Ion Ratio Feature in Skyline 20.2

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Requirements

- Be able to designate certain transitions as "Qualitative"

- Calculate the ratio of the qualitative transition peak areas to the quantitative peak areas

- Calculate the target ion ratio as the average of the ion ratios of the non-excluded external standards

- Specify ion ratio threshold that Skyline uses to indicate whether criteria passed or failed

Designating transitions as "Qualitative"

- In Skyline, users can already right-click on transitions to mark them as non-quantitative

- Non quantitative transitions show up in the Targets tree as grey
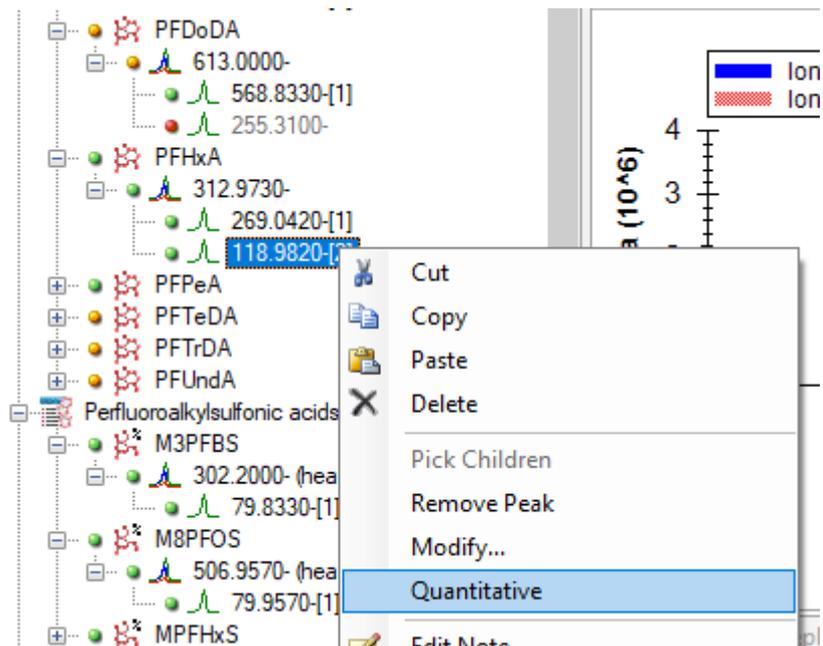
Specifying Ion Ratio Threshold

- Users will be able to specify the ion ratio threshold on the Quantification tab of the Molecule or Peptide settings dialog

- If it turns out that users need to specify different ion ratio thresholds for different molecules, then we might add a `ExplicitQuantificationSettings` thing to the Document Grid where all items on the quantification dialog can be overridden per molecule.
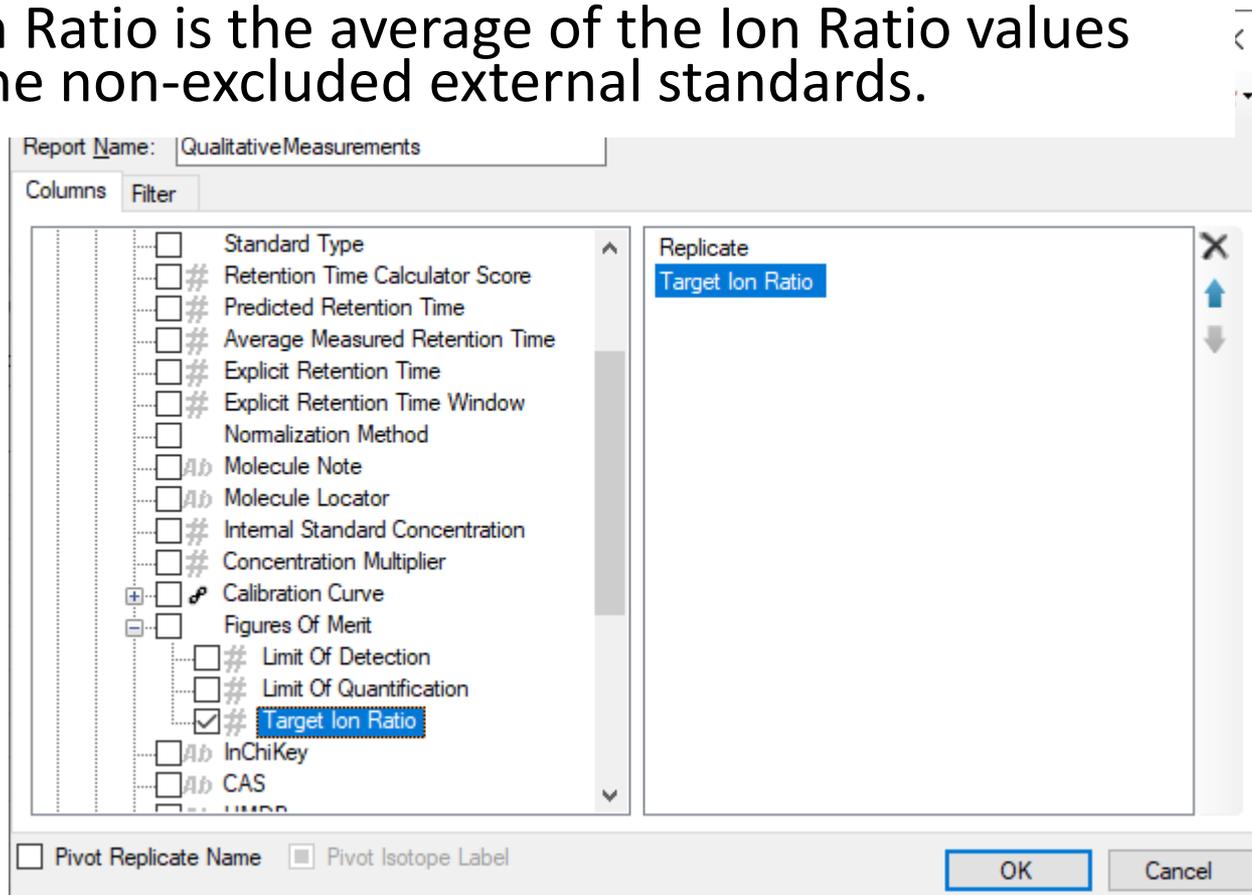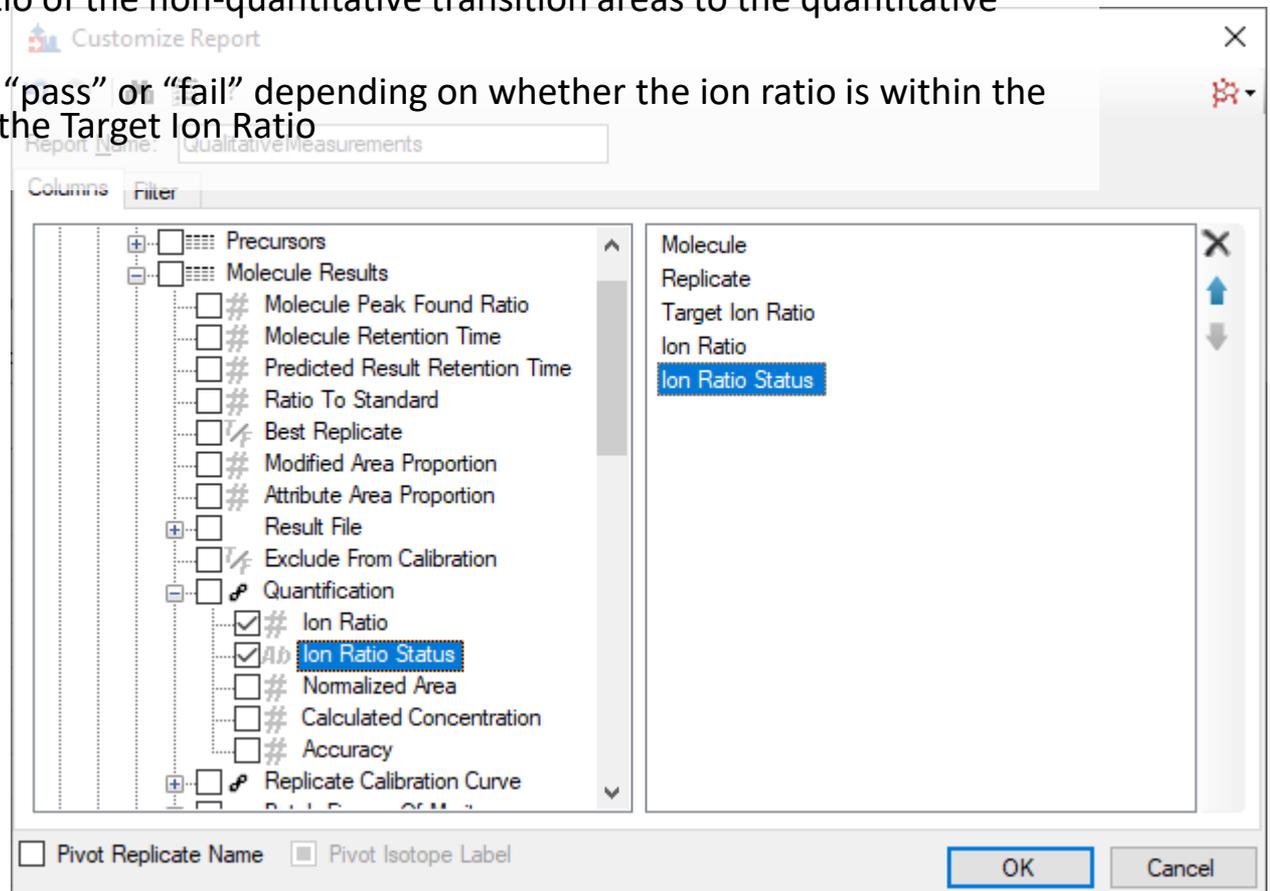
Target Ion Ratio column

- There will be a new "Target Ion Ratio" column available in the document grid under the "Figures of Merit" object.
- The Target Ion Ratio is the average of the Ion Ratio values across all of the non-excluded external standards.

Ion Ratio Result columns

- "Peptide Results" already has a group of columns called "Quantification"

- There will be two new columns under "Quantification": "Ion Ratio" and "Ion Ratio Status"

- Ion Ratio shows the ratio of the non-quantitative transition areas to the quantitative transition areas

- Ion Ratio Status shows "pass" or "fail" depending on whether the ion ratio is within the Ion Ratio Threshold of the Target Ion Ratio

Viewing ion ratio results in the Document Grid