

Supplementary Data 3

Analysis of protein-DNA interactions in chromatin by UV induced cross-linking and mass spectrometry

Stützer *et al.*

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Linker histones + 187bp DNA

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***X. laevis* mononucleosomes and nucleosomal arrays**

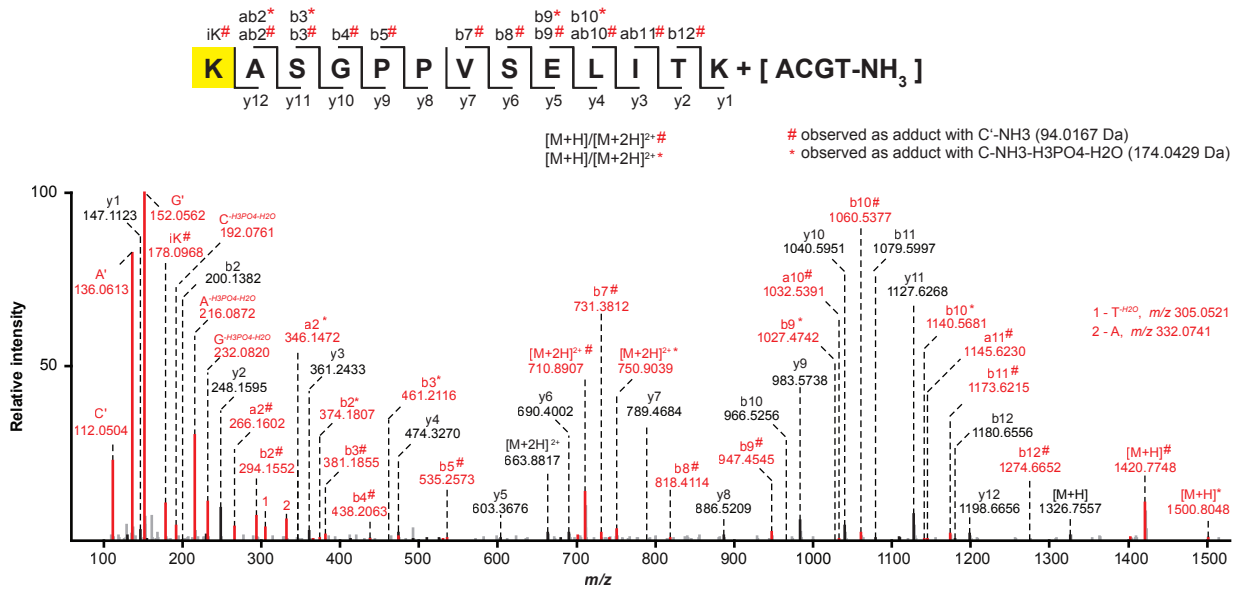
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Linker histone H1.4

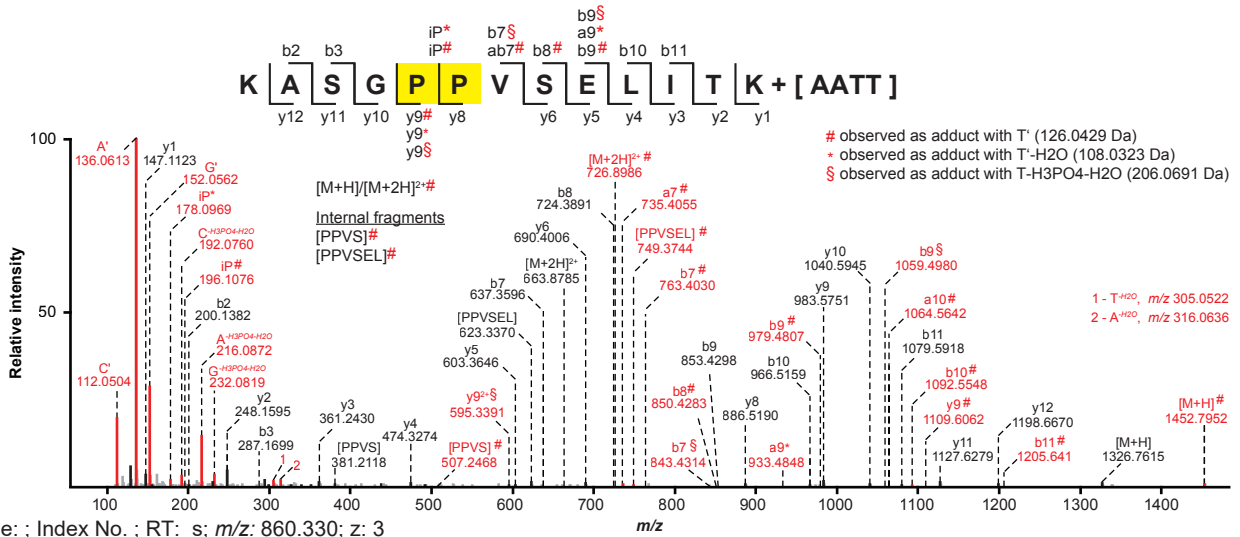
protein	peptide (aa)	cross-link site (aa - base/sugar)	DNA	m/z _{exp}	z	cross-link MW _{exp}	cross-link MW _{calc}	peptide MW _{calc}	DNA MW _{calc}	Δ ppm
H1.4	KASGPPVSELITK (33-45)	Lys33 - C	ACGT-NH3	854.9878	3	2561.9399	2561.9414	1325.7549	1236.1866	-0.59
		Lys33 - C	CGTT-NH3	851.9836	3	2552.9273	2552.9298	1325.7549	1227.1750	-0.99
		Lys33 - C	AACT-NH3	849.6545	3	2545.9400	2545.9465	1325.7549	1220.1917	-2.56
		Lys33 - C	AC-NH3	965.4271	2	1928.8386	1928.8429	1325.7549	603.0880	-2.24
H1.4	KASGPPVSELITK (33-45)	Pro37/38 - T	AATT	860.3301	3	2577.9668	2577.9728	1325.7549	1252.2179	-2.32
		Pro37/38 - T	GGTT-NH3	865.3224	3	2592.9437	2592.9360	1325.7549	1267.1812	2.96
		Pro37/38 - T	AAT	758.9818	3	2273.9219	2273.9268	1325.7549	948.1719	-1.86
		Pro37 - T	T-H3PO4	711.8806	2	1421.7456	1421.7397	1197.6600	224.0797	4.13
H1.4	ASGPPVSELITK (34-45)	Pro37 - T	T-H3PO4	711.8806	2	1421.7456	1421.7397	1197.6600	224.0797	4.13
		Lys45 - C	CC-NH3	769.0228	3	2304.0449	2304.0434	1724.9667	579.0767	0.68
		Lys45 - C	CCC-NH3	865.3712	3	2593.0901	2593.0897	1724.9667	868.1230	0.16
		Lys45 - C	AC-NH3	777.0282	3	2328.0611	2328.0547	1724.9667	603.0880	2.77
H1.4	SGVSLAALKK (54-63)	Lys45 - C	ACCC-NH3	727.5435	4	2906.1427	2906.1473	1724.9667	1181.1807	-1.60
		Lys62 - C	CT-NH3	784.3438	2	1566.6720	1566.6727	972.5963	594.0764	-0.46
		Lys62 - C	ACT-NH3	940.8710	2	1879.7264	1879.7303	972.5963	907.1340	-2.10
		Lys62 - C	CGT-NH3	632.9144	3	1895.7197	1895.7252	972.5963	923.1289	-2.89
H1.4	KALAAAGYDVEK (63-74)	Lys62 - C	CG-NH3	796.8442	2	1591.6728	1591.6792	972.5963	619.0829	-4.03
		Lys63 - C	CG-NH3	618.9192	3	1853.7341	1853.7381	1234.6552	619.0829	-2.13
		Lys63 - C	CCG-NH3	715.2669	3	2142.7772	2142.7844	1234.6552	908.1292	-3.35
		Lys63 - C	CCT-NH3	706.9329	3	2117.7752	2117.7779	1234.6552	883.1227	-1.27
H1.4	ALAAAGYDVEKNNSR (64-78)	Lys63 - C	ACT-NH3	714.9366	3	2141.7863	2141.7892	1234.6552	907.1340	-1.34
		Lys74 - C	CT-NH3	1086.9341	2	2171.8526	2171.8557	1577.7793	594.0764	-1.43
		Lys74 - C	CG-NH3	733.2930	3	2196.8555	2196.8622	1577.7793	619.0829	-3.02
		Lys74 - C	ACC-NH3	824.3106	3	2469.9083	2469.9136	1577.7793	892.1343	-2.14
H1.4	IKLGLK (79-84)	Lys74 - C	ACT-NH3	829.3095	3	2484.9050	2484.9133	1577.7793	907.1340	-3.33
		Lys80 - C	ACG-NH3	802.3120	2	1602.6084	1602.6141	670.4736	932.1405	-3.59
		Lys80 - C	CT-NH3	633.2813	2	1264.5470	1264.5500	670.4736	594.0764	-2.38
		Lys80 - C	CGT-NH3	797.8080	2	1593.6004	1593.6025	670.4736	923.1289	-1.35
H1.4	LGLKSLVSK (81-89)	Lys80 - C	CC-NH3	625.7816	2	1249.5476	1249.5503	670.4736	579.0767	-2.17
		Lys84 - C	ACGT-NH3	1090.9069	2	2179.7982	2179.7926	943.6061	1236.1866	2.53
		Lys84 - C	CGGT-NH3	732.9365	3	2195.7860	2195.7875	943.6061	1252.1815	-0.69
		Lys84 - C	CGT-NH3	934.3757	2	1866.7358	1866.7350	943.6061	923.1289	0.40
H1.4	SLVSKGTLVQTK (85-96)	Lys84 - C	CTT-NH3	921.8704	2	1841.7252	1841.7285	943.6061	898.1224	-1.82
		Lys89 - C	CG-NH3	940.4194	2	1878.8232	1878.8273	1259.7444	619.0829	-2.19
		Lys89 - C	AAC-NH3	726.3054	3	2175.8927	2175.8900	1259.7444	916.1456	1.25
		Lys89 - C	ACCG-NH3	827.9844	3	2480.9297	2480.9312	1259.7444	1221.1869	-0.61
H1.4	GTGASGSFKLNK (97-108)	Lys89 - C	AC-NH3	932.4214	2	1862.8272	1862.8324	1259.7444	603.0880	-2.80
		Lys105 - T	T-H3PO4	464.2390	3	1389.6935	1389.6883	1165.6086	224.0797	3.78
		Lys105 - C	ACCG-NH3	629.7283	4	2514.8819	2514.8904	1293.7036	1221.1869	-3.40
		Lys105 - C	CCG-NH3	734.9493	3	2201.8244	2201.8328	1293.7036	908.1292	-3.81
H1.4	KAASGEAKPK (109-118)	Lys105 - C	ACT-NH3	734.6190	3	2200.8335	2200.8376	1293.7036	907.1340	-1.85
		Lys105 - C	CC-NH3	625.2660	3	1872.7745	1872.7803	1293.7036	579.0767	-3.06
		Lys109 - C	ACCG-NH3	736.5859	3	2206.7342	2206.7419	985.5551	1221.1869	-3.50
		Lys109 - C	AACC-NH3	731.2549	3	2190.7412	2190.7470	985.5551	1205.1920	-2.66
H1.4	AKKPAGAAK (127-135)	Lys128 - C	ACCG-NH3	688.2408	3	2061.6989	2061.7044	840.5176	1221.1869	-2.68
		Lys128 - C	AACC-NH3	682.9091	3	2045.7038	2045.7095	840.5176	1205.1920	-2.80
		Lys128 - C	ACC-NH3	578.5570	3	1732.6475	1732.6519	840.5176	892.1343	-2.53
		Lys128 - C	AAC-NH3	586.5613	3	1756.6604	1756.6632	840.5176	916.1456	-1.58
H1.4	KPAGAAKKPK (129-138)	Lys135 - C	ACC-NH3	629.9267	3	1886.7566	1886.7625	994.6282	892.1343	-3.12
		Lys135 - C	AAC-NH3	637.9318	3	1910.7719	1910.7738	994.6282	916.1456	-0.98
		Lys135 - C	ACCG-NH3	739.6117	3	2215.8116	2215.8150	994.6282	1221.1869	-1.54
		Lys135 - C	CCG-NH3	635.2580	3	1902.7505	1902.7574	994.6282	908.1292	-3.62
H1.4	KATGAATPK (139-147)	Lys139 - C	ACCG-NH3	689.2292	3	2064.6641	2064.6677	843.4809	1221.1869	-1.75
		Lys139 - C	CCGG-NH3	694.5621	3	2080.6628	2080.6626	843.4809	1237.1818	0.09
		Lys139 - C	ACGT-NH3	694.2296	3	2079.6653	2079.6674	843.4809	1236.1866	-1.02
		Lys139 - C	CCGT-NH3	686.2266	3	2055.6563	2055.6561	843.4809	1212.1753	0.09
H1.4	KATGAATPKK (139-148)	Lys147 - C	ACCT-NH3	723.5920	3	2167.7525	2167.7562	971.5759	1196.1804	-1.72
		Lys147 - C	ACCG-NH3	731.9276	3	2192.7593	2192.7627	971.5759	1221.1869	-1.56
		Lys147 - C	ACCC-NH3	718.5917	3	2152.7516	2152.7565	971.5759	1181.1807	-2.29
		Lys156 - C	ACT-NH3	673.6133	3	2017.8164	2017.8208	1110.6868	907.1340	-2.17
H1.4	KAKKPAAAAGAK (156-167)	Lys156 - C	CGT-NH3	678.9455	3	2033.8130	2033.8157	1110.6868	923.1289	-1.32
		Lys156 - C	ACCG-NH3	778.2985	3	2331.8720	2331.8736	1110.6868	1221.1869	-0.69
		Lys156 - C	CT-NH3	569.2610	3	1704.7595	1704.7632	1110.6868	594.0764	-2.14
		Lys167 - C	ACCG-NH3	711.9207	3	2132.7386	2132.7415	911.5547	1221.1869	-1.37
H1.4	KPAAGAAKK (159-168)	Lys167 - C	ACCC-NH3	698.5844	3	2092.7297	2092.7353	911.5547	1181.1807	-2.69
		Lys167 - C	ACC-NH3	602.2365	3	1803.6860	1803.6890	911.5547	892.1343	-1.65
		Lys167 - C	AAC-NH3	610.2402	3	1827.6971	1827.7003	911.5547	916.1456	-1.74
		Lys174/Lys176 - C	ACCG-NH3	516.4416	4	2061.7351	2061.7408	840.5540	1221.1869	-2.79
H1.4	KAKAAKPK (174-181) (likely co-elution of 2 cross-links)	Lys174/Lys176 - C	ACCC-NH3	674.9178	3	2021.7299	2021.7346	840.5540	1181.1807	-2.33
		Lys174/Lys176 - C	ACT-NH3	583.5688	3	1747.6829	1747.6880	840.5540	907.1340	-2.91
		Lys191 - C	ACT-NH3	550.2144	3	1647.6197	1647.6243	740.4903	907.1340	-2.78
		Lys191 - C	ACGT-NH3	659.8982	3	1976.6711	1976.6768	740.4903	1236.1866	-2.89
H1.4	AKAVKPK (190-196)	Lys191 - C	CCG-NH3	550.5467	3	1648.6166	1648.6195	740.4903	908.1292	-1.75
		Lys191 - C	CGT-NH3	555.5461	3	1663.6148	1663.6192	740.4903	923.1289	-2.63
		Lys196 - C	CGT-NH3	654.2748	3	1959.8009	1959.8041	1036.6752	923.1289	-1.62
		Lys196 - C	AACT-NH3	565.2228	4	2256.8599	2256.8668	1036.6752	1220.1917	-3.08
H1.4	AVKPKAAKPK (192-201)	Lys196 - C	ACGT-NH3	569.2213	4	2272.8539	2272.8617	1036.6752	1236.1866	-3.45
		Lys196 - C	ACG-NH3	657.2778	3	1968.8099	1968.8157	1036.6752	932.1405	-2.94
		Lys201 - C	ACCG-NH3	565.9667	4	2259.8355	2259.8412	1038.6544	1221.1869	-2.54
		Lys201 - C	CCT-NH3	961.8959	2	1921.7762	1921.7771	1038.6544	883.1227	-0.50
H1.4	AAKPKTAKPK (197-206)	Lys201 - C	AAC-NH3	652.6061	3	1954.7948	1954.8000	1038.6544	916.1456	-2.65
		Lys201 - C	ACC-NH3	644.6018	3	1930.7819	1930.7887	1038.6544	892.1343	-3.51
		Lys206 - C	ACT-H2O	649.2745	3	1944.8000	1944.8044	1038.6544	906.1500	-2.25
		Lys206 - C	ACCT-H2O	745.6240	3	2233.8485	2233.8507	1038.6544	1195.1964	-0.99
H1.4	TAKPKAAKPK (202-211)	Lys206 - C	CCCG-NH3	746.2853	3	2235.8324	2235.8299	1038.6544	1197.1756	1.11
		Lys206 - C	AACC-NH3	561.9680	4	2243.8407	2243.8463	1038.6544	1205.1920	-2.52

Annotated MS/MS spectra of linker histone H1.4

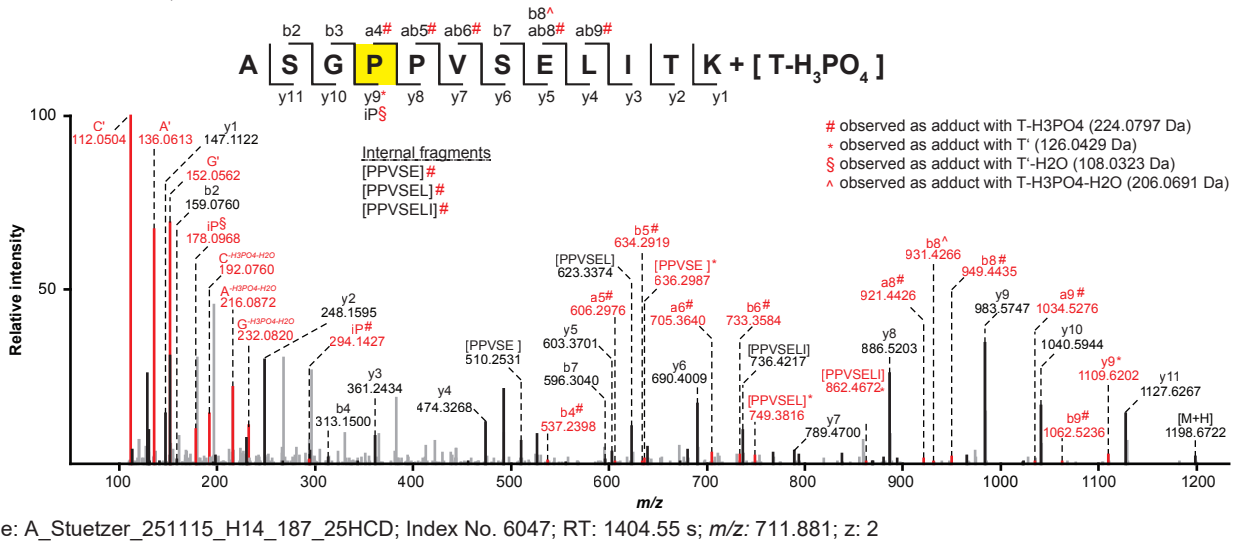
1) Histone H1.4, aa 33-45



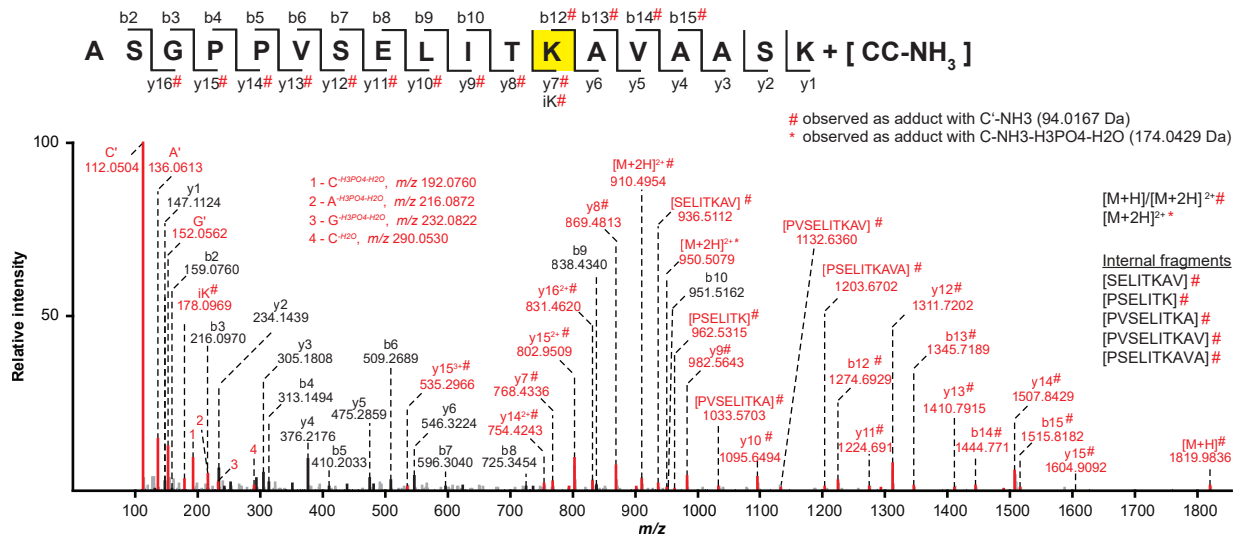
2) Histone H1.4, aa 33-45



3) Histone H1.4, aa 34-45

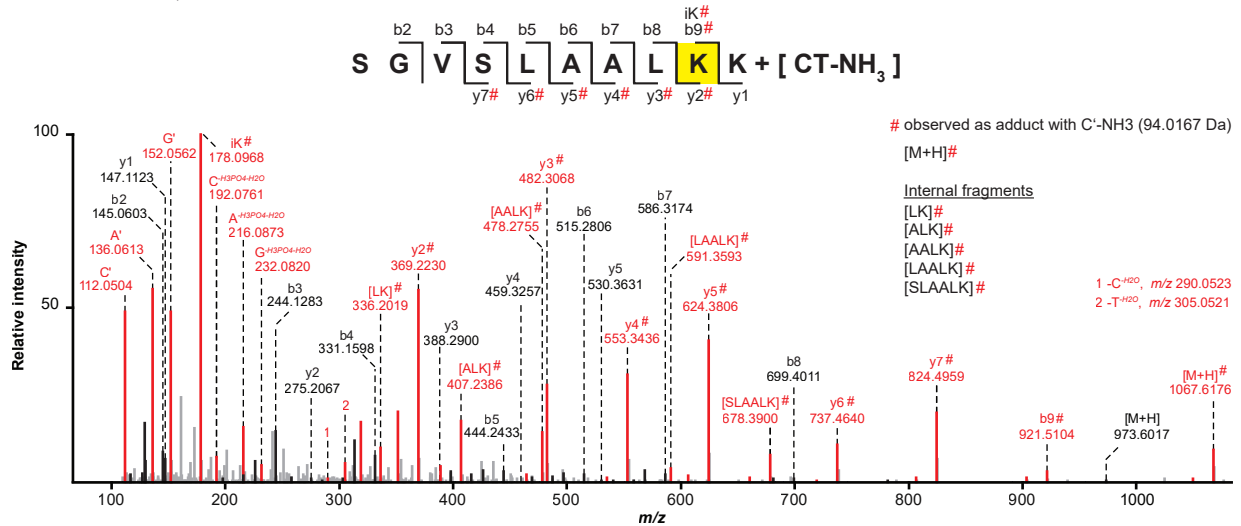


4) Histone H1.4, aa 34-51



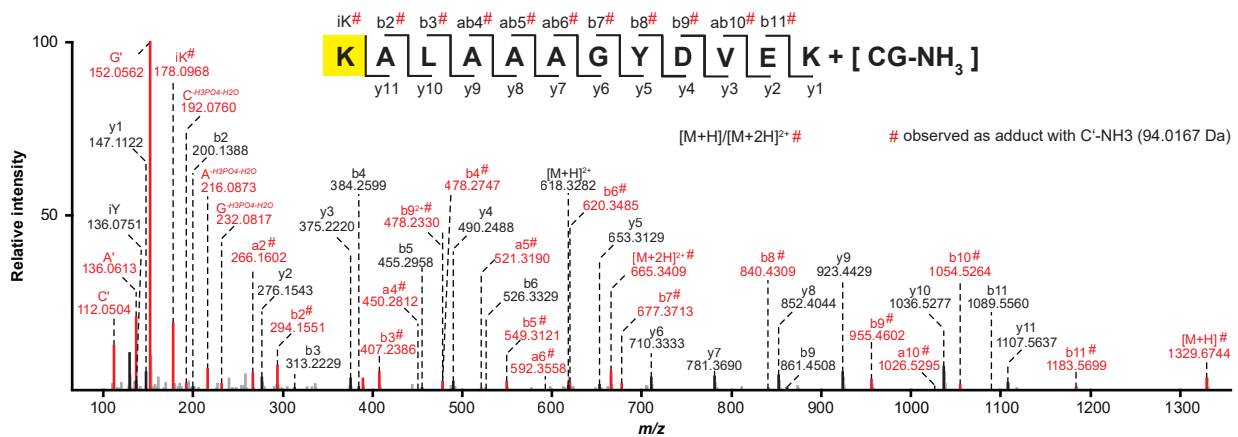
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5) Histone H1.4, aa 54-63



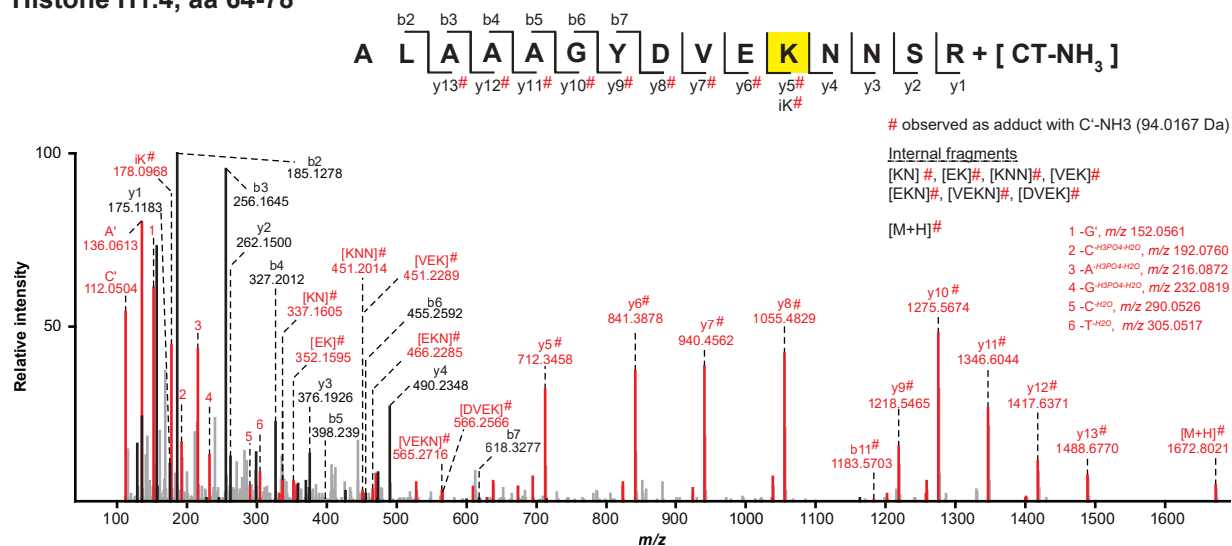
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6) Histone H1.4, aa 63-74



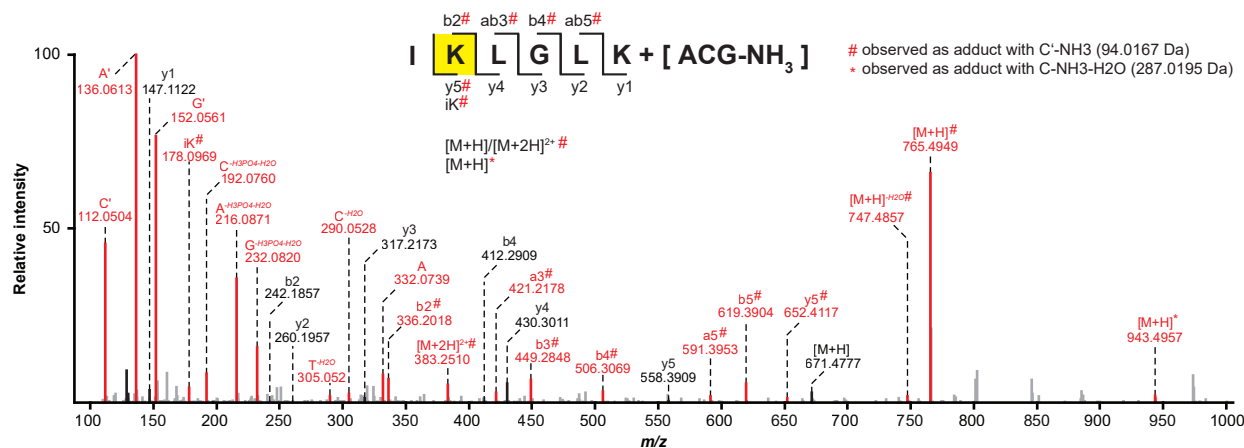
File: A_Stuetzer_251115_H14_187_25HCD; Index No. 5153; RT: 1245.88 s; m/z: 618.919; z: 3

7) Histone H1.4, aa 64-78



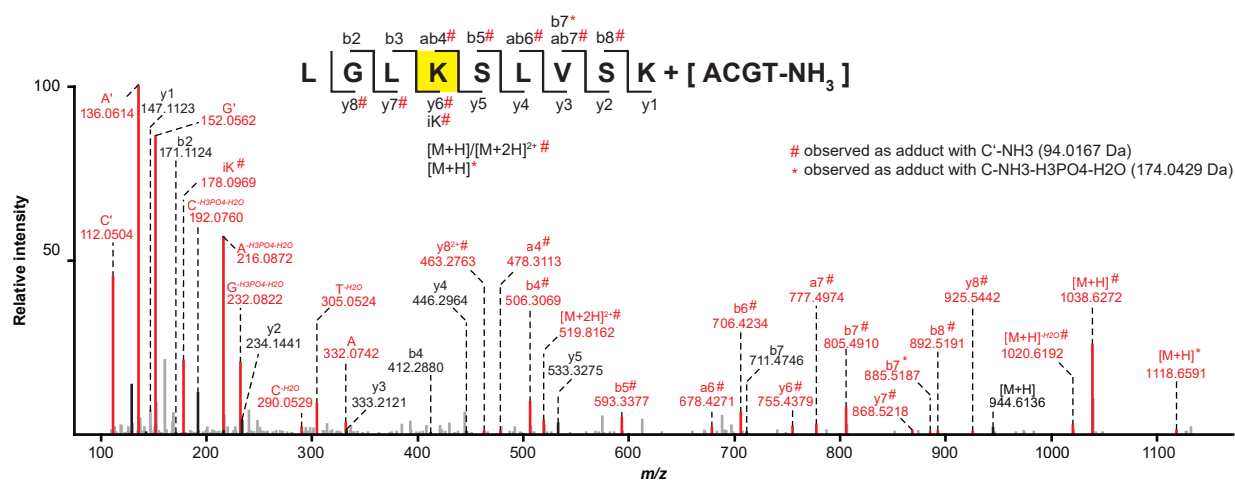
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8) Histone H1.4, aa 79-84



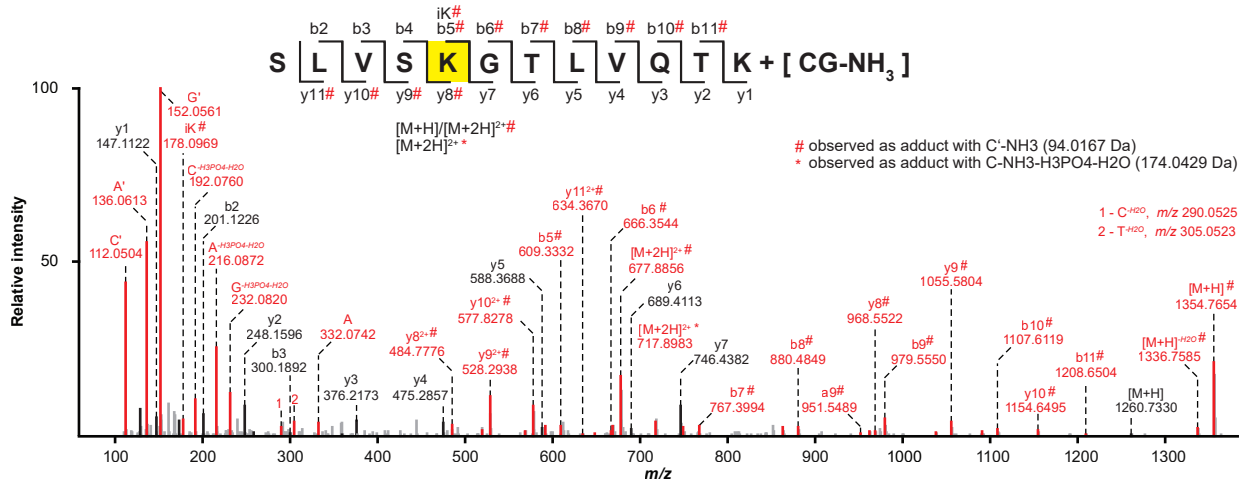
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9) Histone H1.4, aa 81-89



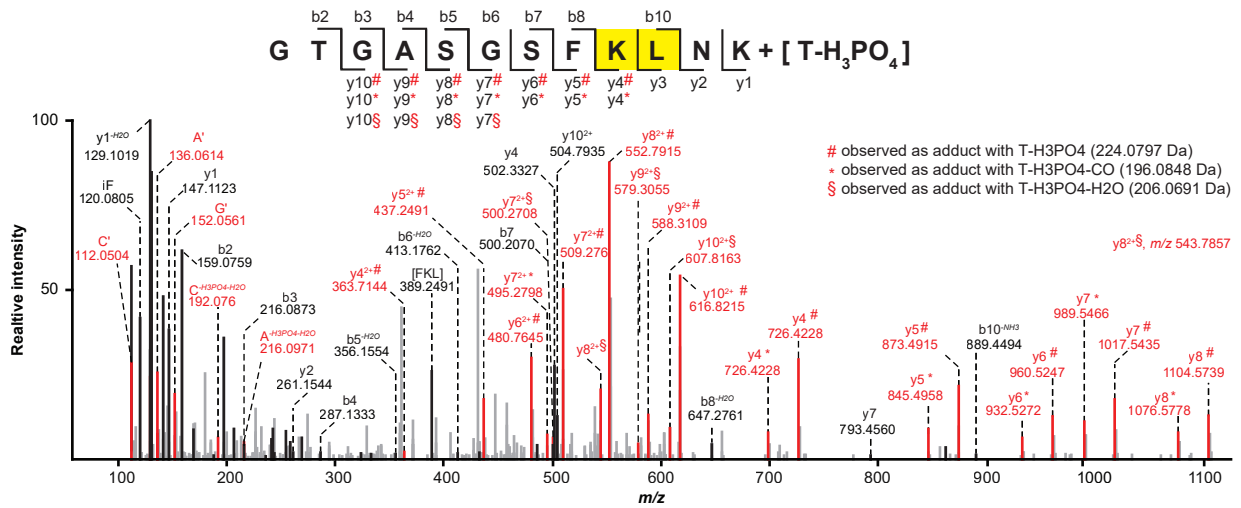
File: A_Stuetzer_251115_H14_187_30HCD; Index No. 6896; RT: 1571.62 s; m/z: 1090.907; z: 2

10) Histone H1.4, aa 85-96



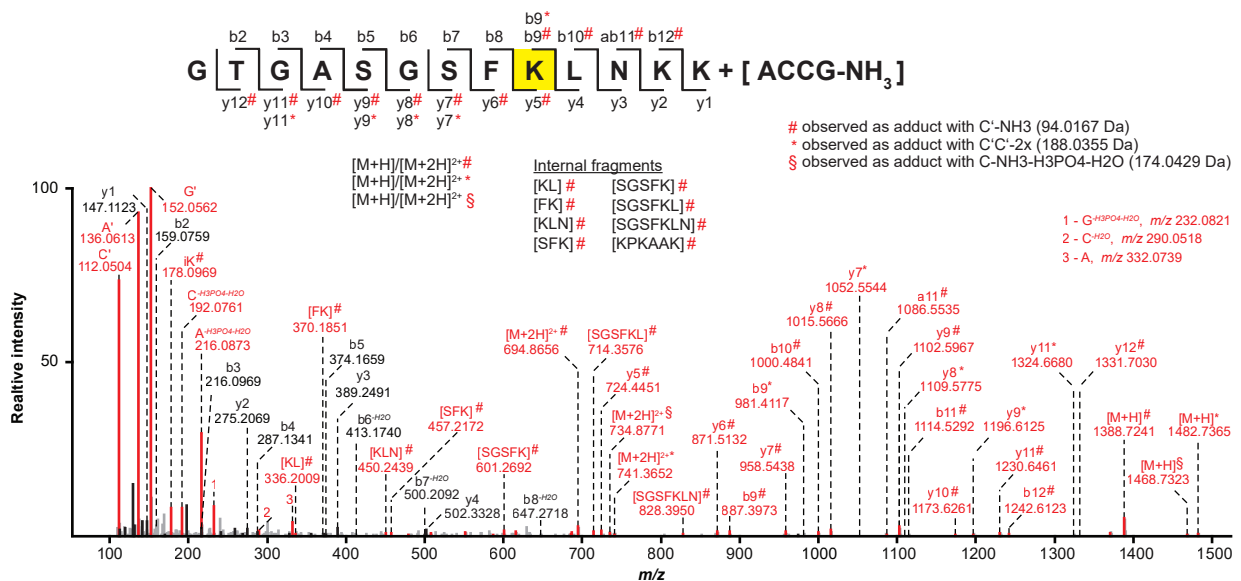
File: A_Stuetzer_251115_H14_187_25HCD; Index No. 5645; RT: 1331.96 s; m/z: 940.4194; z: 2

11) Histone H1.4, aa 97-108



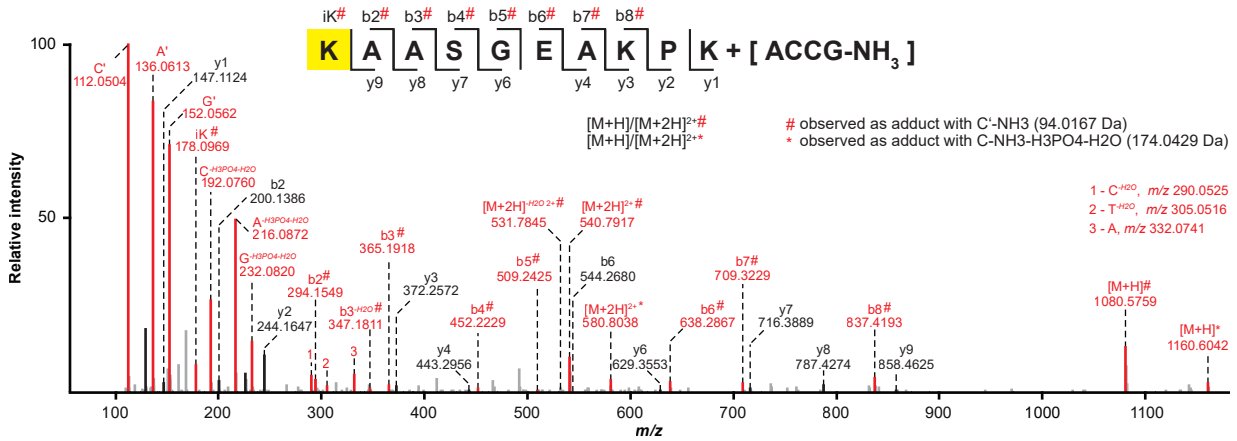
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12) Histone H1.4, aa 97-109



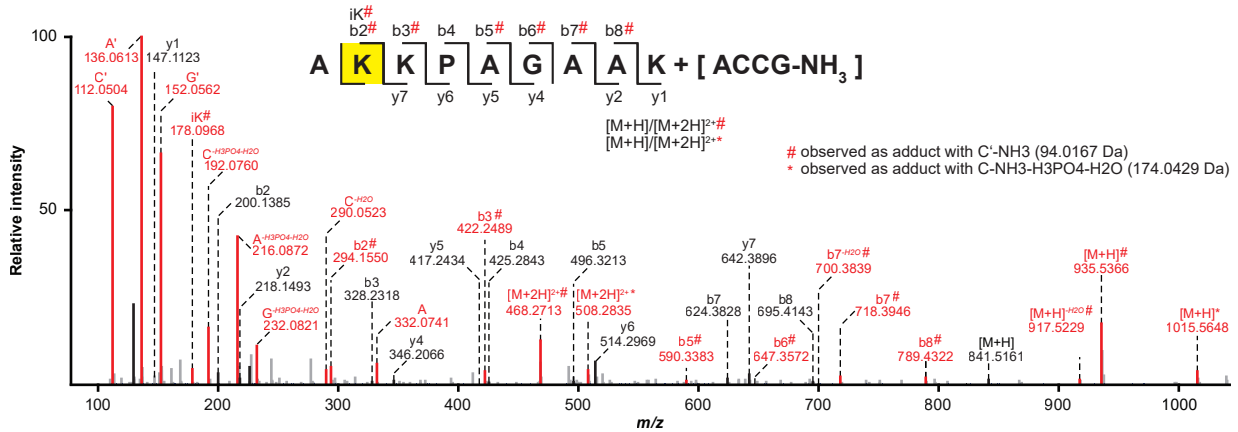
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13) Histone H1.4, aa 109-118



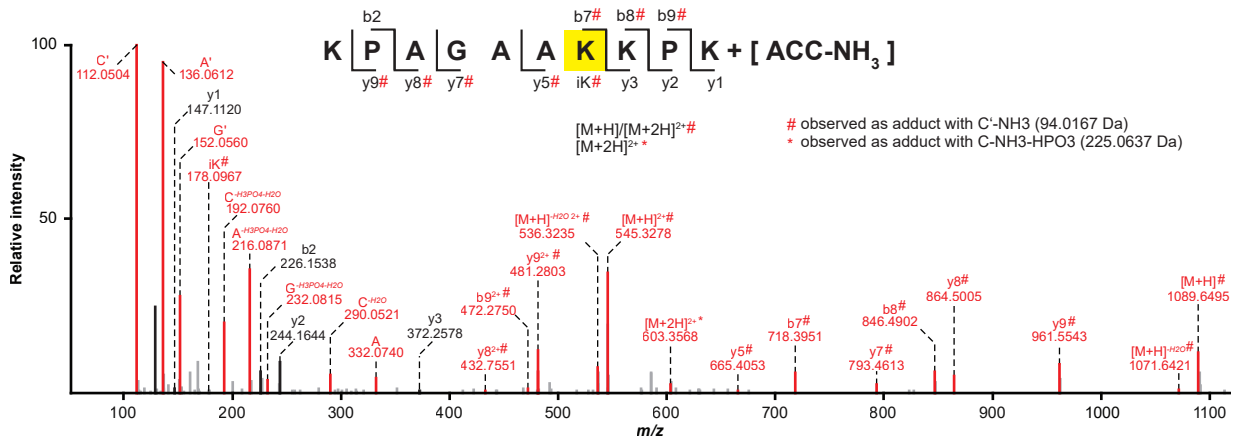
File: A_Stuetzer_251115_H14_187_25HCD; Index No. 3061; RT: 875.201 s; m/z: 736.586; z: 3

14) Histone H1.4, aa 127-135



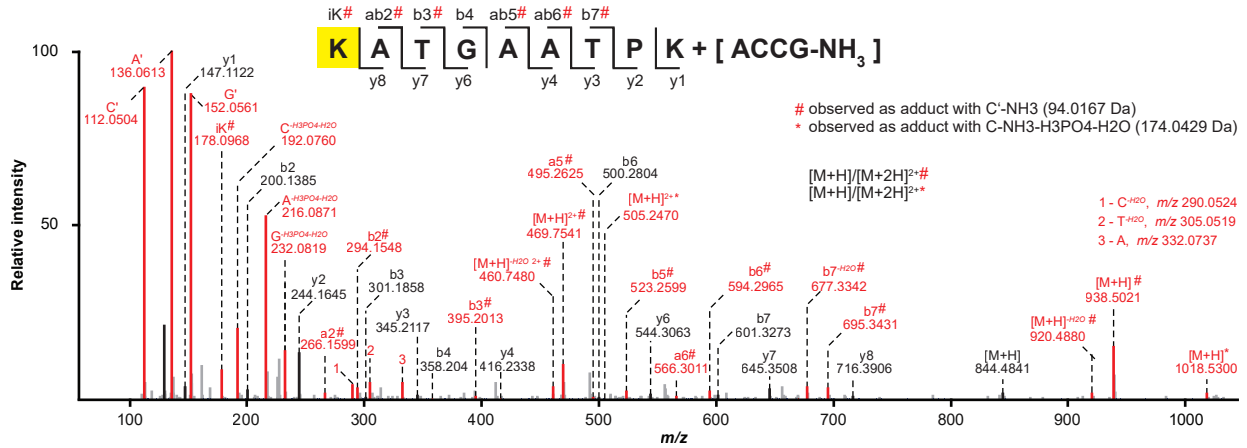
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15) Histone H1.4, aa 129-138

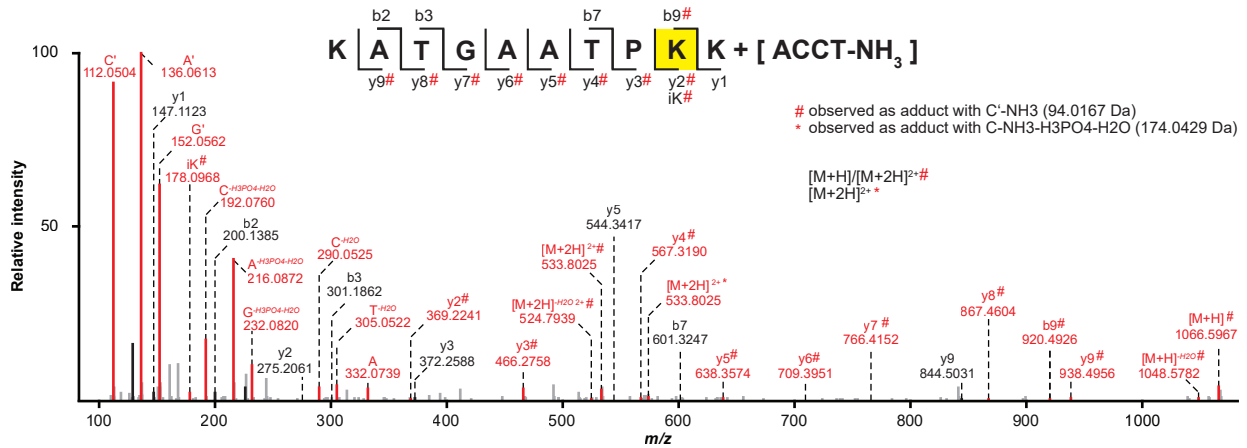


File: A_Stuetzer_251115_H14_187_25HCD; Index No. 2944; RT: 893.932 s; m/z: 629.927; z: 3

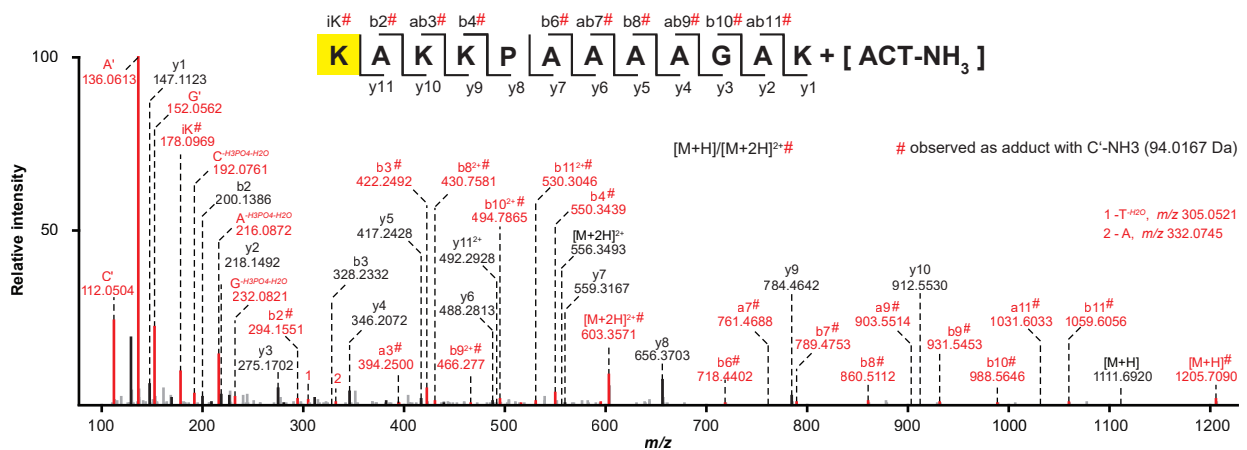
16) Histone H1.4, aa 139-147



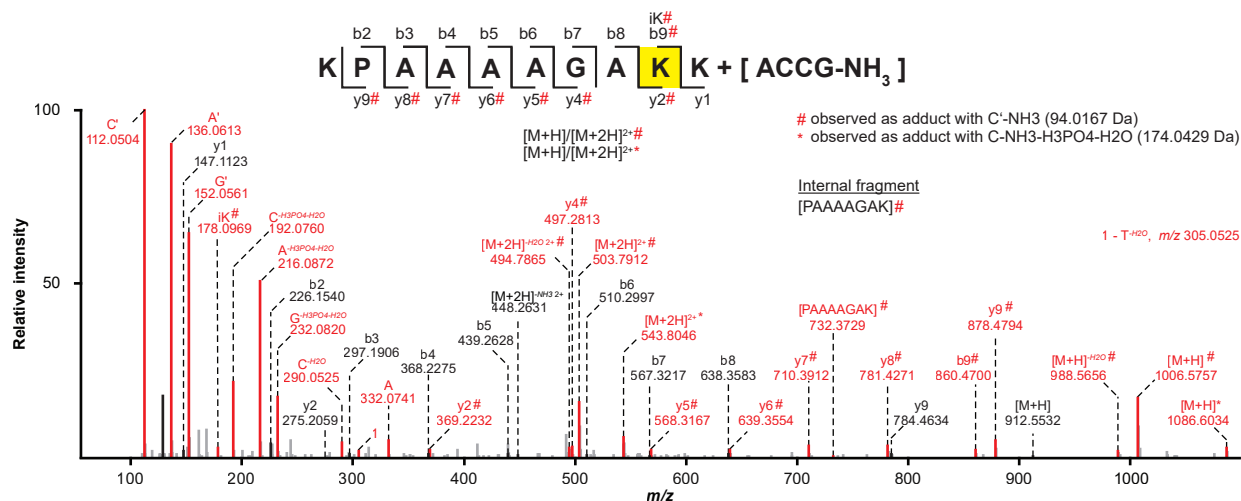
17) Histone H1.4, aa 139-148



18) Histone H1.4, aa 156-167

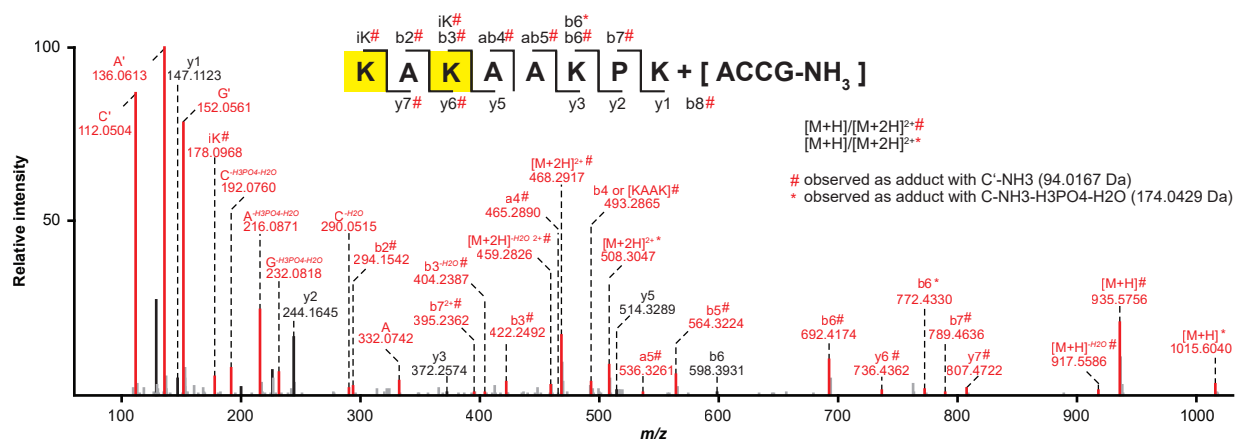


19) Histone H1.4, aa 159-168



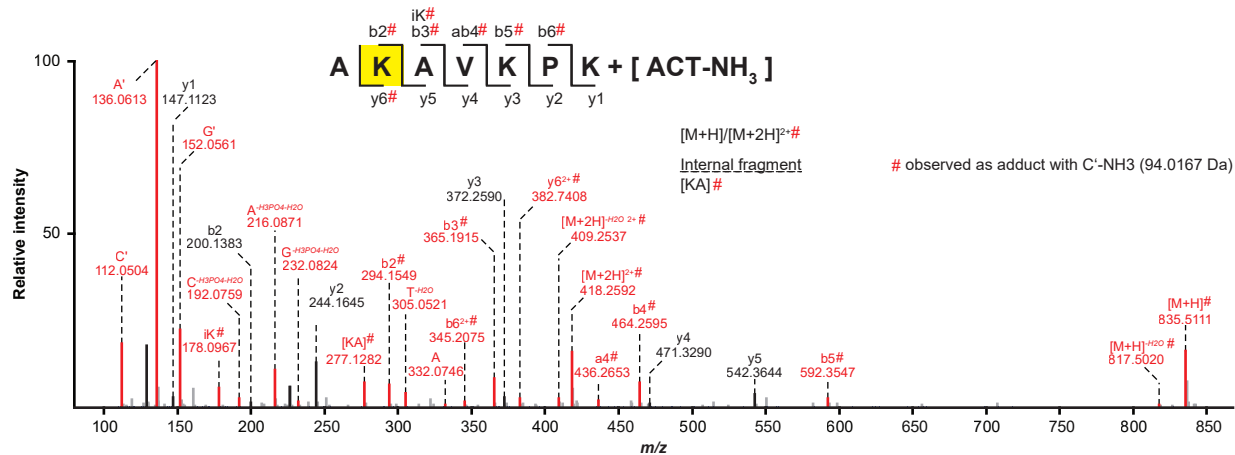
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20) Histone H1.4, aa 174-181



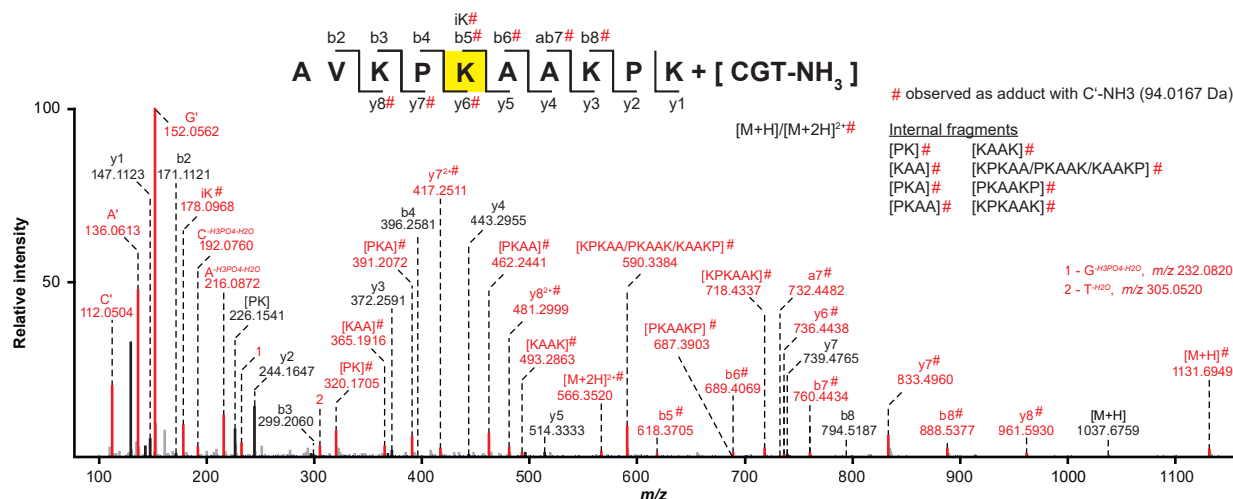
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21) Histone H1.4, aa 190-196



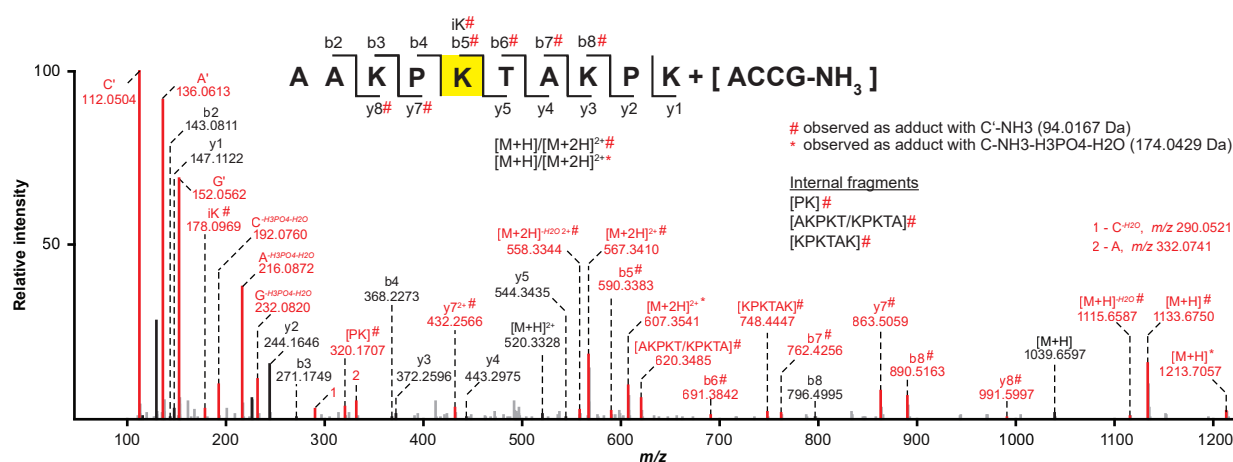
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22) Histone H1.4, aa 192-201



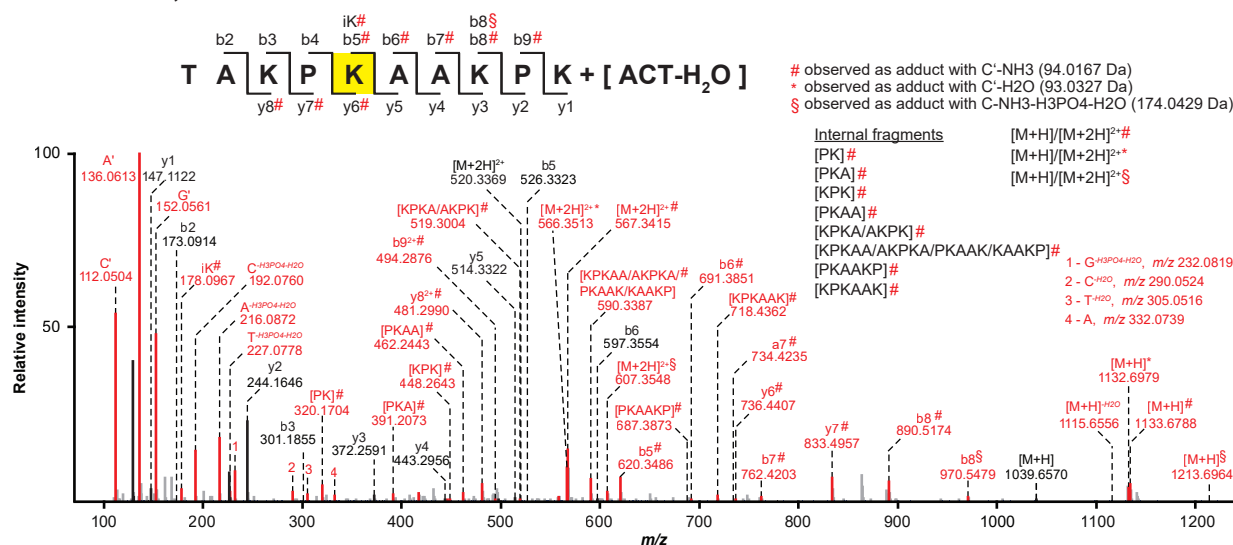
File: ; Index No. ; RT: s; m/z: 550.214; z: 3

23) Histone H1.4, aa 197-206



File: A_Stuetzer_251115_H14_187_25HCD; Index No. 3077; RT: 878.068 s; m/z: 565.967; z: 4

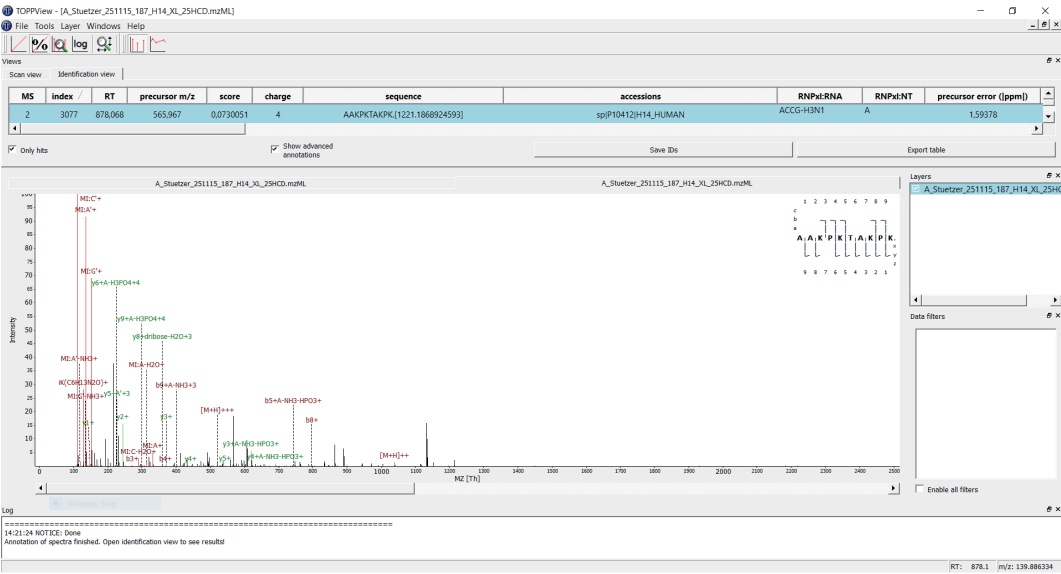
24) Histone H1.4, aa 202-211



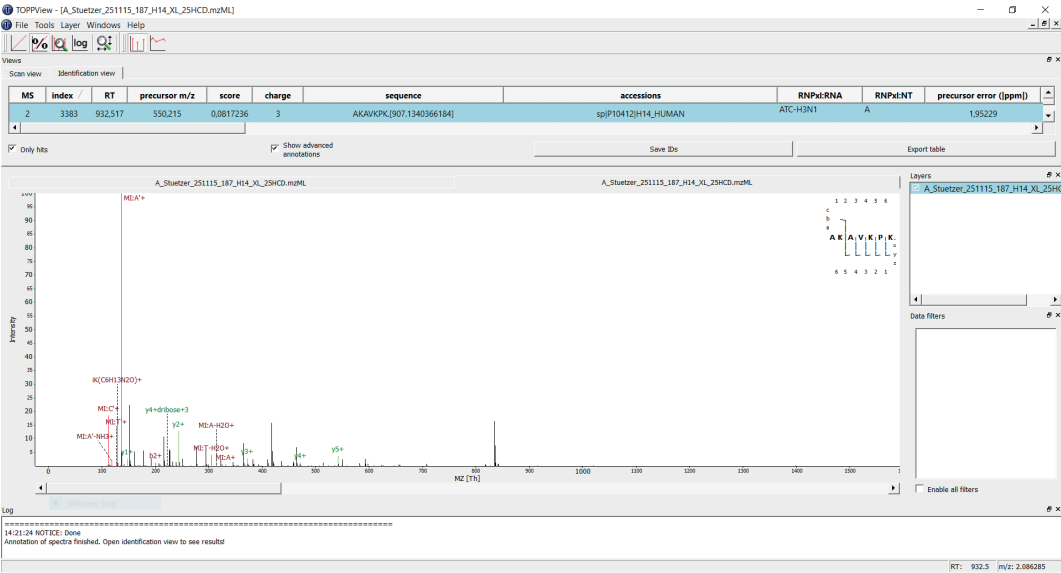
File: ; Index No. ; RT: s; m/z: 649.275; z: 3

TOPPView spectra of Linker histone H1.4

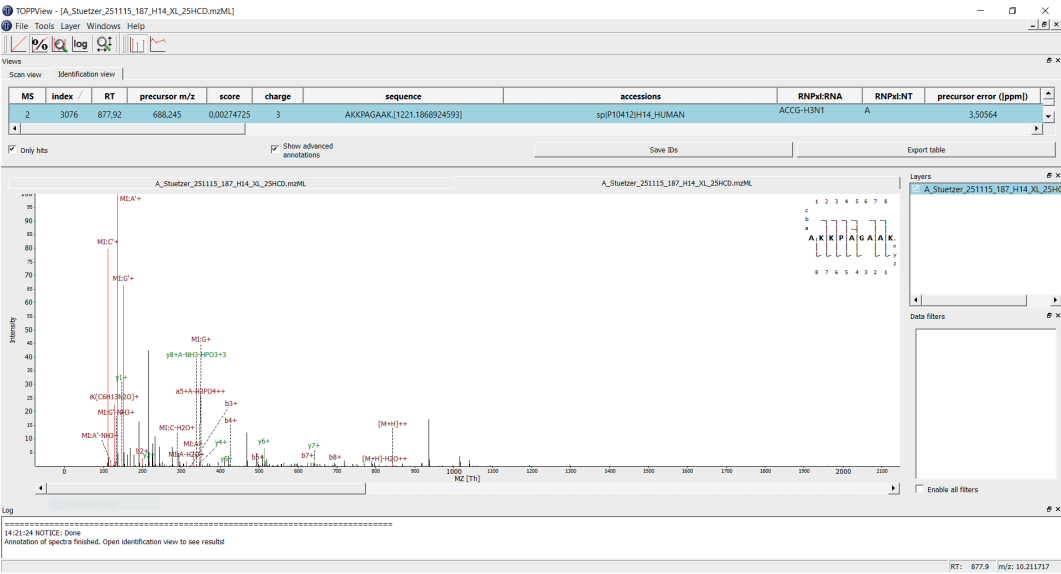
1)



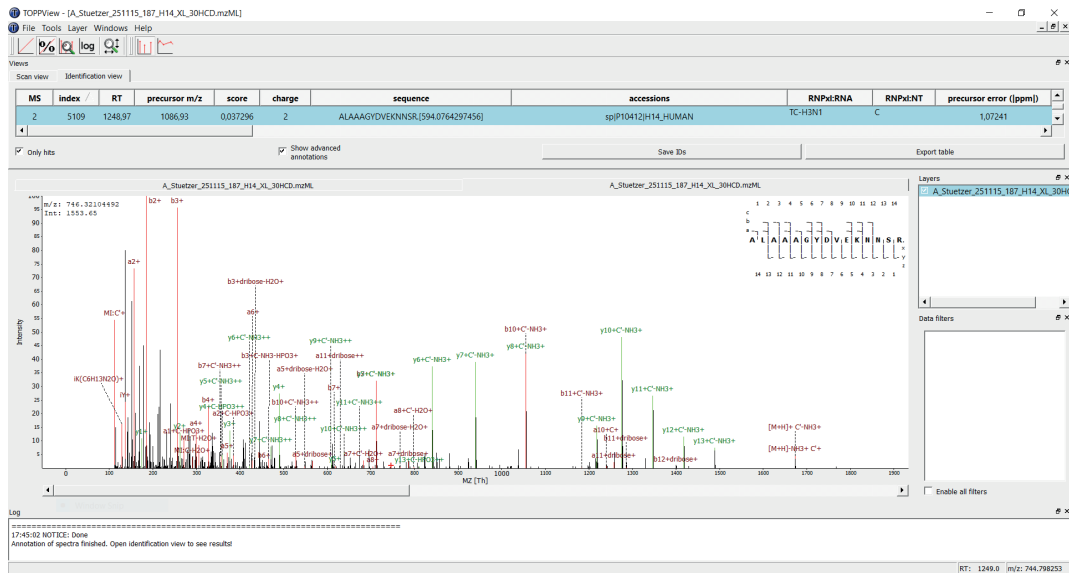
2)



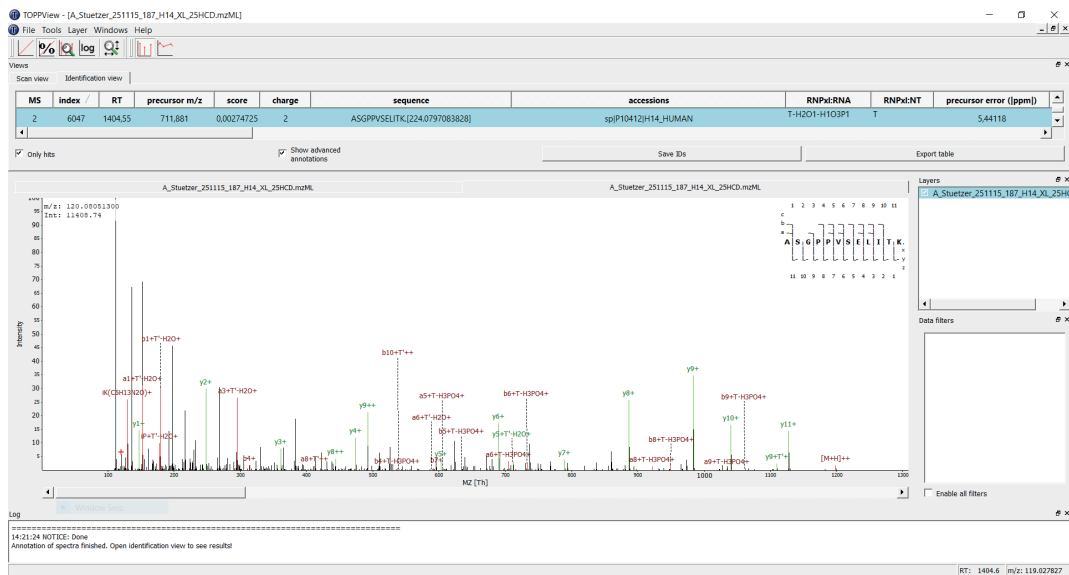
3)



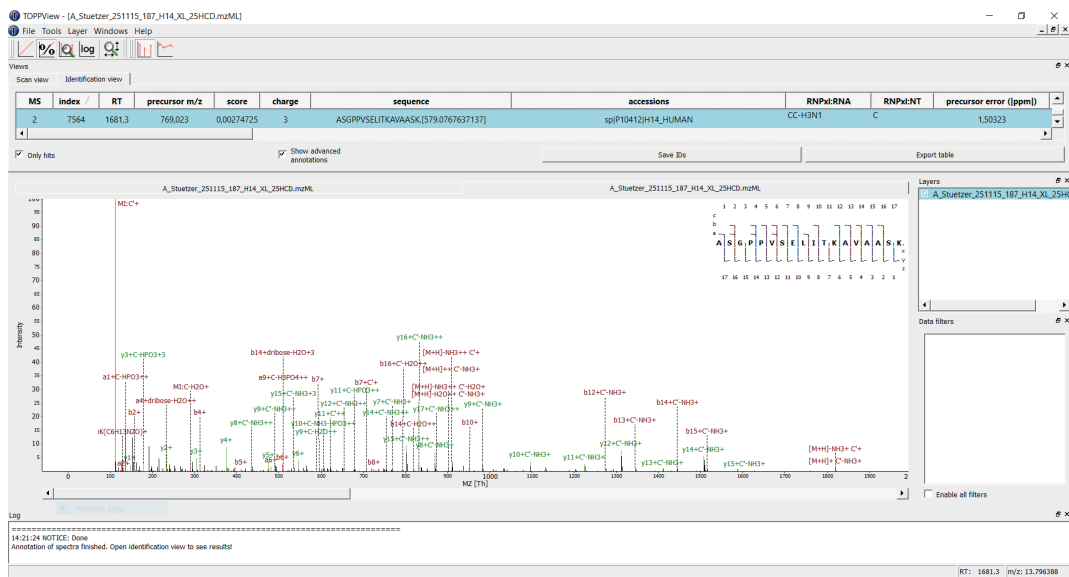
4)



5)



6)



TOPView - [A_Stuetzer_251115_187_H14_XL_20HCD.msML]

File Tools Layers Settings Help

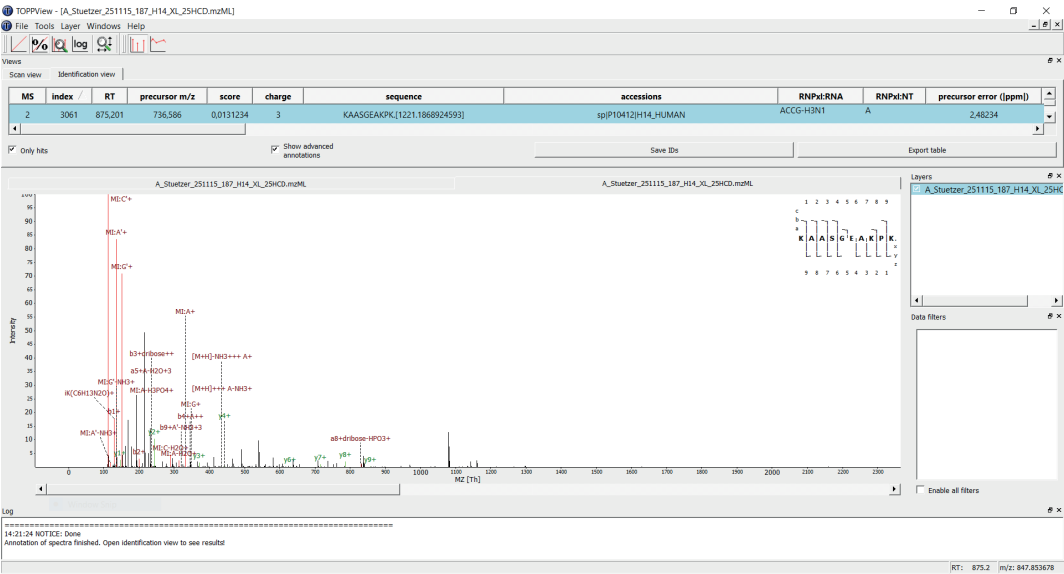
Views: Scan view Identification view

MS	Index	RT	precursor m/z	score	charge	sequence	accessions	RNPe:RNA	RNPe:NT	precursor error (ppm)
2	4436	1096.92	464.239	0.0785563	3	GTGASGSFKLNK[224.0797083828]	sp P10412 H14_HUMAN	T-H201-H103P1	T	4.34446

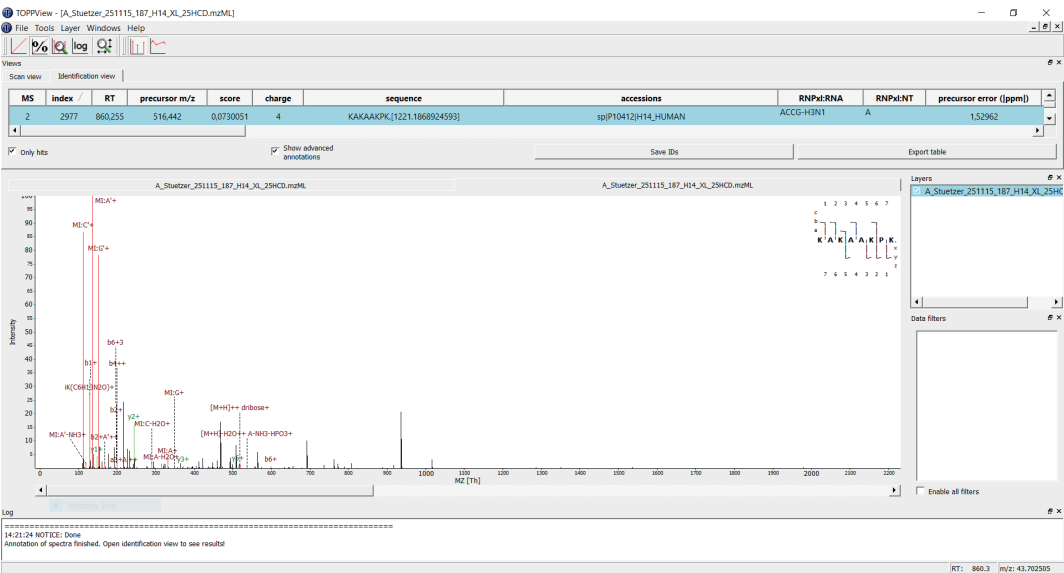
☒ Only hits ☒ Show advanced annotations

[illegible][illegible]

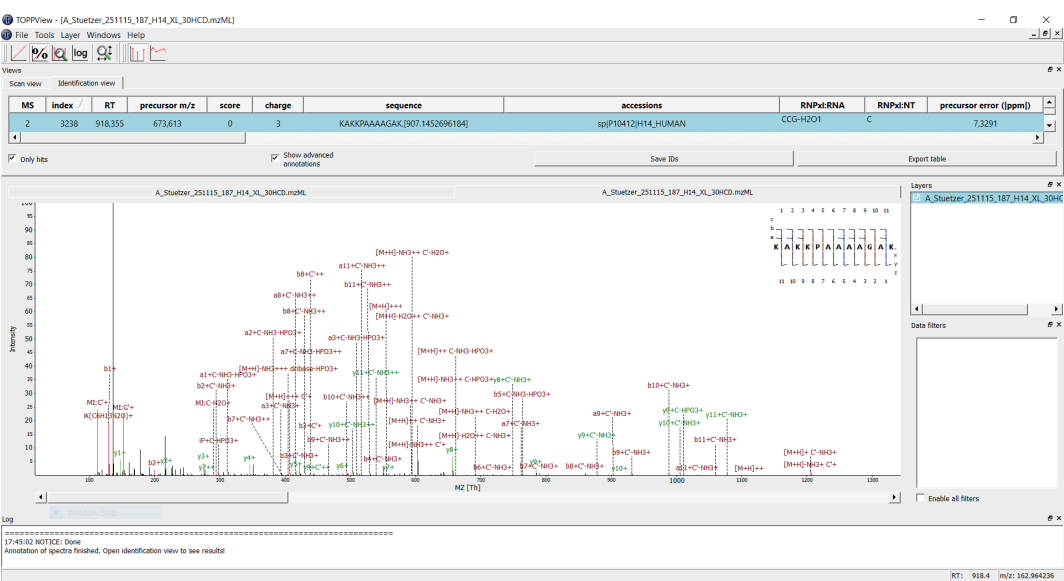
10)



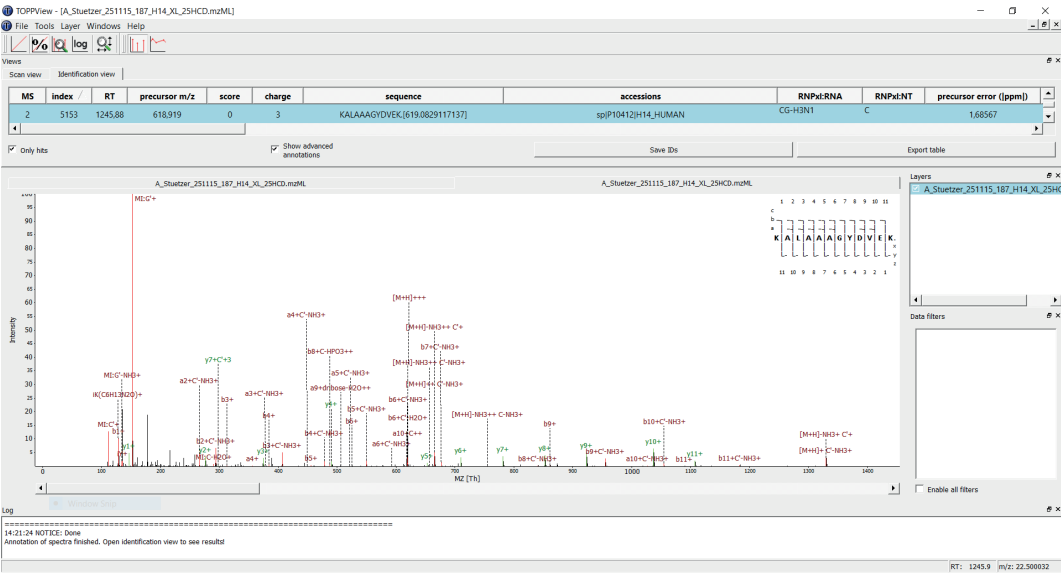
11)



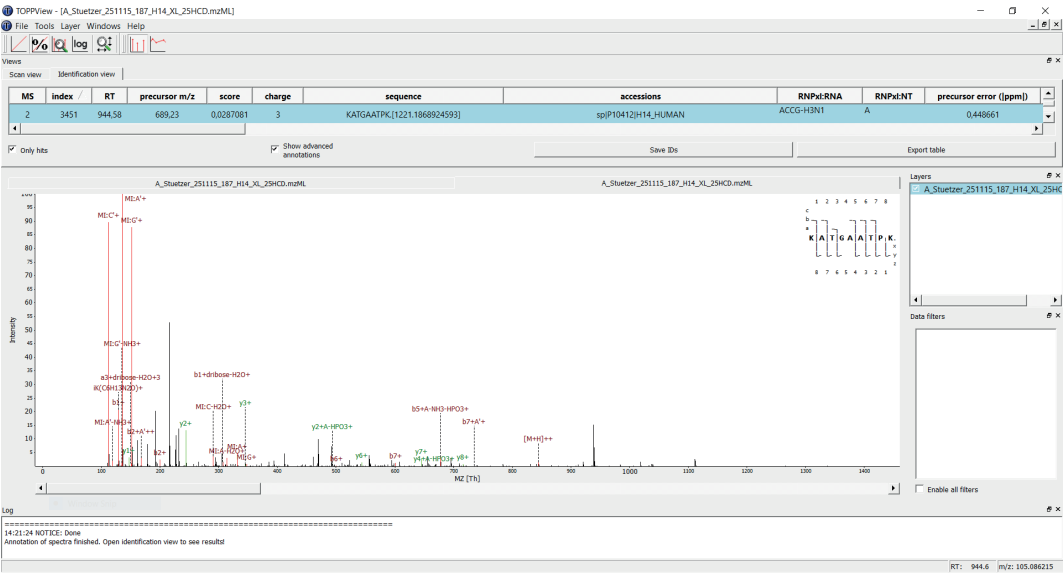
12)



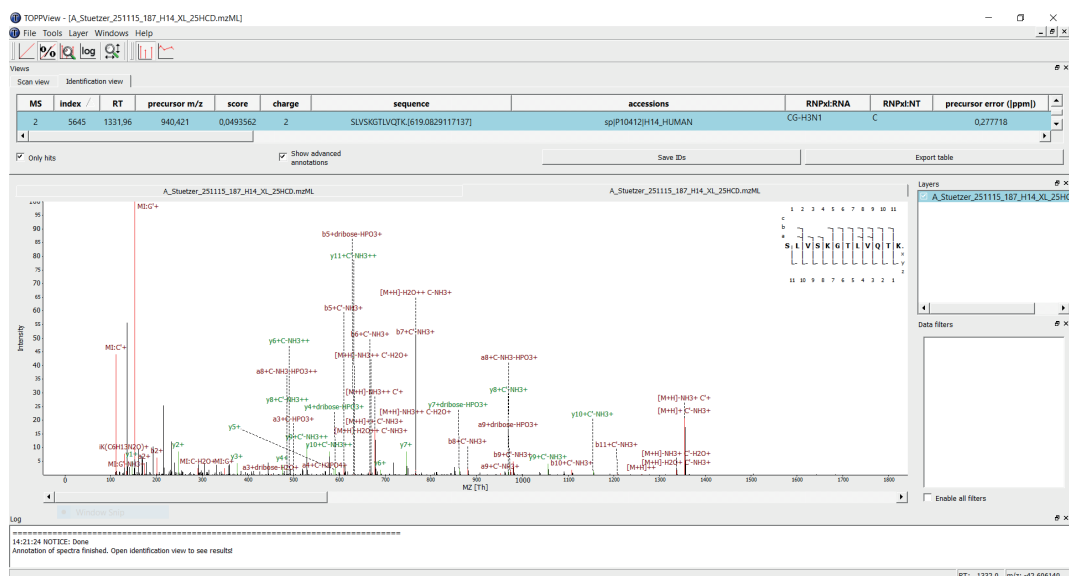
13)



16)



19)

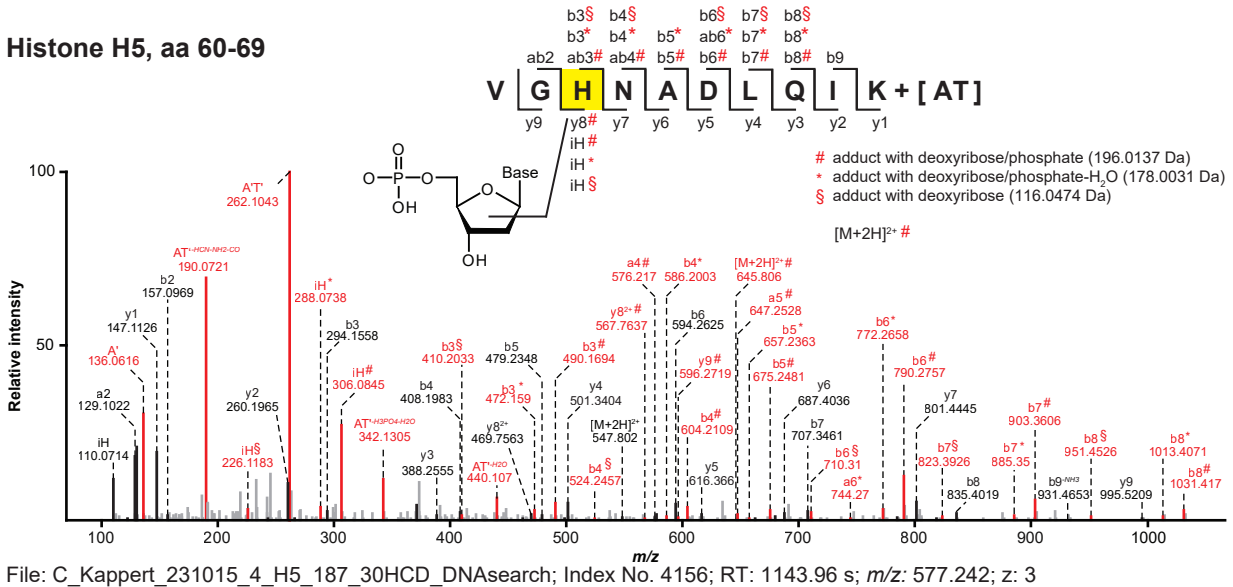


Linker histone H5

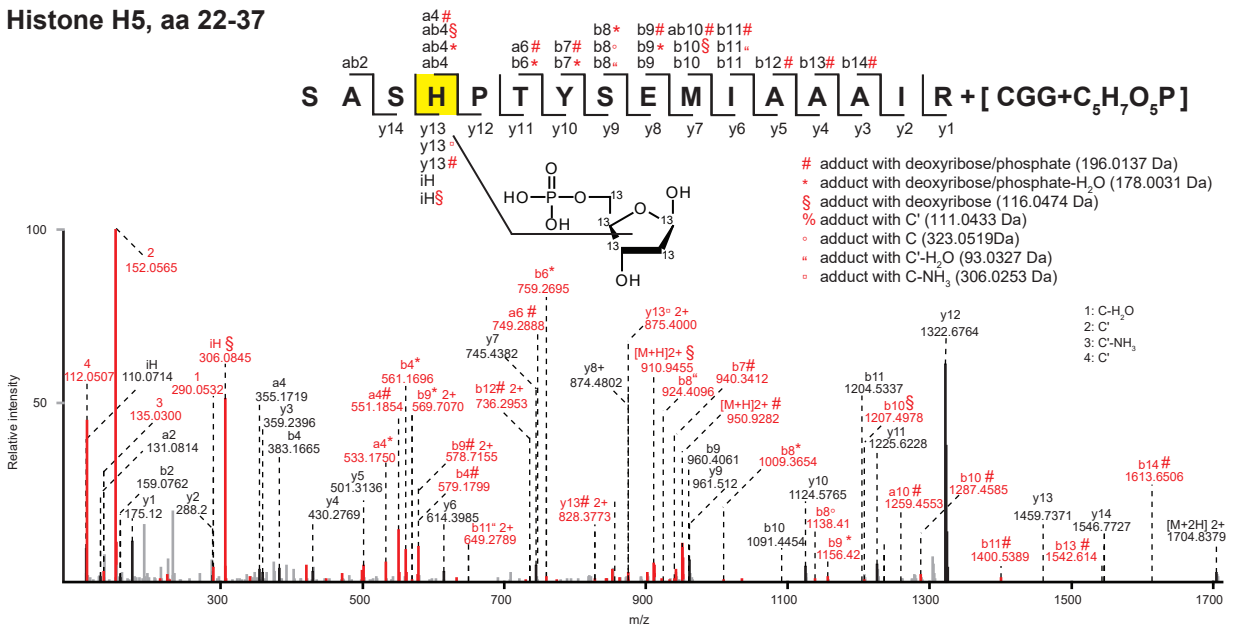
protein	peptide (aa)	cross-link site (aa - base/sugar)	DNA	m/z _{exp}	z	cross-link MW _{exp}	cross-link MW _{calc}	peptide MW _{calc}	DNA MW _{calc}	Δ ppm
H5	SASHPTYSEMAAAIR (22-37)	His25 - deoxyrib.	CGG+C5H7O5P	950.0063	3	2846.9954	2846.9947	1703.8296	1143.1651	0.27
		His25 - deoxyrib.	ACT+C5H7O5P	936.3387	3	2805.9926	2805.9933	1703.8296	1102.1637	-0.22
		His25 - deoxyrib.	C+C5H7O5P	1095.4534	2	2188.8912	2188.8896	1703.8296	485.0600	0.72
		His25 - deoxyrib.	A-C5H5N5 (=C5H9O6P)	950.9295	2	1899.8434	1899.8433	1703.8296	196.0137	0.03
H5	VGHNADLQIK (60-69)	His62 - deoxyrib.	AT	577.2418	3	1728.7019	1728.7017	1703.8296	635.1142	0.12
		His62 - deoxyrib.	CC+C5H7O5P	623.5733	3	1867.6964	1867.6938	1703.8296	774.1063	1.40
		His62 - deoxyrib.	ACC+C5H7O5P	727.9250	3	2180.7515	2180.7515	1703.8296	1087.1640	0.03
		His62 - deoxyrib.	GT+C5H7O5P	962.3581	2	1922.7006	1922.6997	1703.8296	829.1122	0.43

Annotated MS/MS spectra of linker histone H5

1) Histone H5, aa 60-69



2) Histone H5, aa 22-37

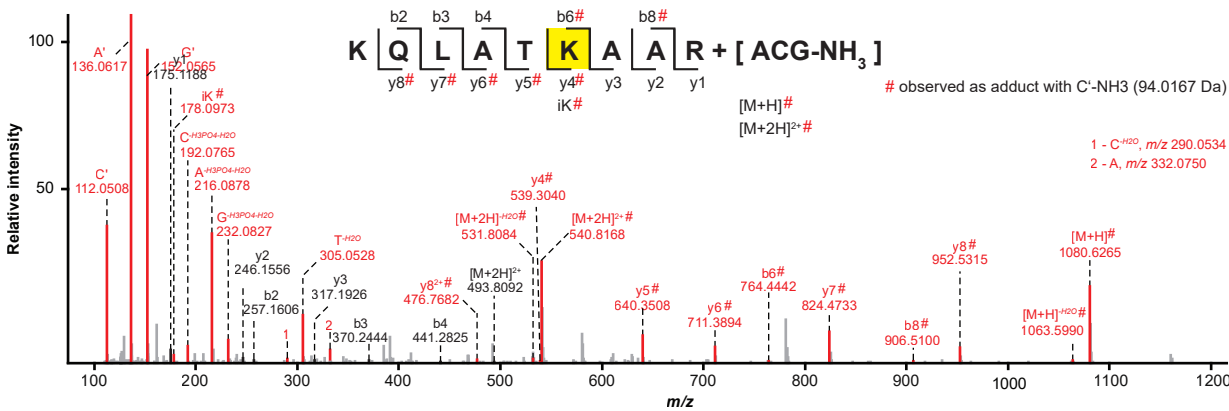


Histone H3

protein	peptide (aa)	cross-link site (aa - base/sugar)	DNA	m/z _{exp}	z	cross-link MW _{exp}	cross-link MW _{calc}	peptide MW _{calc}	DNA MW _{calc}	Δ ppm
H3	KQLATKAAR (18-26)	Lys23 - C	ACG-NH3	640.2553	3	1917.7424	1917.7432	985.6027	932.14053	-0.41
		Lys23 - C	CT-NH3	790.8479	2	1579.6802	1579.6791	985.6027	594.07639	0.69
		Lys23 - C	CCGT-NH3	733.6006	3	2197.7783	2197.7779	985.6027	1212.1753	0.17
		Lys23 - C	CCCG-NH3	728.6011	3	2182.7798	2182.7782	985.6027	1197.1756	0.72
H3	KSAPATGGVK (27-36)	Lys27 - C	ACG-NH3	616.5604	3	1846.6577	1846.6585	914.5180	932.14053	-0.42
		Lys27 - C	AC-NH3	506.8767	3	1517.6066	1517.6060	914.5180	603.08799	0.43
		Lys27 - C	CT-NH3	755.3050	2	1508.5944	1508.5944	914.5180	594.07639	-0.01
		Lys27 - C	CCG-NH3	608.5570	3	1822.6475	1822.6472	914.5180	908.12923	0.18
H3	YRPGTVLR (41-49)	Tyr41 - T	AT	556.5752	3	1666.7021	1666.7013	1031.5871	635.1142	0.49
		Tyr41 - T	TT	829.8544	2	1657.6932	1657.6897	1031.5871	626.1026	2.07
		Tyr41 - T	AATT-HPO3	551.9673	4	2203.8379	2203.8387	1031.5871	1172.2516	-0.35
		Tyr41 - T	ACGT	762.6077	3	2284.7996	2284.8002	1031.5871	1253.2131	-0.25
H3	YQKSTELLIR (54-63)	Lys56 - C	ACT-NH3	719.9533	3	2156.8364	2156.8365	1249.7025	907.13403	-0.04
		Lys56 - C	CT-NH3	922.8987	2	1843.7818	1843.7789	1249.7025	594.07639	1.56
		Lys56 - C	ACCG-NH3	824.6379	3	2470.8902	2470.8893	1249.7025	1221.1869	0.36
		Lys56 - C	CG-NH3	935.4019	2	1868.7882	1868.7854	1249.7025	619.08289	1.49
H3	KLPFQR (64-69)	Lys64 - C	AC-NH3	696.2867	2	1390.5578	1390.5579	787.4699	603.0880	-0.08
		Lys64 - C	CCT	563.5478	3	1687.6199	1687.6192	787.4699	900.14928	0.46
		Lys64 - C	CT-NH3	691.7808	2	1381.5460	1381.5463	787.4699	594.07639	-0.23
		Lys64 - C	ACCG-NH3	670.5587	3	2008.6526	2008.6567	787.4699	1221.1869	-2.05
H3	EIAQDFKTLR (74-83)	Lys79 - C	CT-NH3	965.3860	2	1928.7564	1928.7589	1334.6825	594.07639	-1.30
		Lys79 - C	CCCG-NH3	844.9614	3	2531.8607	2531.8580	1334.6825	1197.1756	1.06
		Lys79 - C	ACGT-NH3	857.9668	3	2570.8769	2570.8690	1334.6825	1236.1866	3.07
		Lys79 - C	CCG-H2O	748.2809	3	2241.8192	2241.8277	1334.6825	907.1452	-3.78
H3	VTIMPKDIQLAR (117-128)	Lys122 - C	CCG-NH3	764.9806	3	2291.9183	2291.9195	1383.7903	908.1292	-0.51
		Lys122 - C	CCTT	863.6687	3	2587.9826	2587.9856	1383.7903	1204.1953	-1.15
		Lys122 - C	ACCC-NH3	856.0003	3	2564.9774	2564.9709	1383.7903	1181.1807	2.53
		Lys122 - C	CCCG-NH3	861.3287	3	2580.9626	2580.9658	1383.7903	1197.1756	-1.25

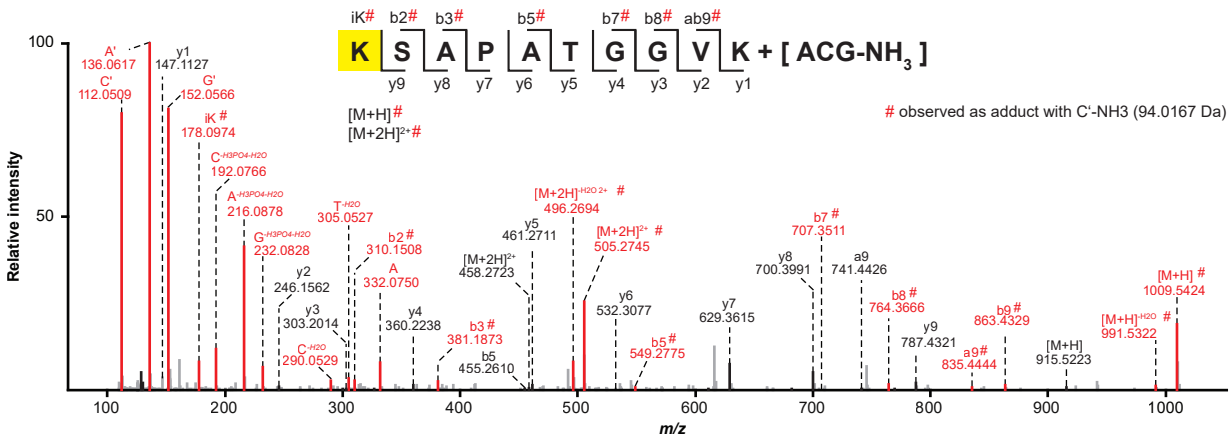
Annotated MS/MS spectra of core histone H3

1) Histone H3, aa 18-26



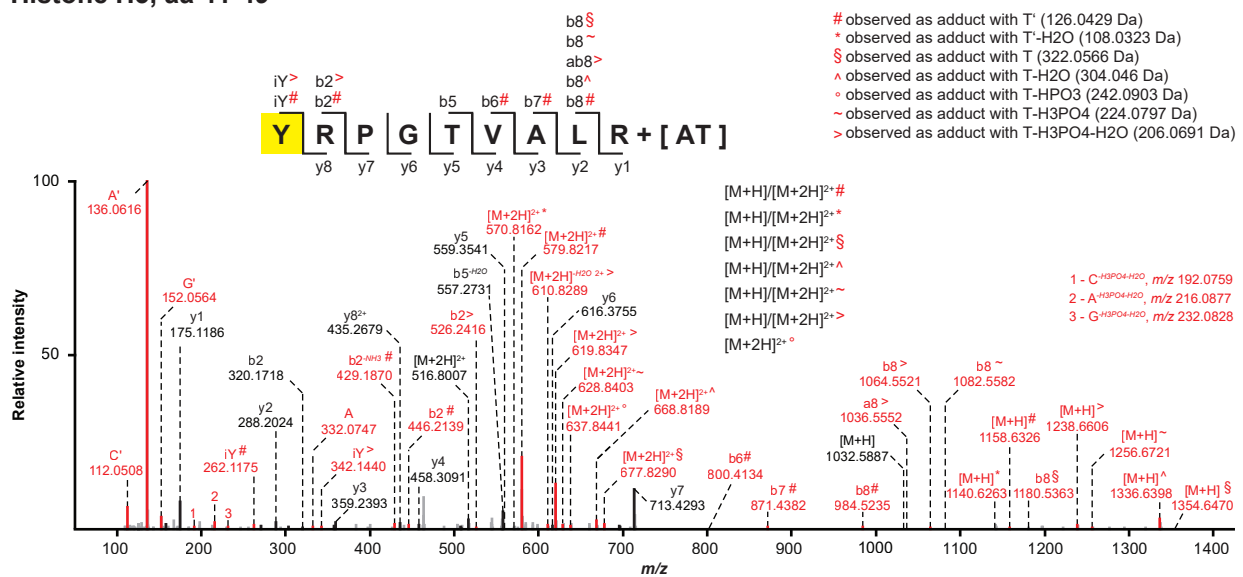
File: A_Stuetzer_180816_12mer_H14_UV_25mM; Index No. 6077; RT: 1162.38 s; m/z: 640.256; z: 3

2) Histone H3, aa 27-36



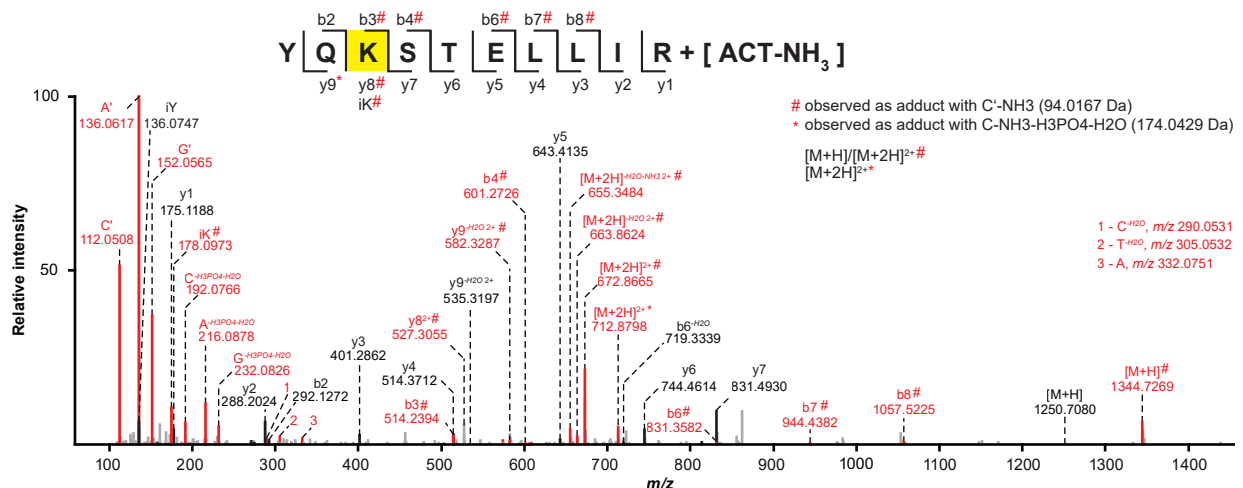
File: A_Stuetzer_180816_12mer_H14_UV_25mM; Index No. 6069; RT: 1161.26 s; m/z: 616.56; z: 3

3) Histone H3, aa 41-49



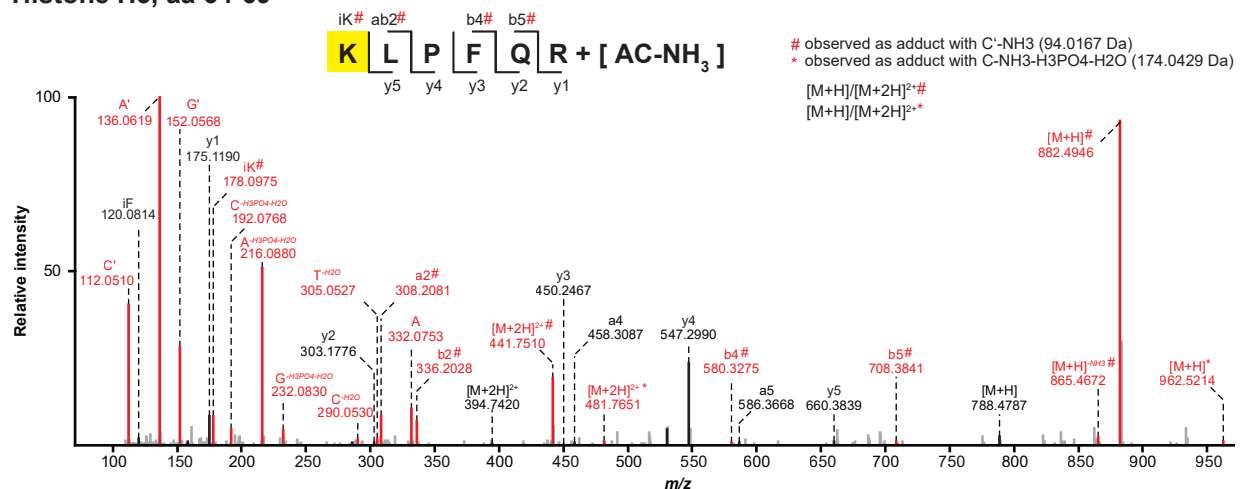
File: A_Stuetzer_180816_12mer_UV_150mM; Index No. 8469; RT: 1551.76 s; m/z: 556.575; z: 3

4) Histone H3, aa 54-63



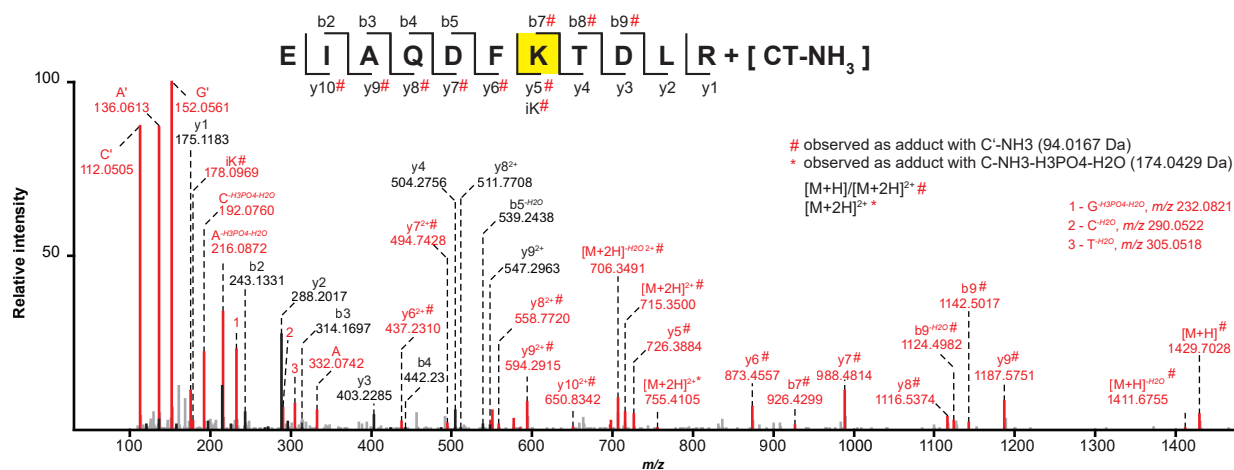
File: A_Stuetzer_180816_12mer_UV_25mM; Index No. 12150; RT: 2092.87 s; m/z: 719.953; z: 3

5) Histone H3, aa 64-69



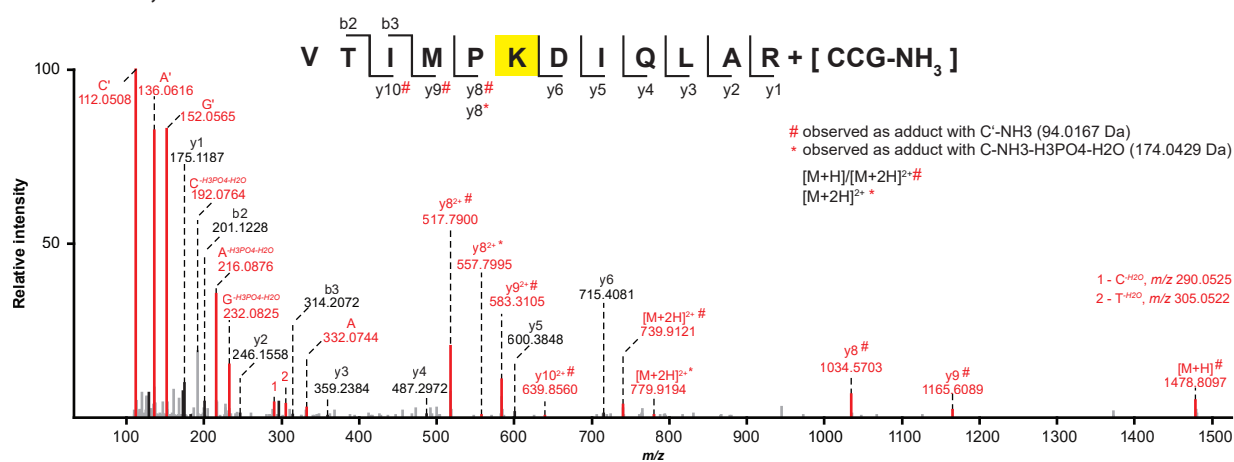
File: A_Stuetzer_180816_12mer_UV_150mM; Index No. 10471; RT: 1849.7 s; m/z: 696.287; z: 2

6) Histone H3, aa 73-83



File: A_Stuetzer_180816_12mer_H14_UV_150mM; Index No. 12808; RT: s; m/z: ; z:

7) Histone H3, aa 117-128



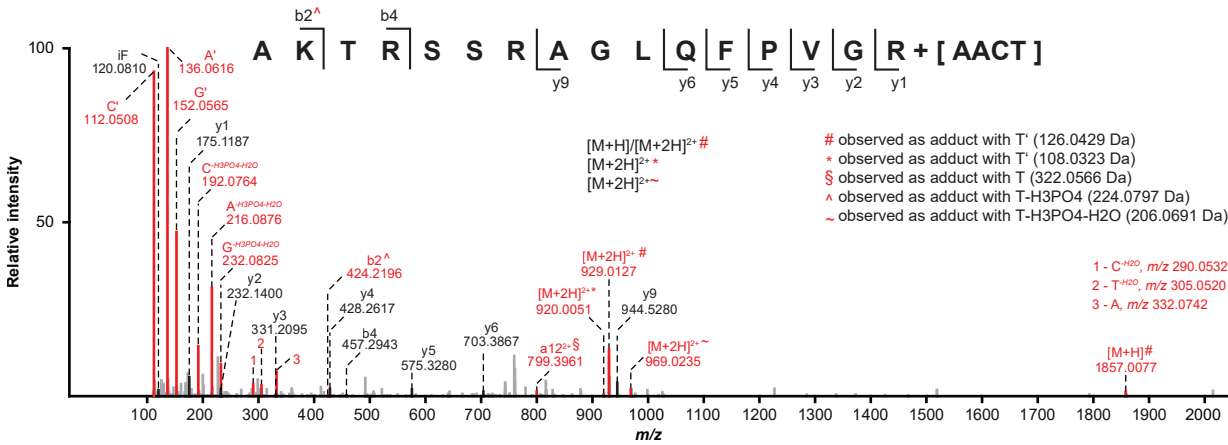
File: A_Stuetzer_180816_12mer_H14_UV_150mM; Index No. 13760; RT: 2335.68 s; m/z: 764.961; z: 3

Histone H2A

protein	peptide (aa)	cross-link site (aa - base/sugar)	DNA	m/z _{exp}	z	cross-link MW _{exp}	cross-link MW _{calc}	peptide MW _{calc}	DNA MW _{calc}	Δ ppm
H2A	AKTRSSRAGLQFPVGR (14-29)	(n/d) - T	AACT	742.8054	4	2967.1903	2967.1877	1729.9695	1237.2182	0.88
		(n/d) - T	CCGT	987.4012	3	2959.1801	2959.1713	1729.9695	1229.2018	2.98
		(n/d) - T	CGT	891.0502	3	2670.1271	2670.1250	1729.9695	940.1555	0.81
H2A	HLQLAVR (82-88)	His82 - deoxyrib.	CCT	579.5580	3	1735.6505	1735.6516	835.5023	900.1493	-0.59
		His82 - deoxyrib.	AAA	598.5699	3	1792.6862	1792.6858	835.5023	957.1835	0.26
		His82 - deoxyrib.	AT	491.2130	3	1470.6155	1470.6165	835.5023	635.1142	-0.67
		His82 - deoxyrib.	ACT	587.5614	3	1759.6607	1759.6629	835.5023	924.1606	-1.21
H2A	NDEELNKLGR (89-99)	Lys95 - C	CCCG-NH3	833.2941	3	2496.8588	2496.8533	1299.6778	1197.1756	2.19
		Lys95 - C	CCC-NH3	723.6083	3	2167.8014	2167.8008	1299.6778	868.1230	0.29
		Lys95 - C	ACCG-NH3	841.2941	3	2520.8588	2520.8646	1299.6778	1221.1869	-2.31
		Lys95 - C	ACCC-NH3	827.9618	3	2480.8619	2480.8584	1299.6778	1181.1807	1.40
H2A	VTIAQGGVLPNIQSVLLPKK (100-119)	Lys118 - C	AC-NH3	893.4549	3	2677.3412	2677.3389	2074.2509	603.0880	0.88
		Lys118 - C	ACC-NH3	989.8029	3	2966.3852	2966.3852	2074.2509	892.1343	0.01
		Lys118 - C	CCG-NH3	995.1349	3	2982.3812	2982.3801	2074.2509	908.1292	0.38
		Lys118 - C	CGT-NH3	1000.1380	3	2997.3905	2997.3798	2074.2509	923.1289	3.58

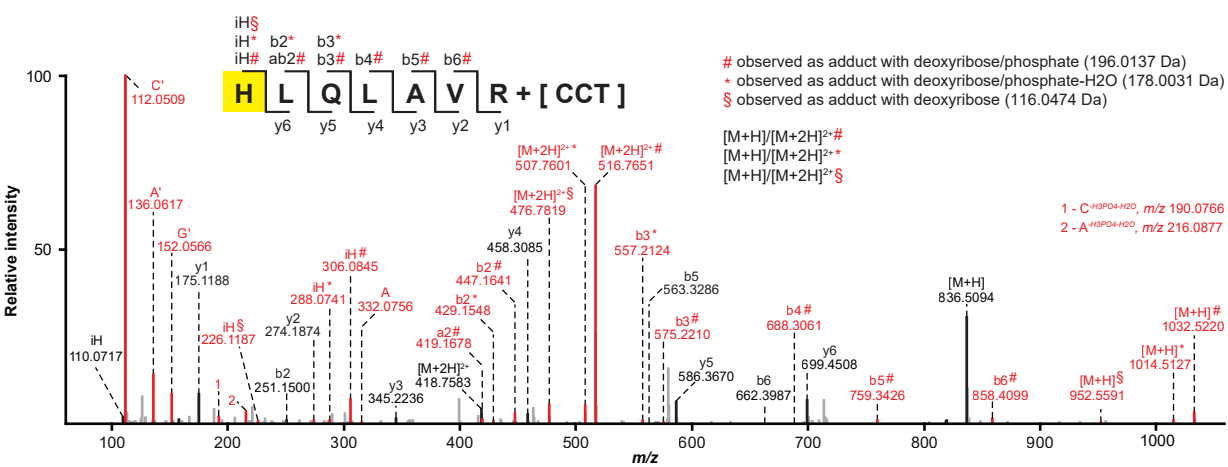
Annotated MS/MS spectra of core histone H2A

1) Histone H2A, aa 14-29



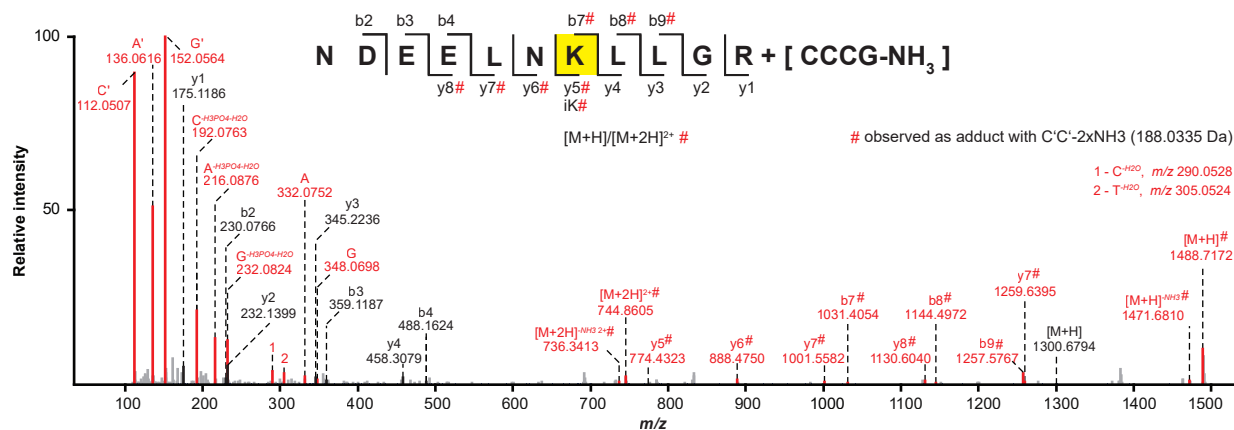
File: A_Stuetzer_180816_12mer_UV_25mM; Index No. 14124; RT: 2390.01 s; m/z: 743.307; z: 4

2) Histone H2A, aa 82-88

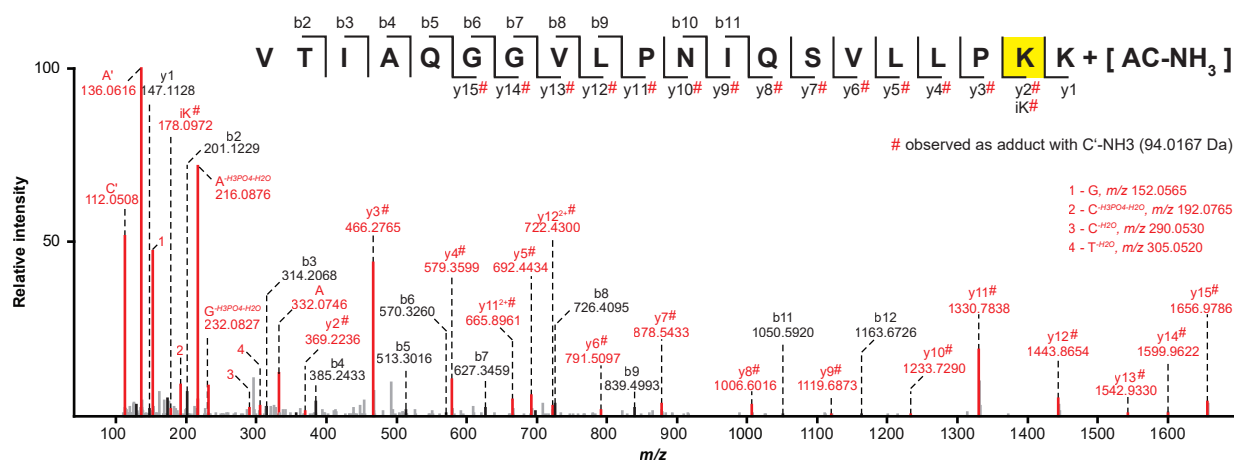


File: A_Stuetzer_180816_12mer_UV_25mM; Index No. 8662; RT: 1579.42 s; m/z: 579.559; z: 3

3) Histone H2A, aa 89-99



4) Histone H2A, aa 100-119

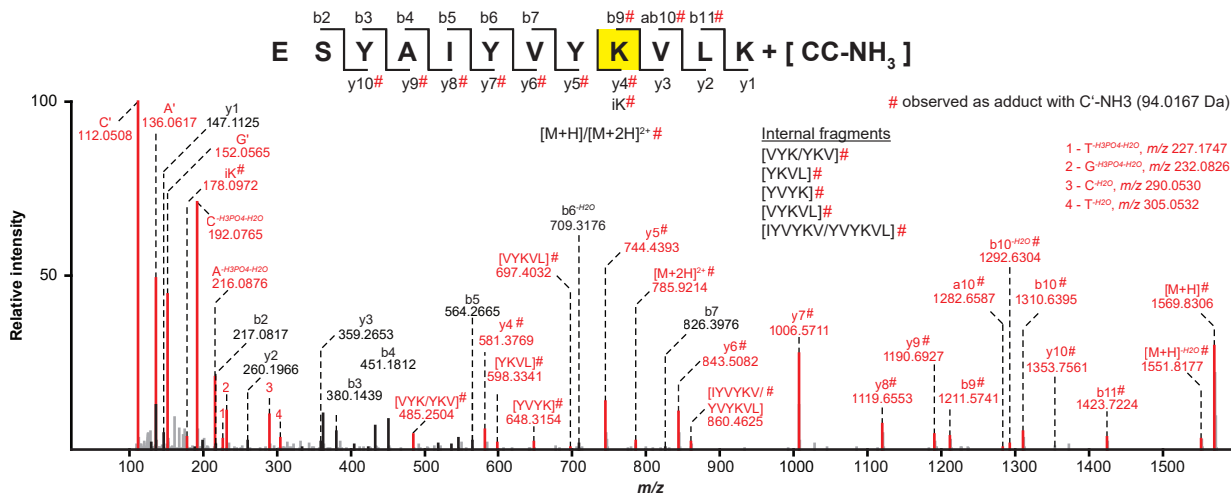


Histone H2B

protein	peptide (aa)	cross-link site (aa - base/sugar)	DNA	m/z _{exp}	z	cross-link MW _{exp}	cross-link MW _{calc}	peptide MW _{calc}	DNA MW _{calc}	Δ ppm
H2B	ESYAIYVYKVLK (32-43)	Lys40 - C	CC-NH3	1027.9506	2	2053.8856	2053.8833	1474.8066	579.0767	1.11
		Lys40 - C	AC-NH3	693.6397	3	2077.8956	2077.8946	1474.8066	603.0880	0.51
		Lys40 - C	CCC-NH3	781.9844	3	2342.9297	2342.9296	1474.8066	868.1230	0.05
		Lys40 - C	CT-NH3	1035.4493	2	2068.8830	2068.8830	1474.8066	594.0764	-0.01
H2B	VLKQVHPDTGISSK (41-54)	Lys43 - C	AC-NH3	704.6492	3	2110.9241	2110.9233	1507.8353	603.0880	0.41
		Lys43 - C	CCGT-NH3	907.6777	3	2720.0096	2720.0105	1507.8353	1212.1753	-0.34
		Lys43 - C	ACC-NH3	800.9990	3	2399.9735	2399.9696	1507.8353	892.1343	1.63
		Lys43 - C	CCGG-NH3	916.0153	3	2745.0224	2745.0170	1507.8353	1237.1818	1.96
H2B	QVHPDTGISSK (44-54)	His46 - deoxyrib.	GGGG	834.9465	3	2501.8160	2501.8086	1167.5879	1334.2207	2.97
H2B	LLLPGLAKHAVSEGTK (97-113)	Lys105 - C	ACT-NH3	890.7191	3	2669.1338	2669.1324	1761.9984	907.1340	0.53
		Lys105 - C	CC-NH3	781.3661	3	2341.0748	2341.0751	1761.9984	579.0767	-0.10
		Lys105 - C	CCCC-NH3	974.0627	3	2919.1646	2919.1677	1761.9984	1157.1694	-1.07
		Lys105 - C	CG-NH3	794.7014	3	2381.0807	2381.0813	1761.9984	619.0829	-0.23
H2B	HAVSEGTKAVTK (106-117)	Lys113 - C	CCGG-NH3	822.2889	3	2463.8432	2463.8431	1226.6614	1237.1818	0.03
		Lys113 - C	CCCG-NH3	808.9543	3	2423.8394	2423.8369	1226.6614	1197.1756	1.02
		Lys113 - C	ACCG-NH3	816.9567	3	2447.8466	2447.8482	1226.6614	1221.1869	-0.66
		Lys113 - C	CCG-NH3	712.6044	3	2134.7897	2134.7906	1226.6614	908.1292	-0.41

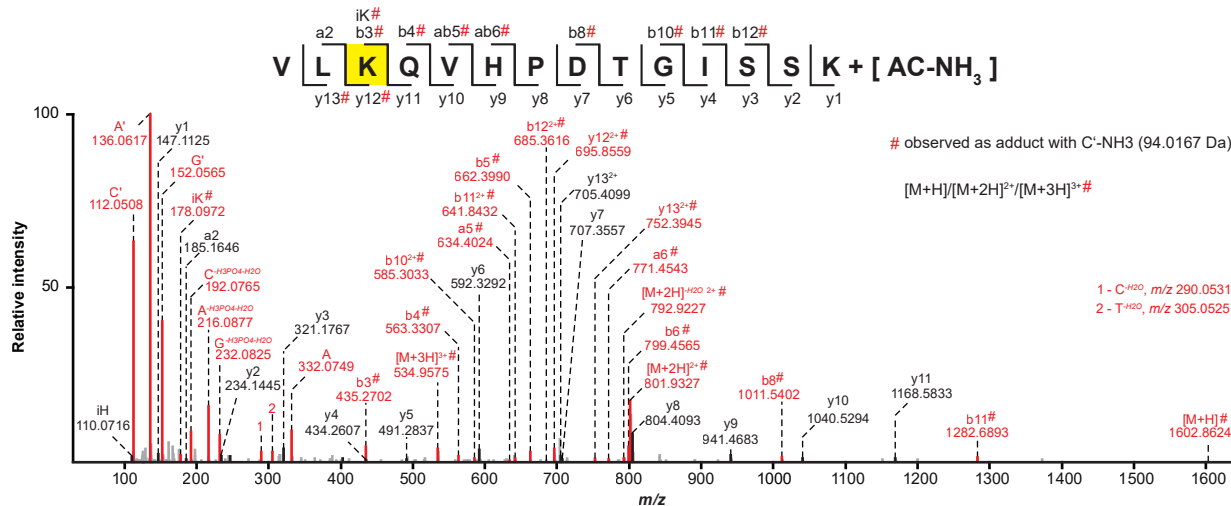
Annotated MS/MS spectra of core histone H2B

1) Histone H2B, aa 32-43



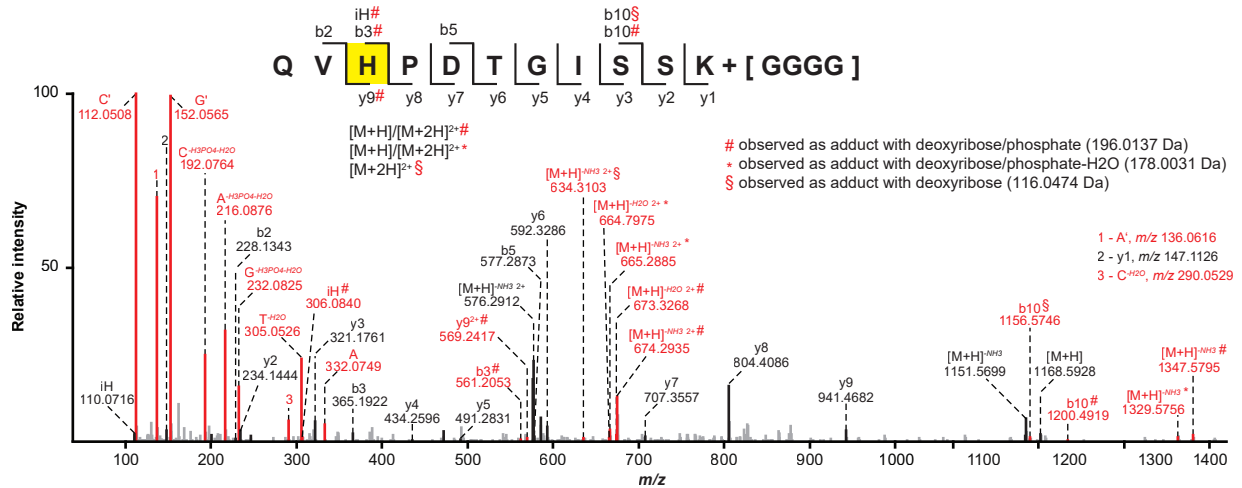
File: A_Stuetzer_180816_12mer_H14_UV_150mM; Index No. 16207; RT: 2705.19 s; m/z: 693.64; z: 3

2) Histone H2B, aa 41-54



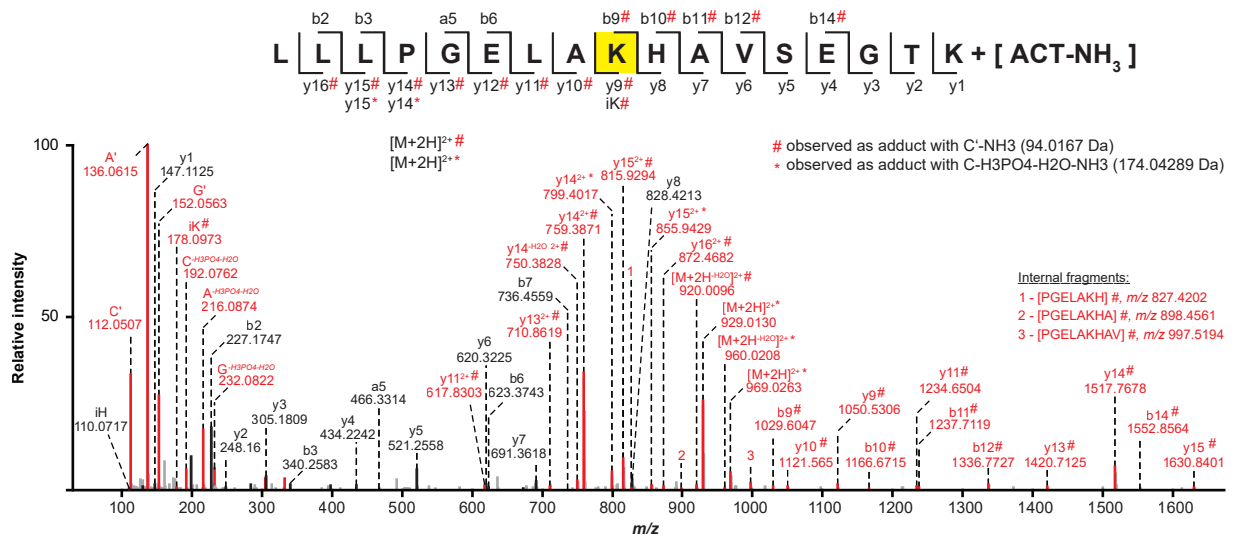
File: A_Stuetzer_180816_12mer_H14_UV_150mM; Index No. 7902; RT: 1465.69 s; m/z: 704.64; z: 3

3) Histone H2B, aa 44-54



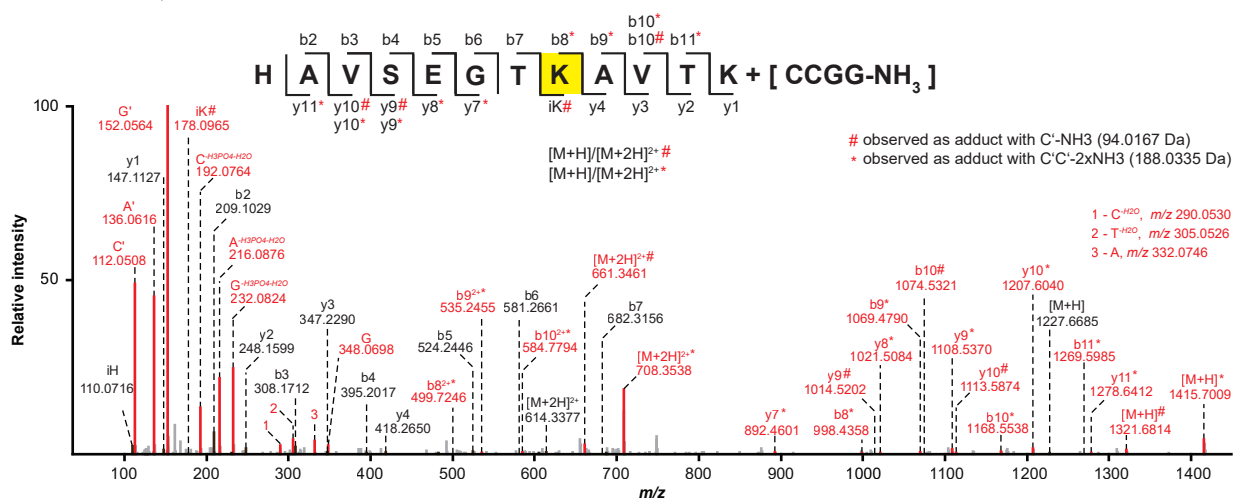
File: ; Index No. ; RT: s; m/z: 834.947; z: 3

4) Histone H2B, aa 97-113



File: A_Stuetzer_180816_12mer_UV_25mM; Index No. 15016; RT: 2524.11 s; m/z: 890.719; z: 3

5) Histone H2B, aa 106-117



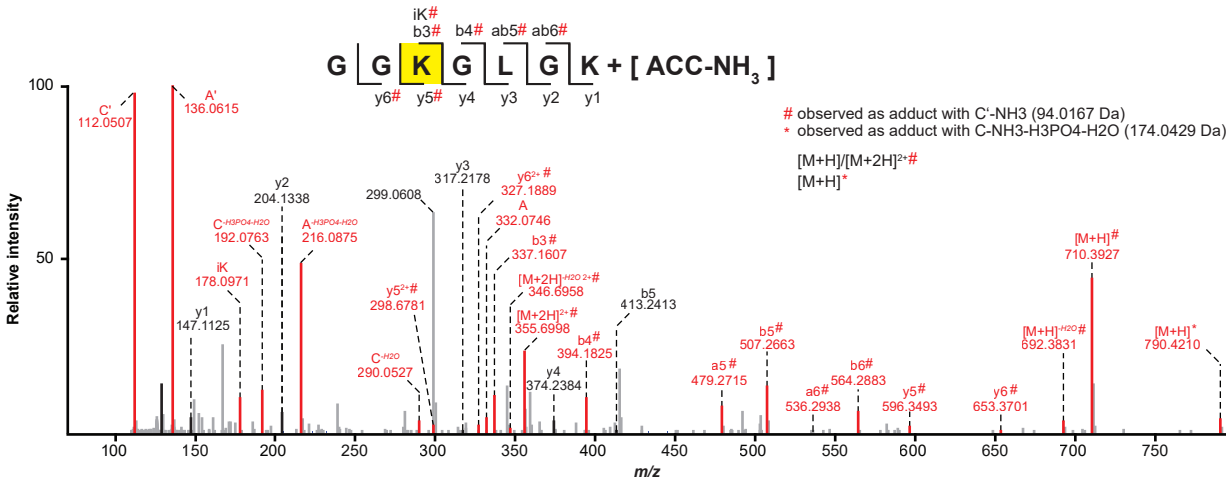
File: A_Stuetzer_180816_12mer_UV_25mM; Index No. ; RT: s; m/z: 822.289; z: 3

Histone H4

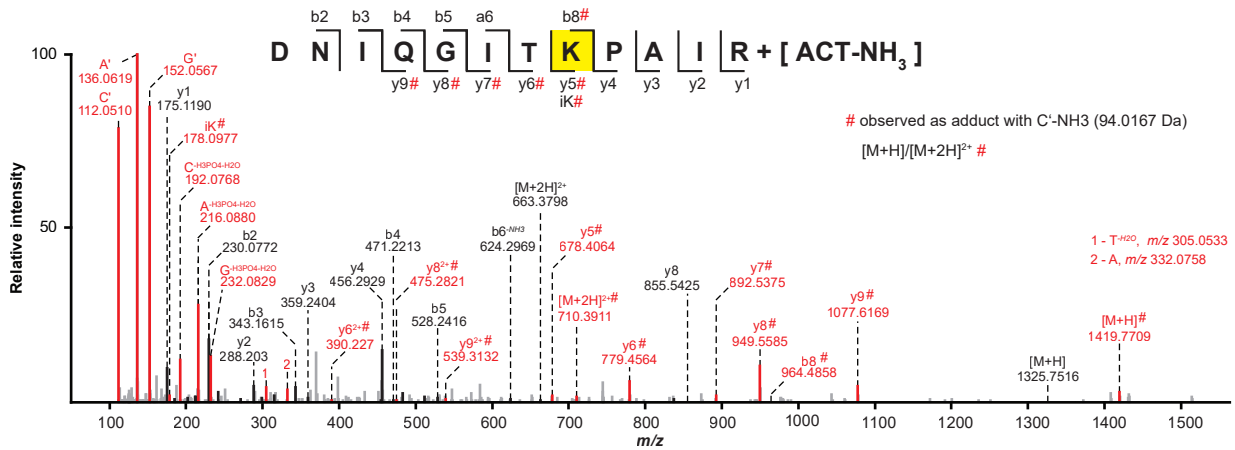
protein	peptide (aa)	cross-link site (aa - base/sugar)	DNA	m/z _{exp}	z	cross-link MW _{exp}	cross-link MW _{calc}	peptide MW _{calc}	DNA MW _{calc}	Δ ppm
H4	GGKGLGK (6-12)	Lys8 - C	ACC-NH3	503.5088	3	1507.5029	1507.5042	615.3699	892.1343	-0.85
		Lys8 - C	AC-NH3	407.1602	3	1218.4571	1218.4579	615.3699	603.0880	-0.61
		Lys8 - C	CCG-NH3	508.8409	3	1523.4992	1523.4991	615.3699	908.1292	0.08
		Lys8 - C	CT-NH3	605.7315	2	1209.4474	1209.4463	615.3699	594.0764	0.90
H4	GLGKGGAK (9-16)	Lys12 - C	ACG-NH3	540.5239	3	1618.5482	1618.5475	686.4070	932.1405	0.44
		Lys12 - C	ACC-NH3	527.1881	3	1578.5408	1578.5413	686.4070	892.1343	-0.30
		Lys12 - C	CCG-NH3	532.5201	3	1594.5368	1594.5362	686.4070	908.1292	0.39
		Lys12 - C	AC-NH3	430.8393	3	1289.4944	1289.4950	686.4070	603.0880	-0.42
H4	DNIQGITKPAIR (24-35)	Lys31 - C	ACT-NH3	744.9653	3	2231.8724	2231.8798	1324.7458	907.1340	-3.31
		Lys31 - C	ACC-NH3	739.9674	3	2216.8787	2216.8801	1324.7458	892.1343	-0.62
		Lys31 - C	CCC-NH3	731.9644	3	2192.8697	2192.8688	1324.7458	868.1230	0.42
		Lys31 - C	CC-NH3	635.6160	3	1903.8245	1903.8225	1324.7458	579.0767	1.08
H4	DAVTYTEHAK (68-77)	His75 - deoxyrib.	CCTT-H2O	774.2497	3	2319.7256	2319.7195	1133.5348	1186.1848	2.63
		His75 - deoxyrib.	AAC-NH3	684.2335	3	2049.6770	2049.6804	1133.5348	916.1456	-1.65
H4	DAVTYTEHAKR (68-78)	Lys77 - C	ACC-NH3	728.2651	3	2181.7718	2181.7702	1289.6359	892.1343	0.74
		Lys77 - C	CCGT-NH3	834.9448	3	2501.8109	2501.8111	1289.6359	1212.1753	-0.09
		Lys77 - C	ACCT-NH3	829.6128	3	2485.8149	2485.8162	1289.6359	1196.1804	-0.53
		Lys77 - C	ACCG-NH3	837.9500	3	2510.8265	2510.8227	1289.6359	1221.1869	1.51
H4	KTVTAMDVVYALK (79-91)	Lys79 - C	AC-NH3	681.3000	3	2040.8765	2040.8776	1437.7896	603.0880	-0.51
		Lys79 - C	CCCC-NH3	865.9927	3	2594.9546	2594.9589	1437.7896	1157.1694	-1.66
		Lys79 - C	CCG-NH3	782.9805	3	2345.9180	2345.9188	1437.7896	908.1292	-0.33
		Lys79 - C	ACC-NH3	777.6490	3	2329.9235	2329.9239	1437.7896	892.1343	-0.16

Annotated MS/MS spectra of core histone H4

1) Histone H4 aa 6-12

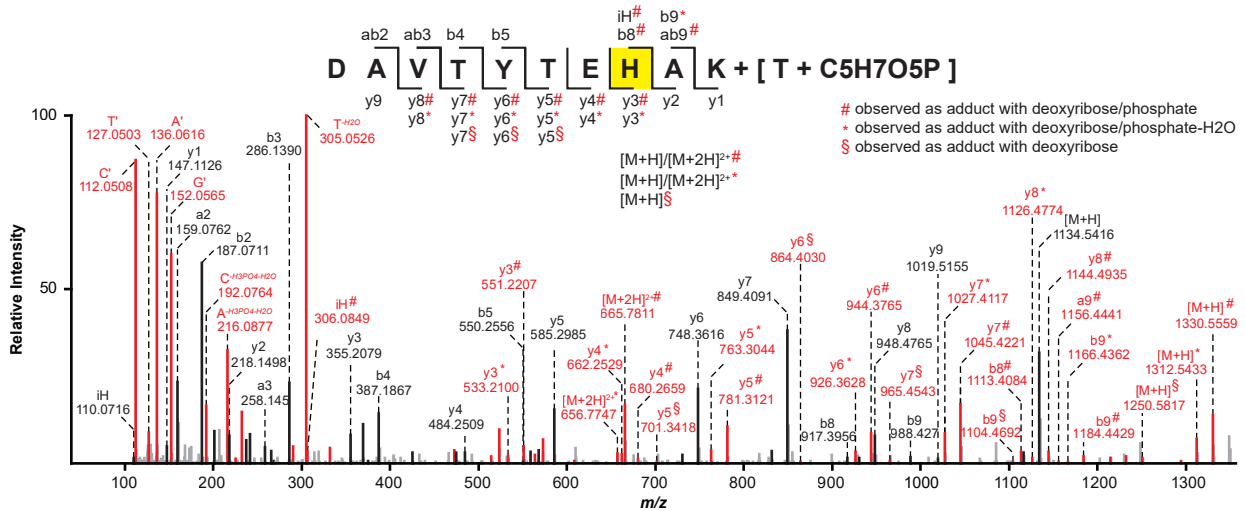


3) Histone H4, aa 24-35



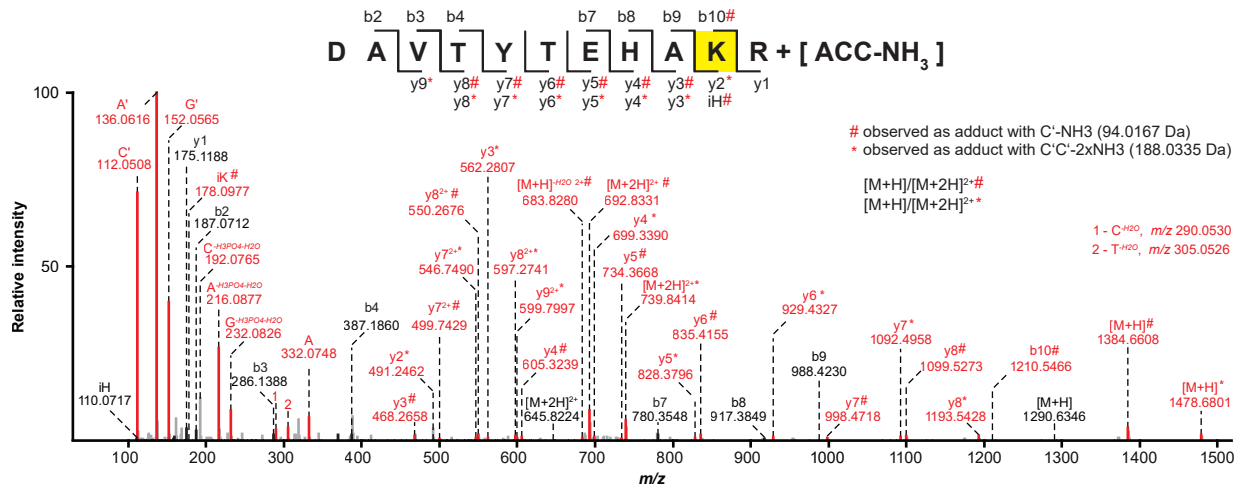
File: A_Stuetzer_180816_12mer_UV_25mM; Index No. 11342; RT: 1973.72 s; m/z: 744.967; z: 3

4) Histone H4, aa 68-77



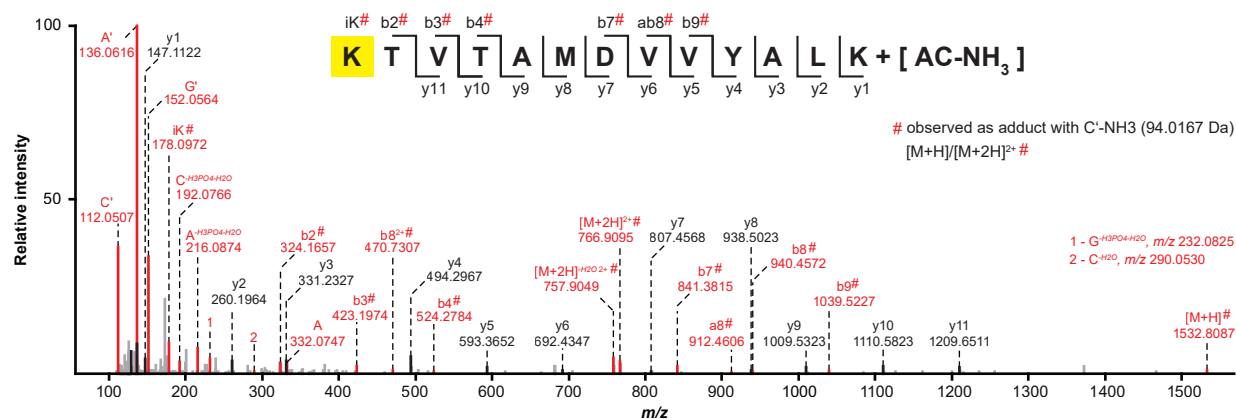
File: A_Stuetzer_180816_12mer_UV_25mM; Index No. 7171; RT: 1353.21 s; m/z: 817.805; z: 2

5) Histone H4, aa 68-78



File: A_Stuetzer_180816_12mer_UV_150mM; Index No. 6619; RT: 1120.26 s; m/z: 540.524; z: 3

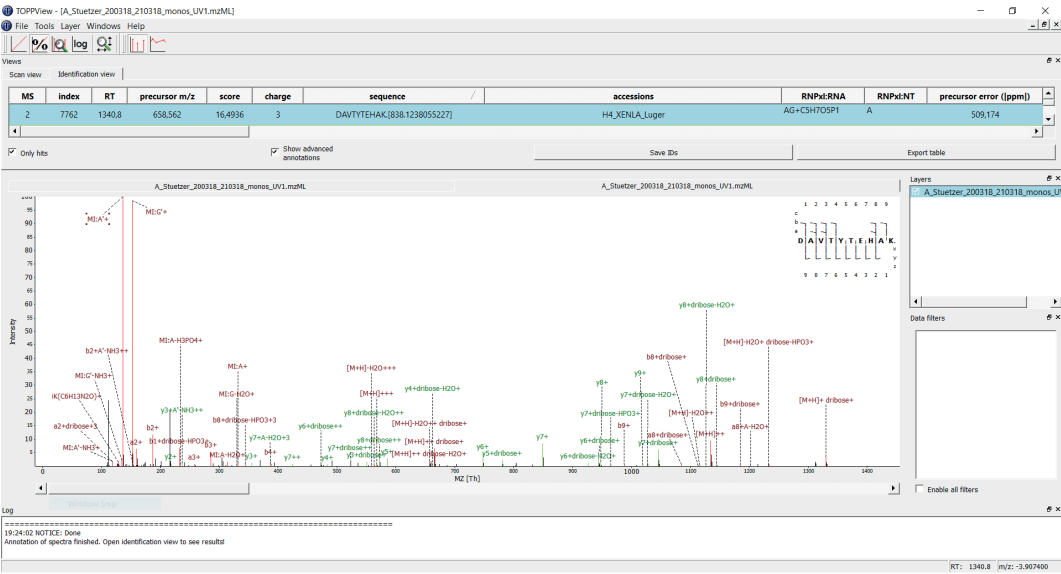
6) Histone H4, aa 79-91



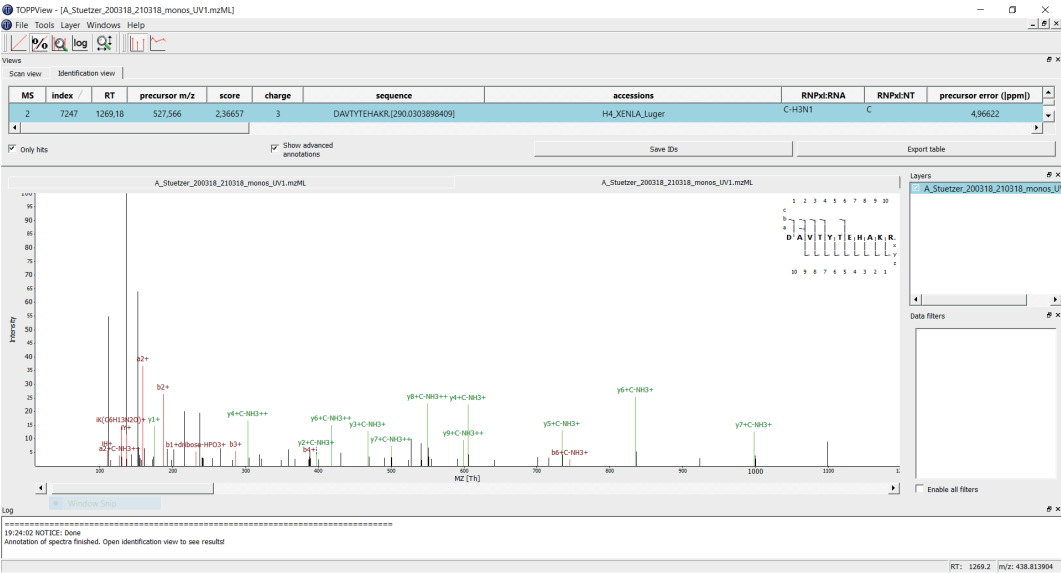
File: ; Index No. ; RT: s; m/z: 681.3; z: 3

TOPPView MS/MS spectra of core histones from *X. laevis* mononucleosomes

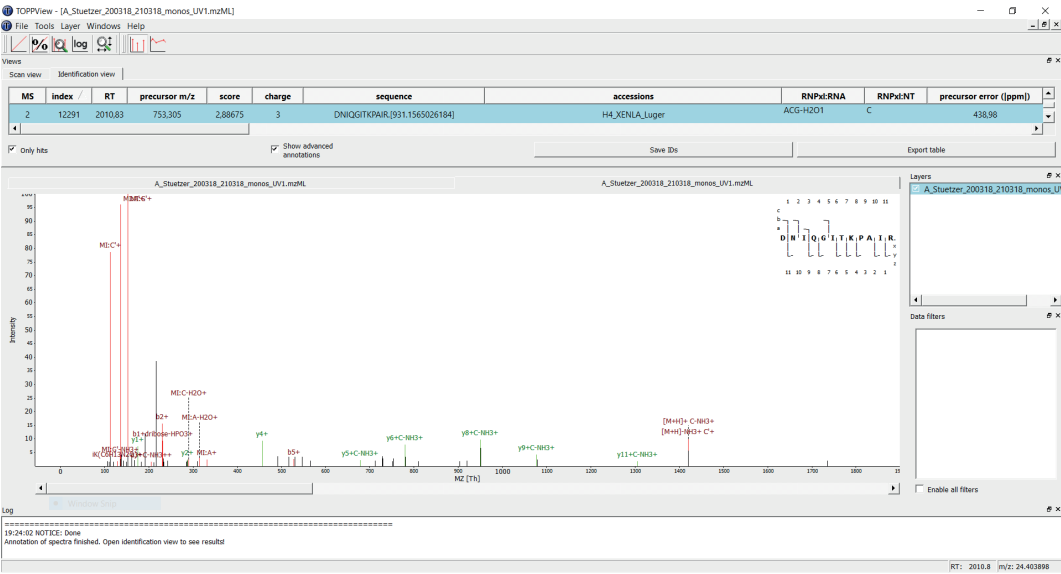
1)



2)



3)



TOPVIEW - [A_Stuetzer_200318_210318_monos_UV1.mzML]
 File Tools Layer Windows Help

File View Tools Layer Windows Help

File View Tools Layer Windows Help

Views: Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPe:RNA	RNPe:NT	precursor error (ppm)
2	13051	2127.67	853.299	0.958968	3	EAQDFKTDLR[1221:1668]924593]	H3_XENLA_Luger	ACCG-F3NT	C	393.428

☐ Only hits
 ☒ Show advanced annotations
Save IDs
Export table

A_Stuetzer_200318_210318_monos_UV1.mzML

TOPView - [A_Stuetzer_200318_210318_monos_UV1.ms.ML]

File Tools Layer Views Help

Views Scan view Identification view

MS	index /	RT	precursor m/z	score	charge	sequence	accessions	RNPeRNA	RNPxNT	precursor error (ppm)
2	18074	2909.59	883.669	0.870859	3	ESYAVYYVKYLK(1172.1691774912)	H2B_XENLA_Luger	CCTC-H3NT	C	380.141

☒ Only MS ☒ Show advanced annotations Save IDs Export table

A_Stuetzer_200318_210318_monos_UV1.ms.ML A_Stuetzer_200318_210318_monos_UV1.ms.ML

Layers A_Stuetzer_200318_210318_monos_UV1.ms.ML

Data filters Enable all filters

Log
19-24-02 NOTICE: Done
Annotation of spectra finished. Open identification view to see results!

RT: 2909.6 m/z: 277.900922

TOPView - [A_Stuetzer_200318_210318_monox_UV1.mzML]

File Tools Layer Help

Views

Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPSxRNA	RNPxLNT	precursor error (ppm)
2	6625	1184.57	612.862	1.84711	3	GKGKLGK(1220.1916434912)	H4_XENIA_Luger	AATC-H3N1	C	0.660587

☒ Only hits ☒ Show advanced annotations

Save IDs Export table

TOPView - [A_Stuetzer_200318_210318_monos_UV1.mvML]

File Tools Layers Settings Layer Names Help

Views Scan view Identification view

MS	index /	RT	precursor m/z	score	charge	sequence	accessions	RNPeRNA	RNPntNT	precursor error (ppm)
2	7418	1292.76	642.206	0.78124	3	GLGKGGAK[1236.1865584912]	H_XENLA_Luger	ACTG-HBNT	C	520.397

☒ Only Hits ☒ Show advanced annotations Save IDs Export table

A_Stuetzer_200318_210318_monos_UV1.mvML A_Stuetzer_200318_210318_monos_UV1.mvML

Layers
A_Stuetzer_200318_210318_monos_UV1.mvML

Data filters

Enable all filters

Log

19:24:02 NOTICE: Done

Annotation of spectra finished. Open identification view to see result

RET: 1292.8 m/z: 107.28595

TOPVIEW - [A_Stuetzer_200318_210318_monos_UV1.mzML]

File Tools Layers Windows Help

Views Scan view Identification view

MS	index /	RT	precursor m/z	score	charge	sequence	accessions	RNPeRNA	RNPcNT	precursor error (ppm)
2	4977	971.134	639.201	4.85831	3	HAVSEGTKI(1087.1640313955)	H2B_XENIA_Luger	ACC+CSHTOSP1	C	1.93126

Only MS ☒ Show advanced annotations Save IDs Export table

A_Stuetzer_200318_210318_monos_UV1.mzML A_Stuetzer_200318_210318_monos_UV1.mzML

Layers
A_Stuetzer_200318_210318_monos_UV1.mzML

Data filters

Enable all filters

Log

19:24:02 NOTICE: Done
Annotation of spectra finished. Open identification view to see result!

[RT: 971.3 m/z: 388.3750]

TOPView - [A_Stuetzer_200318_210318_monos_UV1.msML]

File Tools Layers Windows Help

Views Scan view Identification view

MS	index / RT	precursor m/z	score	charge	sequence	accessions	RNPeRNA	RNPstNT	precursor error (ppm)
2	7765 1341.21	717.94	2.70125	3	HAVSEGTKAWTK[923.1289516184]	H2B_XENIA_Luger	CTG-H3N1	C	468.334

☒ Only MS ☒ Show advanced annotations Save IDs Export table

A_Stuetzer_200318_210318_monos_UV1.msML A_Stuetzer_200318_210318_monos_UV1.msML

Intensity

m/z [Tz]

Layers
A_Stuetzer_200318_210318_monos_UV1.msML

Data filters

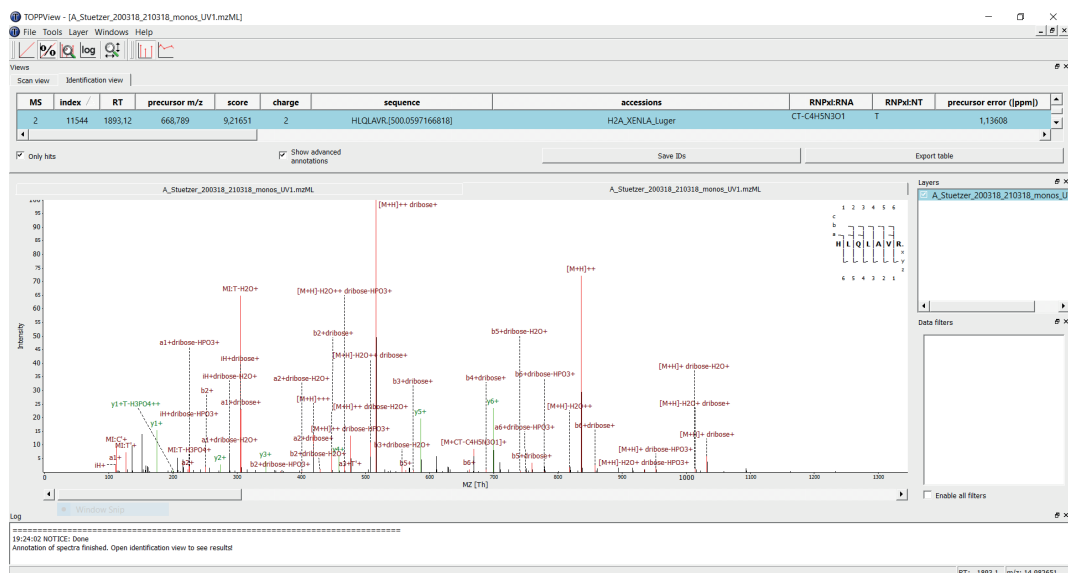
Enable all filters

Log

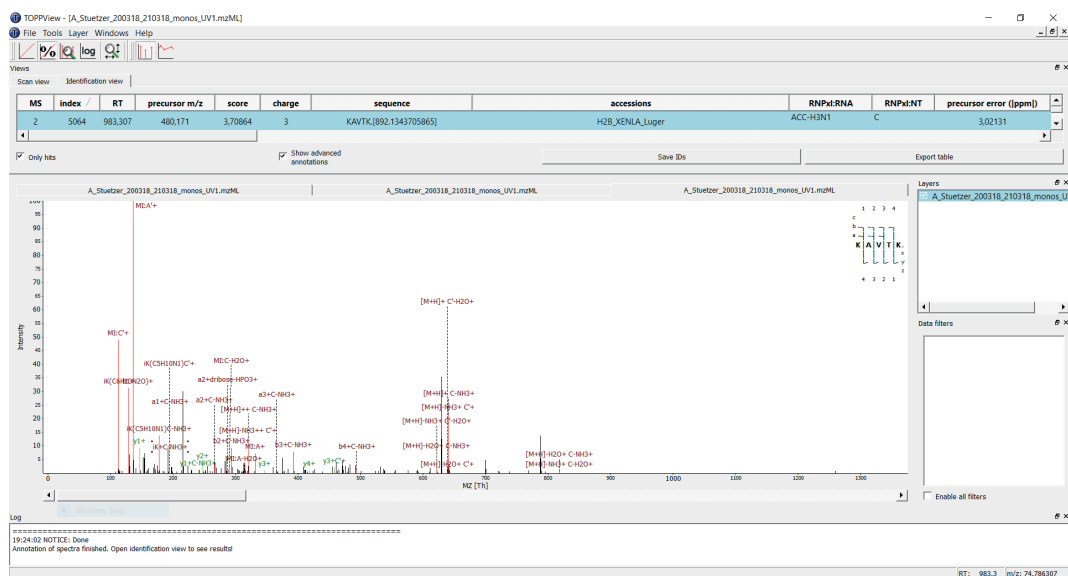
19:24:02 NOTICE: Done
Annodation of spectra finished. Open identification view to see result!

RT: 1341.2 m/z: 1165.5643

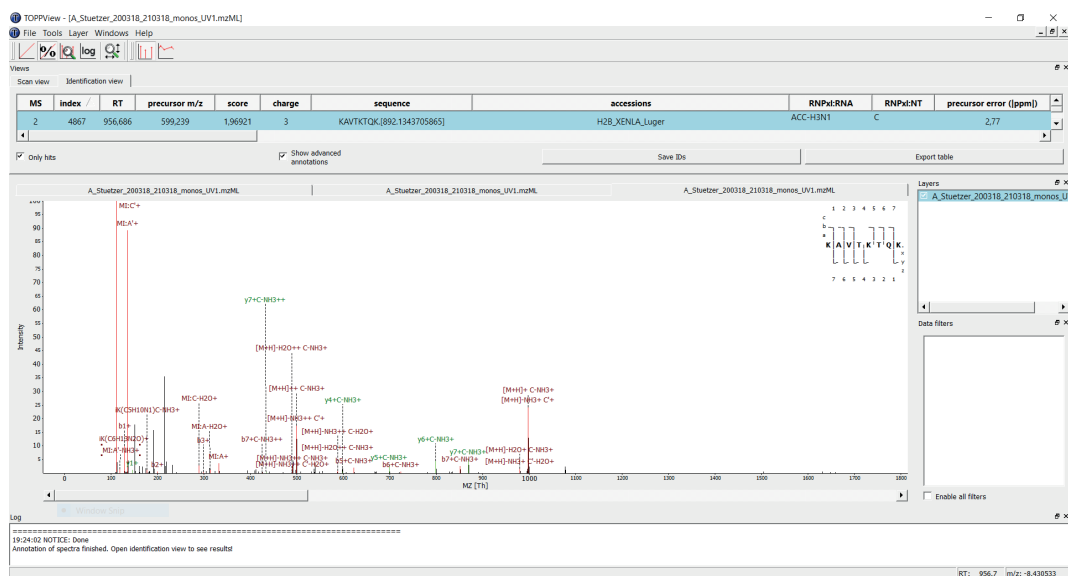
10)



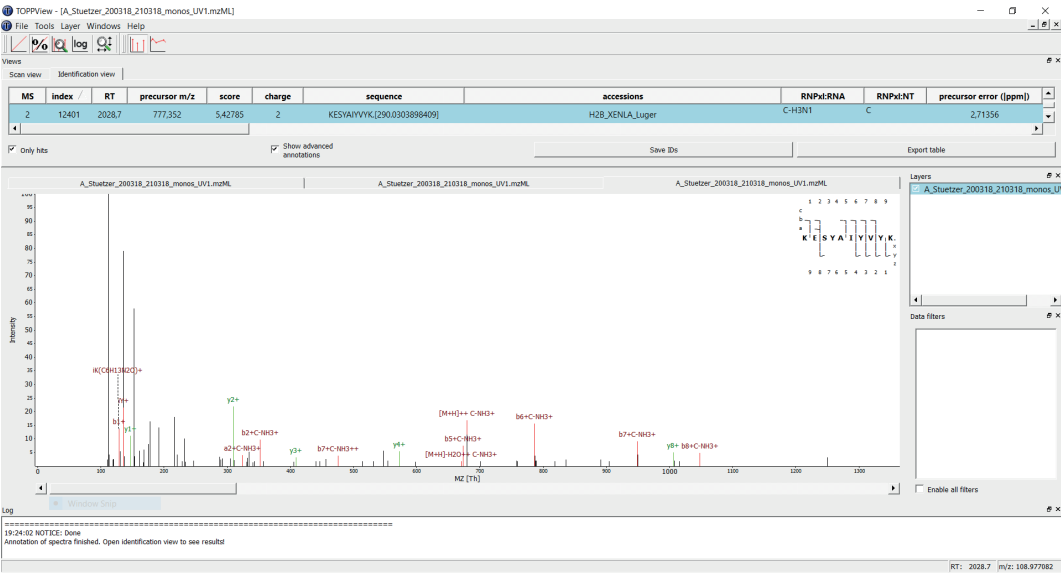
11)



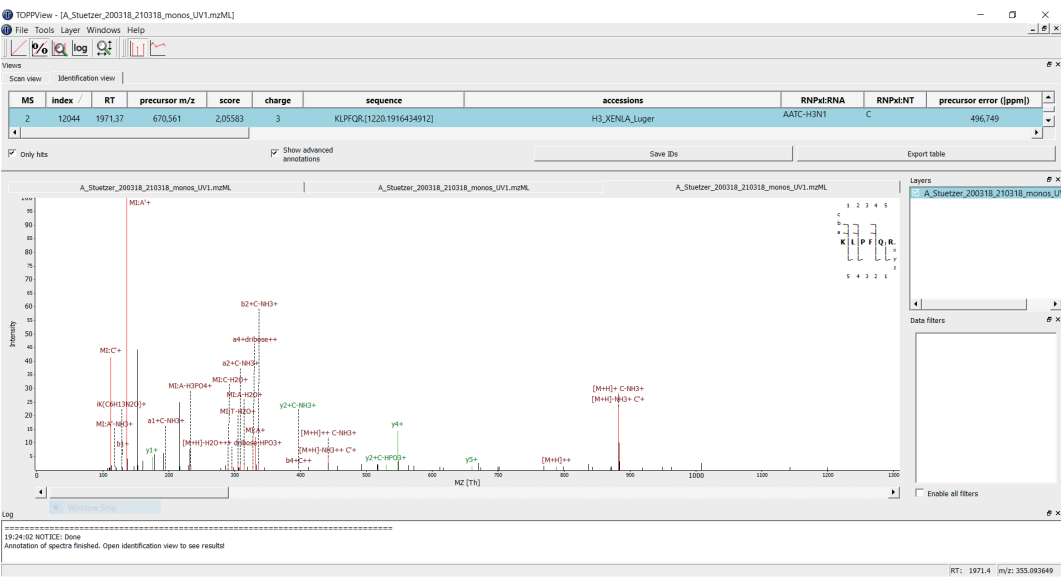
12)



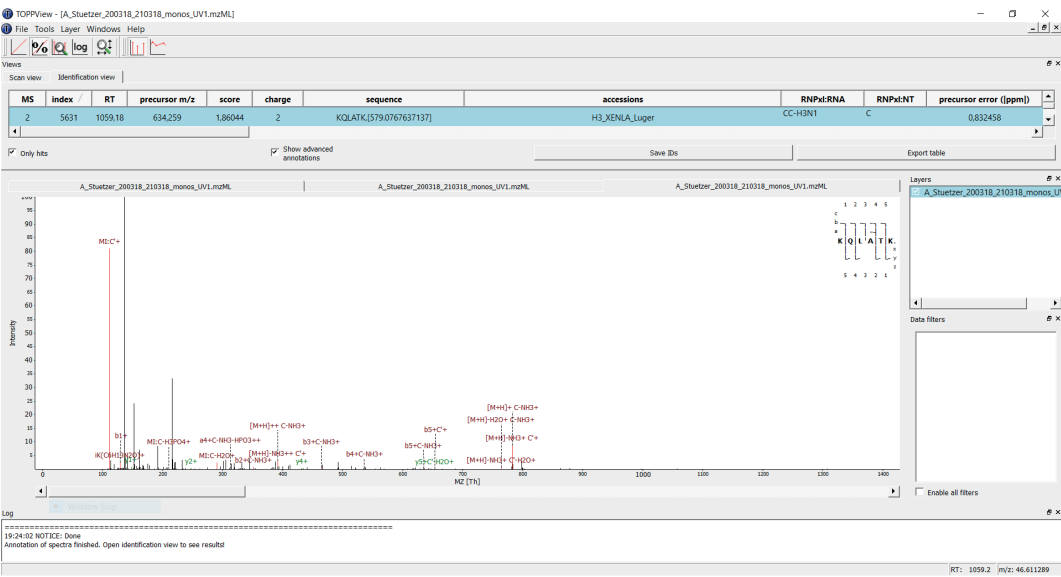
13)



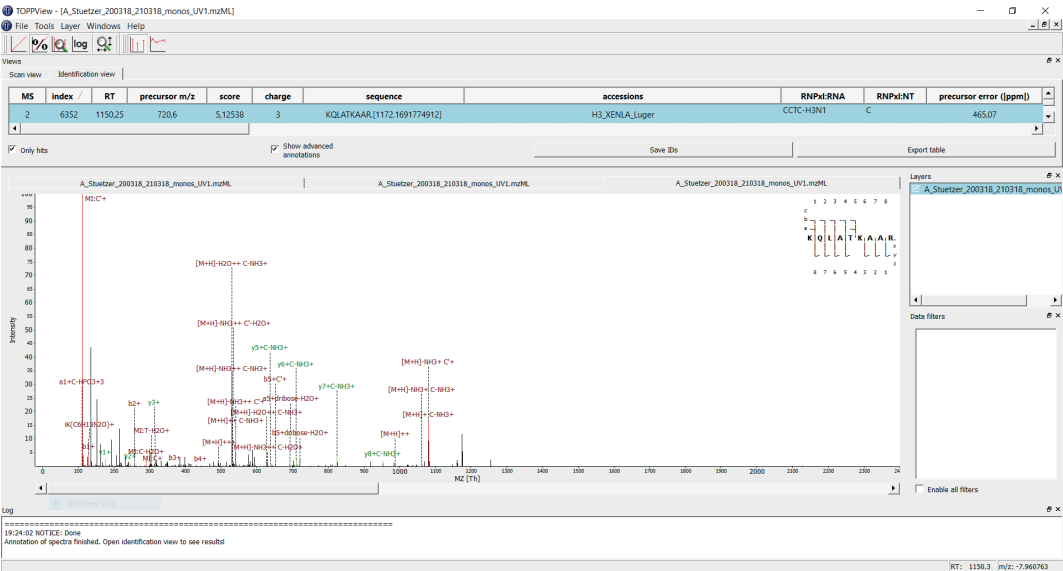
14)



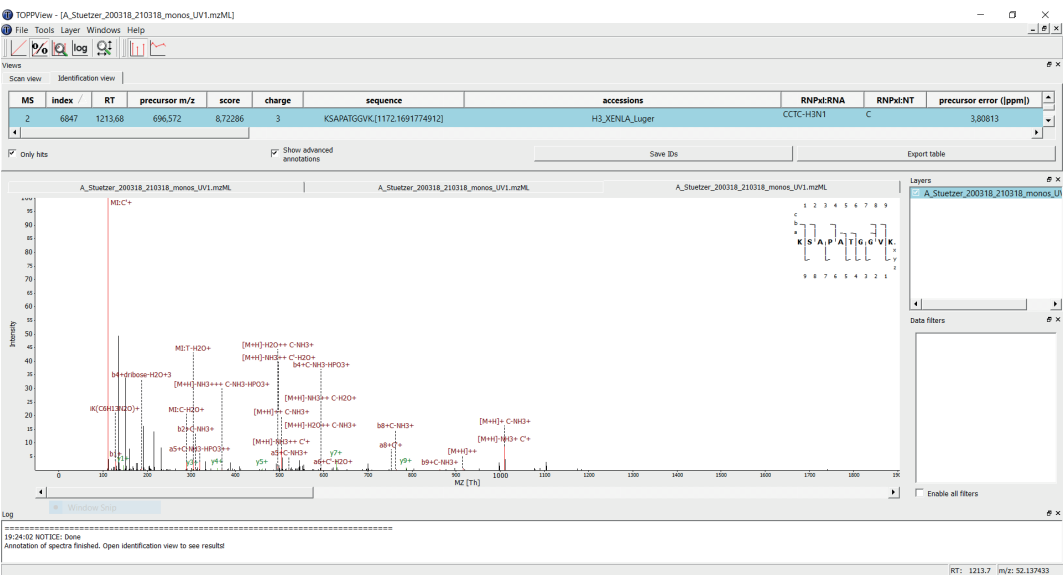
15)



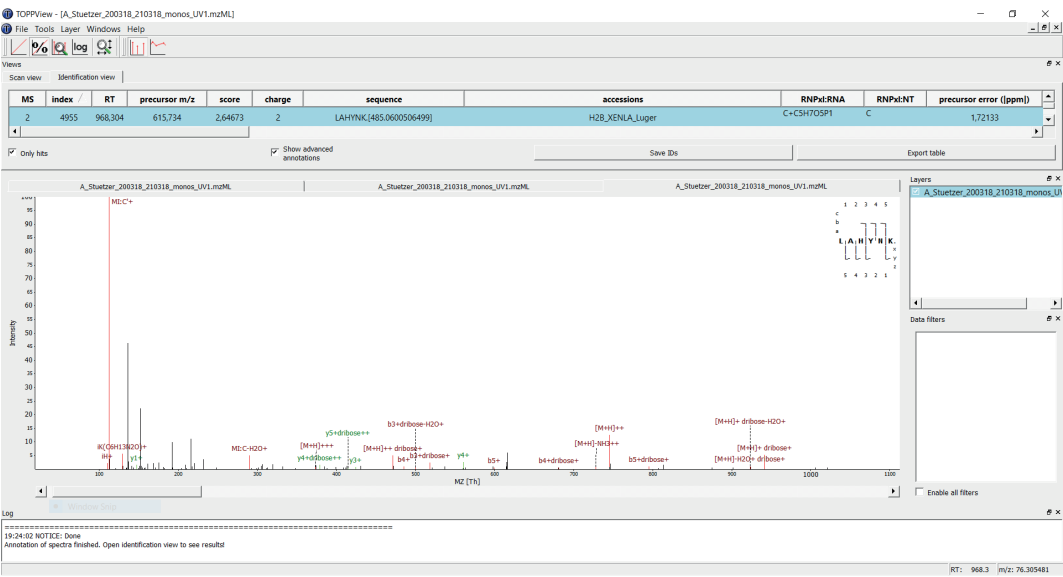
16)



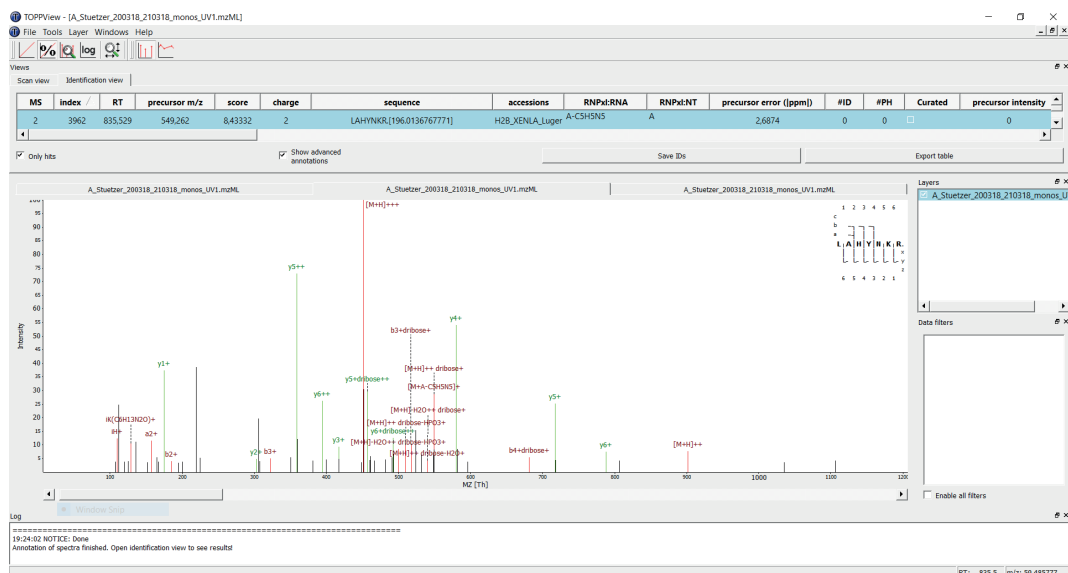
17)



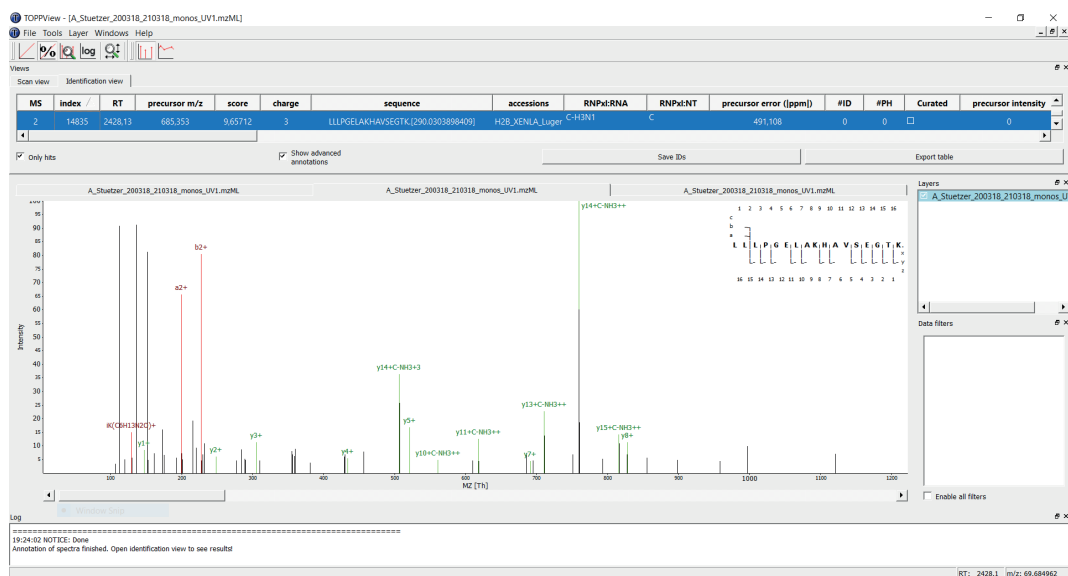
18)



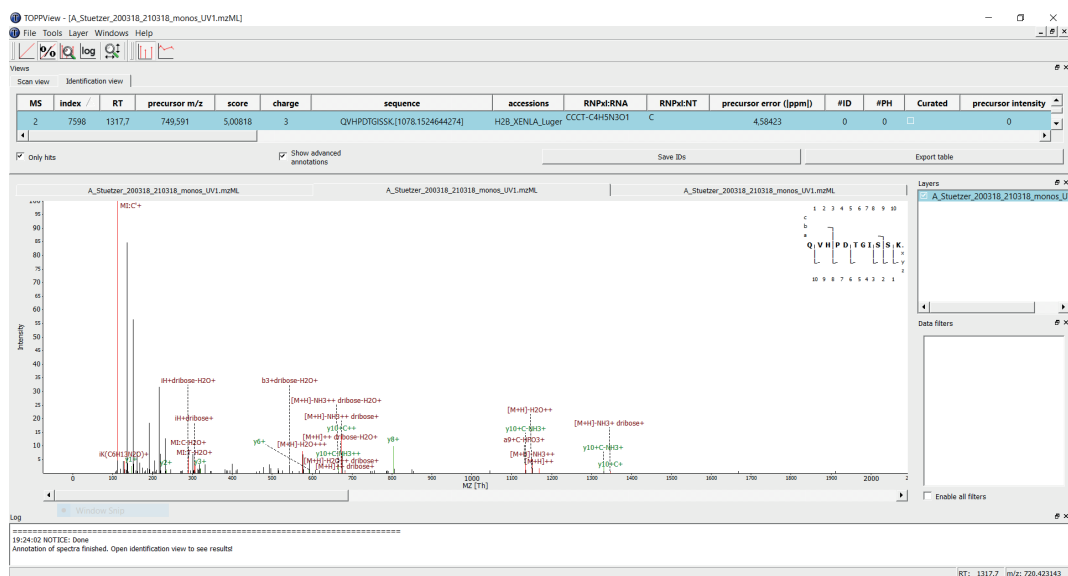
19)



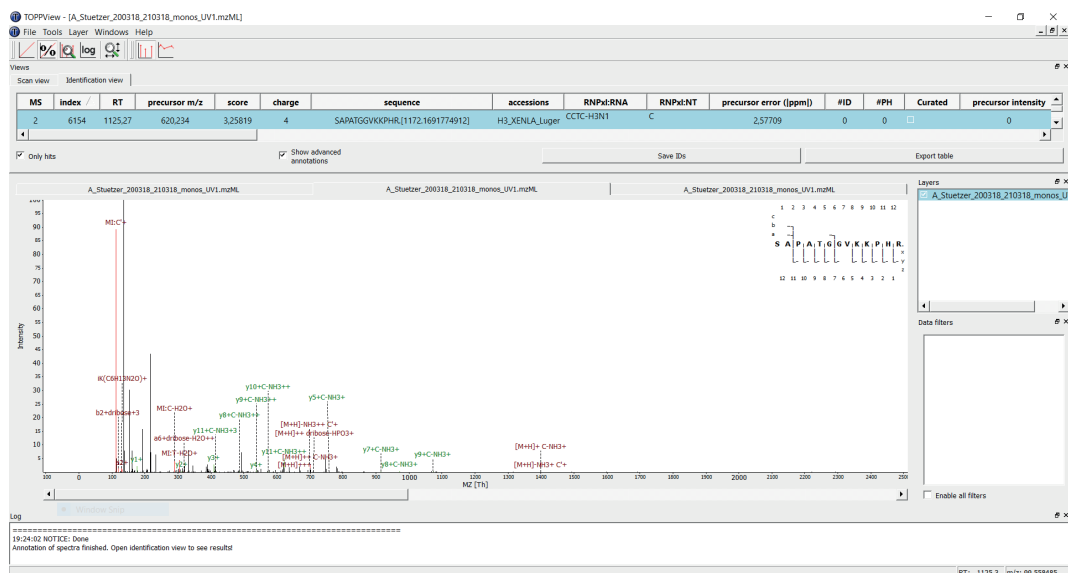
20)



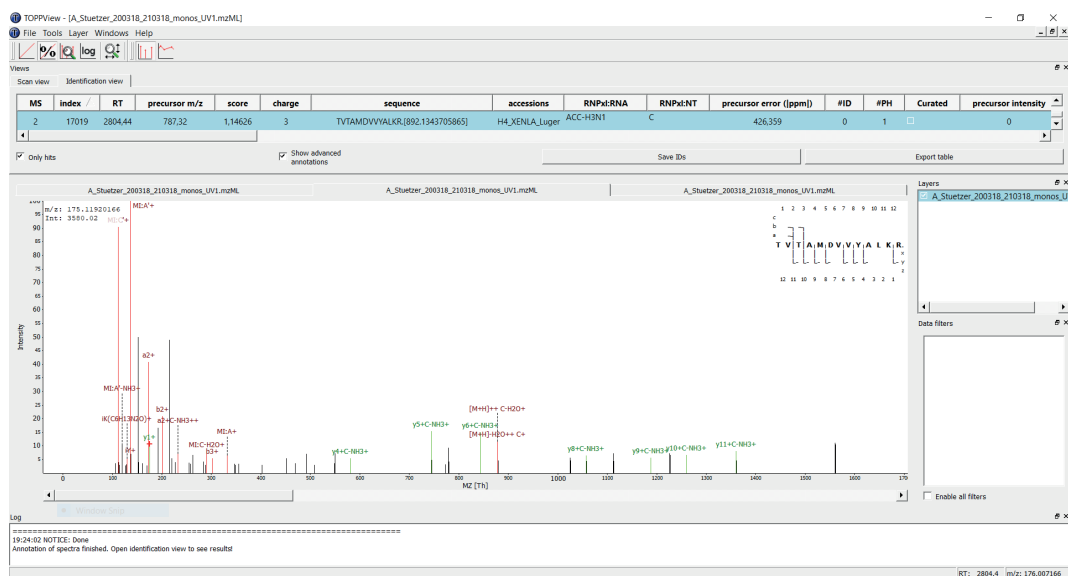
21)



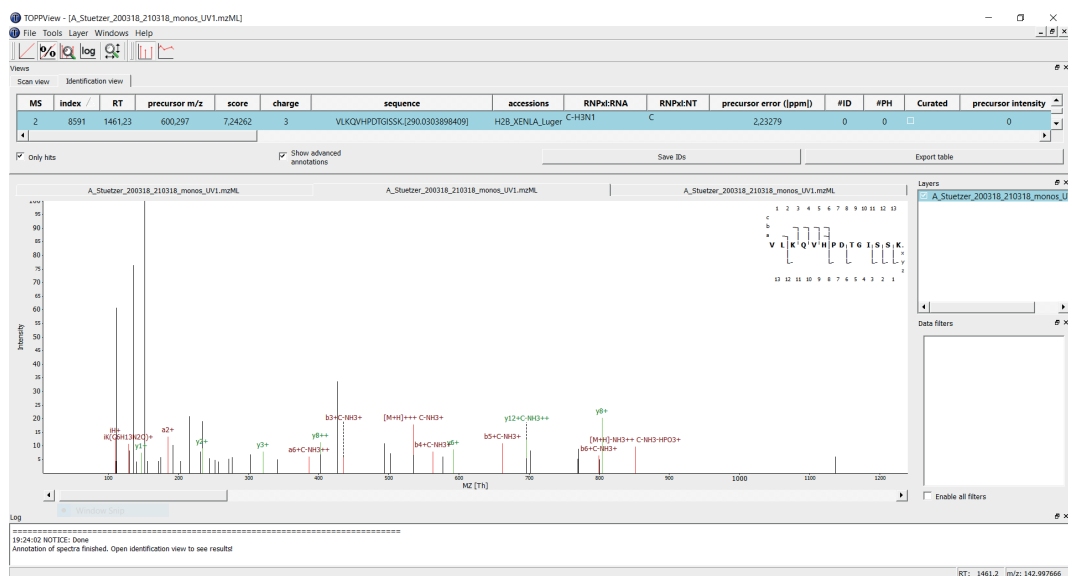
22)



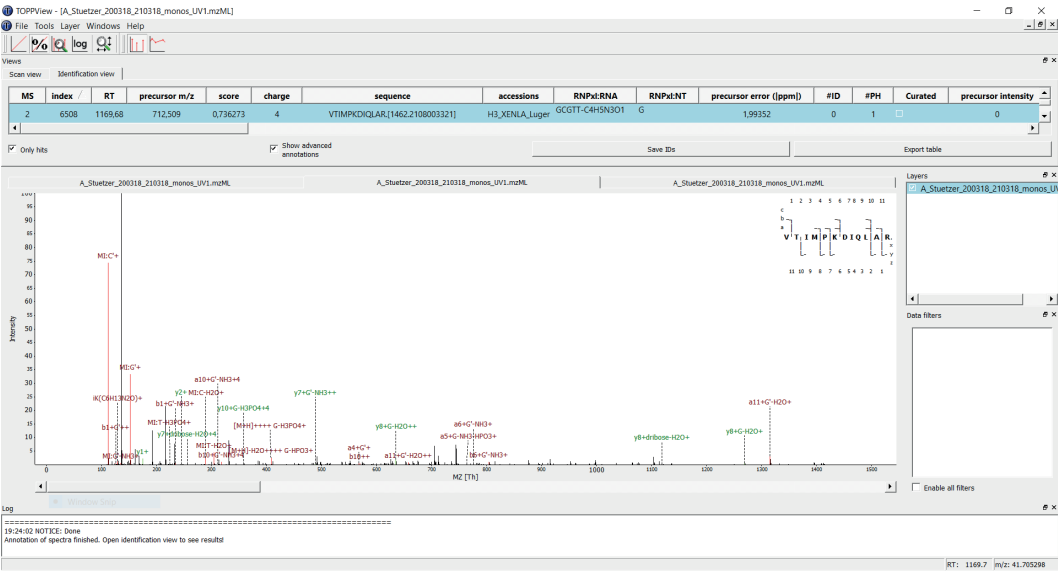
23)



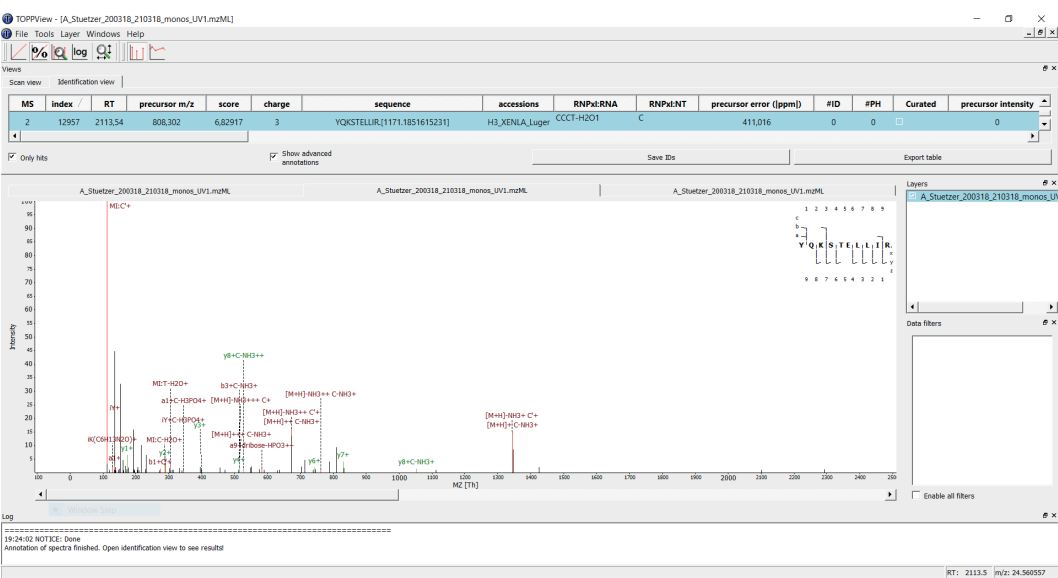
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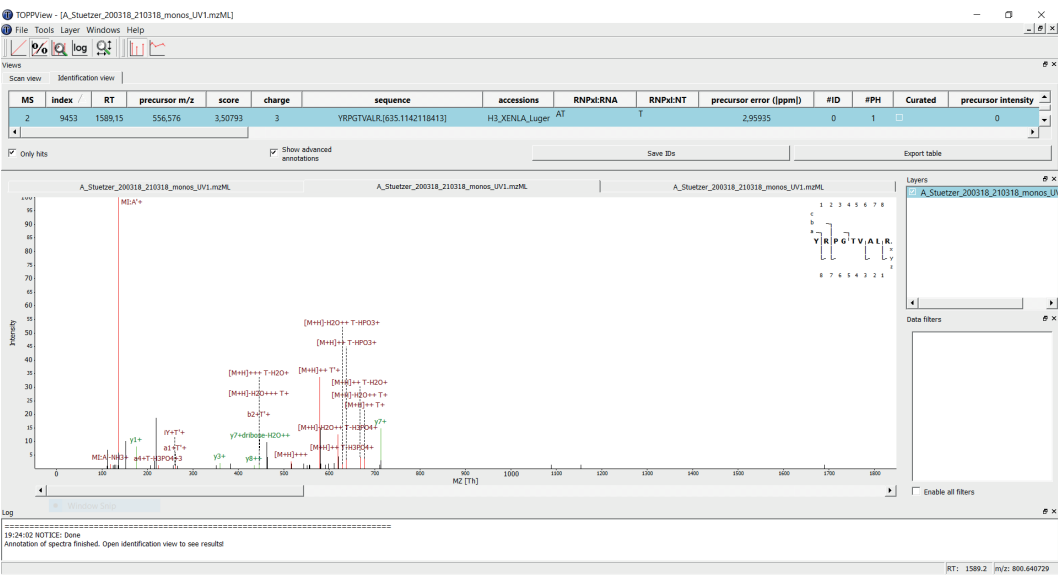
25)



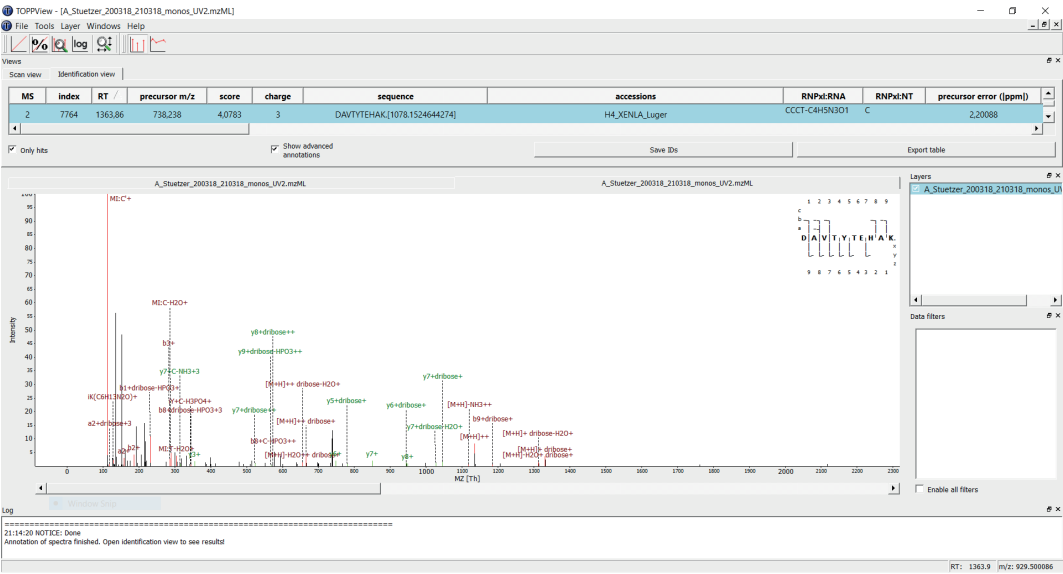
26)



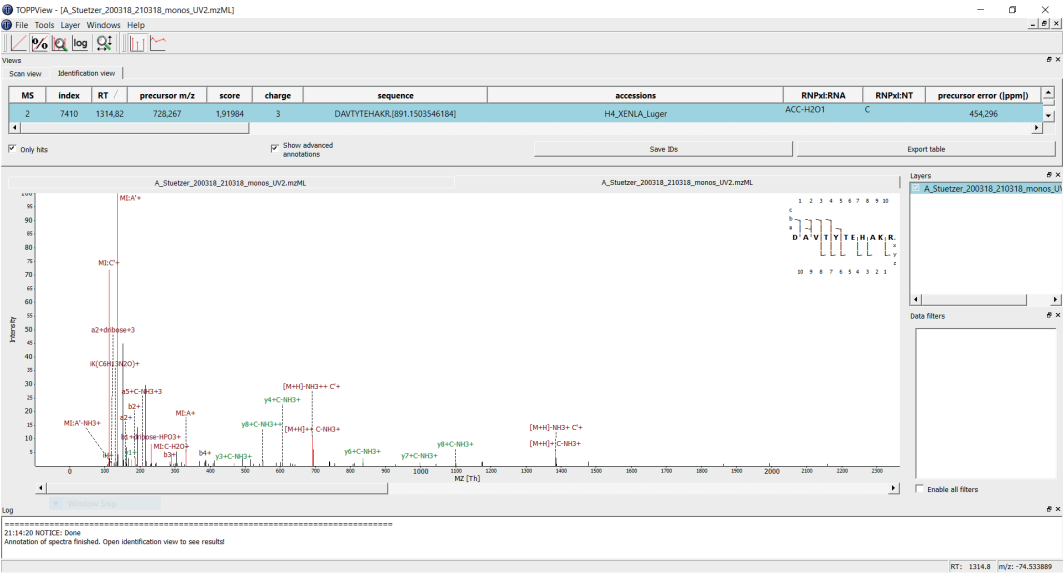
27)



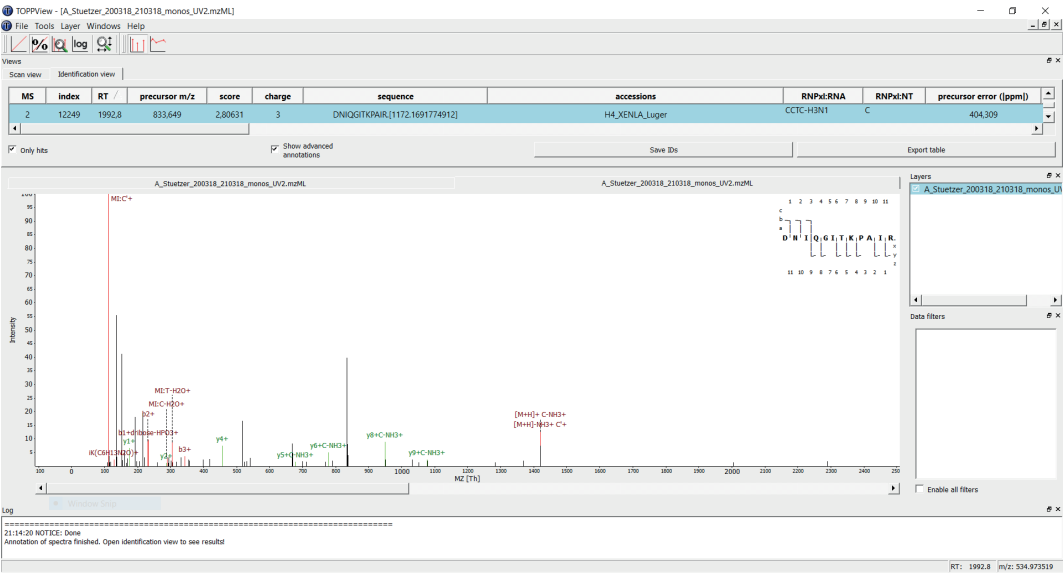
28)



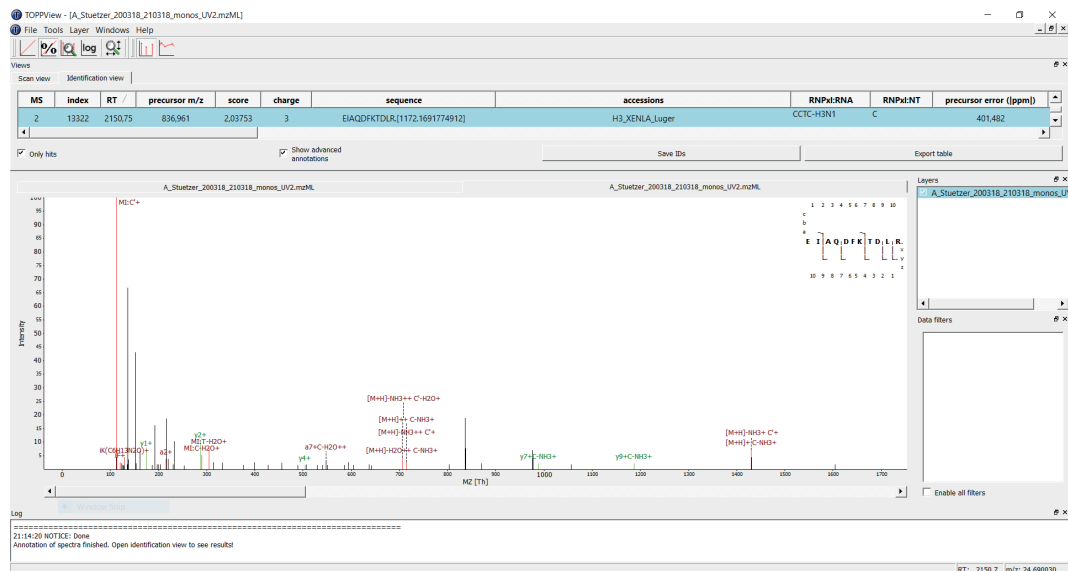
29)



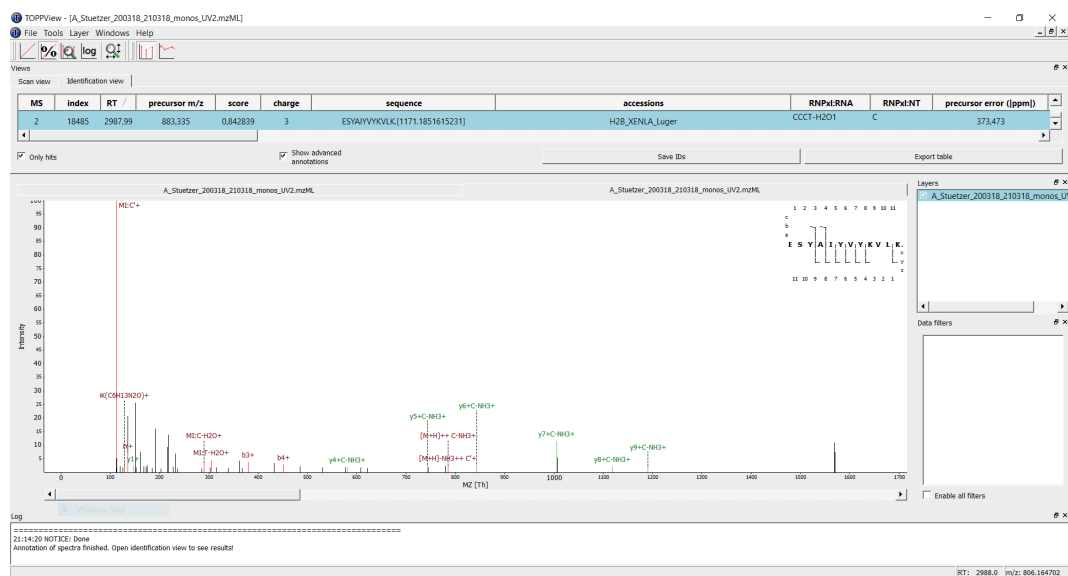
30)



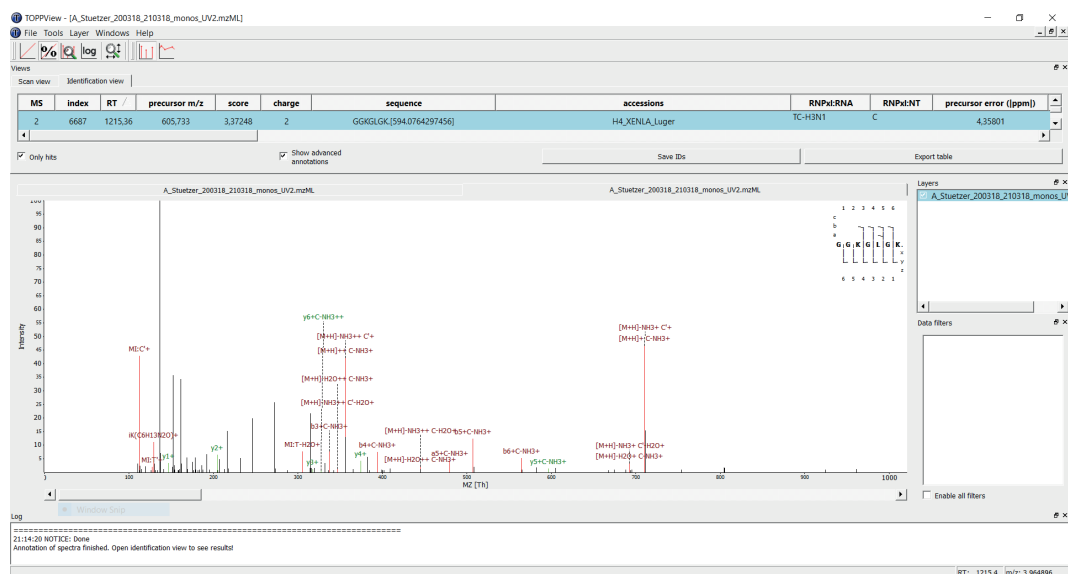
31)



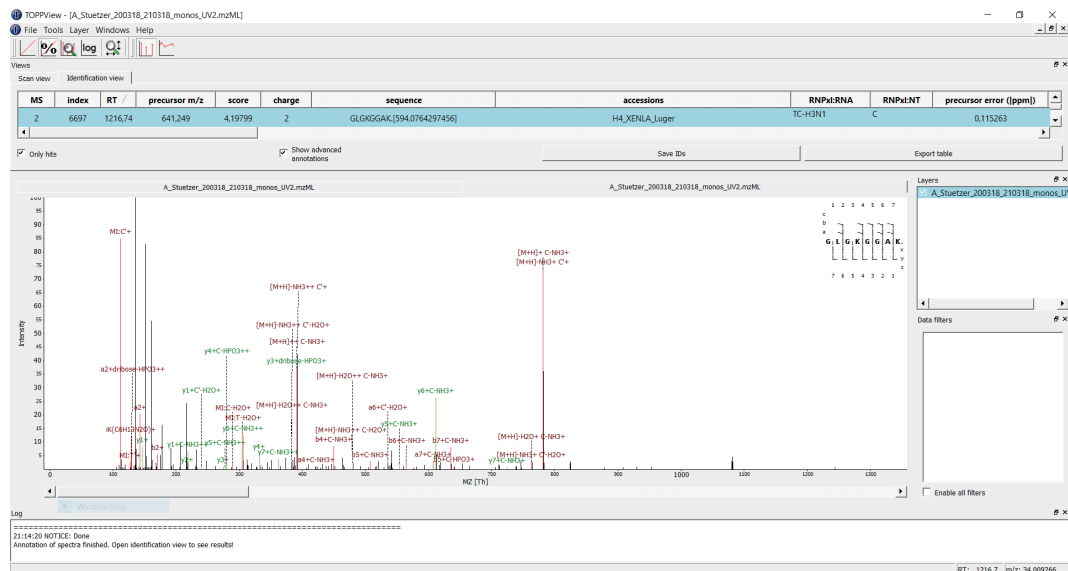
32)



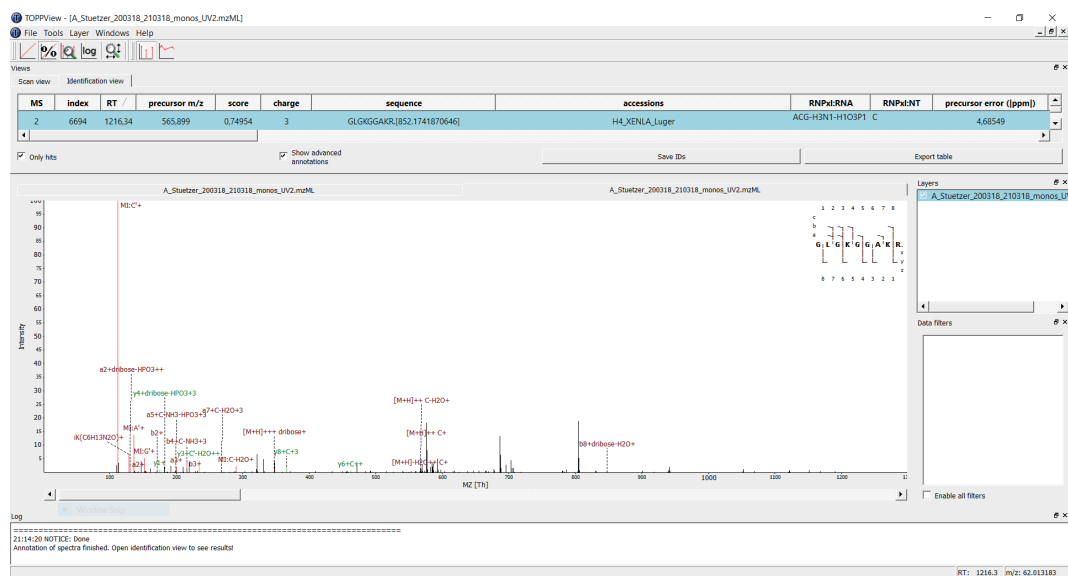
33)



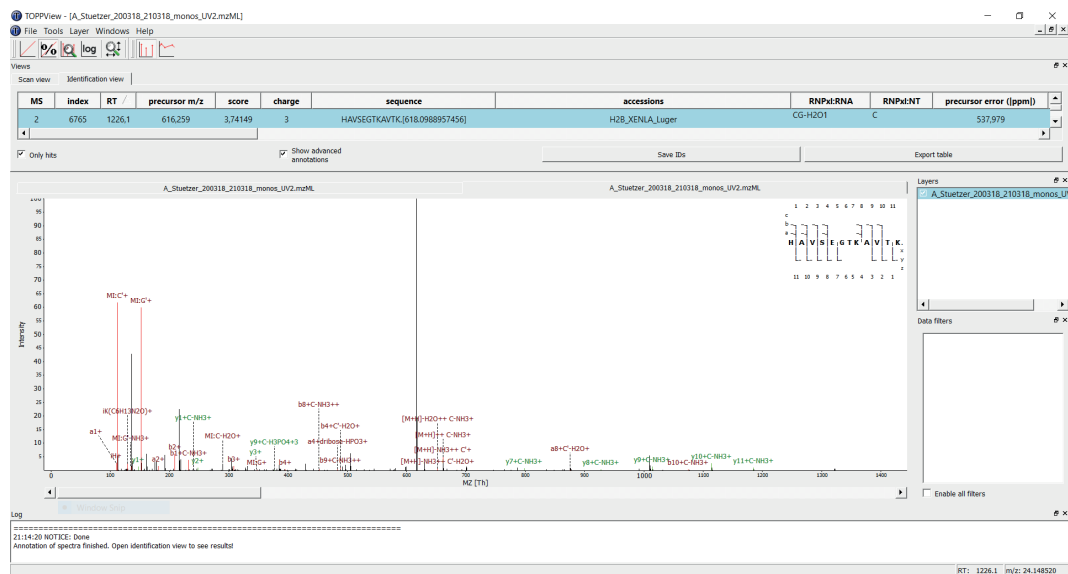
34)



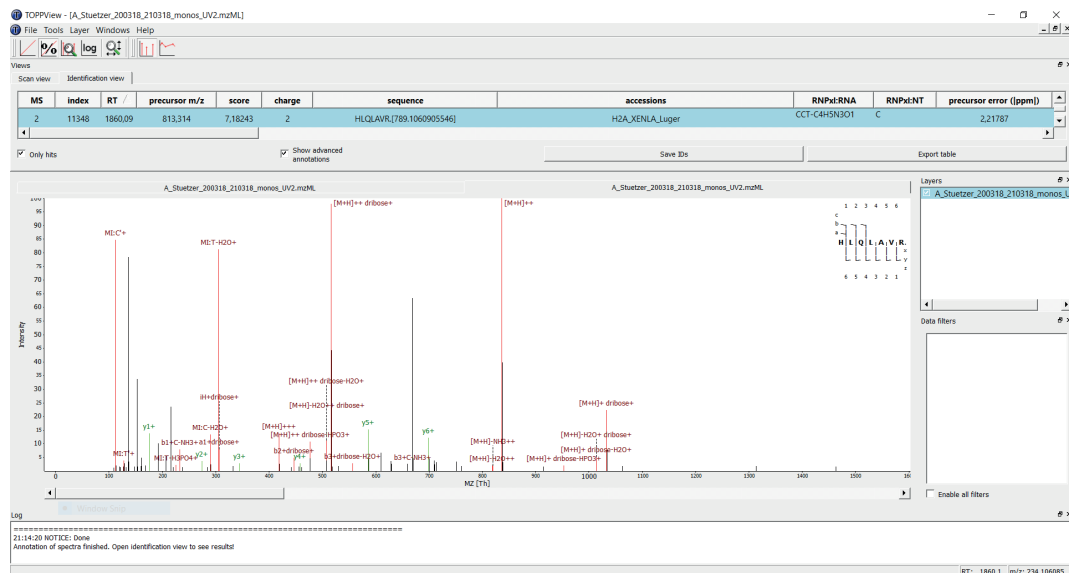
35)



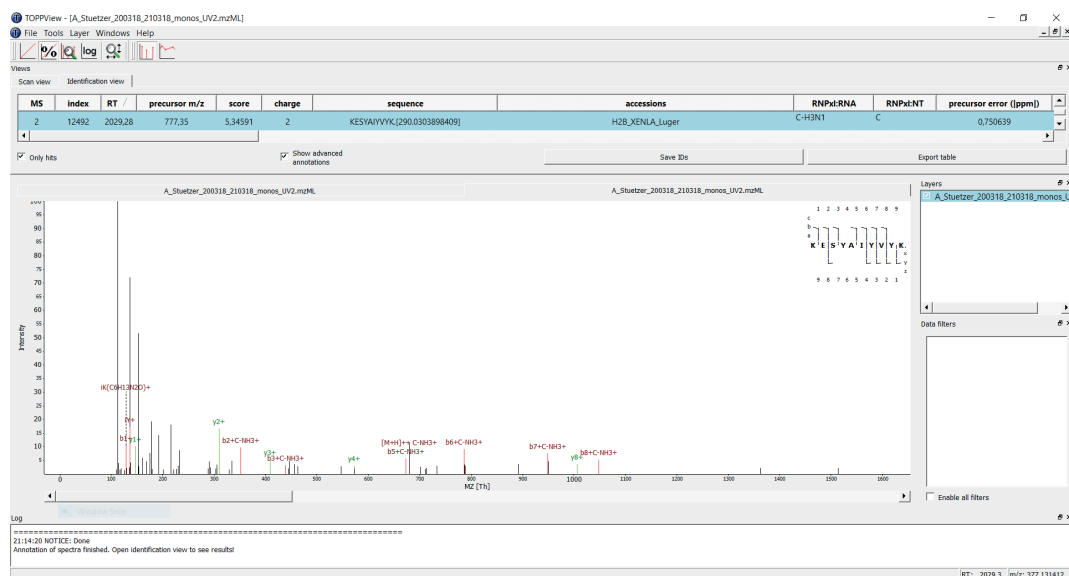
36)



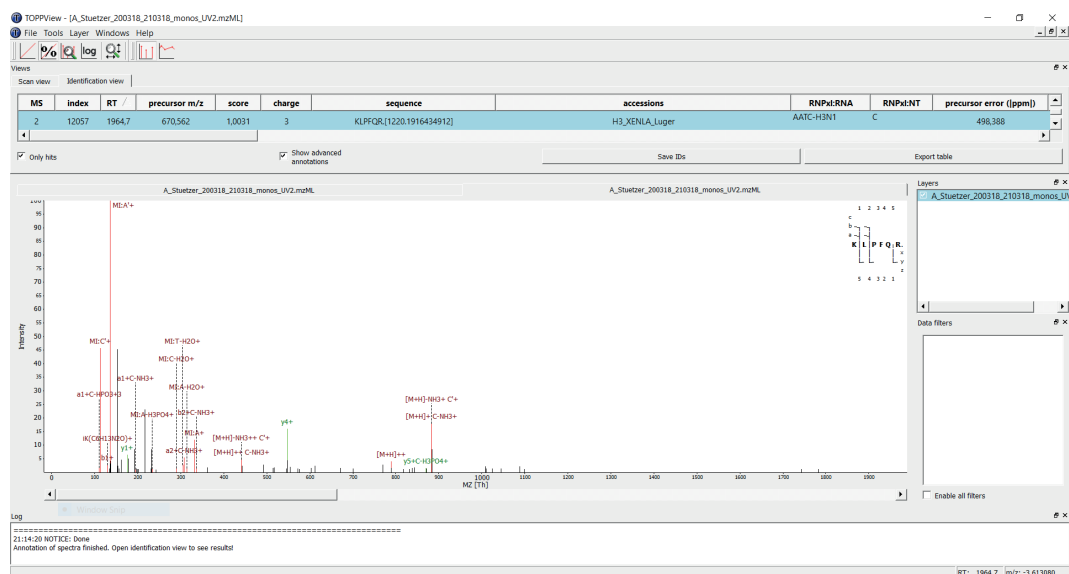
37)



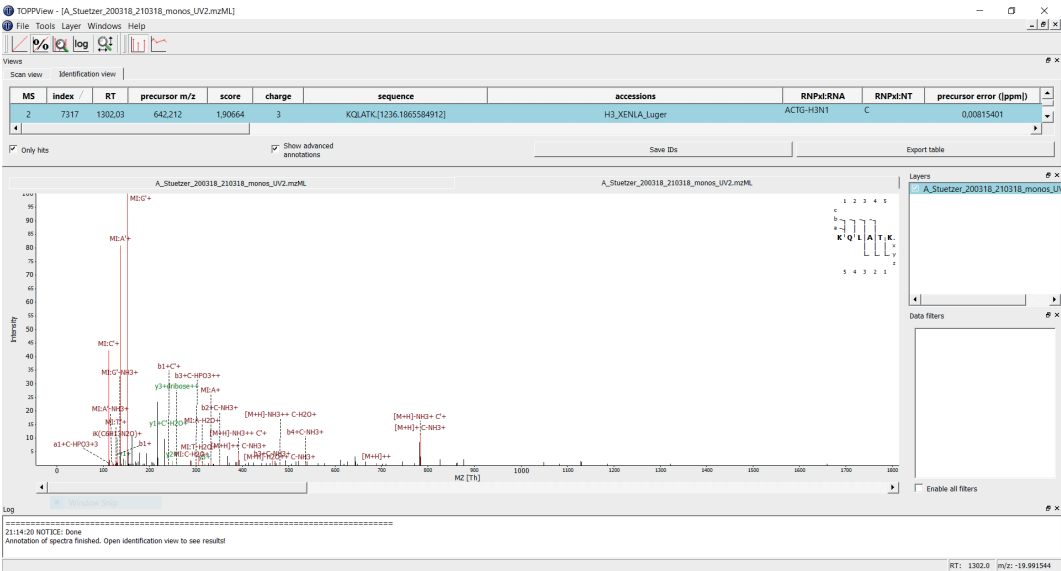
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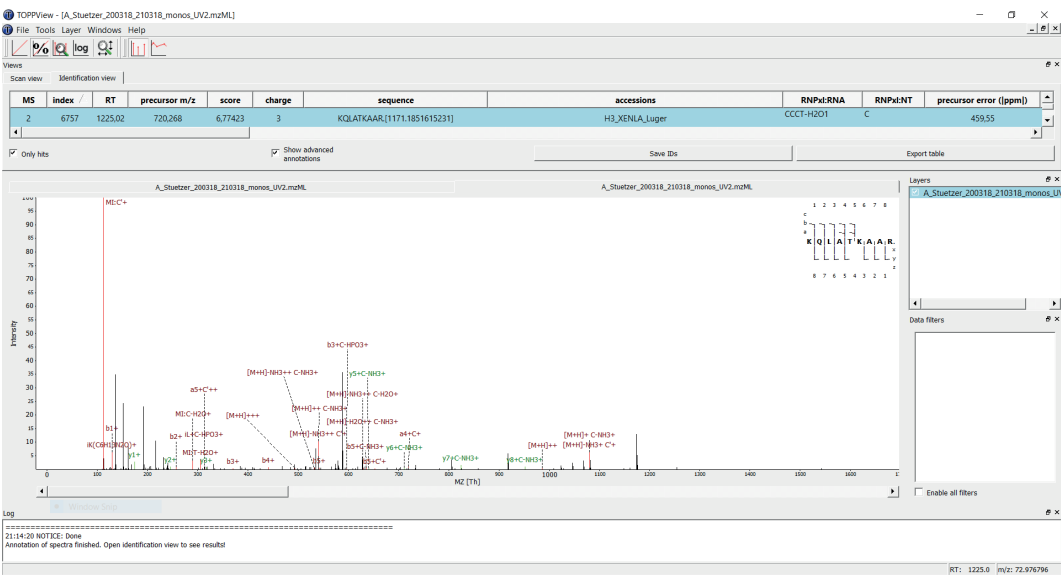
39)



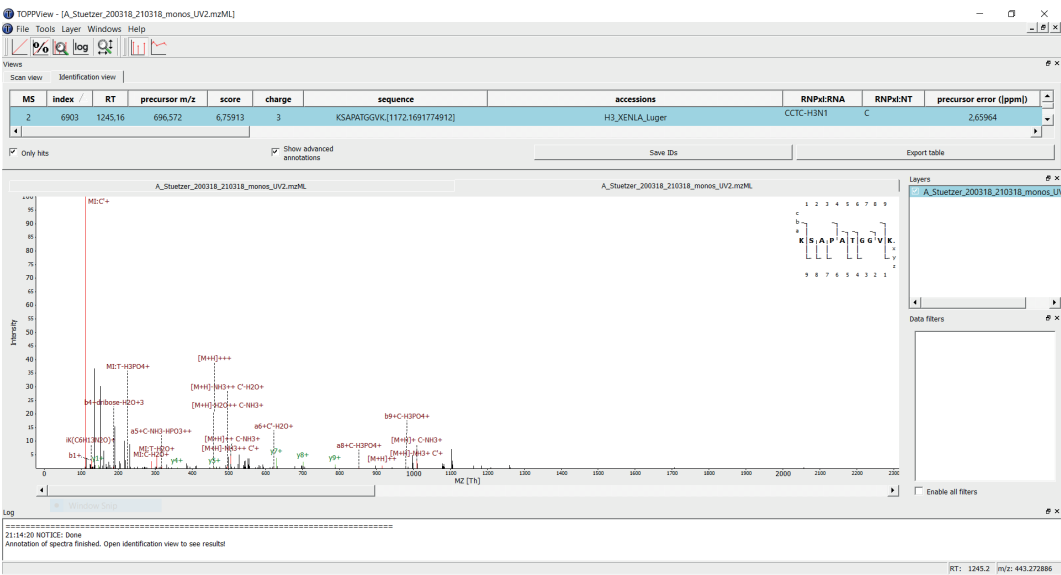
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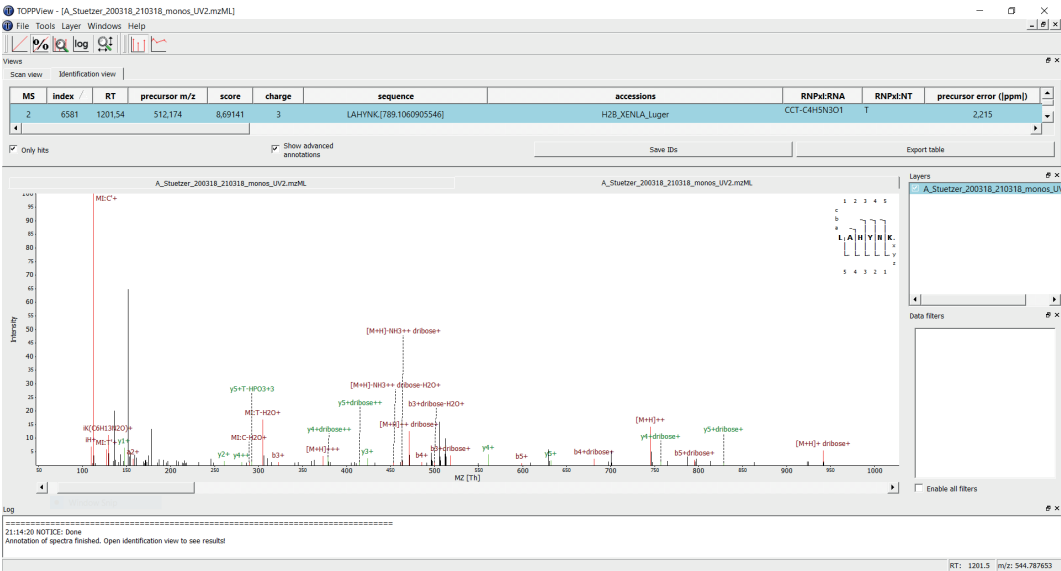
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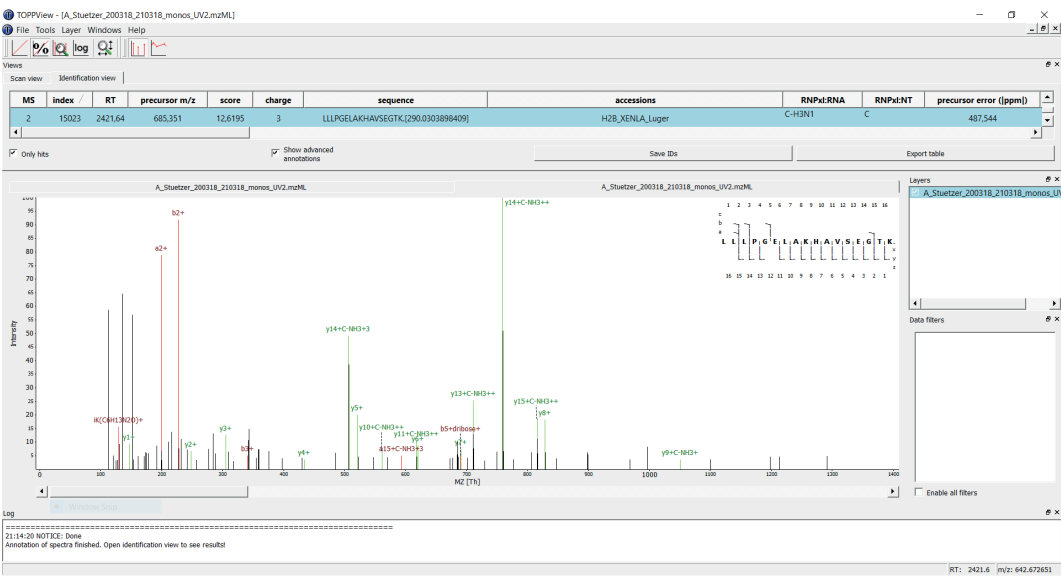
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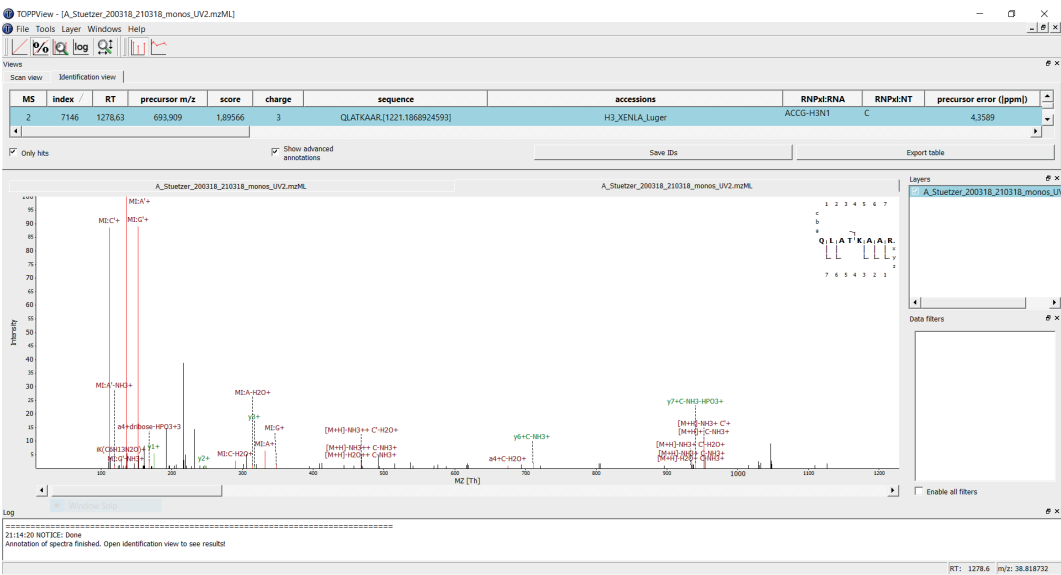
43)



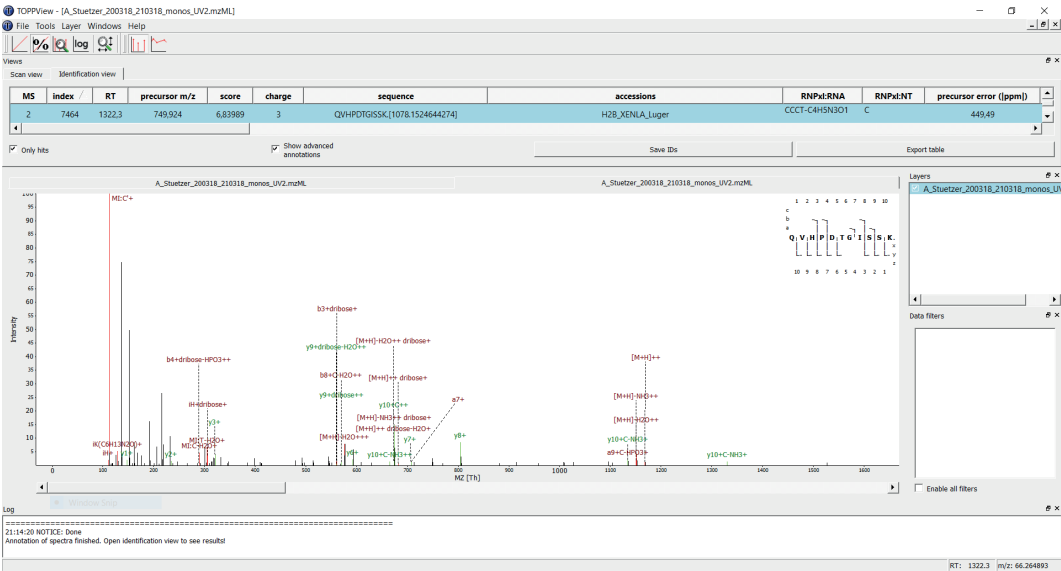
44)



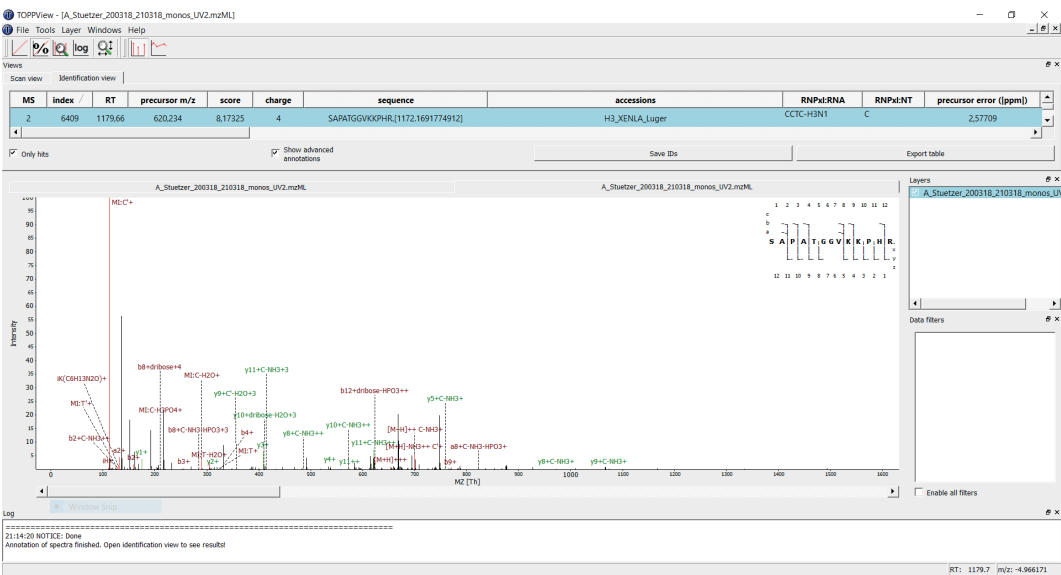
45)



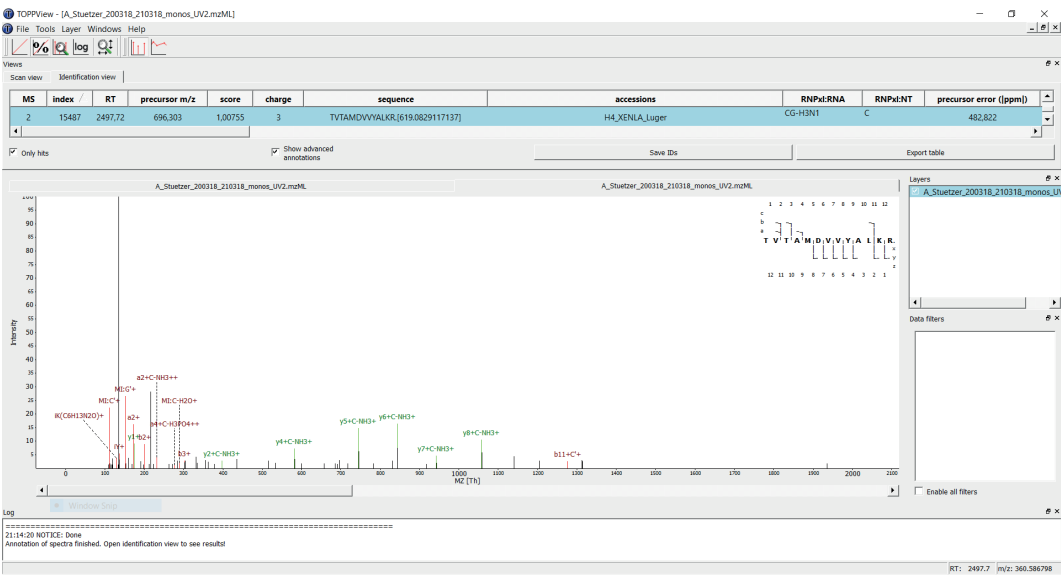
46)



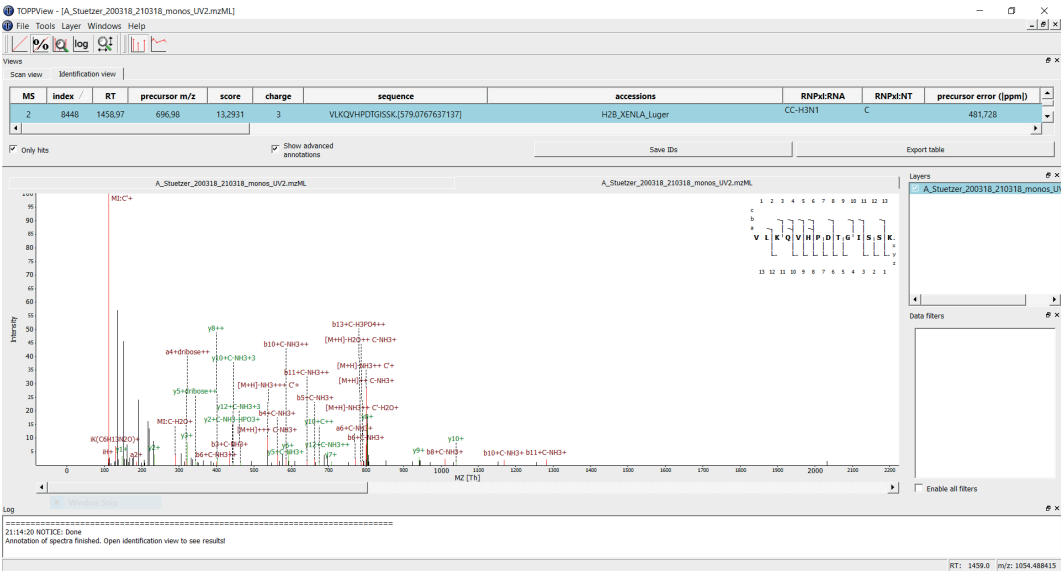
47)



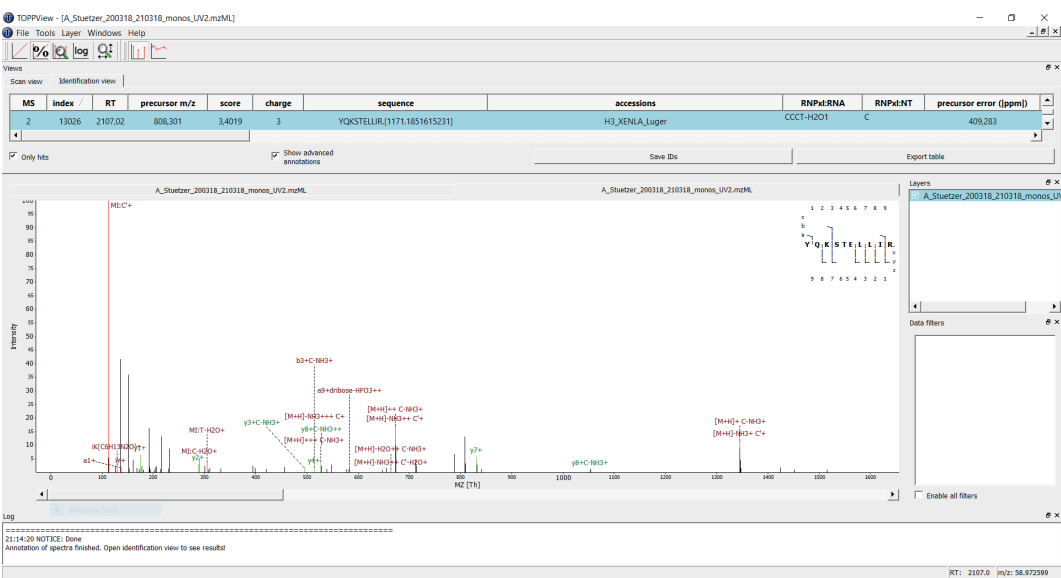
48)



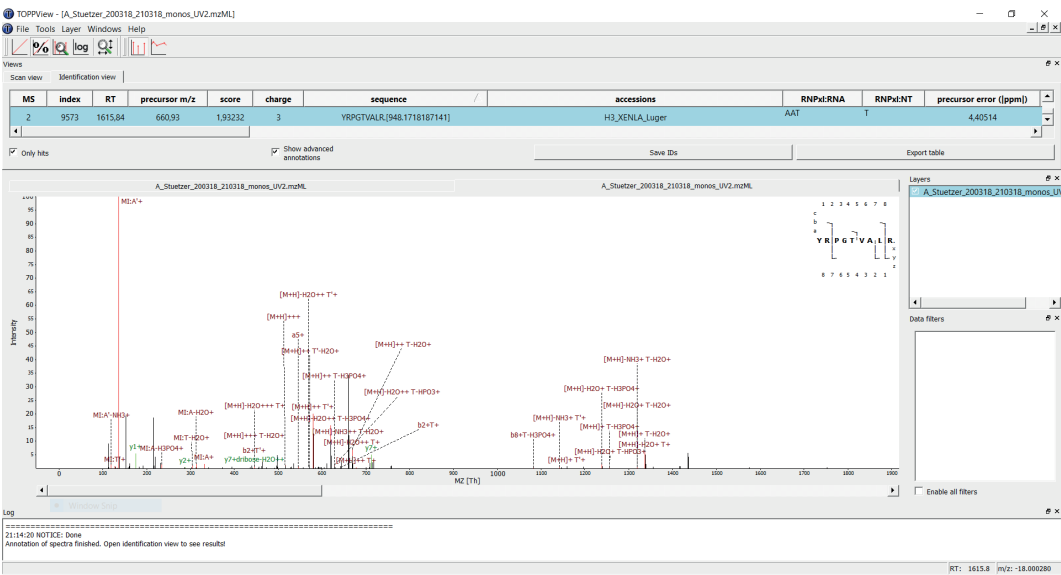
49)



50)

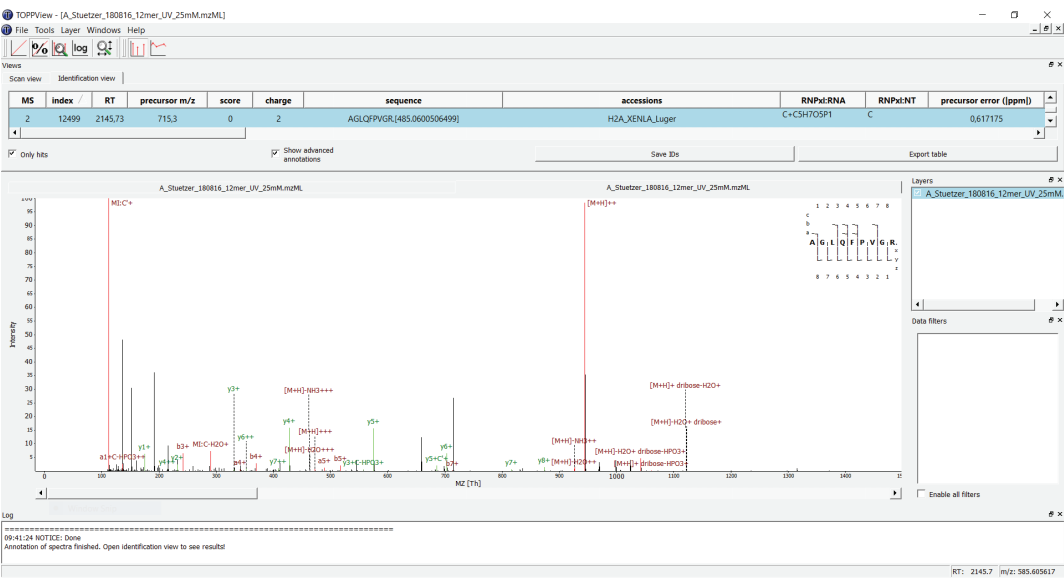


51)

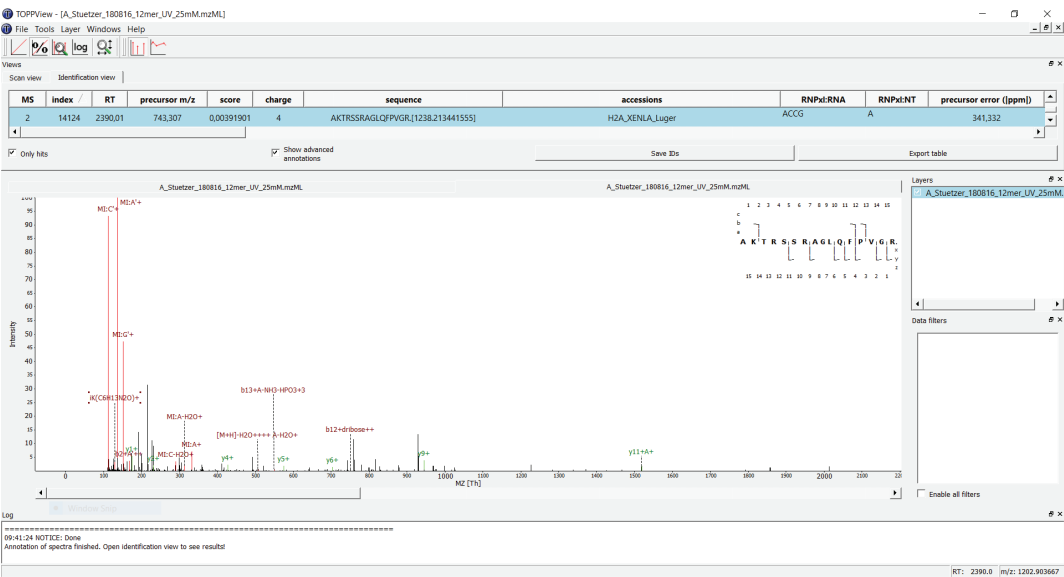


TOPPView MS/MS spectra of core histones from *X. laevis* nucleosomal arrays

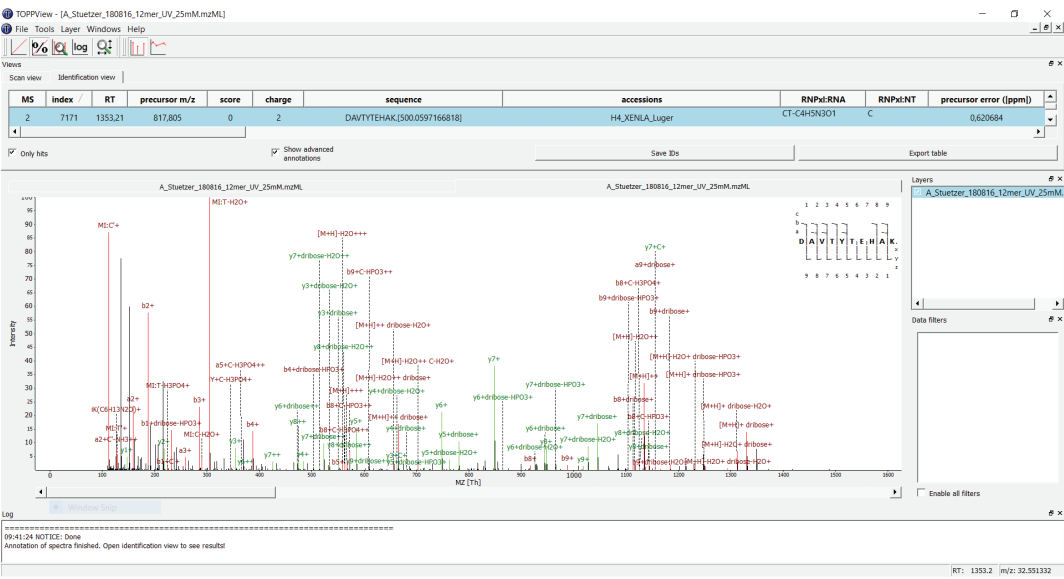
1)



2)



3)



TOPPPView - [A_Stuetzler_180816_12mer_UV_25mM.mzML]

File Tools Layers Layer UV 25nm

VIEWS
Scan view Identification view

MS	index /	RT	precursor m/z	score	charge	sequence	accessions	RNPs:rRNA	RNP:tNT	precursor error (ppm)
2	6975	1323.15	637.249	0.0864368	3	DAVYTEHAKR(619.0829117137)	H4_XENLA_Luger	CG-HSNT	C	2.32436

< Only MS Show advanced annotations Save Dds Export table

A_Stuetzler_180816_12mer_UV_25mM.mzML A_Stuetzler_180816_12mer_UV_25mM.mzML

Layers
A_Stuetzler_180816_12mer_UV_25mM.mzML

Data filters Enable all filters

Log

m/z 1323.15 NOTICE Done
Annotation of spectra finished. Open identification view to see result

[illegible]

TOPVIEW - [A_Stuetzer_180816_12mer_UV_25mM.mzML]

File Tools Layer Settings Help

Scan view Identification view

MS	Index / RT	precursor m/z	score	charge	sequence	accessions	RNPeRNA	RNPNT	precursor error (ppm)
2	10923 1912.12	833.313		0 3	DNIQGITKPAIR[1172.169174912]	H4_XENLA_Luger	CCTC-H3NT	C	1,10059

☒ Only MS ☒ Show advanced annotations Save IDs Export table

A_Stuetzer_180816_12mer_UV_25mM.mzML

A_Stuetzer_180816_12mer_UV_25mM.mzML

Layers
A_Stuetzer_180816_12mer_UV_25mM.mzML

Data filters

Enable all filters

Log

09:41:24 NOTICE: Done
Annotation of spectra finished. Open identification view to see result!

File Tools Layers Layer Views

Views Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPs:RNA	RNPs:NT	precursor error (ppm)
2	12458	2139.57	965.388	0.0141228	2	EIAGDKFTDLR[594.0764297456]	H3_XENLA_Luger	TC-H3NT	C	0.899721

☒ Only Hits ☒ Show advanced annotations

Save IDs Export table

A_Stuetzner_180816_12mer_UV_25nmM.mzML

A_Stuetzner_180816_12mer_UV_25nmM.mzML

Layers

A_Stuetzner_180816_12mer_UV_25nmM.mzML

1 2 3 4 5 6 7 8 9 10
C
D
E
F
G
H
I
J
K
L
M
N
O
P
Q
R
S
T
U
V
W
X
Y
Z

Data filters

Enable all filters

Log

09:41:24 NOTICE: Done

Annotation of spectra finished. Open identification view to see result

RT: 2139.6 m/z: 28.346745

TOPVIEW - [A_Stuetzer_180816_12mer_UV_25mM.mzML]

File Tools Layers Views Help

Views Scan view Identification view

MS	index /	RT	precursor m/z	score	charge	sequence	accessions	RNPeRNA	RNPcNT	precursor error (ppm)
2	12452	2138.66	810.818		2	ESYAVYYK[485.0600506499]	H2B_XENLA_Luger	C+CSH70SP1	C	0.452849

☒ Only Hts ☒ Show advanced annotations Save IDs Export table

A_Stuetzer_180816_12mer_UV_25mM.mzML

A_Stuetzer_180816_12mer_UV_25mM.mzML

Layers
A_Stuetzer_180816_12mer_UV_25mM.mzML

Data filters

☐ Enable all filters

Log

```
=====
09:41:24 NOTICE: Done
Annotation of spectra finished. Open identification view to see result
```

TOPView - [A_Stutzer_180816_12mer_UV_25mM.mzML]

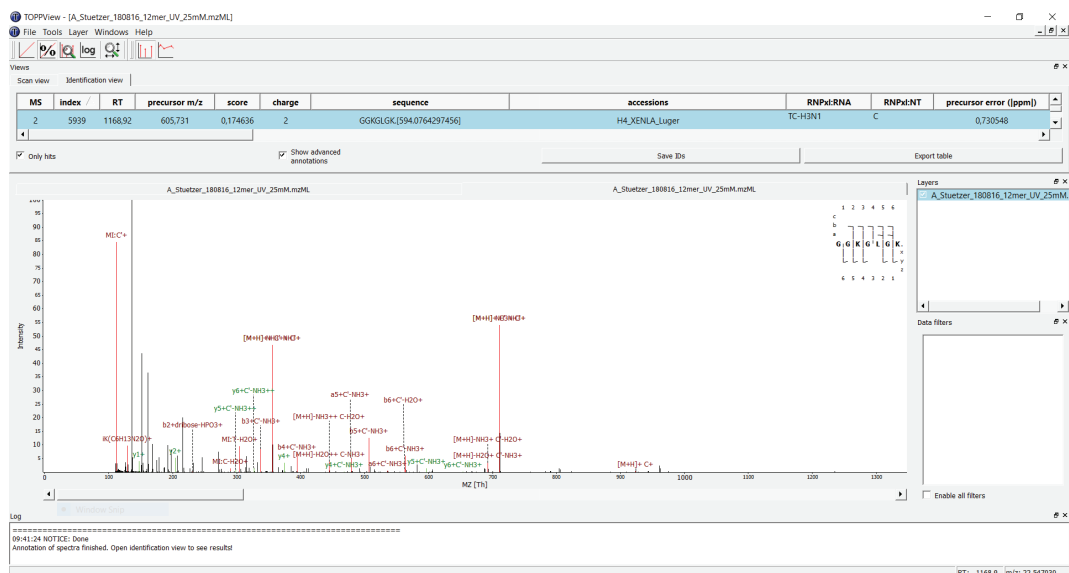
File Tools Layers Views Help

Views Scan view Identification view

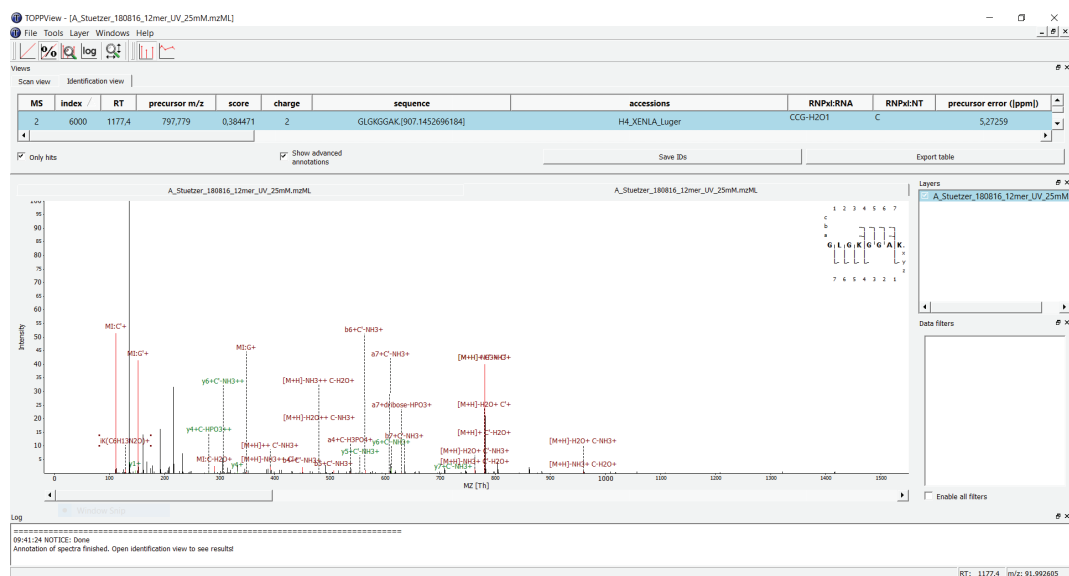
MS	Index / RT	precursor m/z	score	charge	sequence	accessions	RNPs:RNA	RNP:NT	precursor error (ppm)
2	17184 2859.77	891.671	0.241217	3	ESYAVYYVKLK(1197.1756594593)	H2B_XENLA_Luger	CCGC-H3NT	C	2.59189

✓ Only MS ☐ Show advanced annotations Save Ds Export table

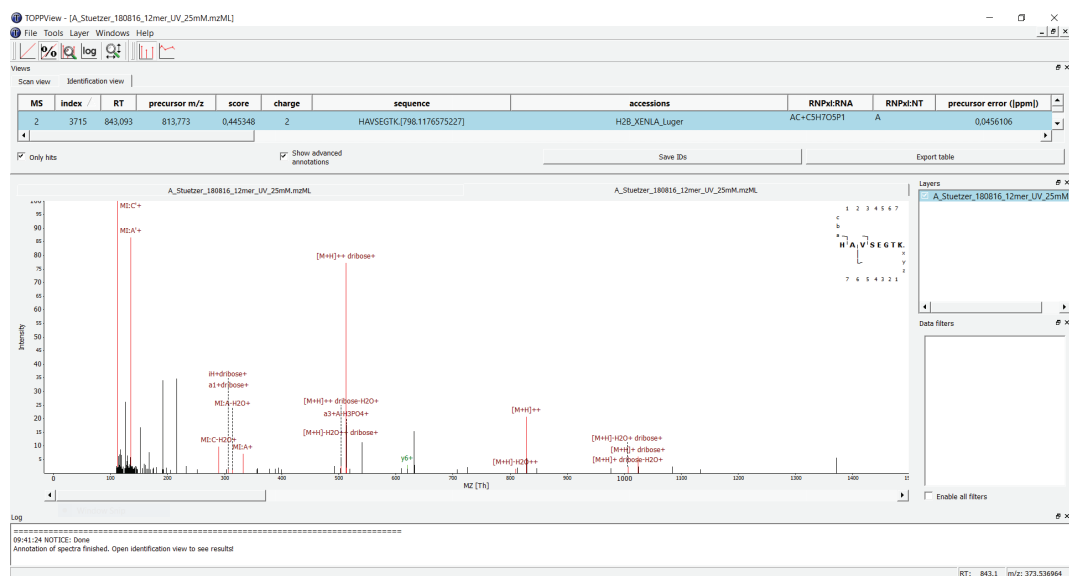
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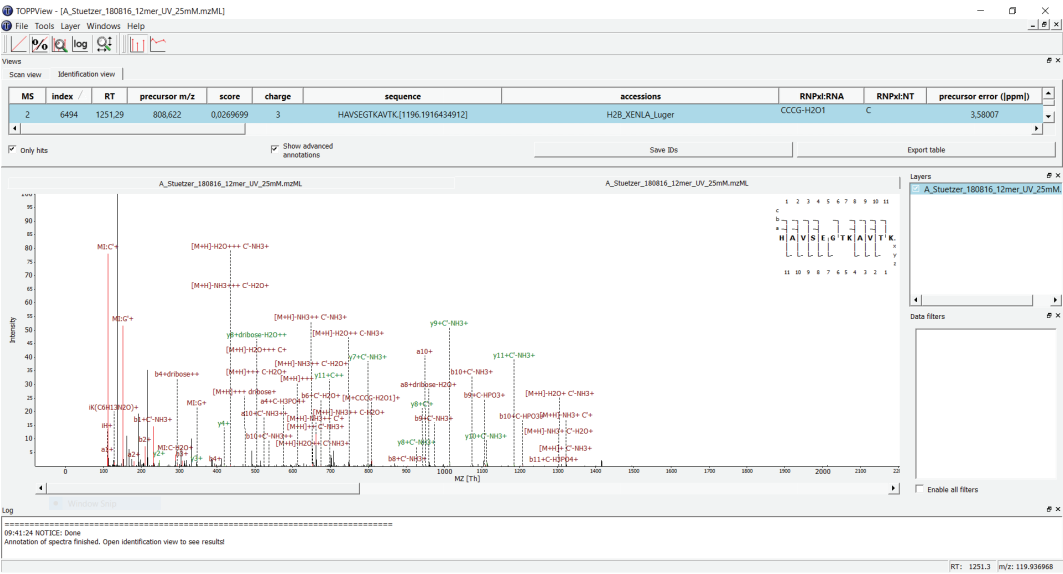
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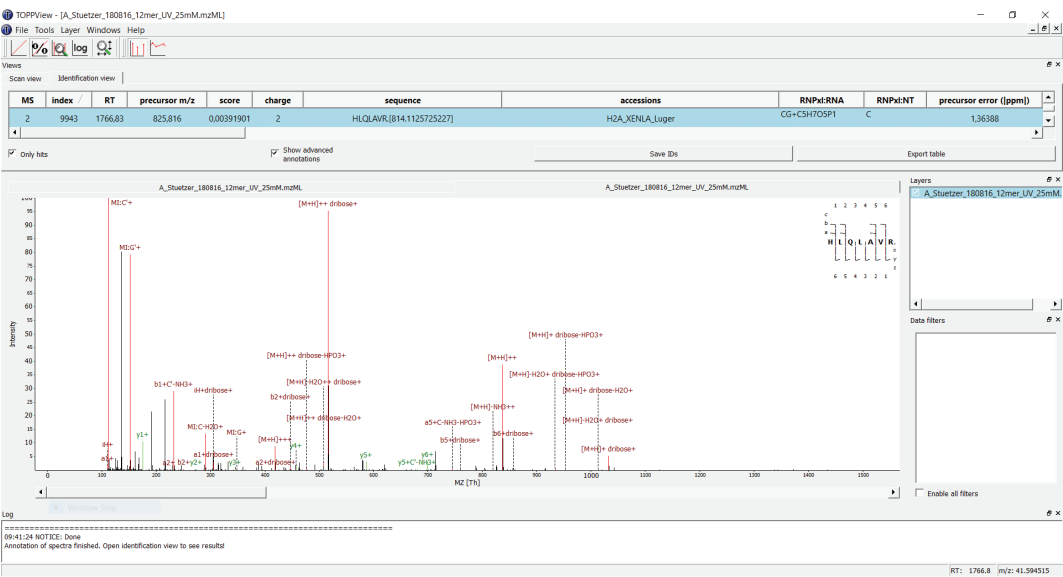
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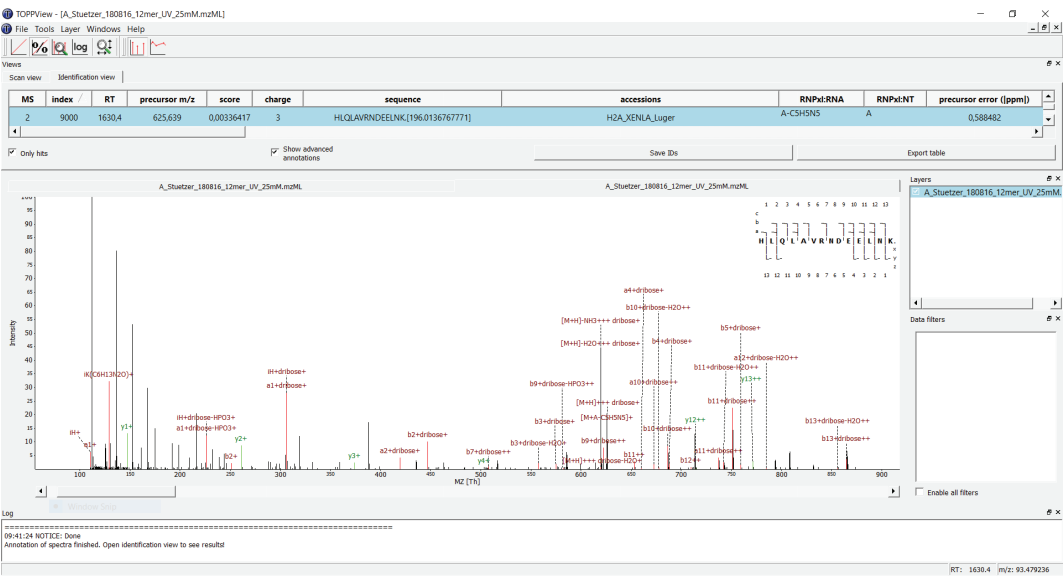
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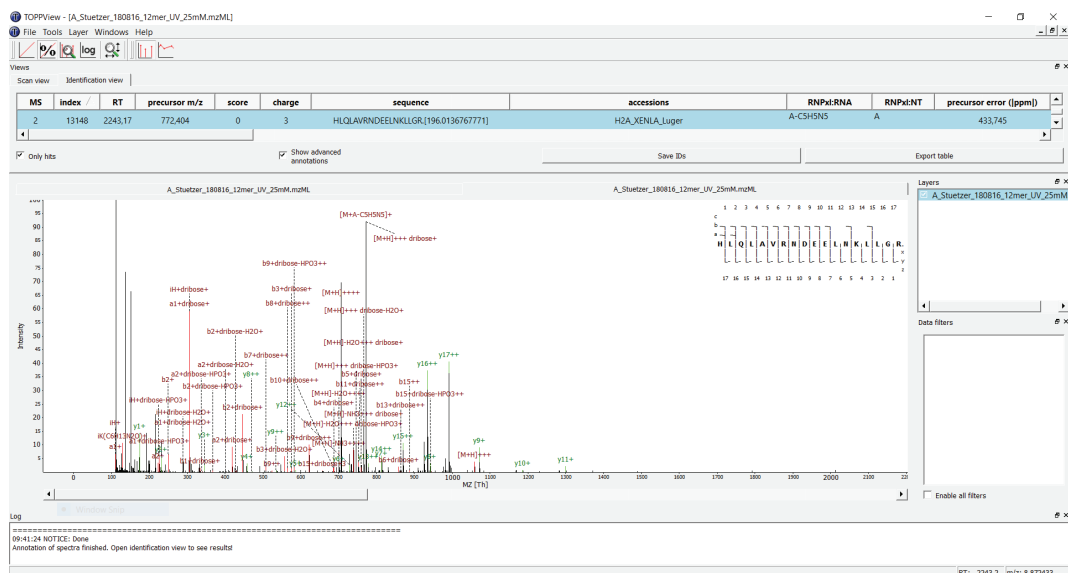
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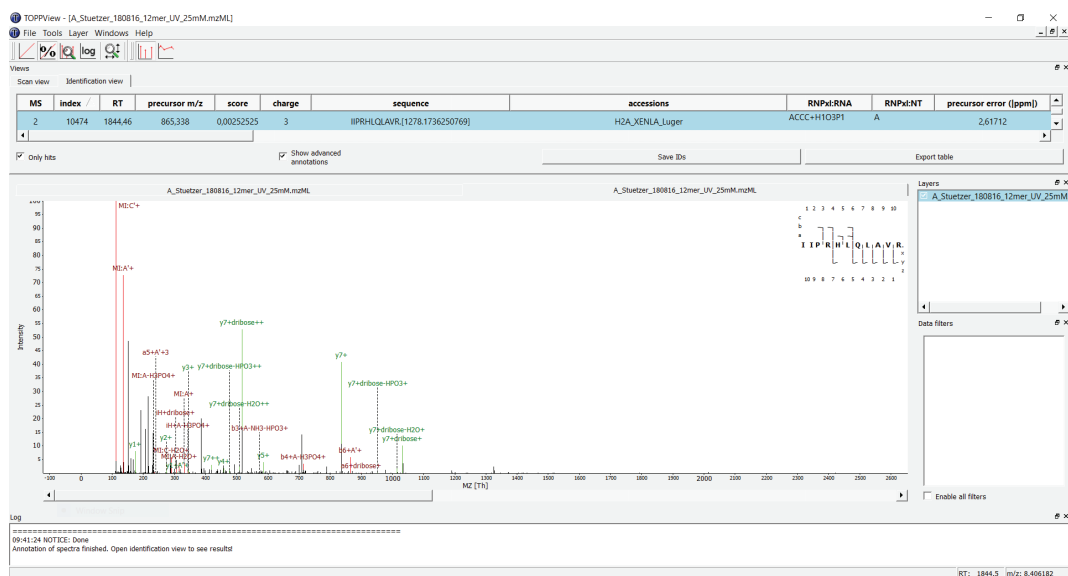
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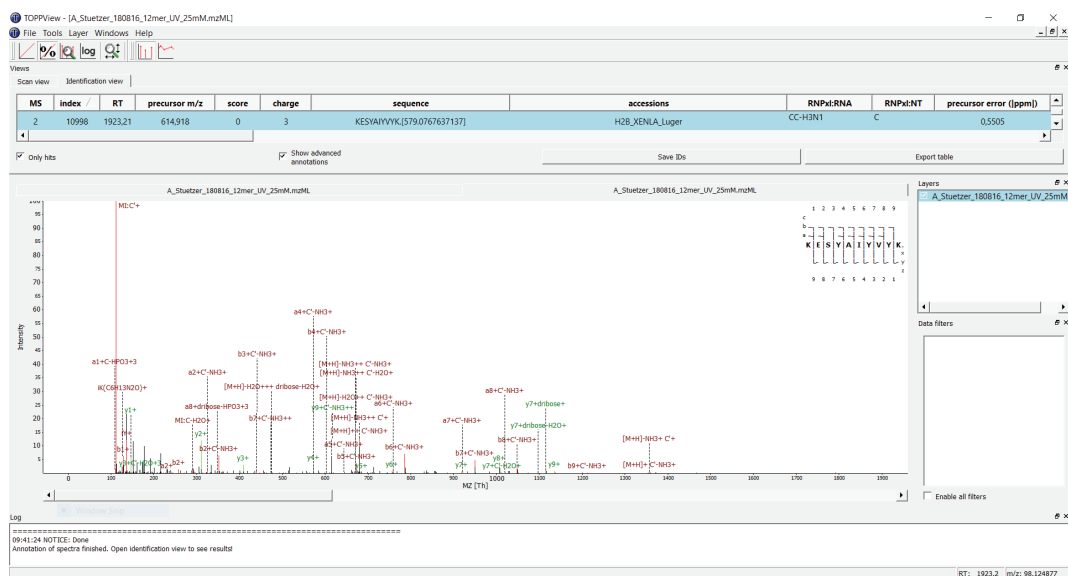
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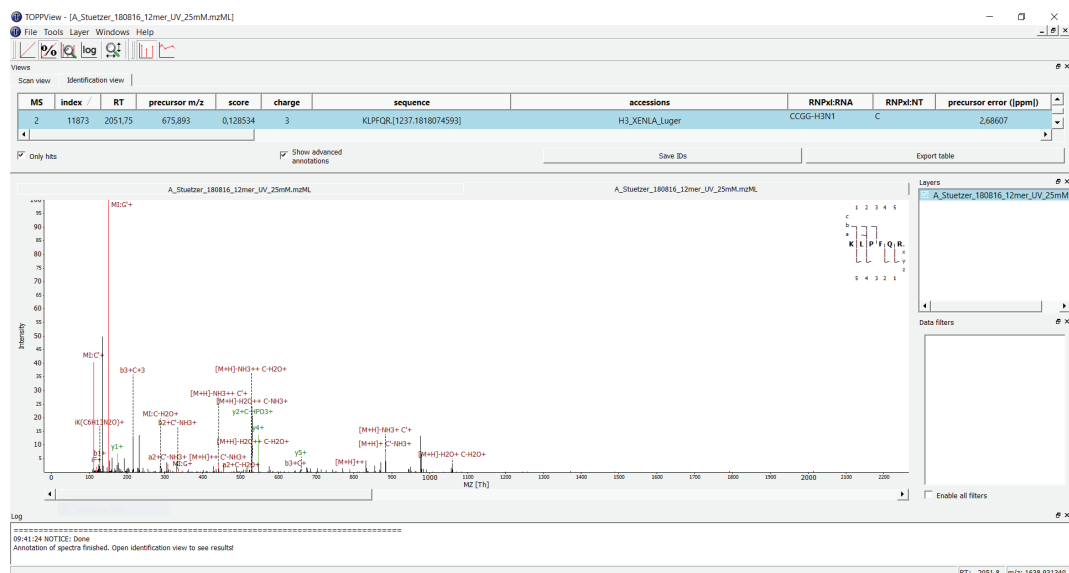
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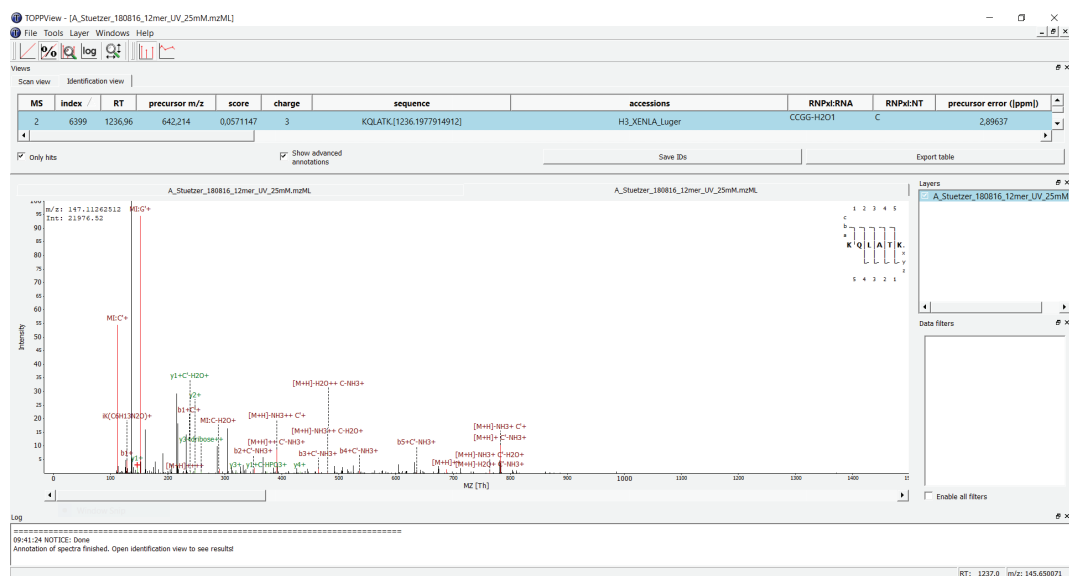
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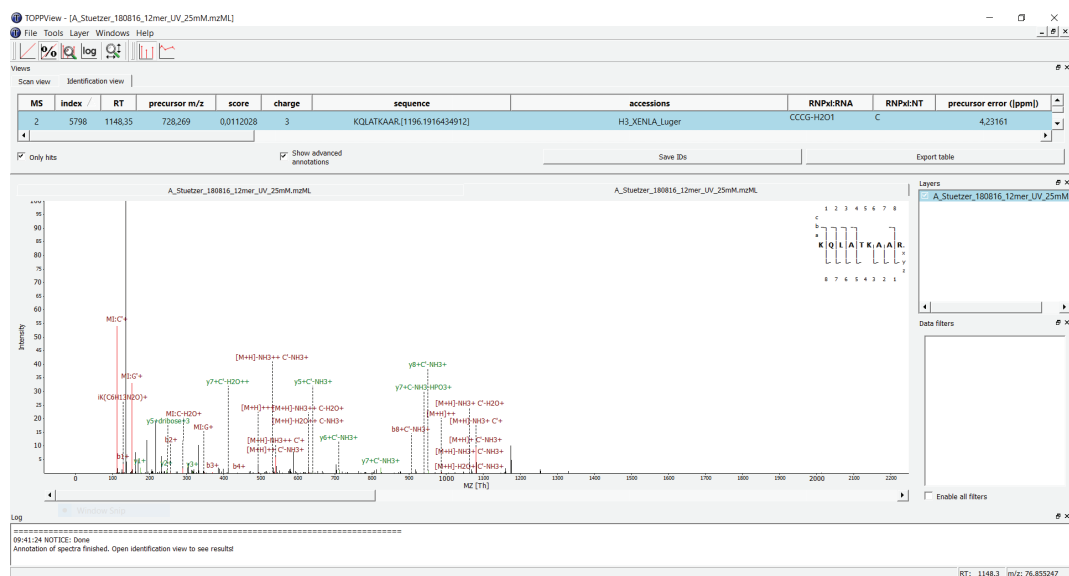
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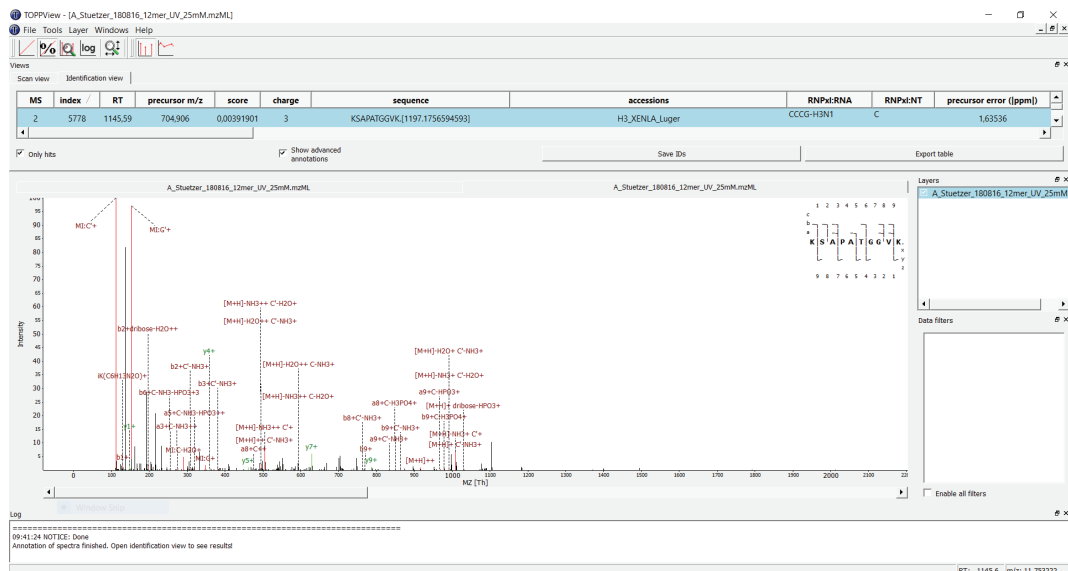
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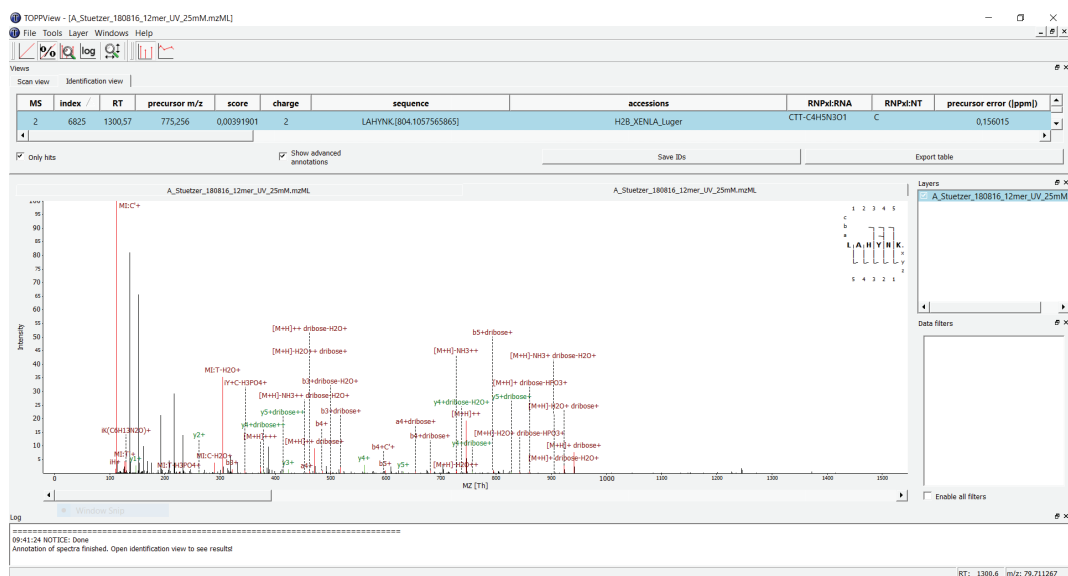
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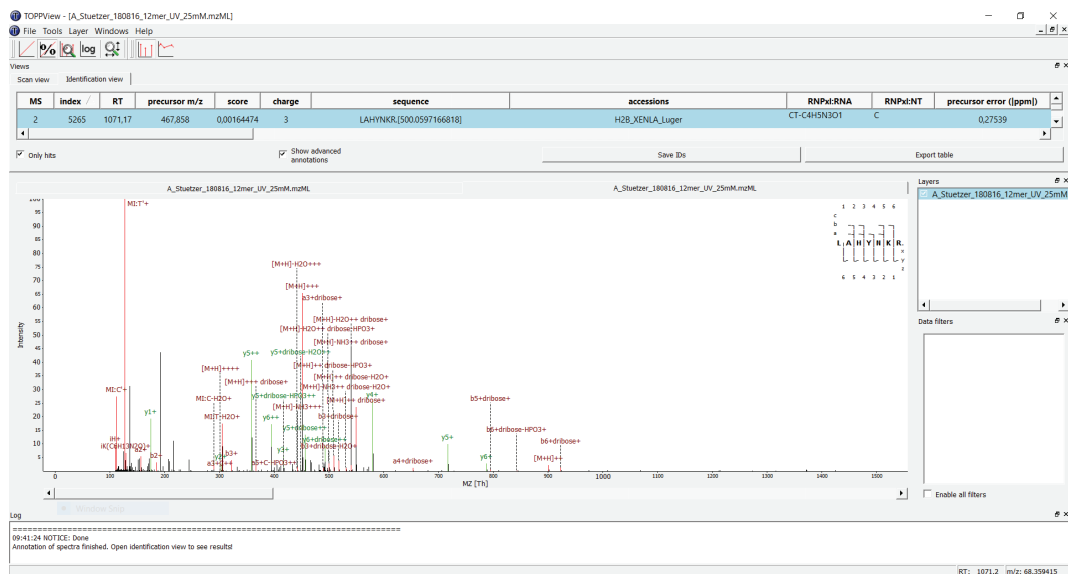
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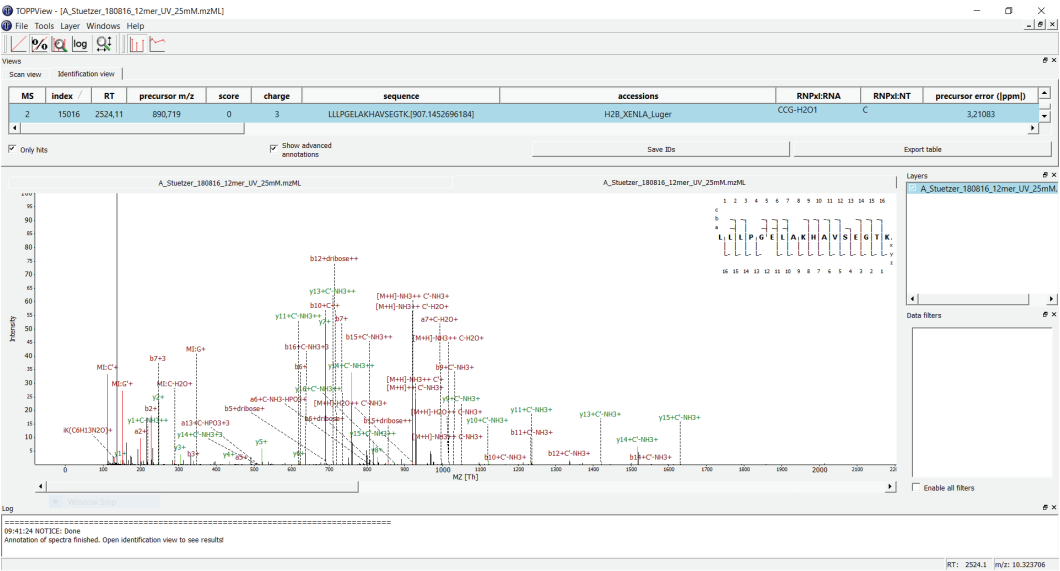
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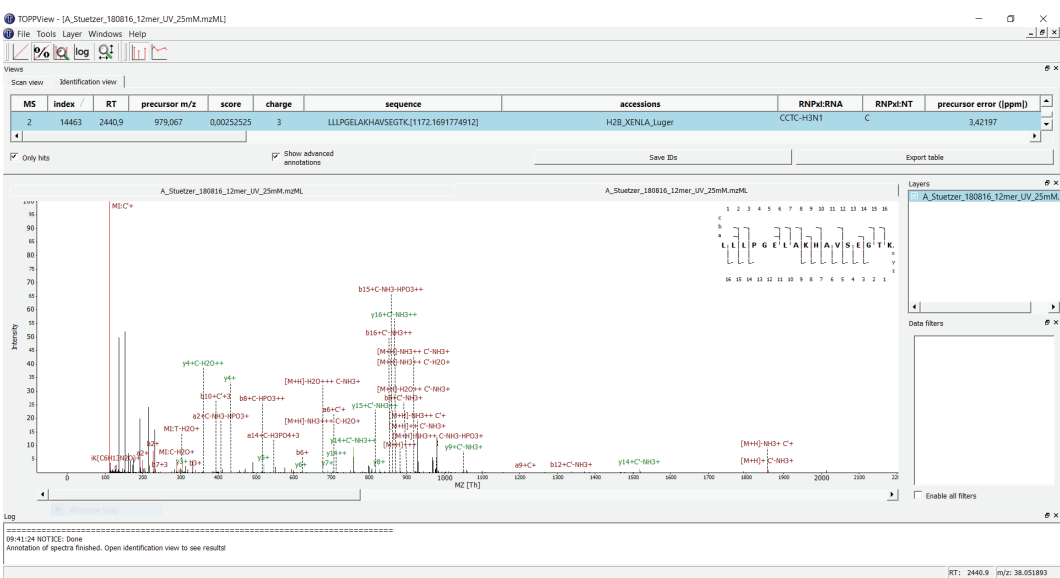
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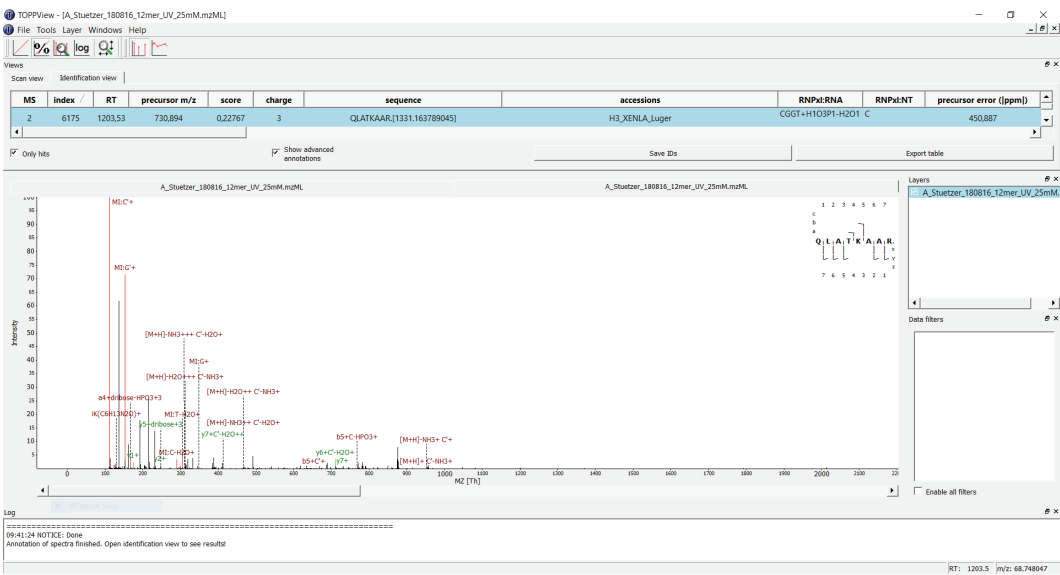
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26)



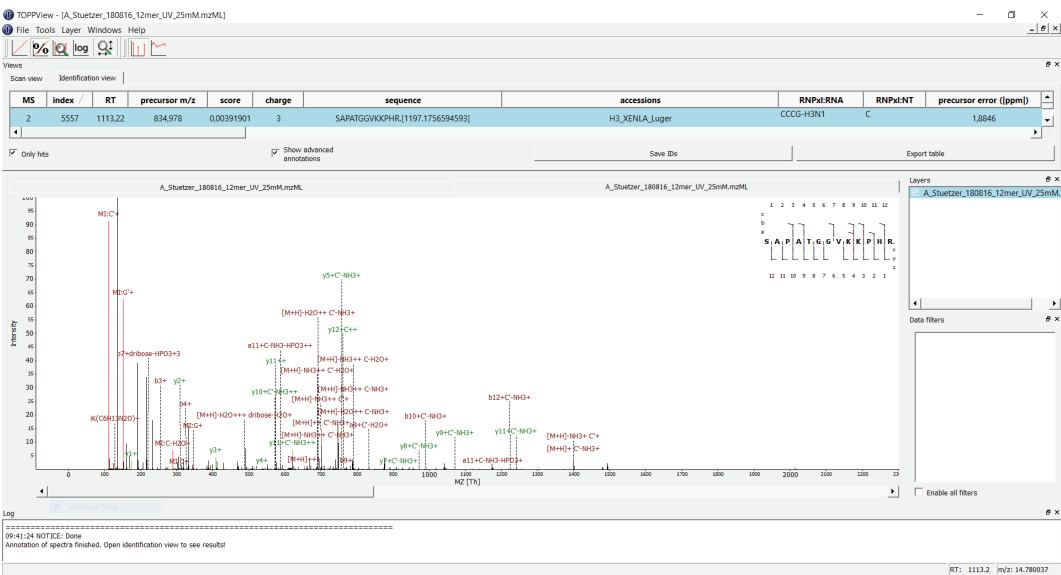
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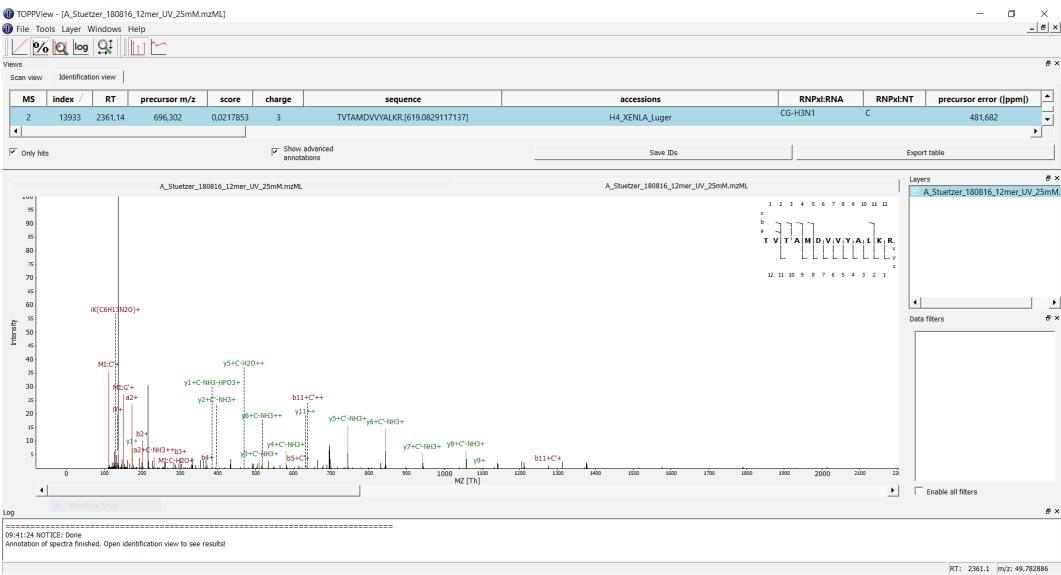
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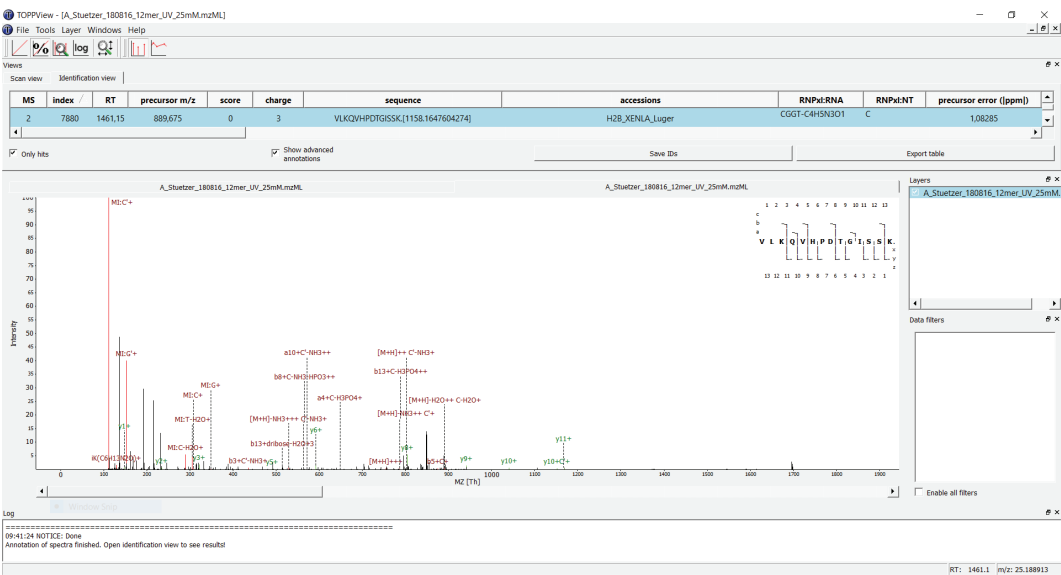
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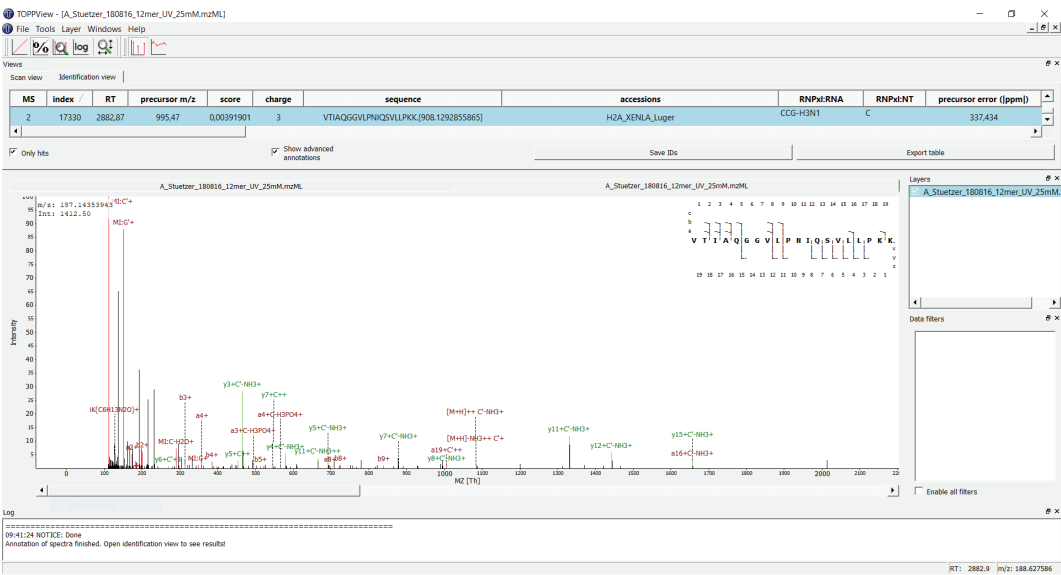
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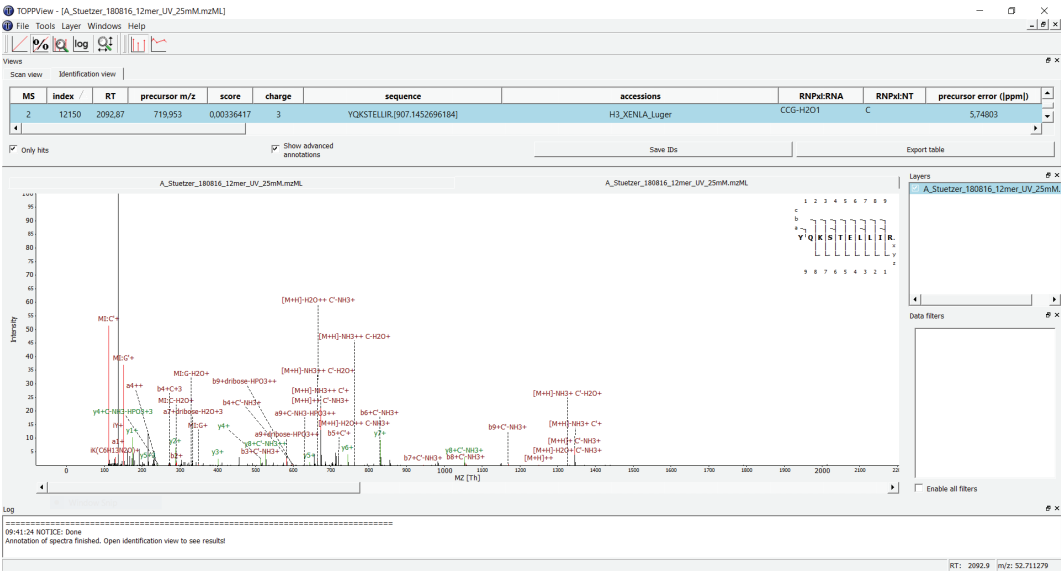
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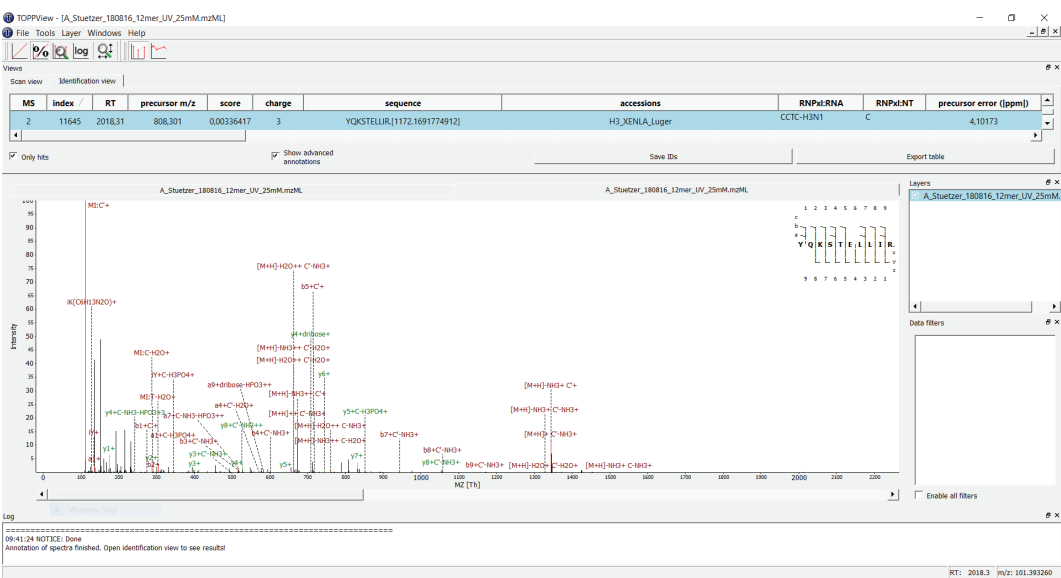
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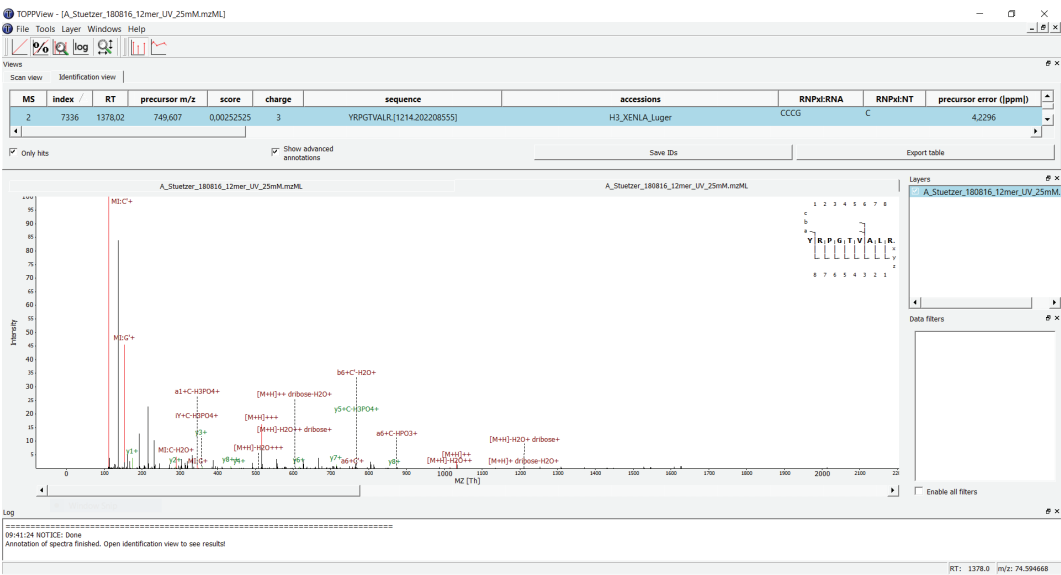
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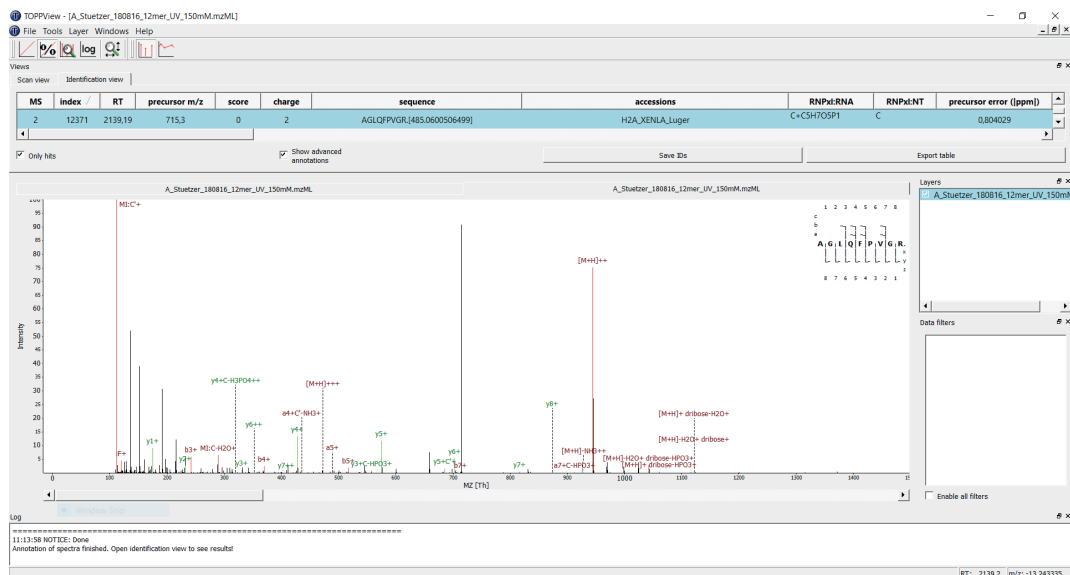
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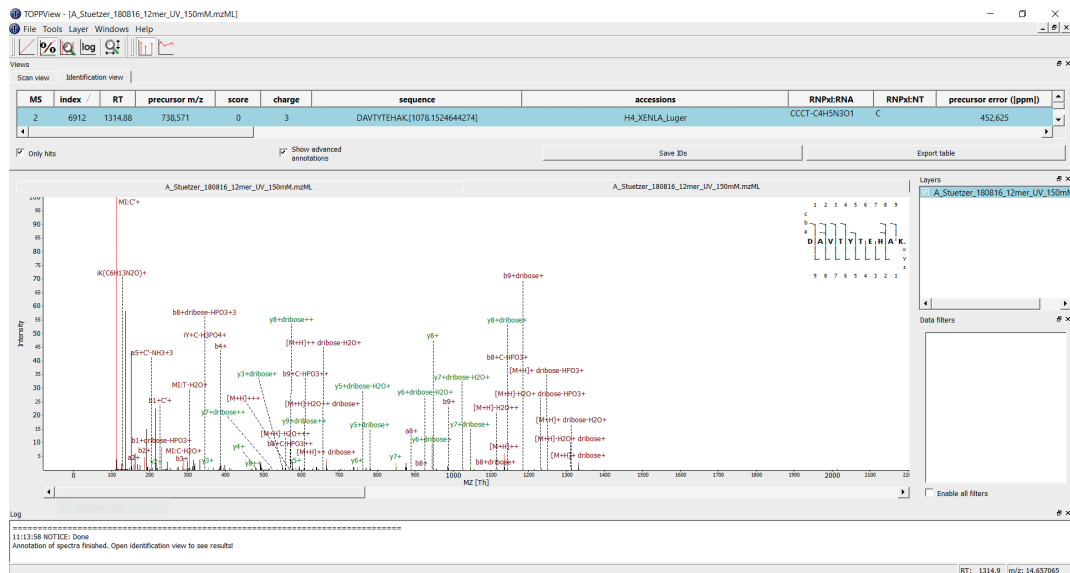
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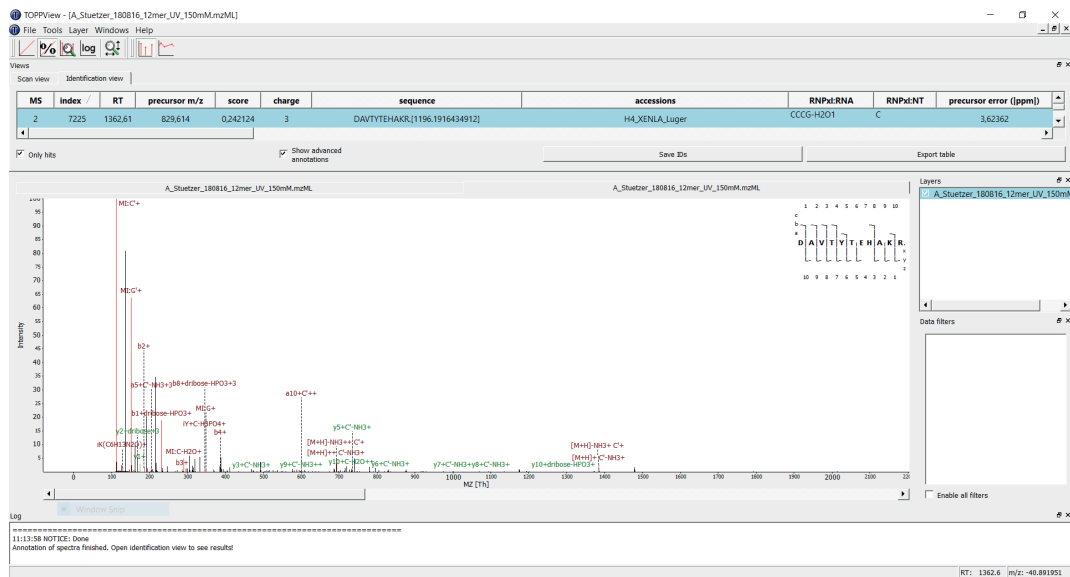
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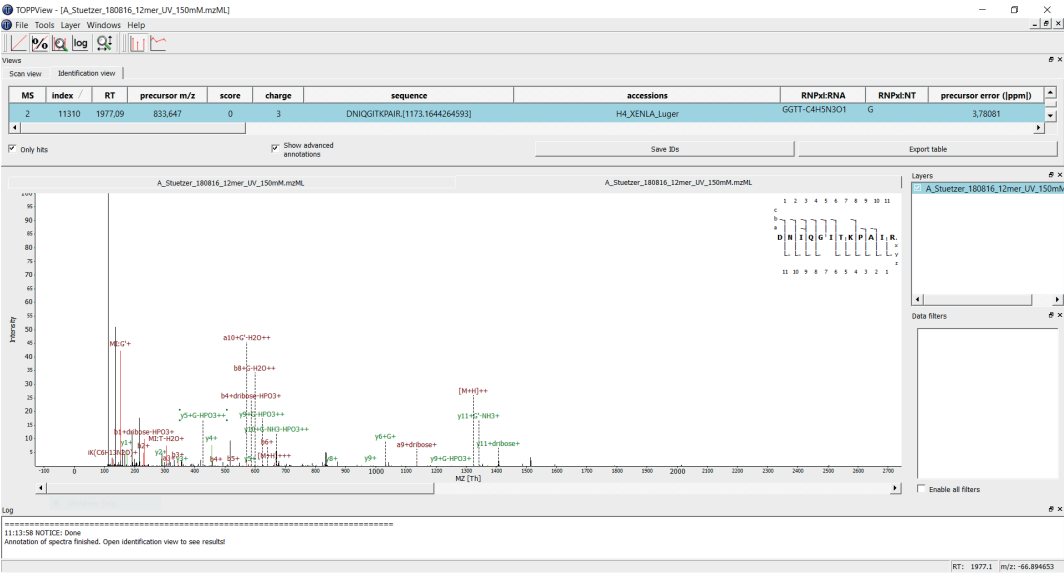
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39)



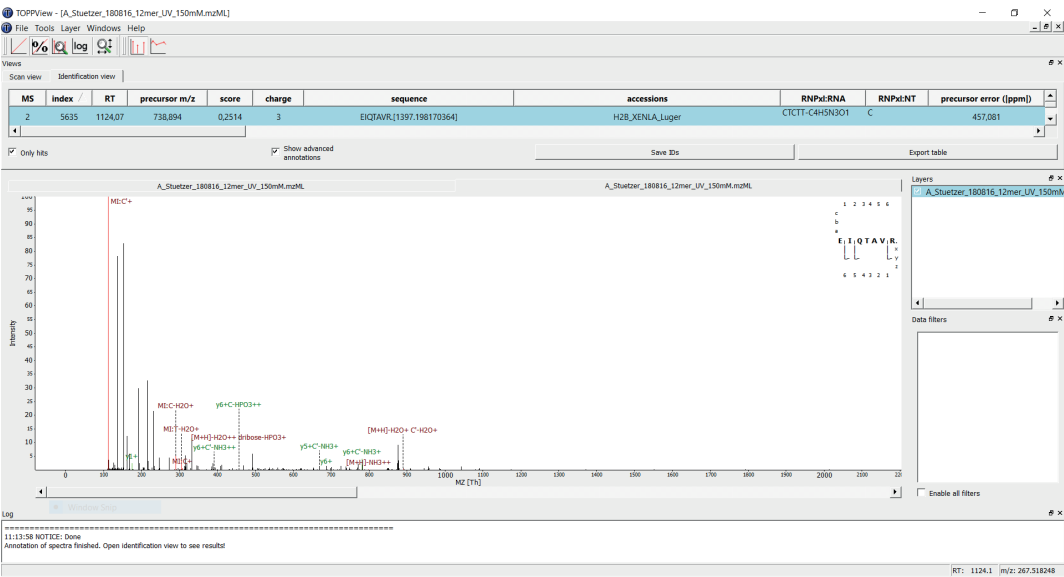
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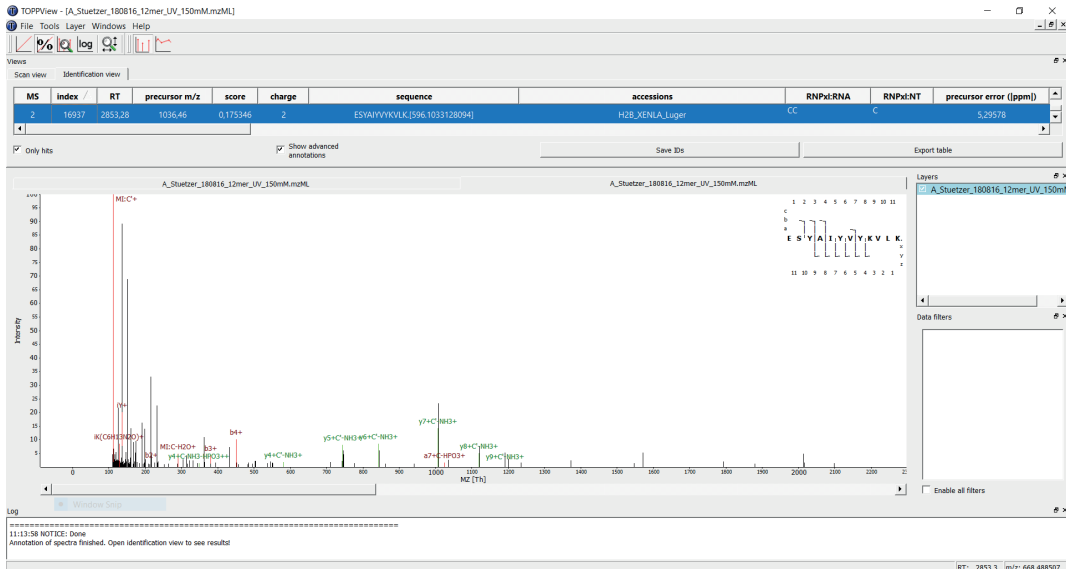
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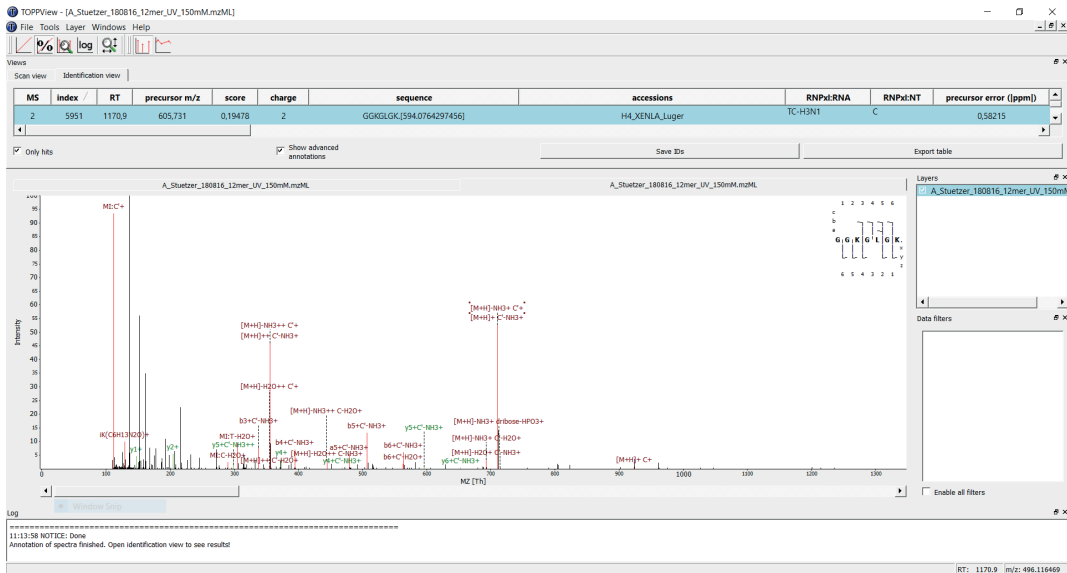
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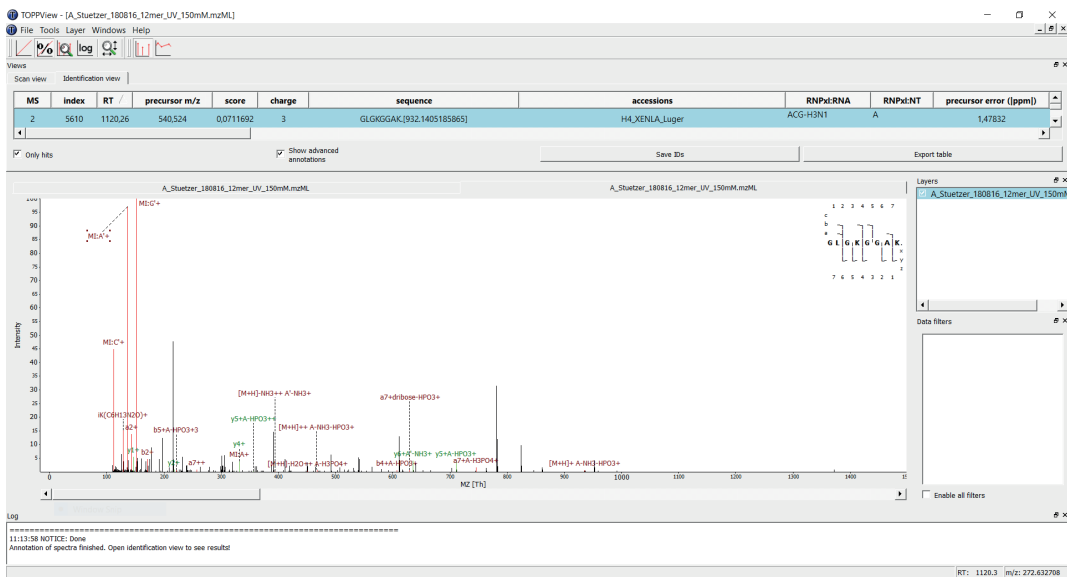
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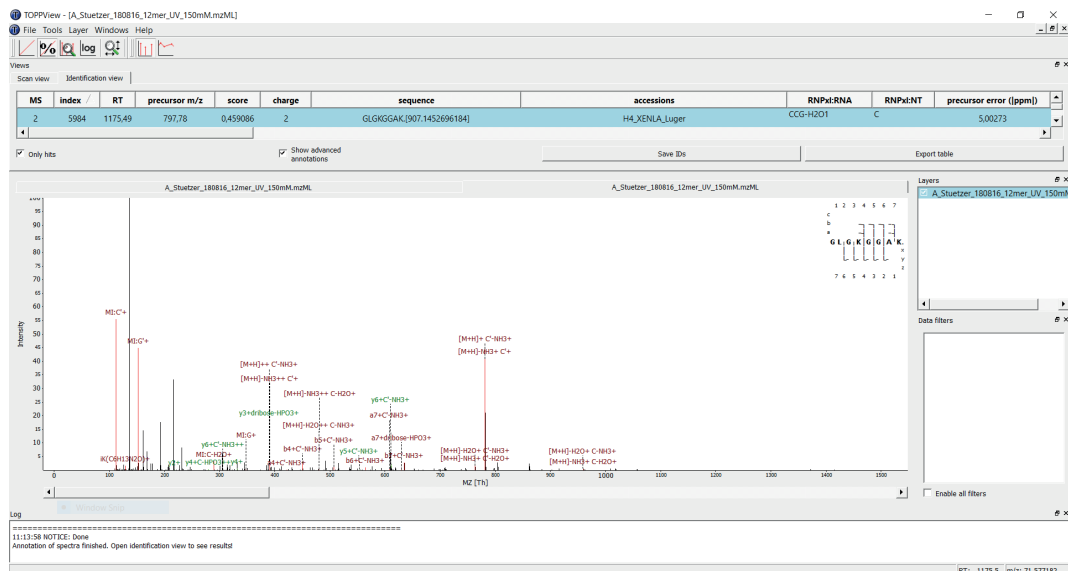
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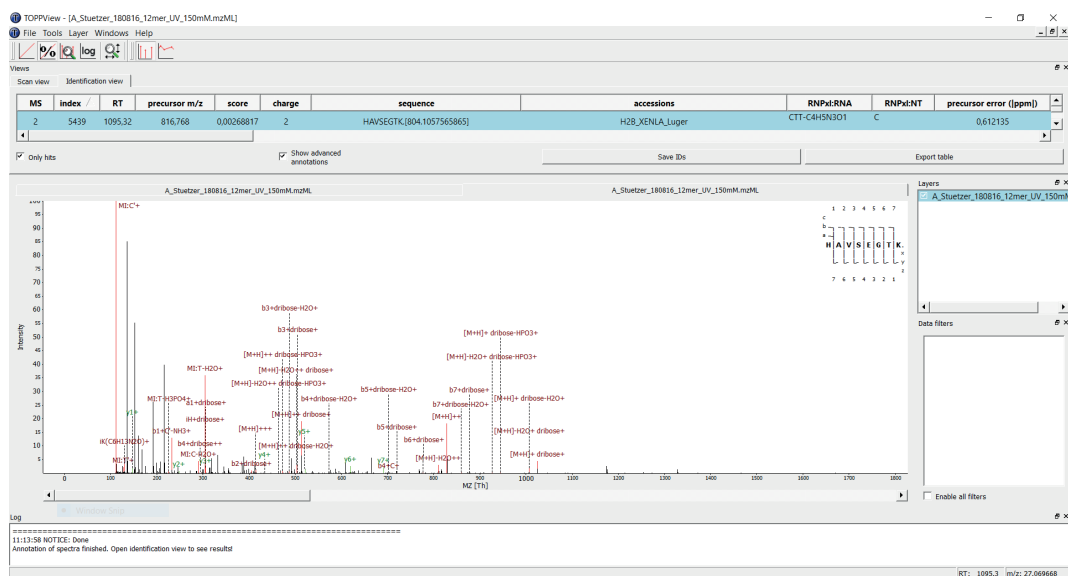
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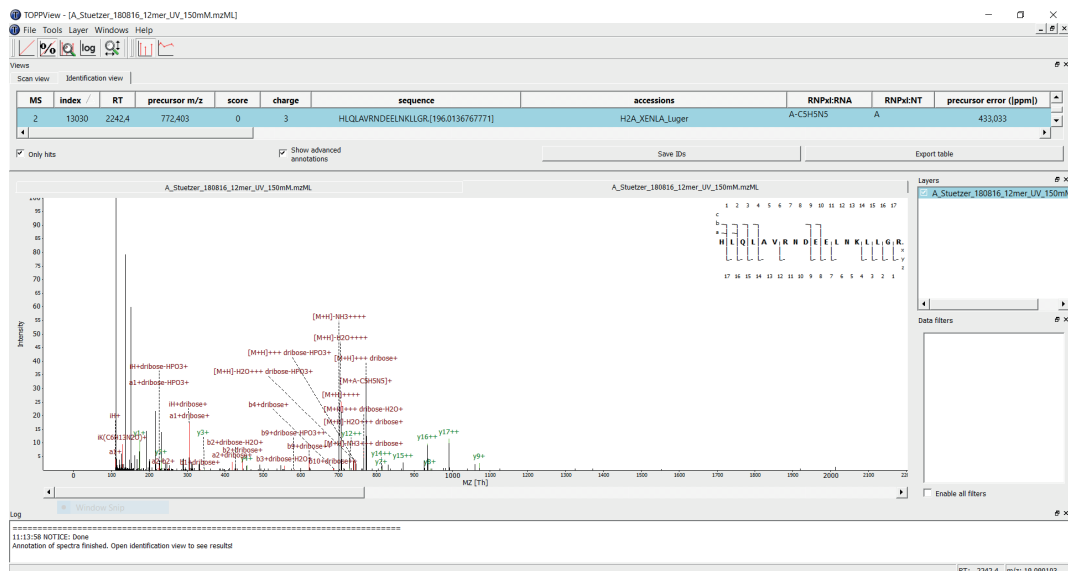
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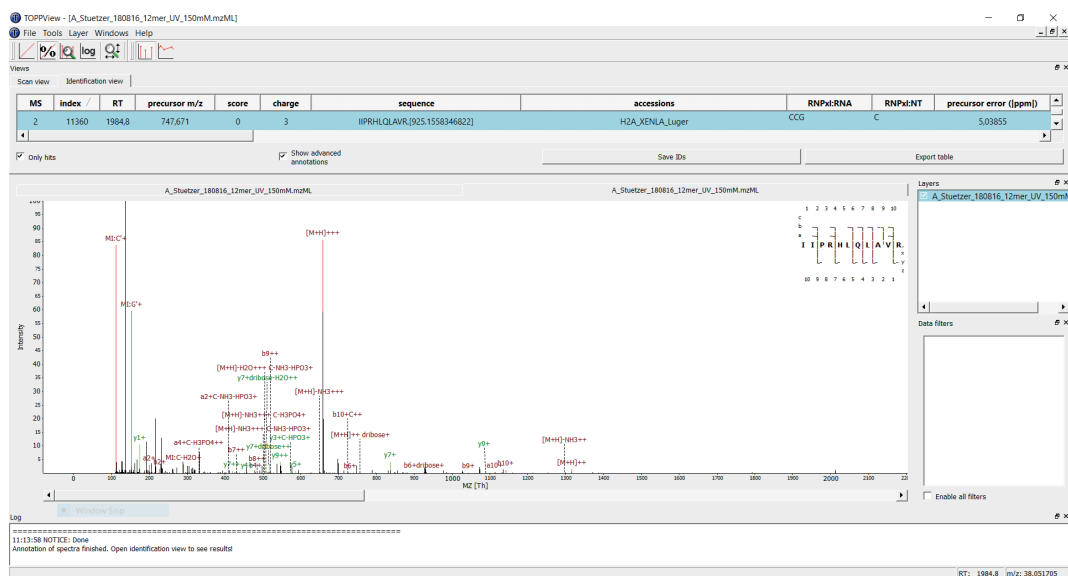
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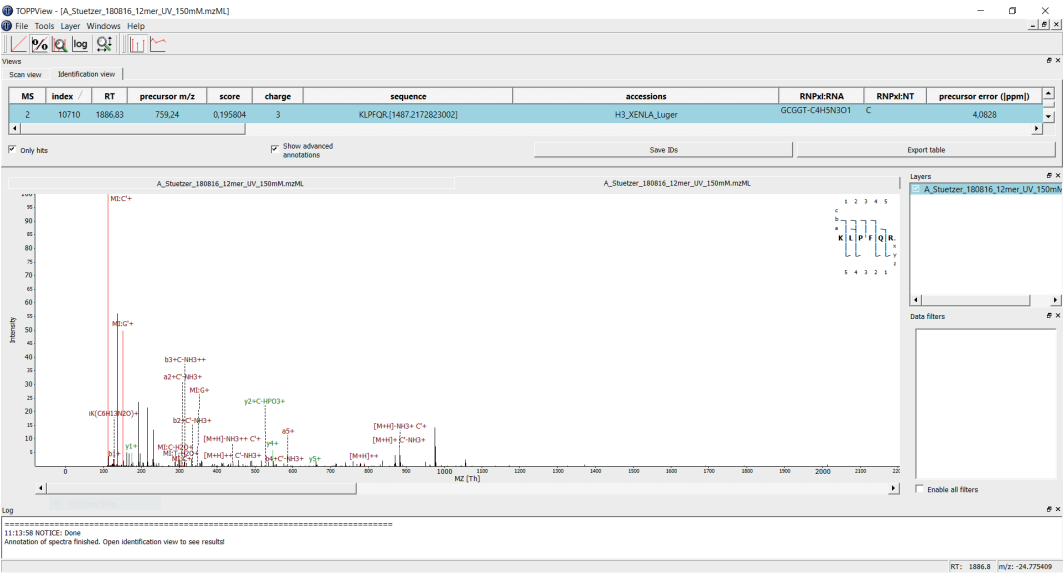
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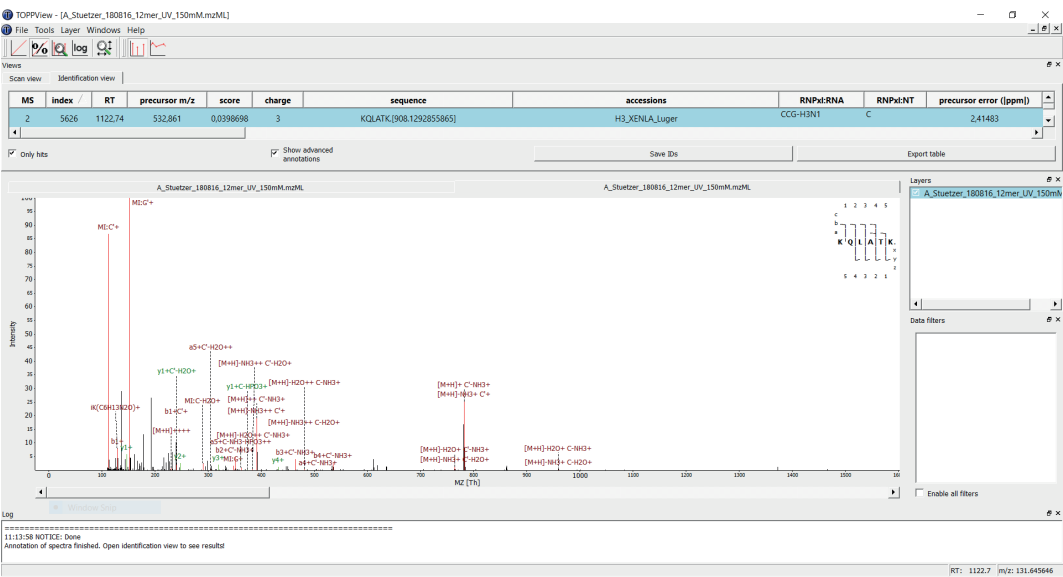
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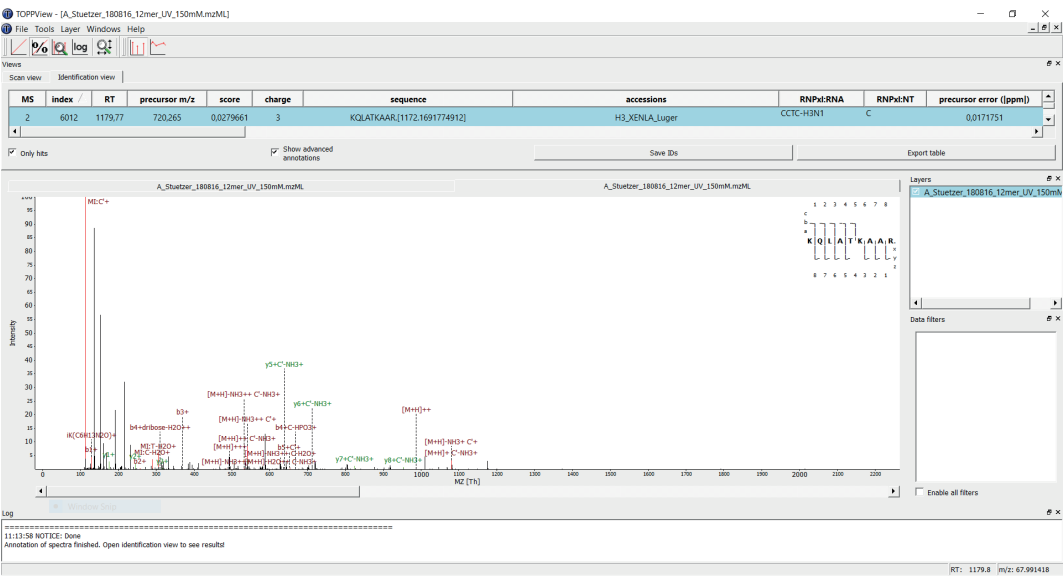
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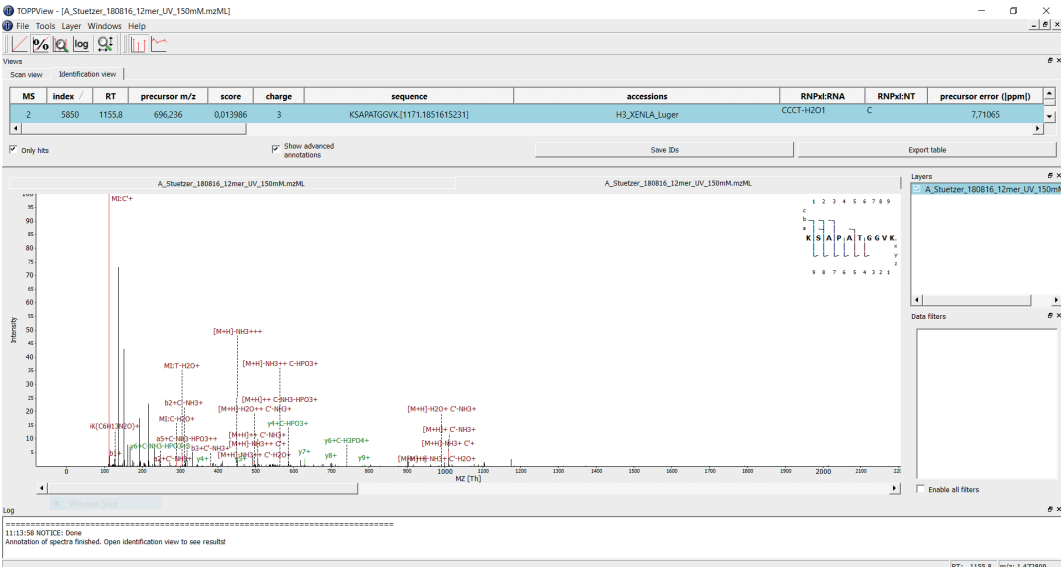
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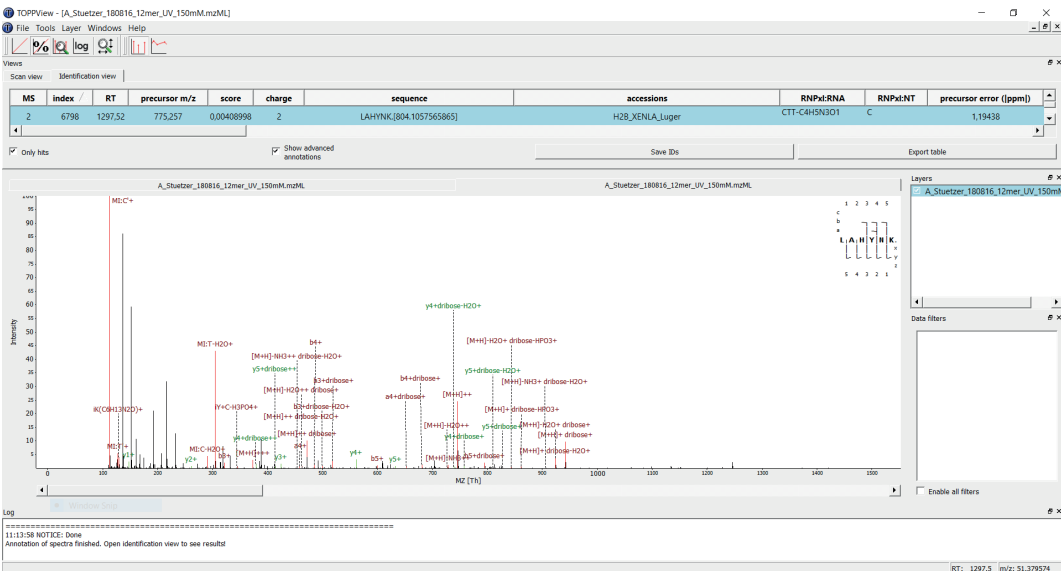
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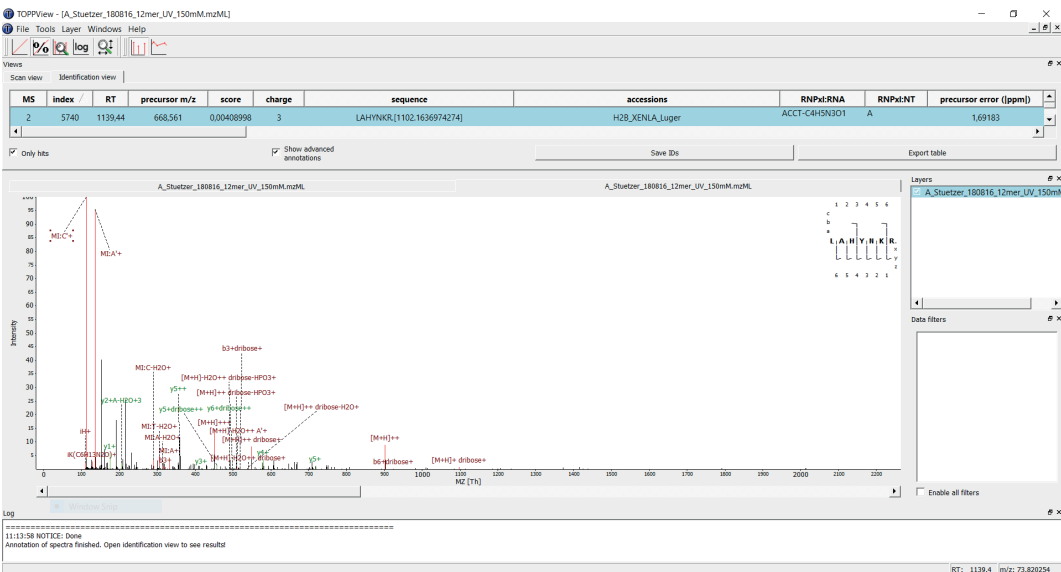
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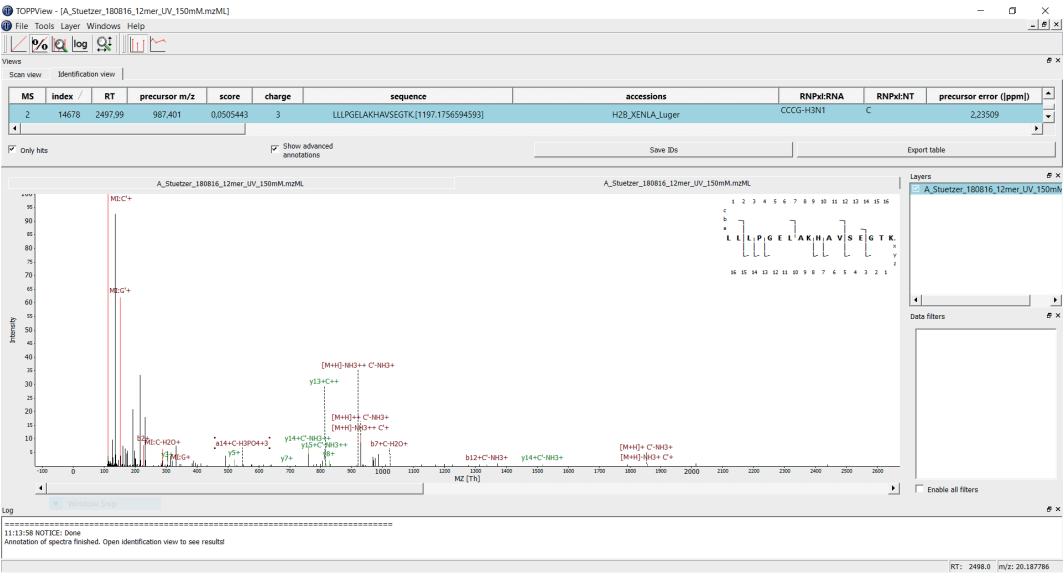
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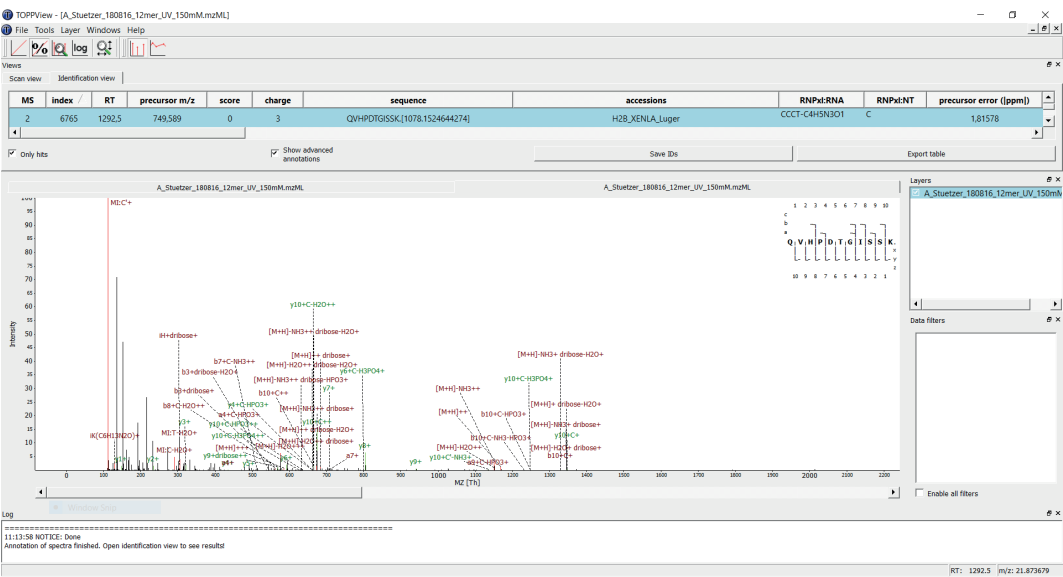
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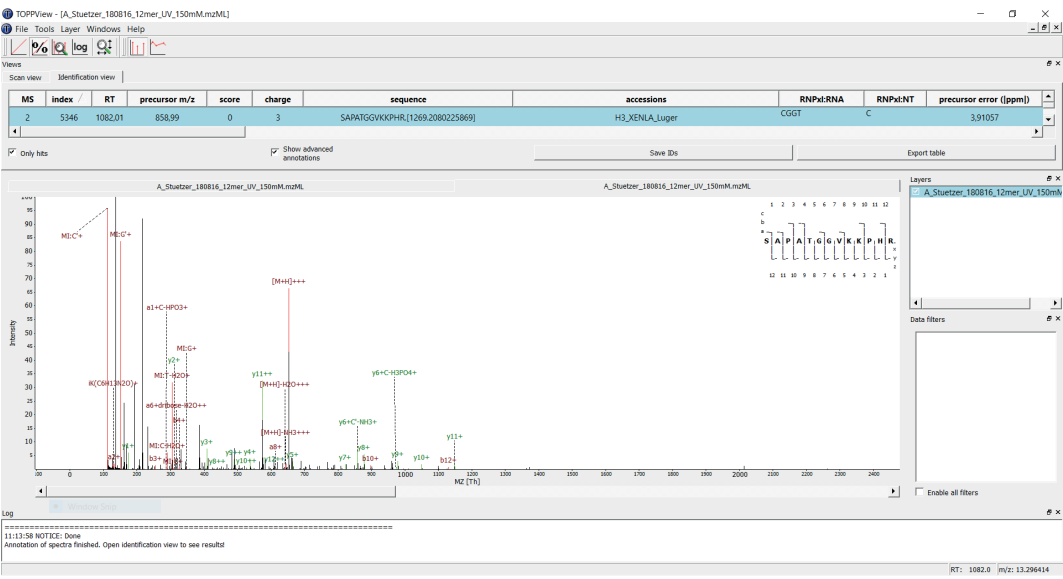
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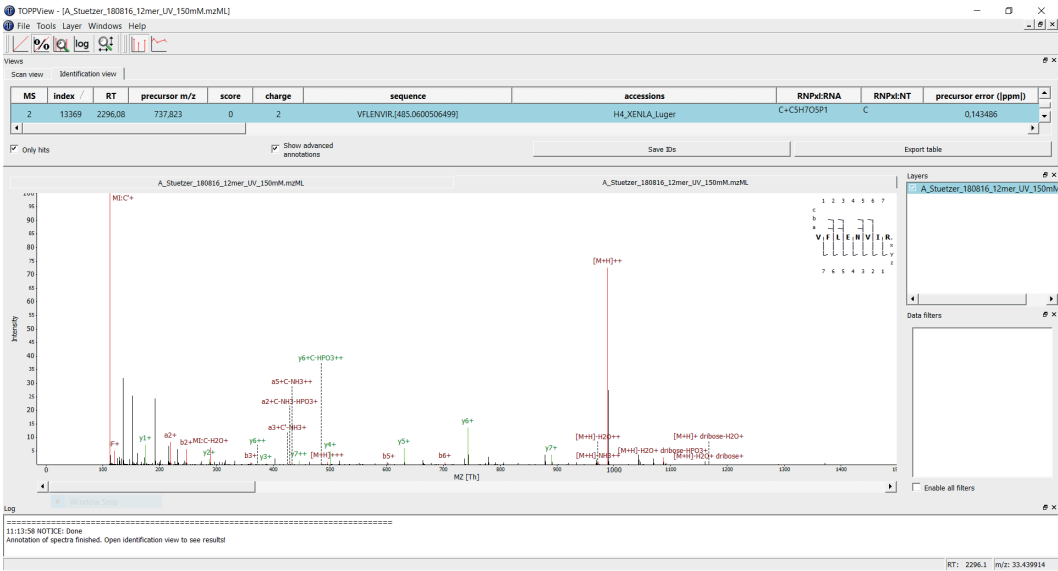
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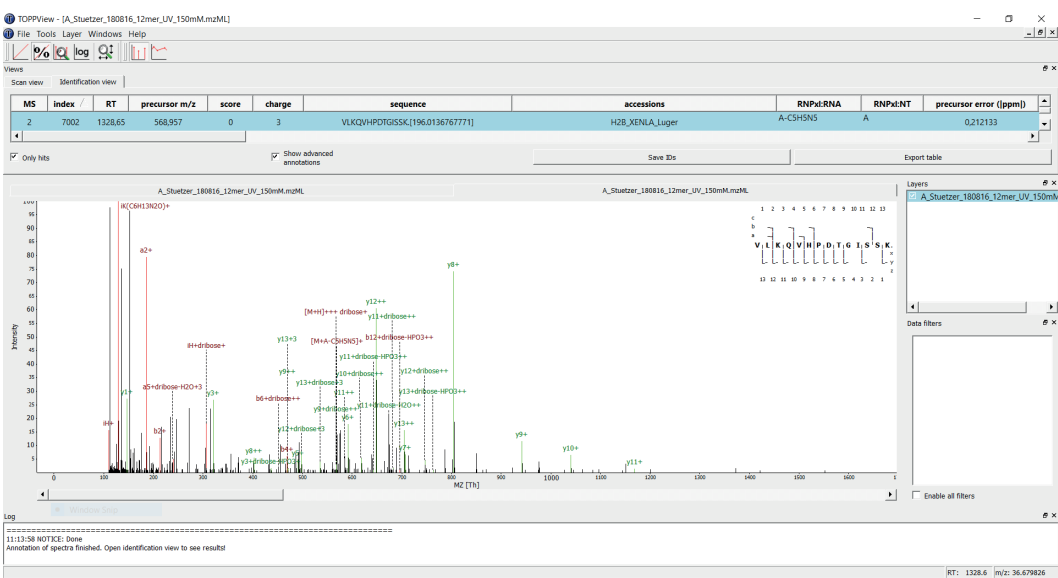
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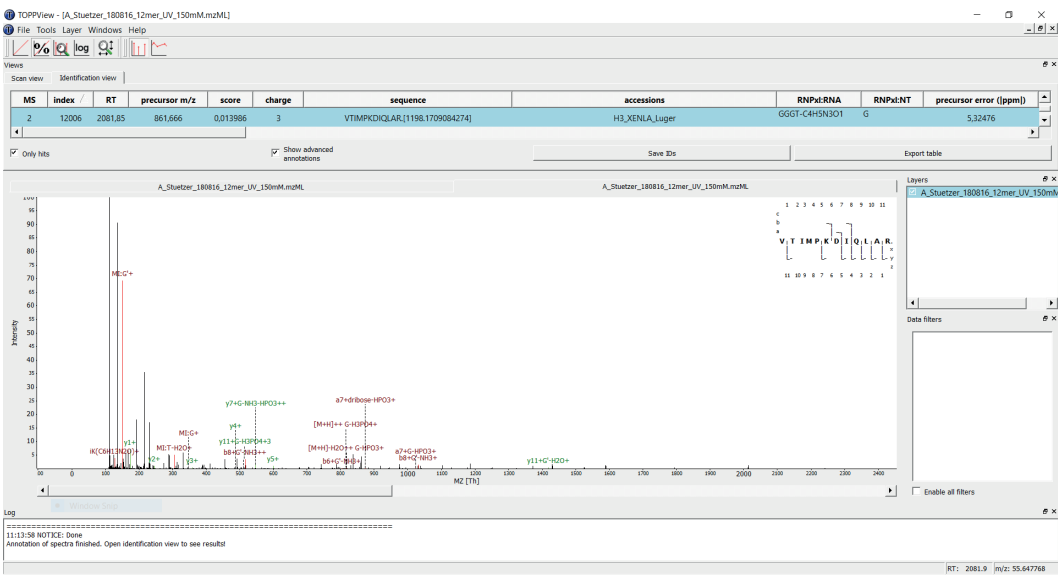
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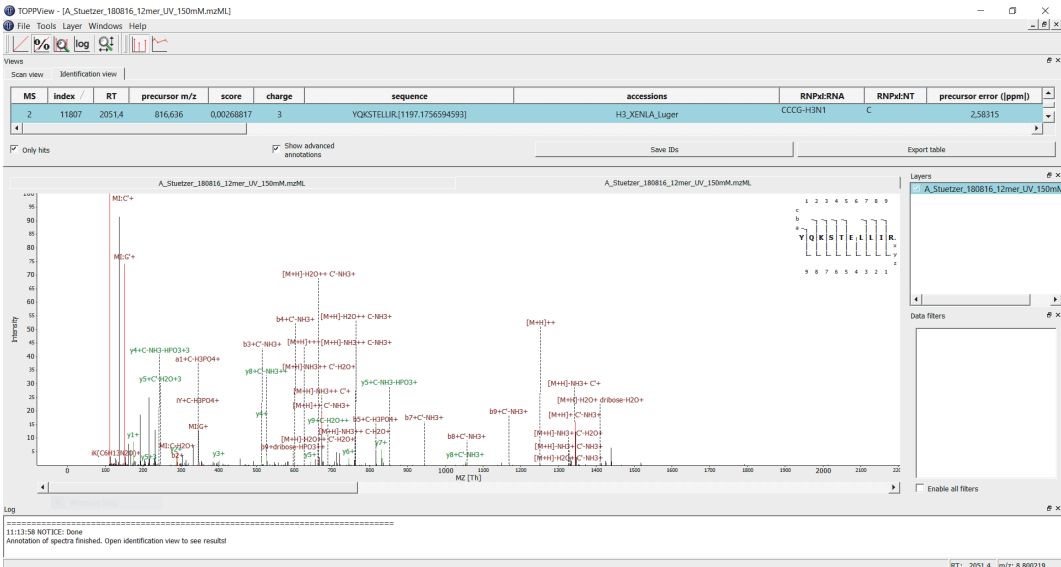
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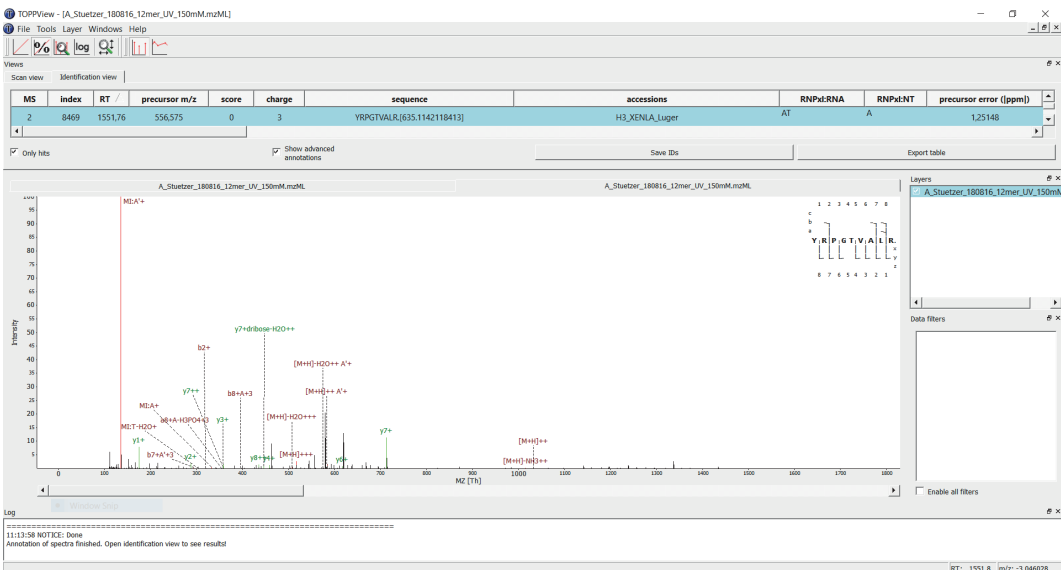
63)



64)



65)



66)

