

Supplementary Data 8

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

Stützer *et al.*

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UV cross-linked HeLa nuclei (chromatin precipitation)

RNP^{xl}search_settings#2

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UV cross-linked HeLa nuclei (chromatin precipitation)

RNP^{xl}search_settingsRNA

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UV cross-linked HeLa nuclei (chromatin precipitation), RNP^{xl}search_settings#1

TopView - [ASutzeur_100118_120118_HelaUV_rep1_sample1.mzML]

File Tools Layer Windows Help

Views

Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPK:RNA	RNPK:NT	precursor error (ppm)
2	11094	1753.85	618.288	2	VVSGNVPEPK [307.056938936600034]	sp Q12830 BPTF_HUMAN	C			1.07778

☒ Only hits ☒ Show advanced annotations Save IDs Export table

ASutzeur_100118_120118_HelaUV_rep1_sample1.mzML ASutzeur_100118_120118_HelaUV_rep1_sample1.mzML

Layers
ASutzeur_100118_120118_HelaUV_rep1_sample1.mzML

Data filters

Enable all filters

Log

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12:18:56 NOTSET Done
Annotation of spectra finished. Open identification view to see result
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TOPView - [AShutzer_100118_120118_HeLaIV_rep2_sample1.mzML]

File Tools Layer Window Help

Views Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPK:RNA	RNPK:NT	precursor error (ppm)
2	11290	1768.3	618.288	0.994559	2	VYSGNVERK[307.056938936600034]	sp Q12830 BPTT_HUMAN	C	C	0.995086

Only hits ☒ Show advanced annotations ☐ Save IDs ☐ Export table

AShutzer_100118_120118_HeLaIV_rep2_sample1.mzML AShutzer_100118_120118_HeLaIV_rep2_sample1.mzML

TOPView - [ASuetzer_100118_120118_HeLaIV_rep2_sample1.mzML]

File Tools Layer Windows Help

100% 100% log Q1 Q2 Q3

Views Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPK:RNA	RNPK:NT	precursor error (ppm)
2	11423	1783.56	618.287	0.994559	2	VYSGNVEPK[307.056938936600034]	sp Q12830 BPTF_HUMAN	C	C	0.418548

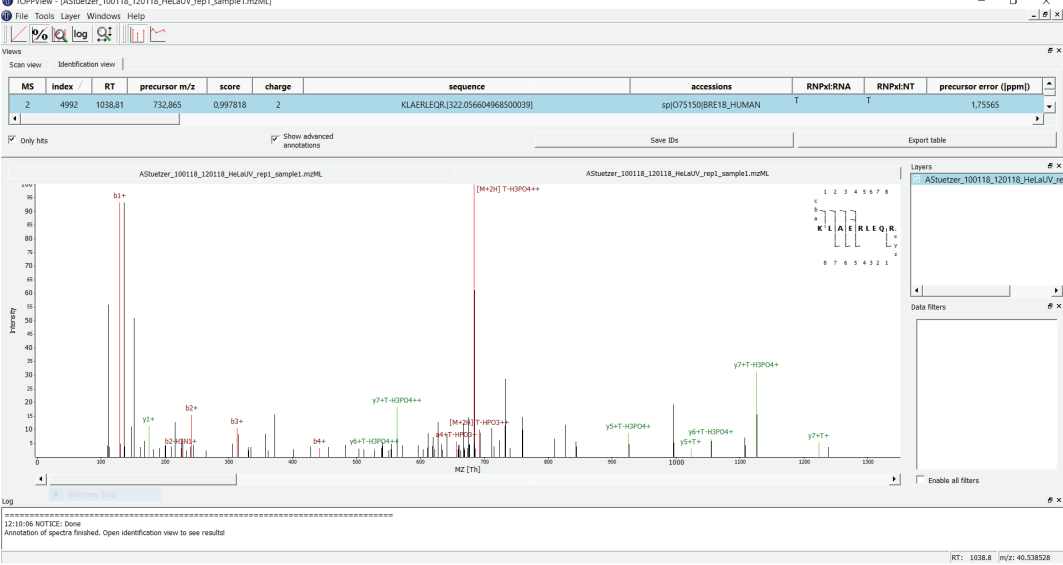
Only hits ☒ Show advanced annotations Save IDs Export table

ASuetzer_100118_120118_HeLaIV_rep2_sample1.mzML ASuetzer_100118_120118_HeLaIV_rep2_sample1.mzML

4) E3 ubiquitin-protein ligase BRE1A



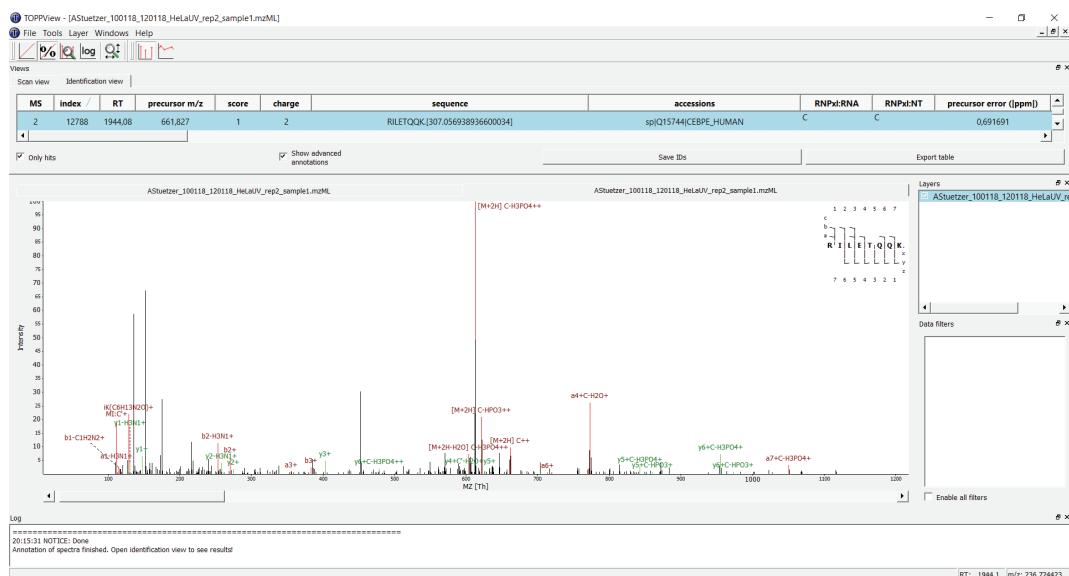
5) E3 ubiquitin-protein ligase BRE1B



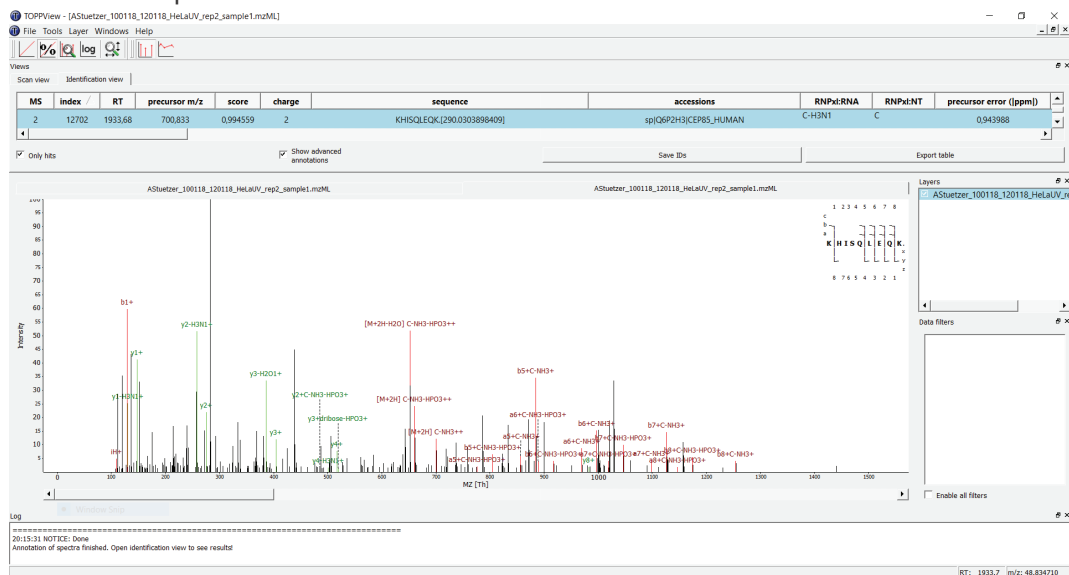
6) Centrosome-associated protein 350



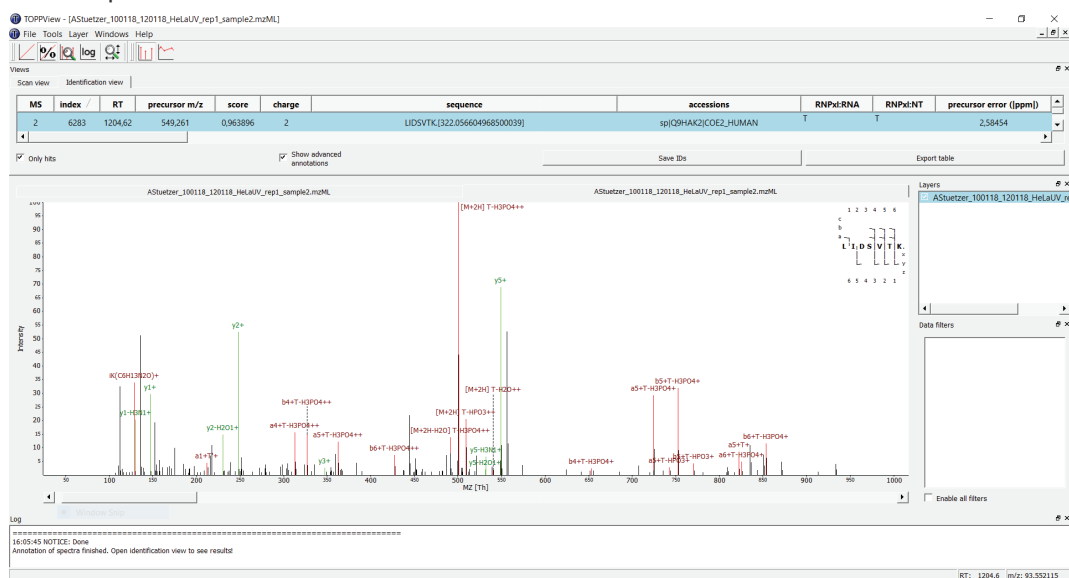
7) CCAAT/enhancer-binding protein epsilon



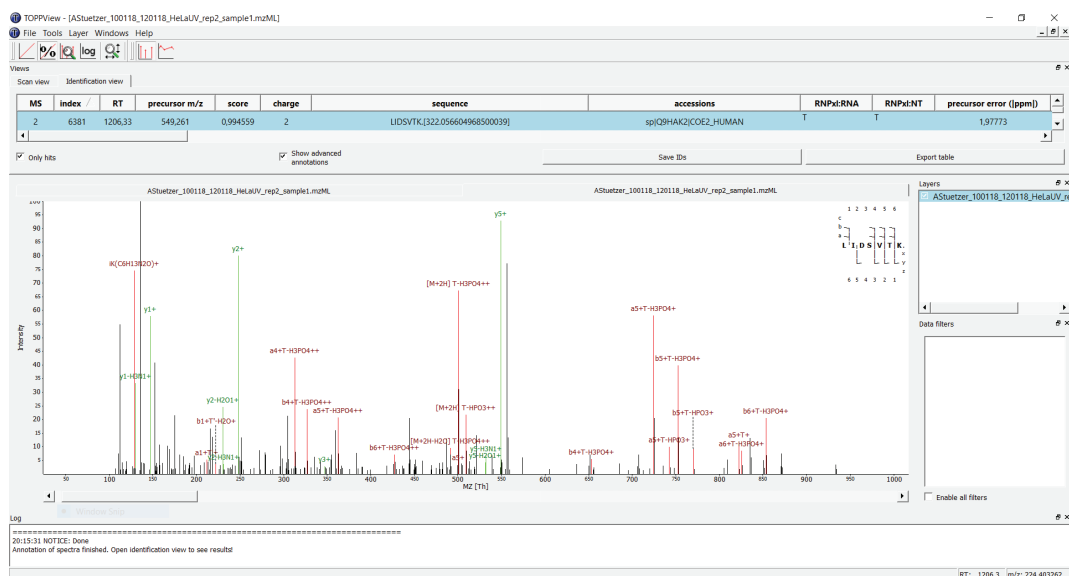
8) Centrosomal protein of 85 kDa



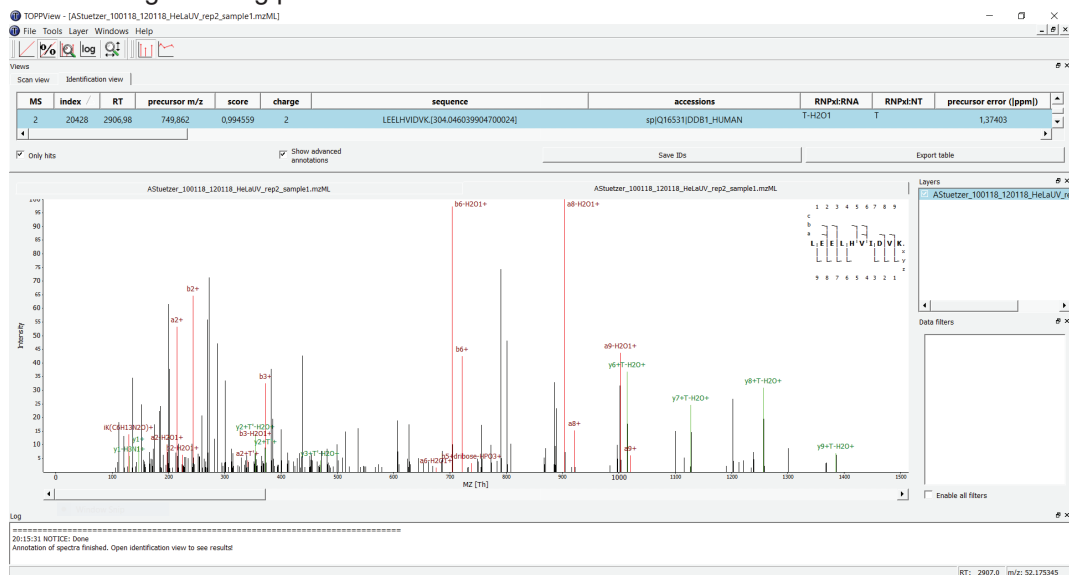
9) Transcription factor COE2



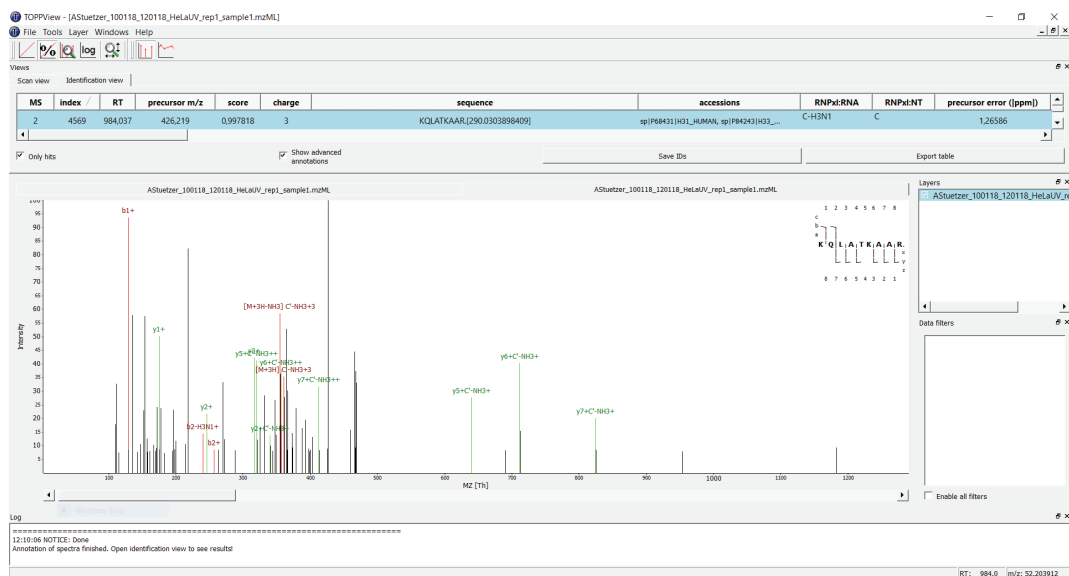
10)



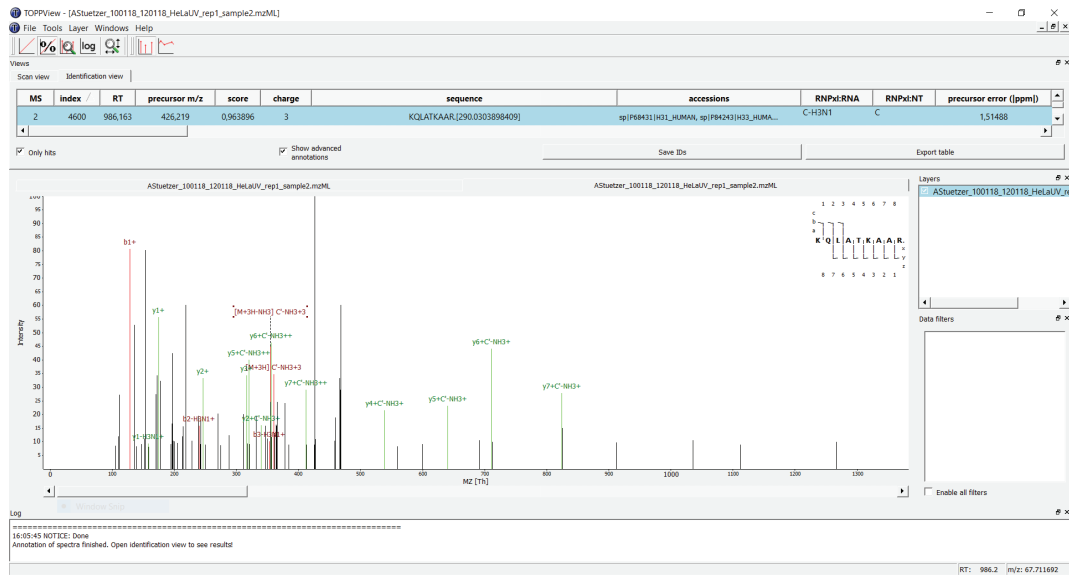
11) DNA damage-binding protein 1



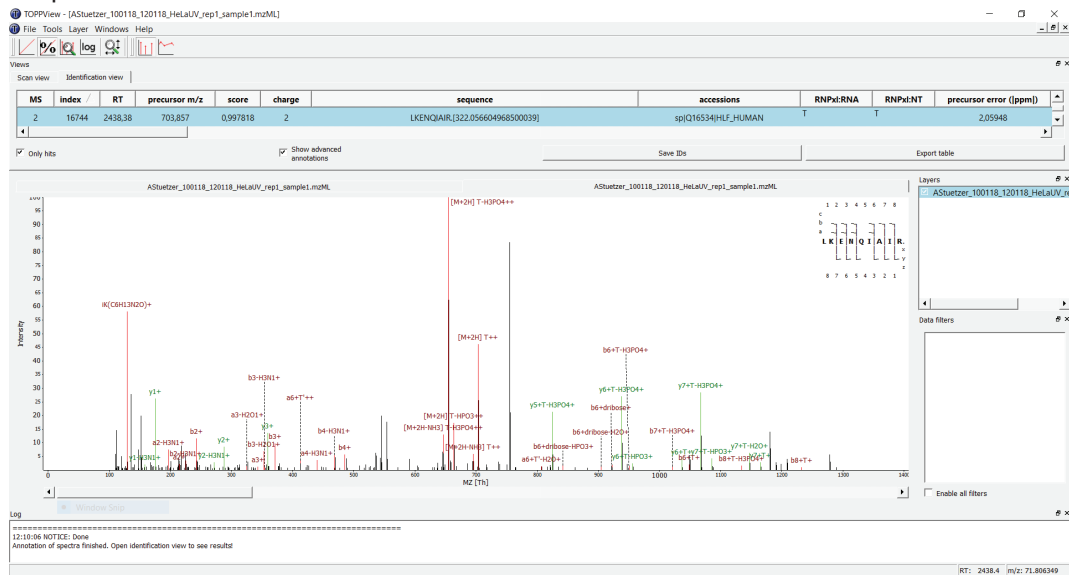
12) Histone H3



13)



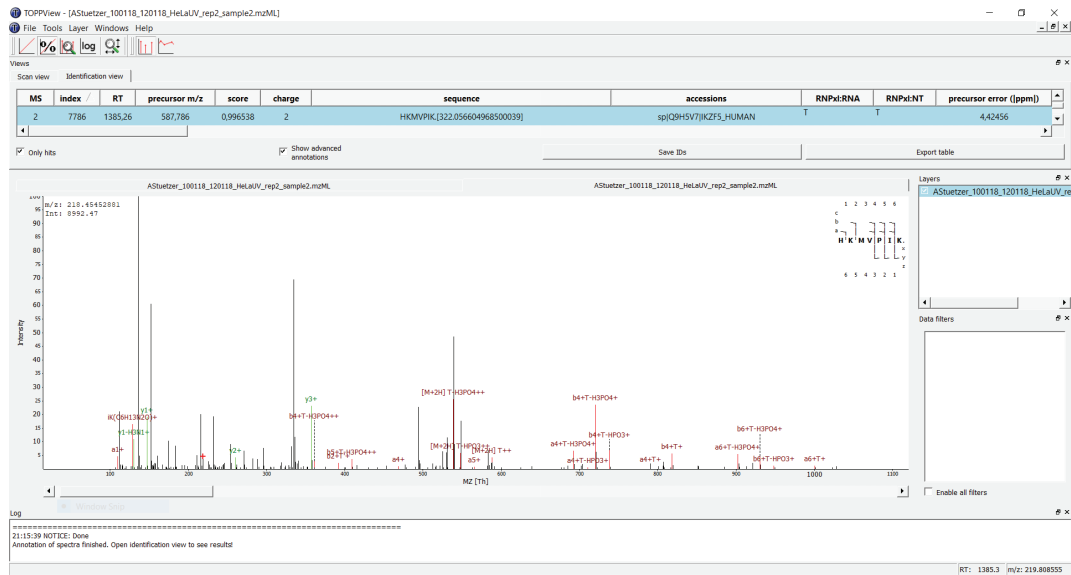
14) Hepatic leukemia factor



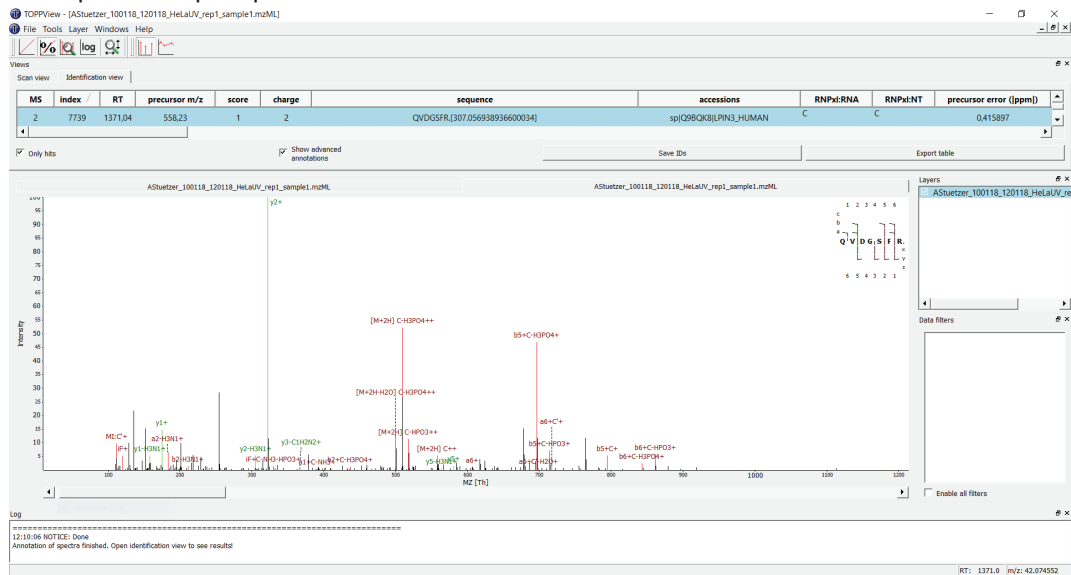
15)



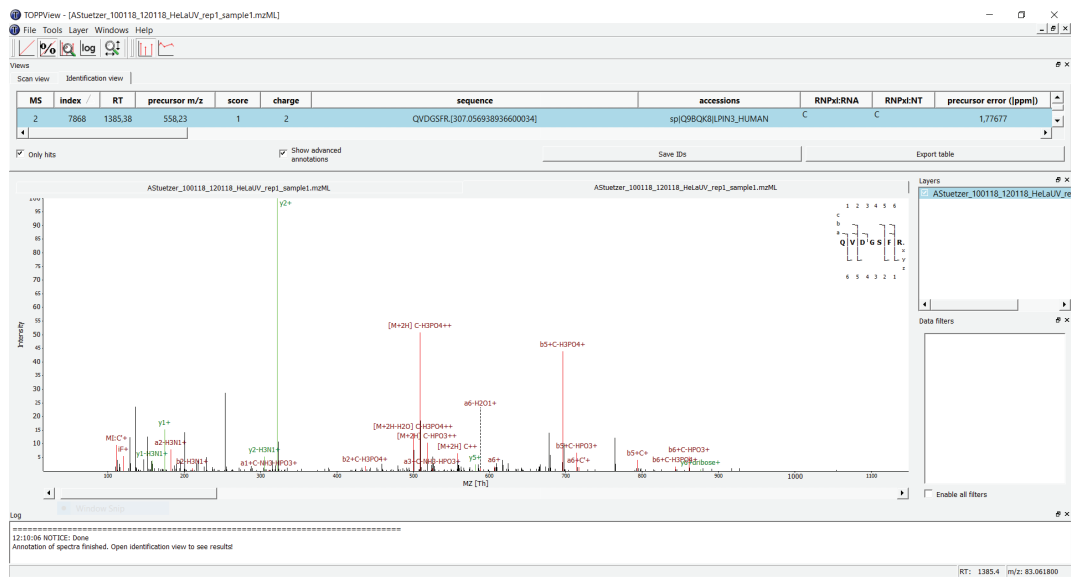
16) Zinc finger protein Pegasus



17) Phosphatidate phosphatase LPIN3



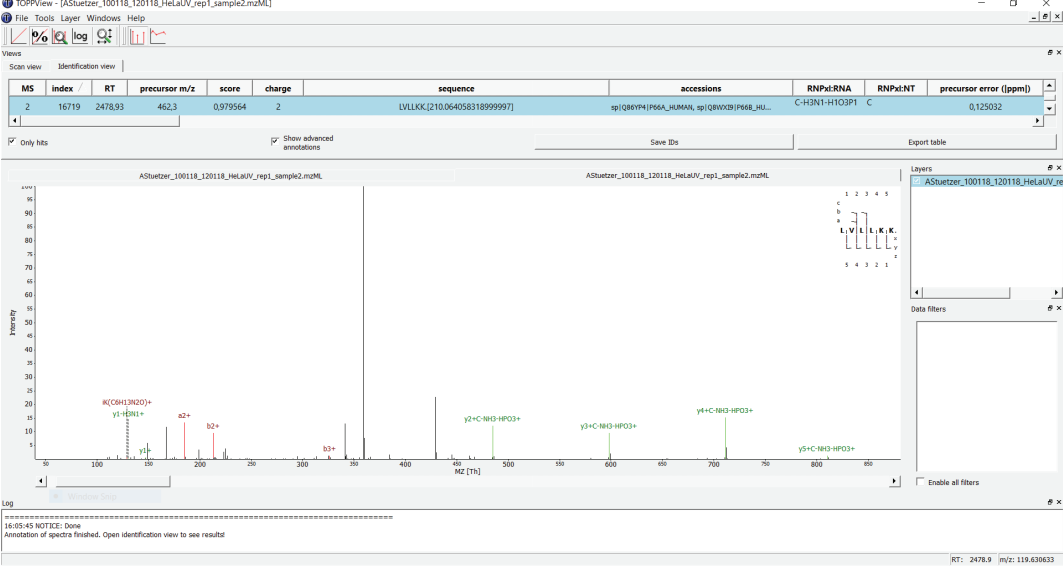
18)



19)



20) Transcriptional repressor p66-alpha



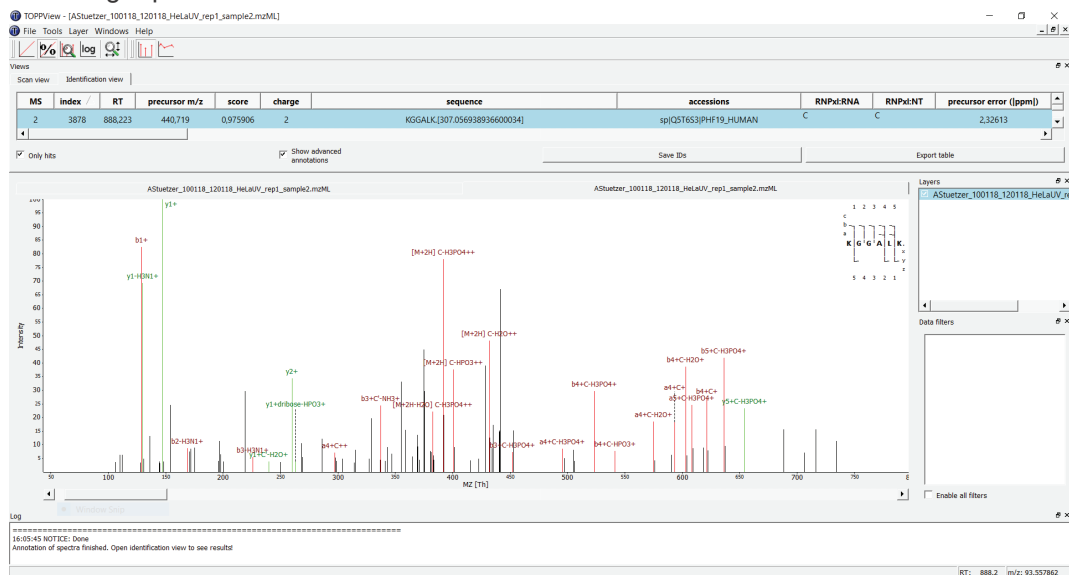
21) Programmed cell death protein 7



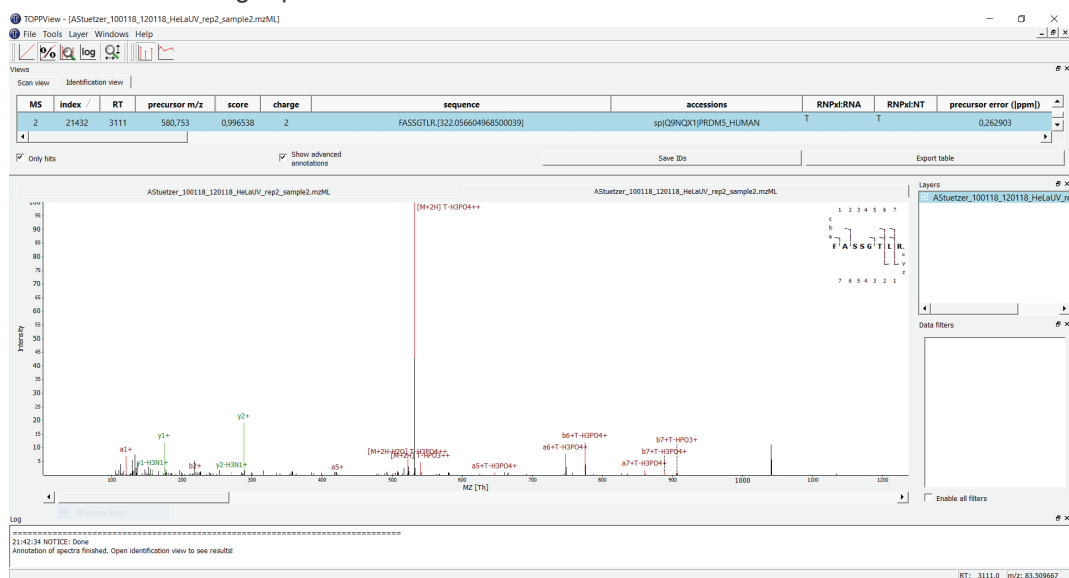
22) PDZ and LIM domain protein 2



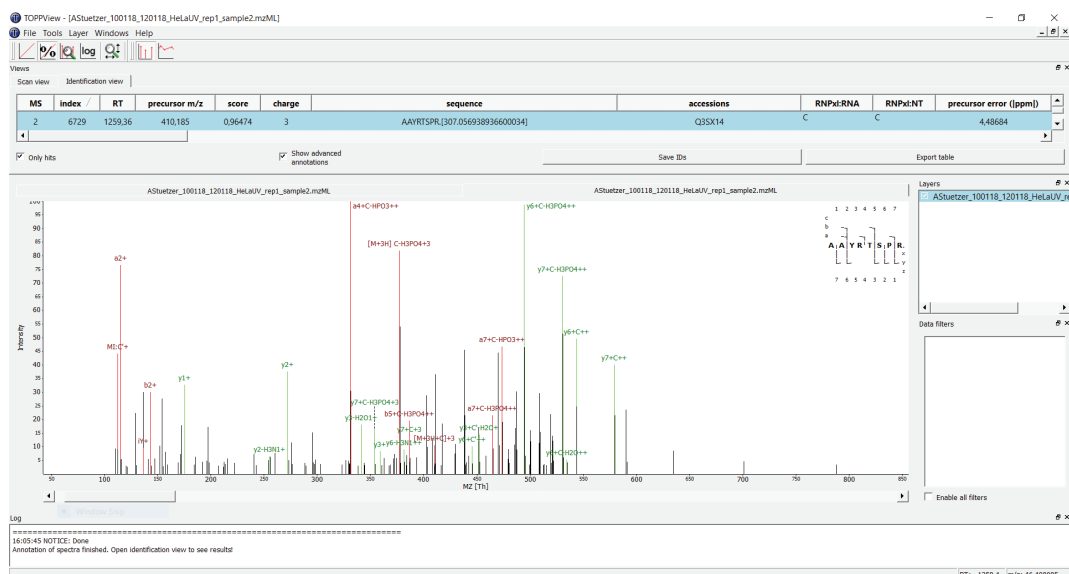
23) PHD finger protein 19



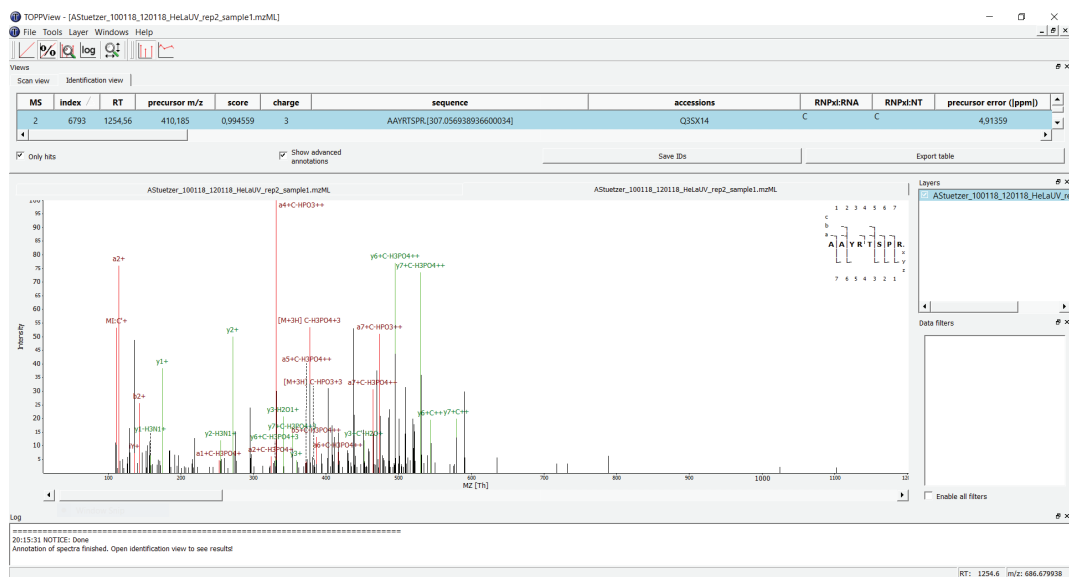
24) PR domain zinc finger protein 5



25) Gelsolin



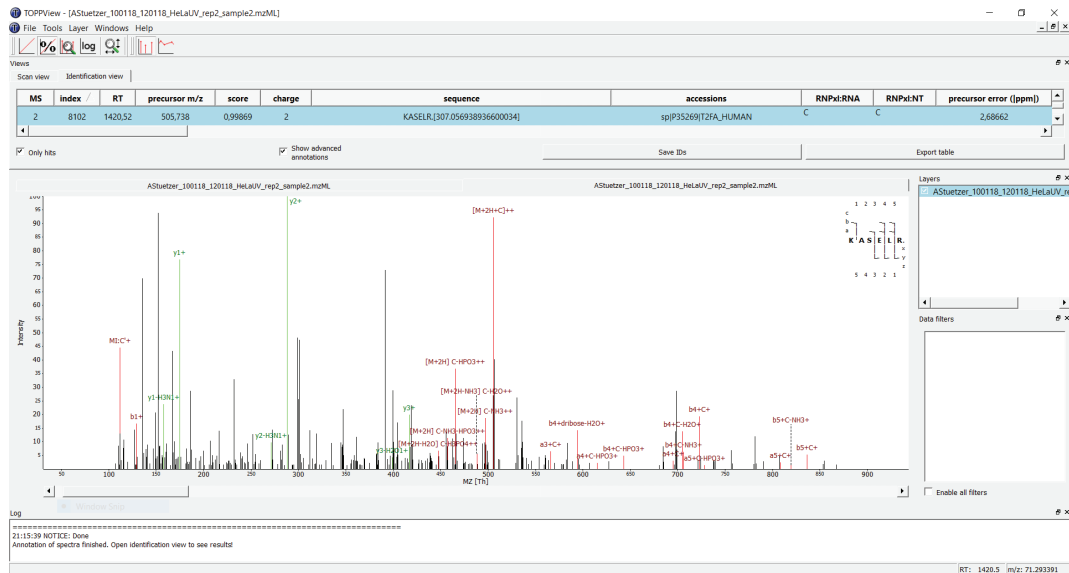
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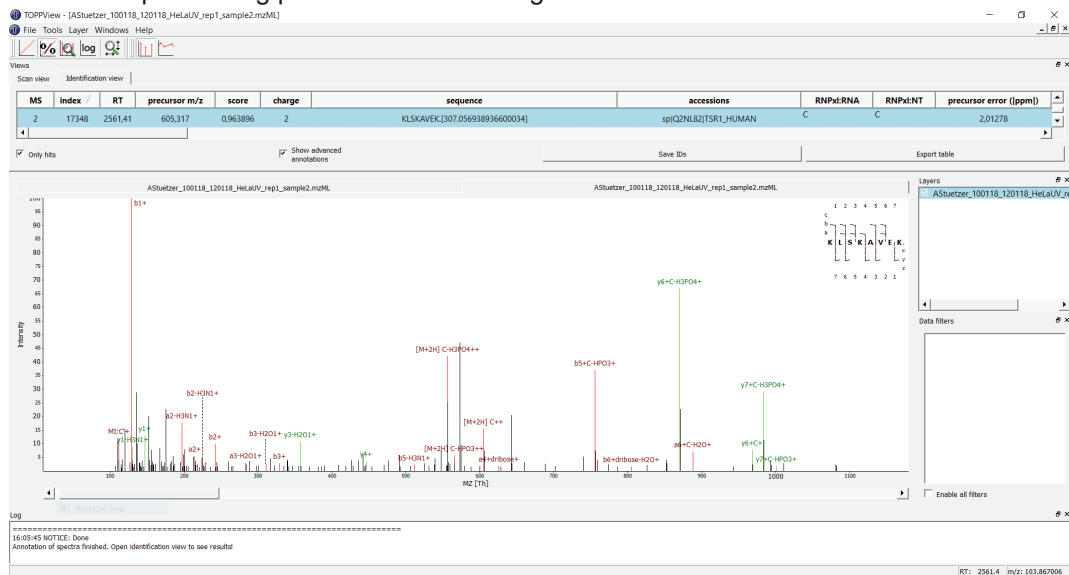
27) DNA-binding protein SMUBP-2



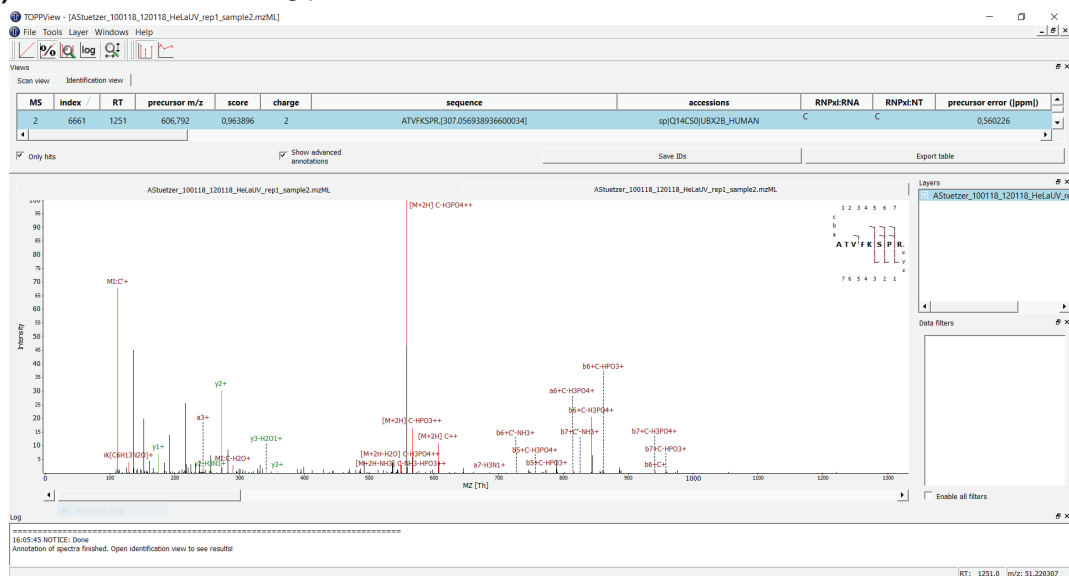
28) General transcription factor IIF subunit 1



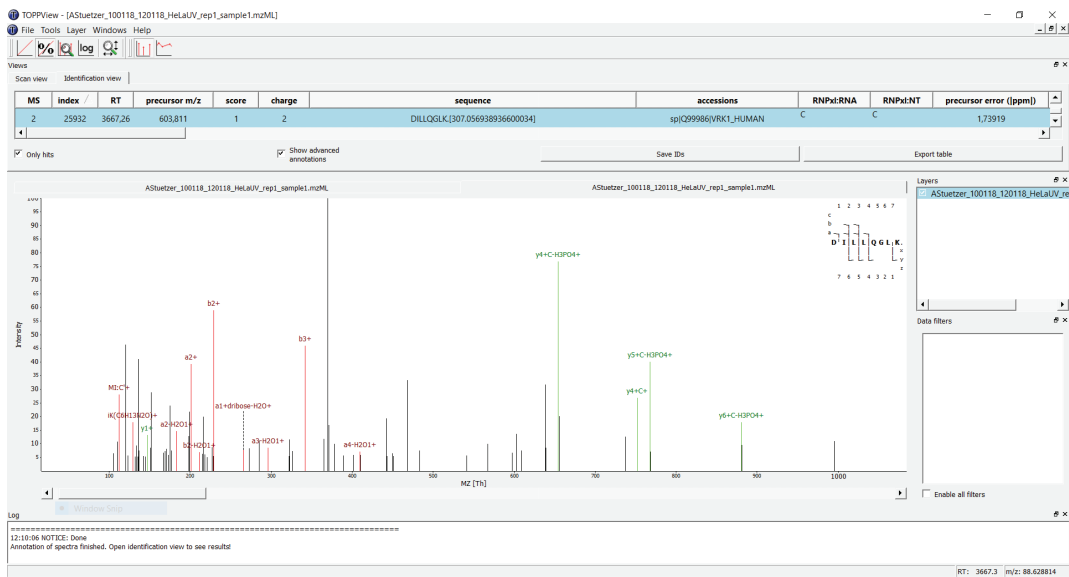
29) Pre-rRNA-processing protein TSR1 homolog



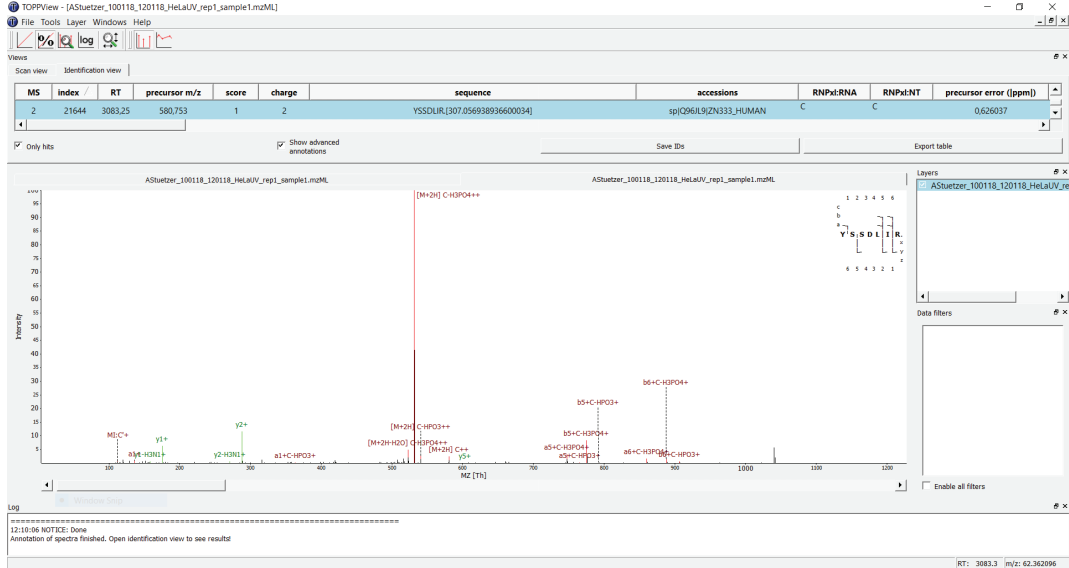
1.30) UBX domain-containing protein 2B



31) Serine/threonine-protein kinase VRK1



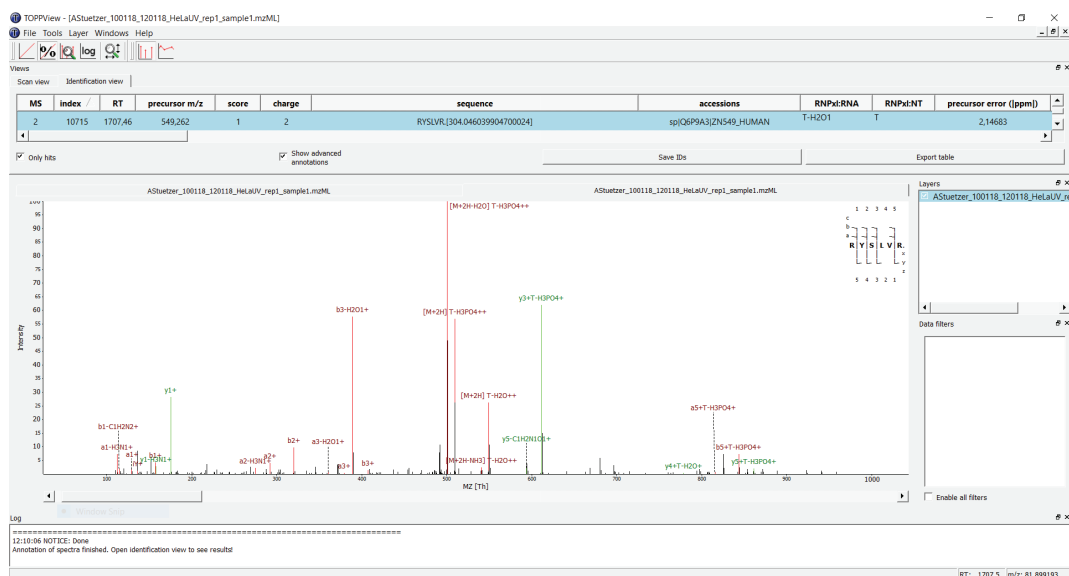
1.32) Zinc finger protein 333



33) Zinc finger protein 469



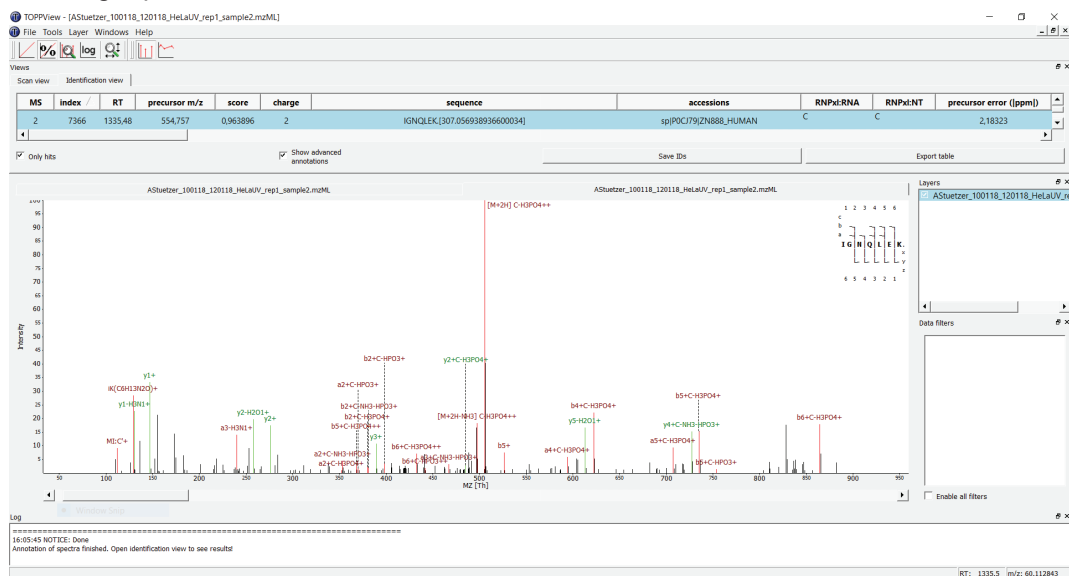
34) Zinc finger protein 549



35)



36) Zinc finger protein 888



UV cross-linked HeLa nuclei (chromatin precipitation), RNP^{xi}search_settings#1

☐ TOPView - ☒ ASuetzer_100118_120118_HeLaUV_rep2_sample2.ms2.ms1
☐ File ☐ 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	8876	1510.22	576.282	0.996538	2	KRQLER[322.056604968500039]	sp Q02040 AK17A_HUMAN	T	T	0.318245

☒ Only hits ☒ Show advanced annotations

ASuetzer_100118_120118_HeLaUV_rep2_sample2.ms2.ms1 ASuetzer_100118_120118_HeLaUV_rep2_sample2.ms2.ms1

Layers

- ASuetzer_100118_120118_HeLaUV_rep2_sample2.ms2.ms1

Data Filters

☐ Enable all filters

Log

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21:15:39 NOTICE: Done
Annotation of spectra finished. Open identification view to see result
  
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RT: 1510.2 m/z: 41.7181/1.7

TCPPView - [ASutetzer_100118_120118_HetAaIV_rep1_sample1.mzML]

File Tools Layer Windows Help

Views

Scan view Identification view

MS	Index	RT	precursor m/z	score	charge	sequence	accessions	RNPs:RNA	RNPs:NT	precursor error (ppm)
2	17290	2508.27	611.804	0.997818	2	IGGGKTARR.[307.056938936600034]	sp P20290 BTF3_HUMAN	C	C	3.94359

Only hits

Show advanced annotations

Save IDs

Export table

ASutetzer_100118_120118_HetAaIV_rep1_sample1.mzML

ASutetzer_100118_120118_HetAaIV_rep1_sample1.mzML

Layers

ASutetzer_100118_120118_HetAaIV_rep1_sample1.mzML

Data filters

Enable all filters

Log

12:10:56 NOTICE: Done

Annotation of spectra finished. Open identification view to see result

TOPPView - [ASuetzer_100118_120118_HetLaUV_rep2_1.mzML] File Edit Tools Layer Windows Help

Views

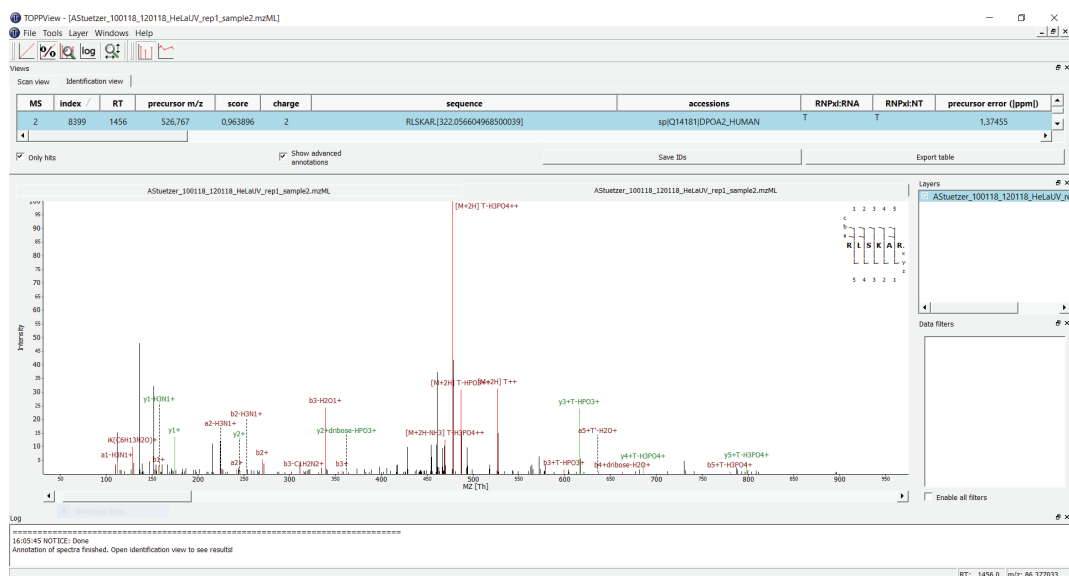
Scan view Identification view

MS	Index	RT	precursor m/z	score	charge	sequence	accessions	RNPs:RNA	RNPs:NT	precursor error (ppm)
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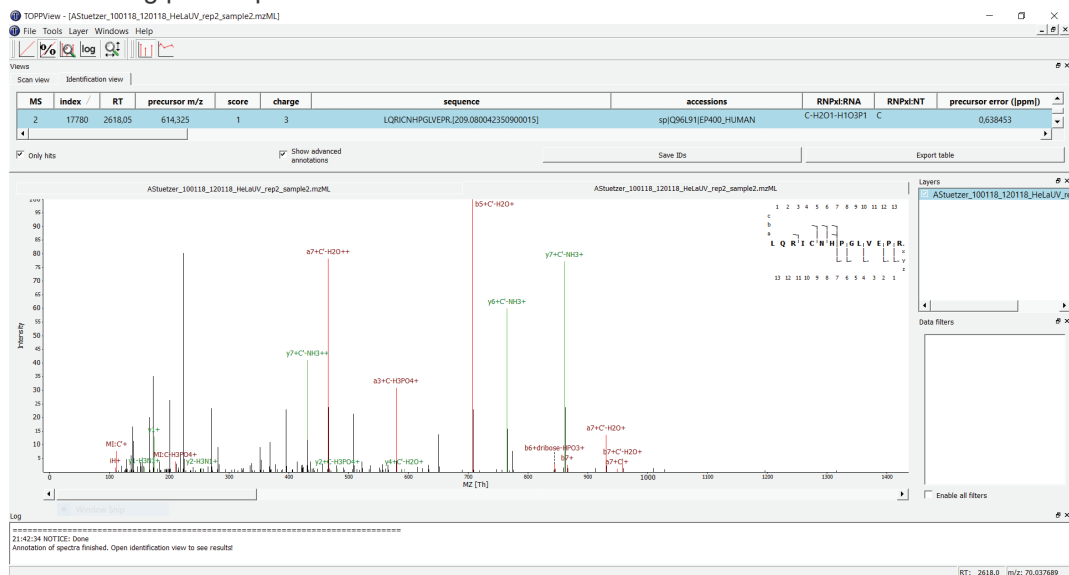
▼ Only hits Show advanced annotations Save IDs Export table

ASuetzer_100118_120118_HetLaUV_rep2_sample1.mzML ASuetzer_100118_120118_HetLaUV_rep2_sample1.mzML

4) DNA polymerase alpha subunit B



5) E1A-binding protein p400



6) Uveal autoantigen with coiled-coil domains and ankyrin repeats



TOPVIEW [ASuetzer_100118_120118_HelLaIV_rep1_sample2.ms.ML]

File Tools Layer Windows Help

Views Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPeRNA	RNPeNT	precursor error (ppm)
2	17907	2636.27	591.134	0.963896	2	VTSILAK[322.056604968500039]	sp Q9BZF9 UACA_HUMAN	T	T	1.9905

☒ Only MS ☒ Show advanced annotations Save IDs Export table

ASuetzer_100118_120118_HelLaIV_rep1_sample2.ms.ML

ASuetzer_100118_120118_HelLaIV_rep1_sample2.ms.ML

Layers ASuetzer_100118_120118_HelLaIV_rep1_sample2.ms.ML

Data filters Enable all filters

Log
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16:05:45 HOFPS Done

Annotation of spectra finished. Open identification view to see result

TOPVIEW - [ASuetzer_100118_120118_HeLaIV_rep2_sample1.mzML]

File Tools Layer Views Help

Views

Scan view Identification view

MS	Index	RT	precursor m/z	score	charge	sequence	accessions	RNPs:RNA	RNPs:NT	precursor error (ppm)
2	18349	2633.95	591.312	0.994559	2	VTSILAKK[322.056604968500039]	sp Q9BZF9 UACA_HUMAN	T	T	0.127318

Only hits ☒ Show advanced annotations

Save IDs Export table

ASuetzer_100118_120118_HeLaIV_rep2_sample1.mzML

Layers

ASuetzer_100118_120118_HeLaIV_rep2_sample1.mzML

Data filters

Enable all filters

Log

20:15:33 NOTICE: Done

Annotation of spectra finished. Open identification view to see result

RT: 2634.8 m/z: 74.444988

TOPVIEW - [ASuetzer_100118_120118_HelaIV_rep2_sample2.ms2.mzML]

File Tools Layer Windows Help

Views Scan view Identification view

MS	index	RT	precursor m/z	score	charge	sequence	accessions	RNPs-RNA	RNP-NT	precursor error (ppm)
2	17902	2633.76	591313	0.996538	2	VTSILAKK(322.056604968500039)	sp Q9BZF9 UACA_HUMAN	T	T	0.750901

☒ Only hits ☒ Show advanced annotations Save IDs Export table

ASuetzer_100118_120118_HelaIV_rep2_sample2.ms2.mzML

ASuetzer_100118_120118_HelaIV_rep2_sample2.ms2.mzML

Layers ASuetzer_100118_120118_HelaIV_rep2_sample2.ms2.mzML

Data filters

Enable all filters

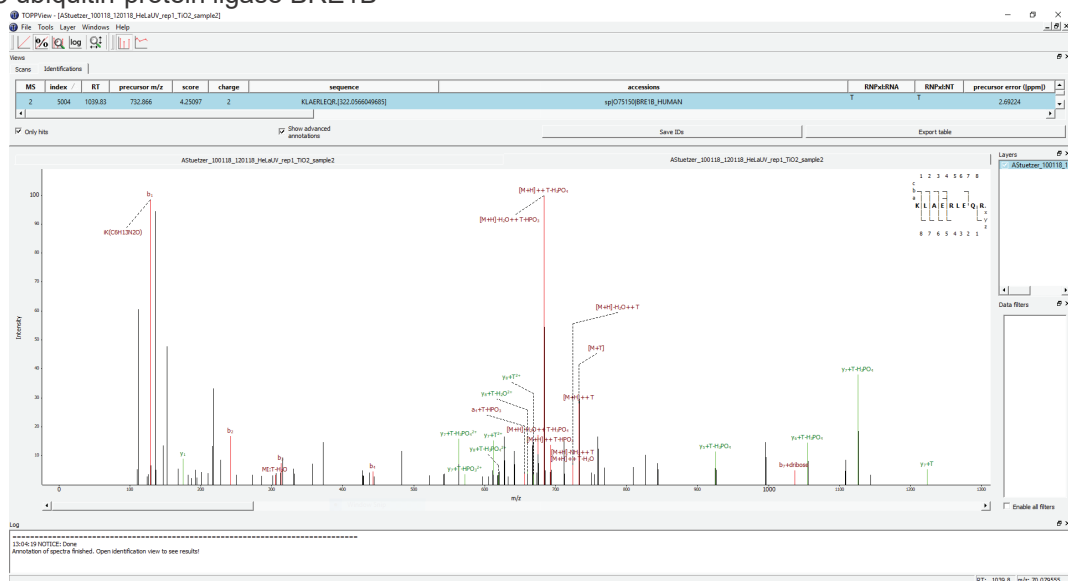
Log

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21:42:34 MSF2SE Done
Annotation of spectra finished. Open identification view to see result
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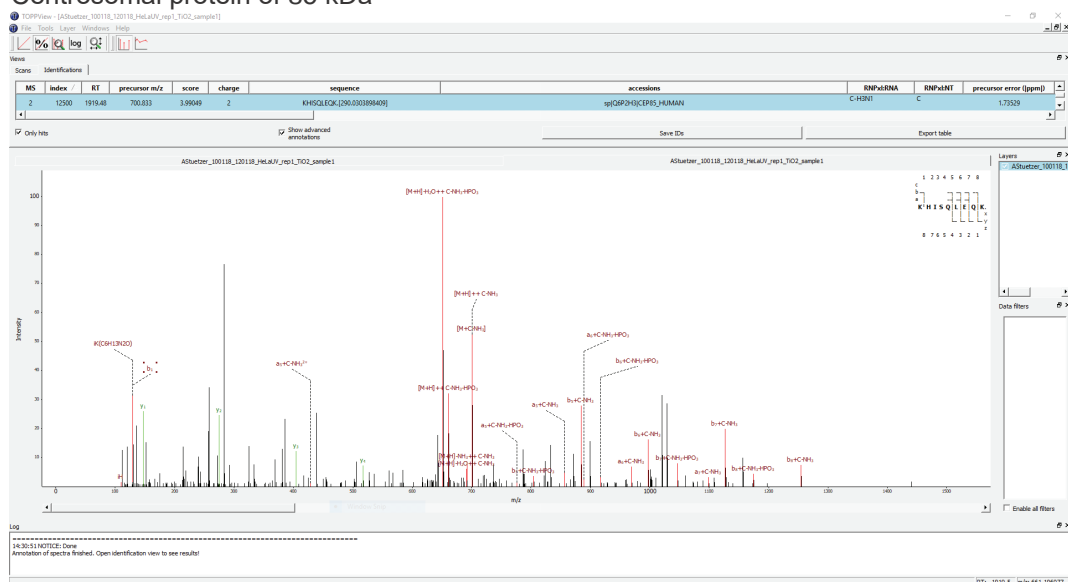

TOPPView spectra - unambiguous cross-link spectrum matches

UV cross-linked HeLa nuclei (chromatin precipitation), RNP^{xl}search_settings#2

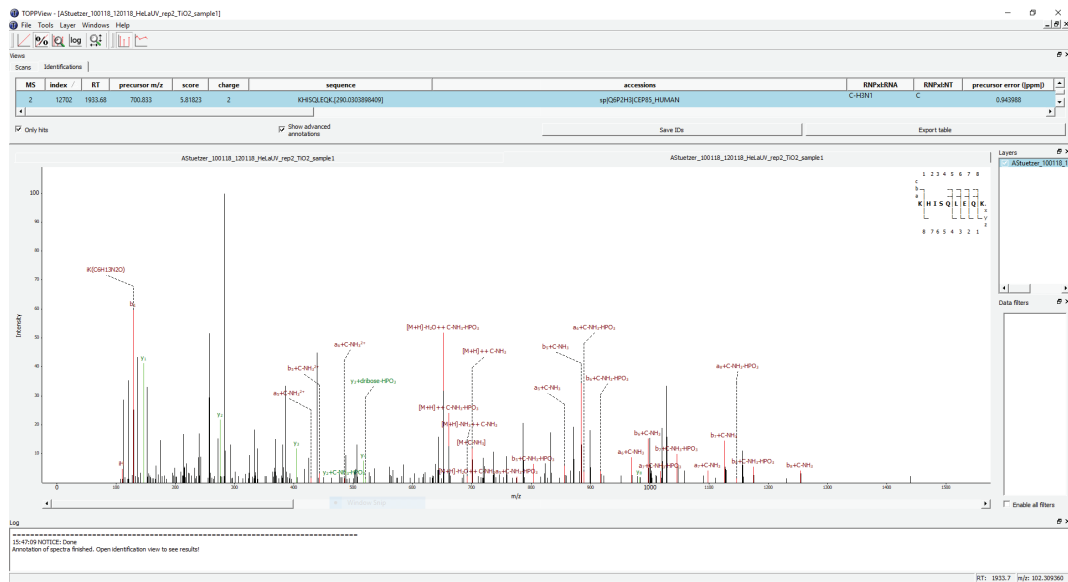
1) E3 ubiquitin-protein ligase BRE1B



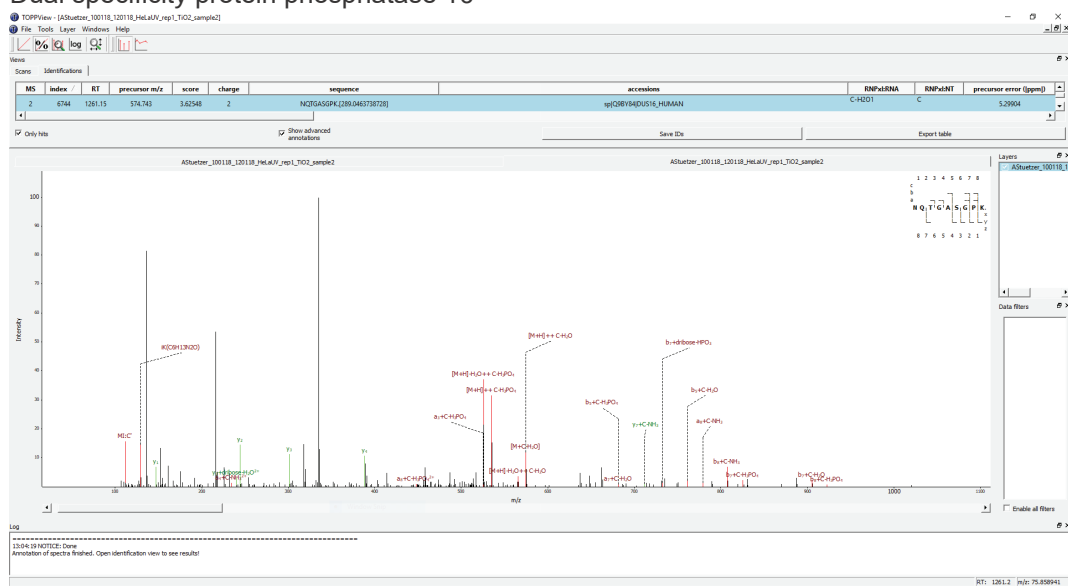
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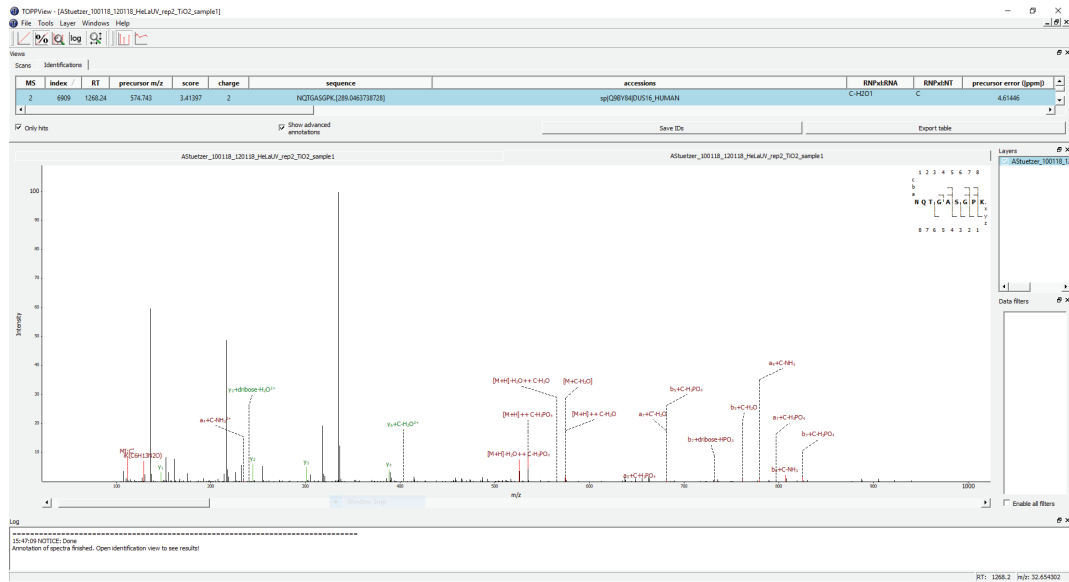
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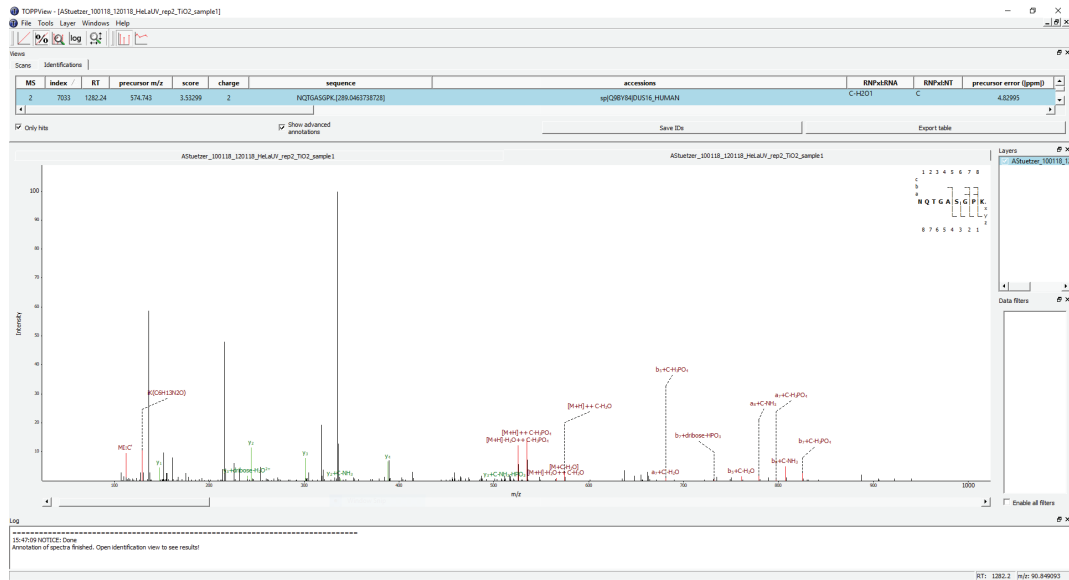
6)



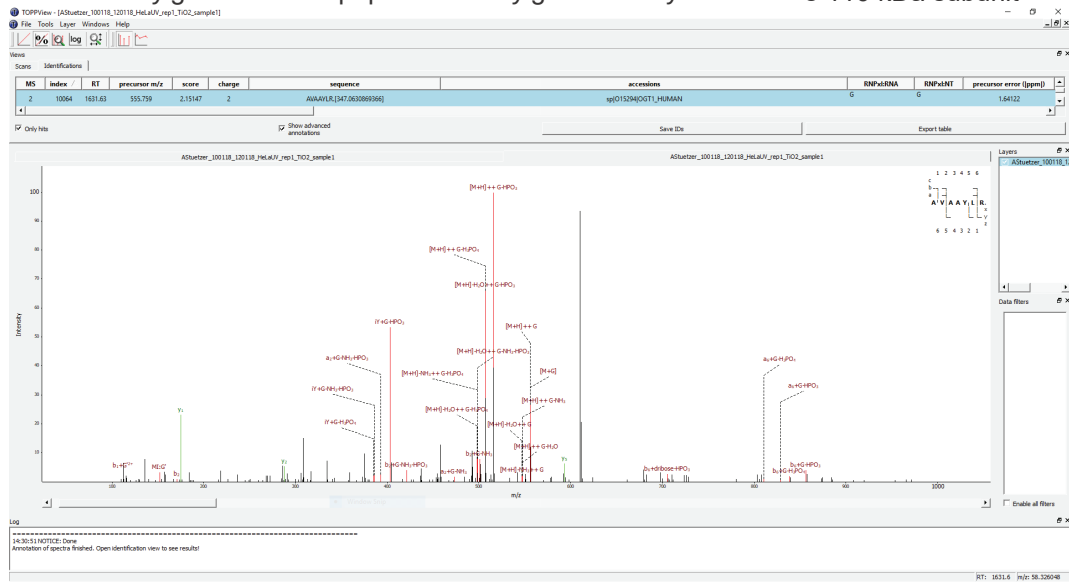
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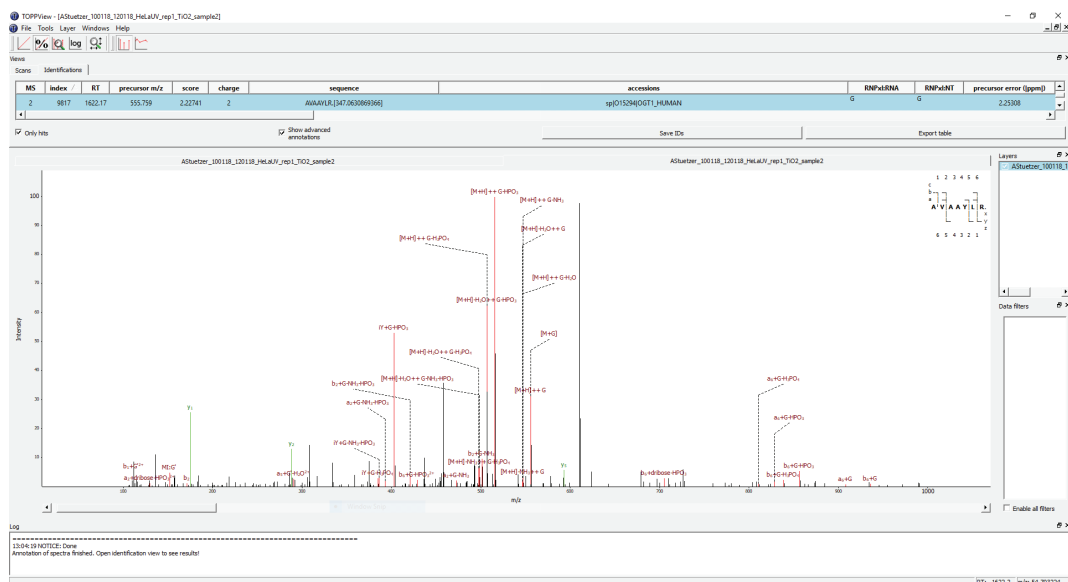
8)



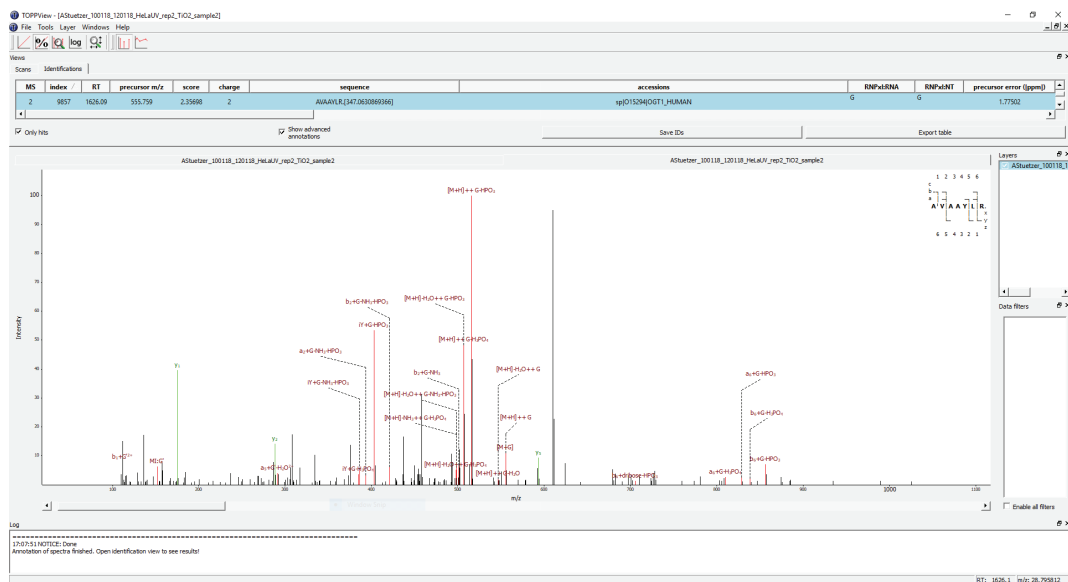
9) UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



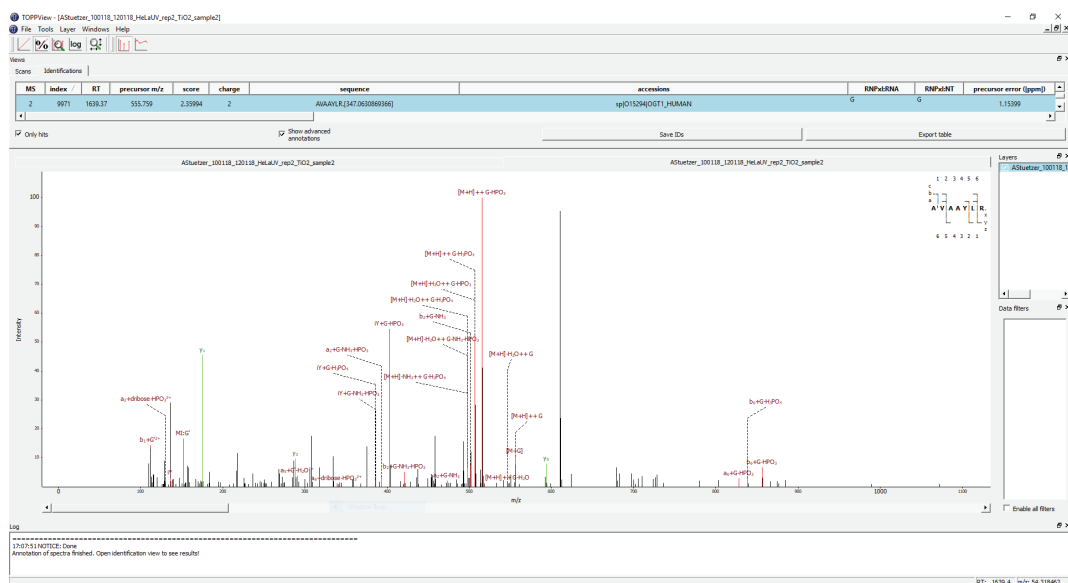
10)



11)



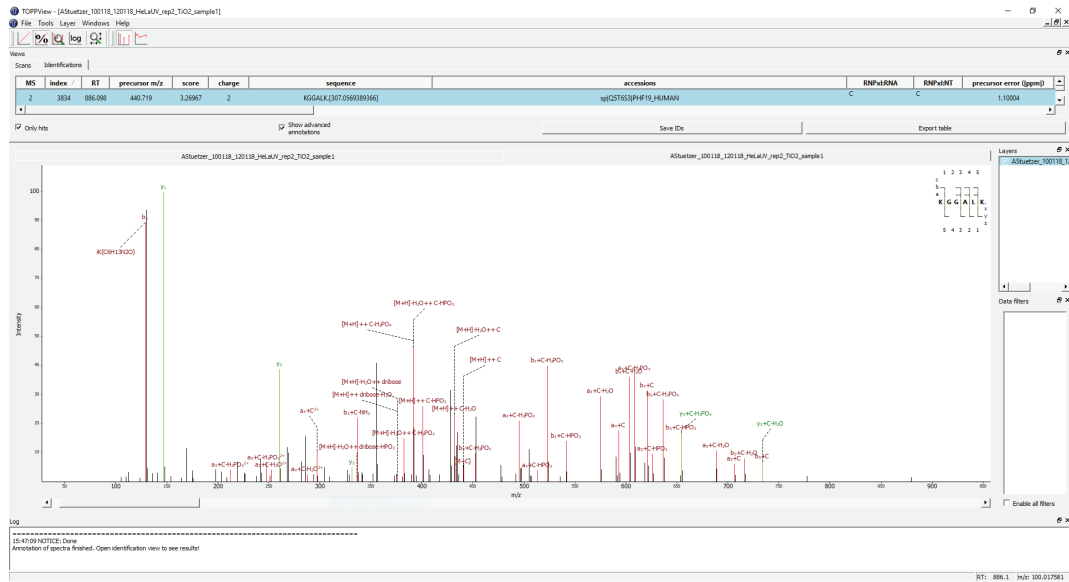
12)



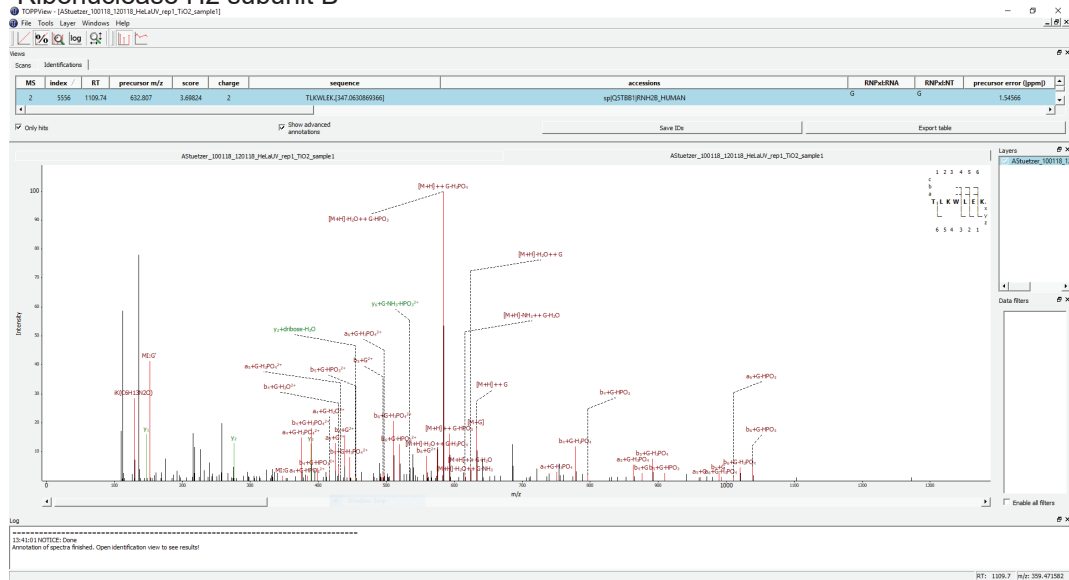
13) PHD finger protein 19



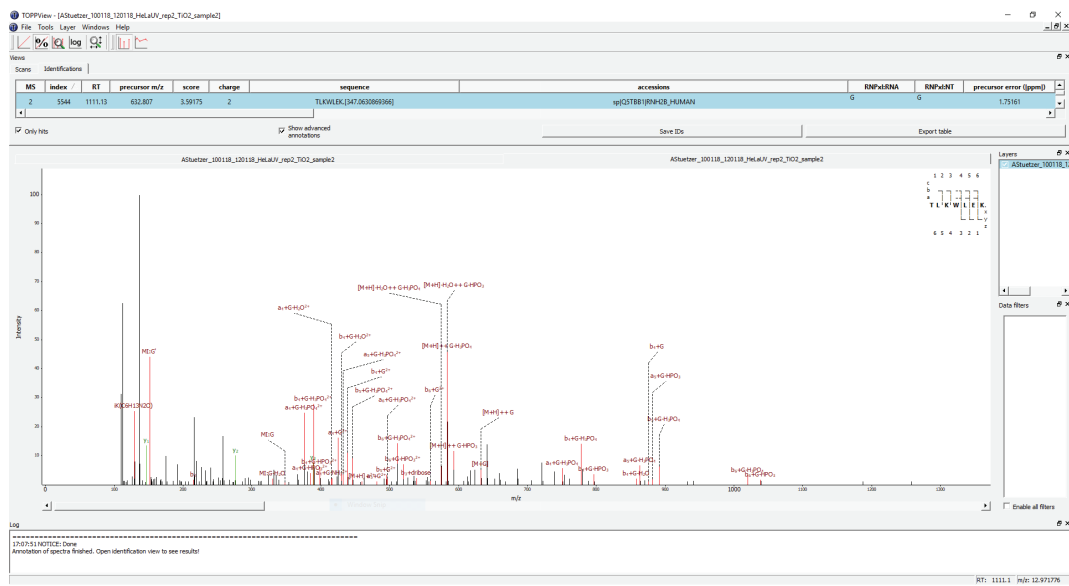
16)



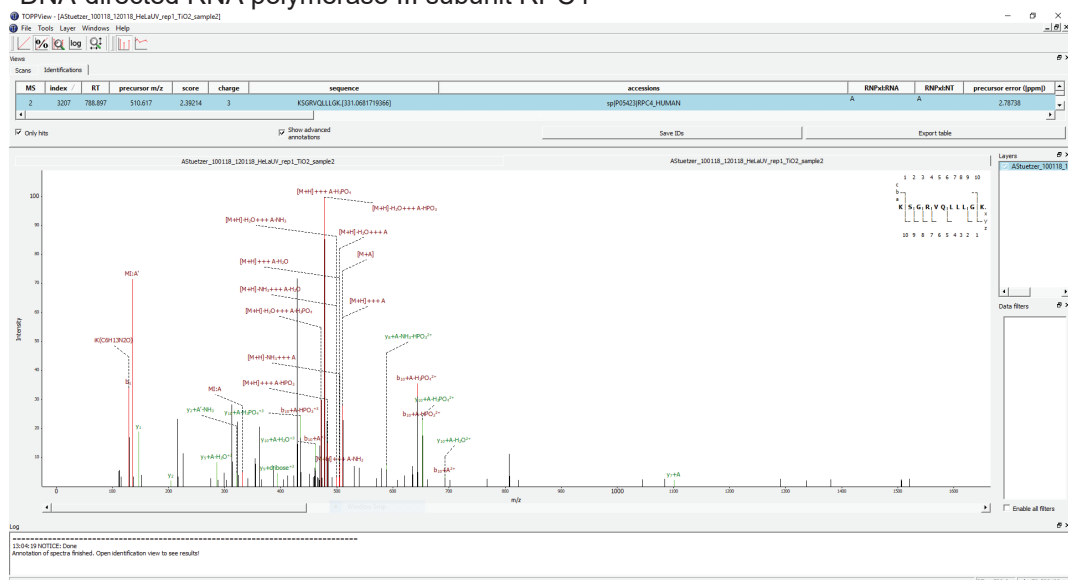
17) Ribonuclease H2 subunit B
 TOPPView - [AStuetzer.100118.120118.HelaUV_rep1.TIG2.sample1]



18)



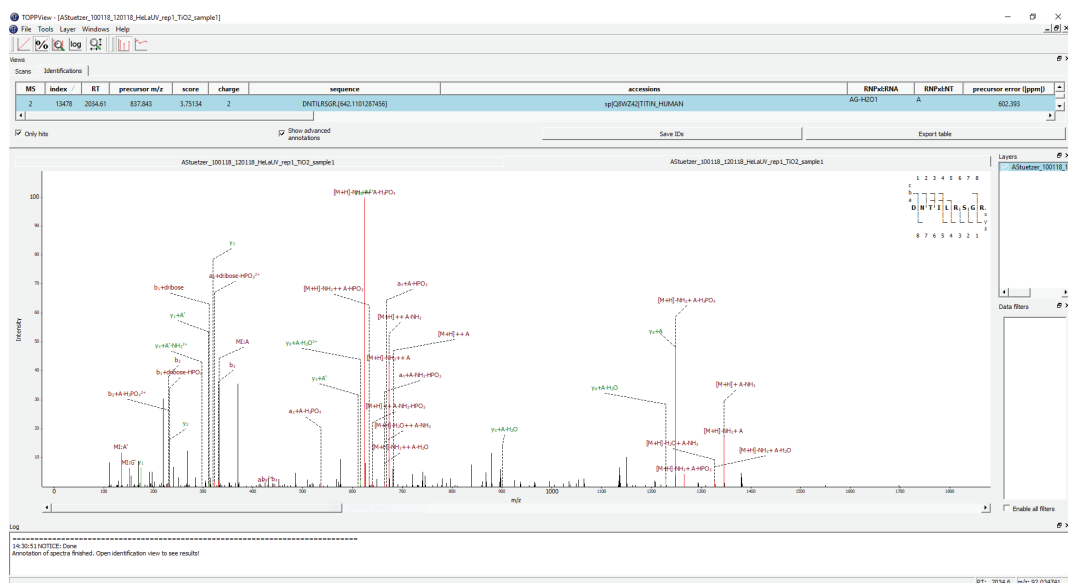
19) DNA-directed RNA polymerase III subunit RPC4



20) Titin



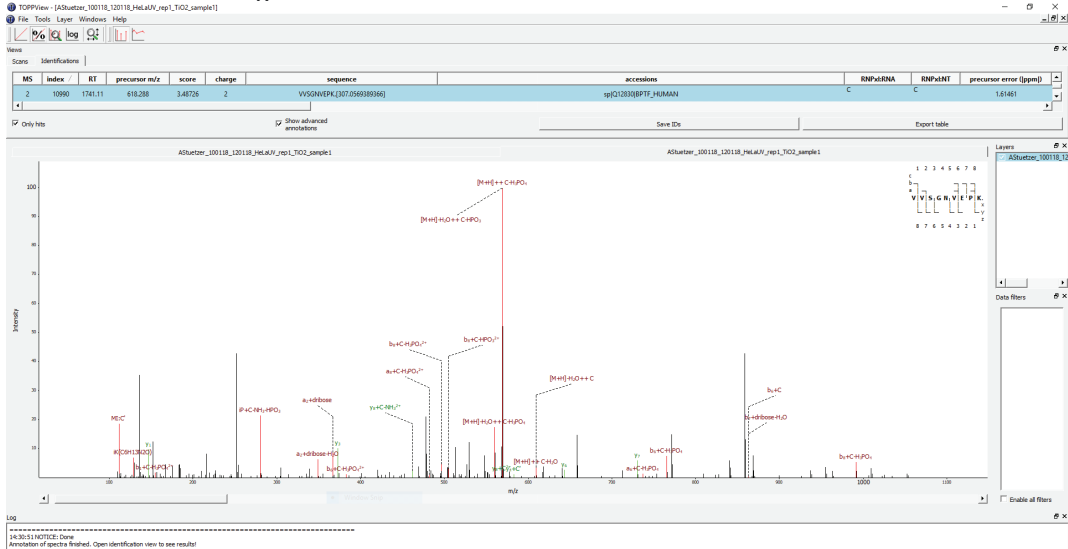
21)



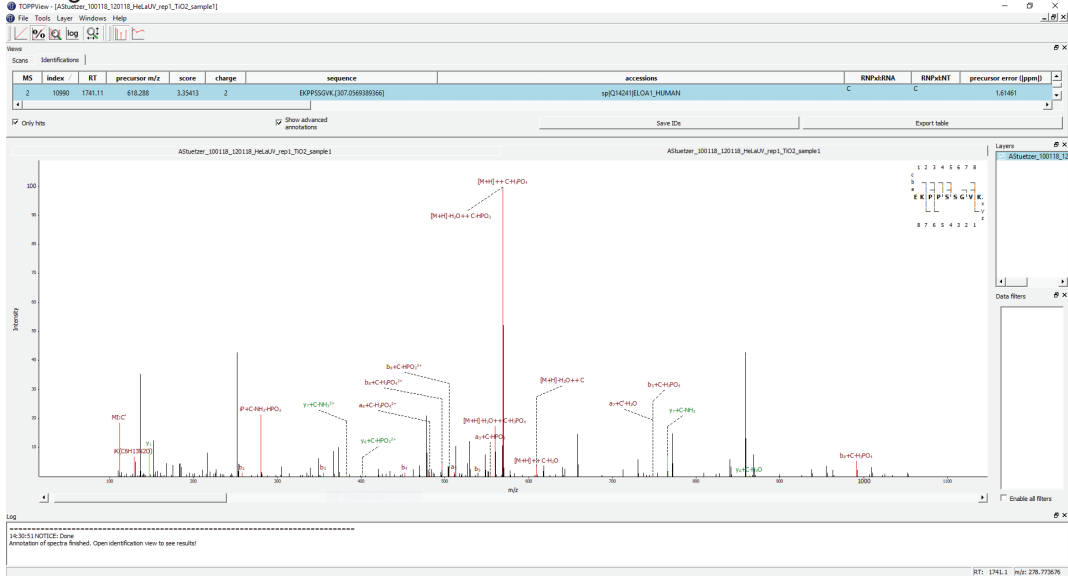
TOPPView spectra - ambiguous cross-link spectrum matches

UV cross-linked HeLa nuclei (chromatin precipitation), RNP^{xl}search_settings#2

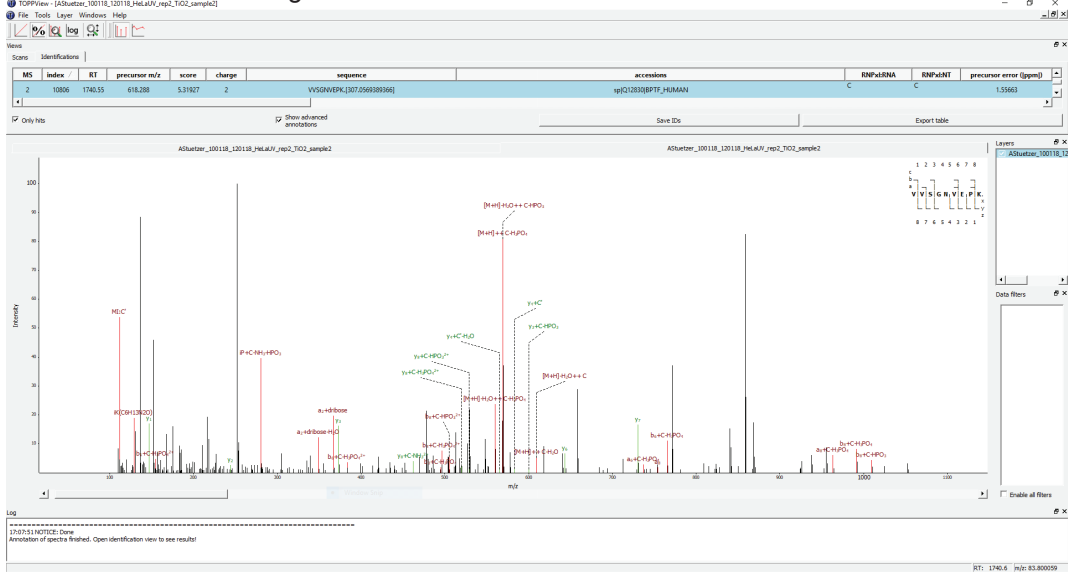
1) Nucleosome-remodeling factor subunit BPTF



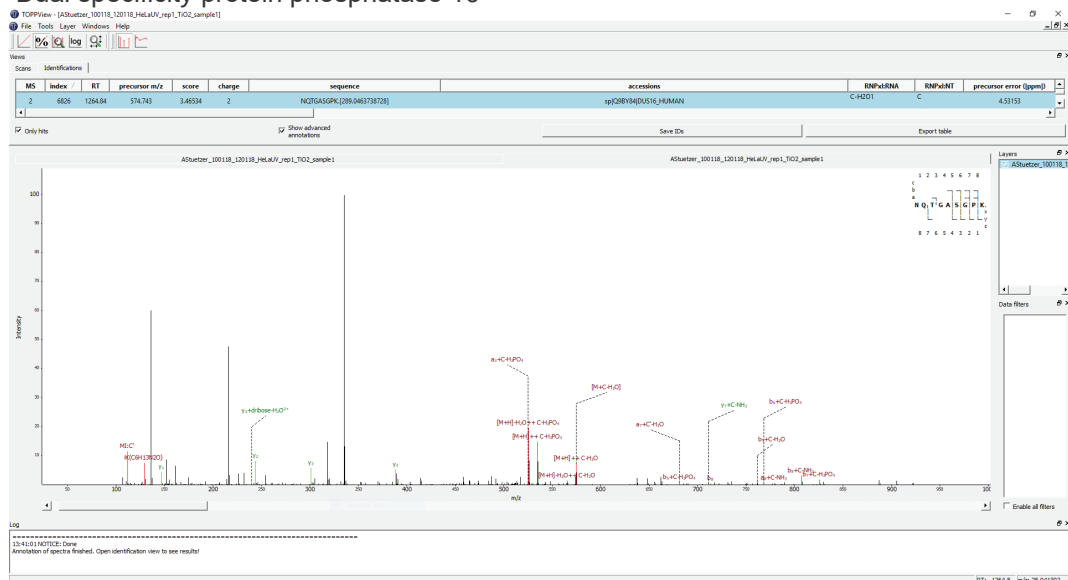
2) Elongin-A



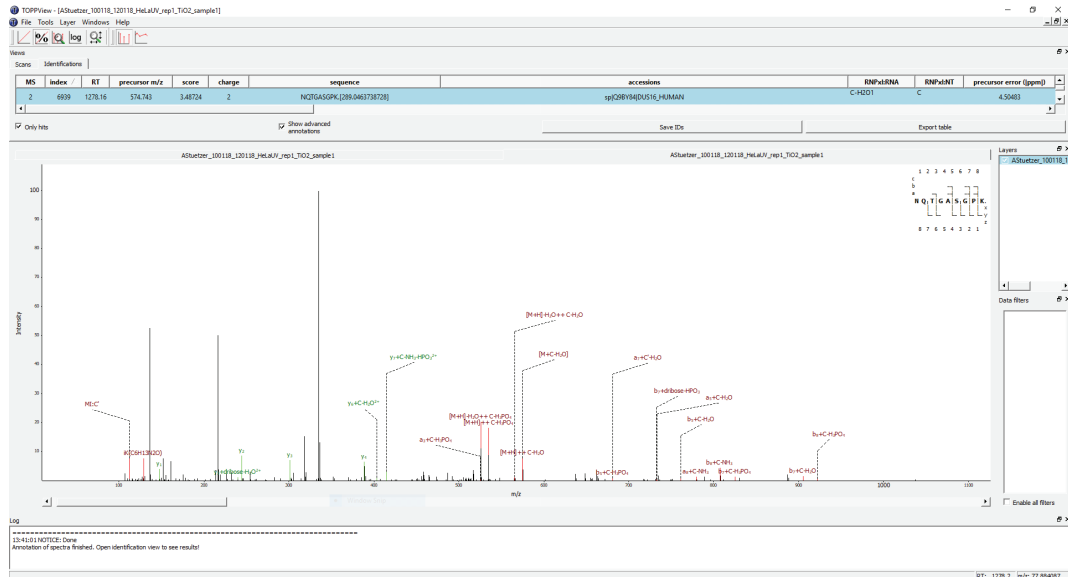
3) Nucleosome-remodeling factor subunit BPTF



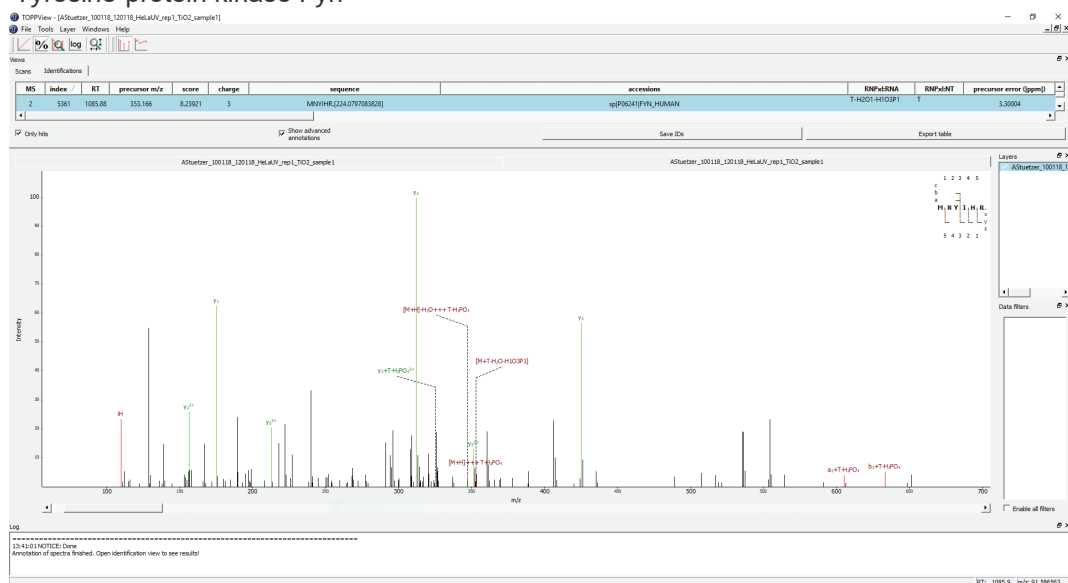
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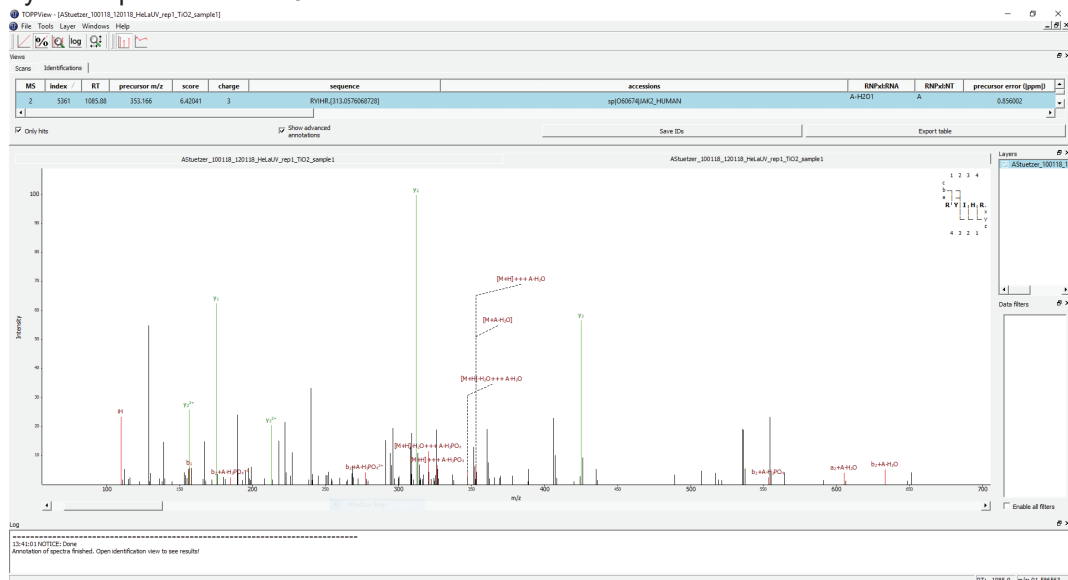
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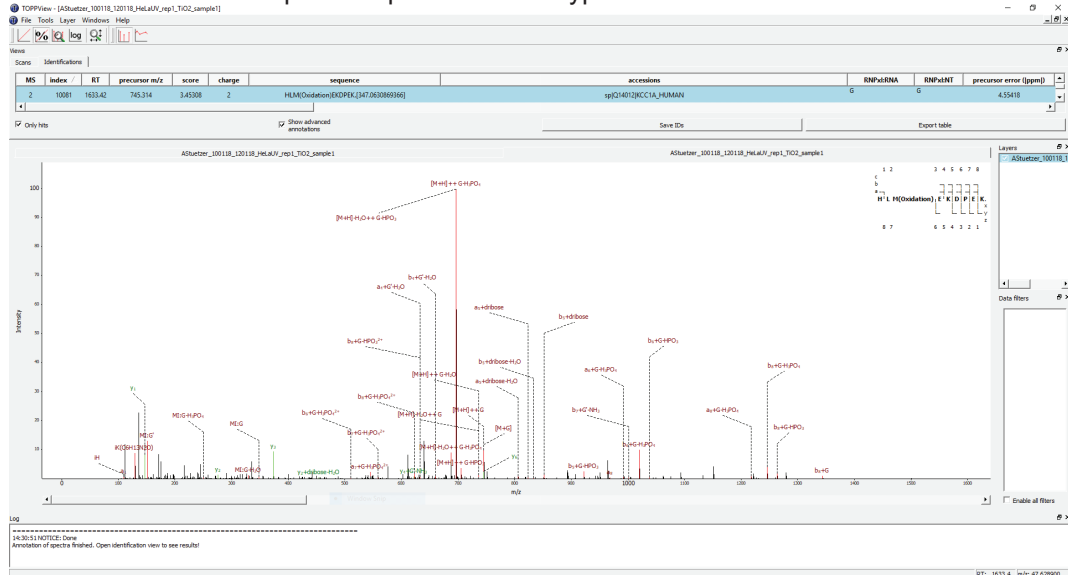
6)



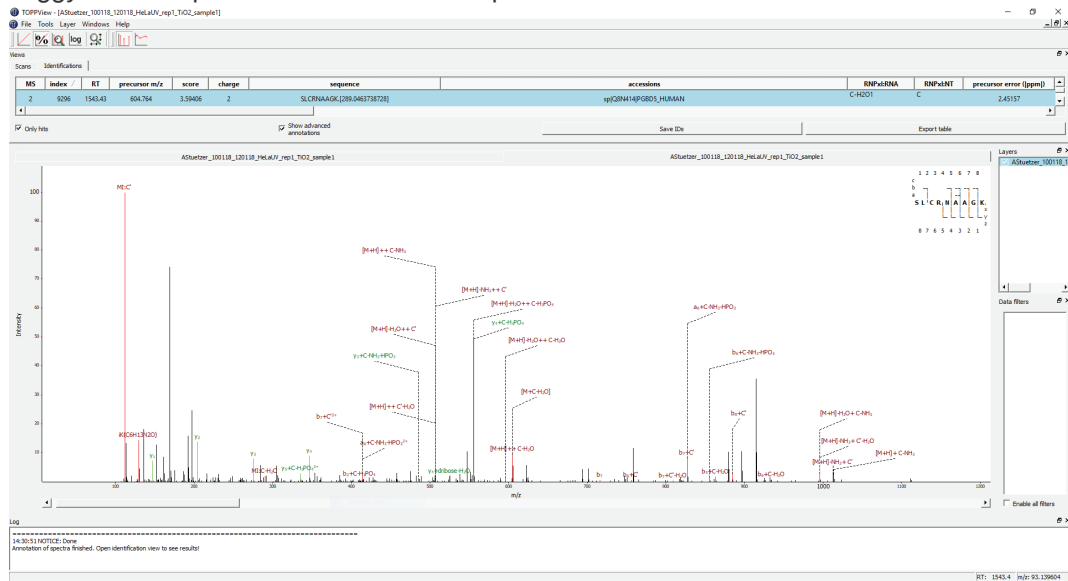
7) Tyrosine-protein kinase JAK2



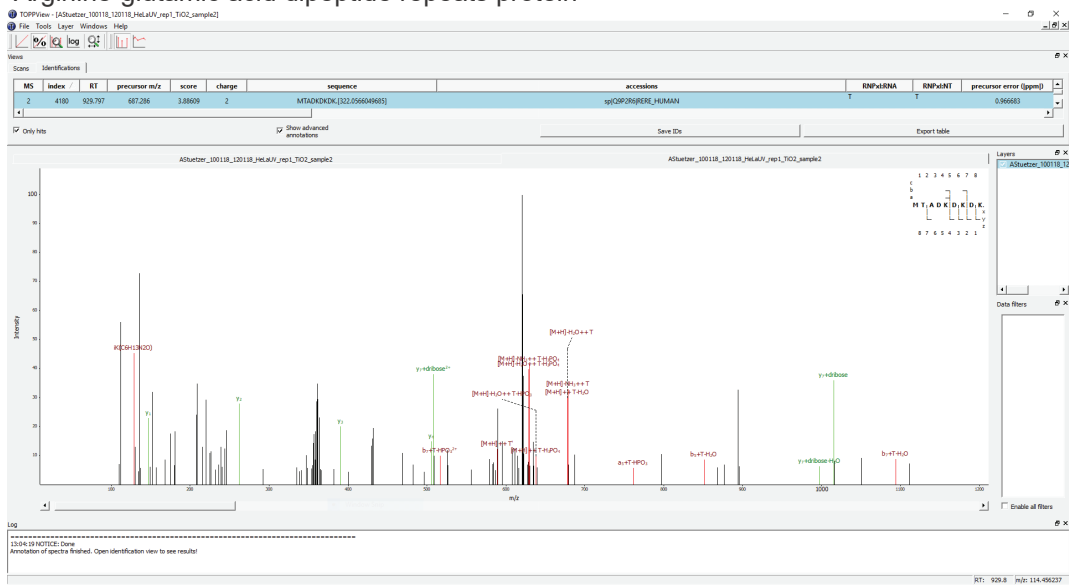
8) Calcium/calmodulin-dependent protein kinase type 1



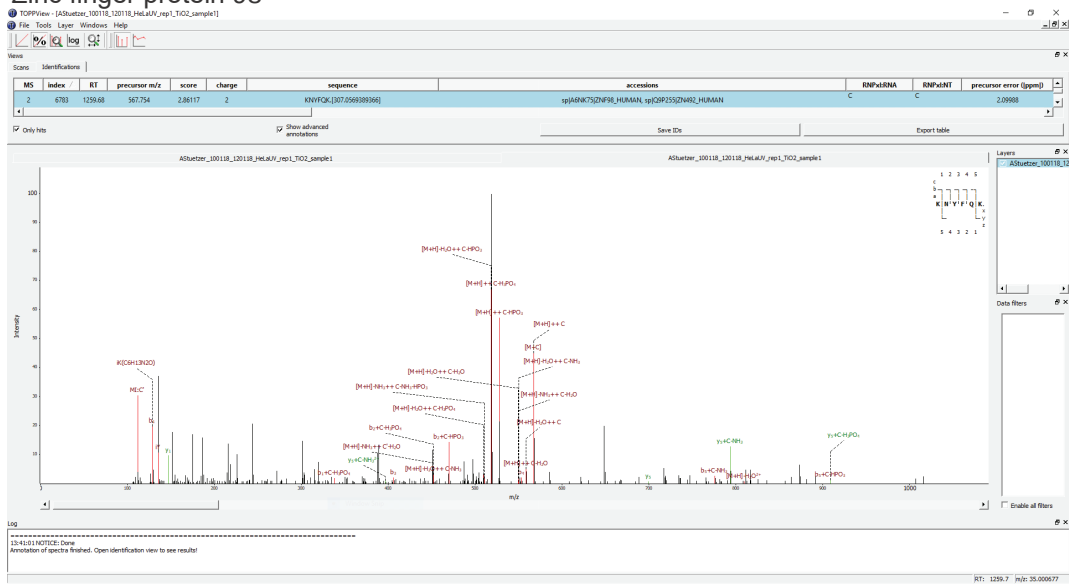
9) PiggyBac transposable element-derived protein 5



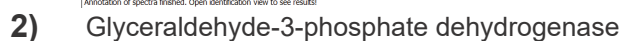
10) Arginine-glutamic acid dipeptide repeats protein

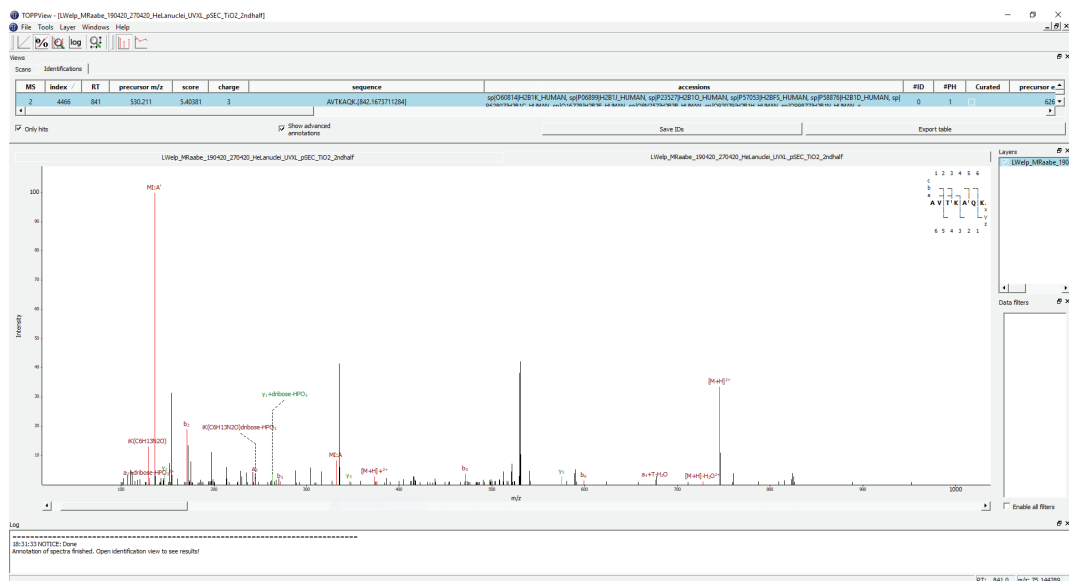
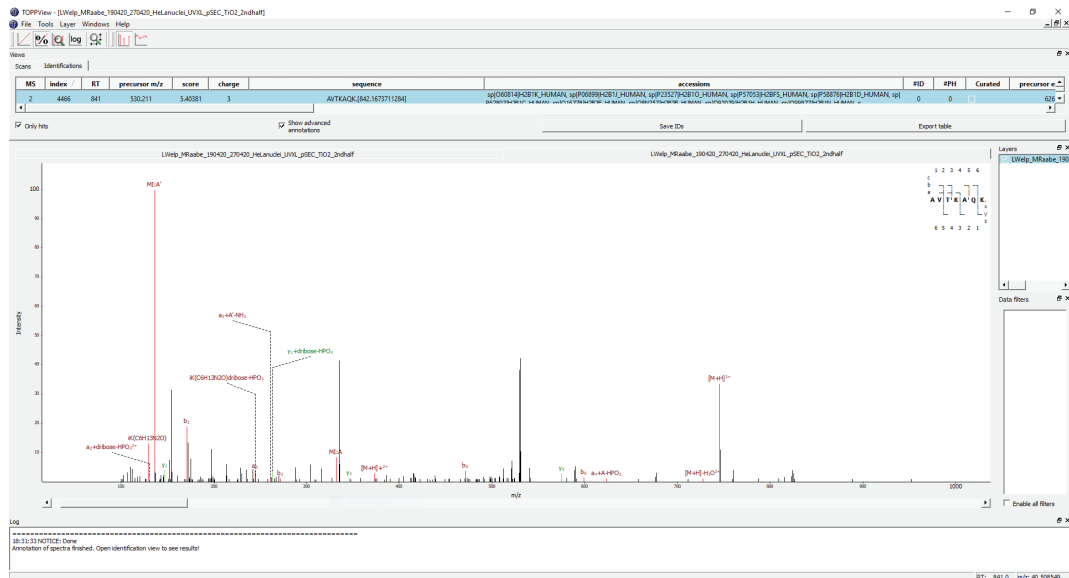
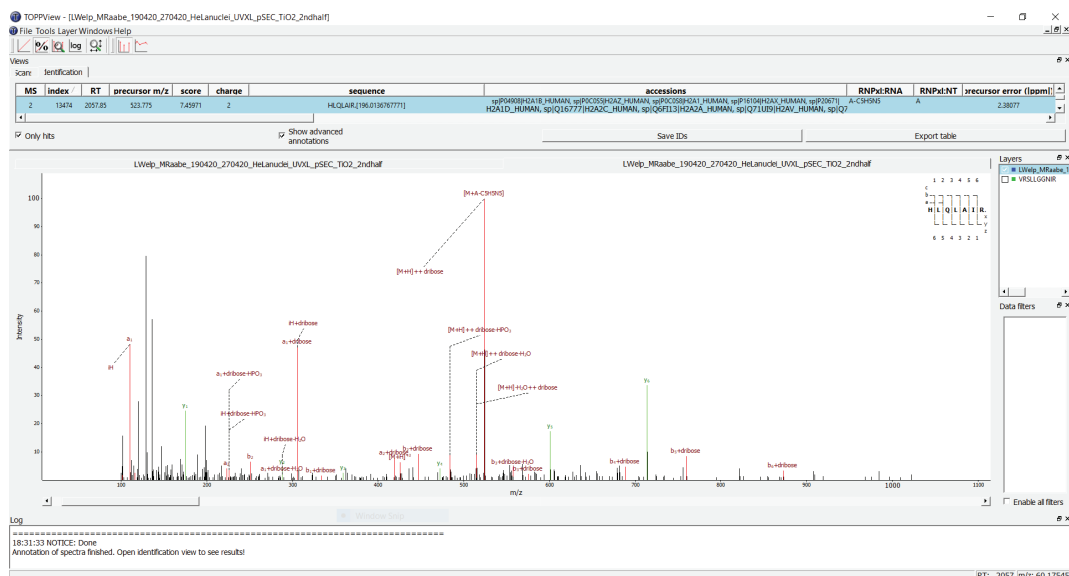


11) Zinc finger protein 98



1) Constitutive coactivator of PPAR-gamma-like protein 1



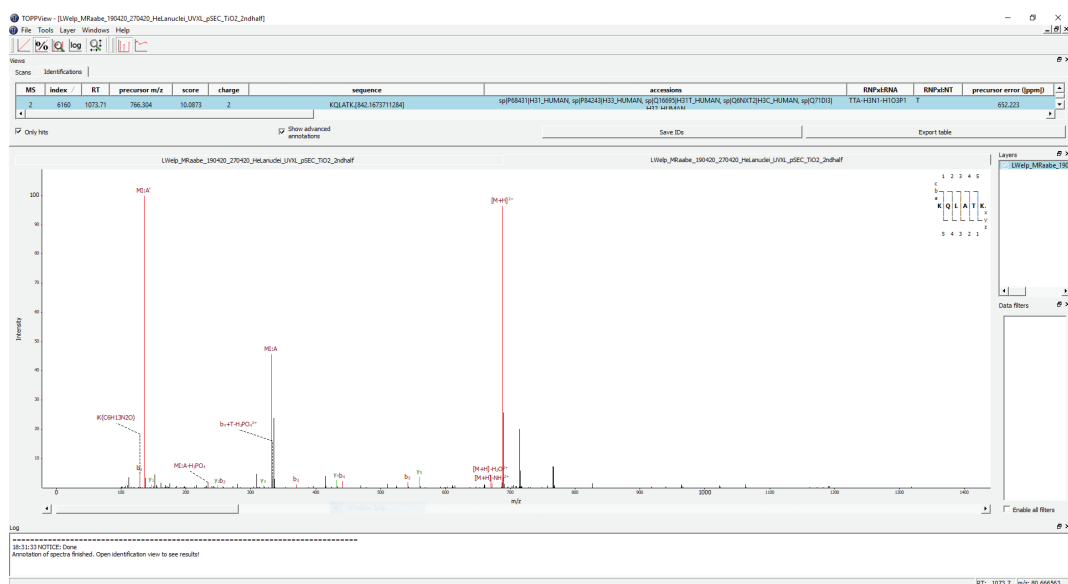


[illegible][illegible][illegible]

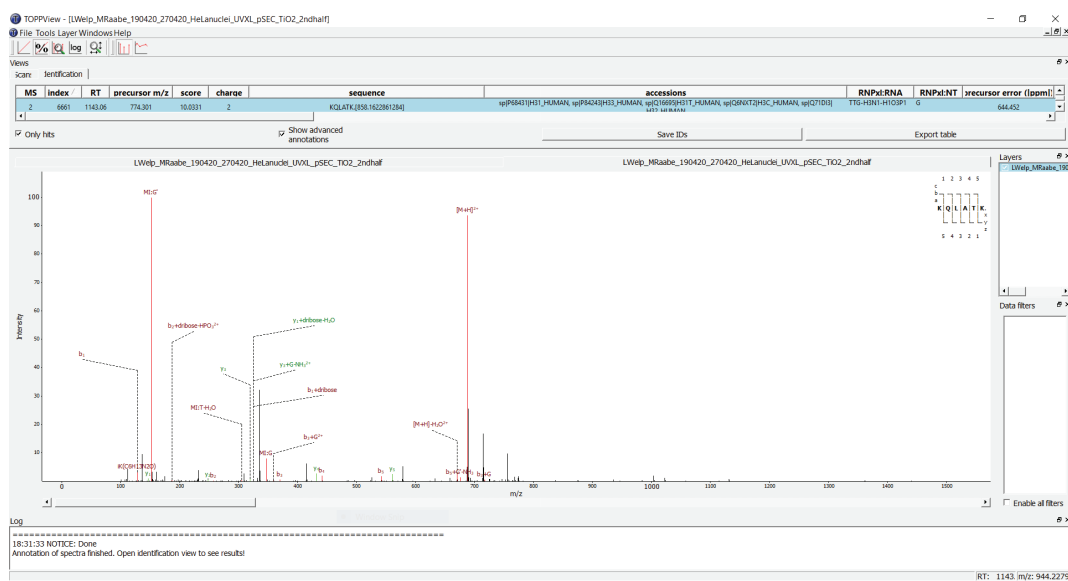
10) Histone H3



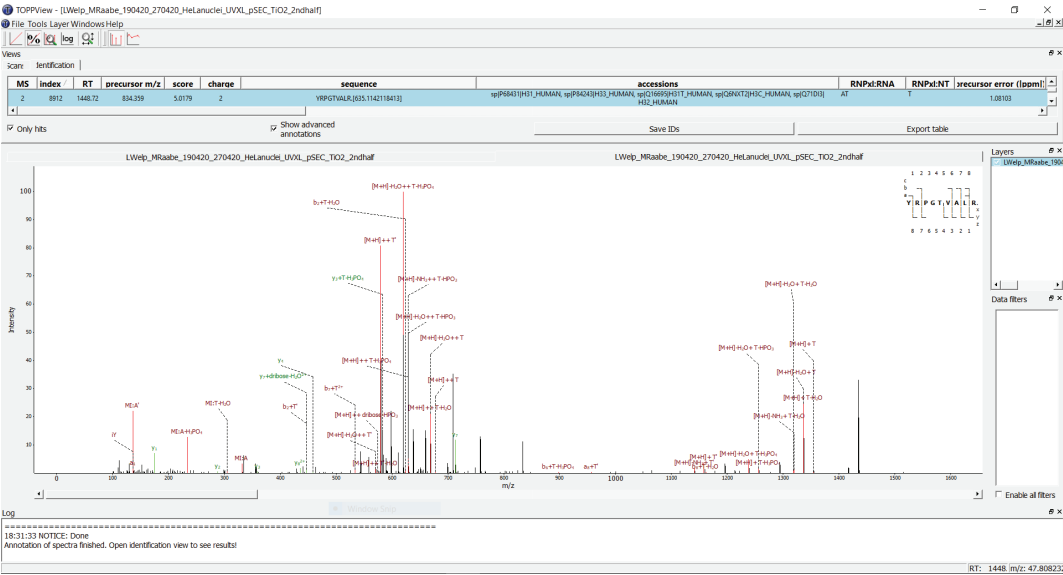
11)



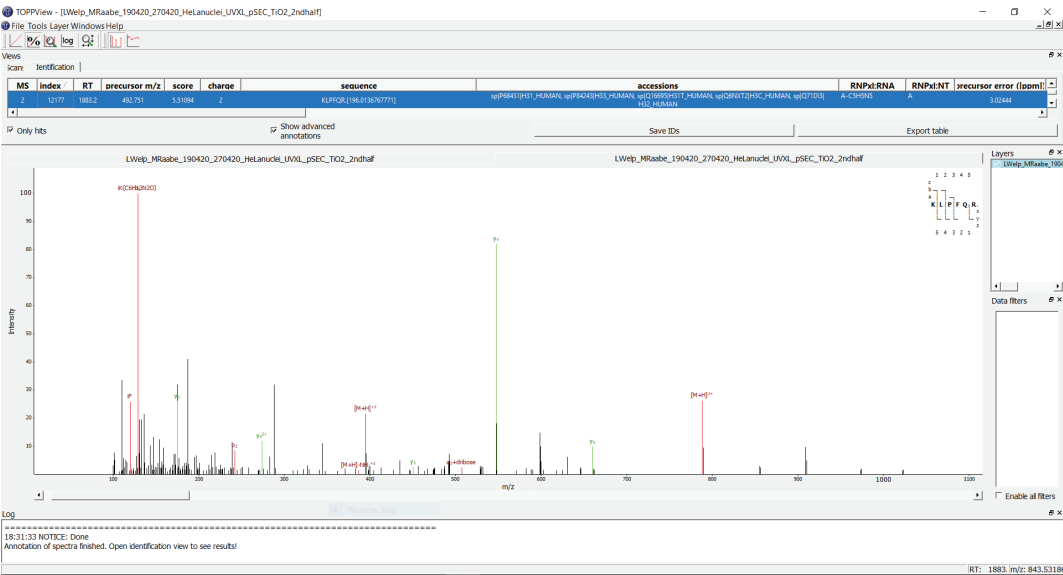
12)



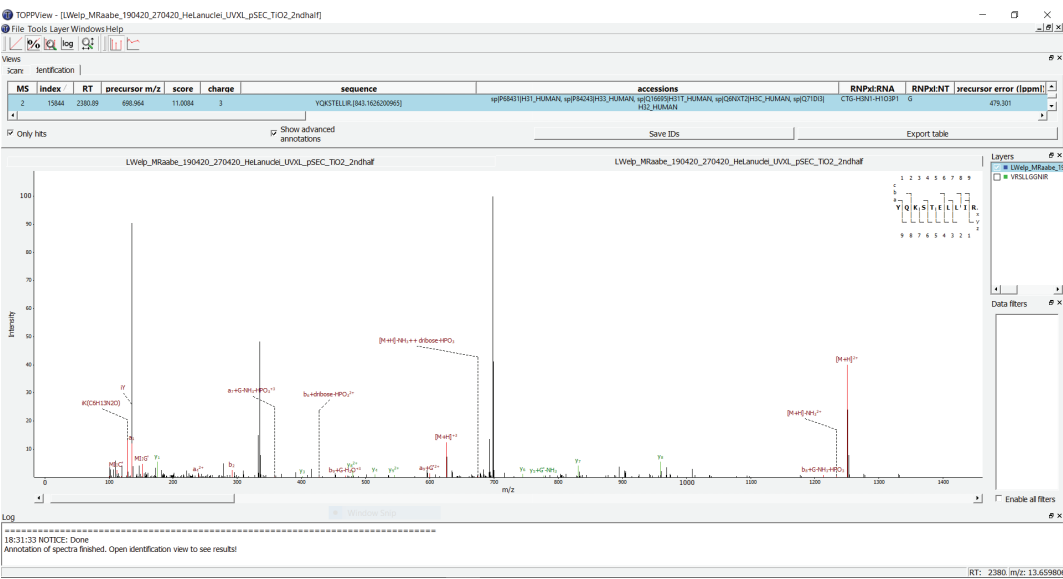
13)



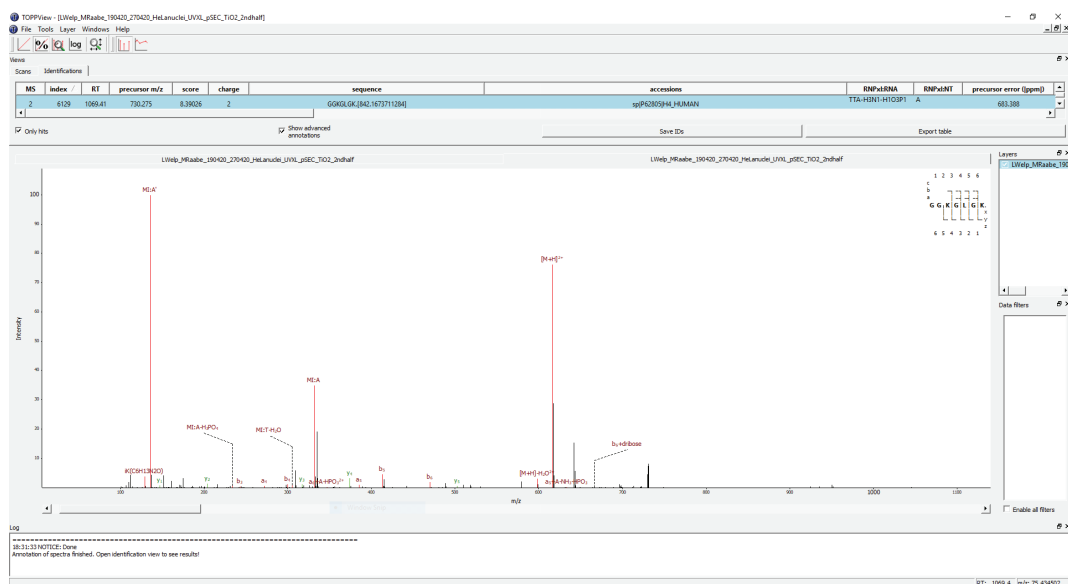
14)



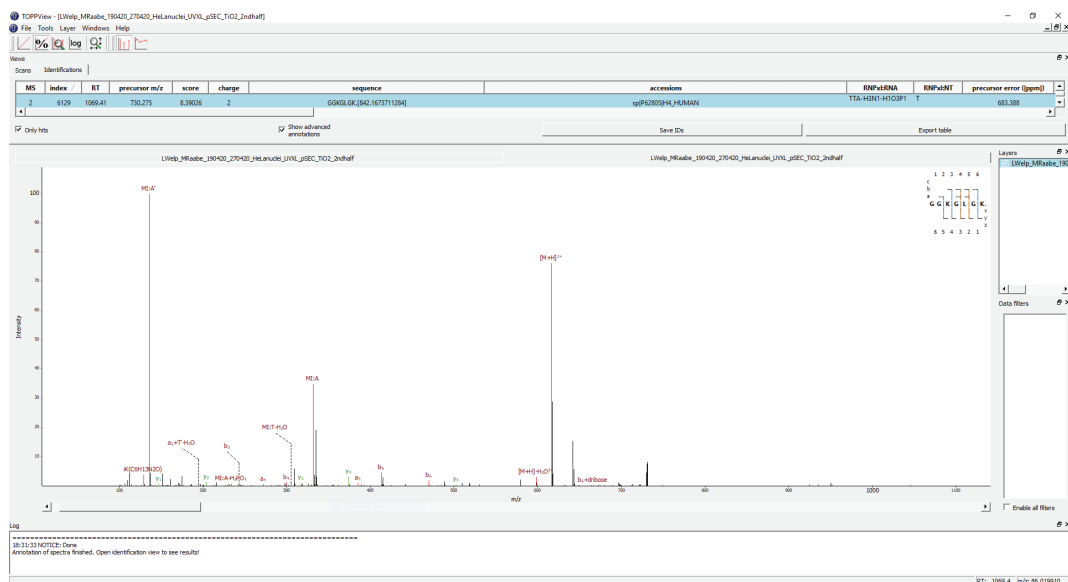
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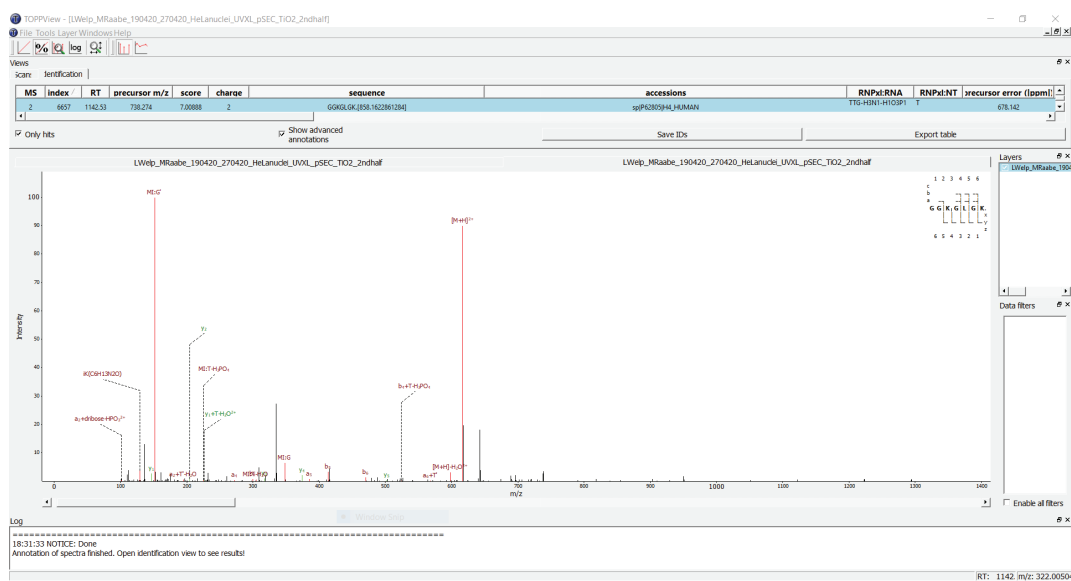
16) Histone H4



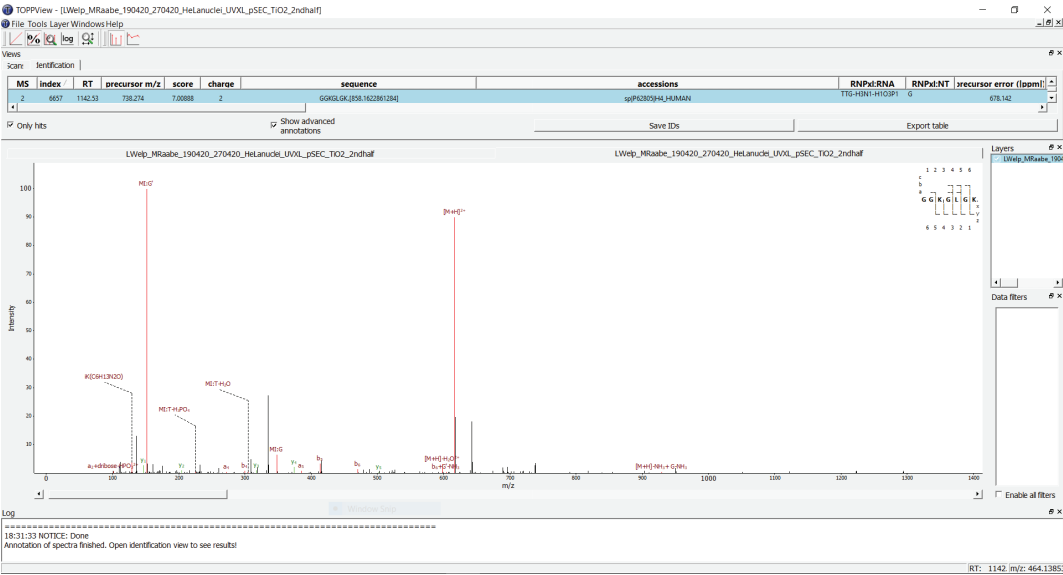
17)



18)



19)



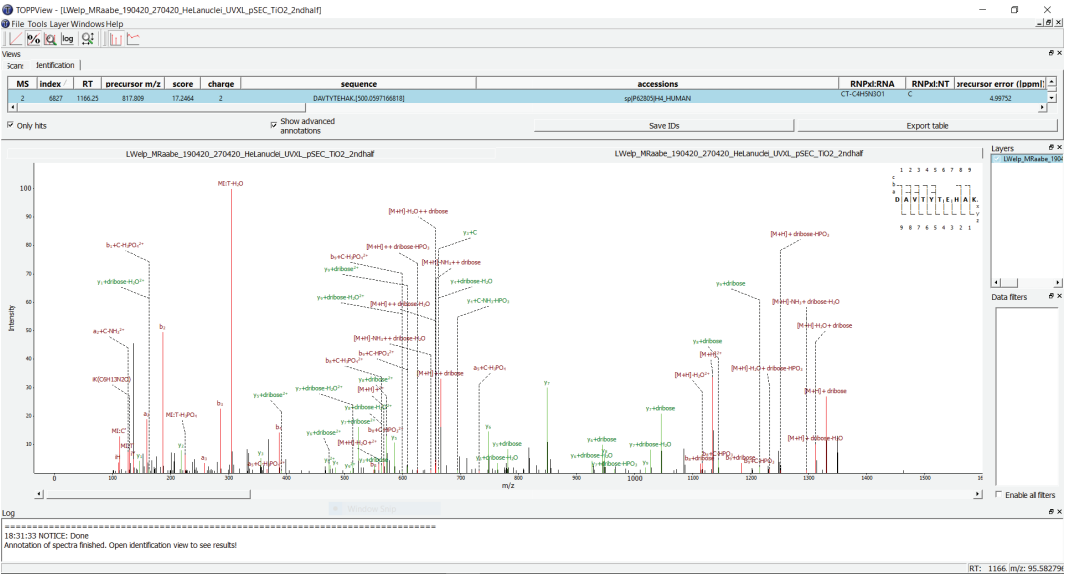
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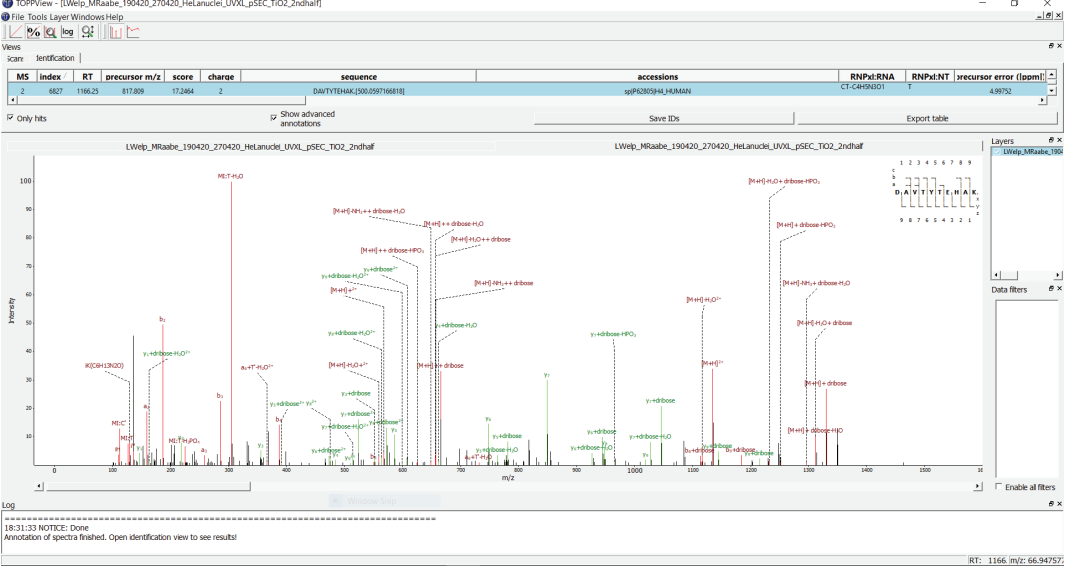
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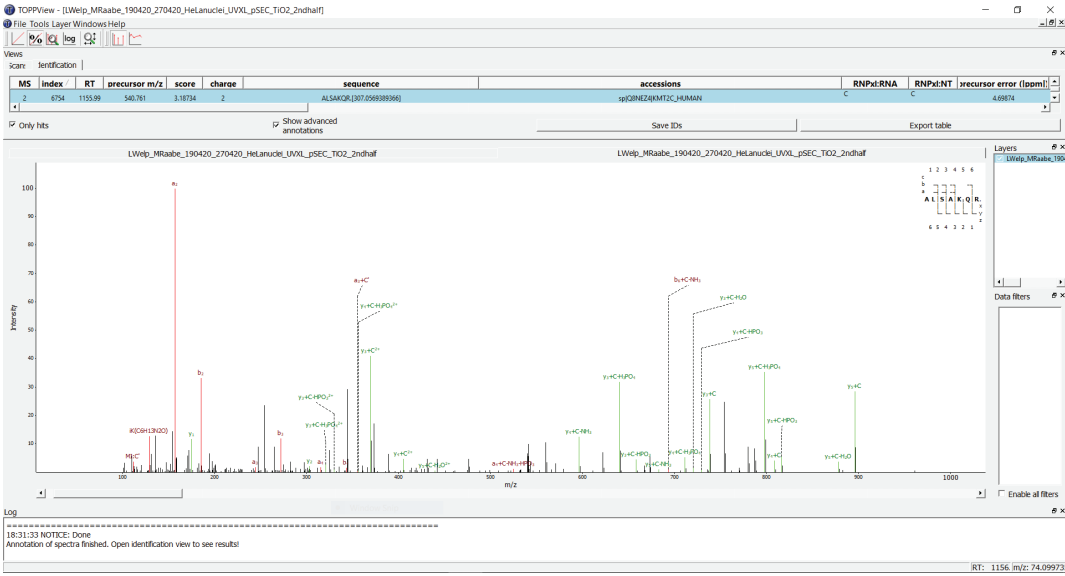
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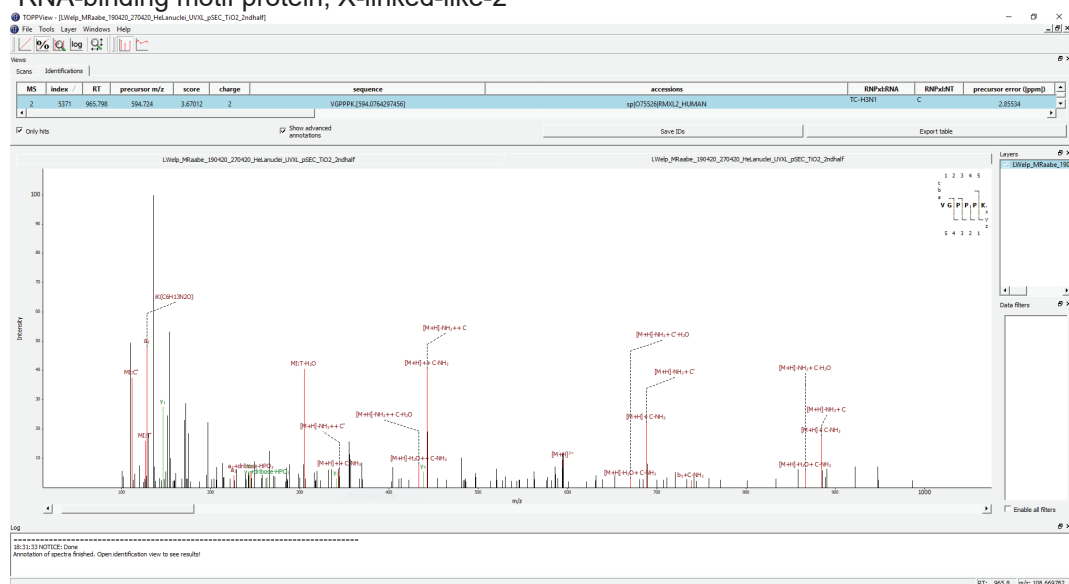
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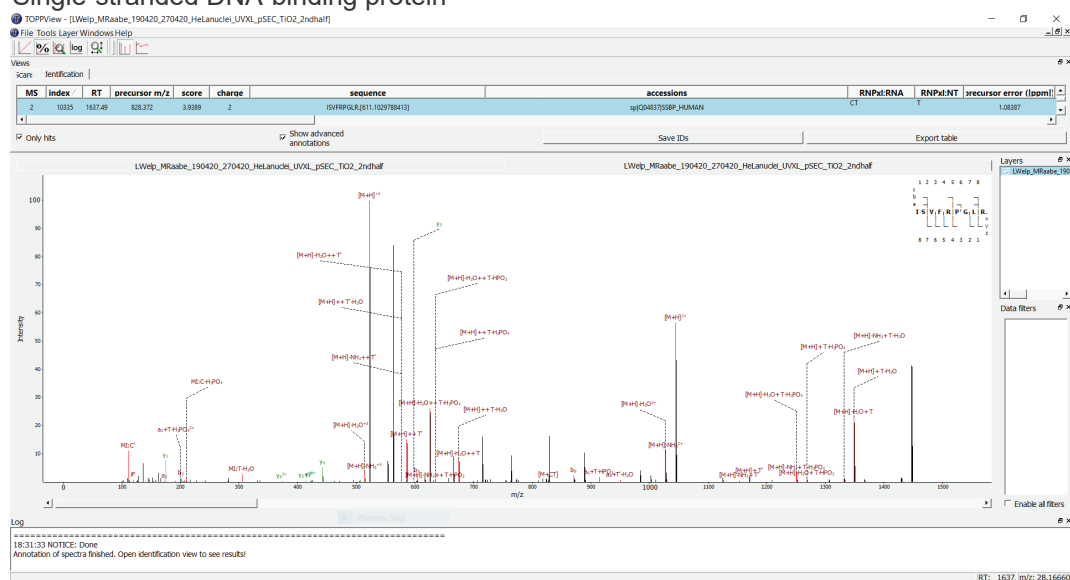
24) Histone-lysine N-methyltransferase 2C



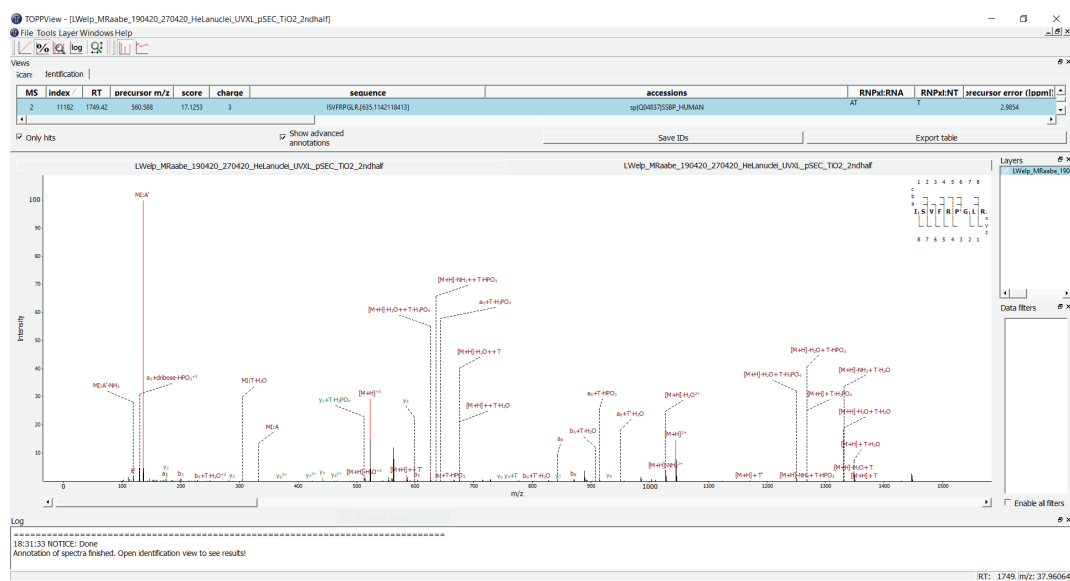
25) RNA-binding motif protein, X-linked-like-2



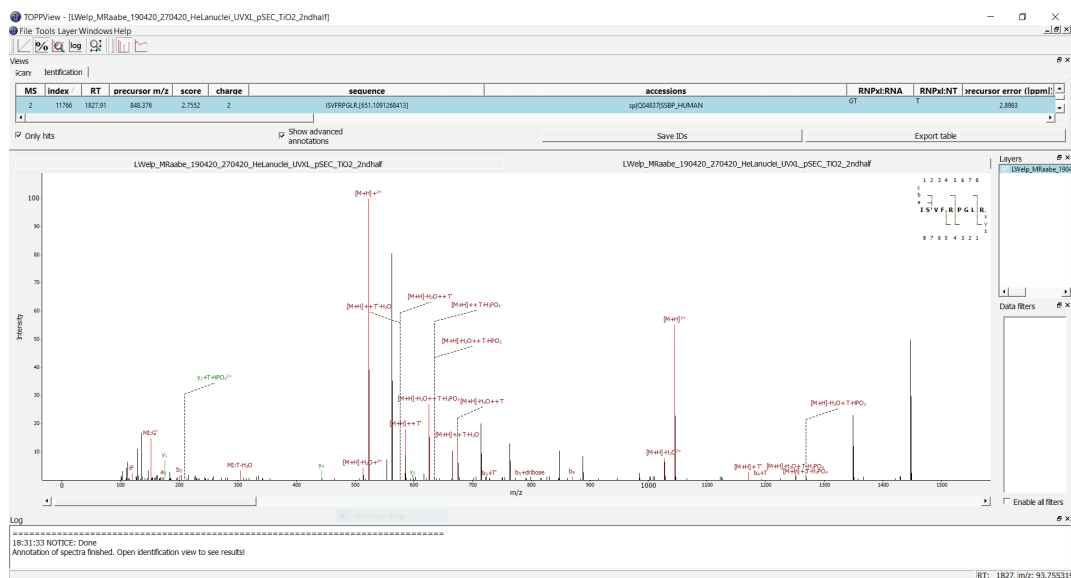
26) Single-stranded DNA-binding protein



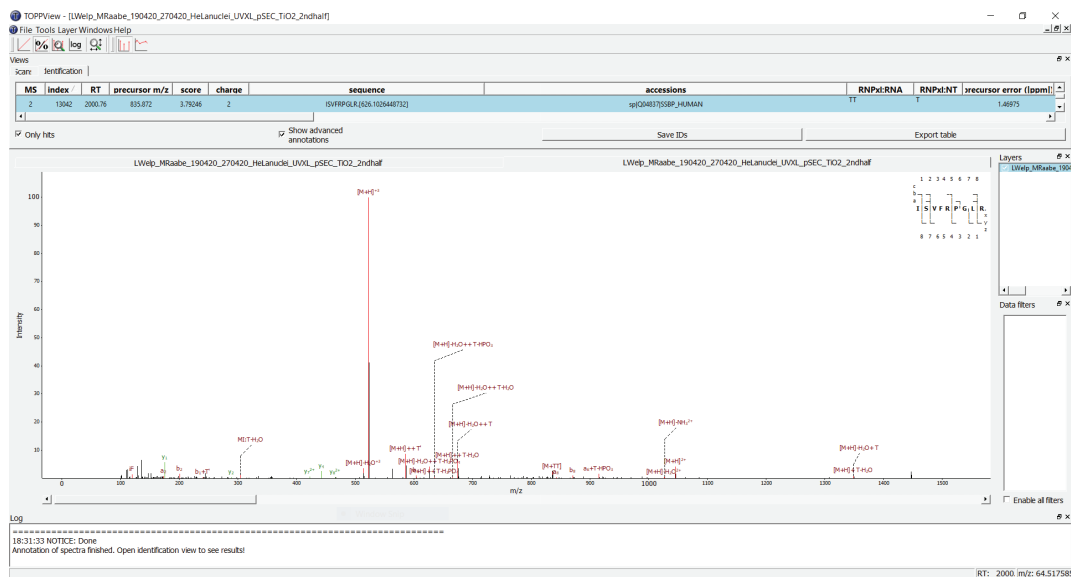
27)



28)



29)



30) Titin



UV cross-linked HeLa nuclei (SEC)

TopPanel - [L]Web_MfAbase_19643_276435_MfAbase_UV01_gSEC_Y022_2ndHalf

File Tools Layer Windows Help

MS Identification

MS	index	RT	precursor m/z	score	charge	sequence	accessions	ENPv4DNA	ENPv4NT	precursor error (ppm)
1	4911	902.734	519.739	13.1624	2	IVGSDHRL[196.0136767771]	sp P07101 HWP_C_HUMAN	A-CH3ND	A	0.55789

☒ Only hit ☒ Show advanced annotations

Save IDs Export table

Web_MfAbase_19643_276435_MfAbase_UV01_gSEC_Y022_2ndHalf

Intensity

m/z

Layers

Web_MfAbase_19643_276435_MfAbase_UV01_gSEC_Y022_2ndHalf

1 2 3 4 5 6 7

8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771

TopView - LTQ/MS_MRM_10420_270420_HelAnucl_UVH_gSEC_TIC2_2ndshf

File Tools Layer Help

View

Score	Identification
MS	Index RT precursor m/z score charge sequence accession RNPdRNA RNPdSNT precursor error (ppm)
2	4997 914.628 519.74 14.8238 2 NGC39HR[196.013670771] spP07191@RBC_HUMAN A-C-HVD A 3.88257

☒ Only MS ☒ Show advanced annotations Save IDs Export table

LTQ/MS_MRM_10420_270420_HelAnucl_UVH_gSEC_TIC2_2ndshf

LTQ/MS_MRM_10420_270420_HelAnucl_UVH_gSEC_TIC2_2ndshf

Layers
LTQ/MS_MRM_10420_270420_HelAnucl_UVH_gSEC_TIC2_2ndshf

Data Filters

☐ Enable all filters

Log

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20-31-31MTCID: Done
Annotation of spectra finished. Open identification view to see results!
    
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[illegible]

[illegible]

TOPView - [LWep_MRaabe_190420_270420_HetAnucl_UVXL_pSEC_TIO2_2ndhalf]

File Tools Layer Windows Help

Views: Scan Identification

MS	Index	RT	precursor m/z	score	charge	sequence	accessions	RNPeI:RNA	RNPeI:NT	recursor error (ppm)
2	7771	1295.19	458.68	5.58676	2	CDVDRL196.013670771	spP60709ACTR_HUMAN, spP63261ACTO_HUMAN	A-C3HG5	A	4.4166

Only hits ☒ Show advanced annotations Save IDs Export table

Log

18:31:33 NOTICE: Done
Annotation of spectra finished. Open identification view to see results!

TOPVIEW - [LWep_MRaabe_190420_270420_HeLa nuclei_UVXL_pSEC_TIO2_2ndhalf]

File Tools Layer Windows Help

Views Scan Identification

MS	Index	RT	precursor m/z	score	charge	sequence	accessions	RNPe:RNA	RNPe:NT	precursor error (ppm)
2	15107	2281.03	571.261	23.624	3	INAHFTPVNELK(196.D13676771)	spP60709 ACTE_HUMAN, spP63201 ACTE_HUMAN, spP60334 ACTE_HUMAN, spP68133 ACTE_HUMAN	A-CHRG	A	2.62073

Only hits

Show advanced annotations

Save IDs

Export table

LWep_MRaabe_190420_270420_HeLa nuclei_UVXL_pSEC_TIO2_2ndhalf

Layers

- LWep_MRaabe_190420_270420_HeLa nuclei_UVXL_pSEC_TIO2_2ndhalf
- MS/MS

Data filters

Enable all filters

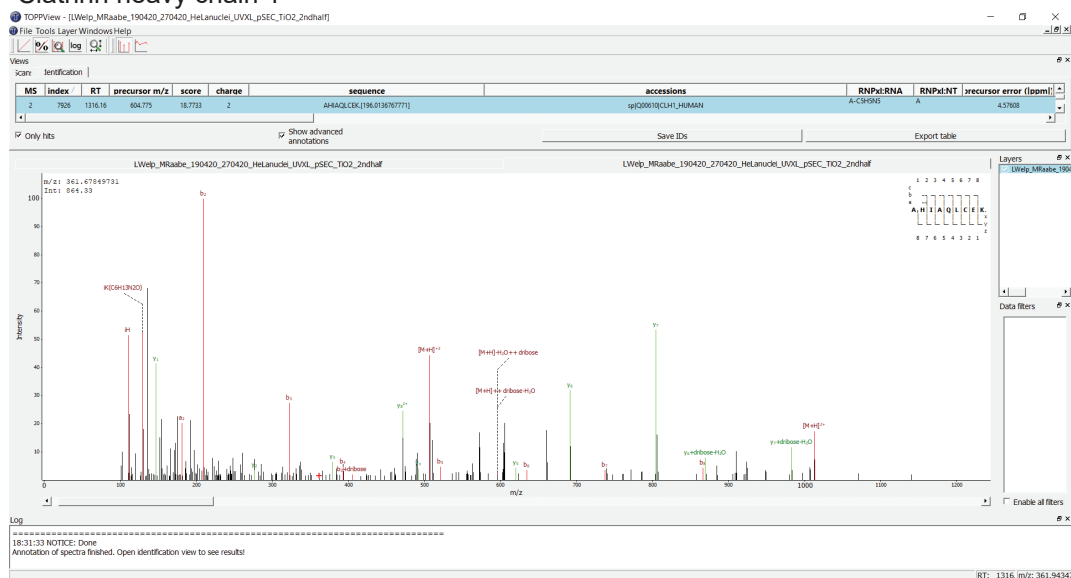
Log

18:31:33 NOTED: Done

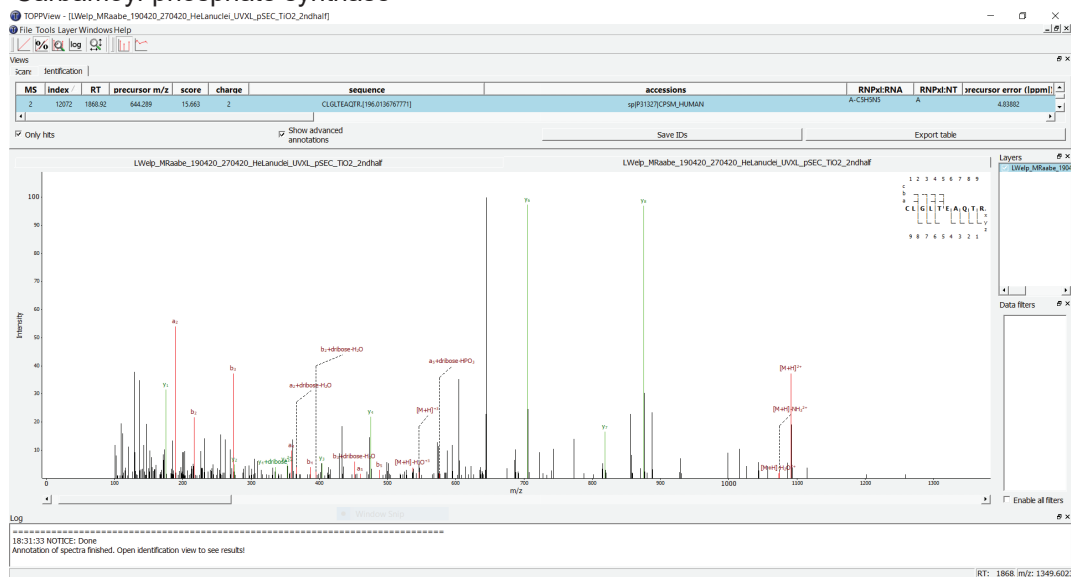
Annotation of spectra finished. Open identification view to see results!

RT: 2281. m/z: 29.792

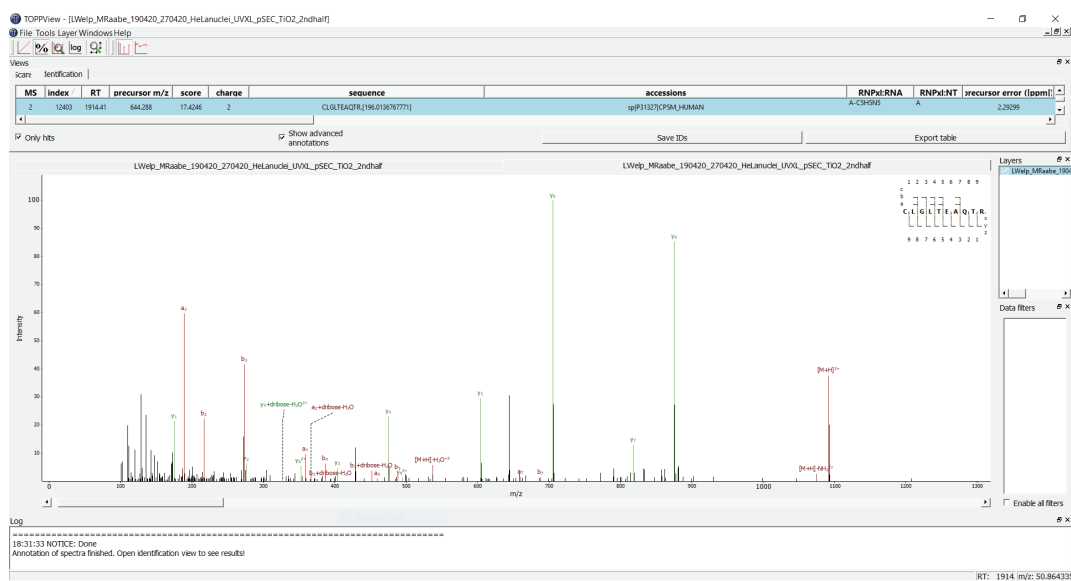
7) Clathrin heavy chain 1



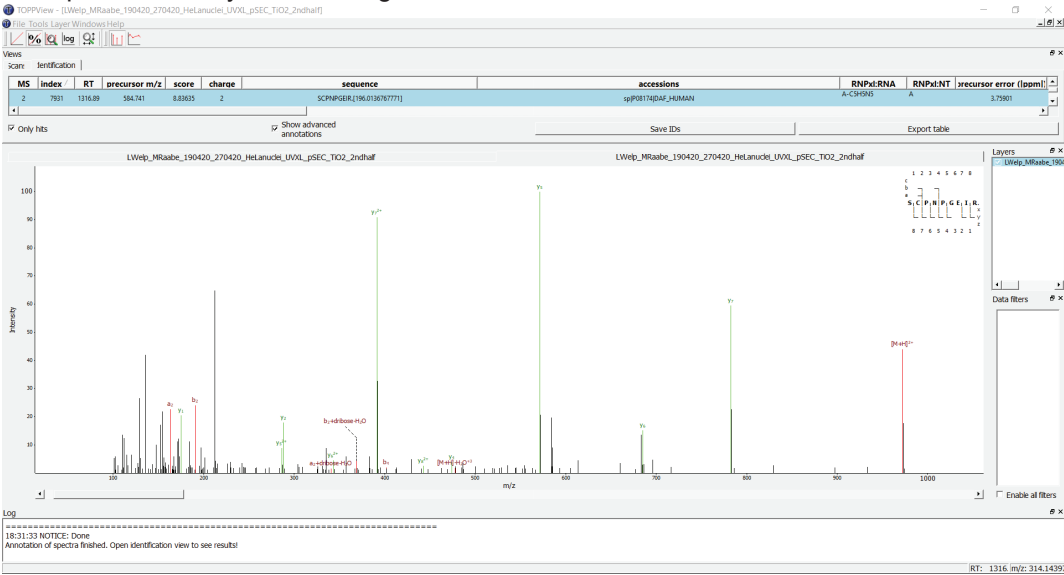
8) Carbamoyl-phosphate synthase



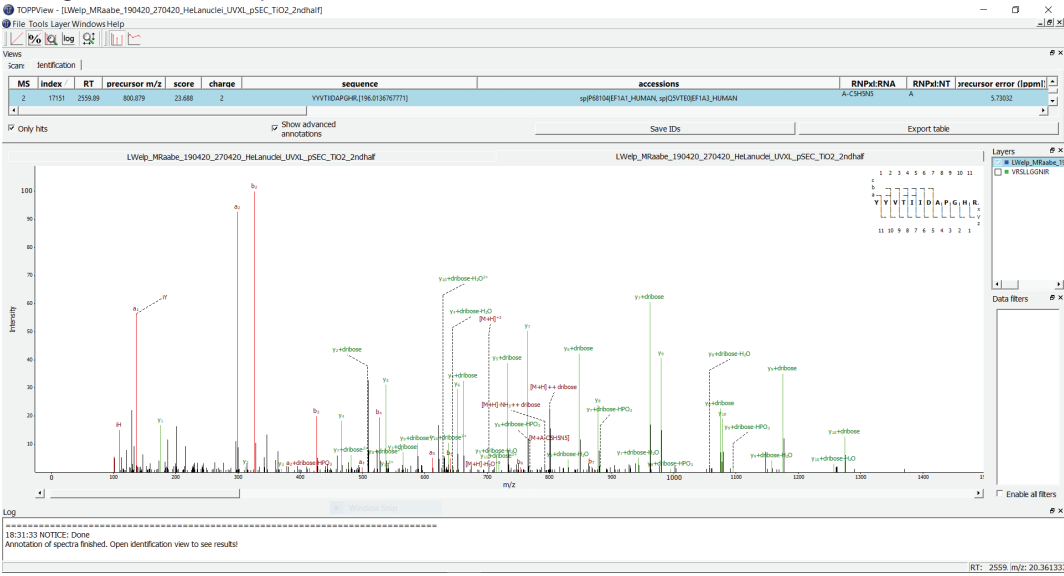
9)



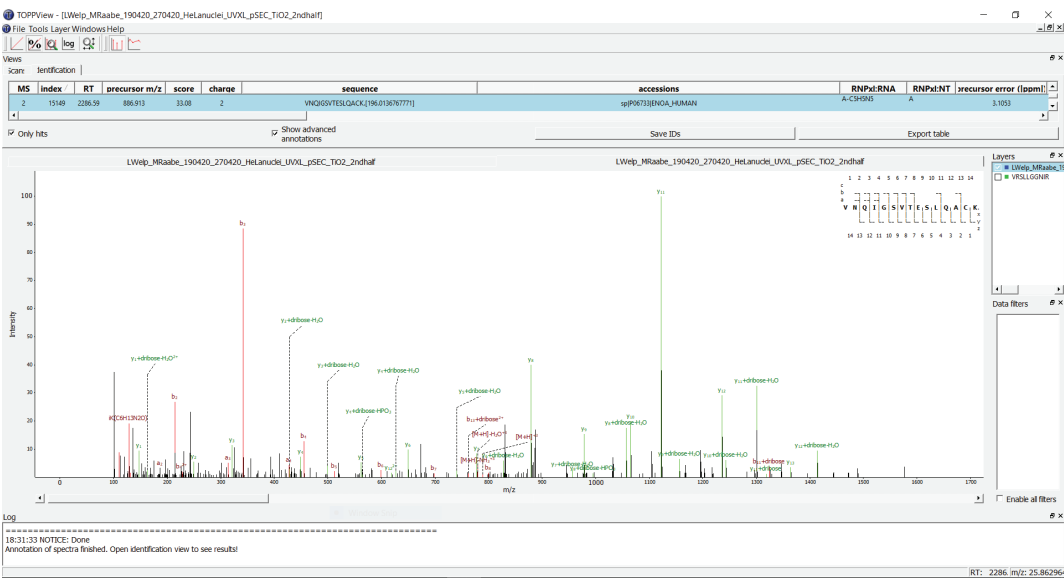
10) Complement decay-accelerating factor



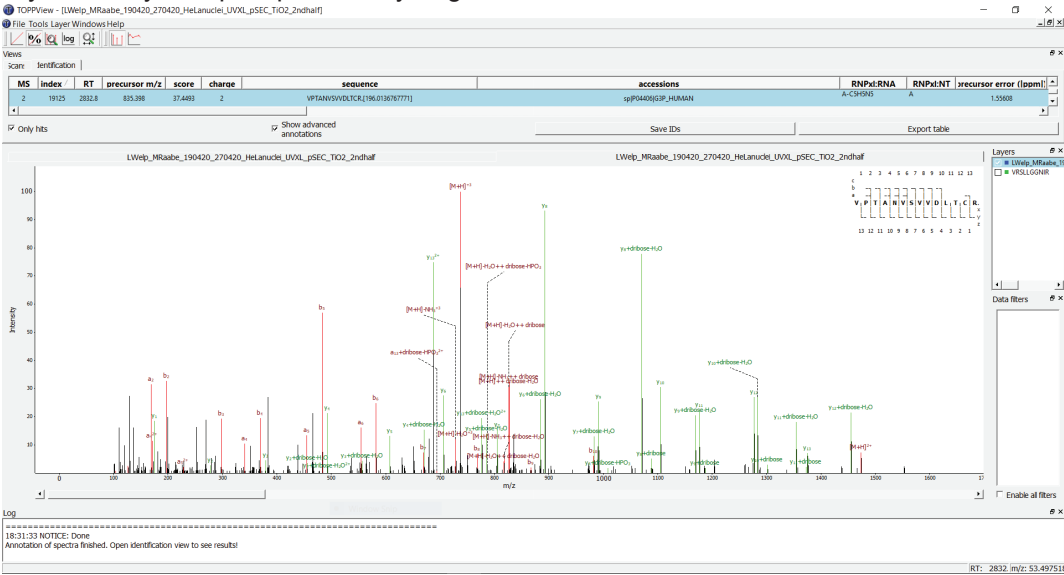
11) Elongation factor 1-alpha 1



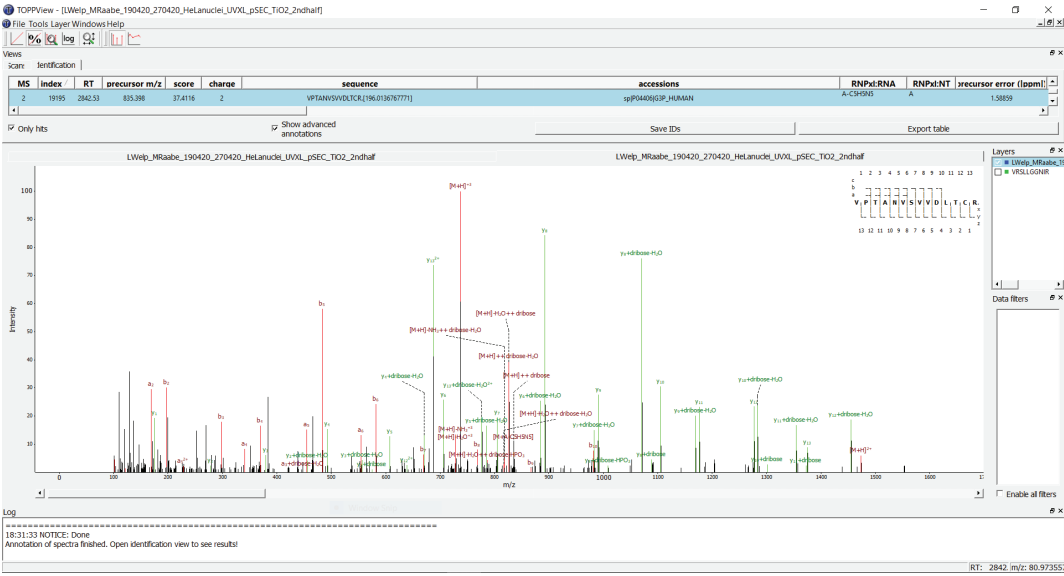
12) Alpha-enolase



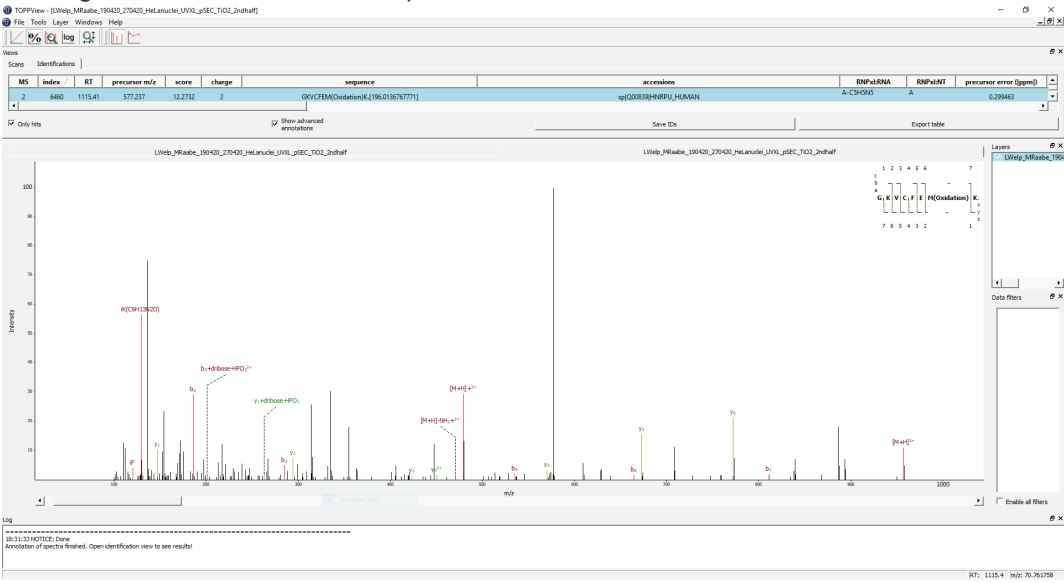
13) Glyceraldehyde-3-phosphate dehydrogenase



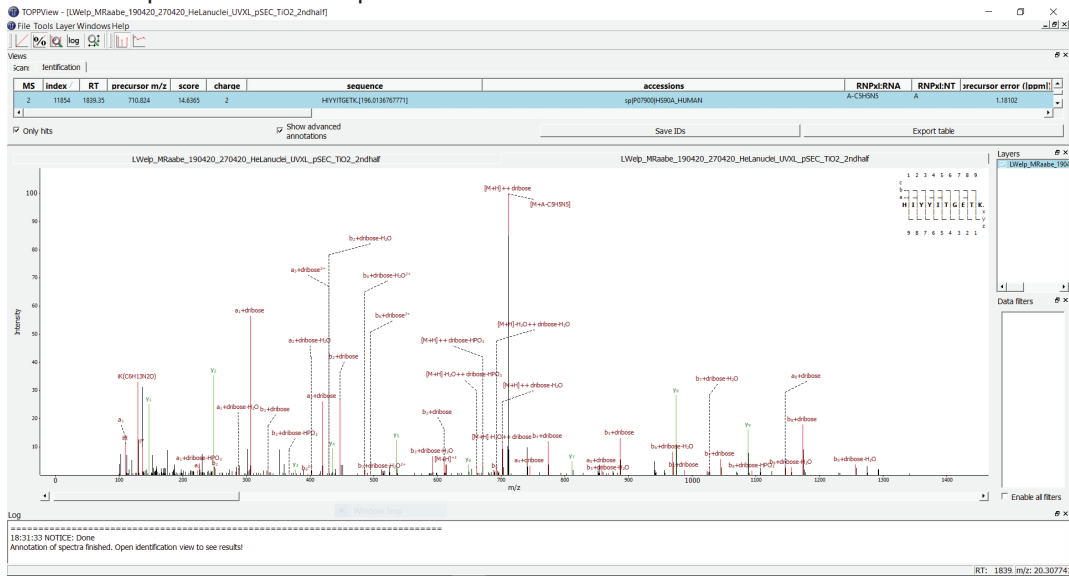
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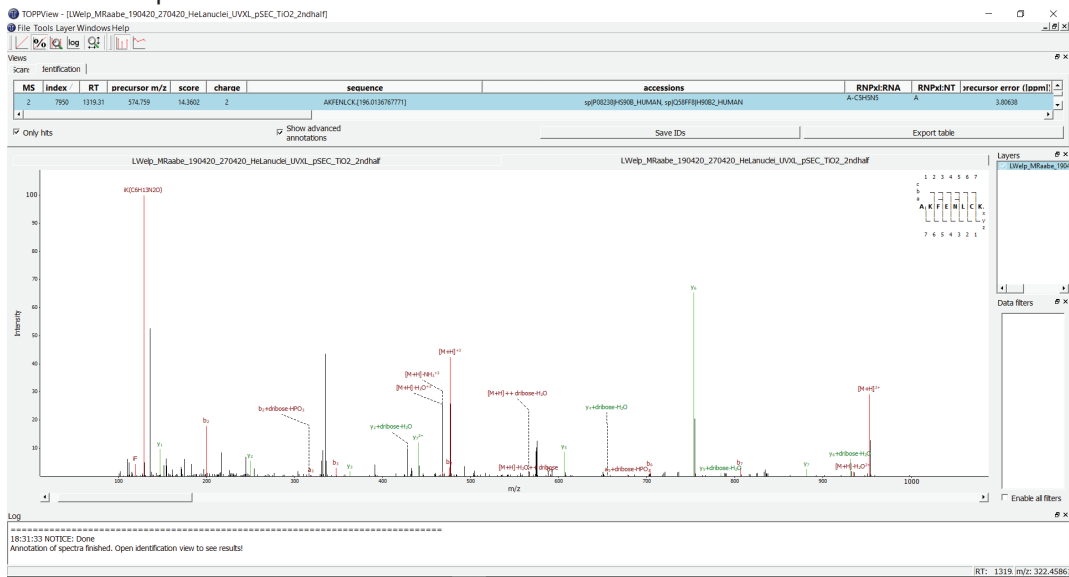
15) Heterogeneous nuclear ribonucleoprotein U



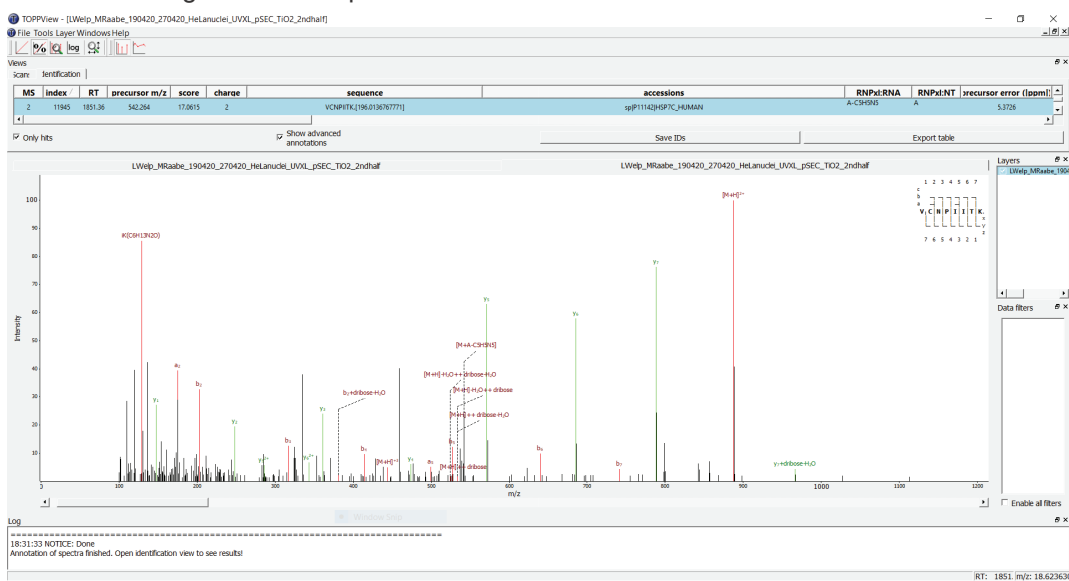
16) Heat shock protein HSP 90-alpha



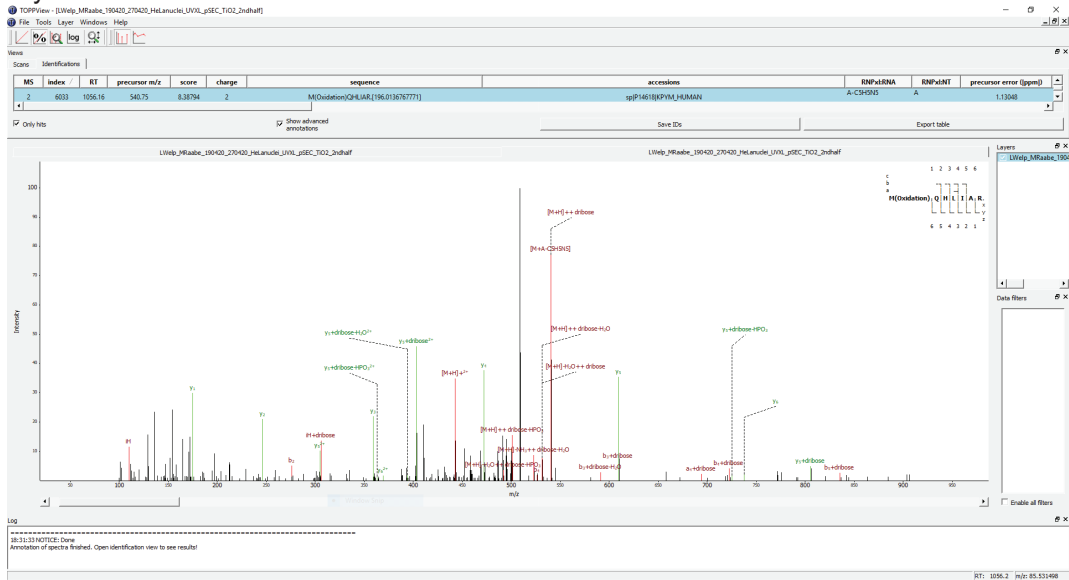
17) Heat shock protein HSP 90-beta



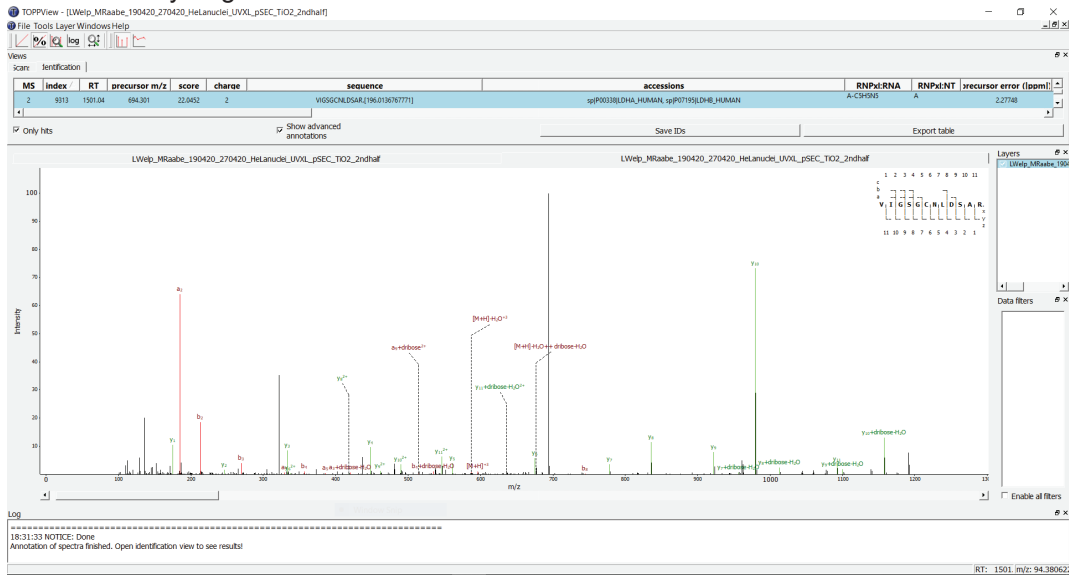
18) Heat shock cognate 71 kDa protein



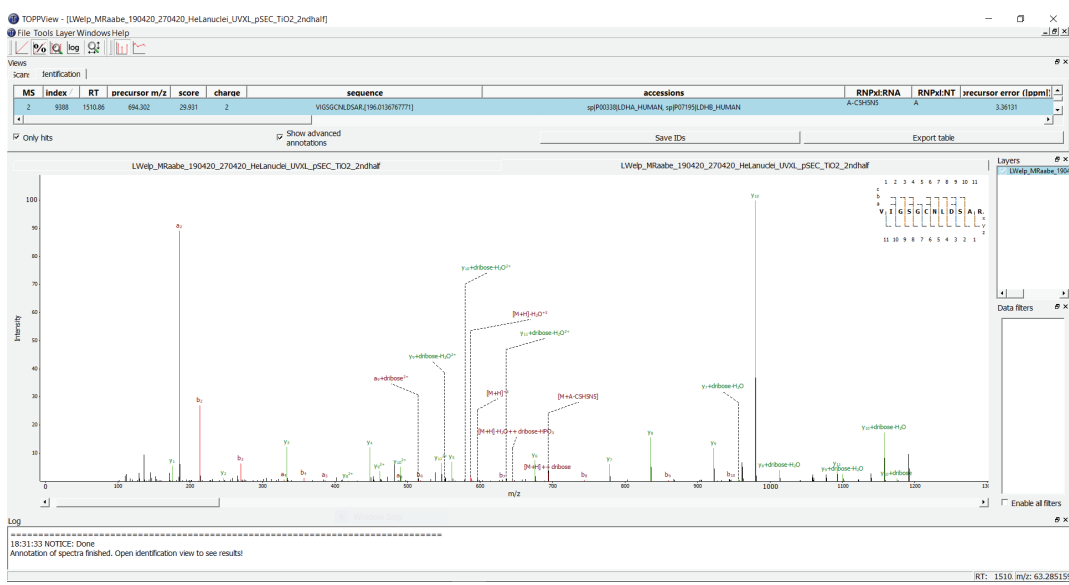
19) Pyruvate kinase PKM



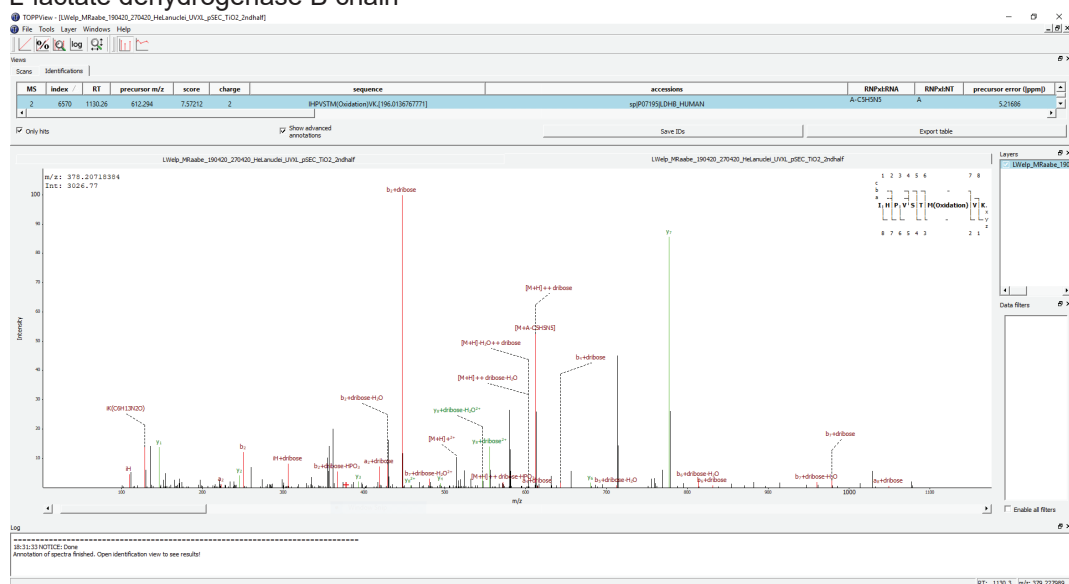
20) L-lactate dehydrogenase A chain



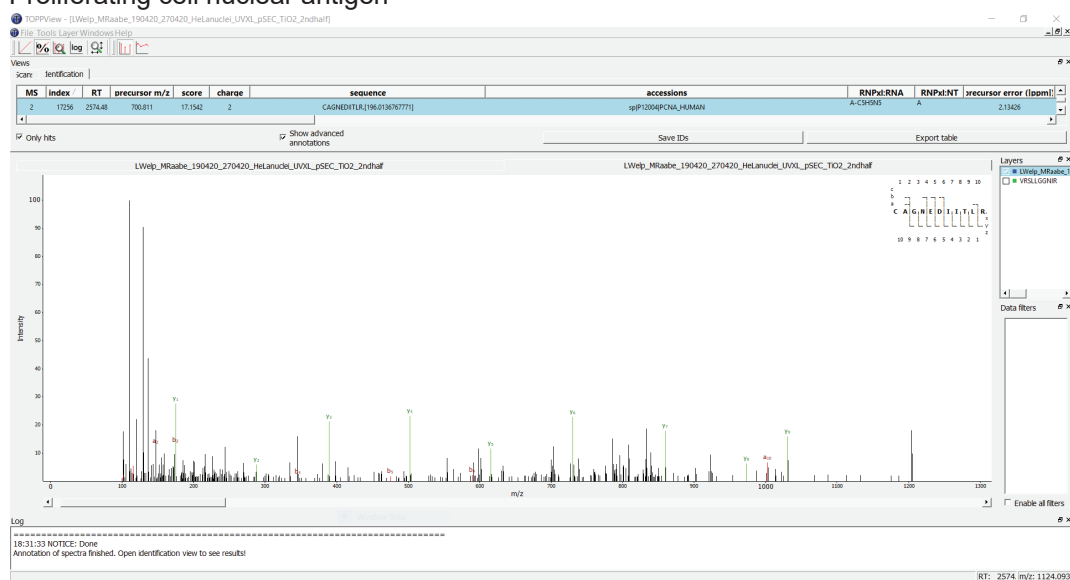
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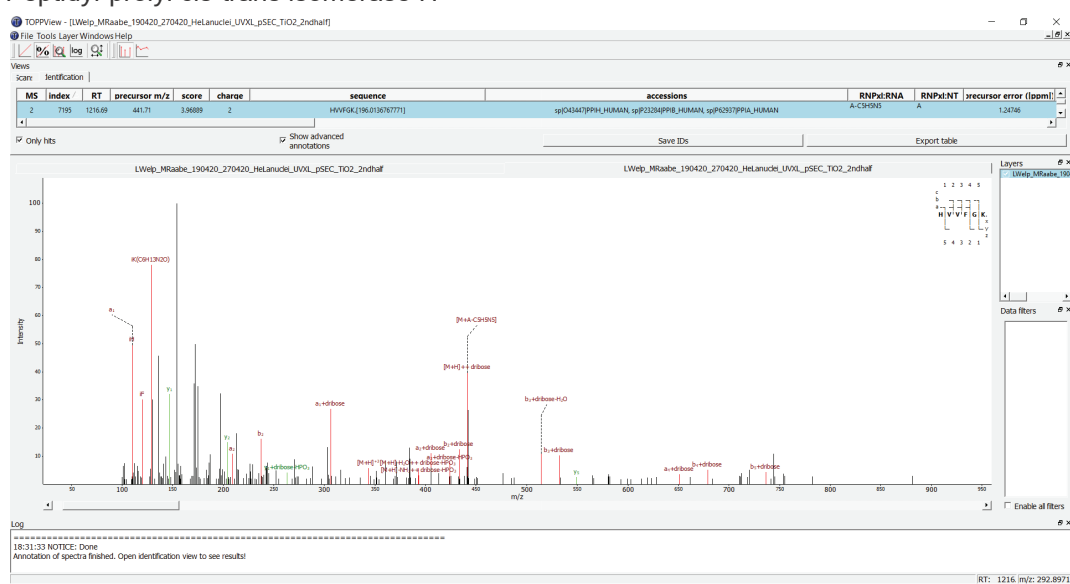
22) L-lactate dehydrogenase B chain



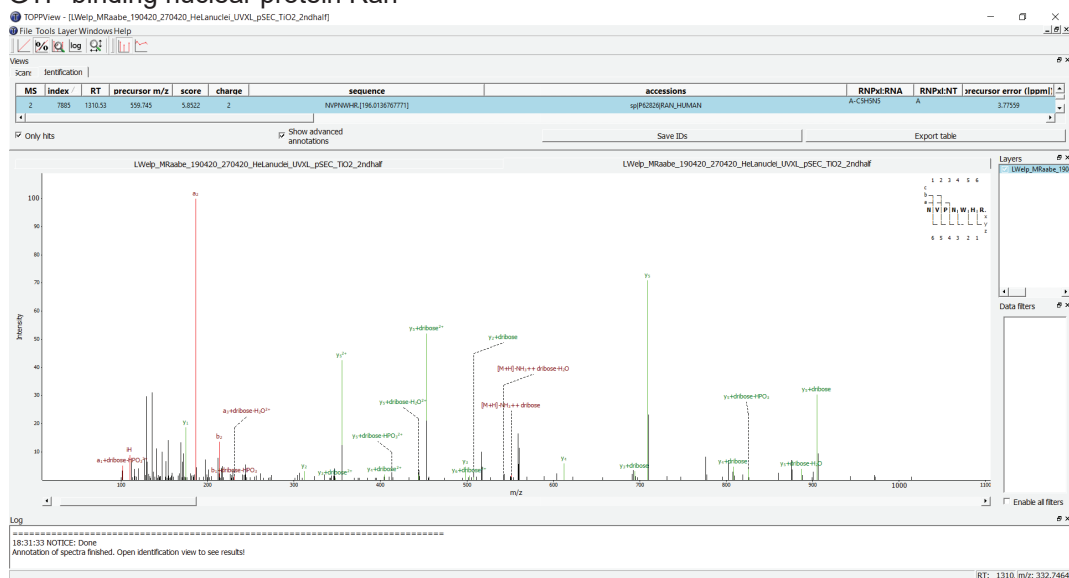
23) Proliferating cell nuclear antigen



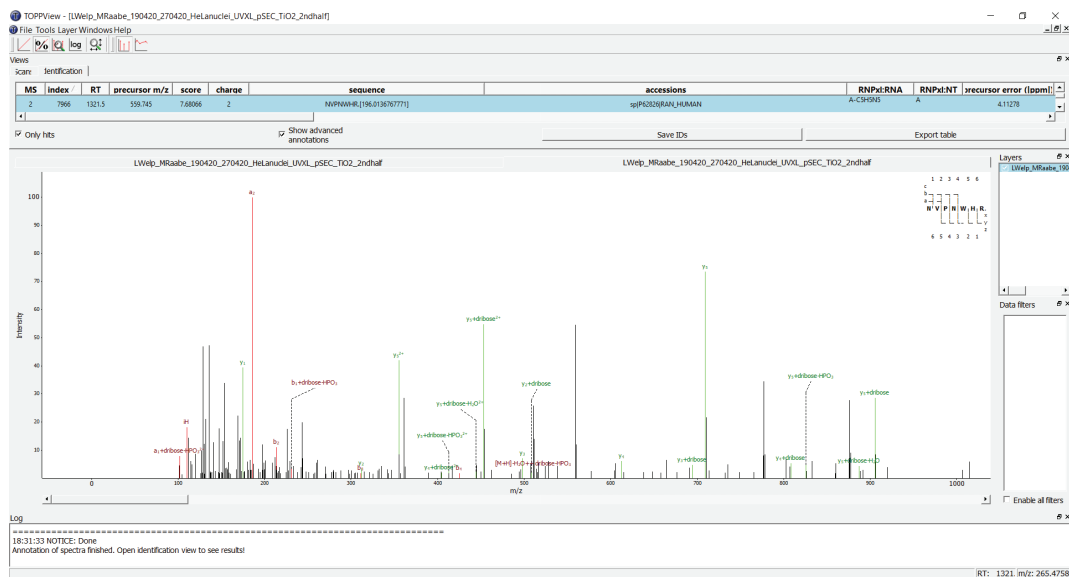
24) Peptidyl-prolyl cis-trans isomerase H



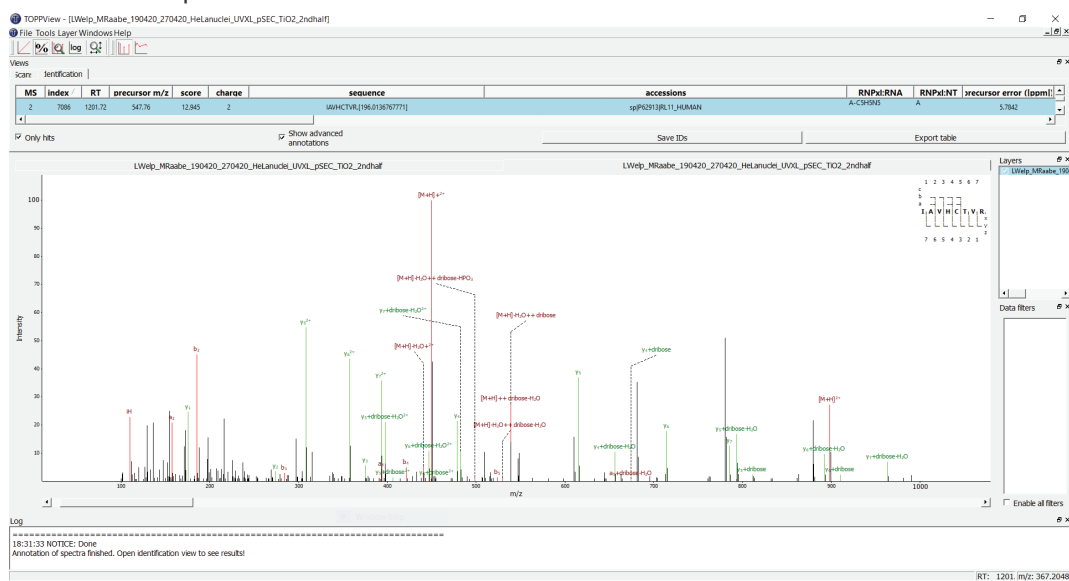
25) GTP-binding nuclear protein Ran



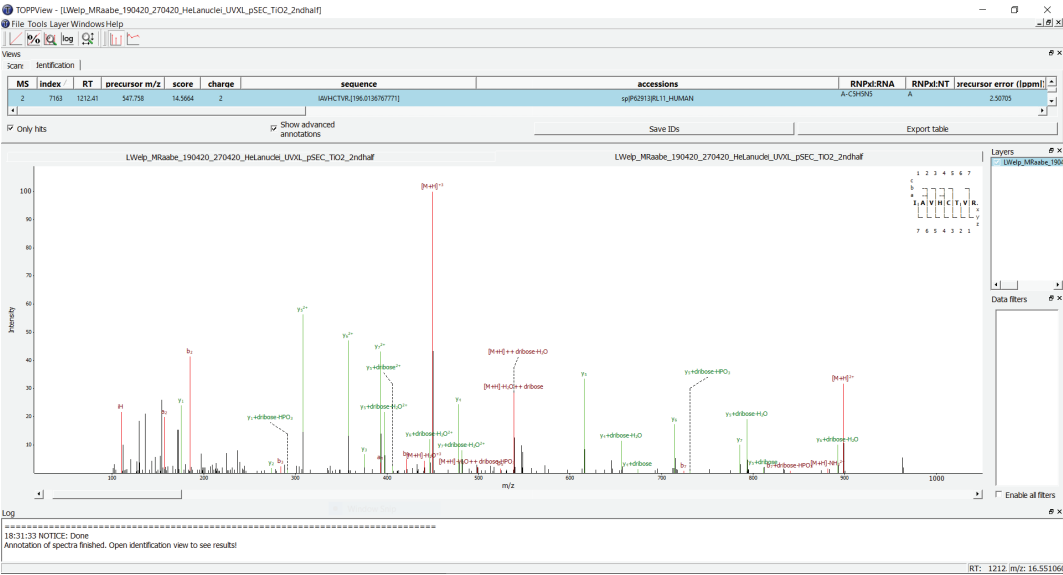
26)



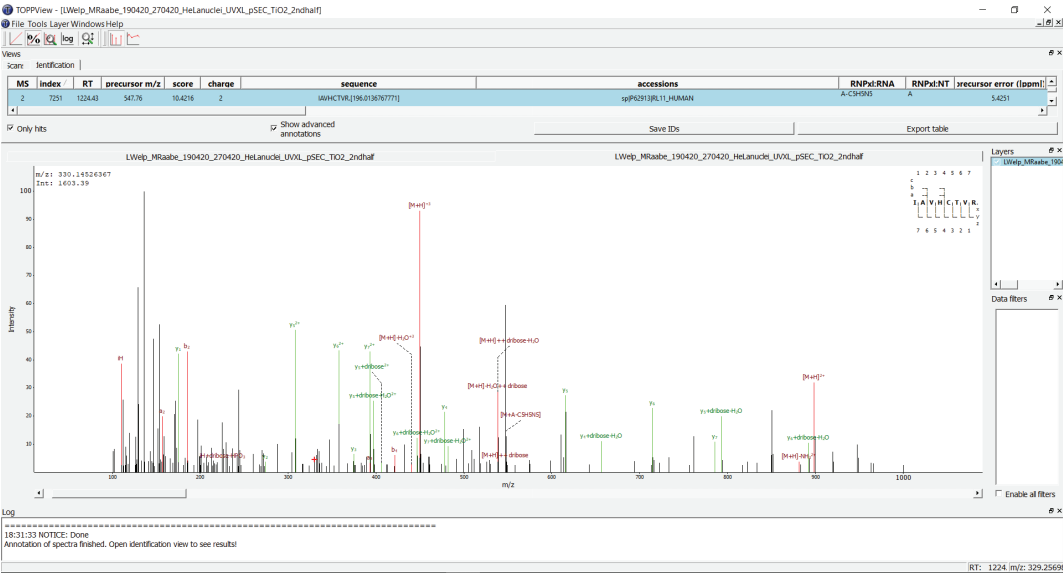
27) 60S ribosomal protein L11



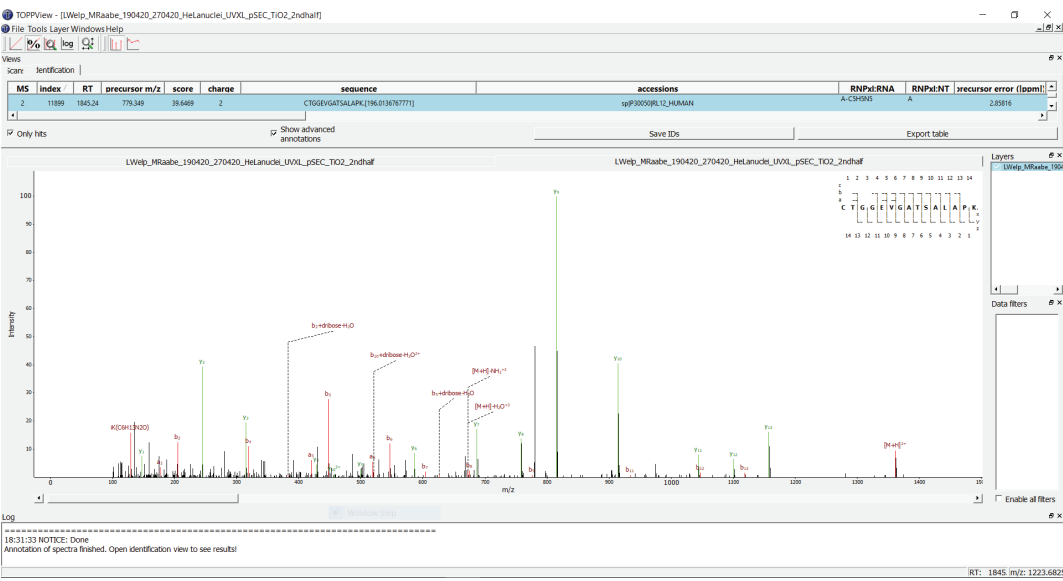
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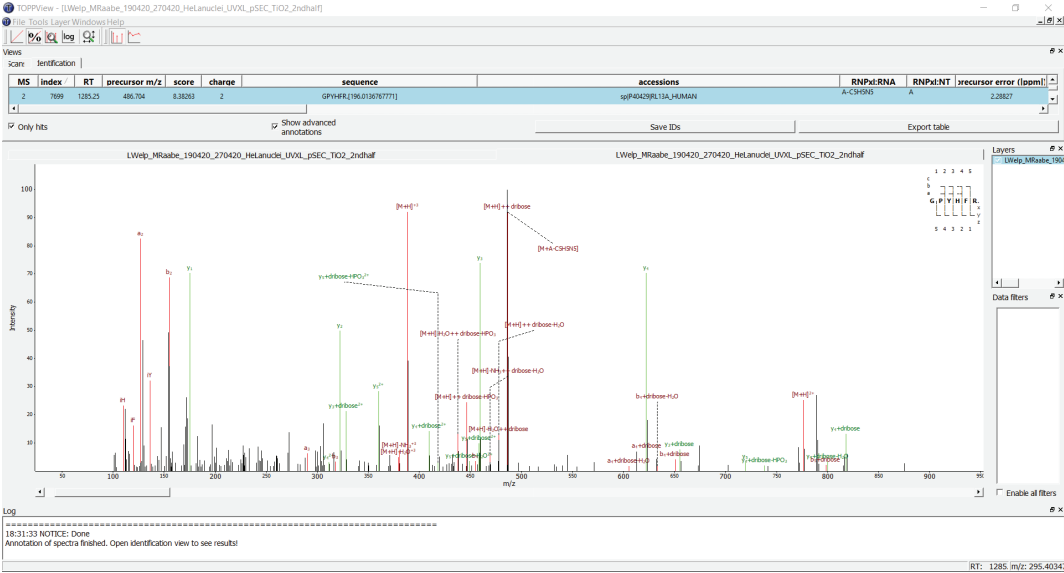
29)



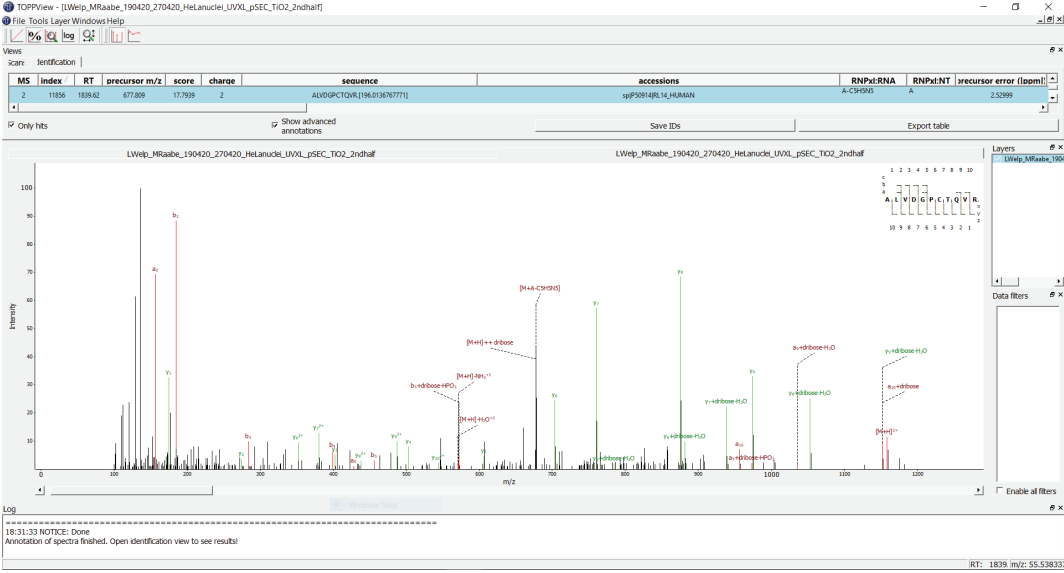
30) 60S ribosomal protein L12



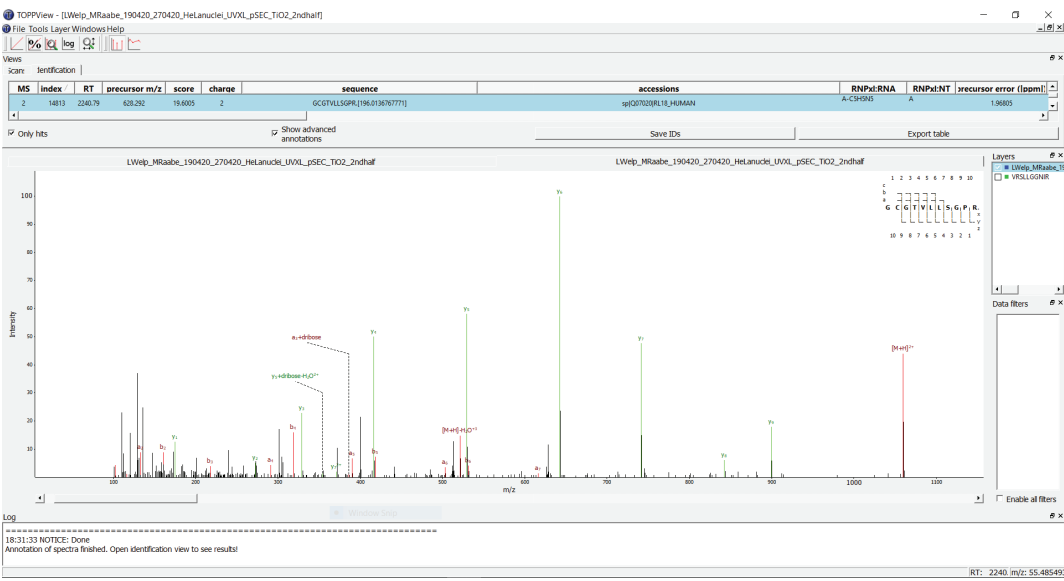
31) 60S ribosomal protein L13a



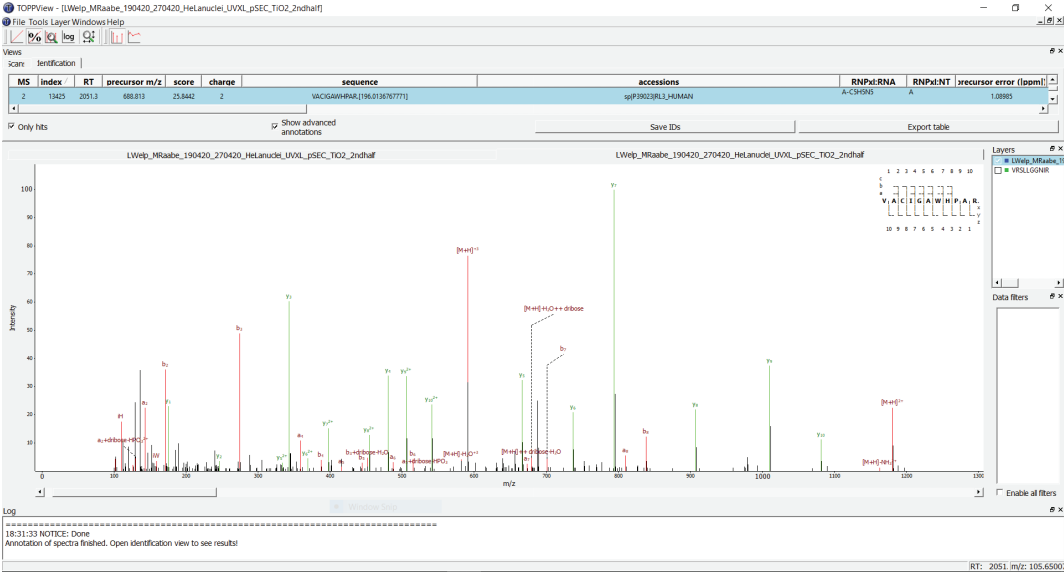
32) 60S ribosomal protein L14



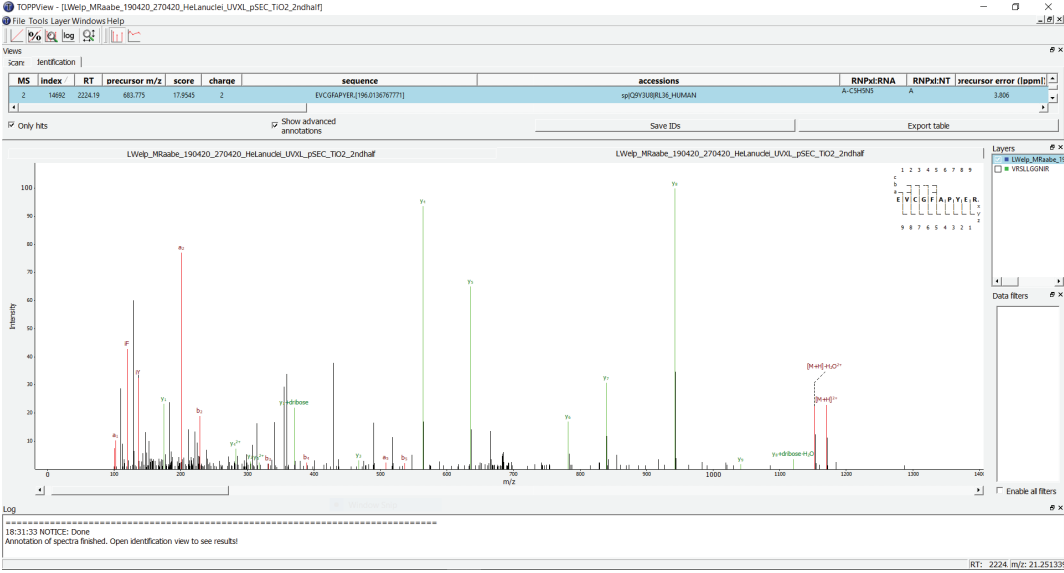
33) 60S ribosomal protein L18



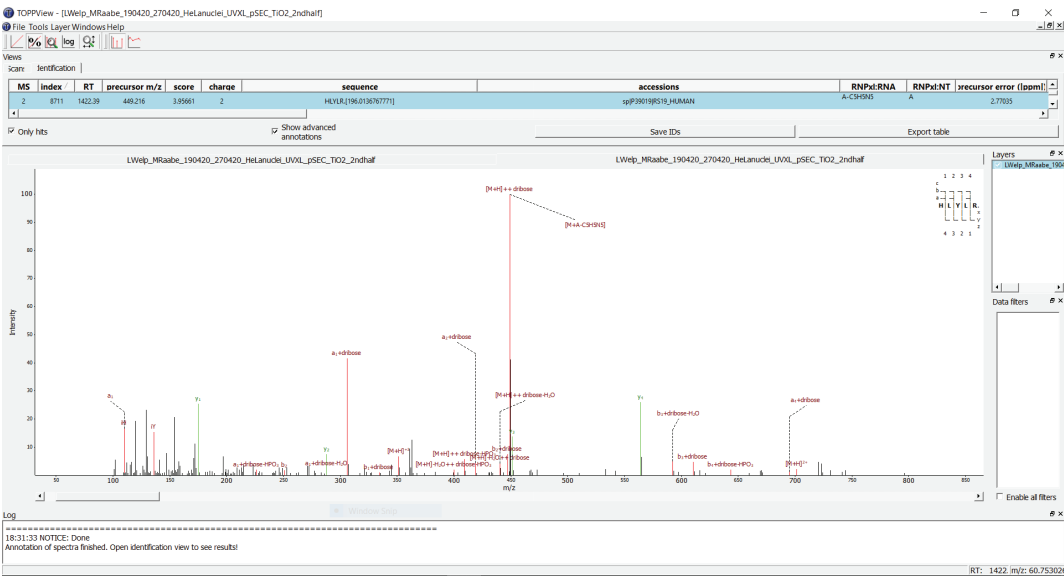
34) 60S ribosomal protein L3



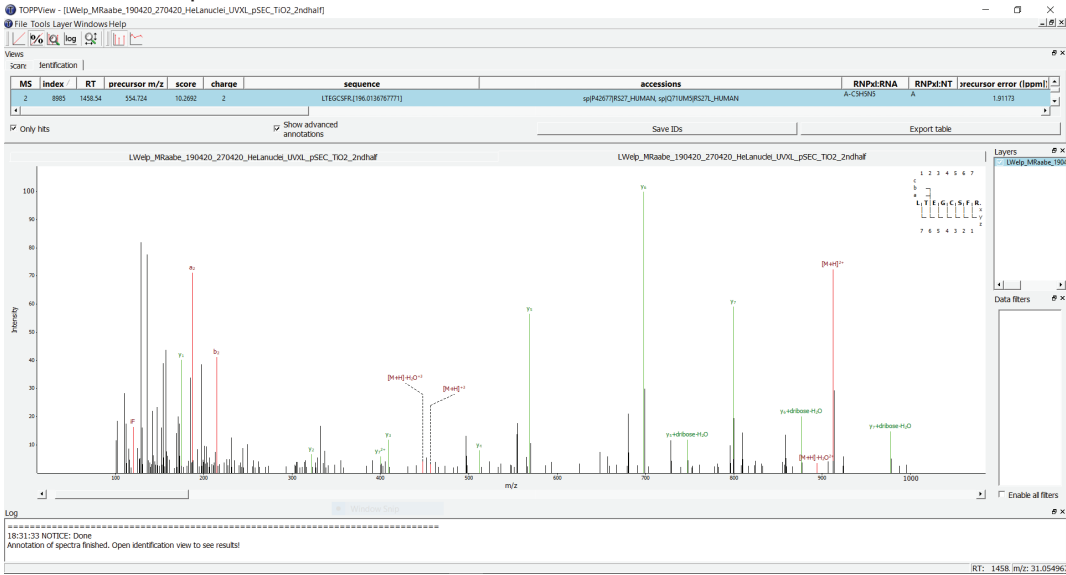
35) 60S ribosomal protein L36



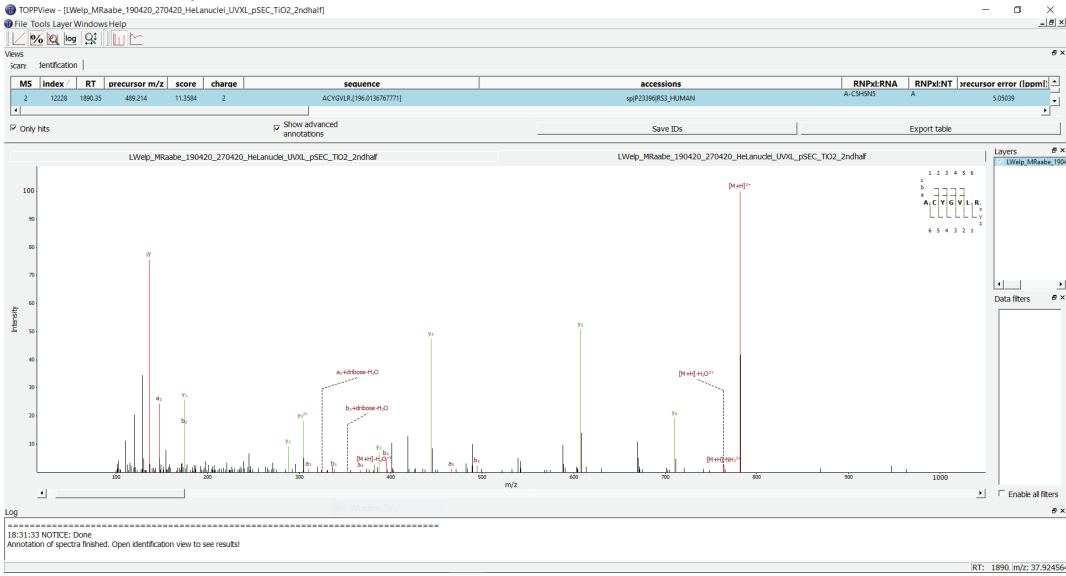
36) 40S ribosomal protein S19



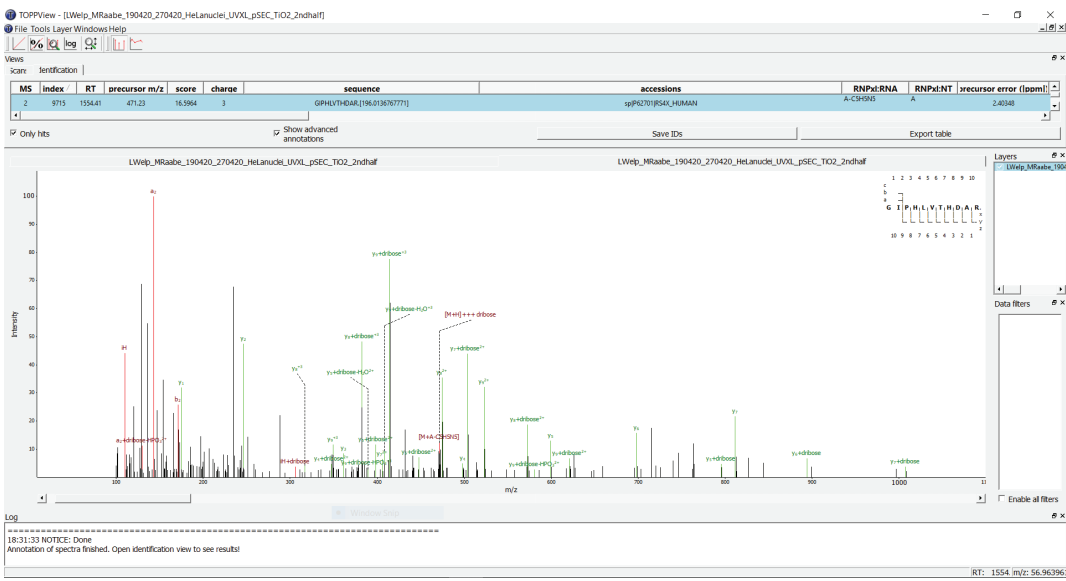
37) 40S ribosomal protein S27



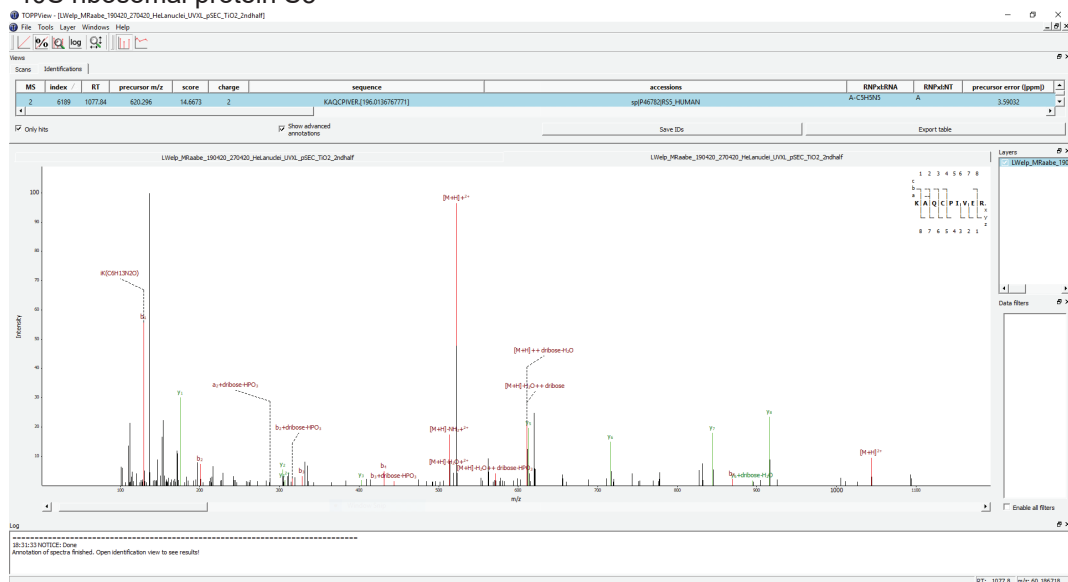
38) 40S ribosomal protein S3



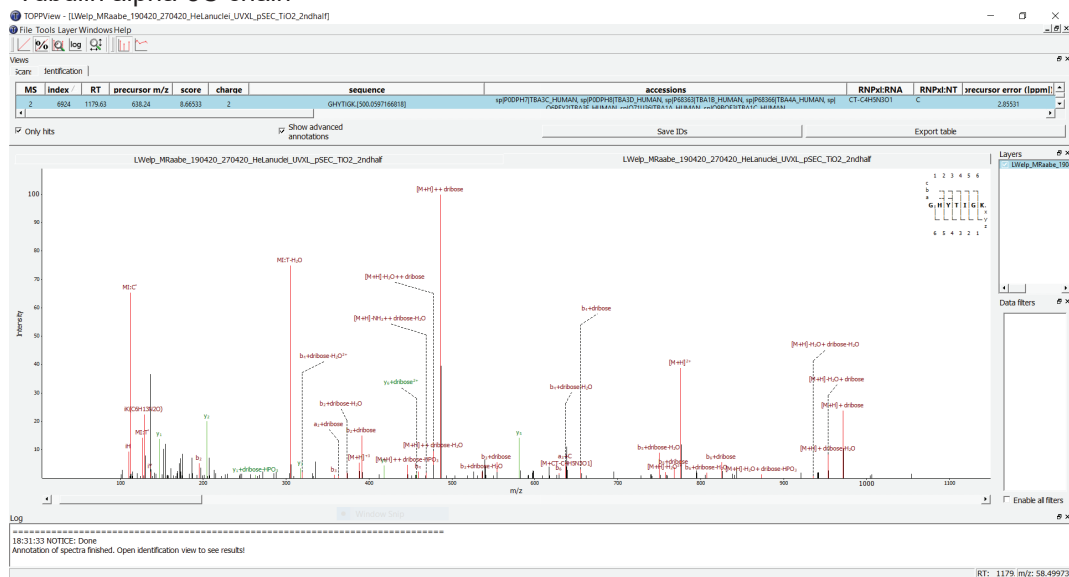
39) 40S ribosomal protein S4, X isoform



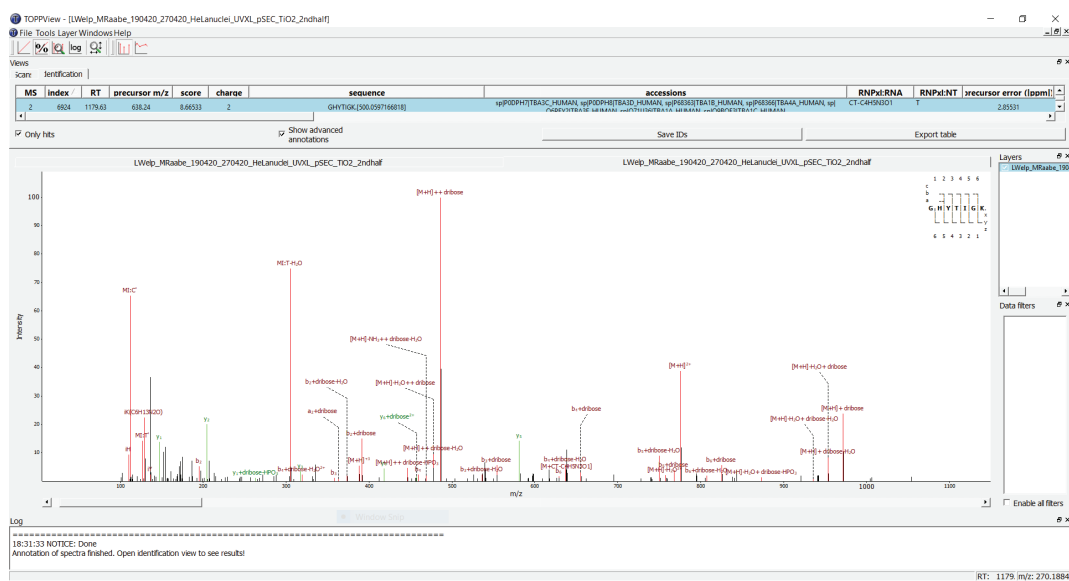
40) 40S ribosomal protein S5



41) Tubulin alpha-3C chain

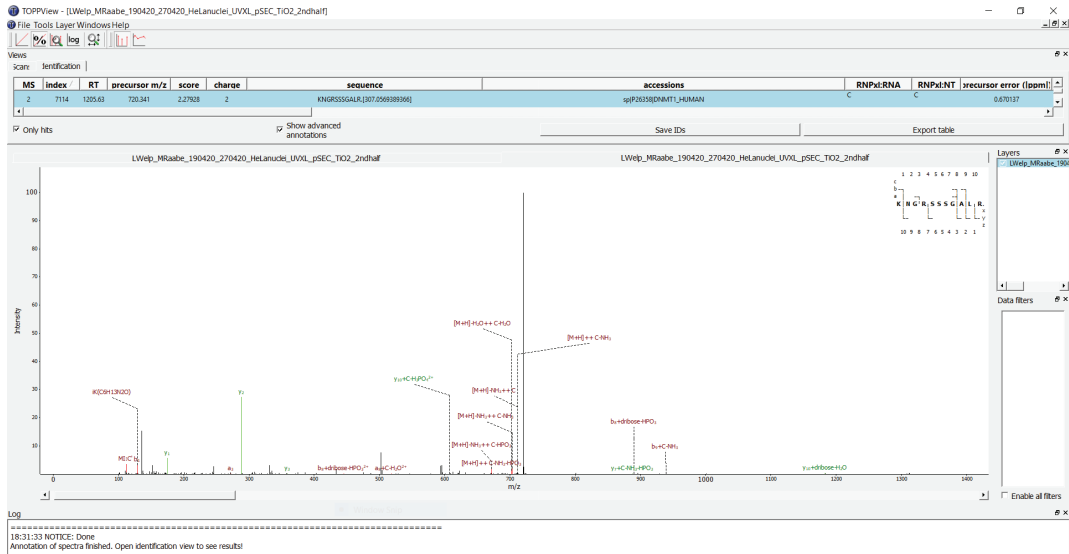


42)

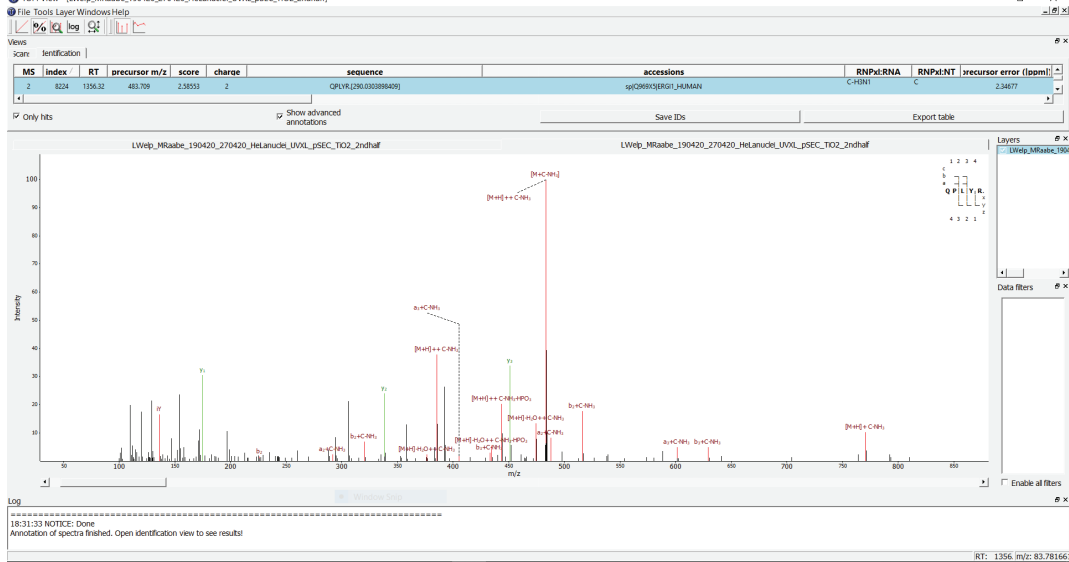


TOPPView spectra - ambiguous cross-link spectrum matches
UV cross-linked HeLa nuclei (SEC)

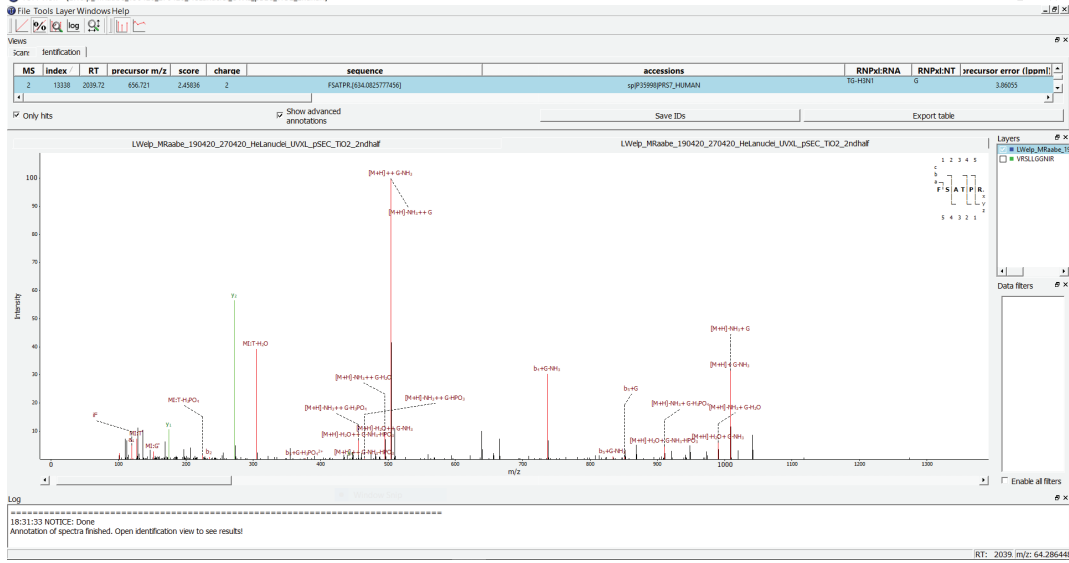
1) DNA (cytosine-5)-methyltransferase



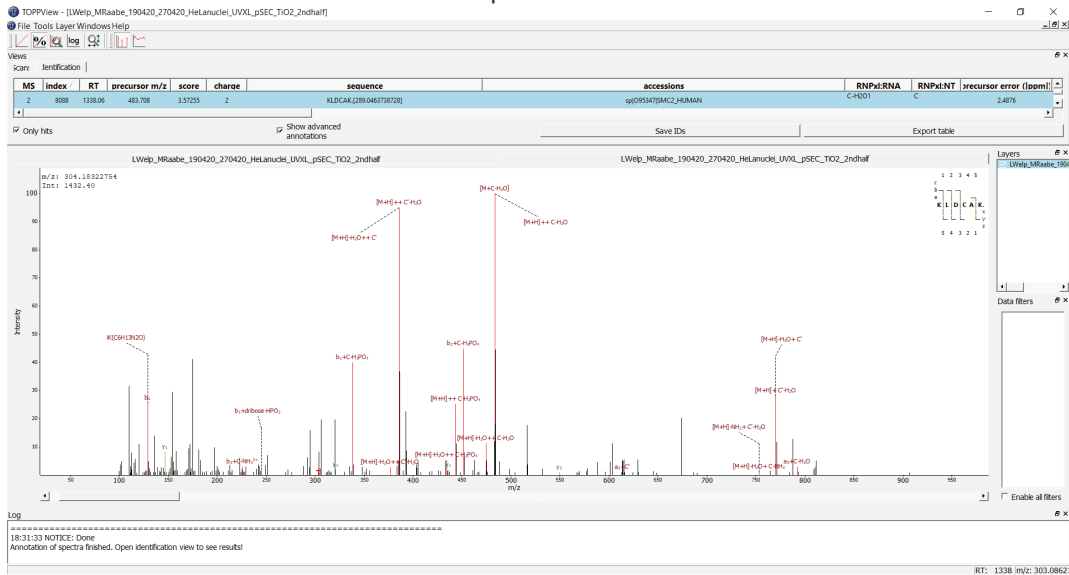
2) Endoplasmic reticulum-Golgi intermediate compartment protein 1



3) 26S proteasome regulatory subunit 7



4) Structural maintenance of chromosomes protein 2



TOPPView spectra - unambiguous cross-link spectrum matches
UV cross-linked HeLa nuclei (chromatin precipitation), RNP^{xl}search_settingsRNA

1) Heterogeneous nuclear ribonucleoprotein M

