

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

Spectrafile	ScanNum	Peptide	sub_pos	status	Sequence	peptide_length	ions_support	support_ions	sum.supportions.intensity	flanking_ions_support	flanking_ions	sum.flanking_ions.intensity	matched_ions	sum.matchedions.intensity	sum.fragmentsions.intensity	maintintensity	average_intensity	median_intensity
e:\data\MSData\2015\CPD_25cm_10\mzML\150111_3_01.mzML	26144	ISYGPWKFVYVLEAFEGTEPK	12	checked	ISYGPWKFVYVLEAFEGTEPK	25	YES	b12,y14	9160.64638	YES	b11,y14,b12,y13	27971.74451	b2,b4,b6,b7,b8,b9,b10,b11,b12,y2,y3,y4,y5,y6,y7,y8,y9,y10,y12,y13,y14	20528.75598	3420939.20965	44857.75000	641.58650	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150110_2_01.mzML	12943	QILEKELNTRAGELR	8	checked	QILEKELNTRAGELR	15	YES	b9,y8,y10,y11	28320.30593	YES	b7,y8,y7	32088.97012	b1,b2,b4,b5,b6,b7,b9,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11	34948.78052	8617742.11253	128488.08032	1131.58879	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150130_3_100mM_01.mzML	12086	ASDQSDNTAWVQDQPGAGPR	8	checked	ASDQSDNTAWVQDQPGAGPR	22	YES	b8,b9,b11	2309.28577	YES	b7,b9	2041.15613	b3,b4,b5,b6,b7,b8,b9,b11,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y13	6248989.69294	1448089.19333	262398.15625	1563.38619	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150120_3_01.mzML	27083	GGGAGFSGLTLELDNPGAKR	11	checked	GGGAGFSGLTLELDNPGAKR	22	YES	b11,y12,y13,y14,y15,y16	52893.24579	YES	y12,b11,y11	27326.19159	b3,b4,b5,b6,b7,b8,b9,b11,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y14,y15,y16	251771.72107	44207.86719	705.15244	0	
e:\data\MSData\2015\CPD_25cm_10\mzML\150125_2_01.mzML	18493	LWFWASAR	8	checked	LWFWASAR	9	YES	y2,y3,y4,y5,y6,y7,y8	87201.62782	YES	y2,y1	15339.23976	b1,b2,b3,y1,y2,y3,y4,y5,y6,y7,y8	130027.42441	2292307.61383	132206.68750	900.03747	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150414_10_500mM_01.mzML	2122	LHS2TKAESEK	2	checked	LHS2TKAESEK	13	YES	b2,b3,b4,b5,b6,y7	44605.26441	NO	b2,y1	34686.19322	b2,b3,b4,b5,b6,y1,y2,y3,y4,y5,y6,y7,y8,y9,y11	416509.70218	2444440.46447	45286.42578	635.24949	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150225_8_01.mzML	7532	LLEDLR	0	skipped	LLEDLR	6	NO		0	NO		b1,b2,b4,y1,y2,y3,y4,y5	174611.05951	15437027.13767	2193327.50000	3020.35945	0	
e:\data\MSData\2015\CPD_50cm_10\mzML\150210_2_01.mzML	22081	NSLFLQMNLSR	4	checked	NSLFLQMNLSR	11	YES	b4,b5,b7,y8,y9,y10	191427.00000	YES	b3,y8,b4,y7	427611.61328	b1,b2,b3,b4,b5,b7,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10	881795.59814	1692326.47102	156364.82813	1445.72963	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150130_3_20mM_01.mzML	12448	ISNSAATGSDSHVANSALGOTPQQDQTLVQR	6	checked	ISNSAATGSDSHVANSALGOTPQQDQTLVQR	32	YES	b6,b7,b8,b9,b10,b11,b12	22504.91760	YES	b5,b6	8842.66626	b3,b4,b5,b6,b7,b8,b9,b10,b11,b12,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y14,y15,y16,y17,y20	317084.30737	5276909.3392	134664.82813	934.21551	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150126_12_30mM_01.mzML	4714	NVSNPC+57.02NHEAVGK	14	NO		14	NO		0	NO		b1,b2,b3,b5,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10	231482.83154	1082907.05520	138082.71875	921.46078	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150126_15_40mM_01.mzML	7488	ADSDQAGATEKEGDPQASAGDETPITSK	16	checked	ADSDQAGATEKEGDPQASAGDETPITSK	31	YES	b18,y16,y18,y19	10019.61511	YES	y16,y15	42817.76611	b3,b4,b5,b6,b7,b8,b9,b10,b11,b12,b13,b14,b15,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y14,y15,y16,y18,y19	524910.01887	762126.72509	91217.79688	1087.40658	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150126_14_50mM_01.mzML	2846	EAGDSASASAPGVK	13	checked	EAGDSASASAPGVK	16	YES	y5,y7,y8,y9,y10,y11,y2,y14	56476.63392	YES	y8	4414.00035	b2,b3,b4,b5,b6,b7,y8,y9,y10,y11,y2,y14	687960.80709	20718.52344	473.44607	0	
e:\data\MSData\2015\CPD_25cm_10\mzML\150118_11_40mM_01.mzML	3487	EQGNQSTSLQNR	6	checked	EQGNQSTSLQNR	13	YES	y8,y9,y10,y11	19230.81787	YES	y8,y7	15179.80518	b2,b3,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11	53623.61555	555884.54841	11339.18457	424.63296	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150505_20_100mM_01.mzML	15911	YGFQFLR	5	checked	YGFQFLR	7	YES	y3,y4,y5,y6	342169.82031	YES	b4,y3,y2	76357.45380	b1,b2,b3,b4,y1,y2,y3,y4,y5,y6	7655160.30710	356793.96875	1724.91219	0	
e:\data\MSData\2015\CPD_50cm_10\mzML\150210_13_01.mzML	29106	TGIEALISQITWAPPQDTSEYSHQVPTGDEPLQRF	0	skipped	TGIEALISQITWAPPQDTSEYSHQVPTGDEPLQRF	39	NO		0	NO		b4,b5,b6,b7,b8,b9,b10,b11,b12,b14,b15,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y13,y15,y16,y17,y20	117926.96419	3000931.78626	40984.57813	653.49352	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150126_14_50mM_01.mzML	2347	AEDM+15.9RETNVAVPGSDQTR	13	checked	AEDM+15.9RETNVAVPGSDQTR	18	YES	y5,y7,y8,y9,y10	99088.17163	YES	y6,y5	26260.49211	b2,b3,b4,b5,b6,y1,b8,b9,b10,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10	323276.67716	521338.42703	53138.42703	689.96225	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150424_16_40mM_01.mzML	3828	YEDENR	7	checked	YEDENR	7	YES	y1,y2,y3,y4,y5,y6	279658.42703	YES	y1	38967.22656	b1,b2,b3,y1,y2,y3,y4,y5,y6	7453859.75510	305118.43750	1651.64187	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150424_16_40mM_01.mzML	6014	SDSELNNEVAR	7	checked	SDSELNNEVAR	12	YES	y6,y7,y8,y9,y10	261580.79785	YES	y6,y5	72925.87109	b2,b3,b4,b5,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10	512029.38883	635364.38970	113427.41406	1046.62921	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150505_20_100mM_01.mzML	3769	EPOGSAVEK	1	checked	EPOGSAVEK	10	YES	b2	1664.32340	YES	y9	472.85000	b2,y1,y2,y3,y4,y5,y6,y7,y8,y9	1522960.38195	600203.94922	901.10016	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150126_14_50mM_01.mzML	4065	NKYEENR	9	checked	NKYEENR	9	YES	y1,y2,y3,y4,y5,y6,y7	405269.73071	YES	y1	121365.79688	b1,b2,b3,b4,b5,b6,y1,y2,y3,y4,y5,y6,y7	464514.63150	18032757.23679	352745.93750	1446.78733	56.37574
e:\data\MSData\2015\CPD_25cm_20\mzML\150126_14_50mM_01.mzML	10086	DPAGETPEAAGTR	0	skipped	DPAGETPEAAGTR	14	NO		0	NO		b2,b3,b4,b5,b6,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12	192525.93436	1658047.21516	49731.89453	591.10418	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150118_11_40mM_01.mzML	9167	EEDQPSAQDETPITSK	4	checked	EEDQPSAQDETPITSK	19	YES	b4,b5,b7,b8	7809.23681	YES	b3,b4	2580.99384	b2,b3,b4,b6,b7,b8,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13	94508.21205	1414200.21248	18506.37655	523.19805	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150129_17_20mM_01.mzML	13173	TLEGLQVEEPPYK	14	checked	TLEGLQVEEPPYK	14	YES	y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11	187544.99377	YES	y1	8358.89648	b2,b3,b4,b5,b7,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11	241436.69220	3465533.20655	147233.62500	788.33785	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150111_19_03.mzML	2397	DSRPSQAAGDNGDEVK	16	checked	DSRPSQAAGDNGDEVK	17	YES	y2,y3,y4,y5,y6,y7,y8,y9,y10,y11	60030.32959	YES	y2,y1	15181.24219	b2,b3,b5,b6,b7,b8,b9,b10,b11,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11	136721.72188	1638891.56872	2853.12704	632.82005	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150111_15_01.mzML	17573	ELTVSNDNEGWHVHC+57.02SDGLK	15	checked	ELTVSNDNEGWHVHC+57.02SDGLK	22	YES	b16,y8,y9,y10,y11,y12,y13,y15,y16	45804.04848	YES	y8,y7	81787.25255	b2,b3,b4,b5,b6,b8,b9,b10,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y15,y16	1664961.47159	178899.65625	1563.09215	0	
e:\data\MSData\2015\CPD_25cm_10\mzML\150111_19_03.mzML	29732	EQAQCEAMQDELEELR	18	checked	EQAQCEAMQDELEELR	18	YES	y6,y7,y8,y9,y10,y11	42449.44088	YES	y6,y5	19153.50195	b2,b3,b4,b5,b6,b7,b8,b9,b10,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11	100668.58357	1022796.82420	18225.70070	489.64003	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150130_3_100mM_01.mzML	15436	GATNIVEALKDQR	6	checked	GATNIVEALKDQR	16	YES	b6,b7,y11,y12,y13	29664.60868	YES	b5,y11,b6,y10	63380.91233	b5,y11,b6,y10	21245.80850	1917098.69502	41826.80959	807.87977	0
e:\data\MSData\2015\CPD_25cm_20\mzML\150130_3_100mM_01.mzML	12809	SDHC+17.02EDTFAGYFAVAIVK	15	checked	SDHC+17.02EDTFAGYFAVAIVK	20	YES	y6,y7,y8,y9,y10,y11	393209.42125	YES	y6,y5	86237.01563	b2,b3,b4,b5,b6,b7,b9,b10,b12,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y15	618460.50086	1123760.52917	162286.06250	1377.53972	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150111_19_03.mzML	26054	VNDVYKDEKSLGLQWPGFEEMK	1	checked	VNDVYKDEKSLGLQWPGFEEMK	25	YES	b2,b3,b4,b5,b6,b7,b9,b10,b11,b12,b13	69621.99310	NO		0	b2,b3,b4,b5,b6,b7,b9,b10,b11,b12,b13,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y15,y16	3002284.90726	60018.42609	600.72949	0	
e:\data\MSData\2015\CPD_25cm_10\mzML\150111_19_03.mzML	28282	AVQSDVLLMKPDAELSSAVYLNPEKDTLPGFLNQDDQDDCNR	47	checked	AVQSDVLLMKPDAELSSAVYLNPEKDTLPGFLNQDDQDDCNR	47	YES	y7,y8,y9,y10,y11,y12,y13,y14,y16,y18,y19,y22	326729.76444	YES	y7,y6	88446.26953	b4,b5,b6,b7,b8,b9,b10,b11,b12,b13,b14,b15,b17,b18,b19,b22,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y14,y16,y18,y19,y22	18003983.37546	164286.06250	1687.82070	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150130_3_100mM_01.mzML	3190	DSEDEVSRDSKEMATK	17	checked	DSEDEVSRDSKEMATK	17	YES	b8,b9,b10,b11,b12,b13,y12	21001.29926	YES		0	b2,b3,b4,b5,b6,b7,b8,b9,b10,b11,b12,b13,y1,y2,y3,y4,y5,y6,y7,y8,y9,y12	5909549.83078	69878.35156	713.92929	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150130_3_100mM_01.mzML	12235	EVQLVGGSGVQPGSGLSR	11	checked	EVQLVGGSGVQPGSGLSR	19	YES	b11,b12,b13,b16,y8,y10,y11,y12,y13,y14,y15,y16,y17	454201.63881	YES	b10,y9,b11,y8	62220.49365	b1,b2,b3,b4,b5,b6,b7,b9,b10,b11,b12,b13,b16,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y14,y15,y16,y17	886991.18837	134026.39063	1553.21558	0	
e:\data\MSData\2015\CPD_25cm_20\mzML\150422_12_100mM_01.mzML	5632	SPYASDHTLSR	13	checked	SPYASDHTLSR	13	YES	y8,y9,y10	39873.87180	YES	b5,y8,y7	48020.08398	b1,b2,b3,y1,y2,y3,y4,y5,y6,y7,y8,y9,y10	375826.32524	12680947.51900	30627.43500	1314.25020	0
e:\data\MSData\2015\CPD_50cm_10\mzML\150210_2_01.mzML	21220	ADIDVSGPVQVDPVPPVNEGPDAK	0	skipped	ADIDVSGPVQVDPVPPVNEGPDAK	25	NO		0	NO		b2,b3,b4,b5,b6,b7,b8,b9,b10,b11,b12,b13,b14,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y14,y15	1739910.97515	2566746.18843	287588.78125	2390.56610	2.17051	
e:\data\MSData\2015\CPD_25cm_20\mzML\150422_8_500mM_01.mzML	14520	SAVGGPQRDLG+57.02DQV+57.02YVSSVSLVPC+57.02AFYWNHVK	8	checked	SAVGGPQRDLG+57.02DQV+57.02YVSSVSLVPC+57.02AFYWNHVK	32	YES	b9,b10,b11,b13,b14,b15,b18,b19	161269.00684	YES		0	b3,b4,b5,b6,b7,b8,b9,b10,b11,b13,b14,b15,b18,b19,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13,y14,y15	10955570.08448	21228755.74678	406509.15625	1774.89988	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150111_19_03.mzML	11218	MA+15.9HKSMPFEVK	0	skipped	MHKSMPFEVK	11	NO		0	NO		b7,b8,y1,y2,y3,y4,y5,y6,y7	769877.96606	36542534.32770	460765.21200	2880.95651	69.90292	
e:\data\MSData\2015\CPD_25cm_10\mzML\150111_9_03.mzML	26504	SVFKPIFGVGVADAPQVLSPTFGAQPDR	10	checked	SVFKPIFGVGVADAPQVLSPTFGAQPDR	30	YES	b10,b11,b12,b13,b14	15717.94775	YES	b9,b10	28326.42822	b3,b4,b5,b6,b7,b8,b9,b10,b11,b12,b13,b14,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13	288342.45166	4370130.28712	59883.81641	938.40032	0
e:\data\MSData\2015\CPD_25cm_10\mzML\150120_10_01.mzML	22140	AAGAGQDQDC+57.02EYLMVGVGVC+57.02DQGVPR	24	checked	AAGAGQDQDC+57.02EYLMVGVGVC+57.02DQGVPR	24	YES	y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13	20043.62398	NO		0	b3,b4,b5,b6,b7,b8,b9,b10,b11,b12,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12,y13	3899114.88949	97193.56250	901.32106	0	
e:\data\MSData\2015\CPD_25cm_10\mzML\150103_8_03.mzML	13217	LWDSKTR	8	checked	LWDSKTR	9	YES	y4,y5,y6,y7,y8	180702.33984	YES	y2,y1	156386.56641	b1,b2,b3,y1,y2,y3,y4,y5,y6,y7,y8	4021652.25304	2			