

# *Trend Responses™ Explained*

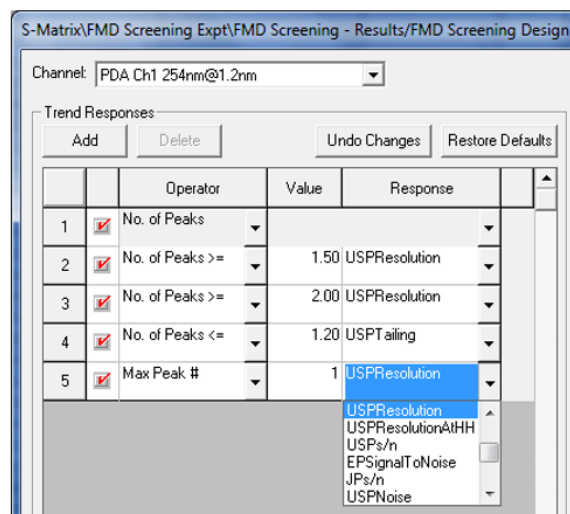


## *Trend Responses*<sup>™</sup> (S-Matrix Patented)

eliminate the requirement for laborious and error-prone peak tracking in initial screening experiments. Flexible Trend Response operators enable you to automatically retrieve data for any separation characteristics you want to evaluate.

**Example** Trend Responses which Fusion QbD can instantly obtain from your experiment chromatograms include:

- No. of Integrated Peaks
- No. of Baseline Resolved Peaks
- No. of Peaks with Acceptable Tailing
- No. of Peaks with Good S/N Ratio



Trend Responses do not require any peak tracking in your chromatograms – only basic integration of your experiment chromatograms is needed. Fusion QbD can automatically compute your defined trend responses from integrated peak data available in the chromatography data software (CDS). From analyses of the trend response data sets Fusion QbD can determine the best performing combination of your chemistry system screening study factors to promote to an optimization study (e.g pH range, Strong Solvent Type, Column, Gradient Slope range).

The table on the following page defines the unique Trend Responses which are utilized in the data analysis. These responses are of two general types: peak count based and peak results based. As the name implies, a *peak count* based response is obtained by counting the number of integrated peaks in each chromatogram that meet a certain criterion. A *peak result* based response is a way of obtaining a result such as resolution or retention time for a specific peak using *indirect* peak tracking. For example, setting the *Max Peak # – RESPONSE* operator to *Max Peak 2 – USP Resolution* will find the 2<sup>nd</sup> largest peak in each chromatogram and obtain the resolution result for the peak.

Note that, as opposed to a pick-the-winner strategy, the trend responses are statistically analyzed and modeled. These models provide quantitative estimates of the study factor effects – it is this quantitation that defines the best column, pH, organic solvent type, and method conditions of any other included study factors.

Peak Count Based Trend Responses	Definition
<p><b>No. of Peaks</b></p>	<p>This will generate a response data set consisting of the number of integrated peaks in each experiment chromatogram.</p> <p>This response is therefore a measure of the overall selectivity of the experiment method associated with each chromatogram.</p>
<p><b>No. of Peaks [VALUE] [RESPONSE]</b></p> <p>Operator options: <math>\geq</math>, <math>&gt;</math>, <math>\leq</math>, <math>&lt;</math>, <math>=</math></p> <p>VALUE: User settable number <math>&gt; 0</math></p> <p>RESPONSE: CDS Computed Result</p>	<p>This will generate a response data set consisting of the number of integrated peaks in each experiment chromatogram with a certain value for the associated response. For example, given the configuration:</p> <p style="padding-left: 40px;">No. of Peaks <math>\geq 1.50</math> – Resolution</p> <p>Fusion QbD will generate a response data set consisting of the number of integrated peaks in each experiment chromatogram with Resolution values of <math>\geq 1.50</math>.</p>
Peak Result Based Trend Responses	Definition
<p><b>Max Peak # [VALUE] [RESPONSE]</b></p> <p>VALUE: User settable integer <math>&gt; 0</math></p> <p>RESPONSE: CDS Computed Result</p>	<p>The “Max Peak #” operator is used to track an individual peak in each chromatogram based on its Peak Area relative to the other integrated peaks in the chromatogram. For example, given the configuration:</p> <p style="padding-left: 40px;">Max Peak # 1 – Resolution</p> <p>Fusion QbD will import the Resolution response data for the largest peak in Area in each chromatogram (pictured on the following page).</p>
<p><b>Post Peak # [VALUE] [RESPONSE]</b></p> <p>VALUE: User settable integer <math>&gt; 0</math></p> <p>RESPONSE: CDS Computed Result</p>	<p>The “Post Peak #” operator is also used to track an individual peak in each chromatogram based on its Peak Area relative to the other integrated peaks in the chromatogram. However, this operator will then bring in the data for the peak which elutes <i>immediately after</i> the tracked peak. For example, given the configuration:</p> <p style="padding-left: 40px;">Post Peak # 1 – Resolution</p> <p>Fusion QbD will import the Resolution response data for the peak which elutes immediately after the largest peak in Area in each chromatogram (pictured on the following page).</p>
<p><b>First Peak [RESPONSE]</b></p> <p>RESPONSE: CDS Computed Result</p>	<p>The “First Peak” operator is used to track the first eluting peak in each experiment chromatogram. For example, given the configuration:</p> <p style="padding-left: 40px;">First Peak – K Prime</p> <p>Fusion QbD will import the K Prime for the first peak in each chromatogram.</p>
<p><b>Last Peak [RESPONSE]</b></p> <p>RESPONSE: CDS Computed Result</p>	<p>The “Last Peak” operator is used to track the last eluting peak in each experiment chromatogram. For example, given the configuration:</p> <p style="padding-left: 40px;">Last Peak – Retention Time</p> <p>Fusion QbD will import the retention time for the last peak in each chromatogram.</p>

Max Peak 1 and Post Peak 1 Peaks

