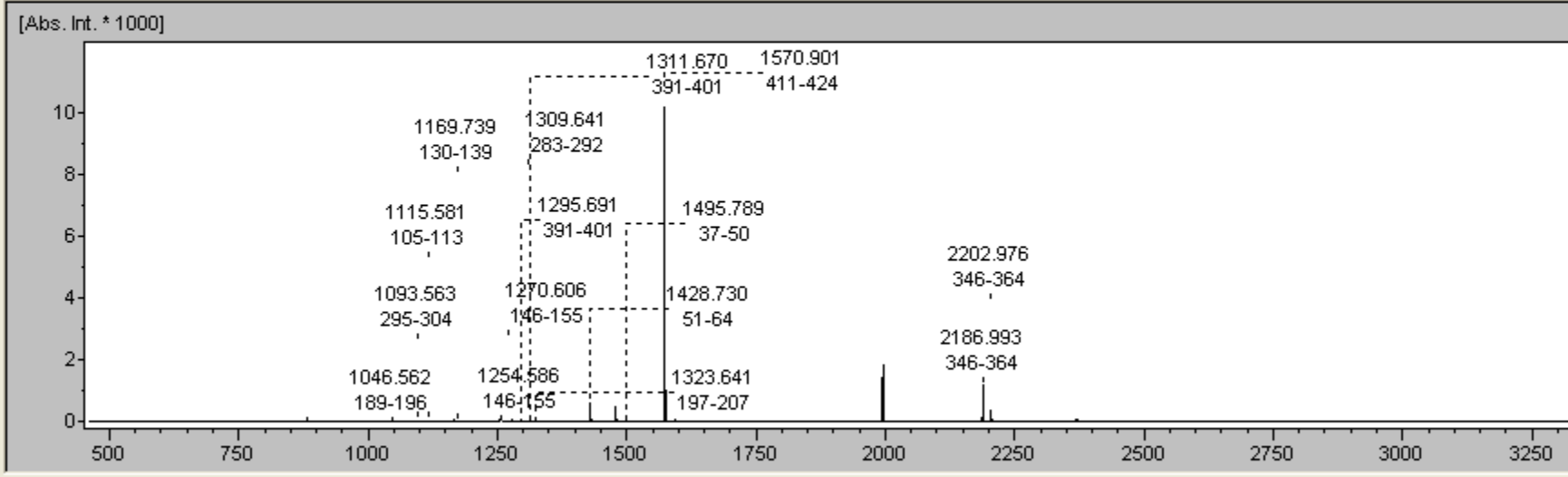
Electronic Supplementary Material (ESI) for Molecular BioSystems.


Fig. 1S. Vimentin protein identifications were confirmed by MS/MS sequencing of selected peptides. Three PMF peaks showing a high intensity were CID fragmented using Argon as collision gas. Accelerating voltages for ion sources 1 and 2 were 8.00 kV and 7.15 kV, respectively, while reflector 1 and reflector 2 voltages were respectively set to 29.50 kV and 14 kV with Lift 1 and Lift 2 set to 19 kV and 2.80 kV, respectively. Lens 10 voltage was 3.60 kV. Fragmented ions were analyzed using the Flex Analysis software v.3.0 and the MS/MS database searching was carried out in the UniProtKB database using the on-line-available MASCOT MS/MS ion search software. Taxonomy was limited to *Homo sapiens*, peptide precursor charge was set to +1, mass tolerance of ±1.2 Da for precursor peptide and ±0.5 Da for fragment peptides were allowed, and the number of accepted missed cleavage sites was set to one. Alkylation of cysteine by carbamidomethylation was selected as fixed modification, while oxidation of methionine was considered as a possible modification. We judged significant peptides with individual ion scores $p<0.05$.




Protein View | Match Errors | MSMS fragments | MSMS Analysis

Protein: Vimentin OS=Homo sapiens GN=VIM PE=1 SV=4 VIME_HUMAN

Peak threshold:

Intensity coverage: 81.2 % (13080 cnts) Sequence coverage MS: 30.0 % Sequence coverage MS/MS: 7.5 % pI: 4.9 MW (kDa):

```
10        20        30        40        50        60        70
MSTRSVSSSS YRRMFGGPGT ASRPSSSRSY VTTSTRTYSL GSALRPSTSR SLYASSPGGV YATRSSAVRL R
90        100       110       120       130       140       150
QDSVDFSLAD AINTEFKNTR TNEKVELQEL NDRFANYIDK VRFLEQQNKI LLAELEQLKG QGKSRLGDLY E
170       180       190       200       210       220       230
VDQLTNDKAR VEVERDNLAE DIMRLREKLQ EEMLQREEAE NTLQSFRQDV DNASLARLDL ERKVESLQEE I
250       260       270       280       290       300       310
EIQELQAQIQ EQHVQIDVDV SKPDLTAALR DVRQQYESVA AKNLQEAEEW YKSKFADLSE AANRNNDALR Q
330       340       350       360       370       380       390
RQVQSLTCEV DALKGTNESL ERQMREMEEN FAVEAANYQD TIGRLQDEIQ NMKEEMARHL REYQDLLNVK M
410       420       430       440       450       460       470
RKLLEGEESR ISLPLPNFSS LNLRETNLDS LPLVDTHSKR TLLIKTVETR DGQVINETSQ HHDDLE
```

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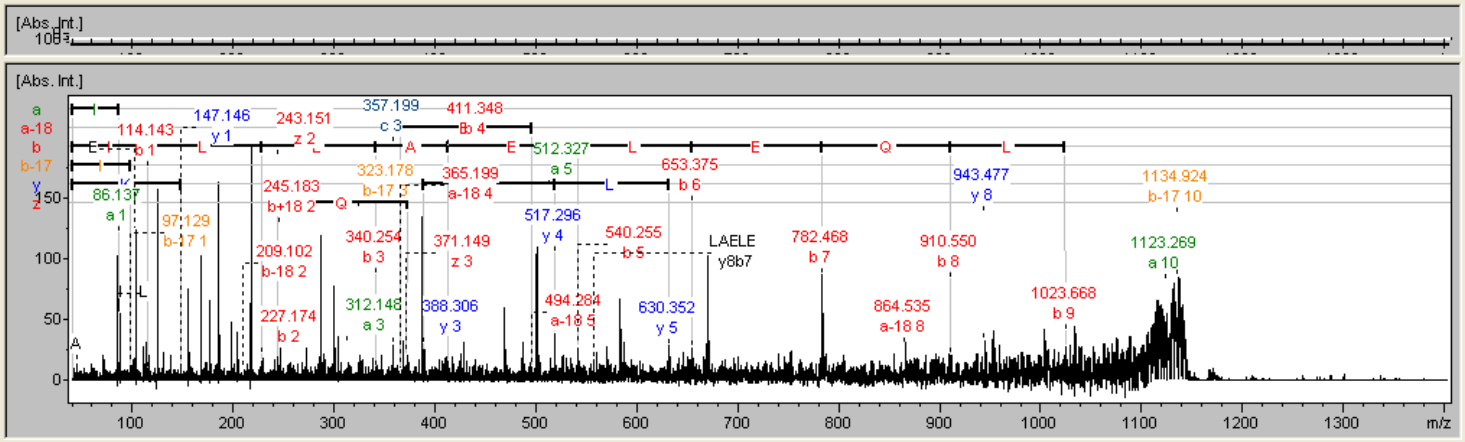
Tree hierarchy

- peak 10
- peak 13
- peak 15
- peak 17
- peak 18
- peak 20
- peak 21
- peak 23
- peak 27
- peak 28
- peak 30
- peak 31
- peak 32
- peak 33
- peak 35
- peak 37
- peak 38
- peak 39
- peak 40
- peak 41
- peak 42
- peak 43
- peak 44
- peak 45
- peak 46
- peak 47
- peak 50
- peak 51
- peak 52
- peak 53
- **Global peptide results**
- **Vimentin OS=Homo sa...**
  - Digest Matches (Score:...
  - Modifications: Global: ...
  - Search Parameter: Ch...
  - peak 9
  - peak 11
  - peak 12
  - MSMS 14
  - peak 16
  - peak 19
  - peak 22
  - peak 24
  - peak 25
  - MSMS 26
  - MSMS 29
  - peak 34
  - peak 36
  - peak 48
  - peak 49




Protein View | Match Errors | MSMS fragments | MSMS Analysis

Sequence: ILLAELEQLK (Peptide Mods: )

Masses: Monoisotopic / Average

MH+(mono): 1169.714 MH+(avg): 1170.421 MS/MS Tol: 0.500 Peaks: 167 Above Threshold: 167

Calculate: Masses Threshold: 0.000 Assigned: 37 Not Assigned: 130

| | I | L | L | A | E | L | E | Q | L | K | Ile | Leu | Leu | Ala | Glu | Leu | Glu | Gln | Leu | Lys |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ion | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| a | I | L | L | A | E | L | E | Q | L | K | 86.096 | 199.180 | 312.265 | 383.302 | 512.344 | 625.428 | 754.471 | 882.529 | 995.614 | 1123.709 |
| a-17 | I | L | L | A | E | L | E | Q | L | K | 69.070 | 182.154 | 295.238 | 366.275 | 495.318 | 608.402 | 737.444 | 865.503 | 978.587 | 1106.682 |
| a-18 | I | L | L | A | E | L | E | Q | L | K | 68.086 | 181.170 | 294.254 | 365.291 | 494.334 | 607.418 | 736.460 | 864.519 | 977.603 | 1105.698 |
| b | I | L | L | A | E | L | E | Q | L | K | 114.091 | 227.175 | 340.259 | 411.297 | 540.339 | 653.423 | 782.466 | 910.524 | 1023.608 | 1151.703 |
| b-17 | I | L | L | A | E | L | E | Q | L | K | 97.065 | 210.149 | 323.233 | 394.270 | 523.313 | 636.397 | 765.439 | 893.498 | 1006.582 | 1134.677 |
| b-18 | I | L | L | A | E | L | E | Q | L | K | 96.081 | 209.165 | 322.249 | 393.286 | 522.329 | 635.413 | 764.455 | 892.514 | 1005.598 | 1133.693 |
| b+18 | I | L | L | A | E | L | E | Q | L | K | 132.102 | 245.186 | 358.270 | 429.307 | 558.350 | 671.434 | 800.476 | 928.535 | 1041.619 | 1169.714 |
| c | I | L | L | A | E | L | E | Q | L | K | 131.118 | 244.202 | 357.286 | 428.323 | 557.366 | 670.450 | 799.492 | 927.551 | 1040.635 | 1168.730 |
| x | I | L | L | A | E | L | E | Q | L | K | 173.092 | 286.176 | 414.235 | 543.277 | 656.361 | 785.404 | 856.441 | 969.525 | 1082.609 | 1195.693 |
| y | I | L | L | A | E | L | E | Q | L | K | 147.113 | 260.197 | 388.255 | 517.298 | 630.382 | 759.425 | 830.462 | 943.546 | 1056.630 | 1169.714 |
| z | I | L | L | A | E | L | E | Q | L | K | 130.086 | 243.170 | 371.229 | 500.271 | 613.356 | 742.398 | 813.435 | 926.519 | 1039.603 | 1152.687 |
| i | I | L | L | A | E | L | E | Q | L | K | 86.096 | 86.096 | 86.096 | 44.049 | 102.054 | 86.096 | 102.054 | 101.070 | 86.096 | 101.107 |
| | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 | Lys | Leu | Gln | Glu | Leu | Glu | Ala | Leu | Leu | Ile |

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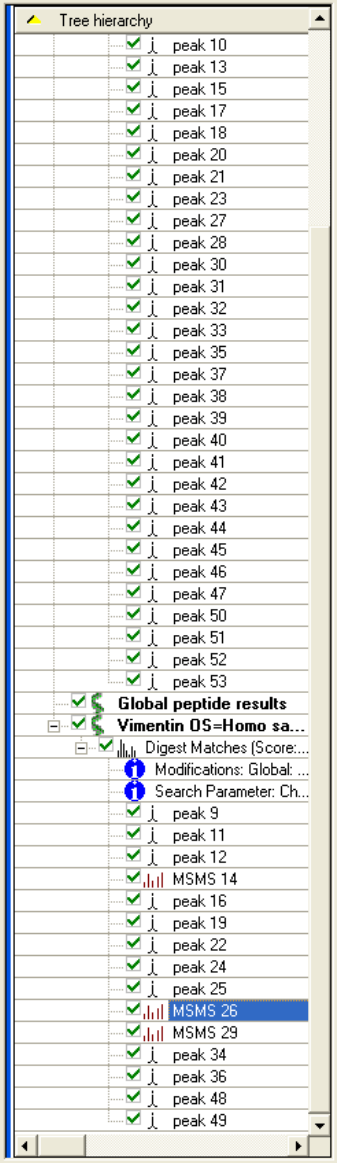


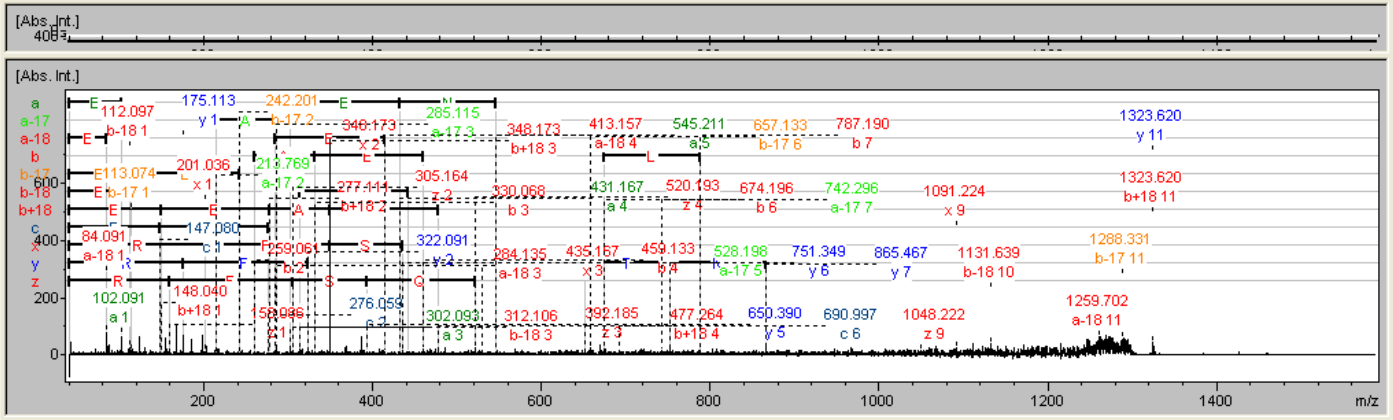


Protein View | Match Errors | MSMS fragments | MSMS Analysis

Sequence: EEAENTLQSFR (Peptide Mods: )

| | | | | | |
|---|---|---|---|---|---|
| Masses: | Monoisotopic / Average | MH+(mono): | 1323.618 | MH+(avg): | 1324.376 |
| Calculate: | Masses | MS/MS Tol: | 0.500 | Threshold: | 0.000 |
| Peaks: | 324 | Above Threshold: | 324 | Assigned: | 57 | Not Assigned: | 267 |

| | E | E | A | E | N | T | L | Q | S | F | R | Glu | Glu | Ala | Glu | Asn | Thr | Leu | Gln | Ser | Phe | Arg |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ion | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| a | E | E | A | E | N | T | L | Q | S | F | R | 102.055 | 231.098 | 302.135 | 431.177 | 545.220 | 646.268 | 759.352 | 887.411 | 974.443 | 1121.511 | 1277.612 |
| a-17 | E | E | A | E | N | T | L | Q | S | F | R | 85.028 | 214.071 | 285.108 | 414.151 | 528.194 | 629.241 | 742.325 | 870.384 | 957.416 | 1104.484 | 1260.586 |
| a-18 | E | E | A | E | N | T | L | Q | S | F | R | 84.044 | 213.087 | 284.124 | 413.167 | 527.210 | 628.257 | 741.341 | 869.400 | 956.432 | 1103.500 | 1259.601 |
| b | E | E | A | E | N | T | L | Q | S | F | R | 130.050 | 259.092 | 330.130 | 459.172 | 573.215 | 674.263 | 787.347 | 915.405 | 1002.437 | 1149.506 | 1305.607 |
| b-17 | E | E | A | E | N | T | L | Q | S | F | R | 113.023 | 242.066 | 313.103 | 442.146 | 556.189 | 657.236 | 770.320 | 898.379 | 985.411 | 1132.479 | 1288.580 |
| b-18 | E | E | A | E | N | T | L | Q | S | F | R | 112.039 | 241.082 | 312.119 | 441.162 | 555.205 | 656.252 | 769.336 | 897.395 | 984.427 | 1131.495 | 1287.596 |
| b+18 | E | E | A | E | N | T | L | Q | S | F | R | 148.060 | 277.103 | 348.140 | 477.183 | 591.226 | 692.273 | 805.357 | 933.416 | 1020.448 | 1167.516 | 1323.618 |
| c | E | E | A | E | N | T | L | Q | S | F | R | 147.076 | 276.119 | 347.156 | 476.199 | 590.242 | 691.289 | 804.373 | 932.432 | 1019.464 | 1166.532 | 1322.634 |
| x | E | E | A | E | N | T | L | Q | S | F | R | 201.098 | 348.167 | 435.199 | 563.257 | 676.341 | 777.389 | 891.432 | 1020.474 | 1091.512 | 1220.554 | 1349.597 |
| y | E | E | A | E | N | T | L | Q | S | F | R | 175.119 | 322.187 | 409.219 | 537.278 | 650.362 | 751.410 | 865.453 | 994.495 | 1065.532 | 1194.575 | 1323.618 |
| z | E | E | A | E | N | T | L | Q | S | F | R | 158.092 | 305.161 | 392.193 | 520.251 | 633.335 | 734.383 | 848.426 | 977.469 | 1048.506 | 1177.548 | 1306.591 |
| i | E | E | A | E | N | T | L | Q | S | F | R | 102.055 | 102.054 | 44.049 | 102.054 | 87.055 | 74.059 | 86.096 | 101.070 | 60.044 | 120.080 | 129.113 |
| | 11 | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 | Arg | Phe | Ser | Gln | Leu | Thr | Asn | Glu | Ala | Glu | Glu |

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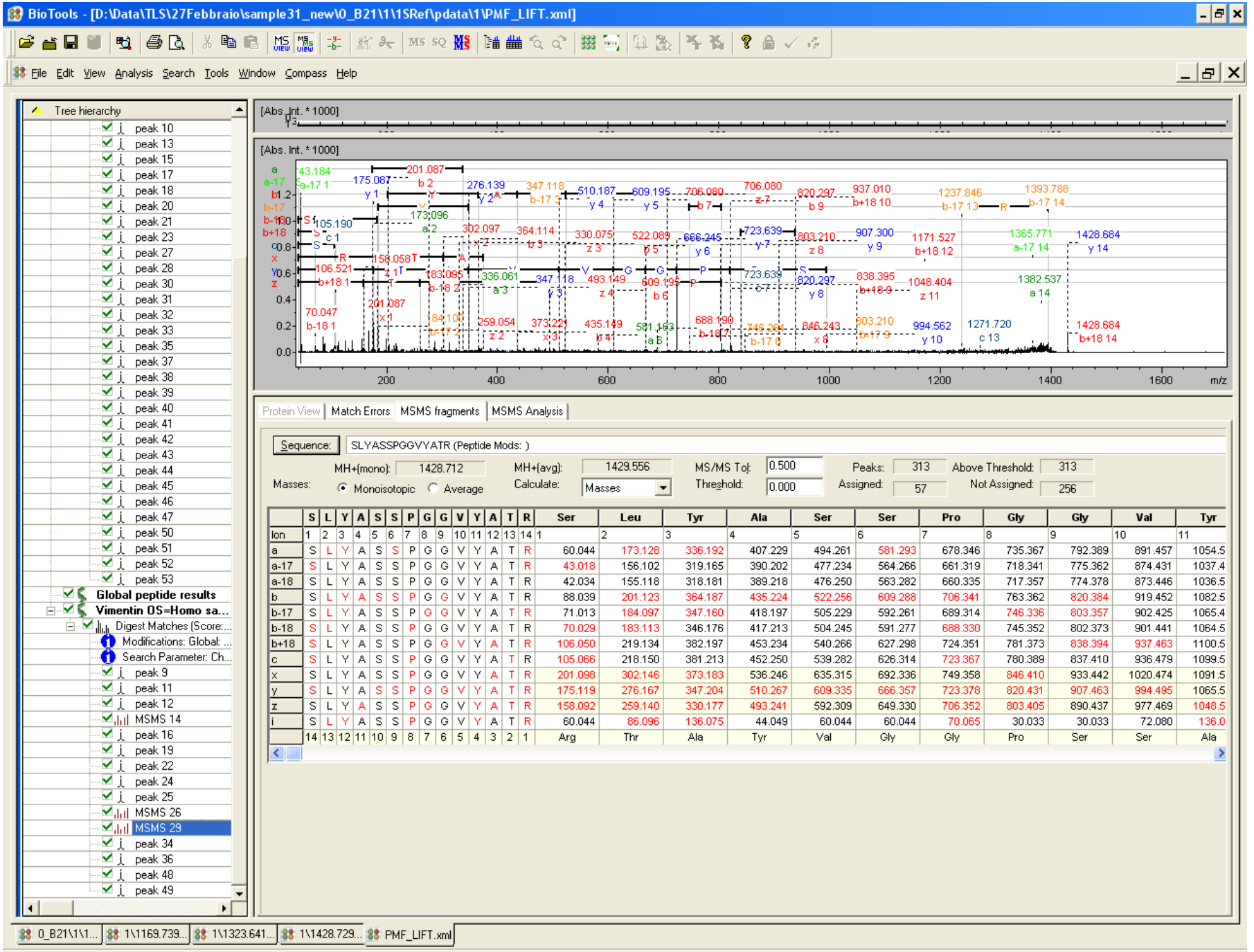
For Help, press F1 | CAP | NUM | bruker07




| | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | Ser | Leu | Tyr | Ala | Ser | Ser | Pro | Gly | Gly | Val | Tyr |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ion | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| a | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 60.044 | 173.128 | 336.192 | 407.229 | 494.261 | 581.293 | 678.346 | 735.367 | 792.389 | 891.457 | 1054.5 |
| a-17 | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 43.018 | 156.102 | 319.165 | 390.202 | 477.234 | 564.266 | 661.319 | 718.341 | 775.362 | 874.431 | 1037.4 |
| a-18 | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 42.034 | 155.118 | 318.181 | 389.218 | 476.250 | 563.282 | 660.335 | 717.357 | 774.378 | 873.446 | 1036.5 |
| b | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 88.039 | 201.123 | 364.187 | 435.224 | 522.256 | 609.288 | 706.341 | 763.362 | 820.384 | 919.452 | 1082.5 |
| b-17 | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 71.013 | 184.097 | 347.160 | 418.197 | 505.229 | 592.261 | 689.314 | 746.336 | 803.357 | 902.425 | 1065.4 |
| b-18 | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 70.029 | 183.113 | 346.176 | 417.213 | 504.245 | 591.277 | 688.330 | 745.352 | 802.373 | 901.441 | 1064.5 |
| b+18 | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 106.050 | 219.134 | 382.197 | 453.234 | 540.266 | 627.298 | 724.351 | 781.373 | 838.394 | 937.463 | 1100.5 |
| c | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 105.066 | 218.150 | 381.213 | 452.250 | 539.282 | 626.314 | 723.367 | 780.389 | 837.410 | 936.479 | 1099.5 |
| x | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 201.098 | 302.146 | 373.183 | 536.246 | 635.315 | 692.336 | 749.358 | 846.410 | 933.442 | 1020.474 | 1091.5 |
| y | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 175.119 | 276.167 | 347.204 | 510.267 | 609.335 | 666.357 | 723.378 | 820.431 | 907.463 | 994.495 | 1065.5 |
| z | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 158.092 | 259.140 | 330.177 | 493.241 | 592.309 | 649.330 | 706.352 | 803.405 | 890.437 | 977.469 | 1048.5 |
| i | S | L | Y | A | S | S | P | G | G | V | Y | A | T | R | 60.044 | 86.096 | 136.075 | 44.049 | 60.044 | 60.044 | 70.065 | 30.033 | 30.033 | 72.080 | 136.0 |
| | 14 | 13 | 12 | 11 | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 | Arg | Thr | Ala | Tyr | Val | Gly | Gly | Pro | Ser | Ser | Ala |