

Column name	description
<i>SpectraFile</i>	path and file name of mzML file containing the assessed peptide spectra
<i>ScanNum</i>	scan number of assessed spectra
<i>Peptide</i>	sequence of assessed peptide with PTM
<i>sub_pos</i>	position of the altered amino acid
<i>status</i>	status indicating if the spectra was evaluated (checked) or not (skipped) by SpectrumAI
<i>Sequence</i>	sequence of assessed peptide without PTM
<i>peptide_length</i>	length of the assessed peptide
<i>ions_support</i>	boolean indicator for presence (YES) or absence (NO) of ion fragments containing the altered amino acid
<i>support_ions</i>	list ion fragments containing the altered amino acid
<i>sum.supportions.intensity</i>	sum of the intensity of the ion fragments containing the altered amino acid
<i>flanking_ions_support</i>	boolean indicator for presence (YES) or absence (NO) of flanking ion fragments neighboring the altered amino acid
<i>flanking_ions</i>	list of flanking ion fragments neighboring the altered amino acid
<i>sum.flanking.ions.intensity</i>	sum of the intensity of the flanking ion fragments neighboring the altered amino acid
<i>matched_ions</i>	list of fragment ions matched in the MS/MS spectra
<i>sum.matchedions.intensity</i>	sum of the intensity of all fragment ions matched in the MS/MS spectra
<i>sum.fragmentions.intensity</i>	sum of the intensity of all fragment ions in the MS/MS spectra
<i>maxintensity</i>	maximal fragment ion intensity
<i>average_intensity</i>	average fragment ion intensity in the MS/MS spectra
<i>median_intensity</i>	medium fragment ion intensity in the MS/MS spectra

