

Response Curve (Experiment 1)

Error category	Error reason	Example case
Internal standard	Internal standard is not set.	File: JHU_DChan_HZhang_ZZhang\ Tissue_TSQVantage_directMRM\ TCGA-glyco-26-peps_response curves_revised160810_2016-08- 10_16-40-42.sky.zip
Internal standard	Internal standard is set to be none.	None
Internal standard	Internal standard is incorrect according to the inferred internal standard.	None
Attribute	Essential attributes have missing values.	None
Attribute	Essential attributes are annotated in unqualified data type.	None
Concentration	More than one concentration levels are needed.	None
Area values of heavy or light Isotope	More than one area values of heavy or light isotope exist for the combination of protein, peptidemodifiedsequence, precursorcharge, productcharge, fragmentation, replicate, concentration, samplegroup, isspike and isotopelabel.	Peptide sequence: ETPAASEAPSSAAK File: UVicPC_Borchers\ MousePlasma_Agilent6490_direct MRM\ 20160720_MousePlasmaExp1Batch 5_refined_2017-12-11_11-50- 02.sky.zip
Fragment ion	In response curve, no fragment ion with both heavy and light isotopes exists.	None

Warning category	Warning reason	Example case
Fragment ion	In response curve, the number of fragment ions with both heavy and light isotopes is less than 3.	Peptide sequence: LNT[+80]SDFQK File: WUSTL_Townsend\ CellLysate_5600TripleTOF_directP RM\ ResponseCurve\ E126_MP_EXP1_RevCurves_20141 215_UPLOAD DOC_2015-06- 08_14-46-49.sky.zip
Bad linear regression fitting	The coefficient of variance of slopes of fragment ions is larger than 0.5.	Peptide sequence: VYPLINR File: WUSTL_Townsend\ CellLysate_5600TripleTOF_directP RM\ ResponseCurve\ E126_MP_EXP1_RevCurves_20141 215_UPLOAD DOC_2015-06- 08_14-46-49.sky.zip
Bad linear regression fitting	The slopes of the fragments ions are 0.	None
Bad linear regression fitting	The fit of the linear regression model is poor due to the low R^2 (coefficient of determination) or large p value of F-test in the process of linear regression.	Peptide sequence: HEDILSILTAVNDDVSR File: WUSTL_Townsend\ CellLysate_5600TripleTOF_directP RM\ ResponseCurve\ E126_MP_EXP1_RevCurves_20141 215_UPLOAD DOC_2015-06- 08_14-46-49.sky.zip
Internal Standard spike peptide concentration	All of the concentrations of the internal standard peptide are zero.	Peptide sequence: LPLPALFK File: UVicPC_Borchers\ MousePlasma_Agilent6490_direct MRM-Exp1\ MousePlasmaV2Exp1B3_refined_2 017-12-11_11-21-51.sky.zip

Repeatability (Experiment 2)

Error category	Error reason	Example case
Internal standard	Internal standard is not set.	File: JHU_DChan_HZhang_ZZhang\ Tissue_TSQVantage_directMRM\ TCGA glyco 26 peps_repeatability_2016-06- 23_11-35-45.sky.zip
Internal standard	Internal standard is set to be none.	None
Internal standard	Internal standard is incorrect according to the inferred internal standard.	None
Attribute	Essential attributes have missing values.	None
Attribute	Essential attributes are using uncontrolled terms.	Chenwei_dataset\ MousePlasmaV2Exp1B3_refined_2 017-12-11_11-21-51.sky.zip
Attribute	Essential attributes are annotated in unqualified data type.	None
Light and Medium isotope	Both light and medium isotope labels are found in the peptide with a specific charge.	None
Area values of heavy or light Isotope	Number of light isotopes or heavy isotopes is not one due to wrongly annotated values in attributes.	Peptide sequence: DFALQNPGVVPR File: UVicPC_Borchers\ MousePlasma_Agilent6490_direct MRM\ MousePlasmaExp2B3_Refined_201 7-12-11_15-09-36.sky.zip

Warning category	Warning reason	Example case
Fragment ion	In repeatability graph, the number of fragment ions with both heavy and light isotopes is less than 3.	Peptide sequence: LLIIDSNLGVQDVENLK File: WUSTL_Townsend\ CellLysate_5600TripleTOF_directPRM\ E130_MP_EXP2_P7_20150105_UPLOAD DOC_2015-06-08_15-23-30.sky.zip
Missing points	In repeatability graph, fragment ion has missing points on the specific day.	Peptide sequence: FFAGIVWQHVEK File: Koomen\ RSLCnano_Quantiva_MRM3\ 082618_iMRM_mAb- Plex2_Exp2_Repeatability_upload_v4_replicates_2018-08-28_09-09-50.sky.zip
Missing points	In repeatability graph, fragment ion doesn't have three concentrations: Hi, Med, and Low on the specific day.	None
Missing points	In repeatability graph, fragment ion has less than 3 replicates for a specific concentration on the specific day.	Peptide sequence: GLDARPEVTR File: Koomen\ RSLCnano_Quantiva_MRM3\ 082618_iMRM_mAb- Plex2_Exp2_Repeatability_upload_v4_replicates_2018-08-28_09-09-50.sky.zip