatically adjusted for the score.

Immediate result after changing to iRT score in the bottom chromatogram window

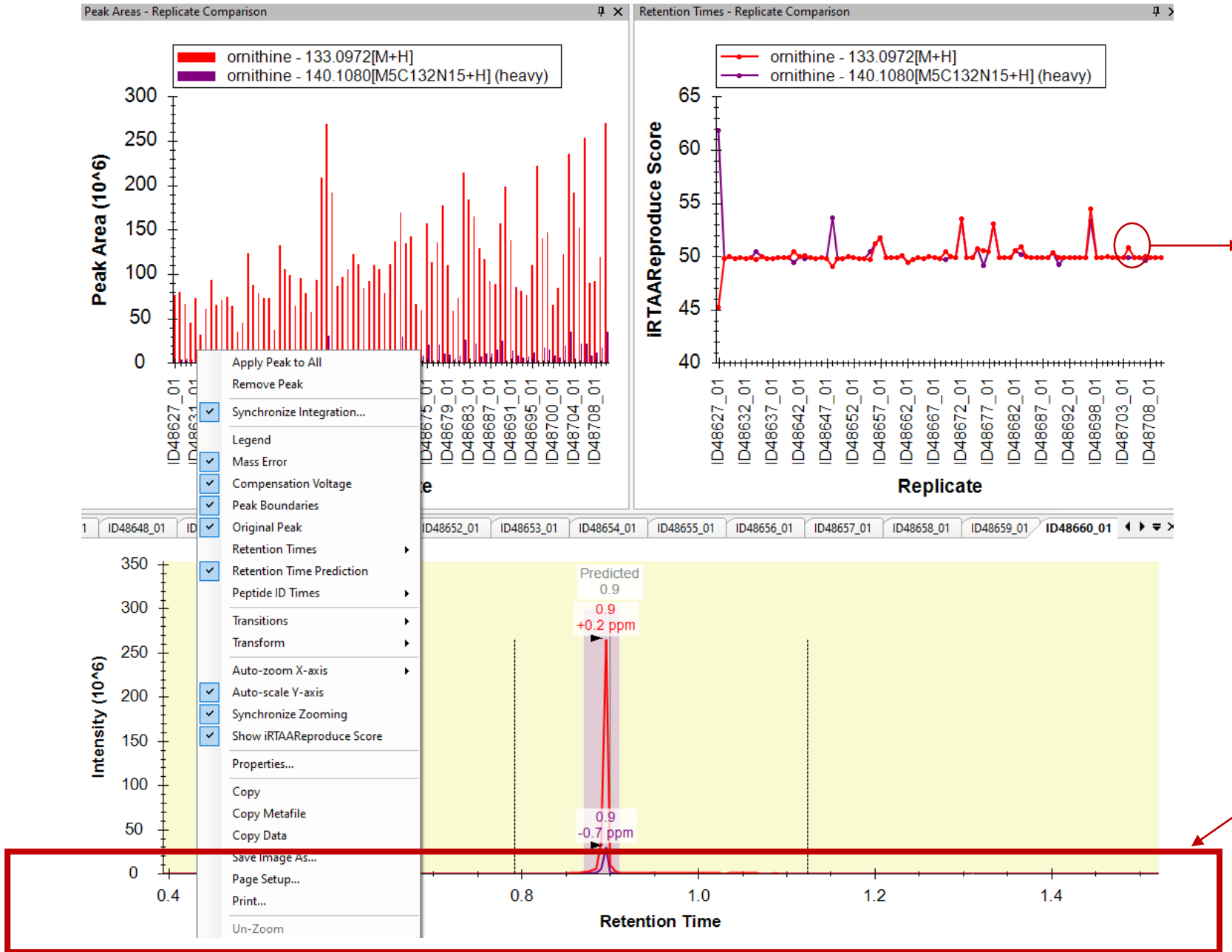


No difference, so not dependent on which window was used to change from RT to iRT score

Problem 2 – Clicking on any data point in “Retention Times – Replicate Comparison” window changes the chromatogram view back to Retention time

- If the window is set to iRT score, I would like the chromatogram window to stay with those units instead of swapping to Retention Time

Immediate result after clicking on a single RT point in the “Retention Times” window

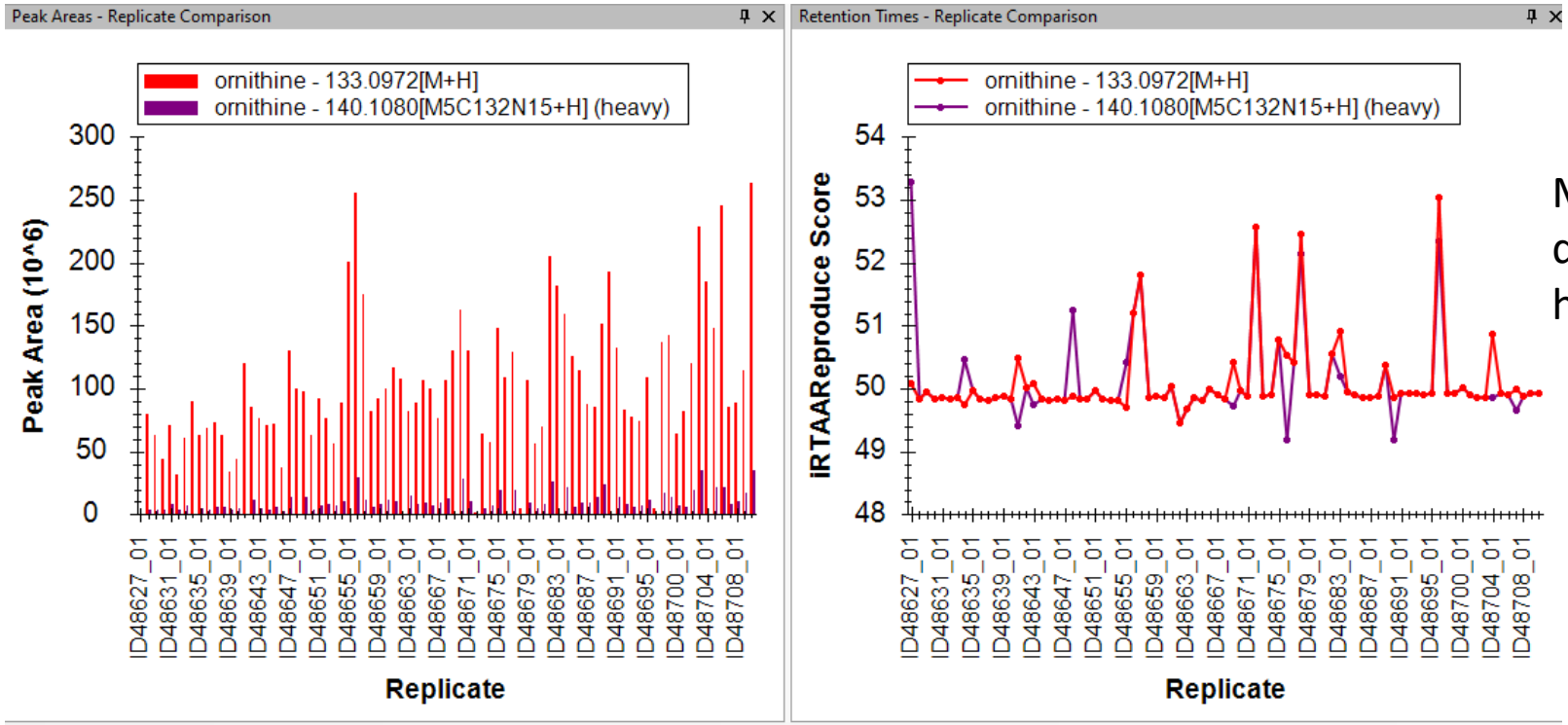


Clicked on a single point here. The units of the chromatogram view then swapped to retention time. The “Show iRTAAReproduce Score” option is still checked. Zooming in or out doesn’t change the x-axis. Changing the “Auto zoom X-axis” option does change the axis.

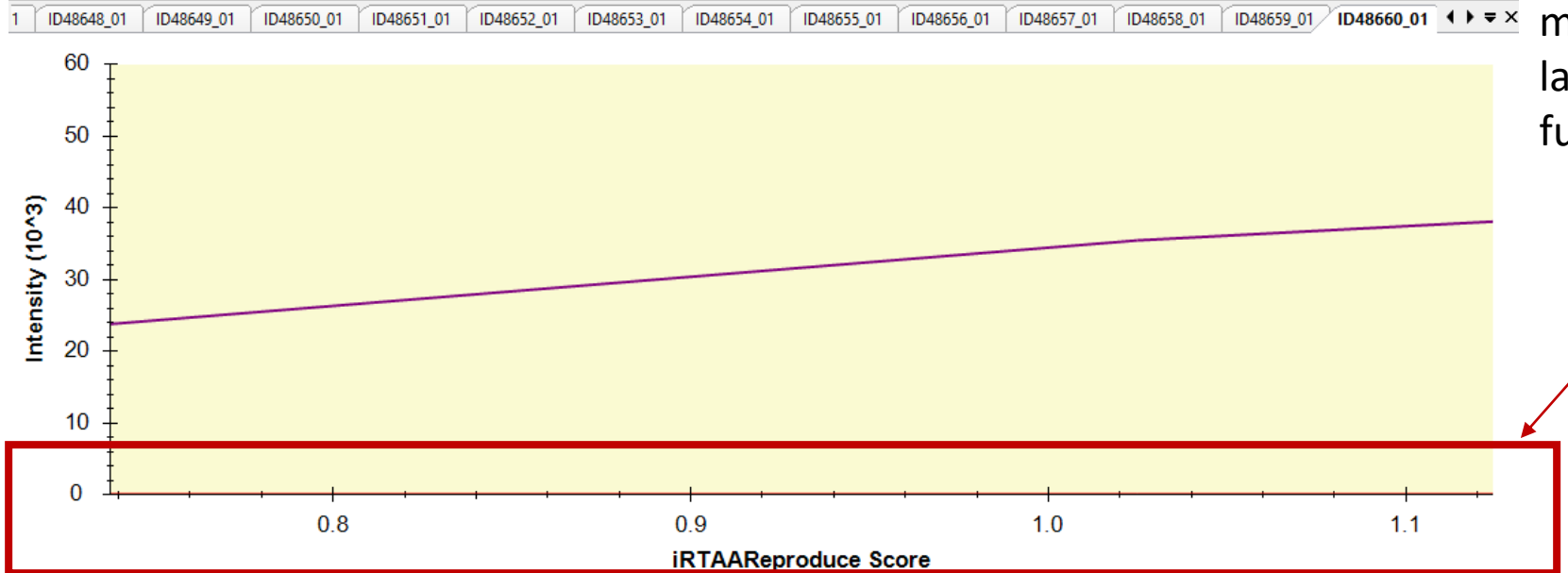
Problem 3 – After trying to integrate the peak in the chromatogram view with bugged X-axis, it changes the X-axis instead of integrating the peak

- This is likely the result of the bug responsible for Problem 2
- No changes to the integration bounds happen, just a change in the X-axis label and the chromatogram shape
- Only happens once per molecule per file

Immediate result after attempting to re-integrate a peak in the chromatogram view



Maybe unrelated: the displayed range in this window has changed



Switched back to the right X-axis label, except now it's the range that was attempted to be integrated on the previous window (e.g. 0.7 to 1.1 min integration has resulted in the label changing and the zoom function)

Notes for the previous slide

- This behavior then happen the first time for each file and molecule that is selected
  - This is annoying because I would have to attempt integration once, rezoom on the best peak on the X-axis, and then I would be able to actually integrate the peak